



Full wwPDB EM Validation Report ⓘ

Apr 1, 2025 – 07:16 pm BST

PDB ID : 6YAC / pdb_00006yac
EMDB ID : EMD-10746
Title : Plant PSI-ferredoxin supercomplex
Authors : Caspy, I.; Nelson, N.; Shkolnisky, Y.; Klaiman, D.; Sheinker, A.
Deposited on : 2020-03-12
Resolution : 2.50 Å (reported)
Based on initial models : 5L8R, 1A70

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.dev117
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.42

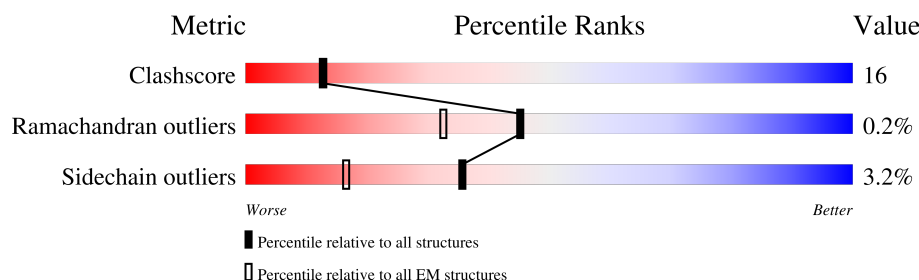
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.50 Å.

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









Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	743	82% 17%
2	B	733	78% 21% .
3	C	80	90% 9% .
4	D	143	77% 22% .
5	E	66	88% 12%
6	F	154	73% 26% .
7	G	97	82% 15% .
8	H	88	68% 30% .
9	I	31	81% 16% .

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Mol	Chain	Length	Quality of chain
10	J	42	
11	K	81	
12	L	157	
13	1	193	
14	2	208	
15	3	221	
16	4	198	
17	N	97	

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
18	CL0	A	1011	X	-	-	-
19	CLA	1	601	X	-	-	-
19	CLA	1	602	X	-	-	-
19	CLA	1	603	X	-	-	-
19	CLA	1	604	X	-	-	-
19	CLA	1	605	X	-	-	-
19	CLA	1	606	X	-	-	-
19	CLA	1	607	X	-	-	-
19	CLA	1	608	X	-	-	-
19	CLA	1	611	X	-	-	-
19	CLA	1	613	X	-	-	-
19	CLA	1	614	X	-	-	-
19	CLA	2	601	X	-	-	-
19	CLA	2	602	X	-	-	-
19	CLA	2	603	X	-	-	-
19	CLA	2	604	X	-	-	-
19	CLA	2	605	X	-	-	-
19	CLA	2	606	X	-	-	-
19	CLA	2	607	X	-	-	-
19	CLA	2	608	X	-	-	-
19	CLA	2	612	X	-	-	-
19	CLA	3	601	X	-	-	-
19	CLA	3	602	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	CLA	3	603	X	-	-	-
19	CLA	3	606	X	-	-	-
19	CLA	3	608	X	-	-	-
19	CLA	3	610	X	-	-	-
19	CLA	3	612	X	-	-	-
19	CLA	3	613	X	-	-	-
19	CLA	3	614	X	-	-	-
19	CLA	3	617	X	-	-	-
19	CLA	4	601	X	-	-	-
19	CLA	4	602	X	-	-	-
19	CLA	4	603	X	-	-	-
19	CLA	4	604	X	-	-	-
19	CLA	4	606	X	-	-	-
19	CLA	4	607	X	-	-	-
19	CLA	4	608	X	-	-	-
19	CLA	4	609	X	-	-	-
19	CLA	4	612	X	-	-	-
19	CLA	4	617	X	-	-	-
19	CLA	A	1012	X	-	-	-
19	CLA	A	1013	X	-	-	-
19	CLA	A	1101	X	-	-	-
19	CLA	A	1102	X	-	-	-
19	CLA	A	1103	X	-	-	-
19	CLA	A	1104	X	-	-	-
19	CLA	A	1105	X	-	-	-
19	CLA	A	1106	X	-	-	-
19	CLA	A	1107	X	-	-	-
19	CLA	A	1108	X	-	-	-
19	CLA	A	1109	X	-	-	-
19	CLA	A	1110	X	-	-	-
19	CLA	A	1111	X	-	-	-
19	CLA	A	1112	X	-	-	-
19	CLA	A	1113	X	-	-	-
19	CLA	A	1114	X	-	-	-
19	CLA	A	1115	X	-	-	-
19	CLA	A	1116	X	-	-	-
19	CLA	A	1117	X	-	-	-
19	CLA	A	1118	X	-	-	-
19	CLA	A	1119	X	-	-	-
19	CLA	A	1120	X	-	-	-
19	CLA	A	1121	X	-	-	-
19	CLA	A	1122	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	CLA	A	1123	X	-	-	-
19	CLA	A	1124	X	-	-	-
19	CLA	A	1125	X	-	-	-
19	CLA	A	1126	X	-	-	-
19	CLA	A	1127	X	-	-	-
19	CLA	A	1128	X	-	-	-
19	CLA	A	1129	X	-	-	-
19	CLA	A	1130	X	-	-	-
19	CLA	A	1131	X	-	-	-
19	CLA	A	1132	X	-	-	-
19	CLA	A	1133	X	-	-	-
19	CLA	A	1134	X	-	-	-
19	CLA	A	1135	X	-	-	-
19	CLA	A	1136	X	-	-	-
19	CLA	A	1137	X	-	-	-
19	CLA	A	1138	X	-	-	-
19	CLA	A	1139	X	-	-	-
19	CLA	A	1140	X	-	-	-
19	CLA	A	1141	X	-	-	-
19	CLA	B	1021	X	-	-	-
19	CLA	B	1022	X	-	-	-
19	CLA	B	1023	X	-	-	-
19	CLA	B	1201	X	-	-	-
19	CLA	B	1202	X	-	-	-
19	CLA	B	1203	X	-	-	-
19	CLA	B	1204	X	-	-	-
19	CLA	B	1205	X	-	-	-
19	CLA	B	1206	X	-	-	-
19	CLA	B	1207	X	-	-	-
19	CLA	B	1208	X	-	-	-
19	CLA	B	1209	X	-	-	-
19	CLA	B	1210	X	-	-	-
19	CLA	B	1211	X	-	-	-
19	CLA	B	1212	X	-	-	-
19	CLA	B	1213	X	-	-	-
19	CLA	B	1214	X	-	-	-
19	CLA	B	1215	X	-	-	-
19	CLA	B	1216	X	-	-	-
19	CLA	B	1217	X	-	-	-
19	CLA	B	1218	X	-	-	-
19	CLA	B	1219	X	-	-	-
19	CLA	B	1220	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	CLA	B	1221	X	-	-	-
19	CLA	B	1222	X	-	-	-
19	CLA	B	1223	X	-	-	-
19	CLA	B	1224	X	-	-	-
19	CLA	B	1225	X	-	-	-
19	CLA	B	1226	X	-	-	-
19	CLA	B	1227	X	-	-	-
19	CLA	B	1228	X	-	-	-
19	CLA	B	1229	X	-	-	-
19	CLA	B	1230	X	-	-	-
19	CLA	B	1231	X	-	-	-
19	CLA	B	1232	X	-	-	-
19	CLA	B	1234	X	-	-	-
19	CLA	B	1235	X	-	-	-
19	CLA	B	1236	X	-	-	-
19	CLA	B	1237	X	-	-	-
19	CLA	B	1238	X	-	-	-
19	CLA	B	1239	X	-	-	-
19	CLA	B	1240	X	-	-	-
19	CLA	F	1301	X	-	-	-
19	CLA	F	1302	X	-	-	-
19	CLA	G	1601	X	-	-	-
19	CLA	G	1602	X	-	-	-
19	CLA	G	1603	X	-	-	-
19	CLA	G	1701	X	-	-	-
19	CLA	J	1901	X	-	-	-
19	CLA	K	1401	X	-	-	-
19	CLA	K	1402	X	-	-	-
19	CLA	K	1403	X	-	-	-
19	CLA	K	1404	X	-	-	-
19	CLA	L	1501	X	-	-	-
19	CLA	L	1502	X	-	-	-
19	CLA	L	1503	X	-	-	-
28	LUT	2	501	X	-	-	-
28	LUT	3	502	X	-	-	-
28	LUT	J	4013	X	-	-	-
29	CHL	1	609	X	-	-	-
29	CHL	1	610	X	-	-	-
29	CHL	1	612	X	-	-	-
29	CHL	2	609	X	-	-	-
29	CHL	2	610	X	-	-	-
29	CHL	2	611	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
29	CHL	2	613	X	-	-	-
29	CHL	2	615	X	-	-	-
29	CHL	3	604	X	-	-	-
29	CHL	3	607	X	-	-	-
29	CHL	3	611	X	-	-	-
29	CHL	4	610	X	-	-	-
29	CHL	4	611	X	-	-	-
29	CHL	4	613	X	-	-	-
29	CHL	4	615	X	-	-	-
30	XAT	2	502	X	-	-	-
30	XAT	4	502	X	-	-	-

2 Entry composition

There are 33 unique types of molecules in this entry. The entry contains 38469 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	743	Total	C	N	O	S	0	0
			5858	3839	998	1003	18		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	733	Total	C	N	O	S	0	0
			5857	3848	998	997	14		

- 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
			612	379	107	115	11		

- Molecule 4 is a protein called PsaD.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	143	Total	C	N	O	S	0	0
			1132	731	194	204	3		

- Molecule 5 is a protein called PsaE.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	E	66	Total	C	N	O	0	0
			528	336	93	99		

- Molecule 6 is a protein called PsaF.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	154	Total	C	N	O	S	0	0
			1206	782	207	215	2		

- Molecule 7 is a protein called PsaG.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	G	97	Total	C	N	O	0	0
			757	492	125	140		

- Molecule 8 is a protein called PsaH.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	H	88	Total	C	N	O	0	0
			673	442	106	125		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	31	Total	C	N	O	S	0	0
			240	165	38	36	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	42	Total	C	N	O	S	0	0
			338	231	51	55	1		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	32	PHE	LEU	conflict	UNP D5MAL3

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	81	Total	C	N	O	S	0	0
			569	362	99	105	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	86	ALA	VAL	conflict	UNP E1C9L3

- Molecule 12 is a protein called PsaL.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	157	Total	C	N	O	S	0	0
			1174	772	189	212	1		

- Molecule 13 is a protein called Lhca1.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	1	193	Total	C	N	O	S	0	0
			1508	982	252	269	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	2	208	Total	C	N	O	S	0	0
			1620	1059	265	292	4		

- Molecule 15 is a protein called Chlorophyll a-b binding protein 3, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	3	221	Total	C	N	O	S	0	0
			1706	1118	278	305	5		

- Molecule 16 is a protein called Chlorophyll a-b binding protein P4, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	4	198	Total	C	N	O	S	0	0
			1559	1022	253	281	3		

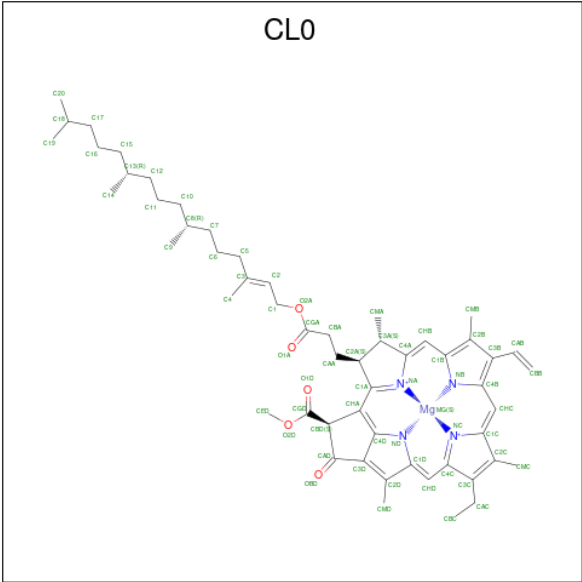
There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
4	89	LYS	ARG	conflict	UNP Q9SQL2
4	128	ASP	ALA	conflict	UNP Q9SQL2
4	149	PHE	SER	conflict	UNP Q9SQL2

- Molecule 17 is a protein called Ferredoxin-1, chloroplastic.

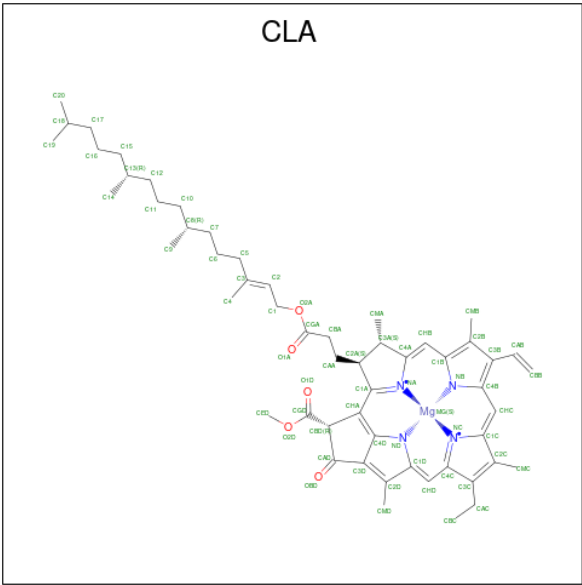
Mol	Chain	Residues	Atoms					AltConf	Trace
17	N	97	Total	C	N	O	S	0	0
			724	448	111	160	5		

- Molecule 18 is CHLOROPHYLL A ISOMER (CCD ID: CL0) (formula: C₅₅H₇₂MgN₄O₅).



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

- Molecule 19 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



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

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Mol	Chain	Residues	Atoms					AltConf
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
19	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
19	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	B	1	Total 58	C 48	Mg 1	N 4	O 5	0
19	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
19	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
19	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
19	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	B	1	Total 50	C 40	Mg 1	N 4	O 5	0
19	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	F	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	F	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
19	G	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
19	G	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
19	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	G	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
19	J	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
19	K	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
19	K	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
19	K	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
19	K	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
19	L	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
19	L	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
19	L	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
19	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	1	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
19	1	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
19	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	1	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
19	1	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
19	1	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
19	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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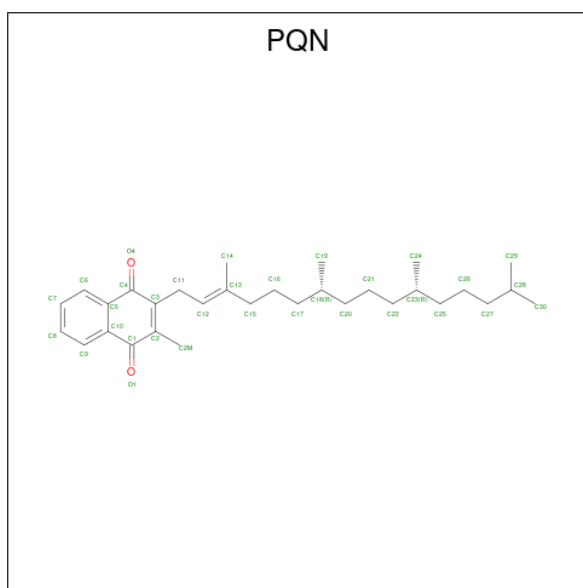
Mol	Chain	Residues	Atoms					AltConf
19	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
19	1	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
19	2	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
19	2	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
19	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	2	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
19	2	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
19	2	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
19	2	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
19	3	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
19	3	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
19	3	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
19	3	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
19	3	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
19	3	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
19	3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	3	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
19	3	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
19	3	1	Total	C	Mg	N	O	0
			42	34	1	4	3	

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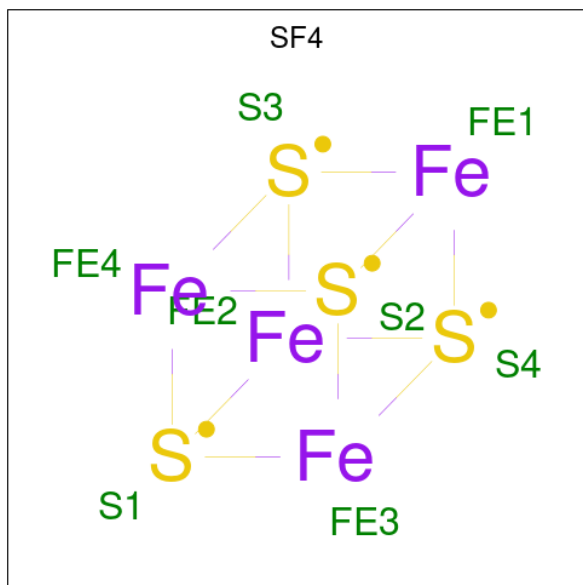
Mol	Chain	Residues	Atoms					AltConf
19	3	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
19	4	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
19	4	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
19	4	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	4	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
19	4	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
19	4	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
19	4	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
19	4	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
19	4	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
19	4	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	4	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

- Molecule 20 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$).



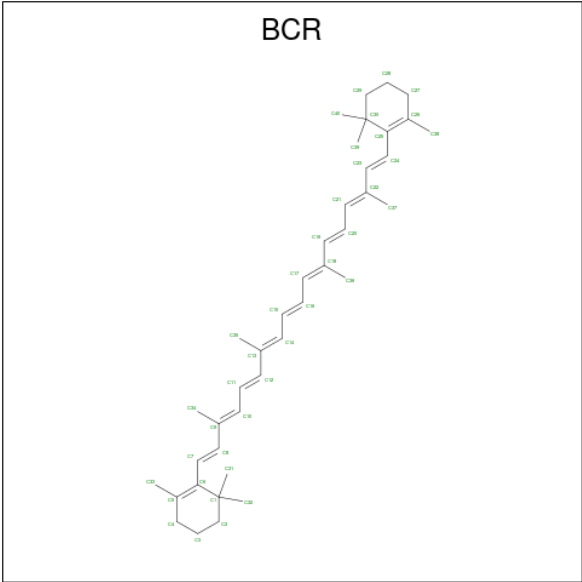
Mol	Chain	Residues	Atoms			AltConf
20	A	1	Total	C	O	0
			33	31	2	
20	B	1	Total	C	O	0
			33	31	2	

- Molecule 21 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



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

- Molecule 22 is BETA-CAROTENE (CCD ID: BCR) (formula: $\text{C}_{40}\text{H}_{56}$).



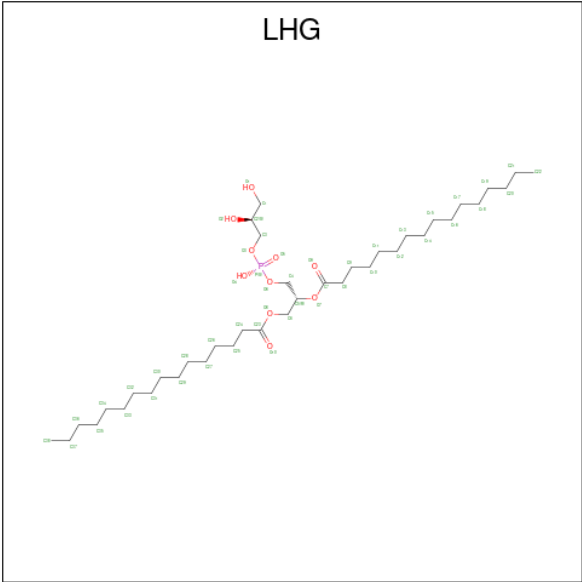
Mol	Chain	Residues	Atoms		AltConf
22	A	1	Total	C	0
			40	40	
22	A	1	Total	C	0
			40	40	
22	A	1	Total	C	0
			40	40	
22	A	1	Total	C	0
			40	40	
22	A	1	Total	C	0
			40	40	
22	A	1	Total	C	0
			40	40	
22	B	1	Total	C	0
			40	40	
22	B	1	Total	C	0
			40	40	
22	B	1	Total	C	0
			40	40	
22	B	1	Total	C	0
			40	40	
22	B	1	Total	C	0
			40	40	
22	F	1	Total	C	0
			40	40	
22	F	1	Total	C	0
			40	40	
22	G	1	Total	C	0
			40	40	

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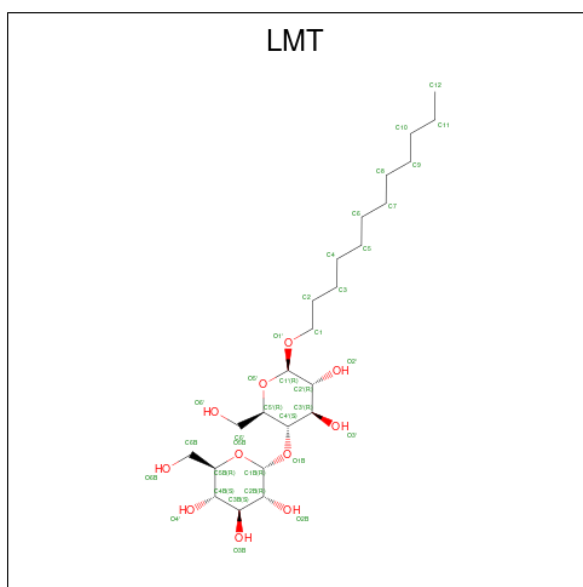
Mol	Chain	Residues	Atoms	AltConf
22	G	1	Total C 40 40	0
22	I	1	Total C 40 40	0
22	I	1	Total C 40 40	0
22	J	1	Total C 40 40	0
22	K	1	Total C 40 40	0
22	K	1	Total C 40 40	0
22	L	1	Total C 40 40	0
22	L	1	Total C 40 40	0
22	1	1	Total C 40 40	0
22	1	1	Total C 40 40	0
22	2	1	Total C 40 40	0
22	3	1	Total C 40 40	0
22	3	1	Total C 40 40	0

- Molecule 23 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).



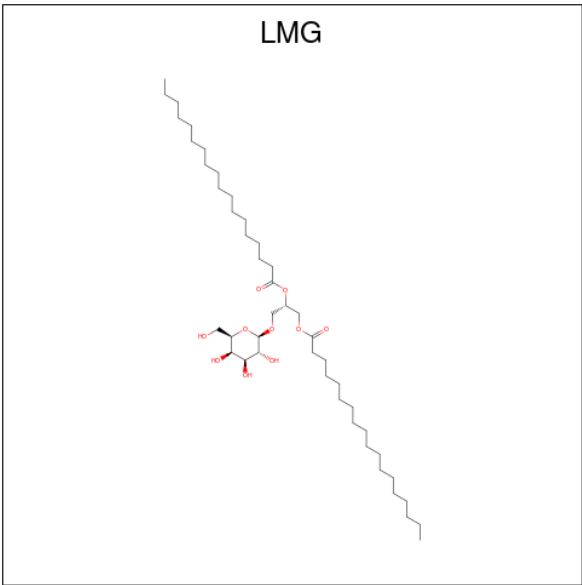
Mol	Chain	Residues	Atoms				AltConf
23	A	1	Total	C	O	P	0
			40	29	10	1	
23	A	1	Total	C	O	P	0
			49	38	10	1	
23	B	1	Total	C	O	P	0
			21	10	10	1	
23	B	1	Total	C	O	P	0
			49	38	10	1	
23	1	1	Total	C	O	P	0
			49	38	10	1	
23	2	1	Total	C	O	P	0
			35	24	10	1	
23	2	1	Total	C	O	P	0
			33	22	10	1	
23	3	1	Total	C	O	P	0
			17	8	8	1	

- Molecule 24 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: C₂₄H₄₆O₁₁).



Mol	Chain	Residues	Atoms			AltConf
24	A	1	Total 35	C 24	O 11	0
24	B	1	Total 32	C 21	O 11	0
24	B	1	Total 31	C 20	O 11	0
24	G	1	Total 35	C 24	O 11	0
24	G	1	Total 31	C 20	O 11	0
24	J	1	Total 25	C 14	O 11	0

- Molecule 25 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



Mol	Chain	Residues	Atoms			AltConf
25	A	1	Total	C	O	0
			50	40	10	
25	B	1	Total	C	O	0
			35	25	10	
25	B	1	Total	C	O	0
			33	23	10	
25	B	1	Total	C	O	0
			34	24	10	
25	F	1	Total	C	O	0
			30	20	10	
25	F	1	Total	C	O	0
			47	37	10	
25	F	1	Total	C	O	0
			36	26	10	
25	F	1	Total	C	O	0
			34	24	10	
25	F	1	Total	C	O	0
			13	7	6	
25	G	1	Total	C	O	0
			49	39	10	
25	G	1	Total	C	O	0
			50	40	10	
25	G	1	Total	C	O	0
			25	15	10	
25	1	1	Total	C	O	0
			46	36	10	
25	2	1	Total	C	O	0
			25	15	10	

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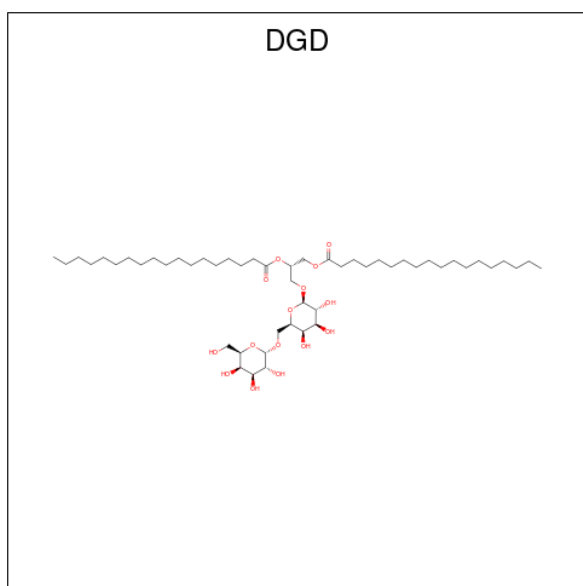
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Mol	Chain	Residues	Atoms			AltConf
25	2	1	Total	C	O	0
			36	26	10	
25	2	1	Total	C	O	0
			30	20	10	
25	2	1	Total	C	O	0
			13	7	6	
25	2	1	Total	C	O	0
			13	7	6	
25	3	1	Total	C	O	0
			30	20	10	

- Molecule 26 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
26	A	1	Total	Ca	0
			1	1	
26	B	1	Total	Ca	0
			1	1	

- Molecule 27 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: C₅₁H₉₆O₁₅).



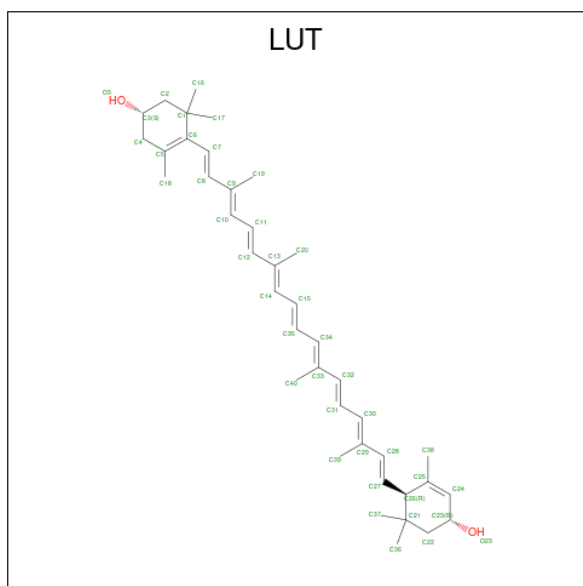
Mol	Chain	Residues	Atoms			AltConf
27	B	1	Total	C	O	0
			61	46	15	
27	F	1	Total	C	O	0
			57	42	15	

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Mol	Chain	Residues	Atoms			AltConf
27	G	1	Total	C	O	0
			47	32	15	
27	J	1	Total	C	O	0
			58	43	15	
27	1	1	Total	C	O	0
			41	26	15	
27	3	1	Total	C	O	0
			51	36	15	
27	4	1	Total	C	O	0
			51	36	15	
27	4	1	Total	C	O	0
			51	36	15	

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



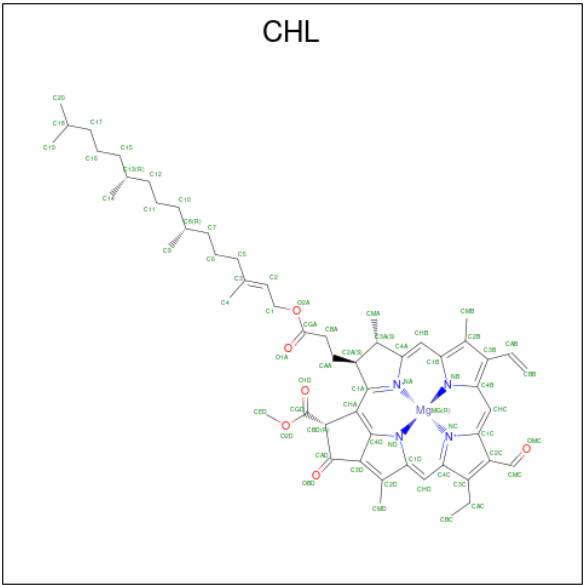
Mol	Chain	Residues	Atoms			AltConf
28	J	1	Total	C	O	0
			42	40	2	
28	1	1	Total	C	O	0
			42	40	2	
28	1	1	Total	C	O	0
			42	40	2	
28	2	1	Total	C	O	0
			42	40	2	
28	3	1	Total	C	O	0
			42	40	2	

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Mol	Chain	Residues	Atoms			AltConf
28	3	1	Total	C	O	0
			42	40	2	
28	4	1	Total	C	O	0
			42	40	2	

- Molecule 29 is CHLOROPHYLL B (CCD ID: CHL) (formula: C₅₅H₇₀MgN₄O₆).



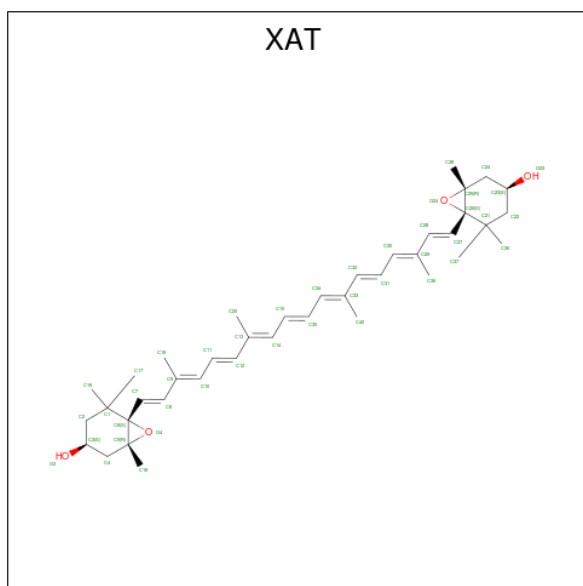
Mol	Chain	Residues	Atoms						AltConf
29	1	1	Total	C	Mg	N	O	0	
			56	45	1	4	6		
29	1	1	Total	C	Mg	N	O	0	
			47	36	1	4	6		
29	1	1	Total	C	Mg	N	O	0	
			61	50	1	4	6		
29	2	1	Total	C	Mg	N	O	0	
			66	55	1	4	6		
29	2	1	Total	C	Mg	N	O	0	
			56	45	1	4	6		
29	2	1	Total	C	Mg	N	O	0	
			48	37	1	4	6		
29	2	1	Total	C	Mg	N	O	0	
			46	35	1	4	6		
29	2	1	Total	C	Mg	N	O	0	
			56	45	1	4	6		
29	3	1	Total	C	Mg	N	O	0	
			66	55	1	4	6		

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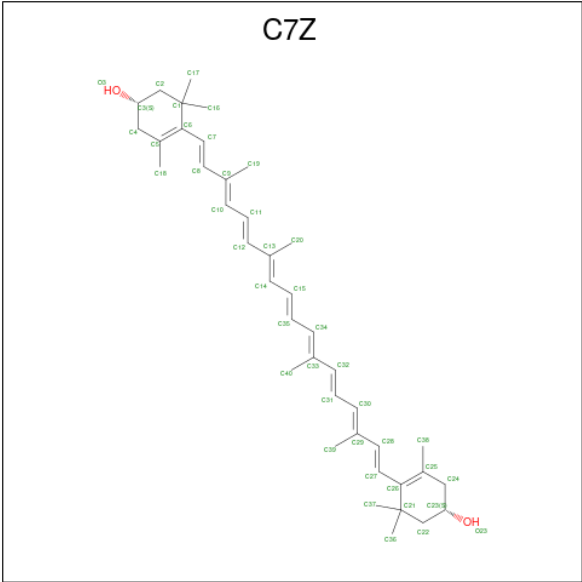
Mol	Chain	Residues	Atoms					AltConf
29	3	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
29	3	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
29	4	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
29	4	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
29	4	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
29	4	1	Total	C	Mg	N	O	0
			43	34	1	4	4	

- Molecule 30 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).



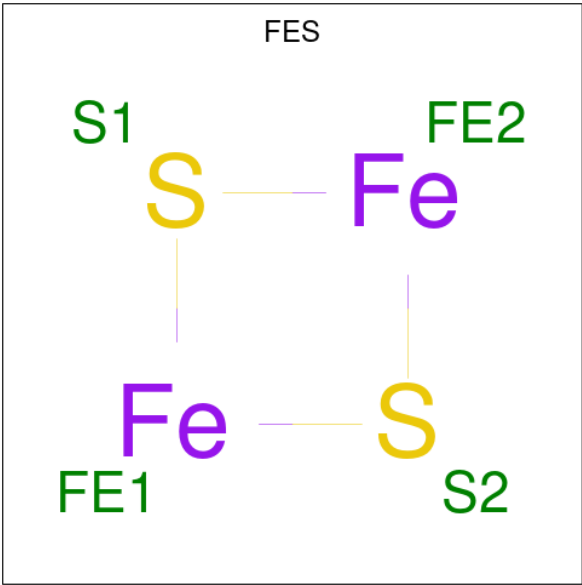
Mol	Chain	Residues	Atoms			AltConf
30	2	1	Total	C	O	0
			44	40	4	
30	4	1	Total	C	O	0
			44	40	4	

- Molecule 31 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
31	4	1	Total	C	O	0
			42	40	2	

- Molecule 32 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe₂S₂).



Mol	Chain	Residues	Atoms			AltConf
32	N	1	Total	Fe	S	0
			4	2	2	

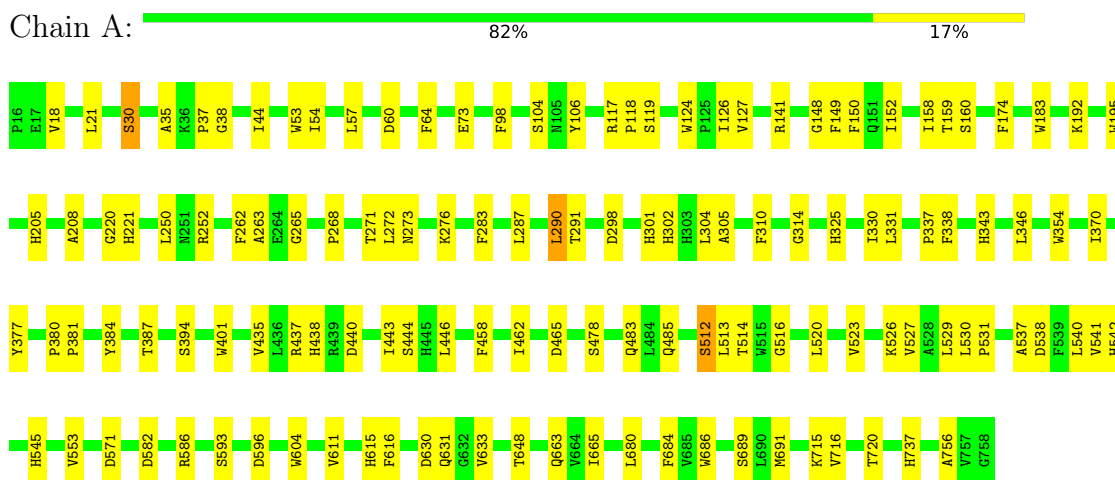
- Molecule 33 is water.

Mol	Chain	Residues	Atoms		AltConf
33	A	13	Total 13	O 13	0
33	B	15	Total 15	O 15	0
33	C	2	Total 2	O 2	0
33	D	1	Total 1	O 1	0
33	F	3	Total 3	O 3	0
33	G	4	Total 4	O 4	0
33	I	1	Total 1	O 1	0
33	J	2	Total 2	O 2	0
33	K	1	Total 1	O 1	0
33	L	3	Total 3	O 3	0
33	1	5	Total 5	O 5	0
33	2	2	Total 2	O 2	0
33	3	3	Total 3	O 3	0
33	4	1	Total 1	O 1	0

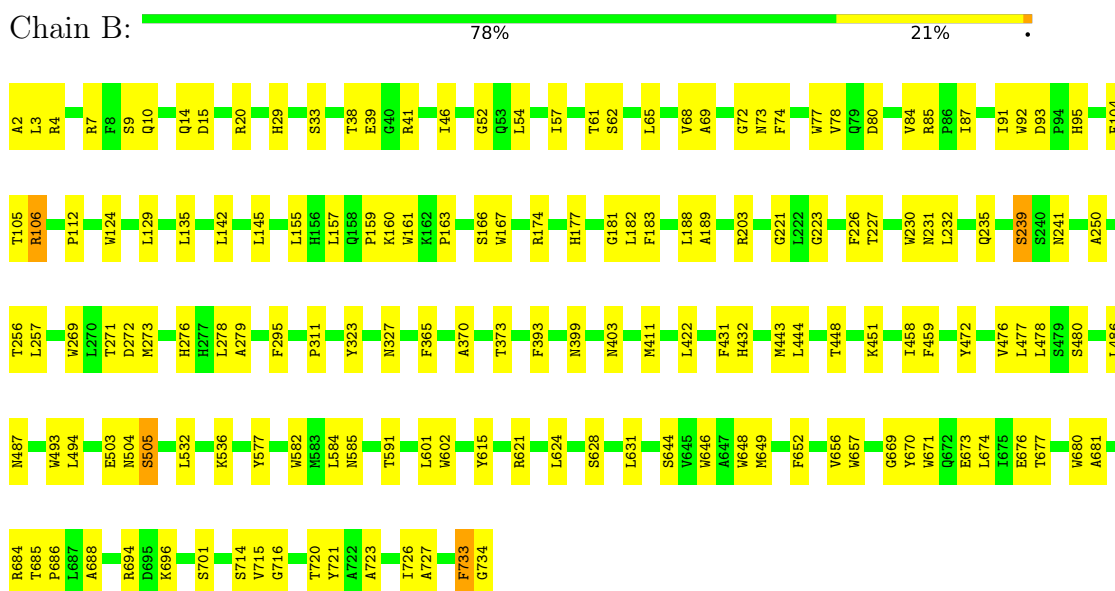
3 Residue-property plots

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

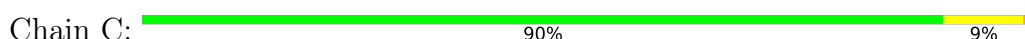
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2



- Molecule 3: Photosystem I iron-sulfur center





- Molecule 4: PsaD

Chain D: 77% 22%



- Molecule 5: PsaE

Chain E: 88% 12%



- Molecule 6: PsaF

Chain F: 73% 26%



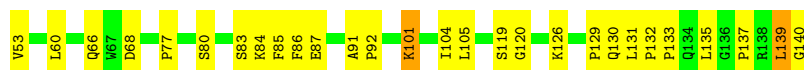
- Molecule 7: PsaG

Chain G: 82% 15%



- Molecule 8: PsaH

Chain H: 68% 30%




- Molecule 9: Photosystem I reaction center subunit VIII

Chain I: 81% 16%



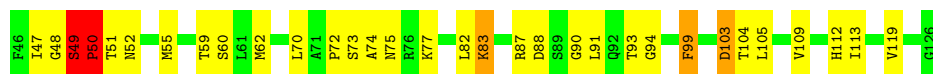
- Molecule 10: Photosystem I reaction center subunit IX

Chain J:  88% 12%



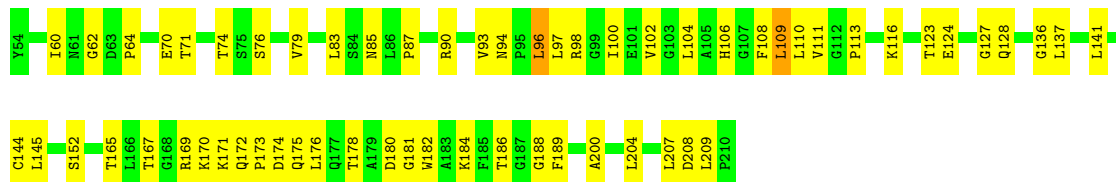
- Molecule 11: Photosystem I reaction center subunit X psaK

Chain K:  60% 33% . .



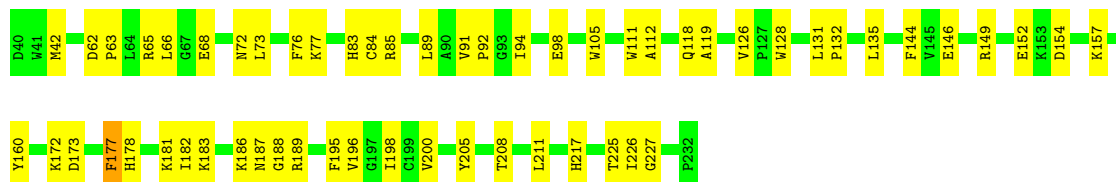
- Molecule 12: PsaL

Chain L:  62% 37% .



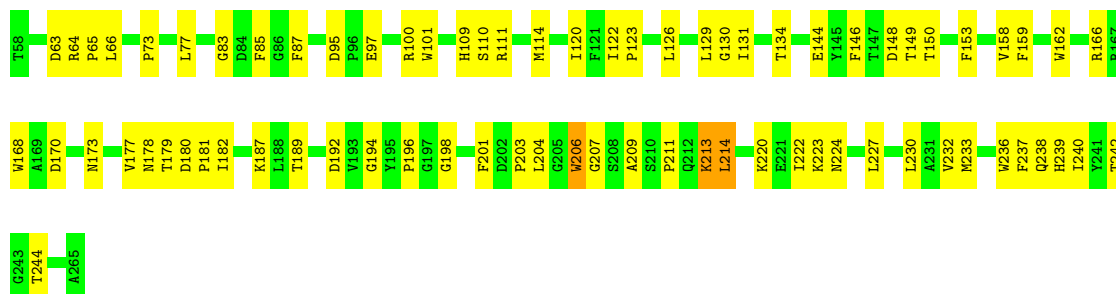
- Molecule 13: Lhca1

Chain 1:  70% 29% .



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

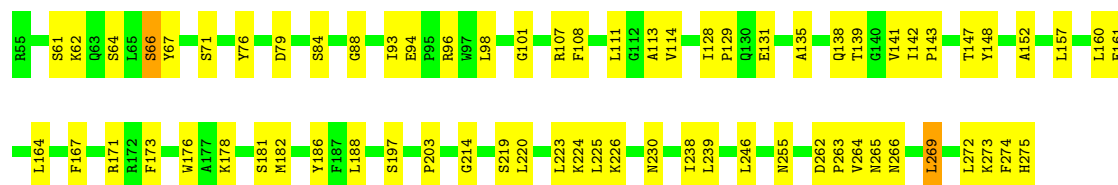
Chain 2:  64% 34% .



- Molecule 15: Chlorophyll a-b binding protein 3, chloroplastic

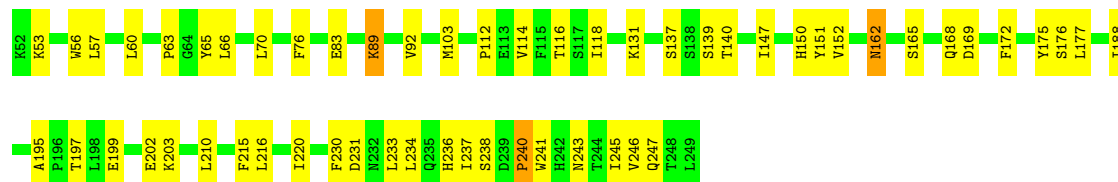
Chain 3:  69% 30% .





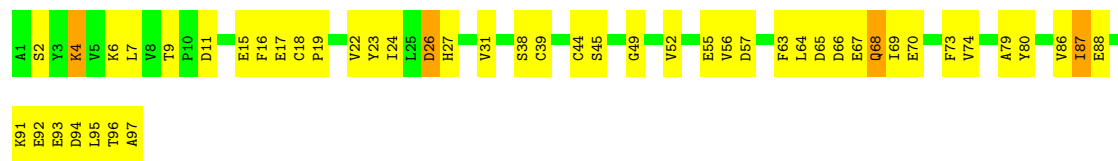
- Molecule 16: Chlorophyll a-b binding protein P4, chloroplastic

Chain 4: 72% 27%



- Molecule 17: Ferredoxin-1, chloroplastic

Chain N: 51% 45%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	269657	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 ($e^-/\text{\AA}^2$)	1.075	Depositor
Minimum defocus (nm)	900	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CL0, C7Z, FES, CA, CHL, DGD, LMG, LMT, CLA, BCR, SF4, LHG, XAT, LUT, PQN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.41	1/6057 (0.0%)	0.49	0/8264
2	B	0.38	0/6069	0.49	0/8286
3	C	0.36	0/625	0.51	0/846
4	D	0.38	0/1163	0.53	0/1572
5	E	0.39	0/540	0.48	0/734
6	F	0.49	1/1234 (0.1%)	0.57	0/1670
7	G	0.36	0/776	0.47	0/1054
8	H	0.36	0/693	0.57	0/942
9	I	0.36	0/246	0.49	0/335
10	J	0.34	0/349	0.43	0/476
11	K	0.71	2/576 (0.3%)	0.66	1/779 (0.1%)
12	L	0.35	0/1207	0.51	0/1651
13	1	0.34	0/1558	0.47	0/2125
14	2	0.38	0/1679	0.52	0/2302
15	3	0.35	0/1760	0.50	0/2390
16	4	0.37	0/1608	0.47	0/2191
17	N	0.42	0/736	0.60	0/1000
All	All	0.40	4/26876 (0.0%)	0.50	1/36617 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	K	50	PRO	N-CA	13.71	1.70	1.47
1	A	117	ARG	C-N	8.93	1.51	1.34
6	F	83	THR	C-N	8.57	1.50	1.34
11	K	49	SER	C-N	6.03	1.45	1.34

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	K	50	PRO	CA-N-CD	-7.88	100.47	111.50

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5858	0	5719	108	0
2	B	5857	0	5653	140	0
3	C	612	0	591	5	0
4	D	1132	0	1141	24	0
5	E	528	0	528	4	0
6	F	1206	0	1231	33	0
7	G	757	0	743	17	0
8	H	673	0	667	27	0
9	I	240	0	264	12	0
10	J	338	0	345	6	0
11	K	569	0	596	37	0
12	L	1174	0	1183	52	0
13	1	1508	0	1489	54	0
14	2	1620	0	1557	70	0
15	3	1706	0	1661	60	0
16	4	1559	0	1527	55	0
17	N	724	0	672	73	0
18	A	65	0	72	6	0
19	1	608	0	565	49	0
19	2	522	0	503	46	0
19	3	578	0	497	37	0
19	4	631	0	600	46	0
19	A	2643	0	2751	183	0
19	B	2610	0	2750	180	0
19	F	130	0	144	8	0
19	G	226	0	212	14	0
19	J	50	0	39	0	0
19	K	199	0	158	19	0
19	L	160	0	136	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	A	33	0	46	0	0
20	B	33	0	46	4	0
21	A	8	0	0	0	0
21	C	16	0	0	0	0
22	1	80	0	105	8	0
22	2	40	0	53	10	0
22	3	80	0	105	6	0
22	A	240	0	316	17	0
22	B	200	0	264	14	0
22	F	80	0	104	5	0
22	G	80	0	105	8	0
22	I	80	0	105	6	0
22	J	40	0	53	1	0
22	K	80	0	106	12	0
22	L	80	0	106	7	0
23	1	49	0	74	8	0
23	2	68	0	76	4	0
23	3	17	0	12	0	0
23	A	89	0	127	5	0
23	B	70	0	86	9	0
24	A	35	0	45	3	0
24	B	63	0	69	4	0
24	G	66	0	77	2	0
24	J	25	0	22	0	0
25	1	46	0	65	3	0
25	2	117	0	114	9	0
25	3	30	0	30	0	0
25	A	50	0	73	5	0
25	B	102	0	114	5	0
25	F	160	0	188	13	0
25	G	124	0	161	8	0
26	A	1	0	0	0	0
26	B	1	0	0	0	0
27	1	41	0	40	1	0
27	3	51	0	60	3	0
27	4	102	0	120	6	0
27	B	61	0	83	7	0
27	F	57	0	75	7	0
27	G	47	0	52	4	0
27	J	58	0	77	4	0
28	1	84	0	110	16	0
28	2	42	0	55	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	3	84	0	110	4	0
28	4	42	0	55	6	0
28	J	42	0	55	4	0
29	1	164	0	133	19	0
29	2	272	0	226	21	0
29	3	164	0	137	18	0
29	4	202	0	151	13	0
30	2	44	0	56	10	0
30	4	44	0	56	6	0
31	4	42	0	0	0	0
32	N	4	0	0	1	0
33	1	5	0	0	2	0
33	2	2	0	0	0	0
33	3	3	0	0	0	0
33	4	1	0	0	0	0
33	A	13	0	0	1	0
33	B	15	0	0	0	0
33	C	2	0	0	0	0
33	D	1	0	0	0	0
33	F	3	0	0	0	0
33	G	4	0	0	1	0
33	I	1	0	0	0	0
33	J	2	0	0	0	0
33	K	1	0	0	0	0
33	L	3	0	0	1	0
All	All	38469	0	38492	1259	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 16.

All (1259) 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)
11:K:50:PRO:N	11:K:50:PRO:CA	1.70	1.36
17:N:73:PHE:CG	17:N:95:LEU:HD23	1.75	1.19
17:N:64:LEU:CD2	17:N:69:ILE:HD11	1.80	1.12
14:2:182:ILE:HG12	19:4:607:CLA:HMB1	1.35	1.09
11:K:49:SER:H	11:K:50:PRO:CD	1.65	1.09
19:K:1401:CLA:HMB1	19:K:1401:CLA:HBB1	1.32	1.08
16:4:220:ILE:HG21	19:4:603:CLA:HAC2	1.08	1.07
17:N:52:VAL:HB	17:N:86:VAL:HG13	1.10	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:A:1135:CLA:HMB1	19:A:1135:CLA:HBB1	1.34	1.06
28:1:501:LUT:H32	19:1:601:CLA:HAB	1.37	1.05
25:2:803:LMG:H122	25:2:803:LMG:HC71	1.39	1.03
11:K:49:SER:N	11:K:50:PRO:HD2	1.70	1.03
19:K:1401:CLA:HBC3	22:K:4002:BCR:C31	1.88	1.03
11:K:49:SER:H	11:K:50:PRO:HD2	0.87	1.03
15:3:265:ASN:HA	15:3:269:LEU:HG	1.40	0.99
17:N:73:PHE:CD1	17:N:95:LEU:HD23	1.97	0.98
17:N:52:VAL:HB	17:N:86:VAL:CG1	1.93	0.97
19:B:1235:CLA:HMB1	19:B:1235:CLA:HBB1	1.49	0.94
16:4:220:ILE:HG21	19:4:603:CLA:CAC	1.96	0.94
14:2:232:VAL:HG21	30:2:502:XAT:H12	1.50	0.94
22:2:503:BCR:H312	19:4:607:CLA:HAB	1.48	0.93
19:A:1136:CLA:HBB1	19:A:1136:CLA:HHC	1.52	0.90
17:N:52:VAL:CB	17:N:86:VAL:HG13	2.03	0.86
17:N:6:LYS:HG2	17:N:86:VAL:HG23	1.57	0.85
17:N:64:LEU:HD22	17:N:69:ILE:HD11	1.58	0.85
14:2:180:ASP:OD1	14:2:181:PRO:HD2	1.78	0.84
17:N:64:LEU:HD23	17:N:69:ILE:HD11	1.57	0.84
16:4:243:ASN:HA	16:4:247:GLN:NE2	1.93	0.84
14:2:179:THR:HB	14:2:187:LYS:HD3	1.60	0.83
12:L:111:VAL:HG21	12:L:200:ALA:HB3	1.59	0.83
16:4:220:ILE:CG2	19:4:603:CLA:HAC2	2.03	0.83
19:B:1022:CLA:H193	19:B:1207:CLA:HMC2	1.61	0.83
19:A:1122:CLA:H43	22:A:4008:BCR:H351	1.61	0.82
16:4:243:ASN:HA	16:4:247:GLN:HE21	1.44	0.82
27:G:5003:DGD:HD5	13:1:132:PRO:HG2	1.62	0.82
17:N:4:LYS:HD3	17:N:15:GLU:HB3	1.61	0.82
13:1:149:ARG:NH2	29:1:612:CHL:O1D	2.13	0.81
28:2:501:LUT:H8	19:2:601:CLA:H52	1.61	0.81
19:A:1119:CLA:H52	19:A:1122:CLA:H42	1.62	0.80
19:B:1211:CLA:H3A	22:B:4006:BCR:H393	1.64	0.79
17:N:57:ASP:HB3	17:N:80:TYR:HB2	1.65	0.79
22:G:4021:BCR:HC8	22:G:4021:BCR:H311	1.65	0.79
1:A:401:TRP:CD1	19:A:1126:CLA:HAB	2.18	0.78
4:D:114:GLU:O	4:D:144:ARG:NH2	2.16	0.78
17:N:9:THR:HG22	17:N:11:ASP:H	1.48	0.78
19:A:1012:CLA:HAB	2:B:582:TRP:CH2	2.18	0.77
1:A:310:PHE:HE1	19:A:1119:CLA:HAB	1.49	0.77
2:B:472:TYR:HB3	6:F:80:ALA:HA	1.65	0.77
2:B:166:SER:HB2	7:G:95:GLN:HE22	1.49	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:394:SER:HB3	19:A:1126:CLA:HMA1	1.64	0.77
2:B:129:LEU:HD23	19:B:1211:CLA:HED2	1.67	0.76
19:A:1135:CLA:H12	19:A:1136:CLA:O1A	1.86	0.76
2:B:61:THR:HG23	2:B:142:LEU:HD13	1.68	0.76
19:G:1701:CLA:HMB2	19:L:1501:CLA:HAA1	1.68	0.76
1:A:44:ILE:HD13	1:A:57:LEU:HA	1.69	0.75
19:K:1401:CLA:HMB1	19:K:1401:CLA:CBB	2.15	0.75
1:A:21:LEU:HA	15:3:88:GLY:HA3	1.67	0.75
13:1:152:GLU:OE1	13:1:157:LYS:HB2	1.85	0.75
28:3:502:LUT:H32	29:3:604:CHL:HAB	1.69	0.75
11:K:59:THR:CG2	19:K:1401:CLA:O1A	2.35	0.74
17:N:18:CYS:HB2	17:N:27:HIS:CD2	2.23	0.74
23:1:801:LHG:H322	16:4:147:ILE:HD12	1.69	0.74
2:B:65:LEU:HD11	22:B:4006:BCR:H292	1.70	0.74
11:K:104:THR:HG21	19:K:1404:CLA:HBB2	1.69	0.74
17:N:64:LEU:HD23	17:N:69:ILE:CD1	2.17	0.74
29:1:609:CHL:H43	16:4:147:ILE:HG22	1.69	0.73
24:B:5006:LMT:H81	25:F:5002:LMG:H381	1.70	0.72
19:2:603:CLA:HMA1	19:2:608:CLA:HBC3	1.70	0.72
19:B:1226:CLA:HBB1	19:B:1226:CLA:HMB1	1.71	0.72
11:K:82:LEU:HB2	11:K:83:LYS:HD2	1.71	0.72
19:B:1201:CLA:HAA2	23:B:5002:LHG:H242	1.72	0.71
1:A:250:LEU:HD23	27:3:803:DGD:HA21	1.72	0.71
22:2:503:BCR:H292	19:2:606:CLA:H2	1.72	0.71
2:B:716:GLY:O	2:B:720:THR:HG22	1.89	0.71
7:G:107:ARG:NH1	24:G:5004:LMT:O6'	2.23	0.71
6:F:220:GLU:HG3	6:F:225:GLU:HB3	1.72	0.71
19:A:1129:CLA:HBA2	23:A:5001:LHG:HC81	1.73	0.71
19:K:1401:CLA:HBC3	22:K:4002:BCR:H313	1.71	0.71
16:4:236:HIS:ND1	16:4:243:ASN:O	2.22	0.70
19:A:1131:CLA:HBB1	19:A:1132:CLA:H2	1.73	0.70
17:N:73:PHE:CG	17:N:95:LEU:CD2	2.68	0.70
19:B:1229:CLA:HAB	19:B:1230:CLA:HMB2	1.74	0.70
19:K:1401:CLA:H2A	19:K:1401:CLA:HED2	1.74	0.70
17:N:39:CYS:N	32:N:101:FES:S1	2.64	0.70
1:A:141:ARG:NH1	6:F:109:TYR:OH	2.23	0.70
16:4:216:LEU:HD22	19:4:603:CLA:HAC1	1.73	0.70
29:2:615:CHL:HHC	29:2:615:CHL:HBB1	1.73	0.70
19:A:1130:CLA:H42	12:L:83:LEU:HD11	1.73	0.69
29:3:607:CHL:HHC	29:3:607:CHL:HBB1	1.74	0.69
1:A:520:LEU:C	1:A:520:LEU:HD23	2.13	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:A:1135:CLA:HMB1	19:A:1135:CLA:CBB	2.17	0.69
19:B:1226:CLA:H61	27:B:5005:DGD:HA92	1.73	0.69
19:B:1219:CLA:HBB2	22:B:4009:BCR:H343	1.75	0.69
19:3:601:CLA:HBB1	19:3:601:CLA:HMB1	1.75	0.69
17:N:18:CYS:HB2	17:N:27:HIS:CG	2.28	0.69
1:A:208:ALA:HB2	1:A:314:GLY:HA3	1.75	0.69
27:4:802:DGD:O5E	27:4:802:DGD:O4E	2.09	0.69
19:A:1103:CLA:HMB1	19:A:1103:CLA:HBB1	1.74	0.68
1:A:252:ARG:NH1	1:A:262:PHE:O	2.26	0.68
1:A:604:TRP:CH2	19:B:1022:CLA:HAB	2.28	0.68
11:K:105:LEU:O	11:K:109:VAL:HG23	1.92	0.68
14:2:158:VAL:HG22	19:4:609:CLA:H43	1.76	0.68
1:A:665:ILE:HD12	2:B:621:ARG:HG3	1.76	0.68
2:B:448:THR:HB	2:B:451:LYS:HG3	1.76	0.68
19:B:1206:CLA:HMB1	19:B:1206:CLA:HBB1	1.74	0.68
19:3:617:CLA:HHC	19:3:617:CLA:HBB1	1.74	0.68
17:N:73:PHE:CD2	17:N:95:LEU:HD23	2.27	0.68
25:2:803:LMG:HC71	25:2:803:LMG:C12	2.20	0.68
19:A:1107:CLA:HMB1	19:A:1107:CLA:HBB1	1.74	0.68
19:A:1110:CLA:HHC	19:A:1110:CLA:HBB1	1.74	0.68
19:A:1136:CLA:HHC	19:A:1136:CLA:CBB	2.24	0.68
2:B:93:ASP:OD1	2:B:95:HIS:ND1	2.27	0.67
14:2:159:PHE:HB3	22:2:503:BCR:H363	1.76	0.67
11:K:77:LYS:HD2	11:K:87:ARG:HH11	1.60	0.67
19:A:1101:CLA:HBB1	19:A:1101:CLA:HMB1	1.76	0.67
7:G:58:LEU:N	33:G:902:HOH:O	2.28	0.67
19:1:611:CLA:HBB1	19:1:611:CLA:HMB1	1.75	0.67
11:K:74:ALA:N	11:K:103:ASP:OD1	2.25	0.67
19:A:1105:CLA:H13	19:A:1107:CLA:H102	1.77	0.67
1:A:283:PHE:CE2	19:A:1116:CLA:HBB1	2.30	0.67
4:D:107:SER:O	4:D:107:SER:OG	2.13	0.67
27:4:801:DGD:HA81	27:4:801:DGD:HB71	1.77	0.67
19:B:1210:CLA:H172	22:B:4005:BCR:H271	1.77	0.67
19:B:1221:CLA:HMB1	19:B:1221:CLA:HBB1	1.77	0.67
14:2:239:HIS:ND1	14:2:244:THR:O	2.27	0.67
19:B:1240:CLA:HMB1	19:B:1240:CLA:HBB1	1.77	0.66
1:A:298:ASP:HB3	19:A:1116:CLA:HMA1	1.76	0.66
19:G:1603:CLA:H11	19:G:1603:CLA:H72	1.77	0.66
2:B:272:ASP:HB3	19:B:1214:CLA:HMA1	1.78	0.66
19:L:1501:CLA:HMB1	19:L:1501:CLA:HBB1	1.78	0.66
29:4:611:CHL:HHC	29:4:611:CHL:HBB1	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:N:16:PHE:HE1	17:N:27:HIS:HB3	1.61	0.66
17:N:18:CYS:HB2	17:N:27:HIS:CE1	2.31	0.66
19:B:1207:CLA:H191	9:I:15:LEU:HD12	1.78	0.66
19:2:604:CLA:HBB1	19:2:604:CLA:HMB1	1.77	0.66
19:B:1023:CLA:H143	22:I:4018:BCR:H323	1.78	0.66
16:4:233:LEU:HG	16:4:234:LEU:HD23	1.77	0.66
19:G:1602:CLA:HMB1	19:G:1602:CLA:HBB1	1.78	0.65
29:2:610:CHL:HBB2	19:2:612:CLA:HBC1	1.79	0.65
2:B:477:LEU:HD21	19:B:1232:CLA:HBC2	1.78	0.65
19:G:1701:CLA:HMB3	22:G:4021:BCR:H372	1.79	0.65
8:H:68:ASP:OD2	12:L:165:THR:HA	1.96	0.65
14:2:85:PHE:HZ	14:2:223:LYS:HE2	1.61	0.65
2:B:656:VAL:HG22	19:B:1239:CLA:HMB3	1.78	0.65
19:B:1235:CLA:HMB1	19:B:1235:CLA:CBB	2.24	0.65
19:B:1219:CLA:H111	22:B:4004:BCR:H401	1.79	0.65
14:2:180:ASP:OD1	14:2:181:PRO:CD	2.46	0.64
14:2:134:THR:OG1	19:2:606:CLA:OBD	2.15	0.64
19:2:605:CLA:H41	19:2:605:CLA:H93	1.79	0.64
19:A:1114:CLA:HHC	19:A:1114:CLA:HBB1	1.80	0.64
12:L:109:LEU:HD13	19:L:1503:CLA:HBC2	1.80	0.64
19:A:1123:CLA:HMB1	19:A:1123:CLA:HBB1	1.80	0.64
14:2:182:ILE:HG12	19:4:607:CLA:CMB	2.22	0.64
6:F:136:GLN:OE1	10:J:38:THR:OG1	2.15	0.64
6:F:203:ALA:O	6:F:207:VAL:HG13	1.98	0.64
29:3:604:CHL:HBB1	29:3:604:CHL:HMB1	1.78	0.64
19:3:617:CLA:H2A	19:3:617:CLA:HED2	1.80	0.64
1:A:387:THR:HG21	1:A:523:VAL:HB	1.80	0.63
2:B:503:GLU:OE1	2:B:505:SER:N	2.30	0.63
19:B:1227:CLA:H191	25:F:5002:LMG:H451	1.80	0.63
13:1:91:VAL:HG23	13:1:92:PRO:HD3	1.80	0.63
1:A:283:PHE:HE2	19:A:1116:CLA:HBB1	1.62	0.63
29:1:609:CHL:H42	16:4:151:TYR:HB2	1.78	0.63
14:2:237:PHE:HA	14:2:240:ILE:HG22	1.81	0.63
15:3:226:LYS:HD3	19:3:602:CLA:HBD	1.80	0.63
17:N:65:ASP:C	17:N:67:GLU:H	2.02	0.63
14:2:236:TRP:HZ2	29:2:610:CHL:H2	1.62	0.63
19:B:1211:CLA:HMB1	19:B:1211:CLA:HBB1	1.80	0.63
19:B:1220:CLA:HAB	19:B:1227:CLA:HMD2	1.79	0.63
29:2:613:CHL:HHC	29:2:613:CHL:HBB1	1.81	0.63
16:4:112:PRO:O	16:4:116:THR:HG22	1.99	0.63
19:B:1201:CLA:HMB1	19:B:1201:CLA:HBB1	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:B:1238:CLA:H61	19:B:1239:CLA:H142	1.81	0.63
27:G:5003:DGD:HD1	13:1:132:PRO:HB2	1.80	0.63
29:2:610:CHL:HBB1	29:2:610:CHL:HMB1	1.80	0.63
29:4:615:CHL:HHC	29:4:615:CHL:HBB1	1.79	0.63
2:B:7:ARG:HH12	9:I:32:LEU:HD12	1.63	0.63
23:B:5001:LHG:O3	23:B:5001:LHG:O1	2.09	0.63
12:L:124:GLU:HA	12:L:127:GLY:H	1.64	0.63
13:1:89:LEU:HG	19:1:601:CLA:HMC1	1.81	0.63
19:1:603:CLA:HBD	19:1:603:CLA:HBA1	1.79	0.63
14:2:196:PRO:HB2	14:2:201:PHE:HD2	1.64	0.62
29:1:610:CHL:HHC	29:1:610:CHL:HBB1	1.80	0.62
14:2:227:LEU:HD11	19:2:603:CLA:H171	1.81	0.62
17:N:92:GLU:O	17:N:95:LEU:HB3	1.99	0.62
1:A:715:LYS:HG3	6:F:228:ALA:HB2	1.80	0.62
19:A:1110:CLA:HBA1	19:A:1110:CLA:HBD	1.80	0.62
2:B:188:LEU:HD11	22:B:4004:BCR:H342	1.81	0.62
14:2:166:ARG:NH2	14:2:177:VAL:O	2.33	0.62
19:B:1204:CLA:H11	22:I:4018:BCR:H281	1.82	0.62
19:A:1135:CLA:C1	19:A:1136:CLA:O1A	2.47	0.62
28:1:501:LUT:C32	19:1:601:CLA:HAB	2.23	0.62
1:A:401:TRP:HD1	19:A:1126:CLA:HAB	1.63	0.62
29:1:612:CHL:HHC	29:1:612:CHL:HBB1	1.81	0.62
19:A:1106:CLA:HMB1	19:A:1106:CLA:HBB1	1.80	0.62
19:K:1401:CLA:CBC	22:K:4002:BCR:H313	2.29	0.62
19:2:603:CLA:HHC	19:2:603:CLA:HBB1	1.82	0.61
25:2:803:LMG:H131	25:2:803:LMG:O7	2.00	0.61
6:F:106:LEU:O	6:F:108:LEU:N	2.34	0.61
22:2:503:BCR:C31	19:4:607:CLA:HAB	2.25	0.61
17:N:49:GLY:O	17:N:74:VAL:N	2.32	0.61
17:N:6:LYS:CG	17:N:86:VAL:HG23	2.30	0.61
19:B:1240:CLA:HBA1	23:B:5001:LHG:HC42	1.82	0.61
19:B:1206:CLA:H91	19:B:1239:CLA:H12	1.81	0.61
19:B:1231:CLA:H62	19:B:1232:CLA:H12	1.80	0.61
19:F:1301:CLA:HBB1	19:F:1301:CLA:HMB1	1.82	0.61
19:A:1137:CLA:H121	22:A:4007:BCR:H392	1.82	0.61
2:B:311:PRO:HG2	23:B:5001:LHG:HC32	1.82	0.61
19:A:1122:CLA:H12	22:A:4007:BCR:H15C	1.82	0.60
19:B:1202:CLA:HHC	19:B:1202:CLA:HBB1	1.82	0.60
19:1:601:CLA:H92	19:1:602:CLA:HMA1	1.82	0.60
15:3:135:ALA:HB3	15:3:138:GLN:HG2	1.83	0.60
2:B:584:LEU:HD11	2:B:714:SER:HB3	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:F:5005:DGD:HE62	23:2:807:LHG:HC62	1.81	0.60
19:B:1222:CLA:HMB1	19:B:1222:CLA:HBB1	1.84	0.60
1:A:64:PHE:CD1	19:A:1103:CLA:HMC2	2.36	0.60
1:A:287:LEU:HD21	1:A:380:PRO:HD2	1.84	0.60
2:B:160:LYS:HE3	2:B:161:TRP:CZ2	2.37	0.60
14:2:111:ARG:NH1	29:2:611:CHL:OBD	2.28	0.60
17:N:16:PHE:CE1	17:N:27:HIS:HB3	2.36	0.60
1:A:183:TRP:HB2	19:A:1109:CLA:HMC3	1.82	0.60
4:D:107:SER:OG	4:D:124:ARG:O	2.14	0.60
12:L:109:LEU:O	33:L:903:HOH:O	2.17	0.60
6:F:205:GLY:HA3	27:F:5005:DGD:HE5	1.83	0.60
19:L:1503:CLA:HBB1	19:L:1503:CLA:HMB1	1.84	0.60
13:1:196:VAL:O	13:1:200:VAL:HG23	2.01	0.60
2:B:487:ASN:OD1	7:G:153:LYS:HB2	2.02	0.60
29:2:611:CHL:HHC	29:2:611:CHL:HBB1	1.83	0.60
15:3:178:LYS:HB2	15:3:181:SER:OG	2.03	0.59
19:B:1223:CLA:HBB1	19:B:1223:CLA:HMB1	1.84	0.59
6:F:138:LEU:HD21	10:J:38:THR:HG21	1.84	0.59
17:N:93:GLU:HA	17:N:96:THR:HB	1.84	0.59
11:K:62:MET:SD	19:K:1403:CLA:HMC2	2.42	0.59
1:A:272:LEU:HD22	11:K:51:THR:HG21	1.83	0.59
19:2:604:CLA:HHD	29:2:609:CHL:HBB2	1.84	0.59
19:3:602:CLA:HED2	29:3:607:CHL:H2	1.84	0.59
17:N:69:ILE:HG22	17:N:69:ILE:O	2.02	0.59
19:1:604:CLA:H71	19:1:605:CLA:HMA1	1.83	0.59
19:4:606:CLA:HBB1	19:4:606:CLA:HMB1	1.85	0.59
1:A:684:PHE:CG	22:A:4011:BCR:H363	2.38	0.59
12:L:182:TRP:O	12:L:186:THR:OG1	2.18	0.59
1:A:663:GLN:HG2	1:A:756:ALA:HB3	1.85	0.59
19:2:606:CLA:HBB1	19:2:606:CLA:HMB1	1.84	0.59
2:B:733:PHE:HB2	8:H:137:PRO:HB2	1.84	0.59
25:B:5007:LMG:O4	13:1:68:GLU:OE1	2.21	0.59
8:H:77:PRO:HG3	12:L:90:ARG:CZ	2.33	0.59
11:K:70:LEU:HA	19:K:1403:CLA:HAA2	1.84	0.59
15:3:214:GLY:HA2	15:3:219:SER:HB3	1.84	0.59
1:A:435:VAL:HA	1:A:438:HIS:CE1	2.38	0.59
15:3:107:ARG:NH1	29:3:611:CHL:OBD	2.35	0.59
2:B:694:ARG:HG3	19:B:1238:CLA:HED3	1.85	0.58
19:B:1215:CLA:CGA	19:B:1215:CLA:H3A	2.32	0.58
6:F:202:LEU:HA	27:F:5005:DGD:HE3	1.85	0.58
13:1:225:THR:OG1	33:1:901:HOH:O	2.17	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:N:49:GLY:HA2	17:N:91:LYS:HB2	1.83	0.58
25:B:5003:LMG:H181	22:F:4016:BCR:H362	1.84	0.58
13:1:118:GLN:NE2	13:1:126:VAL:O	2.36	0.58
16:4:176:SER:OG	16:4:177:LEU:N	2.35	0.58
1:A:604:TRP:HH2	19:B:1022:CLA:HAB	1.67	0.58
19:A:1105:CLA:HMA1	19:A:1106:CLA:HMB3	1.85	0.58
2:B:7:ARG:HH22	9:I:32:LEU:HD12	1.69	0.58
27:F:5005:DGD:O5D	27:F:5005:DGD:O4D	2.17	0.58
2:B:4:ARG:HE	9:I:31:ARG:CZ	2.16	0.58
7:G:146:SER:O	27:G:5003:DGD:O5E	2.17	0.58
1:A:37:PRO:HA	19:A:1101:CLA:HBC1	1.85	0.58
2:B:166:SER:HB2	7:G:95:GLN:NE2	2.17	0.58
19:K:1401:CLA:HBC3	22:K:4002:BCR:H311	1.84	0.58
28:1:502:LUT:H8	19:1:604:CLA:H61	1.84	0.58
2:B:476:VAL:HG12	2:B:477:LEU:H	1.68	0.58
19:2:604:CLA:H71	19:2:605:CLA:HMA1	1.86	0.58
1:A:541:VAL:HG11	1:A:615:HIS:CG	2.39	0.58
19:B:1230:CLA:H91	19:F:1301:CLA:HMA1	1.84	0.58
11:K:59:THR:HG23	19:K:1401:CLA:O1A	2.03	0.58
15:3:67:TYR:CE2	15:3:84:SER:HB2	2.38	0.57
16:4:233:LEU:HD12	16:4:237:ILE:HD11	1.86	0.57
19:A:1102:CLA:HMA2	19:A:1109:CLA:HMD2	1.87	0.57
19:B:1227:CLA:H62	19:B:1240:CLA:H52	1.86	0.57
11:K:77:LYS:HE3	11:K:87:ARG:HE	1.69	0.57
1:A:38:GLY:HA3	1:A:44:ILE:HG22	1.85	0.57
13:1:225:THR:HG22	19:1:603:CLA:HBA2	1.86	0.57
16:4:177:LEU:HD21	16:4:188:ILE:HG22	1.86	0.57
19:A:1123:CLA:HBA1	19:A:1127:CLA:H191	1.86	0.57
8:H:83:SER:O	8:H:87:GLU:HG2	2.05	0.57
19:A:1113:CLA:HAA1	15:3:273:LYS:HE2	1.86	0.57
1:A:159:THR:OG1	33:A:910:HOH:O	2.15	0.57
1:A:290:LEU:HD23	1:A:291:THR:HG23	1.86	0.57
1:A:689:SER:HB3	1:A:737:HIS:HB2	1.86	0.57
5:E:74:VAL:HB	5:E:125:VAL:HG13	1.86	0.57
12:L:102:VAL:HG12	12:L:189:PHE:HD1	1.69	0.57
2:B:459:PHE:HB3	19:B:1234:CLA:H42	1.87	0.57
22:G:4021:BCR:H312	8:H:84:LYS:NZ	2.19	0.57
17:N:64:LEU:CD2	17:N:69:ILE:CD1	2.66	0.57
14:2:181:PRO:HG2	22:2:503:BCR:H313	1.86	0.57
19:A:1105:CLA:HMB1	19:A:1105:CLA:HBB1	1.86	0.56
19:B:1021:CLA:HBB1	19:B:1021:CLA:HMB1	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:B:4009:BCR:H332	25:G:5001:LMG:H392	1.87	0.56
19:G:1603:CLA:H42	25:G:5002:LMG:H222	1.86	0.56
8:H:101:LYS:O	8:H:104:ILE:HG22	2.05	0.56
14:2:66:LEU:HD11	14:2:73:PRO:HD3	1.87	0.56
1:A:304:LEU:HG	19:A:1115:CLA:HAB	1.86	0.56
1:A:545:HIS:HE1	1:A:611:VAL:HG12	1.70	0.56
22:L:4019:BCR:H392	22:L:4019:BCR:H23C	1.86	0.56
13:1:226:ILE:HD12	19:1:603:CLA:C2D	2.36	0.56
22:3:506:BCR:HC7	29:3:611:CHL:HMB2	1.87	0.56
1:A:268:PRO:HG3	1:A:276:LYS:HE3	1.86	0.56
19:A:1136:CLA:HHB	19:A:1137:CLA:O1D	2.05	0.56
19:B:1207:CLA:HMD3	22:I:4018:BCR:H332	1.88	0.56
15:3:238:ILE:HG21	28:3:502:LUT:H12	1.88	0.56
19:A:1122:CLA:HMA1	19:A:1141:CLA:HAB	1.88	0.56
25:G:5002:LMG:H201	25:G:5002:LMG:H141	1.87	0.56
19:A:1113:CLA:CGA	15:3:246:LEU:HD21	2.35	0.56
17:N:65:ASP:HB3	17:N:68:GLN:HG2	1.88	0.56
13:1:66:LEU:HD13	19:1:604:CLA:H42	1.87	0.56
13:1:183:LYS:HD3	19:1:602:CLA:HBA1	1.87	0.56
29:1:609:CHL:O1A	16:4:150:HIS:ND1	2.39	0.56
16:4:168:GLN:HA	16:4:176:SER:HA	1.87	0.56
11:K:104:THR:HG21	19:K:1404:CLA:CBB	2.36	0.56
13:1:172:LYS:HG3	13:1:173:ASP:H	1.71	0.56
28:1:501:LUT:H382	19:1:601:CLA:HBA1	1.88	0.56
19:A:1101:CLA:HBB2	19:A:1109:CLA:H102	1.88	0.56
19:A:1121:CLA:HED1	11:K:77:LYS:HA	1.88	0.56
17:N:18:CYS:SG	17:N:27:HIS:CD2	2.99	0.56
19:A:1013:CLA:H122	19:A:1140:CLA:HBB1	1.88	0.55
17:N:22:VAL:HB	17:N:27:HIS:CD2	2.41	0.55
19:B:1234:CLA:H92	25:F:5002:LMG:H421	1.87	0.55
4:D:104:THR:HA	4:D:128:ASN:O	2.06	0.55
28:J:4013:LUT:H371	28:J:4013:LUT:H28	1.87	0.55
19:2:605:CLA:O2D	19:2:605:CLA:HBA2	2.05	0.55
3:C:2:SER:N	3:C:71:HIS:O	2.39	0.55
8:H:104:ILE:HG23	8:H:105:LEU:N	2.22	0.55
12:L:109:LEU:HG	12:L:110:LEU:N	2.20	0.55
1:A:272:LEU:HD23	11:K:119:VAL:HG11	1.86	0.55
2:B:399:ASN:O	2:B:403:ASN:ND2	2.37	0.55
19:B:1237:CLA:HBC1	20:B:2002:PQN:H191	1.88	0.55
29:4:613:CHL:HBB1	29:4:613:CHL:HHC	1.89	0.55
22:A:4002:BCR:H392	22:K:4001:BCR:HC8	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:B:1207:CLA:HHC	19:B:1207:CLA:HBB1	1.89	0.55
19:B:1213:CLA:C1D	19:B:1214:CLA:HBB2	2.37	0.55
14:2:63:ASP:N	14:2:63:ASP:OD1	2.39	0.55
16:4:162:ASN:O	16:4:165:SER:OG	2.22	0.55
16:4:245:ILE:HD12	19:4:603:CLA:H42	1.87	0.55
19:A:1111:CLA:HMC1	19:A:1111:CLA:HBC2	1.89	0.55
2:B:685:THR:HG23	2:B:688:ALA:HB3	1.88	0.55
19:B:1218:CLA:C1D	22:B:4004:BCR:H402	2.37	0.55
2:B:124:TRP:HB3	2:B:129:LEU:HD12	1.89	0.55
2:B:256:THR:HG23	2:B:271:THR:HB	1.88	0.55
2:B:694:ARG:HH22	9:I:31:ARG:HD3	1.71	0.55
11:K:49:SER:N	11:K:50:PRO:CD	2.44	0.55
29:2:609:CHL:HHC	29:2:609:CHL:HBB1	1.87	0.55
1:A:354:TRP:HB3	19:A:1103:CLA:HAC1	1.89	0.55
2:B:458:ILE:HD13	6:F:151:SER:HB3	1.89	0.55
13:1:85:ARG:HB3	19:1:601:CLA:HBC3	1.88	0.55
29:1:609:CHL:HHC	29:1:609:CHL:HBB1	1.89	0.55
12:L:204:LEU:HD12	12:L:204:LEU:O	2.06	0.55
13:1:183:LYS:O	13:1:187:ASN:ND2	2.32	0.55
6:F:213:TRP:CD1	6:F:214:PRO:HD3	2.42	0.54
13:1:146:GLU:HG2	29:1:612:CHL:C1B	2.38	0.54
2:B:9:SER:HG	27:B:5005:DGD:HO4E	1.53	0.54
2:B:278:LEU:HG	19:B:1213:CLA:HAB	1.89	0.54
19:B:1202:CLA:H8	19:B:1221:CLA:HBA2	1.88	0.54
19:L:1502:CLA:HAC2	22:L:4019:BCR:H382	1.88	0.54
14:2:189:THR:HG22	14:2:189:THR:O	2.07	0.54
14:2:223:LYS:NZ	23:2:801:LHG:O5	2.32	0.54
19:A:1136:CLA:C1A	19:A:1136:CLA:CGA	2.86	0.54
8:H:120:GLY:N	8:H:126:LYS:HE2	2.23	0.54
17:N:6:LYS:HB3	17:N:86:VAL:HA	1.90	0.54
14:2:126:LEU:O	14:2:131:ILE:HB	2.08	0.54
19:B:1208:CLA:HHC	19:B:1208:CLA:HBB1	1.89	0.54
13:1:94:ILE:HG12	28:1:502:LUT:H24	1.90	0.54
22:1:504:BCR:H24C	19:1:613:CLA:HAA1	1.89	0.54
19:2:603:CLA:HMC2	19:2:603:CLA:H8	1.88	0.54
17:N:93:GLU:O	17:N:97:ALA:N	2.37	0.54
19:B:1229:CLA:H8	19:B:1229:CLA:H2	1.89	0.54
14:2:230:LEU:HB3	19:2:603:CLA:HBB2	1.90	0.54
19:A:1112:CLA:HBA2	19:A:1114:CLA:HMB3	1.88	0.54
19:A:1119:CLA:HMB2	19:A:1123:CLA:HMA3	1.90	0.54
19:B:1222:CLA:HAA2	19:B:1223:CLA:OBD	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:2:87:PHE:HB3	19:2:604:CLA:C3D	2.38	0.54
14:2:196:PRO:HD2	19:2:601:CLA:OBD	2.08	0.54
1:A:268:PRO:HA	1:A:271:THR:OG1	2.09	0.53
19:B:1219:CLA:HBB1	19:B:1219:CLA:HMB1	1.89	0.53
6:F:78:ASP:HB3	6:F:82:LEU:O	2.09	0.53
19:A:1109:CLA:H202	23:A:5002:LHG:H212	1.89	0.53
19:A:1111:CLA:H201	19:3:605:CLA:H71	1.90	0.53
2:B:721:TYR:HB2	19:B:1021:CLA:HED3	1.90	0.53
4:D:78:ASN:HA	8:H:53:VAL:HG11	1.90	0.53
23:1:801:LHG:C32	16:4:147:ILE:HD12	2.39	0.53
19:2:604:CLA:HBC1	23:2:801:LHG:H291	1.90	0.53
11:K:88:ASP:OD1	11:K:88:ASP:N	2.39	0.53
14:2:111:ARG:HG2	19:2:601:CLA:C4C	2.39	0.53
19:4:604:CLA:H71	19:4:605:CLA:HMA1	1.90	0.53
1:A:437:ARG:HG2	4:D:87:SER:HB3	1.90	0.53
1:A:586:ARG:NH2	4:D:136:GLU:OE1	2.42	0.53
2:B:631:LEU:HD13	2:B:727:ALA:HB3	1.91	0.53
12:L:113:PRO:HG3	19:L:1503:CLA:CAB	2.38	0.53
19:4:605:CLA:O1D	19:4:605:CLA:H12	2.08	0.53
12:L:116:LYS:HE2	12:L:209:LEU:HD21	1.91	0.53
19:1:601:CLA:CGA	19:1:601:CLA:H3A	2.39	0.53
14:2:159:PHE:HB3	22:2:503:BCR:H16C	1.89	0.53
19:3:601:CLA:H71	19:3:602:CLA:HMA1	1.91	0.53
28:4:501:LUT:H373	19:4:601:CLA:H51	1.91	0.53
19:4:609:CLA:HBC1	27:4:801:DGD:HE2	1.89	0.53
12:L:108:PHE:CD2	12:L:200:ALA:HB2	2.43	0.53
28:1:502:LUT:H381	19:1:606:CLA:HBB1	1.91	0.53
15:3:114:VAL:HG13	19:3:606:CLA:HBC2	1.91	0.53
19:A:1134:CLA:H12	19:K:1402:CLA:H52	1.90	0.53
22:A:4007:BCR:H24C	25:A:5006:LMG:H382	1.91	0.53
2:B:486:LEU:HD12	2:B:494:LEU:HD13	1.91	0.53
2:B:715:VAL:HA	27:B:5005:DGD:HBV2	1.91	0.53
4:D:201:VAL:HG21	4:D:208:PRO:HD3	1.91	0.53
22:2:503:BCR:C8	29:2:615:CHL:HBB2	2.39	0.53
1:A:310:PHE:CE1	19:A:1119:CLA:HAB	2.38	0.53
2:B:166:SER:CB	7:G:95:GLN:HE22	2.20	0.52
19:B:1237:CLA:H152	12:L:141:LEU:HD23	1.91	0.52
10:J:10:VAL:HG13	10:J:12:PRO:HD2	1.90	0.52
28:3:501:LUT:H30	19:3:601:CLA:H61	1.91	0.52
17:N:95:LEU:HD13	17:N:95:LEU:C	2.28	0.52
19:A:1109:CLA:HBB1	19:A:1109:CLA:HHC	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:A:4017:BCR:H362	19:B:1023:CLA:H122	1.91	0.52
2:B:57:ILE:O	2:B:61:THR:HG22	2.09	0.52
12:L:102:VAL:HG12	12:L:189:PHE:CD1	2.45	0.52
15:3:188:LEU:HD12	22:3:503:BCR:H342	1.92	0.52
16:4:241:TRP:CE3	19:4:608:CLA:HMA1	2.44	0.52
17:N:18:CYS:HB2	17:N:27:HIS:NE2	2.24	0.52
29:3:604:CHL:H2	29:3:604:CHL:O1A	2.09	0.52
19:B:1211:CLA:H3A	22:B:4006:BCR:C39	2.37	0.52
4:D:91:LEU:HD22	4:D:95:ALA:HB2	1.92	0.52
6:F:93:LYS:HA	6:F:96:LYS:HE3	1.91	0.52
13:1:154:ASP:HB3	13:1:157:LYS:H	1.73	0.52
6:F:213:TRP:CG	6:F:214:PRO:HD3	2.45	0.52
12:L:128:GLN:HG2	12:L:204:LEU:HD22	1.91	0.52
13:1:111:TRP:CZ2	13:1:119:ALA:HB2	2.43	0.52
19:A:1117:CLA:HMB1	19:A:1117:CLA:HBB1	1.91	0.52
19:A:1130:CLA:HMB1	19:A:1130:CLA:HBB1	1.92	0.52
22:A:4008:BCR:HC7	19:K:1402:CLA:H122	1.91	0.52
16:4:203:LYS:HD3	19:4:602:CLA:HBA2	1.90	0.52
1:A:252:ARG:HH12	1:A:263:ALA:HA	1.74	0.52
19:A:1103:CLA:HMC3	19:A:1128:CLA:HMA1	1.92	0.52
19:A:1111:CLA:HMB1	19:A:1111:CLA:HBB1	1.92	0.52
19:B:1201:CLA:HBC1	27:B:5005:DGD:HAT1	1.92	0.52
13:1:173:ASP:O	13:1:177:PHE:HB2	2.10	0.52
29:1:610:CHL:HBB2	19:1:613:CLA:HBB2	1.92	0.52
15:3:255:ASN:ND2	19:3:603:CLA:O1D	2.41	0.52
16:4:234:LEU:HA	16:4:237:ILE:HG12	1.90	0.52
2:B:370:ALA:HB1	19:B:1224:CLA:HMA1	1.92	0.52
22:1:503:BCR:H271	19:4:606:CLA:NB	2.25	0.52
14:2:150:THR:HG23	16:4:246:VAL:HG11	1.91	0.52
17:N:6:LYS:NZ	17:N:86:VAL:CG2	2.73	0.52
1:A:325:HIS:HB3	1:A:330:ILE:HD11	1.92	0.51
2:B:232:LEU:HA	2:B:235:GLN:HG2	1.92	0.51
14:2:129:LEU:HD23	14:2:130:GLY:N	2.24	0.51
19:B:1209:CLA:HBB1	19:B:1209:CLA:HMB1	1.92	0.51
19:B:1234:CLA:HMB1	19:B:1234:CLA:HBB1	1.92	0.51
6:F:201:PRO:HB3	25:F:5006:LMG:HC1	1.92	0.51
11:K:112:HIS:CE1	22:K:4002:BCR:H14C	2.45	0.51
19:A:1106:CLA:HMC3	19:A:1107:CLA:HMD2	1.91	0.51
15:3:173:PHE:O	15:3:176:TRP:N	2.43	0.51
19:A:1119:CLA:HBA1	19:A:1123:CLA:C3B	2.40	0.51
2:B:2:ALA:O	2:B:3:LEU:HG	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:167:TRP:CZ2	19:B:1208:CLA:HMA1	2.46	0.51
19:B:1229:CLA:CAB	19:B:1230:CLA:HMB2	2.40	0.51
4:D:146:ARG:NH1	4:D:176:GLU:OE2	2.39	0.51
19:3:610:CLA:HMB1	19:3:610:CLA:HBB1	1.92	0.51
19:A:1012:CLA:HAB	2:B:582:TRP:HH2	1.73	0.51
19:4:604:CLA:HBB1	19:4:604:CLA:HMB1	1.92	0.51
17:N:68:GLN:OE1	17:N:68:GLN:HA	2.10	0.51
1:A:483:GLN:HB3	1:A:485:GLN:HE21	1.76	0.51
2:B:73:ASN:HB2	2:B:87:ILE:HB	1.93	0.51
11:K:93:THR:OG1	11:K:94:GLY:N	2.44	0.51
13:1:186:LYS:NZ	23:1:801:LHG:O5	2.28	0.51
1:A:30:SER:O	19:A:1109:CLA:HBB	2.11	0.51
2:B:29:HIS:HB2	19:B:1226:CLA:O1A	2.11	0.51
2:B:279:ALA:HA	19:B:1213:CLA:HMC3	1.93	0.51
6:F:153:ASP:OD2	6:F:154:GLN:N	2.44	0.51
1:A:440:ASP:O	1:A:444:SER:OG	2.27	0.51
13:1:62:ASP:O	13:1:65:ARG:NH1	2.44	0.51
13:1:198:ILE:HG13	28:1:501:LUT:H163	1.93	0.51
22:1:503:BCR:H16C	16:4:152:VAL:HG11	1.93	0.51
19:A:1115:CLA:C4D	19:A:1115:CLA:H12	2.41	0.51
15:3:230:ASN:ND2	29:3:607:CHL:HMD1	2.25	0.51
19:A:1108:CLA:HBB1	19:A:1108:CLA:HMB1	1.92	0.50
2:B:68:VAL:HG21	2:B:124:TRP:HZ3	1.75	0.50
13:1:186:LYS:HG2	23:1:801:LHG:HC81	1.93	0.50
1:A:195:TRP:CZ2	19:A:1111:CLA:HBC3	2.46	0.50
1:A:443:ILE:HG22	2:B:677:THR:HG21	1.92	0.50
2:B:10:GLN:OE1	2:B:14:GLN:NE2	2.36	0.50
19:B:1203:CLA:HMB1	19:B:1203:CLA:HBB1	1.93	0.50
4:D:110:GLU:HG2	4:D:124:ARG:HA	1.93	0.50
15:3:161:GLU:HG3	19:3:613:CLA:CHB	2.41	0.50
15:3:220:LEU:HG	15:3:224:LYS:HE3	1.93	0.50
6:F:106:LEU:HB2	6:F:119:ILE:HG21	1.93	0.50
6:F:205:GLY:HA3	27:F:5005:DGD:C5E	2.42	0.50
27:F:5005:DGD:HA42	27:F:5005:DGD:HB22	1.94	0.50
15:3:171:ARG:NH2	15:3:182:MET:HB3	2.26	0.50
16:4:199:GLU:O	16:4:203:LYS:HG3	2.11	0.50
29:4:610:CHL:HHC	29:4:610:CHL:HBB1	1.93	0.50
19:A:1117:CLA:H192	19:A:1125:CLA:H11	1.94	0.50
2:B:221:GLY:O	24:B:5008:LMT:O2B	2.19	0.50
25:G:5001:LMG:H162	29:1:612:CHL:HBA1	1.93	0.50
12:L:85:ASN:HB3	19:L:1501:CLA:HAC1	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:1:112:ALA:HB3	29:1:610:CHL:HMD3	1.92	0.50
14:2:114:MET:SD	19:2:601:CLA:HAB	2.52	0.50
17:N:93:GLU:HA	17:N:96:THR:CB	2.42	0.50
1:A:582:ASP:OD1	1:A:586:ARG:NH1	2.34	0.50
1:A:689:SER:HB3	1:A:737:HIS:CB	2.42	0.50
6:F:128:ARG:CZ	25:F:5004:LMG:HC5	2.42	0.50
23:1:801:LHG:H342	16:4:147:ILE:HD11	1.92	0.50
30:2:502:XAT:H8	30:2:502:XAT:H161	1.94	0.50
19:4:604:CLA:CGA	19:4:604:CLA:H3A	2.42	0.50
22:A:4002:BCR:H362	22:A:4003:BCR:H10C	1.93	0.50
16:4:238:SER:O	16:4:240:PRO:HD3	2.12	0.50
1:A:21:LEU:HB3	1:A:192:LYS:HD2	1.94	0.49
2:B:422:LEU:HD13	2:B:532:LEU:HA	1.95	0.49
19:B:1237:CLA:H202	22:L:4019:BCR:H391	1.93	0.49
19:L:1501:CLA:HBA1	19:L:1501:CLA:CHA	2.42	0.49
17:N:86:VAL:HG13	17:N:86:VAL:O	2.12	0.49
1:A:331:LEU:O	1:A:343:HIS:HB2	2.12	0.49
2:B:670:TYR:OH	19:B:1023:CLA:OBD	2.24	0.49
25:G:5002:LMG:HC61	33:1:904:HOH:O	2.12	0.49
19:A:1013:CLA:C20	19:A:1140:CLA:H2	2.43	0.49
19:A:1120:CLA:H62	19:A:1121:CLA:H12	1.94	0.49
19:B:1205:CLA:HBA1	19:B:1224:CLA:OBD	2.12	0.49
8:H:84:LYS:HE2	8:H:85:PHE:N	2.26	0.49
16:4:202:GLU:HB3	27:4:801:DGD:O3D	2.12	0.49
4:D:200:GLU:OE2	4:D:200:GLU:HA	2.12	0.49
25:F:5004:LMG:O10	27:J:5001:DGD:O2E	2.30	0.49
14:2:120:ILE:HD11	30:2:502:XAT:H163	1.93	0.49
15:3:152:ALA:HB3	15:3:157:LEU:HG	1.95	0.49
1:A:53:TRP:HE3	1:A:54:ILE:HG13	1.77	0.49
2:B:295:PHE:HE1	19:B:1209:CLA:HMA1	1.77	0.49
25:F:5003:LMG:H121	25:F:5003:LMG:HC91	1.94	0.49
2:B:680:TRP:CZ2	2:B:684:ARG:HG3	2.48	0.49
19:B:1207:CLA:H121	12:L:136:GLY:HA3	1.94	0.49
11:K:77:LYS:CE	11:K:87:ARG:HE	2.24	0.49
1:A:205:HIS:CG	19:A:1111:CLA:HMC2	2.47	0.49
1:A:337:PRO:HG2	19:A:1141:CLA:O1D	2.13	0.49
1:A:691:MET:HB2	19:A:1013:CLA:C1C	2.43	0.49
19:B:1218:CLA:HED1	7:G:86:ASN:HB3	1.94	0.49
12:L:170:LYS:HB2	12:L:170:LYS:NZ	2.26	0.49
14:2:122:ILE:HB	14:2:123:PRO:HD3	1.94	0.49
19:2:603:CLA:ND	19:2:603:CLA:H2	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:3:128:ILE:H	15:3:128:ILE:HD12	1.78	0.49
2:B:694:ARG:HH22	9:I:31:ARG:CD	2.25	0.49
15:3:111:LEU:HD21	22:3:506:BCR:H15C	1.94	0.49
17:N:7:LEU:HD23	17:N:87:ILE:HG13	1.95	0.49
1:A:446:LEU:HD21	1:A:553:VAL:HG12	1.93	0.49
1:A:684:PHE:CD2	22:A:4011:BCR:H363	2.48	0.49
19:2:603:CLA:H192	19:2:603:CLA:HMB1	1.94	0.49
1:A:716:VAL:HG21	19:A:1138:CLA:HMB3	1.94	0.49
2:B:69:ALA:HB2	2:B:135:LEU:HB2	1.94	0.49
2:B:167:TRP:CH2	19:B:1208:CLA:HMA1	2.48	0.49
2:B:226:PHE:HE1	19:G:1601:CLA:HBC1	1.78	0.49
19:B:1237:CLA:H91	19:B:1237:CLA:H151	1.95	0.49
7:G:133:SER:HB2	22:G:4011:BCR:H372	1.95	0.49
30:2:502:XAT:O4	19:2:606:CLA:HMB3	2.13	0.49
15:3:139:THR:HG22	15:3:141:VAL:HG23	1.95	0.49
2:B:432:HIS:CD2	27:J:5001:DGD:HAF1	2.48	0.48
19:B:1222:CLA:H191	19:B:1240:CLA:H122	1.95	0.48
1:A:338:PHE:HB2	23:A:5001:LHG:HC41	1.95	0.48
19:A:1113:CLA:HBD	15:3:273:LYS:HG3	1.94	0.48
7:G:95:GLN:HE21	7:G:103:ALA:CB	2.26	0.48
15:3:93:ILE:O	15:3:93:ILE:HG22	2.12	0.48
11:K:59:THR:HG21	19:K:1401:CLA:O1A	2.11	0.48
16:4:240:PRO:HG2	19:4:608:CLA:HMB3	1.96	0.48
2:B:657:TRP:CE3	19:B:1021:CLA:HMA1	2.47	0.48
15:3:186:TYR:CZ	15:3:188:LEU:HA	2.48	0.48
2:B:696:LYS:HD2	3:C:79:LEU:HD12	1.95	0.48
19:B:1220:CLA:H3A	19:B:1220:CLA:HBA2	1.68	0.48
6:F:173:TRP:CD1	6:F:210:GLY:HA3	2.48	0.48
8:H:86:PHE:CE2	12:L:100:ILE:HG21	2.48	0.48
23:1:801:LHG:H262	23:1:801:LHG:H151	1.95	0.48
17:N:18:CYS:CB	17:N:27:HIS:CD2	2.95	0.48
2:B:177:HIS:CG	19:B:1210:CLA:HMC2	2.48	0.48
2:B:444:LEU:HD22	2:B:615:TYR:CD1	2.48	0.48
19:B:1224:CLA:O1D	19:B:1225:CLA:HMA1	2.14	0.48
19:2:602:CLA:C1D	19:2:607:CLA:H102	2.44	0.48
17:N:2:SER:HG	17:N:17:GLU:HG3	1.79	0.48
28:2:501:LUT:H11	28:2:501:LUT:H191	1.66	0.48
19:4:602:CLA:HMD2	19:4:607:CLA:C1D	2.44	0.48
1:A:343:HIS:HA	1:A:346:LEU:HD12	1.94	0.48
19:B:1205:CLA:O1A	19:B:1224:CLA:HBD	2.13	0.48
19:B:1223:CLA:H72	19:B:1223:CLA:H112	1.67	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:B:1239:CLA:HHC	19:B:1239:CLA:HBB1	1.96	0.48
19:1:605:CLA:H202	29:1:612:CHL:H141	1.95	0.48
17:N:16:PHE:HB2	17:N:31:VAL:HG21	1.96	0.48
4:D:81:SER:O	4:D:124:ARG:NH2	2.47	0.48
11:K:72:PRO:HB2	22:K:4001:BCR:H281	1.96	0.48
14:2:209:ALA:HB3	14:2:213:LYS:HD2	1.96	0.48
19:3:612:CLA:HMB2	19:3:617:CLA:C4B	2.43	0.48
17:N:73:PHE:CE1	17:N:95:LEU:HB2	2.49	0.48
19:A:1138:CLA:H151	19:A:1139:CLA:H43	1.96	0.48
2:B:669:GLY:O	2:B:673:GLU:HG3	2.14	0.48
19:F:1302:CLA:C1B	25:F:5002:LMG:H342	2.43	0.48
14:2:214:LEU:HD12	14:2:214:LEU:O	2.13	0.48
1:A:124:TRP:HD1	24:A:5004:LMT:H2B	1.79	0.47
6:F:99:ILE:HD11	6:F:127:LYS:HG3	1.96	0.47
1:A:158:ILE:HA	19:A:1112:CLA:HED1	1.96	0.47
4:D:110:GLU:HA	4:D:123:MET:O	2.14	0.47
14:2:129:LEU:HD22	14:2:131:ILE:CD1	2.44	0.47
15:3:94:GLU:OE2	15:3:96:ARG:N	2.47	0.47
1:A:593:SER:OG	1:A:596:ASP:OD1	2.29	0.47
19:B:1215:CLA:HMB1	19:B:1215:CLA:HBB1	1.95	0.47
29:1:610:CHL:C2C	19:1:613:CLA:HMC3	2.44	0.47
19:2:602:CLA:H41	19:2:602:CLA:H61	1.55	0.47
19:B:1216:CLA:H41	19:B:1216:CLA:H61	1.68	0.47
19:L:1502:CLA:HMA1	19:L:1503:CLA:HBC1	1.97	0.47
17:N:2:SER:OG	17:N:17:GLU:HG3	2.15	0.47
19:B:1206:CLA:H141	19:B:1206:CLA:H161	1.78	0.47
19:B:1222:CLA:H61	19:B:1234:CLA:H62	1.95	0.47
7:G:133:SER:O	7:G:137:ILE:HD12	2.14	0.47
8:H:139:LEU:HD12	8:H:139:LEU:H	1.80	0.47
28:1:501:LUT:H27	19:1:611:CLA:H43	1.96	0.47
19:2:608:CLA:O2A	15:3:160:LEU:HD13	2.15	0.47
15:3:164:LEU:HD22	22:3:503:BCR:H14C	1.96	0.47
16:4:233:LEU:CD1	16:4:237:ILE:HD11	2.43	0.47
19:B:1238:CLA:H193	19:B:1238:CLA:H161	1.72	0.47
10:J:2:ARG:NH1	14:2:95:ASP:OD2	2.42	0.47
19:2:601:CLA:H41	19:2:602:CLA:HBA2	1.96	0.47
17:N:18:CYS:HA	17:N:19:PRO:HD3	1.81	0.47
19:A:1109:CLA:H3A	19:A:1109:CLA:HBA2	1.51	0.47
19:A:1119:CLA:HBB1	19:A:1119:CLA:HMB1	1.95	0.47
2:B:77:TRP:HA	2:B:84:VAL:HG11	1.95	0.47
19:B:1225:CLA:H142	22:B:4006:BCR:H372	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:K:1401:CLA:HBC3	22:K:4002:BCR:H312	1.87	0.47
22:2:503:BCR:H333	19:4:607:CLA:HMC3	1.96	0.47
29:2:610:CHL:HMD2	25:2:803:LMG:HC92	1.95	0.47
15:3:98:LEU:HD13	29:3:604:CHL:H11	1.97	0.47
19:4:617:CLA:H203	19:4:617:CLA:H162	1.72	0.47
17:N:92:GLU:O	17:N:96:THR:N	2.45	0.47
19:A:1012:CLA:C4	22:A:4011:BCR:H362	2.44	0.47
2:B:239:SER:OG	2:B:241:ASN:OD1	2.29	0.47
2:B:365:PHE:HB3	2:B:602:TRP:CZ3	2.50	0.47
14:2:87:PHE:HB3	19:2:604:CLA:CAD	2.45	0.47
19:4:605:CLA:OBD	19:4:612:CLA:H2	2.14	0.47
19:A:1120:CLA:H3A	25:A:5006:LMG:O9	2.15	0.47
2:B:458:ILE:HG21	6:F:151:SER:HB3	1.96	0.47
7:G:154:PHE:HZ	29:1:610:CHL:HED2	1.80	0.47
28:J:4013:LUT:H381	28:J:4013:LUT:H27	1.78	0.47
12:L:137:LEU:O	12:L:141:LEU:HG	2.14	0.47
13:1:144:PHE:CD2	22:1:504:BCR:H352	2.50	0.47
19:A:1102:CLA:H61	19:A:1102:CLA:H41	1.62	0.47
19:A:1105:CLA:H13	19:A:1107:CLA:H121	1.97	0.47
19:B:1230:CLA:HMA1	27:J:5001:DGD:HA62	1.96	0.47
12:L:173:PRO:O	12:L:175:GLN:NE2	2.40	0.47
6:F:215:ILE:HG12	19:4:605:CLA:H51	1.97	0.46
22:1:503:BCR:H24C	29:4:613:CHL:HBA2	1.97	0.46
15:3:262:ASP:CG	15:3:264:VAL:HG12	2.35	0.46
16:4:137:SER:OG	16:4:140:THR:N	2.30	0.46
19:4:605:CLA:HBA2	19:4:605:CLA:HBD	1.96	0.46
22:A:4017:BCR:H10C	2:B:652:PHE:CZ	2.50	0.46
19:B:1219:CLA:HAB	19:B:1240:CLA:HED3	1.96	0.46
19:B:1237:CLA:H72	19:B:1238:CLA:H43	1.96	0.46
10:J:2:ARG:HD2	14:2:95:ASP:OD2	2.15	0.46
12:L:60:ILE:HA	12:L:70:GLU:HG3	1.96	0.46
14:2:120:ILE:HG12	30:2:502:XAT:H163	1.97	0.46
16:4:56:TRP:CE2	16:4:76:PHE:HD1	2.33	0.46
16:4:103:MET:SD	19:4:601:CLA:HAB	2.55	0.46
2:B:142:LEU:HD11	22:B:4006:BCR:H402	1.96	0.46
12:L:171:LYS:HG2	12:L:172:GLN:N	2.30	0.46
14:2:207:GLY:HA3	19:2:601:CLA:HAA2	1.98	0.46
19:A:1121:CLA:HHC	19:A:1121:CLA:HBB1	1.96	0.46
19:A:1137:CLA:HHC	19:A:1137:CLA:HBB1	1.98	0.46
19:A:1141:CLA:ND	25:A:5006:LMG:H301	2.31	0.46
14:2:120:ILE:CG1	30:2:502:XAT:H163	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:4:501:LUT:H35	28:4:501:LUT:H401	1.77	0.46
19:A:1013:CLA:H61	19:A:1013:CLA:H41	1.60	0.46
19:B:1204:CLA:H3A	19:B:1204:CLA:HBA2	1.64	0.46
19:B:1204:CLA:H41	19:B:1204:CLA:H61	1.50	0.46
19:B:1226:CLA:C6	27:B:5005:DGD:HA92	2.41	0.46
4:D:190:ARG:HH22	4:D:211:LEU:C	2.18	0.46
7:G:125:ILE:HD12	7:G:125:ILE:H	1.81	0.46
15:3:107:ARG:HB3	19:3:601:CLA:HBC3	1.96	0.46
18:A:1011:CL0:H11	18:A:1011:CL0:H15	1.98	0.46
19:A:1013:CLA:HMB1	19:A:1013:CLA:HBB1	1.98	0.46
19:A:1124:CLA:HMB1	19:A:1124:CLA:HBB1	1.97	0.46
2:B:276:HIS:HB2	19:B:1214:CLA:C1B	2.45	0.46
19:B:1222:CLA:H42	19:B:1236:CLA:H42	1.97	0.46
19:2:605:CLA:HMD2	19:2:612:CLA:C1D	2.46	0.46
19:3:610:CLA:H61	19:3:610:CLA:H2	1.61	0.46
19:3:612:CLA:HBB1	19:3:612:CLA:HMB1	1.98	0.46
16:4:70:LEU:HD22	16:4:92:VAL:HG21	1.97	0.46
17:N:24:ILE:HD12	17:N:79:ALA:HB3	1.97	0.46
1:A:465:ASP:OD2	1:A:648:THR:HB	2.15	0.46
19:A:1119:CLA:H91	19:A:1119:CLA:H111	1.61	0.46
19:A:1121:CLA:C3D	22:K:4001:BCR:H271	2.46	0.46
2:B:38:THR:HG22	2:B:39:GLU:H	1.80	0.46
19:B:1224:CLA:CGA	19:B:1224:CLA:H3A	2.43	0.46
19:B:1225:CLA:HMB1	19:B:1225:CLA:HBB1	1.98	0.46
19:B:1229:CLA:H152	19:B:1229:CLA:H111	1.62	0.46
12:L:94:ASN:HB3	12:L:97:LEU:HD23	1.98	0.46
12:L:100:ILE:HD13	12:L:188:GLY:O	2.16	0.46
14:2:189:THR:H	14:2:198:GLY:CA	2.28	0.46
19:2:612:CLA:H41	19:2:612:CLA:H62	1.51	0.46
19:B:1240:CLA:H62	19:B:1240:CLA:H41	1.60	0.46
19:G:1603:CLA:H112	19:G:1603:CLA:H142	1.66	0.46
8:H:80:SER:O	8:H:84:LYS:CB	2.63	0.46
14:2:153:PHE:CE1	25:2:803:LMG:H322	2.51	0.46
28:2:501:LUT:H183	29:2:611:CHL:C2	2.46	0.46
15:3:263:PRO:HB2	19:3:608:CLA:HMA3	1.98	0.46
22:3:506:BCR:H15C	22:3:506:BCR:H351	1.73	0.46
1:A:380:PRO:HA	1:A:381:PRO:HD3	1.87	0.46
19:A:1124:CLA:H3A	19:A:1124:CLA:HBA2	1.62	0.46
2:B:181:GLY:HA3	19:B:1210:CLA:HBB1	1.98	0.46
2:B:221:GLY:HA2	19:B:1212:CLA:HMD1	1.97	0.46
19:B:1237:CLA:H111	19:B:1238:CLA:H72	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:96:LEU:HB2	12:L:184:LYS:HG2	1.97	0.46
12:L:178:THR:OG1	12:L:181:GLY:N	2.49	0.46
29:3:604:CHL:H61	29:3:604:CHL:H41	1.66	0.46
29:4:613:CHL:HBA1	29:4:613:CHL:H3A	1.48	0.46
17:N:63:PHE:CD2	17:N:63:PHE:O	2.68	0.46
17:N:67:GLU:O	17:N:70:GLU:N	2.37	0.46
19:A:1013:CLA:H91	19:A:1013:CLA:H112	1.66	0.46
19:A:1103:CLA:H162	19:A:1103:CLA:H202	1.70	0.46
19:A:1135:CLA:H43	19:A:1136:CLA:O1A	2.15	0.46
2:B:160:LYS:HD3	2:B:161:TRP:CD2	2.51	0.46
2:B:160:LYS:HD3	2:B:161:TRP:CE2	2.51	0.46
2:B:257:LEU:HD22	2:B:493:TRP:HB3	1.98	0.46
19:B:1223:CLA:H13	22:B:4010:BCR:H351	1.96	0.46
19:G:1601:CLA:HAC2	22:G:4011:BCR:H383	1.97	0.46
28:1:501:LUT:H363	19:1:611:CLA:H172	1.98	0.46
19:1:604:CLA:H2A	19:1:604:CLA:HED2	1.97	0.46
15:3:113:ALA:HB2	15:3:238:ILE:HG12	1.97	0.46
15:3:147:THR:OG1	15:3:148:TYR:N	2.49	0.46
17:N:18:CYS:HB2	17:N:27:HIS:ND1	2.31	0.46
1:A:98:PHE:CG	19:A:1105:CLA:HBC3	2.51	0.45
1:A:118:PRO:HB3	1:A:150:PHE:CD2	2.51	0.45
1:A:195:TRP:CZ2	19:A:1108:CLA:HMA1	2.51	0.45
1:A:458:PHE:CZ	1:A:462:ILE:HD11	2.51	0.45
1:A:545:HIS:CE1	1:A:611:VAL:HG12	2.51	0.45
1:A:571:ASP:N	1:A:571:ASP:OD1	2.47	0.45
19:A:1102:CLA:H2A	19:A:1102:CLA:HED2	1.97	0.45
19:A:1106:CLA:HBA2	19:A:1106:CLA:H3A	1.40	0.45
19:A:1109:CLA:H62	19:A:1109:CLA:H41	1.56	0.45
19:A:1123:CLA:HMD2	19:A:1123:CLA:H143	1.98	0.45
19:B:1235:CLA:HBB1	19:B:1235:CLA:CMB	2.35	0.45
23:B:5001:LHG:O2	13:1:72:ASN:OD1	2.19	0.45
6:F:131:ASP:O	6:F:135:LYS:HG3	2.16	0.45
17:N:65:ASP:C	17:N:67:GLU:N	2.68	0.45
2:B:80:ASP:O	2:B:84:VAL:HG12	2.17	0.45
19:B:1202:CLA:HBA1	19:B:1202:CLA:H3A	1.41	0.45
19:B:1203:CLA:H51	27:B:5005:DGD:HB81	1.99	0.45
8:H:86:PHE:CD2	12:L:100:ILE:HG21	2.51	0.45
14:2:101:TRP:CE2	25:2:802:LMG:HC5	2.51	0.45
15:3:197:SER:HB3	15:3:203:PRO:O	2.16	0.45
19:4:606:CLA:H12	29:4:613:CHL:CAD	2.46	0.45
1:A:444:SER:HB3	2:B:681:ALA:HB2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:633:VAL:O	1:A:633:VAL:HG13	2.15	0.45
18:A:1011:CL0:H13	19:A:1012:CLA:OBD	2.16	0.45
19:A:1109:CLA:H161	19:A:1109:CLA:H141	1.70	0.45
19:B:1203:CLA:H92	19:B:1203:CLA:H61	1.72	0.45
19:B:1204:CLA:H92	19:B:1204:CLA:HMC2	1.98	0.45
19:B:1207:CLA:H121	12:L:136:GLY:CA	2.46	0.45
19:B:1216:CLA:H161	19:B:1216:CLA:H203	1.66	0.45
19:B:1238:CLA:H111	19:B:1239:CLA:H13	1.97	0.45
8:H:77:PRO:HG3	12:L:90:ARG:NH1	2.30	0.45
19:1:611:CLA:H152	19:1:611:CLA:H111	1.53	0.45
30:2:502:XAT:H15	30:2:502:XAT:H201	1.80	0.45
22:2:503:BCR:H392	22:2:503:BCR:H282	1.26	0.45
19:2:601:CLA:H142	19:2:601:CLA:H111	1.81	0.45
19:A:1013:CLA:H92	2:B:431:PHE:HE1	1.81	0.45
19:A:1125:CLA:HAB	19:A:1133:CLA:HMA2	1.97	0.45
22:A:4002:BCR:H362	22:A:4003:BCR:C10	2.47	0.45
2:B:203:ARG:HG2	2:B:250:ALA:HB1	1.97	0.45
2:B:671:TRP:CZ2	20:B:2002:PQN:H2M3	2.52	0.45
19:G:1701:CLA:HBB1	12:L:104:LEU:HD11	1.98	0.45
22:1:503:BCR:H16C	16:4:152:VAL:CG1	2.47	0.45
30:4:502:XAT:H15	30:4:502:XAT:H201	1.86	0.45
1:A:516:GLY:HA2	1:A:531:PRO:HB3	1.98	0.45
19:A:1133:CLA:H41	19:A:1133:CLA:H61	1.54	0.45
2:B:20:ARG:NH2	9:I:31:ARG:HH22	2.15	0.45
2:B:91:ILE:HB	2:B:112:PRO:HB2	1.97	0.45
19:B:1235:CLA:H61	22:F:4016:BCR:H343	1.98	0.45
27:3:803:DGD:O5E	27:3:803:DGD:O4E	2.24	0.45
19:A:1103:CLA:H2	19:A:1103:CLA:H62	1.68	0.45
19:A:1114:CLA:H2A	19:A:1114:CLA:HED2	1.98	0.45
19:A:1121:CLA:HMD2	22:K:4001:BCR:H23C	1.99	0.45
19:B:1202:CLA:HBD	19:B:1202:CLA:H122	1.98	0.45
5:E:66:ILE:HG13	5:E:95:GLN:OE1	2.16	0.45
19:G:1602:CLA:O2D	19:G:1602:CLA:HBA2	2.16	0.45
11:K:82:LEU:CB	11:K:83:LYS:HD2	2.45	0.45
19:3:601:CLA:H3A	19:3:601:CLA:HBA2	1.34	0.45
1:A:537:ALA:HA	1:A:540:LEU:HD12	1.98	0.45
19:A:1116:CLA:HBA2	19:A:1116:CLA:H3A	1.46	0.45
2:B:15:ASP:HB3	2:B:20:ARG:HB2	1.99	0.45
19:B:1224:CLA:H111	19:B:1224:CLA:H152	1.72	0.45
19:B:1234:CLA:H71	25:F:5002:LMG:H401	1.99	0.45
27:F:5005:DGD:HG12	23:2:807:LHG:H102	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:47:ILE:HG23	11:K:52:ASN:ND2	2.31	0.45
1:A:630:ASP:OD1	1:A:631:GLN:N	2.49	0.45
19:A:1012:CLA:HBC2	2:B:585:ASN:HB2	1.99	0.45
2:B:443:MET:SD	2:B:451:LYS:HE3	2.56	0.45
13:1:189:ARG:HG2	19:1:604:CLA:C4C	2.47	0.45
19:2:606:CLA:HBD	19:2:606:CLA:HBA1	1.98	0.45
15:3:76:TYR:HB2	29:3:604:CHL:HMD1	1.97	0.45
15:3:161:GLU:HG3	19:3:613:CLA:C1B	2.47	0.45
15:3:246:LEU:C	15:3:246:LEU:HD23	2.37	0.45
22:A:4007:BCR:H15C	22:A:4007:BCR:H351	1.71	0.45
22:A:4017:BCR:HC41	2:B:648:TRP:CZ3	2.51	0.45
5:E:79:GLN:HA	5:E:84:TYR:CG	2.52	0.45
12:L:87:PRO:HG2	19:L:1502:CLA:OBD	2.17	0.45
12:L:167:THR:HG23	12:L:169:ARG:HG3	1.98	0.45
14:2:236:TRP:CZ2	29:2:610:CHL:H2	2.47	0.45
19:A:1126:CLA:H71	19:A:1126:CLA:H112	1.52	0.45
19:B:1222:CLA:H3A	19:B:1222:CLA:HBA2	1.46	0.45
23:B:5002:LHG:H191	23:B:5002:LHG:H162	1.54	0.45
4:D:75:LEU:HD12	4:D:75:LEU:HA	1.87	0.45
19:G:1601:CLA:H41	19:G:1601:CLA:H61	1.46	0.45
14:2:162:TRP:CH2	22:2:503:BCR:HC8	2.51	0.45
19:A:1125:CLA:H161	19:A:1125:CLA:H122	1.83	0.44
22:A:4017:BCR:HC41	2:B:648:TRP:CE3	2.52	0.44
2:B:159:PRO:O	2:B:160:LYS:HB3	2.16	0.44
2:B:323:TYR:O	2:B:327:ASN:HB2	2.17	0.44
19:B:1219:CLA:H41	19:B:1219:CLA:H61	1.50	0.44
19:B:1230:CLA:HMB1	19:B:1230:CLA:HBB1	1.98	0.44
6:F:219:ARG:HE	6:F:219:ARG:HB3	1.68	0.44
13:1:146:GLU:OE1	13:1:149:ARG:NH1	2.48	0.44
13:1:227:GLY:HA3	16:4:139:SER:HB3	1.99	0.44
28:1:501:LUT:H173	19:1:603:CLA:C3B	2.47	0.44
29:2:615:CHL:HHC	29:2:615:CHL:CBB	2.46	0.44
19:4:612:CLA:H141	19:4:612:CLA:H161	1.82	0.44
19:A:1129:CLA:H61	19:A:1129:CLA:H102	1.60	0.44
19:B:1220:CLA:HMA1	19:B:1240:CLA:HED2	1.99	0.44
3:C:61:ASP:HA	3:C:62:PHE:HA	1.85	0.44
14:2:64:ARG:NH2	14:2:77:LEU:O	2.50	0.44
19:A:1139:CLA:H62	19:A:1139:CLA:H41	1.27	0.44
19:B:1238:CLA:H111	19:B:1238:CLA:H152	1.42	0.44
19:F:1302:CLA:H3A	19:F:1302:CLA:HBA1	1.61	0.44
11:K:91:LEU:HD12	15:3:61:SER:HB3	1.97	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:4:610:CHL:CBB	29:4:613:CHL:HBB2	2.47	0.44
1:A:205:HIS:ND1	19:A:1111:CLA:HMC2	2.32	0.44
19:A:1112:CLA:H112	19:A:1112:CLA:H71	1.55	0.44
19:A:1131:CLA:H152	19:A:1131:CLA:H112	1.71	0.44
6:F:110:ALA:HB3	6:F:113:SER:H	1.83	0.44
25:F:5001:LMG:H112	25:F:5001:LMG:H142	1.76	0.44
30:2:502:XAT:H32	19:2:604:CLA:HAB	1.99	0.44
15:3:225:LEU:HG	29:3:607:CHL:HED3	1.99	0.44
19:3:605:CLA:HMD2	19:3:612:CLA:C1D	2.48	0.44
17:N:63:PHE:O	17:N:63:PHE:CG	2.70	0.44
1:A:38:GLY:HA3	1:A:44:ILE:CG2	2.48	0.44
1:A:60:ASP:OD1	23:A:5002:LHG:O2	2.35	0.44
1:A:126:ILE:HG13	1:A:127:VAL:HG13	1.99	0.44
19:L:1502:CLA:C3C	22:L:4019:BCR:H393	2.47	0.44
14:2:150:THR:CG2	16:4:246:VAL:HG11	2.47	0.44
29:2:610:CHL:CMD	25:2:803:LMG:HC72	2.47	0.44
29:2:615:CHL:HBC2	29:2:615:CHL:HHD	1.98	0.44
15:3:101:GLY:HA2	19:3:612:CLA:HED2	2.00	0.44
19:4:602:CLA:HHC	19:4:602:CLA:HBB1	1.98	0.44
17:N:2:SER:HA	17:N:19:PRO:HA	1.99	0.44
22:A:4017:BCR:H10C	2:B:652:PHE:HZ	1.83	0.44
22:K:4001:BCR:H351	22:K:4001:BCR:H15C	1.74	0.44
13:1:76:PHE:C	19:1:604:CLA:HMA1	2.38	0.44
19:4:607:CLA:H91	19:4:607:CLA:H142	1.98	0.44
8:H:132:PRO:HA	8:H:133:PRO:HD3	1.82	0.44
22:I:4020:BCR:H15C	22:I:4020:BCR:H351	1.80	0.44
13:1:217:HIS:CG	19:1:603:CLA:HAA1	2.52	0.44
28:1:501:LUT:H371	19:1:601:CLA:H72	1.99	0.44
19:1:604:CLA:HMD2	29:1:609:CHL:CBB	2.48	0.44
19:2:604:CLA:H142	19:2:604:CLA:H111	1.77	0.44
17:N:91:LYS:HE3	17:N:91:LYS:HB3	1.81	0.44
1:A:680:LEU:HD13	19:A:1012:CLA:H2	2.00	0.44
19:A:1126:CLA:H3A	19:A:1126:CLA:HBA2	1.52	0.44
19:A:1131:CLA:HAA1	22:I:4020:BCR:C16	2.48	0.44
19:B:1206:CLA:H162	19:B:1206:CLA:H193	1.78	0.44
19:B:1227:CLA:H92	19:B:1240:CLA:HMA2	1.99	0.44
19:B:1240:CLA:C4B	19:1:605:CLA:H52	2.48	0.44
19:F:1302:CLA:H11	19:F:1302:CLA:H52	1.62	0.44
22:I:4020:BCR:H24C	22:I:4020:BCR:H371	1.91	0.44
13:1:205:TYR:O	13:1:208:THR:OG1	2.22	0.44
19:2:604:CLA:H92	19:2:605:CLA:H62	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:4:89:LYS:HE2	16:4:89:LYS:HB3	1.63	0.44
19:4:609:CLA:HHC	19:4:609:CLA:HBB1	1.99	0.44
27:4:802:DGD:HG31	27:4:802:DGD:HD2	1.48	0.44
19:A:1102:CLA:H3A	19:A:1102:CLA:HBA2	1.43	0.44
19:A:1104:CLA:O2D	19:A:1104:CLA:HBA2	2.18	0.44
2:B:182:LEU:HD13	19:B:1210:CLA:HBB	1.98	0.44
19:B:1204:CLA:HMB3	19:B:1205:CLA:HMA1	2.00	0.44
19:B:1218:CLA:HED1	7:G:86:ASN:C	2.38	0.44
16:4:65:TYR:CE1	16:4:83:GLU:HG3	2.52	0.44
17:N:22:VAL:HG21	17:N:27:HIS:NE2	2.33	0.44
19:A:1122:CLA:H41	19:A:1122:CLA:H61	1.57	0.43
2:B:54:LEU:HD23	2:B:54:LEU:HA	1.79	0.43
2:B:73:ASN:ND2	2:B:85:ARG:O	2.50	0.43
28:1:502:LUT:H35	28:1:502:LUT:H401	1.90	0.43
19:1:614:CLA:H92	19:1:614:CLA:H62	1.82	0.43
14:2:233:MET:HG2	19:2:604:CLA:H192	1.99	0.43
19:2:605:CLA:H61	19:2:605:CLA:H101	1.55	0.43
29:2:610:CHL:HAA2	29:2:610:CHL:HBD	2.00	0.43
29:3:611:CHL:HHC	29:3:611:CHL:HBB1	2.00	0.43
17:N:23:TYR:HA	17:N:79:ALA:O	2.17	0.43
1:A:291:THR:HG22	1:A:384:TYR:CE2	2.53	0.43
19:A:1125:CLA:H92	19:A:1125:CLA:H61	1.57	0.43
7:G:95:GLN:HE21	7:G:103:ALA:HB3	1.83	0.43
13:1:91:VAL:CG2	13:1:92:PRO:HD3	2.48	0.43
15:3:143:PRO:HD2	19:3:610:CLA:C2B	2.48	0.43
16:4:236:HIS:HA	16:4:243:ASN:HB3	1.99	0.43
19:A:1112:CLA:H143	19:A:1112:CLA:H162	1.82	0.43
2:B:3:LEU:HA	9:I:32:LEU:HB2	2.01	0.43
13:1:146:GLU:HG2	29:1:612:CHL:NB	2.33	0.43
14:2:194:GLY:HA2	29:2:611:CHL:CMD	2.49	0.43
15:3:223:LEU:HB3	19:3:601:CLA:HMA1	2.01	0.43
17:N:91:LYS:HD2	17:N:94:ASP:OD2	2.18	0.43
19:A:1102:CLA:H11	19:A:1102:CLA:H52	1.74	0.43
19:A:1115:CLA:H61	19:A:1115:CLA:H41	1.68	0.43
19:B:1224:CLA:H92	19:B:1224:CLA:H62	1.87	0.43
13:1:73:LEU:HG	13:1:77:LYS:HE3	2.00	0.43
14:2:168:TRP:CE3	19:2:612:CLA:HMA1	2.53	0.43
14:2:180:ASP:HB2	29:2:615:CHL:C4C	2.47	0.43
15:3:129:PRO:HD3	19:3:614:CLA:HMD3	2.00	0.43
17:N:22:VAL:HB	17:N:27:HIS:NE2	2.33	0.43
17:N:93:GLU:C	17:N:95:LEU:H	2.21	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:B:1021:CLA:H102	19:B:1021:CLA:H62	1.73	0.43
19:B:1225:CLA:H3A	19:B:1225:CLA:HBA2	1.28	0.43
11:K:50:PRO:HB2	11:K:51:THR:H	1.66	0.43
12:L:102:VAL:O	12:L:106:HIS:ND1	2.51	0.43
14:2:233:MET:CE	14:2:233:MET:HA	2.47	0.43
1:A:665:ILE:O	2:B:621:ARG:HD3	2.19	0.43
19:A:1115:CLA:CHD	19:A:1116:CLA:HBB2	2.48	0.43
19:B:1207:CLA:H18	19:B:1207:CLA:H151	1.44	0.43
19:2:603:CLA:H62	19:2:603:CLA:H101	1.77	0.43
27:3:803:DGD:HE62	27:3:803:DGD:HE1	1.82	0.43
17:N:45:SER:O	17:N:92:GLU:HG3	2.18	0.43
1:A:401:TRP:HB3	19:A:1126:CLA:HMC3	2.01	0.43
2:B:230:TRP:HZ3	19:B:1213:CLA:H51	1.83	0.43
19:B:1219:CLA:HMB3	19:B:1240:CLA:C1D	2.49	0.43
19:B:1232:CLA:H41	19:B:1232:CLA:H62	1.41	0.43
4:D:170:LYS:HA	4:D:170:LYS:HD3	1.74	0.43
19:G:1701:CLA:HBA1	19:G:1701:CLA:H3A	1.62	0.43
15:3:64:SER:HB2	15:3:79:ASP:HB3	2.01	0.43
17:N:67:GLU:O	17:N:69:ILE:N	2.51	0.43
1:A:221:HIS:HB2	19:A:1112:CLA:C1C	2.49	0.43
2:B:295:PHE:CE1	19:B:1209:CLA:HMA1	2.53	0.43
19:B:1214:CLA:HBA2	19:B:1223:CLA:HBB2	2.01	0.43
6:F:110:ALA:HB3	6:F:113:SER:OG	2.19	0.43
13:1:187:ASN:ND2	19:1:607:CLA:HMD1	2.34	0.43
29:1:610:CHL:C1C	19:1:613:CLA:HMC3	2.48	0.43
30:2:502:XAT:H31	30:2:502:XAT:H391	1.78	0.43
19:3:605:CLA:H93	19:3:605:CLA:H61	1.84	0.43
16:4:57:LEU:HB3	16:4:60:LEU:HB3	2.00	0.43
2:B:684:ARG:HD3	2:B:684:ARG:HA	1.78	0.43
19:B:1221:CLA:H41	19:B:1221:CLA:H61	1.68	0.43
19:B:1239:CLA:H3A	19:B:1239:CLA:HBA2	1.38	0.43
24:B:5006:LMT:H11	25:F:5002:LMG:O10	2.18	0.43
12:L:109:LEU:HD13	19:L:1503:CLA:CBC	2.48	0.43
14:2:220:LYS:O	14:2:224:ASN:OD1	2.37	0.43
1:A:512:SER:OG	1:A:514:THR:HG23	2.19	0.43
18:A:1011:CL0:H72	18:A:1011:CL0:H10	1.60	0.43
19:A:1105:CLA:OBD	24:A:5004:LMT:H22	2.19	0.43
19:A:1110:CLA:HED2	19:A:1111:CLA:HBC1	2.01	0.43
25:A:5006:LMG:H141	25:A:5006:LMG:H172	1.73	0.43
2:B:163:PRO:HG3	19:B:1208:CLA:HMA3	2.01	0.43
2:B:674:LEU:HD12	2:B:674:LEU:HA	1.89	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:B:5007:LMG:H322	25:1:802:LMG:H331	2.01	0.43
25:G:5002:LMG:H141	25:G:5002:LMG:H171	1.90	0.43
11:K:94:GLY:C	19:K:1404:CLA:HAA1	2.39	0.43
12:L:98:ARG:O	12:L:102:VAL:HG23	2.19	0.43
13:1:94:ILE:HG23	13:1:105:TRP:HB3	2.00	0.43
19:3:610:CLA:HBA2	19:3:610:CLA:H3A	1.29	0.43
30:4:502:XAT:H162	29:4:613:CHL:HBB1	2.01	0.43
17:N:24:ILE:HD11	17:N:56:VAL:HG11	2.01	0.43
1:A:538:ASP:O	1:A:542:HIS:ND1	2.36	0.42
19:A:1013:CLA:H122	19:A:1013:CLA:H162	1.80	0.42
19:A:1104:CLA:H12	19:A:1104:CLA:H2A	2.00	0.42
2:B:411:MET:HG3	22:B:4009:BCR:H382	2.00	0.42
19:B:1239:CLA:H143	19:B:1239:CLA:H161	1.73	0.42
13:1:160:TYR:CZ	13:1:181:LYS:HD3	2.54	0.42
15:3:272:LEU:O	15:3:273:LYS:HG2	2.18	0.42
1:A:221:HIS:HB2	19:A:1112:CLA:CHC	2.49	0.42
19:A:1105:CLA:H111	19:A:1105:CLA:H72	1.42	0.42
19:B:1208:CLA:H12	24:G:5004:LMT:H31	2.01	0.42
19:B:1219:CLA:H62	19:B:1219:CLA:H92	1.77	0.42
7:G:119:ASP:HB3	7:G:122:GLY:H	1.83	0.42
22:G:4011:BCR:H351	22:G:4011:BCR:H15C	1.51	0.42
19:1:601:CLA:H61	19:1:601:CLA:H41	1.39	0.42
19:1:601:CLA:H91	19:1:601:CLA:H112	1.84	0.42
14:2:120:ILE:CD1	30:2:502:XAT:H163	2.49	0.42
25:2:802:LMG:HC8	25:2:802:LMG:H112	1.48	0.42
1:A:220:GLY:HA3	19:A:1113:CLA:HAB	2.02	0.42
19:A:1013:CLA:H201	19:A:1140:CLA:H2	2.01	0.42
2:B:231:ASN:HA	19:B:1213:CLA:HAA2	2.00	0.42
23:B:5002:LHG:H172	23:B:5002:LHG:H141	1.76	0.42
4:D:96:GLN:NE2	8:H:66:GLN:HG2	2.33	0.42
5:E:129:LYS:HA	5:E:129:LYS:HD3	1.78	0.42
11:K:90:GLY:HA2	15:3:62:LYS:HD3	2.01	0.42
28:2:501:LUT:H15	28:2:501:LUT:H201	1.76	0.42
15:3:142:ILE:HG23	19:3:610:CLA:HAB	2.01	0.42
19:3:601:CLA:H41	19:3:602:CLA:HMA2	2.00	0.42
16:4:210:LEU:HD23	28:4:501:LUT:H203	2.01	0.42
29:4:610:CHL:HBC3	27:4:802:DGD:O1A	2.18	0.42
19:A:1139:CLA:HBB1	19:A:1139:CLA:HMB1	2.01	0.42
2:B:444:LEU:HD22	2:B:615:TYR:CE1	2.53	0.42
2:B:444:LEU:HD12	2:B:444:LEU:N	2.34	0.42
2:B:733:PHE:CD2	8:H:137:PRO:HD2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:B:1218:CLA:HMD2	22:B:4004:BCR:H24C	2.00	0.42
19:B:1234:CLA:H92	25:F:5002:LMG:C42	2.49	0.42
9:I:21:MET:HG2	22:L:4019:BCR:C10	2.49	0.42
9:I:25:PHE:CE1	9:I:29:GLU:OE1	2.72	0.42
19:1:602:CLA:HED2	19:1:607:CLA:HBA2	2.01	0.42
29:1:609:CHL:H2	23:1:801:LHG:H291	2.02	0.42
15:3:266:ASN:O	19:3:603:CLA:HBD	2.20	0.42
19:3:610:CLA:H122	19:3:610:CLA:H161	1.41	0.42
17:N:18:CYS:CB	17:N:27:HIS:CG	3.01	0.42
19:A:1012:CLA:H91	19:A:1012:CLA:H111	1.63	0.42
2:B:68:VAL:O	2:B:72:GLY:HA3	2.18	0.42
2:B:104:PHE:O	2:B:106:ARG:NH1	2.52	0.42
2:B:189:ALA:HA	19:B:1212:CLA:HAB	2.01	0.42
19:B:1206:CLA:H41	19:B:1206:CLA:H62	1.51	0.42
11:K:104:THR:OG1	19:K:1404:CLA:HAB	2.20	0.42
19:L:1502:CLA:H93	19:L:1502:CLA:H62	1.73	0.42
14:2:230:LEU:HB3	19:2:603:CLA:CBB	2.48	0.42
28:4:501:LUT:H161	19:4:603:CLA:HMB3	2.02	0.42
17:N:22:VAL:HG12	17:N:23:TYR:N	2.34	0.42
1:A:18:VAL:HG13	19:A:1110:CLA:HED3	2.01	0.42
1:A:513:LEU:HB2	1:A:529:LEU:HB3	2.02	0.42
1:A:686:TRP:CE3	18:A:1011:CL0:H4	2.55	0.42
19:A:1105:CLA:C1C	24:A:5004:LMT:H112	2.49	0.42
19:A:1106:CLA:H12	22:J:4012:BCR:H371	2.02	0.42
2:B:105:THR:HG21	8:H:129:PRO:HG3	2.02	0.42
2:B:145:LEU:HD23	2:B:145:LEU:HA	1.87	0.42
2:B:257:LEU:HG	19:B:1214:CLA:HMB2	2.02	0.42
3:C:9:ASP:HB3	4:D:189:PHE:HA	2.02	0.42
19:F:1301:CLA:H171	19:F:1301:CLA:H13	1.74	0.42
13:1:135:LEU:HA	13:1:135:LEU:HD23	1.78	0.42
15:3:226:LYS:HG2	29:3:607:CHL:O1D	2.19	0.42
16:4:175:TYR:CZ	29:4:615:CHL:HBD	2.54	0.42
17:N:6:LYS:HZ2	17:N:86:VAL:CG2	2.33	0.42
18:A:1011:CL0:H61	18:A:1011:CL0:H53	1.70	0.42
19:A:1106:CLA:H91	19:A:1106:CLA:H111	1.72	0.42
2:B:7:ARG:NH1	9:I:32:LEU:HD12	2.32	0.42
2:B:46:ILE:HG12	19:B:1202:CLA:C2C	2.50	0.42
2:B:631:LEU:HD13	2:B:727:ALA:CB	2.49	0.42
19:B:1237:CLA:H192	12:L:110:LEU:HD21	2.01	0.42
4:D:160:PRO:O	8:H:60:LEU:HD12	2.20	0.42
4:D:179:ASN:HA	4:D:180:PRO:HD3	1.87	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:143:ASP:OD1	6:F:143:ASP:N	2.50	0.42
19:G:1602:CLA:HMB1	19:G:1602:CLA:CBB	2.49	0.42
22:1:503:BCR:H373	29:4:613:CHL:HHB	2.02	0.42
14:2:189:THR:H	14:2:198:GLY:HA2	1.84	0.42
28:3:501:LUT:H183	19:3:603:CLA:C3B	2.49	0.42
19:A:1102:CLA:H111	19:A:1102:CLA:H91	1.78	0.42
19:A:1136:CLA:HBB1	19:A:1136:CLA:CHC	2.34	0.42
19:B:1207:CLA:H162	19:B:1207:CLA:H122	1.42	0.42
19:G:1603:CLA:H91	25:G:5002:LMG:H141	2.01	0.42
11:K:55:MET:O	11:K:59:THR:HG22	2.19	0.42
11:K:99:PHE:HE1	11:K:103:ASP:OD2	2.02	0.42
13:1:63:PRO:HB3	25:1:802:LMG:H141	2.01	0.42
13:1:89:LEU:HD23	13:1:89:LEU:HA	1.79	0.42
19:2:603:CLA:HHC	19:2:603:CLA:CBB	2.49	0.42
15:3:66:SER:OG	15:3:67:TYR:N	2.52	0.42
1:A:44:ILE:CD1	1:A:57:LEU:HA	2.43	0.42
18:A:1011:CL0:H66	19:B:1022:CLA:HMB3	2.01	0.42
19:A:1115:CLA:H112	19:A:1115:CLA:H142	1.74	0.42
19:B:1201:CLA:H3A	23:B:5002:LHG:H291	2.02	0.42
19:B:1204:CLA:H193	19:B:1204:CLA:H161	1.87	0.42
19:B:1207:CLA:HBA1	19:B:1207:CLA:H3A	1.83	0.42
7:G:133:SER:CB	22:G:4011:BCR:H372	2.49	0.42
12:L:100:ILE:HD13	12:L:100:ILE:HA	1.88	0.42
13:1:178:HIS:CE1	13:1:182:ILE:HD11	2.54	0.42
28:1:502:LUT:H15	28:1:502:LUT:H201	1.79	0.42
14:2:83:GLY:HA3	14:2:222:ILE:HG21	2.02	0.42
29:2:611:CHL:HBC2	29:2:611:CHL:HHD	2.00	0.42
19:3:601:CLA:HMD3	29:3:611:CHL:CAD	2.50	0.42
16:4:216:LEU:HD22	19:4:603:CLA:HMC1	2.01	0.42
28:4:501:LUT:H201	28:4:501:LUT:H15	1.77	0.42
19:A:1121:CLA:H3A	19:A:1121:CLA:HBA2	1.76	0.42
19:B:1222:CLA:H92	19:B:1234:CLA:H62	2.01	0.42
8:H:80:SER:O	8:H:84:LYS:HB2	2.19	0.42
12:L:90:ARG:HB3	12:L:93:VAL:CG2	2.49	0.42
14:2:97:GLU:H	14:2:97:GLU:HG3	1.68	0.42
1:A:305:ALA:HA	19:A:1115:CLA:HMC3	2.01	0.41
1:A:553:VAL:HG11	19:A:1137:CLA:HMB3	2.02	0.41
19:A:1103:CLA:H91	19:A:1103:CLA:H112	1.84	0.41
19:A:1110:CLA:CGA	19:A:1110:CLA:C1A	2.98	0.41
6:F:172:GLY:HA3	6:F:213:TRP:CZ2	2.55	0.41
19:1:605:CLA:H62	19:1:605:CLA:H41	1.39	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:2:609:CHL:HMD2	22:3:503:BCR:HC42	2.02	0.41
19:4:605:CLA:H41	19:4:605:CLA:H62	1.85	0.41
19:A:1104:CLA:H61	19:A:1104:CLA:H41	1.46	0.41
25:A:5006:LMG:H321	25:A:5006:LMG:H352	1.87	0.41
2:B:676:GLU:HG2	3:C:81:TYR:HE1	1.85	0.41
19:B:1202:CLA:H2	19:B:1202:CLA:H61	1.63	0.41
19:B:1214:CLA:H161	19:B:1214:CLA:H141	1.67	0.41
4:D:169:PRO:HG3	4:D:174:TYR:CE1	2.55	0.41
14:2:203:PRO:HG2	14:2:204:LEU:HD22	2.02	0.41
15:3:239:LEU:HD11	29:3:604:CHL:H18	2.03	0.41
15:3:274:PHE:CG	15:3:275:HIS:N	2.88	0.41
16:4:215:PHE:CE2	30:4:502:XAT:H10	2.55	0.41
19:A:1103:CLA:H151	19:A:1111:CLA:H51	2.03	0.41
19:A:1132:CLA:H141	19:A:1132:CLA:H193	2.03	0.41
19:B:1219:CLA:H43	25:G:5001:LMG:H151	2.01	0.41
19:B:1227:CLA:H162	19:B:1227:CLA:H122	1.71	0.41
19:B:1235:CLA:H193	19:B:1235:CLA:H162	1.65	0.41
28:J:4013:LUT:H191	28:J:4013:LUT:H11	1.73	0.41
27:J:5001:DGD:HAS1	27:J:5001:DGD:HAH2	1.78	0.41
12:L:62:GLY:O	12:L:64:PRO:HD3	2.21	0.41
22:1:503:BCR:HC21	23:1:801:LHG:H241	2.01	0.41
14:2:97:GLU:HA	14:2:100:ARG:HG2	2.02	0.41
14:2:237:PHE:HA	14:2:240:ILE:CG2	2.49	0.41
1:A:302:HIS:HB2	19:A:1116:CLA:C1B	2.50	0.41
19:A:1136:CLA:H71	19:A:1136:CLA:H112	1.65	0.41
19:A:1141:CLA:H93	19:A:1141:CLA:H111	1.74	0.41
2:B:223:GLY:O	2:B:227:THR:HG23	2.20	0.41
2:B:373:THR:HG23	2:B:591:THR:HG21	2.01	0.41
12:L:123:THR:O	12:L:127:GLY:N	2.53	0.41
12:L:144:CYS:HB3	22:L:4019:BCR:H19C	2.02	0.41
28:1:501:LUT:H24	19:1:601:CLA:HBA2	2.02	0.41
14:2:146:PHE:HE2	16:4:241:TRP:HB3	1.85	0.41
19:2:604:CLA:CGA	19:2:604:CLA:H3A	2.40	0.41
15:3:139:THR:CG2	15:3:141:VAL:HG23	2.50	0.41
15:3:157:LEU:HD23	15:3:157:LEU:HA	1.81	0.41
19:3:602:CLA:H62	19:3:602:CLA:H41	1.80	0.41
19:4:612:CLA:HBA1	19:4:612:CLA:H3A	1.72	0.41
1:A:586:ARG:HH21	4:D:136:GLU:CD	2.23	0.41
19:A:1138:CLA:H93	19:A:1138:CLA:H61	1.85	0.41
2:B:74:PHE:O	2:B:78:VAL:HG23	2.20	0.41
2:B:444:LEU:CD2	2:B:615:TYR:CE1	3.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:478:LEU:HA	2:B:486:LEU:HB2	2.01	0.41
19:B:1201:CLA:H3A	19:B:1201:CLA:HBA2	1.73	0.41
19:B:1222:CLA:H41	19:B:1222:CLA:H62	1.43	0.41
20:B:2002:PQN:H172	20:B:2002:PQN:H212	1.76	0.41
19:F:1301:CLA:H3A	19:F:1301:CLA:HBA1	1.73	0.41
12:L:174:ASP:OD1	12:L:176:LEU:HB3	2.20	0.41
13:1:172:LYS:HG3	13:1:173:ASP:N	2.33	0.41
19:1:602:CLA:HMD2	19:1:607:CLA:C1D	2.50	0.41
17:N:6:LYS:HA	17:N:15:GLU:OE1	2.21	0.41
17:N:26:ASP:OD2	17:N:26:ASP:N	2.53	0.41
1:A:616:PHE:HD1	19:A:1135:CLA:HBC2	1.85	0.41
19:A:1104:CLA:HMA1	19:A:1128:CLA:HAB	2.02	0.41
19:A:1112:CLA:H62	19:A:1112:CLA:H93	1.80	0.41
2:B:38:THR:OG1	2:B:41:ARG:NH1	2.53	0.41
2:B:77:TRP:CD1	2:B:84:VAL:HG13	2.55	0.41
19:B:1235:CLA:C4A	19:B:1235:CLA:HBA2	2.47	0.41
12:L:207:LEU:HB3	12:L:208:ASP:H	1.67	0.41
13:1:83:HIS:HD2	28:1:502:LUT:H35	1.85	0.41
13:1:98:GLU:HG2	13:1:211:LEU:HD12	2.03	0.41
16:4:169:ASP:HB3	16:4:172:PHE:O	2.20	0.41
16:4:195:ALA:HB1	16:4:197:THR:HG23	2.02	0.41
17:N:6:LYS:HZ3	17:N:86:VAL:HG21	1.85	0.41
17:N:93:GLU:C	17:N:95:LEU:N	2.74	0.41
1:A:265:GLY:HA2	19:A:1113:CLA:HMD1	2.03	0.41
19:A:1012:CLA:H61	19:A:1012:CLA:H41	1.47	0.41
19:A:1126:CLA:H92	19:A:1126:CLA:H61	1.69	0.41
2:B:269:TRP:O	2:B:273:MET:HG3	2.19	0.41
2:B:503:GLU:OE1	2:B:504:ASN:N	2.54	0.41
19:B:1218:CLA:H111	19:B:1218:CLA:H91	1.87	0.41
11:K:75:ASN:ND2	11:K:87:ARG:O	2.51	0.41
12:L:90:ARG:HB3	12:L:93:VAL:HG21	2.03	0.41
30:4:502:XAT:C32	19:4:605:CLA:HMB2	2.50	0.41
19:4:601:CLA:CHA	19:4:601:CLA:HBA1	2.51	0.41
29:4:613:CHL:H13	29:4:615:CHL:C1C	2.51	0.41
19:4:617:CLA:HBA2	19:4:617:CLA:H3A	1.82	0.41
1:A:440:ASP:HB2	4:D:88:THR:OG1	2.21	0.41
19:A:1120:CLA:H93	19:A:1120:CLA:H111	1.82	0.41
19:A:1134:CLA:H52	19:A:1134:CLA:H11	1.79	0.41
2:B:157:LEU:HD23	2:B:157:LEU:HA	1.94	0.41
19:B:1205:CLA:C1A	19:B:1205:CLA:CGA	2.98	0.41
19:B:1222:CLA:H91	19:B:1222:CLA:H112	1.80	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:B:1228:CLA:H142	19:F:1302:CLA:H122	2.03	0.41
19:B:1240:CLA:H52	19:B:1240:CLA:H11	1.94	0.41
24:B:5006:LMT:H62	25:F:5002:LMG:H381	2.02	0.41
22:G:4021:BCR:H351	22:G:4021:BCR:H15C	1.86	0.41
13:1:128:TRP:NE1	19:1:613:CLA:HED2	2.36	0.41
14:2:146:PHE:CG	25:2:806:LMG:HC3	2.56	0.41
29:3:607:CHL:HHC	29:3:607:CHL:CBB	2.48	0.41
16:4:114:VAL:O	16:4:118:ILE:HG12	2.20	0.41
16:4:131:LYS:HE3	16:4:131:LYS:HB3	1.85	0.41
16:4:215:PHE:CD2	30:4:502:XAT:H12	2.55	0.41
1:A:527:VAL:HG11	1:A:530:LEU:HD23	2.03	0.41
19:A:1101:CLA:H171	19:A:1101:CLA:H13	1.83	0.41
19:A:1115:CLA:H143	19:A:1115:CLA:H161	1.73	0.41
19:A:1116:CLA:H41	19:A:1116:CLA:H62	1.47	0.41
19:A:1116:CLA:HAC1	19:A:1133:CLA:H42	2.03	0.41
2:B:174:ARG:HB2	19:B:1210:CLA:HBC2	2.01	0.41
2:B:365:PHE:CD2	2:B:734:GLY:HA2	2.56	0.41
2:B:685:THR:HA	2:B:686:PRO:HD3	1.93	0.41
19:B:1221:CLA:H51	19:B:1221:CLA:H11	1.92	0.41
19:B:1226:CLA:H143	19:B:1226:CLA:H111	1.82	0.41
19:B:1231:CLA:H142	19:B:1231:CLA:H112	1.74	0.41
25:B:5003:LMG:H201	22:F:4016:BCR:H17C	2.02	0.41
19:1:603:CLA:H92	19:1:603:CLA:H61	1.75	0.41
14:2:222:ILE:HD12	14:2:222:ILE:HA	1.87	0.41
19:2:607:CLA:CBB	15:3:188:LEU:HD21	2.51	0.41
15:3:84:SER:OG	29:3:604:CHL:HAA2	2.21	0.41
19:3:605:CLA:H52	19:3:605:CLA:H11	1.78	0.41
19:3:606:CLA:HMD2	19:3:614:CLA:HAB	2.02	0.41
1:A:35:ALA:O	1:A:37:PRO:HD3	2.21	0.41
1:A:370:ILE:HG22	19:A:1124:CLA:HED2	2.02	0.41
1:A:604:TRP:HE1	19:B:1023:CLA:C1D	2.34	0.41
19:A:1128:CLA:HBB1	19:A:1128:CLA:HMB1	2.02	0.41
2:B:649:MET:HG2	2:B:723:ALA:HB2	2.02	0.41
19:B:1219:CLA:CAB	19:B:1240:CLA:HED3	2.50	0.41
8:H:91:ALA:N	8:H:92:PRO:HD2	2.35	0.41
8:H:130:GLN:O	8:H:131:LEU:HD23	2.20	0.41
14:2:211:PRO:C	14:2:213:LYS:H	2.24	0.41
16:4:57:LEU:HD12	16:4:57:LEU:HA	1.74	0.41
1:A:148:GLY:O	1:A:152:ILE:HG13	2.21	0.40
19:A:1112:CLA:H52	19:A:1112:CLA:H11	1.85	0.40
2:B:624:LEU:O	2:B:628:SER:OG	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:694:ARG:NH1	9:I:29:GLU:O	2.54	0.40
19:B:1229:CLA:H203	22:F:4016:BCR:H16C	2.03	0.40
6:F:214:PRO:HB2	19:4:605:CLA:H102	2.02	0.40
28:J:4013:LUT:C8	28:J:4013:LUT:H181	2.50	0.40
12:L:79:VAL:HG12	12:L:83:LEU:HD12	2.03	0.40
12:L:145:LEU:HD21	22:L:4019:BCR:H24C	2.03	0.40
13:1:84:CYS:HB3	13:1:188:GLY:HA3	2.03	0.40
29:1:610:CHL:CBB	19:1:613:CLA:HBB2	2.51	0.40
19:1:614:CLA:H142	27:1:803:DGD:HA42	2.03	0.40
14:2:204:LEU:C	14:2:206:TRP:H	2.24	0.40
14:2:238:GLN:O	14:2:242:THR:OG1	2.37	0.40
15:3:157:LEU:HD11	19:3:613:CLA:HMD3	2.02	0.40
16:4:63:PRO:HG2	16:4:66:LEU:HD12	2.02	0.40
19:4:605:CLA:HMD2	19:4:612:CLA:C1D	2.50	0.40
17:N:6:LYS:HB3	17:N:86:VAL:HG23	2.03	0.40
19:A:1134:CLA:H92	19:A:1134:CLA:H61	1.68	0.40
2:B:646:TRP:CZ2	2:B:726:ILE:HG21	2.56	0.40
13:1:195:PHE:CE1	28:1:502:LUT:H30	2.56	0.40
19:1:614:CLA:H2	19:1:614:CLA:H93	2.03	0.40
1:A:106:TYR:HA	1:A:150:PHE:CE2	2.56	0.40
19:A:1102:CLA:HBB1	19:A:1109:CLA:C12	2.51	0.40
19:A:1116:CLA:C2C	19:A:1116:CLA:H8	2.51	0.40
2:B:52:GLY:HA3	23:B:5002:LHG:H331	2.02	0.40
2:B:183:PHE:CZ	19:B:1210:CLA:H61	2.57	0.40
19:B:1210:CLA:H143	19:B:1225:CLA:HMD2	2.02	0.40
19:B:1230:CLA:H61	19:B:1230:CLA:H41	1.62	0.40
6:F:128:ARG:NH2	10:J:34:PRO:HD2	2.37	0.40
8:H:120:GLY:CA	8:H:126:LYS:HE2	2.51	0.40
11:K:113:ILE:CG1	22:K:4002:BCR:H333	2.51	0.40
13:1:186:LYS:HB3	19:1:607:CLA:HMD3	2.02	0.40
19:1:604:CLA:CGA	19:1:604:CLA:H3A	2.51	0.40
19:2:604:CLA:H193	19:2:604:CLA:H162	1.91	0.40
19:3:601:CLA:H52	19:3:601:CLA:H11	1.92	0.40
19:4:604:CLA:H3A	19:4:604:CLA:O1A	2.21	0.40
19:4:612:CLA:H91	19:4:612:CLA:H111	1.89	0.40
1:A:720:THR:HG22	6:F:195:GLU:OE1	2.22	0.40
19:A:1113:CLA:HAA1	15:3:273:LYS:CE	2.51	0.40
19:A:1122:CLA:H162	19:A:1122:CLA:H121	1.74	0.40
19:B:1023:CLA:H161	19:B:1023:CLA:H141	1.71	0.40
20:B:2002:PQN:H301	27:B:5005:DGD:HAE2	2.03	0.40
25:B:5003:LMG:H181	22:F:4016:BCR:C36	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:73:SER:HB2	11:K:103:ASP:OD1	2.21	0.40
12:L:71:THR:OG1	12:L:74:THR:HG22	2.22	0.40
13:1:65:ARG:HH21	25:1:802:LMG:HC3	1.86	0.40
14:2:109:HIS:CE1	19:2:612:CLA:HMD1	2.57	0.40
30:4:502:XAT:C31	19:4:604:CLA:HMC2	2.51	0.40
19:4:617:CLA:H141	19:4:617:CLA:H161	1.72	0.40
17:N:6:LYS:NZ	17:N:86:VAL:HG23	2.37	0.40
19:A:1111:CLA:H111	19:A:1111:CLA:H91	1.84	0.40
19:A:1115:CLA:H3A	19:A:1115:CLA:HBA2	1.70	0.40
19:A:1115:CLA:H51	19:A:1115:CLA:H11	1.71	0.40
19:A:1120:CLA:H102	19:A:1121:CLA:H2	2.03	0.40
23:A:5001:LHG:H131	23:A:5001:LHG:H161	1.87	0.40
2:B:494:LEU:HD23	2:B:494:LEU:HA	1.87	0.40
19:B:1207:CLA:H143	12:L:136:GLY:HA2	2.03	0.40
27:G:5003:DGD:O1A	27:G:5003:DGD:O2D	2.37	0.40
8:H:60:LEU:HD23	8:H:60:LEU:HA	1.74	0.40
8:H:83:SER:HA	12:L:97:LEU:HD11	2.03	0.40
8:H:135:LEU:HD23	8:H:140:GLY:HA3	2.03	0.40
13:1:177:PHE:HE1	19:1:601:CLA:HAA2	1.86	0.40
19:1:605:CLA:H93	19:1:605:CLA:H111	1.82	0.40
16:4:210:LEU:HD21	28:4:501:LUT:H191	2.02	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	741/743 (100%)	715 (96%)	26 (4%)	0	100	100
2	B	731/733 (100%)	698 (96%)	33 (4%)	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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	E	64/66 (97%)	61 (95%)	3 (5%)	0	100	100
6	F	152/154 (99%)	145 (95%)	6 (4%)	1 (1%)	19	35
7	G	95/97 (98%)	90 (95%)	5 (5%)	0	100	100
8	H	86/88 (98%)	78 (91%)	8 (9%)	0	100	100
9	I	29/31 (94%)	29 (100%)	0	0	100	100
10	J	40/42 (95%)	40 (100%)	0	0	100	100
11	K	79/81 (98%)	70 (89%)	6 (8%)	3 (4%)	2	3
12	L	155/157 (99%)	143 (92%)	12 (8%)	0	100	100
13	1	191/193 (99%)	175 (92%)	16 (8%)	0	100	100
14	2	206/208 (99%)	178 (86%)	26 (13%)	2 (1%)	13	25
15	3	219/221 (99%)	190 (87%)	29 (13%)	0	100	100
16	4	196/198 (99%)	181 (92%)	15 (8%)	0	100	100
17	N	95/97 (98%)	84 (88%)	9 (10%)	2 (2%)	5	10
All	All	3298/3332 (99%)	3082 (94%)	208 (6%)	8 (0%)	45	64

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
11	K	49	SER
11	K	50	PRO
17	N	66	ASP
14	2	149	THR
17	N	68	GLN
6	F	110	ALA
14	2	178	ASN
11	K	48	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	604/604 (100%)	590 (98%)	14 (2%)	45	72
2	B	598/598 (100%)	583 (98%)	15 (2%)	42	69
3	C	69/69 (100%)	67 (97%)	2 (3%)	37	64
4	D	122/122 (100%)	119 (98%)	3 (2%)	42	69
5	E	58/58 (100%)	57 (98%)	1 (2%)	56	79
6	F	125/126 (99%)	123 (98%)	2 (2%)	58	80
7	G	82/82 (100%)	76 (93%)	6 (7%)	11	24
8	H	71/71 (100%)	68 (96%)	3 (4%)	25	49
9	I	27/27 (100%)	26 (96%)	1 (4%)	29	55
10	J	35/35 (100%)	35 (100%)	0	100	100
11	K	59/59 (100%)	55 (93%)	4 (7%)	13	27
12	L	124/124 (100%)	119 (96%)	5 (4%)	27	51
13	1	158/158 (100%)	155 (98%)	3 (2%)	52	77
14	2	167/167 (100%)	157 (94%)	10 (6%)	16	33
15	3	171/172 (99%)	165 (96%)	6 (4%)	31	57
16	4	164/164 (100%)	158 (96%)	6 (4%)	29	55
17	N	82/82 (100%)	75 (92%)	7 (8%)	8	18
All	All	2716/2718 (100%)	2628 (97%)	88 (3%)	36	60

All (88) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	SER
1	A	73	GLU
1	A	104	SER
1	A	119	SER
1	A	149	PHE
1	A	160	SER
1	A	174	PHE
1	A	273	ASN
1	A	290	LEU
1	A	301	HIS
1	A	377	TYR
1	A	478	SER
1	A	512	SER
1	A	526	LYS
2	B	33	SER

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Mol	Chain	Res	Type
2	B	62	SER
2	B	92	TRP
2	B	106	ARG
2	B	155	LEU
2	B	239	SER
2	B	393	PHE
2	B	480	SER
2	B	505	SER
2	B	536	LYS
2	B	577	TYR
2	B	601	LEU
2	B	644	SER
2	B	701	SER
2	B	733	PHE
3	C	9	ASP
3	C	41	SER
4	D	93	ARG
4	D	149	TYR
4	D	190	ARG
5	E	70	ARG
6	F	100	LYS
6	F	212	SER
7	G	71	SER
7	G	107	ARG
7	G	117	SER
7	G	123	PHE
7	G	146	SER
7	G	147	SER
8	H	101	LYS
8	H	119	SER
8	H	139	LEU
9	I	31	ARG
11	K	60	SER
11	K	83	LYS
11	K	99	PHE
11	K	103	ASP
12	L	76	SER
12	L	96	LEU
12	L	109	LEU
12	L	152	SER
12	L	180	ASP
13	1	42	MET

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Mol	Chain	Res	Type
13	1	131	LEU
13	1	177	PHE
14	2	65	PRO
14	2	110	SER
14	2	144	GLU
14	2	148	ASP
14	2	170	ASP
14	2	173	ASN
14	2	192	ASP
14	2	206	TRP
14	2	213	LYS
14	2	214	LEU
15	3	66	SER
15	3	71	SER
15	3	108	PHE
15	3	131	GLU
15	3	167	PHE
15	3	269	LEU
16	4	53	LYS
16	4	89	LYS
16	4	162	ASN
16	4	230	PHE
16	4	231	ASP
16	4	240	PRO
17	N	4	LYS
17	N	26	ASP
17	N	38	SER
17	N	44	CYS
17	N	55	GLU
17	N	87	ILE
17	N	88	GLU

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

Mol	Chain	Res	Type
7	G	95	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 243 ligands modelled in this entry, 2 are monoatomic - leaving 241 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
28	LUT	1	501	-	42,43,43	2.35	1 (2%)	51,60,60	1.81	10 (19%)
19	CLA	3	602	-	52,60,73	1.53	8 (15%)	60,97,113	2.10	18 (30%)
19	CLA	B	1238	-	65,73,73	1.37	7 (10%)	76,113,113	2.06	18 (23%)
29	CHL	3	604	-	66,74,74	0.89	4 (6%)	73,114,114	1.41	10 (13%)
19	CLA	B	1231	-	60,68,73	1.43	7 (11%)	70,107,113	2.00	16 (22%)
19	CLA	A	1113	-	45,53,73	1.65	8 (17%)	52,89,113	2.19	15 (28%)
19	CLA	1	607	-	46,54,73	1.59	7 (15%)	53,90,113	2.12	13 (24%)
19	CLA	4	605	-	60,68,73	1.48	8 (13%)	70,107,113	2.05	20 (28%)
22	BCR	A	4011	-	41,41,41	1.83	4 (9%)	56,56,56	4.29	17 (30%)
31	C7Z	4	505	-	43,43,43	5.44	17 (39%)	58,60,60	5.32	31 (53%)
19	CLA	G	1603	-	65,73,73	1.37	8 (12%)	76,113,113	2.02	16 (21%)
29	CHL	1	612	-	61,69,74	0.94	3 (4%)	67,108,114	1.27	11 (16%)
19	CLA	3	617	-	60,68,73	1.41	6 (10%)	70,107,113	1.98	18 (25%)
22	BCR	B	4005	-	41,41,41	1.85	5 (12%)	56,56,56	4.27	16 (28%)
19	CLA	B	1202	-	65,73,73	1.36	7 (10%)	76,113,113	1.84	18 (23%)
19	CLA	4	604	-	60,68,73	1.41	7 (11%)	70,107,113	2.18	18 (25%)
19	CLA	A	1121	-	60,68,73	1.44	8 (13%)	70,107,113	1.99	18 (25%)
19	CLA	B	1213	-	60,68,73	1.45	7 (11%)	70,107,113	2.06	17 (24%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	DGD	G	5003	-	48,48,67	0.85	2 (4%)	62,62,81	1.14	3 (4%)
19	CLA	1	613	-	45,53,73	1.64	8 (17%)	52,89,113	2.06	14 (26%)
23	LHG	2	807	-	32,32,48	0.45	0	35,38,54	1.22	2 (5%)
29	CHL	2	609	14	66,74,74	0.97	4 (6%)	73,114,114	1.31	10 (13%)
19	CLA	4	602	-	50,58,73	1.53	8 (16%)	58,95,113	2.33	18 (31%)
22	BCR	B	4006	-	41,41,41	1.88	4 (9%)	56,56,56	4.18	25 (44%)
19	CLA	1	601	-	65,73,73	1.38	7 (10%)	76,113,113	1.98	17 (22%)
29	CHL	2	611	-	48,56,74	1.17	5 (10%)	51,92,114	1.39	10 (19%)
23	LHG	A	5002	-	48,48,48	0.41	0	51,54,54	1.10	3 (5%)
19	CLA	B	1225	-	65,73,73	1.38	8 (12%)	76,113,113	1.89	14 (18%)
20	PQN	B	2002	-	34,34,34	0.32	0	42,45,45	1.18	2 (4%)
19	CLA	1	611	-	65,73,73	1.34	7 (10%)	76,113,113	1.98	16 (21%)
19	CLA	A	1141	-	60,68,73	1.43	7 (11%)	70,107,113	2.16	18 (25%)
25	LMG	F	5003	-	36,36,55	0.71	1 (2%)	44,44,63	1.04	2 (4%)
19	CLA	B	1216	-	65,73,73	1.35	8 (12%)	76,113,113	1.95	17 (22%)
19	CLA	A	1133	-	65,73,73	1.35	7 (10%)	76,113,113	1.99	18 (23%)
19	CLA	A	1137	-	65,73,73	1.39	8 (12%)	76,113,113	1.92	16 (21%)
22	BCR	B	4009	-	41,41,41	1.83	4 (9%)	56,56,56	4.23	16 (28%)
19	CLA	2	607	-	60,68,73	1.42	8 (13%)	70,107,113	2.07	18 (25%)
19	CLA	4	617	-	65,73,73	1.36	7 (10%)	76,113,113	1.94	17 (22%)
19	CLA	2	603	-	65,73,73	1.38	8 (12%)	76,113,113	2.00	17 (22%)
19	CLA	B	1209	-	46,54,73	1.60	7 (15%)	53,90,113	2.20	14 (26%)
19	CLA	3	614	-	42,50,73	1.68	9 (21%)	48,85,113	2.19	16 (33%)
29	CHL	3	611	-	47,55,74	1.17	5 (10%)	50,91,114	1.50	9 (18%)
29	CHL	1	609	13	56,64,74	1.06	6 (10%)	61,102,114	1.31	9 (14%)
29	CHL	2	610	-	56,64,74	0.88	2 (3%)	61,102,114	1.43	15 (24%)
19	CLA	B	1203	2	65,73,73	1.36	7 (10%)	76,113,113	1.87	17 (22%)
22	BCR	F	4016	-	41,41,41	1.84	5 (12%)	56,56,56	4.19	12 (21%)
19	CLA	A	1119	-	65,73,73	1.36	8 (12%)	76,113,113	1.94	15 (19%)
25	LMG	2	803	-	36,36,55	0.68	2 (5%)	44,44,63	1.06	3 (6%)
25	LMG	B	5004	-	33,33,55	0.55	1 (3%)	41,41,63	1.23	4 (9%)
22	BCR	F	4014	-	41,41,41	1.85	4 (9%)	56,56,56	4.28	13 (23%)
32	FES	N	101	17	0,4,4	-	-	-	-	-
19	CLA	B	1223	-	65,73,73	1.38	7 (10%)	76,113,113	1.96	17 (22%)
19	CLA	B	1222	33	65,73,73	1.36	7 (10%)	76,113,113	2.13	16 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	BCR	I	4018	-	41,41,41	1.81	5 (12%)	56,56,56	4.24	21 (37%)
22	BCR	A	4007	-	41,41,41	1.84	4 (9%)	56,56,56	4.41	19 (33%)
19	CLA	A	1138	-	65,73,73	1.35	8 (12%)	76,113,113	1.88	16 (21%)
19	CLA	B	1206	-	65,73,73	1.34	8 (12%)	76,113,113	2.02	14 (18%)
19	CLA	A	1115	-	65,73,73	1.36	7 (10%)	76,113,113	1.96	13 (17%)
23	LHG	A	5001	-	39,39,48	0.44	0	42,45,54	1.12	3 (7%)
19	CLA	A	1103	-	65,73,73	1.34	7 (10%)	76,113,113	2.05	19 (25%)
19	CLA	B	1227	-	65,73,73	1.38	7 (10%)	76,113,113	1.98	14 (18%)
19	CLA	A	1012	-	65,73,73	1.41	7 (10%)	76,113,113	2.10	16 (21%)
27	DGD	4	801	-	52,52,67	0.95	4 (7%)	66,66,81	1.30	8 (12%)
24	LMT	G	5005	-	32,32,36	1.29	6 (18%)	43,43,47	1.13	5 (11%)
19	CLA	A	1118	-	50,58,73	1.56	8 (16%)	58,95,113	2.30	16 (27%)
19	CLA	B	1218	-	65,73,73	1.39	9 (13%)	76,113,113	2.01	19 (25%)
19	CLA	1	605	-	65,73,73	1.36	7 (10%)	76,113,113	2.08	17 (22%)
19	CLA	2	604	-	65,73,73	1.36	7 (10%)	76,113,113	2.08	19 (25%)
22	BCR	A	4003	-	41,41,41	1.83	4 (9%)	56,56,56	4.20	16 (28%)
23	LHG	B	5002	-	48,48,48	0.39	0	51,54,54	1.08	3 (5%)
19	CLA	B	1237	-	65,73,73	1.35	7 (10%)	76,113,113	1.98	16 (21%)
19	CLA	A	1116	-	56,64,73	1.49	7 (12%)	65,102,113	2.05	16 (24%)
19	CLA	B	1217	-	46,54,73	1.65	8 (17%)	53,90,113	2.16	15 (28%)
22	BCR	K	4001	-	41,41,41	1.85	4 (9%)	56,56,56	4.37	14 (25%)
27	DGD	B	5005	-	62,62,67	1.10	6 (9%)	76,76,81	1.09	4 (5%)
19	CLA	B	1229	-	65,73,73	1.37	7 (10%)	76,113,113	2.01	15 (19%)
29	CHL	4	611	-	51,59,74	1.12	4 (7%)	55,96,114	1.74	13 (23%)
19	CLA	A	1111	-	65,73,73	1.34	7 (10%)	76,113,113	2.05	17 (22%)
19	CLA	B	1221	-	65,73,73	1.35	7 (10%)	76,113,113	2.06	16 (21%)
19	CLA	A	1109	-	65,73,73	1.36	8 (12%)	76,113,113	1.98	16 (21%)
25	LMG	A	5006	-	50,50,55	1.06	5 (10%)	58,58,63	1.22	5 (8%)
19	CLA	L	1501	-	50,58,73	1.52	7 (14%)	58,95,113	2.32	19 (32%)
25	LMG	2	806	-	13,13,55	0.53	0	18,18,63	0.55	0
19	CLA	B	1226	-	65,73,73	1.37	8 (12%)	76,113,113	2.09	18 (23%)
19	CLA	B	1230	-	58,66,73	1.44	7 (12%)	67,104,113	2.14	18 (26%)
22	BCR	A	4002	-	41,41,41	1.84	4 (9%)	56,56,56	4.24	22 (39%)
22	BCR	B	4004	-	41,41,41	1.97	4 (9%)	56,56,56	5.07	22 (39%)
28	LUT	1	502	-	42,43,43	2.24	1 (2%)	51,60,60	1.99	14 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	CLA	1	606	-	50,58,73	1.54	8 (16%)	58,95,113	2.23	18 (31%)
22	BCR	1	504	-	41,41,41	1.89	4 (9%)	56,56,56	4.63	22 (39%)
19	CLA	A	1126	-	65,73,73	1.39	7 (10%)	76,113,113	1.97	15 (19%)
19	CLA	K	1402	-	60,68,73	1.44	9 (15%)	70,107,113	2.09	17 (24%)
23	LHG	3	801	-	16,16,48	0.87	1 (6%)	17,20,54	0.67	0
19	CLA	B	1212	-	55,63,73	1.48	8 (14%)	64,101,113	2.21	19 (29%)
19	CLA	3	610	15	65,73,73	1.34	8 (12%)	76,113,113	1.97	17 (22%)
29	CHL	4	613	-	61,69,74	1.00	3 (4%)	67,108,114	1.27	10 (14%)
19	CLA	A	1104	1	65,73,73	1.36	7 (10%)	76,113,113	2.02	18 (23%)
19	CLA	3	606	-	50,58,73	1.56	8 (16%)	58,95,113	2.26	18 (31%)
19	CLA	3	603	-	55,63,73	1.46	8 (14%)	64,101,113	2.12	17 (26%)
19	CLA	B	1208	-	60,68,73	1.42	7 (11%)	70,107,113	2.00	17 (24%)
19	CLA	B	1220	-	55,63,73	1.51	7 (12%)	64,101,113	2.00	17 (26%)
21	SF4	C	3002	3	0,12,12	-	-	-	-	-
22	BCR	J	4012	-	41,41,41	1.83	4 (9%)	56,56,56	4.23	17 (30%)
29	CHL	4	615	-	43,51,74	1.06	2 (4%)	45,86,114	1.52	10 (22%)
19	CLA	A	1120	-	60,68,73	1.40	7 (11%)	70,107,113	2.07	16 (22%)
19	CLA	A	1130	-	55,63,73	1.46	7 (12%)	64,101,113	2.15	18 (28%)
19	CLA	B	1215	-	65,73,73	1.35	7 (10%)	76,113,113	2.17	18 (23%)
28	LUT	J	4013	-	42,43,43	2.27	1 (2%)	51,60,60	1.98	12 (23%)
22	BCR	3	503	-	41,41,41	1.86	4 (9%)	56,56,56	4.39	16 (28%)
29	CHL	2	615	-	56,64,74	0.93	3 (5%)	61,102,114	1.54	11 (18%)
19	CLA	A	1124	33	55,63,73	1.47	8 (14%)	64,101,113	2.20	18 (28%)
19	CLA	A	1114	-	46,54,73	1.63	7 (15%)	53,90,113	2.18	14 (26%)
20	PQN	A	2001	-	34,34,34	0.32	0	42,45,45	1.24	4 (9%)
24	LMT	A	5004	-	36,36,36	1.19	6 (16%)	47,47,47	1.21	4 (8%)
19	CLA	B	1235	-	65,73,73	1.33	8 (12%)	76,113,113	1.99	17 (22%)
19	CLA	4	608	-	46,54,73	1.61	8 (17%)	53,90,113	2.05	12 (22%)
19	CLA	B	1207	-	65,73,73	1.39	8 (12%)	76,113,113	1.99	17 (22%)
19	CLA	B	1211	-	65,73,73	1.34	6 (9%)	76,113,113	2.09	21 (27%)
24	LMT	B	5006	-	33,33,36	1.23	5 (15%)	44,44,47	1.04	4 (9%)
25	LMG	G	5001	-	49,49,55	0.99	4 (8%)	57,57,63	1.25	4 (7%)
19	CLA	3	608	-	48,56,73	1.60	9 (18%)	55,92,113	2.21	16 (29%)
19	CLA	4	612	16	65,73,73	1.37	7 (10%)	76,113,113	1.98	18 (23%)
19	CLA	2	605	-	65,73,73	1.36	7 (10%)	76,113,113	2.11	17 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	CLA	A	1125	-	65,73,73	1.36	7 (10%)	76,113,113	1.96	16 (21%)
28	LUT	4	501	-	42,43,43	2.36	1 (2%)	51,60,60	2.02	16 (31%)
19	CLA	A	1101	-	65,73,73	1.36	8 (12%)	76,113,113	2.19	19 (25%)
19	CLA	4	603	-	65,73,73	1.38	7 (10%)	76,113,113	1.91	17 (22%)
21	SF4	A	3001	1,2	0,12,12	-	-	-	-	-
19	CLA	J	1901	33	50,58,73	1.54	9 (18%)	58,95,113	2.12	16 (27%)
19	CLA	B	1201	-	65,73,73	1.36	8 (12%)	76,113,113	2.05	18 (23%)
19	CLA	A	1110	-	55,63,73	1.48	8 (14%)	64,101,113	2.10	18 (28%)
22	BCR	A	4017	-	41,41,41	1.86	5 (12%)	56,56,56	4.83	18 (32%)
23	LHG	2	801	-	34,34,48	0.49	0	37,40,54	1.18	4 (10%)
19	CLA	4	606	-	50,58,73	1.56	7 (14%)	58,95,113	2.17	16 (27%)
19	CLA	2	601	-	60,68,73	1.42	9 (15%)	70,107,113	2.00	16 (22%)
19	CLA	1	614	13	60,68,73	1.42	9 (15%)	70,107,113	2.11	19 (27%)
22	BCR	2	503	-	41,41,41	1.90	4 (9%)	56,56,56	4.98	24 (42%)
19	CLA	A	1117	-	65,73,73	1.35	7 (10%)	76,113,113	1.96	16 (21%)
19	CLA	A	1131	-	65,73,73	1.40	7 (10%)	76,113,113	1.97	15 (19%)
19	CLA	B	1228	-	60,68,73	1.41	7 (11%)	70,107,113	2.04	14 (20%)
19	CLA	B	1023	-	65,73,73	1.40	7 (10%)	76,113,113	1.97	18 (23%)
19	CLA	2	606	-	50,58,73	1.55	7 (14%)	58,95,113	2.33	17 (29%)
28	LUT	3	501	-	42,43,43	2.37	1 (2%)	51,60,60	2.04	14 (27%)
25	LMG	1	802	-	46,46,55	0.94	3 (6%)	54,54,63	1.10	3 (5%)
22	BCR	G	4011	-	41,41,41	1.85	4 (9%)	56,56,56	4.54	20 (35%)
29	CHL	4	610	-	47,55,74	1.04	3 (6%)	50,91,114	1.44	8 (16%)
19	CLA	A	1132	-	65,73,73	1.41	8 (12%)	76,113,113	2.03	18 (23%)
19	CLA	A	1107	1	65,73,73	1.36	6 (9%)	76,113,113	2.03	20 (26%)
19	CLA	A	1106	1	65,73,73	1.36	7 (10%)	76,113,113	2.02	16 (21%)
19	CLA	G	1601	-	55,63,73	1.48	8 (14%)	64,101,113	2.14	18 (28%)
19	CLA	4	601	16	60,68,73	1.43	7 (11%)	70,107,113	2.08	17 (24%)
19	CLA	A	1134	1	55,63,73	1.49	8 (14%)	64,101,113	2.18	16 (25%)
25	LMG	G	5002	-	50,50,55	1.05	5 (10%)	58,58,63	1.18	3 (5%)
19	CLA	1	604	-	65,73,73	1.38	8 (12%)	76,113,113	1.94	18 (23%)
19	CLA	A	1013	-	65,73,73	1.36	7 (10%)	76,113,113	1.87	18 (23%)
25	LMG	3	802	-	30,30,55	0.57	1 (3%)	38,38,63	1.16	4 (10%)
29	CHL	3	607	-	51,59,74	1.00	3 (5%)	55,96,114	1.30	7 (12%)
25	LMG	2	802	-	25,25,55	0.58	0	33,33,63	1.22	3 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	CLA	A	1139	-	65,73,73	1.37	7 (10%)	76,113,113	2.08	21 (27%)
19	CLA	L	1502	-	60,68,73	1.41	8 (13%)	70,107,113	2.05	17 (24%)
19	CLA	F	1301	-	65,73,73	1.36	7 (10%)	76,113,113	1.99	16 (21%)
19	CLA	B	1234	-	55,63,73	1.50	8 (14%)	64,101,113	2.10	17 (26%)
25	LMG	F	5001	-	30,30,55	0.54	0	38,38,63	1.16	2 (5%)
19	CLA	B	1204	-	65,73,73	1.40	7 (10%)	76,113,113	1.84	12 (15%)
25	LMG	2	804	-	30,30,55	0.52	0	38,38,63	1.20	3 (7%)
29	CHL	1	610	13	47,55,74	1.10	4 (8%)	50,91,114	1.54	9 (18%)
22	BCR	I	4020	-	41,41,41	1.89	5 (12%)	56,56,56	4.45	15 (26%)
22	BCR	L	4020	-	41,41,41	1.87	4 (9%)	56,56,56	4.27	17 (30%)
19	CLA	A	1122	-	65,73,73	1.36	8 (12%)	76,113,113	1.94	16 (21%)
19	CLA	A	1112	-	65,73,73	1.36	8 (12%)	76,113,113	1.98	19 (25%)
25	LMG	2	805	-	13,13,55	0.53	0	18,18,63	0.68	0
19	CLA	1	602	13	46,54,73	1.61	8 (17%)	53,90,113	2.16	13 (24%)
19	CLA	A	1129	-	65,73,73	1.37	8 (12%)	76,113,113	1.98	13 (17%)
19	CLA	3	601	15	55,63,73	1.46	6 (10%)	64,101,113	2.14	17 (26%)
24	LMT	G	5004	-	36,36,36	1.21	6 (16%)	47,47,47	1.20	3 (6%)
19	CLA	A	1140	-	65,73,73	1.37	7 (10%)	76,113,113	1.88	16 (21%)
19	CLA	1	608	-	46,54,73	1.64	8 (17%)	53,90,113	2.27	13 (24%)
19	CLA	A	1123	-	65,73,73	1.37	8 (12%)	76,113,113	2.01	16 (21%)
19	CLA	F	1302	6	65,73,73	1.34	7 (10%)	76,113,113	2.01	15 (19%)
21	SF4	C	3003	3	0,12,12	-	-	-	-	-
24	LMT	B	5008	-	32,32,36	1.27	5 (15%)	43,43,47	0.96	2 (4%)
19	CLA	B	1205	-	65,73,73	1.40	7 (10%)	76,113,113	1.96	14 (18%)
18	CL0	A	1011	-	65,73,73	2.20	17 (26%)	76,113,113	2.43	21 (27%)
22	BCR	A	4008	-	41,41,41	1.85	4 (9%)	56,56,56	4.13	17 (30%)
22	BCR	K	4002	-	41,41,41	1.85	4 (9%)	56,56,56	4.36	17 (30%)
19	CLA	B	1022	-	65,73,73	1.40	7 (10%)	76,113,113	1.96	16 (21%)
19	CLA	A	1136	-	65,73,73	1.33	8 (12%)	76,113,113	2.02	16 (21%)
19	CLA	B	1210	-	65,73,73	1.33	7 (10%)	76,113,113	2.11	20 (26%)
23	LHG	1	801	-	48,48,48	0.40	0	51,54,54	1.14	4 (7%)
19	CLA	4	607	-	60,68,73	1.43	8 (13%)	70,107,113	1.88	15 (21%)
25	LMG	F	5002	-	47,47,55	0.98	3 (6%)	55,55,63	1.22	4 (7%)
27	DGD	F	5005	-	58,58,67	1.05	5 (8%)	72,72,81	1.17	5 (6%)
23	LHG	B	5001	-	20,20,48	0.62	0	23,26,54	1.60	3 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	CLA	1	603	-	55,63,73	1.50	8 (14%)	64,101,113	2.23	18 (28%)
19	CLA	3	612	15	50,58,73	1.53	8 (16%)	58,95,113	2.28	15 (25%)
22	BCR	L	4019	-	41,41,41	1.85	4 (9%)	56,56,56	4.28	16 (28%)
19	CLA	A	1105	-	60,68,73	1.43	6 (10%)	70,107,113	2.07	16 (22%)
19	CLA	A	1127	-	65,73,73	1.36	8 (12%)	76,113,113	2.00	16 (21%)
19	CLA	B	1219	-	65,73,73	1.36	7 (10%)	76,113,113	2.01	18 (23%)
19	CLA	B	1239	-	65,73,73	1.40	9 (13%)	76,113,113	1.99	15 (19%)
22	BCR	3	506	-	41,41,41	1.86	4 (9%)	56,56,56	4.43	16 (28%)
27	DGD	4	802	-	52,52,67	0.90	2 (3%)	66,66,81	1.02	2 (3%)
19	CLA	4	609	16	50,58,73	1.54	8 (16%)	58,95,113	2.28	16 (27%)
30	XAT	4	502	-	39,47,47	0.80	1 (2%)	54,74,74	1.75	15 (27%)
19	CLA	A	1135	-	51,59,73	1.52	8 (15%)	59,96,113	2.25	18 (30%)
19	CLA	K	1401	-	45,53,73	1.61	10 (22%)	52,89,113	2.15	13 (25%)
30	XAT	2	502	-	39,47,47	0.75	1 (2%)	54,74,74	2.42	15 (27%)
19	CLA	A	1128	-	65,73,73	1.37	7 (10%)	76,113,113	2.04	17 (22%)
22	BCR	G	4021	-	41,41,41	1.89	4 (9%)	56,56,56	4.36	18 (32%)
19	CLA	B	1214	-	65,73,73	1.37	7 (10%)	76,113,113	1.98	16 (21%)
27	DGD	1	803	-	42,42,67	0.87	1 (2%)	56,56,81	1.10	3 (5%)
19	CLA	L	1503	33	50,58,73	1.54	9 (18%)	58,95,113	2.27	19 (32%)
24	LMT	J	5003	-	26,26,36	1.34	5 (19%)	37,37,47	1.14	3 (8%)
19	CLA	2	608	-	50,58,73	1.54	8 (16%)	58,95,113	2.20	18 (31%)
22	BCR	B	4010	-	41,41,41	1.86	4 (9%)	56,56,56	4.17	13 (23%)
25	LMG	F	5006	-	13,13,55	0.53	0	18,18,63	0.75	0
19	CLA	2	612	-	55,63,73	1.49	7 (12%)	64,101,113	2.12	14 (21%)
27	DGD	3	803	-	52,52,67	0.86	3 (5%)	66,66,81	1.11	3 (4%)
25	LMG	B	5003	-	35,35,55	0.74	1 (2%)	43,43,63	1.17	5 (11%)
19	CLA	B	1240	-	65,73,73	1.36	7 (10%)	76,113,113	2.07	19 (25%)
25	LMG	B	5007	-	34,34,55	0.49	0	42,42,63	1.18	3 (7%)
19	CLA	B	1236	-	50,58,73	1.56	7 (14%)	58,95,113	2.24	17 (29%)
22	BCR	1	503	-	41,41,41	1.86	4 (9%)	56,56,56	4.23	17 (30%)
19	CLA	2	602	-	52,60,73	1.55	8 (15%)	60,97,113	2.10	18 (30%)
25	LMG	F	5004	-	34,34,55	0.46	0	42,42,63	1.13	2 (4%)
28	LUT	2	501	-	42,43,43	2.39	1 (2%)	51,60,60	2.20	15 (29%)
27	DGD	J	5001	-	59,59,67	1.04	5 (8%)	73,73,81	1.00	2 (2%)
19	CLA	A	1108	-	50,58,73	1.57	7 (14%)	58,95,113	2.19	19 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	CLA	B	1224	-	65,73,73	1.38	7 (10%)	76,113,113	1.95	18 (23%)
19	CLA	G	1602	7	46,54,73	1.59	8 (17%)	53,90,113	2.17	16 (30%)
19	CLA	B	1021	-	65,73,73	1.38	7 (10%)	76,113,113	2.01	18 (23%)
19	CLA	K	1403	11	48,56,73	1.60	9 (18%)	55,92,113	2.35	17 (30%)
19	CLA	A	1102	-	65,73,73	1.34	8 (12%)	76,113,113	2.01	16 (21%)
19	CLA	B	1232	-	55,63,73	1.52	8 (14%)	64,101,113	2.17	18 (28%)
19	CLA	3	605	15	55,63,73	1.53	9 (16%)	64,101,113	2.10	18 (28%)
29	CHL	2	613	-	46,54,74	1.08	3 (6%)	49,90,114	1.37	8 (16%)
25	LMG	G	5006	-	25,25,55	0.56	0	33,33,63	1.32	2 (6%)
19	CLA	K	1404	-	46,54,73	1.65	9 (19%)	53,90,113	1.97	13 (24%)
19	CLA	3	613	-	46,54,73	1.64	8 (17%)	53,90,113	2.18	13 (24%)
19	CLA	G	1701	-	60,68,73	1.42	8 (13%)	70,107,113	2.04	15 (21%)
28	LUT	3	502	-	42,43,43	2.33	1 (2%)	51,60,60	1.99	13 (25%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	LUT	1	501	-	-	2/29/67/67	0/2/2/2
19	CLA	3	602	-	1/1/12/20	9/22/100/115	-
19	CLA	B	1238	-	1/1/15/20	24/37/115/115	-
29	CHL	3	604	-	4/4/20/26	11/39/137/137	-
19	CLA	B	1231	-	1/1/14/20	11/31/109/115	-
19	CLA	A	1113	-	1/1/11/20	7/13/91/115	-
19	CLA	1	607	-	1/1/11/20	4/15/93/115	-
19	CLA	4	605	-	-	15/31/109/115	-
22	BCR	A	4011	-	-	11/29/63/63	0/2/2/2
31	C7Z	4	505	-	-	17/29/67/67	0/2/2/2
19	CLA	G	1603	-	1/1/15/20	17/37/115/115	-
29	CHL	1	612	-	4/4/19/26	6/33/131/137	-
19	CLA	3	617	-	1/1/14/20	14/31/109/115	-
22	BCR	B	4005	-	-	9/29/63/63	0/2/2/2
19	CLA	B	1202	-	1/1/15/20	15/37/115/115	-
19	CLA	4	604	-	1/1/14/20	13/31/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	A	1121	-	1/1/14/20	13/31/109/115	-
19	CLA	B	1213	-	1/1/14/20	6/31/109/115	-
27	DGD	G	5003	-	-	11/36/76/95	0/2/2/2
19	CLA	1	613	-	1/1/11/20	4/13/91/115	-
23	LHG	2	807	-	-	19/37/37/53	-
29	CHL	2	609	14	4/4/20/26	8/39/137/137	-
19	CLA	4	602	-	1/1/12/20	8/19/97/115	-
22	BCR	B	4006	-	-	12/29/63/63	0/2/2/2
19	CLA	1	601	-	1/1/15/20	15/37/115/115	-
29	CHL	2	611	-	3/3/16/26	5/18/116/137	-
23	LHG	A	5002	-	-	39/53/53/53	-
19	CLA	B	1225	-	1/1/15/20	18/37/115/115	-
20	PQN	B	2002	-	-	11/23/43/43	0/2/2/2
19	CLA	1	611	-	1/1/15/20	14/37/115/115	-
19	CLA	A	1141	-	1/1/14/20	11/31/109/115	-
25	LMG	F	5003	-	-	13/31/51/70	0/1/1/1
19	CLA	B	1216	-	1/1/15/20	16/37/115/115	-
19	CLA	A	1133	-	1/1/15/20	21/37/115/115	-
19	CLA	A	1137	-	1/1/15/20	17/37/115/115	-
22	BCR	B	4009	-	-	8/29/63/63	0/2/2/2
19	CLA	2	607	-	1/1/14/20	14/31/109/115	-
19	CLA	4	617	-	1/1/15/20	17/37/115/115	-
19	CLA	2	603	-	1/1/15/20	17/37/115/115	-
19	CLA	B	1209	-	1/1/11/20	6/15/93/115	-
19	CLA	3	614	-	1/1/10/20	3/10/88/115	-
29	CHL	3	611	-	3/3/16/26	1/17/115/137	-
29	CHL	1	609	13	4/4/18/26	4/27/125/137	-
29	CHL	2	610	-	4/4/18/26	3/27/125/137	-
19	CLA	B	1203	2	1/1/15/20	15/37/115/115	-
22	BCR	F	4016	-	-	14/29/63/63	0/2/2/2
19	CLA	A	1119	-	1/1/15/20	14/37/115/115	-
25	LMG	2	803	-	-	14/31/51/70	0/1/1/1
25	LMG	B	5004	-	-	16/28/48/70	0/1/1/1
22	BCR	F	4014	-	-	10/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	FES	N	101	17	-	-	0/1/1/1
19	CLA	B	1223	-	1/1/15/20	16/37/115/115	-
19	CLA	B	1222	33	1/1/15/20	18/37/115/115	-
22	BCR	I	4018	-	-	13/29/63/63	0/2/2/2
22	BCR	A	4007	-	-	4/29/63/63	0/2/2/2
19	CLA	A	1138	-	1/1/15/20	14/37/115/115	-
19	CLA	B	1206	-	1/1/15/20	18/37/115/115	-
19	CLA	A	1115	-	1/1/15/20	23/37/115/115	-
23	LHG	A	5001	-	-	24/44/44/53	-
19	CLA	A	1103	-	1/1/15/20	26/37/115/115	-
19	CLA	B	1227	-	1/1/15/20	14/37/115/115	-
19	CLA	A	1012	-	1/1/15/20	19/37/115/115	-
27	DGD	4	801	-	-	17/40/80/95	0/2/2/2
24	LMT	G	5005	-	-	7/17/57/61	0/2/2/2
19	CLA	A	1118	-	1/1/12/20	4/19/97/115	-
19	CLA	B	1218	-	1/1/15/20	13/37/115/115	-
19	CLA	1	605	-	1/1/15/20	16/37/115/115	-
19	CLA	2	604	-	1/1/15/20	15/37/115/115	-
29	CHL	4	611	-	3/3/17/26	0/21/119/137	-
22	BCR	A	4003	-	-	8/29/63/63	0/2/2/2
19	CLA	B	1237	-	1/1/15/20	20/37/115/115	-
19	CLA	A	1116	-	1/1/13/20	15/27/105/115	-
19	CLA	B	1217	-	1/1/11/20	7/15/93/115	-
22	BCR	K	4001	-	-	9/29/63/63	0/2/2/2
23	LHG	B	5002	-	-	31/53/53/53	-
19	CLA	B	1229	-	1/1/15/20	13/37/115/115	-
27	DGD	B	5005	-	-	25/50/90/95	0/2/2/2
19	CLA	A	1111	-	1/1/15/20	17/37/115/115	-
19	CLA	B	1221	-	1/1/15/20	19/37/115/115	-
19	CLA	A	1109	-	1/1/15/20	10/37/115/115	-
25	LMG	A	5006	-	-	16/45/65/70	0/1/1/1
19	CLA	L	1501	-	1/1/12/20	6/19/97/115	-
25	LMG	2	806	-	-	1/4/24/70	0/1/1/1
19	CLA	B	1226	-	1/1/15/20	24/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	B	1230	-	1/1/13/20	11/29/107/115	-
22	BCR	A	4002	-	-	12/29/63/63	0/2/2/2
22	BCR	B	4004	-	-	8/29/63/63	0/2/2/2
28	LUT	1	502	-	-	2/29/67/67	0/2/2/2
19	CLA	1	606	-	1/1/12/20	7/19/97/115	-
22	BCR	1	504	-	-	14/29/63/63	0/2/2/2
19	CLA	A	1126	-	1/1/15/20	21/37/115/115	-
19	CLA	K	1402	-	1/1/14/20	24/31/109/115	-
23	LHG	3	801	-	-	7/19/19/53	-
19	CLA	B	1212	-	1/1/13/20	12/25/103/115	-
19	CLA	3	610	15	1/1/15/20	20/37/115/115	-
29	CHL	4	613	-	4/4/19/26	8/33/131/137	-
19	CLA	A	1104	1	1/1/15/20	17/37/115/115	-
19	CLA	3	606	-	1/1/12/20	11/19/97/115	-
19	CLA	3	603	-	1/1/13/20	13/25/103/115	-
19	CLA	B	1208	-	1/1/14/20	12/31/109/115	-
19	CLA	B	1220	-	1/1/13/20	9/25/103/115	-
21	SF4	C	3002	3	-	-	0/6/5/5
22	BCR	J	4012	-	-	11/29/63/63	0/2/2/2
29	CHL	4	615	-	3/3/15/26	0/12/110/137	-
19	CLA	A	1120	-	1/1/14/20	12/31/109/115	-
19	CLA	A	1130	-	1/1/13/20	14/25/103/115	-
19	CLA	B	1215	-	1/1/15/20	18/37/115/115	-
28	LUT	J	4013	-	1/1/12/27	4/29/67/67	0/2/2/2
29	CHL	2	615	-	4/4/18/26	8/27/125/137	-
22	BCR	3	503	-	-	12/29/63/63	0/2/2/2
19	CLA	A	1124	33	1/1/13/20	8/25/103/115	-
19	CLA	A	1114	-	1/1/11/20	9/15/93/115	-
20	PQN	A	2001	-	-	4/23/43/43	0/2/2/2
24	LMT	A	5004	-	-	7/21/61/61	0/2/2/2
19	CLA	B	1235	-	1/1/15/20	17/37/115/115	-
19	CLA	4	608	-	1/1/11/20	8/15/93/115	-
19	CLA	B	1207	-	1/1/15/20	19/37/115/115	-
19	CLA	B	1211	-	1/1/15/20	19/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	LMT	B	5006	-	-	9/18/58/61	0/2/2/2
25	LMG	G	5001	-	-	21/44/64/70	0/1/1/1
19	CLA	3	608	-	1/1/11/20	6/17/95/115	-
19	CLA	4	612	16	1/1/15/20	14/37/115/115	-
19	CLA	2	605	-	1/1/15/20	20/37/115/115	-
19	CLA	A	1125	-	1/1/15/20	17/37/115/115	-
28	LUT	4	501	-	-	5/29/67/67	0/2/2/2
19	CLA	A	1101	-	1/1/15/20	21/37/115/115	-
19	CLA	4	603	-	1/1/15/20	15/37/115/115	-
21	SF4	A	3001	1,2	-	-	0/6/5/5
19	CLA	J	1901	33	1/1/12/20	7/19/97/115	-
19	CLA	B	1201	-	1/1/15/20	18/37/115/115	-
19	CLA	A	1110	-	1/1/13/20	7/25/103/115	-
22	BCR	A	4017	-	-	8/29/63/63	0/2/2/2
23	LHG	2	801	-	-	21/39/39/53	-
19	CLA	4	606	-	1/1/12/20	7/19/97/115	-
19	CLA	2	601	-	1/1/14/20	13/31/109/115	-
19	CLA	1	614	13	1/1/14/20	15/31/109/115	-
22	BCR	2	503	-	-	14/29/63/63	0/2/2/2
19	CLA	A	1117	-	1/1/15/20	19/37/115/115	-
19	CLA	A	1131	-	1/1/15/20	14/37/115/115	-
19	CLA	B	1228	-	1/1/14/20	14/31/109/115	-
19	CLA	B	1023	-	1/1/15/20	10/37/115/115	-
19	CLA	2	606	-	1/1/12/20	6/19/97/115	-
28	LUT	3	501	-	-	4/29/67/67	0/2/2/2
25	LMG	1	802	-	-	13/41/61/70	0/1/1/1
22	BCR	G	4011	-	-	10/29/63/63	0/2/2/2
29	CHL	4	610	-	3/3/16/26	7/17/115/137	-
19	CLA	A	1132	-	1/1/15/20	14/37/115/115	-
19	CLA	A	1107	1	1/1/15/20	18/37/115/115	-
19	CLA	A	1106	1	1/1/15/20	17/37/115/115	-
19	CLA	G	1601	-	1/1/13/20	8/25/103/115	-
19	CLA	4	601	16	1/1/14/20	16/31/109/115	-
19	CLA	A	1134	1	1/1/13/20	13/25/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	LMG	G	5002	-	-	20/45/65/70	0/1/1/1
19	CLA	1	604	-	1/1/15/20	16/37/115/115	-
19	CLA	A	1013	-	1/1/15/20	22/37/115/115	-
25	LMG	3	802	-	-	9/25/45/70	0/1/1/1
29	CHL	3	607	-	3/3/17/26	6/21/119/137	-
25	LMG	2	802	-	-	8/20/40/70	0/1/1/1
19	CLA	A	1139	-	1/1/15/20	17/37/115/115	-
19	CLA	L	1502	-	1/1/14/20	15/31/109/115	-
19	CLA	F	1301	-	1/1/15/20	18/37/115/115	-
19	CLA	B	1234	-	1/1/13/20	12/25/103/115	-
25	LMG	F	5001	-	-	9/25/45/70	0/1/1/1
19	CLA	B	1204	-	1/1/15/20	20/37/115/115	-
25	LMG	2	804	-	-	9/25/45/70	0/1/1/1
29	CHL	1	610	13	3/3/16/26	2/17/115/137	-
22	BCR	I	4020	-	-	11/29/63/63	0/2/2/2
22	BCR	L	4020	-	-	9/29/63/63	0/2/2/2
19	CLA	A	1122	-	1/1/15/20	17/37/115/115	-
19	CLA	A	1112	-	1/1/15/20	22/37/115/115	-
25	LMG	2	805	-	-	2/4/24/70	0/1/1/1
19	CLA	1	602	13	1/1/11/20	6/15/93/115	-
19	CLA	A	1129	-	1/1/15/20	18/37/115/115	-
19	CLA	3	601	15	1/1/13/20	10/25/103/115	-
24	LMT	G	5004	-	-	11/21/61/61	0/2/2/2
19	CLA	A	1140	-	1/1/15/20	9/37/115/115	-
19	CLA	1	608	-	1/1/11/20	7/15/93/115	-
19	CLA	A	1123	-	1/1/15/20	16/37/115/115	-
19	CLA	F	1302	6	1/1/15/20	19/37/115/115	-
24	LMT	B	5008	-	-	7/17/57/61	0/2/2/2
21	SF4	C	3003	3	-	-	0/6/5/5
19	CLA	B	1205	-	1/1/15/20	10/37/115/115	-
18	CL0	A	1011	-	3/3/20/25	8/37/135/135	-
22	BCR	A	4008	-	-	13/29/63/63	0/2/2/2
22	BCR	K	4002	-	-	11/29/63/63	0/2/2/2
19	CLA	B	1022	-	1/1/15/20	10/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	A	1136	-	1/1/15/20	19/37/115/115	-
19	CLA	B	1210	-	1/1/15/20	16/37/115/115	-
23	LHG	1	801	-	-	30/53/53/53	-
19	CLA	4	607	-	1/1/14/20	16/31/109/115	-
25	LMG	F	5002	-	-	10/42/62/70	0/1/1/1
27	DGD	F	5005	-	-	20/46/86/95	0/2/2/2
23	LHG	B	5001	-	-	12/23/23/53	-
19	CLA	1	603	-	1/1/13/20	7/25/103/115	-
19	CLA	3	612	15	1/1/12/20	9/19/97/115	-
22	BCR	L	4019	-	-	12/29/63/63	0/2/2/2
19	CLA	A	1105	-	1/1/14/20	18/31/109/115	-
19	CLA	A	1127	-	1/1/15/20	19/37/115/115	-
19	CLA	B	1219	-	1/1/15/20	20/37/115/115	-
19	CLA	B	1239	-	1/1/15/20	19/37/115/115	-
22	BCR	3	506	-	-	14/29/63/63	0/2/2/2
27	DGD	4	802	-	-	16/40/80/95	0/2/2/2
19	CLA	4	609	16	1/1/12/20	10/19/97/115	-
30	XAT	4	502	-	2/2/12/26	6/31/93/93	0/4/4/4
19	CLA	A	1135	-	1/1/12/20	10/21/99/115	-
19	CLA	K	1401	-	1/1/11/20	6/13/91/115	-
30	XAT	2	502	-	1/1/12/26	5/31/93/93	0/4/4/4
19	CLA	A	1128	-	1/1/15/20	13/37/115/115	-
22	BCR	G	4021	-	-	14/29/63/63	0/2/2/2
19	CLA	B	1214	-	1/1/15/20	14/37/115/115	-
27	DGD	1	803	-	-	12/30/70/95	0/2/2/2
19	CLA	L	1503	33	1/1/12/20	6/19/97/115	-
24	LMT	J	5003	-	-	6/11/51/61	0/2/2/2
19	CLA	2	608	-	1/1/12/20	10/19/97/115	-
22	BCR	B	4010	-	-	12/29/63/63	0/2/2/2
25	LMG	F	5006	-	-	1/4/24/70	0/1/1/1
19	CLA	2	612	-	1/1/13/20	11/25/103/115	-
27	DGD	3	803	-	-	10/40/80/95	0/2/2/2
25	LMG	B	5003	-	-	9/30/50/70	0/1/1/1
19	CLA	B	1240	-	1/1/15/20	18/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	LUT	2	501	-	1/1/12/27	5/29/67/67	0/2/2/2
19	CLA	B	1236	-	1/1/12/20	10/19/97/115	-
22	BCR	1	503	-	-	17/29/63/63	0/2/2/2
19	CLA	2	602	-	1/1/12/20	8/22/100/115	-
25	LMG	B	5007	-	-	9/29/49/70	0/1/1/1
25	LMG	F	5004	-	-	9/29/49/70	0/1/1/1
27	DGD	J	5001	-	-	12/47/87/95	0/2/2/2
19	CLA	A	1108	-	1/1/12/20	7/19/97/115	-
19	CLA	B	1224	-	1/1/15/20	15/37/115/115	-
19	CLA	G	1602	7	1/1/11/20	8/15/93/115	-
19	CLA	B	1021	-	1/1/15/20	10/37/115/115	-
19	CLA	K	1403	11	1/1/11/20	9/17/95/115	-
19	CLA	A	1102	-	1/1/15/20	25/37/115/115	-
19	CLA	B	1232	-	1/1/13/20	13/25/103/115	-
29	CHL	2	613	-	3/3/16/26	4/15/113/137	-
19	CLA	3	605	15	-	10/25/103/115	-
25	LMG	G	5006	-	-	10/20/40/70	0/1/1/1
19	CLA	K	1404	-	1/1/11/20	6/15/93/115	-
19	CLA	3	613	-	1/1/11/20	6/15/93/115	-
19	CLA	G	1701	-	1/1/14/20	12/31/109/115	-
28	LUT	3	502	-	1/1/12/27	8/29/67/67	0/2/2/2

All (1364) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	4	505	C7Z	C10-C9	14.87	1.55	1.35
31	4	505	C7Z	C34-C33	14.83	1.55	1.35
31	4	505	C7Z	C14-C13	14.73	1.55	1.35
31	4	505	C7Z	C30-C29	14.67	1.55	1.35
28	3	501	LUT	C24-C25	14.53	1.51	1.33
28	2	501	LUT	C24-C25	14.44	1.51	1.33
28	1	501	LUT	C24-C25	14.19	1.50	1.33
28	4	501	LUT	C24-C25	14.17	1.50	1.33
28	3	502	LUT	C24-C25	14.16	1.50	1.33
28	J	4013	LUT	C24-C25	13.89	1.50	1.33
28	1	502	LUT	C24-C25	13.50	1.49	1.33
31	4	505	C7Z	C25-C26	11.89	1.55	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	4	505	C7Z	C5-C6	10.68	1.52	1.34
18	A	1011	CL0	MG-NA	8.46	2.26	2.06
22	B	4004	BCR	C10-C9	8.30	1.46	1.35
22	2	503	BCR	C10-C9	7.83	1.46	1.35
22	G	4021	BCR	C10-C9	7.65	1.45	1.35
22	1	503	BCR	C10-C9	7.46	1.45	1.35
22	1	504	BCR	C10-C9	7.39	1.45	1.35
22	G	4011	BCR	C10-C9	7.33	1.45	1.35
22	F	4014	BCR	C10-C9	7.17	1.45	1.35
22	3	506	BCR	C10-C9	7.17	1.45	1.35
22	B	4010	BCR	C10-C9	7.15	1.45	1.35
22	K	4001	BCR	C10-C9	7.13	1.45	1.35
22	L	4020	BCR	C10-C9	7.09	1.45	1.35
22	B	4006	BCR	C10-C9	7.08	1.45	1.35
22	L	4019	BCR	C10-C9	7.04	1.45	1.35
22	J	4012	BCR	C10-C9	7.03	1.45	1.35
22	I	4020	BCR	C10-C9	7.02	1.45	1.35
22	B	4005	BCR	C10-C9	6.94	1.45	1.35
22	K	4002	BCR	C10-C9	6.92	1.45	1.35
22	A	4002	BCR	C10-C9	6.91	1.44	1.35
22	A	4008	BCR	C10-C9	6.85	1.44	1.35
22	A	4007	BCR	C10-C9	6.83	1.44	1.35
22	A	4003	BCR	C10-C9	6.82	1.44	1.35
22	3	503	BCR	C10-C9	6.67	1.44	1.35
22	A	4017	BCR	C10-C9	6.66	1.44	1.35
22	B	4009	BCR	C10-C9	6.59	1.44	1.35
19	K	1402	CLA	MG-NA	6.56	2.21	2.06
22	A	4011	BCR	C10-C9	6.50	1.44	1.35
19	K	1404	CLA	MG-NA	6.50	2.21	2.06
22	I	4018	BCR	C10-C9	6.50	1.44	1.35
19	3	605	CLA	MG-NA	6.50	2.21	2.06
19	2	602	CLA	MG-NA	6.49	2.21	2.06
19	K	1403	CLA	MG-NA	6.43	2.21	2.06
19	A	1121	CLA	MG-NA	6.42	2.21	2.06
19	A	1135	CLA	MG-NA	6.40	2.21	2.06
19	B	1234	CLA	MG-NA	6.40	2.21	2.06
19	A	1107	CLA	MG-NA	6.39	2.21	2.06
19	A	1114	CLA	MG-NA	6.38	2.21	2.06
19	A	1123	CLA	MG-NA	6.38	2.21	2.06
19	A	1141	CLA	MG-NA	6.37	2.21	2.06
19	4	605	CLA	MG-NA	6.36	2.21	2.06
19	3	602	CLA	MG-NA	6.35	2.21	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B	1203	CLA	MG-NA	6.34	2.21	2.06
22	F	4016	BCR	C10-C9	6.33	1.44	1.35
19	3	608	CLA	MG-NA	6.33	2.21	2.06
19	B	1218	CLA	MG-NA	6.33	2.21	2.06
19	B	1207	CLA	MG-NA	6.32	2.21	2.06
19	B	1217	CLA	MG-NA	6.32	2.21	2.06
19	1	613	CLA	MG-NA	6.31	2.21	2.06
19	2	603	CLA	MG-NA	6.31	2.21	2.06
19	A	1113	CLA	MG-NA	6.31	2.21	2.06
19	B	1213	CLA	MG-NA	6.31	2.21	2.06
19	B	1223	CLA	MG-NA	6.31	2.21	2.06
19	3	613	CLA	MG-NA	6.30	2.21	2.06
19	3	614	CLA	MG-NA	6.30	2.21	2.06
19	K	1401	CLA	MG-NA	6.30	2.21	2.06
19	F	1301	CLA	MG-NA	6.29	2.21	2.06
19	A	1110	CLA	MG-NA	6.29	2.21	2.06
19	B	1204	CLA	MG-NA	6.27	2.21	2.06
19	L	1503	CLA	MG-NA	6.27	2.21	2.06
19	B	1239	CLA	MG-NA	6.27	2.21	2.06
19	B	1236	CLA	MG-NA	6.26	2.21	2.06
19	G	1602	CLA	MG-NA	6.26	2.21	2.06
19	B	1202	CLA	MG-NA	6.25	2.21	2.06
19	G	1603	CLA	MG-NA	6.25	2.21	2.06
19	B	1229	CLA	MG-NA	6.25	2.21	2.06
19	1	601	CLA	MG-NA	6.25	2.21	2.06
19	A	1116	CLA	MG-NA	6.23	2.21	2.06
19	A	1137	CLA	MG-NA	6.23	2.21	2.06
19	A	1105	CLA	MG-NA	6.23	2.21	2.06
19	1	614	CLA	MG-NA	6.23	2.21	2.06
19	A	1118	CLA	MG-NA	6.22	2.21	2.06
19	B	1240	CLA	MG-NA	6.22	2.21	2.06
19	2	607	CLA	MG-NA	6.22	2.21	2.06
19	B	1212	CLA	MG-NA	6.21	2.21	2.06
19	A	1131	CLA	MG-NA	6.21	2.21	2.06
19	A	1132	CLA	MG-NA	6.21	2.21	2.06
19	J	1901	CLA	MG-NA	6.20	2.21	2.06
19	1	604	CLA	MG-NA	6.20	2.21	2.06
19	B	1022	CLA	MG-NA	6.20	2.21	2.06
19	1	605	CLA	MG-NA	6.19	2.21	2.06
19	4	603	CLA	MG-NA	6.19	2.21	2.06
19	4	612	CLA	MG-NA	6.19	2.21	2.06
19	2	608	CLA	MG-NA	6.19	2.21	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	1108	CLA	MG-NA	6.19	2.21	2.06
19	1	603	CLA	MG-NA	6.19	2.21	2.06
19	G	1601	CLA	MG-NA	6.18	2.21	2.06
19	G	1701	CLA	MG-NA	6.18	2.21	2.06
19	A	1115	CLA	MG-NA	6.18	2.20	2.06
19	A	1128	CLA	MG-NA	6.18	2.20	2.06
19	A	1130	CLA	MG-NA	6.17	2.20	2.06
19	A	1140	CLA	MG-NA	6.16	2.20	2.06
19	A	1012	CLA	MG-NA	6.16	2.20	2.06
19	B	1214	CLA	MG-NA	6.16	2.20	2.06
19	A	1101	CLA	MG-NA	6.16	2.20	2.06
19	B	1209	CLA	MG-NA	6.16	2.20	2.06
19	B	1221	CLA	MG-NA	6.15	2.20	2.06
19	A	1122	CLA	MG-NA	6.15	2.20	2.06
19	B	1235	CLA	MG-NA	6.15	2.20	2.06
19	A	1136	CLA	MG-NA	6.15	2.20	2.06
19	B	1232	CLA	MG-NA	6.15	2.20	2.06
19	A	1104	CLA	MG-NA	6.14	2.20	2.06
19	4	606	CLA	MG-NA	6.14	2.20	2.06
19	B	1023	CLA	MG-NA	6.14	2.20	2.06
19	1	611	CLA	MG-NA	6.14	2.20	2.06
19	A	1109	CLA	MG-NA	6.14	2.20	2.06
19	A	1126	CLA	MG-NA	6.13	2.20	2.06
19	A	1013	CLA	MG-NA	6.13	2.20	2.06
19	A	1112	CLA	MG-NA	6.13	2.20	2.06
19	1	608	CLA	MG-NA	6.12	2.20	2.06
19	B	1021	CLA	MG-NA	6.12	2.20	2.06
19	3	603	CLA	MG-NA	6.12	2.20	2.06
19	2	604	CLA	MG-NA	6.12	2.20	2.06
19	B	1208	CLA	MG-NA	6.12	2.20	2.06
19	1	607	CLA	MG-NA	6.11	2.20	2.06
19	4	608	CLA	MG-NA	6.11	2.20	2.06
19	L	1502	CLA	MG-NA	6.10	2.20	2.06
19	A	1119	CLA	MG-NA	6.10	2.20	2.06
19	B	1230	CLA	MG-NA	6.10	2.20	2.06
19	B	1226	CLA	MG-NA	6.09	2.20	2.06
19	A	1139	CLA	MG-NA	6.09	2.20	2.06
19	A	1120	CLA	MG-NA	6.08	2.20	2.06
19	A	1134	CLA	MG-NA	6.08	2.20	2.06
19	A	1127	CLA	MG-NA	6.07	2.20	2.06
19	B	1227	CLA	MG-NA	6.07	2.20	2.06
19	4	609	CLA	MG-NA	6.07	2.20	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B	1228	CLA	MG-NA	6.07	2.20	2.06
19	B	1216	CLA	MG-NA	6.07	2.20	2.06
19	A	1106	CLA	MG-NA	6.07	2.20	2.06
19	A	1125	CLA	MG-NA	6.06	2.20	2.06
19	4	607	CLA	MG-NA	6.06	2.20	2.06
19	4	604	CLA	MG-NA	6.06	2.20	2.06
19	L	1501	CLA	MG-NA	6.06	2.20	2.06
19	B	1219	CLA	MG-NA	6.06	2.20	2.06
19	2	605	CLA	MG-NA	6.05	2.20	2.06
19	B	1222	CLA	MG-NA	6.05	2.20	2.06
19	1	606	CLA	MG-NA	6.05	2.20	2.06
19	3	617	CLA	MG-NA	6.05	2.20	2.06
19	A	1129	CLA	MG-NA	6.04	2.20	2.06
19	4	602	CLA	MG-NA	6.04	2.20	2.06
19	4	617	CLA	MG-NA	6.04	2.20	2.06
19	B	1237	CLA	MG-NA	6.04	2.20	2.06
19	A	1103	CLA	MG-NA	6.04	2.20	2.06
19	B	1201	CLA	MG-NA	6.02	2.20	2.06
22	I	4020	BCR	C24-C23	6.02	1.51	1.33
19	2	601	CLA	MG-NA	6.02	2.20	2.06
19	B	1225	CLA	MG-NA	6.01	2.20	2.06
19	B	1231	CLA	MG-NA	6.01	2.20	2.06
19	3	601	CLA	MG-NA	6.01	2.20	2.06
19	B	1238	CLA	MG-NA	6.00	2.20	2.06
19	3	612	CLA	MG-NA	6.00	2.20	2.06
19	3	606	CLA	MG-NA	6.00	2.20	2.06
19	A	1111	CLA	MG-NA	6.00	2.20	2.06
19	B	1224	CLA	MG-NA	5.99	2.20	2.06
19	A	1138	CLA	MG-NA	5.99	2.20	2.06
19	2	612	CLA	MG-NA	5.99	2.20	2.06
19	3	610	CLA	MG-NA	5.97	2.20	2.06
19	B	1220	CLA	MG-NA	5.97	2.20	2.06
19	1	602	CLA	MG-NA	5.97	2.20	2.06
19	2	606	CLA	MG-NA	5.97	2.20	2.06
19	A	1124	CLA	MG-NA	5.96	2.20	2.06
19	B	1215	CLA	MG-NA	5.96	2.20	2.06
19	F	1302	CLA	MG-NA	5.96	2.20	2.06
19	A	1102	CLA	MG-NA	5.95	2.20	2.06
19	B	1210	CLA	MG-NA	5.95	2.20	2.06
19	B	1206	CLA	MG-NA	5.94	2.20	2.06
19	A	1133	CLA	MG-NA	5.93	2.20	2.06
19	4	601	CLA	MG-NA	5.91	2.20	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B	1205	CLA	MG-NA	5.89	2.20	2.06
22	3	506	BCR	C24-C23	5.86	1.50	1.33
22	B	4004	BCR	C24-C23	5.86	1.50	1.33
22	1	504	BCR	C24-C23	5.85	1.50	1.33
19	B	1211	CLA	MG-NA	5.85	2.20	2.06
19	A	1117	CLA	MG-NA	5.84	2.20	2.06
22	K	4001	BCR	C24-C23	5.84	1.50	1.33
22	G	4021	BCR	C24-C23	5.81	1.50	1.33
22	A	4017	BCR	C24-C23	5.78	1.50	1.33
22	K	4002	BCR	C24-C23	5.78	1.50	1.33
22	A	4007	BCR	C24-C23	5.76	1.50	1.33
22	2	503	BCR	C24-C23	5.71	1.50	1.33
22	F	4014	BCR	C24-C23	5.68	1.50	1.33
22	I	4018	BCR	C24-C23	5.65	1.50	1.33
22	A	4008	BCR	C24-C23	5.65	1.50	1.33
22	L	4019	BCR	C24-C23	5.65	1.50	1.33
22	B	4010	BCR	C24-C23	5.62	1.50	1.33
22	L	4020	BCR	C24-C23	5.61	1.50	1.33
22	B	4005	BCR	C24-C23	5.60	1.50	1.33
22	F	4016	BCR	C24-C23	5.58	1.49	1.33
22	B	4006	BCR	C24-C23	5.56	1.49	1.33
22	1	503	BCR	C24-C23	5.53	1.49	1.33
22	B	4009	BCR	C24-C23	5.53	1.49	1.33
22	A	4002	BCR	C24-C23	5.52	1.49	1.33
22	G	4011	BCR	C24-C23	5.49	1.49	1.33
22	F	4016	BCR	C11-C12	-5.47	1.20	1.34
22	A	4003	BCR	C24-C23	5.47	1.49	1.33
22	3	503	BCR	C24-C23	5.46	1.49	1.33
22	A	4011	BCR	C11-C12	-5.39	1.20	1.34
22	J	4012	BCR	C24-C23	5.39	1.49	1.33
22	A	4011	BCR	C24-C23	5.39	1.49	1.33
22	B	4005	BCR	C11-C12	-5.36	1.20	1.34
22	A	4003	BCR	C11-C12	-5.30	1.20	1.34
22	3	503	BCR	C11-C12	-5.30	1.20	1.34
22	B	4009	BCR	C11-C12	-5.29	1.20	1.34
22	I	4018	BCR	C11-C12	-5.28	1.21	1.34
22	B	4006	BCR	C11-C12	-5.26	1.21	1.34
22	A	4017	BCR	C11-C12	-5.26	1.21	1.34
22	A	4002	BCR	C11-C12	-5.24	1.21	1.34
22	L	4020	BCR	C11-C12	-5.22	1.21	1.34
22	A	4008	BCR	C11-C12	-5.18	1.21	1.34
18	A	1011	CL0	O2A-C1	5.15	1.60	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	J	4012	BCR	C11-C12	-5.14	1.21	1.34
22	A	4007	BCR	C11-C12	-5.14	1.21	1.34
22	L	4019	BCR	C11-C12	-5.14	1.21	1.34
22	B	4010	BCR	C11-C12	-5.13	1.21	1.34
22	K	4002	BCR	C11-C12	-5.12	1.21	1.34
22	I	4020	BCR	C11-C12	-5.12	1.21	1.34
22	K	4001	BCR	C11-C12	-5.11	1.21	1.34
22	3	506	BCR	C11-C12	-5.06	1.21	1.34
22	G	4011	BCR	C11-C12	-5.04	1.21	1.34
22	F	4014	BCR	C11-C12	-5.03	1.21	1.34
22	1	503	BCR	C11-C12	-4.97	1.21	1.34
22	G	4021	BCR	C11-C12	-4.97	1.21	1.34
22	1	504	BCR	C11-C12	-4.97	1.21	1.34
22	2	503	BCR	C11-C12	-4.90	1.22	1.34
18	A	1011	CL0	C3B-C2B	4.89	1.47	1.40
22	B	4004	BCR	C11-C12	-4.85	1.22	1.34
18	A	1011	CL0	O2D-CGD	4.78	1.44	1.33
22	3	503	BCR	C16-C17	-4.67	1.29	1.43
19	4	605	CLA	MG-ND	-4.63	1.96	2.05
22	A	4011	BCR	C16-C17	-4.57	1.29	1.43
18	A	1011	CL0	CHD-C1D	4.54	1.47	1.38
18	A	1011	CL0	C3C-C2C	4.52	1.46	1.36
22	A	4003	BCR	C16-C17	-4.49	1.29	1.43
22	B	4009	BCR	C16-C17	-4.47	1.29	1.43
22	F	4016	BCR	C16-C17	-4.45	1.29	1.43
22	L	4019	BCR	C16-C17	-4.40	1.29	1.43
22	L	4020	BCR	C16-C17	-4.38	1.29	1.43
19	B	1224	CLA	MG-ND	-4.38	1.97	2.05
22	1	503	BCR	C16-C17	-4.37	1.29	1.43
22	A	4002	BCR	C16-C17	-4.37	1.29	1.43
22	1	504	BCR	C16-C17	-4.37	1.29	1.43
22	A	4017	BCR	C16-C17	-4.36	1.29	1.43
19	B	1213	CLA	MG-ND	-4.32	1.97	2.05
22	B	4010	BCR	C16-C17	-4.32	1.30	1.43
22	G	4011	BCR	C16-C17	-4.32	1.30	1.43
22	A	4008	BCR	C16-C17	-4.30	1.30	1.43
22	K	4002	BCR	C16-C17	-4.29	1.30	1.43
19	4	601	CLA	MG-ND	-4.29	1.97	2.05
22	J	4012	BCR	C16-C17	-4.28	1.30	1.43
27	1	803	DGD	O1G-C1A	4.28	1.45	1.33
19	B	1023	CLA	MG-ND	-4.27	1.97	2.05
22	B	4005	BCR	C16-C17	-4.27	1.30	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	1132	CLA	MG-ND	-4.26	1.97	2.05
19	A	1012	CLA	MG-ND	-4.26	1.97	2.05
19	B	1212	CLA	MG-ND	-4.26	1.97	2.05
27	4	802	DGD	O1G-C1A	4.22	1.45	1.33
22	F	4014	BCR	C16-C17	-4.22	1.30	1.43
19	B	1201	CLA	MG-ND	-4.22	1.97	2.05
22	3	506	BCR	C16-C17	-4.22	1.30	1.43
27	G	5003	DGD	O1G-C1A	4.21	1.45	1.33
19	2	607	CLA	MG-ND	-4.20	1.97	2.05
22	A	4007	BCR	C16-C17	-4.20	1.30	1.43
22	G	4021	BCR	C16-C17	-4.19	1.30	1.43
22	B	4006	BCR	C16-C17	-4.19	1.30	1.43
19	B	1217	CLA	MG-ND	-4.19	1.97	2.05
22	I	4020	BCR	C16-C17	-4.18	1.30	1.43
27	F	5005	DGD	O1G-C1A	4.18	1.45	1.33
22	K	4001	BCR	C16-C17	-4.16	1.30	1.43
22	I	4018	BCR	C16-C17	-4.15	1.30	1.43
27	4	801	DGD	O1G-C1A	4.15	1.45	1.33
19	2	606	CLA	MG-ND	-4.14	1.97	2.05
19	A	1113	CLA	MG-ND	-4.14	1.97	2.05
19	A	1108	CLA	MG-ND	-4.14	1.97	2.05
19	3	601	CLA	MG-ND	-4.14	1.97	2.05
19	2	605	CLA	MG-ND	-4.14	1.97	2.05
19	A	1116	CLA	MG-ND	-4.13	1.97	2.05
19	B	1203	CLA	MG-ND	-4.13	1.97	2.05
19	B	1223	CLA	MG-ND	-4.13	1.97	2.05
18	A	1011	CL0	C1D-ND	-4.13	1.32	1.37
19	3	606	CLA	MG-ND	-4.13	1.97	2.05
19	A	1131	CLA	MG-ND	-4.12	1.97	2.05
19	A	1123	CLA	MG-ND	-4.12	1.97	2.05
19	B	1232	CLA	MG-ND	-4.12	1.97	2.05
19	1	613	CLA	MG-ND	-4.11	1.97	2.05
19	A	1126	CLA	MG-ND	-4.11	1.97	2.05
19	G	1601	CLA	MG-ND	-4.11	1.97	2.05
19	A	1128	CLA	MG-ND	-4.10	1.97	2.05
19	4	606	CLA	MG-ND	-4.10	1.97	2.05
19	3	605	CLA	MG-ND	-4.10	1.97	2.05
19	A	1118	CLA	MG-ND	-4.09	1.97	2.05
19	A	1115	CLA	MG-ND	-4.08	1.97	2.05
19	L	1501	CLA	MG-ND	-4.08	1.97	2.05
19	G	1701	CLA	MG-ND	-4.08	1.97	2.05
19	B	1021	CLA	MG-ND	-4.07	1.97	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	1	604	CLA	MG-ND	-4.07	1.97	2.05
19	B	1219	CLA	MG-ND	-4.07	1.97	2.05
19	2	612	CLA	MG-ND	-4.07	1.97	2.05
19	3	610	CLA	MG-ND	-4.05	1.97	2.05
19	A	1105	CLA	MG-ND	-4.05	1.97	2.05
19	A	1130	CLA	MG-ND	-4.05	1.97	2.05
19	1	607	CLA	MG-ND	-4.05	1.97	2.05
19	B	1211	CLA	MG-ND	-4.05	1.97	2.05
19	B	1214	CLA	MG-ND	-4.04	1.97	2.05
19	B	1228	CLA	MG-ND	-4.04	1.97	2.05
19	B	1240	CLA	MG-ND	-4.04	1.97	2.05
19	1	603	CLA	MG-ND	-4.04	1.97	2.05
19	1	605	CLA	MG-ND	-4.04	1.97	2.05
19	4	603	CLA	MG-ND	-4.03	1.97	2.05
19	4	612	CLA	MG-ND	-4.02	1.97	2.05
19	2	602	CLA	MG-ND	-4.02	1.97	2.05
19	A	1141	CLA	MG-ND	-4.02	1.97	2.05
19	B	1229	CLA	MG-ND	-4.02	1.97	2.05
19	A	1129	CLA	MG-ND	-4.01	1.97	2.05
19	3	602	CLA	MG-ND	-4.01	1.97	2.05
19	A	1137	CLA	MG-ND	-4.01	1.97	2.05
19	B	1221	CLA	MG-ND	-4.00	1.97	2.05
22	B	4004	BCR	C16-C17	-4.00	1.31	1.43
19	L	1502	CLA	MG-ND	-4.00	1.97	2.05
27	J	5001	DGD	O1G-C1A	4.00	1.45	1.33
19	B	1207	CLA	MG-ND	-4.00	1.97	2.05
19	A	1110	CLA	MG-ND	-4.00	1.97	2.05
19	A	1133	CLA	MG-ND	-3.99	1.97	2.05
19	4	609	CLA	MG-ND	-3.99	1.97	2.05
19	3	613	CLA	MG-ND	-3.99	1.97	2.05
22	2	503	BCR	C16-C17	-3.99	1.31	1.43
19	B	1227	CLA	MG-ND	-3.99	1.97	2.05
19	K	1402	CLA	MG-ND	-3.99	1.97	2.05
29	4	613	CHL	C3B-C2B	-3.98	1.34	1.40
19	B	1220	CLA	MG-ND	-3.98	1.97	2.05
19	B	1205	CLA	MG-ND	-3.98	1.97	2.05
19	1	608	CLA	MG-ND	-3.98	1.97	2.05
19	4	607	CLA	MG-ND	-3.97	1.97	2.05
19	B	1231	CLA	MG-ND	-3.97	1.97	2.05
19	B	1236	CLA	MG-ND	-3.97	1.97	2.05
19	B	1225	CLA	C1C-NC	-3.97	1.31	1.37
19	A	1139	CLA	MG-ND	-3.96	1.97	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	1011	CL0	CHD-C4C	3.96	1.48	1.39
19	A	1134	CLA	MG-ND	-3.96	1.97	2.05
19	A	1101	CLA	MG-ND	-3.95	1.98	2.05
19	A	1104	CLA	MG-ND	-3.95	1.98	2.05
19	A	1013	CLA	MG-ND	-3.95	1.98	2.05
19	B	1211	CLA	C1C-NC	-3.95	1.31	1.37
19	A	1112	CLA	MG-ND	-3.95	1.98	2.05
19	B	1022	CLA	MG-ND	-3.95	1.98	2.05
19	4	617	CLA	MG-ND	-3.94	1.98	2.05
27	B	5005	DGD	O1G-C1A	3.94	1.44	1.33
19	1	614	CLA	MG-ND	-3.94	1.98	2.05
19	B	1226	CLA	MG-ND	-3.94	1.98	2.05
19	A	1117	CLA	MG-ND	-3.94	1.98	2.05
19	3	617	CLA	MG-ND	-3.94	1.98	2.05
19	2	604	CLA	MG-ND	-3.94	1.98	2.05
19	K	1404	CLA	MG-ND	-3.94	1.98	2.05
19	1	602	CLA	MG-ND	-3.94	1.98	2.05
19	A	1103	CLA	MG-ND	-3.94	1.98	2.05
19	3	612	CLA	MG-ND	-3.93	1.98	2.05
19	1	611	CLA	MG-ND	-3.93	1.98	2.05
19	1	601	CLA	MG-ND	-3.92	1.98	2.05
19	4	601	CLA	C1C-NC	-3.92	1.31	1.37
19	4	608	CLA	MG-ND	-3.92	1.98	2.05
19	B	1210	CLA	MG-ND	-3.92	1.98	2.05
19	B	1206	CLA	MG-ND	-3.92	1.98	2.05
19	B	1209	CLA	MG-ND	-3.91	1.98	2.05
19	A	1127	CLA	MG-ND	-3.91	1.98	2.05
19	B	1230	CLA	MG-ND	-3.91	1.98	2.05
19	3	608	CLA	MG-ND	-3.91	1.98	2.05
19	A	1107	CLA	MG-ND	-3.91	1.98	2.05
19	2	608	CLA	MG-ND	-3.90	1.98	2.05
19	B	1234	CLA	MG-ND	-3.90	1.98	2.05
19	B	1225	CLA	MG-ND	-3.90	1.98	2.05
19	F	1301	CLA	MG-ND	-3.89	1.98	2.05
19	A	1138	CLA	MG-ND	-3.89	1.98	2.05
19	3	614	CLA	MG-ND	-3.89	1.98	2.05
19	A	1139	CLA	C1C-NC	-3.89	1.32	1.37
19	B	1230	CLA	C1C-NC	-3.88	1.32	1.37
19	A	1120	CLA	MG-ND	-3.88	1.98	2.05
19	A	1106	CLA	MG-ND	-3.88	1.98	2.05
19	B	1215	CLA	MG-ND	-3.88	1.98	2.05
27	3	803	DGD	O1G-C1A	3.88	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	4	505	C7Z	C12-C13	3.88	1.54	1.45
19	4	604	CLA	MG-ND	-3.88	1.98	2.05
19	A	1114	CLA	MG-ND	-3.87	1.98	2.05
19	B	1220	CLA	C1C-NC	-3.87	1.32	1.37
19	B	1237	CLA	MG-ND	-3.87	1.98	2.05
19	A	1116	CLA	C1C-NC	-3.87	1.32	1.37
19	B	1204	CLA	MG-ND	-3.87	1.98	2.05
19	B	1239	CLA	MG-ND	-3.86	1.98	2.05
19	G	1603	CLA	MG-ND	-3.86	1.98	2.05
19	3	603	CLA	MG-ND	-3.86	1.98	2.05
19	B	1216	CLA	MG-ND	-3.85	1.98	2.05
19	B	1202	CLA	MG-ND	-3.85	1.98	2.05
19	B	1219	CLA	C1C-NC	-3.83	1.32	1.37
19	B	1218	CLA	MG-ND	-3.83	1.98	2.05
19	A	1108	CLA	C1C-NC	-3.82	1.32	1.37
19	A	1124	CLA	MG-ND	-3.82	1.98	2.05
19	A	1109	CLA	MG-ND	-3.81	1.98	2.05
19	2	603	CLA	MG-ND	-3.81	1.98	2.05
19	4	602	CLA	MG-ND	-3.81	1.98	2.05
19	A	1140	CLA	MG-ND	-3.81	1.98	2.05
19	A	1111	CLA	MG-ND	-3.81	1.98	2.05
19	A	1121	CLA	MG-ND	-3.81	1.98	2.05
19	1	606	CLA	MG-ND	-3.81	1.98	2.05
19	L	1503	CLA	MG-ND	-3.80	1.98	2.05
19	4	605	CLA	C1C-NC	-3.80	1.32	1.37
19	A	1125	CLA	C1C-NC	-3.79	1.32	1.37
19	A	1122	CLA	MG-ND	-3.79	1.98	2.05
19	A	1105	CLA	C1C-NC	-3.79	1.32	1.37
19	A	1132	CLA	C1C-NC	-3.79	1.32	1.37
19	G	1602	CLA	MG-ND	-3.78	1.98	2.05
19	3	606	CLA	C1C-NC	-3.78	1.32	1.37
19	B	1208	CLA	MG-ND	-3.77	1.98	2.05
19	B	1227	CLA	C1C-NC	-3.77	1.32	1.37
19	B	1021	CLA	C1C-NC	-3.77	1.32	1.37
19	A	1122	CLA	C1C-NC	-3.77	1.32	1.37
19	B	1238	CLA	C1C-NC	-3.76	1.32	1.37
19	2	612	CLA	C1C-NC	-3.76	1.32	1.37
19	K	1403	CLA	MG-ND	-3.76	1.98	2.05
19	2	601	CLA	MG-ND	-3.75	1.98	2.05
19	J	1901	CLA	MG-ND	-3.75	1.98	2.05
19	2	606	CLA	C1C-NC	-3.75	1.32	1.37
31	4	505	C7Z	C35-C34	3.75	1.55	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	1117	CLA	C1C-NC	-3.75	1.32	1.37
19	A	1119	CLA	MG-ND	-3.74	1.98	2.05
19	A	1102	CLA	MG-ND	-3.74	1.98	2.05
19	A	1140	CLA	C1C-NC	-3.74	1.32	1.37
19	1	605	CLA	C1C-NC	-3.74	1.32	1.37
19	2	603	CLA	C1C-NC	-3.74	1.32	1.37
19	1	601	CLA	C1C-NC	-3.72	1.32	1.37
19	A	1131	CLA	C1C-NC	-3.72	1.32	1.37
19	B	1222	CLA	MG-ND	-3.71	1.98	2.05
19	B	1234	CLA	C1C-NC	-3.71	1.32	1.37
19	B	1213	CLA	C1C-NC	-3.71	1.32	1.37
19	G	1601	CLA	C1C-NC	-3.71	1.32	1.37
19	B	1206	CLA	C1C-NC	-3.71	1.32	1.37
19	A	1125	CLA	MG-ND	-3.70	1.98	2.05
19	B	1238	CLA	MG-ND	-3.70	1.98	2.05
31	4	505	C7Z	C31-C30	3.69	1.54	1.43
19	F	1302	CLA	MG-ND	-3.69	1.98	2.05
31	4	505	C7Z	C15-C14	3.69	1.54	1.43
19	B	1239	CLA	C1C-NC	-3.69	1.32	1.37
19	B	1023	CLA	C1C-NC	-3.68	1.32	1.37
19	3	612	CLA	C1C-NC	-3.68	1.32	1.37
19	B	1226	CLA	C1C-NC	-3.68	1.32	1.37
19	A	1012	CLA	C1C-NC	-3.67	1.32	1.37
19	A	1138	CLA	C1C-NC	-3.67	1.32	1.37
19	B	1208	CLA	C1C-NC	-3.66	1.32	1.37
19	3	603	CLA	C1C-NC	-3.66	1.32	1.37
19	A	1129	CLA	C1C-NC	-3.66	1.32	1.37
31	4	505	C7Z	C11-C10	3.66	1.54	1.43
19	A	1111	CLA	C1C-NC	-3.65	1.32	1.37
29	1	609	CHL	C3B-C2B	-3.65	1.35	1.40
19	4	602	CLA	C1C-NC	-3.64	1.32	1.37
19	G	1701	CLA	C1C-NC	-3.64	1.32	1.37
19	A	1118	CLA	C1C-NC	-3.64	1.32	1.37
19	1	602	CLA	C1C-NC	-3.63	1.32	1.37
19	A	1106	CLA	C1C-NC	-3.63	1.32	1.37
19	2	605	CLA	C1C-NC	-3.63	1.32	1.37
19	3	601	CLA	C1C-NC	-3.63	1.32	1.37
19	B	1223	CLA	C1C-NC	-3.63	1.32	1.37
19	A	1124	CLA	C1C-NC	-3.62	1.32	1.37
19	B	1214	CLA	C1C-NC	-3.62	1.32	1.37
19	A	1109	CLA	C1C-NC	-3.62	1.32	1.37
29	3	611	CHL	C3B-C2B	-3.62	1.35	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B	1231	CLA	C1C-NC	-3.61	1.32	1.37
19	A	1104	CLA	C1C-NC	-3.61	1.32	1.37
19	A	1115	CLA	C1C-NC	-3.60	1.32	1.37
19	3	617	CLA	C1C-NC	-3.60	1.32	1.37
19	A	1101	CLA	C1C-NC	-3.60	1.32	1.37
19	A	1127	CLA	C1C-NC	-3.60	1.32	1.37
19	A	1103	CLA	C1C-NC	-3.60	1.32	1.37
19	A	1126	CLA	C1C-NC	-3.60	1.32	1.37
19	B	1228	CLA	C1C-NC	-3.60	1.32	1.37
19	L	1502	CLA	C1C-NC	-3.59	1.32	1.37
19	4	609	CLA	C1C-NC	-3.59	1.32	1.37
19	4	603	CLA	C1C-NC	-3.59	1.32	1.37
19	B	1205	CLA	C1C-NC	-3.59	1.32	1.37
19	B	1222	CLA	C1C-NC	-3.58	1.32	1.37
19	F	1301	CLA	C1C-NC	-3.58	1.32	1.37
19	A	1130	CLA	C1C-NC	-3.58	1.32	1.37
19	B	1215	CLA	C1C-NC	-3.58	1.32	1.37
19	B	1207	CLA	C1C-NC	-3.57	1.32	1.37
19	F	1302	CLA	C1C-NC	-3.57	1.32	1.37
19	B	1229	CLA	C1C-NC	-3.57	1.32	1.37
19	2	601	CLA	C1C-NC	-3.57	1.32	1.37
19	B	1216	CLA	C1C-NC	-3.56	1.32	1.37
19	B	1224	CLA	C1C-NC	-3.56	1.32	1.37
19	B	1240	CLA	C1C-NC	-3.55	1.32	1.37
19	A	1107	CLA	C1C-NC	-3.55	1.32	1.37
19	4	607	CLA	C1C-NC	-3.55	1.32	1.37
19	1	603	CLA	C1C-NC	-3.54	1.32	1.37
19	B	1201	CLA	C1C-NC	-3.54	1.32	1.37
19	4	606	CLA	C1C-NC	-3.53	1.32	1.37
19	B	1210	CLA	C1C-NC	-3.52	1.32	1.37
19	A	1128	CLA	C1C-NC	-3.52	1.32	1.37
19	4	617	CLA	C1C-NC	-3.52	1.32	1.37
19	A	1120	CLA	C1C-NC	-3.52	1.32	1.37
19	A	1133	CLA	C1C-NC	-3.52	1.32	1.37
19	A	1113	CLA	C1C-NC	-3.52	1.32	1.37
19	G	1603	CLA	C1C-NC	-3.51	1.32	1.37
19	B	1204	CLA	C1C-NC	-3.51	1.32	1.37
19	A	1119	CLA	C1C-NC	-3.51	1.32	1.37
19	4	612	CLA	C1C-NC	-3.50	1.32	1.37
19	3	608	CLA	C1C-NC	-3.50	1.32	1.37
19	B	1212	CLA	C1C-NC	-3.49	1.32	1.37
19	3	610	CLA	C1C-NC	-3.49	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	1114	CLA	C1C-NC	-3.49	1.32	1.37
19	A	1123	CLA	C1C-NC	-3.49	1.32	1.37
19	A	1135	CLA	MG-ND	-3.49	1.98	2.05
19	B	1209	CLA	C1C-NC	-3.48	1.32	1.37
19	1	608	CLA	C1C-NC	-3.48	1.32	1.37
19	3	605	CLA	C1C-NC	-3.48	1.32	1.37
19	1	607	CLA	C1C-NC	-3.48	1.32	1.37
19	A	1112	CLA	C1C-NC	-3.46	1.32	1.37
19	B	1218	CLA	C1C-NC	-3.46	1.32	1.37
19	B	1237	CLA	C1C-NC	-3.46	1.32	1.37
19	A	1013	CLA	C1C-NC	-3.45	1.32	1.37
19	2	602	CLA	C1C-NC	-3.44	1.32	1.37
19	B	1221	CLA	C1C-NC	-3.44	1.32	1.37
19	B	1235	CLA	MG-ND	-3.44	1.99	2.05
19	2	604	CLA	C1C-NC	-3.43	1.32	1.37
19	A	1137	CLA	C1C-NC	-3.42	1.32	1.37
19	1	614	CLA	C1C-NC	-3.42	1.32	1.37
19	B	1217	CLA	C1C-NC	-3.42	1.32	1.37
19	A	1134	CLA	C1C-NC	-3.42	1.32	1.37
19	K	1401	CLA	MG-ND	-3.41	1.99	2.05
19	3	613	CLA	C1C-NC	-3.41	1.32	1.37
19	2	607	CLA	C1C-NC	-3.40	1.32	1.37
19	A	1110	CLA	C1C-NC	-3.40	1.32	1.37
19	B	1232	CLA	C1C-NC	-3.39	1.32	1.37
19	2	601	CLA	CBB-CAB	3.39	1.51	1.29
19	A	1121	CLA	C1C-NC	-3.39	1.32	1.37
19	L	1503	CLA	C1C-NC	-3.39	1.32	1.37
19	L	1503	CLA	CBB-CAB	3.38	1.51	1.29
19	A	1141	CLA	C1C-NC	-3.38	1.32	1.37
19	B	1236	CLA	C1C-NC	-3.38	1.32	1.37
19	1	611	CLA	C1C-NC	-3.38	1.32	1.37
19	L	1501	CLA	C1C-NC	-3.38	1.32	1.37
19	2	606	CLA	CBB-CAB	3.37	1.51	1.29
19	1	607	CLA	CBB-CAB	3.37	1.51	1.29
19	A	1136	CLA	MG-ND	-3.37	1.99	2.05
19	G	1602	CLA	C1C-NC	-3.37	1.32	1.37
27	J	5001	DGD	CAA-C9A	-3.37	1.32	1.51
19	K	1402	CLA	CBB-CAB	3.37	1.51	1.29
27	B	5005	DGD	CDB-CCB	-3.37	1.32	1.51
19	4	608	CLA	C1C-NC	-3.37	1.32	1.37
19	3	601	CLA	CBB-CAB	3.36	1.51	1.29
19	K	1404	CLA	CBB-CAB	3.36	1.51	1.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	1	601	CLA	CBB-CAB	3.36	1.51	1.29
29	2	610	CHL	CBB-CAB	3.35	1.51	1.29
19	3	613	CLA	CBB-CAB	3.35	1.51	1.29
19	1	603	CLA	CBB-CAB	3.35	1.51	1.29
19	1	613	CLA	C1C-NC	-3.35	1.32	1.37
19	2	608	CLA	C1C-NC	-3.35	1.32	1.37
19	B	1215	CLA	CBB-CAB	3.35	1.51	1.29
19	3	603	CLA	CBB-CAB	3.35	1.51	1.29
19	1	614	CLA	CBB-CAB	3.34	1.51	1.29
19	3	612	CLA	CBB-CAB	3.34	1.51	1.29
19	2	608	CLA	CBB-CAB	3.34	1.51	1.29
19	3	614	CLA	CBB-CAB	3.34	1.51	1.29
19	3	602	CLA	C1C-NC	-3.34	1.32	1.37
19	A	1119	CLA	CBB-CAB	3.34	1.51	1.29
19	3	608	CLA	CBB-CAB	3.34	1.51	1.29
19	3	606	CLA	CBB-CAB	3.34	1.51	1.29
19	B	1205	CLA	C3B-C2B	-3.34	1.35	1.40
19	4	606	CLA	CBB-CAB	3.34	1.51	1.29
19	1	613	CLA	CBB-CAB	3.34	1.51	1.29
19	K	1403	CLA	CBB-CAB	3.34	1.51	1.29
27	J	5001	DGD	CGA-CFA	-3.34	1.32	1.51
19	A	1012	CLA	CBB-CAB	3.34	1.51	1.29
19	4	602	CLA	CBB-CAB	3.33	1.51	1.29
19	B	1201	CLA	CBB-CAB	3.33	1.51	1.29
19	B	1217	CLA	CBB-CAB	3.33	1.51	1.29
19	L	1502	CLA	CBB-CAB	3.33	1.51	1.29
19	1	605	CLA	CBB-CAB	3.33	1.51	1.29
19	A	1108	CLA	CBB-CAB	3.33	1.51	1.29
19	B	1223	CLA	CBB-CAB	3.33	1.51	1.29
27	B	5005	DGD	CGB-CFB	-3.33	1.32	1.51
19	1	604	CLA	CBB-CAB	3.33	1.51	1.29
18	A	1011	CL0	OBD-CAD	3.33	1.28	1.22
19	K	1401	CLA	CBB-CAB	3.33	1.51	1.29
19	A	1136	CLA	CBB-CAB	3.33	1.51	1.29
19	G	1602	CLA	CBB-CAB	3.33	1.51	1.29
19	A	1128	CLA	CBB-CAB	3.33	1.51	1.29
19	1	611	CLA	CBB-CAB	3.33	1.51	1.29
19	2	602	CLA	CBB-CAB	3.33	1.51	1.29
19	B	1221	CLA	CBB-CAB	3.33	1.51	1.29
19	G	1601	CLA	CBB-CAB	3.32	1.51	1.29
19	L	1501	CLA	CBB-CAB	3.32	1.51	1.29
19	1	606	CLA	CBB-CAB	3.32	1.51	1.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B	1222	CLA	CBB-CAB	3.32	1.51	1.29
19	B	1228	CLA	CBB-CAB	3.32	1.51	1.29
19	4	604	CLA	C1C-NC	-3.32	1.32	1.37
19	2	612	CLA	CBB-CAB	3.32	1.51	1.29
19	B	1213	CLA	CBB-CAB	3.32	1.51	1.29
25	1	802	LMG	C19-C18	-3.32	1.32	1.51
29	4	615	CHL	CBB-CAB	3.32	1.51	1.29
19	A	1118	CLA	CBB-CAB	3.32	1.51	1.29
19	4	612	CLA	CBB-CAB	3.32	1.51	1.29
19	J	1901	CLA	CBB-CAB	3.32	1.51	1.29
19	3	602	CLA	CBB-CAB	3.32	1.51	1.29
19	A	1120	CLA	CBB-CAB	3.32	1.51	1.29
19	F	1301	CLA	CBB-CAB	3.32	1.51	1.29
19	1	606	CLA	C1C-NC	-3.32	1.32	1.37
27	J	5001	DGD	CDA-CCA	-3.31	1.33	1.51
19	K	1402	CLA	C1C-NC	-3.31	1.32	1.37
19	4	604	CLA	CBB-CAB	3.31	1.51	1.29
19	A	1110	CLA	CBB-CAB	3.31	1.51	1.29
19	B	1230	CLA	CBB-CAB	3.31	1.51	1.29
19	A	1135	CLA	CBB-CAB	3.31	1.51	1.29
19	A	1138	CLA	CBB-CAB	3.31	1.51	1.29
19	4	608	CLA	CBB-CAB	3.31	1.51	1.29
19	A	1114	CLA	C3B-C2B	-3.31	1.35	1.40
19	B	1023	CLA	CBB-CAB	3.31	1.51	1.29
19	A	1129	CLA	CBB-CAB	3.31	1.51	1.29
19	A	1123	CLA	CBB-CAB	3.31	1.51	1.29
19	1	608	CLA	CBB-CAB	3.31	1.51	1.29
19	B	1239	CLA	CBB-CAB	3.31	1.51	1.29
19	A	1124	CLA	CBB-CAB	3.31	1.51	1.29
29	3	607	CHL	CBB-CAB	3.31	1.51	1.29
31	4	505	C7Z	C28-C29	3.31	1.53	1.45
19	B	1205	CLA	CBB-CAB	3.31	1.51	1.29
19	A	1106	CLA	CBB-CAB	3.31	1.51	1.29
19	2	604	CLA	CBB-CAB	3.31	1.51	1.29
19	A	1126	CLA	CBB-CAB	3.31	1.51	1.29
19	A	1111	CLA	CBB-CAB	3.31	1.51	1.29
19	A	1132	CLA	CBB-CAB	3.30	1.51	1.29
19	B	1211	CLA	CBB-CAB	3.30	1.51	1.29
19	G	1603	CLA	CBB-CAB	3.30	1.51	1.29
19	4	607	CLA	CBB-CAB	3.30	1.51	1.29
19	1	602	CLA	CBB-CAB	3.30	1.51	1.29
29	4	611	CHL	CBB-CAB	3.30	1.51	1.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B	1235	CLA	CBB-CAB	3.30	1.51	1.29
19	A	1013	CLA	CBB-CAB	3.30	1.51	1.29
19	G	1701	CLA	CBB-CAB	3.30	1.51	1.29
19	B	1212	CLA	CBB-CAB	3.30	1.51	1.29
19	2	605	CLA	CBB-CAB	3.30	1.51	1.29
19	A	1103	CLA	CBB-CAB	3.30	1.51	1.29
19	A	1137	CLA	CBB-CAB	3.30	1.51	1.29
19	B	1209	CLA	CBB-CAB	3.30	1.51	1.29
25	B	5003	LMG	C19-C18	-3.30	1.33	1.51
19	A	1134	CLA	CBB-CAB	3.29	1.51	1.29
19	A	1125	CLA	CBB-CAB	3.29	1.51	1.29
19	B	1203	CLA	CBB-CAB	3.29	1.51	1.29
19	B	1206	CLA	CBB-CAB	3.29	1.51	1.29
19	B	1225	CLA	CBB-CAB	3.29	1.51	1.29
19	A	1131	CLA	CBB-CAB	3.29	1.51	1.29
19	4	601	CLA	CBB-CAB	3.29	1.51	1.29
19	4	609	CLA	CBB-CAB	3.29	1.51	1.29
19	3	605	CLA	CBB-CAB	3.29	1.51	1.29
19	A	1113	CLA	CBB-CAB	3.29	1.51	1.29
19	A	1109	CLA	CBB-CAB	3.29	1.51	1.29
29	2	615	CHL	CBB-CAB	3.29	1.51	1.29
19	B	1236	CLA	CBB-CAB	3.29	1.51	1.29
19	A	1122	CLA	CBB-CAB	3.29	1.51	1.29
19	B	1204	CLA	CBB-CAB	3.29	1.51	1.29
19	B	1207	CLA	CBB-CAB	3.28	1.51	1.29
19	B	1237	CLA	CBB-CAB	3.28	1.51	1.29
19	A	1115	CLA	CBB-CAB	3.28	1.51	1.29
19	4	605	CLA	CBB-CAB	3.28	1.51	1.29
19	B	1240	CLA	CBB-CAB	3.28	1.51	1.29
27	B	5005	DGD	CAB-C9B	-3.28	1.33	1.51
25	F	5002	LMG	C43-C42	-3.28	1.33	1.51
27	4	802	DGD	CAB-C9B	-3.28	1.33	1.51
19	A	1127	CLA	CBB-CAB	3.28	1.51	1.29
25	A	5006	LMG	C25-C24	-3.28	1.33	1.51
19	A	1101	CLA	CBB-CAB	3.28	1.51	1.29
19	A	1140	CLA	CBB-CAB	3.27	1.51	1.29
19	A	1104	CLA	CBB-CAB	3.27	1.51	1.29
19	B	1219	CLA	CBB-CAB	3.27	1.51	1.29
25	G	5002	LMG	C22-C21	-3.27	1.33	1.51
19	2	607	CLA	CBB-CAB	3.27	1.51	1.29
25	A	5006	LMG	C22-C21	-3.27	1.33	1.51
19	B	1238	CLA	CBB-CAB	3.27	1.51	1.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	F	5002	LMG	C40-C39	-3.27	1.33	1.51
27	4	801	DGD	CAA-C9A	-3.27	1.33	1.51
19	4	603	CLA	CBB-CAB	3.27	1.51	1.29
19	3	610	CLA	CBB-CAB	3.27	1.51	1.29
19	A	1114	CLA	CBB-CAB	3.27	1.51	1.29
19	A	1141	CLA	CBB-CAB	3.27	1.51	1.29
31	4	505	C7Z	C8-C9	3.27	1.53	1.45
19	B	1232	CLA	CBB-CAB	3.26	1.50	1.29
19	B	1226	CLA	CBB-CAB	3.26	1.50	1.29
19	B	1234	CLA	CBB-CAB	3.26	1.50	1.29
19	B	1210	CLA	CBB-CAB	3.26	1.50	1.29
19	4	617	CLA	CBB-CAB	3.26	1.50	1.29
29	1	612	CHL	CBB-CAB	3.26	1.50	1.29
19	B	1218	CLA	CBB-CAB	3.26	1.50	1.29
25	G	5002	LMG	C40-C39	-3.26	1.33	1.51
19	A	1121	CLA	CBB-CAB	3.26	1.50	1.29
19	B	1229	CLA	CBB-CAB	3.26	1.50	1.29
19	B	1022	CLA	CBB-CAB	3.26	1.50	1.29
19	A	1105	CLA	CBB-CAB	3.25	1.50	1.29
25	1	802	LMG	C22-C21	-3.25	1.33	1.51
19	A	1117	CLA	CBB-CAB	3.25	1.50	1.29
19	A	1130	CLA	CBB-CAB	3.25	1.50	1.29
19	2	603	CLA	CBB-CAB	3.25	1.50	1.29
19	A	1133	CLA	CBB-CAB	3.25	1.50	1.29
19	3	614	CLA	C1C-NC	-3.25	1.32	1.37
19	B	1203	CLA	C1C-NC	-3.25	1.32	1.37
25	G	5002	LMG	C19-C18	-3.25	1.33	1.51
25	F	5002	LMG	C37-C36	-3.25	1.33	1.51
25	A	5006	LMG	C37-C36	-3.25	1.33	1.51
19	A	1139	CLA	CBB-CAB	3.25	1.50	1.29
19	B	1208	CLA	CBB-CAB	3.25	1.50	1.29
19	F	1302	CLA	CBB-CAB	3.25	1.50	1.29
25	G	5001	LMG	C19-C18	-3.25	1.33	1.51
19	A	1102	CLA	C1C-NC	-3.25	1.33	1.37
19	B	1021	CLA	CBB-CAB	3.24	1.50	1.29
19	B	1227	CLA	CBB-CAB	3.24	1.50	1.29
27	B	5005	DGD	CAA-C9A	-3.24	1.33	1.51
19	B	1216	CLA	CBB-CAB	3.24	1.50	1.29
19	A	1112	CLA	CBB-CAB	3.24	1.50	1.29
19	3	617	CLA	CBB-CAB	3.24	1.50	1.29
19	1	604	CLA	C1C-NC	-3.24	1.33	1.37
25	F	5003	LMG	C37-C36	-3.23	1.33	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B	1231	CLA	CBB-CAB	3.23	1.50	1.29
19	A	1107	CLA	CBB-CAB	3.23	1.50	1.29
31	4	505	C7Z	C32-C33	3.23	1.52	1.45
27	F	5005	DGD	CAA-C9A	-3.23	1.33	1.51
25	A	5006	LMG	C19-C18	-3.23	1.33	1.51
29	3	604	CHL	CBB-CAB	3.23	1.50	1.29
19	A	1102	CLA	CBB-CAB	3.22	1.50	1.29
18	A	1011	CL0	C1C-NC	-3.22	1.33	1.37
19	B	1022	CLA	C1C-NC	-3.22	1.33	1.37
19	B	1224	CLA	CBB-CAB	3.22	1.50	1.29
19	B	1220	CLA	CBB-CAB	3.22	1.50	1.29
29	2	609	CHL	CBB-CAB	3.22	1.50	1.29
27	F	5005	DGD	CDA-CCA	-3.21	1.33	1.51
19	A	1116	CLA	CBB-CAB	3.21	1.50	1.29
29	2	611	CHL	CBB-CAB	3.20	1.50	1.29
18	A	1011	CL0	CBB-CAB	3.20	1.50	1.29
27	F	5005	DGD	CGA-CFA	-3.20	1.33	1.51
29	4	615	CHL	C4B-NB	3.20	1.38	1.35
25	1	802	LMG	C25-C24	-3.19	1.33	1.51
25	G	5001	LMG	C43-C42	-3.19	1.33	1.51
19	A	1134	CLA	C3B-C2B	-3.18	1.36	1.40
19	B	1202	CLA	CBB-CAB	3.18	1.50	1.29
25	G	5002	LMG	C37-C36	-3.17	1.33	1.51
29	2	613	CHL	C4B-NB	3.17	1.38	1.35
29	3	611	CHL	CBB-CAB	3.17	1.50	1.29
25	G	5001	LMG	C37-C36	-3.17	1.33	1.51
19	B	1232	CLA	C3B-C2B	-3.17	1.36	1.40
19	J	1901	CLA	C1C-NC	-3.16	1.33	1.37
19	B	1239	CLA	C3B-C2B	-3.16	1.36	1.40
19	A	1137	CLA	C3B-C2B	-3.16	1.36	1.40
19	A	1135	CLA	C1C-NC	-3.15	1.33	1.37
19	B	1214	CLA	CBB-CAB	3.15	1.50	1.29
29	4	611	CHL	C3B-C2B	-3.15	1.36	1.40
19	B	1202	CLA	C1C-NC	-3.14	1.33	1.37
19	B	1235	CLA	C1C-NC	-3.12	1.33	1.37
29	2	613	CHL	CBB-CAB	3.12	1.50	1.29
19	A	1102	CLA	C3B-C2B	-3.12	1.36	1.40
29	2	609	CHL	C3B-C2B	-3.12	1.36	1.40
29	1	610	CHL	CBB-CAB	3.11	1.49	1.29
19	A	1136	CLA	C1C-NC	-3.11	1.33	1.37
19	1	608	CLA	C3B-C2B	-3.11	1.36	1.40
19	K	1401	CLA	C1C-NC	-3.11	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	3	617	CLA	C3B-C2B	-3.11	1.36	1.40
25	G	5001	LMG	C40-C39	-3.11	1.34	1.51
29	4	610	CHL	CBB-CAB	3.10	1.49	1.29
31	4	505	C7Z	C27-C26	3.09	1.56	1.45
19	B	1202	CLA	C3B-C2B	-3.08	1.36	1.40
19	B	1217	CLA	C3B-C2B	-3.08	1.36	1.40
19	K	1403	CLA	C1C-NC	-3.07	1.33	1.37
29	4	613	CHL	CBB-CAB	3.05	1.49	1.29
29	1	609	CHL	C4B-NB	3.04	1.37	1.35
29	3	607	CHL	C4B-NB	3.03	1.37	1.35
19	B	1218	CLA	C3B-C2B	-3.01	1.36	1.40
19	4	607	CLA	C3B-C2B	-3.00	1.36	1.40
19	A	1140	CLA	C3B-C2B	-3.00	1.36	1.40
31	4	505	C7Z	C7-C6	3.00	1.55	1.45
19	K	1404	CLA	C1C-NC	-3.00	1.33	1.37
29	2	615	CHL	C4B-NB	2.99	1.37	1.35
19	K	1404	CLA	C3B-C2B	-2.99	1.36	1.40
19	A	1121	CLA	CHC-C1C	2.98	1.42	1.35
19	G	1603	CLA	C3B-C2B	-2.98	1.36	1.40
29	1	610	CHL	C3B-C2B	-2.97	1.36	1.40
19	2	603	CLA	C3B-C2B	-2.97	1.36	1.40
19	4	603	CLA	C3B-C2B	-2.97	1.36	1.40
19	B	1238	CLA	C3B-C2B	-2.97	1.36	1.40
19	B	1207	CLA	C3B-C2B	-2.96	1.36	1.40
19	1	603	CLA	C3B-C2B	-2.95	1.36	1.40
29	2	609	CHL	C4B-NB	2.95	1.37	1.35
24	B	5008	LMT	O3'-C3'	-2.94	1.36	1.43
29	2	609	CHL	C3A-C2A	-2.94	1.46	1.54
19	A	1012	CLA	C3B-C2B	-2.93	1.36	1.40
18	A	1011	CL0	MG-NC	2.93	2.13	2.06
19	A	1121	CLA	C3B-C2B	-2.92	1.36	1.40
19	B	1208	CLA	C3B-C2B	-2.92	1.36	1.40
19	A	1110	CLA	C3B-C2B	-2.91	1.36	1.40
29	1	609	CHL	CBB-CAB	2.90	1.48	1.29
19	A	1132	CLA	C3B-C2B	-2.90	1.36	1.40
24	G	5004	LMT	O3'-C3'	-2.90	1.36	1.43
19	A	1131	CLA	C3B-C2B	-2.90	1.36	1.40
19	A	1109	CLA	C3B-C2B	-2.90	1.36	1.40
19	4	608	CLA	C3B-C2B	-2.89	1.36	1.40
29	4	610	CHL	C4B-NB	2.89	1.37	1.35
29	4	611	CHL	C4B-NB	2.88	1.37	1.35
19	B	1204	CLA	C3B-C2B	-2.88	1.36	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B	1202	CLA	CHC-C1C	2.86	1.42	1.35
29	3	611	CHL	C4B-NB	2.84	1.37	1.35
19	4	602	CLA	C3B-C2B	-2.84	1.36	1.40
19	4	609	CLA	C3B-C2B	-2.83	1.36	1.40
19	F	1302	CLA	C3B-C2B	-2.82	1.36	1.40
18	A	1011	CL0	C1B-CHB	2.82	1.48	1.41
19	B	1022	CLA	C3B-C2B	-2.82	1.36	1.40
19	1	602	CLA	C3B-C2B	-2.82	1.36	1.40
29	2	611	CHL	C3B-C2B	-2.81	1.36	1.40
19	J	1901	CLA	CHC-C1C	2.81	1.42	1.35
19	B	1214	CLA	C3B-C2B	-2.81	1.36	1.40
29	1	610	CHL	C4B-NB	2.81	1.37	1.35
19	A	1136	CLA	CHC-C1C	2.81	1.42	1.35
29	2	611	CHL	C3A-C2A	-2.81	1.46	1.54
19	3	606	CLA	C3B-C2B	-2.80	1.36	1.40
19	A	1102	CLA	CHC-C1C	2.80	1.42	1.35
24	G	5005	LMT	O3'-C3'	-2.79	1.36	1.43
19	2	601	CLA	CHC-C1C	2.79	1.42	1.35
29	1	612	CHL	C3B-C2B	-2.78	1.36	1.40
19	K	1404	CLA	CHC-C1C	2.78	1.42	1.35
29	1	612	CHL	C4B-NB	2.78	1.37	1.35
29	4	613	CHL	C4B-NB	2.78	1.37	1.35
19	A	1135	CLA	CHC-C1C	2.78	1.42	1.35
19	A	1137	CLA	CHC-C1C	2.78	1.42	1.35
19	3	617	CLA	CHC-C1C	2.78	1.42	1.35
19	3	614	CLA	CHC-C1C	2.77	1.42	1.35
19	B	1232	CLA	CHC-C1C	2.77	1.42	1.35
19	K	1401	CLA	CHC-C1C	2.77	1.42	1.35
29	2	613	CHL	C3B-C2B	-2.76	1.36	1.40
24	G	5005	LMT	O2B-C2B	-2.76	1.36	1.43
19	B	1237	CLA	C3B-C2B	-2.76	1.36	1.40
29	3	604	CHL	C4B-NB	2.74	1.37	1.35
19	4	607	CLA	CHC-C1C	2.73	1.42	1.35
24	B	5006	LMT	O3'-C3'	-2.73	1.36	1.43
19	B	1235	CLA	CHC-C1C	2.72	1.42	1.35
19	B	1217	CLA	CHC-C1C	2.72	1.41	1.35
19	3	605	CLA	C3B-C2B	-2.72	1.36	1.40
19	B	1208	CLA	CHC-C1C	2.71	1.41	1.35
19	3	608	CLA	C3B-C2B	-2.71	1.36	1.40
19	A	1119	CLA	CHC-C1C	2.70	1.41	1.35
19	1	601	CLA	CHC-C1C	2.70	1.41	1.35
19	B	1218	CLA	CHC-C1C	2.69	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	1	613	CLA	CHC-C1C	2.69	1.41	1.35
19	A	1125	CLA	C3B-C2B	-2.69	1.36	1.40
19	1	604	CLA	C3B-C2B	-2.69	1.36	1.40
19	K	1403	CLA	CHC-C1C	2.69	1.41	1.35
19	G	1701	CLA	C3B-C2B	-2.68	1.36	1.40
19	1	614	CLA	C3B-C2B	-2.68	1.36	1.40
19	1	604	CLA	CHC-C1C	2.68	1.41	1.35
19	2	608	CLA	C3B-C2B	-2.68	1.36	1.40
19	2	607	CLA	CHC-C1C	2.67	1.41	1.35
19	1	601	CLA	C3B-C2B	-2.67	1.36	1.40
29	2	611	CHL	C4B-NB	2.67	1.37	1.35
19	B	1203	CLA	CHC-C1C	2.67	1.41	1.35
19	4	601	CLA	C3B-C2B	-2.67	1.36	1.40
19	A	1125	CLA	CHC-C1C	2.66	1.41	1.35
19	A	1112	CLA	CHC-C1C	2.66	1.41	1.35
19	1	602	CLA	CHC-C1C	2.66	1.41	1.35
19	B	1227	CLA	C3B-C2B	-2.66	1.36	1.40
19	A	1122	CLA	CHC-C1C	2.65	1.41	1.35
19	G	1602	CLA	CHC-C1C	2.65	1.41	1.35
19	2	602	CLA	C3B-C2B	-2.65	1.36	1.40
19	3	602	CLA	CHC-C1C	2.65	1.41	1.35
19	A	1128	CLA	C3B-C2B	-2.64	1.36	1.40
19	A	1126	CLA	C3B-C2B	-2.64	1.36	1.40
19	B	1213	CLA	C3B-C2B	-2.63	1.36	1.40
19	1	603	CLA	CHC-C1C	2.63	1.41	1.35
24	A	5004	LMT	O3B-C3B	-2.63	1.36	1.43
19	B	1216	CLA	CHC-C1C	2.63	1.41	1.35
19	4	608	CLA	CHC-C1C	2.63	1.41	1.35
19	A	1013	CLA	CHC-C1C	2.62	1.41	1.35
19	A	1122	CLA	C3B-C2B	-2.62	1.36	1.40
19	1	606	CLA	C3B-C2B	-2.62	1.36	1.40
19	3	608	CLA	CHC-C1C	2.62	1.41	1.35
19	A	1109	CLA	CHC-C1C	2.62	1.41	1.35
29	4	610	CHL	C3B-C2B	-2.62	1.36	1.40
19	B	1210	CLA	CHC-C1C	2.61	1.41	1.35
19	1	614	CLA	CHC-C1C	2.61	1.41	1.35
19	2	602	CLA	CHC-C1C	2.61	1.41	1.35
19	2	608	CLA	CHC-C1C	2.61	1.41	1.35
19	3	601	CLA	CHC-C1C	2.61	1.41	1.35
19	B	1239	CLA	CHC-C1C	2.61	1.41	1.35
24	G	5004	LMT	O2'-C2'	-2.61	1.36	1.43
19	L	1502	CLA	CHC-C1C	2.60	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	1126	CLA	CHC-C1C	2.60	1.41	1.35
19	A	1106	CLA	CHC-C1C	2.60	1.41	1.35
19	3	613	CLA	CHC-C1C	2.59	1.41	1.35
19	J	1901	CLA	C3B-C2B	-2.59	1.36	1.40
19	4	617	CLA	C3B-C2B	-2.59	1.36	1.40
19	A	1111	CLA	CHC-C1C	2.59	1.41	1.35
19	A	1124	CLA	CHC-C1C	2.59	1.41	1.35
19	A	1140	CLA	CHC-C1C	2.59	1.41	1.35
19	B	1023	CLA	C3B-C2B	-2.59	1.36	1.40
18	A	1011	CL0	C4B-CHC	2.58	1.48	1.41
29	4	611	CHL	C3A-C2A	-2.58	1.47	1.54
27	3	803	DGD	CAB-C9B	-2.58	1.33	1.51
19	A	1129	CLA	C3B-C2B	-2.58	1.36	1.40
19	A	1118	CLA	C3B-C2B	-2.57	1.36	1.40
25	2	803	LMG	C19-C18	-2.57	1.33	1.51
19	1	611	CLA	CHC-C1C	2.57	1.41	1.35
19	L	1503	CLA	CHC-C1C	2.57	1.41	1.35
19	B	1234	CLA	CHC-C1C	2.57	1.41	1.35
19	L	1501	CLA	CHC-C1C	2.57	1.41	1.35
24	B	5006	LMT	O2'-C2'	-2.56	1.36	1.43
24	J	5003	LMT	O3'-C3'	-2.56	1.36	1.43
19	3	606	CLA	CHC-C1C	2.56	1.41	1.35
29	2	610	CHL	C4B-NB	2.56	1.37	1.35
19	B	1238	CLA	CHC-C1C	2.56	1.41	1.35
29	2	615	CHL	C3B-C2B	-2.56	1.36	1.40
19	B	1220	CLA	C3B-C2B	-2.56	1.36	1.40
19	3	602	CLA	C3B-C2B	-2.56	1.36	1.40
19	A	1110	CLA	CHC-C1C	2.56	1.41	1.35
19	2	604	CLA	CHC-C1C	2.56	1.41	1.35
19	B	1219	CLA	CHC-C1C	2.56	1.41	1.35
19	B	1207	CLA	CHC-C1C	2.55	1.41	1.35
18	A	1011	CL0	C4D-CHA	2.55	1.47	1.38
19	B	1022	CLA	CHC-C1C	2.55	1.41	1.35
19	A	1138	CLA	CHC-C1C	2.55	1.41	1.35
19	B	1226	CLA	C3B-C2B	-2.54	1.36	1.40
19	3	605	CLA	CHC-C1C	2.54	1.41	1.35
24	A	5004	LMT	O3'-C3'	-2.54	1.37	1.43
29	1	610	CHL	C3A-C2A	-2.54	1.47	1.54
19	B	1201	CLA	CHC-C1C	2.54	1.41	1.35
19	B	1229	CLA	CHC-C1C	2.53	1.41	1.35
19	1	606	CLA	CHC-C1C	2.53	1.41	1.35
19	K	1402	CLA	C3B-C2B	-2.53	1.36	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	1	608	CLA	CHC-C1C	2.53	1.41	1.35
19	4	617	CLA	CHC-C1C	2.53	1.41	1.35
19	A	1108	CLA	CHC-C1C	2.53	1.41	1.35
19	3	603	CLA	C3B-C2B	-2.52	1.36	1.40
19	B	1223	CLA	CHC-C1C	2.52	1.41	1.35
30	4	502	XAT	O24-C25	-2.51	1.42	1.46
19	B	1204	CLA	CHC-C1C	2.51	1.41	1.35
19	2	606	CLA	C3B-C2B	-2.51	1.36	1.40
19	B	1237	CLA	CHC-C1C	2.51	1.41	1.35
19	A	1141	CLA	CHC-C1C	2.51	1.41	1.35
19	4	605	CLA	C3D-C4D	-2.51	1.38	1.44
19	B	1236	CLA	CHC-C1C	2.50	1.41	1.35
19	B	1223	CLA	C3D-C4D	-2.50	1.38	1.44
19	G	1603	CLA	CHC-C1C	2.50	1.41	1.35
19	3	603	CLA	CHC-C1C	2.50	1.41	1.35
19	B	1231	CLA	C3B-C2B	-2.50	1.36	1.40
24	B	5008	LMT	O2B-C2B	-2.50	1.37	1.43
19	1	607	CLA	CHC-C1C	2.50	1.41	1.35
19	B	1224	CLA	C3B-C2B	-2.50	1.36	1.40
19	F	1302	CLA	CHC-C1C	2.49	1.41	1.35
19	A	1134	CLA	CHC-C1C	2.49	1.41	1.35
19	B	1220	CLA	CHC-C1C	2.49	1.41	1.35
24	B	5008	LMT	O3B-C3B	-2.49	1.37	1.43
19	2	603	CLA	CHC-C1C	2.48	1.41	1.35
19	A	1103	CLA	CHC-C1C	2.48	1.41	1.35
19	A	1136	CLA	C3B-C2B	-2.48	1.36	1.40
19	B	1225	CLA	CHC-C1C	2.48	1.41	1.35
19	B	1023	CLA	CHC-C1C	2.48	1.41	1.35
19	4	604	CLA	CHC-C1C	2.48	1.41	1.35
24	A	5004	LMT	O4'-C4B	-2.47	1.37	1.43
19	4	603	CLA	CHC-C1C	2.47	1.41	1.35
19	3	610	CLA	CHC-C1C	2.47	1.41	1.35
19	B	1212	CLA	CHC-C1C	2.47	1.41	1.35
19	B	1215	CLA	CHC-C1C	2.47	1.41	1.35
19	B	1221	CLA	CHC-C1C	2.46	1.41	1.35
19	3	612	CLA	CHC-C1C	2.46	1.41	1.35
19	B	1209	CLA	CHC-C1C	2.46	1.41	1.35
19	4	609	CLA	CHC-C1C	2.46	1.41	1.35
19	4	602	CLA	CHC-C1C	2.46	1.41	1.35
19	A	1115	CLA	C3B-C2B	-2.46	1.37	1.40
24	J	5003	LMT	O3B-C3B	-2.46	1.37	1.43
19	K	1403	CLA	C3B-C2B	-2.45	1.37	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	1113	CLA	CHC-C1C	2.45	1.41	1.35
19	A	1116	CLA	C3B-C2B	-2.45	1.37	1.40
19	A	1107	CLA	CHC-C1C	2.44	1.41	1.35
19	A	1139	CLA	CHC-C1C	2.44	1.41	1.35
19	4	601	CLA	CHC-C1C	2.44	1.41	1.35
19	B	1210	CLA	C3B-C2B	-2.44	1.37	1.40
19	A	1130	CLA	CHC-C1C	2.43	1.41	1.35
19	A	1114	CLA	CHC-C1C	2.43	1.41	1.35
19	B	1228	CLA	CHC-C1C	2.43	1.41	1.35
19	A	1120	CLA	CHC-C1C	2.43	1.41	1.35
19	A	1133	CLA	CHC-C1C	2.43	1.41	1.35
19	B	1231	CLA	CHC-C1C	2.43	1.41	1.35
19	4	612	CLA	CHC-C1C	2.43	1.41	1.35
19	A	1127	CLA	CHC-C1C	2.43	1.41	1.35
19	4	606	CLA	CHC-C1C	2.43	1.41	1.35
19	A	1116	CLA	CHC-C1C	2.43	1.41	1.35
19	B	1205	CLA	CHC-C1C	2.43	1.41	1.35
19	4	612	CLA	C3B-C2B	-2.42	1.37	1.40
19	A	1138	CLA	C3B-C2B	-2.42	1.37	1.40
19	B	1236	CLA	C3D-C4D	-2.42	1.38	1.44
19	B	1214	CLA	CHC-C1C	2.42	1.41	1.35
19	B	1222	CLA	CHC-C1C	2.41	1.41	1.35
19	A	1141	CLA	C3B-C2B	-2.41	1.37	1.40
19	A	1101	CLA	CHC-C1C	2.41	1.41	1.35
19	1	604	CLA	C3D-C4D	-2.40	1.38	1.44
19	A	1123	CLA	CHC-C1C	2.40	1.41	1.35
19	A	1135	CLA	C3B-C2B	-2.40	1.37	1.40
19	A	1119	CLA	C3B-C2B	-2.40	1.37	1.40
19	2	605	CLA	CHC-C1C	2.40	1.41	1.35
19	B	1224	CLA	CHC-C1C	2.40	1.41	1.35
19	B	1224	CLA	C3D-C4D	-2.40	1.38	1.44
24	B	5008	LMT	O4'-C4B	-2.40	1.37	1.43
19	A	1111	CLA	C3B-C2B	-2.39	1.37	1.40
19	K	1404	CLA	C1C-C2C	2.39	1.49	1.44
19	A	1117	CLA	CHC-C1C	2.39	1.41	1.35
19	A	1113	CLA	C3B-C2B	-2.38	1.37	1.40
19	A	1013	CLA	C3B-C2B	-2.38	1.37	1.40
19	A	1132	CLA	CHC-C1C	2.38	1.41	1.35
19	1	613	CLA	C3B-C2B	-2.38	1.37	1.40
19	B	1236	CLA	C3B-C2B	-2.38	1.37	1.40
19	3	613	CLA	C3B-C2B	-2.38	1.37	1.40
19	B	1211	CLA	CHC-C1C	2.38	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B	1225	CLA	C4B-NB	-2.37	1.33	1.35
19	G	1601	CLA	CHC-C1C	2.37	1.41	1.35
19	2	606	CLA	CHC-C1C	2.37	1.41	1.35
19	B	1220	CLA	C3D-C4D	-2.36	1.38	1.44
19	B	1206	CLA	C3B-C2B	-2.36	1.37	1.40
24	G	5004	LMT	O2B-C2B	-2.36	1.37	1.43
24	G	5005	LMT	O3B-C3B	-2.36	1.37	1.43
19	A	1101	CLA	C3D-C4D	-2.36	1.38	1.44
19	A	1137	CLA	C3D-C4D	-2.36	1.38	1.44
19	F	1301	CLA	CHC-C1C	2.35	1.41	1.35
19	4	605	CLA	C4B-NB	-2.35	1.33	1.35
19	2	607	CLA	C3B-C2B	-2.35	1.37	1.40
19	2	612	CLA	CHC-C1C	2.35	1.41	1.35
19	B	1230	CLA	C3D-C4D	-2.35	1.38	1.44
19	B	1226	CLA	CHC-C1C	2.35	1.41	1.35
19	B	1228	CLA	C3B-C2B	-2.35	1.37	1.40
19	K	1402	CLA	CHC-C1C	2.35	1.41	1.35
19	B	1022	CLA	C3D-C4D	-2.35	1.38	1.44
19	A	1105	CLA	CHC-C1C	2.35	1.41	1.35
19	A	1115	CLA	CHC-C1C	2.35	1.41	1.35
19	4	606	CLA	C3B-C2B	-2.34	1.37	1.40
30	2	502	XAT	O24-C25	-2.34	1.42	1.46
19	A	1115	CLA	C3D-C4D	-2.34	1.38	1.44
27	F	5005	DGD	O5D-C1E	2.34	1.44	1.40
24	B	5008	LMT	O2'-C2'	-2.34	1.37	1.43
19	A	1131	CLA	CHC-C1C	2.34	1.41	1.35
19	1	605	CLA	C3B-C2B	-2.34	1.37	1.40
24	B	5006	LMT	O2B-C2B	-2.34	1.37	1.43
19	B	1227	CLA	CHC-C1C	2.34	1.41	1.35
19	B	1212	CLA	C3B-C2B	-2.34	1.37	1.40
19	K	1401	CLA	C3B-C2B	-2.33	1.37	1.40
24	G	5005	LMT	O2'-C2'	-2.33	1.37	1.43
19	B	1225	CLA	C3D-C4D	-2.33	1.38	1.44
19	A	1124	CLA	C3B-C2B	-2.33	1.37	1.40
19	4	605	CLA	C3B-C2B	-2.33	1.37	1.40
19	4	617	CLA	C3D-C4D	-2.33	1.38	1.44
19	B	1215	CLA	C3B-C2B	-2.33	1.37	1.40
19	A	1119	CLA	C3D-C4D	-2.33	1.38	1.44
19	B	1231	CLA	C3D-C4D	-2.33	1.38	1.44
19	B	1214	CLA	C3D-C4D	-2.33	1.38	1.44
19	B	1229	CLA	C3B-C2B	-2.33	1.37	1.40
19	A	1120	CLA	C3D-C4D	-2.32	1.38	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	1106	CLA	C3B-C2B	-2.32	1.37	1.40
19	G	1701	CLA	CHC-C1C	2.31	1.40	1.35
19	2	612	CLA	C3D-C4D	-2.31	1.39	1.44
19	L	1502	CLA	C3B-C2B	-2.31	1.37	1.40
19	3	605	CLA	C3D-C4D	-2.31	1.39	1.44
19	A	1118	CLA	CHC-C1C	2.31	1.40	1.35
19	B	1235	CLA	C3B-C2B	-2.31	1.37	1.40
24	B	5006	LMT	O3B-C3B	-2.31	1.37	1.43
19	K	1403	CLA	C3D-C4D	-2.31	1.39	1.44
19	B	1021	CLA	C3D-C4D	-2.30	1.39	1.44
19	B	1203	CLA	C3D-C4D	-2.30	1.39	1.44
19	A	1120	CLA	C3B-C2B	-2.30	1.37	1.40
19	B	1213	CLA	CHC-C1C	2.30	1.40	1.35
19	A	1128	CLA	CHC-C1C	2.30	1.40	1.35
22	I	4018	BCR	C12-C13	-2.30	1.41	1.45
19	B	1021	CLA	CHC-C1C	2.30	1.40	1.35
19	A	1012	CLA	C3D-C4D	-2.30	1.39	1.44
19	B	1240	CLA	C3D-C4D	-2.30	1.39	1.44
19	A	1107	CLA	C3D-C4D	-2.29	1.39	1.44
19	4	603	CLA	C3D-C4D	-2.29	1.39	1.44
19	B	1204	CLA	C3D-C4D	-2.29	1.39	1.44
19	2	605	CLA	C3B-C2B	-2.29	1.37	1.40
19	A	1108	CLA	C3D-C4D	-2.29	1.39	1.44
19	1	607	CLA	C3B-C2B	-2.29	1.37	1.40
24	A	5004	LMT	O2'-C2'	-2.29	1.37	1.43
19	B	1227	CLA	C3D-C4D	-2.29	1.39	1.44
19	B	1230	CLA	CHC-C1C	2.29	1.40	1.35
19	G	1601	CLA	C3D-C4D	-2.29	1.39	1.44
19	B	1219	CLA	C3D-C4D	-2.29	1.39	1.44
19	A	1117	CLA	C3B-C2B	-2.29	1.37	1.40
19	A	1129	CLA	CHC-C1C	2.28	1.40	1.35
19	A	1106	CLA	C3D-C4D	-2.28	1.39	1.44
24	J	5003	LMT	O2B-C2B	-2.28	1.37	1.43
19	A	1104	CLA	C3D-C4D	-2.28	1.39	1.44
19	B	1229	CLA	C3D-C4D	-2.28	1.39	1.44
19	3	614	CLA	C3B-C2B	-2.28	1.37	1.40
19	A	1012	CLA	CHC-C1C	2.28	1.40	1.35
19	B	1221	CLA	C3D-C4D	-2.28	1.39	1.44
29	3	604	CHL	C1D-ND	-2.27	1.35	1.37
19	A	1126	CLA	C3D-C4D	-2.27	1.39	1.44
19	A	1129	CLA	C3D-C4D	-2.27	1.39	1.44
19	B	1209	CLA	C3D-C4D	-2.27	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	1104	CLA	C3B-C2B	-2.27	1.37	1.40
19	A	1127	CLA	C3B-C2B	-2.27	1.37	1.40
19	B	1240	CLA	CHC-C1C	2.26	1.40	1.35
19	1	613	CLA	C3D-C4D	-2.26	1.39	1.44
19	4	605	CLA	CHC-C1C	2.26	1.40	1.35
19	3	614	CLA	C1C-C2C	2.26	1.48	1.44
19	A	1116	CLA	C3D-C4D	-2.26	1.39	1.44
19	J	1901	CLA	C1C-C2C	2.26	1.48	1.44
19	2	612	CLA	C3B-C2B	-2.26	1.37	1.40
19	B	1216	CLA	C3B-C2B	-2.26	1.37	1.40
19	B	1206	CLA	C3D-C4D	-2.25	1.39	1.44
19	B	1225	CLA	C3B-C2B	-2.25	1.37	1.40
19	A	1124	CLA	C3D-C4D	-2.25	1.39	1.44
19	A	1133	CLA	C3D-C4D	-2.25	1.39	1.44
19	2	602	CLA	C1C-C2C	2.24	1.48	1.44
19	1	605	CLA	CHC-C1C	2.24	1.40	1.35
19	A	1104	CLA	CHC-C1C	2.24	1.40	1.35
19	A	1117	CLA	C3D-C4D	-2.24	1.39	1.44
19	B	1211	CLA	C3D-C4D	-2.24	1.39	1.44
19	B	1216	CLA	C3D-C4D	-2.24	1.39	1.44
19	B	1210	CLA	C3D-C4D	-2.24	1.39	1.44
19	B	1205	CLA	C3D-C4D	-2.24	1.39	1.44
19	B	1218	CLA	C3D-C4D	-2.24	1.39	1.44
19	A	1123	CLA	C3D-C4D	-2.24	1.39	1.44
19	A	1121	CLA	C1C-C2C	2.24	1.48	1.44
19	2	601	CLA	C3B-C2B	-2.23	1.37	1.40
19	A	1125	CLA	C3D-C4D	-2.23	1.39	1.44
19	B	1206	CLA	CHC-C1C	2.23	1.40	1.35
19	A	1133	CLA	C3B-C2B	-2.23	1.37	1.40
19	L	1501	CLA	C3D-C4D	-2.23	1.39	1.44
19	3	602	CLA	C1C-C2C	2.23	1.48	1.44
19	B	1228	CLA	C3D-C4D	-2.23	1.39	1.44
19	1	611	CLA	C3D-C4D	-2.23	1.39	1.44
19	A	1128	CLA	C3D-C4D	-2.23	1.39	1.44
19	A	1140	CLA	C3D-C4D	-2.23	1.39	1.44
19	A	1130	CLA	C3D-C4D	-2.22	1.39	1.44
19	A	1121	CLA	C3D-C4D	-2.22	1.39	1.44
19	A	1114	CLA	C3D-C4D	-2.22	1.39	1.44
19	B	1202	CLA	C3D-C4D	-2.22	1.39	1.44
19	A	1127	CLA	C3D-C4D	-2.22	1.39	1.44
19	2	608	CLA	C3D-C4D	-2.22	1.39	1.44
19	B	1232	CLA	C3D-C4D	-2.22	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	1139	CLA	C3D-C4D	-2.21	1.39	1.44
19	B	1238	CLA	C3D-C4D	-2.21	1.39	1.44
24	G	5005	LMT	O4'-C4B	-2.21	1.37	1.43
19	B	1207	CLA	C3D-C4D	-2.21	1.39	1.44
23	3	801	LHG	O7-C7	-2.21	1.34	1.42
19	4	601	CLA	C3D-C4D	-2.21	1.39	1.44
19	B	1232	CLA	C1C-C2C	2.21	1.48	1.44
19	B	1222	CLA	C3B-C2B	-2.20	1.37	1.40
18	A	1011	CL0	C3D-C4D	-2.20	1.39	1.44
19	1	605	CLA	C3D-C4D	-2.20	1.39	1.44
19	B	1215	CLA	C3D-C4D	-2.20	1.39	1.44
19	A	1105	CLA	C3D-C4D	-2.20	1.39	1.44
19	A	1135	CLA	C1C-C2C	2.20	1.48	1.44
19	B	1213	CLA	C3D-C4D	-2.20	1.39	1.44
24	A	5004	LMT	O2B-C2B	-2.20	1.37	1.43
24	G	5004	LMT	O3B-C3B	-2.20	1.37	1.43
24	J	5003	LMT	O2'-C2'	-2.20	1.37	1.43
19	L	1502	CLA	C3D-C4D	-2.19	1.39	1.44
19	A	1138	CLA	C3D-C4D	-2.19	1.39	1.44
19	B	1234	CLA	C3D-C4D	-2.19	1.39	1.44
19	B	1023	CLA	C3D-C4D	-2.19	1.39	1.44
19	B	1237	CLA	C3D-C4D	-2.19	1.39	1.44
19	1	607	CLA	C3D-C4D	-2.19	1.39	1.44
19	A	1130	CLA	C3B-C2B	-2.19	1.37	1.40
19	B	1239	CLA	C3D-C4D	-2.18	1.39	1.44
19	K	1402	CLA	C3D-C4D	-2.18	1.39	1.44
19	B	1223	CLA	C3B-C2B	-2.18	1.37	1.40
19	4	604	CLA	C3D-C4D	-2.18	1.39	1.44
19	A	1111	CLA	C3D-C4D	-2.18	1.39	1.44
19	A	1141	CLA	C3D-C4D	-2.18	1.39	1.44
19	1	608	CLA	C3D-C4D	-2.18	1.39	1.44
19	B	1021	CLA	C3B-C2B	-2.18	1.37	1.40
19	2	603	CLA	C1A-CHA	2.18	1.52	1.43
19	3	613	CLA	C1A-CHA	2.18	1.52	1.43
19	4	608	CLA	C3D-C4D	-2.18	1.39	1.44
19	B	1207	CLA	C1C-C2C	2.17	1.48	1.44
19	K	1403	CLA	C1C-C2C	2.17	1.48	1.44
19	A	1132	CLA	C3D-C4D	-2.17	1.39	1.44
19	K	1402	CLA	MG-NC	2.17	2.11	2.06
19	3	612	CLA	C3B-C2B	-2.17	1.37	1.40
19	A	1112	CLA	C3D-C4D	-2.17	1.39	1.44
19	L	1503	CLA	C3D-C4D	-2.17	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	F	1302	CLA	C3D-C4D	-2.17	1.39	1.44
19	A	1113	CLA	C3D-C4D	-2.17	1.39	1.44
19	B	1221	CLA	C3B-C2B	-2.16	1.37	1.40
19	A	1013	CLA	C3D-C4D	-2.16	1.39	1.44
19	K	1401	CLA	C1C-C2C	2.16	1.48	1.44
19	A	1131	CLA	C3D-C4D	-2.16	1.39	1.44
19	G	1602	CLA	C3D-C4D	-2.16	1.39	1.44
19	4	606	CLA	C3D-C4D	-2.16	1.39	1.44
19	A	1139	CLA	C3B-C2B	-2.16	1.37	1.40
24	J	5003	LMT	O4'-C4B	-2.16	1.37	1.43
29	2	611	CHL	C1D-ND	-2.16	1.35	1.37
19	2	605	CLA	C3D-C4D	-2.16	1.39	1.44
19	A	1134	CLA	C3D-C4D	-2.16	1.39	1.44
19	G	1601	CLA	C3B-C2B	-2.15	1.37	1.40
19	3	608	CLA	C1C-C2C	2.15	1.48	1.44
24	A	5004	LMT	O1'-C1'	-2.15	1.36	1.40
19	4	604	CLA	C3B-C2B	-2.15	1.37	1.40
19	B	1201	CLA	C1C-C2C	2.15	1.48	1.44
19	B	1212	CLA	C1C-C2C	2.15	1.48	1.44
19	A	1102	CLA	C1C-C2C	2.15	1.48	1.44
19	4	612	CLA	C3D-C4D	-2.15	1.39	1.44
19	3	612	CLA	C3D-C4D	-2.15	1.39	1.44
27	4	801	DGD	O5D-C1E	2.14	1.43	1.40
19	A	1110	CLA	C3D-C4D	-2.14	1.39	1.44
19	2	601	CLA	C1C-C2C	2.14	1.48	1.44
19	1	606	CLA	C3D-C4D	-2.14	1.39	1.44
19	G	1602	CLA	C3B-C2B	-2.13	1.37	1.40
19	3	610	CLA	C3D-C4D	-2.13	1.39	1.44
19	A	1112	CLA	C3B-C2B	-2.13	1.37	1.40
24	B	5006	LMT	O4'-C4B	-2.13	1.38	1.43
19	G	1603	CLA	C1A-CHA	2.13	1.51	1.43
19	3	610	CLA	C3B-C2B	-2.13	1.37	1.40
19	K	1404	CLA	C1A-CHA	2.12	1.51	1.43
19	B	1201	CLA	C3B-C2B	-2.12	1.37	1.40
19	B	1217	CLA	C3D-C4D	-2.12	1.39	1.44
19	1	608	CLA	C1B-NB	2.12	1.37	1.35
19	B	1226	CLA	C3D-C4D	-2.12	1.39	1.44
19	1	602	CLA	C3D-C4D	-2.12	1.39	1.44
19	2	601	CLA	C3D-C4D	-2.12	1.39	1.44
19	4	607	CLA	C3D-C4D	-2.12	1.39	1.44
19	4	608	CLA	C1C-C2C	2.12	1.48	1.44
19	2	604	CLA	C3B-C2B	-2.12	1.37	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	2	602	CLA	C1A-CHA	2.12	1.51	1.43
19	B	1203	CLA	C3B-C2B	-2.12	1.37	1.40
19	1	614	CLA	C3D-C4D	-2.12	1.39	1.44
19	A	1101	CLA	C4B-NB	-2.11	1.33	1.35
19	A	1122	CLA	C3D-C4D	-2.11	1.39	1.44
19	B	1208	CLA	C3D-C4D	-2.11	1.39	1.44
19	A	1109	CLA	C3D-C4D	-2.11	1.39	1.44
19	A	1136	CLA	C1C-C2C	2.11	1.48	1.44
19	A	1102	CLA	C3D-C4D	-2.11	1.39	1.44
19	3	608	CLA	C3D-C4D	-2.10	1.39	1.44
19	B	1219	CLA	C3B-C2B	-2.10	1.37	1.40
19	4	602	CLA	C3D-C4D	-2.10	1.39	1.44
24	G	5004	LMT	O4'-C4B	-2.10	1.38	1.43
22	I	4020	BCR	C1-C6	-2.10	1.50	1.53
19	L	1501	CLA	C3B-C2B	-2.10	1.37	1.40
19	B	1218	CLA	C1C-C2C	2.10	1.48	1.44
19	1	613	CLA	C1C-C2C	2.10	1.48	1.44
19	4	609	CLA	C1A-CHA	2.10	1.51	1.43
19	A	1103	CLA	C3B-C2B	-2.10	1.37	1.40
19	B	1239	CLA	C1A-CHA	2.10	1.51	1.43
19	B	1222	CLA	C3D-C4D	-2.10	1.39	1.44
25	3	802	LMG	O1-C1	2.09	1.43	1.40
19	A	1103	CLA	C3D-C4D	-2.09	1.39	1.44
19	A	1118	CLA	C3D-C4D	-2.09	1.39	1.44
19	3	606	CLA	C3D-C4D	-2.09	1.39	1.44
19	B	1226	CLA	C1A-CHA	2.09	1.51	1.43
19	K	1402	CLA	C1C-C2C	2.09	1.48	1.44
19	2	607	CLA	C3D-C4D	-2.09	1.39	1.44
22	A	4017	BCR	C12-C13	-2.09	1.41	1.45
19	F	1301	CLA	C3D-C4D	-2.09	1.39	1.44
24	G	5005	LMT	O1'-C1'	-2.08	1.36	1.40
19	B	1201	CLA	C3D-C4D	-2.08	1.39	1.44
19	G	1603	CLA	C3D-C4D	-2.08	1.39	1.44
19	4	607	CLA	C1C-C2C	2.08	1.48	1.44
19	L	1502	CLA	C1A-CHA	2.08	1.51	1.43
19	A	1122	CLA	C1A-CHA	2.08	1.51	1.43
19	A	1118	CLA	C1A-CHA	2.08	1.51	1.43
19	1	614	CLA	C1C-C2C	2.08	1.48	1.44
19	B	1218	CLA	C1A-CHA	2.08	1.51	1.43
19	1	601	CLA	C1A-CHA	2.08	1.51	1.43
19	G	1701	CLA	C1A-CHA	2.08	1.51	1.43
19	2	603	CLA	C3D-C4D	-2.08	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	1	603	CLA	C1A-CHA	2.07	1.51	1.43
19	A	1108	CLA	C1A-CHA	2.07	1.51	1.43
19	B	1234	CLA	C3B-C2B	-2.07	1.37	1.40
19	G	1701	CLA	C3D-C4D	-2.07	1.39	1.44
19	A	1127	CLA	C1A-CHA	2.07	1.51	1.43
19	3	601	CLA	C3D-C4D	-2.07	1.39	1.44
31	4	505	C7Z	C24-C25	2.07	1.54	1.51
22	F	4016	BCR	C12-C13	-2.07	1.41	1.45
19	A	1129	CLA	C4B-NB	-2.07	1.33	1.35
19	B	1240	CLA	C3B-C2B	-2.07	1.37	1.40
19	A	1109	CLA	C1C-C2C	2.07	1.48	1.44
19	L	1503	CLA	C3B-C2B	-2.07	1.37	1.40
24	G	5004	LMT	O1'-C1'	-2.07	1.36	1.40
29	1	609	CHL	C1D-ND	-2.07	1.35	1.37
19	3	614	CLA	C3D-C4D	-2.07	1.39	1.44
19	B	1235	CLA	C3D-C4D	-2.07	1.39	1.44
19	3	602	CLA	C3D-C4D	-2.06	1.39	1.44
19	A	1136	CLA	C3D-C4D	-2.06	1.39	1.44
19	A	1123	CLA	MG-NC	2.06	2.11	2.06
19	2	608	CLA	C1C-C2C	2.06	1.48	1.44
19	B	1212	CLA	C3D-C4D	-2.06	1.39	1.44
29	3	611	CHL	CHC-C1C	2.06	1.40	1.35
19	A	1132	CLA	C1A-CHA	2.06	1.51	1.43
19	2	606	CLA	C3D-C4D	-2.05	1.39	1.44
19	J	1901	CLA	C1A-CHA	2.05	1.51	1.43
19	3	608	CLA	C1A-CHA	2.05	1.51	1.43
18	A	1011	CL0	C1D-C2D	2.05	1.49	1.45
19	L	1503	CLA	C1A-CHA	2.05	1.51	1.43
19	3	612	CLA	C1A-CHA	2.05	1.51	1.43
19	A	1112	CLA	C1C-C2C	2.05	1.48	1.44
27	G	5003	DGD	CAB-C9B	-2.05	1.33	1.49
19	A	1137	CLA	C1C-C2C	2.04	1.48	1.44
19	B	1216	CLA	C1A-CHA	2.04	1.51	1.43
19	A	1123	CLA	C4B-NB	-2.04	1.33	1.35
27	B	5005	DGD	CDA-CCA	-2.04	1.33	1.49
19	A	1134	CLA	C1A-CHA	2.04	1.51	1.43
19	3	603	CLA	C3D-C4D	-2.04	1.39	1.44
19	3	614	CLA	C1A-CHA	2.04	1.51	1.43
19	1	611	CLA	C3B-C2B	-2.04	1.37	1.40
25	2	803	LMG	O1-C1	2.04	1.43	1.40
19	B	1206	CLA	C1A-CHA	2.03	1.51	1.43
19	1	602	CLA	C1C-C2C	2.03	1.48	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	1	603	CLA	C3D-C4D	-2.03	1.39	1.44
19	3	610	CLA	C1A-CHA	2.03	1.51	1.43
19	K	1404	CLA	MG-NC	2.03	2.11	2.06
19	A	1119	CLA	CHD-C1D	2.03	1.42	1.38
19	G	1602	CLA	C1C-C2C	2.03	1.48	1.44
19	1	606	CLA	C1A-CHA	2.03	1.51	1.43
25	B	5004	LMG	O1-C1	2.03	1.43	1.40
19	B	1209	CLA	C3B-C2B	-2.03	1.37	1.40
19	4	609	CLA	C3D-C4D	-2.03	1.39	1.44
19	B	1230	CLA	C3B-C2B	-2.03	1.37	1.40
19	3	613	CLA	C1C-C2C	2.02	1.48	1.44
19	A	1101	CLA	C3B-C2B	-2.02	1.37	1.40
19	K	1403	CLA	MG-NC	2.02	2.11	2.06
19	2	601	CLA	C1B-NB	2.02	1.37	1.35
19	B	1234	CLA	C1C-C2C	2.02	1.48	1.44
19	3	603	CLA	C1A-CHA	2.02	1.51	1.43
25	A	5006	LMG	C40-C39	-2.02	1.33	1.49
19	B	1235	CLA	C1C-C2C	2.02	1.48	1.44
29	3	611	CHL	C1A-CHA	-2.02	1.34	1.43
19	4	602	CLA	C1A-CHA	2.02	1.51	1.43
19	3	606	CLA	C1A-CHA	2.02	1.51	1.43
29	1	609	CHL	C3A-C2A	-2.02	1.48	1.54
19	1	604	CLA	C1C-C2C	2.02	1.48	1.44
19	A	1113	CLA	C1A-CHA	2.02	1.51	1.43
29	3	607	CHL	C1D-ND	-2.02	1.35	1.37
19	A	1110	CLA	C1A-CHA	2.02	1.51	1.43
19	A	1135	CLA	C3D-C4D	-2.02	1.39	1.44
19	2	607	CLA	C1C-C2C	2.02	1.48	1.44
29	3	604	CHL	C3A-C2A	-2.02	1.48	1.54
19	A	1138	CLA	C1A-CHA	2.02	1.51	1.43
19	G	1601	CLA	C1A-CHA	2.02	1.51	1.43
19	B	1217	CLA	C1C-C2C	2.01	1.48	1.44
29	1	609	CHL	CHC-C1C	2.01	1.40	1.35
25	G	5002	LMG	C43-C42	-2.01	1.33	1.49
19	B	1239	CLA	C1C-C2C	2.01	1.48	1.44
27	J	5001	DGD	CAB-C9B	-2.01	1.33	1.49
19	K	1401	CLA	C1B-NB	2.01	1.37	1.35
27	3	803	DGD	CAA-C9A	-2.01	1.33	1.49
19	3	605	CLA	MG-NC	2.01	2.11	2.06
19	K	1401	CLA	MG-NC	2.01	2.11	2.06
19	3	605	CLA	C1A-CHA	2.00	1.51	1.43
19	1	614	CLA	C1A-CHA	2.00	1.51	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	F	1301	CLA	C1A-CHA	2.00	1.51	1.43
19	J	1901	CLA	C3D-C4D	-2.00	1.39	1.44
19	2	604	CLA	C1A-CHA	2.00	1.51	1.43
19	L	1503	CLA	C1C-C2C	2.00	1.48	1.44
19	A	1124	CLA	C1A-CHA	2.00	1.51	1.43
22	B	4005	BCR	C12-C13	-2.00	1.41	1.45
27	4	801	DGD	CDA-CCA	-2.00	1.33	1.49
19	K	1401	CLA	C3D-C4D	-2.00	1.39	1.44

All (3279) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	4004	BCR	C11-C10-C9	19.37	154.96	127.31
22	A	4017	BCR	C16-C15-C14	18.15	160.66	123.47
22	1	504	BCR	C10-C11-C12	17.64	178.27	123.22
22	G	4021	BCR	C10-C11-C12	17.50	177.83	123.22
22	I	4018	BCR	C10-C11-C12	17.47	177.72	123.22
22	B	4004	BCR	C10-C11-C12	17.44	177.64	123.22
22	A	4008	BCR	C10-C11-C12	17.44	177.63	123.22
22	3	503	BCR	C10-C11-C12	17.35	177.38	123.22
22	F	4016	BCR	C10-C11-C12	17.29	177.18	123.22
22	2	503	BCR	C10-C11-C12	17.25	177.06	123.22
22	B	4006	BCR	C10-C11-C12	17.21	176.93	123.22
22	G	4011	BCR	C10-C11-C12	17.18	176.84	123.22
22	1	503	BCR	C10-C11-C12	17.15	176.75	123.22
22	K	4001	BCR	C10-C11-C12	17.09	176.55	123.22
22	B	4010	BCR	C10-C11-C12	17.04	176.40	123.22
22	A	4007	BCR	C10-C11-C12	16.99	176.23	123.22
22	A	4003	BCR	C10-C11-C12	16.98	176.20	123.22
22	3	506	BCR	C10-C11-C12	16.98	176.19	123.22
22	J	4012	BCR	C10-C11-C12	16.86	175.84	123.22
22	F	4014	BCR	C10-C11-C12	16.76	175.51	123.22
22	B	4009	BCR	C10-C11-C12	16.64	175.16	123.22
22	L	4019	BCR	C10-C11-C12	16.58	174.97	123.22
22	K	4002	BCR	C10-C11-C12	16.57	174.94	123.22
22	A	4002	BCR	C10-C11-C12	16.49	174.68	123.22
22	L	4020	BCR	C10-C11-C12	16.43	174.49	123.22
22	B	4005	BCR	C10-C11-C12	16.43	174.48	123.22
22	I	4020	BCR	C10-C11-C12	16.38	174.33	123.22
22	A	4017	BCR	C10-C11-C12	16.28	174.01	123.22
22	1	504	BCR	C16-C15-C14	15.94	156.12	123.47
22	A	4011	BCR	C10-C11-C12	15.94	172.95	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	I	4020	BCR	C11-C10-C9	14.91	148.59	127.31
22	A	4017	BCR	C11-C10-C9	14.80	148.43	127.31
22	G	4011	BCR	C16-C15-C14	14.80	153.79	123.47
22	A	4011	BCR	C11-C10-C9	14.66	148.23	127.31
22	B	4005	BCR	C11-C10-C9	14.40	147.86	127.31
22	F	4014	BCR	C11-C10-C9	14.04	147.35	127.31
22	B	4004	BCR	C21-C20-C19	13.83	166.37	123.22
22	3	503	BCR	C16-C15-C14	13.79	151.72	123.47
22	A	4007	BCR	C16-C15-C14	13.74	151.63	123.47
22	K	4001	BCR	C11-C10-C9	13.63	146.77	127.31
22	3	506	BCR	C16-C15-C14	13.55	151.23	123.47
22	K	4002	BCR	C11-C10-C9	13.53	146.62	127.31
22	L	4020	BCR	C11-C10-C9	13.41	146.44	127.31
22	G	4011	BCR	C21-C20-C19	13.34	164.84	123.22
22	1	503	BCR	C11-C10-C9	13.27	146.25	127.31
22	J	4012	BCR	C11-C10-C9	13.25	146.23	127.31
22	A	4002	BCR	C11-C10-C9	13.25	146.22	127.31
22	B	4009	BCR	C11-C10-C9	13.25	146.22	127.31
22	3	506	BCR	C11-C10-C9	13.24	146.20	127.31
22	L	4019	BCR	C11-C10-C9	13.15	146.08	127.31
22	G	4021	BCR	C16-C15-C14	13.01	150.12	123.47
22	2	503	BCR	C16-C15-C14	12.97	150.04	123.47
22	B	4010	BCR	C11-C10-C9	12.95	145.79	127.31
22	1	504	BCR	C21-C20-C19	12.80	163.18	123.22
22	B	4006	BCR	C11-C10-C9	12.79	145.57	127.31
22	3	506	BCR	C21-C20-C19	12.78	163.10	123.22
22	A	4011	BCR	C11-C12-C13	12.77	162.29	126.42
22	I	4020	BCR	C16-C15-C14	12.75	149.58	123.47
22	I	4018	BCR	C16-C15-C14	12.61	149.31	123.47
22	K	4001	BCR	C21-C20-C19	12.59	162.50	123.22
22	G	4021	BCR	C11-C10-C9	12.54	145.21	127.31
31	4	505	C7Z	C38-C25-C26	-12.52	110.47	124.53
22	2	503	BCR	C11-C10-C9	12.49	145.13	127.31
22	A	4017	BCR	C21-C20-C19	12.42	161.97	123.22
22	1	504	BCR	C11-C10-C9	12.38	144.98	127.31
31	4	505	C7Z	C31-C30-C29	-12.36	109.67	127.31
22	F	4016	BCR	C11-C10-C9	12.31	144.88	127.31
22	A	4007	BCR	C11-C10-C9	12.28	144.83	127.31
22	L	4019	BCR	C16-C15-C14	12.22	148.51	123.47
22	G	4011	BCR	C11-C10-C9	12.21	144.74	127.31
22	A	4003	BCR	C21-C20-C19	12.20	161.30	123.22
22	A	4003	BCR	C11-C10-C9	12.13	144.62	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	L	4020	BCR	C11-C12-C13	12.06	160.28	126.42
22	2	503	BCR	C29-C30-C25	-12.03	91.96	110.48
31	4	505	C7Z	C18-C5-C6	-12.02	111.03	124.53
22	B	4009	BCR	C11-C12-C13	12.01	160.16	126.42
22	A	4008	BCR	C11-C10-C9	11.96	144.37	127.31
22	A	4007	BCR	C21-C20-C19	11.93	160.44	123.22
22	A	4003	BCR	C11-C12-C13	11.92	159.89	126.42
22	B	4005	BCR	C11-C12-C13	11.86	159.73	126.42
22	K	4002	BCR	C21-C20-C19	11.72	159.79	123.22
22	L	4019	BCR	C11-C12-C13	11.72	159.34	126.42
22	J	4012	BCR	C21-C20-C19	11.70	159.74	123.22
22	K	4002	BCR	C11-C12-C13	11.70	159.29	126.42
22	K	4002	BCR	C16-C15-C14	11.68	147.39	123.47
22	I	4020	BCR	C21-C20-C19	11.66	159.61	123.22
22	F	4014	BCR	C16-C15-C14	11.64	147.31	123.47
22	K	4001	BCR	C16-C15-C14	11.57	147.18	123.47
22	3	503	BCR	C11-C12-C13	11.52	158.77	126.42
22	F	4016	BCR	C21-C20-C19	11.51	159.14	123.22
22	A	4002	BCR	C11-C12-C13	11.49	158.69	126.42
22	F	4016	BCR	C16-C15-C14	11.48	146.98	123.47
22	2	503	BCR	C21-C20-C19	11.42	158.87	123.22
22	A	4007	BCR	C11-C12-C13	11.40	158.44	126.42
22	J	4012	BCR	C11-C12-C13	11.38	158.38	126.42
22	F	4014	BCR	C11-C12-C13	11.35	158.29	126.42
22	B	4010	BCR	C16-C15-C14	11.25	146.52	123.47
22	2	503	BCR	C11-C12-C13	11.24	158.00	126.42
22	L	4020	BCR	C21-C20-C19	11.21	158.19	123.22
22	I	4020	BCR	C11-C12-C13	11.17	157.81	126.42
22	3	506	BCR	C11-C12-C13	11.16	157.75	126.42
22	L	4019	BCR	C21-C20-C19	11.11	157.90	123.22
22	B	4006	BCR	C11-C12-C13	11.02	157.38	126.42
22	3	503	BCR	C11-C10-C9	10.98	142.99	127.31
22	1	503	BCR	C21-C20-C19	10.97	157.44	123.22
22	K	4001	BCR	C11-C12-C13	10.90	157.04	126.42
30	2	502	XAT	O4-C5-C4	-10.88	105.21	113.38
31	4	505	C7Z	C15-C14-C13	-10.82	111.86	127.31
31	4	505	C7Z	C20-C13-C14	-10.82	107.77	122.92
22	A	4008	BCR	C11-C12-C13	10.76	156.64	126.42
22	1	503	BCR	C11-C12-C13	10.73	156.57	126.42
22	A	4002	BCR	C21-C20-C19	10.65	156.45	123.22
22	B	4005	BCR	C16-C15-C14	10.63	145.26	123.47
22	A	4008	BCR	C21-C20-C19	10.62	156.35	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	1	503	BCR	C16-C15-C14	10.61	145.21	123.47
22	B	4009	BCR	C16-C15-C14	10.53	145.05	123.47
22	B	4010	BCR	C11-C12-C13	10.45	155.76	126.42
22	F	4016	BCR	C11-C12-C13	10.43	155.71	126.42
22	B	4010	BCR	C21-C20-C19	10.41	155.69	123.22
22	I	4018	BCR	C21-C20-C19	10.39	155.65	123.22
22	G	4021	BCR	C21-C20-C19	10.38	155.60	123.22
22	A	4011	BCR	C21-C20-C19	10.33	155.45	123.22
22	B	4004	BCR	C16-C15-C14	10.31	144.59	123.47
19	F	1301	CLA	C4A-NA-C1A	10.27	111.32	106.71
22	L	4020	BCR	C16-C15-C14	10.23	144.44	123.47
22	1	504	BCR	C11-C12-C13	10.22	155.12	126.42
22	G	4011	BCR	C11-C12-C13	10.20	155.07	126.42
22	G	4021	BCR	C11-C12-C13	10.17	154.99	126.42
31	4	505	C7Z	C39-C29-C30	-10.17	108.68	122.92
22	I	4018	BCR	C11-C10-C9	10.14	141.78	127.31
22	B	4005	BCR	C21-C20-C19	10.12	154.79	123.22
31	4	505	C7Z	C11-C10-C9	-10.08	112.93	127.31
19	A	1105	CLA	C4A-NA-C1A	9.92	111.17	106.71
22	A	4011	BCR	C16-C15-C14	9.90	143.75	123.47
22	3	503	BCR	C21-C20-C19	9.85	153.96	123.22
22	3	503	BCR	C20-C19-C18	9.83	154.03	126.42
19	2	605	CLA	C4A-NA-C1A	9.81	111.12	106.71
22	F	4014	BCR	C21-C20-C19	9.80	153.79	123.22
22	G	4021	BCR	C20-C19-C18	9.79	153.92	126.42
19	B	1201	CLA	C4A-NA-C1A	9.79	111.11	106.71
19	B	1211	CLA	C4A-NA-C1A	9.78	111.11	106.71
19	B	1229	CLA	C4A-NA-C1A	9.76	111.10	106.71
19	2	606	CLA	C4A-NA-C1A	9.76	111.09	106.71
19	G	1603	CLA	C4A-NA-C1A	9.70	111.07	106.71
19	B	1206	CLA	C4A-NA-C1A	9.69	111.06	106.71
19	A	1139	CLA	C4A-NA-C1A	9.61	111.03	106.71
19	A	1118	CLA	C4A-NA-C1A	9.61	111.03	106.71
19	3	613	CLA	C4A-NA-C1A	9.60	111.02	106.71
22	B	4009	BCR	C21-C20-C19	9.59	153.13	123.22
19	A	1124	CLA	C4A-NA-C1A	9.57	111.01	106.71
22	B	4009	BCR	C20-C19-C18	9.56	153.28	126.42
19	3	610	CLA	C4A-NA-C1A	9.55	111.00	106.71
31	4	505	C7Z	C40-C33-C34	-9.54	109.56	122.92
22	I	4018	BCR	C20-C19-C18	9.53	153.20	126.42
19	A	1134	CLA	C4A-NA-C1A	9.53	110.99	106.71
19	3	612	CLA	C4A-NA-C1A	9.49	110.97	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	4	612	CLA	C4A-NA-C1A	9.47	110.97	106.71
19	4	609	CLA	C4A-NA-C1A	9.38	110.92	106.71
19	G	1701	CLA	C4A-NA-C1A	9.38	110.92	106.71
19	A	1131	CLA	C4A-NA-C1A	9.34	110.90	106.71
19	1	603	CLA	C4A-NA-C1A	9.34	110.90	106.71
22	A	4017	BCR	C11-C12-C13	9.32	152.61	126.42
19	1	602	CLA	C4A-NA-C1A	9.28	110.88	106.71
19	A	1104	CLA	C4A-NA-C1A	9.28	110.88	106.71
22	F	4014	BCR	C20-C19-C18	9.27	152.45	126.42
19	A	1115	CLA	C4A-NA-C1A	9.26	110.87	106.71
19	B	1205	CLA	C4A-NA-C1A	9.26	110.87	106.71
19	B	1023	CLA	C4A-NA-C1A	9.26	110.87	106.71
19	B	1228	CLA	C4A-NA-C1A	9.26	110.87	106.71
22	A	4002	BCR	C16-C15-C14	9.25	142.43	123.47
19	B	1021	CLA	C4A-NA-C1A	9.24	110.86	106.71
19	1	605	CLA	C4A-NA-C1A	9.22	110.85	106.71
19	1	608	CLA	C4A-NA-C1A	9.22	110.85	106.71
19	3	601	CLA	C4A-NA-C1A	9.20	110.84	106.71
19	A	1140	CLA	C4A-NA-C1A	9.20	110.84	106.71
31	4	505	C7Z	C35-C34-C33	-9.16	114.24	127.31
22	J	4012	BCR	C16-C15-C14	9.16	142.23	123.47
22	A	4008	BCR	C16-C15-C14	9.15	142.21	123.47
22	B	4006	BCR	C16-C15-C14	9.12	142.16	123.47
31	4	505	C7Z	C1-C6-C5	-9.11	109.78	122.61
19	A	1127	CLA	C4A-NA-C1A	9.10	110.80	106.71
19	A	1120	CLA	C4A-NA-C1A	9.05	110.78	106.71
19	B	1221	CLA	C4A-NA-C1A	9.05	110.78	106.71
19	B	1226	CLA	C4A-NA-C1A	9.05	110.77	106.71
19	L	1502	CLA	C4A-NA-C1A	9.04	110.77	106.71
19	B	1222	CLA	C4A-NA-C1A	9.03	110.77	106.71
31	4	505	C7Z	C19-C9-C10	-9.03	110.27	122.92
22	A	4011	BCR	C20-C19-C18	9.02	151.76	126.42
19	A	1012	CLA	C4A-NA-C1A	9.02	110.76	106.71
19	4	602	CLA	C4A-NA-C1A	9.02	110.76	106.71
19	A	1111	CLA	C4A-NA-C1A	9.01	110.76	106.71
19	A	1108	CLA	C4A-NA-C1A	9.01	110.75	106.71
19	A	1101	CLA	C4A-NA-C1A	8.99	110.75	106.71
19	G	1601	CLA	C4A-NA-C1A	8.98	110.74	106.71
22	B	4010	BCR	C20-C19-C18	8.98	151.64	126.42
19	1	601	CLA	C4A-NA-C1A	8.97	110.74	106.71
19	A	1107	CLA	C4A-NA-C1A	8.97	110.74	106.71
19	B	1239	CLA	C4A-NA-C1A	8.97	110.74	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	1103	CLA	C4A-NA-C1A	8.96	110.73	106.71
19	A	1122	CLA	C4A-NA-C1A	8.94	110.73	106.71
19	B	1216	CLA	C4A-NA-C1A	8.92	110.72	106.71
19	A	1126	CLA	C4A-NA-C1A	8.92	110.72	106.71
19	B	1240	CLA	C4A-NA-C1A	8.91	110.71	106.71
19	B	1227	CLA	C4A-NA-C1A	8.91	110.71	106.71
19	B	1237	CLA	C4A-NA-C1A	8.91	110.71	106.71
19	B	1215	CLA	C4A-NA-C1A	8.90	110.71	106.71
19	2	607	CLA	C4A-NA-C1A	8.90	110.71	106.71
22	B	4005	BCR	C20-C19-C18	8.88	151.37	126.42
19	1	606	CLA	C4A-NA-C1A	8.87	110.69	106.71
19	A	1135	CLA	C4A-NA-C1A	8.86	110.69	106.71
19	3	603	CLA	C4A-NA-C1A	8.86	110.69	106.71
19	K	1402	CLA	C4A-NA-C1A	8.84	110.68	106.71
19	A	1130	CLA	C4A-NA-C1A	8.84	110.68	106.71
19	A	1117	CLA	C4A-NA-C1A	8.83	110.68	106.71
19	2	612	CLA	C4A-NA-C1A	8.83	110.67	106.71
22	F	4016	BCR	C20-C19-C18	8.82	151.19	126.42
19	B	1210	CLA	C4A-NA-C1A	8.80	110.66	106.71
19	A	1128	CLA	C4A-NA-C1A	8.79	110.66	106.71
19	F	1302	CLA	C4A-NA-C1A	8.79	110.66	106.71
19	A	1132	CLA	C4A-NA-C1A	8.79	110.66	106.71
19	A	1129	CLA	C4A-NA-C1A	8.77	110.65	106.71
19	1	607	CLA	C4A-NA-C1A	8.77	110.65	106.71
19	3	608	CLA	C4A-NA-C1A	8.76	110.65	106.71
19	G	1602	CLA	C4A-NA-C1A	8.76	110.64	106.71
19	A	1141	CLA	C4A-NA-C1A	8.75	110.64	106.71
19	2	601	CLA	C4A-NA-C1A	8.74	110.64	106.71
19	B	1231	CLA	C4A-NA-C1A	8.73	110.63	106.71
19	A	1106	CLA	C4A-NA-C1A	8.73	110.63	106.71
19	4	601	CLA	C4A-NA-C1A	8.70	110.62	106.71
19	3	614	CLA	C4A-NA-C1A	8.70	110.62	106.71
19	4	603	CLA	C4A-NA-C1A	8.70	110.62	106.71
19	A	1112	CLA	C4A-NA-C1A	8.69	110.61	106.71
19	2	603	CLA	C4A-NA-C1A	8.69	110.61	106.71
19	B	1230	CLA	C4A-NA-C1A	8.69	110.61	106.71
19	B	1235	CLA	C4A-NA-C1A	8.69	110.61	106.71
19	B	1238	CLA	C4A-NA-C1A	8.69	110.61	106.71
19	B	1212	CLA	C4A-NA-C1A	8.69	110.61	106.71
19	A	1109	CLA	C4A-NA-C1A	8.68	110.61	106.71
19	A	1110	CLA	C4A-NA-C1A	8.67	110.61	106.71
19	1	614	CLA	C4A-NA-C1A	8.66	110.60	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	1116	CLA	C4A-NA-C1A	8.66	110.60	106.71
19	B	1224	CLA	C4A-NA-C1A	8.65	110.59	106.71
19	B	1022	CLA	C4A-NA-C1A	8.63	110.59	106.71
19	A	1133	CLA	C4A-NA-C1A	8.62	110.58	106.71
19	L	1503	CLA	C4A-NA-C1A	8.61	110.58	106.71
19	A	1114	CLA	C4A-NA-C1A	8.60	110.57	106.71
19	K	1401	CLA	C4A-NA-C1A	8.59	110.57	106.71
19	1	611	CLA	C4A-NA-C1A	8.56	110.55	106.71
19	B	1209	CLA	C4A-NA-C1A	8.54	110.55	106.71
19	4	606	CLA	C4A-NA-C1A	8.54	110.54	106.71
19	4	604	CLA	C4A-NA-C1A	8.52	110.53	106.71
19	B	1232	CLA	C4A-NA-C1A	8.51	110.53	106.71
19	B	1214	CLA	C4A-NA-C1A	8.50	110.53	106.71
19	3	606	CLA	C4A-NA-C1A	8.50	110.53	106.71
19	A	1113	CLA	C4A-NA-C1A	8.49	110.53	106.71
19	A	1102	CLA	C4A-NA-C1A	8.49	110.52	106.71
19	A	1123	CLA	C4A-NA-C1A	8.47	110.51	106.71
19	B	1217	CLA	C4A-NA-C1A	8.46	110.51	106.71
22	A	4017	BCR	C15-C14-C13	-8.46	115.24	127.31
22	L	4019	BCR	C20-C19-C18	8.45	150.16	126.42
19	B	1213	CLA	C4A-NA-C1A	8.44	110.50	106.71
19	2	608	CLA	C4A-NA-C1A	8.43	110.50	106.71
22	B	4006	BCR	C21-C20-C19	8.43	149.52	123.22
19	B	1207	CLA	C4A-NA-C1A	8.43	110.49	106.71
19	K	1403	CLA	C4A-NA-C1A	8.43	110.49	106.71
19	3	602	CLA	C4A-NA-C1A	8.42	110.49	106.71
22	A	4008	BCR	C20-C19-C18	8.41	150.05	126.42
19	A	1136	CLA	C4A-NA-C1A	8.41	110.49	106.71
19	B	1236	CLA	C4A-NA-C1A	8.41	110.49	106.71
19	A	1125	CLA	C4A-NA-C1A	8.38	110.47	106.71
19	B	1225	CLA	C4A-NA-C1A	8.35	110.46	106.71
19	A	1138	CLA	C4A-NA-C1A	8.34	110.46	106.71
19	3	617	CLA	C4A-NA-C1A	8.34	110.46	106.71
19	A	1013	CLA	C4A-NA-C1A	8.33	110.45	106.71
19	L	1501	CLA	C4A-NA-C1A	8.33	110.45	106.71
19	B	1234	CLA	C4A-NA-C1A	8.28	110.43	106.71
19	B	1220	CLA	C4A-NA-C1A	8.27	110.42	106.71
19	B	1218	CLA	C4A-NA-C1A	8.23	110.41	106.71
19	4	607	CLA	C4A-NA-C1A	8.21	110.39	106.71
19	3	605	CLA	C4A-NA-C1A	8.18	110.39	106.71
19	4	605	CLA	C4A-NA-C1A	8.18	110.38	106.71
19	2	604	CLA	C4A-NA-C1A	8.11	110.35	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	4	608	CLA	C4A-NA-C1A	8.10	110.35	106.71
22	I	4018	BCR	C11-C12-C13	8.09	149.14	126.42
19	B	1219	CLA	C4A-NA-C1A	8.09	110.34	106.71
22	L	4020	BCR	C20-C19-C18	8.07	149.10	126.42
22	K	4002	BCR	C20-C19-C18	8.06	149.07	126.42
22	A	4003	BCR	C16-C15-C14	8.06	139.97	123.47
22	1	503	BCR	C20-C19-C18	8.03	148.98	126.42
22	B	4004	BCR	C19-C18-C17	7.94	131.13	118.94
19	B	1204	CLA	C4A-NA-C1A	7.94	110.28	106.71
19	B	1223	CLA	C4A-NA-C1A	7.94	110.27	106.71
19	2	602	CLA	C4A-NA-C1A	7.87	110.25	106.71
22	B	4004	BCR	C8-C9-C10	7.85	130.98	118.94
22	A	4002	BCR	C20-C19-C18	7.81	148.34	126.42
19	J	1901	CLA	C4A-NA-C1A	7.73	110.18	106.71
19	4	617	CLA	C4A-NA-C1A	7.65	110.15	106.71
28	J	4013	LUT	C21-C26-C27	7.65	122.37	112.70
19	A	1137	CLA	C4A-NA-C1A	7.64	110.14	106.71
19	1	613	CLA	C4A-NA-C1A	7.58	110.11	106.71
22	2	503	BCR	C20-C19-C18	7.58	147.71	126.42
19	A	1119	CLA	C4A-NA-C1A	7.57	110.11	106.71
19	B	1210	CLA	O2D-CGD-CBD	7.56	124.71	111.27
22	B	4004	BCR	C11-C12-C13	7.44	147.31	126.42
19	B	1208	CLA	C4A-NA-C1A	7.39	110.03	106.71
19	1	604	CLA	C4A-NA-C1A	7.35	110.01	106.71
22	A	4003	BCR	C20-C19-C18	7.29	146.91	126.42
19	A	1121	CLA	C4A-NA-C1A	7.28	109.98	106.71
19	K	1404	CLA	C4A-NA-C1A	7.27	109.97	106.71
22	J	4012	BCR	C20-C19-C18	7.27	146.83	126.42
19	B	1202	CLA	C4A-NA-C1A	7.23	109.95	106.71
22	2	503	BCR	C40-C30-C29	-7.21	80.07	108.91
22	A	4007	BCR	C20-C19-C18	7.11	146.38	126.42
19	B	1203	CLA	C4A-NA-C1A	7.09	109.89	106.71
22	B	4004	BCR	C12-C13-C14	7.08	129.81	118.94
22	I	4020	BCR	C20-C19-C18	7.05	146.22	126.42
22	3	506	BCR	C20-C19-C18	7.03	146.17	126.42
19	A	1111	CLA	O2D-CGD-CBD	7.00	123.71	111.27
31	4	505	C7Z	C39-C29-C28	-6.98	107.07	118.08
22	K	4001	BCR	C20-C19-C18	6.88	145.76	126.42
19	K	1403	CLA	CMD-C2D-C1D	6.83	136.75	124.71
22	1	504	BCR	C20-C19-C18	6.70	145.22	126.42
19	1	608	CLA	O2D-CGD-CBD	6.60	123.00	111.27
19	B	1215	CLA	O2A-C1-C2	6.60	125.98	108.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	1238	CLA	O2A-C1-C2	6.58	125.92	108.64
19	1	614	CLA	O2D-CGD-CBD	6.56	122.93	111.27
19	4	617	CLA	O2D-CGD-CBD	6.53	122.87	111.27
19	2	604	CLA	O2A-C1-C2	6.51	125.76	108.64
19	A	1128	CLA	O2D-CGD-CBD	6.50	122.82	111.27
31	4	505	C7Z	C19-C9-C8	-6.49	107.86	118.08
19	A	1101	CLA	O2D-CGD-CBD	6.43	122.69	111.27
19	B	1222	CLA	O2D-CGD-CBD	6.39	122.62	111.27
18	A	1011	CL0	CMD-C2D-C1D	6.38	135.96	124.71
19	B	1226	CLA	O2D-CGD-CBD	6.38	122.61	111.27
19	B	1212	CLA	O2D-CGD-CBD	6.38	122.60	111.27
19	4	604	CLA	O2D-CGD-CBD	6.33	122.52	111.27
19	B	1205	CLA	O2D-CGD-CBD	6.28	122.42	111.27
19	A	1132	CLA	O2D-CGD-CBD	6.27	122.40	111.27
18	A	1011	CL0	C2D-C1D-ND	6.26	114.72	110.10
19	A	1137	CLA	O2D-CGD-CBD	6.26	122.39	111.27
22	G	4011	BCR	C20-C19-C18	6.21	143.87	126.42
19	B	1232	CLA	O2A-C1-C2	6.20	124.92	108.64
28	3	502	LUT	C21-C26-C27	6.19	120.53	112.70
19	A	1102	CLA	O2D-CGD-CBD	6.18	122.25	111.27
19	B	1207	CLA	O2D-CGD-CBD	6.16	122.22	111.27
19	A	1123	CLA	O2D-CGD-CBD	6.14	122.18	111.27
19	B	1240	CLA	O2D-CGD-CBD	6.12	122.14	111.27
19	B	1238	CLA	CMD-C2D-C1D	6.11	135.48	124.71
18	A	1011	CL0	C4A-NA-C1A	6.10	109.45	106.71
19	A	1106	CLA	O2A-C1-C2	6.10	124.66	108.64
19	A	1141	CLA	O2D-CGD-CBD	6.09	122.10	111.27
19	A	1101	CLA	O2A-C1-C2	6.05	124.53	108.64
22	2	503	BCR	C39-C30-C25	6.05	120.11	110.30
19	A	1130	CLA	CMD-C2D-C1D	6.04	135.37	124.71
19	B	1222	CLA	O2A-C1-C2	5.96	124.31	108.64
28	2	501	LUT	C21-C26-C27	5.95	120.22	112.70
19	A	1113	CLA	CMD-C2D-C1D	5.93	135.17	124.71
19	B	1218	CLA	O2D-CGD-CBD	5.91	121.77	111.27
19	A	1112	CLA	O2D-CGD-CBD	5.89	121.73	111.27
19	4	604	CLA	CMD-C2D-C1D	5.88	135.07	124.71
19	2	608	CLA	CMD-C2D-C1D	5.87	135.06	124.71
19	4	602	CLA	O2D-CGD-CBD	5.87	121.70	111.27
19	B	1221	CLA	O2D-CGD-CBD	5.87	121.69	111.27
19	1	603	CLA	O2A-C1-C2	5.86	124.05	108.64
19	A	1129	CLA	O2D-CGD-CBD	5.86	121.68	111.27
19	1	608	CLA	CMD-C2D-C1D	5.84	135.01	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	1012	CLA	O2A-C1-C2	5.84	123.98	108.64
19	2	603	CLA	CMD-C2D-C1D	5.83	134.99	124.71
22	A	4017	BCR	C20-C19-C18	5.83	142.79	126.42
19	A	1120	CLA	CMD-C2D-C1D	5.82	134.97	124.71
31	4	505	C7Z	C7-C6-C5	-5.82	107.36	121.46
19	F	1302	CLA	CMD-C2D-C1D	5.80	134.93	124.71
19	B	1213	CLA	O2A-C1-C2	5.80	123.87	108.64
19	1	605	CLA	O2A-C1-C2	5.79	123.85	108.64
19	B	1202	CLA	O2D-CGD-CBD	5.79	121.55	111.27
19	A	1121	CLA	CMD-C2D-C1D	5.78	134.91	124.71
19	A	1141	CLA	CMD-C2D-C1D	5.78	134.90	124.71
19	4	602	CLA	CMD-C2D-C1D	5.78	134.90	124.71
31	4	505	C7Z	C12-C13-C14	-5.77	110.08	118.94
18	A	1011	CL0	CHD-C1D-ND	-5.77	119.16	124.45
19	A	1110	CLA	CMD-C2D-C1D	5.76	134.87	124.71
19	L	1501	CLA	O2D-CGD-CBD	5.76	121.50	111.27
19	B	1208	CLA	CMD-C2D-C1D	5.76	134.86	124.71
28	3	501	LUT	C21-C26-C27	5.75	119.98	112.70
19	B	1230	CLA	O2D-CGD-CBD	5.75	121.49	111.27
19	1	604	CLA	CMD-C2D-C1D	5.74	134.82	124.71
19	B	1218	CLA	CMD-C2D-C1D	5.72	134.80	124.71
19	B	1223	CLA	O2D-CGD-CBD	5.72	121.44	111.27
19	F	1301	CLA	O2A-C1-C2	5.71	123.63	108.64
19	A	1118	CLA	O2D-CGD-CBD	5.71	121.41	111.27
19	B	1208	CLA	O2A-C1-C2	5.70	123.62	108.64
19	1	613	CLA	CMD-C2D-C1D	5.70	134.76	124.71
19	2	605	CLA	CMD-C2D-C1D	5.70	134.76	124.71
19	A	1101	CLA	CMD-C2D-C1D	5.69	134.75	124.71
19	A	1102	CLA	CMD-C2D-C1D	5.69	134.73	124.71
19	B	1202	CLA	CMD-C2D-C1D	5.68	134.72	124.71
19	B	1217	CLA	O2D-CGD-CBD	5.67	121.35	111.27
19	A	1114	CLA	CMD-C2D-C1D	5.67	134.71	124.71
19	B	1236	CLA	O2D-CGD-CBD	5.67	121.33	111.27
19	4	605	CLA	O2A-C1-C2	5.66	123.50	108.64
19	B	1213	CLA	O2D-CGD-CBD	5.65	121.31	111.27
19	B	1231	CLA	O2D-CGD-CBD	5.65	121.30	111.27
19	K	1402	CLA	O2D-CGD-CBD	5.64	121.30	111.27
19	B	1236	CLA	O2A-C1-C2	5.64	123.45	108.64
19	B	1227	CLA	O2D-CGD-CBD	5.63	121.27	111.27
19	4	601	CLA	CMD-C2D-C1D	5.63	134.63	124.71
19	B	1234	CLA	O2D-CGD-CBD	5.62	121.26	111.27
22	B	4004	BCR	C34-C9-C10	-5.62	115.05	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	3	606	CLA	CMD-C2D-C1D	5.62	134.62	124.71
19	G	1601	CLA	O2A-C1-C2	5.61	123.38	108.64
19	A	1012	CLA	O2D-CGD-CBD	5.61	121.23	111.27
19	A	1121	CLA	O2A-C1-C2	5.61	123.38	108.64
19	A	1125	CLA	O2A-C1-C2	5.61	123.37	108.64
19	1	602	CLA	CMD-C2D-C1D	5.60	134.58	124.71
19	A	1106	CLA	O2D-CGD-CBD	5.60	121.22	111.27
19	1	606	CLA	O2A-C1-C2	5.60	123.35	108.64
19	4	601	CLA	O2A-C1-C2	5.59	123.34	108.64
31	4	505	C7Z	C7-C8-C9	-5.59	117.79	126.23
22	B	4004	BCR	C15-C14-C13	5.59	135.29	127.31
19	3	608	CLA	CMD-C2D-C1D	5.59	134.56	124.71
19	2	612	CLA	O2A-C1-C2	5.59	123.32	108.64
19	A	1133	CLA	O2D-CGD-CBD	5.58	121.19	111.27
19	B	1214	CLA	CMD-C2D-C1D	5.58	134.56	124.71
19	A	1135	CLA	O2D-CGD-CBD	5.58	121.18	111.27
28	2	501	LUT	C11-C10-C9	-5.57	119.36	127.31
19	2	604	CLA	O2D-CGD-CBD	5.57	121.17	111.27
19	B	1232	CLA	CMD-C2D-C1D	5.57	134.52	124.71
19	3	613	CLA	CMD-C2D-C1D	5.55	134.50	124.71
19	B	1209	CLA	O2D-CGD-CBD	5.55	121.12	111.27
19	A	1139	CLA	CMD-C2D-C1D	5.54	134.49	124.71
19	4	602	CLA	O2A-C1-C2	5.54	123.21	108.64
19	J	1901	CLA	CMD-C2D-C1D	5.54	134.48	124.71
19	A	1124	CLA	O2D-CGD-CBD	5.54	121.11	111.27
19	B	1211	CLA	CMD-C2D-C1D	5.53	134.46	124.71
31	4	505	C7Z	C40-C33-C32	-5.53	109.37	118.08
19	A	1140	CLA	CMD-C2D-C1D	5.52	134.45	124.71
19	2	606	CLA	CMD-C2D-C1D	5.51	134.43	124.71
19	B	1240	CLA	O2A-C1-C2	5.51	123.11	108.64
19	3	612	CLA	O2D-CGD-CBD	5.50	121.05	111.27
19	3	606	CLA	O2A-C1-C2	5.50	123.08	108.64
19	B	1212	CLA	O2A-C1-C2	5.50	123.08	108.64
19	B	1239	CLA	CMD-C2D-C1D	5.49	134.40	124.71
19	4	609	CLA	O2A-C1-C2	5.49	123.07	108.64
19	1	614	CLA	O2A-C1-C2	5.49	123.06	108.64
19	A	1109	CLA	CMD-C2D-C1D	5.48	134.38	124.71
19	3	614	CLA	CMD-C2D-C1D	5.48	134.37	124.71
18	A	1011	CL0	O2D-CGD-CBD	5.48	121.00	111.27
19	B	1209	CLA	CMD-C2D-C1D	5.47	134.35	124.71
19	4	603	CLA	O2A-C1-C2	5.47	123.01	108.64
19	3	605	CLA	CMD-C2D-C1D	5.47	134.35	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	G	1602	CLA	O2D-CGD-CBD	5.47	120.98	111.27
19	B	1230	CLA	O2A-C1-C2	5.46	122.98	108.64
19	K	1401	CLA	CMD-C2D-C1D	5.45	134.32	124.71
19	B	1235	CLA	CMD-C2D-C1D	5.45	134.31	124.71
19	L	1501	CLA	CMD-C2D-C1D	5.44	134.30	124.71
31	4	505	C7Z	C4-C5-C6	-5.44	108.72	120.85
19	A	1107	CLA	O2A-C1-C2	5.44	122.93	108.64
19	A	1112	CLA	CMD-C2D-C1D	5.44	134.29	124.71
19	3	610	CLA	CMD-C2D-C1D	5.44	134.29	124.71
19	A	1137	CLA	CMD-C2D-C1D	5.43	134.29	124.71
19	B	1236	CLA	CMD-C2D-C1D	5.43	134.28	124.71
19	A	1119	CLA	CMD-C2D-C1D	5.43	134.28	124.71
19	A	1130	CLA	O2A-C1-C2	5.43	122.90	108.64
19	1	605	CLA	O2D-CGD-CBD	5.42	120.91	111.27
19	4	609	CLA	O2D-CGD-CBD	5.42	120.91	111.27
19	3	601	CLA	CMD-C2D-C1D	5.42	134.27	124.71
19	B	1219	CLA	CMD-C2D-C1D	5.42	134.26	124.71
19	B	1225	CLA	CMD-C2D-C1D	5.42	134.26	124.71
19	L	1503	CLA	CMD-C2D-C1D	5.42	134.26	124.71
19	1	611	CLA	O2D-CGD-CBD	5.41	120.89	111.27
19	3	605	CLA	O2A-C1-C2	5.41	122.86	108.64
19	B	1239	CLA	O2A-C1-C2	5.41	122.85	108.64
18	A	1011	CL0	C2C-C1C-NC	5.41	115.04	109.97
19	G	1601	CLA	CMD-C2D-C1D	5.40	134.24	124.71
19	B	1223	CLA	CMD-C2D-C1D	5.40	134.23	124.71
19	A	1116	CLA	CMD-C2D-C1D	5.40	134.22	124.71
19	A	1136	CLA	O2A-C1-C2	5.40	122.81	108.64
19	1	605	CLA	CMD-C2D-C1D	5.39	134.21	124.71
19	B	1201	CLA	O2D-CGD-CBD	5.39	120.84	111.27
19	B	1219	CLA	O2A-C1-C2	5.38	122.78	108.64
19	B	1237	CLA	CMD-C2D-C1D	5.38	134.19	124.71
19	A	1124	CLA	CMD-C2D-C1D	5.38	134.19	124.71
19	B	1228	CLA	O2A-C1-C2	5.37	122.75	108.64
19	A	1132	CLA	O2A-C1-C2	5.37	122.75	108.64
19	A	1115	CLA	O2A-C1-C2	5.37	122.74	108.64
19	A	1136	CLA	CMD-C2D-C1D	5.36	134.15	124.71
19	B	1215	CLA	O2D-CGD-CBD	5.35	120.78	111.27
19	A	1140	CLA	O2D-CGD-CBD	5.34	120.76	111.27
19	3	617	CLA	CMD-C2D-C1D	5.34	134.13	124.71
19	A	1135	CLA	CMD-C2D-C1D	5.34	134.13	124.71
19	B	1211	CLA	O2D-CGD-CBD	5.33	120.74	111.27
19	A	1107	CLA	O2D-CGD-CBD	5.33	120.74	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	4	607	CLA	O2A-C1-C2	5.33	122.64	108.64
19	B	1229	CLA	O2D-CGD-CBD	5.33	120.73	111.27
19	G	1701	CLA	O2D-CGD-CBD	5.33	120.73	111.27
19	2	607	CLA	CMD-C2D-C1D	5.33	134.10	124.71
19	A	1102	CLA	O2A-C1-C2	5.33	122.63	108.64
19	A	1133	CLA	CMD-C2D-C1D	5.33	134.10	124.71
28	3	501	LUT	C21-C26-C25	5.32	120.95	111.42
19	1	614	CLA	CMD-C2D-C1D	5.32	134.09	124.71
19	A	1133	CLA	O2A-C1-C2	5.32	122.62	108.64
19	A	1105	CLA	CMD-C2D-C1D	5.32	134.09	124.71
19	B	1240	CLA	CMD-C2D-C1D	5.32	134.09	124.71
19	B	1235	CLA	O2D-CGD-CBD	5.32	120.71	111.27
19	2	601	CLA	CMD-C2D-C1D	5.31	134.08	124.71
19	4	612	CLA	O2A-C1-C2	5.31	122.59	108.64
19	A	1127	CLA	O2D-CGD-CBD	5.31	120.70	111.27
19	B	1220	CLA	CMD-C2D-C1D	5.31	134.07	124.71
19	B	1224	CLA	CMD-C2D-C1D	5.31	134.07	124.71
19	A	1104	CLA	CMD-C2D-C1D	5.31	134.07	124.71
19	B	1227	CLA	O2A-C1-C2	5.30	122.56	108.64
19	B	1217	CLA	CMD-C2D-C1D	5.30	134.05	124.71
19	B	1203	CLA	O2A-C1-C2	5.29	122.55	108.64
19	4	606	CLA	CMD-C2D-C1D	5.29	134.03	124.71
19	1	606	CLA	CMD-C2D-C1D	5.29	134.03	124.71
22	A	4017	BCR	C19-C18-C17	5.29	127.05	118.94
19	A	1012	CLA	C1-C2-C3	-5.28	116.90	126.04
19	J	1901	CLA	O2D-CGD-CBD	5.28	120.65	111.27
19	A	1103	CLA	O2D-CGD-CBD	5.28	120.65	111.27
19	2	605	CLA	O2D-CGD-CBD	5.28	120.65	111.27
19	2	608	CLA	O2D-CGD-CBD	5.27	120.63	111.27
19	A	1114	CLA	O2D-CGD-CBD	5.27	120.63	111.27
19	2	604	CLA	CMD-C2D-C1D	5.26	133.98	124.71
19	B	1239	CLA	O2D-CGD-CBD	5.26	120.61	111.27
19	K	1402	CLA	CMD-C2D-C1D	5.25	133.97	124.71
19	A	1122	CLA	O2A-C1-C2	5.25	122.44	108.64
19	2	607	CLA	O2D-CGD-CBD	5.25	120.59	111.27
19	B	1214	CLA	O2A-C1-C2	5.25	122.43	108.64
19	G	1701	CLA	CMD-C2D-C1D	5.25	133.96	124.71
19	A	1119	CLA	O2A-C1-C2	5.25	122.42	108.64
19	L	1502	CLA	O2A-C1-C2	5.24	122.42	108.64
19	1	611	CLA	CMD-C2D-C1D	5.24	133.94	124.71
18	A	1011	CL0	C1C-C2C-C3C	-5.24	101.45	106.96
19	A	1115	CLA	O2D-CGD-CBD	5.24	120.57	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	5001	LHG	O7-C7-C8	5.23	120.72	111.09
19	A	1134	CLA	CMD-C2D-C1D	5.23	133.93	124.71
28	1	501	LUT	C21-C26-C25	5.23	120.78	111.42
22	B	4006	BCR	C19-C18-C17	5.23	126.96	118.94
19	1	603	CLA	CMD-C2D-C1D	5.22	133.92	124.71
22	2	503	BCR	C39-C30-C29	-5.22	88.01	108.91
19	B	1213	CLA	CMD-C2D-C1D	5.22	133.92	124.71
19	1	604	CLA	O2D-CGD-CBD	5.22	120.55	111.27
19	A	1117	CLA	O2D-CGD-CBD	5.22	120.54	111.27
19	A	1134	CLA	O2D-CGD-CBD	5.22	120.54	111.27
19	2	605	CLA	O2A-C1-C2	5.21	122.32	108.64
19	B	1207	CLA	CMD-C2D-C1D	5.20	133.88	124.71
19	B	1221	CLA	O2A-C1-C2	5.20	122.31	108.64
19	B	1229	CLA	CMD-C2D-C1D	5.20	133.88	124.71
19	B	1201	CLA	O2A-C1-C2	5.20	122.30	108.64
30	2	502	XAT	O4-C5-C18	-5.20	108.83	115.06
19	A	1109	CLA	O2A-C1-C2	5.20	122.29	108.64
19	A	1136	CLA	O2D-CGD-CBD	5.20	120.50	111.27
19	B	1022	CLA	O2D-CGD-CBD	5.19	120.49	111.27
28	4	501	LUT	C21-C26-C25	5.19	120.71	111.42
19	B	1231	CLA	CMD-C2D-C1D	5.18	133.85	124.71
19	4	604	CLA	O2A-C1-C2	5.18	122.26	108.64
19	B	1232	CLA	O2D-CGD-CBD	5.18	120.48	111.27
19	A	1103	CLA	O2A-C1-C2	5.18	122.26	108.64
19	A	1113	CLA	O2D-CGD-CBD	5.18	120.47	111.27
19	2	601	CLA	O2A-C1-C2	5.18	122.25	108.64
19	L	1501	CLA	O2A-C1-C2	5.18	122.24	108.64
19	3	617	CLA	O2D-CGD-CBD	5.18	120.47	111.27
19	A	1106	CLA	CMD-C2D-C1D	5.18	133.84	124.71
22	2	503	BCR	C40-C30-C25	5.17	118.69	110.30
19	B	1238	CLA	O2D-CGD-CBD	5.17	120.45	111.27
19	A	1125	CLA	CMD-C2D-C1D	5.17	133.82	124.71
19	A	1110	CLA	O2A-C1-C2	5.16	122.19	108.64
19	4	605	CLA	CMD-C2D-C1D	5.15	133.78	124.71
19	2	606	CLA	O2A-C1-C2	5.15	122.16	108.64
19	A	1108	CLA	CMD-C2D-C1D	5.14	133.77	124.71
19	K	1404	CLA	CMD-C2D-C1D	5.14	133.77	124.71
19	2	602	CLA	CMD-C2D-C1D	5.14	133.76	124.71
19	G	1602	CLA	CMD-C2D-C1D	5.13	133.76	124.71
19	1	601	CLA	CMD-C2D-C1D	5.13	133.76	124.71
19	A	1138	CLA	CMD-C2D-C1D	5.13	133.76	124.71
19	A	1116	CLA	O2D-CGD-CBD	5.13	120.38	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	L	1502	CLA	CMD-C2D-C1D	5.13	133.75	124.71
19	B	1021	CLA	CMD-C2D-C1D	5.13	133.75	124.71
19	3	605	CLA	O2D-CGD-CBD	5.13	120.38	111.27
19	G	1603	CLA	O2D-CGD-CBD	5.12	120.37	111.27
19	3	601	CLA	O2D-CGD-CBD	5.12	120.37	111.27
19	3	603	CLA	CMD-C2D-C1D	5.12	133.74	124.71
19	A	1103	CLA	CMD-C2D-C1D	5.12	133.73	124.71
19	B	1228	CLA	CMD-C2D-C1D	5.11	133.72	124.71
19	A	1126	CLA	CMD-C2D-C1D	5.11	133.72	124.71
19	B	1226	CLA	O2A-C1-C2	5.11	122.07	108.64
19	1	613	CLA	O2D-CGD-CBD	5.11	120.35	111.27
22	K	4002	BCR	C33-C5-C6	-5.11	118.79	124.53
19	A	1115	CLA	CMD-C2D-C1D	5.10	133.71	124.71
19	G	1603	CLA	O2A-C1-C2	5.10	122.05	108.64
19	A	1123	CLA	CMD-C2D-C1D	5.10	133.71	124.71
19	A	1135	CLA	O2A-C1-C2	5.10	122.04	108.64
19	A	1118	CLA	CMD-C2D-C1D	5.09	133.69	124.71
19	A	1128	CLA	O2A-C1-C2	5.09	122.02	108.64
22	I	4018	BCR	C12-C13-C14	5.09	126.75	118.94
19	B	1230	CLA	CMD-C2D-C1D	5.09	133.68	124.71
19	A	1127	CLA	O2A-C1-C2	5.08	122.00	108.64
19	B	1215	CLA	CMD-C2D-C1D	5.08	133.67	124.71
19	A	1126	CLA	O2D-CGD-CBD	5.08	120.30	111.27
19	B	1022	CLA	O2A-C1-C2	5.08	121.98	108.64
19	B	1214	CLA	O2D-CGD-CBD	5.08	120.29	111.27
19	3	602	CLA	O2D-CGD-CBD	5.08	120.29	111.27
19	B	1237	CLA	O2D-CGD-CBD	5.08	120.29	111.27
19	A	1139	CLA	O2A-C1-C2	5.08	121.97	108.64
29	4	611	CHL	C2C-C3C-C4C	5.07	110.11	106.49
19	2	607	CLA	O2A-C1-C2	5.07	121.96	108.64
19	A	1104	CLA	O2A-C1-C2	5.07	121.96	108.64
19	4	606	CLA	O2A-C1-C2	5.07	121.95	108.64
19	F	1302	CLA	O2D-CGD-CBD	5.06	120.27	111.27
19	B	1207	CLA	O2A-C1-C2	5.06	121.95	108.64
22	3	503	BCR	C33-C5-C6	-5.06	118.84	124.53
19	1	607	CLA	O2D-CGD-CBD	5.06	120.27	111.27
28	1	502	LUT	C21-C26-C25	5.06	120.48	111.42
19	A	1107	CLA	CMD-C2D-C1D	5.06	133.63	124.71
19	4	609	CLA	CMD-C2D-C1D	5.05	133.62	124.71
19	3	606	CLA	C1-C2-C3	-5.05	118.58	126.75
19	L	1503	CLA	O2A-C1-C2	5.05	121.91	108.64
19	B	1216	CLA	CMD-C2D-C1D	5.05	133.61	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	1120	CLA	O2D-CGD-CBD	5.05	120.23	111.27
19	A	1141	CLA	O2A-C1-C2	5.04	121.88	108.64
19	4	603	CLA	O2D-CGD-CBD	5.04	120.22	111.27
19	4	617	CLA	CMD-C2D-C1D	5.03	133.59	124.71
18	A	1011	CL0	O2A-CGA-O1A	-5.03	110.90	123.59
19	B	1203	CLA	CMD-C2D-C1D	5.03	133.57	124.71
19	3	612	CLA	CMD-C2D-C1D	5.03	133.57	124.71
19	B	1206	CLA	O2D-CGD-CBD	5.02	120.20	111.27
19	B	1208	CLA	O2D-CGD-CBD	5.02	120.19	111.27
19	A	1122	CLA	O2D-CGD-CBD	5.02	120.19	111.27
19	A	1122	CLA	CMD-C2D-C1D	5.02	133.56	124.71
19	B	1234	CLA	O2A-C1-C2	5.01	121.80	108.64
19	2	612	CLA	O2D-CGD-CBD	5.00	120.15	111.27
19	4	608	CLA	CMD-C2D-C1D	4.99	133.51	124.71
19	B	1211	CLA	O2A-C1-C2	4.99	121.75	108.64
19	B	1227	CLA	CMD-C2D-C1D	4.99	133.50	124.71
19	A	1132	CLA	CMD-C2D-C1D	4.99	133.50	124.71
19	A	1131	CLA	O2A-C1-C2	4.98	121.74	108.64
28	3	502	LUT	C31-C30-C29	-4.98	120.20	127.31
19	B	1234	CLA	CMD-C2D-C1D	4.98	133.50	124.71
19	B	1224	CLA	O2D-CGD-CBD	4.98	120.12	111.27
19	2	612	CLA	CMD-C2D-C1D	4.98	133.48	124.71
19	A	1117	CLA	CMD-C2D-C1D	4.97	133.48	124.71
19	B	1212	CLA	CMD-C2D-C1D	4.97	133.46	124.71
19	B	1204	CLA	O2D-CGD-CBD	4.96	120.09	111.27
19	3	603	CLA	O2D-CGD-CBD	4.96	120.08	111.27
19	B	1225	CLA	O2A-C1-C2	4.96	121.67	108.64
19	4	612	CLA	CMD-C2D-C1D	4.96	133.45	124.71
19	B	1220	CLA	O2A-C1-C2	4.95	121.64	108.64
19	B	1226	CLA	CMD-C2D-C1D	4.95	133.43	124.71
28	2	501	LUT	C22-C23-C24	-4.94	106.12	111.74
19	B	1204	CLA	CMD-C2D-C1D	4.94	133.42	124.71
19	B	1216	CLA	O2D-CGD-CBD	4.94	120.04	111.27
19	4	608	CLA	O2D-CGD-CBD	4.93	120.04	111.27
19	K	1403	CLA	O2D-CGD-CBD	4.93	120.03	111.27
19	B	1022	CLA	CMD-C2D-C1D	4.93	133.41	124.71
19	B	1221	CLA	CMD-C2D-C1D	4.93	133.41	124.71
19	A	1131	CLA	O2D-CGD-CBD	4.93	120.03	111.27
19	A	1126	CLA	O2A-C1-C2	4.92	121.58	108.64
19	B	1223	CLA	O2A-C1-C2	4.92	121.58	108.64
19	A	1134	CLA	O2A-C1-C2	4.92	121.57	108.64
19	3	612	CLA	O2A-C1-C2	4.92	121.56	108.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	1201	CLA	CMD-C2D-C1D	4.92	133.38	124.71
19	A	1131	CLA	CMD-C2D-C1D	4.91	133.37	124.71
19	B	1023	CLA	O2A-C1-C2	4.91	121.55	108.64
28	2	501	LUT	C21-C26-C25	4.91	120.22	111.42
19	A	1129	CLA	CMD-C2D-C1D	4.91	133.37	124.71
19	3	608	CLA	O2D-CGD-CBD	4.91	119.99	111.27
18	A	1011	CL0	C1D-ND-C4D	-4.91	102.85	106.33
19	A	1116	CLA	O2A-C1-C2	4.90	121.52	108.64
19	3	602	CLA	CMD-C2D-C1D	4.89	133.34	124.71
19	A	1104	CLA	O2D-CGD-CBD	4.88	119.95	111.27
19	1	603	CLA	O2D-CGD-CBD	4.88	119.95	111.27
19	A	1124	CLA	O2A-C1-C2	4.88	121.45	108.64
22	B	4006	BCR	C33-C5-C6	-4.88	119.05	124.53
19	A	1119	CLA	O2D-CGD-CBD	4.85	119.89	111.27
19	1	601	CLA	O2D-CGD-CBD	4.85	119.89	111.27
19	A	1111	CLA	CMD-C2D-C1D	4.85	133.26	124.71
19	1	601	CLA	O2A-C1-C2	4.85	121.38	108.64
19	2	603	CLA	O2A-C1-C2	4.85	121.38	108.64
22	B	4006	BCR	C20-C19-C18	4.84	140.02	126.42
19	2	602	CLA	O2A-C1-C2	4.84	121.36	108.64
25	F	5002	LMG	O7-C10-C11	4.84	121.93	111.50
19	B	1219	CLA	O2D-CGD-CBD	4.83	119.85	111.27
19	2	608	CLA	O2A-C1-C2	4.83	121.33	108.64
19	B	1210	CLA	CMD-C2D-C1D	4.83	133.23	124.71
19	K	1401	CLA	O2D-CGD-CBD	4.83	119.85	111.27
19	B	1205	CLA	CMD-C2D-C1D	4.82	133.21	124.71
19	A	1109	CLA	O2D-CGD-CBD	4.82	119.83	111.27
19	B	1222	CLA	CMD-C2D-C1D	4.82	133.20	124.71
19	A	1123	CLA	O2A-C1-C2	4.82	121.29	108.64
19	A	1137	CLA	O2A-C1-C2	4.81	121.28	108.64
19	B	1210	CLA	O2A-C1-C2	4.81	121.28	108.64
28	1	501	LUT	C22-C23-C24	-4.80	106.28	111.74
19	A	1127	CLA	CMD-C2D-C1D	4.80	133.16	124.71
19	B	1206	CLA	CMD-C2D-C1D	4.79	133.16	124.71
19	B	1023	CLA	O2D-CGD-CBD	4.79	119.79	111.27
19	B	1228	CLA	O2D-CGD-CBD	4.79	119.78	111.27
31	4	505	C7Z	C20-C13-C12	-4.78	110.54	118.08
19	B	1203	CLA	O2D-CGD-CBD	4.78	119.76	111.27
19	A	1105	CLA	O2D-CGD-CBD	4.77	119.75	111.27
19	B	1021	CLA	O2D-CGD-CBD	4.77	119.75	111.27
19	J	1901	CLA	O2A-C1-C2	4.77	121.18	108.64
19	A	1013	CLA	O2D-CGD-CBD	4.77	119.74	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B	5005	DGD	O2G-C1B-C2B	4.76	121.76	111.50
19	A	1129	CLA	O2A-C1-C2	4.75	121.11	108.64
29	4	611	CHL	C3C-C4C-NC	-4.74	105.25	110.57
29	3	604	CHL	C1-O2A-CGA	4.74	128.87	116.44
19	3	602	CLA	O2A-C1-C2	4.72	121.03	108.64
22	G	4011	BCR	C19-C18-C17	4.71	126.18	118.94
19	A	1125	CLA	O2D-CGD-CBD	4.71	119.64	111.27
22	1	504	BCR	C15-C14-C13	-4.70	120.60	127.31
19	B	1235	CLA	O2A-C1-C2	4.70	120.99	108.64
22	I	4020	BCR	C23-C22-C21	4.70	126.16	118.94
19	L	1503	CLA	O2D-CGD-CBD	4.69	119.61	111.27
19	1	604	CLA	O2A-C1-C2	4.69	120.96	108.64
19	1	607	CLA	CMD-C2D-C1D	4.68	132.97	124.71
19	1	606	CLA	O2D-CGD-CBD	4.68	119.59	111.27
19	B	1206	CLA	O2A-C1-C2	4.68	120.93	108.64
19	A	1013	CLA	CMD-C2D-C1D	4.68	132.96	124.71
29	3	604	CHL	CHD-C1D-ND	-4.68	120.16	124.45
19	4	603	CLA	CMD-C2D-C1D	4.68	132.95	124.71
19	F	1302	CLA	O2A-C1-C2	4.67	120.91	108.64
19	A	1108	CLA	O2D-CGD-CBD	4.66	119.54	111.27
19	A	1130	CLA	O2D-CGD-CBD	4.65	119.53	111.27
22	B	4004	BCR	C35-C13-C14	-4.64	116.42	122.92
20	B	2002	PQN	C11-C12-C13	-4.63	119.08	126.79
19	4	605	CLA	O2D-CGD-CBD	4.63	119.50	111.27
19	L	1501	CLA	C1-C2-C3	-4.63	119.26	126.75
19	B	1222	CLA	C1-C2-C3	-4.63	118.04	126.04
19	4	607	CLA	O2D-CGD-CBD	4.63	119.49	111.27
19	B	1023	CLA	CMD-C2D-C1D	4.62	132.86	124.71
30	4	502	XAT	C38-C25-C24	4.62	119.47	114.28
28	J	4013	LUT	C11-C10-C9	-4.60	120.74	127.31
19	G	1603	CLA	CMD-C2D-C1D	4.60	132.82	124.71
19	A	1012	CLA	CMD-C2D-C1D	4.60	132.81	124.71
19	K	1402	CLA	O2A-C1-C2	4.59	120.71	108.64
19	G	1601	CLA	O2D-CGD-CBD	4.59	119.42	111.27
19	L	1503	CLA	C1-C2-C3	-4.59	119.33	126.75
19	3	603	CLA	O2A-C1-C2	4.58	120.67	108.64
19	B	1231	CLA	O2A-C1-C2	4.58	120.67	108.64
29	4	611	CHL	CHD-C1D-ND	-4.58	120.25	124.45
19	2	606	CLA	O2D-CGD-CBD	4.58	119.40	111.27
19	2	601	CLA	O2D-CGD-CBD	4.56	119.38	111.27
19	K	1404	CLA	O2D-CGD-CBD	4.56	119.37	111.27
19	3	610	CLA	O2D-CGD-CBD	4.55	119.36	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	1120	CLA	O2A-C1-C2	4.55	120.60	108.64
29	2	615	CHL	CHD-C1D-ND	-4.55	120.27	124.45
19	3	601	CLA	O2A-C1-C2	4.54	120.58	108.64
23	1	801	LHG	O7-C7-C8	4.54	121.28	111.50
19	A	1128	CLA	CMD-C2D-C1D	4.54	132.71	124.71
19	F	1301	CLA	O2D-CGD-CBD	4.54	119.33	111.27
19	2	603	CLA	O2D-CGD-CBD	4.54	119.33	111.27
19	4	606	CLA	O2D-CGD-CBD	4.53	119.32	111.27
19	B	1225	CLA	O2D-CGD-CBD	4.51	119.29	111.27
19	1	605	CLA	C1-C2-C3	-4.51	118.24	126.04
19	3	614	CLA	O2D-CGD-CBD	4.51	119.29	111.27
19	B	1237	CLA	O2A-C1-C2	4.51	120.50	108.64
22	A	4003	BCR	C36-C18-C17	-4.51	116.61	122.92
19	G	1701	CLA	O2A-C1-C2	4.50	120.47	108.64
19	3	617	CLA	O2A-C1-C2	4.50	120.47	108.64
25	G	5001	LMG	O7-C10-C11	4.50	121.20	111.50
19	B	1021	CLA	O2A-C1-C2	4.50	120.45	108.64
19	A	1105	CLA	O2A-C1-C2	4.49	120.43	108.64
28	3	502	LUT	C7-C8-C9	-4.49	119.45	126.23
19	1	611	CLA	O2A-C1-C2	4.48	120.41	108.64
19	A	1121	CLA	O2D-CGD-CBD	4.48	119.23	111.27
25	B	5007	LMG	O7-C10-C11	4.48	121.15	111.50
22	2	503	BCR	C33-C5-C6	-4.48	119.50	124.53
19	F	1301	CLA	CMD-C2D-C1D	4.48	132.60	124.71
22	I	4020	BCR	C19-C18-C17	4.48	125.81	118.94
22	K	4001	BCR	C19-C18-C17	4.46	125.79	118.94
28	4	501	LUT	C35-C34-C33	-4.46	120.94	127.31
28	2	501	LUT	C15-C14-C13	-4.46	120.95	127.31
19	3	610	CLA	O2A-C1-C2	4.46	120.35	108.64
19	4	601	CLA	O2D-CGD-CBD	4.46	119.19	111.27
28	2	501	LUT	C18-C5-C6	-4.45	119.53	124.53
22	G	4011	BCR	C15-C14-C13	-4.44	120.97	127.31
19	4	602	CLA	C1-C2-C3	-4.43	119.58	126.75
19	A	1138	CLA	O2D-CGD-CBD	4.42	119.13	111.27
19	B	1204	CLA	O2A-C1-C2	4.42	120.24	108.64
19	2	602	CLA	O2D-CGD-CBD	4.41	119.11	111.27
23	2	807	LHG	O7-C7-C8	4.41	121.01	111.50
19	4	607	CLA	CMD-C2D-C1D	4.40	132.47	124.71
22	A	4002	BCR	C23-C24-C25	-4.40	114.85	127.20
28	1	502	LUT	C21-C26-C27	4.39	118.25	112.70
19	3	613	CLA	O2D-CGD-CBD	4.36	119.02	111.27
27	G	5003	DGD	O2G-C1B-C2B	4.36	120.89	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	1	602	CLA	O2D-CGD-CBD	4.36	119.01	111.27
19	B	1224	CLA	O2A-C1-C2	4.35	120.07	108.64
19	A	1108	CLA	O2A-C1-C2	4.35	120.07	108.64
28	1	502	LUT	C7-C8-C9	-4.35	119.66	126.23
19	B	1220	CLA	O2D-CGD-CBD	4.35	118.99	111.27
19	3	606	CLA	O2D-CGD-CBD	4.34	118.99	111.27
19	A	1118	CLA	O2A-C1-C2	4.34	120.05	108.64
25	B	5004	LMG	O7-C10-C11	4.34	120.86	111.50
29	2	609	CHL	CHD-C1D-ND	-4.34	120.47	124.45
19	B	1021	CLA	C1-C2-C3	-4.32	118.57	126.04
19	B	1203	CLA	C1-C2-C3	-4.32	118.57	126.04
22	J	4012	BCR	C33-C5-C6	-4.31	119.69	124.53
23	B	5002	LHG	O7-C7-C8	4.31	120.78	111.50
19	L	1502	CLA	O2D-CGD-CBD	4.31	118.92	111.27
19	A	1101	CLA	C1-C2-C3	-4.30	118.60	126.04
18	A	1011	CL0	O2A-CGA-CBA	4.30	125.39	111.91
22	3	503	BCR	C23-C24-C25	-4.28	115.18	127.20
29	1	610	CHL	CHD-C1D-ND	-4.28	120.52	124.45
22	B	4005	BCR	C33-C5-C6	-4.27	119.73	124.53
19	A	1117	CLA	O2A-C1-C2	4.26	119.84	108.64
19	A	1139	CLA	O2D-CGD-CBD	4.26	118.84	111.27
22	I	4018	BCR	C3-C4-C5	-4.24	106.50	114.08
27	1	803	DGD	O2G-C1B-C2B	4.24	120.63	111.50
25	F	5004	LMG	O7-C10-C11	4.23	120.62	111.50
29	2	609	CHL	C3C-C4C-NC	-4.23	105.82	110.57
19	A	1134	CLA	C1-C2-C3	-4.21	118.77	126.04
23	2	801	LHG	O7-C7-C8	4.21	120.56	111.50
19	4	617	CLA	O2A-C1-C2	4.20	119.67	108.64
25	G	5002	LMG	O7-C10-C11	4.19	120.53	111.50
22	I	4020	BCR	C36-C18-C17	-4.18	117.07	122.92
25	1	802	LMG	O7-C10-C11	4.17	120.50	111.50
19	K	1403	CLA	O2A-C1-C2	4.17	123.60	109.49
28	1	502	LUT	C15-C14-C13	-4.17	121.36	127.31
19	B	1216	CLA	O2A-C1-C2	4.17	119.59	108.64
29	3	611	CHL	CHD-C1D-ND	-4.16	120.63	124.45
22	G	4011	BCR	C36-C18-C17	-4.16	117.10	122.92
27	4	802	DGD	O2G-C1B-C2B	4.16	120.46	111.50
28	3	501	LUT	C22-C23-C24	-4.15	107.01	111.74
19	3	608	CLA	CMA-C3A-C4A	4.15	122.93	111.77
27	J	5001	DGD	O2G-C1B-C2B	4.15	120.44	111.50
23	A	5001	LHG	O7-C7-C8	4.15	120.44	111.50
22	2	503	BCR	C28-C27-C26	-4.14	106.68	114.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	2	803	LMG	O7-C10-C11	4.13	120.41	111.50
28	4	501	LUT	C15-C14-C13	-4.12	121.42	127.31
19	B	1215	CLA	C1-C2-C3	-4.11	118.93	126.04
22	B	4004	BCR	C20-C19-C18	4.10	137.94	126.42
22	B	4004	BCR	C36-C18-C19	-4.10	111.62	118.08
27	3	803	DGD	O2G-C1B-C2B	4.09	120.32	111.50
27	F	5005	DGD	O2G-C1B-C2B	4.09	120.32	111.50
22	I	4020	BCR	C37-C22-C21	-4.07	117.22	122.92
19	A	1102	CLA	CHD-C1D-ND	-4.07	120.72	124.45
22	B	4004	BCR	C36-C18-C17	-4.06	117.23	122.92
19	A	1126	CLA	C1-C2-C3	-4.06	119.02	126.04
19	4	612	CLA	O2D-CGD-CBD	4.06	118.48	111.27
24	A	5004	LMT	C3'-C4'-C5'	-4.05	101.64	110.93
28	4	501	LUT	C22-C23-C24	-4.05	107.14	111.74
29	4	613	CHL	C1-O2A-CGA	4.04	127.05	116.44
19	4	604	CLA	CHD-C1D-ND	-4.03	120.75	124.45
19	A	1141	CLA	C1-C2-C3	-4.03	119.07	126.04
23	A	5002	LHG	O7-C7-C8	4.03	120.19	111.50
19	B	1205	CLA	O2A-C1-C2	4.03	119.22	108.64
28	3	501	LUT	C35-C34-C33	-4.02	121.57	127.31
19	F	1302	CLA	CHD-C1D-ND	-4.02	120.76	124.45
19	1	602	CLA	C2D-C1D-ND	4.01	113.06	110.10
30	2	502	XAT	C18-C5-C4	4.00	118.78	114.28
29	4	610	CHL	CHD-C1D-ND	-3.99	120.78	124.45
28	3	502	LUT	C21-C26-C25	3.99	118.57	111.42
22	A	4003	BCR	C19-C18-C17	3.99	125.07	118.94
19	B	1238	CLA	CHD-C1D-ND	-3.99	120.79	124.45
19	K	1403	CLA	CHD-C1D-ND	-3.98	120.80	124.45
22	K	4001	BCR	C36-C18-C17	-3.98	117.35	122.92
25	A	5006	LMG	O7-C10-C11	3.97	120.06	111.50
22	2	503	BCR	C38-C26-C25	-3.97	120.07	124.53
22	B	4006	BCR	C36-C18-C17	-3.97	117.36	122.92
29	2	613	CHL	CHD-C1D-ND	-3.97	120.81	124.45
31	4	505	C7Z	C32-C33-C34	-3.96	112.86	118.94
22	B	4006	BCR	C23-C22-C21	-3.96	112.87	118.94
29	2	615	CHL	C4D-CHA-C1A	3.96	126.06	121.25
30	4	502	XAT	C31-C30-C29	-3.95	121.67	127.31
22	A	4017	BCR	C36-C18-C17	-3.94	117.40	122.92
19	B	1208	CLA	CHD-C1D-ND	-3.94	120.83	124.45
30	2	502	XAT	C38-C25-C24	3.94	118.71	114.28
28	4	501	LUT	C18-C5-C6	-3.94	120.10	124.53
19	A	1118	CLA	C1-C2-C3	-3.94	120.38	126.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	1	601	CLA	C1-C2-C3	-3.93	119.25	126.04
19	A	1138	CLA	O2A-C1-C2	3.93	118.96	108.64
29	3	604	CHL	C4D-CHA-C1A	3.93	126.03	121.25
22	K	4001	BCR	C33-C5-C6	-3.92	120.12	124.53
19	2	606	CLA	C1-C2-C3	-3.92	120.41	126.75
30	2	502	XAT	C31-C30-C29	-3.92	121.72	127.31
18	A	1011	CL0	O2A-C1-C2	3.92	118.93	108.64
19	A	1136	CLA	C1-C2-C3	-3.91	119.28	126.04
28	1	501	LUT	C21-C26-C27	3.91	117.64	112.70
19	4	601	CLA	OBD-CAD-C3D	-3.90	119.14	128.52
19	B	1215	CLA	O2A-CGA-CBA	3.89	124.12	111.91
19	A	1127	CLA	C1-C2-C3	-3.89	119.31	126.04
22	B	4006	BCR	C23-C24-C25	-3.89	116.27	127.20
19	F	1302	CLA	C1-C2-C3	-3.89	119.31	126.04
28	3	501	LUT	C18-C5-C6	-3.88	120.17	124.53
25	2	802	LMG	O7-C10-C11	3.88	121.62	110.80
25	F	5003	LMG	O7-C10-C11	3.88	119.86	111.50
30	4	502	XAT	C18-C5-C4	3.87	118.64	114.28
22	G	4021	BCR	C33-C5-C6	-3.87	120.18	124.53
22	G	4011	BCR	C33-C5-C6	-3.87	120.19	124.53
25	2	804	LMG	O7-C10-C11	3.85	119.80	111.50
28	J	4013	LUT	C21-C26-C25	3.85	118.31	111.42
31	4	505	C7Z	C21-C26-C25	-3.85	117.19	122.61
19	4	609	CLA	C1-C2-C3	-3.85	120.53	126.75
19	A	1109	CLA	CHD-C1D-ND	-3.85	120.92	124.45
19	K	1402	CLA	C2C-C1C-NC	3.83	113.56	109.97
19	B	1215	CLA	CAA-C2A-C1A	-3.83	99.41	111.97
19	A	1102	CLA	C1-C2-C3	-3.82	119.43	126.04
19	1	606	CLA	C1-C2-C3	-3.82	120.57	126.75
19	G	1603	CLA	C1-C2-C3	-3.81	119.45	126.04
22	2	503	BCR	C40-C30-C39	3.81	120.21	108.53
19	G	1701	CLA	C2C-C1C-NC	3.80	113.53	109.97
19	2	603	CLA	C1-C2-C3	-3.80	119.47	126.04
22	L	4020	BCR	C33-C5-C6	-3.80	120.26	124.53
19	A	1121	CLA	C1-C2-C3	-3.80	119.47	126.04
19	2	605	CLA	C1-C2-C3	-3.77	119.52	126.04
25	3	802	LMG	O7-C10-C11	3.77	119.63	111.50
29	1	609	CHL	CHD-C1D-ND	-3.77	120.99	124.45
22	A	4003	BCR	C33-C5-C6	-3.77	120.30	124.53
28	1	501	LUT	C18-C5-C6	-3.76	120.30	124.53
29	2	610	CHL	C3C-C4C-NC	-3.75	106.36	110.57
19	B	1218	CLA	CHD-C1D-ND	-3.75	121.01	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	J	4012	BCR	C19-C18-C17	3.75	124.69	118.94
19	4	601	CLA	CHD-C1D-ND	-3.74	121.01	124.45
19	A	1111	CLA	O2D-CGD-O1D	-3.74	116.52	123.84
19	2	606	CLA	CAA-C2A-C3A	-3.74	102.53	112.78
19	A	1131	CLA	C1-C2-C3	-3.74	119.58	126.04
19	B	1202	CLA	CHD-C1D-ND	-3.73	121.03	124.45
19	A	1132	CLA	C1-C2-C3	-3.73	119.59	126.04
19	B	1209	CLA	CHD-C1D-ND	-3.73	121.03	124.45
29	3	607	CHL	CHD-C1D-ND	-3.73	121.03	124.45
27	F	5005	DGD	O5D-C1E-C2E	3.73	114.12	108.30
30	2	502	XAT	C17-C1-C16	3.72	112.86	107.37
29	2	610	CHL	CHD-C1D-ND	-3.72	121.04	124.45
27	4	801	DGD	O2G-C1B-C2B	3.72	119.51	111.50
19	B	1206	CLA	C1-C2-C3	-3.71	119.63	126.04
19	A	1117	CLA	CHD-C1D-ND	-3.71	121.05	124.45
19	B	1022	CLA	CHD-C1D-ND	-3.71	121.05	124.45
18	A	1011	CL0	C3D-C2D-C1D	-3.70	100.78	105.83
19	A	1119	CLA	CHD-C1D-ND	-3.70	121.05	124.45
19	B	1226	CLA	C1-C2-C3	-3.70	119.64	126.04
22	1	504	BCR	C38-C26-C25	-3.69	120.38	124.53
22	I	4018	BCR	C35-C13-C14	-3.69	117.75	122.92
25	F	5001	LMG	O7-C10-C11	3.69	119.44	111.50
29	3	611	CHL	C3C-C4C-NC	-3.68	106.44	110.57
19	B	1215	CLA	CHD-C1D-ND	-3.68	121.08	124.45
19	A	1113	CLA	CHD-C1D-ND	-3.67	121.08	124.45
22	A	4017	BCR	C33-C5-C6	-3.67	120.41	124.53
19	4	605	CLA	C2C-C1C-NC	3.67	113.41	109.97
22	3	506	BCR	C33-C5-C6	-3.67	120.41	124.53
19	A	1140	CLA	CHD-C1D-ND	-3.66	121.09	124.45
19	J	1901	CLA	C1-C2-C3	-3.66	120.83	126.75
22	F	4014	BCR	C23-C22-C21	-3.66	113.32	118.94
28	3	502	LUT	C18-C5-C6	-3.66	120.42	124.53
22	B	4006	BCR	C27-C26-C25	-3.66	117.42	122.73
25	B	5003	LMG	O7-C10-C11	3.65	119.36	111.50
19	B	1226	CLA	CHD-C1D-ND	-3.64	121.11	124.45
22	1	504	BCR	C19-C18-C17	3.63	124.51	118.94
19	A	1129	CLA	O2D-CGD-O1D	-3.63	116.75	123.84
24	G	5004	LMT	C3'-C4'-C5'	-3.63	102.61	110.93
19	A	1109	CLA	C2D-C1D-ND	3.62	112.78	110.10
19	B	1240	CLA	C2C-C1C-NC	3.62	113.36	109.97
19	B	1211	CLA	CHD-C1D-ND	-3.62	121.13	124.45
29	4	613	CHL	CHD-C1D-ND	-3.62	121.13	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	G	5006	LMG	O7-C10-C11	3.62	120.88	110.80
22	1	504	BCR	C36-C18-C17	-3.61	117.86	122.92
19	B	1236	CLA	CHD-C1D-ND	-3.61	121.14	124.45
19	B	1218	CLA	O2A-C1-C2	3.60	118.11	108.64
29	1	610	CHL	C3C-C4C-NC	-3.60	106.53	110.57
31	4	505	C7Z	C27-C26-C25	-3.60	112.73	121.46
19	B	1208	CLA	C1-C2-C3	-3.60	119.81	126.04
19	3	613	CLA	C2C-C1C-NC	3.60	113.34	109.97
19	A	1112	CLA	CHD-C1D-ND	-3.59	121.16	124.45
22	A	4002	BCR	C36-C18-C17	-3.58	117.91	122.92
19	A	1120	CLA	CHD-C1D-ND	-3.58	121.17	124.45
29	2	611	CHL	CHD-C1D-ND	-3.58	121.17	124.45
19	A	1104	CLA	CAA-C2A-C3A	-3.57	102.99	112.78
19	4	608	CLA	CHD-C1D-ND	-3.57	121.17	124.45
19	A	1110	CLA	O2D-CGD-CBD	3.57	117.61	111.27
30	4	502	XAT	O4-C5-C18	-3.57	110.78	115.06
19	A	1111	CLA	CHD-C1D-ND	-3.57	121.18	124.45
19	A	1119	CLA	C1-C2-C3	-3.56	119.88	126.04
19	B	1239	CLA	CHD-C1D-ND	-3.56	121.18	124.45
22	1	504	BCR	C33-C5-C4	3.56	120.45	113.62
29	2	615	CHL	C1-O2A-CGA	3.56	125.78	116.44
19	A	1135	CLA	C1-C2-C3	-3.56	119.89	126.04
29	4	610	CHL	C3C-C4C-NC	-3.56	106.58	110.57
29	2	609	CHL	C2C-C3C-C4C	3.55	109.02	106.49
22	B	4006	BCR	C30-C25-C26	-3.55	117.61	122.61
19	A	1125	CLA	CHD-C1D-ND	-3.55	121.19	124.45
19	A	1123	CLA	C2C-C1C-NC	3.54	113.29	109.97
19	L	1501	CLA	CHD-C1D-ND	-3.54	121.20	124.45
28	J	4013	LUT	C2-C3-C4	-3.54	105.46	110.30
22	B	4005	BCR	C23-C24-C25	-3.54	117.27	127.20
19	A	1105	CLA	C1-C2-C3	-3.53	119.93	126.04
22	A	4002	BCR	C19-C18-C17	3.53	124.36	118.94
19	B	1225	CLA	CHD-C1D-ND	-3.53	121.21	124.45
19	G	1601	CLA	C1-C2-C3	-3.52	119.95	126.04
19	B	1222	CLA	CHD-C1D-ND	-3.52	121.22	124.45
29	1	610	CHL	C4D-CHA-C1A	3.52	125.53	121.25
19	A	1012	CLA	CHD-C1D-ND	-3.51	121.22	124.45
22	B	4009	BCR	C28-C27-C26	-3.51	107.80	114.08
29	4	615	CHL	CMA-C3A-C4A	3.51	121.20	111.77
19	A	1140	CLA	O2A-C1-C2	3.51	117.85	108.64
19	L	1502	CLA	C1-C2-C3	-3.50	119.98	126.04
25	G	5006	LMG	O8-C28-C29	3.50	120.55	111.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	2	608	CLA	CHD-C1D-ND	-3.50	121.24	124.45
19	A	1112	CLA	O2A-C1-C2	3.49	117.82	108.64
19	A	1128	CLA	CHD-C1D-ND	-3.49	121.25	124.45
30	4	502	XAT	C7-C8-C9	-3.49	120.11	125.53
28	4	501	LUT	C31-C30-C29	-3.49	122.33	127.31
19	B	1207	CLA	C1-C2-C3	-3.49	120.01	126.04
19	3	608	CLA	O2A-C1-C2	3.48	121.27	109.49
19	A	1125	CLA	C1-C2-C3	-3.48	120.02	126.04
19	B	1217	CLA	CHD-C1D-ND	-3.48	121.26	124.45
19	B	1210	CLA	O2D-CGD-O1D	-3.47	117.04	123.84
22	B	4010	BCR	C23-C24-C25	-3.47	117.45	127.20
19	A	1138	CLA	CHD-C1D-ND	-3.47	121.27	124.45
22	A	4002	BCR	C27-C26-C25	-3.47	117.69	122.73
19	1	604	CLA	CHD-C1D-ND	-3.46	121.27	124.45
19	B	1219	CLA	CHD-C1D-ND	-3.46	121.28	124.45
19	B	1229	CLA	O2A-C1-C2	3.46	117.72	108.64
19	A	1128	CLA	O2D-CGD-O1D	-3.45	117.08	123.84
20	A	2001	PQN	C14-C13-C15	3.45	121.08	115.27
22	A	4007	BCR	C27-C26-C25	-3.45	117.72	122.73
22	A	4008	BCR	C15-C14-C13	3.45	132.24	127.31
19	3	603	CLA	C1-C2-C3	-3.45	120.07	126.04
19	B	1213	CLA	CHD-C1D-ND	-3.45	121.28	124.45
19	A	1126	CLA	CHD-C1D-ND	-3.45	121.28	124.45
19	1	611	CLA	C1-C2-C3	-3.45	120.08	126.04
28	J	4013	LUT	C15-C14-C13	-3.45	122.39	127.31
19	1	608	CLA	O2D-CGD-O1D	-3.45	117.10	123.84
19	2	604	CLA	CHD-C1D-ND	-3.44	121.29	124.45
19	3	605	CLA	C1-C2-C3	-3.44	120.09	126.04
29	3	611	CHL	C2C-C3C-C4C	3.44	108.94	106.49
19	4	602	CLA	CHD-C1D-ND	-3.43	121.30	124.45
19	1	603	CLA	CAA-C2A-C3A	-3.43	103.38	112.78
19	G	1601	CLA	C2C-C1C-NC	3.43	113.19	109.97
19	B	1224	CLA	CHD-C1D-ND	-3.43	121.30	124.45
19	B	1231	CLA	CHD-C1D-ND	-3.43	121.31	124.45
19	J	1901	CLA	CHD-C1D-ND	-3.42	121.31	124.45
22	A	4007	BCR	C33-C5-C6	-3.42	120.69	124.53
19	A	1129	CLA	C2C-C1C-NC	3.42	113.18	109.97
19	A	1105	CLA	C2C-C1C-NC	3.42	113.18	109.97
19	A	1123	CLA	C1-C2-C3	-3.42	120.13	126.04
22	A	4002	BCR	C33-C5-C6	-3.42	120.69	124.53
19	A	1133	CLA	CHD-C1D-ND	-3.42	121.31	124.45
29	1	612	CHL	C3C-C4C-NC	-3.41	106.75	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	2	612	CLA	C2C-C1C-NC	3.41	113.17	109.97
19	A	1106	CLA	CHD-C1D-ND	-3.41	121.32	124.45
22	L	4020	BCR	C36-C18-C17	-3.41	118.15	122.92
19	A	1134	CLA	CHD-C1D-ND	-3.41	121.32	124.45
19	A	1115	CLA	C1-C2-C3	-3.40	120.16	126.04
19	A	1123	CLA	O2D-CGD-O1D	-3.40	117.19	123.84
19	A	1139	CLA	CHD-C1D-ND	-3.40	121.33	124.45
19	A	1130	CLA	CHD-C1D-ND	-3.40	121.33	124.45
19	2	604	CLA	C1-C2-C3	-3.39	120.17	126.04
22	A	4011	BCR	C12-C13-C14	-3.39	113.73	118.94
22	F	4014	BCR	C23-C24-C25	-3.39	117.68	127.20
25	2	802	LMG	O8-C28-C29	3.39	120.26	111.38
19	A	1124	CLA	CHD-C1D-ND	-3.39	121.34	124.45
19	A	1118	CLA	C2C-C1C-NC	3.39	113.14	109.97
19	A	1122	CLA	CHD-C1D-ND	-3.39	121.34	124.45
19	1	614	CLA	C1-C2-C3	-3.38	120.19	126.04
19	A	1101	CLA	C2C-C1C-NC	3.38	113.14	109.97
19	B	1206	CLA	C2C-C1C-NC	3.38	113.14	109.97
19	B	1213	CLA	C2C-C1C-NC	3.38	113.14	109.97
19	A	1013	CLA	CHD-C1D-ND	-3.37	121.35	124.45
19	B	1237	CLA	CHD-C1D-ND	-3.37	121.35	124.45
19	A	1012	CLA	C2C-C1C-NC	3.37	113.13	109.97
22	I	4020	BCR	C33-C5-C6	-3.37	120.74	124.53
19	4	612	CLA	C1-C2-C3	-3.37	120.21	126.04
28	2	501	LUT	C7-C8-C9	-3.37	121.14	126.23
22	K	4001	BCR	C37-C22-C21	-3.37	118.21	122.92
22	J	4012	BCR	C36-C18-C17	-3.37	118.21	122.92
19	4	602	CLA	C2C-C1C-NC	3.36	113.12	109.97
29	4	615	CHL	CHD-C1D-ND	-3.36	121.36	124.45
19	K	1403	CLA	CMD-C2D-C3D	-3.36	119.88	127.61
19	3	617	CLA	CHD-C1D-ND	-3.36	121.36	124.45
19	1	605	CLA	C2C-C1C-NC	3.36	113.12	109.97
29	4	611	CHL	C4D-CHA-C1A	3.36	125.34	121.25
22	G	4021	BCR	C36-C18-C17	-3.36	118.22	122.92
30	2	502	XAT	C15-C14-C13	-3.35	122.53	127.31
22	1	504	BCR	C4-C5-C6	-3.35	117.86	122.73
19	A	1110	CLA	CHD-C1D-ND	-3.35	121.38	124.45
28	4	501	LUT	C21-C26-C27	3.34	116.93	112.70
19	A	1128	CLA	C1-C2-C3	-3.34	120.26	126.04
29	2	615	CHL	C1B-CHB-C4A	-3.34	123.51	130.12
22	A	4011	BCR	C23-C24-C25	-3.33	117.84	127.20
19	A	1131	CLA	C2C-C1C-NC	3.33	113.09	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	4	601	CLA	C1-C2-C3	-3.33	120.29	126.04
22	1	503	BCR	C33-C5-C6	-3.33	120.79	124.53
22	3	503	BCR	C35-C13-C12	3.33	123.32	118.08
29	1	610	CHL	CMA-C3A-C4A	3.32	120.71	111.77
19	A	1114	CLA	CMA-C3A-C4A	3.32	120.71	111.77
29	4	610	CHL	C2C-C3C-C4C	3.32	108.86	106.49
27	4	801	DGD	C3G-O3G-C1D	-3.32	107.25	113.74
19	3	601	CLA	CHD-C1D-ND	-3.32	121.41	124.45
19	G	1603	CLA	C2D-C1D-ND	3.32	112.55	110.10
19	A	1121	CLA	CHD-C1D-ND	-3.31	121.41	124.45
19	B	1214	CLA	C2C-C1C-NC	3.31	113.07	109.97
22	A	4007	BCR	C30-C25-C26	-3.31	117.95	122.61
19	B	1206	CLA	CHD-C1D-ND	-3.31	121.41	124.45
22	A	4007	BCR	C19-C18-C17	3.31	124.02	118.94
22	B	4010	BCR	C33-C5-C6	-3.31	120.81	124.53
19	1	603	CLA	CHD-C1D-ND	-3.31	121.41	124.45
22	G	4011	BCR	C23-C22-C21	3.31	124.02	118.94
19	A	1136	CLA	C2D-C1D-ND	3.31	112.54	110.10
19	L	1503	CLA	C2C-C1C-NC	3.30	113.07	109.97
19	A	1013	CLA	O2A-C1-C2	3.30	117.32	108.64
24	G	5004	LMT	C1'-O5'-C5'	-3.30	107.20	113.69
22	2	503	BCR	C19-C18-C17	3.30	124.01	118.94
22	2	503	BCR	C30-C25-C26	3.30	127.26	122.61
19	A	1114	CLA	C2C-C1C-NC	3.30	113.06	109.97
19	2	606	CLA	C2C-C1C-NC	3.30	113.06	109.97
19	G	1603	CLA	C2C-C1C-NC	3.30	113.06	109.97
19	4	606	CLA	C1-C2-C3	-3.29	121.43	126.75
30	2	502	XAT	C5-C4-C3	-3.29	106.24	112.75
19	B	1207	CLA	O2D-CGD-O1D	-3.29	117.41	123.84
19	A	1136	CLA	CHD-C1D-ND	-3.27	121.45	124.45
19	3	612	CLA	CHD-C1D-ND	-3.27	121.45	124.45
19	B	1229	CLA	O2A-CGA-CBA	3.27	122.17	111.91
19	B	1204	CLA	CHD-C1D-ND	-3.27	121.45	124.45
22	A	4002	BCR	C35-C13-C12	3.27	123.23	118.08
19	F	1301	CLA	C2C-C1C-NC	3.27	113.03	109.97
19	A	1134	CLA	C2C-C1C-NC	3.27	113.03	109.97
29	1	609	CHL	C1-O2A-CGA	3.27	125.01	116.44
19	A	1118	CLA	CHD-C1D-ND	-3.26	121.45	124.45
19	A	1103	CLA	CHD-C1D-ND	-3.26	121.45	124.45
19	K	1403	CLA	CMA-C3A-C4A	3.26	120.54	111.77
19	B	1230	CLA	C1-C2-C3	-3.26	120.40	126.04
19	4	604	CLA	O2D-CGD-O1D	-3.26	117.46	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	1	609	CHL	CMA-C3A-C4A	3.26	120.53	111.77
19	B	1226	CLA	C2C-C1C-NC	3.26	113.02	109.97
19	A	1136	CLA	C1D-ND-C4D	-3.26	104.02	106.33
19	B	1021	CLA	CHD-C1D-ND	-3.26	121.46	124.45
19	B	1228	CLA	C1-C2-C3	-3.25	120.42	126.04
19	1	603	CLA	C1-C2-C3	-3.24	120.44	126.04
19	B	1204	CLA	C2C-C1C-NC	3.24	113.01	109.97
19	4	609	CLA	C2C-C1C-NC	3.23	113.00	109.97
19	B	1232	CLA	CHD-C1D-ND	-3.23	121.48	124.45
19	B	1222	CLA	O2D-CGD-O1D	-3.23	117.52	123.84
18	A	1011	CL0	CMB-C2B-C3B	3.23	130.72	124.68
19	L	1502	CLA	C2D-C1D-ND	3.23	112.48	110.10
19	A	1141	CLA	CHD-C1D-ND	-3.23	121.49	124.45
29	2	609	CHL	C1-O2A-CGA	3.22	124.90	116.44
19	2	601	CLA	CHD-C1D-ND	-3.22	121.49	124.45
19	3	610	CLA	C2C-C1C-NC	3.22	112.99	109.97
25	3	802	LMG	O8-C28-C29	3.22	122.01	111.91
19	4	617	CLA	CHD-C1D-ND	-3.22	121.50	124.45
22	A	4003	BCR	C28-C27-C26	-3.22	108.33	114.08
19	A	1104	CLA	C2C-C1C-NC	3.22	112.98	109.97
19	A	1124	CLA	C1-C2-C3	-3.21	120.48	126.04
19	1	606	CLA	C2C-C1C-NC	3.21	112.98	109.97
19	B	1228	CLA	CHD-C1D-ND	-3.21	121.50	124.45
19	B	1230	CLA	C2C-C1C-NC	3.20	112.97	109.97
19	3	606	CLA	C2C-C1C-NC	3.20	112.97	109.97
19	A	1129	CLA	C1-C2-C3	-3.20	120.51	126.04
19	B	1221	CLA	C1-O2A-CGA	3.20	124.84	116.44
19	A	1110	CLA	C1-C2-C3	-3.20	120.51	126.04
19	B	1219	CLA	CMB-C2B-C3B	3.20	130.66	124.68
22	A	4007	BCR	C23-C24-C25	-3.19	118.23	127.20
19	A	1125	CLA	C2D-C1D-ND	3.19	112.46	110.10
19	2	606	CLA	CHD-C1D-ND	-3.19	121.52	124.45
19	1	613	CLA	CHD-C1D-ND	-3.19	121.52	124.45
19	1	607	CLA	C2C-C1C-NC	3.19	112.96	109.97
19	3	605	CLA	C2C-C1C-NC	3.19	112.96	109.97
19	2	603	CLA	CHD-C1D-ND	-3.18	121.53	124.45
22	3	506	BCR	C36-C18-C17	-3.18	118.47	122.92
19	A	1137	CLA	O2D-CGD-O1D	-3.18	117.62	123.84
28	3	501	LUT	C7-C8-C9	-3.18	121.43	126.23
19	B	1223	CLA	CHD-C1D-ND	-3.18	121.53	124.45
19	L	1502	CLA	CHD-C1D-ND	-3.18	121.53	124.45
19	B	1209	CLA	O2D-CGD-O1D	-3.18	117.63	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	1	606	CLA	CHD-C1D-ND	-3.17	121.54	124.45
19	A	1141	CLA	C2C-C1C-NC	3.17	112.94	109.97
19	B	1021	CLA	C2C-C1C-NC	3.17	112.94	109.97
19	A	1129	CLA	CHD-C1D-ND	-3.17	121.54	124.45
19	G	1603	CLA	CMA-C3A-C4A	3.17	120.29	111.77
28	J	4013	LUT	C31-C30-C29	-3.17	122.79	127.31
28	1	502	LUT	C11-C10-C9	-3.17	122.79	127.31
25	G	5001	LMG	O8-C28-C29	3.16	121.84	111.91
19	1	611	CLA	CHD-C1D-ND	-3.16	121.55	124.45
22	B	4010	BCR	C23-C22-C21	-3.16	114.09	118.94
19	K	1403	CLA	C2C-C1C-NC	3.16	112.93	109.97
19	B	1230	CLA	CHD-C1D-ND	-3.16	121.55	124.45
22	I	4018	BCR	C31-C1-C6	-3.16	105.17	110.30
19	B	1223	CLA	C1-C2-C3	-3.16	120.58	126.04
22	I	4018	BCR	C33-C5-C6	-3.16	120.98	124.53
31	4	505	C7Z	C38-C25-C24	-3.15	108.51	114.36
19	A	1103	CLA	C1-C2-C3	-3.15	120.59	126.04
19	2	604	CLA	CMB-C2B-C3B	3.15	130.57	124.68
19	4	604	CLA	C1-C2-C3	-3.15	120.60	126.04
29	3	604	CHL	C3C-C4C-NC	-3.15	107.04	110.57
19	A	1119	CLA	CMB-C2B-C3B	3.14	130.56	124.68
19	A	1139	CLA	CMA-C3A-C4A	3.14	120.22	111.77
29	4	611	CHL	CMA-C3A-C4A	3.14	120.22	111.77
19	4	612	CLA	CHD-C1D-ND	-3.14	121.57	124.45
19	A	1135	CLA	C2D-C1D-ND	3.14	112.42	110.10
19	A	1107	CLA	CHD-C1D-ND	-3.14	121.57	124.45
19	B	1210	CLA	CHD-C1D-ND	-3.14	121.57	124.45
19	B	1220	CLA	CHD-C1D-ND	-3.14	121.57	124.45
19	B	1206	CLA	C1C-C2C-C3C	-3.13	103.66	106.96
29	1	612	CHL	C1-O2A-CGA	3.13	124.67	116.44
19	A	1137	CLA	CHD-C1D-ND	-3.13	121.58	124.45
22	I	4018	BCR	C23-C24-C25	-3.13	118.41	127.20
19	A	1107	CLA	C2C-C1C-NC	3.13	112.90	109.97
19	B	1228	CLA	C2C-C1C-NC	3.13	112.90	109.97
19	1	608	CLA	C2C-C1C-NC	3.13	112.90	109.97
19	B	1214	CLA	O2A-CGA-CBA	3.13	121.73	111.91
29	3	607	CHL	C4D-CHA-C1A	3.13	125.06	121.25
29	1	610	CHL	C1B-CHB-C4A	-3.13	123.92	130.12
19	1	608	CLA	CHD-C1D-ND	-3.13	121.58	124.45
19	3	603	CLA	C2C-C1C-NC	3.13	112.90	109.97
19	B	1240	CLA	CHD-C1D-ND	-3.13	121.58	124.45
19	3	601	CLA	CMB-C2B-C3B	3.12	130.52	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	4017	BCR	C34-C9-C10	-3.12	118.55	122.92
19	3	617	CLA	C2D-C1D-ND	3.12	112.41	110.10
29	3	607	CHL	CMA-C3A-C4A	3.12	120.17	111.77
19	B	1224	CLA	C2C-C1C-NC	3.12	112.90	109.97
19	B	1212	CLA	CHD-C1D-ND	-3.12	121.58	124.45
19	B	1226	CLA	O2D-CGD-O1D	-3.12	117.74	123.84
19	B	1221	CLA	O2D-CGD-O1D	-3.12	117.74	123.84
19	B	1239	CLA	C1-C2-C3	-3.12	120.65	126.04
19	B	1205	CLA	CHD-C1D-ND	-3.12	121.59	124.45
29	1	609	CHL	C3C-C4C-NC	-3.12	107.07	110.57
19	A	1120	CLA	C2C-C1C-NC	3.12	112.89	109.97
19	B	1227	CLA	C2C-C1C-NC	3.11	112.89	109.97
19	A	1106	CLA	C1-C2-C3	-3.11	120.66	126.04
19	L	1503	CLA	CHD-C1D-ND	-3.11	121.59	124.45
19	A	1101	CLA	CHD-C1D-ND	-3.11	121.59	124.45
25	F	5001	LMG	O8-C28-C29	3.11	119.54	111.38
19	3	608	CLA	C2C-C1C-NC	3.11	112.89	109.97
19	B	1216	CLA	CMB-C2B-C3B	3.11	130.50	124.68
19	B	1239	CLA	C2D-C1D-ND	3.11	112.39	110.10
19	B	1218	CLA	O2D-CGD-O1D	-3.11	117.76	123.84
19	A	1115	CLA	C2C-C1C-NC	3.11	112.88	109.97
19	3	606	CLA	CHD-C1D-ND	-3.10	121.60	124.45
22	A	4003	BCR	C12-C13-C14	-3.10	114.18	118.94
19	4	608	CLA	CMA-C3A-C4A	3.10	120.11	111.77
22	1	503	BCR	C36-C18-C17	-3.10	118.58	122.92
22	A	4008	BCR	C36-C18-C17	-3.10	118.58	122.92
19	K	1401	CLA	C2D-C1D-ND	3.10	112.39	110.10
19	1	601	CLA	CHD-C1D-ND	-3.09	121.61	124.45
19	A	1117	CLA	C2C-C1C-NC	3.09	112.87	109.97
28	1	502	LUT	C18-C5-C6	-3.09	121.05	124.53
19	4	606	CLA	C2C-C1C-NC	3.09	112.87	109.97
19	A	1137	CLA	C1-C2-C3	-3.09	120.69	126.04
19	2	605	CLA	CHD-C1D-ND	-3.09	121.61	124.45
31	4	505	C7Z	C21-C26-C27	-3.09	107.03	115.78
29	4	611	CHL	C1-C2-C3	-3.09	121.75	126.75
22	A	4008	BCR	C19-C18-C17	3.09	123.68	118.94
19	3	602	CLA	C2D-C1D-ND	3.09	112.38	110.10
19	K	1402	CLA	CMA-C3A-C4A	3.08	120.06	111.77
28	3	502	LUT	C2-C3-C4	-3.08	106.08	110.30
19	A	1108	CLA	C2D-C1D-ND	3.08	112.38	110.10
22	A	4008	BCR	C38-C26-C25	-3.08	121.07	124.53
19	A	1101	CLA	C1C-C2C-C3C	-3.08	103.72	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	J	4012	BCR	C33-C5-C4	3.08	119.53	113.62
19	B	1211	CLA	CMB-C2B-C3B	3.07	130.43	124.68
19	4	609	CLA	C2D-C1D-ND	3.07	112.37	110.10
19	B	1219	CLA	C2C-C1C-NC	3.07	112.85	109.97
19	A	1127	CLA	C2C-C1C-NC	3.07	112.85	109.97
30	2	502	XAT	C40-C33-C34	-3.07	118.63	122.92
19	L	1501	CLA	CMB-C2B-C3B	3.07	130.42	124.68
22	A	4002	BCR	C12-C13-C14	-3.07	114.24	118.94
22	L	4020	BCR	C27-C26-C25	-3.06	118.29	122.73
19	1	603	CLA	C2D-C1D-ND	3.06	112.36	110.10
19	1	614	CLA	O2D-CGD-O1D	-3.06	117.86	123.84
19	4	608	CLA	C2D-C1D-ND	3.06	112.36	110.10
19	A	1132	CLA	C2C-C1C-NC	3.06	112.84	109.97
22	A	4002	BCR	C38-C26-C27	3.06	119.49	113.62
19	4	606	CLA	CHD-C1D-ND	-3.06	121.64	124.45
22	G	4021	BCR	C30-C25-C26	-3.06	118.31	122.61
19	A	1133	CLA	C2C-C1C-NC	3.06	112.83	109.97
19	A	1115	CLA	CHD-C1D-ND	-3.05	121.65	124.45
29	2	609	CHL	CHB-C4A-NA	3.05	128.74	124.51
19	B	1207	CLA	C2D-C1D-ND	3.05	112.35	110.10
19	A	1141	CLA	O2D-CGD-O1D	-3.05	117.87	123.84
22	1	503	BCR	C38-C26-C25	-3.05	121.10	124.53
19	A	1103	CLA	C2D-C1D-ND	3.05	112.35	110.10
29	4	611	CHL	C1B-CHB-C4A	-3.05	124.08	130.12
19	F	1302	CLA	C2C-C1C-NC	3.05	112.83	109.97
19	B	1210	CLA	O1D-CGD-CBD	-3.05	118.25	124.48
19	K	1401	CLA	CHD-C1D-ND	-3.05	121.65	124.45
19	B	1221	CLA	C2C-C1C-NC	3.05	112.83	109.97
19	3	603	CLA	C2D-C1D-ND	3.04	112.35	110.10
19	A	1012	CLA	C1C-C2C-C3C	-3.04	103.76	106.96
22	G	4021	BCR	C27-C26-C25	-3.04	118.31	122.73
19	2	607	CLA	C2C-C1C-NC	3.04	112.82	109.97
19	A	1113	CLA	C2C-C1C-NC	3.04	112.82	109.97
19	3	610	CLA	CHD-C1D-ND	-3.03	121.67	124.45
19	B	1222	CLA	C2C-C1C-NC	3.03	112.81	109.97
19	2	605	CLA	C2D-C1D-ND	3.03	112.34	110.10
19	A	1104	CLA	CHD-C1D-ND	-3.03	121.67	124.45
19	B	1229	CLA	CHD-C1D-ND	-3.03	121.67	124.45
19	B	1211	CLA	C1-C2-C3	-3.03	120.81	126.04
19	B	1231	CLA	C2C-C1C-NC	3.03	112.81	109.97
19	1	603	CLA	O2A-CGA-CBA	3.03	121.41	111.91
19	B	1229	CLA	C2D-C1D-ND	3.03	112.33	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	2	605	CLA	C2C-C1C-NC	3.03	112.81	109.97
19	1	602	CLA	CHD-C1D-ND	-3.03	121.67	124.45
20	B	2002	PQN	C14-C13-C15	3.03	120.36	115.27
19	2	602	CLA	C2D-C1D-ND	3.02	112.33	110.10
19	B	1202	CLA	O2A-C1-C2	3.02	116.58	108.64
19	A	1104	CLA	O2D-CGD-O1D	-3.02	117.93	123.84
19	B	1213	CLA	O2D-CGD-O1D	-3.02	117.93	123.84
19	B	1235	CLA	C2C-C1C-NC	3.02	112.80	109.97
22	L	4020	BCR	C19-C18-C17	3.02	123.58	118.94
19	F	1302	CLA	C1C-C2C-C3C	-3.02	103.78	106.96
19	K	1401	CLA	C2C-C1C-NC	3.02	112.80	109.97
22	J	4012	BCR	C15-C14-C13	3.02	131.62	127.31
19	A	1139	CLA	C2D-C1D-ND	3.02	112.33	110.10
19	2	612	CLA	C1C-C2C-C3C	-3.02	103.79	106.96
19	3	612	CLA	C1-C2-C3	-3.02	121.87	126.75
19	L	1501	CLA	C1C-C2C-C3C	-3.01	103.79	106.96
19	A	1135	CLA	C2C-C1C-NC	3.01	112.80	109.97
19	B	1205	CLA	C2C-C1C-NC	3.01	112.80	109.97
19	K	1401	CLA	CMA-C3A-C4A	3.01	119.87	111.77
22	A	4011	BCR	C3-C4-C5	-3.01	108.70	114.08
19	A	1141	CLA	CMA-C3A-C4A	3.01	119.85	111.77
19	4	604	CLA	CMA-C3A-C4A	3.01	119.85	111.77
19	A	1012	CLA	O2D-CGD-O1D	-3.00	117.96	123.84
19	G	1603	CLA	O2D-CGD-O1D	-3.00	117.97	123.84
25	F	5002	LMG	C8-O7-C10	-3.00	110.40	117.79
19	A	1111	CLA	C2C-C1C-NC	3.00	112.78	109.97
19	2	603	CLA	C2C-C1C-NC	3.00	112.78	109.97
19	B	1204	CLA	C1-C2-C3	-3.00	120.85	126.04
19	B	1223	CLA	C2C-C1C-NC	3.00	112.78	109.97
19	K	1401	CLA	C1D-ND-C4D	-3.00	104.20	106.33
19	4	617	CLA	O2D-CGD-O1D	-3.00	117.98	123.84
19	G	1701	CLA	C1C-C2C-C3C	-3.00	103.81	106.96
22	F	4014	BCR	C37-C22-C23	3.00	122.80	118.08
19	B	1201	CLA	C2D-C1D-ND	3.00	112.31	110.10
19	3	608	CLA	C2D-C1D-ND	3.00	112.31	110.10
19	1	605	CLA	CHD-C1D-ND	-3.00	121.70	124.45
19	B	1229	CLA	C2C-C1C-NC	3.00	112.78	109.97
19	1	614	CLA	C2C-C1C-NC	3.00	112.78	109.97
19	B	1222	CLA	CAA-C2A-C3A	-2.99	104.58	112.78
19	A	1138	CLA	CMB-C2B-C3B	2.99	130.28	124.68
19	B	1202	CLA	C1-O2A-CGA	2.99	124.30	116.44
27	4	801	DGD	O3G-C1D-C2D	2.99	112.97	108.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	I	4018	BCR	C33-C5-C4	2.99	119.36	113.62
27	4	801	DGD	O6D-C5D-C6D	2.99	112.70	106.67
22	L	4019	BCR	C28-C27-C26	-2.99	108.74	114.08
22	3	503	BCR	C34-C9-C10	-2.99	118.73	122.92
19	A	1119	CLA	O2D-CGD-O1D	-2.99	117.99	123.84
19	B	1226	CLA	CMB-C2B-C1B	-2.99	123.87	128.46
19	B	1232	CLA	C1-C2-C3	-2.99	120.88	126.04
19	B	1235	CLA	C2D-C1D-ND	2.99	112.31	110.10
19	A	1139	CLA	C2C-C1C-NC	2.99	112.77	109.97
29	2	611	CHL	C4D-CHA-C1A	2.99	124.89	121.25
19	B	1216	CLA	C1-C2-C3	-2.99	120.88	126.04
22	B	4006	BCR	C37-C22-C23	2.99	122.78	118.08
22	B	4006	BCR	C34-C9-C10	-2.99	118.74	122.92
19	3	612	CLA	C2C-C1C-NC	2.99	112.77	109.97
19	A	1105	CLA	CHD-C1D-ND	-2.99	121.71	124.45
19	B	1203	CLA	CHD-C1D-ND	-2.98	121.71	124.45
29	4	615	CHL	C3C-C4C-NC	-2.98	107.22	110.57
19	B	1201	CLA	C1-C2-C3	-2.98	120.88	126.04
19	1	607	CLA	CMA-C3A-C4A	2.98	119.79	111.77
19	B	1022	CLA	C2C-C1C-NC	2.98	112.77	109.97
19	B	1226	CLA	CMB-C2B-C3B	2.98	130.26	124.68
19	4	612	CLA	C2C-C1C-NC	2.98	112.76	109.97
19	4	607	CLA	C1-O2A-CGA	2.98	124.25	116.44
22	1	503	BCR	C33-C5-C4	2.97	119.33	113.62
19	L	1501	CLA	CMA-C3A-C4A	2.97	119.77	111.77
19	A	1136	CLA	CMA-C3A-C4A	2.97	119.76	111.77
22	G	4011	BCR	C33-C5-C4	2.97	119.33	113.62
19	2	602	CLA	C2C-C1C-NC	2.97	112.76	109.97
19	A	1111	CLA	O2A-C1-C2	2.97	116.44	108.64
22	B	4009	BCR	C36-C18-C17	-2.97	118.76	122.92
19	A	1139	CLA	C1C-C2C-C3C	-2.97	103.83	106.96
19	B	1205	CLA	O2D-CGD-O1D	-2.97	118.03	123.84
29	2	611	CHL	C1B-CHB-C4A	-2.97	124.23	130.12
22	A	4003	BCR	C27-C26-C25	-2.97	118.42	122.73
19	B	1239	CLA	O2D-CGD-O1D	-2.97	118.03	123.84
28	2	501	LUT	C30-C31-C32	-2.97	113.96	123.22
19	4	604	CLA	C2C-C1C-NC	2.97	112.75	109.97
19	2	604	CLA	C2C-C1C-NC	2.96	112.75	109.97
19	B	1210	CLA	C2D-C1D-ND	2.96	112.29	110.10
19	A	1132	CLA	O2D-CGD-O1D	-2.96	118.05	123.84
19	A	1103	CLA	CAA-C2A-C3A	-2.96	104.67	112.78
19	4	603	CLA	CMA-C3A-C4A	2.96	119.73	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	1209	CLA	C2C-C1C-NC	2.96	112.75	109.97
19	G	1602	CLA	CHD-C1D-ND	-2.96	121.73	124.45
25	B	5004	LMG	O8-C28-C29	2.96	121.19	111.91
19	B	1232	CLA	C1-O2A-CGA	2.96	124.20	116.44
19	3	614	CLA	CHD-C1D-ND	-2.96	121.74	124.45
22	L	4020	BCR	C38-C26-C27	2.96	119.29	113.62
19	A	1103	CLA	O2D-CGD-O1D	-2.95	118.06	123.84
19	1	602	CLA	C1D-ND-C4D	-2.95	104.24	106.33
19	3	601	CLA	C2D-C1D-ND	2.95	112.28	110.10
19	2	607	CLA	O2A-CGA-CBA	2.95	121.17	111.91
19	A	1122	CLA	C2D-C1D-ND	2.95	112.28	110.10
19	1	611	CLA	C2C-C1C-NC	2.95	112.73	109.97
19	3	603	CLA	CHD-C1D-ND	-2.95	121.75	124.45
19	B	1234	CLA	C2C-C1C-NC	2.95	112.73	109.97
19	B	1235	CLA	CMA-C3A-C4A	2.95	119.69	111.77
29	2	610	CHL	C2C-C3C-C4C	2.94	108.59	106.49
19	A	1128	CLA	C2C-C1C-NC	2.94	112.73	109.97
19	B	1023	CLA	C2D-C1D-ND	2.94	112.27	110.10
29	1	610	CHL	C2C-C3C-C4C	2.94	108.59	106.49
19	B	1226	CLA	O2A-CGA-CBA	2.94	121.14	111.91
19	B	1229	CLA	CMA-C3A-C4A	2.94	119.68	111.77
29	2	615	CHL	CMA-C3A-C4A	2.94	119.67	111.77
29	2	615	CHL	C3C-C4C-NC	-2.94	107.28	110.57
19	K	1402	CLA	O2A-CGA-CBA	2.94	121.12	111.91
19	A	1111	CLA	C1C-C2C-C3C	-2.94	103.87	106.96
19	B	1214	CLA	CHD-C1D-ND	-2.94	121.76	124.45
19	A	1107	CLA	CMB-C2B-C3B	2.93	130.17	124.68
19	B	1204	CLA	O2D-CGD-O1D	-2.93	118.10	123.84
28	4	501	LUT	C38-C25-C24	-2.93	117.28	123.56
19	B	1214	CLA	C1-O2A-CGA	2.93	124.14	116.44
19	A	1139	CLA	C1-C2-C3	-2.93	120.97	126.04
19	A	1118	CLA	C2D-C1D-ND	2.93	112.26	110.10
19	B	1234	CLA	C2D-C1D-ND	2.93	112.26	110.10
19	2	603	CLA	C2D-C1D-ND	2.93	112.26	110.10
19	A	1102	CLA	C2D-C1D-ND	2.93	112.26	110.10
19	3	612	CLA	O2A-CGA-CBA	2.93	121.09	111.91
19	A	1103	CLA	CMB-C2B-C3B	2.93	130.15	124.68
19	A	1130	CLA	C2C-C1C-NC	2.92	112.71	109.97
19	2	608	CLA	C2C-C1C-NC	2.92	112.71	109.97
19	A	1108	CLA	CHD-C1D-ND	-2.92	121.77	124.45
19	B	1227	CLA	CHD-C1D-ND	-2.92	121.77	124.45
22	3	506	BCR	C33-C5-C4	2.92	119.23	113.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	4	607	CLA	C2D-C1D-ND	2.92	112.26	110.10
19	2	607	CLA	CHD-C1D-ND	-2.92	121.77	124.45
19	A	1116	CLA	C2C-C1C-NC	2.92	112.71	109.97
19	B	1235	CLA	CHD-C1D-ND	-2.92	121.77	124.45
19	1	614	CLA	C2D-C1D-ND	2.92	112.25	110.10
29	2	611	CHL	CMA-C3A-C4A	2.91	119.61	111.77
22	L	4020	BCR	C23-C24-C25	-2.91	119.02	127.20
19	A	1124	CLA	C2D-C1D-ND	2.91	112.25	110.10
29	4	611	CHL	CHD-C4C-C3C	2.91	129.12	124.84
19	A	1114	CLA	O2D-CGD-O1D	-2.91	118.15	123.84
19	B	1215	CLA	C2C-C1C-NC	2.91	112.70	109.97
19	4	603	CLA	C2C-C1C-NC	2.91	112.70	109.97
19	B	1223	CLA	O2D-CGD-O1D	-2.91	118.15	123.84
19	4	604	CLA	CAA-C2A-C3A	-2.91	104.81	112.78
19	B	1212	CLA	C1-C2-C3	-2.91	121.01	126.04
19	K	1404	CLA	C2C-C1C-NC	2.91	112.69	109.97
19	B	1023	CLA	CHD-C1D-ND	-2.91	121.78	124.45
19	B	1214	CLA	O2D-CGD-O1D	-2.91	118.16	123.84
19	B	1236	CLA	C2C-C1C-NC	2.90	112.69	109.97
19	B	1240	CLA	C1C-C2C-C3C	-2.90	103.90	106.96
28	3	502	LUT	C35-C34-C33	-2.90	123.17	127.31
19	A	1117	CLA	C1C-C2C-C3C	-2.90	103.91	106.96
29	3	611	CHL	CHB-C4A-NA	2.90	128.52	124.51
22	K	4002	BCR	C35-C13-C12	2.90	122.65	118.08
19	J	1901	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
19	A	1114	CLA	CHD-C1D-ND	-2.90	121.79	124.45
19	3	601	CLA	C1-O2A-CGA	2.90	124.05	116.44
22	F	4014	BCR	C33-C5-C6	-2.90	121.27	124.53
19	B	1212	CLA	C2D-C1D-ND	2.90	112.24	110.10
19	2	603	CLA	O2A-CGA-CBA	2.90	121.01	111.91
19	3	602	CLA	C1-C2-C3	-2.90	121.03	126.04
22	L	4019	BCR	C34-C9-C10	-2.90	118.86	122.92
18	A	1011	CL0	C1-O2A-CGA	2.90	124.05	116.44
19	B	1236	CLA	C1-C2-C3	-2.90	122.06	126.75
19	B	1236	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
19	3	614	CLA	C2D-C1D-ND	2.90	112.24	110.10
19	A	1138	CLA	C1-C2-C3	-2.90	121.03	126.04
28	3	502	LUT	C39-C29-C30	-2.90	118.87	122.92
24	B	5006	LMT	C1'-O5'-C5'	-2.90	108.00	113.69
27	4	801	DGD	O1G-C1A-C2A	2.90	120.99	111.91
22	A	4007	BCR	C38-C26-C27	2.89	119.18	113.62
28	1	502	LUT	C22-C23-C24	-2.89	108.45	111.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	1219	CLA	CMA-C3A-C4A	2.89	119.55	111.77
19	B	1237	CLA	O2A-CGA-CBA	2.89	120.98	111.91
29	2	610	CHL	CHD-C4C-C3C	2.89	129.09	124.84
22	L	4020	BCR	C12-C13-C14	-2.89	114.51	118.94
19	B	1229	CLA	CAA-CBA-CGA	-2.89	104.82	113.25
19	B	1212	CLA	C1C-C2C-C3C	-2.89	103.92	106.96
19	B	1201	CLA	CHD-C1D-ND	-2.88	121.81	124.45
29	4	615	CHL	C4D-CHA-C1A	2.88	124.75	121.25
22	K	4001	BCR	C33-C5-C4	2.88	119.15	113.62
19	B	1202	CLA	O2D-CGD-O1D	-2.88	118.21	123.84
19	A	1131	CLA	C1C-C2C-C3C	-2.88	103.93	106.96
19	A	1129	CLA	C1C-C2C-C3C	-2.88	103.93	106.96
19	3	613	CLA	CHD-C1D-ND	-2.88	121.81	124.45
28	1	502	LUT	C35-C34-C33	-2.88	123.20	127.31
19	A	1109	CLA	CMA-C3A-C4A	2.88	119.51	111.77
19	A	1112	CLA	O2D-CGD-O1D	-2.88	118.21	123.84
19	2	605	CLA	CAA-C2A-C3A	-2.88	104.90	112.78
19	F	1301	CLA	C2D-C1D-ND	2.88	112.22	110.10
19	4	609	CLA	C1C-C2C-C3C	-2.87	103.93	106.96
19	A	1124	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
22	L	4020	BCR	C35-C13-C12	2.87	122.60	118.08
19	4	602	CLA	C1C-C2C-C3C	-2.87	103.94	106.96
19	B	1201	CLA	CMB-C2B-C3B	2.87	130.05	124.68
29	3	611	CHL	C4D-CHA-C1A	2.87	124.74	121.25
19	B	1238	CLA	CMA-C3A-C4A	2.87	119.49	111.77
19	B	1234	CLA	O2A-CGA-CBA	2.87	120.91	111.91
19	B	1237	CLA	C1-C2-C3	-2.87	121.08	126.04
19	A	1132	CLA	CHD-C1D-ND	-2.87	121.82	124.45
19	L	1501	CLA	C2C-C1C-NC	2.87	112.66	109.97
31	4	505	C7Z	C2-C3-C4	2.87	114.23	110.30
19	3	613	CLA	CMA-C3A-C4A	2.87	119.48	111.77
19	A	1123	CLA	CMA-C3A-C4A	2.87	119.48	111.77
19	A	1116	CLA	CHD-C1D-ND	-2.87	121.82	124.45
22	A	4008	BCR	C4-C5-C6	-2.86	118.57	122.73
19	L	1502	CLA	C2C-C1C-NC	2.86	112.66	109.97
22	B	4005	BCR	C19-C18-C17	2.86	123.33	118.94
19	B	1234	CLA	CHD-C1D-ND	-2.86	121.82	124.45
19	3	603	CLA	O2A-CGA-CBA	2.86	120.89	111.91
19	A	1123	CLA	CHD-C1D-ND	-2.86	121.83	124.45
19	A	1121	CLA	C2D-C1D-ND	2.86	112.21	110.10
19	B	1209	CLA	CMA-C3A-C4A	2.86	119.45	111.77
29	2	611	CHL	C3C-C4C-NC	-2.86	107.37	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	G	1601	CLA	C1C-C2C-C3C	-2.86	103.95	106.96
19	2	606	CLA	C1C-C2C-C3C	-2.86	103.95	106.96
19	3	602	CLA	CHD-C1D-ND	-2.85	121.83	124.45
19	A	1133	CLA	C1C-C2C-C3C	-2.85	103.96	106.96
19	4	605	CLA	C1C-C2C-C3C	-2.85	103.96	106.96
19	1	604	CLA	CMA-C3A-C4A	2.85	119.44	111.77
19	A	1110	CLA	C2D-C1D-ND	2.85	112.21	110.10
19	2	605	CLA	O2D-CGD-O1D	-2.85	118.26	123.84
22	A	4017	BCR	C35-C13-C14	-2.85	118.93	122.92
19	B	1203	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
19	B	1203	CLA	C2D-C1D-ND	2.85	112.20	110.10
19	G	1601	CLA	CHD-C1D-ND	-2.85	121.84	124.45
19	A	1125	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
19	A	1013	CLA	CMB-C2B-C3B	2.84	130.00	124.68
28	2	501	LUT	C35-C34-C33	-2.84	123.25	127.31
19	B	1208	CLA	C2D-C1D-ND	2.84	112.20	110.10
19	4	602	CLA	C2D-C1D-ND	2.84	112.20	110.10
29	2	613	CHL	C3C-C4C-NC	-2.84	107.39	110.57
19	2	608	CLA	C1-C2-C3	-2.84	122.16	126.75
19	3	608	CLA	CHD-C1D-ND	-2.84	121.85	124.45
29	1	612	CHL	CHB-C4A-NA	2.84	128.43	124.51
19	4	617	CLA	C1C-C2C-C3C	-2.84	103.97	106.96
23	B	5001	LHG	C5-O7-C7	-2.84	112.61	117.90
19	3	617	CLA	C1-C2-C3	-2.83	121.14	126.04
19	A	1118	CLA	C1C-C2C-C3C	-2.83	103.98	106.96
19	A	1013	CLA	CAA-C2A-C3A	-2.83	105.02	112.78
22	3	506	BCR	C37-C22-C21	-2.83	118.95	122.92
19	A	1108	CLA	C2C-C1C-NC	2.83	112.63	109.97
19	2	602	CLA	CMA-C3A-C4A	2.83	119.39	111.77
19	B	1213	CLA	O2A-CGA-CBA	2.83	120.80	111.91
19	K	1402	CLA	C1C-C2C-C3C	-2.83	103.98	106.96
19	1	611	CLA	CMB-C2B-C3B	2.83	129.98	124.68
19	4	605	CLA	CHA-C4D-ND	2.83	138.42	132.50
19	A	1101	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
19	A	1130	CLA	C1-C2-C3	-2.83	121.15	126.04
19	A	1106	CLA	CMB-C2B-C3B	2.83	129.97	124.68
19	1	614	CLA	CHD-C1D-ND	-2.83	121.86	124.45
19	4	609	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
29	4	610	CHL	CMA-C3A-C4A	2.83	119.37	111.77
19	B	1218	CLA	CMA-C3A-C4A	2.83	119.37	111.77
19	B	1235	CLA	C1D-ND-C4D	-2.83	104.33	106.33
22	B	4009	BCR	C35-C13-C12	2.83	122.53	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	1135	CLA	CMA-C3A-C4A	2.83	119.37	111.77
23	1	801	LHG	C5-O7-C7	-2.83	110.83	117.79
19	4	607	CLA	CHD-C1D-ND	-2.82	121.86	124.45
19	B	1207	CLA	CHD-C1D-ND	-2.82	121.86	124.45
29	2	615	CHL	CHC-C1C-NC	2.82	128.49	124.20
19	B	1223	CLA	CMB-C2B-C3B	2.82	129.96	124.68
19	4	601	CLA	C2C-C1C-NC	2.82	112.61	109.97
19	B	1211	CLA	O2A-CGA-CBA	2.82	120.75	111.91
19	A	1106	CLA	C2C-C1C-NC	2.82	112.61	109.97
19	B	1212	CLA	C2C-C1C-NC	2.82	112.61	109.97
27	4	802	DGD	O1G-C1A-C2A	2.82	120.75	111.91
19	B	1217	CLA	C2D-C1D-ND	2.82	112.18	110.10
29	2	610	CHL	CHB-C4A-NA	2.81	128.40	124.51
25	F	5003	LMG	O8-C28-C29	2.81	120.74	111.91
19	1	604	CLA	C1-C2-C3	-2.81	121.18	126.04
19	B	1212	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
19	3	601	CLA	C2C-C1C-NC	2.81	112.61	109.97
19	B	1215	CLA	CMB-C2B-C3B	2.81	129.93	124.68
19	B	1232	CLA	CAA-C2A-C3A	-2.81	105.09	112.78
19	3	617	CLA	C2C-C1C-NC	2.81	112.60	109.97
19	2	612	CLA	CHD-C1D-ND	-2.81	121.88	124.45
19	B	1205	CLA	C1C-C2C-C3C	-2.81	104.01	106.96
22	J	4012	BCR	C12-C13-C14	-2.81	114.64	118.94
19	B	1238	CLA	C1-O2A-CGA	2.80	123.80	116.44
19	1	611	CLA	CMA-C3A-C4A	2.80	119.31	111.77
19	A	1120	CLA	C1C-C2C-C3C	-2.80	104.01	106.96
19	A	1111	CLA	C2D-C1D-ND	2.80	112.17	110.10
19	B	1238	CLA	C2D-C1D-ND	2.80	112.17	110.10
19	3	602	CLA	C2C-C1C-NC	2.80	112.60	109.97
22	1	503	BCR	C19-C18-C17	2.80	123.24	118.94
19	B	1021	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
19	A	1107	CLA	CMA-C3A-C4A	2.80	119.30	111.77
25	2	804	LMG	O8-C28-C29	2.80	120.69	111.91
23	1	801	LHG	O8-C23-C24	2.80	120.69	111.91
19	2	607	CLA	CMA-C3A-C4A	2.80	119.29	111.77
19	A	1110	CLA	CMA-C3A-C4A	2.80	119.29	111.77
19	B	1201	CLA	C2C-C1C-NC	2.79	112.59	109.97
19	4	603	CLA	CHD-C1D-ND	-2.79	121.89	124.45
19	2	604	CLA	O2D-CGD-O1D	-2.79	118.38	123.84
19	A	1119	CLA	CMB-C2B-C1B	-2.79	124.17	128.46
19	A	1117	CLA	C1-C2-C3	-2.79	121.21	126.04
19	B	1204	CLA	C1C-C2C-C3C	-2.79	104.02	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	4003	BCR	C35-C13-C12	2.79	122.48	118.08
22	3	506	BCR	C19-C18-C17	2.79	123.23	118.94
28	3	502	LUT	C10-C11-C12	-2.79	114.51	123.22
19	B	1226	CLA	C1C-C2C-C3C	-2.79	104.03	106.96
22	A	4003	BCR	C33-C5-C4	2.79	118.97	113.62
19	A	1127	CLA	CHD-C1D-ND	-2.79	121.89	124.45
22	A	4011	BCR	C34-C9-C10	-2.78	119.02	122.92
19	A	1120	CLA	O2D-CGD-O1D	-2.78	118.40	123.84
27	J	5001	DGD	O1G-C1A-C2A	2.78	120.64	111.91
22	A	4017	BCR	C12-C13-C14	2.78	123.21	118.94
29	3	607	CHL	C1B-CHB-C4A	-2.78	124.61	130.12
19	1	607	CLA	CHD-C1D-ND	-2.78	121.90	124.45
19	B	1224	CLA	C2D-C1D-ND	2.78	112.15	110.10
19	K	1402	CLA	O2D-CGD-O1D	-2.77	118.41	123.84
19	3	612	CLA	O2D-CGD-O1D	-2.77	118.41	123.84
25	F	5004	LMG	O8-C28-C29	2.77	120.61	111.91
19	A	1108	CLA	CMB-C2B-C3B	2.77	129.87	124.68
19	F	1302	CLA	C2D-C1D-ND	2.77	112.15	110.10
19	L	1501	CLA	CMB-C2B-C1B	-2.77	124.20	128.46
29	1	609	CHL	C2C-C3C-C4C	2.77	108.47	106.49
19	B	1237	CLA	C2C-C1C-NC	2.77	112.57	109.97
28	3	501	LUT	C11-C10-C9	-2.77	123.35	127.31
19	3	614	CLA	C2C-C1C-NC	2.77	112.57	109.97
19	B	1221	CLA	C1C-C2C-C3C	-2.77	104.04	106.96
19	A	1140	CLA	C2D-C1D-ND	2.77	112.15	110.10
19	G	1602	CLA	C2D-C1D-ND	2.77	112.15	110.10
22	B	4006	BCR	C15-C14-C13	2.77	131.26	127.31
22	I	4020	BCR	C28-C27-C26	-2.77	109.13	114.08
19	A	1104	CLA	C2D-C1D-ND	2.77	112.14	110.10
19	L	1503	CLA	O2A-CGA-CBA	2.77	120.59	111.91
19	4	603	CLA	C1C-C2C-C3C	-2.77	104.05	106.96
22	B	4004	BCR	C30-C25-C26	-2.77	118.72	122.61
19	A	1103	CLA	C2C-C1C-NC	2.77	112.56	109.97
19	A	1109	CLA	O2A-CGA-CBA	2.77	120.59	111.91
19	A	1130	CLA	CMB-C2B-C3B	2.77	129.85	124.68
19	A	1134	CLA	C2D-C1D-ND	2.76	112.14	110.10
19	B	1223	CLA	CHA-C4D-ND	2.76	138.28	132.50
19	A	1115	CLA	O2D-CGD-O1D	-2.76	118.44	123.84
19	B	1235	CLA	O2A-CGA-CBA	2.76	120.57	111.91
19	B	1218	CLA	CED-O2D-CGD	-2.76	109.70	115.94
19	B	1210	CLA	CMB-C2B-C3B	2.76	129.84	124.68
19	A	1131	CLA	C2D-C1D-ND	2.76	112.14	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	1012	CLA	CAA-C2A-C3A	-2.76	105.23	112.78
19	B	1230	CLA	O2D-CGD-O1D	-2.76	118.45	123.84
19	A	1122	CLA	CMA-C3A-C4A	2.76	119.18	111.77
19	A	1109	CLA	C1D-ND-C4D	-2.76	104.38	106.33
19	A	1104	CLA	C1C-C2C-C3C	-2.76	104.06	106.96
19	B	1222	CLA	CMB-C2B-C3B	2.76	129.83	124.68
27	F	5005	DGD	O1G-C1A-C2A	2.76	120.56	111.91
19	3	610	CLA	CMA-C3A-C4A	2.75	119.18	111.77
19	4	606	CLA	C1C-C2C-C3C	-2.75	104.06	106.96
25	F	5002	LMG	O8-C28-C29	2.75	120.55	111.91
19	G	1602	CLA	C2C-C1C-NC	2.75	112.55	109.97
29	4	613	CHL	C3C-C4C-NC	-2.75	107.49	110.57
19	B	1023	CLA	C1-C2-C3	-2.75	121.29	126.04
19	A	1135	CLA	C1D-ND-C4D	-2.75	104.38	106.33
19	1	613	CLA	CMA-C3A-C4A	2.75	119.16	111.77
19	B	1240	CLA	O2D-CGD-O1D	-2.75	118.47	123.84
29	2	610	CHL	CMA-C3A-C4A	2.75	119.16	111.77
19	L	1502	CLA	CMA-C3A-C4A	2.75	119.16	111.77
19	A	1112	CLA	O2A-CGA-CBA	2.75	120.53	111.91
31	4	505	C7Z	C28-C27-C26	-2.75	119.49	127.20
29	2	615	CHL	CHD-C4C-C3C	2.75	128.88	124.84
19	B	1221	CLA	CHD-C1D-ND	-2.75	121.93	124.45
19	B	1209	CLA	C1C-C2C-C3C	-2.75	104.07	106.96
19	B	1235	CLA	C1C-C2C-C3C	-2.75	104.07	106.96
29	3	604	CHL	C1B-CHB-C4A	-2.74	124.68	130.12
19	A	1101	CLA	C1-O2A-CGA	2.74	123.64	116.44
19	B	1227	CLA	O2D-CGD-O1D	-2.74	118.47	123.84
19	B	1232	CLA	C2D-C1D-ND	2.74	112.13	110.10
19	1	606	CLA	C2D-C1D-ND	2.74	112.13	110.10
19	2	607	CLA	C2D-C1D-ND	2.74	112.13	110.10
19	B	1216	CLA	O2D-CGD-O1D	-2.74	118.47	123.84
19	3	610	CLA	C1C-C2C-C3C	-2.74	104.07	106.96
19	K	1404	CLA	C2D-C1D-ND	2.74	112.12	110.10
19	4	604	CLA	C2D-C1D-ND	2.74	112.12	110.10
19	K	1404	CLA	CHD-C1D-ND	-2.74	121.93	124.45
28	3	501	LUT	C35-C15-C14	-2.74	117.86	123.47
19	A	1107	CLA	O2D-CGD-O1D	-2.74	118.48	123.84
19	B	1224	CLA	O2A-CGA-CBA	2.74	120.51	111.91
19	2	602	CLA	O2A-CGA-CBA	2.74	120.51	111.91
18	A	1011	CL0	O2D-CGD-O1D	-2.74	118.48	123.84
19	A	1132	CLA	C2D-C1D-ND	2.74	112.12	110.10
19	2	612	CLA	C1-C2-C3	-2.74	121.31	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	3	503	BCR	C33-C5-C4	2.74	118.88	113.62
19	A	1127	CLA	O2D-CGD-O1D	-2.74	118.48	123.84
31	4	505	C7Z	C8-C9-C10	-2.74	114.74	118.94
25	B	5007	LMG	O8-C28-C29	2.74	120.50	111.91
19	B	1224	CLA	C1-C2-C3	-2.73	121.31	126.04
22	B	4004	BCR	C35-C13-C12	-2.73	113.77	118.08
22	3	506	BCR	C38-C26-C25	-2.73	121.46	124.53
22	B	4009	BCR	C12-C13-C14	-2.73	114.75	118.94
19	B	1239	CLA	C2C-C1C-NC	2.73	112.53	109.97
19	A	1101	CLA	CMB-C2B-C3B	2.73	129.79	124.68
19	A	1128	CLA	CMB-C2B-C1B	-2.73	124.26	128.46
19	3	617	CLA	CAA-C2A-C3A	-2.73	105.30	112.78
29	2	615	CHL	C1-C2-C3	-2.73	121.32	126.04
19	A	1114	CLA	C1C-C2C-C3C	-2.73	104.09	106.96
19	2	607	CLA	O2D-CGD-O1D	-2.73	118.50	123.84
28	1	501	LUT	C38-C25-C24	-2.73	117.72	123.56
19	L	1503	CLA	CMA-C3A-C4A	2.73	119.11	111.77
19	B	1022	CLA	CAA-C2A-C3A	-2.73	105.31	112.78
19	A	1131	CLA	CHD-C1D-ND	-2.73	121.95	124.45
22	F	4014	BCR	C28-C27-C26	-2.73	109.21	114.08
19	A	1109	CLA	O2D-CGD-O1D	-2.73	118.51	123.84
19	B	1021	CLA	CAA-C2A-C3A	-2.73	105.31	112.78
29	1	612	CHL	CHD-C1D-ND	-2.73	121.95	124.45
29	1	612	CHL	C2C-C3C-C4C	2.73	108.43	106.49
19	1	611	CLA	O2D-CGD-O1D	-2.73	118.51	123.84
19	B	1208	CLA	C1D-ND-C4D	-2.73	104.40	106.33
19	B	1021	CLA	C1C-C2C-C3C	-2.72	104.09	106.96
19	A	1123	CLA	C1C-C2C-C3C	-2.72	104.09	106.96
27	B	5005	DGD	O1G-C1A-C2A	2.72	120.45	111.91
19	2	608	CLA	CMA-C3A-C4A	2.72	119.08	111.77
19	A	1105	CLA	O2D-CGD-O1D	-2.72	118.52	123.84
22	K	4002	BCR	C36-C18-C17	-2.72	119.11	122.92
19	4	605	CLA	CHA-C1A-NA	-2.72	120.17	126.40
19	3	605	CLA	CHD-C1D-ND	-2.72	121.96	124.45
19	A	1114	CLA	C2D-C1D-ND	2.72	112.11	110.10
19	A	1134	CLA	C1C-C2C-C3C	-2.72	104.10	106.96
19	B	1222	CLA	C1C-C2C-C3C	-2.72	104.10	106.96
19	B	1231	CLA	C1C-C2C-C3C	-2.71	104.10	106.96
19	L	1501	CLA	O2D-CGD-O1D	-2.71	118.53	123.84
27	F	5005	DGD	O6E-C5E-C4E	2.71	114.62	109.69
19	B	1219	CLA	CMB-C2B-C1B	-2.71	124.29	128.46
19	A	1105	CLA	C1C-C2C-C3C	-2.71	104.10	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	1013	CLA	C2D-C1D-ND	2.71	112.10	110.10
19	B	1202	CLA	C2D-C1D-ND	2.71	112.10	110.10
19	3	605	CLA	CHA-C4D-ND	2.71	138.18	132.50
19	F	1301	CLA	C1C-C2C-C3C	-2.71	104.10	106.96
19	1	608	CLA	C1C-C2C-C3C	-2.71	104.10	106.96
23	A	5001	LHG	C5-O7-C7	-2.71	111.11	117.79
25	1	802	LMG	O8-C28-C29	2.71	120.42	111.91
19	G	1602	CLA	CMA-C3A-C4A	2.71	119.06	111.77
19	B	1230	CLA	O2A-CGA-CBA	2.71	120.42	111.91
19	B	1237	CLA	O2D-CGD-O1D	-2.71	118.54	123.84
19	A	1119	CLA	C2C-C1C-NC	2.71	112.51	109.97
19	A	1124	CLA	C2C-C1C-NC	2.71	112.51	109.97
19	2	605	CLA	CHA-C4D-ND	2.71	138.17	132.50
19	4	602	CLA	O2D-CGD-O1D	-2.71	118.54	123.84
19	A	1135	CLA	CHD-C1D-ND	-2.71	121.97	124.45
19	1	605	CLA	C1C-C2C-C3C	-2.71	104.11	106.96
19	B	1216	CLA	CHD-C1D-ND	-2.71	121.97	124.45
25	G	5001	LMG	C9-C8-C7	-2.71	105.39	111.79
19	B	1214	CLA	C1C-C2C-C3C	-2.70	104.11	106.96
19	B	1214	CLA	CHA-C4D-ND	2.70	138.16	132.50
22	A	4011	BCR	C35-C13-C12	2.70	122.34	118.08
19	3	614	CLA	CMA-C3A-C4A	2.70	119.03	111.77
19	B	1236	CLA	C1C-C2C-C3C	-2.70	104.12	106.96
25	G	5002	LMG	C8-O7-C10	-2.70	111.14	117.79
19	1	604	CLA	O2A-CGA-CBA	2.70	120.38	111.91
19	B	1215	CLA	C1C-C2C-C3C	-2.70	104.12	106.96
22	B	4004	BCR	C2-C1-C6	2.70	114.64	110.48
19	B	1220	CLA	O2D-CGD-O1D	-2.70	118.56	123.84
22	F	4014	BCR	C36-C18-C17	-2.70	119.14	122.92
19	1	601	CLA	C2D-C1D-ND	2.70	112.09	110.10
19	B	1221	CLA	CMB-C2B-C3B	2.70	129.72	124.68
19	B	1239	CLA	C1C-C2C-C3C	-2.70	104.12	106.96
19	K	1403	CLA	CHA-C4D-ND	2.70	138.14	132.50
19	B	1210	CLA	C2C-C1C-NC	2.70	112.50	109.97
19	3	606	CLA	O2D-CGD-O1D	-2.69	118.57	123.84
19	B	1203	CLA	CMB-C2B-C3B	2.69	129.72	124.68
19	4	605	CLA	CMB-C2B-C3B	2.69	129.72	124.68
22	F	4016	BCR	C33-C5-C6	-2.69	121.50	124.53
19	B	1217	CLA	CMA-C3A-C4A	2.69	119.01	111.77
19	A	1121	CLA	O2A-CGA-CBA	2.69	120.36	111.91
19	A	1108	CLA	CMA-C3A-C4A	2.69	119.01	111.77
19	L	1503	CLA	CAA-C2A-C3A	-2.69	105.41	112.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	1126	CLA	C2C-C1C-NC	2.69	112.49	109.97
19	B	1238	CLA	CMD-C2D-C3D	-2.69	121.43	127.61
22	K	4002	BCR	C12-C13-C14	-2.69	114.81	118.94
19	1	601	CLA	CMA-C3A-C4A	2.69	119.00	111.77
19	K	1402	CLA	CHD-C1D-ND	-2.69	121.98	124.45
19	A	1113	CLA	C1C-C2C-C3C	-2.69	104.13	106.96
22	B	4009	BCR	C23-C24-C25	-2.69	119.66	127.20
19	3	612	CLA	C2D-C1D-ND	2.69	112.08	110.10
19	A	1136	CLA	O2A-CGA-CBA	2.69	120.34	111.91
19	1	604	CLA	C6-C5-C3	-2.69	106.41	113.45
19	B	1207	CLA	C2C-C1C-NC	2.68	112.49	109.97
19	A	1112	CLA	C2D-C1D-ND	2.68	112.08	110.10
19	L	1503	CLA	C1C-C2C-C3C	-2.68	104.14	106.96
19	A	1140	CLA	CMA-C3A-C4A	2.68	118.98	111.77
29	2	613	CHL	CMA-C3A-C4A	2.68	118.97	111.77
19	4	617	CLA	O2A-CGA-CBA	2.68	120.31	111.91
19	1	606	CLA	C1C-C2C-C3C	-2.68	104.14	106.96
24	A	5004	LMT	C3B-C4B-C5B	-2.68	105.46	110.24
25	B	5003	LMG	O8-C28-C29	2.68	120.31	111.91
29	2	611	CHL	CHD-C4C-C3C	2.68	128.77	124.84
22	B	4005	BCR	C36-C18-C17	-2.68	119.17	122.92
19	B	1229	CLA	C1C-C2C-C3C	-2.68	104.14	106.96
19	B	1235	CLA	C1-C2-C3	-2.68	121.42	126.04
19	B	1203	CLA	CHA-C4D-ND	2.68	138.10	132.50
19	A	1101	CLA	O1D-CGD-CBD	-2.67	119.01	124.48
19	4	603	CLA	C2D-C1D-ND	2.67	112.08	110.10
28	1	501	LUT	C35-C34-C33	-2.67	123.49	127.31
19	A	1134	CLA	O2D-CGD-O1D	-2.67	118.61	123.84
19	G	1601	CLA	C2D-C1D-ND	2.67	112.07	110.10
19	B	1214	CLA	C1-C2-C3	-2.67	121.42	126.04
19	K	1403	CLA	C1C-C2C-C3C	-2.67	104.15	106.96
19	3	606	CLA	CAA-C2A-C3A	-2.67	105.46	112.78
19	2	601	CLA	O2D-CGD-O1D	-2.67	118.62	123.84
19	G	1603	CLA	CHD-C1D-ND	-2.67	122.00	124.45
19	L	1502	CLA	CMB-C2B-C3B	2.67	129.67	124.68
19	2	608	CLA	C1C-C2C-C3C	-2.67	104.15	106.96
19	B	1225	CLA	C2C-C1C-NC	2.67	112.47	109.97
22	G	4021	BCR	C38-C26-C27	2.67	118.74	113.62
19	A	1107	CLA	C1C-C2C-C3C	-2.67	104.15	106.96
22	I	4018	BCR	C27-C26-C25	-2.67	118.86	122.73
22	A	4007	BCR	C34-C9-C10	-2.67	119.19	122.92
29	4	615	CHL	C4A-NA-C1A	2.66	107.90	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	G	5005	LMT	C3B-C4B-C5B	-2.66	105.49	110.24
30	2	502	XAT	C38-C25-C26	-2.66	117.80	122.26
19	2	612	CLA	O2A-CGA-CBA	2.66	120.27	111.91
19	A	1133	CLA	O2D-CGD-O1D	-2.66	118.63	123.84
19	A	1105	CLA	CMA-C3A-C4A	2.66	118.93	111.77
19	4	609	CLA	CHD-C1D-ND	-2.66	122.01	124.45
19	B	1221	CLA	C2D-C1D-ND	2.66	112.06	110.10
19	B	1212	CLA	CMB-C2B-C3B	2.66	129.66	124.68
19	G	1603	CLA	C1C-C2C-C3C	-2.66	104.16	106.96
19	3	606	CLA	CHA-C4D-ND	2.66	138.06	132.50
19	3	612	CLA	C1C-C2C-C3C	-2.66	104.16	106.96
19	A	1116	CLA	O2A-CGA-CBA	2.66	120.25	111.91
19	B	1230	CLA	C1C-C2C-C3C	-2.66	104.16	106.96
19	B	1237	CLA	C1C-C2C-C3C	-2.66	104.16	106.96
19	2	605	CLA	C1C-C2C-C3C	-2.66	104.16	106.96
19	B	1022	CLA	C1-C2-C3	-2.66	121.45	126.04
19	B	1234	CLA	C1C-C2C-C3C	-2.65	104.17	106.96
19	2	606	CLA	C2D-C1D-ND	2.65	112.06	110.10
25	G	5002	LMG	O8-C28-C29	2.65	120.24	111.91
22	1	504	BCR	C30-C25-C24	2.65	123.28	115.78
19	K	1401	CLA	C1C-C2C-C3C	-2.65	104.17	106.96
19	B	1212	CLA	O1D-CGD-CBD	-2.65	119.06	124.48
19	F	1302	CLA	O2D-CGD-O1D	-2.65	118.65	123.84
19	1	606	CLA	CMA-C3A-C4A	2.65	118.90	111.77
19	A	1013	CLA	C6-C5-C3	-2.65	106.51	113.45
19	B	1219	CLA	C1-C2-C3	-2.65	121.46	126.04
19	A	1135	CLA	C1C-C2C-C3C	-2.65	104.17	106.96
19	A	1127	CLA	CMB-C2B-C3B	2.65	129.63	124.68
19	2	602	CLA	CHD-C1D-ND	-2.65	122.02	124.45
19	A	1102	CLA	O1D-CGD-CBD	-2.65	119.07	124.48
19	A	1133	CLA	C2D-C1D-ND	2.65	112.06	110.10
29	1	612	CHL	C4A-NA-C1A	2.65	107.90	106.71
19	A	1106	CLA	O2D-CGD-O1D	-2.65	118.66	123.84
19	B	1231	CLA	O2D-CGD-O1D	-2.65	118.67	123.84
19	B	1203	CLA	C2C-C1C-NC	2.65	112.45	109.97
19	4	608	CLA	C2C-C1C-NC	2.65	112.45	109.97
19	B	1208	CLA	O2D-CGD-O1D	-2.64	118.67	123.84
19	B	1227	CLA	C2D-C1D-ND	2.64	112.05	110.10
19	B	1023	CLA	C2C-C1C-NC	2.64	112.45	109.97
19	B	1210	CLA	O2A-CGA-CBA	2.64	120.20	111.91
19	1	607	CLA	C1C-C2C-C3C	-2.64	104.18	106.96
19	A	1136	CLA	O2D-CGD-O1D	-2.64	118.67	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	1125	CLA	C1C-C2C-C3C	-2.64	104.18	106.96
22	B	4005	BCR	C12-C13-C14	-2.64	114.89	118.94
19	A	1113	CLA	O2D-CGD-O1D	-2.64	118.68	123.84
19	2	607	CLA	C1-O2A-CGA	2.64	123.37	116.44
28	3	501	LUT	C38-C25-C24	-2.64	117.91	123.56
28	1	501	LUT	C16-C1-C6	-2.64	106.02	110.30
19	A	1141	CLA	C1C-C2C-C3C	-2.64	104.18	106.96
19	A	1102	CLA	O2D-CGD-O1D	-2.64	118.68	123.84
22	2	503	BCR	C36-C18-C17	-2.64	119.23	122.92
19	B	1211	CLA	C2D-C1D-ND	2.64	112.05	110.10
19	A	1130	CLA	C1C-C2C-C3C	-2.64	104.18	106.96
19	B	1232	CLA	O2D-CGD-O1D	-2.64	118.68	123.84
19	B	1206	CLA	C2D-C1D-ND	2.64	112.05	110.10
19	B	1225	CLA	CMB-C2B-C3B	2.64	129.61	124.68
22	A	4007	BCR	C36-C18-C17	-2.64	119.23	122.92
19	A	1137	CLA	CHA-C4D-ND	2.64	138.01	132.50
19	4	608	CLA	C1D-ND-C4D	-2.64	104.46	106.33
19	A	1112	CLA	CMB-C2B-C3B	2.63	129.61	124.68
19	A	1136	CLA	C2C-C1C-NC	2.63	112.44	109.97
19	B	1238	CLA	C2C-C1C-NC	2.63	112.44	109.97
19	1	602	CLA	C3D-C2D-C1D	-2.63	102.24	105.83
19	B	1213	CLA	C1C-C2C-C3C	-2.63	104.19	106.96
19	2	605	CLA	CMA-C3A-C4A	2.63	118.85	111.77
19	B	1221	CLA	CHA-C4D-ND	2.63	138.00	132.50
19	A	1116	CLA	CHA-C4D-ND	2.63	138.00	132.50
19	1	608	CLA	CHA-C4D-ND	2.63	138.00	132.50
19	A	1124	CLA	C1C-C2C-C3C	-2.63	104.19	106.96
19	A	1110	CLA	CAA-C2A-C3A	-2.63	105.58	112.78
19	A	1118	CLA	O2D-CGD-O1D	-2.63	118.70	123.84
19	A	1128	CLA	O2A-CGA-CBA	2.63	120.16	111.91
19	B	1216	CLA	C2C-C1C-NC	2.63	112.43	109.97
29	2	613	CHL	C4D-CHA-C1A	2.63	124.45	121.25
19	A	1110	CLA	C2C-C1C-NC	2.63	112.43	109.97
19	2	607	CLA	CHA-C4D-ND	2.63	137.99	132.50
22	A	4008	BCR	C33-C5-C4	2.63	118.66	113.62
19	A	1137	CLA	C2D-C1D-ND	2.62	112.04	110.10
19	3	602	CLA	CMA-C3A-C4A	2.62	118.83	111.77
19	A	1105	CLA	C2D-C1D-ND	2.62	112.04	110.10
19	B	1219	CLA	CAA-CBA-CGA	-2.62	105.59	113.25
19	A	1115	CLA	C1C-C2C-C3C	-2.62	104.20	106.96
19	2	602	CLA	C6-C5-C3	-2.62	110.33	114.62
19	2	607	CLA	C1C-C2C-C3C	-2.62	104.20	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	1238	CLA	O2D-CGD-O1D	-2.62	118.72	123.84
19	2	601	CLA	CMA-C3A-C4A	2.62	118.81	111.77
28	1	502	LUT	C3-C4-C5	-2.62	106.64	111.85
29	4	615	CHL	C2C-C3C-C4C	2.62	108.36	106.49
19	A	1107	CLA	O2A-CGA-CBA	2.62	120.12	111.91
19	G	1601	CLA	CHA-C4D-ND	2.62	137.97	132.50
19	B	1238	CLA	C1D-ND-C4D	-2.62	104.48	106.33
22	B	4005	BCR	C33-C5-C4	2.62	118.64	113.62
19	B	1231	CLA	C1-C2-C3	-2.62	121.52	126.04
19	G	1701	CLA	CHD-C1D-ND	-2.62	122.05	124.45
19	4	617	CLA	C2C-C1C-NC	2.62	112.42	109.97
19	B	1202	CLA	CHA-C4D-ND	2.61	137.97	132.50
19	A	1138	CLA	C1C-C2C-C3C	-2.61	104.21	106.96
19	L	1502	CLA	C1C-C2C-C3C	-2.61	104.21	106.96
19	4	601	CLA	C2D-C1D-ND	2.61	112.03	110.10
22	B	4004	BCR	C34-C9-C8	-2.61	113.96	118.08
19	B	1229	CLA	O2D-CGD-O1D	-2.61	118.73	123.84
19	A	1116	CLA	O2D-CGD-O1D	-2.61	118.74	123.84
22	A	4008	BCR	C23-C24-C25	-2.61	119.88	127.20
19	B	1223	CLA	C2D-C1D-ND	2.61	112.03	110.10
19	2	601	CLA	C2D-C1D-ND	2.61	112.03	110.10
19	A	1131	CLA	O2D-CGD-O1D	-2.61	118.74	123.84
19	A	1121	CLA	CMA-C3A-C4A	2.61	118.78	111.77
25	A	5006	LMG	O8-C28-C29	2.61	120.09	111.91
22	2	503	BCR	C33-C5-C4	2.61	118.62	113.62
19	4	617	CLA	O1D-CGD-CBD	-2.61	119.15	124.48
19	B	1225	CLA	O2A-CGA-CBA	2.60	120.08	111.91
19	A	1013	CLA	C1C-C2C-C3C	-2.60	104.22	106.96
19	A	1117	CLA	CMB-C2B-C3B	2.60	129.55	124.68
19	B	1201	CLA	O2D-CGD-O1D	-2.60	118.75	123.84
19	A	1135	CLA	O2D-CGD-O1D	-2.60	118.75	123.84
19	G	1602	CLA	C1C-C2C-C3C	-2.60	104.22	106.96
19	A	1118	CLA	CMA-C3A-C4A	2.60	118.76	111.77
19	G	1601	CLA	O2A-CGA-CBA	2.60	120.06	111.91
19	F	1301	CLA	CHD-C1D-ND	-2.60	122.07	124.45
19	F	1302	CLA	CAA-C2A-C1A	-2.60	103.46	111.97
19	A	1108	CLA	OBD-CAD-C3D	-2.60	122.27	128.52
19	1	608	CLA	C2D-C1D-ND	2.60	112.02	110.10
22	B	4006	BCR	C12-C13-C14	-2.60	114.96	118.94
19	A	1117	CLA	O2A-CGA-CBA	2.60	120.05	111.91
22	F	4016	BCR	C38-C26-C25	-2.59	121.61	124.53
22	A	4017	BCR	C23-C24-C25	-2.59	119.91	127.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	1130	CLA	CMD-C2D-C3D	-2.59	121.65	127.61
19	2	604	CLA	CMB-C2B-C1B	-2.59	124.48	128.46
19	A	1119	CLA	C1-O2A-CGA	2.59	123.25	116.44
22	1	504	BCR	C37-C22-C21	-2.59	119.29	122.92
19	1	607	CLA	C2D-C1D-ND	2.59	112.02	110.10
22	2	503	BCR	C29-C28-C27	-2.59	105.58	111.38
19	A	1103	CLA	CMB-C2B-C1B	-2.59	124.48	128.46
19	B	1224	CLA	C1C-C2C-C3C	-2.59	104.23	106.96
19	3	608	CLA	C1C-C2C-C3C	-2.59	104.23	106.96
19	B	1232	CLA	CMA-C3A-C4A	2.59	118.74	111.77
19	A	1104	CLA	CHA-C4D-ND	2.59	137.92	132.50
19	2	608	CLA	C1-O2A-CGA	2.59	123.24	116.44
19	B	1240	CLA	CMB-C2B-C3B	2.59	129.52	124.68
19	3	610	CLA	CMB-C2B-C3B	2.59	129.52	124.68
22	B	4006	BCR	C33-C5-C4	2.59	118.59	113.62
29	2	610	CHL	C4D-CHA-C1A	2.59	124.40	121.25
19	4	612	CLA	C2D-C1D-ND	2.59	112.01	110.10
22	B	4009	BCR	C33-C5-C6	-2.59	121.62	124.53
19	A	1106	CLA	C1-O2A-CGA	2.59	123.23	116.44
22	K	4002	BCR	C33-C5-C4	2.59	118.58	113.62
19	G	1601	CLA	O2D-CGD-O1D	-2.58	118.78	123.84
23	2	801	LHG	C5-O7-C7	-2.58	111.43	117.79
19	3	613	CLA	C1C-C2C-C3C	-2.58	104.24	106.96
19	K	1403	CLA	C1D-ND-C4D	-2.58	104.50	106.33
19	4	603	CLA	C1-C2-C3	-2.58	121.57	126.04
19	2	604	CLA	O2A-CGA-CBA	2.58	120.02	111.91
19	A	1115	CLA	CMA-C3A-C4A	2.58	118.72	111.77
19	B	1022	CLA	C1C-C2C-C3C	-2.58	104.24	106.96
19	3	606	CLA	C1C-C2C-C3C	-2.58	104.24	106.96
19	A	1122	CLA	C2C-C1C-NC	2.58	112.39	109.97
19	A	1141	CLA	CHA-C4D-ND	2.58	137.90	132.50
19	B	1215	CLA	O2D-CGD-O1D	-2.58	118.79	123.84
19	A	1128	CLA	C1C-C2C-C3C	-2.58	104.24	106.96
19	B	1223	CLA	C1C-C2C-C3C	-2.58	104.24	106.96
22	1	504	BCR	C1-C6-C5	-2.58	118.98	122.61
19	1	614	CLA	O1D-CGD-CBD	-2.58	119.21	124.48
29	1	612	CHL	CHD-C4C-C3C	2.58	128.63	124.84
25	1	802	LMG	C8-O7-C10	-2.58	111.45	117.79
22	B	4004	BCR	C33-C5-C6	-2.58	121.64	124.53
27	3	803	DGD	C3G-C2G-C1G	-2.57	105.70	111.79
19	3	601	CLA	CMB-C2B-C1B	-2.57	124.51	128.46
22	I	4018	BCR	C34-C9-C10	-2.57	119.32	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	I	4020	BCR	C31-C1-C6	-2.57	106.12	110.30
19	B	1226	CLA	CAA-C2A-C3A	-2.57	105.73	112.78
22	B	4006	BCR	C38-C26-C27	2.57	118.56	113.62
19	B	1228	CLA	CHA-C4D-ND	2.57	137.88	132.50
22	B	4005	BCR	C34-C9-C10	-2.57	119.32	122.92
19	B	1226	CLA	CMA-C3A-C4A	2.57	118.69	111.77
19	B	1232	CLA	CHA-C4D-ND	2.57	137.88	132.50
19	B	1223	CLA	O2A-CGA-CBA	2.57	119.97	111.91
28	1	502	LUT	C30-C31-C32	-2.57	115.20	123.22
19	3	617	CLA	C1D-ND-C4D	-2.57	104.51	106.33
31	4	505	C7Z	C1-C2-C3	2.57	119.44	113.64
19	4	608	CLA	C1C-C2C-C3C	-2.57	104.26	106.96
19	2	604	CLA	C1-O2A-CGA	2.57	123.18	116.44
19	B	1207	CLA	CHA-C4D-ND	2.57	137.87	132.50
19	B	1237	CLA	CMA-C3A-C4A	2.57	118.67	111.77
19	A	1108	CLA	CHA-C4D-ND	2.57	137.87	132.50
22	L	4019	BCR	C38-C26-C27	2.57	118.55	113.62
19	B	1216	CLA	C2D-C1D-ND	2.56	111.99	110.10
19	1	605	CLA	C2D-C1D-ND	2.56	111.99	110.10
19	B	1219	CLA	C1C-C2C-C3C	-2.56	104.26	106.96
19	4	617	CLA	CAA-CBA-CGA	-2.56	105.76	113.25
19	B	1201	CLA	C1C-C2C-C3C	-2.56	104.26	106.96
19	1	614	CLA	C1C-C2C-C3C	-2.56	104.26	106.96
29	3	604	CHL	CMA-C3A-C4A	2.56	118.66	111.77
19	A	1112	CLA	CMA-C3A-C4A	2.56	118.66	111.77
19	4	604	CLA	C1C-C2C-C3C	-2.56	104.27	106.96
22	A	4017	BCR	C27-C26-C25	-2.56	119.02	122.73
22	2	503	BCR	C23-C24-C25	-2.56	120.02	127.20
29	2	610	CHL	C1B-CHB-C4A	-2.56	125.05	130.12
19	A	1138	CLA	C2C-C1C-NC	2.56	112.37	109.97
19	1	603	CLA	C2C-C1C-NC	2.56	112.37	109.97
19	A	1106	CLA	C1C-C2C-C3C	-2.56	104.27	106.96
22	A	4002	BCR	C30-C25-C26	-2.56	119.01	122.61
19	1	613	CLA	C2C-C1C-NC	2.56	112.37	109.97
22	B	4005	BCR	C8-C9-C10	2.56	122.86	118.94
19	K	1404	CLA	C1C-C2C-C3C	-2.55	104.27	106.96
19	A	1120	CLA	C2D-C1D-ND	2.55	111.99	110.10
19	G	1602	CLA	O2D-CGD-O1D	-2.55	118.84	123.84
19	B	1224	CLA	C6-C5-C3	-2.55	106.76	113.45
19	A	1130	CLA	C2D-C1D-ND	2.55	111.98	110.10
19	A	1127	CLA	C1C-C2C-C3C	-2.55	104.27	106.96
19	K	1402	CLA	CHA-C4D-ND	2.55	137.84	132.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	4	605	CLA	C1-O2A-CGA	2.55	123.14	116.44
19	4	612	CLA	OBD-CAD-C3D	-2.55	122.38	128.52
19	A	1113	CLA	CHA-C4D-ND	2.55	137.84	132.50
22	3	503	BCR	C38-C26-C27	2.55	118.52	113.62
19	A	1123	CLA	CHA-C4D-ND	2.55	137.83	132.50
19	B	1228	CLA	C2D-C1D-ND	2.55	111.98	110.10
19	A	1130	CLA	CHA-C4D-ND	2.55	137.83	132.50
19	A	1114	CLA	CHA-C4D-ND	2.54	137.82	132.50
22	A	4008	BCR	C34-C9-C10	-2.54	119.36	122.92
19	3	614	CLA	CHA-C4D-ND	2.54	137.82	132.50
19	A	1013	CLA	C2C-C1C-NC	2.54	112.35	109.97
22	1	504	BCR	C33-C5-C6	-2.54	121.67	124.53
19	B	1228	CLA	C1C-C2C-C3C	-2.54	104.28	106.96
19	A	1118	CLA	O2A-CGA-CBA	2.54	119.88	111.91
22	K	4002	BCR	C38-C26-C27	2.54	118.50	113.62
19	1	604	CLA	CMD-C2D-C3D	-2.54	121.77	127.61
19	A	1013	CLA	CHA-C4D-ND	2.54	137.81	132.50
19	A	1117	CLA	O2D-CGD-O1D	-2.54	118.87	123.84
29	2	610	CHL	C1-O2A-CGA	2.54	123.11	116.44
19	B	1218	CLA	C2D-C1D-ND	2.54	111.98	110.10
19	1	606	CLA	C1-O2A-CGA	2.54	123.11	116.44
19	1	601	CLA	O2A-CGA-CBA	2.54	119.88	111.91
19	A	1110	CLA	CHA-C4D-ND	2.54	137.81	132.50
19	B	1227	CLA	C1-C2-C3	-2.54	121.65	126.04
19	B	1021	CLA	CMB-C2B-C3B	2.54	129.43	124.68
19	J	1901	CLA	CHA-C4D-ND	2.54	137.81	132.50
19	A	1125	CLA	C2C-C1C-NC	2.54	112.35	109.97
19	A	1107	CLA	C2D-C1D-ND	2.53	111.97	110.10
19	1	605	CLA	CMA-C3A-C4A	2.53	118.58	111.77
19	B	1223	CLA	CMB-C2B-C1B	-2.53	124.57	128.46
19	4	604	CLA	CMD-C2D-C3D	-2.53	121.79	127.61
19	4	612	CLA	C1C-C2C-C3C	-2.53	104.29	106.96
19	A	1012	CLA	CHA-C4D-ND	2.53	137.80	132.50
19	B	1224	CLA	CHA-C4D-ND	2.53	137.80	132.50
19	B	1023	CLA	O2A-CGA-CBA	2.53	119.86	111.91
19	B	1216	CLA	C1-O2A-CGA	2.53	123.09	116.44
19	1	604	CLA	CHA-C4D-ND	2.53	137.80	132.50
19	G	1701	CLA	C2D-C1D-ND	2.53	111.97	110.10
19	B	1240	CLA	C1-O2A-CGA	2.53	123.09	116.44
22	1	503	BCR	C35-C13-C12	2.53	122.06	118.08
19	B	1228	CLA	O2D-CGD-O1D	-2.53	118.89	123.84
19	A	1126	CLA	O2D-CGD-O1D	-2.53	118.89	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	1236	CLA	C1-O2A-CGA	2.53	123.08	116.44
19	G	1602	CLA	CHA-C4D-ND	2.53	137.79	132.50
19	1	611	CLA	C2D-C1D-ND	2.53	111.97	110.10
19	3	605	CLA	C2D-C1D-ND	2.53	111.97	110.10
19	2	602	CLA	CHA-C4D-ND	2.53	137.78	132.50
19	4	617	CLA	C2D-C1D-ND	2.53	111.97	110.10
28	3	502	LUT	C22-C23-C24	-2.53	108.87	111.74
19	2	608	CLA	CMD-C2D-C3D	-2.52	121.81	127.61
19	B	1237	CLA	C2D-C1D-ND	2.52	111.96	110.10
19	A	1136	CLA	C1C-C2C-C3C	-2.52	104.30	106.96
19	B	1211	CLA	CHA-C4D-ND	2.52	137.78	132.50
19	A	1113	CLA	CMD-C2D-C3D	-2.52	121.82	127.61
19	A	1119	CLA	CMD-C2D-C3D	-2.52	121.82	127.61
19	3	601	CLA	CHA-C4D-ND	2.52	137.77	132.50
19	B	1208	CLA	CAA-C2A-C3A	-2.52	105.88	112.78
19	A	1101	CLA	CHA-C4D-ND	2.52	137.77	132.50
19	B	1227	CLA	C1C-C2C-C3C	-2.52	104.31	106.96
19	G	1701	CLA	CHA-C4D-ND	2.52	137.77	132.50
19	1	614	CLA	CHA-C4D-ND	2.52	137.77	132.50
19	A	1107	CLA	CMB-C2B-C1B	-2.52	124.59	128.46
19	B	1221	CLA	C6-C5-C3	-2.52	106.85	113.45
29	3	607	CHL	C3C-C4C-NC	-2.52	107.75	110.57
19	2	604	CLA	C1C-C2C-C3C	-2.52	104.31	106.96
28	1	502	LUT	C18-C5-C4	2.52	119.02	114.36
22	1	503	BCR	C29-C28-C27	2.52	117.00	111.38
19	B	1203	CLA	C1C-C2C-C3C	-2.52	104.31	106.96
22	2	503	BCR	C24-C25-C26	-2.52	115.37	121.46
29	4	613	CHL	C4D-CHA-C1A	2.52	124.31	121.25
19	A	1111	CLA	CMB-C2B-C3B	2.52	129.38	124.68
23	B	5002	LHG	O8-C23-C24	2.51	119.80	111.91
19	1	604	CLA	C1C-C2C-C3C	-2.51	104.31	106.96
19	3	617	CLA	C1C-C2C-C3C	-2.51	104.31	106.96
19	B	1240	CLA	CHA-C4D-ND	2.51	137.76	132.50
19	L	1503	CLA	CHA-C4D-ND	2.51	137.76	132.50
19	2	608	CLA	CHA-C4D-ND	2.51	137.76	132.50
30	2	502	XAT	C19-C9-C10	-2.51	119.40	122.92
19	G	1701	CLA	O2A-CGA-CBA	2.51	119.79	111.91
19	B	1023	CLA	CMA-C3A-C4A	2.51	118.53	111.77
22	F	4016	BCR	C38-C26-C27	2.51	118.44	113.62
19	B	1213	CLA	CHA-C4D-ND	2.51	137.75	132.50
19	B	1209	CLA	CMB-C2B-C3B	2.51	129.38	124.68
19	2	604	CLA	C2D-C1D-ND	2.51	111.95	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	1212	CLA	CHA-C4D-ND	2.51	137.75	132.50
19	A	1131	CLA	CHA-C4D-ND	2.51	137.75	132.50
19	B	1213	CLA	C1-O2A-CGA	2.51	123.03	116.44
19	B	1234	CLA	O2D-CGD-O1D	-2.51	118.93	123.84
19	1	613	CLA	CHA-C4D-ND	2.51	137.74	132.50
19	A	1139	CLA	CMB-C2B-C3B	2.51	129.37	124.68
19	A	1109	CLA	C1C-C2C-C3C	-2.51	104.32	106.96
19	B	1239	CLA	C1-O2A-CGA	2.51	123.02	116.44
19	1	601	CLA	C2C-C1C-NC	2.51	112.32	109.97
19	A	1130	CLA	CMB-C2B-C1B	-2.51	124.61	128.46
19	A	1135	CLA	CHA-C4D-ND	2.51	137.74	132.50
19	B	1023	CLA	O2D-CGD-O1D	-2.51	118.94	123.84
19	K	1404	CLA	CHA-C1A-NA	-2.50	120.66	126.40
23	A	5001	LHG	O8-C23-C24	2.50	119.77	111.91
19	3	612	CLA	CMA-C3A-C4A	2.50	118.50	111.77
23	2	801	LHG	O8-C23-C24	2.50	119.76	111.91
19	B	1208	CLA	CMD-C2D-C3D	-2.50	121.86	127.61
19	A	1108	CLA	CAA-C2A-C3A	-2.50	105.92	112.78
19	A	1140	CLA	C1D-ND-C4D	-2.50	104.56	106.33
19	B	1225	CLA	O2D-CGD-O1D	-2.50	118.95	123.84
28	3	501	LUT	C15-C14-C13	-2.50	123.74	127.31
19	F	1301	CLA	C1-C2-C3	-2.50	121.72	126.04
19	K	1403	CLA	O2D-CGD-O1D	-2.50	118.95	123.84
19	4	601	CLA	C1C-C2C-C3C	-2.50	104.33	106.96
19	B	1201	CLA	CHA-C4D-ND	2.50	137.73	132.50
19	B	1219	CLA	O2D-CGD-O1D	-2.50	118.95	123.84
19	B	1235	CLA	O2D-CGD-O1D	-2.50	118.95	123.84
19	L	1503	CLA	C1-O2A-CGA	2.50	123.00	116.44
19	3	605	CLA	O2D-CGD-O1D	-2.50	118.95	123.84
19	A	1108	CLA	C1C-C2C-C3C	-2.50	104.33	106.96
19	3	601	CLA	C1C-C2C-C3C	-2.50	104.33	106.96
19	1	604	CLA	C2C-C1C-NC	2.50	112.31	109.97
19	A	1121	CLA	CHA-C4D-ND	2.50	137.73	132.50
19	4	606	CLA	O2A-CGA-CBA	2.50	119.75	111.91
19	3	605	CLA	C1C-C2C-C3C	-2.50	104.33	106.96
19	4	602	CLA	CHA-C4D-ND	2.50	137.72	132.50
22	A	4007	BCR	C33-C5-C4	2.50	118.41	113.62
19	B	1216	CLA	CMB-C2B-C1B	-2.50	124.63	128.46
19	A	1133	CLA	CMB-C2B-C3B	2.50	129.35	124.68
29	4	613	CHL	CMA-C3A-C4A	2.50	118.48	111.77
19	B	1219	CLA	CHA-C4D-ND	2.50	137.72	132.50
19	A	1141	CLA	CMD-C2D-C3D	-2.49	121.88	127.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	I	4018	BCR	C38-C26-C27	2.49	118.41	113.62
22	3	503	BCR	C15-C14-C13	-2.49	123.75	127.31
19	A	1128	CLA	CHA-C4D-ND	2.49	137.72	132.50
19	A	1120	CLA	CMD-C2D-C3D	-2.49	121.88	127.61
19	B	1234	CLA	CMB-C2B-C3B	2.49	129.34	124.68
24	J	5003	LMT	C1'-O5'-C5'	-2.49	108.80	113.69
22	B	4004	BCR	C30-C25-C24	2.49	122.83	115.78
19	1	602	CLA	CHA-C4D-ND	2.49	137.71	132.50
19	A	1013	CLA	O2D-CGD-O1D	-2.49	118.97	123.84
19	4	605	CLA	CMB-C2B-C1B	-2.49	124.63	128.46
19	3	603	CLA	CMA-C3A-C4A	2.49	118.47	111.77
22	L	4020	BCR	C30-C25-C26	-2.49	119.10	122.61
19	2	606	CLA	CHA-C4D-ND	2.49	137.71	132.50
19	3	603	CLA	C1C-C2C-C3C	-2.49	104.34	106.96
19	B	1217	CLA	CHA-C4D-ND	2.49	137.71	132.50
19	4	601	CLA	CHA-C4D-ND	2.49	137.71	132.50
19	A	1104	CLA	C1-C2-C3	-2.49	121.73	126.04
19	B	1217	CLA	O2D-CGD-O1D	-2.49	118.97	123.84
19	A	1132	CLA	CHA-C4D-ND	2.49	137.71	132.50
19	2	602	CLA	CHA-C1A-NA	-2.49	120.70	126.40
24	G	5005	LMT	C1'-O5'-C5'	-2.49	108.80	113.69
22	J	4012	BCR	C3-C4-C5	-2.49	109.63	114.08
23	A	5002	LHG	O8-C23-C24	2.49	119.72	111.91
24	J	5003	LMT	C3'-C4'-C5'	-2.49	105.22	110.93
19	K	1404	CLA	CHA-C4D-ND	2.49	137.70	132.50
19	B	1240	CLA	O1D-CGD-CBD	-2.49	119.39	124.48
25	2	803	LMG	O8-C28-C29	2.49	119.71	111.91
22	3	503	BCR	C27-C26-C25	-2.49	119.12	122.73
19	4	606	CLA	CHA-C4D-ND	2.49	137.70	132.50
31	4	505	C7Z	C31-C32-C33	-2.49	119.43	126.42
22	G	4011	BCR	C35-C13-C14	-2.49	119.44	122.92
22	J	4012	BCR	C29-C28-C27	2.49	116.93	111.38
19	4	607	CLA	C1C-C2C-C3C	-2.49	104.34	106.96
22	B	4009	BCR	C33-C5-C4	2.49	118.39	113.62
19	A	1119	CLA	C1C-C2C-C3C	-2.48	104.34	106.96
19	4	604	CLA	CHA-C4D-ND	2.48	137.70	132.50
19	A	1105	CLA	CHA-C4D-ND	2.48	137.69	132.50
19	F	1301	CLA	O2D-CGD-O1D	-2.48	118.98	123.84
29	4	611	CHL	CHC-C1C-NC	2.48	127.97	124.20
19	G	1602	CLA	CMB-C2B-C3B	2.48	129.32	124.68
19	1	603	CLA	CHA-C4D-ND	2.48	137.69	132.50
19	3	608	CLA	CHA-C4D-ND	2.48	137.69	132.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	G	5003	DGD	O1G-C1A-C2A	2.48	119.69	111.91
19	B	1021	CLA	CHA-C4D-ND	2.48	137.69	132.50
19	B	1211	CLA	CMB-C2B-C1B	-2.48	124.65	128.46
19	A	1120	CLA	O2A-CGA-CBA	2.48	119.69	111.91
19	B	1205	CLA	CHA-C4D-ND	2.48	137.69	132.50
19	4	609	CLA	CHA-C4D-ND	2.48	137.68	132.50
28	4	501	LUT	C10-C11-C12	-2.48	115.48	123.22
19	L	1501	CLA	C2D-C1D-ND	2.48	111.93	110.10
19	3	614	CLA	C1C-C2C-C3C	-2.48	104.35	106.96
19	1	613	CLA	CMD-C2D-C3D	-2.48	121.92	127.61
22	K	4002	BCR	C27-C26-C25	-2.48	119.14	122.73
19	A	1103	CLA	CHA-C4D-ND	2.48	137.68	132.50
19	B	1229	CLA	CHA-C4D-ND	2.48	137.68	132.50
19	B	1220	CLA	C2C-C1C-NC	2.48	112.29	109.97
19	A	1013	CLA	CMB-C2B-C1B	-2.48	124.66	128.46
19	B	1201	CLA	CMB-C2B-C1B	-2.48	124.66	128.46
19	A	1102	CLA	C1C-C2C-C3C	-2.48	104.35	106.96
19	A	1126	CLA	C2D-C1D-ND	2.48	111.93	110.10
19	F	1302	CLA	CMD-C2D-C3D	-2.47	121.92	127.61
19	4	608	CLA	O2D-CGD-O1D	-2.47	119.00	123.84
19	1	605	CLA	CHA-C4D-ND	2.47	137.67	132.50
22	B	4009	BCR	C27-C26-C25	-2.47	119.14	122.73
28	4	501	LUT	C20-C13-C12	2.47	121.97	118.08
19	1	611	CLA	C1C-C2C-C3C	-2.47	104.36	106.96
19	2	601	CLA	C1D-ND-C4D	-2.47	104.58	106.33
22	1	504	BCR	C3-C4-C5	-2.47	109.67	114.08
19	1	601	CLA	CMB-C2B-C3B	2.47	129.30	124.68
19	2	608	CLA	C2D-C1D-ND	2.47	111.92	110.10
19	A	1102	CLA	C1D-ND-C4D	-2.47	104.58	106.33
19	2	608	CLA	O2D-CGD-O1D	-2.47	119.01	123.84
22	A	4017	BCR	C33-C5-C4	2.47	118.36	113.62
19	B	1217	CLA	C1C-C2C-C3C	-2.46	104.36	106.96
19	A	1117	CLA	C2D-C1D-ND	2.46	111.92	110.10
19	A	1110	CLA	C1C-C2C-C3C	-2.46	104.37	106.96
19	J	1901	CLA	C2C-C1C-NC	2.46	112.28	109.97
19	A	1113	CLA	CMA-C3A-C4A	2.46	118.39	111.77
19	4	612	CLA	CHA-C4D-ND	2.46	137.65	132.50
19	4	605	CLA	C2D-C1D-ND	2.46	111.92	110.10
19	B	1022	CLA	O2D-CGD-O1D	-2.46	119.03	123.84
19	3	608	CLA	CAA-C2A-C3A	-2.46	106.04	112.78
19	A	1138	CLA	CMB-C2B-C1B	-2.46	124.69	128.46
29	4	610	CHL	CHD-C4C-C3C	2.46	128.45	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	4	606	CLA	CMB-C2B-C3B	2.46	129.28	124.68
19	B	1207	CLA	C1C-C2C-C3C	-2.46	104.37	106.96
19	A	1112	CLA	C1-C2-C3	-2.46	121.80	126.04
22	G	4011	BCR	C38-C26-C25	-2.46	121.77	124.53
19	A	1101	CLA	O2A-CGA-CBA	2.46	119.61	111.91
19	A	1138	CLA	C2D-C1D-ND	2.45	111.91	110.10
28	1	502	LUT	C15-C35-C34	-2.45	118.45	123.47
19	1	608	CLA	CMD-C2D-C3D	-2.45	121.97	127.61
22	K	4001	BCR	C23-C22-C21	2.45	122.71	118.94
19	B	1211	CLA	CMA-C3A-C4A	2.45	118.37	111.77
19	B	1209	CLA	CHA-C4D-ND	2.45	137.63	132.50
19	A	1110	CLA	CMD-C2D-C3D	-2.45	121.97	127.61
19	3	612	CLA	CMB-C2B-C3B	2.45	129.26	124.68
19	A	1120	CLA	CHA-C4D-ND	2.45	137.62	132.50
19	4	617	CLA	C1-C2-C3	-2.45	121.81	126.04
19	A	1123	CLA	CMB-C2B-C3B	2.45	129.26	124.68
19	B	1232	CLA	O2A-CGA-CBA	2.45	119.60	111.91
19	A	1128	CLA	CMB-C2B-C3B	2.45	129.26	124.68
29	4	613	CHL	C4A-NA-C1A	2.45	107.81	106.71
19	A	1101	CLA	CMD-C2D-C3D	-2.45	121.98	127.61
29	2	609	CHL	CHD-C4C-C3C	2.45	128.44	124.84
19	A	1106	CLA	CHA-C4D-ND	2.45	137.62	132.50
19	K	1402	CLA	C2D-C1D-ND	2.45	111.91	110.10
22	B	4010	BCR	C37-C22-C23	2.45	121.93	118.08
22	L	4019	BCR	C37-C22-C23	2.45	121.93	118.08
19	B	1210	CLA	C1-C2-C3	-2.45	121.81	126.04
27	1	803	DGD	C2G-O2G-C1B	-2.45	111.77	117.79
19	B	1235	CLA	CHA-C4D-ND	2.45	137.62	132.50
19	4	605	CLA	CMA-C3A-C4A	2.45	118.35	111.77
28	4	501	LUT	C7-C8-C9	-2.45	122.54	126.23
19	B	1209	CLA	C2D-C1D-ND	2.45	111.91	110.10
19	3	613	CLA	C2D-C1D-ND	2.45	111.91	110.10
29	4	610	CHL	CHB-C4A-NA	2.44	127.89	124.51
19	4	603	CLA	CHA-C4D-ND	2.44	137.61	132.50
22	L	4019	BCR	C27-C26-C25	-2.44	119.18	122.73
19	B	1212	CLA	O2A-CGA-CBA	2.44	119.58	111.91
19	B	1213	CLA	CMA-C3A-C4A	2.44	118.34	111.77
19	B	1204	CLA	CHA-C4D-ND	2.44	137.61	132.50
19	4	604	CLA	CMB-C2B-C3B	2.44	129.25	124.68
28	2	501	LUT	C39-C29-C28	2.44	121.92	118.08
22	G	4011	BCR	C30-C25-C24	2.44	122.69	115.78
19	B	1230	CLA	CMB-C2B-C3B	2.44	129.25	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	1218	CLA	C1-C2-C3	-2.44	121.82	126.04
19	4	607	CLA	C2C-C1C-NC	2.44	112.26	109.97
19	2	603	CLA	CHA-C4D-ND	2.44	137.60	132.50
19	2	603	CLA	C1C-C2C-C3C	-2.44	104.39	106.96
18	A	1011	CL0	CAA-C2A-C3A	-2.44	106.10	112.78
19	K	1401	CLA	O2D-CGD-O1D	-2.44	119.07	123.84
19	1	605	CLA	C1-O2A-CGA	2.44	122.84	116.44
22	G	4011	BCR	C29-C28-C27	2.44	116.82	111.38
22	K	4002	BCR	C34-C9-C10	-2.44	119.51	122.92
19	A	1106	CLA	CMB-C2B-C1B	-2.44	124.72	128.46
19	B	1225	CLA	C2D-C1D-ND	2.44	111.90	110.10
19	3	613	CLA	CHA-C4D-ND	2.44	137.59	132.50
22	I	4020	BCR	C33-C5-C4	2.43	118.29	113.62
19	1	606	CLA	O2D-CGD-O1D	-2.43	119.08	123.84
19	B	1218	CLA	CMD-C2D-C3D	-2.43	122.02	127.61
19	A	1101	CLA	CAA-C2A-C3A	-2.43	106.11	112.78
19	B	1021	CLA	OBD-CAD-C3D	-2.43	122.66	128.52
19	1	604	CLA	CMB-C2B-C1B	-2.43	124.72	128.46
30	4	502	XAT	C38-C25-C26	-2.43	118.19	122.26
19	B	1238	CLA	C1-C2-C3	-2.43	121.84	126.04
27	B	5005	DGD	O2G-C1B-O1B	-2.43	117.83	123.70
19	B	1218	CLA	C1C-C2C-C3C	-2.43	104.40	106.96
22	J	4012	BCR	C31-C1-C6	-2.43	106.36	110.30
19	A	1125	CLA	C1D-ND-C4D	-2.43	104.61	106.33
19	A	1128	CLA	C2D-C1D-ND	2.43	111.89	110.10
19	1	602	CLA	C2C-C1C-NC	2.43	112.25	109.97
19	2	608	CLA	O2A-CGA-CBA	2.43	119.52	111.91
28	J	4013	LUT	C35-C34-C33	-2.43	123.85	127.31
19	B	1022	CLA	CMB-C2B-C3B	2.43	129.22	124.68
19	A	1117	CLA	CAA-C2A-C3A	-2.43	106.14	112.78
19	4	604	CLA	C1D-ND-C4D	-2.43	104.61	106.33
28	2	501	LUT	C15-C35-C34	-2.42	118.51	123.47
18	A	1011	CL0	C1-C2-C3	-2.42	121.85	126.04
19	L	1503	CLA	CMB-C2B-C3B	2.42	129.21	124.68
20	A	2001	PQN	C2M-C2-C3	-2.42	120.45	124.40
22	A	4002	BCR	C15-C14-C13	2.42	130.77	127.31
19	A	1120	CLA	CMA-C3A-C4A	2.42	118.28	111.77
19	B	1203	CLA	CMB-C2B-C1B	-2.42	124.74	128.46
19	A	1127	CLA	O2A-CGA-CBA	2.42	119.51	111.91
29	4	610	CHL	C1-O2A-CGA	2.42	124.09	116.11
19	B	1206	CLA	O2D-CGD-O1D	-2.42	119.11	123.84
19	B	1217	CLA	C2C-C1C-NC	2.42	112.24	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	1	611	CLA	CHA-C4D-ND	2.42	137.56	132.50
19	B	1218	CLA	CHA-C4D-ND	2.42	137.56	132.50
19	K	1403	CLA	CMC-C2C-C1C	2.42	128.72	125.04
22	A	4011	BCR	C2-C1-C6	2.42	114.20	110.48
29	1	612	CHL	CMA-C3A-C4A	2.42	118.27	111.77
19	A	1112	CLA	C2C-C1C-NC	2.42	112.24	109.97
19	A	1116	CLA	C1C-C2C-C3C	-2.42	104.42	106.96
23	A	5002	LHG	C5-O7-C7	-2.42	111.84	117.79
19	B	1205	CLA	O1D-CGD-CBD	-2.41	119.55	124.48
19	3	617	CLA	CHA-C4D-ND	2.41	137.55	132.50
19	K	1402	CLA	C1-O2A-CGA	2.41	122.77	116.44
19	A	1132	CLA	O1D-CGD-CBD	-2.41	119.55	124.48
19	4	604	CLA	O2A-CGA-CBA	2.41	119.48	111.91
19	B	1238	CLA	C1C-C2C-C3C	-2.41	104.42	106.96
19	G	1701	CLA	CMA-C3A-C4A	2.41	118.25	111.77
19	B	1212	CLA	C1-O2A-CGA	2.41	122.77	116.44
19	B	1210	CLA	C1C-C2C-C3C	-2.41	104.42	106.96
19	B	1203	CLA	C1-O2A-CGA	2.41	122.76	116.44
19	B	1237	CLA	CHA-C4D-ND	2.41	137.53	132.50
19	B	1208	CLA	CMA-C3A-C4A	2.41	118.24	111.77
19	4	602	CLA	CMD-C2D-C3D	-2.41	122.08	127.61
19	1	604	CLA	CMB-C2B-C3B	2.41	129.18	124.68
25	2	802	LMG	O7-C10-O9	-2.40	117.89	123.70
19	A	1124	CLA	CMB-C2B-C3B	2.40	129.18	124.68
29	2	613	CHL	C1B-CHB-C4A	-2.40	125.36	130.12
19	B	1239	CLA	C1D-ND-C4D	-2.40	104.63	106.33
19	A	1118	CLA	CHA-C4D-ND	2.40	137.53	132.50
19	A	1119	CLA	CHA-C4D-ND	2.40	137.53	132.50
22	K	4001	BCR	C30-C25-C26	-2.40	119.23	122.61
19	3	612	CLA	CHA-C4D-ND	2.40	137.52	132.50
19	B	1214	CLA	CMD-C2D-C3D	-2.40	122.09	127.61
19	J	1901	CLA	C2D-C1D-ND	2.40	111.87	110.10
23	2	807	LHG	O8-C23-C24	2.40	119.44	111.91
19	B	1234	CLA	CHA-C1A-NA	-2.40	120.90	126.40
19	B	1231	CLA	CMB-C2B-C3B	2.40	129.17	124.68
19	A	1112	CLA	CHA-C4D-ND	2.40	137.52	132.50
19	F	1301	CLA	O2A-CGA-CBA	2.40	119.43	111.91
19	2	612	CLA	O2D-CGD-O1D	-2.40	119.15	123.84
19	B	1222	CLA	C2D-C1D-ND	2.40	111.87	110.10
19	B	1240	CLA	C2D-C1D-ND	2.40	111.87	110.10
19	B	1209	CLA	CMD-C2D-C3D	-2.40	122.10	127.61
19	B	1231	CLA	CHA-C4D-ND	2.39	137.51	132.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	1227	CLA	CHA-C4D-ND	2.39	137.50	132.50
19	A	1112	CLA	C1C-C2C-C3C	-2.39	104.44	106.96
22	2	503	BCR	C34-C9-C10	-2.39	119.57	122.92
19	B	1211	CLA	C2C-C1C-NC	2.39	112.21	109.97
22	F	4014	BCR	C35-C13-C12	2.39	121.85	118.08
19	1	604	CLA	O2D-CGD-O1D	-2.39	119.16	123.84
19	3	602	CLA	CHA-C4D-ND	2.39	137.50	132.50
28	2	501	LUT	C19-C9-C10	-2.39	119.57	122.92
19	3	606	CLA	CMB-C2B-C3B	2.39	129.15	124.68
29	1	610	CHL	CHC-C1C-NC	2.39	127.83	124.20
19	B	1239	CLA	CHA-C4D-ND	2.39	137.50	132.50
19	K	1401	CLA	CHA-C4D-ND	2.39	137.50	132.50
19	1	603	CLA	CBA-CAA-C2A	2.39	120.91	113.86
19	3	602	CLA	C1C-C2C-C3C	-2.39	104.44	106.96
19	B	1234	CLA	CHA-C4D-ND	2.39	137.50	132.50
22	A	4003	BCR	C15-C14-C13	2.39	130.72	127.31
29	1	610	CHL	CHD-C4C-C3C	2.39	128.35	124.84
19	A	1107	CLA	CHA-C4D-ND	2.39	137.49	132.50
19	A	1126	CLA	CHA-C4D-ND	2.39	137.49	132.50
19	1	611	CLA	CMB-C2B-C1B	-2.39	124.80	128.46
22	B	4005	BCR	C35-C13-C12	2.39	121.84	118.08
19	B	1216	CLA	CHA-C4D-ND	2.38	137.48	132.50
19	1	606	CLA	O2A-CGA-CBA	2.38	119.38	111.91
19	2	602	CLA	C1-C2-C3	-2.38	121.92	126.04
19	A	1128	CLA	CMA-C3A-C4A	2.38	118.17	111.77
19	B	1230	CLA	CHA-C4D-ND	2.38	137.48	132.50
19	A	1122	CLA	CAA-C2A-C3A	-2.38	106.26	112.78
19	B	1215	CLA	CMB-C2B-C1B	-2.38	124.81	128.46
19	3	610	CLA	CHA-C4D-ND	2.38	137.48	132.50
19	A	1122	CLA	C1D-ND-C4D	-2.38	104.64	106.33
19	A	1138	CLA	O2D-CGD-O1D	-2.38	119.19	123.84
19	A	1126	CLA	C1-O2A-CGA	2.38	122.68	116.44
19	B	1202	CLA	C2C-C1C-NC	2.38	112.20	109.97
19	A	1121	CLA	CMD-C2D-C3D	-2.38	122.15	127.61
19	B	1207	CLA	CMA-C3A-C4A	2.38	118.16	111.77
19	4	612	CLA	O2A-CGA-CBA	2.38	119.36	111.91
19	L	1501	CLA	CHA-C4D-ND	2.37	137.47	132.50
19	A	1012	CLA	OBD-CAD-C3D	-2.37	122.81	128.52
19	A	1126	CLA	C1C-C2C-C3C	-2.37	104.46	106.96
19	3	613	CLA	CMD-C2D-C3D	-2.37	122.15	127.61
22	G	4021	BCR	C19-C18-C17	2.37	122.58	118.94
22	K	4002	BCR	C30-C25-C26	-2.37	119.27	122.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	1102	CLA	CMD-C2D-C3D	-2.37	122.16	127.61
19	A	1123	CLA	CHA-C1A-NA	-2.37	120.97	126.40
22	L	4020	BCR	C33-C5-C4	2.37	118.17	113.62
19	A	1124	CLA	CHA-C4D-ND	2.37	137.46	132.50
19	B	1204	CLA	CMA-C3A-C4A	2.37	118.15	111.77
19	1	601	CLA	CHA-C4D-ND	2.37	137.46	132.50
19	4	601	CLA	CAA-C2A-C3A	-2.37	106.29	112.78
19	1	605	CLA	O2D-CGD-O1D	-2.37	119.20	123.84
19	L	1503	CLA	C2D-C1D-ND	2.37	111.85	110.10
19	1	601	CLA	CHA-C1A-NA	-2.37	120.97	126.40
19	A	1111	CLA	CAA-C2A-C1A	-2.37	104.21	111.97
19	A	1103	CLA	C1-O2A-CGA	2.37	122.66	116.44
24	B	5008	LMT	C3'-C4'-C5'	-2.37	105.50	110.93
19	J	1901	CLA	O2A-CGA-CBA	2.37	119.34	111.91
19	B	1209	CLA	C1D-ND-C4D	-2.37	104.65	106.33
18	A	1011	CL0	C4-C3-C5	2.37	119.25	115.27
19	A	1116	CLA	C2D-C1D-ND	2.37	111.85	110.10
22	B	4010	BCR	C28-C27-C26	-2.37	109.85	114.08
18	A	1011	CL0	CHA-C4D-ND	2.36	137.44	132.50
19	A	1139	CLA	CHA-C4D-ND	2.36	137.44	132.50
25	F	5002	LMG	O7-C10-O9	-2.36	117.99	123.70
19	3	601	CLA	O1D-CGD-CBD	-2.36	119.65	124.48
19	A	1130	CLA	O2A-CGA-CBA	2.36	119.32	111.91
19	A	1117	CLA	CMA-C3A-C4A	2.36	118.12	111.77
19	A	1121	CLA	CHA-C1A-NA	-2.36	120.99	126.40
19	B	1208	CLA	CHA-C4D-ND	2.36	137.44	132.50
19	A	1127	CLA	CHA-C4D-ND	2.36	137.43	132.50
19	B	1226	CLA	O1D-CGD-CBD	-2.36	119.66	124.48
19	B	1216	CLA	O2A-CGA-CBA	2.36	119.31	111.91
19	B	1210	CLA	CED-O2D-CGD	-2.36	110.60	115.94
29	4	611	CHL	C3A-C2A-C1A	2.36	104.87	101.34
19	1	602	CLA	O2D-CGD-O1D	-2.36	119.23	123.84
19	A	1115	CLA	CHA-C4D-ND	2.36	137.43	132.50
19	A	1125	CLA	O2A-CGA-CBA	2.36	119.31	111.91
22	G	4011	BCR	C23-C24-C25	-2.36	120.58	127.20
19	4	612	CLA	CMA-C3A-C4A	2.36	118.11	111.77
22	3	506	BCR	C30-C25-C24	2.36	122.45	115.78
19	A	1103	CLA	CAA-C2A-C1A	-2.36	104.25	111.97
19	A	1114	CLA	CMD-C2D-C3D	-2.36	122.20	127.61
19	A	1137	CLA	CHA-C1A-NA	-2.35	121.00	126.40
19	A	1105	CLA	CMB-C2B-C3B	2.35	129.08	124.68
19	A	1135	CLA	O2A-CGA-CBA	2.35	119.30	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	1207	CLA	CMC-C2C-C1C	2.35	128.62	125.04
19	2	612	CLA	CHA-C4D-ND	2.35	137.42	132.50
19	4	606	CLA	C2D-C1D-ND	2.35	111.84	110.10
19	B	1236	CLA	C2D-C1D-ND	2.35	111.84	110.10
19	B	1211	CLA	O2D-CGD-O1D	-2.35	119.24	123.84
27	3	803	DGD	O1G-C1A-C2A	2.35	119.28	111.91
19	F	1302	CLA	C1D-ND-C4D	-2.35	104.67	106.33
19	B	1236	CLA	CHA-C4D-ND	2.35	137.41	132.50
19	K	1402	CLA	CHA-C1A-NA	-2.35	121.02	126.40
19	B	1217	CLA	O1D-CGD-CBD	-2.35	119.68	124.48
19	4	609	CLA	CBC-CAC-C3C	-2.35	105.96	112.43
19	A	1137	CLA	C2C-C1C-NC	2.35	112.17	109.97
19	A	1136	CLA	CHA-C4D-ND	2.35	137.41	132.50
19	B	1022	CLA	CHA-C4D-ND	2.35	137.41	132.50
22	3	503	BCR	C12-C13-C14	-2.35	115.34	118.94
19	A	1109	CLA	C2C-C1C-NC	2.35	112.17	109.97
19	B	1214	CLA	OBD-CAD-C3D	-2.34	122.88	128.52
29	4	615	CHL	C1B-CHB-C4A	-2.34	125.47	130.12
19	B	1224	CLA	CMB-C2B-C3B	2.34	129.06	124.68
19	A	1133	CLA	CHA-C4D-ND	2.34	137.40	132.50
19	G	1603	CLA	CHA-C4D-ND	2.34	137.40	132.50
19	B	1219	CLA	O2A-CGA-CBA	2.34	119.25	111.91
19	1	606	CLA	CHA-C4D-ND	2.34	137.39	132.50
24	B	5008	LMT	C3B-C4B-C5B	-2.34	106.06	110.24
19	K	1404	CLA	CMA-C3A-C4A	2.34	118.06	111.77
19	1	602	CLA	CMA-C3A-C4A	2.34	118.06	111.77
25	B	5003	LMG	O7-C10-O9	-2.34	118.05	123.70
31	4	505	C7Z	C24-C25-C26	-2.34	115.64	120.85
28	4	501	LUT	C35-C15-C14	-2.34	118.68	123.47
19	F	1302	CLA	CHA-C4D-ND	2.34	137.39	132.50
19	B	1211	CLA	CAA-C2A-C3A	-2.34	106.38	112.78
19	4	605	CLA	CGD-CBD-CAD	-2.34	103.17	110.73
19	A	1109	CLA	CHA-C4D-ND	2.34	137.39	132.50
19	A	1132	CLA	O2A-CGA-CBA	2.34	119.24	111.91
19	A	1137	CLA	O2A-CGA-CBA	2.34	119.24	111.91
19	B	1219	CLA	CMD-C2D-C3D	-2.33	122.24	127.61
19	B	1220	CLA	CAA-C2A-C1A	-2.33	104.33	111.97
19	A	1129	CLA	CMB-C2B-C3B	2.33	129.04	124.68
19	B	1208	CLA	C1-O2A-CGA	2.33	122.57	116.44
19	A	1107	CLA	C1-C2-C3	-2.33	122.01	126.04
30	2	502	XAT	C24-C23-C22	-2.33	106.27	110.77
19	A	1105	CLA	C6-C5-C3	-2.33	107.34	113.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	1121	CLA	O2D-CGD-O1D	-2.33	119.28	123.84
27	4	801	DGD	O6E-C5E-C4E	2.33	113.93	109.69
19	A	1134	CLA	CHA-C4D-ND	2.33	137.38	132.50
19	A	1111	CLA	CHA-C4D-ND	2.33	137.38	132.50
22	L	4019	BCR	C35-C13-C12	2.33	121.75	118.08
19	B	1202	CLA	CMD-C2D-C3D	-2.33	122.25	127.61
22	1	504	BCR	C34-C9-C10	-2.33	119.66	122.92
19	2	602	CLA	C1-O2A-CGA	2.33	122.56	116.44
22	A	4017	BCR	C8-C9-C10	2.33	122.52	118.94
22	1	504	BCR	C8-C7-C6	-2.33	120.66	127.20
19	1	607	CLA	CHA-C4D-ND	2.33	137.37	132.50
29	4	613	CHL	CHB-C4A-NA	2.33	127.73	124.51
19	1	613	CLA	O2D-CGD-O1D	-2.33	119.29	123.84
29	4	611	CHL	C4A-NA-C1A	2.33	107.75	106.71
19	1	607	CLA	O2D-CGD-O1D	-2.33	119.29	123.84
19	B	1212	CLA	CMA-C3A-C4A	2.33	118.02	111.77
19	A	1108	CLA	CMB-C2B-C1B	-2.33	124.89	128.46
29	3	604	CHL	CHC-C1C-NC	2.32	127.73	124.20
19	B	1225	CLA	CHA-C4D-ND	2.32	137.36	132.50
19	B	1223	CLA	CHA-C1A-NA	-2.32	121.08	126.40
19	1	603	CLA	C1D-ND-C4D	-2.32	104.68	106.33
19	A	1132	CLA	C1C-C2C-C3C	-2.32	104.51	106.96
19	L	1503	CLA	CMD-C2D-C3D	-2.32	122.27	127.61
19	B	1210	CLA	C6-C5-C3	-2.32	107.36	113.45
19	2	607	CLA	C1-C2-C3	-2.32	122.03	126.04
30	4	502	XAT	C32-C33-C34	2.32	122.50	118.94
19	4	601	CLA	CHA-C1A-NA	-2.32	121.08	126.40
19	2	607	CLA	CMB-C2B-C3B	2.32	129.02	124.68
29	2	613	CHL	C2C-C3C-C4C	2.32	108.14	106.49
19	B	1210	CLA	CMB-C2B-C1B	-2.32	124.90	128.46
19	B	1021	CLA	O2A-CGA-CBA	2.32	119.19	111.91
22	L	4019	BCR	C33-C5-C6	-2.32	121.92	124.53
25	B	5007	LMG	C8-O7-C10	-2.32	112.08	117.79
22	A	4011	BCR	C4-C5-C6	-2.32	119.36	122.73
19	2	603	CLA	CMD-C2D-C3D	-2.32	122.28	127.61
19	A	1133	CLA	CAA-C2A-C3A	-2.32	106.43	112.78
19	B	1225	CLA	C1C-C2C-C3C	-2.32	104.52	106.96
19	3	610	CLA	O2D-CGD-O1D	-2.32	119.31	123.84
19	A	1132	CLA	CMA-C3A-C4A	2.32	118.00	111.77
19	2	606	CLA	CBA-CAA-C2A	2.32	120.70	113.86
24	B	5006	LMT	O5B-C5B-C4B	2.32	113.90	109.69
19	A	1105	CLA	O2A-CGA-CBA	2.32	119.17	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	J	4013	LUT	C19-C9-C10	-2.32	119.68	122.92
18	A	1011	CL0	CMC-C2C-C1C	2.31	128.56	125.04
19	3	602	CLA	O2A-CGA-CBA	2.31	119.17	111.91
19	K	1403	CLA	O2A-CGA-CBA	2.31	119.16	111.91
19	3	610	CLA	O2A-CGA-CBA	2.31	119.16	111.91
19	A	1102	CLA	CHA-C4D-ND	2.31	137.33	132.50
19	F	1301	CLA	CHA-C4D-ND	2.31	137.33	132.50
19	4	602	CLA	O1D-CGD-CBD	-2.31	119.75	124.48
19	1	613	CLA	C1C-C2C-C3C	-2.31	104.53	106.96
19	B	1220	CLA	CHA-C4D-ND	2.31	137.33	132.50
19	A	1109	CLA	C1-O2A-CGA	2.31	122.50	116.44
19	2	603	CLA	CMA-C3A-C4A	2.31	117.98	111.77
29	4	613	CHL	C2C-C3C-C4C	2.31	108.13	106.49
19	4	603	CLA	C1-O2A-CGA	2.31	122.50	116.44
19	A	1012	CLA	O2A-CGA-CBA	2.30	119.14	111.91
19	G	1603	CLA	C1D-ND-C4D	-2.30	104.70	106.33
19	A	1111	CLA	O1D-CGD-CBD	-2.30	119.77	124.48
19	2	604	CLA	CHA-C4D-ND	2.30	137.32	132.50
19	B	1206	CLA	CBC-CAC-C3C	-2.30	106.08	112.43
22	I	4018	BCR	C30-C25-C26	-2.30	119.37	122.61
19	A	1126	CLA	CMB-C2B-C3B	2.30	128.99	124.68
19	A	1138	CLA	CHA-C4D-ND	2.30	137.31	132.50
19	4	603	CLA	C1D-ND-C4D	-2.30	104.70	106.33
29	1	612	CHL	C1B-CHB-C4A	-2.30	125.56	130.12
19	B	1221	CLA	O2A-CGA-CBA	2.30	119.12	111.91
19	A	1137	CLA	C1C-C2C-C3C	-2.30	104.54	106.96
19	L	1502	CLA	CHA-C4D-ND	2.30	137.30	132.50
22	B	4010	BCR	C33-C5-C4	2.30	118.03	113.62
19	4	617	CLA	CHA-C4D-ND	2.30	137.30	132.50
19	B	1234	CLA	O1D-CGD-CBD	-2.30	119.79	124.48
19	2	606	CLA	O2D-CGD-O1D	-2.29	119.35	123.84
19	3	610	CLA	CMD-C2D-C3D	-2.29	122.33	127.61
19	B	1202	CLA	CHA-C1A-NA	-2.29	121.14	126.40
19	B	1227	CLA	O2A-CGA-CBA	2.29	119.11	111.91
22	A	4017	BCR	C30-C25-C26	-2.29	119.38	122.61
30	4	502	XAT	C27-C28-C29	2.29	129.09	125.53
19	4	608	CLA	CHA-C4D-ND	2.29	137.30	132.50
19	A	1110	CLA	O2A-CGA-CBA	2.29	119.10	111.91
19	B	1220	CLA	O2A-CGA-CBA	2.29	119.10	111.91
19	B	1206	CLA	CHA-C4D-ND	2.29	137.29	132.50
19	2	601	CLA	CHA-C4D-ND	2.29	137.29	132.50
19	A	1126	CLA	O2A-CGA-CBA	2.29	119.10	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	1	603	CLA	CHA-C1A-NA	-2.29	121.15	126.40
19	B	1238	CLA	O2A-CGA-CBA	2.29	119.10	111.91
28	1	501	LUT	C2-C3-C4	-2.29	107.17	110.30
19	J	1901	CLA	CMD-C2D-C3D	-2.29	122.34	127.61
19	B	1211	CLA	C1C-C2C-C3C	-2.29	104.55	106.96
22	1	503	BCR	C38-C26-C27	2.29	118.02	113.62
19	B	1240	CLA	C1-C2-C3	-2.29	122.08	126.04
19	A	1122	CLA	CHA-C4D-ND	2.29	137.29	132.50
22	1	503	BCR	C34-C9-C10	-2.29	119.72	122.92
19	B	1238	CLA	CHA-C4D-ND	2.29	137.28	132.50
19	B	1216	CLA	C1C-C2C-C3C	-2.29	104.55	106.96
19	B	1021	CLA	CHA-C1A-NA	-2.29	121.16	126.40
19	3	605	CLA	CHA-C1A-NA	-2.29	121.16	126.40
22	A	4007	BCR	C31-C1-C6	-2.29	106.59	110.30
19	B	1240	CLA	CMA-C3A-C4A	2.29	117.92	111.77
30	4	502	XAT	C26-C27-C28	-2.29	121.16	125.99
19	2	605	CLA	CMD-C2D-C3D	-2.29	122.36	127.61
19	3	606	CLA	O2A-CGA-CBA	2.28	119.08	111.91
19	B	1217	CLA	CMC-C2C-C1C	2.28	128.52	125.04
19	1	601	CLA	C2A-C1A-CHA	2.28	127.85	123.86
19	B	1221	CLA	CHA-C1A-NA	-2.28	121.17	126.40
19	A	1140	CLA	C2C-C1C-NC	2.28	112.11	109.97
28	3	502	LUT	C31-C32-C33	-2.28	120.01	126.42
30	4	502	XAT	C15-C14-C13	-2.28	124.06	127.31
19	3	606	CLA	C2D-C1D-ND	2.28	111.78	110.10
19	B	1202	CLA	O2A-CGA-CBA	2.28	119.06	111.91
29	4	615	CHL	CHB-C4A-NA	2.28	127.66	124.51
19	A	1106	CLA	C2D-C1D-ND	2.28	111.78	110.10
19	B	1215	CLA	C2D-C1D-ND	2.28	111.78	110.10
22	I	4020	BCR	C38-C26-C25	-2.28	121.97	124.53
19	A	1133	CLA	C1-O2A-CGA	2.28	122.42	116.44
22	K	4002	BCR	C23-C24-C25	-2.28	120.81	127.20
19	B	1215	CLA	C1D-ND-C4D	-2.27	104.72	106.33
27	4	801	DGD	O5D-C6D-C5D	2.27	113.26	109.05
19	G	1701	CLA	O2D-CGD-O1D	-2.27	119.39	123.84
19	A	1131	CLA	CMA-C3A-C4A	2.27	117.89	111.77
19	B	1223	CLA	C3D-C2D-C1D	-2.27	102.73	105.83
19	A	1141	CLA	O2A-CGA-CBA	2.27	119.04	111.91
19	A	1140	CLA	O1D-CGD-CBD	-2.27	119.83	124.48
19	B	1023	CLA	CAC-C3C-C4C	2.27	127.76	124.81
19	A	1113	CLA	CMB-C2B-C3B	2.27	128.93	124.68
19	A	1122	CLA	C1C-C2C-C3C	-2.27	104.57	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	3	602	CLA	CHA-C1A-NA	-2.27	121.19	126.40
19	2	603	CLA	C3D-C2D-C1D	-2.27	102.73	105.83
19	A	1108	CLA	C3D-C2D-C1D	-2.27	102.73	105.83
19	3	602	CLA	C6-C5-C3	-2.27	110.91	114.62
19	A	1013	CLA	O2A-CGA-CBA	2.27	119.03	111.91
19	A	1122	CLA	O2A-CGA-CBA	2.27	119.03	111.91
22	J	4012	BCR	C35-C13-C12	2.27	121.65	118.08
19	2	612	CLA	CMB-C2B-C3B	2.27	128.93	124.68
19	B	1228	CLA	O2A-CGA-CBA	2.27	119.03	111.91
19	A	1101	CLA	C2D-C1D-ND	2.27	111.78	110.10
24	G	5004	LMT	O5B-C5B-C4B	2.27	113.81	109.69
19	B	1210	CLA	C1D-ND-C4D	-2.27	104.72	106.33
19	A	1113	CLA	C2D-C1D-ND	2.27	111.78	110.10
19	A	1115	CLA	C2D-C1D-ND	2.27	111.78	110.10
19	3	610	CLA	C2D-C1D-ND	2.27	111.78	110.10
19	A	1140	CLA	O2D-CGD-O1D	-2.27	119.41	123.84
22	A	4011	BCR	C33-C5-C4	2.27	117.97	113.62
19	A	1110	CLA	C1D-ND-C4D	-2.27	104.72	106.33
19	L	1502	CLA	C3D-C2D-C1D	-2.27	102.74	105.83
19	3	617	CLA	O2A-CGA-CBA	2.27	119.02	111.91
19	A	1103	CLA	C1C-C2C-C3C	-2.26	104.58	106.96
19	1	613	CLA	C2D-C1D-ND	2.26	111.77	110.10
19	B	1226	CLA	CHA-C4D-ND	2.26	137.24	132.50
30	2	502	XAT	C39-C29-C30	-2.26	119.75	122.92
19	2	601	CLA	CMD-C2D-C3D	-2.26	122.41	127.61
19	A	1129	CLA	CHA-C4D-ND	2.26	137.23	132.50
19	B	1023	CLA	CHA-C4D-ND	2.26	137.23	132.50
29	3	604	CHL	CMB-C2B-C1B	-2.26	124.98	128.46
29	2	610	CHL	CMA-C3A-C2A	2.26	122.96	113.83
19	1	603	CLA	O2D-CGD-O1D	-2.26	119.41	123.84
19	B	1023	CLA	C1C-C2C-C3C	-2.26	104.58	106.96
22	K	4001	BCR	C34-C9-C10	-2.26	119.75	122.92
19	A	1140	CLA	CMD-C2D-C3D	-2.26	122.41	127.61
19	A	1139	CLA	CAA-C2A-C3A	-2.26	106.58	112.78
19	B	1222	CLA	O1D-CGD-CBD	-2.26	119.86	124.48
29	2	609	CHL	C1B-CHB-C4A	-2.26	125.64	130.12
19	A	1125	CLA	CMA-C3A-C4A	2.26	117.85	111.77
22	B	4006	BCR	C1-C6-C7	2.26	122.18	115.78
19	A	1124	CLA	CAA-C2A-C1A	-2.26	104.57	111.97
19	B	1218	CLA	OBD-CAD-C3D	-2.26	123.08	128.52
19	3	603	CLA	C1D-ND-C4D	-2.26	104.73	106.33
19	3	610	CLA	C1-C2-C3	-2.26	122.14	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	1125	CLA	CHA-C4D-ND	2.26	137.22	132.50
19	4	605	CLA	C1-C2-C3	-2.26	122.14	126.04
19	1	613	CLA	CMB-C2B-C3B	2.26	128.90	124.68
19	B	1221	CLA	CMB-C2B-C1B	-2.26	124.99	128.46
19	A	1111	CLA	C1D-ND-C4D	-2.26	104.73	106.33
29	2	610	CHL	C4A-NA-C1A	2.26	107.72	106.71
19	3	605	CLA	CMD-C2D-C3D	-2.26	122.43	127.61
22	L	4019	BCR	C36-C18-C17	-2.26	119.76	122.92
19	1	608	CLA	O1D-CGD-CBD	-2.25	119.87	124.48
19	G	1701	CLA	O1D-CGD-CBD	-2.25	119.87	124.48
19	1	603	CLA	CMA-C3A-C4A	2.25	117.83	111.77
19	4	609	CLA	CMA-C3A-C4A	2.25	117.83	111.77
19	B	1222	CLA	CMB-C2B-C1B	-2.25	125.01	128.46
19	4	607	CLA	CHA-C4D-ND	2.25	137.21	132.50
19	B	1207	CLA	C1D-ND-C4D	-2.25	104.74	106.33
19	L	1502	CLA	C1D-ND-C4D	-2.25	104.74	106.33
19	B	1210	CLA	CHA-C1A-NA	-2.25	121.25	126.40
19	B	1232	CLA	CMD-C2D-C3D	-2.25	122.44	127.61
19	4	609	CLA	O2A-CGA-CBA	2.25	118.96	111.91
19	1	606	CLA	C1D-ND-C4D	-2.25	104.74	106.33
19	1	602	CLA	CBA-CAA-C2A	-2.25	107.23	113.86
19	B	1223	CLA	CMA-C3A-C4A	2.25	117.81	111.77
19	2	606	CLA	CHA-C1A-NA	-2.25	121.25	126.40
19	1	605	CLA	O1D-CGD-CBD	-2.25	119.89	124.48
19	B	1022	CLA	C1-O2A-CGA	2.24	122.33	116.44
19	A	1123	CLA	C2D-C1D-ND	2.24	111.76	110.10
19	B	1220	CLA	CMD-C2D-C3D	-2.24	122.45	127.61
19	B	1228	CLA	CMB-C2B-C3B	2.24	128.88	124.68
19	4	605	CLA	O2D-CGD-O1D	-2.24	119.45	123.84
19	A	1118	CLA	O1D-CGD-CBD	-2.24	119.89	124.48
19	A	1134	CLA	CMA-C3A-C4A	2.24	117.80	111.77
19	A	1131	CLA	O2A-CGA-CBA	2.24	118.94	111.91
19	B	1231	CLA	O2A-CGA-CBA	2.24	118.94	111.91
19	A	1128	CLA	CAA-C2A-C3A	-2.24	106.64	112.78
22	G	4011	BCR	C37-C22-C21	-2.24	119.78	122.92
19	G	1601	CLA	CHA-C1A-NA	-2.24	121.27	126.40
19	3	614	CLA	CHA-C1A-NA	-2.24	121.27	126.40
29	3	611	CHL	CHC-C1C-NC	2.24	127.60	124.20
19	B	1205	CLA	C1-C2-C3	-2.24	122.17	126.04
19	B	1021	CLA	C2D-C1D-ND	2.24	111.75	110.10
22	2	503	BCR	C2-C3-C4	-2.24	106.38	111.38
19	2	601	CLA	CMB-C2B-C3B	2.24	128.87	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	J	1901	CLA	C1C-C2C-C3C	-2.24	104.60	106.96
19	A	1139	CLA	C1D-ND-C4D	-2.24	104.75	106.33
22	I	4018	BCR	C1-C6-C7	2.24	122.11	115.78
19	B	1236	CLA	CMD-C2D-C3D	-2.24	122.47	127.61
19	A	1110	CLA	CHA-C1A-NA	-2.24	121.28	126.40
28	J	4013	LUT	C18-C5-C6	-2.24	122.02	124.53
22	A	4007	BCR	C28-C27-C26	-2.24	110.09	114.08
19	1	601	CLA	O2D-CGD-O1D	-2.23	119.47	123.84
19	A	1138	CLA	C11-C10-C8	-2.23	108.70	115.92
19	B	1218	CLA	C2C-C1C-NC	2.23	112.06	109.97
19	4	605	CLA	OBD-CAD-C3D	-2.23	123.14	128.52
19	A	1112	CLA	CHA-C1A-NA	-2.23	121.28	126.40
19	3	613	CLA	CHA-C1A-NA	-2.23	121.28	126.40
19	4	602	CLA	C1-O2A-CGA	2.23	122.30	116.44
19	B	1023	CLA	CAA-C2A-C3A	-2.23	106.66	112.78
19	A	1141	CLA	C2D-C1D-ND	2.23	111.75	110.10
19	3	606	CLA	CMD-C2D-C3D	-2.23	122.48	127.61
19	B	1232	CLA	C1C-C2C-C3C	-2.23	104.61	106.96
19	3	612	CLA	CAA-CBA-CGA	-2.23	106.73	113.25
29	1	609	CHL	C4D-CHA-C1A	2.23	123.96	121.25
22	I	4018	BCR	C1-C6-C5	-2.23	119.47	122.61
28	J	4013	LUT	C37-C21-C22	-2.23	105.21	109.44
19	3	608	CLA	O2D-CGD-O1D	-2.23	119.48	123.84
19	B	1201	CLA	CMA-C3A-C4A	2.23	117.77	111.77
19	B	1236	CLA	CHA-C1A-NA	-2.23	121.29	126.40
19	A	1108	CLA	O2A-CGA-CBA	2.23	118.90	111.91
19	B	1240	CLA	CMB-C2B-C1B	-2.23	125.04	128.46
19	4	602	CLA	C1D-ND-C4D	-2.23	104.75	106.33
19	G	1601	CLA	CMB-C2B-C3B	2.23	128.85	124.68
28	4	501	LUT	C11-C10-C9	-2.23	124.13	127.31
22	F	4016	BCR	C12-C13-C14	-2.23	115.52	118.94
19	A	1140	CLA	C1-O2A-CGA	2.23	122.29	116.44
19	1	607	CLA	CHA-C1A-NA	-2.23	121.30	126.40
19	1	602	CLA	C1C-C2C-C3C	-2.23	104.61	106.96
19	A	1109	CLA	C3D-C2D-C1D	-2.23	102.79	105.83
19	2	602	CLA	C1C-C2C-C3C	-2.23	104.62	106.96
19	3	603	CLA	CHA-C4D-ND	2.23	137.15	132.50
28	1	502	LUT	C39-C29-C28	2.23	121.58	118.08
19	A	1104	CLA	C11-C12-C13	-2.23	108.73	115.92
19	B	1210	CLA	C16-C15-C13	-2.22	108.73	115.92
19	L	1502	CLA	CMB-C2B-C1B	-2.22	125.05	128.46
19	B	1218	CLA	CHA-C1A-NA	-2.22	121.30	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	1103	CLA	C3D-C2D-C1D	-2.22	102.80	105.83
28	1	501	LUT	C8-C7-C6	-2.22	120.96	127.20
19	A	1117	CLA	CHA-C4D-ND	2.22	137.15	132.50
19	A	1127	CLA	C1-O2A-CGA	2.22	122.28	116.44
19	A	1103	CLA	C6-C5-C3	-2.22	107.63	113.45
19	4	601	CLA	C3D-C2D-C1D	-2.22	102.80	105.83
25	B	5003	LMG	C7-O1-C1	-2.22	109.40	113.74
19	1	601	CLA	CAA-C2A-C3A	-2.22	106.69	112.78
19	A	1127	CLA	CAA-C2A-C3A	-2.22	106.69	112.78
22	B	4006	BCR	C7-C6-C5	-2.22	116.08	121.46
19	K	1403	CLA	C2D-C1D-ND	2.22	111.74	110.10
19	2	605	CLA	O2A-CGA-CBA	2.22	118.87	111.91
23	B	5001	LHG	O7-C7-O9	-2.22	118.55	122.96
19	B	1222	CLA	CHA-C4D-ND	2.22	137.14	132.50
19	G	1602	CLA	C1D-ND-C4D	-2.22	104.76	106.33
30	2	502	XAT	C16-C1-C6	-2.22	104.06	110.05
19	3	601	CLA	CHA-C1A-NA	-2.22	121.32	126.40
29	4	615	CHL	CHC-C1C-NC	2.22	127.57	124.20
29	2	610	CHL	CMB-C2B-C1B	-2.22	125.06	128.46
19	3	602	CLA	C1D-ND-C4D	-2.22	104.76	106.33
22	A	4007	BCR	C15-C14-C13	-2.22	124.15	127.31
24	B	5006	LMT	C3'-C4'-C5'	-2.22	105.84	110.93
19	2	604	CLA	CMD-C2D-C3D	-2.22	122.52	127.61
20	A	2001	PQN	C21-C22-C23	-2.22	108.76	115.92
31	4	505	C7Z	C18-C5-C4	-2.22	110.25	114.36
19	3	608	CLA	C1D-ND-C4D	-2.21	104.76	106.33
19	A	1012	CLA	C4-C3-C2	-2.21	118.00	123.68
19	4	601	CLA	O2A-CGA-CBA	2.21	118.86	111.91
19	A	1139	CLA	CMD-C2D-C3D	-2.21	122.52	127.61
19	A	1104	CLA	O2A-CGA-CBA	2.21	118.85	111.91
19	A	1113	CLA	CAA-CBA-CGA	-2.21	106.63	112.51
22	1	503	BCR	C1-C6-C7	2.21	122.04	115.78
25	B	5004	LMG	O6-C5-C6	2.21	111.94	106.44
19	4	612	CLA	O2D-CGD-O1D	-2.21	119.51	123.84
19	B	1022	CLA	CHA-C1A-NA	-2.21	121.33	126.40
27	1	803	DGD	O1G-C1A-C2A	2.21	118.85	111.91
19	4	606	CLA	O2D-CGD-O1D	-2.21	119.51	123.84
19	3	603	CLA	O1D-CGD-CBD	-2.21	119.96	124.48
19	A	1107	CLA	C1-O2A-CGA	2.21	122.25	116.44
19	B	1225	CLA	CMD-C2D-C3D	-2.21	122.53	127.61
19	2	606	CLA	CMB-C2B-C3B	2.21	128.81	124.68
19	A	1140	CLA	CHA-C4D-ND	2.21	137.12	132.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	1123	CLA	O2A-CGA-CBA	2.21	118.84	111.91
22	G	4011	BCR	C34-C9-C10	-2.21	119.83	122.92
22	A	4002	BCR	C37-C22-C23	2.21	121.56	118.08
19	B	1202	CLA	C1C-C2C-C3C	-2.21	104.63	106.96
19	3	617	CLA	O1D-CGD-CBD	-2.21	119.96	124.48
19	A	1127	CLA	C2D-C1D-ND	2.21	111.73	110.10
19	B	1208	CLA	O2A-CGA-CBA	2.21	118.84	111.91
19	A	1141	CLA	CHA-C1A-NA	-2.21	121.34	126.40
19	L	1501	CLA	O1D-CGD-CBD	-2.21	119.97	124.48
19	B	1201	CLA	C3D-C2D-C1D	-2.21	102.82	105.83
19	K	1401	CLA	CMD-C2D-C3D	-2.21	122.54	127.61
19	B	1240	CLA	CHA-C1A-NA	-2.21	121.34	126.40
19	2	607	CLA	CHA-C1A-NA	-2.21	121.34	126.40
19	B	1235	CLA	CMD-C2D-C3D	-2.21	122.54	127.61
19	A	1121	CLA	C1D-ND-C4D	-2.21	104.77	106.33
19	1	603	CLA	C1C-C2C-C3C	-2.21	104.64	106.96
22	G	4021	BCR	C15-C14-C13	-2.20	124.16	127.31
19	B	1234	CLA	CMA-C3A-C4A	2.20	117.70	111.77
19	2	602	CLA	O2D-CGD-O1D	-2.20	119.53	123.84
30	4	502	XAT	C39-C29-C30	-2.20	119.84	122.92
22	A	4011	BCR	C15-C14-C13	2.20	130.45	127.31
19	1	605	CLA	CMD-C2D-C3D	-2.20	122.55	127.61
19	B	1220	CLA	CAA-CBA-CGA	-2.20	106.82	113.25
19	B	1224	CLA	O1D-CGD-CBD	-2.20	119.98	124.48
19	A	1122	CLA	O1D-CGD-CBD	-2.20	119.98	124.48
19	A	1118	CLA	C3D-C2D-C1D	-2.20	102.83	105.83
19	A	1137	CLA	O1D-CGD-CBD	-2.20	119.98	124.48
19	A	1124	CLA	O2A-CGA-CBA	2.20	118.81	111.91
25	A	5006	LMG	C1-C2-C3	2.20	114.58	110.00
19	J	1901	CLA	CMA-C3A-C4A	2.20	117.68	111.77
19	A	1130	CLA	CMA-C3A-C4A	2.20	117.68	111.77
19	B	1237	CLA	CMD-C2D-C3D	-2.20	122.56	127.61
19	3	614	CLA	C3D-C2D-C1D	-2.20	102.83	105.83
19	3	608	CLA	C3D-C2D-C1D	-2.20	102.83	105.83
19	L	1501	CLA	CMD-C2D-C3D	-2.20	122.56	127.61
22	F	4016	BCR	C23-C24-C25	-2.20	121.03	127.20
19	3	605	CLA	CMA-C3A-C4A	2.19	117.67	111.77
24	B	5006	LMT	C6B-C5B-C4B	-2.19	107.86	113.00
19	B	1213	CLA	CMB-C2B-C3B	2.19	128.78	124.68
19	A	1125	CLA	C3D-C2D-C1D	-2.19	102.84	105.83
19	4	601	CLA	CMD-C2D-C3D	-2.19	122.57	127.61
19	B	1220	CLA	C1C-C2C-C3C	-2.19	104.65	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	1232	CLA	C2C-C1C-NC	2.19	112.03	109.97
19	B	1216	CLA	CAA-C2A-C3A	-2.19	106.77	112.78
19	B	1219	CLA	CHA-C1A-NA	-2.19	121.38	126.40
19	F	1302	CLA	CMA-C3A-C4A	2.19	117.66	111.77
19	B	1203	CLA	CHA-C1A-NA	-2.19	121.38	126.40
19	B	1213	CLA	CBA-CAA-C2A	2.19	120.33	113.86
19	B	1211	CLA	CMD-C2D-C3D	-2.19	122.58	127.61
24	J	5003	LMT	C3B-C4B-C5B	-2.19	106.34	110.24
19	B	1211	CLA	O1D-CGD-CBD	-2.19	120.01	124.48
19	B	1205	CLA	C2D-C1D-ND	2.18	111.71	110.10
29	2	613	CHL	CHB-C4A-NA	2.18	127.53	124.51
22	B	4004	BCR	C8-C7-C6	2.18	133.34	127.20
19	3	617	CLA	O2D-CGD-O1D	-2.18	119.57	123.84
19	A	1135	CLA	CHA-C1A-NA	-2.18	121.40	126.40
19	1	607	CLA	CMB-C2B-C3B	2.18	128.76	124.68
19	4	607	CLA	CHA-C1A-NA	-2.18	121.40	126.40
19	4	603	CLA	CHA-C1A-NA	-2.18	121.40	126.40
19	4	604	CLA	O1D-CGD-CBD	-2.18	120.02	124.48
22	A	4011	BCR	C32-C1-C6	-2.18	106.76	110.30
19	B	1229	CLA	C3D-C2D-C1D	-2.18	102.85	105.83
19	A	1124	CLA	C1D-ND-C4D	-2.18	104.78	106.33
19	4	617	CLA	CMA-C3A-C4A	2.18	117.64	111.77
29	2	610	CHL	CHC-C1C-NC	2.18	127.51	124.20
19	A	1133	CLA	O2A-CGA-CBA	2.18	118.75	111.91
19	2	607	CLA	C3D-C2D-C1D	-2.18	102.85	105.83
19	A	1108	CLA	O2D-CGD-O1D	-2.18	119.58	123.84
19	B	1237	CLA	CMB-C2B-C3B	2.18	128.76	124.68
19	B	1231	CLA	C2D-C1D-ND	2.18	111.71	110.10
19	B	1234	CLA	C1D-ND-C4D	-2.18	104.79	106.33
19	B	1220	CLA	CMA-C3A-C4A	2.18	117.63	111.77
19	1	607	CLA	OBD-CAD-C3D	-2.18	123.28	128.52
19	3	608	CLA	CMD-C2D-C3D	-2.18	122.61	127.61
30	4	502	XAT	C40-C33-C34	-2.18	119.87	122.92
28	J	4013	LUT	C8-C9-C10	2.18	122.28	118.94
19	B	1023	CLA	CHA-C1A-NA	-2.18	121.41	126.40
29	2	615	CHL	CMB-C2B-C1B	-2.18	125.12	128.46
22	A	4002	BCR	C31-C1-C6	-2.18	106.77	110.30
19	1	606	CLA	CAA-C2A-C3A	-2.18	106.82	112.78
19	B	1208	CLA	C2C-C1C-NC	2.18	112.01	109.97
19	A	1102	CLA	C1-O2A-CGA	2.18	122.15	116.44
19	A	1141	CLA	O1D-CGD-CBD	-2.18	120.03	124.48
19	A	1118	CLA	CAA-CBA-CGA	-2.18	106.89	113.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	3	606	CLA	OBD-CAD-C3D	-2.18	123.28	128.52
19	B	1231	CLA	O1D-CGD-CBD	-2.17	120.03	124.48
19	B	1206	CLA	CMB-C2B-C3B	2.17	128.75	124.68
19	1	614	CLA	C1-O2A-CGA	2.17	122.15	116.44
19	A	1108	CLA	CHA-C1A-NA	-2.17	121.42	126.40
19	A	1129	CLA	CHA-C1A-NA	-2.17	121.42	126.40
19	A	1120	CLA	CMB-C2B-C3B	2.17	128.74	124.68
19	A	1129	CLA	C2D-C1D-ND	2.17	111.70	110.10
22	1	504	BCR	C38-C26-C27	2.17	117.79	113.62
19	2	604	CLA	CHA-C1A-NA	-2.17	121.43	126.40
22	I	4018	BCR	C4-C5-C6	-2.17	119.58	122.73
19	2	606	CLA	CMD-C2D-C3D	-2.17	122.62	127.61
29	2	609	CHL	CHC-C1C-NC	2.17	127.50	124.20
19	A	1124	CLA	CAA-C2A-C3A	-2.17	106.84	112.78
19	B	1240	CLA	O2A-CGA-CBA	2.17	118.72	111.91
29	3	604	CHL	CBA-CAA-C2A	2.17	120.26	113.86
19	3	608	CLA	CHA-C1A-NA	-2.17	121.43	126.40
19	B	1210	CLA	CHA-C4D-ND	2.17	137.03	132.50
19	J	1901	CLA	CHA-C1A-NA	-2.17	121.43	126.40
25	B	5004	LMG	C1-O6-C5	2.17	117.94	113.69
19	4	607	CLA	CMA-C3A-C4A	2.17	117.60	111.77
19	B	1215	CLA	CHA-C4D-ND	2.17	137.03	132.50
19	B	1215	CLA	CMD-C2D-C3D	-2.17	122.63	127.61
19	B	1202	CLA	CMA-C3A-C4A	2.17	117.59	111.77
19	A	1112	CLA	O1D-CGD-CBD	-2.17	120.05	124.48
19	B	1218	CLA	CAA-CBA-CGA	-2.16	106.93	113.25
19	2	605	CLA	C3D-C2D-C1D	-2.16	102.88	105.83
28	2	501	LUT	C11-C12-C13	-2.16	120.34	126.42
22	F	4016	BCR	C34-C9-C10	-2.16	119.89	122.92
19	A	1101	CLA	CMB-C2B-C1B	-2.16	125.14	128.46
19	3	602	CLA	O1D-CGD-CBD	-2.16	120.06	124.48
19	4	612	CLA	C1D-ND-C4D	-2.16	104.80	106.33
19	B	1235	CLA	CAA-C2A-C3A	-2.16	106.86	112.78
19	B	1230	CLA	O1D-CGD-CBD	-2.16	120.06	124.48
28	1	502	LUT	C38-C25-C24	-2.16	118.93	123.56
29	3	604	CHL	C2C-C3C-C4C	2.16	108.03	106.49
22	3	506	BCR	C34-C9-C10	-2.16	119.89	122.92
19	L	1501	CLA	O2A-CGA-CBA	2.16	118.69	111.91
22	L	4020	BCR	C8-C7-C6	-2.16	121.13	127.20
19	B	1236	CLA	CMB-C2B-C3B	2.16	128.72	124.68
19	1	611	CLA	O2A-CGA-CBA	2.16	118.69	111.91
19	A	1135	CLA	O1D-CGD-CBD	-2.16	120.06	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	1213	CLA	CAC-C3C-C4C	2.16	127.61	124.81
19	2	601	CLA	OBD-CAD-C3D	-2.16	123.32	128.52
30	4	502	XAT	O24-C25-C38	-2.16	112.47	115.06
19	A	1139	CLA	C1-O2A-CGA	2.16	122.11	116.44
19	A	1113	CLA	CHA-C1A-NA	-2.16	121.46	126.40
19	A	1116	CLA	CHA-C1A-NA	-2.16	121.46	126.40
19	A	1102	CLA	C2C-C1C-NC	2.16	111.99	109.97
19	A	1134	CLA	C1D-ND-C4D	-2.16	104.80	106.33
19	A	1111	CLA	C1-O2A-CGA	2.16	122.10	116.44
22	G	4021	BCR	C33-C5-C4	2.16	117.76	113.62
22	G	4021	BCR	C37-C22-C21	-2.16	119.90	122.92
19	A	1112	CLA	CMD-C2D-C3D	-2.16	122.66	127.61
19	A	1107	CLA	CAA-CBA-CGA	-2.15	106.96	113.25
28	3	501	LUT	C10-C11-C12	-2.15	116.50	123.22
19	A	1132	CLA	C3D-C2D-C1D	-2.15	102.89	105.83
30	4	502	XAT	C19-C9-C10	-2.15	119.91	122.92
19	A	1103	CLA	CMA-C3A-C4A	2.15	117.56	111.77
19	2	602	CLA	C2A-C1A-CHA	2.15	127.62	123.86
19	B	1204	CLA	CMD-C2D-C3D	-2.15	122.67	127.61
19	4	603	CLA	O1D-CGD-CBD	-2.15	120.08	124.48
29	2	611	CHL	CHC-C1C-NC	2.15	127.47	124.20
19	3	606	CLA	C3D-C2D-C1D	-2.15	102.90	105.83
19	B	1211	CLA	CAA-CBA-CGA	-2.15	106.97	113.25
19	A	1141	CLA	CMB-C2B-C3B	2.15	128.70	124.68
19	K	1404	CLA	C3D-C2D-C1D	-2.15	102.90	105.83
19	B	1209	CLA	CMB-C2B-C1B	-2.15	125.16	128.46
19	A	1120	CLA	C1D-ND-C4D	-2.15	104.81	106.33
19	B	1239	CLA	CMD-C2D-C3D	-2.15	122.68	127.61
19	A	1133	CLA	C1-C2-C3	-2.15	122.33	126.04
19	L	1502	CLA	O2A-CGA-CBA	2.15	118.64	111.91
19	3	617	CLA	CMA-C3A-C4A	2.15	117.54	111.77
19	4	607	CLA	C1D-ND-C4D	-2.15	104.81	106.33
19	L	1503	CLA	CHA-C1A-NA	-2.15	121.48	126.40
19	A	1139	CLA	OBD-CAD-C3D	-2.14	123.36	128.52
19	A	1128	CLA	O1D-CGD-CBD	-2.14	120.10	124.48
19	1	614	CLA	CHA-C1A-NA	-2.14	121.49	126.40
22	A	4002	BCR	C33-C5-C4	2.14	117.73	113.62
19	A	1107	CLA	CHA-C1A-NA	-2.14	121.49	126.40
19	4	605	CLA	C3D-C2D-C1D	-2.14	102.91	105.83
19	4	601	CLA	O2D-CGD-O1D	-2.14	119.65	123.84
29	4	615	CHL	CMB-C2B-C1B	-2.14	125.17	128.46
19	A	1115	CLA	C1-O2A-CGA	2.14	122.06	116.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	3	503	BCR	C36-C18-C17	-2.14	119.92	122.92
19	3	602	CLA	O2D-CGD-O1D	-2.14	119.65	123.84
24	G	5005	LMT	O5B-C5B-C6B	2.14	111.76	106.44
29	4	611	CHL	CHB-C4A-NA	2.14	127.47	124.51
22	A	4011	BCR	C37-C22-C23	2.14	121.45	118.08
29	4	610	CHL	CMB-C2B-C1B	-2.14	125.17	128.46
19	A	1120	CLA	CHA-C1A-NA	-2.14	121.50	126.40
19	A	1126	CLA	C6-C5-C3	-2.14	107.85	113.45
19	B	1207	CLA	C1-O2A-CGA	2.14	122.06	116.44
29	3	607	CHL	CMB-C2B-C1B	-2.14	125.18	128.46
19	B	1201	CLA	O2A-CGA-CBA	2.14	118.62	111.91
19	3	601	CLA	C3D-C2D-C1D	-2.14	102.91	105.83
19	A	1102	CLA	CAA-C2A-C1A	-2.14	104.97	111.97
19	4	606	CLA	CHA-C1A-NA	-2.14	121.51	126.40
19	A	1106	CLA	O1D-CGD-CBD	-2.14	120.11	124.48
19	4	606	CLA	CMD-C2D-C3D	-2.14	122.70	127.61
25	3	802	LMG	O8-C28-O10	-2.14	118.20	123.59
22	G	4021	BCR	C1-C6-C7	2.13	121.82	115.78
19	B	1230	CLA	CAA-CBA-CGA	-2.13	107.02	113.25
28	J	4013	LUT	C15-C35-C34	-2.13	119.10	123.47
24	G	5005	LMT	C3'-C4'-C5'	-2.13	106.03	110.93
19	3	614	CLA	CAA-C2A-C3A	-2.13	108.93	114.26
28	2	501	LUT	C40-C33-C32	2.13	121.44	118.08
19	L	1501	CLA	C1D-ND-C4D	-2.13	104.82	106.33
19	A	1112	CLA	CED-O2D-CGD	-2.13	111.11	115.94
19	A	1105	CLA	CMD-C2D-C3D	-2.13	122.71	127.61
19	A	1116	CLA	CMD-C2D-C3D	-2.13	122.71	127.61
19	3	602	CLA	C3D-C2D-C1D	-2.13	102.92	105.83
19	B	1212	CLA	CMB-C2B-C1B	-2.13	125.19	128.46
19	B	1218	CLA	O2A-CGA-CBA	2.13	118.59	111.91
27	B	5005	DGD	O6D-C5D-C6D	2.13	110.97	106.67
19	B	1219	CLA	C1-O2A-CGA	2.13	122.03	116.44
19	2	603	CLA	CHA-C1A-NA	-2.13	121.52	126.40
19	2	603	CLA	CAA-C2A-C3A	-2.13	106.95	112.78
29	2	611	CHL	C1-O2A-CGA	2.13	122.91	116.73
19	B	1239	CLA	C3D-C2D-C1D	-2.13	102.93	105.83
19	4	609	CLA	C3D-C2D-C1D	-2.13	102.93	105.83
23	1	801	LHG	O7-C7-O9	-2.13	118.56	123.70
22	B	4006	BCR	C35-C13-C12	2.13	121.43	118.08
19	2	602	CLA	C3D-C2D-C1D	-2.13	102.93	105.83
19	K	1403	CLA	OBD-CAD-C3D	-2.12	123.41	128.52
19	1	601	CLA	C1C-C2C-C3C	-2.12	104.72	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	4	501	LUT	C31-C32-C33	-2.12	120.45	126.42
19	A	1138	CLA	O2A-CGA-CBA	2.12	118.57	111.91
19	4	602	CLA	O2A-CGA-CBA	2.12	118.57	111.91
22	A	4007	BCR	C30-C25-C24	2.12	121.78	115.78
19	A	1122	CLA	CHA-C1A-NA	-2.12	121.54	126.40
19	B	1220	CLA	C2D-C1D-ND	2.12	111.67	110.10
19	A	1114	CLA	C1D-ND-C4D	-2.12	104.83	106.33
19	2	603	CLA	C1D-ND-C4D	-2.12	104.83	106.33
19	2	612	CLA	C2D-C1D-ND	2.12	111.67	110.10
19	4	607	CLA	O2A-CGA-CBA	2.12	118.56	111.91
19	A	1137	CLA	C3D-C2D-C1D	-2.12	102.94	105.83
22	1	504	BCR	C35-C13-C14	-2.12	119.95	122.92
19	A	1101	CLA	CHA-C1A-NA	-2.12	121.55	126.40
19	4	603	CLA	O2D-CGD-O1D	-2.12	119.70	123.84
19	B	1208	CLA	C1C-C2C-C3C	-2.12	104.73	106.96
19	A	1013	CLA	CHA-C1A-NA	-2.12	121.55	126.40
19	L	1503	CLA	O2D-CGD-O1D	-2.12	119.70	123.84
29	3	611	CHL	CMB-C2B-C1B	-2.12	125.21	128.46
19	3	605	CLA	CAC-C3C-C4C	2.12	127.56	124.81
19	2	604	CLA	C1D-ND-C4D	-2.12	104.83	106.33
19	G	1601	CLA	OBD-CAD-C3D	-2.12	123.43	128.52
22	B	4006	BCR	C8-C9-C10	2.12	122.19	118.94
29	1	610	CHL	CMB-C2B-C1B	-2.12	125.21	128.46
19	G	1603	CLA	CHA-C1A-NA	-2.12	121.55	126.40
19	B	1230	CLA	CMA-C3A-C4A	2.12	117.46	111.77
19	3	603	CLA	CHA-C1A-NA	-2.12	121.55	126.40
19	1	606	CLA	CMD-C2D-C3D	-2.11	122.75	127.61
19	3	617	CLA	CMD-C2D-C3D	-2.11	122.75	127.61
19	A	1111	CLA	CMB-C2B-C1B	-2.11	125.21	128.46
19	A	1136	CLA	CMD-C2D-C3D	-2.11	122.75	127.61
28	3	501	LUT	C30-C31-C32	-2.11	116.62	123.22
19	A	1121	CLA	C3D-C2D-C1D	-2.11	102.95	105.83
25	B	5003	LMG	O1-C1-C2	2.11	111.60	108.30
19	3	605	CLA	CAA-C2A-C3A	-2.11	106.99	112.78
29	2	611	CHL	CMB-C2B-C1B	-2.11	125.22	128.46
19	A	1140	CLA	O2A-CGA-CBA	2.11	118.53	111.91
19	A	1132	CLA	CAA-C2A-C3A	-2.11	107.00	112.78
29	1	609	CHL	CHB-C4A-NA	2.11	127.43	124.51
29	2	611	CHL	CHB-C4A-NA	2.11	127.43	124.51
19	2	608	CLA	CHA-C1A-NA	-2.11	121.56	126.40
19	1	614	CLA	CMA-C3A-C4A	2.11	117.44	111.77
19	A	1124	CLA	CMD-C2D-C3D	-2.11	122.76	127.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	1131	CLA	C3D-C2D-C1D	-2.11	102.95	105.83
22	A	4002	BCR	C34-C9-C10	-2.11	119.97	122.92
19	B	1214	CLA	CHA-C1A-NA	-2.11	121.57	126.40
19	2	606	CLA	C3D-C2D-C1D	-2.11	102.95	105.83
19	G	1602	CLA	O1D-CGD-CBD	-2.11	120.17	124.48
19	B	1236	CLA	C1D-ND-C4D	-2.11	104.84	106.33
19	3	610	CLA	C11-C10-C8	-2.11	109.11	115.92
19	A	1106	CLA	CMD-C2D-C3D	-2.11	122.77	127.61
19	G	1602	CLA	CMB-C2B-C1B	-2.11	125.23	128.46
22	1	503	BCR	C3-C4-C5	-2.11	110.32	114.08
19	B	1211	CLA	C3D-C2D-C1D	-2.11	102.96	105.83
19	B	1213	CLA	CMD-C2D-C3D	-2.11	122.77	127.61
22	A	4008	BCR	C31-C1-C6	-2.11	106.88	110.30
19	F	1301	CLA	CMB-C2B-C3B	2.11	128.62	124.68
19	A	1137	CLA	CMD-C2D-C3D	-2.11	122.77	127.61
19	A	1133	CLA	O1D-CGD-CBD	-2.10	120.18	124.48
19	2	612	CLA	CAA-CBA-CGA	-2.10	107.10	113.25
19	A	1104	CLA	C1D-ND-C4D	-2.10	104.84	106.33
19	A	1127	CLA	CMA-C3A-C4A	2.10	117.43	111.77
29	2	615	CHL	C4A-NA-C1A	2.10	107.65	106.71
19	B	1212	CLA	CHA-C1A-NA	-2.10	121.58	126.40
29	1	609	CHL	CMB-C2B-C1B	-2.10	125.23	128.46
19	G	1601	CLA	C3D-C2D-C1D	-2.10	102.96	105.83
28	3	502	LUT	C35-C15-C14	-2.10	119.17	123.47
29	3	611	CHL	CHA-C1A-NA	-2.10	121.58	126.40
19	B	1214	CLA	CMA-C3A-C4A	2.10	117.42	111.77
19	B	1230	CLA	CAA-C2A-C1A	-2.10	105.09	111.97
22	B	4009	BCR	C34-C9-C10	-2.10	119.98	122.92
19	B	1228	CLA	CMA-C3A-C4A	2.10	117.42	111.77
29	1	612	CHL	CHC-C1C-NC	2.10	127.39	124.20
19	K	1404	CLA	O2D-CGD-O1D	-2.10	119.73	123.84
19	4	605	CLA	O2A-CGA-CBA	2.10	118.50	111.91
22	B	4006	BCR	C28-C27-C26	-2.10	110.33	114.08
19	B	1230	CLA	CMD-C2D-C3D	-2.10	122.78	127.61
19	B	1236	CLA	O2A-CGA-CBA	2.10	118.50	111.91
29	1	612	CHL	CMB-C2B-C1B	-2.10	125.24	128.46
29	2	613	CHL	CMB-C2B-C1B	-2.10	125.24	128.46
19	B	1238	CLA	CAA-C2A-C1A	-2.10	105.09	111.97
25	2	803	LMG	C8-O7-C10	-2.10	112.62	117.79
19	A	1121	CLA	C1-O2A-CGA	2.10	121.95	116.44
19	A	1141	CLA	CAC-C3C-C4C	2.10	127.53	124.81
19	B	1217	CLA	CHA-C1A-NA	-2.10	121.59	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	1	611	CLA	CMD-C2D-C3D	-2.10	122.79	127.61
19	3	617	CLA	CHA-C1A-NA	-2.10	121.60	126.40
29	4	611	CHL	CMB-C2B-C1B	-2.10	125.24	128.46
29	2	610	CHL	C1-C2-C3	-2.10	122.42	126.04
19	B	1217	CLA	C3D-C2D-C1D	-2.09	102.97	105.83
19	3	614	CLA	CMD-C2D-C3D	-2.09	122.80	127.61
19	2	601	CLA	C1-C2-C3	-2.09	122.42	126.04
19	B	1202	CLA	C1D-ND-C4D	-2.09	104.85	106.33
19	G	1603	CLA	C3D-C2D-C1D	-2.09	102.97	105.83
19	A	1125	CLA	CHA-C1A-NA	-2.09	121.60	126.40
19	4	617	CLA	CMB-C2B-C3B	2.09	128.59	124.68
19	A	1119	CLA	C7-C6-C5	-2.09	107.67	113.36
20	A	2001	PQN	C11-C12-C13	-2.09	123.31	126.79
22	A	4008	BCR	C37-C22-C23	2.09	121.37	118.08
19	B	1237	CLA	CHA-C1A-NA	-2.09	121.61	126.40
19	4	607	CLA	O2D-CGD-O1D	-2.09	119.75	123.84
19	G	1701	CLA	CMD-C2D-C3D	-2.09	122.80	127.61
19	4	605	CLA	CHD-C1D-ND	-2.09	122.53	124.45
19	B	1240	CLA	CMD-C2D-C3D	-2.09	122.80	127.61
19	G	1601	CLA	CMD-C2D-C3D	-2.09	122.80	127.61
19	B	1205	CLA	O2A-CGA-CBA	2.09	118.47	111.91
19	K	1404	CLA	CMC-C2C-C1C	2.09	128.22	125.04
19	A	1108	CLA	C1-C2-C3	-2.09	123.37	126.75
19	A	1140	CLA	C7-C6-C5	-2.09	107.68	113.36
19	K	1403	CLA	C1-O2A-CGA	2.09	121.93	116.44
19	A	1116	CLA	OBD-CAD-C3D	-2.09	123.49	128.52
19	A	1139	CLA	O2A-CGA-CBA	2.09	118.46	111.91
19	2	605	CLA	C1D-ND-C4D	-2.09	104.85	106.33
19	3	614	CLA	O2D-CGD-O1D	-2.09	119.75	123.84
28	4	501	LUT	C20-C13-C14	-2.09	120.00	122.92
19	1	613	CLA	CHA-C1A-NA	-2.09	121.62	126.40
19	4	617	CLA	CHA-C1A-NA	-2.09	121.62	126.40
19	A	1130	CLA	CHA-C1A-NA	-2.09	121.62	126.40
29	1	609	CHL	C1B-CHB-C4A	-2.09	125.98	130.12
19	A	1135	CLA	CMD-C2D-C3D	-2.09	122.81	127.61
29	2	609	CHL	CMB-C2B-C1B	-2.09	125.26	128.46
22	3	506	BCR	C30-C25-C26	-2.09	119.67	122.61
19	B	1205	CLA	C16-C15-C13	-2.09	109.18	115.92
19	3	601	CLA	CMD-C2D-C3D	-2.08	122.82	127.61
19	L	1501	CLA	CHA-C1A-NA	-2.08	121.62	126.40
19	B	1234	CLA	C3D-C2D-C1D	-2.08	102.99	105.83
28	4	501	LUT	C39-C29-C30	-2.08	120.00	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	1130	CLA	C3D-C2D-C1D	-2.08	102.99	105.83
19	3	603	CLA	C3D-C2D-C1D	-2.08	102.99	105.83
22	G	4021	BCR	C37-C22-C23	2.08	121.36	118.08
28	3	502	LUT	C28-C29-C30	2.08	122.14	118.94
25	A	5006	LMG	O7-C10-O9	-2.08	118.67	123.70
19	A	1109	CLA	CMD-C2D-C3D	-2.08	122.83	127.61
19	A	1139	CLA	C3D-C2D-C1D	-2.08	102.99	105.83
19	A	1012	CLA	C2D-C1D-ND	2.08	111.64	110.10
28	3	501	LUT	C40-C33-C34	-2.08	120.01	122.92
19	A	1132	CLA	CHA-C1A-NA	-2.08	121.64	126.40
19	1	614	CLA	O2A-CGA-CBA	2.08	118.43	111.91
19	L	1503	CLA	CMB-C2B-C1B	-2.08	125.27	128.46
25	2	804	LMG	C8-O7-C10	-2.08	112.68	117.79
29	4	613	CHL	CHC-C1C-NC	2.08	127.36	124.20
29	2	609	CHL	C4D-CHA-C1A	2.08	123.78	121.25
19	B	1201	CLA	CMC-C2C-C1C	2.08	128.20	125.04
19	3	603	CLA	CAA-C2A-C3A	-2.08	107.09	112.78
19	G	1701	CLA	CHA-C1A-NA	-2.07	121.65	126.40
19	B	1218	CLA	C1D-ND-C4D	-2.07	104.86	106.33
19	F	1301	CLA	C1-O2A-CGA	2.07	121.89	116.44
19	B	1231	CLA	CMD-C2D-C3D	-2.07	122.84	127.61
22	B	4009	BCR	C38-C26-C27	2.07	117.60	113.62
19	K	1401	CLA	CHA-C1A-NA	-2.07	121.65	126.40
25	3	802	LMG	C8-O7-C10	-2.07	112.69	117.79
19	B	1022	CLA	OBD-CAD-C3D	-2.07	123.53	128.52
19	A	1130	CLA	O2D-CGD-O1D	-2.07	119.78	123.84
19	B	1202	CLA	O1D-CGD-CBD	-2.07	120.24	124.48
19	B	1023	CLA	CMB-C2B-C3B	2.07	128.56	124.68
19	1	614	CLA	C1D-ND-C4D	-2.07	104.86	106.33
19	A	1104	CLA	CMD-C2D-C3D	-2.07	122.85	127.61
27	4	801	DGD	C3E-C4E-C5E	2.07	113.93	110.24
19	B	1203	CLA	O2A-CGA-CBA	2.07	118.41	111.91
22	B	4004	BCR	C33-C5-C4	2.07	117.59	113.62
19	3	605	CLA	C1D-ND-C4D	-2.07	104.86	106.33
19	A	1110	CLA	CMC-C2C-C1C	2.07	128.19	125.04
19	A	1114	CLA	CHA-C1A-NA	-2.07	121.66	126.40
19	B	1213	CLA	C2D-C1D-ND	2.07	111.63	110.10
19	A	1133	CLA	CMD-C2D-C3D	-2.07	122.85	127.61
22	B	4005	BCR	C37-C22-C23	2.07	121.34	118.08
19	B	1227	CLA	O1D-CGD-CBD	-2.07	120.26	124.48
19	A	1121	CLA	C1C-C2C-C3C	-2.07	104.78	106.96
25	A	5006	LMG	C8-O7-C10	-2.07	112.70	117.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	4	613	CHL	CMB-C2B-C1B	-2.07	125.29	128.46
19	4	612	CLA	CHA-C1A-NA	-2.06	121.67	126.40
19	A	1113	CLA	C3D-C2D-C1D	-2.06	103.02	105.83
19	4	612	CLA	CMB-C2B-C3B	2.06	128.54	124.68
22	A	4008	BCR	C12-C13-C14	-2.06	115.78	118.94
19	A	1012	CLA	CHA-C1A-NA	-2.06	121.68	126.40
19	1	604	CLA	C2D-C1D-ND	2.06	111.62	110.10
19	4	606	CLA	CMB-C2B-C1B	-2.06	125.30	128.46
19	B	1230	CLA	C2D-C1D-ND	2.06	111.62	110.10
19	4	602	CLA	C3D-C2D-C1D	-2.06	103.02	105.83
19	3	613	CLA	C2A-C1A-CHA	2.06	127.46	123.86
19	B	1215	CLA	CMA-C3A-C4A	2.06	117.31	111.77
19	1	614	CLA	C3D-C2D-C1D	-2.06	103.02	105.83
19	A	1132	CLA	CAC-C3C-C4C	2.06	127.48	124.81
19	1	608	CLA	C3D-C2D-C1D	-2.06	103.02	105.83
19	B	1202	CLA	C3D-C2D-C1D	-2.06	103.02	105.83
19	G	1602	CLA	CHA-C1A-NA	-2.06	121.69	126.40
19	1	614	CLA	CMD-C2D-C3D	-2.06	122.89	127.61
19	B	1021	CLA	CMB-C2B-C1B	-2.06	125.31	128.46
19	B	1229	CLA	C1D-ND-C4D	-2.06	104.88	106.33
22	I	4018	BCR	C8-C9-C10	2.05	122.09	118.94
19	B	1224	CLA	C3D-C2D-C1D	-2.05	103.03	105.83
19	3	614	CLA	CMB-C2B-C3B	2.05	128.52	124.68
19	B	1232	CLA	C3D-C2D-C1D	-2.05	103.03	105.83
19	F	1301	CLA	CMA-C3A-C4A	2.05	117.29	111.77
19	B	1231	CLA	CHA-C1A-NA	-2.05	121.70	126.40
19	3	610	CLA	CMB-C2B-C1B	-2.05	125.31	128.46
19	A	1111	CLA	CHA-C1A-NA	-2.05	121.70	126.40
19	K	1402	CLA	O1D-CGD-CBD	-2.05	120.29	124.48
19	1	604	CLA	O1D-CGD-CBD	-2.05	120.29	124.48
19	A	1121	CLA	CAA-CBA-CGA	-2.05	107.26	113.25
19	3	601	CLA	O2A-CGA-CBA	2.05	118.34	111.91
19	B	1224	CLA	CMD-C2D-C3D	-2.05	122.90	127.61
19	1	605	CLA	CMB-C2B-C3B	2.05	128.51	124.68
19	B	1203	CLA	C3D-C2D-C1D	-2.05	103.03	105.83
22	G	4011	BCR	C24-C25-C26	-2.05	116.50	121.46
19	A	1122	CLA	O2D-CGD-O1D	-2.05	119.83	123.84
19	B	1232	CLA	CHA-C1A-NA	-2.05	121.71	126.40
23	B	5002	LHG	C6-C5-C4	-2.05	106.94	111.79
28	2	501	LUT	C28-C29-C30	-2.05	115.80	118.94
19	1	605	CLA	C1D-ND-C4D	-2.05	104.88	106.33
19	B	1207	CLA	CMD-C2D-C3D	-2.04	122.91	127.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	1117	CLA	CMB-C2B-C1B	-2.04	125.32	128.46
22	A	4003	BCR	C38-C26-C27	2.04	117.54	113.62
19	A	1133	CLA	C3D-C2D-C1D	-2.04	103.05	105.83
19	B	1216	CLA	C6-C7-C8	-2.04	109.33	115.92
22	B	4006	BCR	C40-C30-C39	-2.04	102.27	108.53
19	G	1601	CLA	CMA-C3A-C4A	2.04	117.25	111.77
22	A	4002	BCR	C23-C22-C21	-2.04	115.81	118.94
27	F	5005	DGD	C6D-O5D-C1E	2.04	117.72	113.74
19	A	1112	CLA	C3D-C2D-C1D	-2.04	103.05	105.83
19	A	1107	CLA	C1D-ND-C4D	-2.04	104.89	106.33
22	G	4021	BCR	C7-C6-C5	-2.04	116.53	121.46
19	4	612	CLA	C1-O2A-CGA	2.04	121.79	116.44
19	A	1124	CLA	C3D-C2D-C1D	-2.04	103.05	105.83
29	3	611	CHL	CMA-C3A-C4A	2.04	117.25	111.77
27	G	5003	DGD	O5D-C1E-C2E	2.04	111.48	108.30
19	A	1134	CLA	CHA-C1A-NA	-2.04	121.73	126.40
19	B	1022	CLA	CMD-C2D-C3D	-2.04	122.93	127.61
19	3	613	CLA	O2D-CGD-O1D	-2.04	119.86	123.84
19	B	1212	CLA	C3D-C2D-C1D	-2.04	103.05	105.83
19	A	1104	CLA	CMB-C2B-C3B	2.04	128.49	124.68
29	3	607	CHL	C1-O2A-CGA	2.03	121.78	116.44
24	G	5005	LMT	O5'-C1'-O1'	-2.03	105.16	109.97
19	4	609	CLA	CHA-C1A-NA	-2.03	121.74	126.40
19	J	1901	CLA	CMB-C2B-C3B	2.03	128.48	124.68
19	B	1226	CLA	C2D-C1D-ND	2.03	111.60	110.10
19	B	1211	CLA	CHA-C1A-NA	-2.03	121.74	126.40
19	4	603	CLA	O2A-CGA-CBA	2.03	118.29	111.91
22	J	4012	BCR	C23-C24-C25	-2.03	121.49	127.20
19	1	603	CLA	C3D-C2D-C1D	-2.03	103.06	105.83
30	2	502	XAT	O24-C25-C24	2.03	114.91	113.38
19	A	1135	CLA	C3D-C2D-C1D	-2.03	103.06	105.83
19	B	1220	CLA	CMB-C2B-C3B	2.03	128.48	124.68
19	K	1402	CLA	CMD-C2D-C3D	-2.03	122.94	127.61
19	3	606	CLA	CHA-C1A-NA	-2.03	121.75	126.40
24	A	5004	LMT	O5B-C5B-C6B	2.03	111.48	106.44
19	G	1603	CLA	C11-C10-C8	-2.03	109.36	115.92
19	A	1139	CLA	CMB-C2B-C1B	-2.03	125.35	128.46
19	B	1235	CLA	O1D-CGD-CBD	-2.03	120.34	124.48
19	A	1116	CLA	C3D-C2D-C1D	-2.03	103.06	105.83
19	B	1201	CLA	OBD-CAD-C3D	-2.03	123.64	128.52
29	2	610	CHL	C3A-C2A-C1A	2.02	104.37	101.34
19	A	1013	CLA	C1-O2A-CGA	2.02	121.75	116.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	1011	CL0	C2A-C3A-C4A	2.02	105.14	101.87
22	L	4019	BCR	C38-C26-C25	-2.02	122.26	124.53
19	B	1222	CLA	O2A-CGA-CBA	2.02	118.25	111.91
19	A	1139	CLA	CHA-C1A-NA	-2.02	121.77	126.40
25	G	5001	LMG	O8-C28-O10	-2.02	118.49	123.59
19	B	1023	CLA	C1D-ND-C4D	-2.02	104.90	106.33
19	B	1224	CLA	CHA-C1A-NA	-2.02	121.77	126.40
30	4	502	XAT	O24-C25-C24	-2.02	111.86	113.38
19	B	1206	CLA	CBA-CAA-C2A	-2.02	107.90	113.86
19	3	605	CLA	O2A-CGA-CBA	2.02	118.25	111.91
19	L	1502	CLA	CHA-C1A-NA	-2.02	121.77	126.40
19	A	1107	CLA	CMD-C2D-C3D	-2.02	122.97	127.61
19	4	608	CLA	C3D-C2D-C1D	-2.02	103.08	105.83
19	3	614	CLA	C1D-ND-C4D	-2.02	104.90	106.33
19	A	1110	CLA	CBA-CAA-C2A	2.02	119.82	113.86
19	2	608	CLA	O1D-CGD-CBD	-2.02	120.36	124.48
19	A	1131	CLA	CHA-C1A-NA	-2.02	121.78	126.40
19	A	1104	CLA	C3D-C2D-C1D	-2.02	103.08	105.83
19	B	1220	CLA	C1D-ND-C4D	-2.02	104.90	106.33
19	2	608	CLA	C1D-ND-C4D	-2.02	104.90	106.33
22	L	4019	BCR	C12-C13-C14	-2.02	115.85	118.94
19	A	1138	CLA	CMA-C3A-C4A	2.02	117.19	111.77
19	2	604	CLA	CAC-C3C-C4C	2.02	127.42	124.81
19	B	1217	CLA	CMD-C2D-C3D	-2.02	122.98	127.61
19	1	613	CLA	O1D-CGD-CBD	-2.02	120.36	124.48
19	G	1602	CLA	CMD-C2D-C3D	-2.01	122.98	127.61
19	B	1227	CLA	CMA-C3A-C4A	2.01	117.19	111.77
19	B	1021	CLA	CMD-C2D-C3D	-2.01	122.98	127.61
19	A	1134	CLA	C3D-C2D-C1D	-2.01	103.08	105.83
19	K	1402	CLA	C3D-C2D-C1D	-2.01	103.08	105.83
19	2	607	CLA	CAA-CBA-CGA	-2.01	107.37	113.25
19	B	1224	CLA	O2D-CGD-O1D	-2.01	119.90	123.84
19	F	1301	CLA	CHA-C1A-NA	-2.01	121.79	126.40
19	A	1123	CLA	CMD-C2D-C3D	-2.01	122.98	127.61
28	1	501	LUT	C1-C6-C5	-2.01	119.78	122.61
22	B	4010	BCR	C32-C1-C6	-2.01	107.04	110.30
19	1	606	CLA	CHA-C1A-NA	-2.01	121.79	126.40
22	A	4002	BCR	C28-C27-C26	-2.01	110.49	114.08
22	3	506	BCR	C35-C13-C12	2.01	121.24	118.08
19	A	1134	CLA	CMD-C2D-C3D	-2.01	122.99	127.61
19	2	601	CLA	O2A-CGA-CBA	2.01	118.21	111.91
19	B	1238	CLA	C3D-C2D-C1D	-2.01	103.09	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	1	504	BCR	C24-C25-C26	-2.01	116.60	121.46
19	B	1207	CLA	O1D-CGD-CBD	-2.01	120.38	124.48
19	A	1013	CLA	C4-C3-C2	-2.01	118.53	123.68
19	1	608	CLA	CHA-C1A-NA	-2.01	121.80	126.40
23	2	801	LHG	O8-C23-O10	-2.00	118.53	123.59
19	B	1226	CLA	CMD-C2D-C3D	-2.00	123.00	127.61
28	3	501	LUT	C8-C7-C6	-2.00	121.57	127.20
19	A	1136	CLA	C3D-C2D-C1D	-2.00	103.10	105.83
22	K	4002	BCR	C19-C18-C17	2.00	122.02	118.94
19	2	601	CLA	CAC-C3C-C4C	2.00	127.41	124.81
19	A	1114	CLA	C3D-C2D-C1D	-2.00	103.10	105.83
19	B	1225	CLA	CMA-C3A-C4A	2.00	117.15	111.77
19	4	602	CLA	CHA-C1A-NA	-2.00	121.81	126.40
19	A	1116	CLA	CMA-C3A-C4A	2.00	117.15	111.77
24	A	5004	LMT	O5B-C1B-C2B	2.00	114.58	110.35

All (200) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
18	A	1011	CL0	ND
18	A	1011	CL0	NA
18	A	1011	CL0	NC
19	A	1012	CLA	ND
19	A	1013	CLA	ND
19	A	1101	CLA	ND
19	A	1102	CLA	ND
19	A	1103	CLA	ND
19	A	1104	CLA	ND
19	A	1105	CLA	ND
19	A	1106	CLA	ND
19	A	1107	CLA	ND
19	A	1108	CLA	ND
19	A	1109	CLA	ND
19	A	1110	CLA	ND
19	A	1111	CLA	ND
19	A	1112	CLA	ND
19	A	1113	CLA	ND
19	A	1114	CLA	ND
19	A	1115	CLA	ND
19	A	1116	CLA	ND
19	A	1117	CLA	ND
19	A	1118	CLA	ND

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Mol	Chain	Res	Type	Atom
19	A	1119	CLA	ND
19	A	1120	CLA	ND
19	A	1121	CLA	ND
19	A	1122	CLA	ND
19	A	1123	CLA	ND
19	A	1124	CLA	ND
19	A	1125	CLA	ND
19	A	1126	CLA	ND
19	A	1127	CLA	ND
19	A	1128	CLA	ND
19	A	1129	CLA	ND
19	A	1130	CLA	ND
19	A	1131	CLA	ND
19	A	1132	CLA	ND
19	A	1133	CLA	ND
19	A	1134	CLA	ND
19	A	1135	CLA	ND
19	A	1136	CLA	ND
19	A	1137	CLA	ND
19	A	1138	CLA	ND
19	A	1139	CLA	ND
19	A	1140	CLA	ND
19	A	1141	CLA	ND
19	B	1021	CLA	ND
19	B	1022	CLA	ND
19	B	1023	CLA	ND
19	B	1201	CLA	ND
19	B	1202	CLA	ND
19	B	1203	CLA	ND
19	B	1204	CLA	ND
19	B	1205	CLA	ND
19	B	1206	CLA	ND
19	B	1207	CLA	ND
19	B	1208	CLA	ND
19	B	1209	CLA	ND
19	B	1210	CLA	ND
19	B	1211	CLA	ND
19	B	1212	CLA	ND
19	B	1213	CLA	ND
19	B	1214	CLA	ND
19	B	1215	CLA	ND
19	B	1216	CLA	ND

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Mol	Chain	Res	Type	Atom
19	B	1217	CLA	ND
19	B	1218	CLA	ND
19	B	1219	CLA	ND
19	B	1220	CLA	ND
19	B	1221	CLA	ND
19	B	1222	CLA	ND
19	B	1223	CLA	ND
19	B	1224	CLA	ND
19	B	1225	CLA	ND
19	B	1226	CLA	ND
19	B	1227	CLA	ND
19	B	1228	CLA	ND
19	B	1229	CLA	ND
19	B	1230	CLA	ND
19	B	1231	CLA	ND
19	B	1232	CLA	ND
19	B	1234	CLA	ND
19	B	1235	CLA	ND
19	B	1236	CLA	ND
19	B	1237	CLA	ND
19	B	1238	CLA	ND
19	B	1239	CLA	ND
19	B	1240	CLA	ND
19	F	1301	CLA	ND
19	F	1302	CLA	ND
19	G	1601	CLA	ND
19	G	1602	CLA	ND
19	G	1603	CLA	ND
19	G	1701	CLA	ND
19	J	1901	CLA	ND
19	K	1401	CLA	ND
19	K	1402	CLA	ND
19	K	1403	CLA	ND
19	K	1404	CLA	ND
19	L	1501	CLA	ND
19	L	1502	CLA	ND
19	L	1503	CLA	ND
19	1	601	CLA	ND
19	1	602	CLA	ND
19	1	603	CLA	ND
19	1	604	CLA	ND
19	1	605	CLA	ND

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Mol	Chain	Res	Type	Atom
19	1	606	CLA	ND
19	1	607	CLA	ND
19	1	608	CLA	ND
19	1	611	CLA	ND
19	1	613	CLA	ND
19	1	614	CLA	ND
19	2	601	CLA	ND
19	2	602	CLA	ND
19	2	603	CLA	ND
19	2	604	CLA	ND
19	2	605	CLA	ND
19	2	606	CLA	ND
19	2	607	CLA	ND
19	2	608	CLA	ND
19	2	612	CLA	ND
19	3	601	CLA	ND
19	3	602	CLA	ND
19	3	603	CLA	ND
19	3	606	CLA	ND
19	3	608	CLA	ND
19	3	610	CLA	ND
19	3	612	CLA	ND
19	3	613	CLA	ND
19	3	614	CLA	ND
19	3	617	CLA	ND
19	4	601	CLA	ND
19	4	602	CLA	ND
19	4	603	CLA	ND
19	4	604	CLA	ND
19	4	606	CLA	ND
19	4	607	CLA	ND
19	4	608	CLA	ND
19	4	609	CLA	ND
19	4	612	CLA	ND
19	4	617	CLA	ND
28	J	4013	LUT	C26
28	2	501	LUT	C26
28	3	502	LUT	C26
29	1	609	CHL	ND
29	1	609	CHL	NA
29	1	609	CHL	NC
29	1	609	CHL	C8

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Mol	Chain	Res	Type	Atom
29	1	610	CHL	ND
29	1	610	CHL	NA
29	1	610	CHL	NC
29	1	612	CHL	ND
29	1	612	CHL	NA
29	1	612	CHL	NC
29	1	612	CHL	C8
29	2	609	CHL	ND
29	2	609	CHL	NA
29	2	609	CHL	NC
29	2	609	CHL	C8
29	2	610	CHL	ND
29	2	610	CHL	NA
29	2	610	CHL	NC
29	2	610	CHL	C8
29	2	611	CHL	ND
29	2	611	CHL	NA
29	2	611	CHL	NC
29	2	613	CHL	ND
29	2	613	CHL	NA
29	2	613	CHL	NC
29	2	615	CHL	ND
29	2	615	CHL	NA
29	2	615	CHL	NC
29	2	615	CHL	C8
29	3	604	CHL	ND
29	3	604	CHL	NA
29	3	604	CHL	NC
29	3	604	CHL	C8
29	3	607	CHL	ND
29	3	607	CHL	NA
29	3	607	CHL	NC
29	3	611	CHL	ND
29	3	611	CHL	NA
29	3	611	CHL	NC
29	4	610	CHL	ND
29	4	610	CHL	NA
29	4	610	CHL	NC
29	4	611	CHL	ND
29	4	611	CHL	NA
29	4	611	CHL	NC
29	4	613	CHL	ND

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Mol	Chain	Res	Type	Atom
29	4	613	CHL	NA
29	4	613	CHL	NC
29	4	613	CHL	C8
29	4	615	CHL	ND
29	4	615	CHL	NA
29	4	615	CHL	NC
30	2	502	XAT	C5
30	4	502	XAT	C26
30	4	502	XAT	C6

All (2925) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
19	A	1012	CLA	C2-C3-C5-C6
19	A	1012	CLA	C4-C3-C5-C6
19	A	1013	CLA	C2-C1-O2A-CGA
19	A	1013	CLA	C2-C3-C5-C6
19	A	1013	CLA	C4-C3-C5-C6
19	A	1102	CLA	C3A-C2A-CAA-CBA
19	A	1103	CLA	C1A-C2A-CAA-CBA
19	A	1103	CLA	C3A-C2A-CAA-CBA
19	A	1103	CLA	CHA-CBD-CGD-O1D
19	A	1103	CLA	CHA-CBD-CGD-O2D
19	A	1103	CLA	CAD-CBD-CGD-O1D
19	A	1103	CLA	CAD-CBD-CGD-O2D
19	A	1104	CLA	C1A-C2A-CAA-CBA
19	A	1104	CLA	CBD-CGD-O2D-CED
19	A	1105	CLA	C2-C1-O2A-CGA
19	A	1106	CLA	C3A-C2A-CAA-CBA
19	A	1107	CLA	C1A-C2A-CAA-CBA
19	A	1108	CLA	CHA-CBD-CGD-O1D
19	A	1109	CLA	C1A-C2A-CAA-CBA
19	A	1109	CLA	C3A-C2A-CAA-CBA
19	A	1109	CLA	C2-C3-C5-C6
19	A	1109	CLA	C4-C3-C5-C6
19	A	1110	CLA	C1A-C2A-CAA-CBA
19	A	1110	CLA	C3A-C2A-CAA-CBA
19	A	1113	CLA	C1A-C2A-CAA-CBA
19	A	1113	CLA	C3A-C2A-CAA-CBA
19	A	1113	CLA	CHA-CBD-CGD-O1D
19	A	1113	CLA	CHA-CBD-CGD-O2D
19	A	1114	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
19	A	1114	CLA	CBA-CGA-O2A-C1
19	A	1116	CLA	C3A-C2A-CAA-CBA
19	A	1117	CLA	CHA-CBD-CGD-O1D
19	A	1117	CLA	CHA-CBD-CGD-O2D
19	A	1120	CLA	C1A-C2A-CAA-CBA
19	A	1120	CLA	CHA-CBD-CGD-O1D
19	A	1120	CLA	CHA-CBD-CGD-O2D
19	A	1122	CLA	CHA-CBD-CGD-O1D
19	A	1122	CLA	CHA-CBD-CGD-O2D
19	A	1122	CLA	C2-C3-C5-C6
19	A	1122	CLA	C4-C3-C5-C6
19	A	1123	CLA	C2-C1-O2A-CGA
19	A	1126	CLA	C1A-C2A-CAA-CBA
19	A	1126	CLA	C3A-C2A-CAA-CBA
19	A	1126	CLA	CBD-CGD-O2D-CED
19	A	1127	CLA	CHA-CBD-CGD-O1D
19	A	1127	CLA	CHA-CBD-CGD-O2D
19	A	1128	CLA	CHA-CBD-CGD-O1D
19	A	1128	CLA	CHA-CBD-CGD-O2D
19	A	1129	CLA	O1A-CGA-O2A-C1
19	A	1130	CLA	C1A-C2A-CAA-CBA
19	A	1130	CLA	C2-C3-C5-C6
19	A	1130	CLA	C4-C3-C5-C6
19	A	1133	CLA	C2-C3-C5-C6
19	A	1133	CLA	C4-C3-C5-C6
19	A	1134	CLA	CHA-CBD-CGD-O1D
19	A	1134	CLA	CHA-CBD-CGD-O2D
19	A	1135	CLA	C2-C3-C5-C6
19	A	1135	CLA	C4-C3-C5-C6
19	A	1138	CLA	CHA-CBD-CGD-O1D
19	A	1138	CLA	CHA-CBD-CGD-O2D
19	A	1139	CLA	C1A-C2A-CAA-CBA
19	A	1139	CLA	C3A-C2A-CAA-CBA
19	B	1021	CLA	CHA-CBD-CGD-O1D
19	B	1021	CLA	CHA-CBD-CGD-O2D
19	B	1021	CLA	CBD-CGD-O2D-CED
19	B	1202	CLA	C3A-C2A-CAA-CBA
19	B	1204	CLA	C1A-C2A-CAA-CBA
19	B	1204	CLA	CHA-CBD-CGD-O1D
19	B	1204	CLA	C2-C3-C5-C6
19	B	1204	CLA	C4-C3-C5-C6
19	B	1205	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
19	B	1206	CLA	C14-C13-C15-C16
19	B	1207	CLA	C4-C3-C5-C6
19	B	1210	CLA	C1A-C2A-CAA-CBA
19	B	1212	CLA	CHA-CBD-CGD-O1D
19	B	1212	CLA	CHA-CBD-CGD-O2D
19	B	1213	CLA	C2-C1-O2A-CGA
19	B	1214	CLA	CBA-CGA-O2A-C1
19	B	1214	CLA	O1A-CGA-O2A-C1
19	B	1215	CLA	C1A-C2A-CAA-CBA
19	B	1217	CLA	CBA-CGA-O2A-C1
19	B	1217	CLA	CHA-CBD-CGD-O2D
19	B	1218	CLA	CHA-CBD-CGD-O1D
19	B	1218	CLA	CHA-CBD-CGD-O2D
19	B	1219	CLA	C2-C1-O2A-CGA
19	B	1219	CLA	CHA-CBD-CGD-O1D
19	B	1219	CLA	CHA-CBD-CGD-O2D
19	B	1219	CLA	CBD-CGD-O2D-CED
19	B	1219	CLA	C2-C3-C5-C6
19	B	1219	CLA	C4-C3-C5-C6
19	B	1221	CLA	C1A-C2A-CAA-CBA
19	B	1221	CLA	C2-C1-O2A-CGA
19	B	1222	CLA	C1A-C2A-CAA-CBA
19	B	1222	CLA	C2-C3-C5-C6
19	B	1222	CLA	C4-C3-C5-C6
19	B	1223	CLA	C1A-C2A-CAA-CBA
19	B	1223	CLA	C3A-C2A-CAA-CBA
19	B	1224	CLA	C1A-C2A-CAA-CBA
19	B	1224	CLA	C3A-C2A-CAA-CBA
19	B	1224	CLA	CBD-CGD-O2D-CED
19	B	1225	CLA	C1A-C2A-CAA-CBA
19	B	1225	CLA	C3A-C2A-CAA-CBA
19	B	1228	CLA	C1A-C2A-CAA-CBA
19	B	1232	CLA	CBD-CGD-O2D-CED
19	B	1232	CLA	C2-C3-C5-C6
19	B	1232	CLA	C4-C3-C5-C6
19	B	1238	CLA	CBD-CGD-O2D-CED
19	B	1239	CLA	C3A-C2A-CAA-CBA
19	B	1239	CLA	C2-C3-C5-C6
19	B	1239	CLA	C4-C3-C5-C6
19	F	1301	CLA	C2-C1-O2A-CGA
19	F	1302	CLA	CHA-CBD-CGD-O1D
19	F	1302	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
19	F	1302	CLA	CBD-CGD-O2D-CED
19	G	1601	CLA	C1A-C2A-CAA-CBA
19	G	1601	CLA	C3A-C2A-CAA-CBA
19	G	1601	CLA	C4-C3-C5-C6
19	G	1602	CLA	CHA-CBD-CGD-O1D
19	G	1602	CLA	CHA-CBD-CGD-O2D
19	G	1603	CLA	C1A-C2A-CAA-CBA
19	G	1701	CLA	C2-C1-O2A-CGA
19	G	1701	CLA	CHA-CBD-CGD-O1D
19	G	1701	CLA	CHA-CBD-CGD-O2D
19	J	1901	CLA	CBD-CGD-O2D-CED
19	K	1401	CLA	C1A-C2A-CAA-CBA
19	K	1401	CLA	C3A-C2A-CAA-CBA
19	K	1401	CLA	CBD-CGD-O2D-CED
19	K	1402	CLA	C1A-C2A-CAA-CBA
19	K	1402	CLA	C2-C3-C5-C6
19	K	1402	CLA	C4-C3-C5-C6
19	K	1403	CLA	CBA-CGA-O2A-C1
19	K	1403	CLA	O1A-CGA-O2A-C1
19	K	1403	CLA	CBD-CGD-O2D-CED
19	K	1404	CLA	CBD-CGD-O2D-CED
19	L	1501	CLA	C1A-C2A-CAA-CBA
19	L	1501	CLA	CHA-CBD-CGD-O1D
19	L	1501	CLA	CHA-CBD-CGD-O2D
19	L	1502	CLA	C1A-C2A-CAA-CBA
19	L	1502	CLA	C3A-C2A-CAA-CBA
19	L	1503	CLA	C1A-C2A-CAA-CBA
19	L	1503	CLA	CBA-CGA-O2A-C1
19	1	601	CLA	C4-C3-C5-C6
19	1	602	CLA	CBA-CGA-O2A-C1
19	1	603	CLA	C1A-C2A-CAA-CBA
19	1	605	CLA	CBD-CGD-O2D-CED
19	1	606	CLA	CHA-CBD-CGD-O1D
19	1	606	CLA	CHA-CBD-CGD-O2D
19	1	611	CLA	CBD-CGD-O2D-CED
19	1	614	CLA	C6-C7-C8-C9
19	2	601	CLA	C1A-C2A-CAA-CBA
19	2	601	CLA	C3A-C2A-CAA-CBA
19	2	602	CLA	CBD-CGD-O2D-CED
19	2	602	CLA	C2-C3-C5-C6
19	2	602	CLA	C4-C3-C5-C6
19	2	603	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
19	2	603	CLA	CHA-CBD-CGD-O2D
19	2	604	CLA	C3A-C2A-CAA-CBA
19	2	604	CLA	CHA-CBD-CGD-O2D
19	2	605	CLA	C3A-C2A-CAA-CBA
19	2	605	CLA	CHA-CBD-CGD-O1D
19	2	605	CLA	CHA-CBD-CGD-O2D
19	2	606	CLA	C1A-C2A-CAA-CBA
19	2	606	CLA	C3A-C2A-CAA-CBA
19	2	606	CLA	CBD-CGD-O2D-CED
19	2	607	CLA	CBA-CGA-O2A-C1
19	2	607	CLA	O1A-CGA-O2A-C1
19	2	607	CLA	CBD-CGD-O2D-CED
19	2	608	CLA	CBD-CGD-O2D-CED
19	2	612	CLA	C1A-C2A-CAA-CBA
19	2	612	CLA	C3A-C2A-CAA-CBA
19	2	612	CLA	C2-C1-O2A-CGA
19	2	612	CLA	C2-C3-C5-C6
19	2	612	CLA	C4-C3-C5-C6
19	3	601	CLA	C1A-C2A-CAA-CBA
19	3	601	CLA	C3A-C2A-CAA-CBA
19	3	601	CLA	CBD-CGD-O2D-CED
19	3	602	CLA	C2-C3-C5-C6
19	3	602	CLA	C4-C3-C5-C6
19	3	603	CLA	CBD-CGD-O2D-CED
19	3	603	CLA	C2-C3-C5-C6
19	3	603	CLA	C4-C3-C5-C6
19	3	606	CLA	CAD-CBD-CGD-O1D
19	3	606	CLA	CAD-CBD-CGD-O2D
19	3	608	CLA	C1A-C2A-CAA-CBA
19	3	610	CLA	C3A-C2A-CAA-CBA
19	3	610	CLA	CBD-CGD-O2D-CED
19	3	612	CLA	C3A-C2A-CAA-CBA
19	3	612	CLA	C2-C1-O2A-CGA
19	3	612	CLA	CBD-CGD-O2D-CED
19	3	613	CLA	C1A-C2A-CAA-CBA
19	3	614	CLA	C1A-C2A-CAA-CBA
19	3	614	CLA	CBD-CGD-O2D-CED
19	3	617	CLA	CBD-CGD-O2D-CED
19	4	601	CLA	C1A-C2A-CAA-CBA
19	4	602	CLA	CHA-CBD-CGD-O1D
19	4	602	CLA	CHA-CBD-CGD-O2D
19	4	603	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
19	4	605	CLA	C1A-C2A-CAA-CBA
19	4	606	CLA	C2-C1-O2A-CGA
19	4	606	CLA	CBD-CGD-O2D-CED
19	4	607	CLA	C1A-C2A-CAA-CBA
19	4	607	CLA	C3A-C2A-CAA-CBA
19	4	607	CLA	CBD-CGD-O2D-CED
19	4	608	CLA	CHA-CBD-CGD-O1D
19	4	608	CLA	CHA-CBD-CGD-O2D
19	4	608	CLA	CBD-CGD-O2D-CED
19	4	609	CLA	CHA-CBD-CGD-O1D
19	4	609	CLA	CHA-CBD-CGD-O2D
19	4	609	CLA	CAD-CBD-CGD-O1D
19	4	612	CLA	CBA-CGA-O2A-C1
19	4	612	CLA	O1A-CGA-O2A-C1
19	4	617	CLA	C2-C1-O2A-CGA
22	A	4002	BCR	C1-C6-C7-C8
22	A	4002	BCR	C11-C10-C9-C8
22	A	4002	BCR	C11-C10-C9-C34
22	A	4002	BCR	C10-C11-C12-C13
22	A	4002	BCR	C11-C12-C13-C14
22	A	4002	BCR	C11-C12-C13-C35
22	A	4003	BCR	C21-C22-C23-C24
22	A	4003	BCR	C37-C22-C23-C24
22	A	4008	BCR	C11-C10-C9-C8
22	A	4008	BCR	C11-C10-C9-C34
22	A	4011	BCR	C17-C18-C19-C20
22	A	4011	BCR	C36-C18-C19-C20
22	A	4017	BCR	C11-C10-C9-C8
22	A	4017	BCR	C11-C10-C9-C34
22	A	4017	BCR	C10-C11-C12-C13
22	B	4004	BCR	C23-C24-C25-C26
22	B	4004	BCR	C23-C24-C25-C30
22	B	4005	BCR	C11-C10-C9-C8
22	B	4005	BCR	C11-C10-C9-C34
22	B	4005	BCR	C17-C18-C19-C20
22	B	4005	BCR	C36-C18-C19-C20
22	B	4005	BCR	C21-C22-C23-C24
22	B	4005	BCR	C37-C22-C23-C24
22	B	4006	BCR	C1-C6-C7-C8
22	B	4006	BCR	C5-C6-C7-C8
22	B	4006	BCR	C7-C8-C9-C10
22	B	4006	BCR	C7-C8-C9-C34

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Mol	Chain	Res	Type	Atoms
22	B	4009	BCR	C11-C10-C9-C8
22	B	4009	BCR	C11-C10-C9-C34
22	B	4010	BCR	C7-C8-C9-C34
22	B	4010	BCR	C11-C10-C9-C8
22	B	4010	BCR	C11-C10-C9-C34
22	B	4010	BCR	C10-C11-C12-C13
22	B	4010	BCR	C17-C18-C19-C20
22	B	4010	BCR	C36-C18-C19-C20
22	F	4014	BCR	C7-C8-C9-C10
22	F	4014	BCR	C7-C8-C9-C34
22	F	4014	BCR	C11-C10-C9-C8
22	F	4014	BCR	C11-C10-C9-C34
22	F	4016	BCR	C7-C8-C9-C10
22	F	4016	BCR	C7-C8-C9-C34
22	F	4016	BCR	C11-C10-C9-C8
22	F	4016	BCR	C11-C10-C9-C34
22	F	4016	BCR	C10-C11-C12-C13
22	F	4016	BCR	C36-C18-C19-C20
22	G	4011	BCR	C10-C11-C12-C13
22	G	4011	BCR	C23-C24-C25-C26
22	G	4021	BCR	C7-C8-C9-C10
22	G	4021	BCR	C7-C8-C9-C34
22	G	4021	BCR	C11-C10-C9-C8
22	G	4021	BCR	C11-C10-C9-C34
22	G	4021	BCR	C9-C10-C11-C12
22	G	4021	BCR	C10-C11-C12-C13
22	G	4021	BCR	C37-C22-C23-C24
22	I	4018	BCR	C5-C6-C7-C8
22	I	4018	BCR	C7-C8-C9-C10
22	I	4018	BCR	C7-C8-C9-C34
22	I	4018	BCR	C11-C10-C9-C8
22	I	4018	BCR	C11-C10-C9-C34
22	I	4018	BCR	C10-C11-C12-C13
22	J	4012	BCR	C1-C6-C7-C8
22	J	4012	BCR	C7-C8-C9-C10
22	J	4012	BCR	C7-C8-C9-C34
22	J	4012	BCR	C11-C12-C13-C14
22	J	4012	BCR	C11-C12-C13-C35
22	J	4012	BCR	C21-C22-C23-C24
22	J	4012	BCR	C37-C22-C23-C24
22	K	4001	BCR	C1-C6-C7-C8
22	K	4001	BCR	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
22	K	4001	BCR	C7-C8-C9-C10
22	K	4001	BCR	C7-C8-C9-C34
22	K	4001	BCR	C11-C10-C9-C8
22	K	4001	BCR	C11-C10-C9-C34
22	K	4002	BCR	C1-C6-C7-C8
22	K	4002	BCR	C11-C10-C9-C8
22	K	4002	BCR	C11-C10-C9-C34
22	K	4002	BCR	C10-C11-C12-C13
22	K	4002	BCR	C13-C14-C15-C16
22	K	4002	BCR	C21-C22-C23-C24
22	K	4002	BCR	C37-C22-C23-C24
22	L	4019	BCR	C7-C8-C9-C10
22	L	4019	BCR	C7-C8-C9-C34
22	L	4019	BCR	C11-C10-C9-C8
22	L	4019	BCR	C11-C10-C9-C34
22	L	4019	BCR	C23-C24-C25-C26
22	L	4019	BCR	C23-C24-C25-C30
22	L	4020	BCR	C7-C8-C9-C10
22	L	4020	BCR	C7-C8-C9-C34
22	L	4020	BCR	C11-C10-C9-C8
22	L	4020	BCR	C11-C10-C9-C34
22	1	503	BCR	C1-C6-C7-C8
22	1	503	BCR	C5-C6-C7-C8
22	1	503	BCR	C11-C10-C9-C8
22	1	503	BCR	C11-C10-C9-C34
22	1	503	BCR	C10-C11-C12-C13
22	1	503	BCR	C11-C12-C13-C14
22	1	503	BCR	C11-C12-C13-C35
22	1	503	BCR	C23-C24-C25-C26
22	1	503	BCR	C23-C24-C25-C30
22	1	504	BCR	C7-C8-C9-C10
22	1	504	BCR	C7-C8-C9-C34
22	1	504	BCR	C11-C10-C9-C8
22	1	504	BCR	C11-C10-C9-C34
22	1	504	BCR	C21-C22-C23-C24
22	1	504	BCR	C37-C22-C23-C24
22	2	503	BCR	C11-C10-C9-C8
22	2	503	BCR	C11-C10-C9-C34
22	2	503	BCR	C36-C18-C19-C20
22	2	503	BCR	C21-C22-C23-C24
22	2	503	BCR	C37-C22-C23-C24
22	3	503	BCR	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
22	3	503	BCR	C7-C8-C9-C34
22	3	503	BCR	C11-C10-C9-C8
22	3	503	BCR	C11-C10-C9-C34
22	3	503	BCR	C36-C18-C19-C20
22	3	506	BCR	C5-C6-C7-C8
22	3	506	BCR	C7-C8-C9-C10
22	3	506	BCR	C7-C8-C9-C34
22	3	506	BCR	C23-C24-C25-C26
22	3	506	BCR	C23-C24-C25-C30
23	A	5001	LHG	O1-C1-C2-C3
23	A	5001	LHG	C4-O6-P-O4
23	A	5001	LHG	C4-O6-P-O5
23	A	5002	LHG	O1-C1-C2-C3
23	A	5002	LHG	O2-C2-C3-O3
23	A	5002	LHG	C3-O3-P-O5
23	A	5002	LHG	C3-O3-P-O6
23	A	5002	LHG	C4-O6-P-O4
23	A	5002	LHG	C4-O6-P-O5
23	B	5001	LHG	C4-O6-P-O3
23	B	5001	LHG	C4-O6-P-O4
23	B	5001	LHG	C4-O6-P-O5
23	B	5001	LHG	O9-C7-O7-C5
23	B	5001	LHG	C8-C7-O7-C5
23	B	5002	LHG	C8-C7-O7-C5
23	1	801	LHG	O1-C1-C2-C3
23	1	801	LHG	O2-C2-C3-O3
23	1	801	LHG	C4-O6-P-O5
23	2	801	LHG	O1-C1-C2-C3
23	2	801	LHG	C4-O6-P-O3
23	2	801	LHG	C4-O6-P-O4
23	2	801	LHG	C4-O6-P-O5
23	2	801	LHG	C8-C7-O7-C5
23	2	807	LHG	C1-C2-C3-O3
23	2	807	LHG	C4-O6-P-O4
23	3	801	LHG	C4-O6-P-O4
24	B	5006	LMT	C2'-C1'-O1'-C1
24	B	5006	LMT	O5'-C1'-O1'-C1
24	G	5005	LMT	C2'-C1'-O1'-C1
24	G	5005	LMT	O5'-C1'-O1'-C1
24	G	5005	LMT	C2-C1-O1'-C1'
25	A	5006	LMG	O6-C1-O1-C7
25	A	5006	LMG	O9-C10-O7-C8

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Mol	Chain	Res	Type	Atoms
25	B	5003	LMG	O9-C10-O7-C8
25	B	5003	LMG	C11-C10-O7-C8
25	B	5004	LMG	O6-C1-O1-C7
25	B	5004	LMG	O9-C10-O7-C8
25	B	5004	LMG	C11-C10-O7-C8
25	F	5002	LMG	O6-C1-O1-C7
25	F	5002	LMG	C11-C10-O7-C8
25	F	5004	LMG	C11-C10-O7-C8
25	G	5001	LMG	C11-C10-O7-C8
25	G	5002	LMG	O6-C1-O1-C7
25	G	5002	LMG	O1-C7-C8-O7
25	G	5002	LMG	C11-C10-O7-C8
25	G	5006	LMG	C2-C1-O1-C7
25	G	5006	LMG	O6-C1-O1-C7
25	G	5006	LMG	O9-C10-O7-C8
25	G	5006	LMG	C11-C10-O7-C8
25	2	802	LMG	O9-C10-O7-C8
25	2	802	LMG	C11-C10-O7-C8
25	2	803	LMG	O6-C1-O1-C7
25	2	803	LMG	C8-C7-O1-C1
25	2	803	LMG	C11-C10-O7-C8
25	3	802	LMG	C2-C1-O1-C7
25	3	802	LMG	O6-C1-O1-C7
25	3	802	LMG	O9-C10-O7-C8
25	3	802	LMG	C11-C10-O7-C8
27	B	5005	DGD	C2B-C1B-O2G-C2G
27	B	5005	DGD	O1B-C1B-O2G-C2G
27	B	5005	DGD	C2D-C1D-O3G-C3G
27	B	5005	DGD	O6D-C1D-O3G-C3G
27	F	5005	DGD	C2D-C1D-O3G-C3G
27	F	5005	DGD	O6D-C1D-O3G-C3G
27	G	5003	DGD	C2D-C1D-O3G-C3G
27	G	5003	DGD	O6D-C1D-O3G-C3G
27	J	5001	DGD	O6E-C1E-O5D-C6D
27	1	803	DGD	C2D-C1D-O3G-C3G
27	1	803	DGD	O6D-C1D-O3G-C3G
27	1	803	DGD	O6E-C1E-O5D-C6D
27	3	803	DGD	O6D-C1D-O3G-C3G
27	3	803	DGD	C5D-C6D-O5D-C1E
27	4	802	DGD	C2B-C1B-O2G-C2G
27	4	802	DGD	O6D-C1D-O3G-C3G
28	J	4013	LUT	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
28	J	4013	LUT	C7-C8-C9-C19
28	J	4013	LUT	C21-C26-C27-C28
28	2	501	LUT	C21-C26-C27-C28
28	2	501	LUT	C31-C32-C33-C34
28	2	501	LUT	C31-C32-C33-C40
28	3	502	LUT	C7-C8-C9-C10
28	3	502	LUT	C7-C8-C9-C19
28	3	502	LUT	C21-C26-C27-C28
28	3	502	LUT	C27-C28-C29-C30
28	3	502	LUT	C27-C28-C29-C39
28	3	502	LUT	C29-C30-C31-C32
28	3	502	LUT	C31-C32-C33-C40
29	2	609	CHL	O2A-C1-C2-C3
29	2	613	CHL	C1A-C2A-CAA-CBA
29	2	615	CHL	CHA-CBD-CGD-O1D
29	2	615	CHL	CHA-CBD-CGD-O2D
29	3	604	CHL	C2-C1-O2A-CGA
29	3	604	CHL	C2-C3-C5-C6
29	3	604	CHL	C4-C3-C5-C6
29	3	607	CHL	C1A-C2A-CAA-CBA
29	4	610	CHL	CHA-CBD-CGD-O1D
29	4	613	CHL	C1A-C2A-CAA-CBA
29	4	613	CHL	C3A-C2A-CAA-CBA
30	2	502	XAT	C1-C6-C7-C8
30	2	502	XAT	C7-C8-C9-C10
30	2	502	XAT	C7-C8-C9-C19
31	4	505	C7Z	C5-C6-C7-C8
31	4	505	C7Z	C7-C8-C9-C19
31	4	505	C7Z	C11-C10-C9-C8
31	4	505	C7Z	C11-C10-C9-C19
31	4	505	C7Z	C20-C13-C14-C15
31	4	505	C7Z	C40-C33-C34-C35
31	4	505	C7Z	C32-C33-C34-C35
31	4	505	C7Z	C39-C29-C30-C31
31	4	505	C7Z	C27-C28-C29-C30
19	L	1503	CLA	O1D-CGD-O2D-CED
19	3	613	CLA	O1D-CGD-O2D-CED
19	3	614	CLA	O1D-CGD-O2D-CED
19	A	1104	CLA	O1D-CGD-O2D-CED
19	A	1121	CLA	O1D-CGD-O2D-CED
19	K	1404	CLA	O1D-CGD-O2D-CED
19	1	602	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
19	2	605	CLA	O1D-CGD-O2D-CED
19	3	608	CLA	O1D-CGD-O2D-CED
19	4	606	CLA	O1D-CGD-O2D-CED
19	4	607	CLA	O1D-CGD-O2D-CED
19	A	1012	CLA	CBD-CGD-O2D-CED
19	A	1102	CLA	CBD-CGD-O2D-CED
19	A	1103	CLA	CBD-CGD-O2D-CED
19	A	1107	CLA	CBD-CGD-O2D-CED
19	A	1109	CLA	CBD-CGD-O2D-CED
19	A	1114	CLA	CBD-CGD-O2D-CED
19	A	1115	CLA	CBD-CGD-O2D-CED
19	A	1116	CLA	CBD-CGD-O2D-CED
19	A	1121	CLA	CBD-CGD-O2D-CED
19	A	1129	CLA	CBD-CGD-O2D-CED
19	A	1131	CLA	CBD-CGD-O2D-CED
19	A	1132	CLA	CBD-CGD-O2D-CED
19	A	1136	CLA	CBD-CGD-O2D-CED
19	A	1137	CLA	CBD-CGD-O2D-CED
19	A	1139	CLA	CBD-CGD-O2D-CED
19	A	1140	CLA	CBD-CGD-O2D-CED
19	A	1141	CLA	CBD-CGD-O2D-CED
19	B	1022	CLA	CBD-CGD-O2D-CED
19	B	1201	CLA	CBD-CGD-O2D-CED
19	B	1206	CLA	CBD-CGD-O2D-CED
19	B	1207	CLA	CBD-CGD-O2D-CED
19	B	1208	CLA	CBD-CGD-O2D-CED
19	B	1209	CLA	CBD-CGD-O2D-CED
19	B	1226	CLA	CBD-CGD-O2D-CED
19	B	1227	CLA	CBD-CGD-O2D-CED
19	B	1229	CLA	CBD-CGD-O2D-CED
19	G	1601	CLA	CBD-CGD-O2D-CED
19	G	1602	CLA	CBD-CGD-O2D-CED
19	G	1701	CLA	CBD-CGD-O2D-CED
19	L	1503	CLA	CBD-CGD-O2D-CED
19	1	602	CLA	CBD-CGD-O2D-CED
19	1	603	CLA	CBD-CGD-O2D-CED
19	1	606	CLA	CBD-CGD-O2D-CED
19	1	608	CLA	CBD-CGD-O2D-CED
19	1	613	CLA	CBD-CGD-O2D-CED
19	2	601	CLA	CBD-CGD-O2D-CED
19	2	605	CLA	CBD-CGD-O2D-CED
19	2	612	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
19	3	606	CLA	CBD-CGD-O2D-CED
19	3	608	CLA	CBD-CGD-O2D-CED
19	3	613	CLA	CBD-CGD-O2D-CED
19	4	602	CLA	CBD-CGD-O2D-CED
19	A	1104	CLA	O1A-CGA-O2A-C1
19	A	1121	CLA	O1A-CGA-O2A-C1
19	J	1901	CLA	O1A-CGA-O2A-C1
19	L	1503	CLA	O1A-CGA-O2A-C1
19	1	606	CLA	O1A-CGA-O2A-C1
25	F	5002	LMG	O10-C28-O8-C9
25	2	804	LMG	O10-C28-O8-C9
19	A	1114	CLA	O1A-CGA-O2A-C1
19	B	1217	CLA	O1A-CGA-O2A-C1
19	K	1404	CLA	O1A-CGA-O2A-C1
19	1	602	CLA	O1A-CGA-O2A-C1
19	B	1201	CLA	O1D-CGD-O2D-CED
19	B	1206	CLA	O1D-CGD-O2D-CED
19	B	1226	CLA	O1D-CGD-O2D-CED
19	1	606	CLA	O1D-CGD-O2D-CED
19	3	601	CLA	O1D-CGD-O2D-CED
19	3	610	CLA	O1D-CGD-O2D-CED
19	B	1209	CLA	CBA-CGA-O2A-C1
19	G	1602	CLA	CBA-CGA-O2A-C1
19	K	1404	CLA	CBA-CGA-O2A-C1
27	B	5005	DGD	C2G-C1G-O1G-C1A
27	1	803	DGD	C2G-C1G-O1G-C1A
19	A	1126	CLA	O1D-CGD-O2D-CED
19	A	1137	CLA	O1D-CGD-O2D-CED
19	B	1219	CLA	O1D-CGD-O2D-CED
19	J	1901	CLA	O1D-CGD-O2D-CED
19	K	1403	CLA	O1D-CGD-O2D-CED
19	2	602	CLA	O1D-CGD-O2D-CED
19	2	606	CLA	O1D-CGD-O2D-CED
19	2	607	CLA	O1D-CGD-O2D-CED
19	A	1101	CLA	CBA-CGA-O2A-C1
19	A	1121	CLA	CBA-CGA-O2A-C1
19	A	1122	CLA	CBA-CGA-O2A-C1
19	A	1129	CLA	CBA-CGA-O2A-C1
19	J	1901	CLA	CBA-CGA-O2A-C1
19	A	1119	CLA	CBD-CGD-O2D-CED
19	A	1120	CLA	CBD-CGD-O2D-CED
19	A	1135	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
19	B	1212	CLA	CBD-CGD-O2D-CED
19	B	1222	CLA	CBD-CGD-O2D-CED
19	B	1231	CLA	CBD-CGD-O2D-CED
19	B	1234	CLA	CBD-CGD-O2D-CED
19	B	1235	CLA	CBD-CGD-O2D-CED
19	B	1236	CLA	CBD-CGD-O2D-CED
19	B	1237	CLA	CBD-CGD-O2D-CED
19	B	1239	CLA	CBD-CGD-O2D-CED
19	G	1603	CLA	CBD-CGD-O2D-CED
19	K	1402	CLA	CBD-CGD-O2D-CED
19	1	604	CLA	CBD-CGD-O2D-CED
19	2	603	CLA	CBD-CGD-O2D-CED
19	A	1101	CLA	O1A-CGA-O2A-C1
19	A	1122	CLA	O1A-CGA-O2A-C1
19	B	1227	CLA	O1A-CGA-O2A-C1
19	B	1237	CLA	O1A-CGA-O2A-C1
19	F	1302	CLA	O1A-CGA-O2A-C1
19	G	1701	CLA	O1A-CGA-O2A-C1
19	2	601	CLA	O1A-CGA-O2A-C1
19	2	602	CLA	O1A-CGA-O2A-C1
19	2	603	CLA	O1A-CGA-O2A-C1
19	3	602	CLA	O1A-CGA-O2A-C1
19	3	603	CLA	O1A-CGA-O2A-C1
19	3	610	CLA	O1A-CGA-O2A-C1
19	4	606	CLA	O1A-CGA-O2A-C1
25	B	5003	LMG	O10-C28-O8-C9
25	B	5004	LMG	O10-C28-O8-C9
25	G	5002	LMG	O10-C28-O8-C9
25	G	5006	LMG	O10-C28-O8-C9
25	2	803	LMG	O10-C28-O8-C9
19	B	1209	CLA	O1A-CGA-O2A-C1
19	G	1602	CLA	O1A-CGA-O2A-C1
19	B	1021	CLA	O1D-CGD-O2D-CED
19	B	1224	CLA	O1D-CGD-O2D-CED
19	F	1302	CLA	O1D-CGD-O2D-CED
19	K	1401	CLA	O1D-CGD-O2D-CED
19	3	603	CLA	O1D-CGD-O2D-CED
19	4	603	CLA	O1D-CGD-O2D-CED
19	B	1207	CLA	C15-C16-C17-C18
19	A	1111	CLA	C4C-C3C-CAC-CBC
19	B	1232	CLA	O1D-CGD-O2D-CED
19	B	1238	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
19	1	611	CLA	O1D-CGD-O2D-CED
19	2	608	CLA	O1D-CGD-O2D-CED
19	4	608	CLA	O1D-CGD-O2D-CED
24	G	5004	LMT	O5B-C1B-O1B-C4'
27	4	801	DGD	O6D-C5D-C6D-O5D
19	B	1203	CLA	CBD-CGD-O2D-CED
19	4	601	CLA	CBD-CGD-O2D-CED
19	4	604	CLA	CBD-CGD-O2D-CED
19	A	1140	CLA	O1D-CGD-O2D-CED
19	1	605	CLA	O1D-CGD-O2D-CED
19	3	612	CLA	O1D-CGD-O2D-CED
19	3	617	CLA	O1D-CGD-O2D-CED
25	F	5002	LMG	O9-C10-O7-C8
25	F	5004	LMG	O9-C10-O7-C8
25	G	5001	LMG	O9-C10-O7-C8
25	G	5002	LMG	O9-C10-O7-C8
25	2	803	LMG	O9-C10-O7-C8
27	F	5005	DGD	O1B-C1B-O2G-C2G
27	4	802	DGD	O1B-C1B-O2G-C2G
19	3	613	CLA	O1A-CGA-O2A-C1
19	A	1101	CLA	C3-C5-C6-C7
19	A	1105	CLA	C3-C5-C6-C7
19	A	1106	CLA	C3-C5-C6-C7
19	A	1110	CLA	C3-C5-C6-C7
19	A	1121	CLA	C3-C5-C6-C7
19	A	1125	CLA	C3-C5-C6-C7
19	A	1137	CLA	C3-C5-C6-C7
19	B	1203	CLA	C3-C5-C6-C7
19	B	1211	CLA	C3-C5-C6-C7
19	B	1215	CLA	C3-C5-C6-C7
19	B	1219	CLA	C3-C5-C6-C7
19	B	1223	CLA	C3-C5-C6-C7
19	B	1228	CLA	C3-C5-C6-C7
19	B	1237	CLA	C3-C5-C6-C7
19	B	1238	CLA	C3-C5-C6-C7
19	1	601	CLA	C3-C5-C6-C7
19	1	611	CLA	C3-C5-C6-C7
19	2	605	CLA	C3-C5-C6-C7
19	3	601	CLA	C3-C5-C6-C7
19	3	605	CLA	C3-C5-C6-C7
19	3	617	CLA	C3-C5-C6-C7
19	A	1104	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
19	A	1108	CLA	CBA-CGA-O2A-C1
19	A	1118	CLA	CBA-CGA-O2A-C1
19	B	1211	CLA	CBA-CGA-O2A-C1
19	B	1227	CLA	CBA-CGA-O2A-C1
19	B	1237	CLA	CBA-CGA-O2A-C1
19	1	606	CLA	CBA-CGA-O2A-C1
19	2	602	CLA	CBA-CGA-O2A-C1
19	2	603	CLA	CBA-CGA-O2A-C1
19	3	602	CLA	CBA-CGA-O2A-C1
19	4	606	CLA	CBA-CGA-O2A-C1
25	F	5002	LMG	C29-C28-O8-C9
25	G	5006	LMG	C29-C28-O8-C9
25	2	803	LMG	C29-C28-O8-C9
25	2	804	LMG	C29-C28-O8-C9
25	A	5006	LMG	C11-C10-O7-C8
27	F	5005	DGD	C2B-C1B-O2G-C2G
19	G	1601	CLA	O1D-CGD-O2D-CED
19	G	1602	CLA	O1D-CGD-O2D-CED
19	G	1701	CLA	O1D-CGD-O2D-CED
19	3	606	CLA	O1D-CGD-O2D-CED
19	4	617	CLA	CBD-CGD-O2D-CED
19	A	1111	CLA	C2C-C3C-CAC-CBC
19	4	609	CLA	O1A-CGA-O2A-C1
19	A	1131	CLA	O1D-CGD-O2D-CED
19	3	613	CLA	CBA-CGA-O2A-C1
19	4	608	CLA	CBA-CGA-O2A-C1
19	2	602	CLA	C3-C5-C6-C7
19	A	1102	CLA	C4-C3-C5-C6
19	A	1104	CLA	C4-C3-C5-C6
19	B	1240	CLA	C4-C3-C5-C6
19	4	601	CLA	C4-C3-C5-C6
19	A	1104	CLA	C2-C3-C5-C6
19	B	1207	CLA	C2-C3-C5-C6
19	G	1601	CLA	C2-C3-C5-C6
19	1	601	CLA	C2-C3-C5-C6
19	A	1127	CLA	CBD-CGD-O2D-CED
19	B	1228	CLA	CBD-CGD-O2D-CED
19	A	1105	CLA	C2A-CAA-CBA-CGA
19	A	1113	CLA	C2A-CAA-CBA-CGA
19	A	1121	CLA	C2A-CAA-CBA-CGA
19	B	1201	CLA	C2A-CAA-CBA-CGA
19	B	1214	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
19	B	1221	CLA	C2A-CAA-CBA-CGA
19	B	1239	CLA	C2A-CAA-CBA-CGA
19	2	601	CLA	C2A-CAA-CBA-CGA
19	2	602	CLA	C2A-CAA-CBA-CGA
19	3	610	CLA	C2A-CAA-CBA-CGA
19	4	606	CLA	C2A-CAA-CBA-CGA
19	4	608	CLA	C2A-CAA-CBA-CGA
29	2	610	CHL	C2A-CAA-CBA-CGA
29	3	604	CHL	C2A-CAA-CBA-CGA
19	A	1107	CLA	O1D-CGD-O2D-CED
25	A	5006	LMG	C17-C18-C19-C20
25	G	5001	LMG	C35-C36-C37-C38
25	G	5001	LMG	C38-C39-C40-C41
25	G	5002	LMG	C17-C18-C19-C20
25	G	5002	LMG	C35-C36-C37-C38
27	B	5005	DGD	C8A-C9A-CAA-CBA
27	F	5005	DGD	C8A-C9A-CAA-CBA
19	A	1109	CLA	C3-C5-C6-C7
19	A	1119	CLA	C3-C5-C6-C7
19	A	1126	CLA	C3-C5-C6-C7
19	B	1205	CLA	C3-C5-C6-C7
19	F	1302	CLA	C3-C5-C6-C7
19	1	605	CLA	C3-C5-C6-C7
19	3	603	CLA	C3-C5-C6-C7
19	3	610	CLA	C3-C5-C6-C7
19	A	1105	CLA	CBA-CGA-O2A-C1
19	A	1126	CLA	CBA-CGA-O2A-C1
19	A	1127	CLA	CBA-CGA-O2A-C1
19	B	1206	CLA	CBA-CGA-O2A-C1
19	B	1208	CLA	CBA-CGA-O2A-C1
19	B	1232	CLA	CBA-CGA-O2A-C1
19	F	1302	CLA	CBA-CGA-O2A-C1
19	G	1603	CLA	CBA-CGA-O2A-C1
19	G	1701	CLA	CBA-CGA-O2A-C1
19	K	1402	CLA	CBA-CGA-O2A-C1
19	L	1501	CLA	CBA-CGA-O2A-C1
19	2	601	CLA	CBA-CGA-O2A-C1
19	2	606	CLA	CBA-CGA-O2A-C1
19	2	612	CLA	CBA-CGA-O2A-C1
19	3	603	CLA	CBA-CGA-O2A-C1
19	3	610	CLA	CBA-CGA-O2A-C1
19	4	617	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
25	B	5003	LMG	C29-C28-O8-C9
25	B	5004	LMG	C29-C28-O8-C9
25	F	5003	LMG	C29-C28-O8-C9
25	G	5002	LMG	C29-C28-O8-C9
27	F	5005	DGD	C2A-C1A-O1G-C1G
27	4	802	DGD	C2A-C1A-O1G-C1G
19	A	1117	CLA	CBD-CGD-O2D-CED
19	A	1128	CLA	CBD-CGD-O2D-CED
19	A	1130	CLA	CBD-CGD-O2D-CED
19	1	614	CLA	CBD-CGD-O2D-CED
19	3	605	CLA	CBD-CGD-O2D-CED
19	A	1115	CLA	O1D-CGD-O2D-CED
19	A	1139	CLA	O1D-CGD-O2D-CED
19	B	1209	CLA	O1D-CGD-O2D-CED
19	B	1227	CLA	O1D-CGD-O2D-CED
19	2	612	CLA	O1D-CGD-O2D-CED
23	B	5002	LHG	O9-C7-O7-C5
23	2	801	LHG	O9-C7-O7-C5
24	A	5004	LMT	C4B-C5B-C6B-O6B
24	G	5004	LMT	C4B-C5B-C6B-O6B
19	A	1118	CLA	O1A-CGA-O2A-C1
19	A	1126	CLA	O1A-CGA-O2A-C1
19	B	1206	CLA	O1A-CGA-O2A-C1
19	B	1208	CLA	O1A-CGA-O2A-C1
19	B	1211	CLA	O1A-CGA-O2A-C1
19	B	1232	CLA	O1A-CGA-O2A-C1
19	G	1603	CLA	O1A-CGA-O2A-C1
19	L	1501	CLA	O1A-CGA-O2A-C1
19	2	606	CLA	O1A-CGA-O2A-C1
19	4	617	CLA	O1A-CGA-O2A-C1
27	4	802	DGD	O1A-C1A-O1G-C1G
19	4	608	CLA	O1A-CGA-O2A-C1
19	1	613	CLA	O1D-CGD-O2D-CED
25	2	805	LMG	O6-C5-C6-O5
19	A	1013	CLA	CBD-CGD-O2D-CED
19	A	1125	CLA	CBD-CGD-O2D-CED
19	B	1215	CLA	CBD-CGD-O2D-CED
19	1	601	CLA	CBD-CGD-O2D-CED
19	2	604	CLA	CBD-CGD-O2D-CED
19	4	605	CLA	CBD-CGD-O2D-CED
19	4	609	CLA	CBD-CGD-O2D-CED
19	A	1103	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
19	A	1114	CLA	O1D-CGD-O2D-CED
19	A	1129	CLA	O1D-CGD-O2D-CED
19	A	1132	CLA	O1D-CGD-O2D-CED
19	2	601	CLA	O1D-CGD-O2D-CED
23	A	5001	LHG	O2-C2-C3-O3
23	B	5001	LHG	O2-C2-C3-O3
23	B	5002	LHG	O2-C2-C3-O3
23	2	807	LHG	O2-C2-C3-O3
19	B	1226	CLA	C3-C5-C6-C7
19	1	614	CLA	C3-C5-C6-C7
19	B	1222	CLA	CBA-CGA-O2A-C1
19	2	605	CLA	CBA-CGA-O2A-C1
19	4	609	CLA	CBA-CGA-O2A-C1
23	A	5001	LHG	C13-C14-C15-C16
19	A	1108	CLA	O1A-CGA-O2A-C1
19	A	1127	CLA	O1A-CGA-O2A-C1
19	K	1402	CLA	O1A-CGA-O2A-C1
24	B	5008	LMT	O5B-C5B-C6B-O6B
24	G	5004	LMT	O5B-C5B-C6B-O6B
24	B	5006	LMT	C4B-C5B-C6B-O6B
19	A	1102	CLA	O1D-CGD-O2D-CED
19	B	1022	CLA	O1D-CGD-O2D-CED
19	B	1207	CLA	O1D-CGD-O2D-CED
19	4	602	CLA	O1D-CGD-O2D-CED
23	2	807	LHG	C8-C7-O7-C5
25	F	5001	LMG	C11-C10-O7-C8
19	1	607	CLA	CBA-CGA-O2A-C1
19	1	608	CLA	CBA-CGA-O2A-C1
19	A	1134	CLA	CBD-CGD-O2D-CED
19	B	1217	CLA	CBD-CGD-O2D-CED
24	B	5006	LMT	O5B-C5B-C6B-O6B
24	G	5004	LMT	O5'-C5'-C6'-O6'
27	F	5005	DGD	O1A-C1A-O1G-C1G
24	A	5004	LMT	O5B-C5B-C6B-O6B
25	2	802	LMG	C4-C5-C6-O5
19	A	1012	CLA	O1D-CGD-O2D-CED
19	1	608	CLA	O1D-CGD-O2D-CED
19	A	1139	CLA	C3-C5-C6-C7
19	B	1232	CLA	C3-C5-C6-C7
19	K	1402	CLA	C3-C5-C6-C7
29	4	613	CHL	C3-C5-C6-C7
19	A	1123	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
19	2	604	CLA	CBA-CGA-O2A-C1
19	A	1116	CLA	O1D-CGD-O2D-CED
19	A	1141	CLA	O1D-CGD-O2D-CED
19	A	1105	CLA	O1A-CGA-O2A-C1
19	2	612	CLA	O1A-CGA-O2A-C1
25	F	5003	LMG	O10-C28-O8-C9
24	B	5008	LMT	O5'-C5'-C6'-O6'
24	J	5003	LMT	O5B-C5B-C6B-O6B
19	A	1116	CLA	C4-C3-C5-C6
19	A	1139	CLA	C4-C3-C5-C6
19	B	1206	CLA	C4-C3-C5-C6
19	B	1225	CLA	C4-C3-C5-C6
19	B	1230	CLA	C4-C3-C5-C6
19	1	605	CLA	C4-C3-C5-C6
19	A	1116	CLA	C2-C3-C5-C6
19	A	1139	CLA	C2-C3-C5-C6
19	B	1206	CLA	C2-C3-C5-C6
19	B	1225	CLA	C2-C3-C5-C6
19	B	1230	CLA	C2-C3-C5-C6
19	1	605	CLA	C2-C3-C5-C6
19	A	1141	CLA	C2A-CAA-CBA-CGA
19	B	1225	CLA	C2A-CAA-CBA-CGA
19	1	607	CLA	C2A-CAA-CBA-CGA
29	2	611	CHL	C2A-CAA-CBA-CGA
29	4	613	CHL	C2A-CAA-CBA-CGA
19	B	1208	CLA	O1D-CGD-O2D-CED
19	A	1123	CLA	O1A-CGA-O2A-C1
19	B	1222	CLA	O1A-CGA-O2A-C1
19	2	605	CLA	O1A-CGA-O2A-C1
24	B	5008	LMT	C4B-C5B-C6B-O6B
24	B	5008	LMT	O5'-C1'-O1'-C1
25	B	5003	LMG	O6-C1-O1-C7
25	G	5001	LMG	O6-C1-O1-C7
19	2	603	CLA	C3-C5-C6-C7
19	B	1202	CLA	CBA-CGA-O2A-C1
19	2	608	CLA	CBA-CGA-O2A-C1
19	4	603	CLA	CBA-CGA-O2A-C1
19	4	605	CLA	CBA-CGA-O2A-C1
27	G	5003	DGD	C2A-C1A-O1G-C1G
27	3	803	DGD	C2A-C1A-O1G-C1G
19	A	1136	CLA	O1D-CGD-O2D-CED
24	G	5004	LMT	C2B-C1B-O1B-C4'

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Mol	Chain	Res	Type	Atoms
19	A	1109	CLA	O1D-CGD-O2D-CED
19	B	1229	CLA	O1D-CGD-O2D-CED
19	B	1235	CLA	O1D-CGD-O2D-CED
19	1	603	CLA	O1D-CGD-O2D-CED
19	B	1202	CLA	O1A-CGA-O2A-C1
19	2	604	CLA	O1A-CGA-O2A-C1
19	B	1222	CLA	O1D-CGD-O2D-CED
19	G	1603	CLA	O1D-CGD-O2D-CED
19	1	604	CLA	O1D-CGD-O2D-CED
19	2	603	CLA	O1D-CGD-O2D-CED
23	B	5001	LHG	C24-C23-O8-C6
19	B	1202	CLA	CBD-CGD-O2D-CED
19	B	1204	CLA	CBD-CGD-O2D-CED
19	F	1301	CLA	CBD-CGD-O2D-CED
19	A	1119	CLA	O1D-CGD-O2D-CED
23	A	5001	LHG	C1-C2-C3-O3
23	A	5002	LHG	C1-C2-C3-O3
23	B	5001	LHG	C1-C2-C3-O3
23	2	801	LHG	C1-C2-C3-O3
24	B	5008	LMT	C4'-C5'-C6'-O6'
25	2	805	LMG	C4-C5-C6-O5
19	A	1013	CLA	O1A-CGA-O2A-C1
19	B	1235	CLA	O1A-CGA-O2A-C1
27	G	5003	DGD	O1A-C1A-O1G-C1G
27	3	803	DGD	O1A-C1A-O1G-C1G
19	A	1127	CLA	C3-C5-C6-C7
19	B	1206	CLA	C3-C5-C6-C7
19	A	1120	CLA	O1D-CGD-O2D-CED
19	A	1013	CLA	CBA-CGA-O2A-C1
19	A	1120	CLA	CBA-CGA-O2A-C1
19	A	1130	CLA	CBA-CGA-O2A-C1
19	A	1134	CLA	CBA-CGA-O2A-C1
19	A	1141	CLA	CBA-CGA-O2A-C1
19	B	1204	CLA	CBA-CGA-O2A-C1
19	B	1219	CLA	CBA-CGA-O2A-C1
19	B	1220	CLA	CBA-CGA-O2A-C1
19	B	1230	CLA	CBA-CGA-O2A-C1
19	B	1235	CLA	CBA-CGA-O2A-C1
19	3	605	CLA	CBA-CGA-O2A-C1
19	3	606	CLA	CBA-CGA-O2A-C1
19	3	612	CLA	CBA-CGA-O2A-C1
19	3	617	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
19	4	602	CLA	CBA-CGA-O2A-C1
27	J	5001	DGD	C2A-C1A-O1G-C1G
27	4	801	DGD	C2A-C1A-O1G-C1G
19	A	1124	CLA	CBD-CGD-O2D-CED
24	J	5003	LMT	C4B-C5B-C6B-O6B
22	L	4019	BCR	C13-C14-C15-C16
22	2	503	BCR	C19-C20-C21-C22
22	3	503	BCR	C13-C14-C15-C16
19	A	1122	CLA	C10-C11-C12-C13
19	B	1202	CLA	C15-C16-C17-C18
19	B	1222	CLA	C15-C16-C17-C18
25	2	804	LMG	O6-C5-C6-O5
19	A	1101	CLA	C10-C11-C12-C13
19	A	1133	CLA	C15-C16-C17-C18
19	A	1141	CLA	C8-C10-C11-C12
19	B	1206	CLA	C15-C16-C17-C18
19	B	1214	CLA	C15-C16-C17-C18
19	B	1237	CLA	C8-C10-C11-C12
19	G	1603	CLA	C8-C10-C11-C12
19	4	601	CLA	C10-C11-C12-C13
24	J	5003	LMT	C2'-C1'-O1'-C1
25	A	5006	LMG	C2-C1-O1-C7
25	G	5001	LMG	C2-C1-O1-C7
27	F	5005	DGD	C2E-C1E-O5D-C6D
27	4	802	DGD	C2D-C1D-O3G-C3G
23	A	5002	LHG	O7-C5-C6-O8
19	3	606	CLA	O1A-CGA-O2A-C1
19	A	1102	CLA	C2-C3-C5-C6
19	B	1240	CLA	C2-C3-C5-C6
19	4	601	CLA	C2-C3-C5-C6
19	A	1013	CLA	C11-C10-C8-C9
19	A	1102	CLA	C11-C10-C8-C9
19	A	1102	CLA	C14-C13-C15-C16
19	A	1107	CLA	C6-C7-C8-C9
19	A	1112	CLA	C6-C7-C8-C9
19	A	1112	CLA	C14-C13-C15-C16
19	A	1115	CLA	C11-C10-C8-C9
19	A	1115	CLA	C11-C12-C13-C14
19	A	1115	CLA	C14-C13-C15-C16
19	A	1120	CLA	C11-C10-C8-C9
19	A	1125	CLA	C11-C10-C8-C9
19	A	1132	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
19	A	1137	CLA	C6-C7-C8-C9
19	A	1138	CLA	C6-C7-C8-C9
19	A	1138	CLA	C11-C12-C13-C14
19	A	1140	CLA	C6-C7-C8-C9
19	A	1141	CLA	C11-C10-C8-C9
19	B	1022	CLA	C6-C7-C8-C9
19	B	1023	CLA	C14-C13-C15-C16
19	B	1203	CLA	C6-C7-C8-C9
19	B	1208	CLA	C11-C10-C8-C9
19	B	1211	CLA	C14-C13-C15-C16
19	B	1214	CLA	C11-C10-C8-C9
19	B	1214	CLA	C14-C13-C15-C16
19	B	1216	CLA	C14-C13-C15-C16
19	B	1221	CLA	C14-C13-C15-C16
19	B	1222	CLA	C6-C7-C8-C9
19	B	1225	CLA	C11-C12-C13-C14
19	B	1226	CLA	C11-C12-C13-C14
19	B	1237	CLA	C14-C13-C15-C16
19	B	1239	CLA	C11-C10-C8-C9
19	F	1301	CLA	C6-C7-C8-C9
19	F	1302	CLA	C11-C12-C13-C14
19	L	1502	CLA	C6-C7-C8-C9
19	1	604	CLA	C14-C13-C15-C16
19	2	607	CLA	C6-C7-C8-C9
19	4	601	CLA	C6-C7-C8-C9
19	4	605	CLA	C11-C10-C8-C9
19	4	612	CLA	C14-C13-C15-C16
19	4	617	CLA	C14-C13-C15-C16
19	K	1402	CLA	O1D-CGD-O2D-CED
19	A	1123	CLA	CBD-CGD-O2D-CED
19	B	1228	CLA	C8-C10-C11-C12
19	A	1109	CLA	C2A-CAA-CBA-CGA
19	3	603	CLA	C2A-CAA-CBA-CGA
22	A	4002	BCR	C36-C18-C19-C20
22	A	4007	BCR	C36-C18-C19-C20
22	A	4008	BCR	C37-C22-C23-C24
22	A	4011	BCR	C37-C22-C23-C24
22	B	4006	BCR	C37-C22-C23-C24
22	B	4009	BCR	C7-C8-C9-C34
22	F	4014	BCR	C36-C18-C19-C20
22	G	4021	BCR	C36-C18-C19-C20
22	I	4018	BCR	C36-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
22	K	4001	BCR	C37-C22-C23-C24
22	L	4019	BCR	C37-C22-C23-C24
22	1	503	BCR	C7-C8-C9-C34
22	1	503	BCR	C36-C18-C19-C20
28	4	501	LUT	C27-C28-C29-C39
31	4	505	C7Z	C31-C32-C33-C40
31	4	505	C7Z	C27-C28-C29-C39
22	F	4016	BCR	C17-C18-C19-C20
22	G	4021	BCR	C17-C18-C19-C20
22	G	4021	BCR	C21-C22-C23-C24
22	L	4019	BCR	C21-C22-C23-C24
22	1	503	BCR	C7-C8-C9-C10
22	3	503	BCR	C7-C8-C9-C10
23	2	807	LHG	O9-C7-O7-C5
25	F	5001	LMG	O9-C10-O7-C8
23	B	5002	LHG	C23-C24-C25-C26
25	3	802	LMG	C10-C11-C12-C13
19	A	1130	CLA	O1A-CGA-O2A-C1
19	B	1230	CLA	O1A-CGA-O2A-C1
19	3	605	CLA	O1A-CGA-O2A-C1
19	3	612	CLA	O1A-CGA-O2A-C1
27	J	5001	DGD	O1A-C1A-O1G-C1G
27	4	801	DGD	O1A-C1A-O1G-C1G
19	B	1207	CLA	C13-C15-C16-C17
19	B	1211	CLA	C13-C15-C16-C17
19	B	1218	CLA	C5-C6-C7-C8
19	B	1219	CLA	C5-C6-C7-C8
19	2	601	CLA	C10-C11-C12-C13
19	2	603	CLA	C15-C16-C17-C18
19	3	610	CLA	C15-C16-C17-C18
19	4	612	CLA	C10-C11-C12-C13
20	A	2001	PQN	C18-C20-C21-C22
27	J	5001	DGD	CDA-CEA-CFA-CGA
19	2	601	CLA	C3-C5-C6-C7
24	A	5004	LMT	C2B-C1B-O1B-C4'
19	A	1116	CLA	CBA-CGA-O2A-C1
19	B	1231	CLA	CBA-CGA-O2A-C1
19	1	604	CLA	CBA-CGA-O2A-C1
19	A	1107	CLA	C13-C15-C16-C17
19	A	1109	CLA	C13-C15-C16-C17
19	A	1111	CLA	C15-C16-C17-C18
19	A	1115	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
19	A	1119	CLA	C8-C10-C11-C12
19	A	1133	CLA	C8-C10-C11-C12
19	A	1133	CLA	C10-C11-C12-C13
19	B	1205	CLA	C8-C10-C11-C12
19	B	1219	CLA	C8-C10-C11-C12
19	B	1226	CLA	C15-C16-C17-C18
19	B	1230	CLA	C5-C6-C7-C8
19	B	1239	CLA	C10-C11-C12-C13
19	G	1701	CLA	C10-C11-C12-C13
19	1	601	CLA	C8-C10-C11-C12
19	3	605	CLA	C5-C6-C7-C8
19	3	610	CLA	C13-C15-C16-C17
23	A	5002	LHG	C7-C8-C9-C10
23	2	807	LHG	C7-C8-C9-C10
25	B	5004	LMG	C28-C29-C30-C31
27	4	801	DGD	C1A-C2A-C3A-C4A
19	A	1134	CLA	O1A-CGA-O2A-C1
25	F	5004	LMG	O6-C5-C6-O5
19	A	1012	CLA	C8-C10-C11-C12
19	A	1101	CLA	C8-C10-C11-C12
19	A	1104	CLA	C13-C15-C16-C17
19	A	1106	CLA	C5-C6-C7-C8
19	A	1107	CLA	C10-C11-C12-C13
19	A	1109	CLA	C10-C11-C12-C13
19	A	1112	CLA	C8-C10-C11-C12
19	A	1115	CLA	C10-C11-C12-C13
19	A	1117	CLA	C8-C10-C11-C12
19	A	1121	CLA	C10-C11-C12-C13
19	A	1123	CLA	C15-C16-C17-C18
19	A	1126	CLA	C5-C6-C7-C8
19	A	1127	CLA	C8-C10-C11-C12
19	B	1203	CLA	C5-C6-C7-C8
19	B	1214	CLA	C10-C11-C12-C13
19	B	1219	CLA	C13-C15-C16-C17
19	B	1225	CLA	C5-C6-C7-C8
19	B	1228	CLA	C10-C11-C12-C13
19	B	1240	CLA	C15-C16-C17-C18
19	2	605	CLA	C5-C6-C7-C8
19	2	605	CLA	C15-C16-C17-C18
19	4	617	CLA	C15-C16-C17-C18
29	2	615	CHL	C2C-C3C-CAC-CBC
19	B	1237	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
19	B	1220	CLA	O1A-CGA-O2A-C1
25	A	5006	LMG	C28-C29-C30-C31
25	F	5003	LMG	C28-C29-C30-C31
19	A	1135	CLA	O1D-CGD-O2D-CED
19	B	1236	CLA	O1D-CGD-O2D-CED
19	A	1012	CLA	C15-C16-C17-C18
19	A	1013	CLA	C10-C11-C12-C13
19	A	1101	CLA	C5-C6-C7-C8
19	A	1103	CLA	C13-C15-C16-C17
19	A	1106	CLA	C8-C10-C11-C12
19	A	1111	CLA	C10-C11-C12-C13
19	A	1111	CLA	C13-C15-C16-C17
19	A	1112	CLA	C15-C16-C17-C18
19	A	1117	CLA	C13-C15-C16-C17
19	A	1128	CLA	C10-C11-C12-C13
19	B	1207	CLA	C5-C6-C7-C8
19	B	1214	CLA	C8-C10-C11-C12
19	B	1218	CLA	C15-C16-C17-C18
19	B	1224	CLA	C13-C15-C16-C17
19	B	1227	CLA	C8-C10-C11-C12
19	B	1237	CLA	C10-C11-C12-C13
19	1	603	CLA	C5-C6-C7-C8
19	4	612	CLA	C5-C6-C7-C8
19	1	608	CLA	O1A-CGA-O2A-C1
19	B	1212	CLA	O1D-CGD-O2D-CED
19	B	1239	CLA	O1D-CGD-O2D-CED
27	F	5005	DGD	O6E-C5E-C6E-O5E
19	A	1101	CLA	C2-C1-O2A-CGA
19	A	1103	CLA	C2-C1-O2A-CGA
19	A	1112	CLA	C2-C1-O2A-CGA
19	A	1118	CLA	C2-C1-O2A-CGA
19	A	1120	CLA	C2-C1-O2A-CGA
19	A	1126	CLA	C2-C1-O2A-CGA
19	A	1137	CLA	C2-C1-O2A-CGA
19	B	1022	CLA	C2-C1-O2A-CGA
19	B	1220	CLA	C2-C1-O2A-CGA
19	B	1229	CLA	C2-C1-O2A-CGA
19	B	1230	CLA	C2-C1-O2A-CGA
19	B	1236	CLA	C2-C1-O2A-CGA
19	B	1238	CLA	C2-C1-O2A-CGA
19	J	1901	CLA	C2-C1-O2A-CGA
19	2	604	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
19	3	602	CLA	C2-C1-O2A-CGA
19	3	610	CLA	C2-C1-O2A-CGA
19	3	617	CLA	C2-C1-O2A-CGA
19	4	605	CLA	C2-C1-O2A-CGA
19	4	607	CLA	C2-C1-O2A-CGA
19	B	1022	CLA	C8-C10-C11-C12
19	B	1212	CLA	C5-C6-C7-C8
19	K	1402	CLA	C8-C10-C11-C12
19	K	1402	CLA	C10-C11-C12-C13
25	F	5003	LMG	C10-C11-C12-C13
19	A	1108	CLA	CBD-CGD-O2D-CED
19	A	1133	CLA	CBD-CGD-O2D-CED
27	J	5001	DGD	C2B-C1B-O2G-C2G
19	A	1122	CLA	C13-C15-C16-C17
19	B	1239	CLA	C15-C16-C17-C18
19	A	1101	CLA	C6-C7-C8-C10
19	A	1101	CLA	C12-C13-C15-C16
19	A	1105	CLA	C11-C10-C8-C7
19	A	1112	CLA	C6-C7-C8-C10
19	A	1129	CLA	C6-C7-C8-C10
19	A	1136	CLA	C11-C10-C8-C7
19	B	1201	CLA	C11-C10-C8-C7
19	B	1201	CLA	C12-C13-C15-C16
19	B	1203	CLA	C11-C10-C8-C7
19	B	1206	CLA	C11-C12-C13-C15
19	B	1207	CLA	C12-C13-C15-C16
19	B	1210	CLA	C11-C10-C8-C7
19	B	1210	CLA	C11-C12-C13-C15
19	B	1231	CLA	C6-C7-C8-C10
19	B	1238	CLA	C11-C12-C13-C15
19	1	611	CLA	C11-C10-C8-C7
19	3	610	CLA	C12-C13-C15-C16
20	B	2002	PQN	C21-C22-C23-C25
19	A	1102	CLA	C3-C5-C6-C7
19	A	1116	CLA	C3-C5-C6-C7
19	A	1120	CLA	O1A-CGA-O2A-C1
19	B	1204	CLA	O1A-CGA-O2A-C1
19	B	1219	CLA	O1A-CGA-O2A-C1
19	4	602	CLA	O1A-CGA-O2A-C1
19	4	603	CLA	O1A-CGA-O2A-C1
19	4	605	CLA	O1A-CGA-O2A-C1
22	A	4017	BCR	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
22	3	506	BCR	C19-C20-C21-C22
19	A	1106	CLA	C2A-CAA-CBA-CGA
19	A	1130	CLA	C2A-CAA-CBA-CGA
19	B	1219	CLA	C2A-CAA-CBA-CGA
19	G	1603	CLA	C2A-CAA-CBA-CGA
19	L	1503	CLA	C2A-CAA-CBA-CGA
19	2	608	CLA	C2A-CAA-CBA-CGA
19	B	1231	CLA	O1D-CGD-O2D-CED
19	4	601	CLA	O1D-CGD-O2D-CED
19	4	604	CLA	O1D-CGD-O2D-CED
19	A	1131	CLA	C5-C6-C7-C8
19	A	1137	CLA	C13-C15-C16-C17
19	B	1210	CLA	C13-C15-C16-C17
19	B	1229	CLA	C15-C16-C17-C18
19	2	603	CLA	C13-C15-C16-C17
19	4	603	CLA	C5-C6-C7-C8
19	4	607	CLA	C8-C10-C11-C12
25	A	5006	LMG	C19-C20-C21-C22
25	2	802	LMG	O6-C5-C6-O5
19	A	1141	CLA	O1A-CGA-O2A-C1
19	3	617	CLA	O1A-CGA-O2A-C1
19	B	1213	CLA	CBD-CGD-O2D-CED
19	1	611	CLA	C13-C15-C16-C17
19	4	617	CLA	C10-C11-C12-C13
22	A	4008	BCR	C10-C11-C12-C13
22	B	4006	BCR	C10-C11-C12-C13
22	K	4001	BCR	C10-C11-C12-C13
22	L	4019	BCR	C10-C11-C12-C13
19	B	1234	CLA	O1D-CGD-O2D-CED
23	2	801	LHG	O2-C2-C3-O3
19	A	1112	CLA	C3-C5-C6-C7
19	A	1103	CLA	C8-C10-C11-C12
19	A	1140	CLA	C10-C11-C12-C13
19	B	1208	CLA	C5-C6-C7-C8
19	B	1237	CLA	C15-C16-C17-C18
19	B	1239	CLA	C5-C6-C7-C8
19	F	1301	CLA	C5-C6-C7-C8
19	L	1502	CLA	C10-C11-C12-C13
19	2	601	CLA	C5-C6-C7-C8
19	2	603	CLA	C10-C11-C12-C13
19	4	605	CLA	C5-C6-C7-C8
29	2	610	CHL	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
27	B	5005	DGD	C2A-C1A-O1G-C1G
19	2	608	CLA	O1A-CGA-O2A-C1
19	A	1119	CLA	C13-C15-C16-C17
19	A	1120	CLA	C8-C10-C11-C12
19	A	1126	CLA	C15-C16-C17-C18
19	A	1132	CLA	C8-C10-C11-C12
19	B	1201	CLA	C8-C10-C11-C12
19	B	1201	CLA	C13-C15-C16-C17
19	B	1216	CLA	C8-C10-C11-C12
19	B	1224	CLA	C15-C16-C17-C18
19	B	1226	CLA	C10-C11-C12-C13
19	B	1237	CLA	C13-C15-C16-C17
19	F	1302	CLA	C13-C15-C16-C17
19	K	1402	CLA	C5-C6-C7-C8
19	1	607	CLA	O1A-CGA-O2A-C1
19	B	1203	CLA	O1D-CGD-O2D-CED
19	4	617	CLA	O1D-CGD-O2D-CED
25	F	5001	LMG	C4-C5-C6-O5
19	A	1117	CLA	C5-C6-C7-C8
19	A	1121	CLA	C8-C10-C11-C12
19	A	1125	CLA	C5-C6-C7-C8
19	A	1129	CLA	C15-C16-C17-C18
19	A	1136	CLA	C8-C10-C11-C12
19	A	1137	CLA	C8-C10-C11-C12
19	B	1202	CLA	C13-C15-C16-C17
19	B	1204	CLA	C15-C16-C17-C18
19	B	1231	CLA	C8-C10-C11-C12
19	G	1603	CLA	C5-C6-C7-C8
19	1	601	CLA	C15-C16-C17-C18
19	1	614	CLA	C5-C6-C7-C8
23	A	5001	LHG	C3-O3-P-O6
23	A	5001	LHG	C4-O6-P-O3
23	A	5002	LHG	C4-O6-P-O3
23	B	5002	LHG	C3-O3-P-O6
23	1	801	LHG	C3-O3-P-O6
23	2	807	LHG	C3-O3-P-O6
23	2	807	LHG	C4-O6-P-O3
23	3	801	LHG	C4-O6-P-O3
19	B	1218	CLA	CBA-CGA-O2A-C1
19	F	1301	CLA	CBA-CGA-O2A-C1
19	4	605	CLA	O1D-CGD-O2D-CED
19	A	1127	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
19	A	1141	CLA	C5-C6-C7-C8
19	B	1206	CLA	C13-C15-C16-C17
19	1	605	CLA	C15-C16-C17-C18
19	4	617	CLA	C5-C6-C7-C8
23	A	5001	LHG	C7-C8-C9-C10
23	2	807	LHG	C23-C24-C25-C26
19	A	1127	CLA	O1D-CGD-O2D-CED
23	B	5002	LHG	C1-C2-C3-O3
23	1	801	LHG	C1-C2-C3-O3
27	J	5001	DGD	O1B-C1B-O2G-C2G
19	B	1229	CLA	C5-C6-C7-C8
19	1	614	CLA	C8-C10-C11-C12
19	4	603	CLA	C8-C10-C11-C12
19	2	603	CLA	C2A-CAA-CBA-CGA
19	4	607	CLA	C2A-CAA-CBA-CGA
19	A	1110	CLA	C6-C7-C8-C9
19	B	1204	CLA	C16-C17-C18-C20
19	G	1603	CLA	C16-C17-C18-C20
19	4	604	CLA	C11-C12-C13-C14
27	4	802	DGD	O6E-C5E-C6E-O5E
19	A	1129	CLA	C3-C5-C6-C7
19	B	1230	CLA	C3-C5-C6-C7
19	B	1234	CLA	C3-C5-C6-C7
19	A	1124	CLA	CBA-CGA-O2A-C1
19	B	1240	CLA	CBA-CGA-O2A-C1
19	A	1102	CLA	C5-C6-C7-C8
19	1	604	CLA	O1A-CGA-O2A-C1
22	L	4020	BCR	C19-C20-C21-C22
25	F	5003	LMG	C30-C31-C32-C33
25	G	5002	LMG	C16-C17-C18-C19
25	F	5003	LMG	C11-C10-O7-C8
19	B	1211	CLA	C5-C6-C7-C8
19	B	1211	CLA	C15-C16-C17-C18
22	B	4004	BCR	C11-C10-C9-C34
22	G	4011	BCR	C11-C10-C9-C34
22	3	506	BCR	C11-C10-C9-C34
23	1	801	LHG	C30-C31-C32-C33
25	G	5002	LMG	C29-C30-C31-C32
19	A	1117	CLA	O1D-CGD-O2D-CED
19	B	1207	CLA	C16-C17-C18-C19
19	B	1221	CLA	C16-C17-C18-C19
19	B	1226	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
19	B	1232	CLA	C6-C7-C8-C9
19	3	603	CLA	C6-C7-C8-C10
19	A	1112	CLA	CBA-CGA-O2A-C1
25	B	5004	LMG	C11-C12-C13-C14
19	1	601	CLA	O1D-CGD-O2D-CED
19	1	614	CLA	O1D-CGD-O2D-CED
25	F	5003	LMG	O9-C10-O7-C8
19	4	617	CLA	C13-C15-C16-C17
23	1	801	LHG	C23-C24-C25-C26
23	A	5002	LHG	C27-C28-C29-C30
19	A	1013	CLA	O1D-CGD-O2D-CED
19	A	1130	CLA	O1D-CGD-O2D-CED
19	A	1116	CLA	O1A-CGA-O2A-C1
19	B	1231	CLA	O1A-CGA-O2A-C1
19	F	1301	CLA	O1A-CGA-O2A-C1
27	B	5005	DGD	C6A-C7A-C8A-C9A
24	A	5004	LMT	O5B-C1B-O1B-C4'
19	B	1228	CLA	O1D-CGD-O2D-CED
19	A	1134	CLA	C5-C6-C7-C8
29	3	604	CHL	C5-C6-C7-C8
23	B	5002	LHG	C11-C12-C13-C14
23	1	801	LHG	C13-C14-C15-C16
27	F	5005	DGD	C2A-C3A-C4A-C5A
19	A	1128	CLA	O1D-CGD-O2D-CED
22	B	4004	BCR	C11-C10-C9-C8
22	G	4011	BCR	C11-C10-C9-C8
22	3	506	BCR	C11-C10-C9-C8
24	B	5008	LMT	C2'-C1'-O1'-C1
31	4	505	C7Z	C12-C13-C14-C15
23	A	5002	LHG	C10-C11-C12-C13
23	A	5002	LHG	C11-C12-C13-C14
23	B	5002	LHG	C31-C32-C33-C34
25	B	5003	LMG	C11-C12-C13-C14
27	B	5005	DGD	C2A-C3A-C4A-C5A
19	A	1120	CLA	C5-C6-C7-C8
19	F	1302	CLA	C8-C10-C11-C12
19	4	604	CLA	C8-C10-C11-C12
19	B	1218	CLA	O1A-CGA-O2A-C1
19	A	1115	CLA	C16-C17-C18-C20
19	A	1117	CLA	C16-C17-C18-C19
19	A	1123	CLA	C16-C17-C18-C20
19	A	1129	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
19	B	1235	CLA	C16-C17-C18-C20
19	G	1603	CLA	C16-C17-C18-C19
19	K	1402	CLA	C11-C12-C13-C15
19	3	605	CLA	O1D-CGD-O2D-CED
19	A	1103	CLA	C4-C3-C5-C6
19	B	1234	CLA	C4-C3-C5-C6
19	A	1105	CLA	C6-C7-C8-C9
19	A	1106	CLA	C14-C13-C15-C16
19	B	1201	CLA	C14-C13-C15-C16
19	B	1210	CLA	C11-C10-C8-C9
19	B	1221	CLA	C11-C12-C13-C14
19	B	1225	CLA	C14-C13-C15-C16
19	K	1402	CLA	C6-C7-C8-C9
19	L	1502	CLA	C11-C10-C8-C9
19	1	611	CLA	C6-C7-C8-C9
20	B	2002	PQN	C21-C22-C23-C24
23	A	5002	LHG	C13-C14-C15-C16
19	B	1223	CLA	C13-C15-C16-C17
19	A	1119	CLA	C2A-CAA-CBA-CGA
19	B	1237	CLA	C2A-CAA-CBA-CGA
19	2	604	CLA	O1D-CGD-O2D-CED
22	A	4008	BCR	C7-C8-C9-C34
22	1	504	BCR	C11-C12-C13-C35
22	3	506	BCR	C37-C22-C23-C24
31	4	505	C7Z	C11-C12-C13-C20
23	B	5001	LHG	O1-C1-C2-C3
22	A	4008	BCR	C7-C8-C9-C10
22	K	4001	BCR	C21-C22-C23-C24
22	1	504	BCR	C11-C12-C13-C14
22	3	506	BCR	C21-C22-C23-C24
28	3	502	LUT	C31-C32-C33-C34
19	F	1301	CLA	C3-C5-C6-C7
25	2	804	LMG	O9-C10-O7-C8
19	B	1216	CLA	C10-C11-C12-C13
19	1	611	CLA	C8-C10-C11-C12
25	2	804	LMG	C11-C10-O7-C8
23	A	5002	LHG	C26-C27-C28-C29
23	1	801	LHG	C11-C12-C13-C14
23	2	807	LHG	C9-C10-C11-C12
25	G	5002	LMG	C12-C13-C14-C15
25	B	5004	LMG	C10-C11-C12-C13
27	4	802	DGD	C1A-C2A-C3A-C4A

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Mol	Chain	Res	Type	Atoms
19	4	609	CLA	O1D-CGD-O2D-CED
23	A	5001	LHG	C11-C12-C13-C14
25	2	803	LMG	O6-C5-C6-O5
19	A	1012	CLA	C16-C17-C18-C19
19	A	1012	CLA	C16-C17-C18-C20
19	A	1102	CLA	C16-C17-C18-C19
19	A	1107	CLA	C16-C17-C18-C19
19	A	1107	CLA	C16-C17-C18-C20
19	A	1110	CLA	C6-C7-C8-C10
19	A	1112	CLA	C16-C17-C18-C19
19	B	1212	CLA	C6-C7-C8-C10
19	B	1219	CLA	C16-C17-C18-C19
19	B	1219	CLA	C16-C17-C18-C20
19	B	1240	CLA	C16-C17-C18-C19
19	K	1402	CLA	C11-C12-C13-C14
19	3	601	CLA	C6-C7-C8-C10
29	4	613	CHL	C11-C12-C13-C15
19	A	1013	CLA	C5-C6-C7-C8
19	A	1129	CLA	C5-C6-C7-C8
23	A	5001	LHG	C15-C16-C17-C18
23	A	5002	LHG	C33-C34-C35-C36
23	2	801	LHG	C10-C11-C12-C13
19	A	1105	CLA	CBD-CGD-O2D-CED
23	B	5001	LHG	O10-C23-O8-C6
19	A	1125	CLA	O1D-CGD-O2D-CED
24	G	5004	LMT	C6-C7-C8-C9
25	3	802	LMG	C11-C12-C13-C14
23	2	801	LHG	C11-C12-C13-C14
25	F	5003	LMG	C33-C34-C35-C36
24	A	5004	LMT	O5'-C5'-C6'-O6'
19	B	1201	CLA	CBA-CGA-O2A-C1
23	A	5002	LHG	C24-C23-O8-C6
27	1	803	DGD	O6D-C5D-C6D-O5D
19	B	1215	CLA	O1D-CGD-O2D-CED
19	A	1101	CLA	C3A-C2A-CAA-CBA
19	A	1104	CLA	C3A-C2A-CAA-CBA
19	A	1130	CLA	C3A-C2A-CAA-CBA
19	A	1135	CLA	C3A-C2A-CAA-CBA
19	B	1210	CLA	C3A-C2A-CAA-CBA
19	B	1221	CLA	C3A-C2A-CAA-CBA
19	B	1228	CLA	C3A-C2A-CAA-CBA
19	G	1602	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
19	J	1901	CLA	C3A-C2A-CAA-CBA
19	K	1402	CLA	C3A-C2A-CAA-CBA
19	K	1403	CLA	C3A-C2A-CAA-CBA
19	L	1501	CLA	C3A-C2A-CAA-CBA
19	1	602	CLA	C3A-C2A-CAA-CBA
19	1	603	CLA	C3A-C2A-CAA-CBA
19	3	605	CLA	C3A-C2A-CAA-CBA
19	3	613	CLA	C3A-C2A-CAA-CBA
19	3	617	CLA	C3A-C2A-CAA-CBA
29	2	613	CHL	C3A-C2A-CAA-CBA
29	3	607	CHL	C3A-C2A-CAA-CBA
19	A	1137	CLA	C10-C11-C12-C13
19	4	603	CLA	C15-C16-C17-C18
23	2	807	LHG	C11-C10-C9-C8
25	G	5001	LMG	C15-C16-C17-C18
19	A	1112	CLA	C16-C17-C18-C20
19	A	1126	CLA	C16-C17-C18-C19
19	A	1131	CLA	C16-C17-C18-C19
19	A	1131	CLA	C16-C17-C18-C20
19	B	1207	CLA	C16-C17-C18-C20
19	B	1212	CLA	C6-C7-C8-C9
19	B	1221	CLA	C16-C17-C18-C20
19	B	1222	CLA	C16-C17-C18-C19
19	B	1222	CLA	C16-C17-C18-C20
19	B	1232	CLA	C6-C7-C8-C10
19	1	603	CLA	C6-C7-C8-C10
29	1	612	CHL	C11-C12-C13-C15
25	2	806	LMG	O6-C5-C6-O5
19	3	602	CLA	CBD-CGD-O2D-CED
23	A	5002	LHG	C31-C32-C33-C34
27	J	5001	DGD	C2B-C3B-C4B-C5B
29	3	607	CHL	O2A-C1-C2-C3
19	1	611	CLA	C4-C3-C5-C6
19	4	604	CLA	CBA-CGA-O2A-C1
19	A	1103	CLA	C2-C3-C5-C6
19	1	611	CLA	C2-C3-C5-C6
23	1	801	LHG	O1-C1-C2-O2
23	2	801	LHG	O1-C1-C2-O2
19	A	1124	CLA	O1A-CGA-O2A-C1
19	B	1240	CLA	O1A-CGA-O2A-C1
27	B	5005	DGD	O1A-C1A-O1G-C1G
25	F	5001	LMG	O6-C5-C6-O5

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Mol	Chain	Res	Type	Atoms
18	A	1011	CL0	C16-C17-C18-C19
19	A	1115	CLA	C16-C17-C18-C19
19	A	1117	CLA	C16-C17-C18-C20
19	A	1129	CLA	C16-C17-C18-C20
19	B	1204	CLA	C16-C17-C18-C19
19	4	604	CLA	C11-C12-C13-C15
19	B	1218	CLA	C8-C10-C11-C12
19	B	1238	CLA	C13-C15-C16-C17
19	1	605	CLA	C10-C11-C12-C13
19	A	1104	CLA	C3-C5-C6-C7
19	B	1202	CLA	C3-C5-C6-C7
24	G	5004	LMT	C4'-C5'-C6'-O6'
19	A	1112	CLA	O1A-CGA-O2A-C1
19	A	1106	CLA	C2-C1-O2A-CGA
19	A	1107	CLA	C2-C1-O2A-CGA
19	A	1108	CLA	C2-C1-O2A-CGA
19	A	1139	CLA	C2-C1-O2A-CGA
19	B	1204	CLA	C2-C1-O2A-CGA
19	B	1206	CLA	C2-C1-O2A-CGA
19	B	1214	CLA	C2-C1-O2A-CGA
19	B	1225	CLA	C2-C1-O2A-CGA
19	B	1227	CLA	C2-C1-O2A-CGA
19	B	1232	CLA	C2-C1-O2A-CGA
19	F	1302	CLA	C2-C1-O2A-CGA
19	1	611	CLA	C2-C1-O2A-CGA
19	2	601	CLA	C2-C1-O2A-CGA
19	4	602	CLA	C2-C1-O2A-CGA
27	F	5005	DGD	C3A-C4A-C5A-C6A
19	B	1226	CLA	C16-C17-C18-C20
22	A	4002	BCR	C5-C6-C7-C8
22	A	4008	BCR	C23-C24-C25-C26
22	A	4008	BCR	C23-C24-C25-C30
22	B	4005	BCR	C1-C6-C7-C8
22	B	4005	BCR	C5-C6-C7-C8
22	B	4006	BCR	C23-C24-C25-C26
22	B	4006	BCR	C23-C24-C25-C30
22	B	4009	BCR	C23-C24-C25-C26
22	B	4009	BCR	C23-C24-C25-C30
22	B	4010	BCR	C1-C6-C7-C8
22	B	4010	BCR	C5-C6-C7-C8
22	G	4011	BCR	C23-C24-C25-C30
22	I	4018	BCR	C1-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
22	I	4020	BCR	C23-C24-C25-C26
22	I	4020	BCR	C23-C24-C25-C30
22	J	4012	BCR	C5-C6-C7-C8
22	K	4002	BCR	C5-C6-C7-C8
22	L	4020	BCR	C1-C6-C7-C8
22	L	4020	BCR	C5-C6-C7-C8
22	1	504	BCR	C23-C24-C25-C26
22	1	504	BCR	C23-C24-C25-C30
22	2	503	BCR	C1-C6-C7-C8
22	2	503	BCR	C5-C6-C7-C8
22	2	503	BCR	C23-C24-C25-C26
22	2	503	BCR	C23-C24-C25-C30
22	3	503	BCR	C1-C6-C7-C8
22	3	506	BCR	C1-C6-C7-C8
28	1	501	LUT	C1-C6-C7-C8
28	1	501	LUT	C5-C6-C7-C8
23	A	5002	LHG	C32-C33-C34-C35
18	A	1011	CL0	CBA-CGA-O2A-C1
19	B	1212	CLA	CBA-CGA-O2A-C1
19	B	1226	CLA	CBA-CGA-O2A-C1
19	B	1228	CLA	CBA-CGA-O2A-C1
19	1	601	CLA	CBA-CGA-O2A-C1
27	1	803	DGD	C2A-C1A-O1G-C1G
19	A	1129	CLA	C8-C10-C11-C12
19	B	1224	CLA	C5-C6-C7-C8
19	B	1227	CLA	C15-C16-C17-C18
19	F	1302	CLA	C5-C6-C7-C8
19	L	1502	CLA	C8-C10-C11-C12
19	1	601	CLA	C5-C6-C7-C8
19	4	607	CLA	C10-C11-C12-C13
20	B	2002	PQN	C23-C25-C26-C27
23	A	5002	LHG	C8-C7-O7-C5
27	B	5005	DGD	C7A-C8A-C9A-CAA
23	B	5002	LHG	C14-C15-C16-C17
19	A	1136	CLA	C10-C11-C12-C13
23	B	5002	LHG	C16-C17-C18-C19
19	B	1226	CLA	C4-C3-C5-C6
19	3	617	CLA	C4-C3-C5-C6
19	A	1134	CLA	O1D-CGD-O2D-CED
19	A	1012	CLA	C6-C7-C8-C10
19	A	1102	CLA	C12-C13-C15-C16
19	A	1106	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
19	A	1107	CLA	C6-C7-C8-C10
19	A	1107	CLA	C11-C12-C13-C15
19	A	1112	CLA	C12-C13-C15-C16
19	A	1115	CLA	C12-C13-C15-C16
19	A	1123	CLA	C2-C3-C5-C6
19	A	1137	CLA	C6-C7-C8-C10
19	A	1137	CLA	C11-C10-C8-C7
19	A	1138	CLA	C6-C7-C8-C10
19	A	1138	CLA	C11-C10-C8-C7
19	A	1140	CLA	C6-C7-C8-C10
19	A	1141	CLA	C11-C10-C8-C7
19	B	1201	CLA	C11-C12-C13-C15
19	B	1219	CLA	C11-C12-C13-C15
19	B	1221	CLA	C11-C12-C13-C15
19	B	1226	CLA	C11-C12-C13-C15
19	B	1234	CLA	C2-C3-C5-C6
19	F	1302	CLA	C11-C12-C13-C15
19	K	1402	CLA	C6-C7-C8-C10
19	L	1502	CLA	C6-C7-C8-C10
19	L	1502	CLA	C11-C10-C8-C7
19	1	611	CLA	C6-C7-C8-C10
19	2	607	CLA	C6-C7-C8-C10
19	4	603	CLA	C11-C12-C13-C15
19	4	603	CLA	C12-C13-C15-C16
19	4	604	CLA	C11-C10-C8-C7
20	B	2002	PQN	C17-C18-C20-C21
29	3	604	CHL	C12-C13-C15-C16
19	B	1201	CLA	O1A-CGA-O2A-C1
19	4	604	CLA	O1A-CGA-O2A-C1
23	A	5002	LHG	O10-C23-O8-C6
29	2	611	CHL	C2C-C3C-CAC-CBC
19	A	1102	CLA	C10-C11-C12-C13
19	A	1122	CLA	C5-C6-C7-C8
19	B	1207	CLA	C8-C10-C11-C12
19	A	1130	CLA	C6-C7-C8-C9
19	L	1502	CLA	C11-C12-C13-C15
19	1	605	CLA	C16-C17-C18-C19
27	G	5003	DGD	C1B-C2B-C3B-C4B
23	A	5002	LHG	C28-C29-C30-C31
25	G	5002	LMG	C31-C32-C33-C34
19	B	1022	CLA	C2A-CAA-CBA-CGA
19	B	1204	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
19	A	1123	CLA	C10-C11-C12-C13
19	A	1133	CLA	C13-C15-C16-C17
25	G	5001	LMG	C16-C17-C18-C19
27	1	803	DGD	O1A-C1A-O1G-C1G
19	B	1235	CLA	C15-C16-C17-C18
19	A	1138	CLA	CBD-CGD-O2D-CED
19	B	1210	CLA	CBA-CGA-O2A-C1
19	B	1211	CLA	C16-C17-C18-C19
19	B	1237	CLA	C16-C17-C18-C19
19	F	1302	CLA	C16-C17-C18-C20
19	4	603	CLA	C16-C17-C18-C20
19	B	1217	CLA	O1D-CGD-O2D-CED
23	A	5001	LHG	C11-C10-C9-C8
23	A	5002	LHG	C30-C31-C32-C33
27	3	803	DGD	O6E-C5E-C6E-O5E
22	J	4012	BCR	C10-C11-C12-C13
22	2	503	BCR	C18-C19-C20-C21
23	2	801	LHG	C9-C10-C11-C12
25	2	804	LMG	C4-C5-C6-O5
27	4	801	DGD	C4E-C5E-C6E-O5E
19	A	1013	CLA	C15-C16-C17-C18
19	B	1023	CLA	C8-C10-C11-C12
19	B	1222	CLA	C5-C6-C7-C8
19	B	1222	CLA	C8-C10-C11-C12
19	B	1240	CLA	C8-C10-C11-C12
19	B	1228	CLA	O1A-CGA-O2A-C1
23	A	5002	LHG	O9-C7-O7-C5
25	B	5004	LMG	C2-C1-O1-C7
19	4	603	CLA	C10-C11-C12-C13
27	F	5005	DGD	O2G-C2G-C3G-O3G
27	4	801	DGD	C5A-C6A-C7A-C8A
18	A	1011	CL0	O1A-CGA-O2A-C1
19	A	1105	CLA	C10-C11-C12-C13
19	B	1238	CLA	C5-C6-C7-C8
19	A	1123	CLA	C4-C3-C5-C6
19	B	1216	CLA	C4-C3-C5-C6
19	B	1229	CLA	C4-C3-C5-C6
19	B	1226	CLA	C2-C3-C5-C6
19	3	617	CLA	C2-C3-C5-C6
23	2	801	LHG	C11-C10-C9-C8
19	A	1012	CLA	C6-C7-C8-C9
19	A	1012	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
19	A	1012	CLA	C14-C13-C15-C16
19	A	1101	CLA	C14-C13-C15-C16
19	A	1107	CLA	C11-C12-C13-C14
19	A	1123	CLA	C11-C10-C8-C9
19	A	1137	CLA	C11-C10-C8-C9
19	A	1138	CLA	C11-C10-C8-C9
19	B	1201	CLA	C11-C10-C8-C9
19	B	1204	CLA	C14-C13-C15-C16
19	B	1207	CLA	C14-C13-C15-C16
19	B	1208	CLA	C6-C7-C8-C9
19	B	1219	CLA	C11-C12-C13-C14
19	B	1230	CLA	C11-C10-C8-C9
19	B	1231	CLA	C6-C7-C8-C9
19	B	1238	CLA	C6-C7-C8-C9
19	B	1238	CLA	C11-C12-C13-C14
19	F	1301	CLA	C11-C12-C13-C14
19	1	611	CLA	C11-C10-C8-C9
19	3	610	CLA	C14-C13-C15-C16
19	4	603	CLA	C11-C12-C13-C14
19	4	603	CLA	C14-C13-C15-C16
19	4	604	CLA	C11-C10-C8-C9
19	B	1225	CLA	CBD-CGD-O2D-CED
24	G	5005	LMT	O5B-C5B-C6B-O6B
23	B	5002	LHG	C17-C18-C19-C20
22	G	4011	BCR	C37-C22-C23-C24
30	4	502	XAT	C7-C8-C9-C19
30	4	502	XAT	C27-C28-C29-C39
19	B	1205	CLA	C15-C16-C17-C18
20	B	2002	PQN	C25-C26-C27-C28
22	G	4011	BCR	C21-C22-C23-C24
19	B	1212	CLA	O1A-CGA-O2A-C1
19	1	601	CLA	O1A-CGA-O2A-C1
18	A	1011	CL0	C1A-C2A-CAA-CBA
19	A	1101	CLA	C1A-C2A-CAA-CBA
19	A	1102	CLA	C1A-C2A-CAA-CBA
19	A	1106	CLA	C1A-C2A-CAA-CBA
19	A	1116	CLA	C1A-C2A-CAA-CBA
19	A	1119	CLA	C1A-C2A-CAA-CBA
19	A	1132	CLA	C1A-C2A-CAA-CBA
19	A	1133	CLA	C1A-C2A-CAA-CBA
19	A	1135	CLA	C1A-C2A-CAA-CBA
19	A	1141	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
19	B	1201	CLA	C1A-C2A-CAA-CBA
19	B	1202	CLA	C1A-C2A-CAA-CBA
19	B	1208	CLA	C1A-C2A-CAA-CBA
19	B	1209	CLA	C1A-C2A-CAA-CBA
19	B	1226	CLA	C1A-C2A-CAA-CBA
19	B	1229	CLA	C1A-C2A-CAA-CBA
19	B	1236	CLA	C1A-C2A-CAA-CBA
19	B	1239	CLA	C1A-C2A-CAA-CBA
19	G	1602	CLA	C1A-C2A-CAA-CBA
19	J	1901	CLA	C1A-C2A-CAA-CBA
19	K	1403	CLA	C1A-C2A-CAA-CBA
19	1	602	CLA	C1A-C2A-CAA-CBA
19	2	604	CLA	C1A-C2A-CAA-CBA
19	2	605	CLA	C1A-C2A-CAA-CBA
19	2	607	CLA	C1A-C2A-CAA-CBA
19	3	605	CLA	C1A-C2A-CAA-CBA
19	3	606	CLA	C1A-C2A-CAA-CBA
19	3	610	CLA	C1A-C2A-CAA-CBA
19	3	612	CLA	C1A-C2A-CAA-CBA
19	3	617	CLA	C1A-C2A-CAA-CBA
29	2	611	CHL	C1A-C2A-CAA-CBA
18	A	1011	CL0	C16-C17-C18-C20
19	A	1102	CLA	C16-C17-C18-C20
19	A	1130	CLA	C6-C7-C8-C10
19	B	1211	CLA	C16-C17-C18-C20
19	B	1237	CLA	C16-C17-C18-C20
19	B	1240	CLA	C16-C17-C18-C20
19	F	1302	CLA	C16-C17-C18-C19
19	3	603	CLA	C6-C7-C8-C9
19	4	603	CLA	C16-C17-C18-C19
24	G	5004	LMT	C11-C10-C9-C8
27	B	5005	DGD	CCB-CDB-CEB-CFB
22	2	503	BCR	C13-C14-C15-C16
19	B	1201	CLA	C5-C6-C7-C8
19	B	1213	CLA	C8-C10-C11-C12
19	B	1221	CLA	C10-C11-C12-C13
19	B	1232	CLA	C5-C6-C7-C8
23	A	5001	LHG	C25-C26-C27-C28
27	G	5003	DGD	C2A-C3A-C4A-C5A
27	4	802	DGD	C2B-C3B-C4B-C5B
23	A	5001	LHG	C23-C24-C25-C26
25	F	5001	LMG	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
25	G	5001	LMG	C10-C11-C12-C13
25	B	5004	LMG	O6-C5-C6-O5
19	A	1106	CLA	C13-C15-C16-C17
19	B	1023	CLA	C5-C6-C7-C8
19	4	601	CLA	C8-C10-C11-C12
23	A	5002	LHG	O6-C4-C5-C6
19	A	1108	CLA	O1D-CGD-O2D-CED
19	A	1123	CLA	O1D-CGD-O2D-CED
19	F	1301	CLA	O1D-CGD-O2D-CED
23	1	801	LHG	C24-C25-C26-C27
19	A	1110	CLA	C5-C6-C7-C8
19	A	1122	CLA	C15-C16-C17-C18
19	L	1502	CLA	C5-C6-C7-C8
27	4	802	DGD	O6D-C5D-C6D-O5D
25	G	5001	LMG	C31-C32-C33-C34
19	A	1126	CLA	C8-C10-C11-C12
19	1	614	CLA	C10-C11-C12-C13
19	A	1115	CLA	CBA-CGA-O2A-C1
19	A	1137	CLA	CBA-CGA-O2A-C1
27	1	803	DGD	O6E-C5E-C6E-O5E
19	A	1117	CLA	C4-C3-C5-C6
19	A	1117	CLA	C2-C3-C5-C6
19	B	1229	CLA	C2-C3-C5-C6
19	A	1101	CLA	C15-C16-C17-C18
19	A	1138	CLA	C15-C16-C17-C18
27	B	5005	DGD	O6D-C5D-C6D-O5D
24	G	5004	LMT	C7-C8-C9-C10
19	B	1226	CLA	O1A-CGA-O2A-C1
23	A	5002	LHG	C12-C13-C14-C15
23	B	5002	LHG	C30-C31-C32-C33
19	A	1133	CLA	C2A-CAA-CBA-CGA
19	B	1228	CLA	C2A-CAA-CBA-CGA
19	A	1133	CLA	C16-C17-C18-C19
19	B	1229	CLA	C3-C5-C6-C7
19	4	605	CLA	C3-C5-C6-C7
23	2	807	LHG	C4-C5-C6-O8
25	B	5007	LMG	O1-C7-C8-C9
25	F	5004	LMG	C7-C8-C9-O8
25	G	5001	LMG	O1-C7-C8-C9
19	B	1225	CLA	C15-C16-C17-C18
23	1	801	LHG	C35-C36-C37-C38
27	4	801	DGD	C6A-C7A-C8A-C9A

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Mol	Chain	Res	Type	Atoms
25	F	5004	LMG	C4-C5-C6-O5
27	4	802	DGD	C5D-C6D-O5D-C1E
19	B	1202	CLA	O1D-CGD-O2D-CED
27	F	5005	DGD	CFA-CGA-CHA-CIA
19	B	1221	CLA	C15-C16-C17-C18
19	B	1227	CLA	C5-C6-C7-C8
25	B	5007	LMG	O6-C5-C6-O5
19	B	1210	CLA	O1A-CGA-O2A-C1
19	A	1126	CLA	C16-C17-C18-C20
27	F	5005	DGD	O6E-C1E-O5D-C6D
19	A	1133	CLA	C5-C6-C7-C8
19	A	1106	CLA	CBD-CGD-O2D-CED
23	A	5001	LHG	O1-C1-C2-O2
23	A	5002	LHG	O1-C1-C2-O2
19	2	605	CLA	C10-C11-C12-C13
25	G	5001	LMG	C28-C29-C30-C31
18	A	1011	CL0	CAA-CBA-CGA-O2A
23	A	5002	LHG	C35-C36-C37-C38
19	B	1023	CLA	C13-C15-C16-C17
19	B	1225	CLA	C13-C15-C16-C17
24	J	5003	LMT	O5'-C5'-C6'-O6'
25	F	5006	LMG	O6-C5-C6-O5
25	G	5001	LMG	O6-C5-C6-O5
27	B	5005	DGD	O6E-C5E-C6E-O5E
19	G	1701	CLA	C3-C5-C6-C7
19	A	1121	CLA	C4-C3-C5-C6
19	3	610	CLA	C4-C3-C5-C6
29	1	612	CHL	C4-C3-C5-C6
29	2	615	CHL	C4-C3-C5-C6
23	B	5002	LHG	C29-C30-C31-C32
19	A	1133	CLA	O1D-CGD-O2D-CED
23	2	801	LHG	C7-C8-C9-C10
19	A	1105	CLA	C11-C12-C13-C15
19	A	1122	CLA	C16-C17-C18-C19
19	L	1502	CLA	C11-C12-C13-C14
19	1	614	CLA	CBA-CGA-O2A-C1
25	A	5006	LMG	O6-C5-C6-O5
19	F	1301	CLA	C8-C10-C11-C12
19	4	612	CLA	C8-C10-C11-C12
25	F	5004	LMG	C9-C8-O7-C10
25	1	802	LMG	O6-C5-C6-O5
19	1	604	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
19	A	1105	CLA	C8-C10-C11-C12
19	2	604	CLA	C15-C16-C17-C18
19	A	1133	CLA	C2-C1-O2A-CGA
19	B	1207	CLA	C2-C1-O2A-CGA
19	B	1239	CLA	C2-C1-O2A-CGA
19	4	601	CLA	C2-C1-O2A-CGA
19	4	609	CLA	C2-C1-O2A-CGA
25	G	5002	LMG	O6-C5-C6-O5
19	A	1107	CLA	C3-C5-C6-C7
19	A	1103	CLA	C15-C16-C17-C18
19	A	1139	CLA	C10-C11-C12-C13
27	4	801	DGD	C2A-C3A-C4A-C5A
19	A	1136	CLA	CBA-CGA-O2A-C1
19	B	1229	CLA	CBA-CGA-O2A-C1
19	B	1234	CLA	CBA-CGA-O2A-C1
23	B	5002	LHG	C24-C23-O8-C6
19	B	1220	CLA	CAA-CBA-CGA-O2A
19	1	605	CLA	C16-C17-C18-C20
19	2	607	CLA	C11-C12-C13-C14
24	B	5006	LMT	C4'-C5'-C6'-O6'
19	A	1112	CLA	C13-C15-C16-C17
19	A	1125	CLA	C8-C10-C11-C12
19	2	607	CLA	C8-C10-C11-C12
19	A	1124	CLA	O1D-CGD-O2D-CED
19	A	1115	CLA	O1A-CGA-O2A-C1
19	A	1137	CLA	O1A-CGA-O2A-C1
19	B	1216	CLA	C13-C15-C16-C17
25	G	5002	LMG	C2-C1-O1-C7
27	J	5001	DGD	C2E-C1E-O5D-C6D
27	1	803	DGD	C2E-C1E-O5D-C6D
27	3	803	DGD	C2D-C1D-O3G-C3G
25	1	802	LMG	O7-C10-C11-C12
23	2	807	LHG	O7-C5-C6-O8
25	B	5007	LMG	O1-C7-C8-O7
19	B	1225	CLA	O1D-CGD-O2D-CED
19	A	1105	CLA	C2C-C3C-CAC-CBC
25	A	5006	LMG	C22-C23-C24-C25
19	F	1301	CLA	C10-C11-C12-C13
19	A	1127	CLA	C4-C3-C5-C6
19	B	1211	CLA	C4-C3-C5-C6
19	4	607	CLA	C4-C3-C5-C6
19	B	1213	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
19	B	1235	CLA	C5-C6-C7-C8
19	A	1012	CLA	C12-C13-C15-C16
19	A	1013	CLA	C12-C13-C15-C16
19	A	1102	CLA	C11-C12-C13-C15
19	A	1112	CLA	C11-C10-C8-C7
19	A	1117	CLA	C11-C10-C8-C7
19	A	1120	CLA	C11-C10-C8-C7
19	A	1121	CLA	C2-C3-C5-C6
19	A	1123	CLA	C11-C10-C8-C7
19	A	1125	CLA	C11-C10-C8-C7
19	A	1129	CLA	C12-C13-C15-C16
19	A	1136	CLA	C11-C12-C13-C15
19	A	1138	CLA	C12-C13-C15-C16
19	B	1023	CLA	C11-C12-C13-C15
19	B	1204	CLA	C11-C12-C13-C15
19	B	1204	CLA	C12-C13-C15-C16
19	B	1208	CLA	C6-C7-C8-C10
19	B	1208	CLA	C11-C10-C8-C7
19	B	1211	CLA	C6-C7-C8-C10
19	B	1214	CLA	C11-C10-C8-C7
19	B	1216	CLA	C12-C13-C15-C16
19	B	1218	CLA	C11-C12-C13-C15
19	B	1221	CLA	C12-C13-C15-C16
19	B	1225	CLA	C12-C13-C15-C16
19	B	1226	CLA	C6-C7-C8-C10
19	B	1227	CLA	C11-C12-C13-C15
19	B	1230	CLA	C11-C10-C8-C7
19	B	1231	CLA	C11-C10-C8-C7
19	B	1238	CLA	C6-C7-C8-C10
19	B	1239	CLA	C11-C10-C8-C7
19	F	1301	CLA	C11-C12-C13-C15
19	F	1302	CLA	C11-C10-C8-C7
19	K	1402	CLA	C11-C10-C8-C7
19	1	604	CLA	C11-C12-C13-C15
19	2	603	CLA	C6-C7-C8-C10
19	4	601	CLA	C6-C7-C8-C10
19	4	601	CLA	C11-C10-C8-C7
19	4	605	CLA	C6-C7-C8-C10
19	4	607	CLA	C2-C3-C5-C6
20	A	2001	PQN	C17-C18-C20-C21
20	B	2002	PQN	C16-C17-C18-C20
29	1	612	CHL	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
29	2	615	CHL	C2-C3-C5-C6
29	3	604	CHL	C11-C12-C13-C15
23	A	5002	LHG	C18-C19-C20-C21
19	A	1102	CLA	C11-C12-C13-C14
19	A	1103	CLA	C11-C12-C13-C14
19	A	1104	CLA	C11-C12-C13-C14
19	A	1117	CLA	C11-C10-C8-C9
19	A	1126	CLA	C6-C7-C8-C9
19	A	1126	CLA	C11-C12-C13-C14
19	A	1129	CLA	C6-C7-C8-C9
19	A	1129	CLA	C14-C13-C15-C16
19	A	1136	CLA	C11-C12-C13-C14
19	A	1138	CLA	C14-C13-C15-C16
19	B	1201	CLA	C11-C12-C13-C14
19	B	1204	CLA	C11-C12-C13-C14
19	B	1207	CLA	C6-C7-C8-C9
19	B	1216	CLA	C11-C10-C8-C9
19	B	1226	CLA	C6-C7-C8-C9
19	B	1226	CLA	C14-C13-C15-C16
19	B	1227	CLA	C11-C12-C13-C14
19	B	1235	CLA	C6-C7-C8-C9
19	B	1237	CLA	C11-C10-C8-C9
19	F	1302	CLA	C11-C10-C8-C9
19	1	604	CLA	C11-C12-C13-C14
19	2	605	CLA	C11-C12-C13-C14
19	4	605	CLA	C6-C7-C8-C9
19	4	607	CLA	C6-C7-C8-C9
20	A	2001	PQN	C19-C18-C20-C21
29	3	604	CHL	C11-C12-C13-C14
22	3	503	BCR	C15-C16-C17-C18
19	B	1023	CLA	CBD-CGD-O2D-CED
27	B	5005	DGD	C5A-C6A-C7A-C8A
25	2	802	LMG	C29-C28-O8-C9
19	B	1214	CLA	C13-C15-C16-C17
19	A	1116	CLA	C2A-CAA-CBA-CGA
19	A	1129	CLA	C2A-CAA-CBA-CGA
19	B	1224	CLA	C2A-CAA-CBA-CGA
19	B	1238	CLA	C15-C16-C17-C18
19	A	1123	CLA	C16-C17-C18-C19
19	B	1218	CLA	C16-C17-C18-C20
19	2	607	CLA	C11-C12-C13-C15
22	A	4008	BCR	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
22	B	4009	BCR	C7-C8-C9-C10
22	B	4010	BCR	C7-C8-C9-C10
22	3	503	BCR	C17-C18-C19-C20
28	4	501	LUT	C27-C28-C29-C30
19	G	1601	CLA	C3-C5-C6-C7
20	B	2002	PQN	C15-C16-C17-C18
25	1	802	LMG	C11-C10-O7-C8
25	1	802	LMG	C29-C28-O8-C9
19	B	1216	CLA	C15-C16-C17-C18
23	B	5002	LHG	C32-C33-C34-C35
19	B	1235	CLA	C16-C17-C18-C19
23	1	801	LHG	O6-C4-C5-C6
23	3	801	LHG	O6-C4-C5-C6
19	B	1212	CLA	C3-C5-C6-C7
27	1	803	DGD	C4D-C5D-C6D-O5D
19	B	1240	CLA	C10-C11-C12-C13
19	4	612	CLA	C4-C3-C5-C6
19	A	1127	CLA	C2-C3-C5-C6
19	B	1211	CLA	C2-C3-C5-C6
19	3	610	CLA	C2-C3-C5-C6
27	4	802	DGD	C4D-C5D-C6D-O5D
19	B	1205	CLA	C16-C17-C18-C20
27	B	5005	DGD	C4B-C5B-C6B-C7B
19	A	1128	CLA	C13-C15-C16-C17
19	A	1138	CLA	O1D-CGD-O2D-CED
19	1	614	CLA	O1A-CGA-O2A-C1
18	A	1011	CL0	C3A-C2A-CAA-CBA
19	A	1115	CLA	C3A-C2A-CAA-CBA
19	A	1119	CLA	C3A-C2A-CAA-CBA
19	A	1121	CLA	C3A-C2A-CAA-CBA
19	A	1134	CLA	C3A-C2A-CAA-CBA
19	B	1201	CLA	C3A-C2A-CAA-CBA
19	B	1204	CLA	C3A-C2A-CAA-CBA
19	B	1215	CLA	C3A-C2A-CAA-CBA
19	B	1222	CLA	C3A-C2A-CAA-CBA
19	B	1232	CLA	C3A-C2A-CAA-CBA
19	2	608	CLA	C3A-C2A-CAA-CBA
25	2	804	LMG	C11-C12-C13-C14
22	B	4010	BCR	C9-C10-C11-C12
22	F	4016	BCR	C9-C10-C11-C12
31	4	505	C7Z	C9-C10-C11-C12
24	B	5006	LMT	C2-C1-O1'-C1'

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Mol	Chain	Res	Type	Atoms
24	B	5008	LMT	C2-C1-O1'-C1'
24	G	5004	LMT	C2-C1-O1'-C1'
19	B	1229	CLA	O1A-CGA-O2A-C1
19	A	1105	CLA	C11-C12-C13-C14
19	A	1134	CLA	C6-C7-C8-C9
19	A	1125	CLA	CBA-CGA-O2A-C1
19	A	1128	CLA	CBA-CGA-O2A-C1
19	A	1140	CLA	C15-C16-C17-C18
19	B	1021	CLA	C5-C6-C7-C8
19	B	1021	CLA	C8-C10-C11-C12
19	B	1240	CLA	C5-C6-C7-C8
19	1	605	CLA	C13-C15-C16-C17
23	A	5002	LHG	C4-C5-C6-O8
23	1	801	LHG	C4-C5-C6-O8
23	3	801	LHG	C4-C5-C6-O8
25	G	5002	LMG	O1-C7-C8-C9
25	2	803	LMG	O1-C7-C8-C9
27	F	5005	DGD	C1G-C2G-C3G-O3G
27	3	803	DGD	O1G-C1G-C2G-C3G
28	3	501	LUT	C21-C26-C27-C28
19	A	1133	CLA	C16-C17-C18-C20
19	3	601	CLA	C6-C7-C8-C9
19	4	612	CLA	C2-C3-C5-C6
23	B	5002	LHG	C34-C35-C36-C37
19	A	1136	CLA	O1A-CGA-O2A-C1
25	2	802	LMG	O10-C28-O8-C9
23	B	5002	LHG	C19-C20-C21-C22
19	2	604	CLA	C3-C5-C6-C7
23	A	5002	LHG	O6-C4-C5-O7
23	B	5002	LHG	O6-C4-C5-O7
25	1	802	LMG	O9-C10-O7-C8
25	B	5003	LMG	C28-C29-C30-C31
24	A	5004	LMT	C1-C2-C3-C4
19	B	1236	CLA	CBA-CGA-O2A-C1
29	4	613	CHL	C11-C12-C13-C14
19	B	1021	CLA	C13-C15-C16-C17
19	F	1301	CLA	C13-C15-C16-C17
25	B	5007	LMG	O7-C10-C11-C12
19	A	1132	CLA	C13-C15-C16-C17
19	B	1234	CLA	O1A-CGA-O2A-C1
23	B	5002	LHG	O10-C23-O8-C6
25	1	802	LMG	O10-C28-O8-C9

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Mol	Chain	Res	Type	Atoms
24	B	5006	LMT	C6-C7-C8-C9
23	3	801	LHG	O7-C5-C6-O8
25	F	5004	LMG	O7-C8-C9-O8
25	1	802	LMG	O7-C8-C9-O8
19	B	1240	CLA	CAA-CBA-CGA-O2A
25	G	5001	LMG	C11-C12-C13-C14
19	A	1122	CLA	C16-C17-C18-C20
19	A	1134	CLA	C6-C7-C8-C10
19	B	1238	CLA	C16-C17-C18-C19
19	3	617	CLA	C11-C12-C13-C15
25	G	5002	LMG	C30-C31-C32-C33
23	A	5002	LHG	C34-C35-C36-C37
19	B	1216	CLA	C2-C1-O2A-CGA
19	B	1222	CLA	C2-C1-O2A-CGA
27	4	801	DGD	C5B-C6B-C7B-C8B
29	2	615	CHL	CAA-CBA-CGA-O2A
19	A	1103	CLA	C14-C13-C15-C16
19	A	1111	CLA	C11-C10-C8-C9
19	A	1115	CLA	C6-C7-C8-C9
19	A	1127	CLA	C11-C10-C8-C9
19	A	1128	CLA	C11-C10-C8-C9
19	B	1203	CLA	C11-C10-C8-C9
19	B	1203	CLA	C11-C12-C13-C14
19	B	1211	CLA	C11-C10-C8-C9
19	B	1215	CLA	C14-C13-C15-C16
19	B	1240	CLA	C11-C10-C8-C9
19	B	1240	CLA	C14-C13-C15-C16
19	G	1603	CLA	C11-C12-C13-C14
19	2	603	CLA	C11-C10-C8-C9
19	2	605	CLA	C14-C13-C15-C16
19	3	610	CLA	C6-C7-C8-C9
19	3	610	CLA	C11-C12-C13-C14
29	3	604	CHL	C14-C13-C15-C16
23	A	5001	LHG	C26-C27-C28-C29
23	A	5002	LHG	C11-C10-C9-C8
23	1	801	LHG	C28-C29-C30-C31
19	A	1111	CLA	C8-C10-C11-C12
19	B	1221	CLA	C5-C6-C7-C8
19	A	1111	CLA	C16-C17-C18-C20
19	A	1124	CLA	C6-C7-C8-C9
19	B	1203	CLA	C16-C17-C18-C19
19	B	1223	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
29	1	612	CHL	C11-C12-C13-C14
22	A	4003	BCR	C5-C6-C7-C8
22	A	4003	BCR	C23-C24-C25-C26
22	A	4008	BCR	C1-C6-C7-C8
22	A	4008	BCR	C5-C6-C7-C8
22	F	4016	BCR	C23-C24-C25-C26
22	F	4016	BCR	C23-C24-C25-C30
22	J	4012	BCR	C23-C24-C25-C26
22	J	4012	BCR	C23-C24-C25-C30
22	L	4019	BCR	C5-C6-C7-C8
28	2	501	LUT	C1-C6-C7-C8
28	2	501	LUT	C5-C6-C7-C8
19	B	1227	CLA	C10-C11-C12-C13
19	3	602	CLA	O1D-CGD-O2D-CED
22	A	4007	BCR	C17-C18-C19-C20
22	B	4006	BCR	C21-C22-C23-C24
22	F	4014	BCR	C17-C18-C19-C20
22	2	503	BCR	C17-C18-C19-C20
23	1	801	LHG	C25-C26-C27-C28
23	A	5001	LHG	C16-C17-C18-C19
19	A	1134	CLA	C3-C5-C6-C7
19	A	1107	CLA	C8-C10-C11-C12
19	B	1203	CLA	C8-C10-C11-C12
19	3	617	CLA	C10-C11-C12-C13
23	B	5002	LHG	O6-C4-C5-C6
23	B	5002	LHG	C13-C14-C15-C16
24	J	5003	LMT	C2-C1-O1'-C1'
19	A	1103	CLA	C11-C12-C13-C15
19	A	1104	CLA	C11-C12-C13-C15
19	A	1105	CLA	C6-C7-C8-C10
19	A	1115	CLA	C6-C7-C8-C10
19	A	1115	CLA	C11-C10-C8-C7
19	A	1126	CLA	C11-C12-C13-C15
19	A	1128	CLA	C11-C10-C8-C7
19	A	1131	CLA	C12-C13-C15-C16
19	A	1133	CLA	C6-C7-C8-C10
19	A	1137	CLA	C11-C12-C13-C15
19	A	1138	CLA	C11-C12-C13-C15
19	A	1139	CLA	C6-C7-C8-C10
19	B	1022	CLA	C11-C12-C13-C15
19	B	1203	CLA	C11-C12-C13-C15
19	B	1205	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
19	B	1206	CLA	C11-C10-C8-C7
19	B	1211	CLA	C11-C10-C8-C7
19	B	1214	CLA	C12-C13-C15-C16
19	B	1215	CLA	C12-C13-C15-C16
19	B	1222	CLA	C6-C7-C8-C10
19	B	1223	CLA	C6-C7-C8-C10
19	B	1226	CLA	C12-C13-C15-C16
19	B	1235	CLA	C6-C7-C8-C10
19	B	1237	CLA	C6-C7-C8-C10
19	B	1237	CLA	C11-C10-C8-C7
19	B	1237	CLA	C12-C13-C15-C16
19	F	1301	CLA	C6-C7-C8-C10
19	1	605	CLA	C6-C7-C8-C10
19	1	614	CLA	C6-C7-C8-C10
19	2	604	CLA	C6-C7-C8-C10
19	2	605	CLA	C11-C12-C13-C15
19	2	607	CLA	C11-C10-C8-C7
19	4	607	CLA	C6-C7-C8-C10
19	4	612	CLA	C12-C13-C15-C16
19	4	617	CLA	C6-C7-C8-C10
29	2	609	CHL	C11-C12-C13-C15
19	4	607	CLA	C3-C5-C6-C7
19	B	1023	CLA	O1D-CGD-O2D-CED
22	B	4009	BCR	C19-C20-C21-C22
22	F	4016	BCR	C19-C20-C21-C22
22	3	503	BCR	C19-C20-C21-C22
19	1	603	CLA	C6-C7-C8-C9
19	4	601	CLA	C11-C12-C13-C14
19	B	1216	CLA	CBA-CGA-O2A-C1
23	A	5002	LHG	C16-C17-C18-C19
19	A	1013	CLA	C8-C10-C11-C12
19	A	1116	CLA	C5-C6-C7-C8
19	4	617	CLA	C8-C10-C11-C12
19	A	1132	CLA	C2A-CAA-CBA-CGA
19	2	603	CLA	C5-C6-C7-C8
22	I	4020	BCR	C11-C10-C9-C34
30	4	502	XAT	C40-C33-C34-C35
19	1	604	CLA	C3-C5-C6-C7
25	B	5007	LMG	C32-C33-C34-C35
19	B	1205	CLA	C16-C17-C18-C19
19	B	1218	CLA	C16-C17-C18-C19
23	2	807	LHG	C25-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
19	A	1131	CLA	C13-C15-C16-C17
19	A	1118	CLA	CAD-CBD-CGD-O2D
19	A	1124	CLA	CAD-CBD-CGD-O2D
19	B	1230	CLA	CAD-CBD-CGD-O2D
19	1	604	CLA	CAD-CBD-CGD-O2D
19	2	607	CLA	CAD-CBD-CGD-O2D
25	F	5003	LMG	C9-C8-O7-C10
27	F	5005	DGD	C1G-C2G-O2G-C1B
27	J	5001	DGD	C1G-C2G-O2G-C1B
29	2	609	CHL	CAD-CBD-CGD-O2D
19	A	1102	CLA	C8-C10-C11-C12
19	A	1102	CLA	C15-C16-C17-C18
19	4	607	CLA	C5-C6-C7-C8
24	G	5005	LMT	C1-C2-C3-C4
27	4	801	DGD	C4D-C5D-C6D-O5D
23	1	801	LHG	C29-C30-C31-C32
23	2	807	LHG	C2-C3-O3-P
25	F	5001	LMG	C7-C8-C9-O8
25	F	5002	LMG	O1-C7-C8-C9
27	B	5005	DGD	C1G-C2G-C3G-O3G
27	4	802	DGD	O1G-C1G-C2G-C3G
19	B	1216	CLA	O1A-CGA-O2A-C1
23	B	5002	LHG	C28-C29-C30-C31
25	F	5003	LMG	C29-C30-C31-C32
23	1	801	LHG	O6-C4-C5-O7
23	3	801	LHG	O6-C4-C5-O7
19	B	1224	CLA	CAA-CBA-CGA-O2A
27	1	803	DGD	O1G-C1A-C2A-C3A
19	A	1128	CLA	O1A-CGA-O2A-C1
19	A	1105	CLA	C4C-C3C-CAC-CBC
19	A	1106	CLA	CHA-CBD-CGD-O1D
19	A	1106	CLA	CHA-CBD-CGD-O2D
19	A	1108	CLA	CHA-CBD-CGD-O2D
19	A	1114	CLA	CHA-CBD-CGD-O1D
19	A	1114	CLA	CHA-CBD-CGD-O2D
19	A	1126	CLA	CHA-CBD-CGD-O1D
19	B	1201	CLA	CHA-CBD-CGD-O1D
19	B	1201	CLA	CHA-CBD-CGD-O2D
19	B	1204	CLA	CHA-CBD-CGD-O2D
19	B	1207	CLA	CHA-CBD-CGD-O1D
19	B	1207	CLA	CHA-CBD-CGD-O2D
19	B	1217	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
19	B	1221	CLA	CHA-CBD-CGD-O1D
19	B	1221	CLA	CHA-CBD-CGD-O2D
19	B	1227	CLA	CHA-CBD-CGD-O1D
19	B	1240	CLA	CHA-CBD-CGD-O1D
19	B	1240	CLA	CHA-CBD-CGD-O2D
19	K	1402	CLA	CHA-CBD-CGD-O1D
19	1	608	CLA	CHA-CBD-CGD-O1D
19	1	614	CLA	CHA-CBD-CGD-O1D
19	1	614	CLA	CHA-CBD-CGD-O2D
19	2	604	CLA	CHA-CBD-CGD-O1D
19	4	605	CLA	CHA-CBD-CGD-O1D
19	4	605	CLA	CHA-CBD-CGD-O2D
29	3	607	CHL	CHA-CBD-CGD-O2D
29	4	610	CHL	CHA-CBD-CGD-O2D
19	A	1125	CLA	O1A-CGA-O2A-C1
24	G	5005	LMT	C5-C6-C7-C8
19	K	1403	CLA	O2A-C1-C2-C3
23	1	801	LHG	O7-C5-C6-O8
27	3	803	DGD	O1G-C1G-C2G-O2G
27	4	802	DGD	O1G-C1G-C2G-O2G
19	B	1215	CLA	CBA-CGA-O2A-C1
19	A	1124	CLA	C6-C7-C8-C10
23	2	807	LHG	O1-C1-C2-O2
19	B	1238	CLA	C4-C3-C5-C6
27	F	5005	DGD	C9A-CAA-CBA-CCA
19	B	1236	CLA	O1A-CGA-O2A-C1
27	G	5003	DGD	O1B-C1B-O2G-C2G
19	A	1132	CLA	C5-C6-C7-C8
19	2	612	CLA	C5-C6-C7-C8
19	A	1103	CLA	C6-C7-C8-C9
19	A	1119	CLA	C11-C10-C8-C9
19	A	1122	CLA	C11-C10-C8-C9
19	A	1133	CLA	C6-C7-C8-C9
19	A	1139	CLA	C6-C7-C8-C9
19	A	1139	CLA	C14-C13-C15-C16
19	1	601	CLA	C14-C13-C15-C16
29	2	609	CHL	C11-C12-C13-C14
27	1	803	DGD	C2A-C3A-C4A-C5A
29	4	610	CHL	C2C-C3C-CAC-CBC
19	A	1102	CLA	O1A-CGA-O2A-C1
22	1	503	BCR	C37-C22-C23-C24
30	2	502	XAT	C27-C28-C29-C39

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Mol	Chain	Res	Type	Atoms
23	B	5002	LHG	O1-C1-C2-C3
19	A	1136	CLA	C15-C16-C17-C18
22	A	4002	BCR	C17-C18-C19-C20
22	A	4011	BCR	C21-C22-C23-C24
22	1	503	BCR	C17-C18-C19-C20
22	1	503	BCR	C21-C22-C23-C24
19	A	1112	CLA	C1A-C2A-CAA-CBA
19	B	1220	CLA	C1A-C2A-CAA-CBA
19	F	1302	CLA	C1A-C2A-CAA-CBA
19	1	608	CLA	C1A-C2A-CAA-CBA
19	A	1115	CLA	C2-C1-O2A-CGA
19	A	1116	CLA	C2-C1-O2A-CGA
19	B	1231	CLA	C2-C1-O2A-CGA
19	G	1601	CLA	C2-C1-O2A-CGA
19	2	608	CLA	C2-C1-O2A-CGA
22	G	4021	BCR	C13-C14-C15-C16
22	1	504	BCR	C13-C14-C15-C16
31	4	505	C7Z	C33-C34-C35-C15
19	A	1105	CLA	O1D-CGD-O2D-CED
23	1	801	LHG	C4-O6-P-O3
23	1	801	LHG	C2-C3-O3-P
23	A	5001	LHG	C3-O3-P-O5
23	B	5002	LHG	C3-O3-P-O5
23	1	801	LHG	C3-O3-P-O5
23	2	807	LHG	C3-O3-P-O5
19	A	1101	CLA	C16-C17-C18-C19
19	B	1215	CLA	C16-C17-C18-C20
25	F	5003	LMG	C11-C12-C13-C14
24	J	5003	LMT	O5'-C1'-O1'-C1
19	B	1023	CLA	C15-C16-C17-C18
19	B	1222	CLA	C10-C11-C12-C13
19	A	1117	CLA	CBA-CGA-O2A-C1
24	A	5004	LMT	C9-C10-C11-C12
24	B	5006	LMT	O5'-C5'-C6'-O6'
19	A	1135	CLA	C2A-CAA-CBA-CGA
29	4	610	CHL	C2A-CAA-CBA-CGA
19	B	1235	CLA	C13-C15-C16-C17
23	1	801	LHG	C33-C34-C35-C36
19	2	605	CLA	C16-C17-C18-C19
19	4	607	CLA	C11-C12-C13-C15
19	4	612	CLA	C16-C17-C18-C19
19	B	1207	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
19	B	1227	CLA	CAD-CBD-CGD-O1D
19	3	606	CLA	C2C-C3C-CAC-CBC
19	B	1222	CLA	C3-C5-C6-C7
24	G	5005	LMT	O1'-C1-C2-C3
19	A	1102	CLA	CBA-CGA-O2A-C1
19	A	1107	CLA	CBA-CGA-O2A-C1
29	2	609	CHL	C4-C3-C5-C6
19	A	1012	CLA	C11-C12-C13-C15
19	A	1013	CLA	C6-C7-C8-C10
19	A	1101	CLA	C11-C10-C8-C7
19	A	1102	CLA	C6-C7-C8-C10
19	A	1103	CLA	C6-C7-C8-C10
19	A	1111	CLA	C3A-C2A-CAA-CBA
19	A	1111	CLA	C6-C7-C8-C10
19	A	1112	CLA	C11-C12-C13-C15
19	A	1129	CLA	C11-C10-C8-C7
19	A	1131	CLA	C11-C12-C13-C15
19	A	1132	CLA	C12-C13-C15-C16
19	A	1133	CLA	C11-C12-C13-C15
19	A	1133	CLA	C12-C13-C15-C16
19	A	1139	CLA	C12-C13-C15-C16
19	B	1203	CLA	C6-C7-C8-C10
19	B	1206	CLA	C12-C13-C15-C16
19	B	1211	CLA	C12-C13-C15-C16
19	B	1215	CLA	C11-C10-C8-C7
19	B	1221	CLA	C6-C7-C8-C10
19	B	1225	CLA	C11-C12-C13-C15
19	B	1226	CLA	C11-C10-C8-C7
19	B	1229	CLA	C12-C13-C15-C16
19	B	1238	CLA	C12-C13-C15-C16
19	1	601	CLA	C12-C13-C15-C16
19	1	604	CLA	C6-C7-C8-C10
19	1	611	CLA	C11-C12-C13-C15
19	3	610	CLA	C11-C12-C13-C15
19	4	605	CLA	C3A-C2A-CAA-CBA
19	4	605	CLA	C11-C10-C8-C7
19	4	617	CLA	C12-C13-C15-C16
28	J	4013	LUT	C25-C26-C27-C28
28	4	501	LUT	C25-C26-C27-C28
29	2	611	CHL	C3A-C2A-CAA-CBA
25	F	5002	LMG	C34-C35-C36-C37
27	4	802	DGD	C5A-C6A-C7A-C8A

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Mol	Chain	Res	Type	Atoms
22	I	4020	BCR	C19-C20-C21-C22
22	1	504	BCR	C19-C20-C21-C22
27	J	5001	DGD	O6D-C5D-C6D-O5D
19	B	1209	CLA	CAA-CBA-CGA-O2A
19	4	612	CLA	C15-C16-C17-C18
27	G	5003	DGD	C2B-C1B-O2G-C2G
19	B	1211	CLA	C8-C10-C11-C12
19	A	1012	CLA	C2A-CAA-CBA-CGA
19	B	1023	CLA	C2A-CAA-CBA-CGA
19	B	1214	CLA	C16-C17-C18-C20
25	A	5006	LMG	C12-C13-C14-C15
25	3	802	LMG	O1-C7-C8-C9
25	F	5002	LMG	O1-C7-C8-O7
25	G	5001	LMG	O1-C7-C8-O7
25	3	802	LMG	O1-C7-C8-O7
27	B	5005	DGD	O2G-C2G-C3G-O3G
25	B	5007	LMG	C8-C7-O1-C1
25	1	802	LMG	C8-C7-O1-C1
19	B	1210	CLA	C8-C10-C11-C12
19	A	1107	CLA	O1A-CGA-O2A-C1
19	A	1139	CLA	O1A-CGA-O2A-C1
19	A	1139	CLA	CBA-CGA-O2A-C1
23	2	801	LHG	C24-C23-O8-C6
19	B	1216	CLA	C2-C3-C5-C6
19	2	607	CLA	C10-C11-C12-C13
19	A	1013	CLA	C6-C7-C8-C9
19	A	1101	CLA	C6-C7-C8-C9
19	A	1112	CLA	C11-C12-C13-C14
19	A	1131	CLA	C14-C13-C15-C16
19	A	1137	CLA	C11-C12-C13-C14
19	B	1022	CLA	C11-C12-C13-C14
19	B	1206	CLA	C11-C10-C8-C9
19	B	1206	CLA	C11-C12-C13-C14
19	B	1211	CLA	C6-C7-C8-C9
19	B	1218	CLA	C11-C12-C13-C14
19	B	1223	CLA	C6-C7-C8-C9
19	B	1231	CLA	C11-C10-C8-C9
19	B	1237	CLA	C6-C7-C8-C9
19	B	1239	CLA	C14-C13-C15-C16
19	K	1402	CLA	C11-C10-C8-C9
19	1	605	CLA	C6-C7-C8-C9
19	2	604	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
19	2	605	CLA	C11-C10-C8-C9
19	2	607	CLA	C11-C10-C8-C9
19	3	617	CLA	C6-C7-C8-C9
19	4	617	CLA	C6-C7-C8-C9
29	1	612	CHL	C6-C7-C8-C9
19	A	1117	CLA	O1A-CGA-O2A-C1
19	4	612	CLA	C3-C5-C6-C7
19	B	1223	CLA	C16-C17-C18-C20
19	B	1231	CLA	C11-C12-C13-C14
19	A	1119	CLA	O1A-CGA-O2A-C1
19	4	608	CLA	CAA-CBA-CGA-O2A
29	2	610	CHL	CAA-CBA-CGA-O2A
27	J	5001	DGD	C5B-C6B-C7B-C8B
22	B	4006	BCR	C18-C19-C20-C21
22	K	4002	BCR	C18-C19-C20-C21
31	4	505	C7Z	C10-C11-C12-C13
19	A	1106	CLA	O1D-CGD-O2D-CED
28	3	501	LUT	C29-C30-C31-C32
19	A	1111	CLA	C16-C17-C18-C19
19	A	1136	CLA	C16-C17-C18-C19
19	3	605	CLA	C6-C7-C8-C9
30	4	502	XAT	C27-C28-C29-C30
27	B	5005	DGD	C9B-CAB-CBB-CCB
23	1	801	LHG	C11-C10-C9-C8
25	G	5002	LMG	C15-C16-C17-C18
19	A	1012	CLA	C13-C15-C16-C17
19	B	1203	CLA	C10-C11-C12-C13
19	B	1238	CLA	C10-C11-C12-C13
19	A	1132	CLA	C4-C3-C5-C6
19	A	1141	CLA	C10-C11-C12-C13
25	G	5006	LMG	O10-C28-C29-C30
25	2	802	LMG	O9-C10-C11-C12
23	1	801	LHG	C10-C11-C12-C13
25	G	5001	LMG	C42-C43-C44-C45
25	G	5001	LMG	C33-C34-C35-C36
29	1	610	CHL	CAA-CBA-CGA-O2A
25	F	5001	LMG	C7-C8-O7-C10
25	G	5001	LMG	C7-C8-O7-C10
25	2	803	LMG	C7-C8-O7-C10
27	B	5005	DGD	C3G-C2G-O2G-C1B
19	A	1115	CLA	C2A-CAA-CBA-CGA
19	1	601	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
23	A	5001	LHG	O9-C7-O7-C5
19	B	1224	CLA	C2-C1-O2A-CGA
19	1	606	CLA	C2-C1-O2A-CGA
19	2	603	CLA	C2-C1-O2A-CGA
29	1	612	CHL	C2-C1-O2A-CGA
19	F	1301	CLA	CAA-CBA-CGA-O2A
19	B	1210	CLA	C3-C5-C6-C7
23	2	801	LHG	C26-C27-C28-C29
22	A	4003	BCR	C1-C6-C7-C8
22	A	4003	BCR	C23-C24-C25-C30
22	A	4017	BCR	C5-C6-C7-C8
22	L	4019	BCR	C1-C6-C7-C8
28	3	501	LUT	C1-C6-C7-C8
28	3	501	LUT	C5-C6-C7-C8
31	4	505	C7Z	C25-C26-C27-C28
19	B	1238	CLA	C2-C3-C5-C6
23	2	801	LHG	O10-C23-O8-C6
24	B	5006	LMT	C5-C6-C7-C8
19	B	1219	CLA	C10-C11-C12-C13
19	4	603	CLA	C13-C15-C16-C17
19	B	1203	CLA	C16-C17-C18-C20
19	B	1234	CLA	C6-C7-C8-C9
19	A	1117	CLA	C2A-CAA-CBA-CGA
22	I	4020	BCR	C11-C10-C9-C8
27	4	802	DGD	O2G-C2G-C3G-O3G
25	1	802	LMG	C22-C23-C24-C25
23	B	5001	LHG	C3-O3-P-O6
23	B	5002	LHG	C4-O6-P-O3
23	2	801	LHG	C3-O3-P-O6
23	3	801	LHG	C3-O3-P-O6
19	A	1131	CLA	C15-C16-C17-C18
25	2	803	LMG	C7-C8-C9-O8
19	A	1117	CLA	C11-C12-C13-C15
19	3	610	CLA	C6-C7-C8-C10
19	A	1105	CLA	C11-C10-C8-C9
19	A	1136	CLA	C11-C10-C8-C9
19	B	1023	CLA	C11-C12-C13-C14
19	B	1226	CLA	C11-C10-C8-C9
19	B	1229	CLA	C14-C13-C15-C16
19	B	1238	CLA	C14-C13-C15-C16
19	1	604	CLA	C6-C7-C8-C9
19	4	601	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
20	B	2002	PQN	C16-C17-C18-C19
20	B	2002	PQN	C19-C18-C20-C21
25	G	5006	LMG	O8-C28-C29-C30
25	2	802	LMG	O7-C10-C11-C12
23	A	5001	LHG	C8-C7-O7-C5
22	A	4002	BCR	C19-C20-C21-C22
19	A	1106	CLA	C16-C17-C18-C19
27	F	5005	DGD	C7A-C8A-C9A-CAA
19	B	1202	CLA	C10-C11-C12-C13
25	1	802	LMG	C31-C32-C33-C34
22	A	4011	BCR	C7-C8-C9-C34
19	A	1136	CLA	C13-C15-C16-C17
22	I	4018	BCR	C17-C18-C19-C20
25	A	5006	LMG	C36-C37-C38-C39
25	G	5002	LMG	C28-C29-C30-C31
25	1	802	LMG	C10-C11-C12-C13
23	1	801	LHG	C34-C35-C36-C37
19	4	607	CLA	C11-C12-C13-C14
19	4	612	CLA	C16-C17-C18-C20
19	3	608	CLA	CBA-CGA-O2A-C1
19	B	1239	CLA	C13-C15-C16-C17
25	B	5004	LMG	C29-C30-C31-C32
19	A	1119	CLA	CBA-CGA-O2A-C1
19	B	1235	CLA	C2A-CAA-CBA-CGA
19	B	1228	CLA	C11-C12-C13-C14
19	3	605	CLA	C6-C7-C8-C10
22	B	4009	BCR	C13-C14-C15-C16
22	F	4014	BCR	C13-C14-C15-C16
22	G	4011	BCR	C9-C10-C11-C12
22	I	4018	BCR	C19-C20-C21-C22
22	1	503	BCR	C19-C20-C21-C22
28	4	501	LUT	C29-C30-C31-C32
27	4	801	DGD	O1B-C1B-O2G-C2G
19	B	1215	CLA	O1A-CGA-O2A-C1
19	B	1216	CLA	CBD-CGD-O2D-CED
27	B	5005	DGD	CDB-CEB-CFB-CGB
19	3	617	CLA	C11-C12-C13-C14
19	A	1111	CLA	C4-C3-C5-C6
19	A	1106	CLA	C10-C11-C12-C13
19	A	1136	CLA	C2-C1-O2A-CGA
19	B	1202	CLA	C2-C1-O2A-CGA
29	4	613	CHL	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
19	B	1238	CLA	C8-C10-C11-C12
19	A	1101	CLA	C16-C17-C18-C20
19	A	1127	CLA	C16-C17-C18-C20
19	B	1238	CLA	C16-C17-C18-C20
19	4	617	CLA	C16-C17-C18-C20
19	B	1205	CLA	C5-C6-C7-C8
19	A	1013	CLA	C2A-CAA-CBA-CGA
19	B	1204	CLA	C2A-CAA-CBA-CGA
19	2	604	CLA	C2A-CAA-CBA-CGA
25	2	803	LMG	O1-C7-C8-O7
23	1	801	LHG	C9-C10-C11-C12
25	2	803	LMG	C13-C14-C15-C16
23	A	5001	LHG	C2-C3-O3-P
23	2	801	LHG	C2-C3-O3-P
19	A	1107	CLA	C3A-C2A-CAA-CBA
19	B	1220	CLA	C3A-C2A-CAA-CBA
19	F	1302	CLA	C3A-C2A-CAA-CBA
19	G	1701	CLA	C3A-C2A-CAA-CBA
19	3	608	CLA	C3A-C2A-CAA-CBA
22	A	4002	BCR	C9-C10-C11-C12
22	A	4011	BCR	C19-C20-C21-C22
22	F	4016	BCR	C13-C14-C15-C16
19	B	1224	CLA	C4-C3-C5-C6
19	A	1107	CLA	C11-C10-C8-C9
19	A	1123	CLA	C11-C12-C13-C14
19	A	1129	CLA	C11-C12-C13-C14
19	A	1133	CLA	C14-C13-C15-C16
19	B	1202	CLA	C11-C10-C8-C9
19	B	1218	CLA	C14-C13-C15-C16
19	B	1228	CLA	C11-C10-C8-C9
19	1	601	CLA	C11-C12-C13-C14
19	A	1104	CLA	C16-C17-C18-C19
19	A	1123	CLA	C8-C10-C11-C12
27	4	801	DGD	C2B-C3B-C4B-C5B
19	A	1104	CLA	C5-C6-C7-C8
22	A	4007	BCR	C16-C17-C18-C36
22	A	4011	BCR	C11-C10-C9-C34
22	A	4011	BCR	C16-C17-C18-C36
22	A	4017	BCR	C16-C17-C18-C36
22	B	4004	BCR	C35-C13-C14-C15
22	B	4004	BCR	C16-C17-C18-C36
22	B	4006	BCR	C11-C10-C9-C34

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Mol	Chain	Res	Type	Atoms
22	F	4016	BCR	C16-C17-C18-C36
22	G	4011	BCR	C16-C17-C18-C36
22	I	4018	BCR	C35-C13-C14-C15
22	I	4020	BCR	C16-C17-C18-C36
22	I	4020	BCR	C20-C21-C22-C37
22	1	504	BCR	C16-C17-C18-C36
22	3	506	BCR	C16-C17-C18-C36
25	A	5006	LMG	O1-C7-C8-C9
19	A	1103	CLA	C3-C5-C6-C7
19	G	1603	CLA	C3-C5-C6-C7
19	K	1403	CLA	C2A-CAA-CBA-CGA
19	B	1220	CLA	CAA-CBA-CGA-O1A
19	B	1214	CLA	C16-C17-C18-C19
19	B	1234	CLA	C6-C7-C8-C10
19	1	604	CLA	C16-C17-C18-C20
19	B	1216	CLA	O1D-CGD-O2D-CED
25	F	5002	LMG	C13-C14-C15-C16
29	2	613	CHL	CAA-CBA-CGA-O1A
25	F	5001	LMG	C9-C8-O7-C10
19	A	1121	CLA	C1A-C2A-CAA-CBA
19	A	1134	CLA	C1A-C2A-CAA-CBA
19	A	1137	CLA	C1A-C2A-CAA-CBA
19	G	1701	CLA	C1A-C2A-CAA-CBA
19	2	603	CLA	C1A-C2A-CAA-CBA
19	2	608	CLA	C1A-C2A-CAA-CBA
29	1	609	CHL	C1A-C2A-CAA-CBA
29	4	610	CHL	C1A-C2A-CAA-CBA
19	A	1013	CLA	C11-C10-C8-C7
19	A	1125	CLA	C11-C12-C13-C15
19	A	1127	CLA	C11-C12-C13-C15
19	A	1133	CLA	C11-C10-C8-C7
19	B	1202	CLA	C12-C13-C15-C16
19	B	1207	CLA	C6-C7-C8-C10
19	B	1223	CLA	C11-C10-C8-C7
19	B	1223	CLA	C12-C13-C15-C16
19	1	604	CLA	C12-C13-C15-C16
19	2	605	CLA	C6-C7-C8-C10
19	1	613	CLA	CAA-CBA-CGA-O1A
19	3	606	CLA	C4C-C3C-CAC-CBC
23	B	5002	LHG	C11-C10-C9-C8
22	G	4021	BCR	C15-C16-C17-C18
19	A	1131	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
19	1	613	CLA	CAA-CBA-CGA-O2A
19	2	604	CLA	C10-C11-C12-C13
19	B	1217	CLA	C2A-CAA-CBA-CGA
19	A	1125	CLA	C10-C11-C12-C13
19	B	1224	CLA	C8-C10-C11-C12
19	1	604	CLA	C8-C10-C11-C12
19	A	1126	CLA	CAA-CBA-CGA-O2A
19	B	1215	CLA	CAA-CBA-CGA-O2A
19	A	1136	CLA	C16-C17-C18-C20
19	A	1139	CLA	C13-C15-C16-C17
19	A	1113	CLA	CAA-CBA-CGA-O2A
19	A	1105	CLA	C5-C6-C7-C8
19	B	1226	CLA	C8-C10-C11-C12
19	1	601	CLA	C10-C11-C12-C13
19	2	605	CLA	C13-C15-C16-C17
25	F	5002	LMG	C40-C41-C42-C43
22	A	4007	BCR	C16-C17-C18-C19
22	A	4011	BCR	C16-C17-C18-C19
22	A	4017	BCR	C16-C17-C18-C19
22	B	4004	BCR	C12-C13-C14-C15
22	B	4004	BCR	C16-C17-C18-C19
22	B	4006	BCR	C11-C10-C9-C8
22	F	4016	BCR	C16-C17-C18-C19
22	G	4011	BCR	C16-C17-C18-C19
22	I	4018	BCR	C12-C13-C14-C15
22	I	4020	BCR	C16-C17-C18-C19
22	I	4020	BCR	C20-C21-C22-C23
22	1	504	BCR	C16-C17-C18-C19
22	3	506	BCR	C16-C17-C18-C19
30	4	502	XAT	C32-C33-C34-C35
25	A	5006	LMG	O1-C7-C8-O7
27	G	5003	DGD	O1G-C1G-C2G-O2G
22	A	4002	BCR	C15-C16-C17-C18
22	A	4008	BCR	C19-C20-C21-C22
22	F	4014	BCR	C19-C20-C21-C22
22	K	4002	BCR	C19-C20-C21-C22
22	1	503	BCR	C9-C10-C11-C12
22	3	506	BCR	C15-C16-C17-C18
19	A	1119	CLA	C16-C17-C18-C20
19	4	604	CLA	C4-C3-C5-C6
20	B	2002	PQN	C14-C13-C15-C16
19	A	1121	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
19	A	1127	CLA	C2-C1-O2A-CGA
19	B	1234	CLA	C2-C1-O2A-CGA
19	B	1235	CLA	C2-C1-O2A-CGA
19	4	604	CLA	C2-C1-O2A-CGA
29	2	609	CHL	C2-C1-O2A-CGA
19	B	1224	CLA	C2-C3-C5-C6
29	4	613	CHL	C10-C11-C12-C13
19	A	1113	CLA	CAA-CBA-CGA-O1A
25	A	5006	LMG	C14-C15-C16-C17
27	B	5005	DGD	CAA-CBA-CCA-CDA
19	B	1210	CLA	C11-C12-C13-C14
19	G	1603	CLA	C15-C16-C17-C18
19	K	1402	CLA	C2A-CAA-CBA-CGA
19	K	1404	CLA	C2A-CAA-CBA-CGA
19	4	601	CLA	C11-C12-C13-C15
29	2	613	CHL	CAA-CBA-CGA-O2A
18	A	1011	CL0	CAA-CBA-CGA-O1A
19	3	608	CLA	O1A-CGA-O2A-C1
22	A	4017	BCR	C1-C6-C7-C8
22	B	4010	BCR	C23-C24-C25-C30
22	G	4021	BCR	C1-C6-C7-C8
22	L	4020	BCR	C23-C24-C25-C30
28	1	502	LUT	C1-C6-C7-C8
28	1	502	LUT	C5-C6-C7-C8
28	4	501	LUT	C1-C6-C7-C8
23	1	801	LHG	C19-C20-C21-C22
19	A	1103	CLA	C5-C6-C7-C8
23	A	5001	LHG	C17-C18-C19-C20
19	A	1131	CLA	CBA-CGA-O2A-C1
19	A	1101	CLA	C4-C3-C5-C6
19	A	1115	CLA	C4-C3-C5-C6
19	B	1210	CLA	C4-C3-C5-C6
19	A	1119	CLA	C10-C11-C12-C13
19	B	1204	CLA	C10-C11-C12-C13
19	A	1132	CLA	C2-C3-C5-C6
19	B	1223	CLA	CBD-CGD-O2D-CED
25	B	5004	LMG	C8-C7-O1-C1
25	F	5004	LMG	C8-C7-O1-C1
27	3	803	DGD	C2G-C3G-O3G-C1D
23	1	801	LHG	C24-C23-O8-C6
25	1	802	LMG	O9-C10-C11-C12
19	B	1216	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
20	A	2001	PQN	C26-C27-C28-C30
23	B	5002	LHG	C35-C36-C37-C38
27	B	5005	DGD	C1B-C2B-C3B-C4B
19	B	1208	CLA	C2A-CAA-CBA-CGA
27	4	801	DGD	O1G-C1A-C2A-C3A
23	1	801	LHG	O10-C23-O8-C6
25	G	5001	LMG	C14-C15-C16-C17
25	B	5007	LMG	C31-C32-C33-C34
23	2	807	LHG	O8-C23-C24-C25
19	A	1101	CLA	C2-C3-C5-C6
19	B	1210	CLA	C2-C3-C5-C6
19	B	1240	CLA	C12-C13-C15-C16
19	2	603	CLA	C11-C10-C8-C7
20	B	2002	PQN	C12-C13-C15-C16
19	B	1238	CLA	CBA-CGA-O2A-C1
19	B	1215	CLA	C13-C15-C16-C17
23	B	5001	LHG	O1-C1-C2-O2
23	B	5002	LHG	O1-C1-C2-O2
27	B	5005	DGD	C5B-C6B-C7B-C8B
25	G	5006	LMG	O7-C10-C11-C12
22	I	4018	BCR	C9-C10-C11-C12
19	B	1210	CLA	C16-C17-C18-C19
19	1	607	CLA	O1D-CGD-O2D-CED
25	B	5007	LMG	O9-C10-C11-C12
19	B	1215	CLA	C8-C10-C11-C12
19	G	1603	CLA	C10-C11-C12-C13
19	B	1208	CLA	C3-C5-C6-C7
19	B	1236	CLA	CAA-CBA-CGA-O2A
27	J	5001	DGD	C6B-C7B-C8B-C9B
29	2	611	CHL	C4C-C3C-CAC-CBC
19	A	1106	CLA	C16-C17-C18-C20
19	A	1127	CLA	C16-C17-C18-C19
19	B	1228	CLA	C11-C12-C13-C15
19	4	617	CLA	C16-C17-C18-C19
19	1	614	CLA	CAA-CBA-CGA-O2A
19	3	602	CLA	CAA-CBA-CGA-O2A
25	B	5004	LMG	O8-C28-C29-C30
19	A	1122	CLA	C2C-C3C-CAC-CBC
19	A	1126	CLA	C4-C3-C5-C6
19	A	1131	CLA	C4-C3-C5-C6
19	B	1203	CLA	C4-C3-C5-C6
19	B	1212	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
19	B	1215	CLA	C4-C3-C5-C6
19	1	614	CLA	C4-C3-C5-C6
19	2	605	CLA	C4-C3-C5-C6
25	G	5006	LMG	O9-C10-C11-C12
19	1	604	CLA	C16-C17-C18-C19
19	A	1012	CLA	C11-C12-C13-C14
19	A	1101	CLA	C11-C10-C8-C9
19	A	1102	CLA	C6-C7-C8-C9
19	A	1111	CLA	C6-C7-C8-C9
19	A	1117	CLA	C11-C12-C13-C14
19	A	1126	CLA	C14-C13-C15-C16
19	A	1127	CLA	C11-C12-C13-C14
19	A	1129	CLA	C11-C10-C8-C9
19	A	1133	CLA	C11-C12-C13-C14
19	B	1215	CLA	C11-C10-C8-C9
19	B	1221	CLA	C6-C7-C8-C9
19	B	1223	CLA	C14-C13-C15-C16
19	G	1701	CLA	C6-C7-C8-C9
25	2	803	LMG	C11-C12-C13-C14
19	F	1301	CLA	C3A-C2A-CAA-CBA
19	4	612	CLA	C3A-C2A-CAA-CBA
29	1	609	CHL	C3A-C2A-CAA-CBA
19	A	1115	CLA	CAA-CBA-CGA-O2A
19	3	601	CLA	CAA-CBA-CGA-O2A
19	B	1218	CLA	CBD-CGD-O2D-CED
19	A	1110	CLA	CAD-CBD-CGD-O2D
19	A	1123	CLA	CAD-CBD-CGD-O2D
19	A	1137	CLA	CAD-CBD-CGD-O2D
19	B	1211	CLA	CAD-CBD-CGD-O2D
19	B	1234	CLA	CAD-CBD-CGD-O2D
19	B	1240	CLA	CAD-CBD-CGD-O2D
19	K	1402	CLA	CAD-CBD-CGD-O2D
19	K	1403	CLA	CAD-CBD-CGD-O2D
19	4	604	CLA	CAD-CBD-CGD-O2D
19	4	609	CLA	CAD-CBD-CGD-O2D
19	A	1104	CLA	C16-C17-C18-C20
19	L	1502	CLA	C2A-CAA-CBA-CGA
25	B	5007	LMG	O9-C10-O7-C8
19	B	1235	CLA	CAA-CBA-CGA-O2A
19	A	1112	CLA	O1D-CGD-O2D-CED
19	B	1022	CLA	C4-C3-C5-C6
19	B	1212	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
19	A	1136	CLA	CAA-CBA-CGA-O2A
19	B	1238	CLA	CAA-CBA-CGA-O2A
19	K	1402	CLA	CAA-CBA-CGA-O2A
25	F	5003	LMG	O7-C10-C11-C12
25	G	5001	LMG	O8-C28-C29-C30
25	2	803	LMG	O7-C10-C11-C12
22	I	4020	BCR	C7-C8-C9-C10
30	2	502	XAT	C27-C28-C29-C30
30	4	502	XAT	C7-C8-C9-C10
19	A	1116	CLA	C11-C10-C8-C9
25	1	802	LMG	C7-C8-C9-O8
27	3	803	DGD	C3A-C4A-C5A-C6A
23	A	5001	LHG	O6-C4-C5-O7
23	A	5002	LHG	O8-C23-C24-C25
25	A	5006	LMG	O7-C10-C11-C12
19	A	1101	CLA	C13-C15-C16-C17
19	A	1103	CLA	O2A-C1-C2-C3
19	4	604	CLA	C2A-CAA-CBA-CGA
19	2	601	CLA	CAA-CBA-CGA-O2A
19	A	1112	CLA	CBD-CGD-O2D-CED
19	A	1013	CLA	CHA-CBD-CGD-O1D
19	A	1013	CLA	CHA-CBD-CGD-O2D
19	A	1104	CLA	CHA-CBD-CGD-O1D
19	A	1104	CLA	CHA-CBD-CGD-O2D
19	A	1125	CLA	CHA-CBD-CGD-O1D
19	A	1125	CLA	CHA-CBD-CGD-O2D
19	A	1126	CLA	CHA-CBD-CGD-O2D
19	A	1132	CLA	CHA-CBD-CGD-O1D
19	A	1132	CLA	CHA-CBD-CGD-O2D
19	A	1135	CLA	CHA-CBD-CGD-O1D
19	A	1135	CLA	CHA-CBD-CGD-O2D
19	A	1136	CLA	CHA-CBD-CGD-O1D
19	A	1136	CLA	CHA-CBD-CGD-O2D
19	B	1205	CLA	CHA-CBD-CGD-O1D
19	B	1205	CLA	CHA-CBD-CGD-O2D
19	B	1213	CLA	CHA-CBD-CGD-O2D
19	B	1220	CLA	CHA-CBD-CGD-O1D
19	B	1220	CLA	CHA-CBD-CGD-O2D
19	B	1224	CLA	CHA-CBD-CGD-O1D
19	B	1224	CLA	CHA-CBD-CGD-O2D
19	B	1225	CLA	CHA-CBD-CGD-O1D
19	B	1225	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
19	B	1227	CLA	CHA-CBD-CGD-O2D
19	B	1228	CLA	CHA-CBD-CGD-O2D
19	B	1235	CLA	CHA-CBD-CGD-O1D
19	B	1235	CLA	CHA-CBD-CGD-O2D
19	B	1236	CLA	CHA-CBD-CGD-O1D
19	B	1236	CLA	CHA-CBD-CGD-O2D
19	B	1237	CLA	CHA-CBD-CGD-O1D
19	B	1237	CLA	CHA-CBD-CGD-O2D
19	G	1603	CLA	CHA-CBD-CGD-O1D
19	G	1603	CLA	CHA-CBD-CGD-O2D
19	K	1401	CLA	CHA-CBD-CGD-O1D
19	K	1401	CLA	CHA-CBD-CGD-O2D
19	K	1402	CLA	CHA-CBD-CGD-O2D
19	L	1502	CLA	CHA-CBD-CGD-O1D
19	L	1502	CLA	CHA-CBD-CGD-O2D
19	1	608	CLA	CHA-CBD-CGD-O2D
19	3	603	CLA	CHA-CBD-CGD-O1D
19	3	603	CLA	CHA-CBD-CGD-O2D
19	3	606	CLA	CHA-CBD-CGD-O1D
19	3	606	CLA	CHA-CBD-CGD-O2D
19	3	612	CLA	CHA-CBD-CGD-O1D
19	3	612	CLA	CHA-CBD-CGD-O2D
29	1	610	CHL	CHA-CBD-CGD-O2D
29	3	607	CHL	CHA-CBD-CGD-O1D
19	A	1128	CLA	C5-C6-C7-C8
19	A	1112	CLA	CAA-CBA-CGA-O2A
25	B	5003	LMG	O8-C28-C29-C30
25	F	5004	LMG	C33-C34-C35-C36
22	A	4011	BCR	C11-C10-C9-C8
19	B	1210	CLA	CAA-CBA-CGA-O2A
27	4	801	DGD	O2G-C1B-C2B-C3B
29	4	610	CHL	CAA-CBA-CGA-O2A
23	A	5001	LHG	O7-C5-C6-O8
27	4	801	DGD	O2G-C2G-C3G-O3G
29	2	615	CHL	CAA-CBA-CGA-O1A
19	A	1111	CLA	CAA-CBA-CGA-O2A
19	A	1131	CLA	C2A-CAA-CBA-CGA
19	A	1122	CLA	C4C-C3C-CAC-CBC
27	4	801	DGD	C2B-C1B-O2G-C2G
19	B	1226	CLA	CAA-CBA-CGA-O2A
19	B	1239	CLA	CAA-CBA-CGA-O2A
19	A	1112	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
19	B	1236	CLA	CAA-CBA-CGA-O1A
19	A	1013	CLA	C11-C12-C13-C15
19	A	1102	CLA	C11-C10-C8-C7
19	A	1103	CLA	C12-C13-C15-C16
19	B	1021	CLA	C12-C13-C15-C16
19	B	1215	CLA	C2-C3-C5-C6
19	B	1239	CLA	C6-C7-C8-C10
19	A	1127	CLA	C13-C15-C16-C17
23	A	5002	LHG	O7-C7-C8-C9
24	G	5004	LMT	C3-C4-C5-C6
27	B	5005	DGD	C4A-C5A-C6A-C7A
19	A	1013	CLA	C14-C13-C15-C16
19	A	1125	CLA	C11-C12-C13-C14
19	B	1021	CLA	C14-C13-C15-C16
19	B	1202	CLA	C14-C13-C15-C16
19	B	1240	CLA	CAA-CBA-CGA-O1A
19	B	1223	CLA	O1D-CGD-O2D-CED
19	A	1134	CLA	C2A-CAA-CBA-CGA
29	2	615	CHL	C4C-C3C-CAC-CBC
19	1	605	CLA	CAA-CBA-CGA-O2A
22	A	4003	BCR	C36-C18-C19-C20
19	B	1216	CLA	C16-C17-C18-C19
23	2	807	LHG	O1-C1-C2-C3
19	B	1223	CLA	O1A-CGA-O2A-C1
25	B	5004	LMG	O10-C28-C29-C30
22	A	4003	BCR	C17-C18-C19-C20
22	A	4011	BCR	C7-C8-C9-C10
22	B	4010	BCR	C21-C22-C23-C24
22	F	4014	BCR	C21-C22-C23-C24
19	A	1012	CLA	C1A-C2A-CAA-CBA
19	A	1111	CLA	C1A-C2A-CAA-CBA
19	A	1115	CLA	C1A-C2A-CAA-CBA
19	A	1117	CLA	C1A-C2A-CAA-CBA
19	A	1124	CLA	C1A-C2A-CAA-CBA
19	B	1232	CLA	C1A-C2A-CAA-CBA
19	F	1301	CLA	C1A-C2A-CAA-CBA
19	4	609	CLA	C1A-C2A-CAA-CBA
19	4	617	CLA	C1A-C2A-CAA-CBA
29	2	609	CHL	C1A-C2A-CAA-CBA
19	A	1140	CLA	C16-C17-C18-C20
23	A	5002	LHG	O9-C7-C8-C9
19	A	1122	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
19	B	1223	CLA	CBA-CGA-O2A-C1
19	K	1402	CLA	CAA-CBA-CGA-O1A
19	3	602	CLA	CAA-CBA-CGA-O1A
25	2	804	LMG	O1-C7-C8-C9
27	G	5003	DGD	O1G-C1G-C2G-C3G
19	F	1301	CLA	C2A-CAA-CBA-CGA
19	3	601	CLA	C2A-CAA-CBA-CGA
19	A	1111	CLA	CAA-CBA-CGA-O1A
19	A	1112	CLA	CAA-CBA-CGA-O1A
19	B	1235	CLA	CAA-CBA-CGA-O1A
19	1	605	CLA	CAA-CBA-CGA-O1A
19	B	1230	CLA	C8-C10-C11-C12
19	A	1114	CLA	CAA-CBA-CGA-O2A
19	1	611	CLA	CAA-CBA-CGA-O2A
27	F	5005	DGD	O1G-C1A-C2A-C3A
19	B	1238	CLA	CAA-CBA-CGA-O1A
19	1	614	CLA	CAA-CBA-CGA-O1A
19	3	601	CLA	CAA-CBA-CGA-O1A
25	B	5003	LMG	O10-C28-C29-C30
25	G	5002	LMG	C21-C22-C23-C24
19	A	1125	CLA	C15-C16-C17-C18
19	A	1138	CLA	C5-C6-C7-C8
19	A	1139	CLA	C8-C10-C11-C12
23	B	5002	LHG	C4-O6-P-O5
19	A	1115	CLA	CAA-CBA-CGA-O1A
29	4	610	CHL	CAA-CBA-CGA-O1A
19	B	1215	CLA	C5-C6-C7-C8
22	F	4014	BCR	C23-C24-C25-C30
22	G	4021	BCR	C5-C6-C7-C8
22	L	4020	BCR	C23-C24-C25-C26
22	3	503	BCR	C23-C24-C25-C30
19	A	1136	CLA	CAA-CBA-CGA-O1A
19	B	1210	CLA	CAA-CBA-CGA-O1A
19	B	1221	CLA	CAA-CBA-CGA-O2A
29	3	604	CHL	CAA-CBA-CGA-O2A
19	A	1115	CLA	C4C-C3C-CAC-CBC
22	B	4005	BCR	C10-C11-C12-C13
19	2	601	CLA	CAA-CBA-CGA-O1A
25	F	5003	LMG	O9-C10-C11-C12
25	G	5001	LMG	O10-C28-C29-C30
25	3	802	LMG	O7-C10-C11-C12
23	A	5002	LHG	O10-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
25	A	5006	LMG	O9-C10-C11-C12
19	B	1202	CLA	CAD-CBD-CGD-O1D
19	B	1213	CLA	CAD-CBD-CGD-O1D
19	B	1226	CLA	CAD-CBD-CGD-O1D
19	B	1234	CLA	CAD-CBD-CGD-O1D
19	1	605	CLA	CAD-CBD-CGD-O1D
29	3	611	CHL	CAD-CBD-CGD-O1D
19	B	1238	CLA	O1A-CGA-O2A-C1
19	B	1206	CLA	CAA-CBA-CGA-O2A
23	2	801	LHG	O7-C7-C8-C9
19	A	1013	CLA	C11-C12-C13-C14
19	A	1127	CLA	C6-C7-C8-C9
19	A	1132	CLA	C11-C12-C13-C14
19	B	1239	CLA	C6-C7-C8-C9
23	A	5002	LHG	C24-C25-C26-C27
19	A	1116	CLA	CAA-CBA-CGA-O2A
19	A	1125	CLA	CAA-CBA-CGA-O2A
19	A	1130	CLA	CAA-CBA-CGA-O2A
19	B	1207	CLA	CAA-CBA-CGA-O2A
19	B	1219	CLA	CAA-CBA-CGA-O2A
19	A	1128	CLA	CAA-CBA-CGA-O2A
19	A	1140	CLA	CAA-CBA-CGA-O2A
19	L	1502	CLA	CAA-CBA-CGA-O2A
19	4	606	CLA	CAA-CBA-CGA-O2A
25	2	804	LMG	O7-C10-C11-C12
29	3	607	CHL	CAA-CBA-CGA-O2A
19	A	1130	CLA	C5-C6-C7-C8
19	3	610	CLA	C10-C11-C12-C13
19	B	1226	CLA	CAA-CBA-CGA-O1A
19	B	1239	CLA	CAA-CBA-CGA-O1A
27	4	801	DGD	O1B-C1B-C2B-C3B
22	I	4020	BCR	C7-C8-C9-C34
19	A	1012	CLA	C3A-C2A-CAA-CBA
19	A	1111	CLA	C2-C3-C5-C6
19	A	1122	CLA	C6-C7-C8-C10
19	B	1022	CLA	C6-C7-C8-C10
19	B	1225	CLA	C6-C7-C8-C10
19	B	1238	CLA	C11-C10-C8-C7
19	G	1603	CLA	C3A-C2A-CAA-CBA
19	4	601	CLA	C3A-C2A-CAA-CBA
29	1	609	CHL	C2-C3-C5-C6
29	2	609	CHL	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
19	B	1206	CLA	CAA-CBA-CGA-O1A
19	A	1102	CLA	CAA-CBA-CGA-O2A
19	2	608	CLA	CAA-CBA-CGA-O2A
19	3	603	CLA	CAA-CBA-CGA-O2A
23	B	5002	LHG	O8-C23-C24-C25
25	B	5004	LMG	O7-C10-C11-C12
25	F	5001	LMG	O7-C10-C11-C12
25	G	5002	LMG	O8-C28-C29-C30
27	G	5003	DGD	O1G-C1A-C2A-C3A
19	4	601	CLA	C3-C5-C6-C7
22	2	503	BCR	C11-C12-C13-C14
19	A	1102	CLA	CAA-CBA-CGA-O1A
19	A	1130	CLA	CAA-CBA-CGA-O1A
19	B	1221	CLA	CAA-CBA-CGA-O1A
23	B	5002	LHG	O10-C23-C24-C25
22	A	4008	BCR	C13-C14-C15-C16
22	K	4002	BCR	C9-C10-C11-C12
19	A	1119	CLA	C16-C17-C18-C19
19	A	1103	CLA	CAA-CBA-CGA-O2A
19	4	602	CLA	CAA-CBA-CGA-O2A
19	A	1103	CLA	O1A-CGA-O2A-C1
19	A	1103	CLA	CAA-CBA-CGA-O1A
19	A	1114	CLA	CAA-CBA-CGA-O1A
19	A	1116	CLA	CAA-CBA-CGA-O1A
19	A	1125	CLA	CAA-CBA-CGA-O1A
19	A	1140	CLA	CAA-CBA-CGA-O1A
19	2	608	CLA	CAA-CBA-CGA-O1A
27	F	5005	DGD	O1A-C1A-C2A-C3A
19	B	1021	CLA	CAA-CBA-CGA-O2A
19	B	1211	CLA	CAA-CBA-CGA-O2A
29	1	609	CHL	CAA-CBA-CGA-O2A
19	1	605	CLA	C5-C6-C7-C8
23	2	801	LHG	O9-C7-C8-C9
29	3	604	CHL	CAA-CBA-CGA-O1A
19	B	1223	CLA	C2A-CAA-CBA-CGA
19	2	612	CLA	C2A-CAA-CBA-CGA
19	A	1128	CLA	CAA-CBA-CGA-O1A
25	B	5004	LMG	O9-C10-C11-C12
19	A	1135	CLA	CAA-CBA-CGA-O2A
19	K	1404	CLA	CAA-CBA-CGA-O2A

There are no ring outliers.

222 monomers are involved in 798 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
28	1	501	LUT	9	0
19	3	602	CLA	5	0
19	B	1238	CLA	7	0
29	3	604	CHL	8	0
19	B	1231	CLA	2	0
19	A	1113	CLA	6	0
19	1	607	CLA	4	0
19	4	605	CLA	9	0
22	A	4011	BCR	3	0
19	G	1603	CLA	4	0
29	1	612	CHL	6	0
19	3	617	CLA	3	0
22	B	4005	BCR	1	0
19	B	1202	CLA	6	0
19	4	604	CLA	5	0
19	A	1121	CLA	7	0
19	B	1213	CLA	5	0
27	G	5003	DGD	4	0
19	1	613	CLA	6	0
23	2	807	LHG	2	0
29	2	609	CHL	3	0
19	4	602	CLA	3	0
22	B	4006	BCR	5	0
19	1	601	CLA	12	0
29	2	611	CHL	5	0
23	A	5002	LHG	2	0
19	B	1225	CLA	5	0
20	B	2002	PQN	4	0
19	1	611	CLA	4	0
19	A	1141	CLA	4	0
25	F	5003	LMG	1	0
19	B	1216	CLA	2	0
19	A	1133	CLA	3	0
19	A	1137	CLA	4	0
22	B	4009	BCR	3	0
19	2	607	CLA	2	0
19	4	617	CLA	3	0
19	2	603	CLA	10	0
19	B	1209	CLA	3	0
19	3	614	CLA	2	0
29	3	611	CHL	4	0
29	1	609	CHL	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	2	610	CHL	7	0
19	B	1203	CLA	3	0
22	F	4016	BCR	5	0
19	A	1119	CLA	7	0
25	2	803	LMG	6	0
32	N	101	FES	1	0
19	B	1223	CLA	5	0
19	B	1222	CLA	9	0
22	I	4018	BCR	3	0
22	A	4007	BCR	4	0
19	A	1138	CLA	3	0
19	B	1206	CLA	5	0
19	A	1115	CLA	9	0
23	A	5001	LHG	3	0
19	A	1103	CLA	8	0
19	B	1227	CLA	5	0
19	A	1012	CLA	8	0
27	4	801	DGD	3	0
19	B	1218	CLA	5	0
19	1	605	CLA	5	0
19	2	604	CLA	12	0
22	A	4003	BCR	2	0
23	B	5002	LHG	5	0
19	B	1237	CLA	7	0
19	A	1116	CLA	9	0
22	K	4001	BCR	5	0
27	B	5005	DGD	7	0
19	B	1229	CLA	5	0
29	4	611	CHL	1	0
19	A	1111	CLA	9	0
19	B	1221	CLA	4	0
19	A	1109	CLA	10	0
25	A	5006	LMG	5	0
19	L	1501	CLA	4	0
25	2	806	LMG	1	0
19	B	1226	CLA	5	0
19	B	1230	CLA	6	0
22	A	4002	BCR	3	0
22	B	4004	BCR	4	0
28	1	502	LUT	7	0
19	1	606	CLA	1	0
22	1	504	BCR	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	A	1126	CLA	7	0
19	K	1402	CLA	2	0
19	B	1212	CLA	2	0
19	3	610	CLA	6	0
29	4	613	CHL	8	0
19	A	1104	CLA	4	0
19	3	606	CLA	2	0
19	3	603	CLA	3	0
19	B	1208	CLA	5	0
19	B	1220	CLA	3	0
22	J	4012	BCR	1	0
29	4	615	CHL	3	0
19	A	1120	CLA	4	0
19	A	1130	CLA	2	0
19	B	1215	CLA	2	0
28	J	4013	LUT	4	0
22	3	503	BCR	3	0
29	2	615	CHL	5	0
19	A	1124	CLA	3	0
19	A	1114	CLA	3	0
24	A	5004	LMT	3	0
19	B	1235	CLA	6	0
19	4	608	CLA	2	0
19	B	1207	CLA	10	0
19	B	1211	CLA	4	0
24	B	5006	LMT	3	0
25	G	5001	LMG	3	0
19	3	608	CLA	1	0
19	4	612	CLA	5	0
19	2	605	CLA	6	0
19	A	1125	CLA	4	0
28	4	501	LUT	6	0
19	A	1101	CLA	4	0
19	4	603	CLA	7	0
19	B	1201	CLA	5	0
19	A	1110	CLA	5	0
22	A	4017	BCR	5	0
23	2	801	LHG	2	0
19	4	606	CLA	3	0
19	2	601	CLA	7	0
19	1	614	CLA	3	0
22	2	503	BCR	10	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	A	1117	CLA	2	0
19	A	1131	CLA	3	0
19	B	1228	CLA	1	0
19	B	1023	CLA	5	0
19	2	606	CLA	5	0
28	3	501	LUT	2	0
25	1	802	LMG	3	0
22	G	4011	BCR	4	0
29	4	610	CHL	3	0
19	A	1132	CLA	2	0
19	A	1107	CLA	4	0
19	A	1106	CLA	6	0
19	G	1601	CLA	3	0
19	4	601	CLA	3	0
19	A	1134	CLA	3	0
25	G	5002	LMG	5	0
19	1	604	CLA	8	0
19	A	1013	CLA	9	0
29	3	607	CHL	6	0
25	2	802	LMG	2	0
19	A	1139	CLA	3	0
19	L	1502	CLA	5	0
19	F	1301	CLA	4	0
19	B	1234	CLA	7	0
25	F	5001	LMG	1	0
19	B	1204	CLA	6	0
29	1	610	CHL	7	0
22	I	4020	BCR	3	0
19	A	1122	CLA	6	0
19	A	1112	CLA	8	0
19	1	602	CLA	4	0
19	A	1129	CLA	2	0
19	3	601	CLA	9	0
24	G	5004	LMT	2	0
19	A	1140	CLA	3	0
19	A	1123	CLA	5	0
19	F	1302	CLA	4	0
24	B	5008	LMT	1	0
19	B	1205	CLA	4	0
18	A	1011	CL0	6	0
22	A	4008	BCR	2	0
22	K	4002	BCR	7	0

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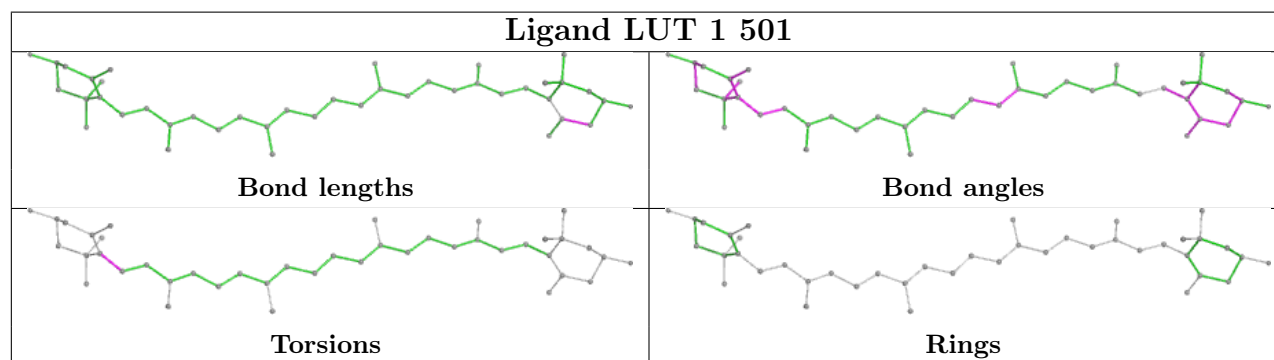
Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	B	1022	CLA	4	0
19	A	1136	CLA	9	0
19	B	1210	CLA	7	0
23	1	801	LHG	8	0
19	4	607	CLA	7	0
25	F	5002	LMG	8	0
27	F	5005	DGD	7	0
23	B	5001	LHG	4	0
19	1	603	CLA	6	0
19	3	612	CLA	4	0
22	L	4019	BCR	7	0
19	A	1105	CLA	8	0
19	A	1127	CLA	1	0
19	B	1219	CLA	9	0
19	B	1239	CLA	7	0
22	3	506	BCR	3	0
27	4	802	DGD	3	0
19	4	609	CLA	3	0
30	4	502	XAT	6	0
19	A	1135	CLA	6	0
19	K	1401	CLA	11	0
30	2	502	XAT	10	0
19	A	1128	CLA	3	0
22	G	4021	BCR	4	0
19	B	1214	CLA	6	0
27	1	803	DGD	1	0
19	L	1503	CLA	5	0
19	2	608	CLA	2	0
22	B	4010	BCR	1	0
25	F	5006	LMG	1	0
19	2	612	CLA	5	0
27	3	803	DGD	3	0
25	B	5003	LMG	3	0
19	B	1240	CLA	12	0
25	B	5007	LMG	2	0
19	B	1236	CLA	1	0
22	1	503	BCR	6	0
19	2	602	CLA	3	0
25	F	5004	LMG	2	0
28	2	501	LUT	4	0
27	J	5001	DGD	4	0
19	A	1108	CLA	2	0

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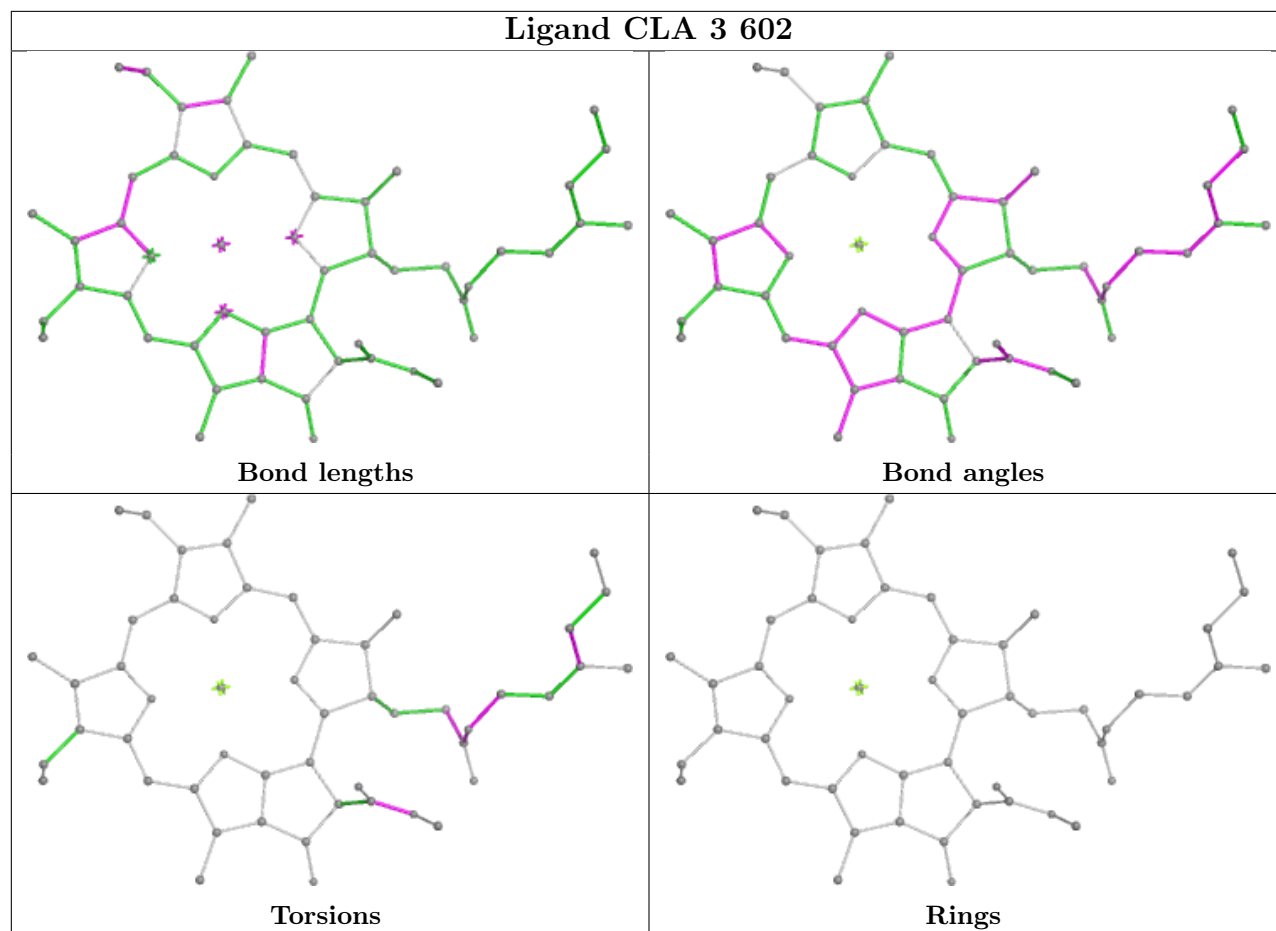
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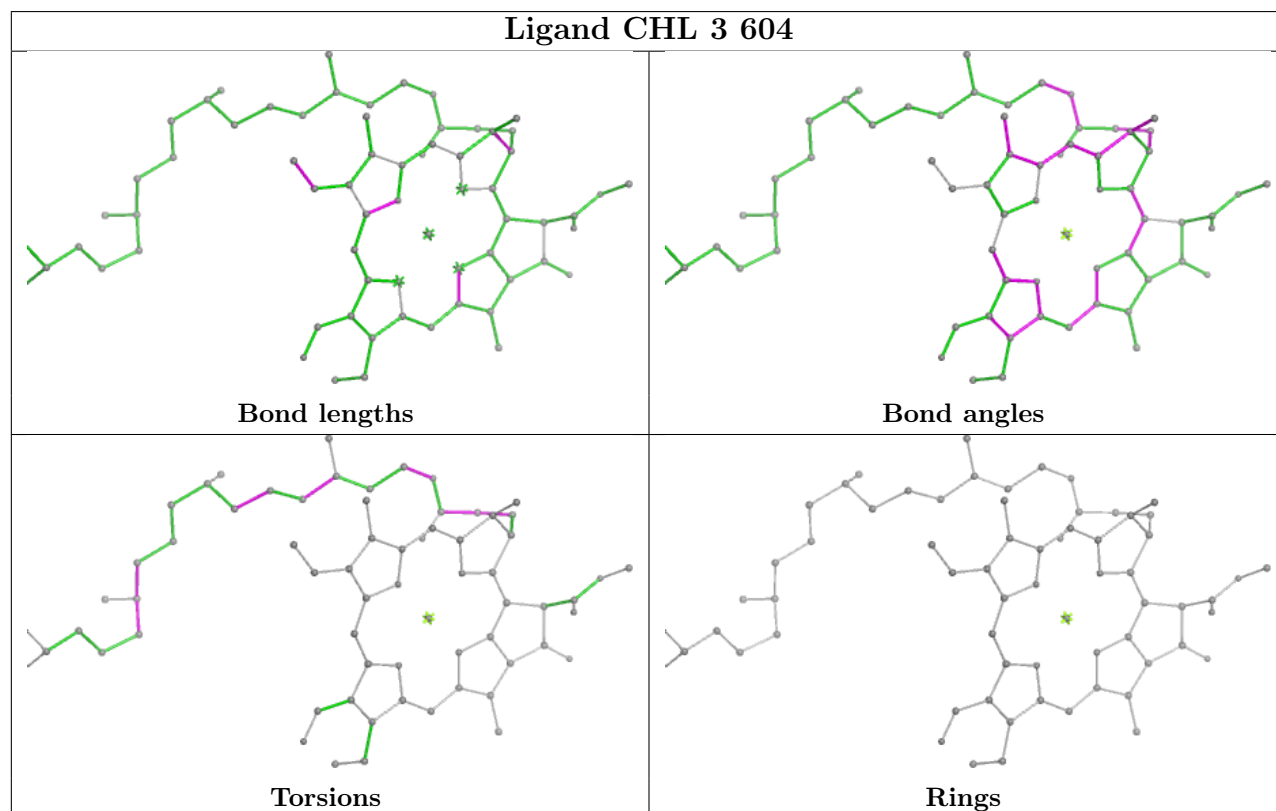
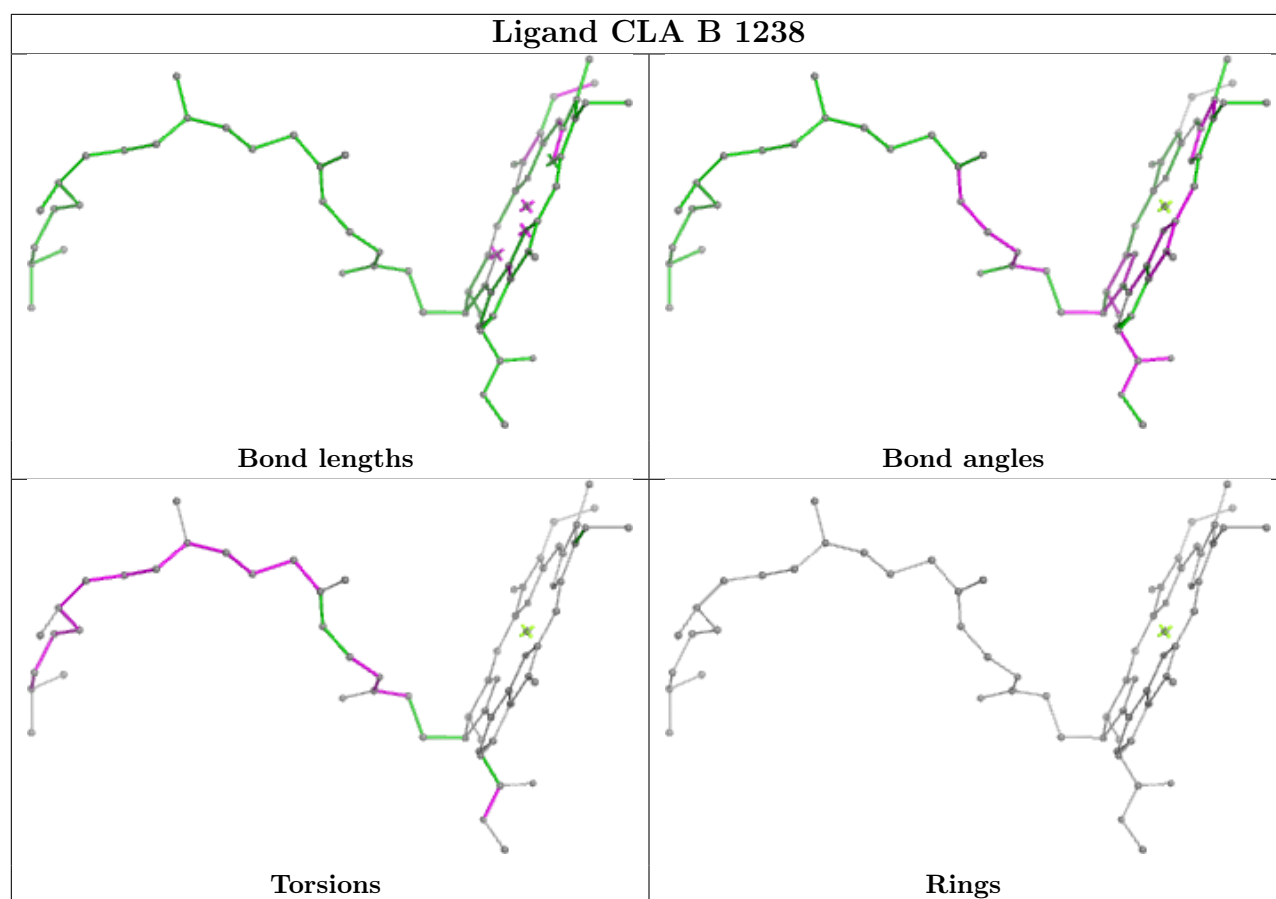
Mol	Chain	Res	Type	Clashes	Symm-Clashes
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19	G	1602	CLA	3	0
19	B	1021	CLA	4	0
19	K	1403	CLA	2	0
19	A	1102	CLA	7	0
19	B	1232	CLA	3	0
19	3	605	CLA	4	0
29	2	613	CHL	1	0
19	K	1404	CLA	4	0
19	3	613	CLA	3	0
19	G	1701	CLA	4	0
28	3	502	LUT	2	0

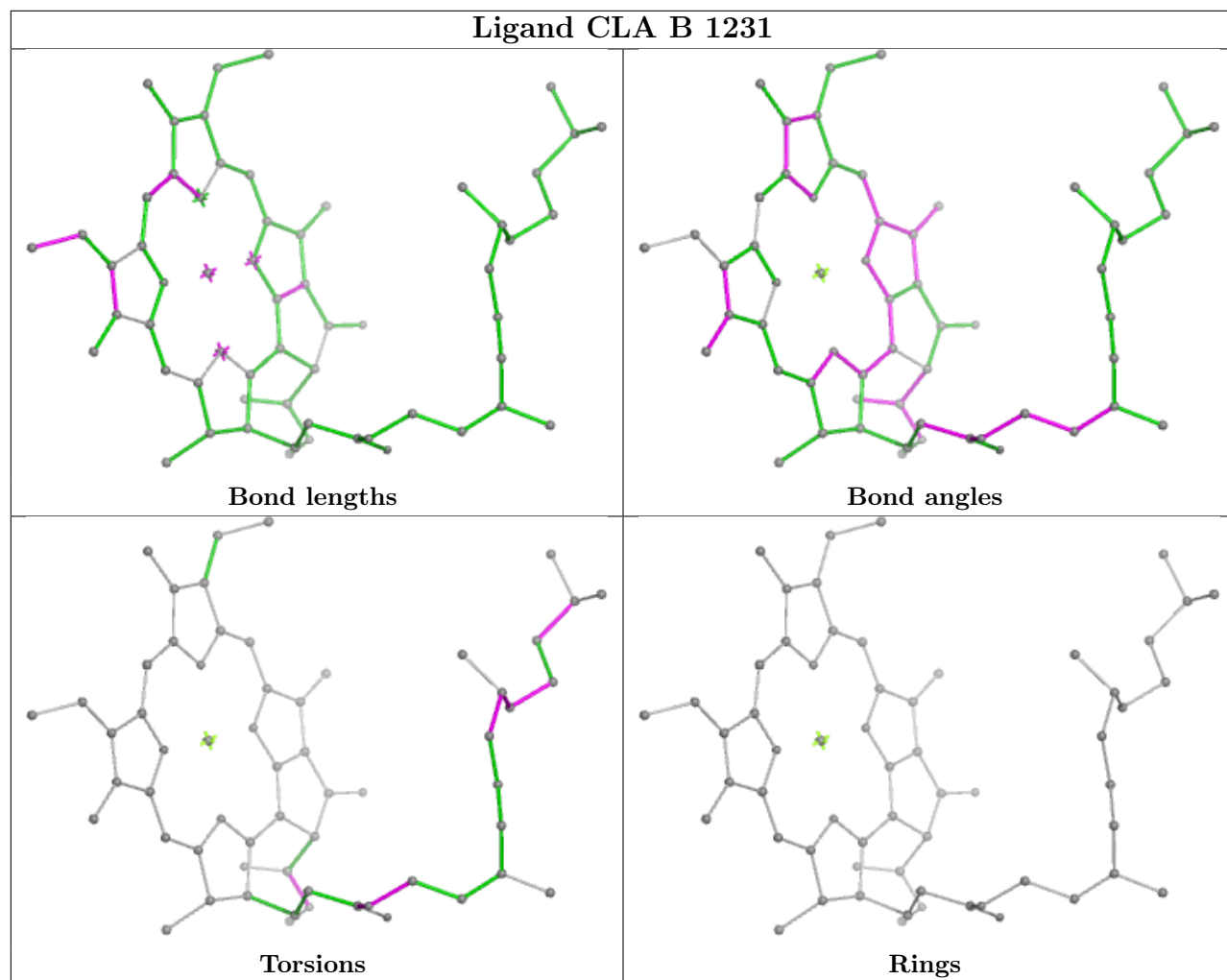
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

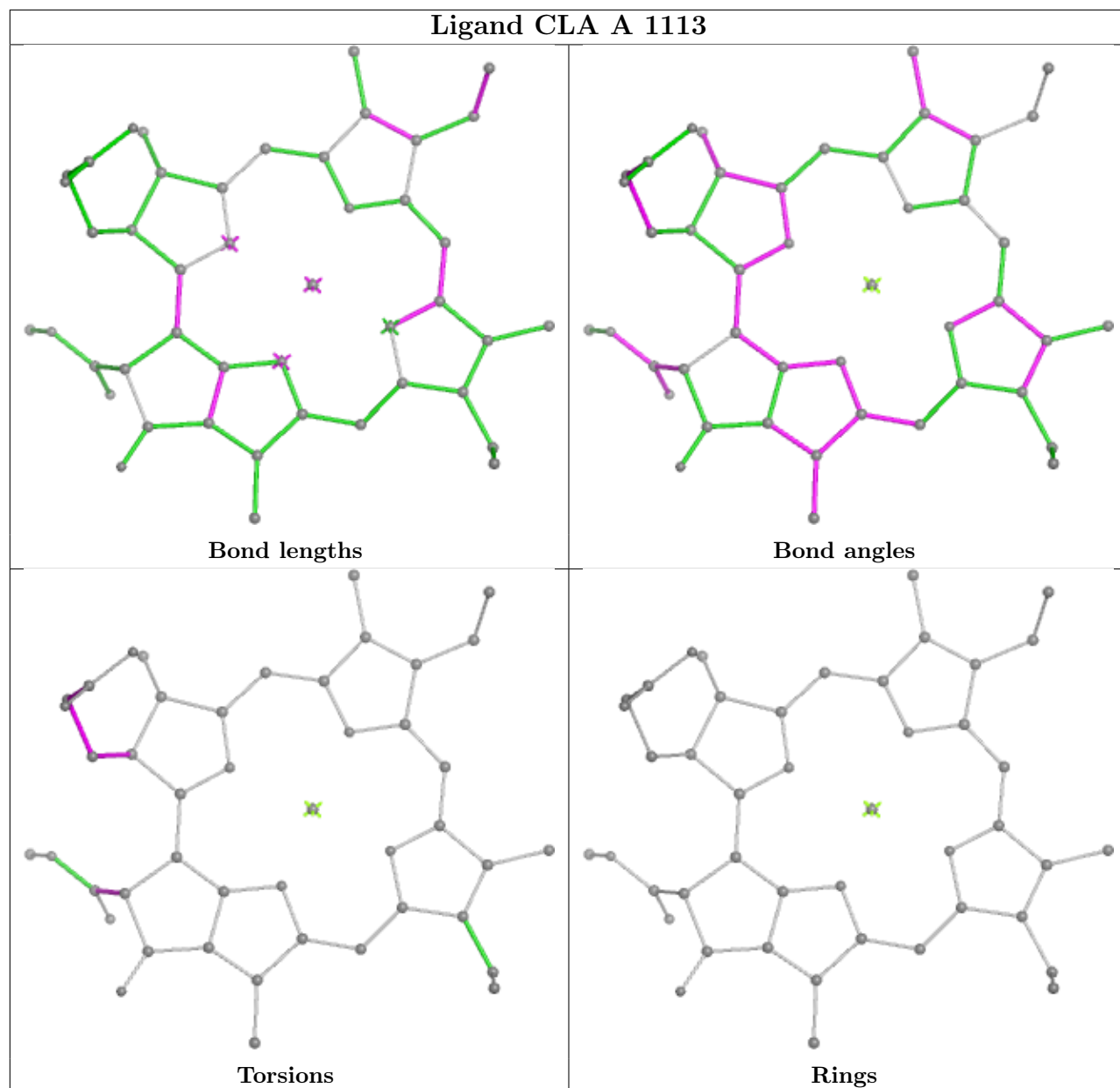


Ligand CLA 3 602

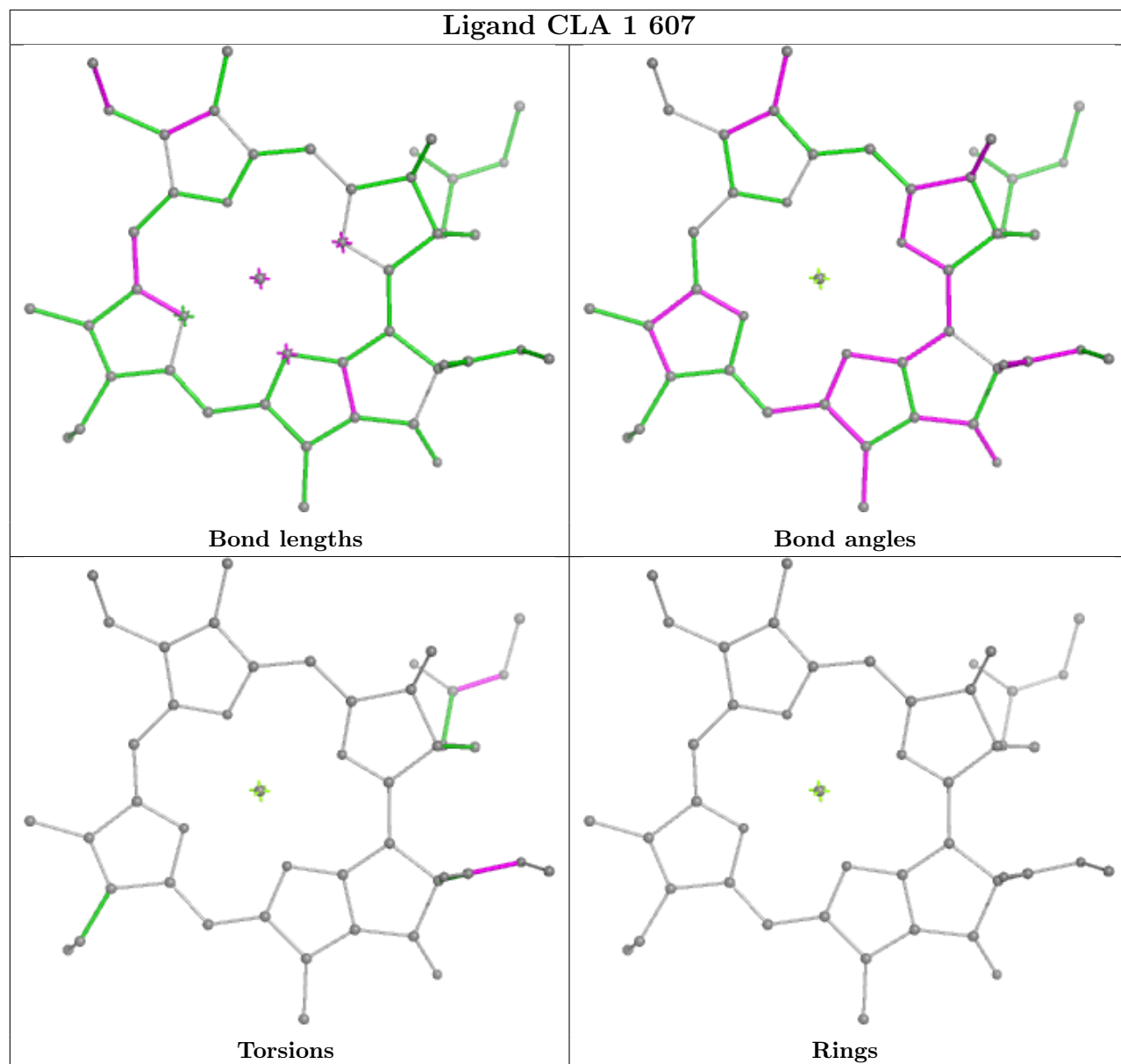




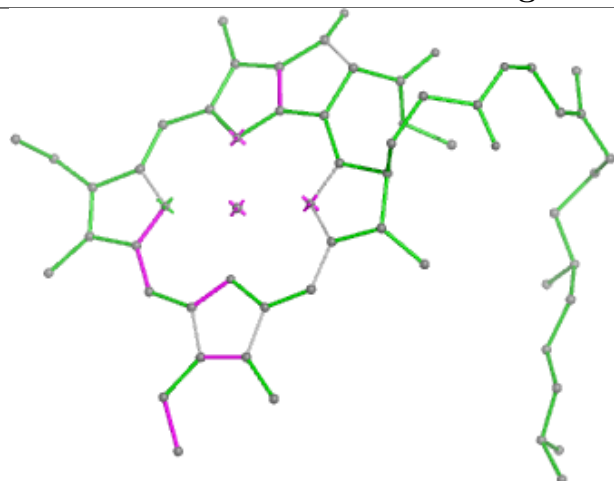




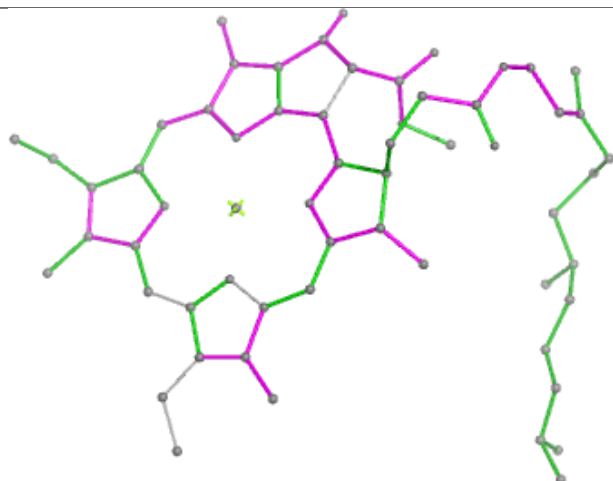
Ligand CLA 1 607



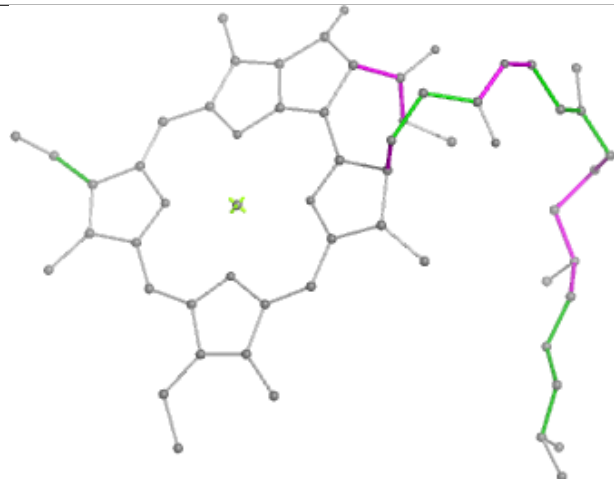
Ligand CLA 4 605



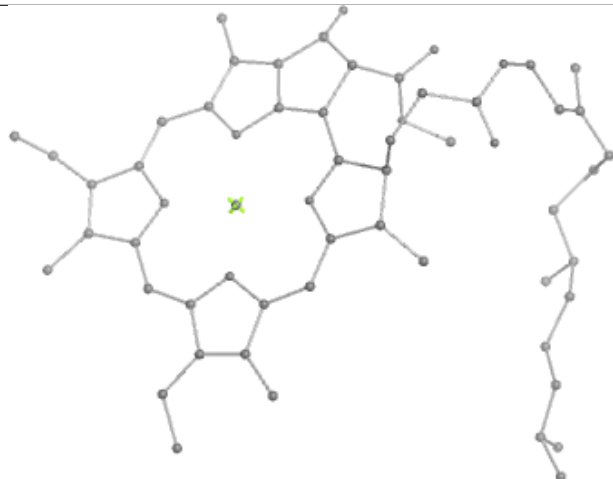
Bond lengths



Bond angles

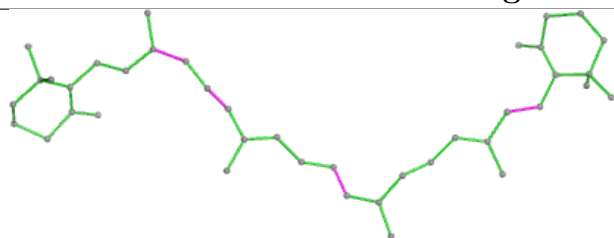


Torsions

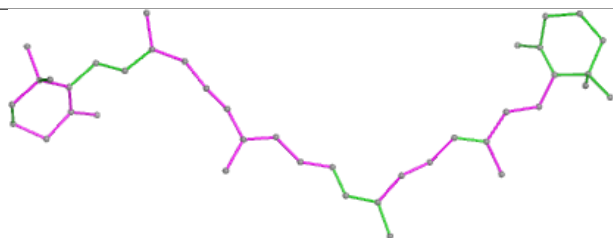


Rings

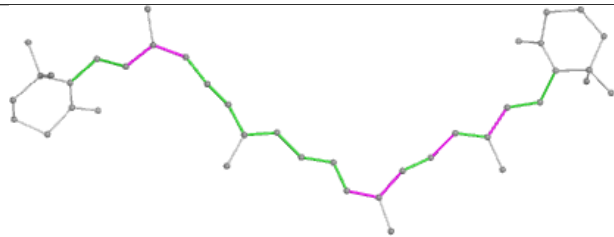
Ligand BCR A 4011



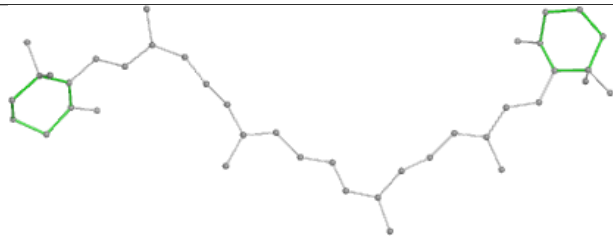
Bond lengths



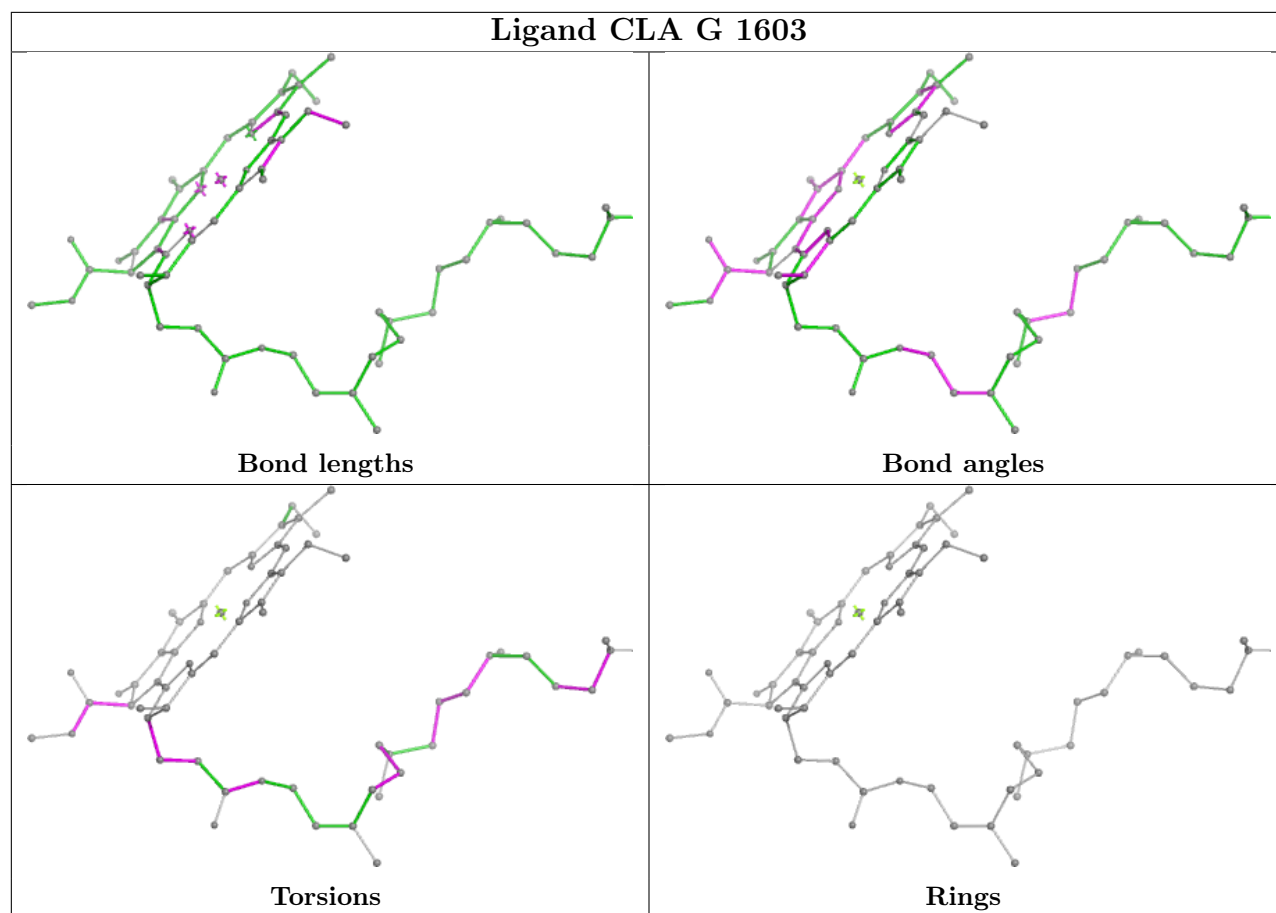
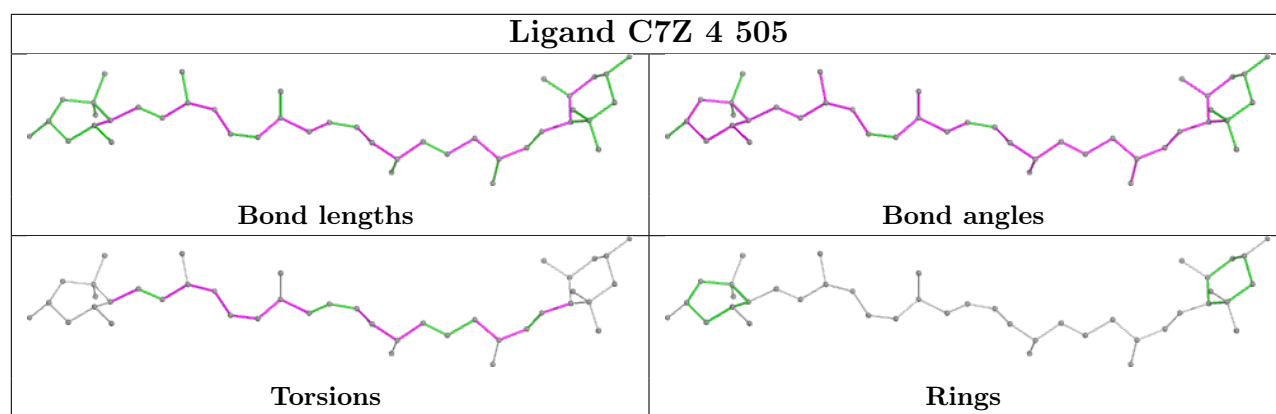
Bond angles



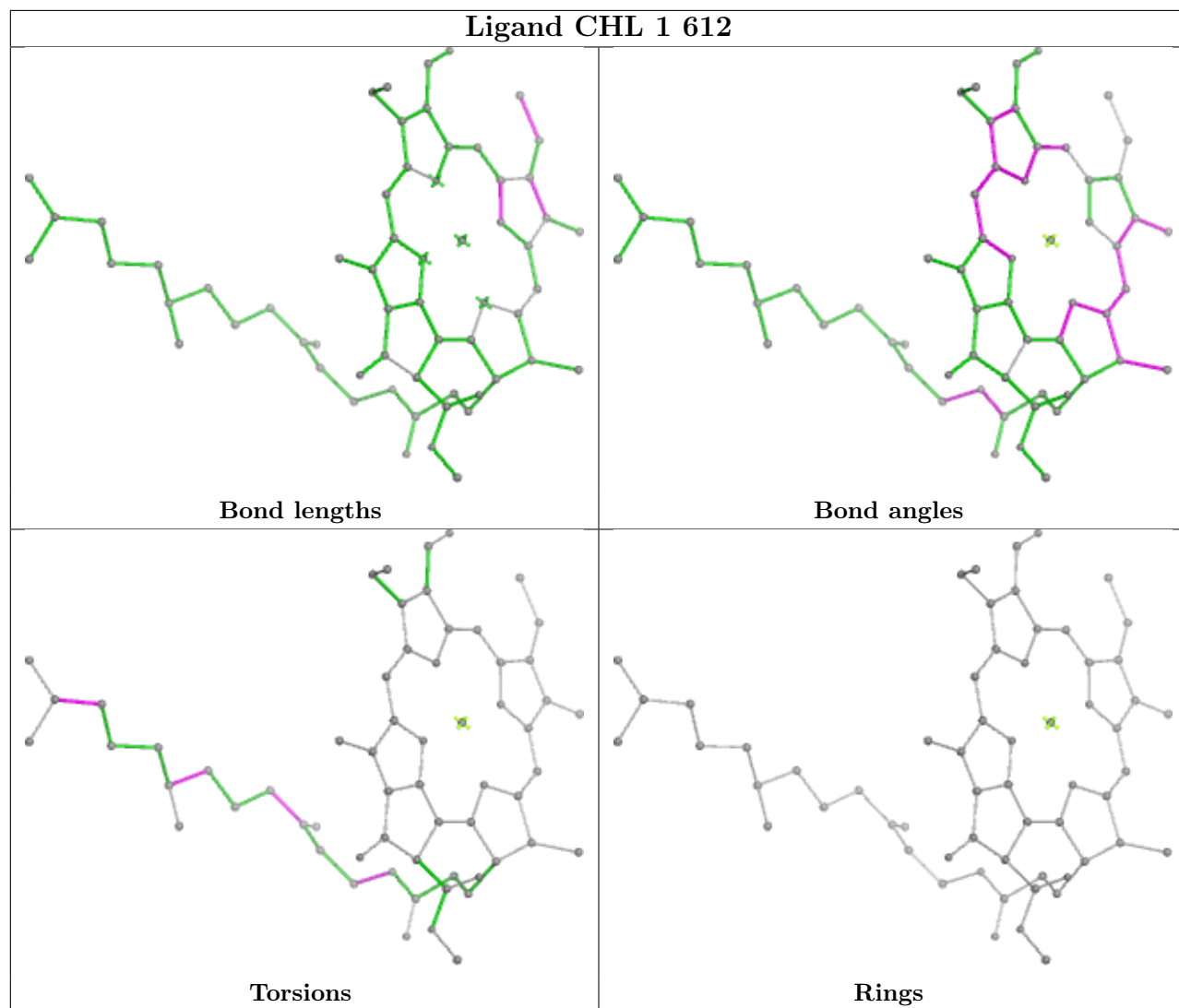
Torsions



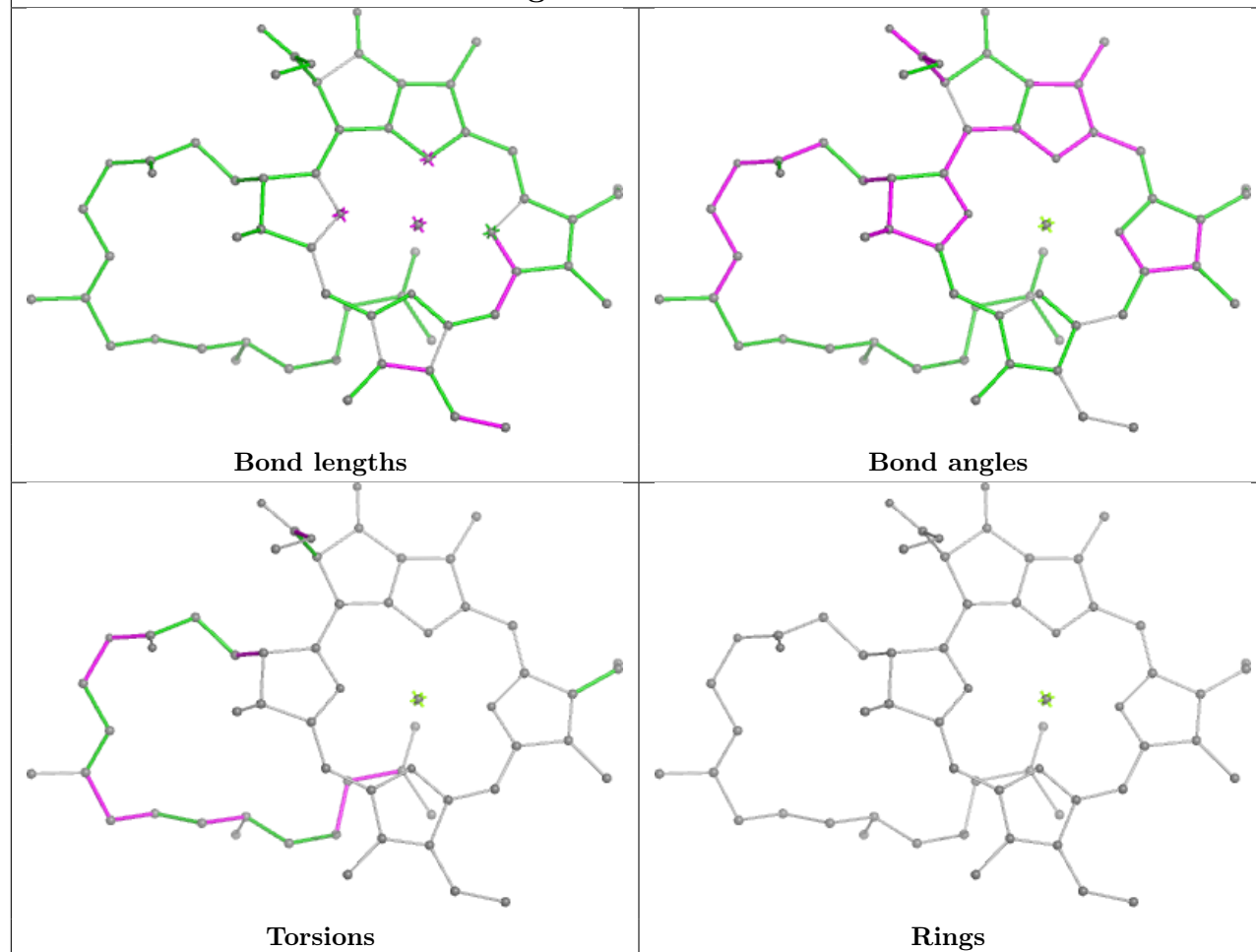
Rings



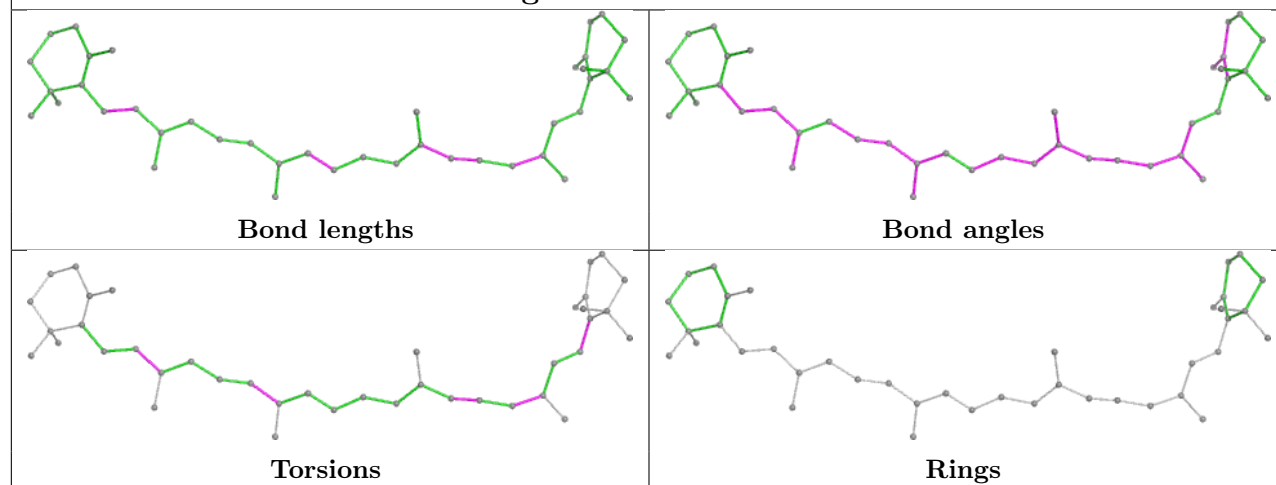
Ligand CHL 1 612

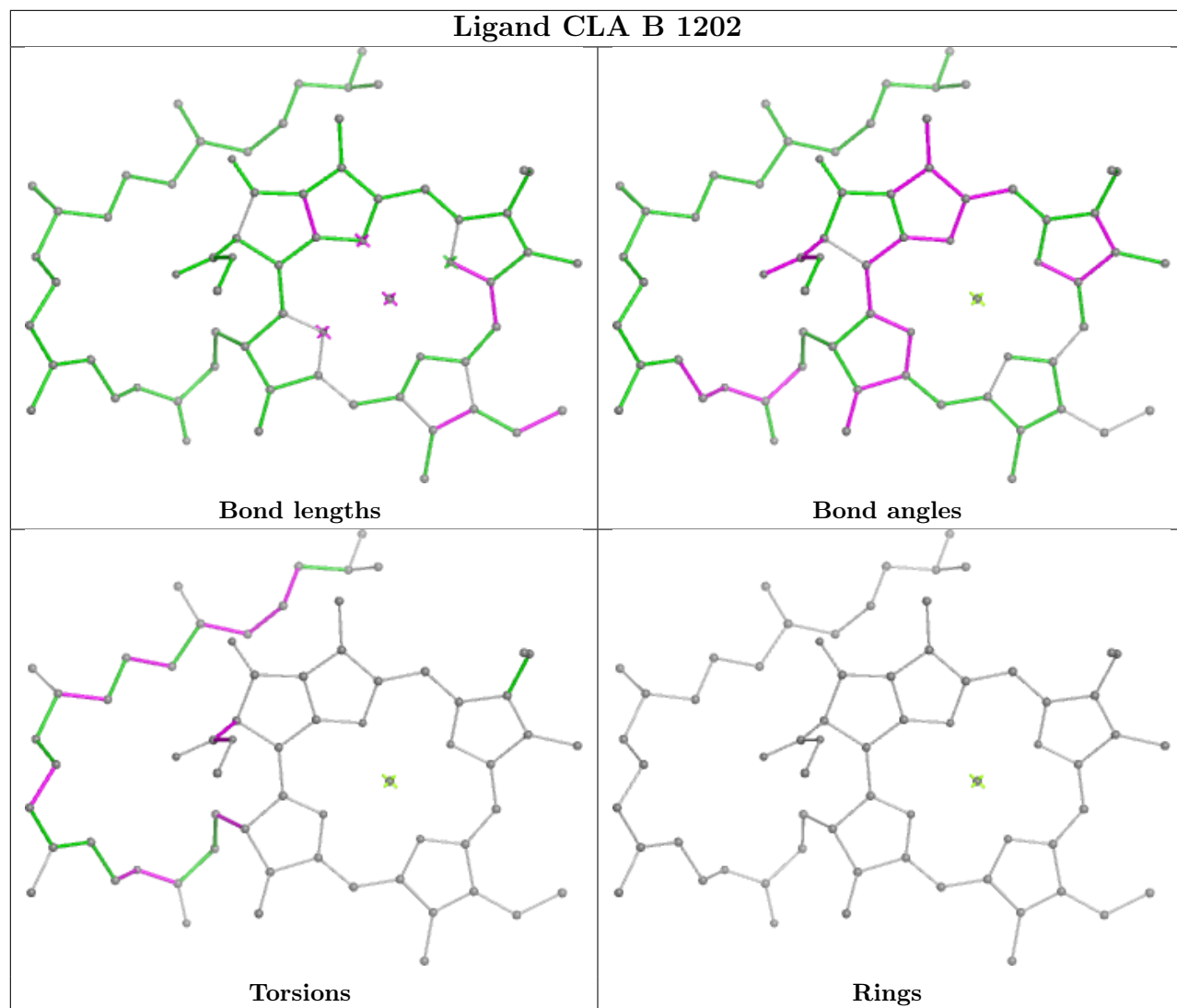


Ligand CLA 3 617

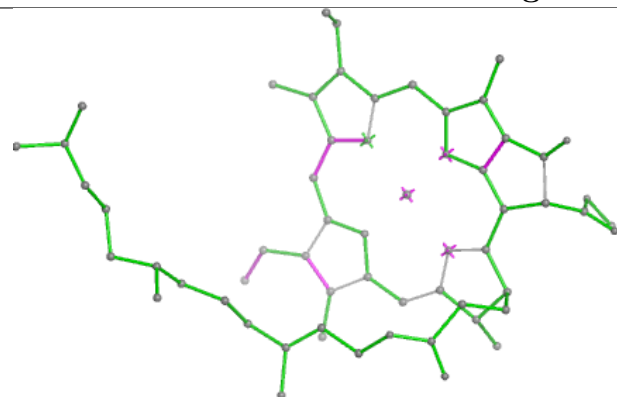


Ligand BCR B 4005

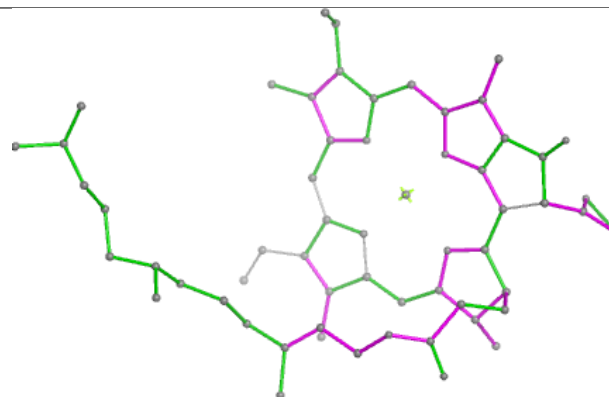




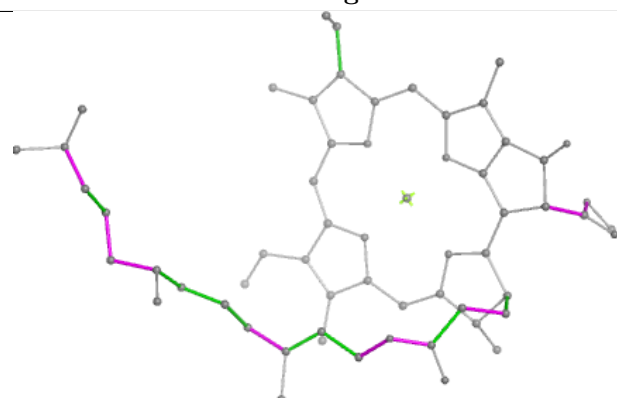
Ligand CLA 4 604



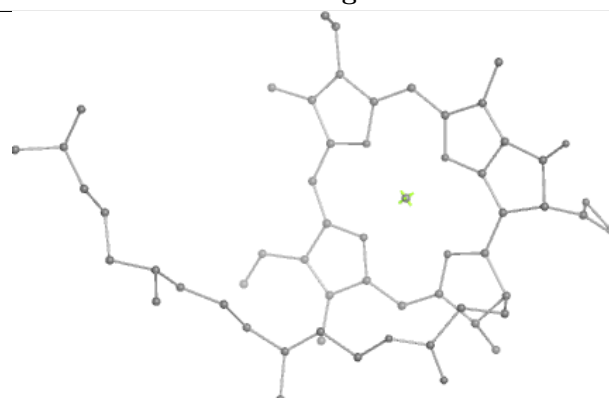
Bond lengths



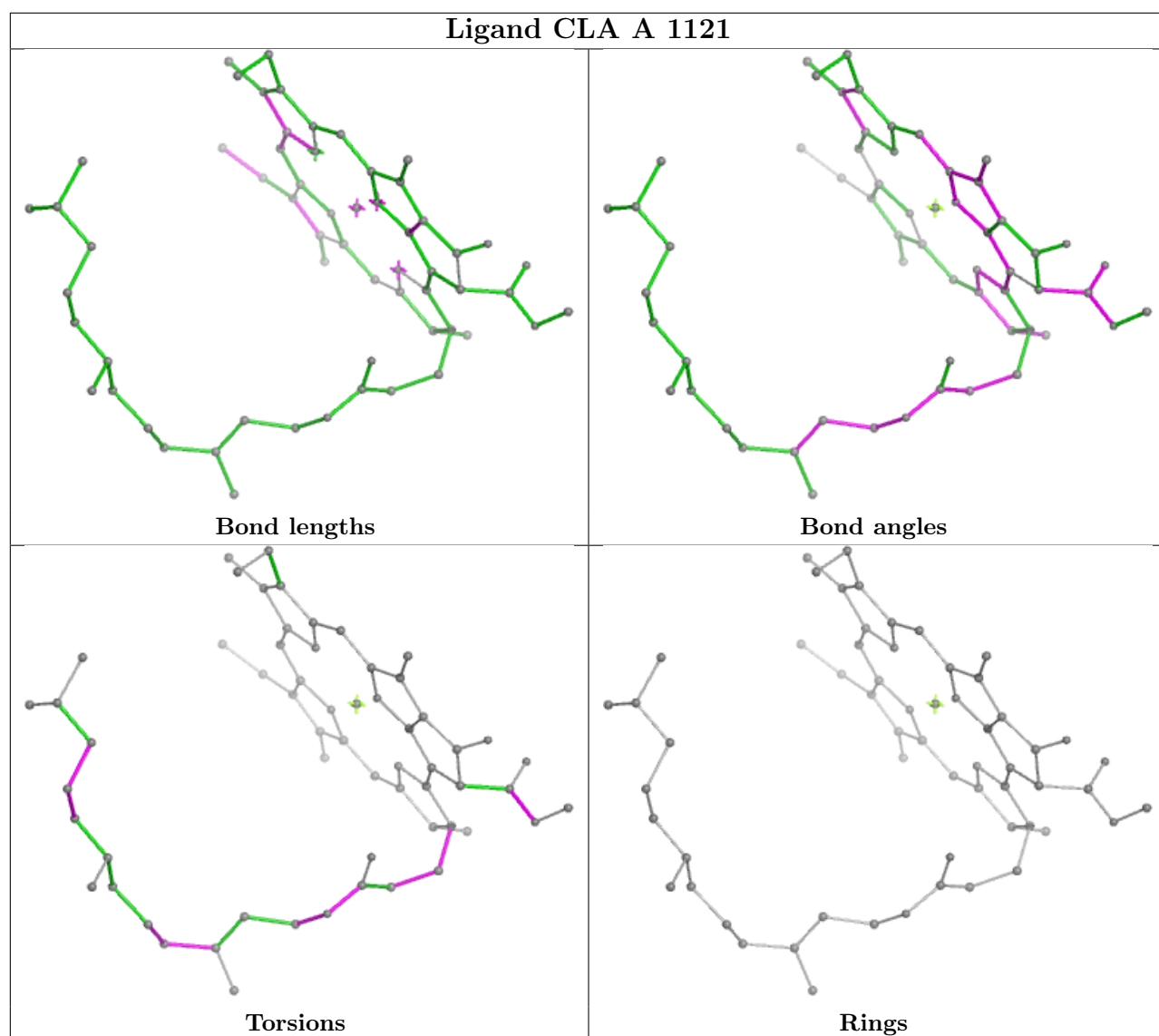
Bond angles

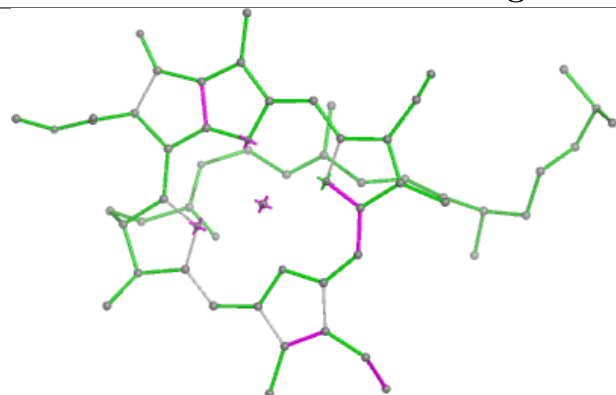
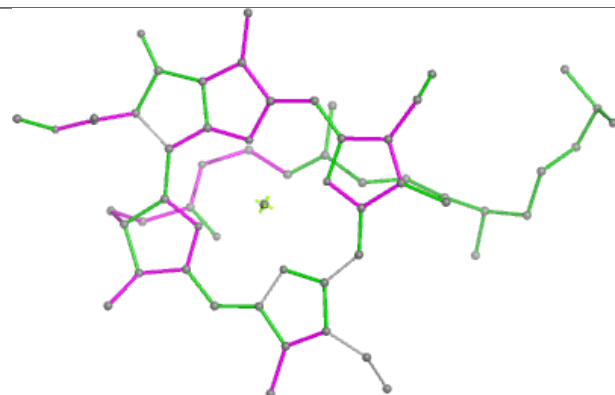
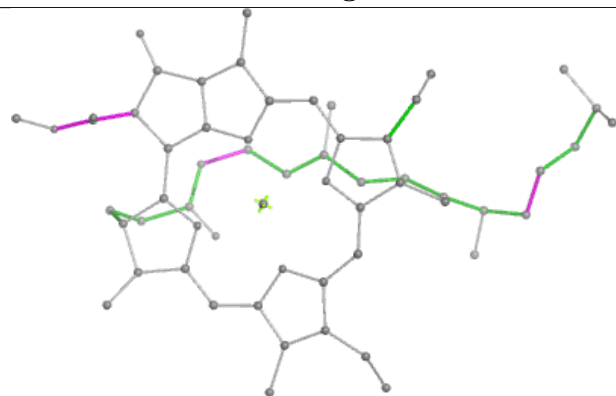
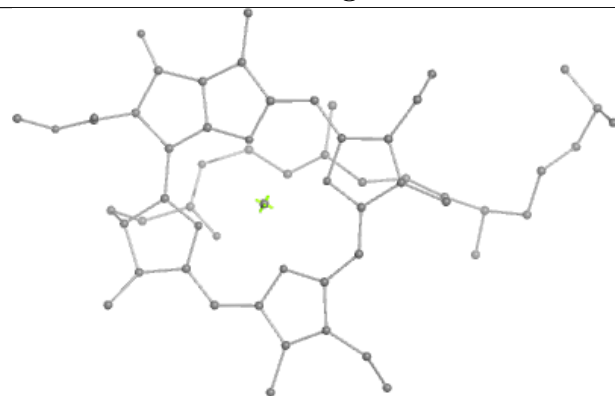
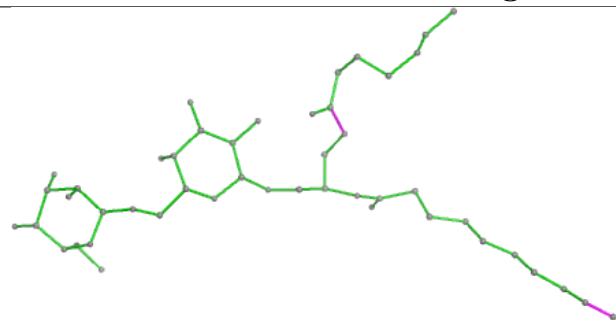
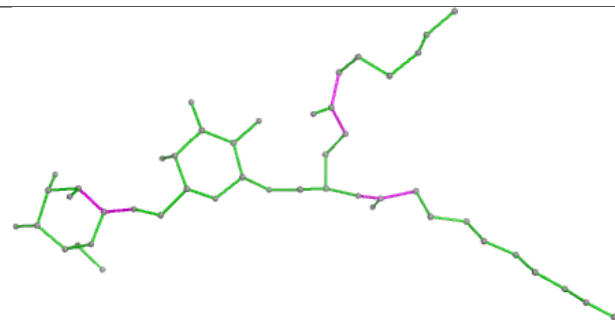
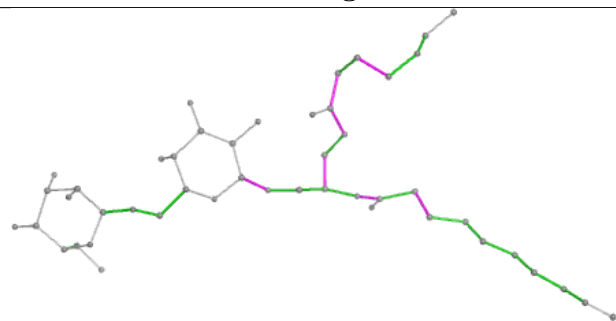
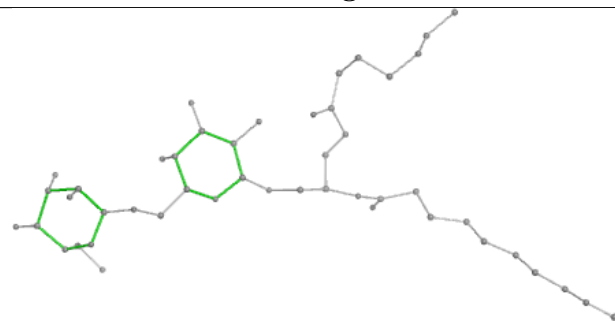


Torsions

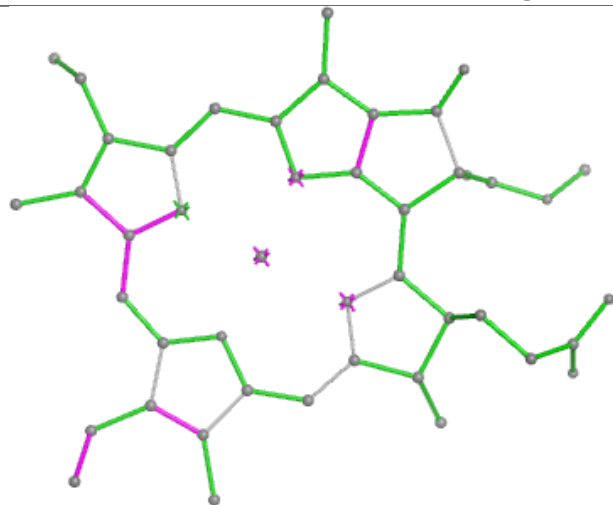


Rings

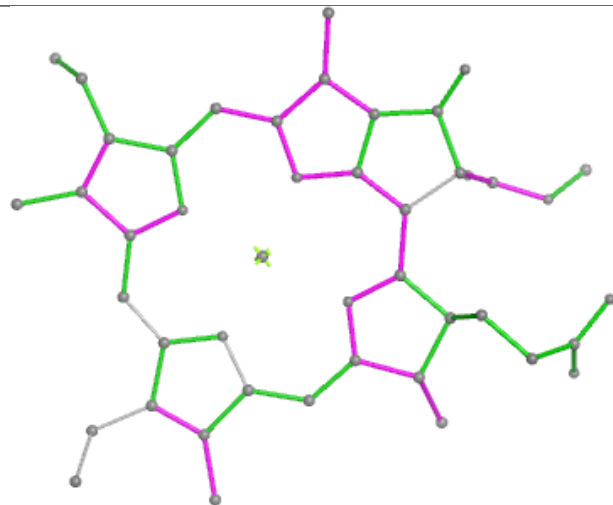


Ligand CLA B 1213**Bond lengths****Bond angles****Torsions****Rings****Ligand DGD G 5003****Bond lengths****Bond angles****Torsions****Rings**

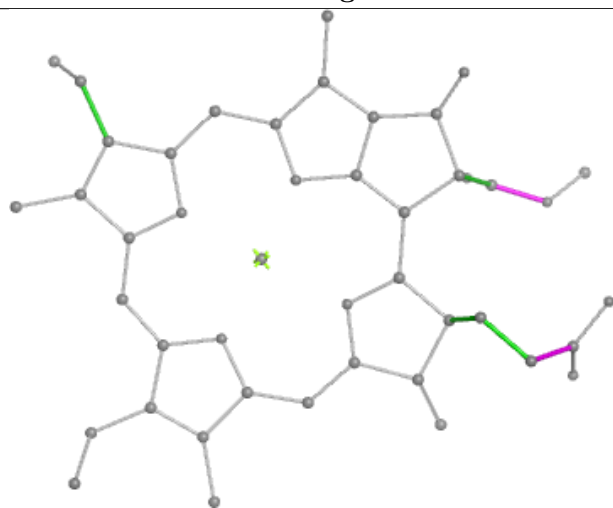
Ligand CLA 1 613



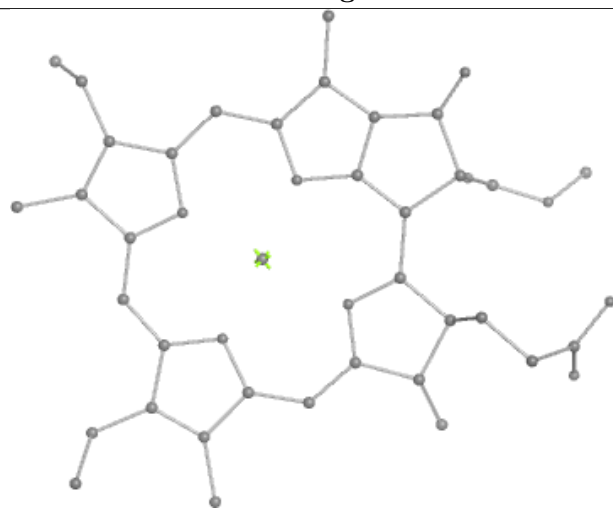
Bond lengths



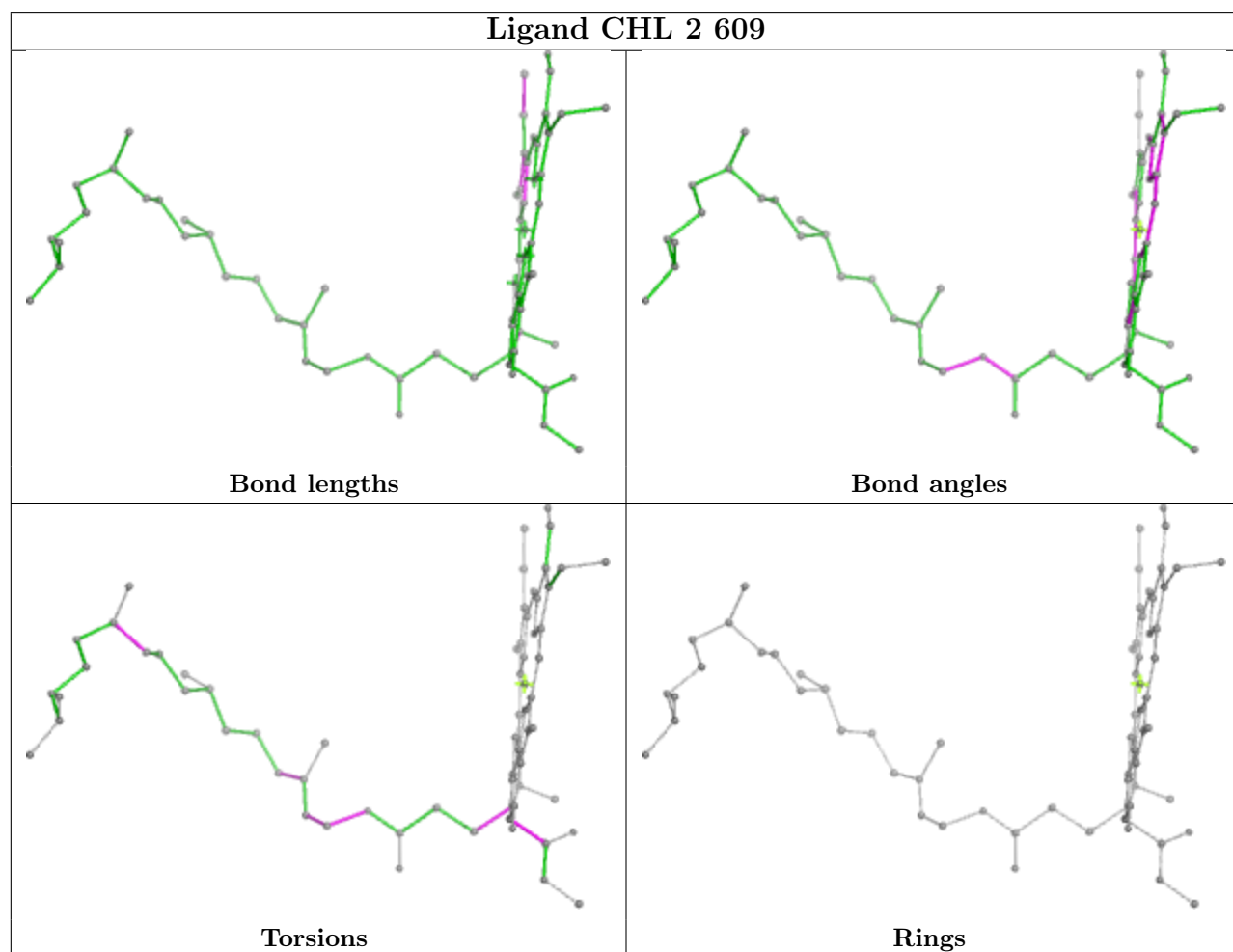
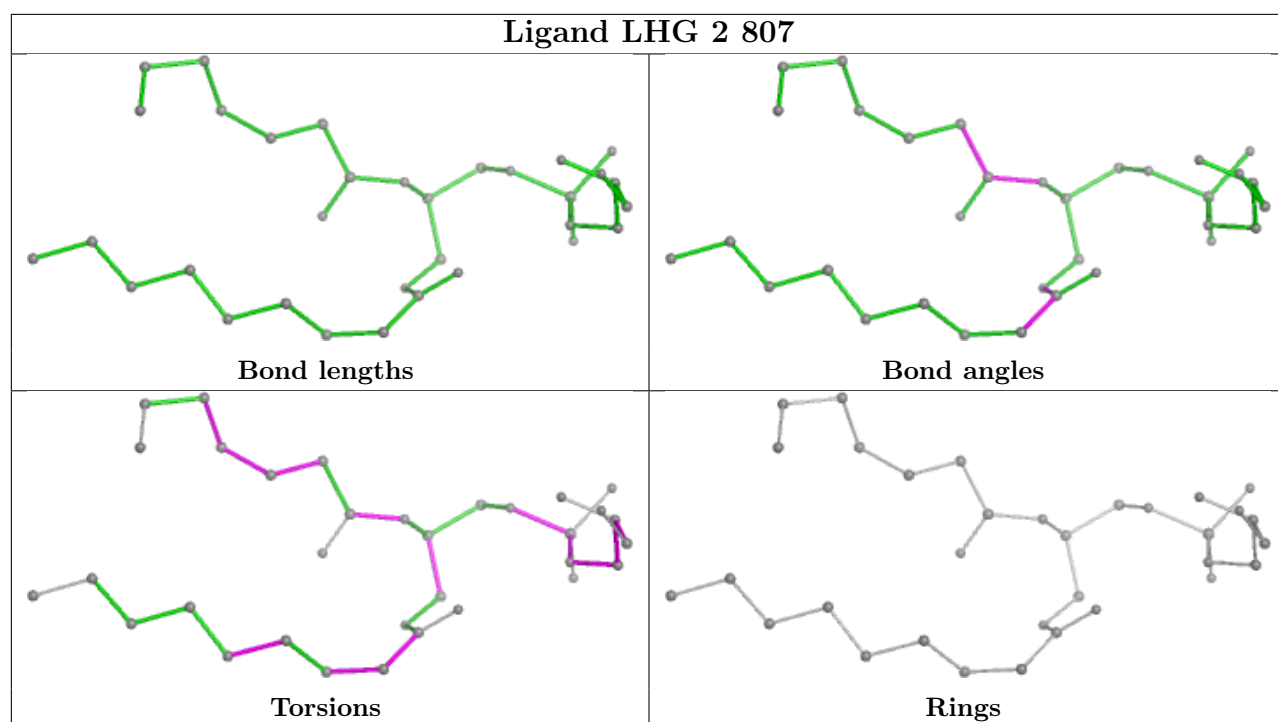
Bond angles

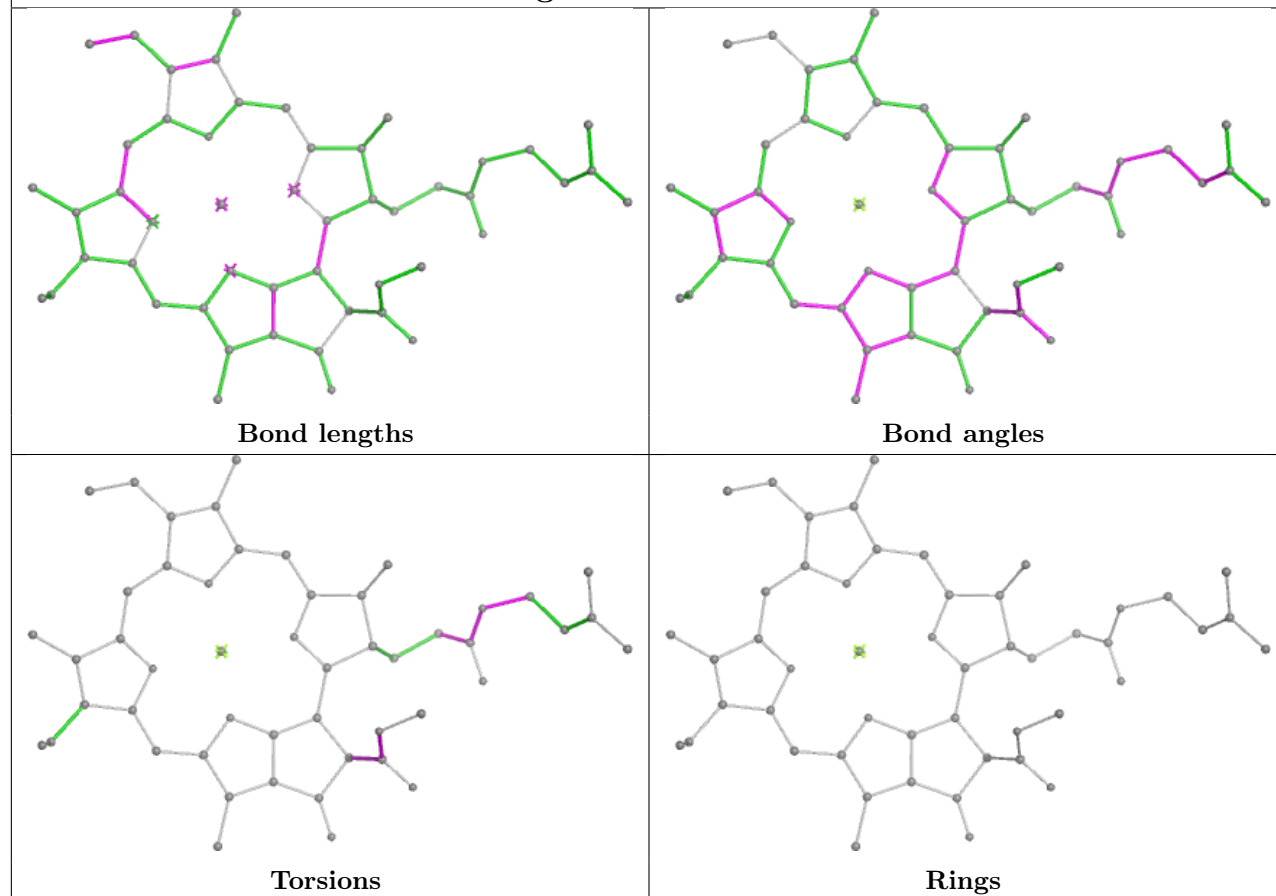
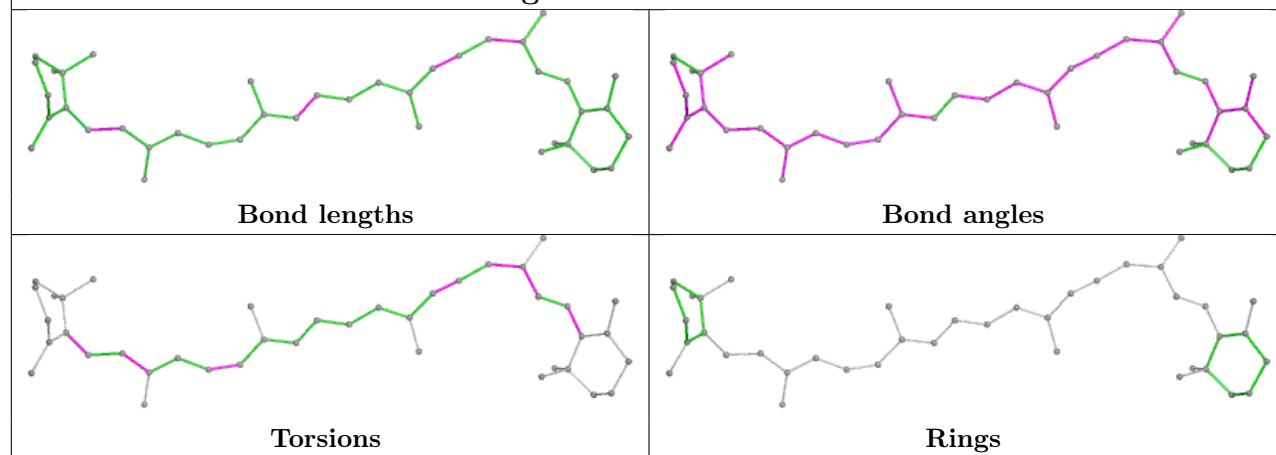


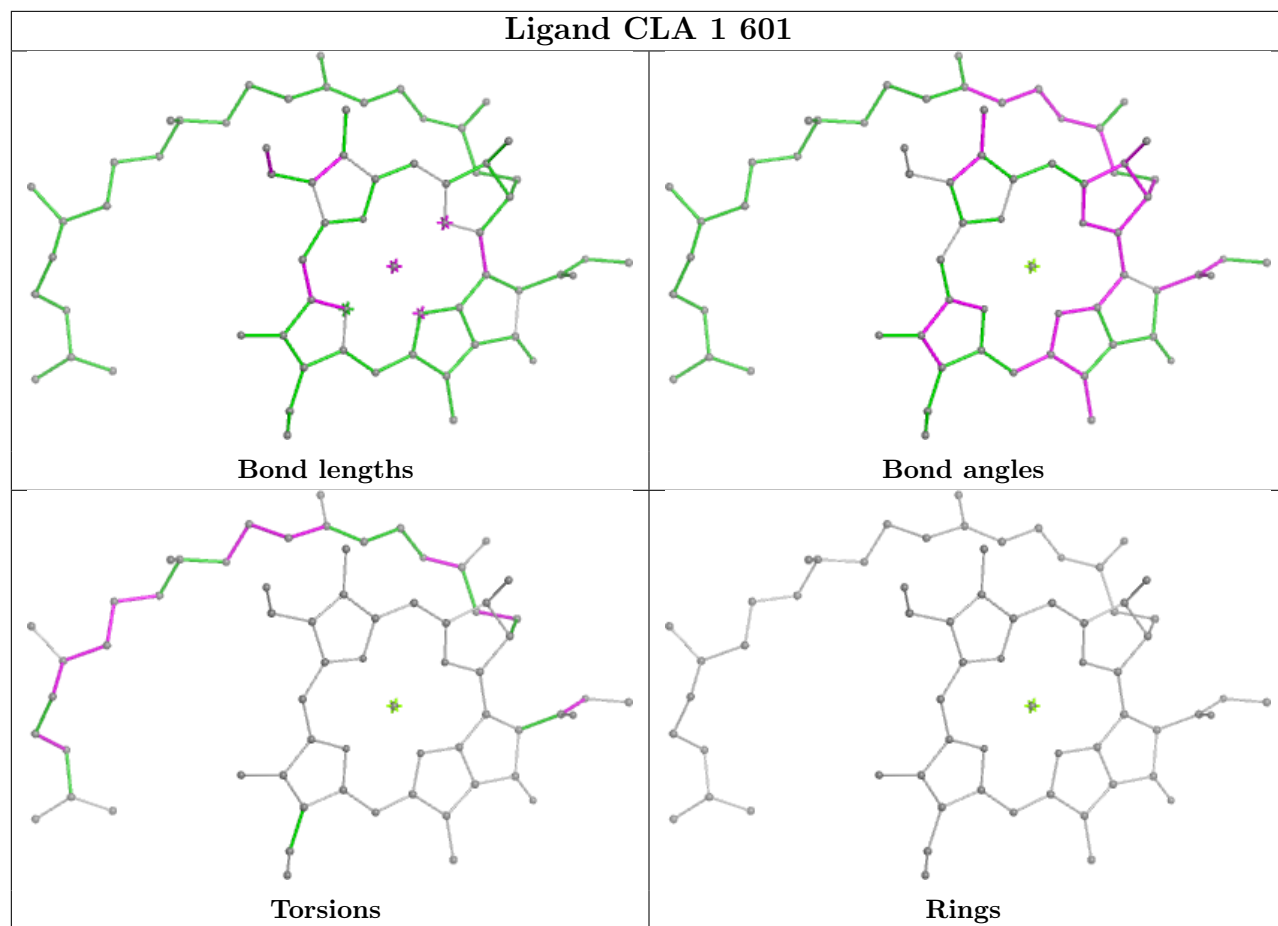
Torsions



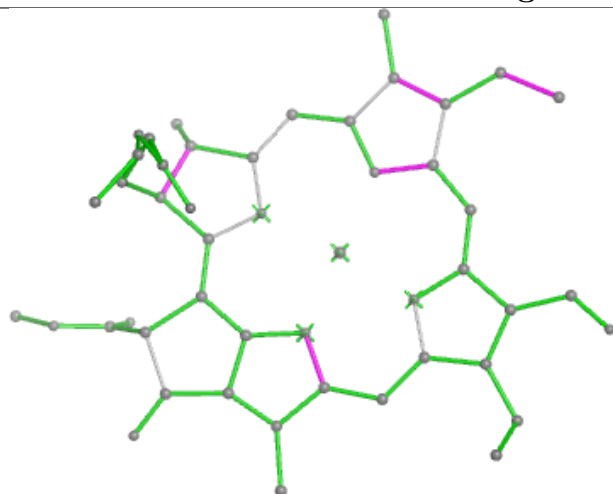
Rings



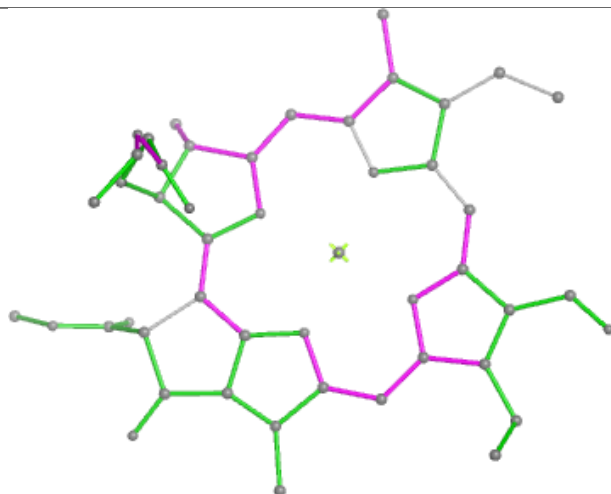
Ligand CLA 4 602**Ligand BCR B 4006**



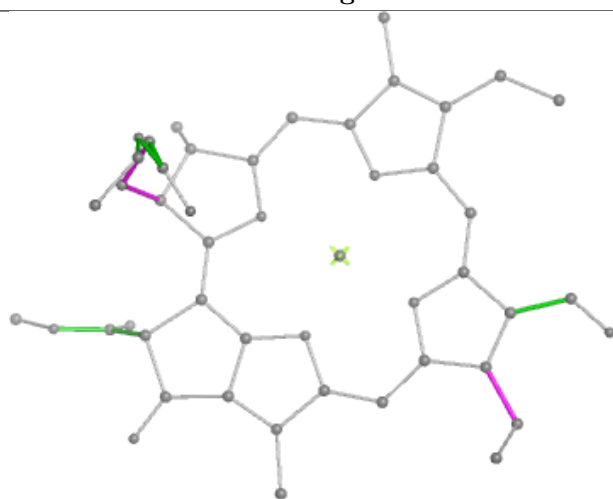
Ligand CHL 2 611



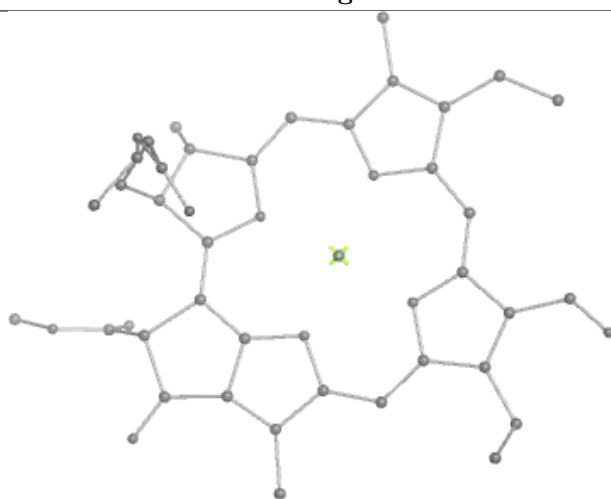
Bond lengths



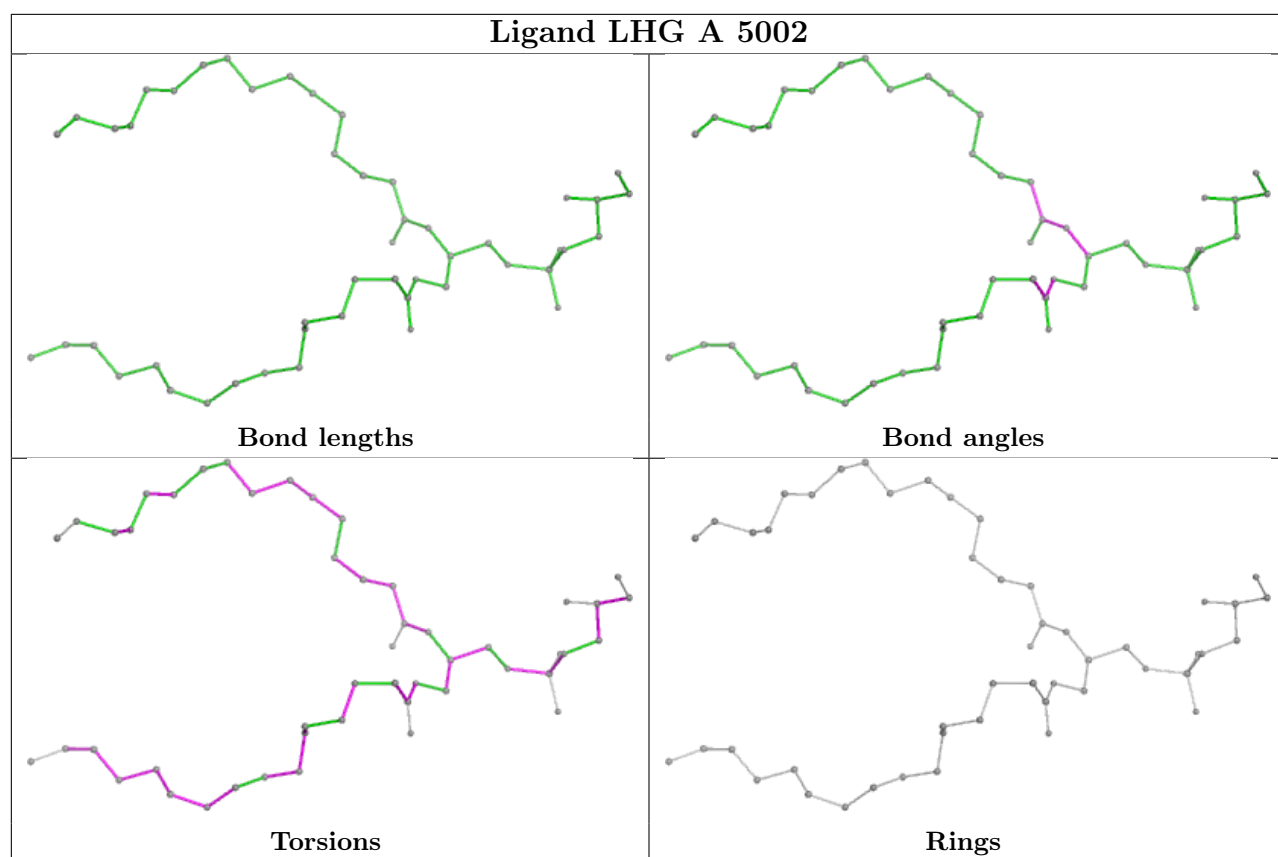
Bond angles

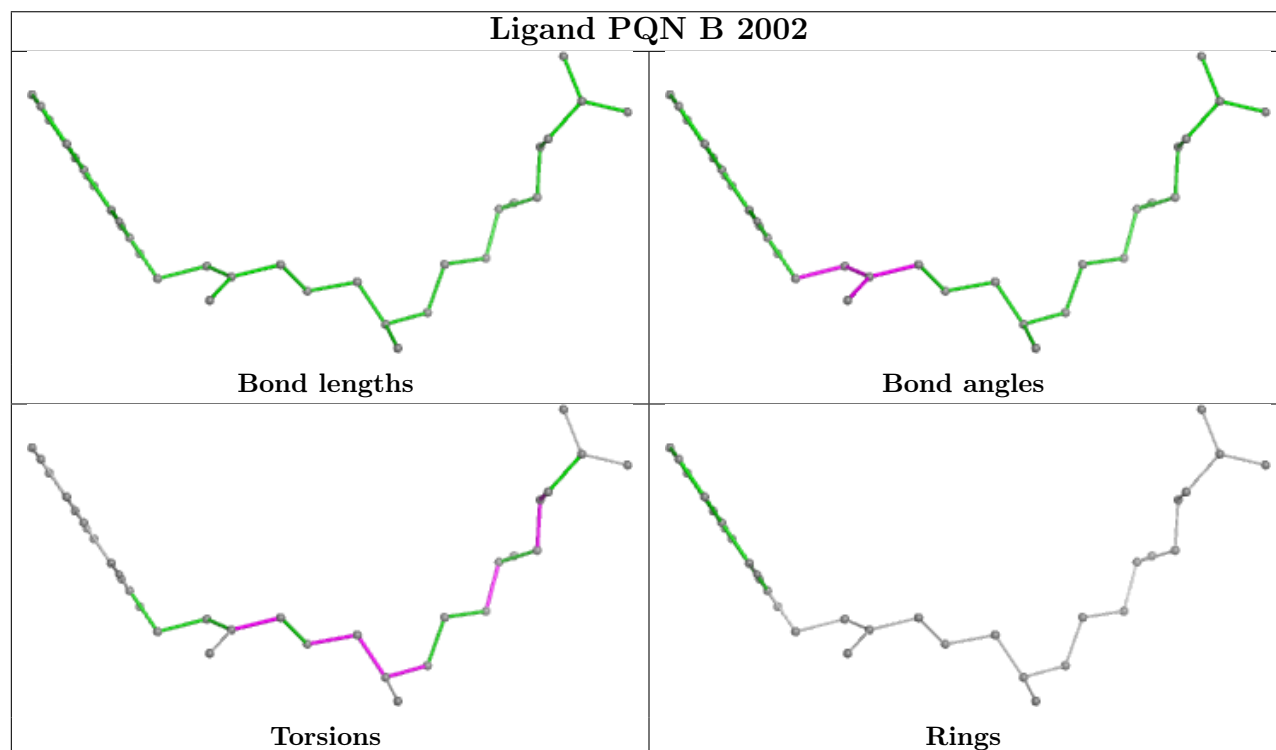
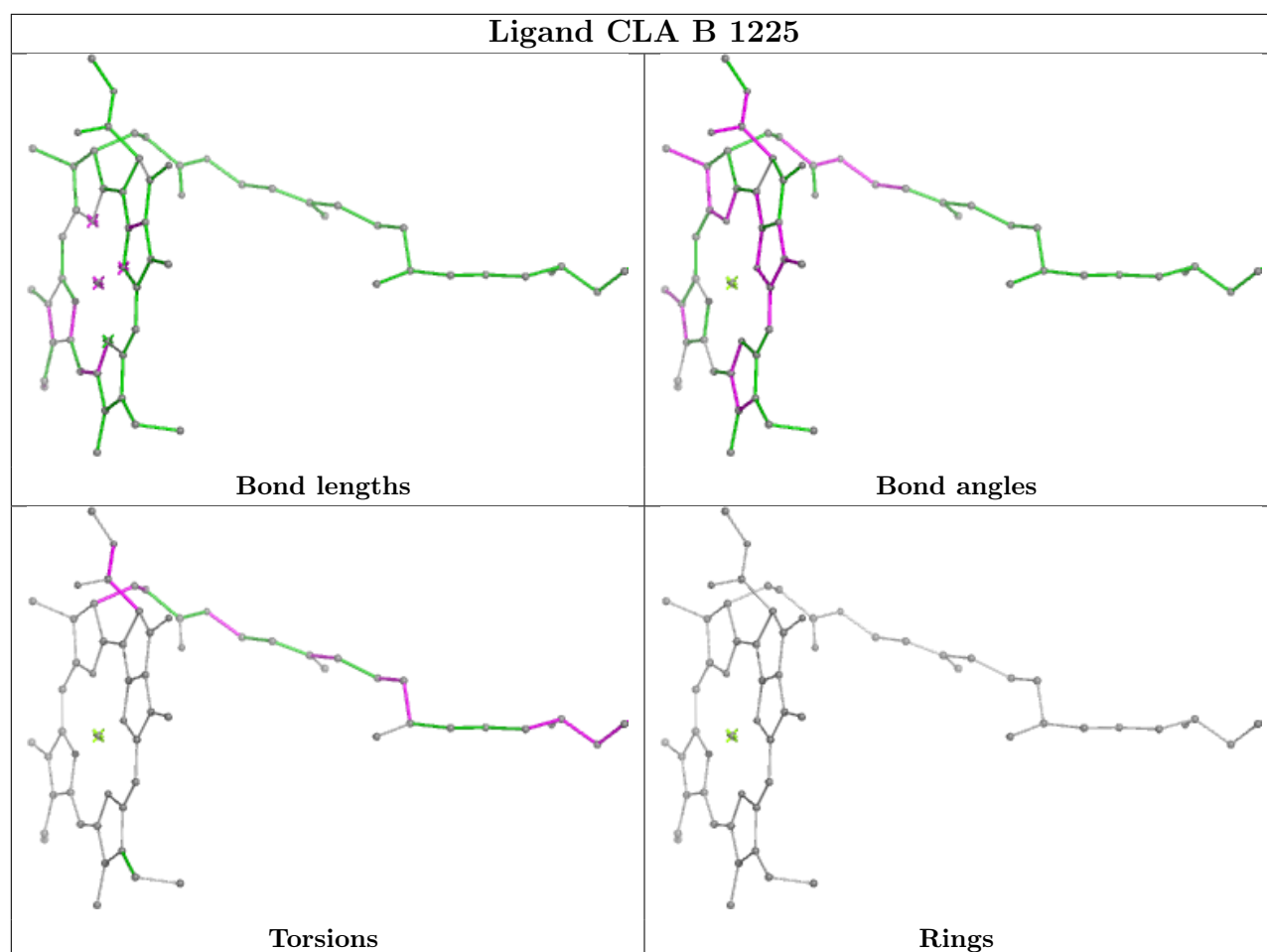


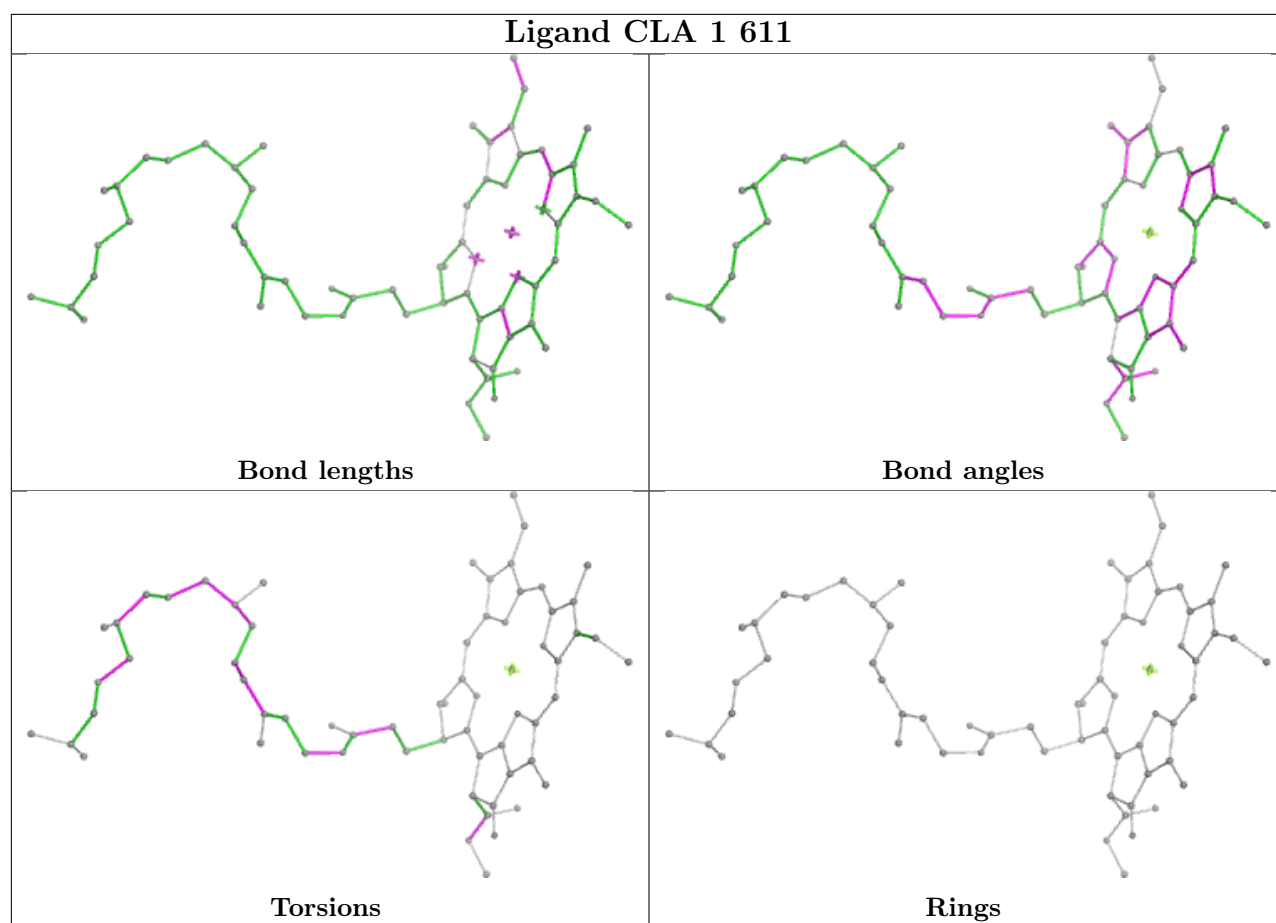
Torsions



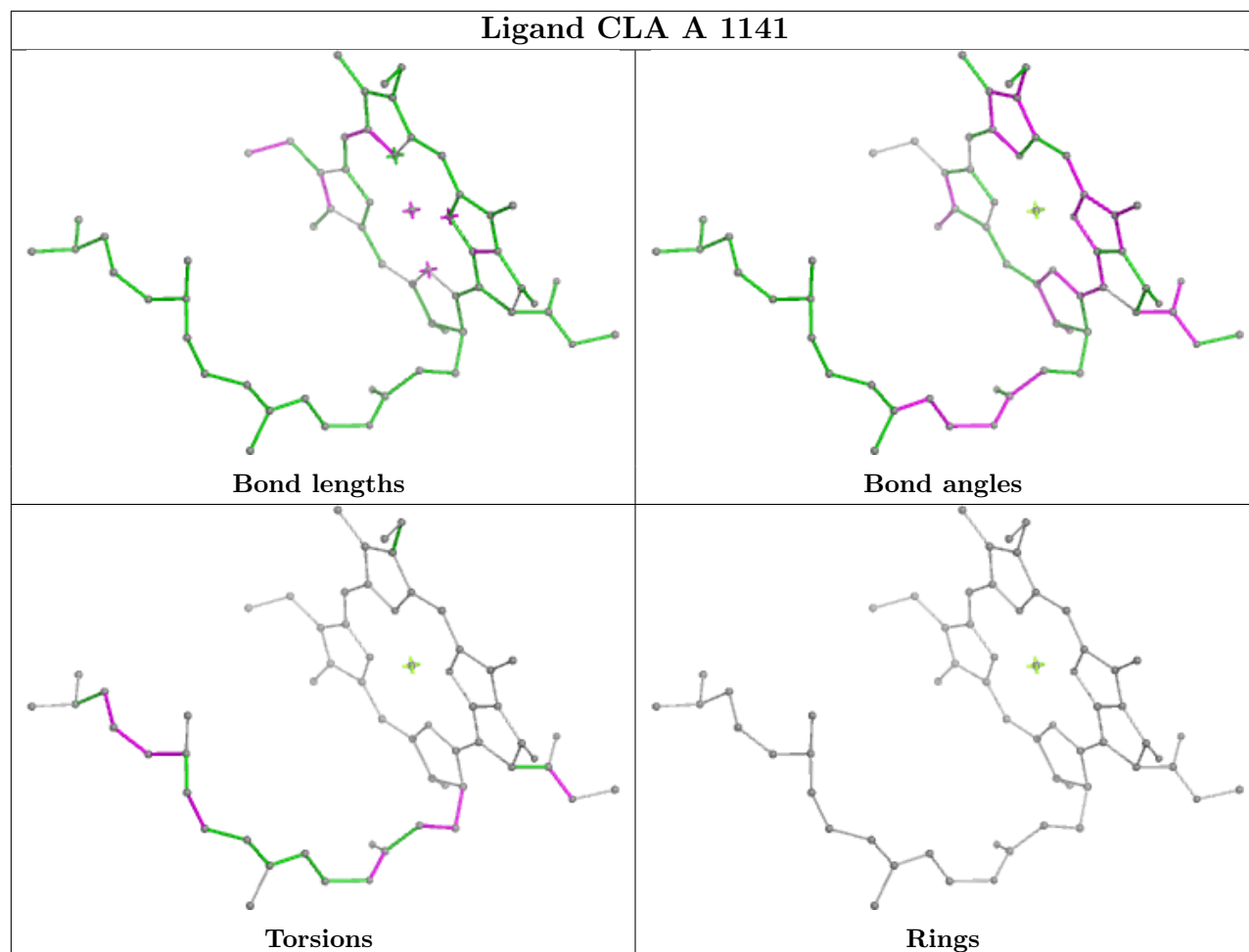
Rings



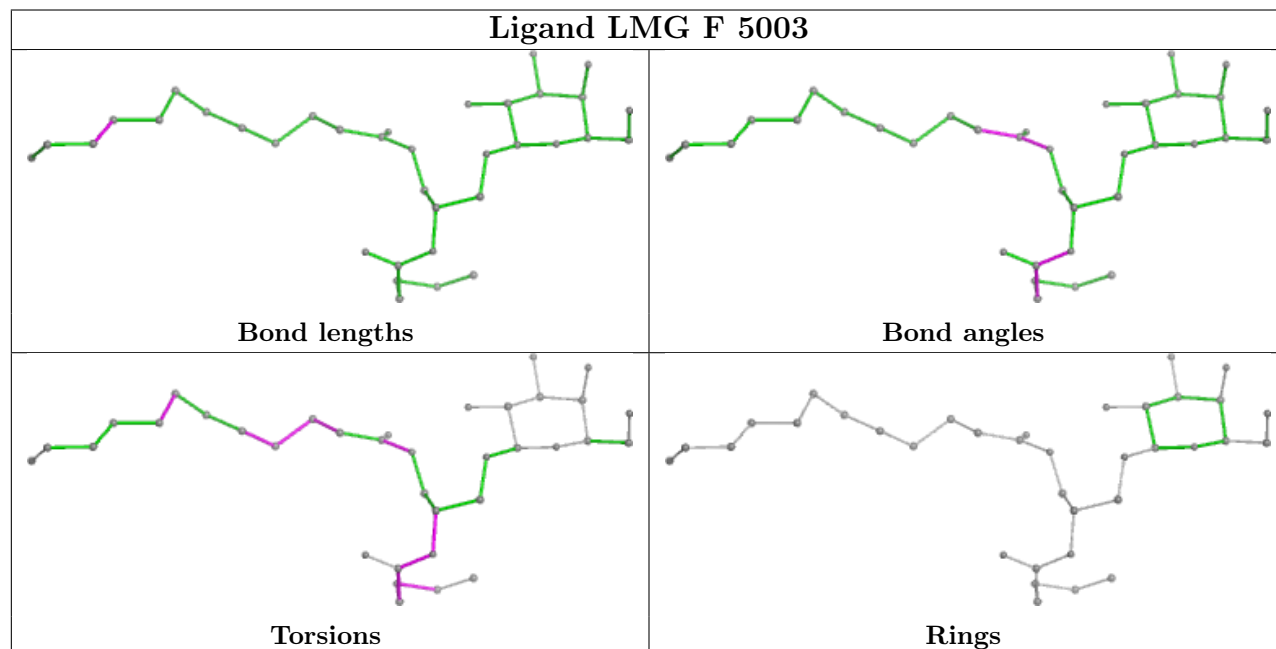


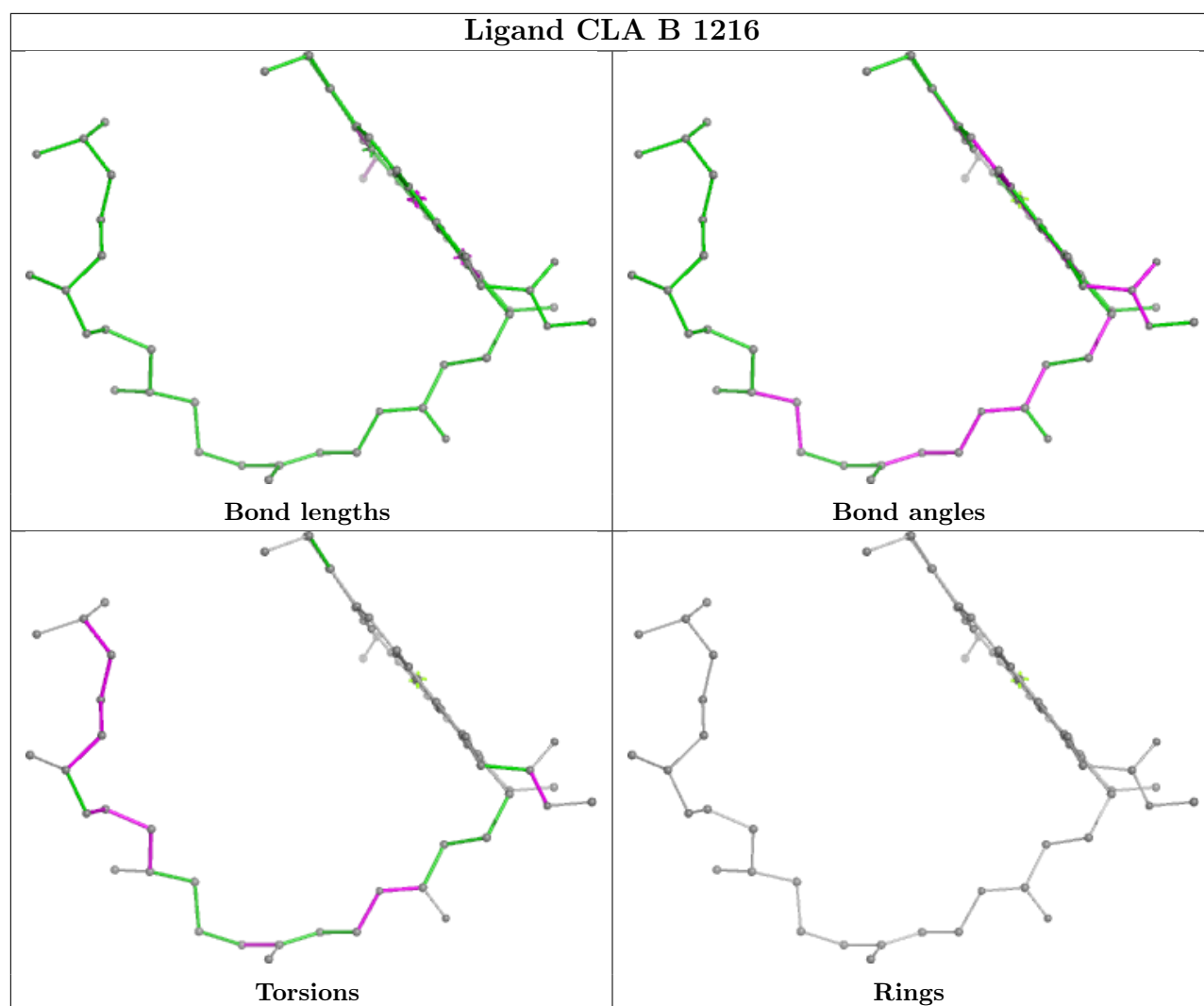


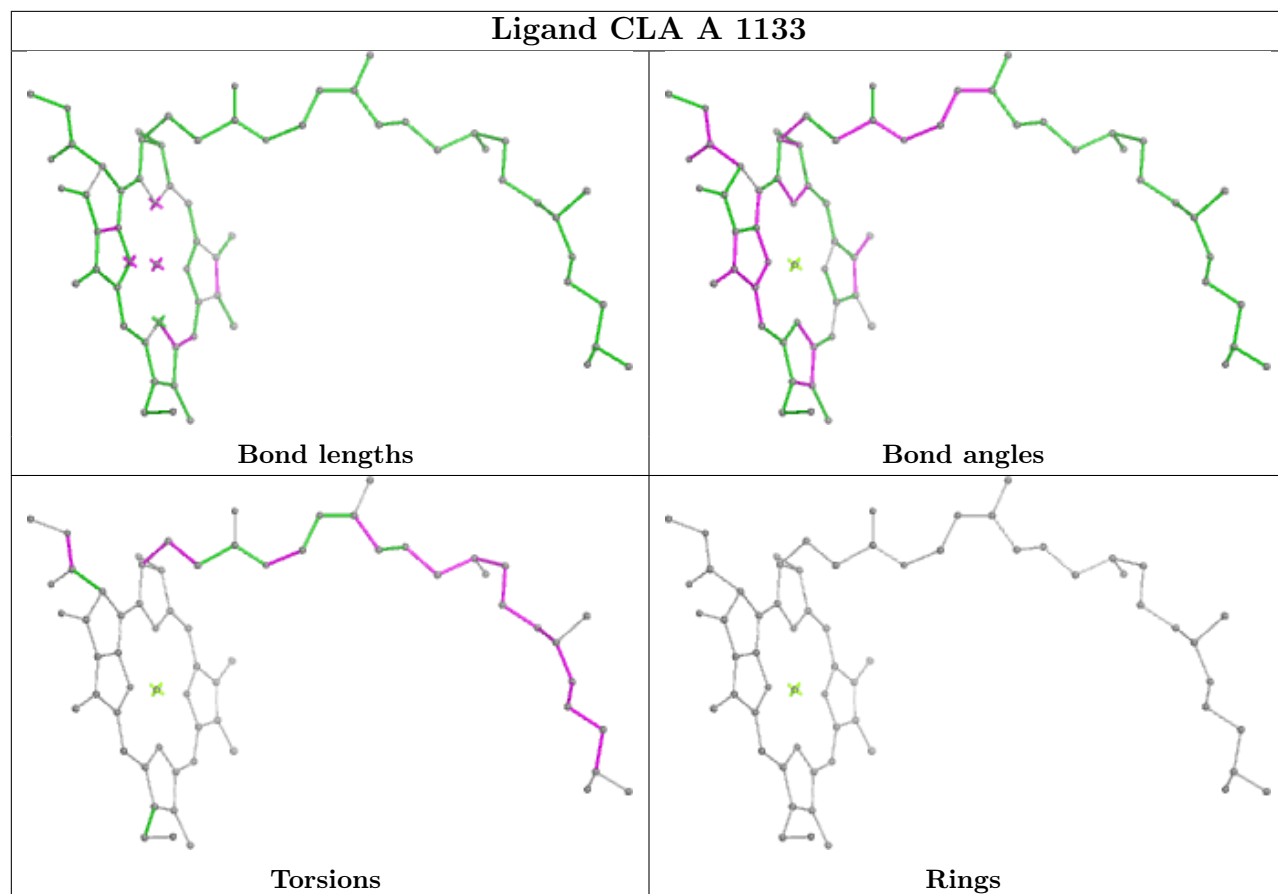
Ligand CLA A 1141

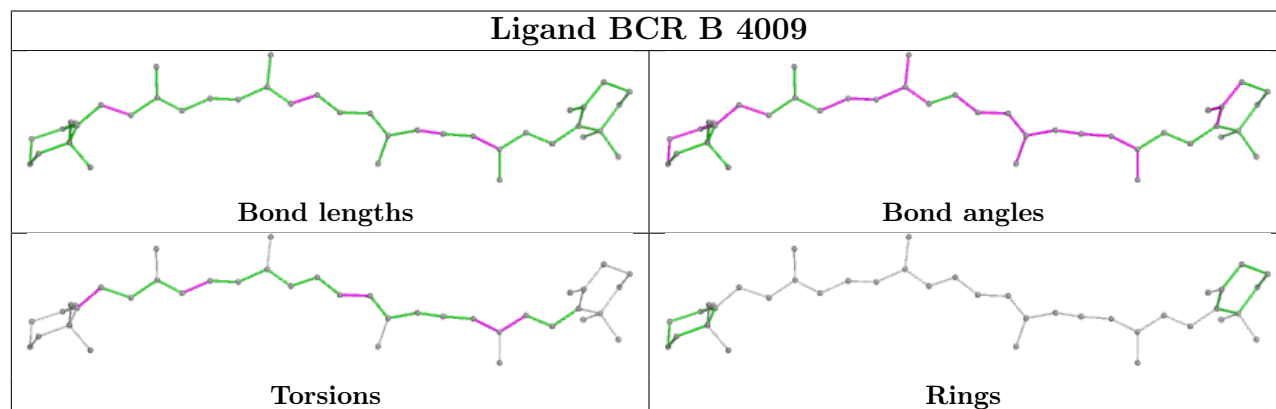
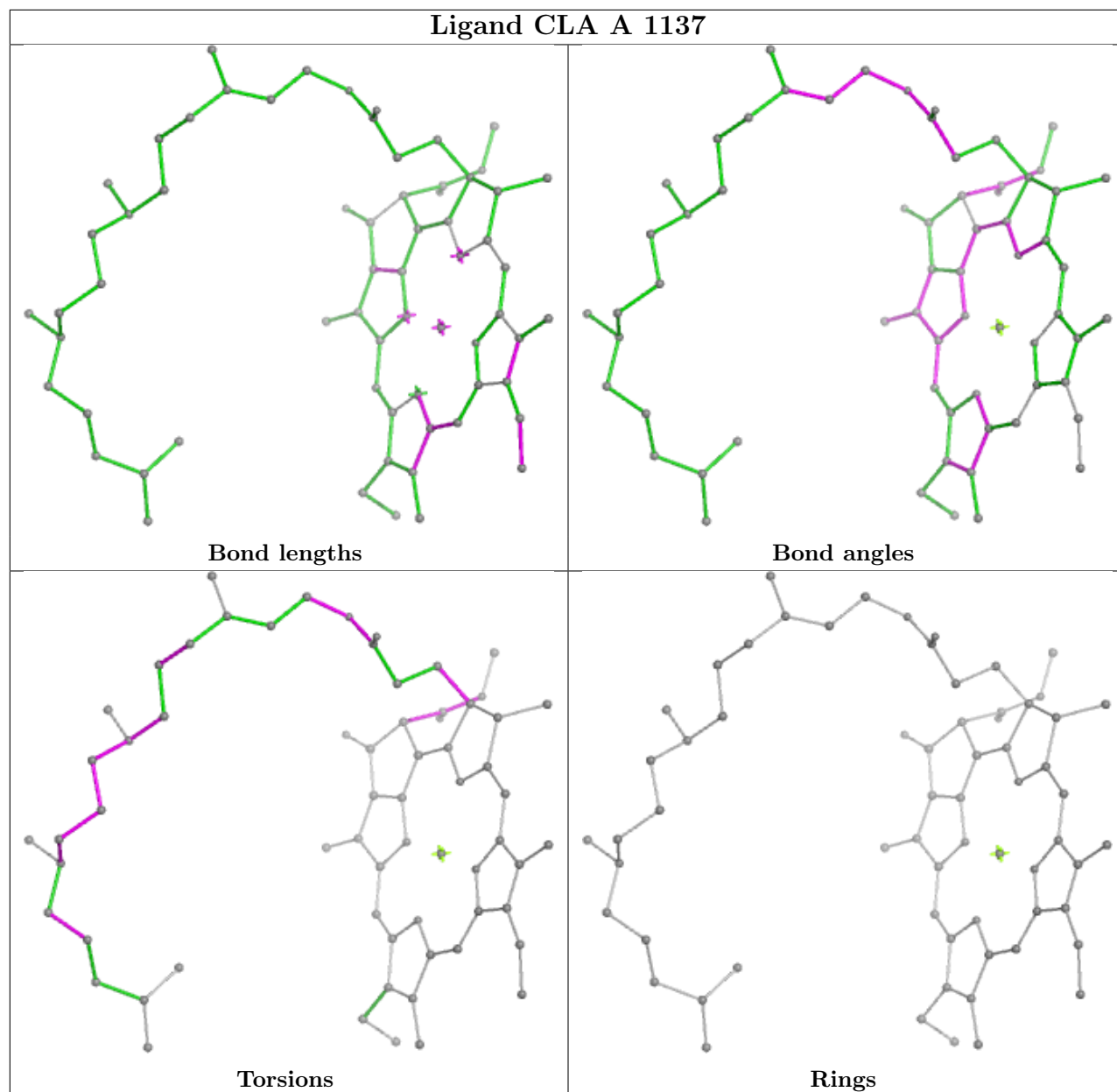


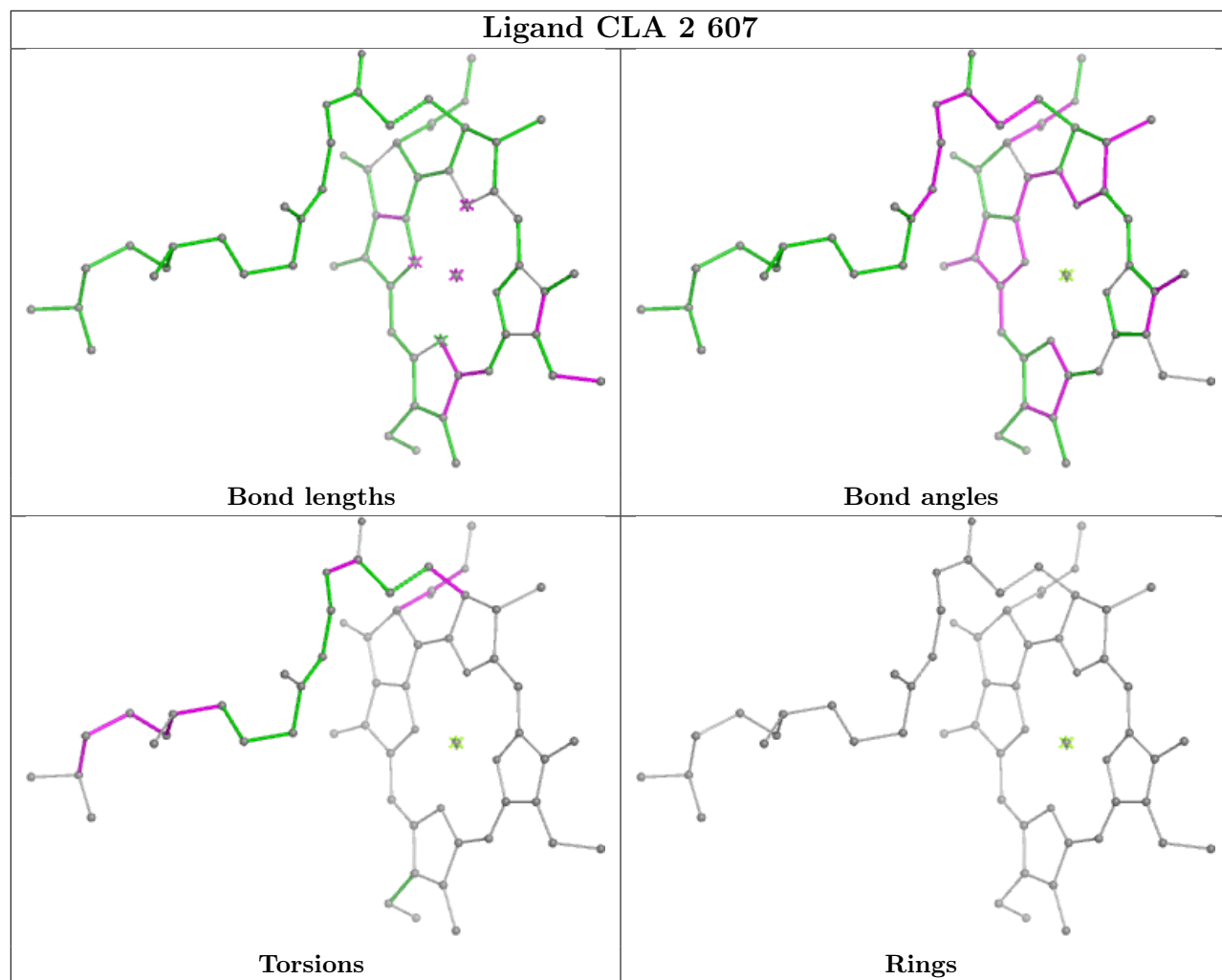
Ligand LMG F 5003

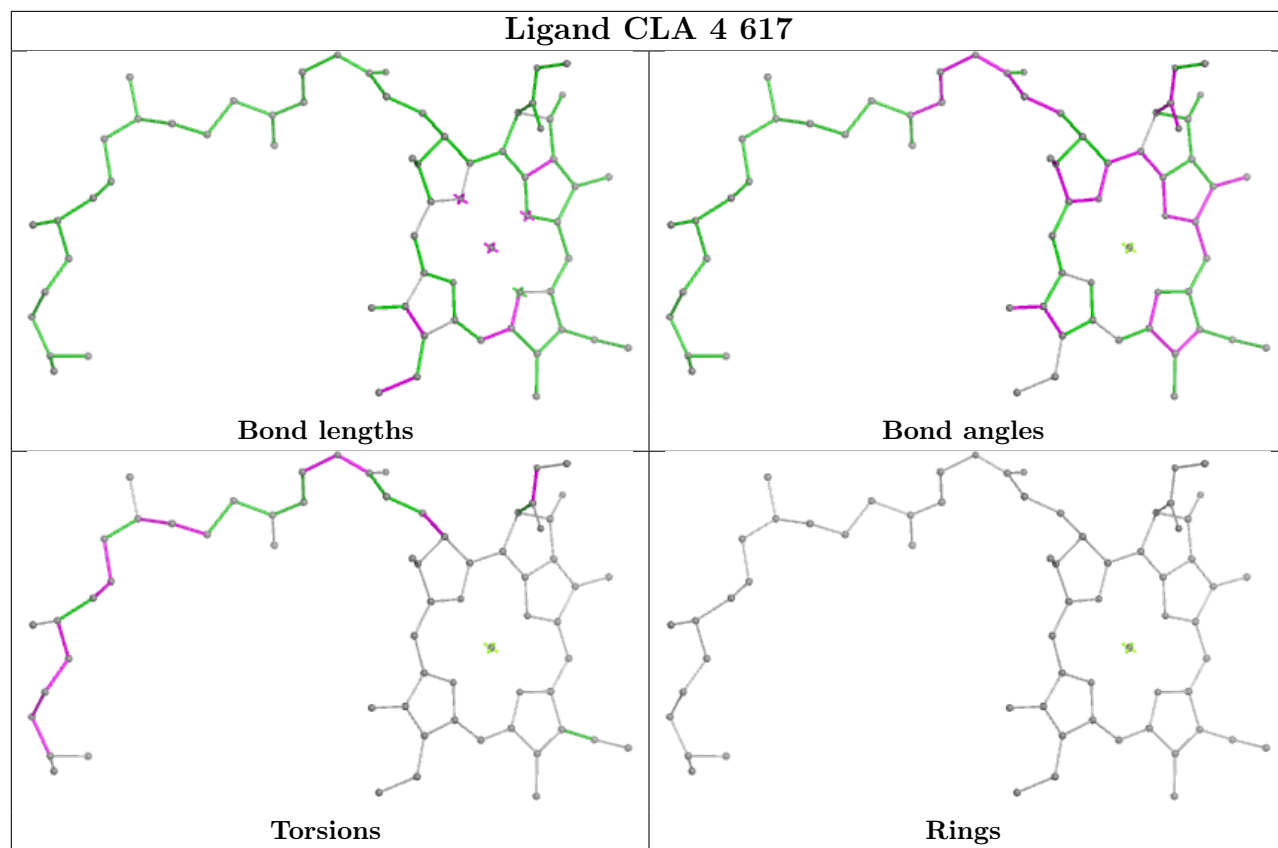




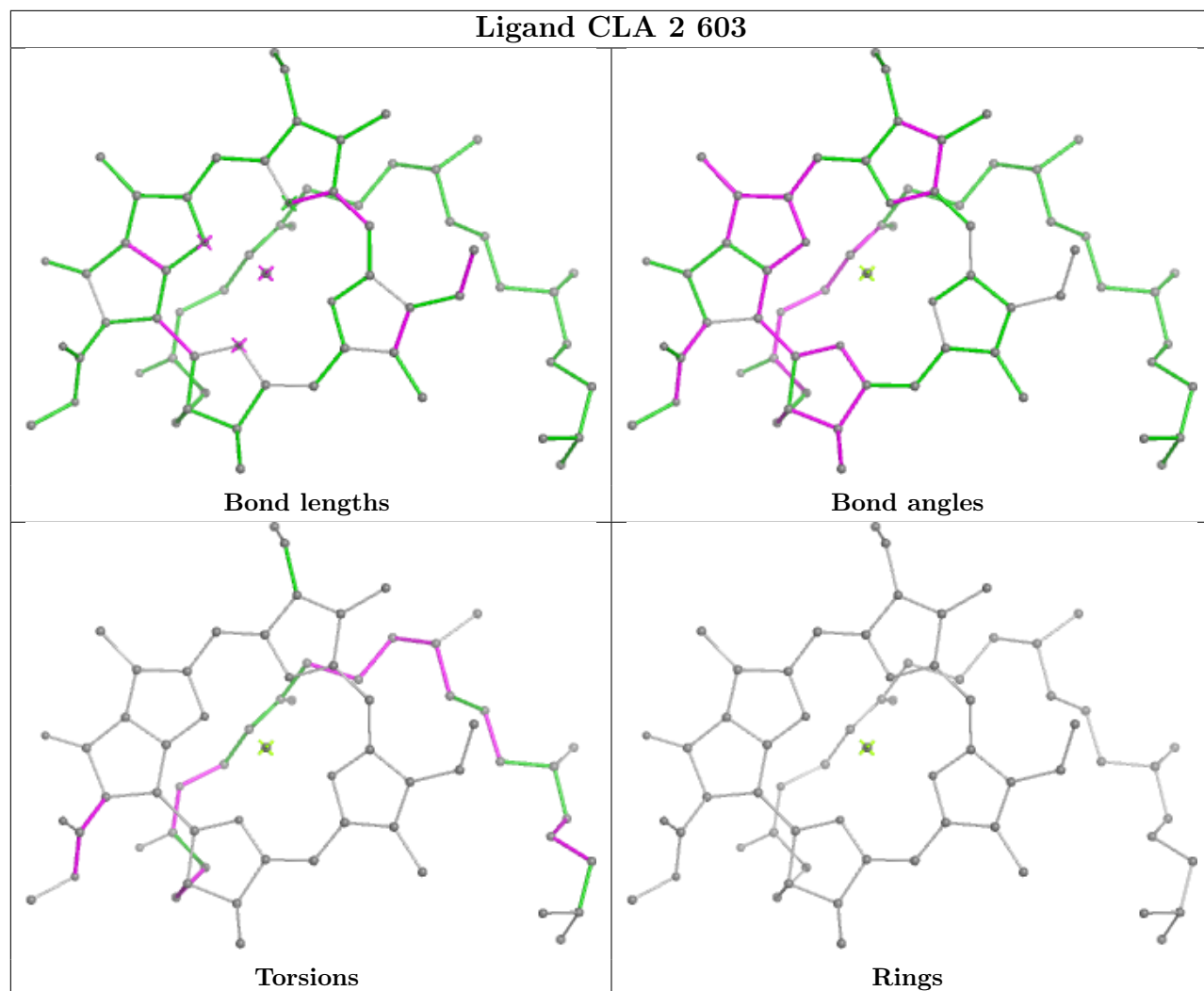


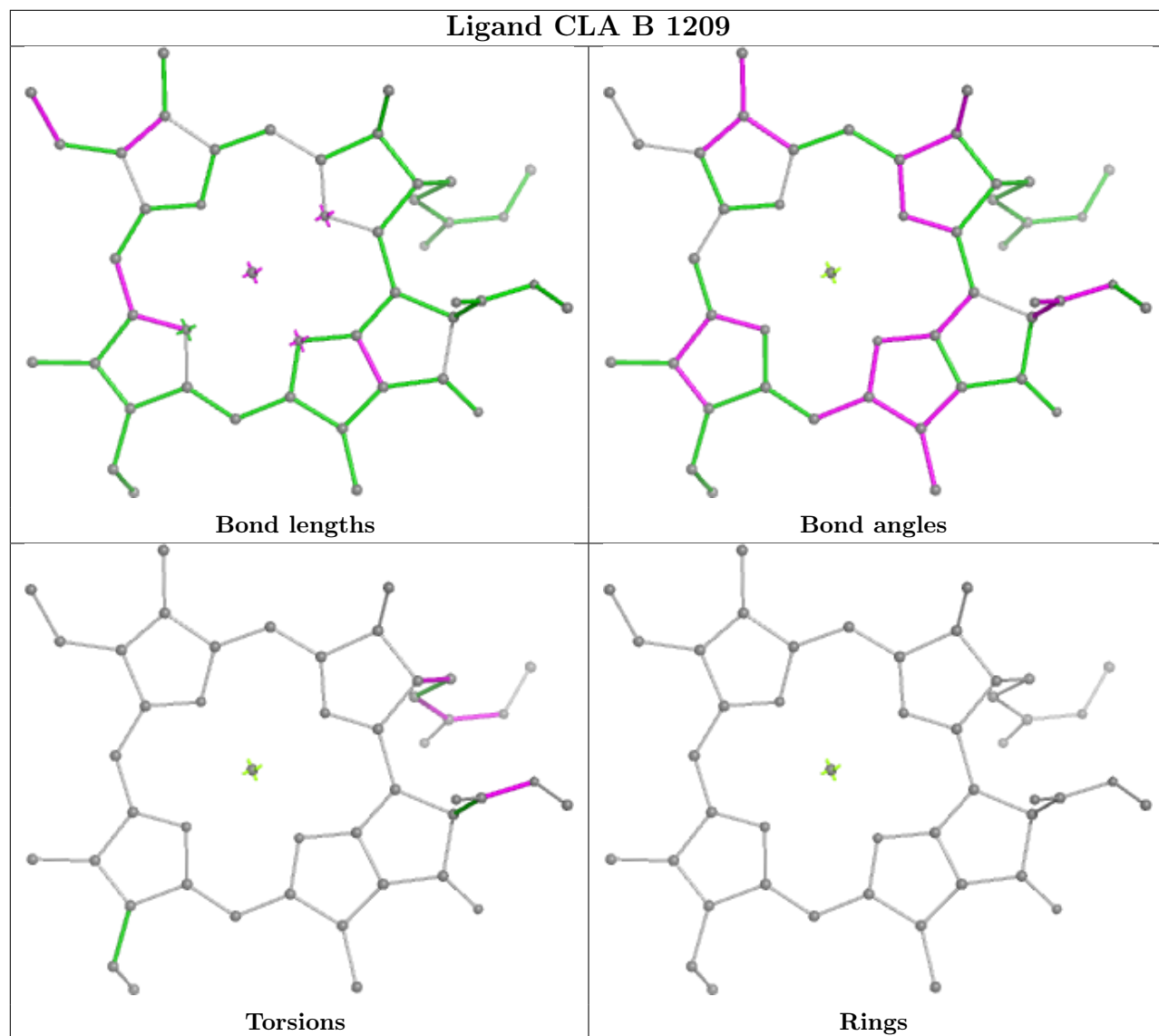




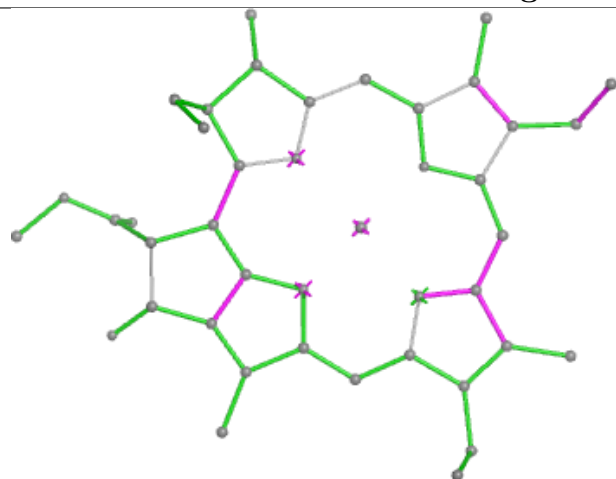


Ligand CLA 2 603

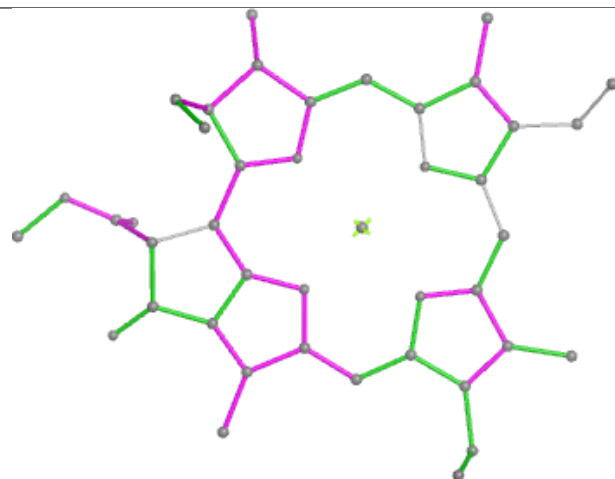




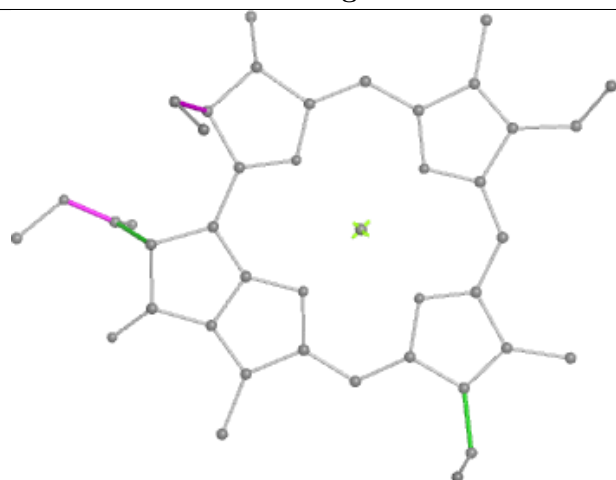
Ligand CLA 3 614



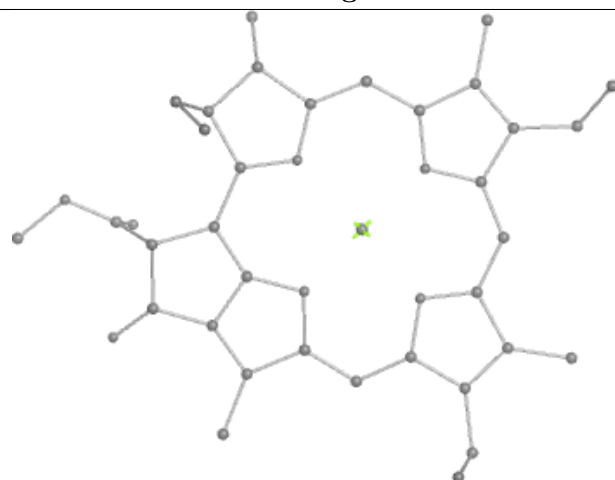
Bond lengths



Bond angles

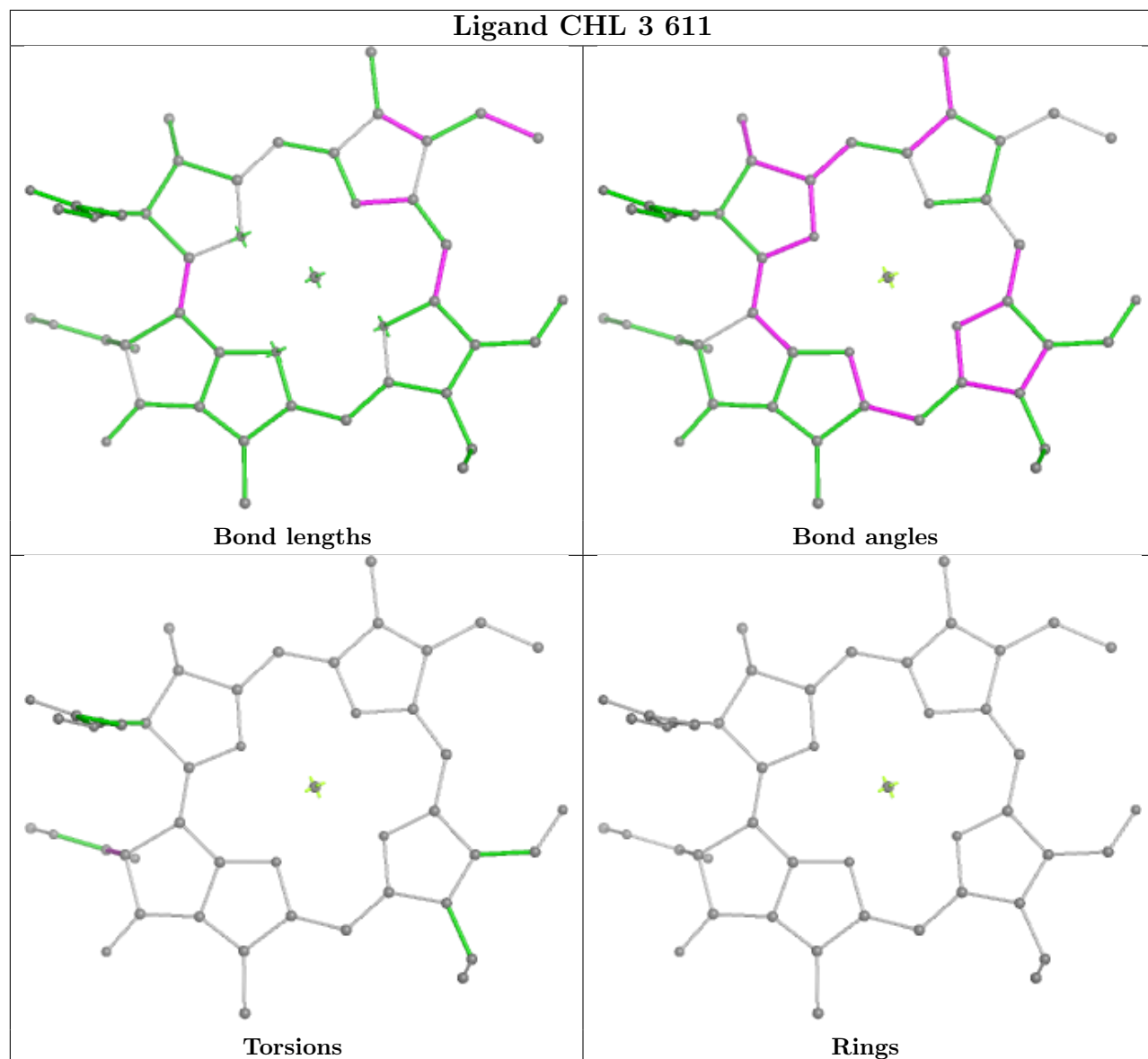


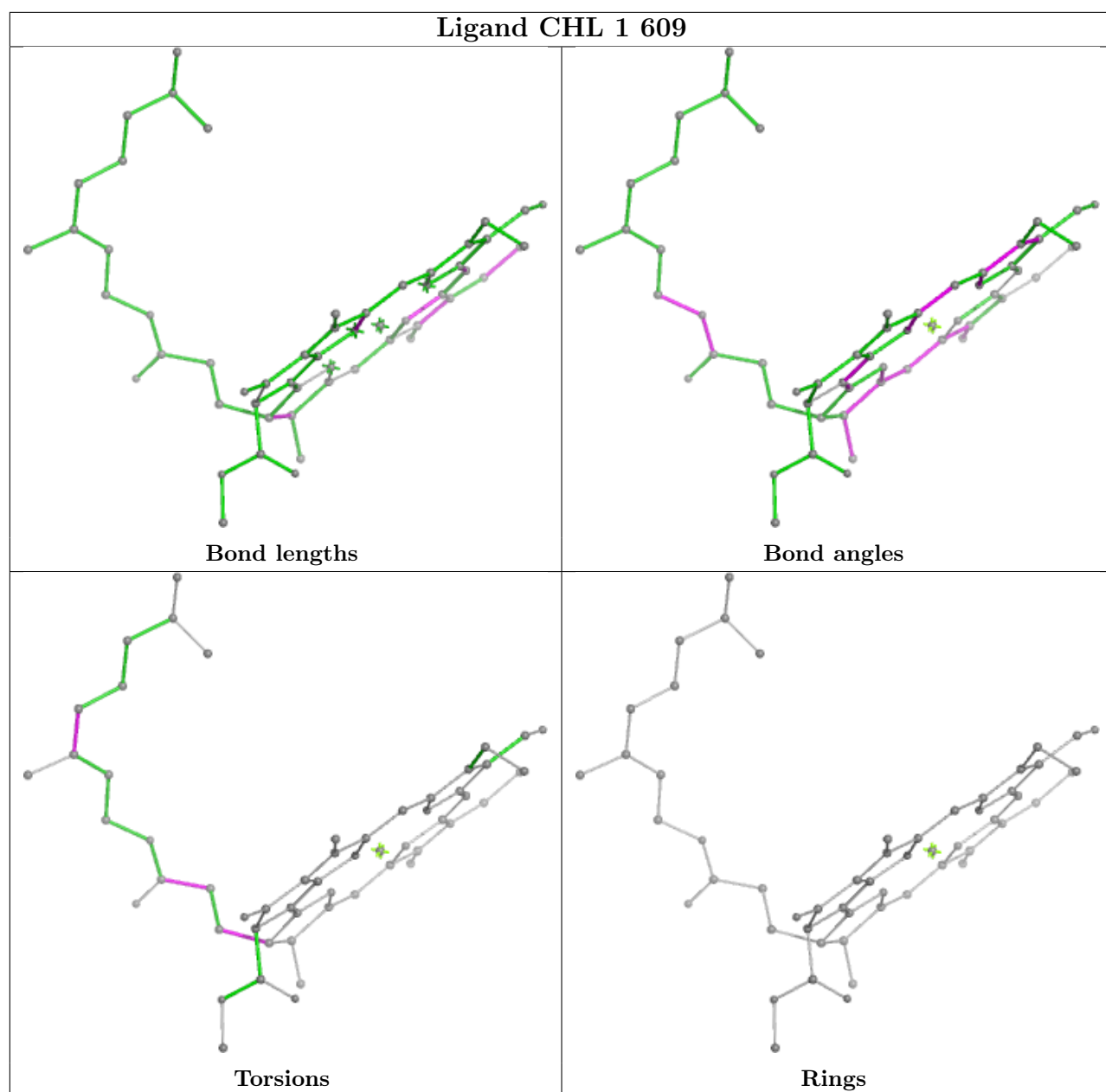
Torsions



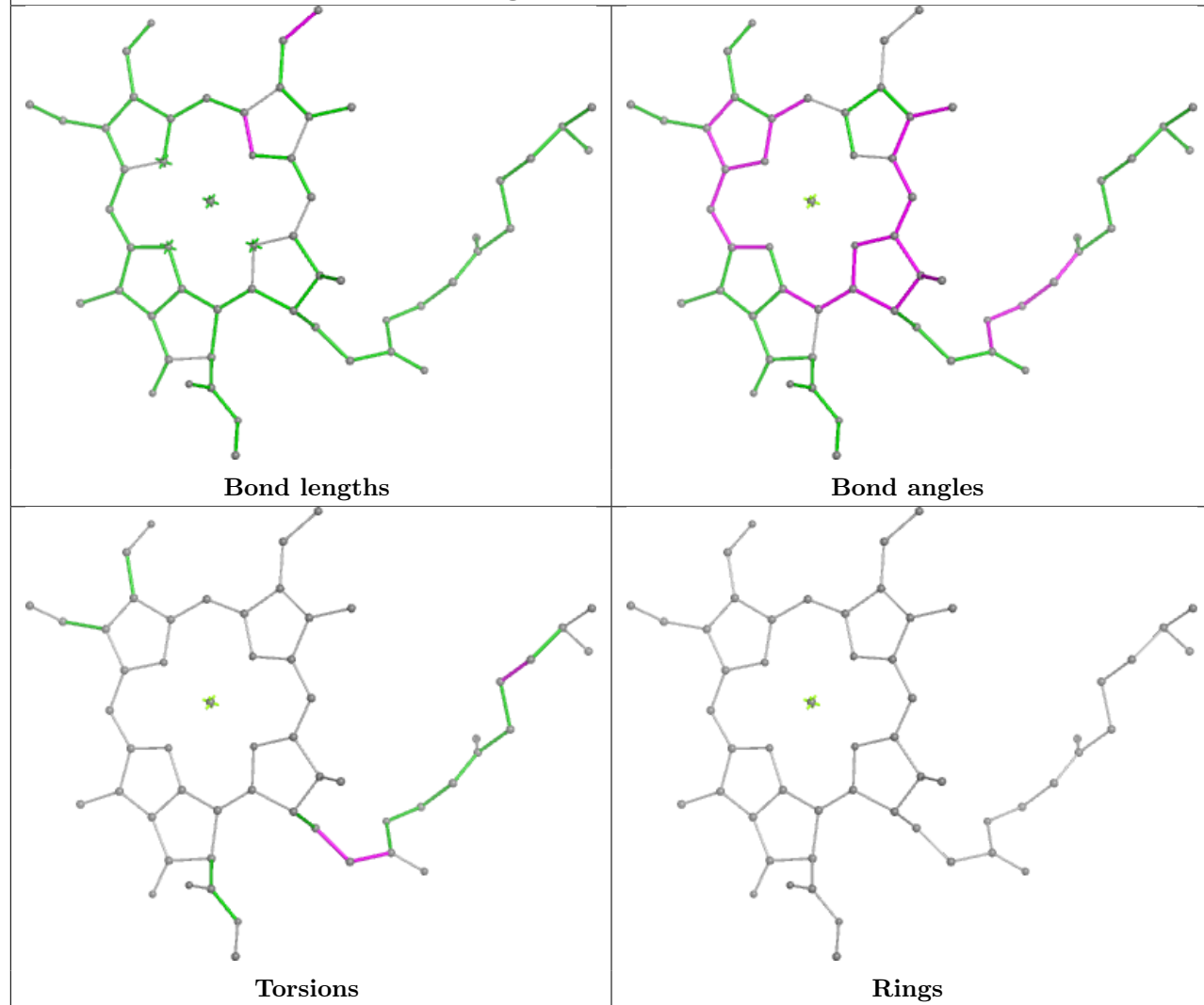
Rings

Ligand CHL 3 611

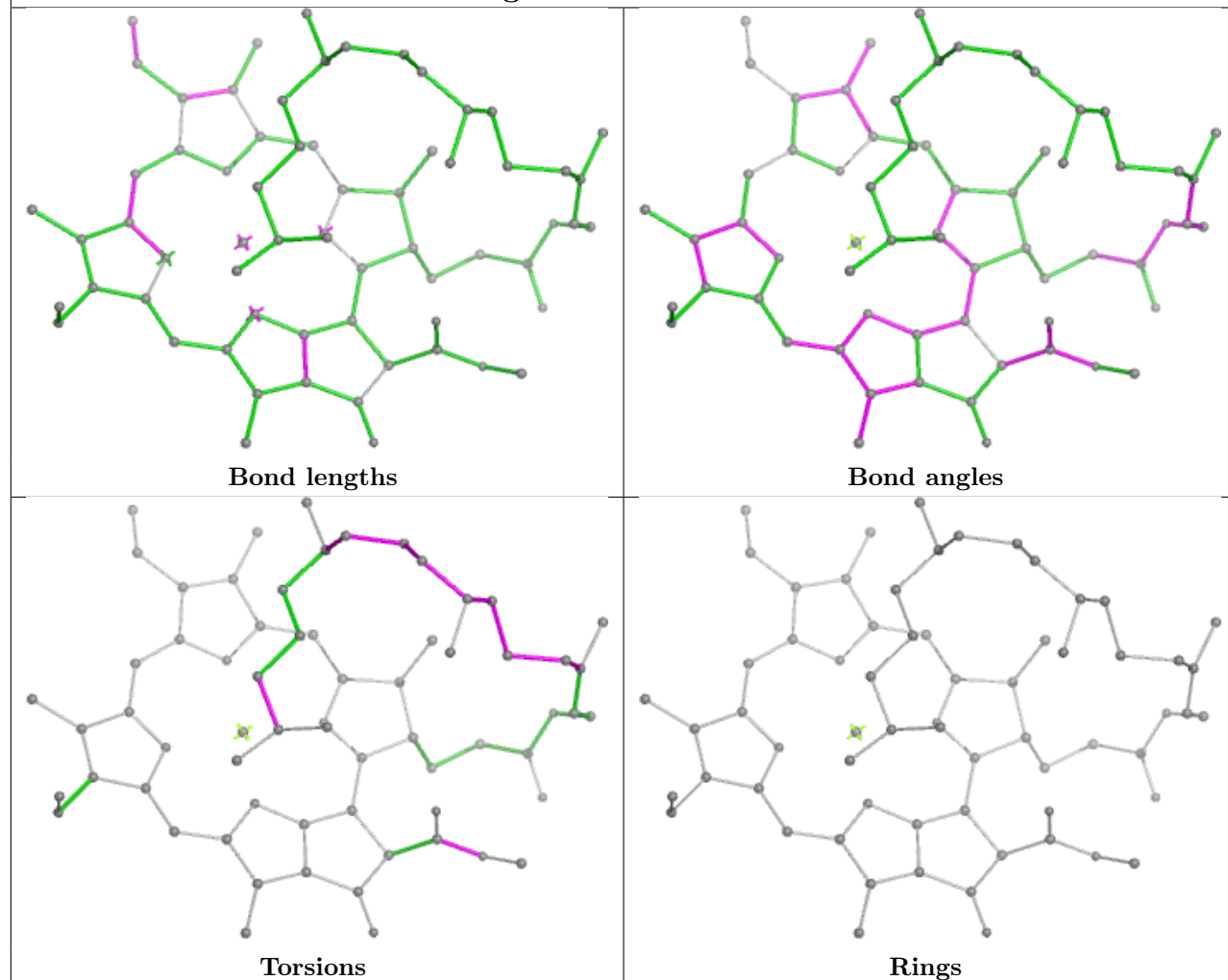




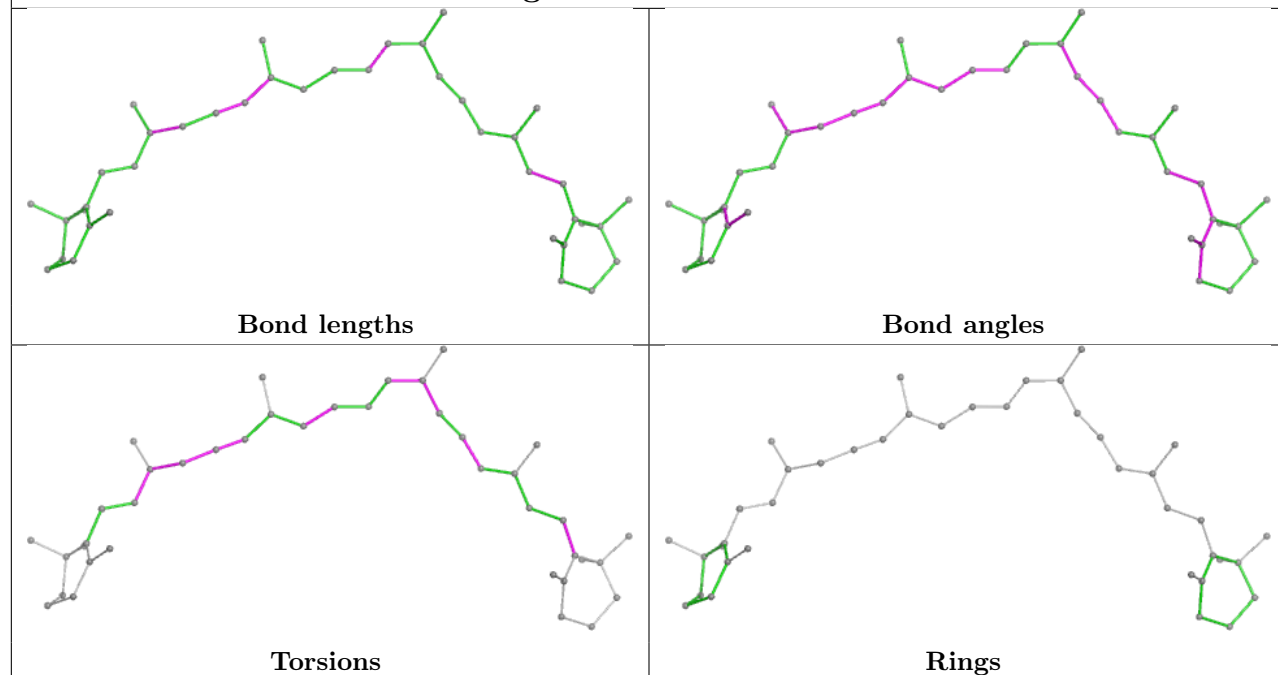
Ligand CHL 2 610



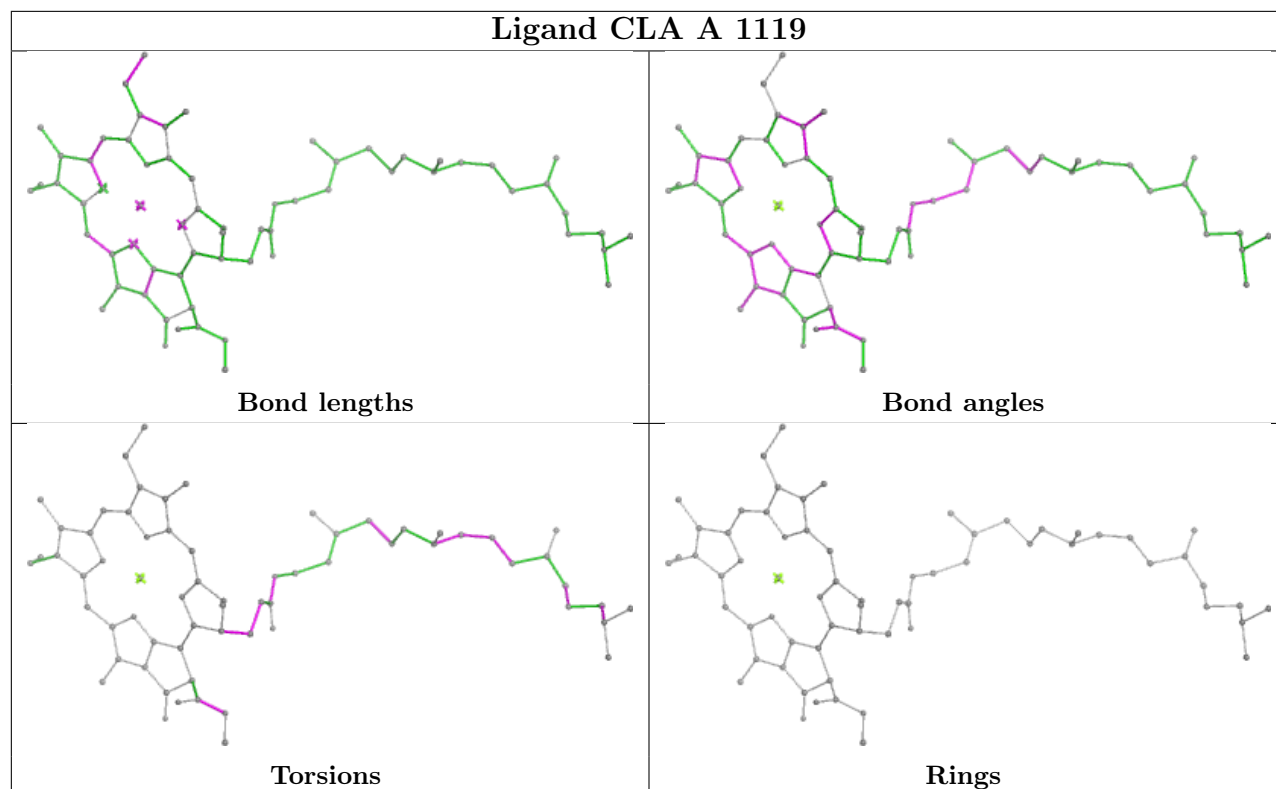
Ligand CLA B 1203



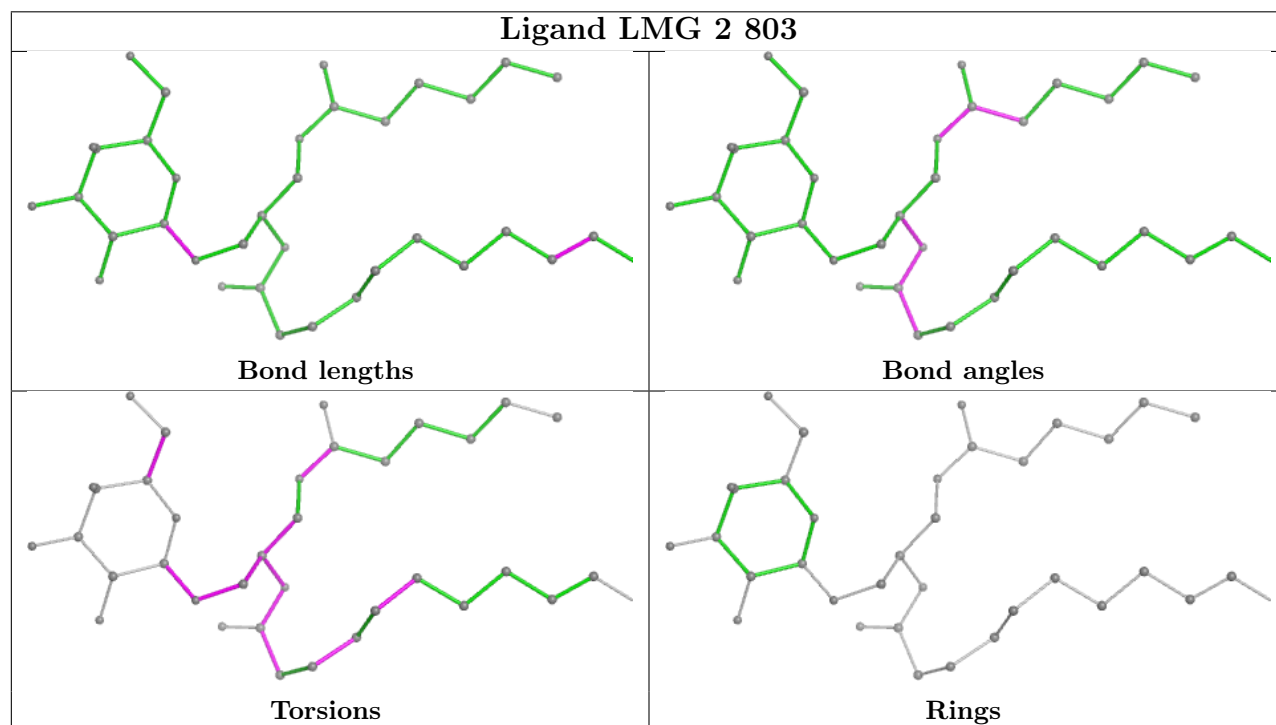
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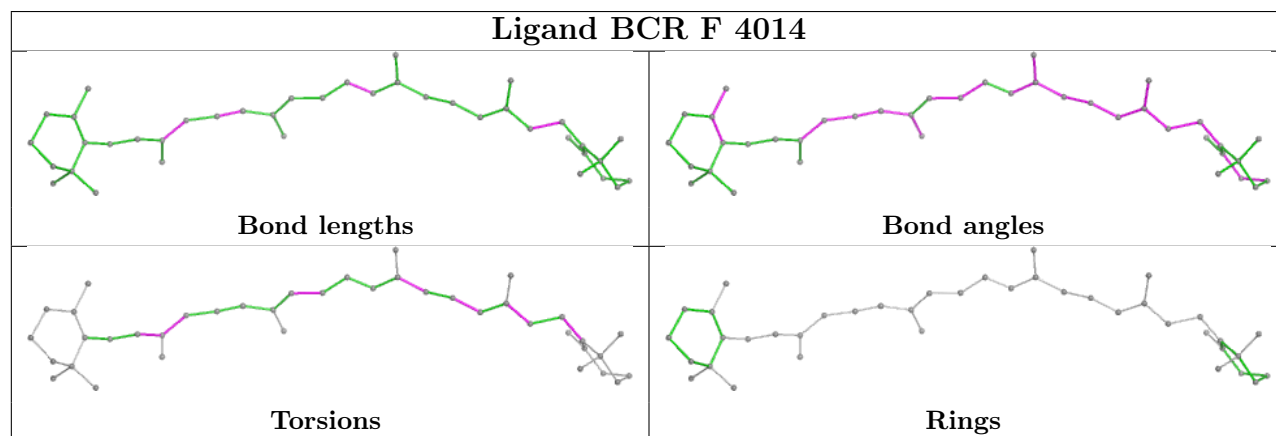
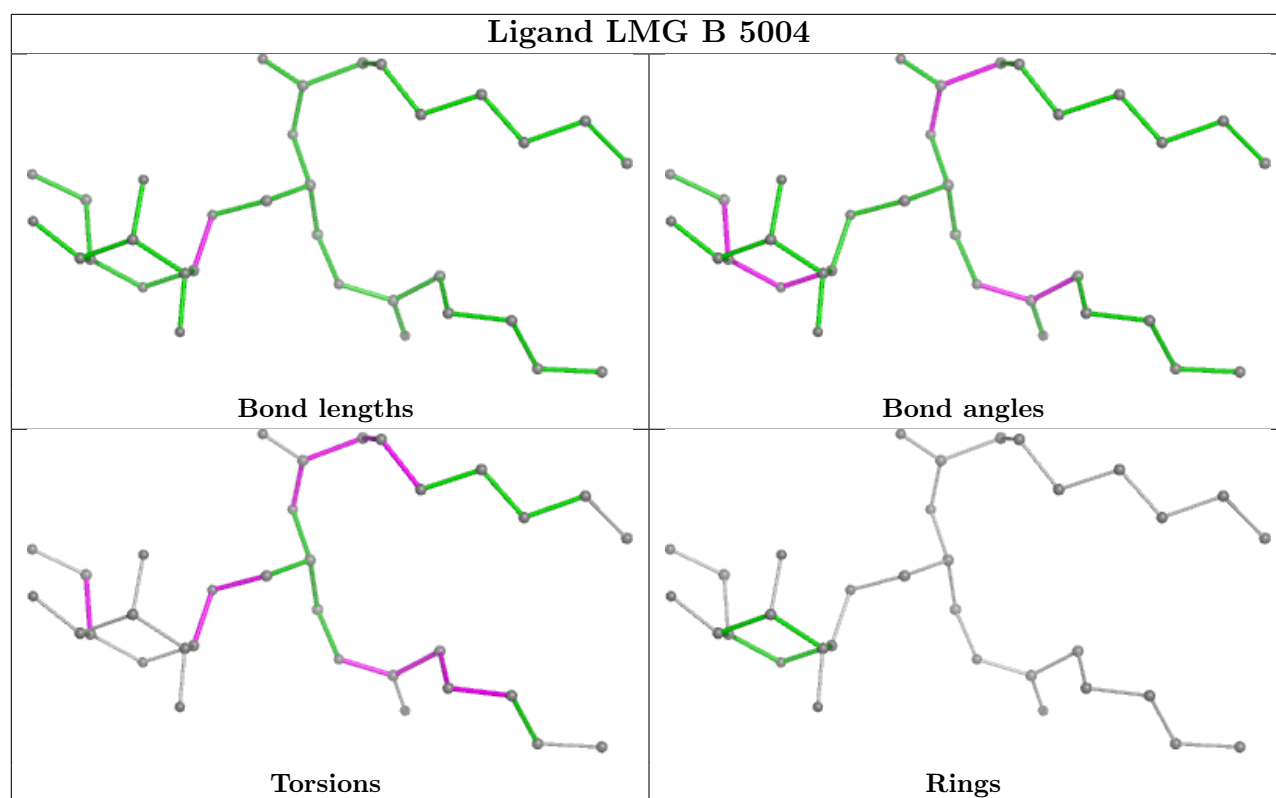


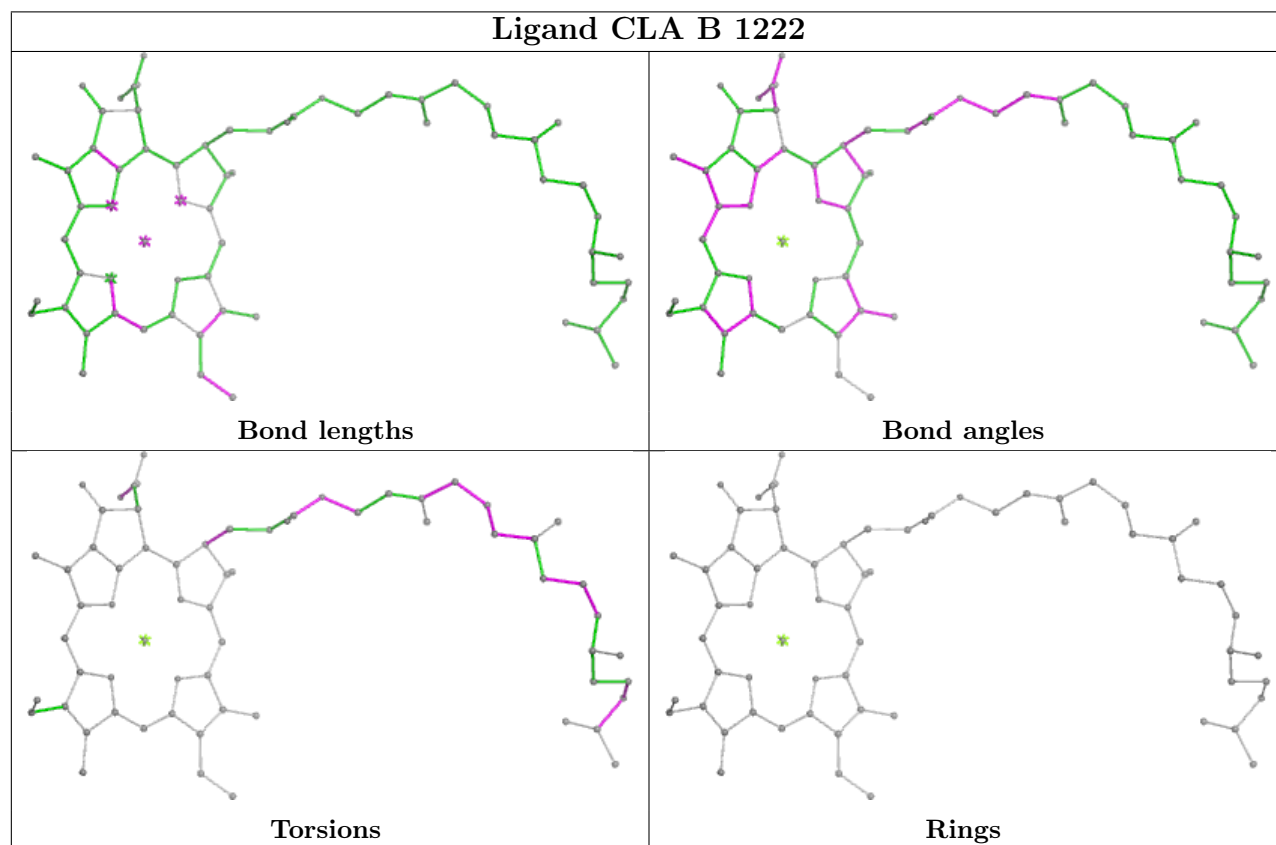
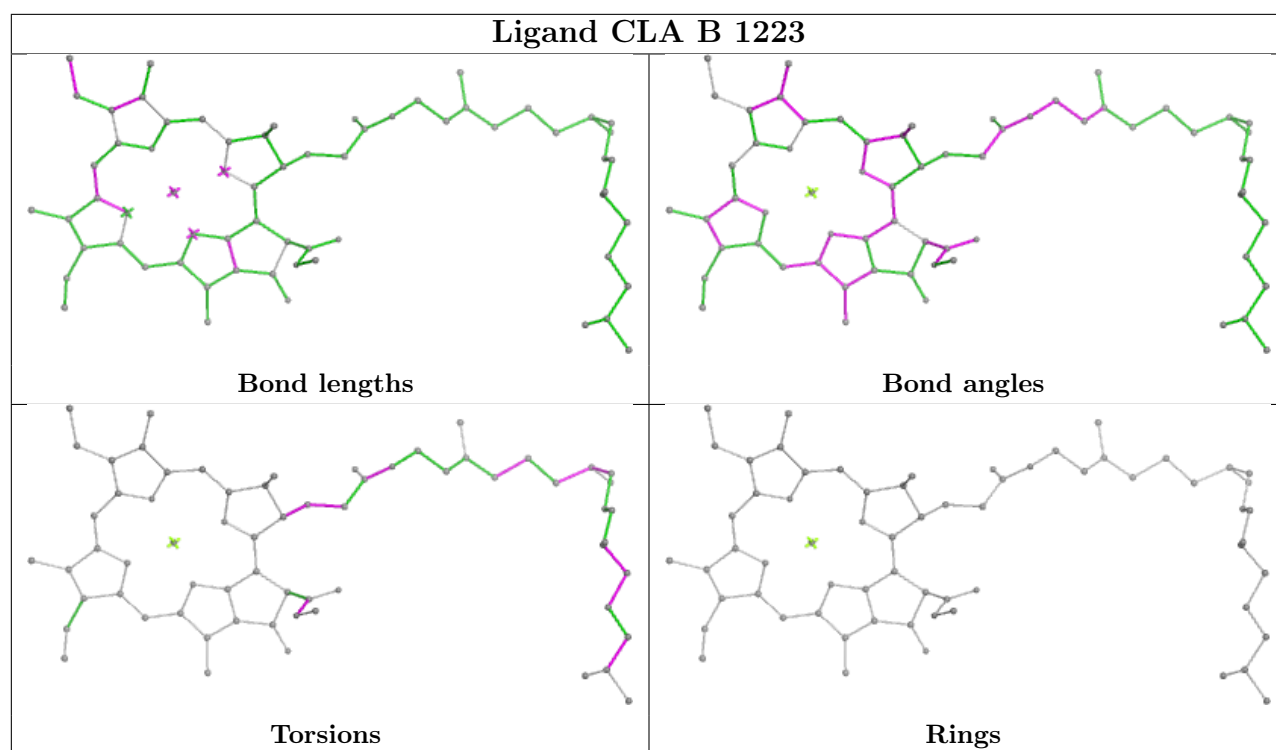
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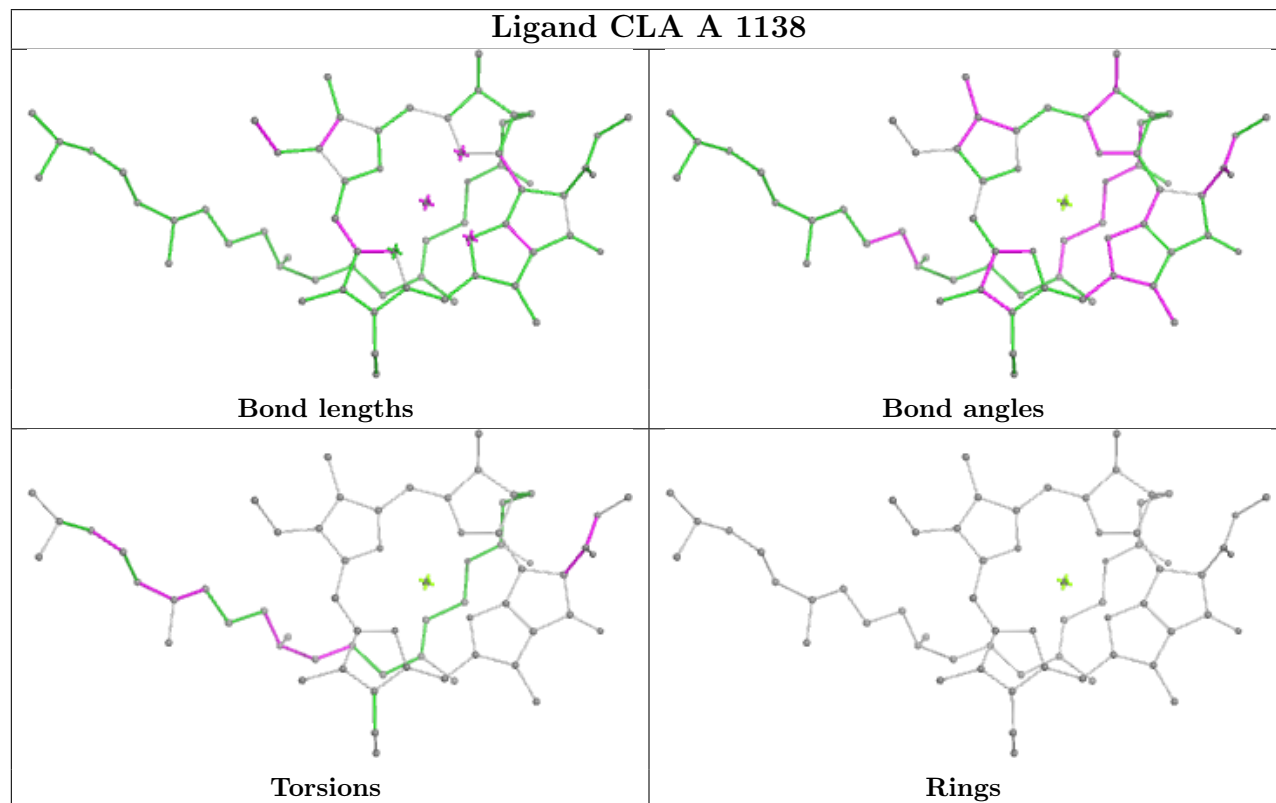
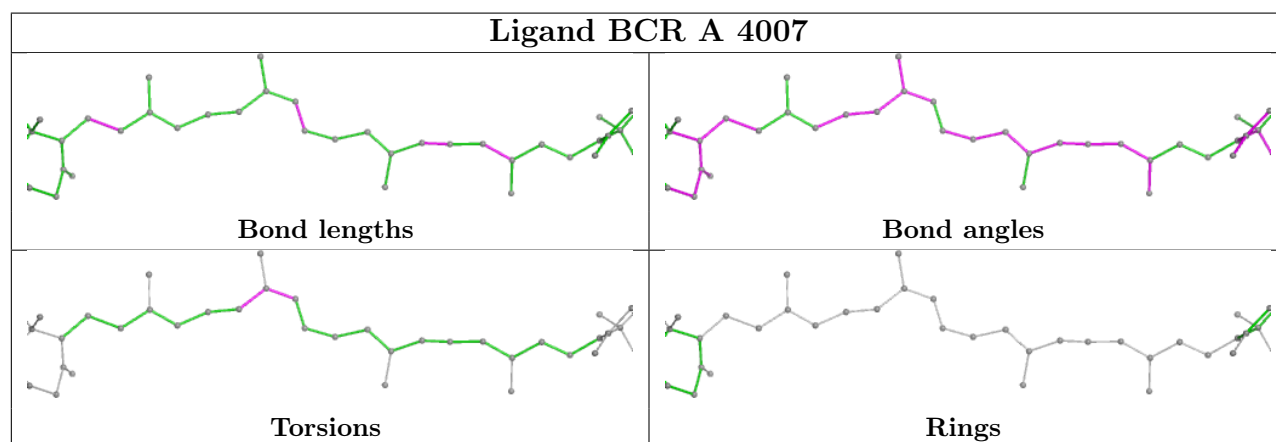
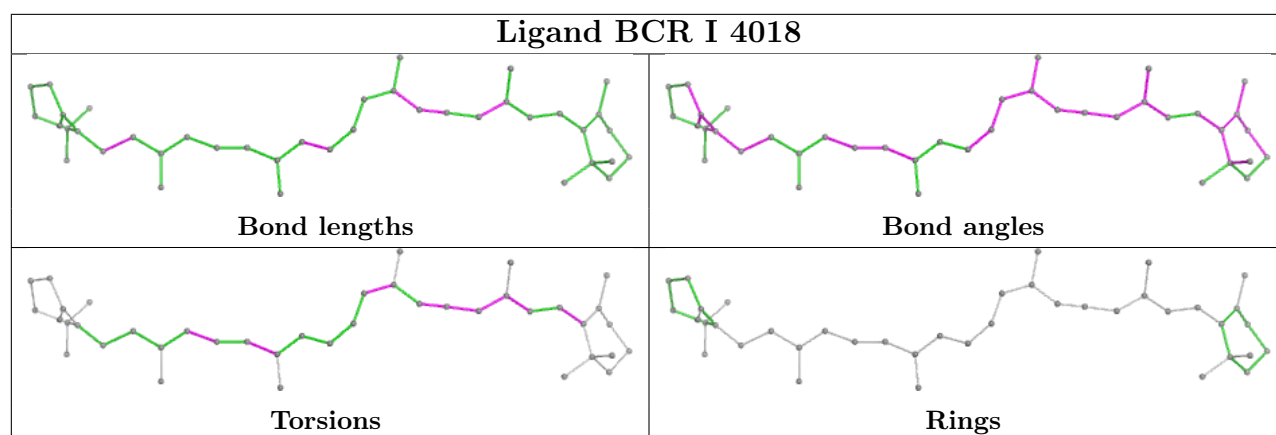


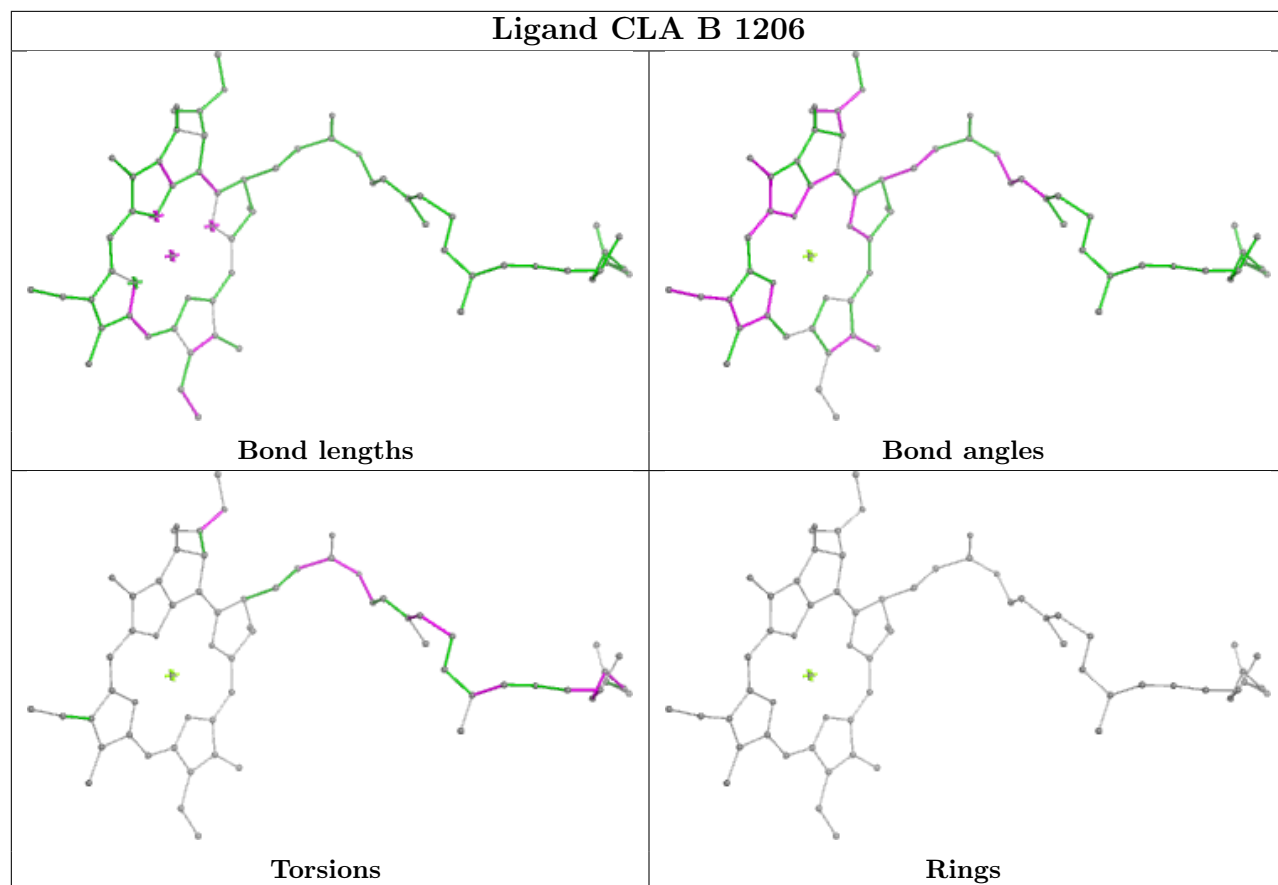
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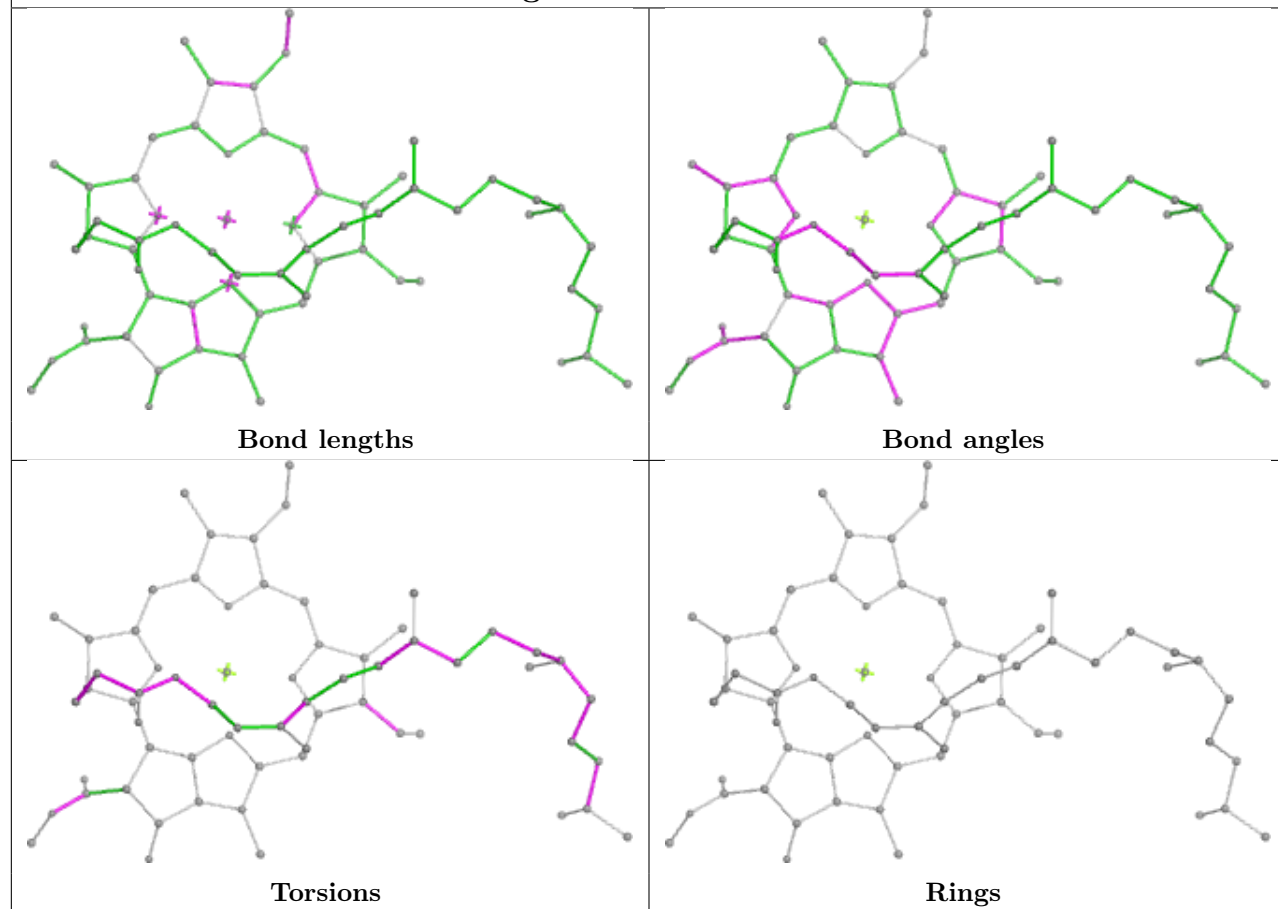
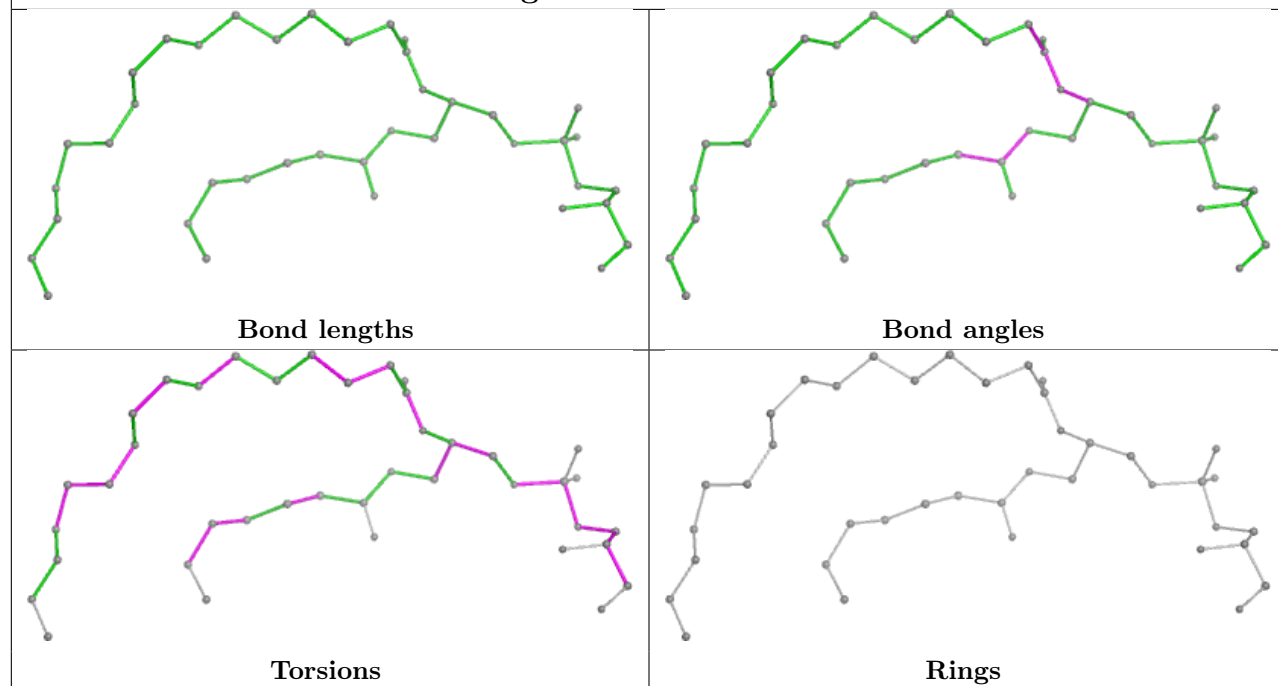


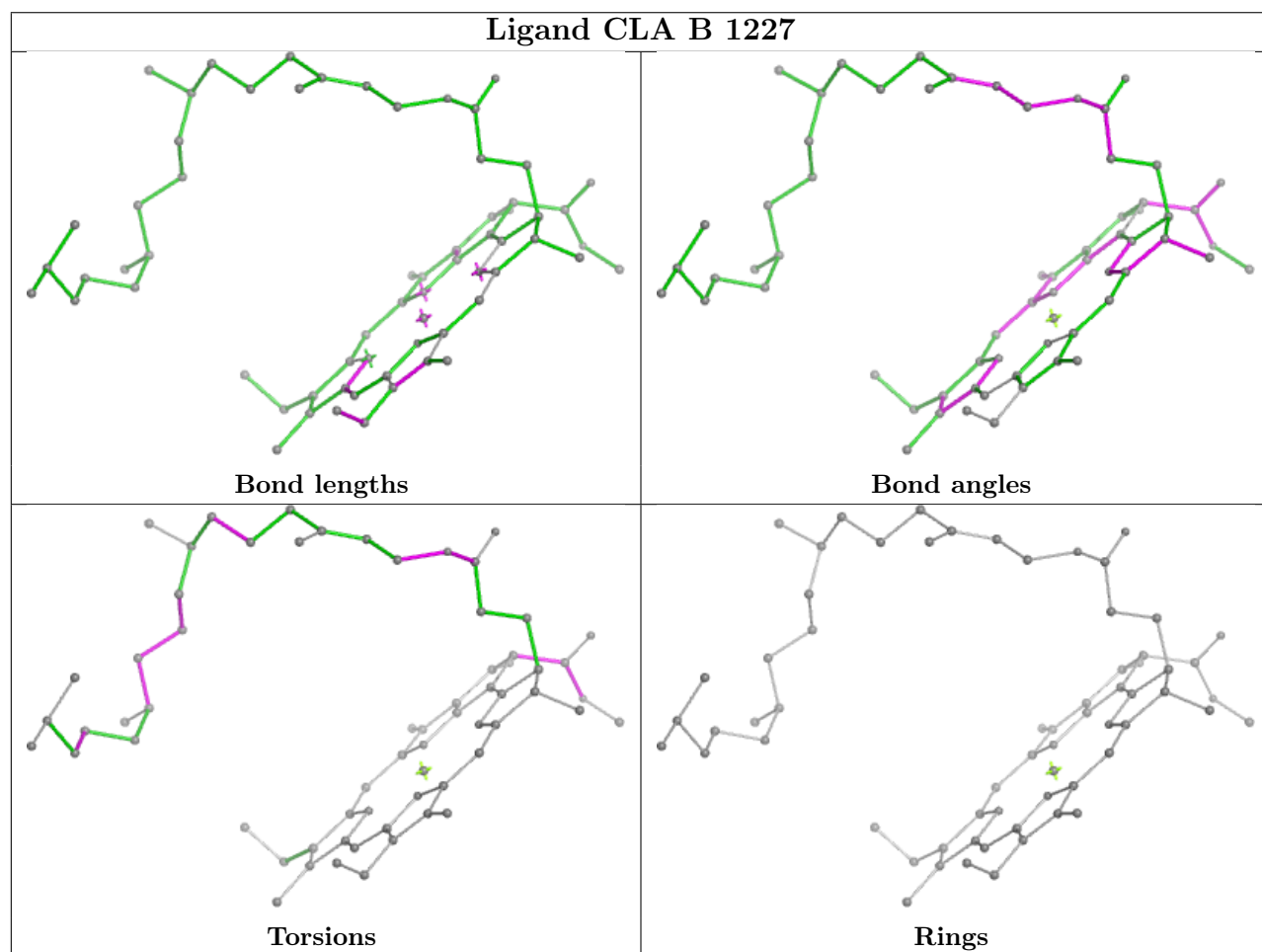
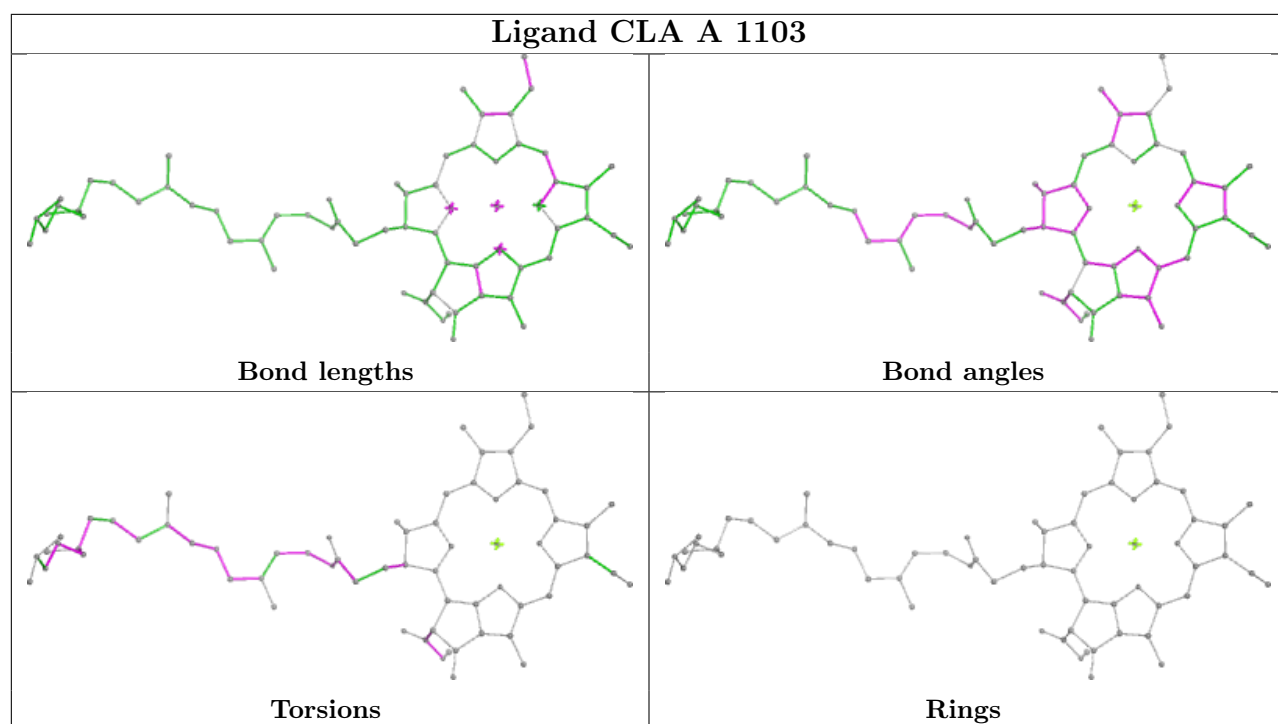


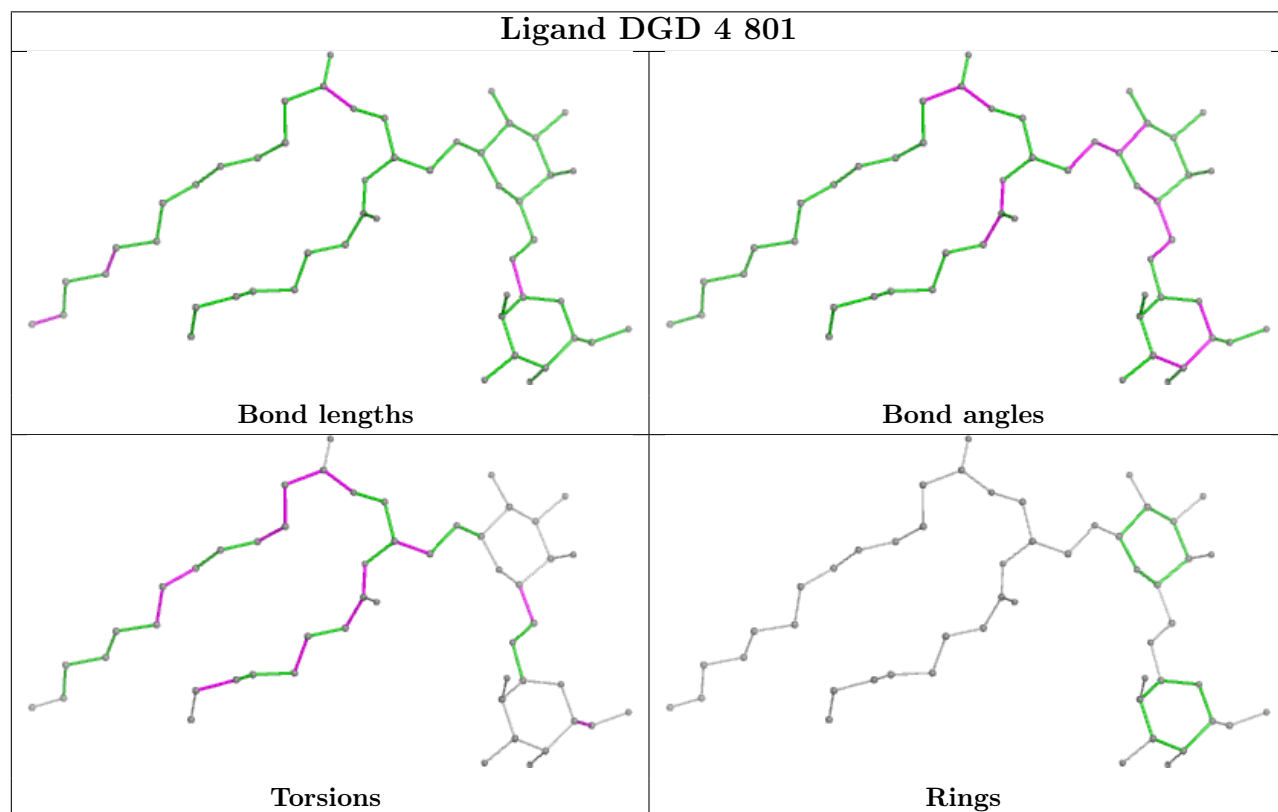
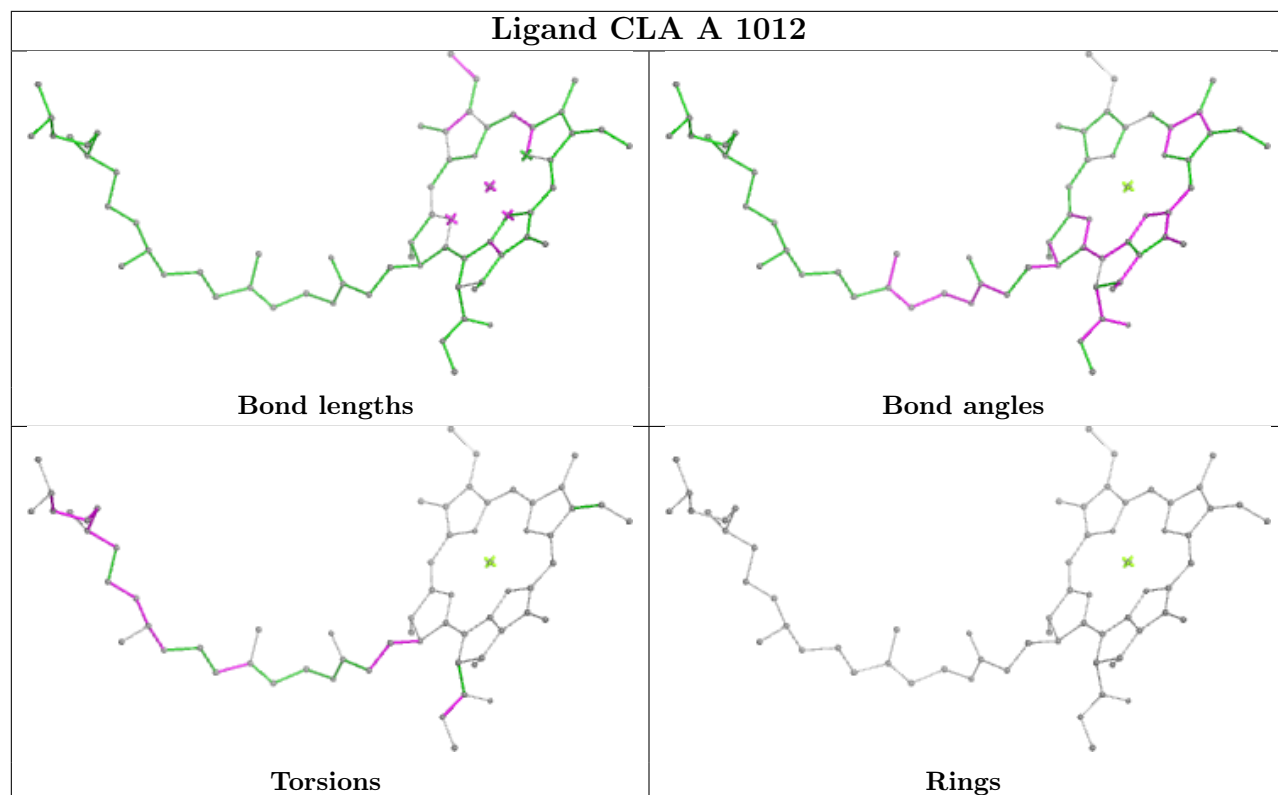




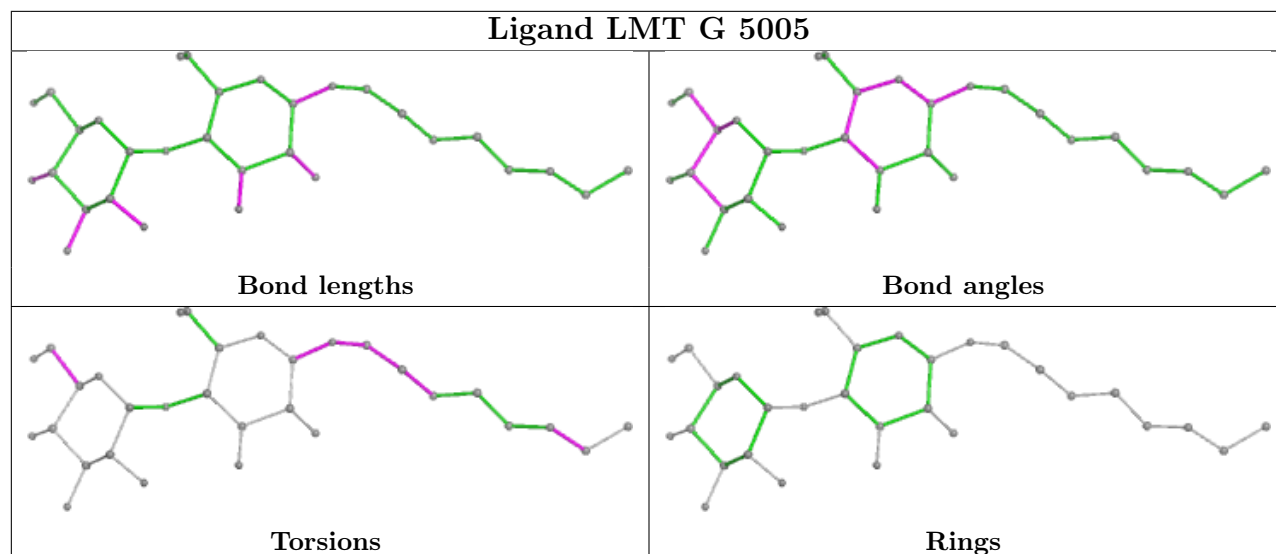


Ligand CLA A 1115**Ligand LHG A 5001**

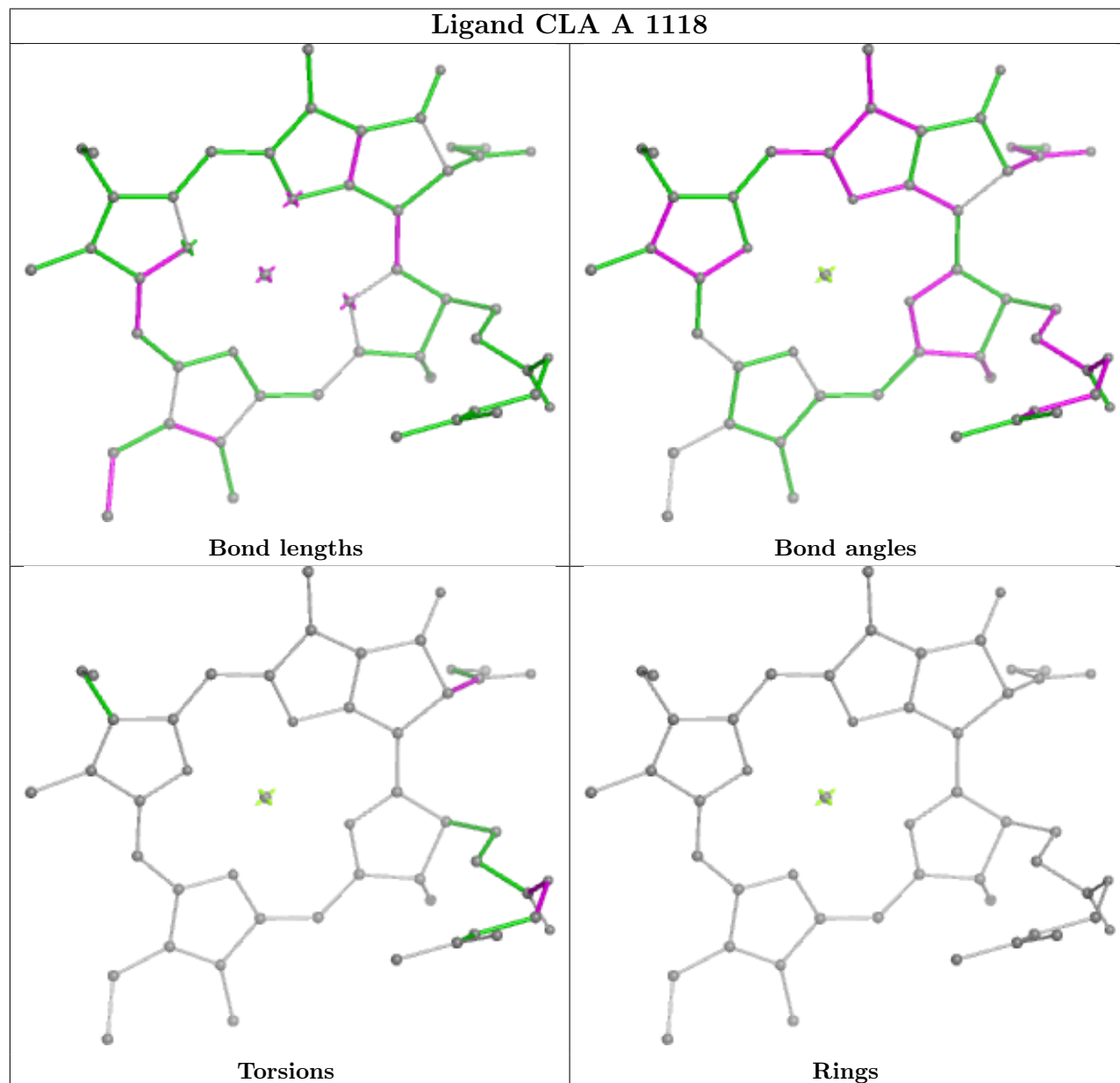


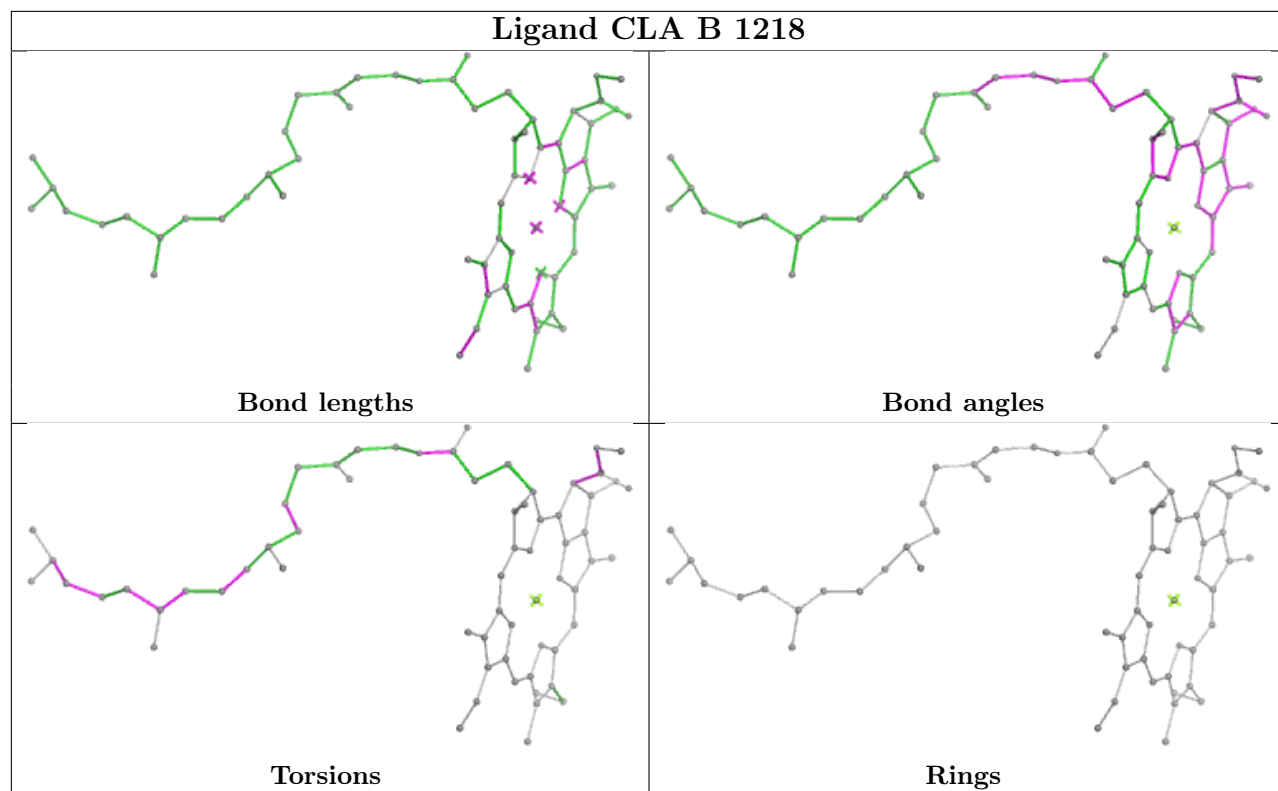


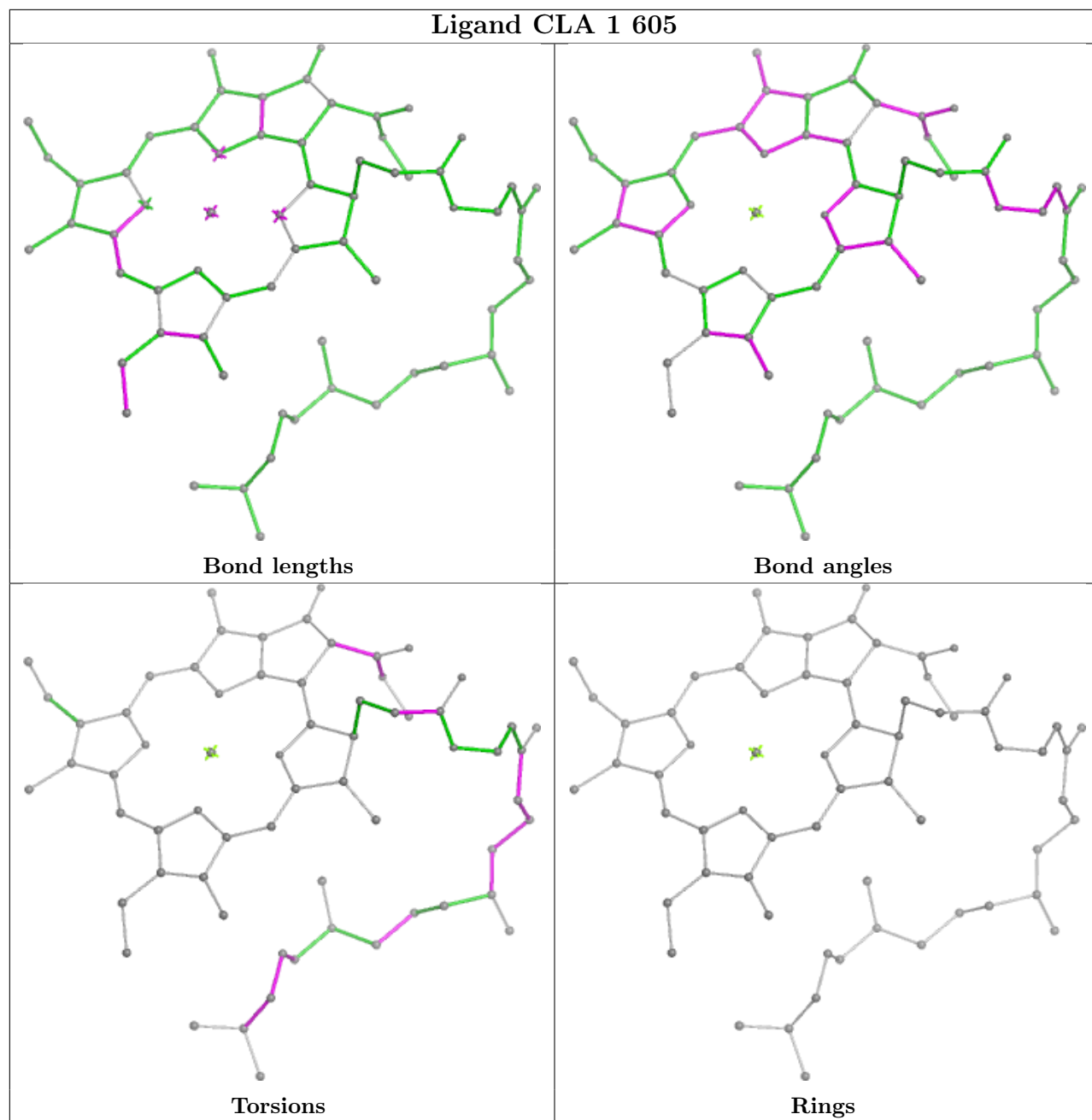
Ligand LMT G 5005



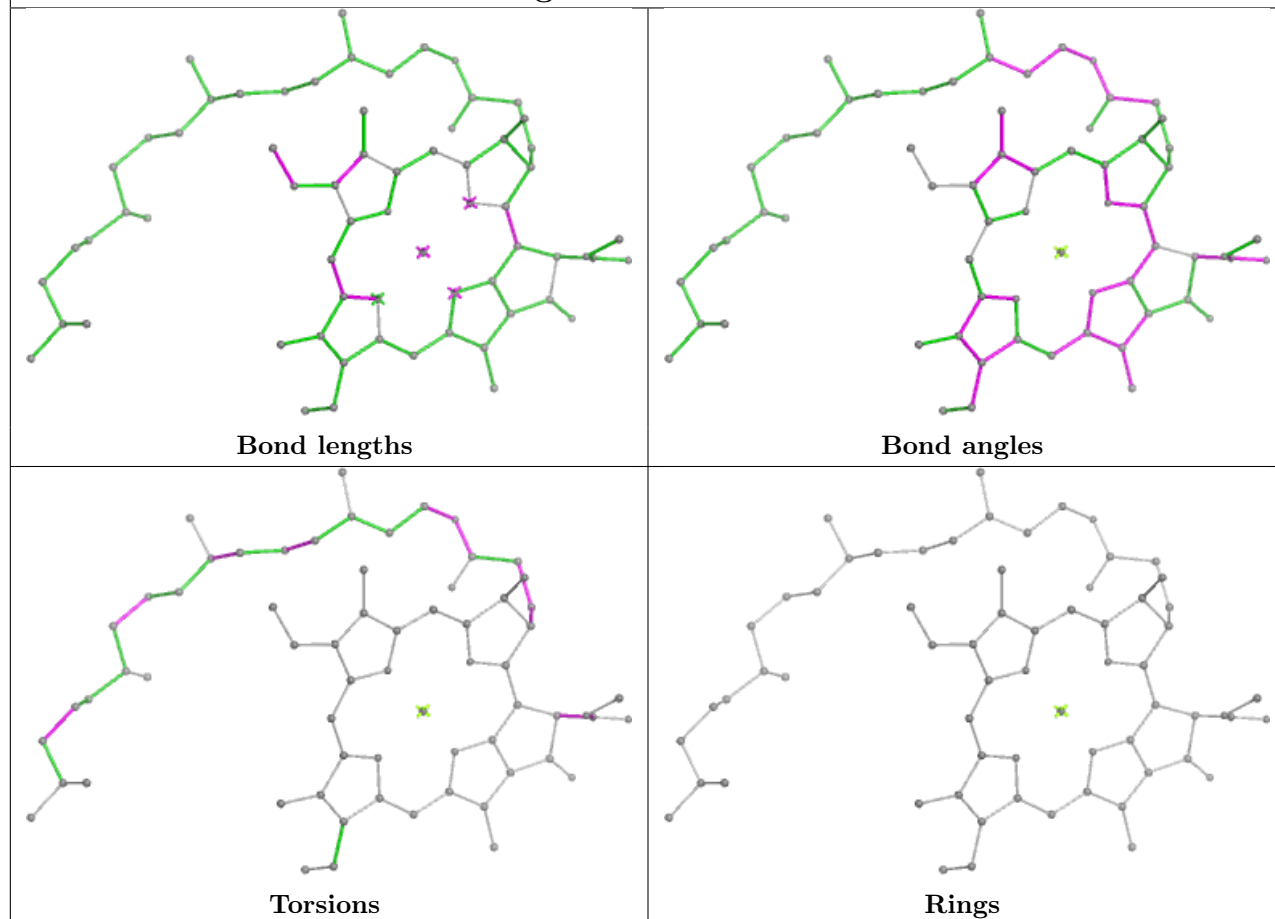
Ligand CLA A 1118



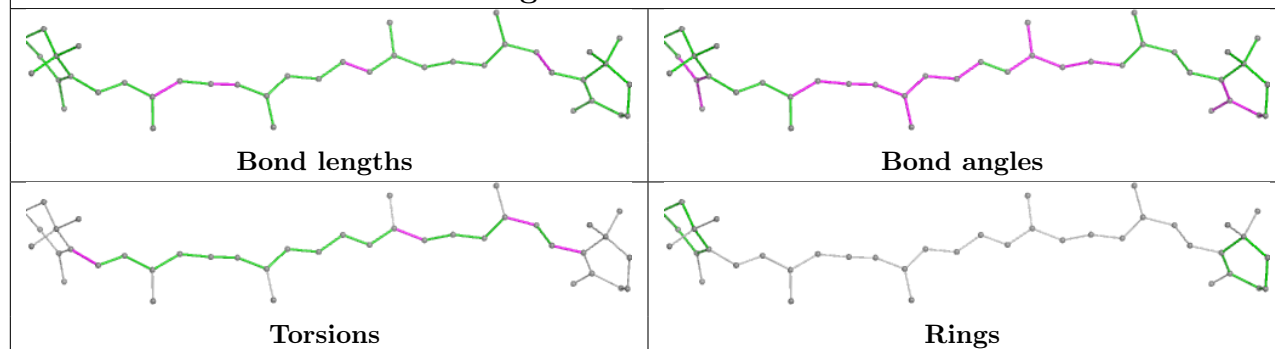


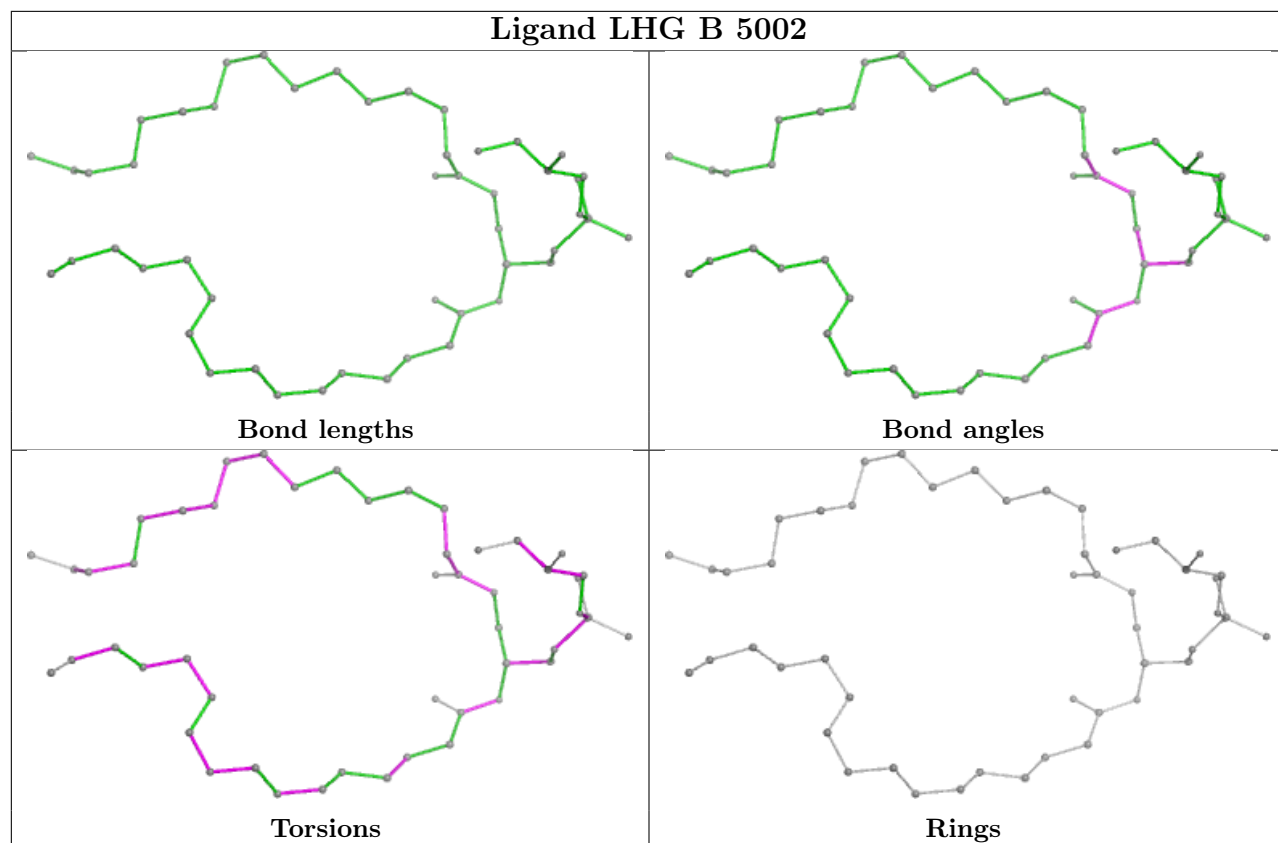


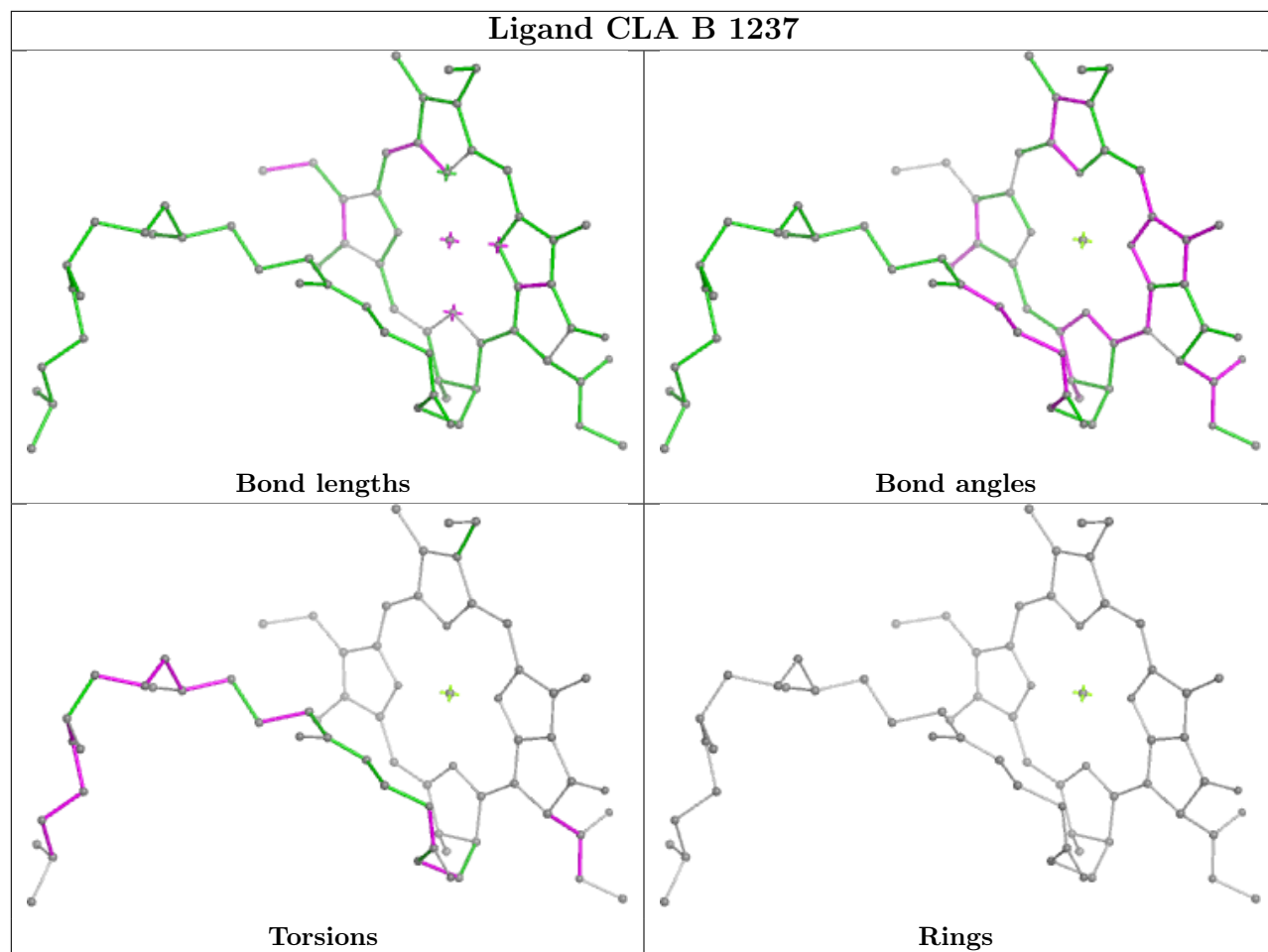
Ligand CLA 2 604

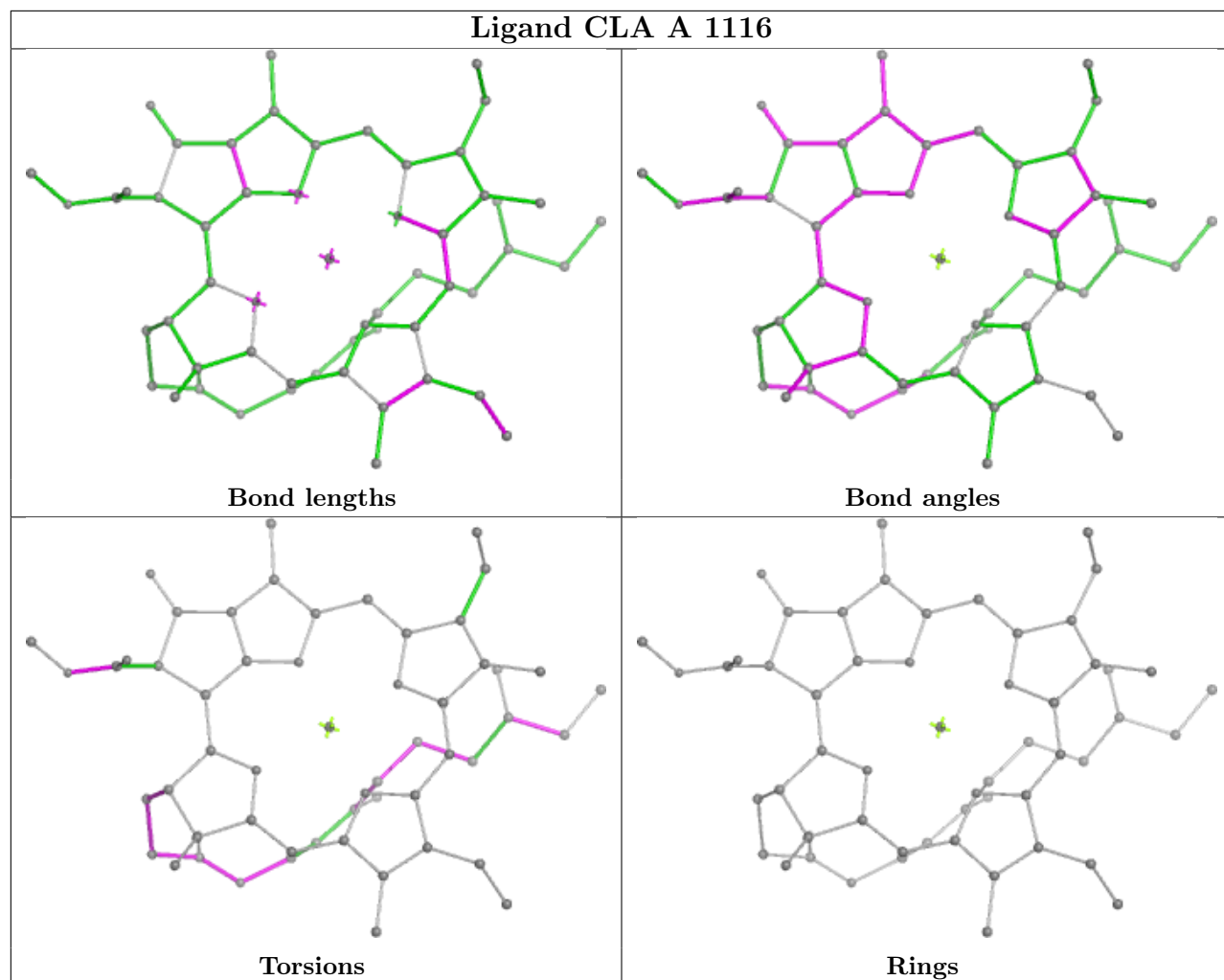


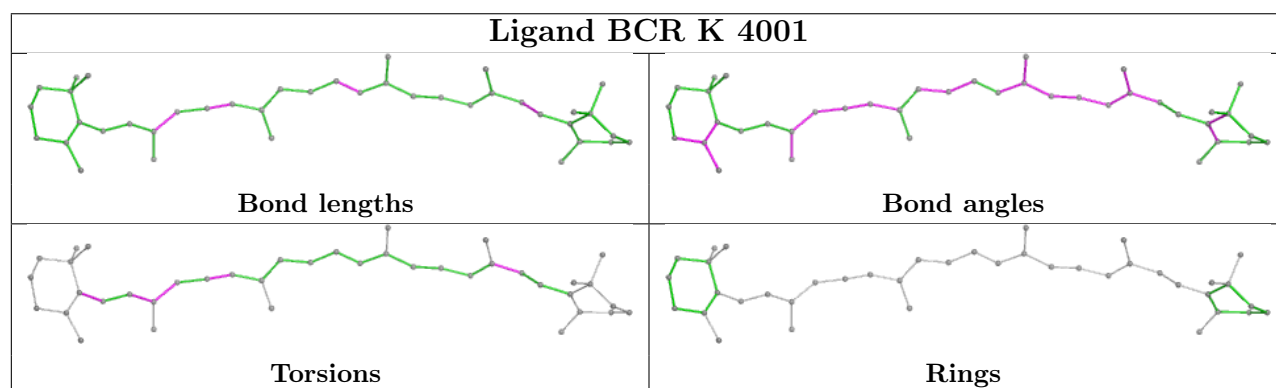
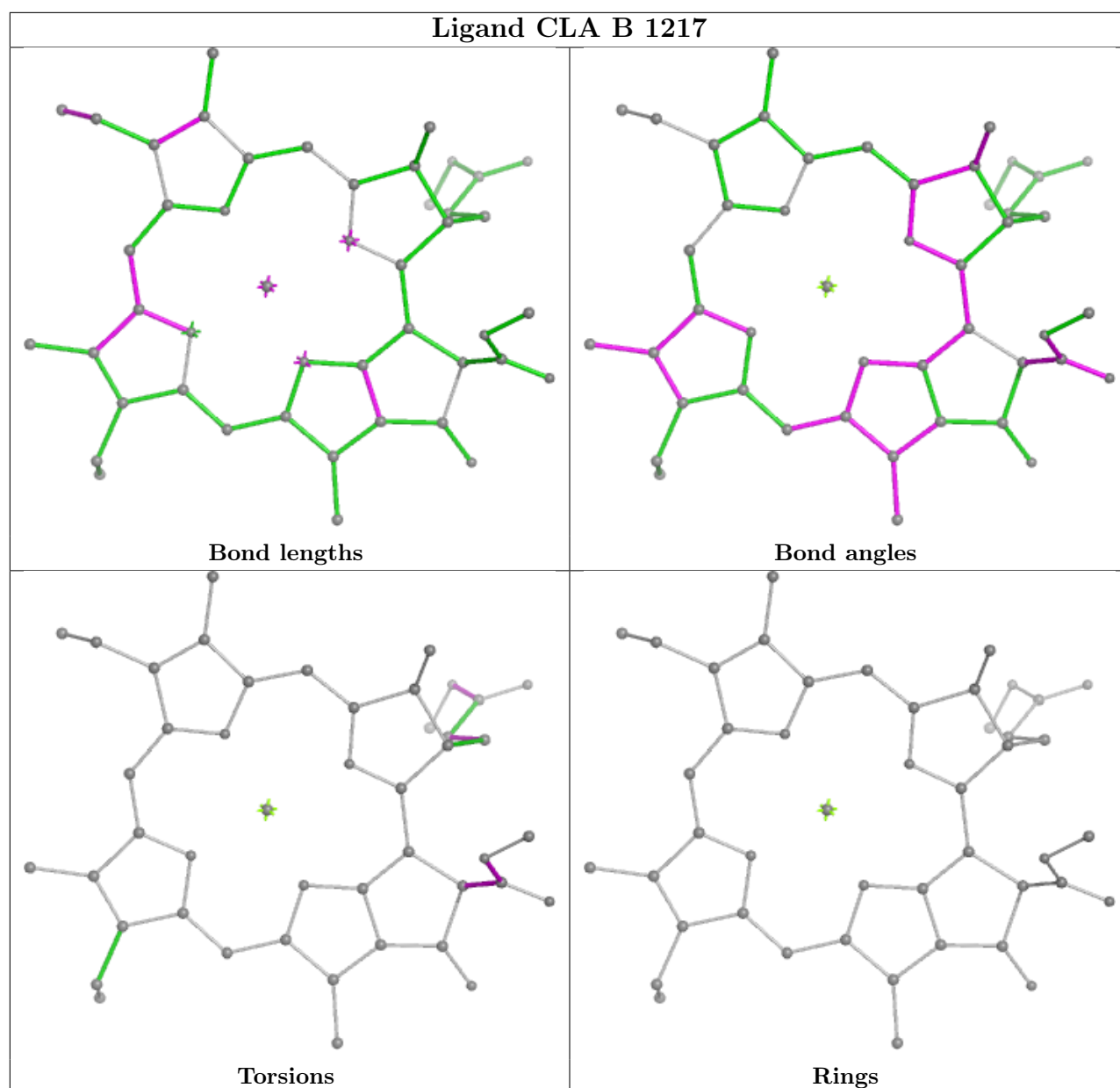
Ligand BCR A 4003

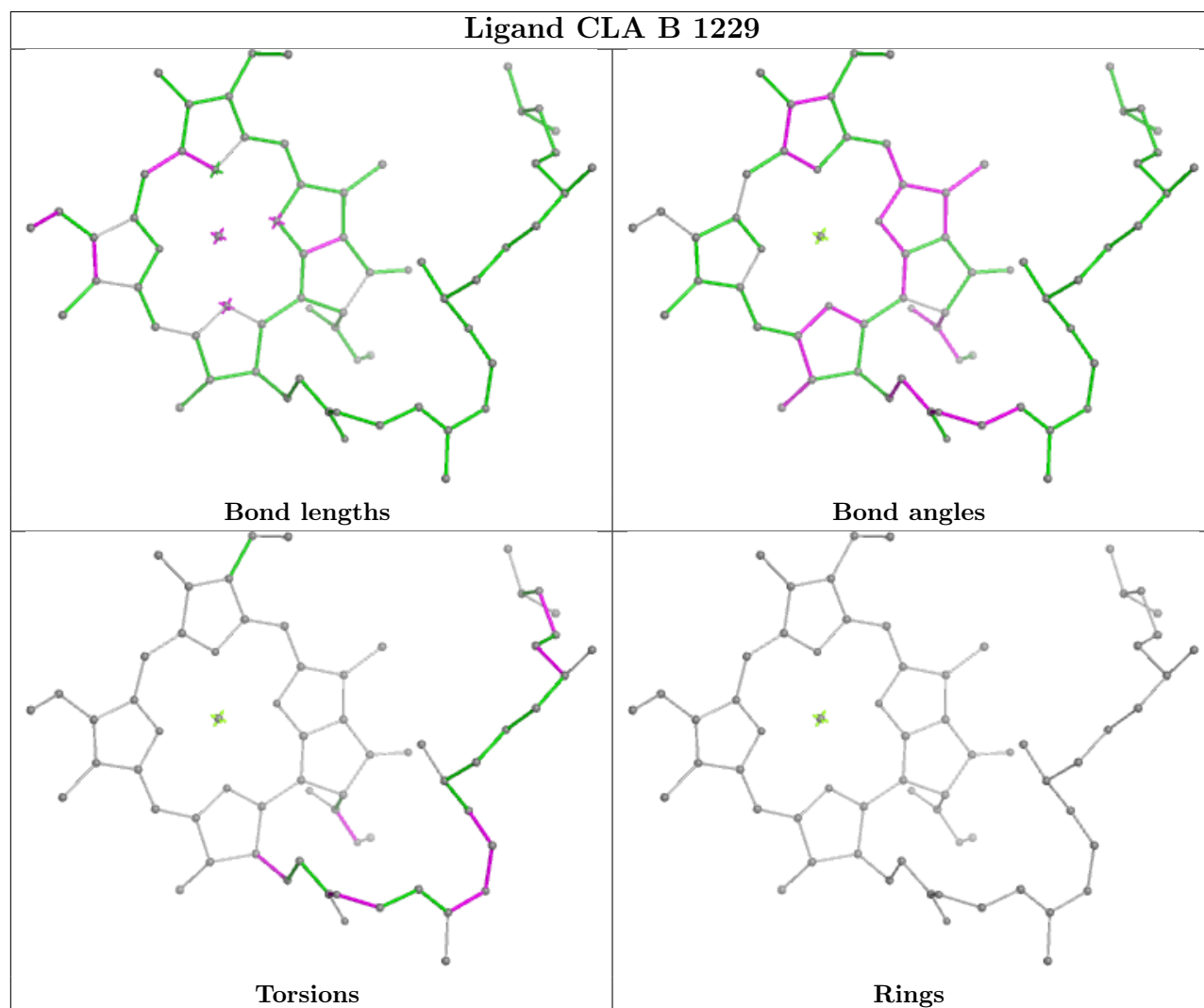
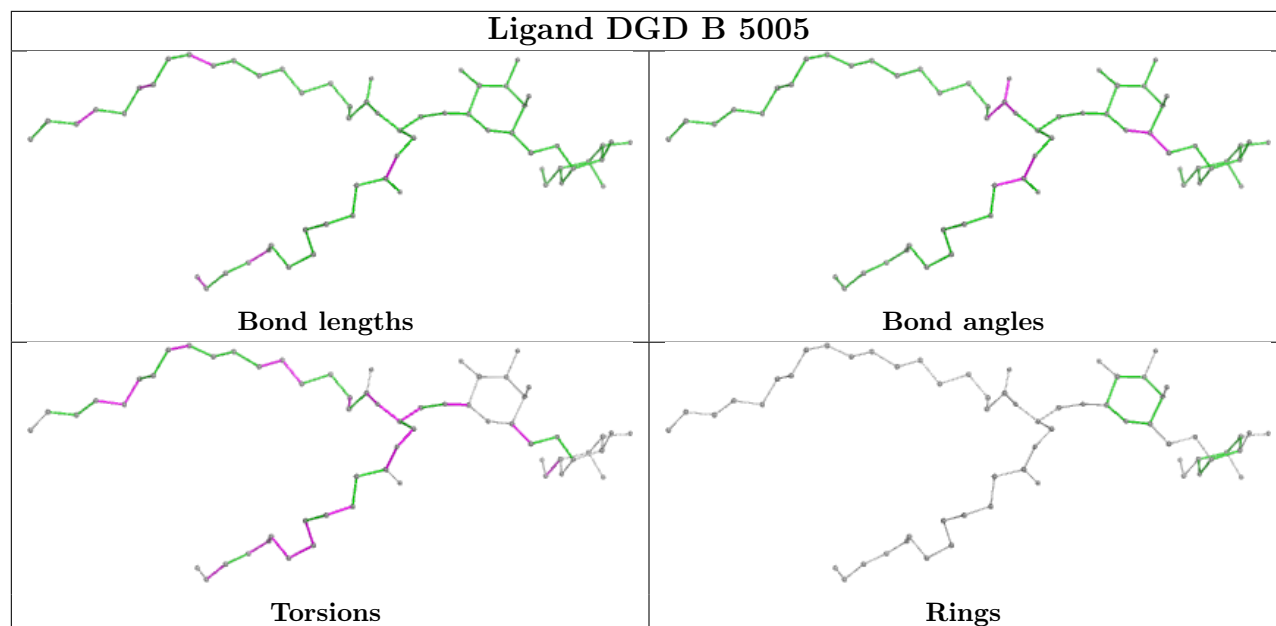




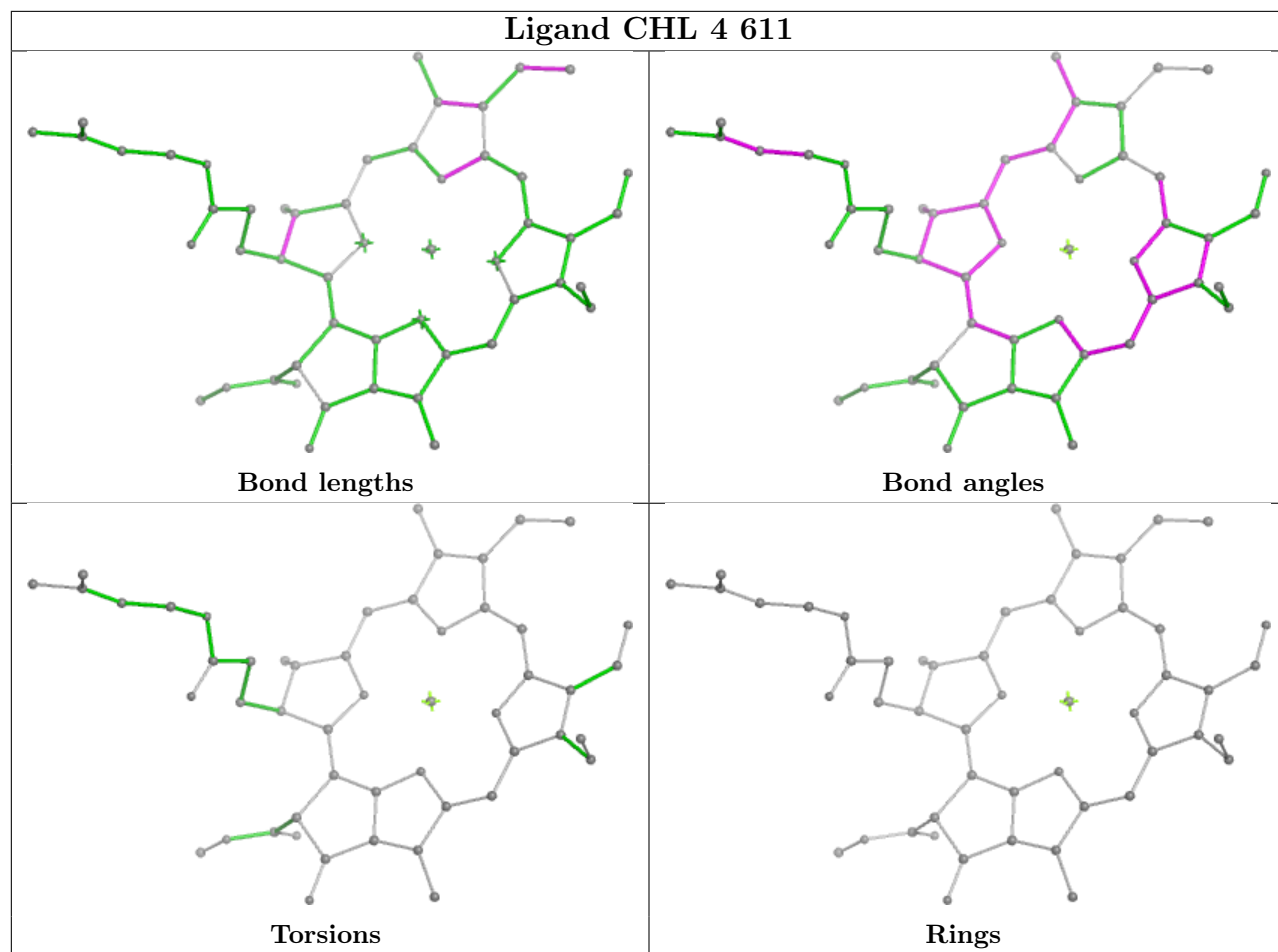


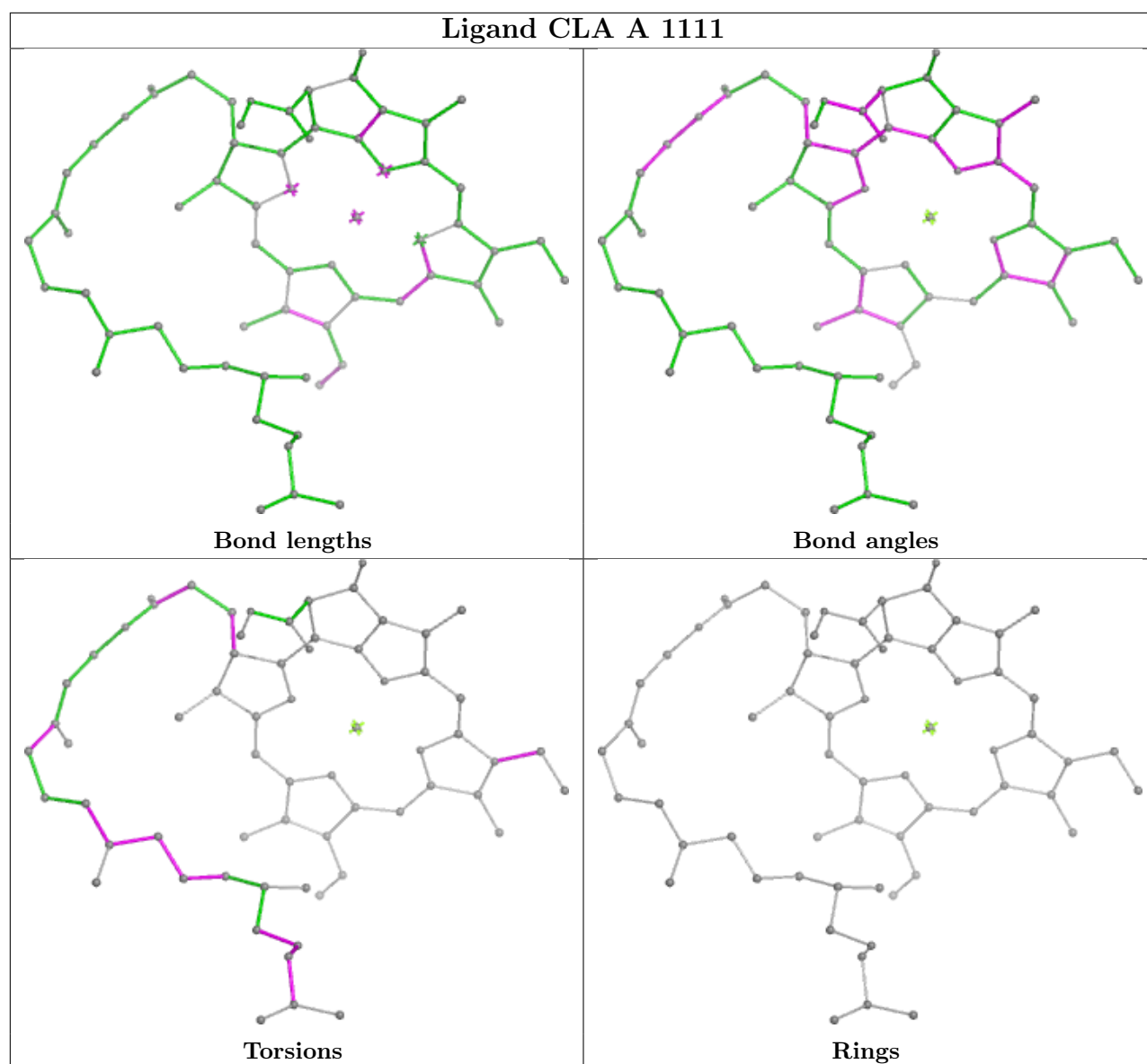


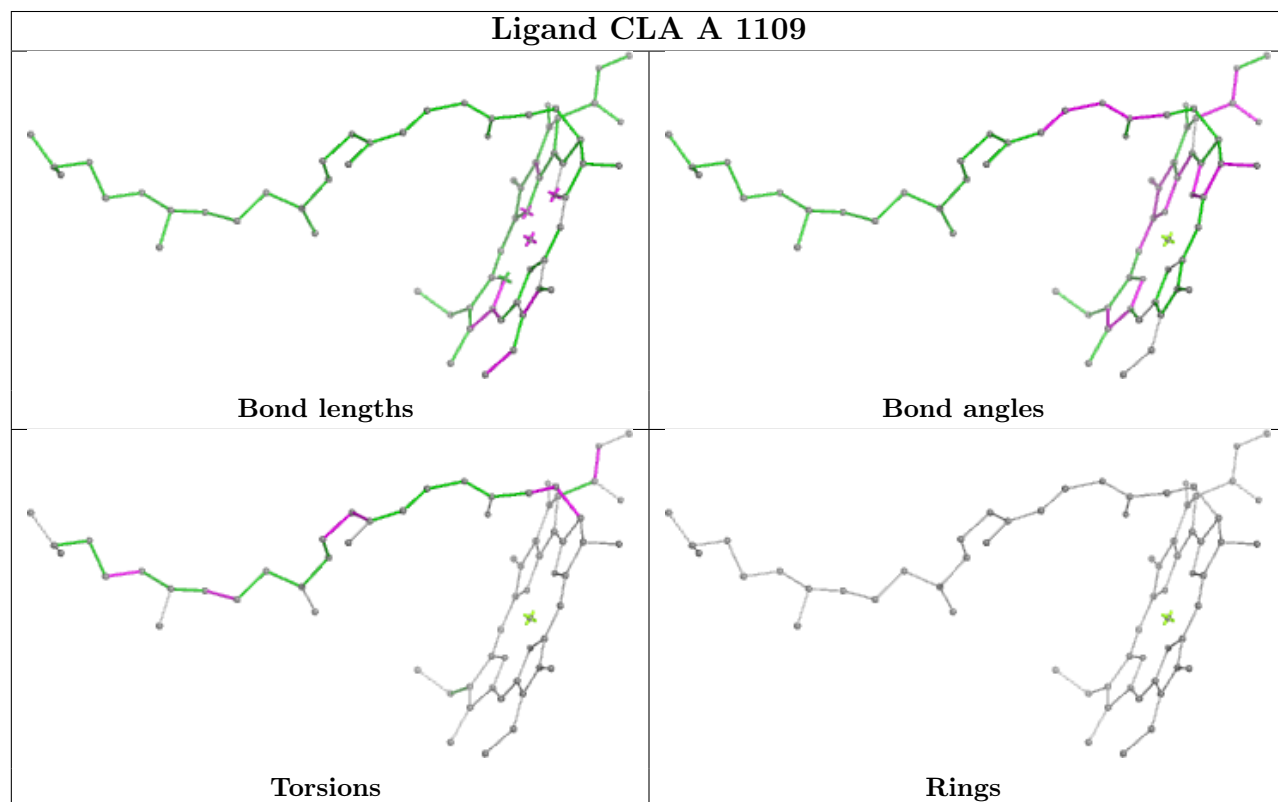
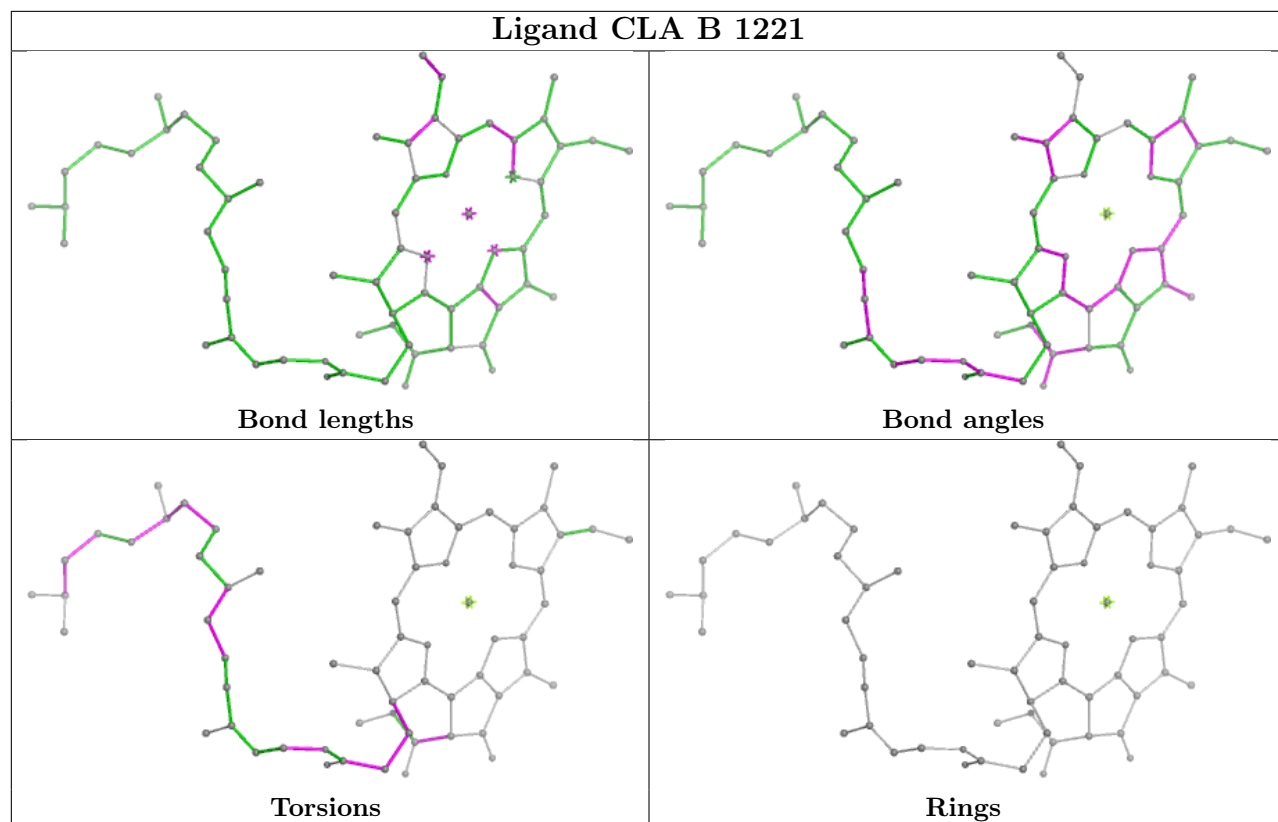




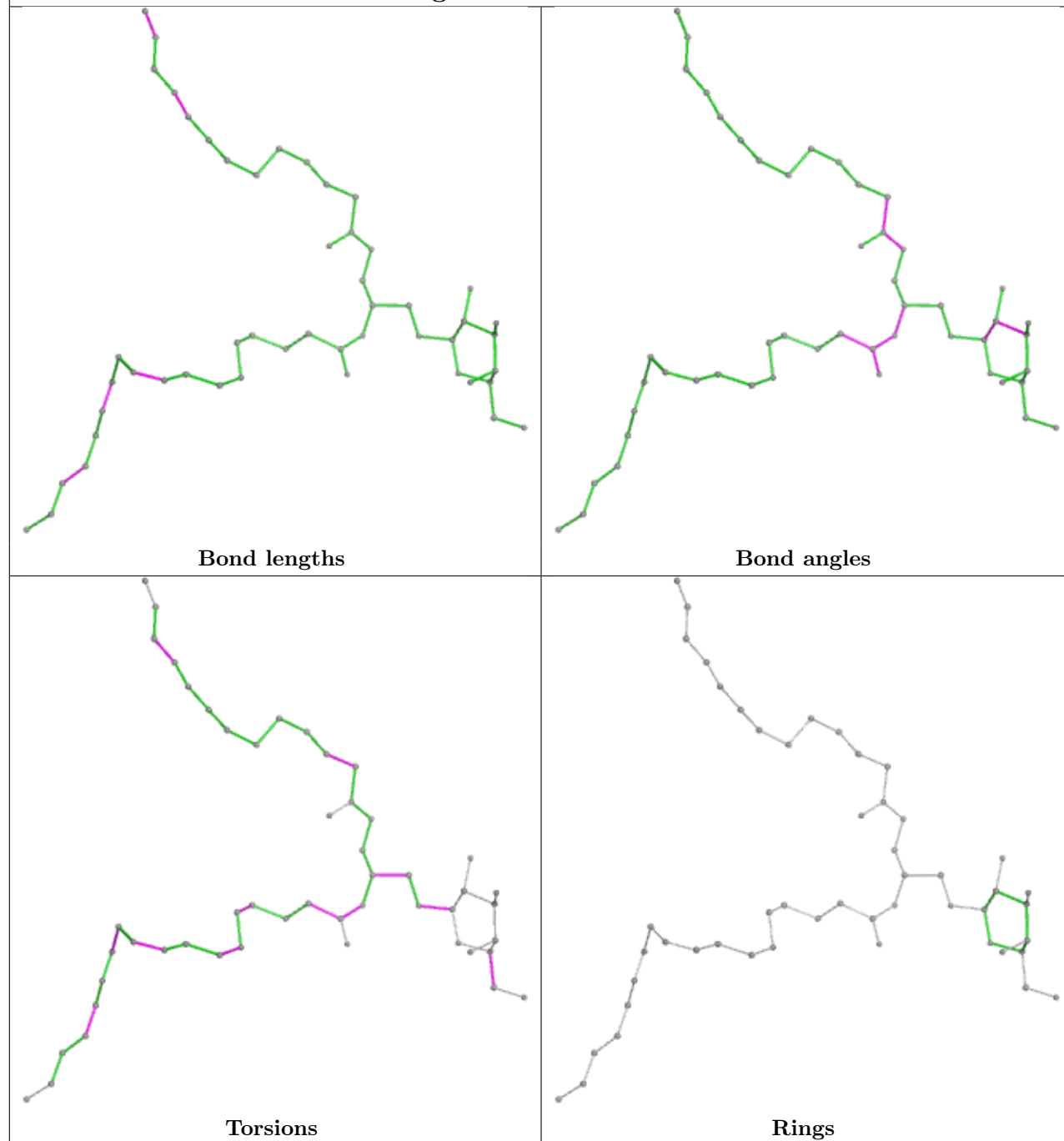
Ligand CHL 4 611

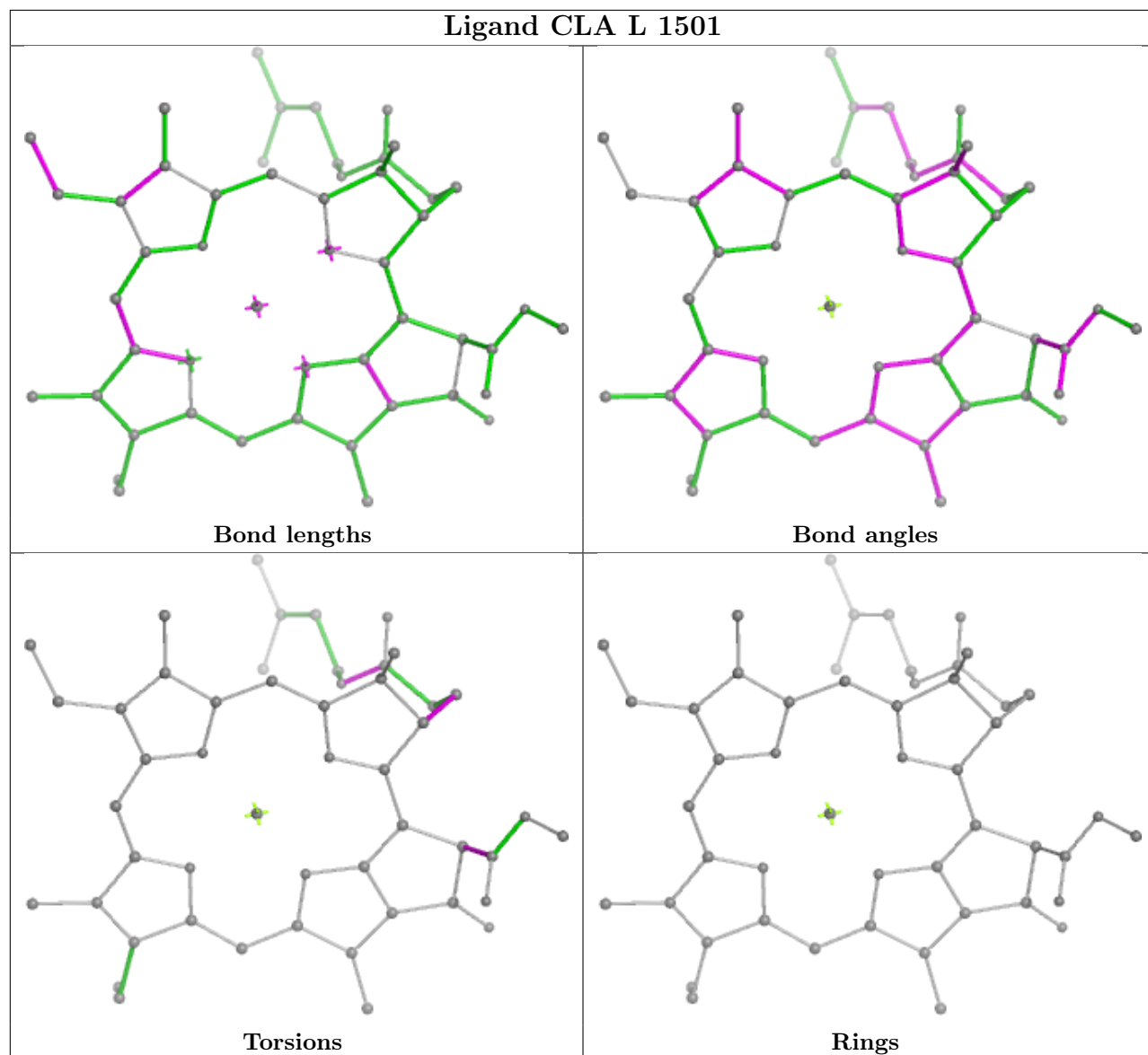


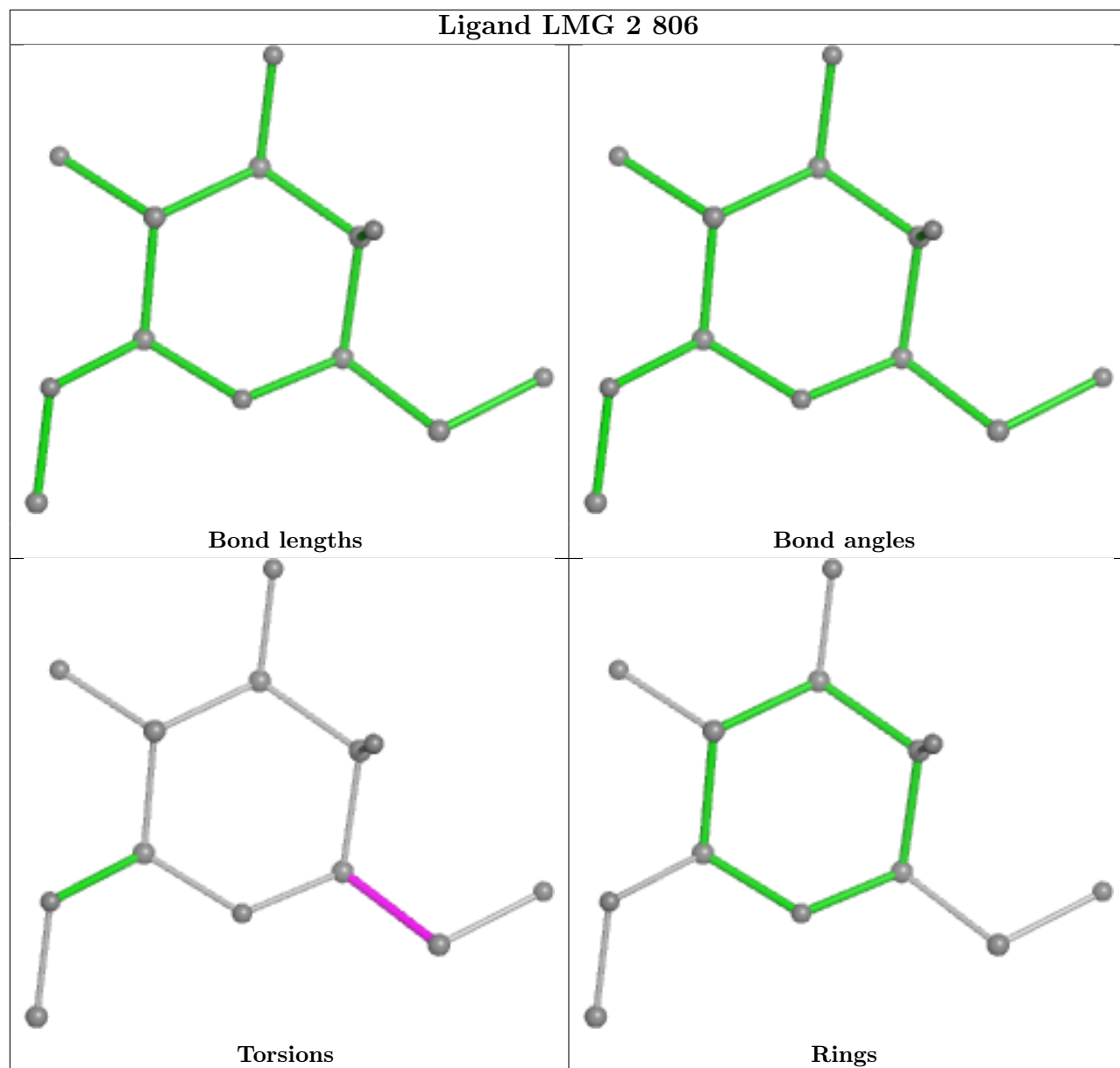


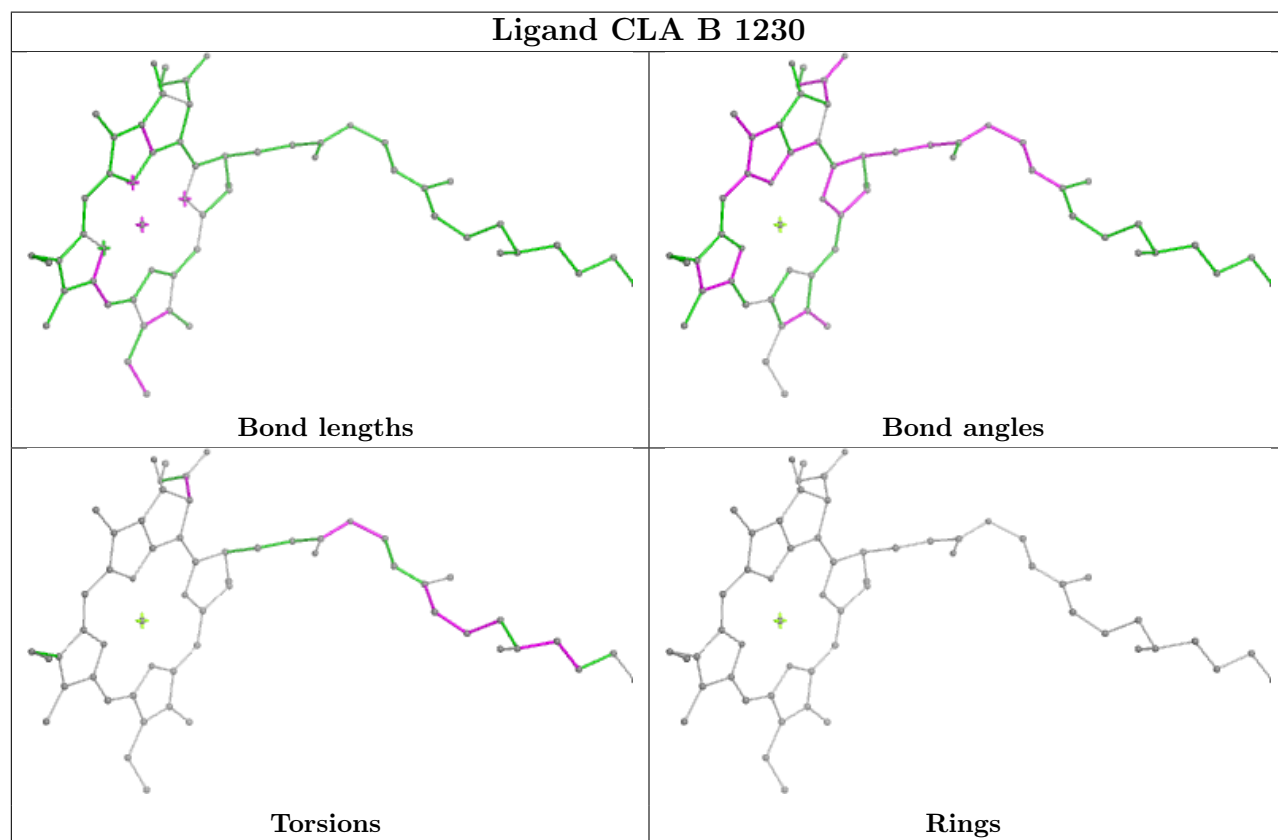
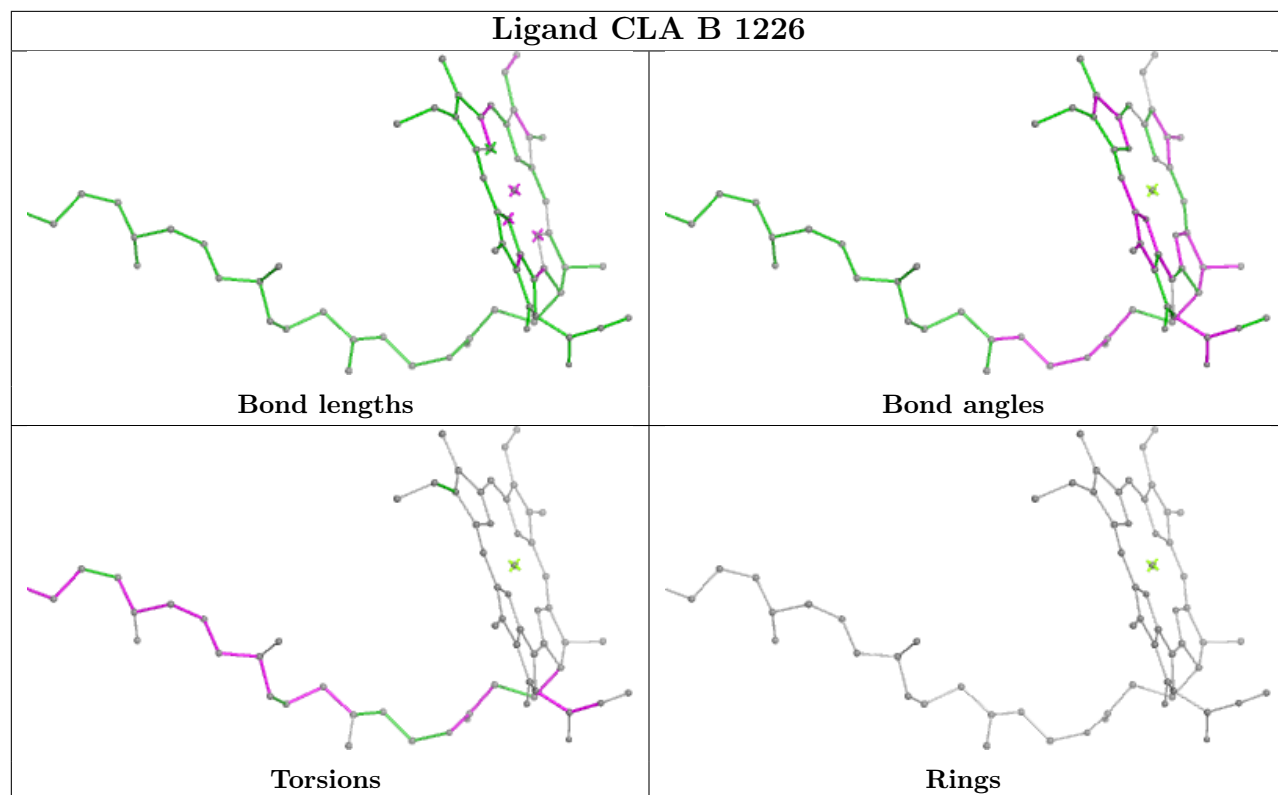


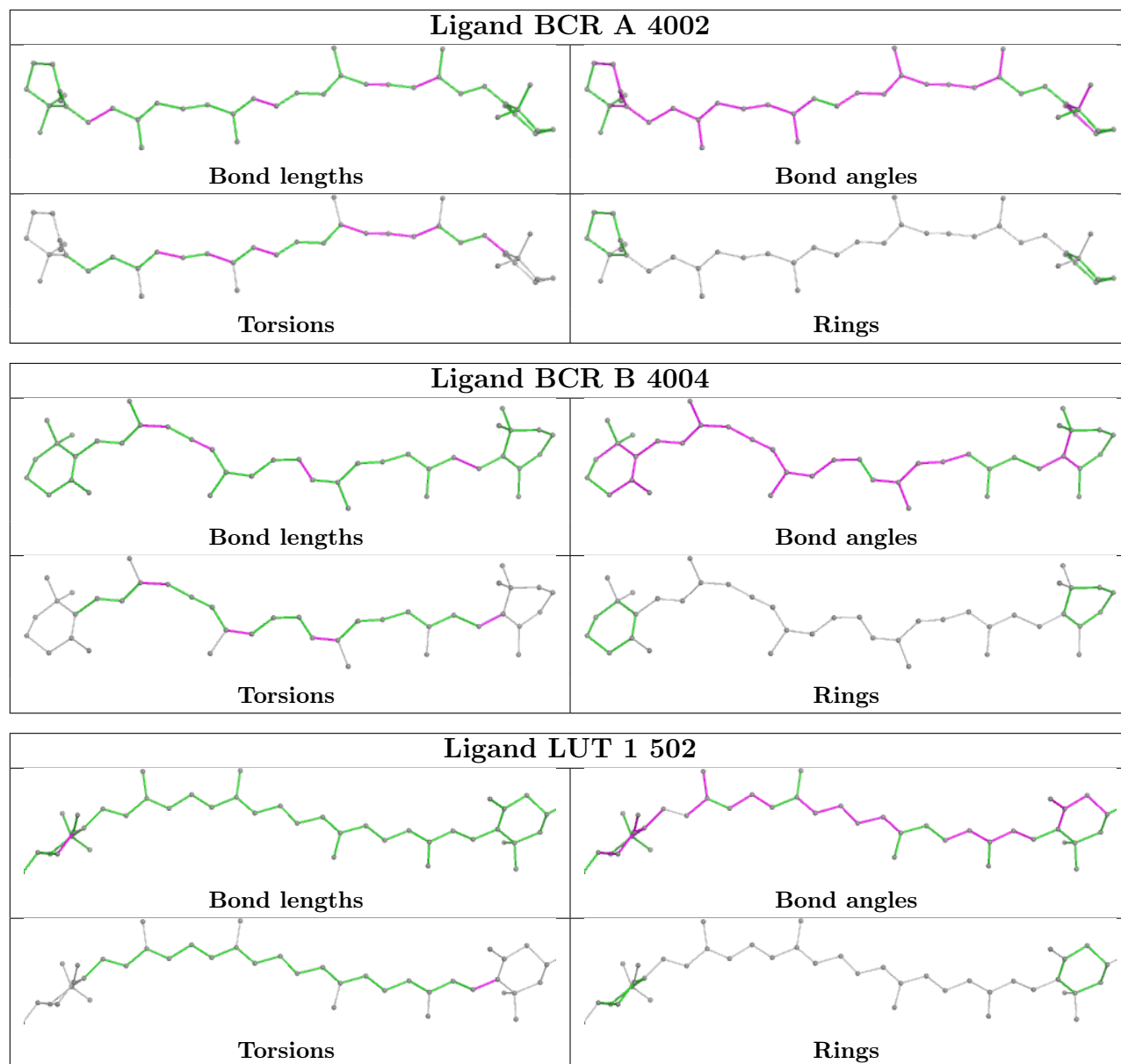
Ligand LMG A 5006



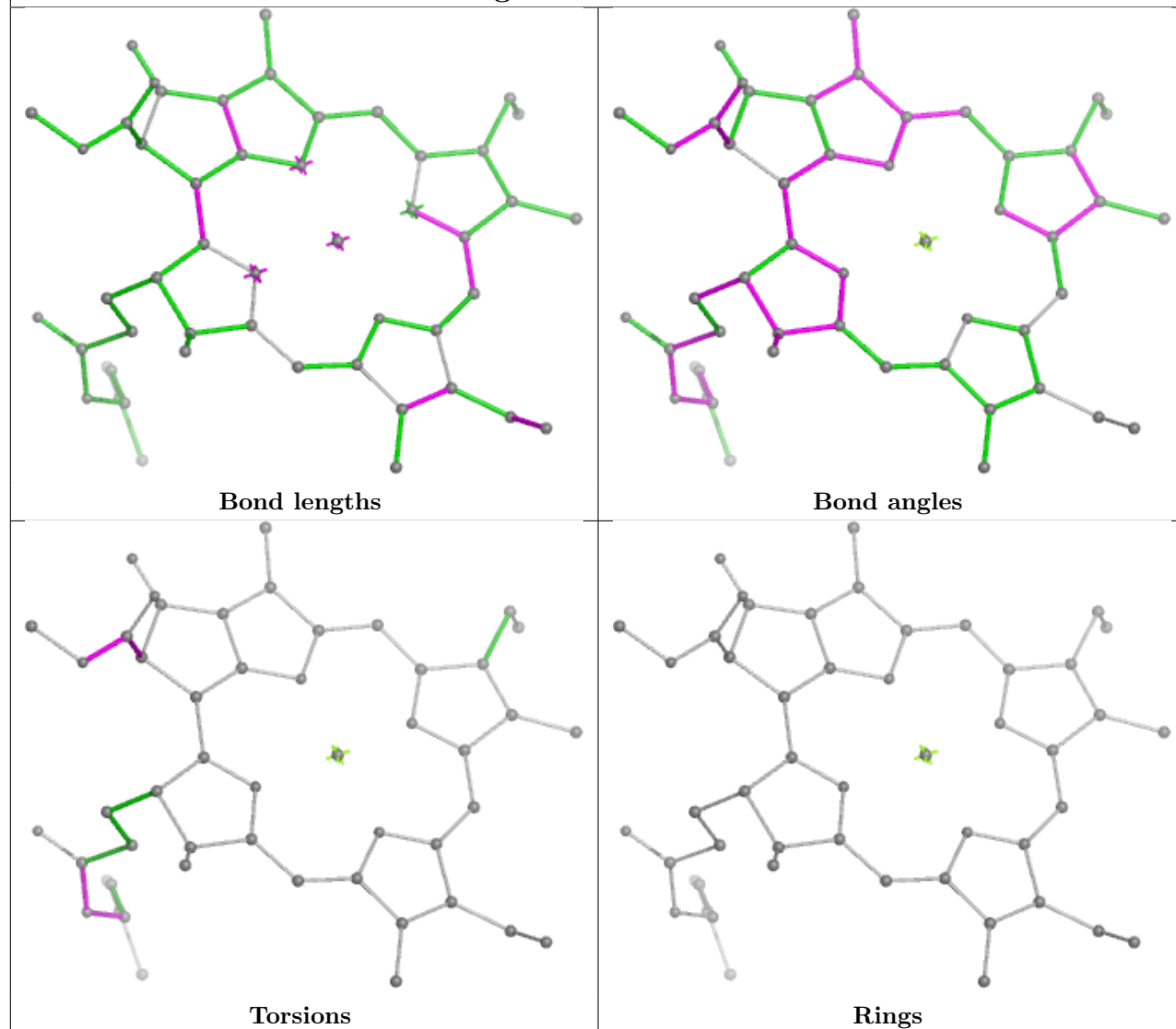




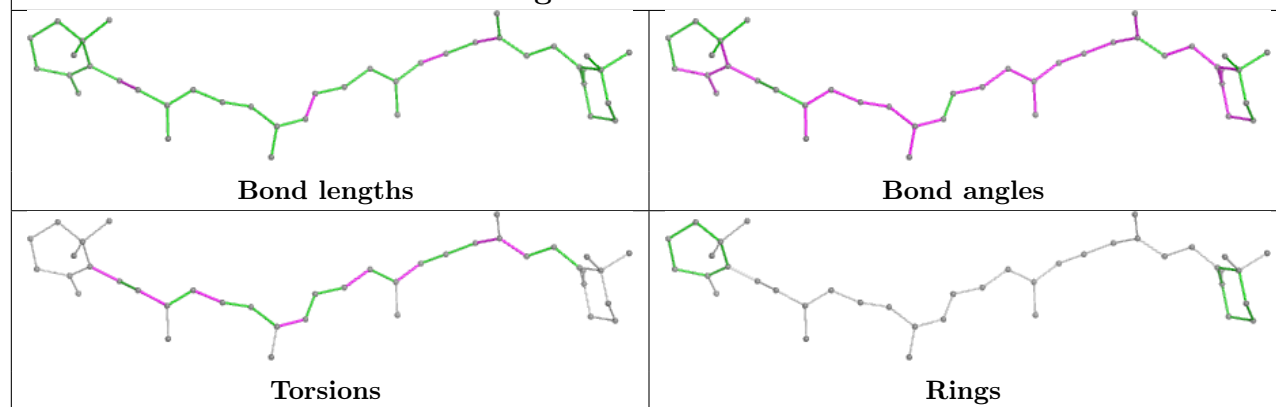


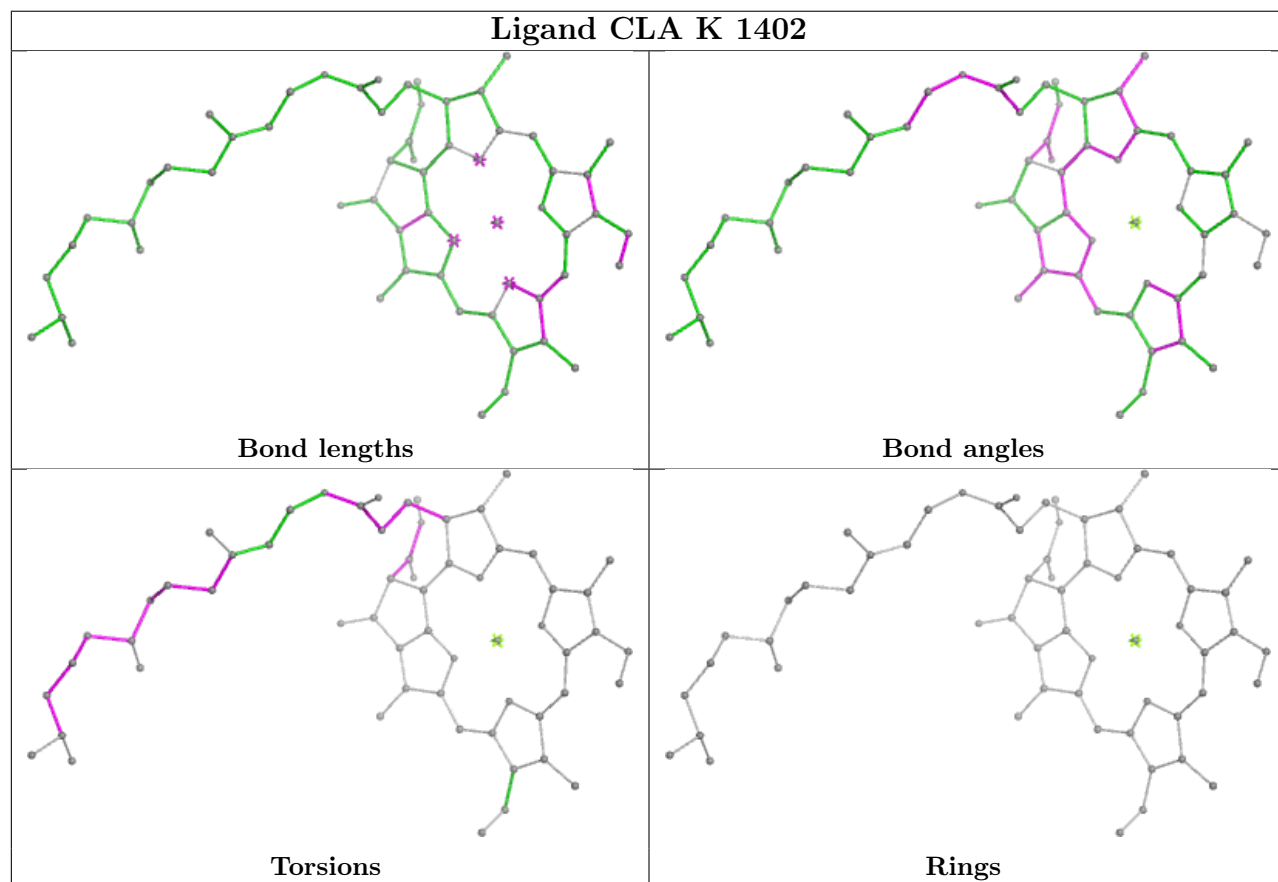
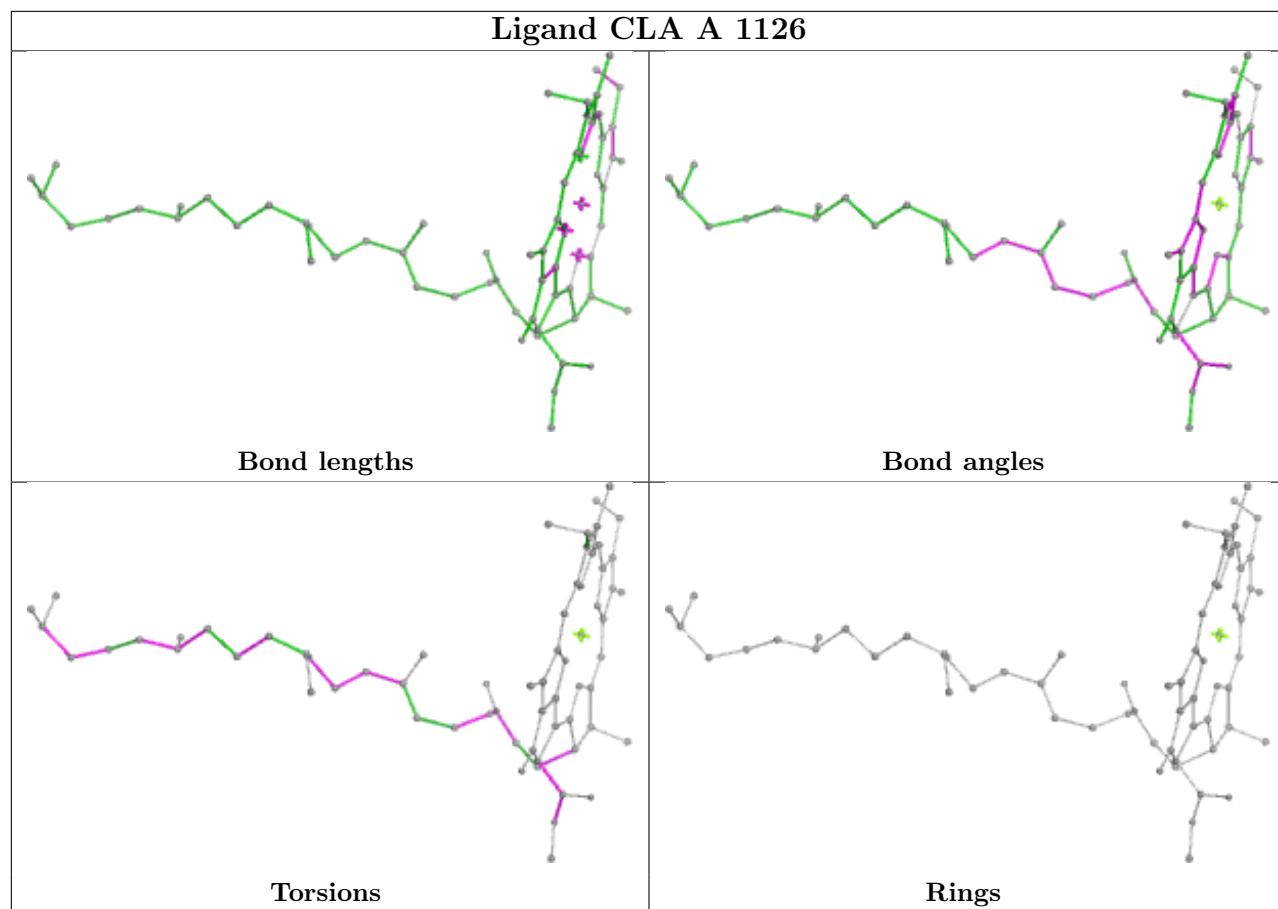


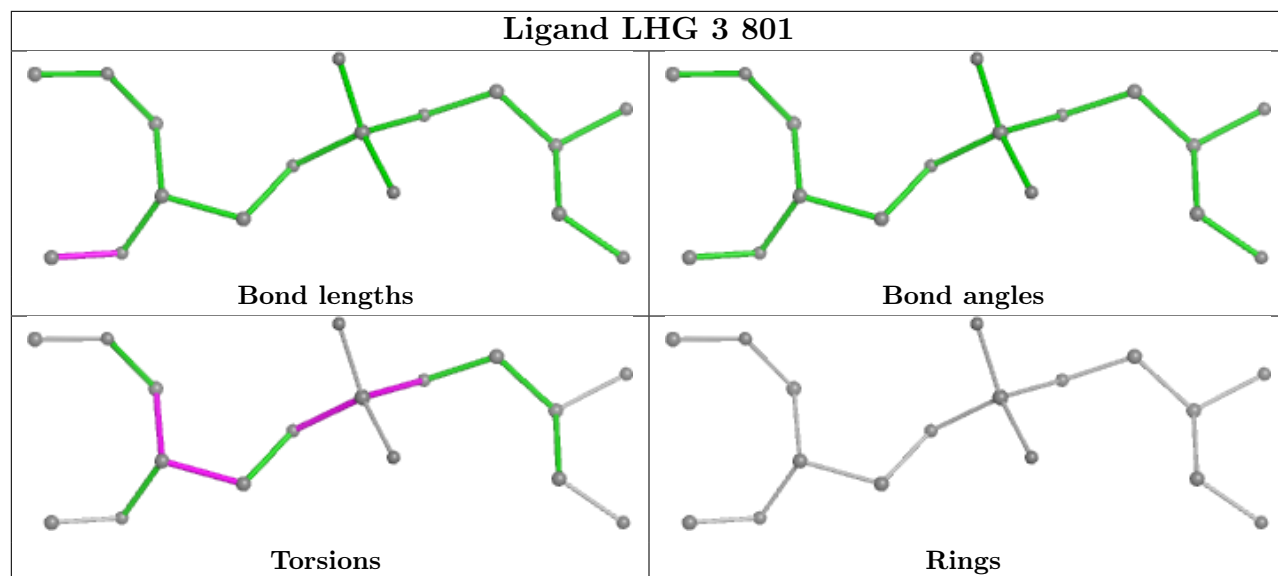
Ligand CLA 1 606

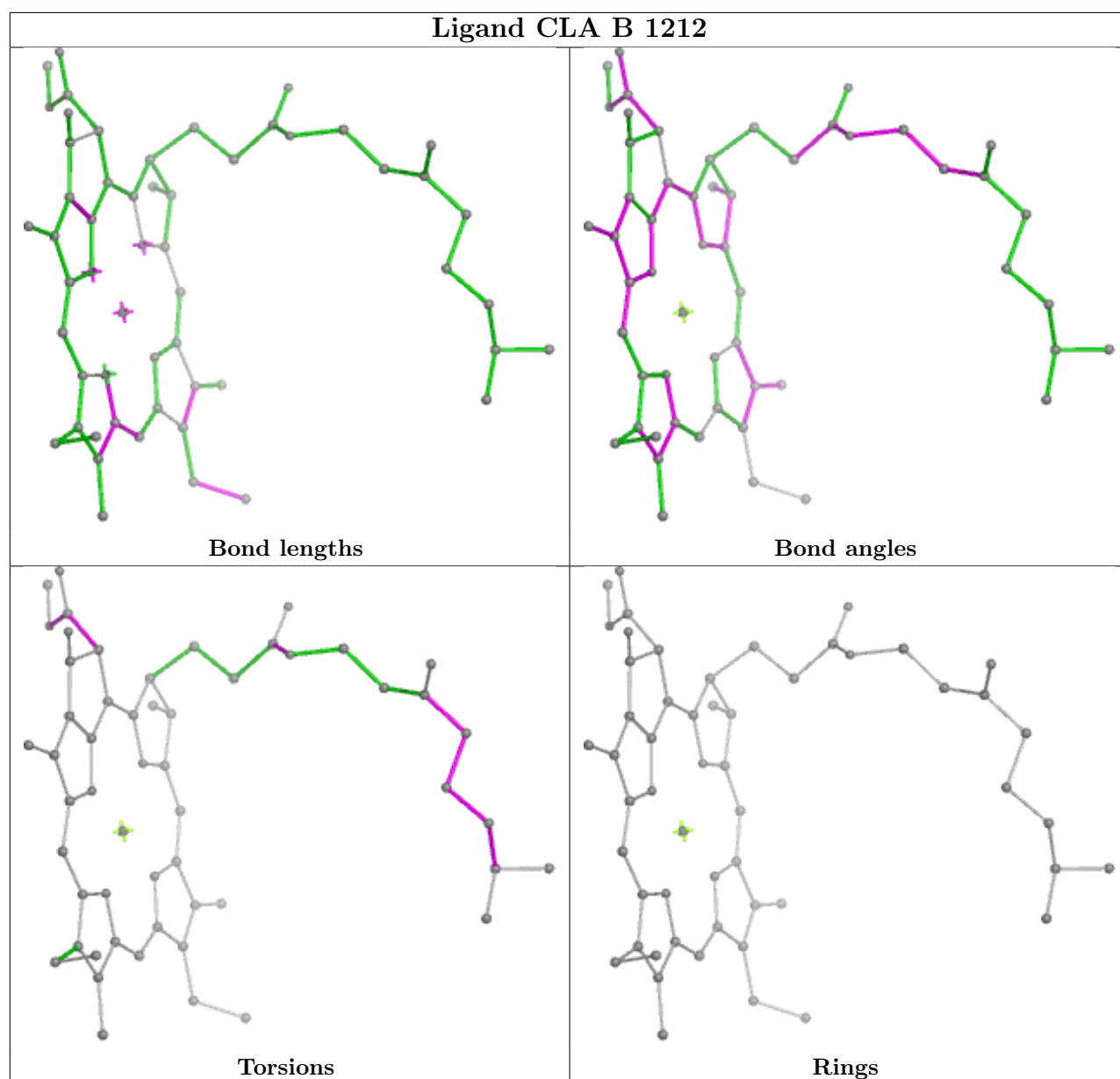


Ligand BCR 1 504

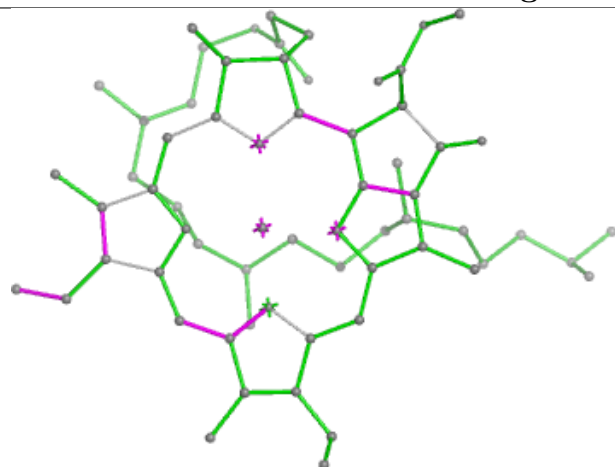




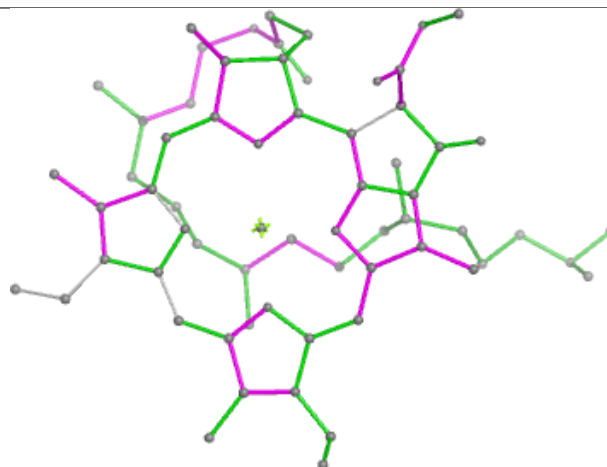




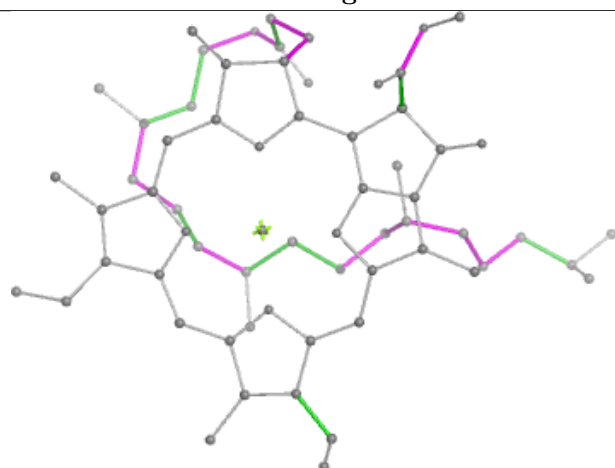
Ligand CLA 3 610



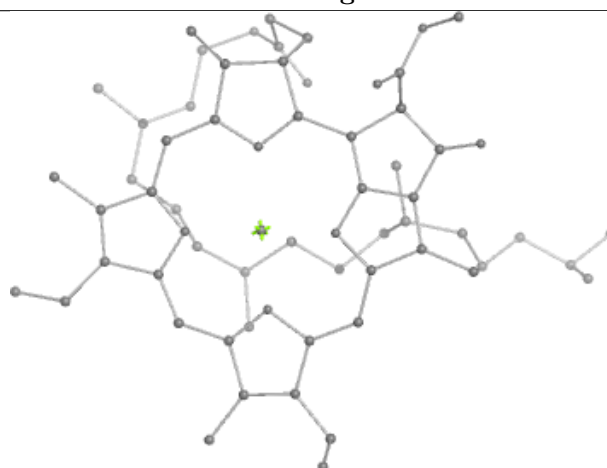
Bond lengths



Bond angles

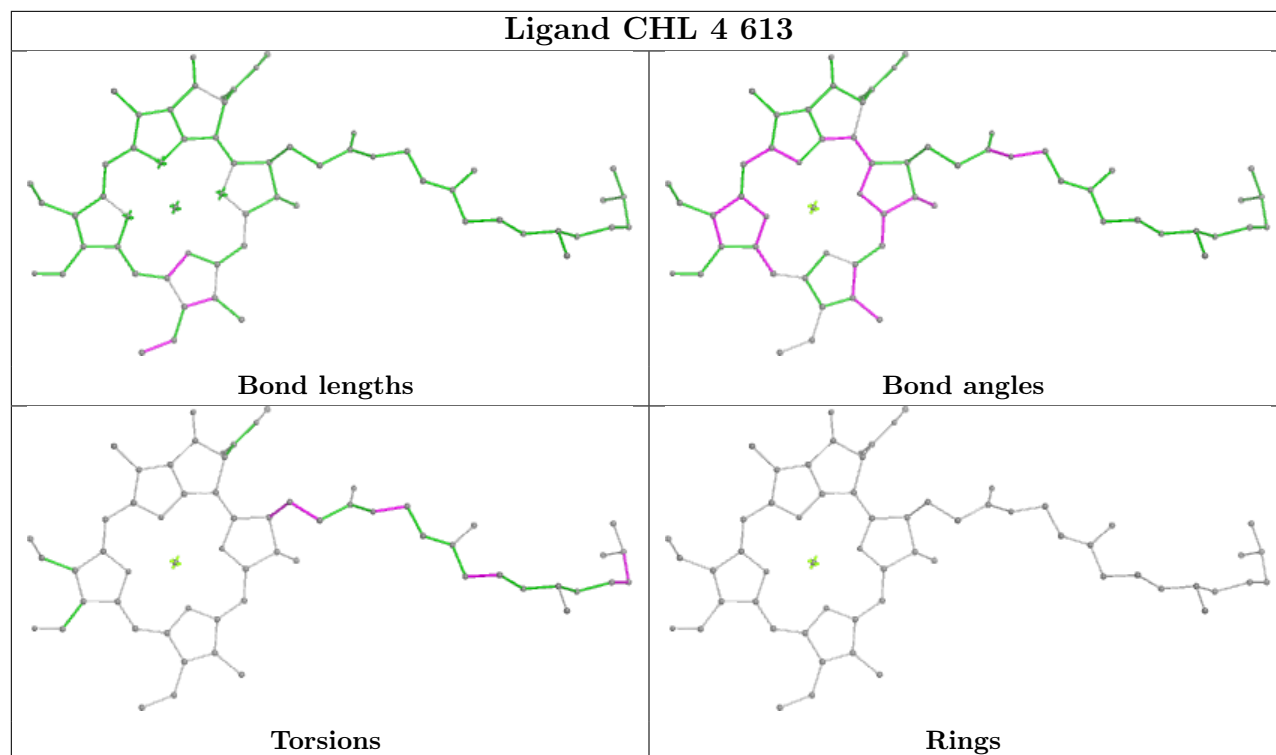


Torsions

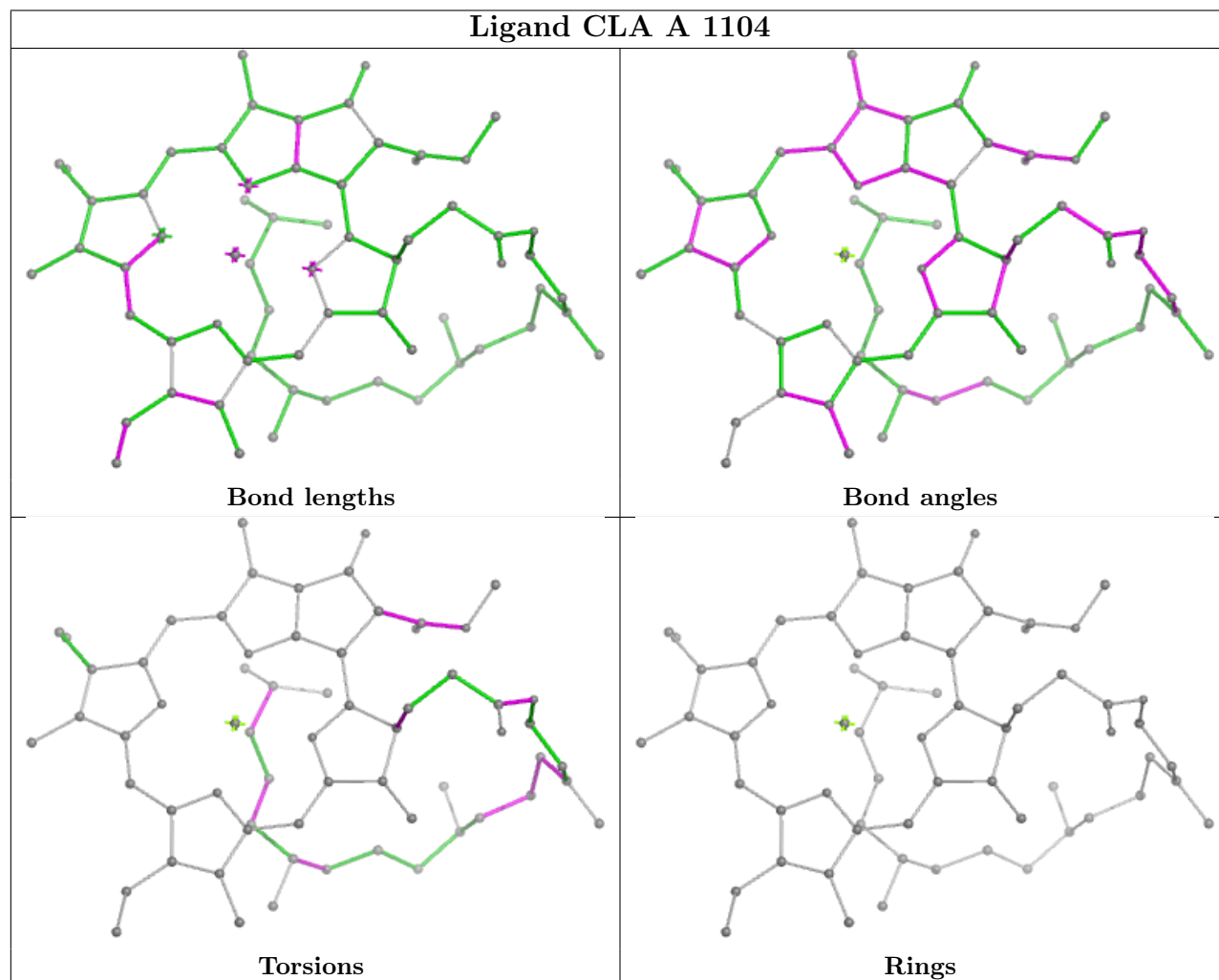


Rings

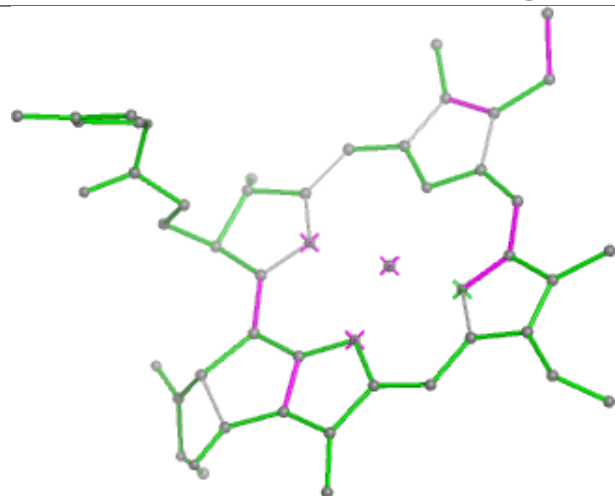
Ligand CHL 4 613



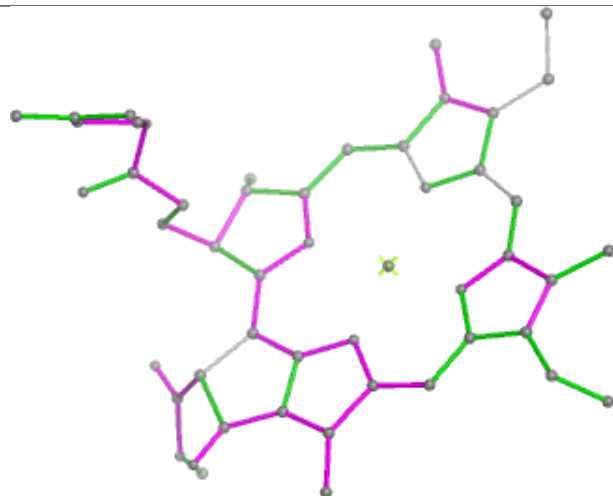
Ligand CLA A 1104



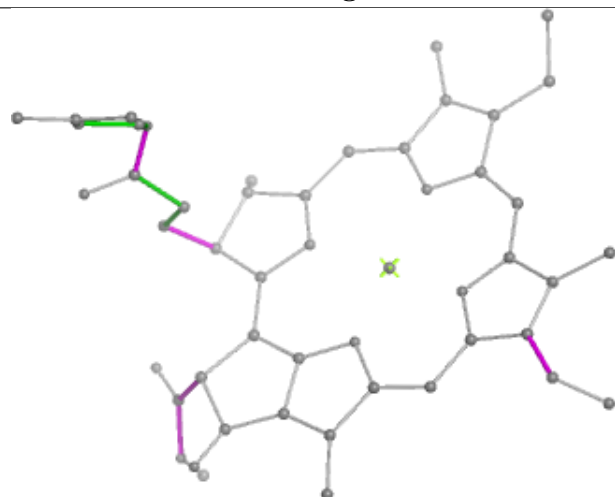
Ligand CLA 3 606



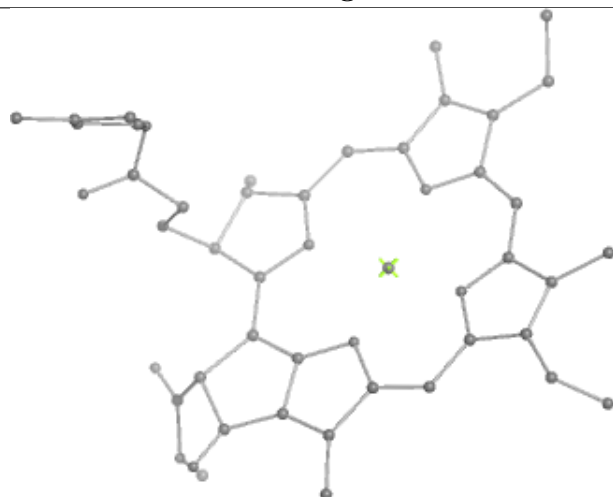
Bond lengths



Bond angles

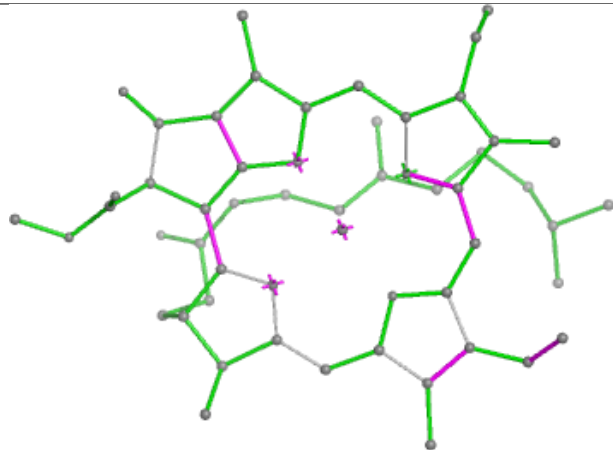


Torsions

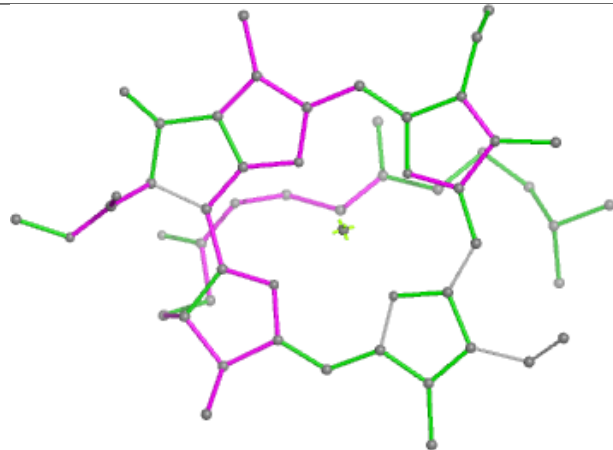


Rings

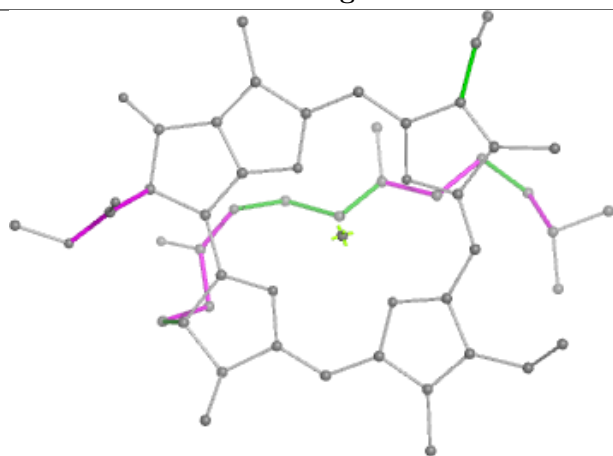
Ligand CLA 3 603



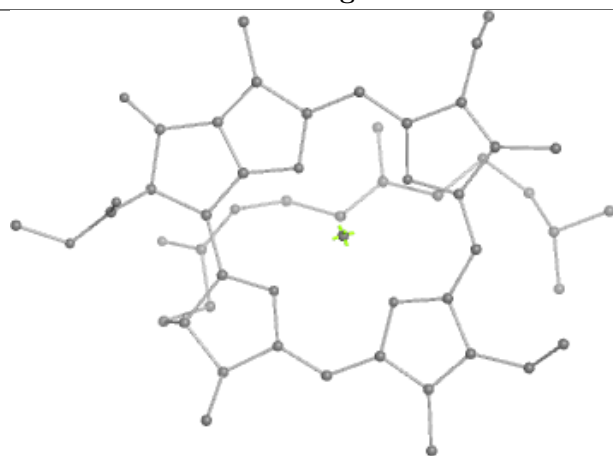
Bond lengths



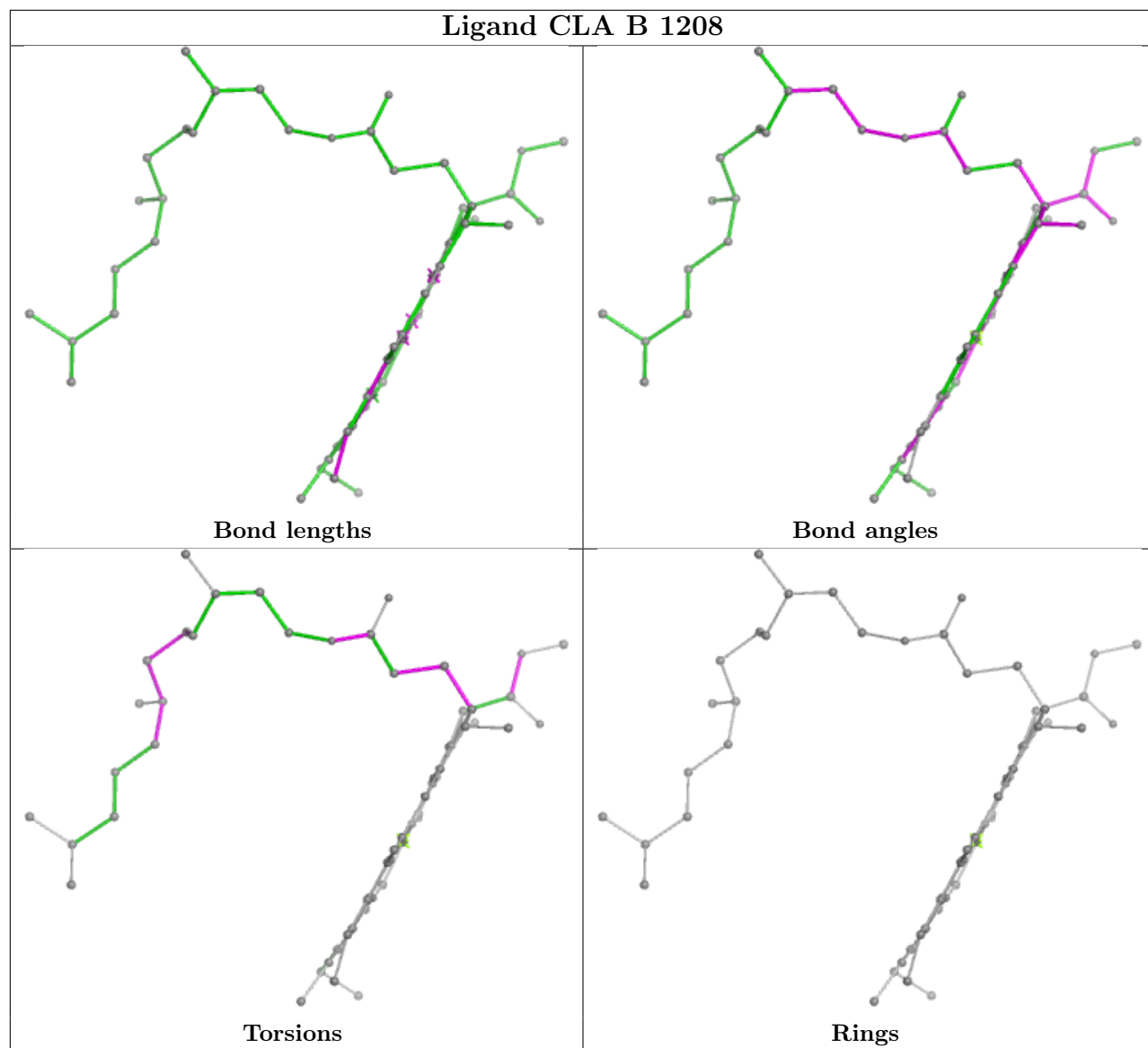
Bond angles

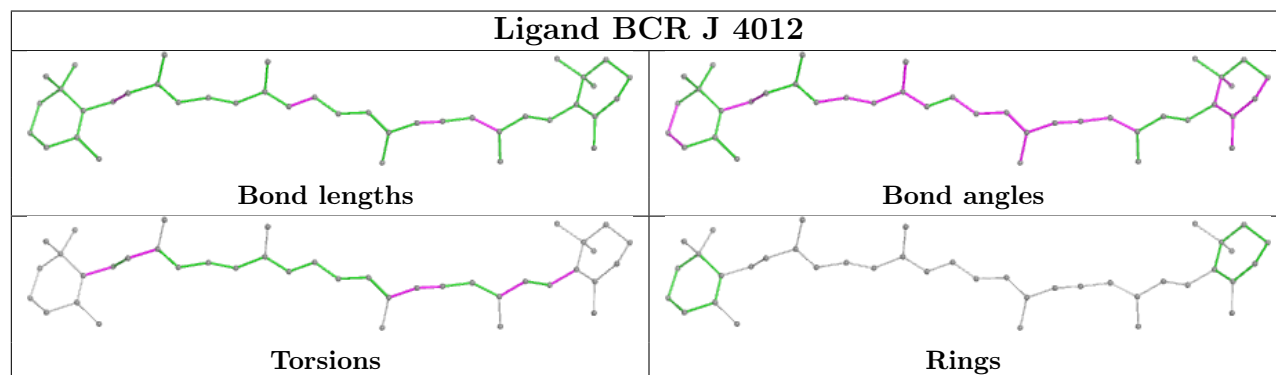
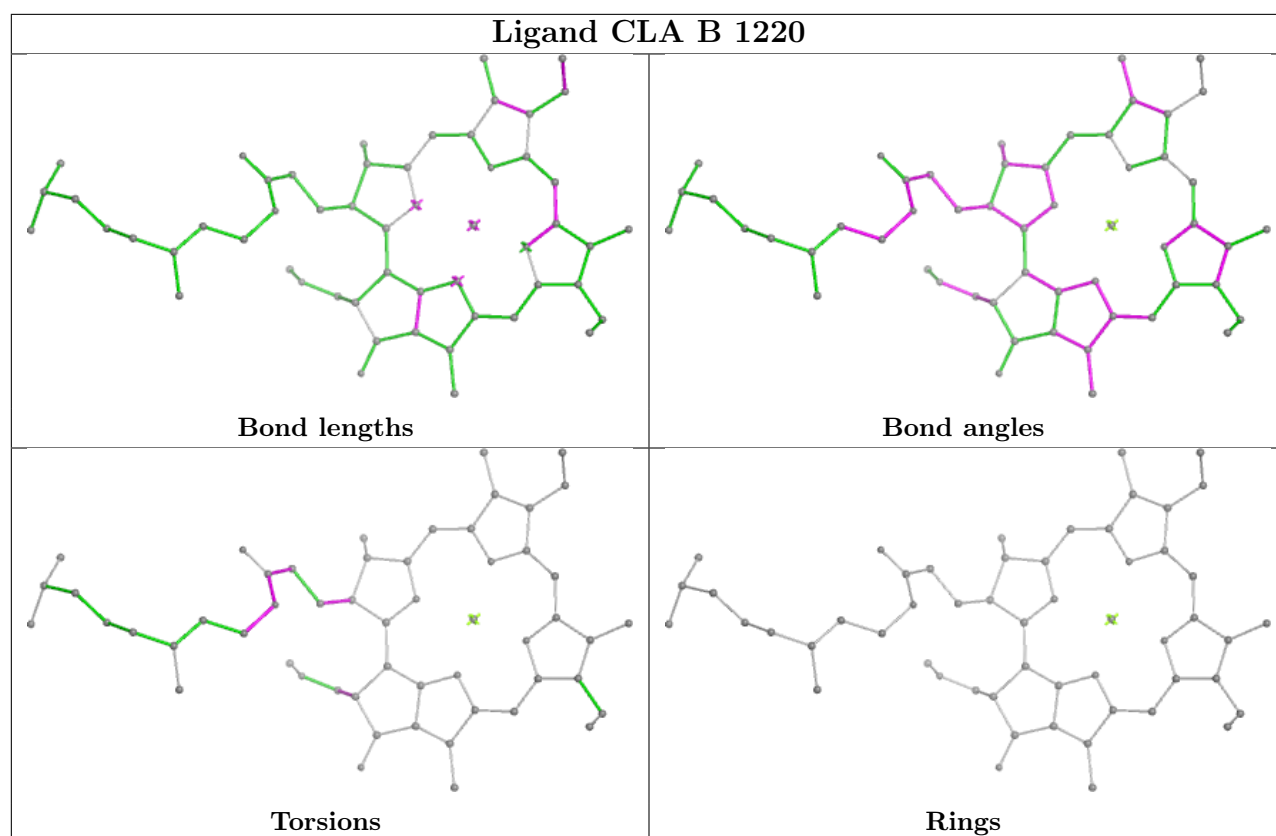


Torsions

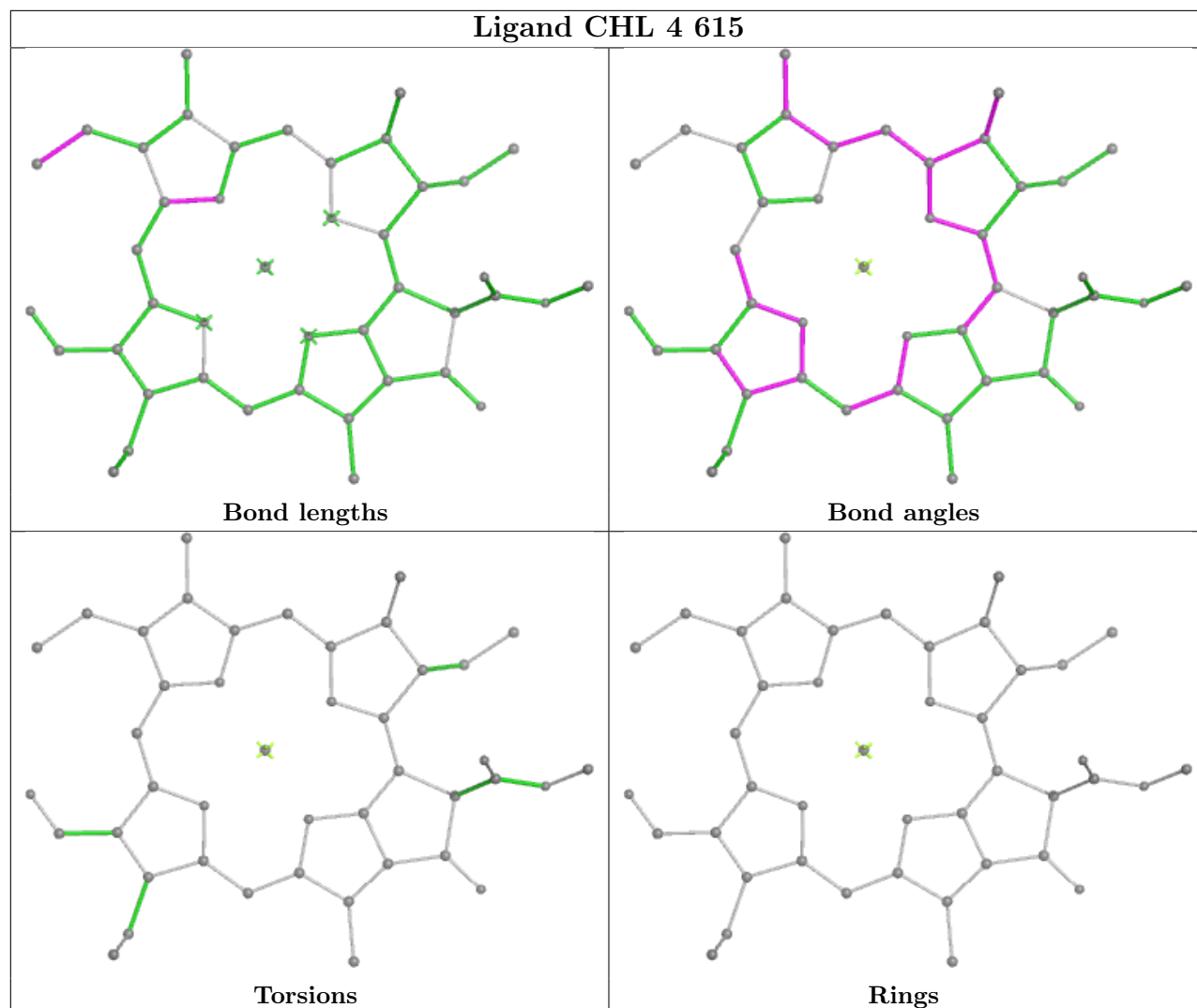


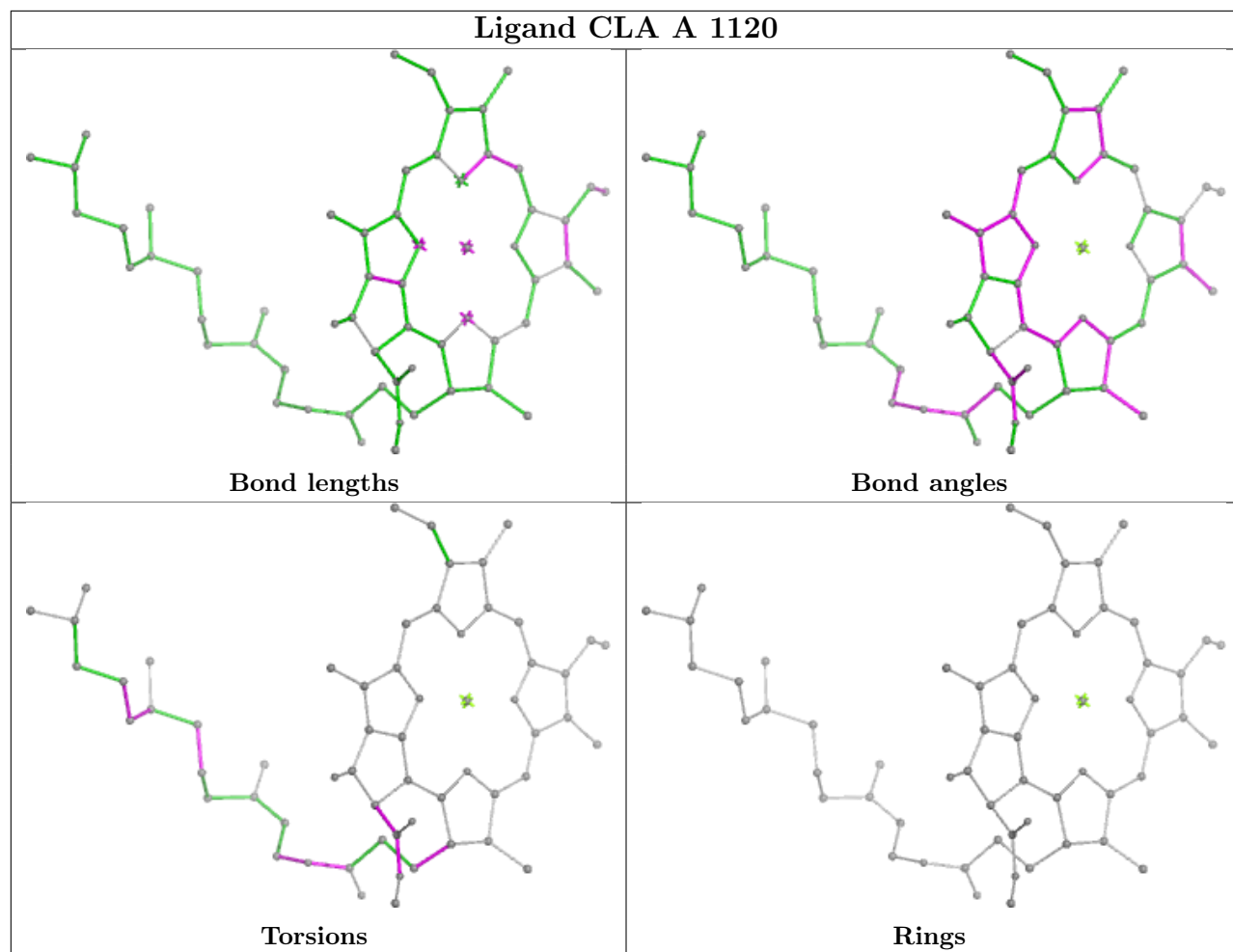
Rings

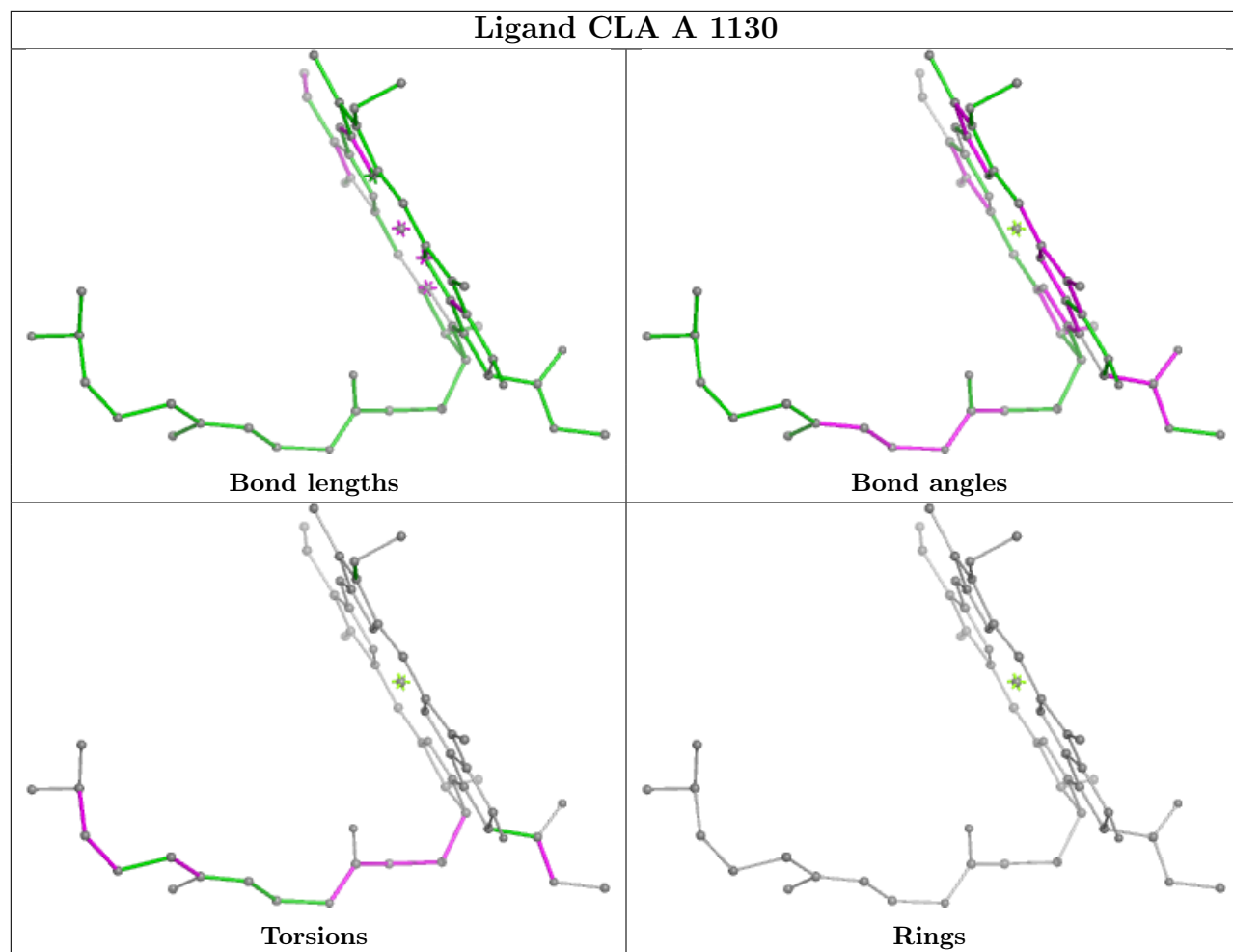


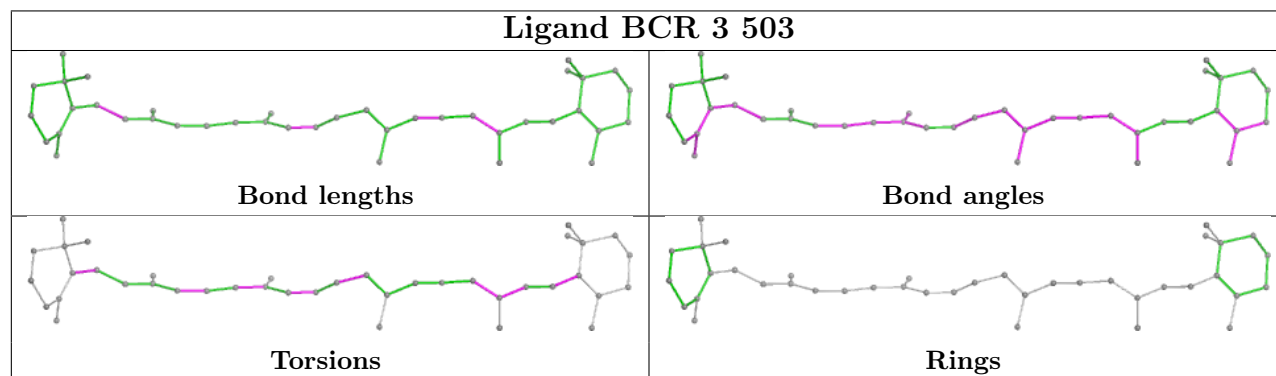
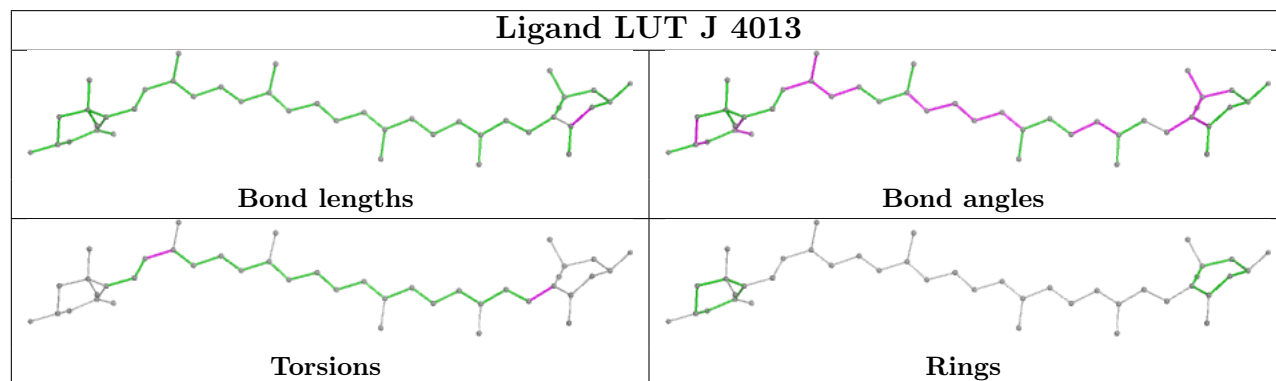
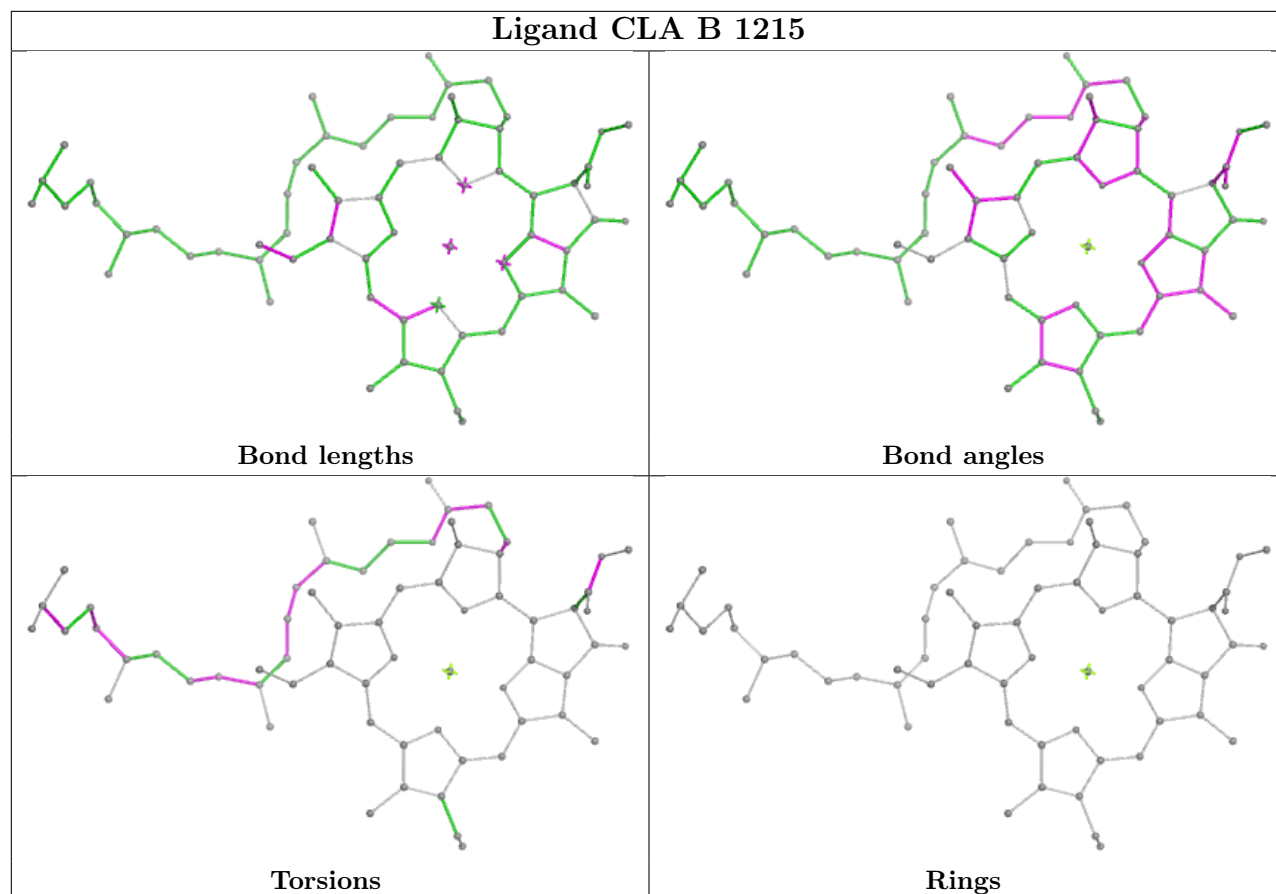


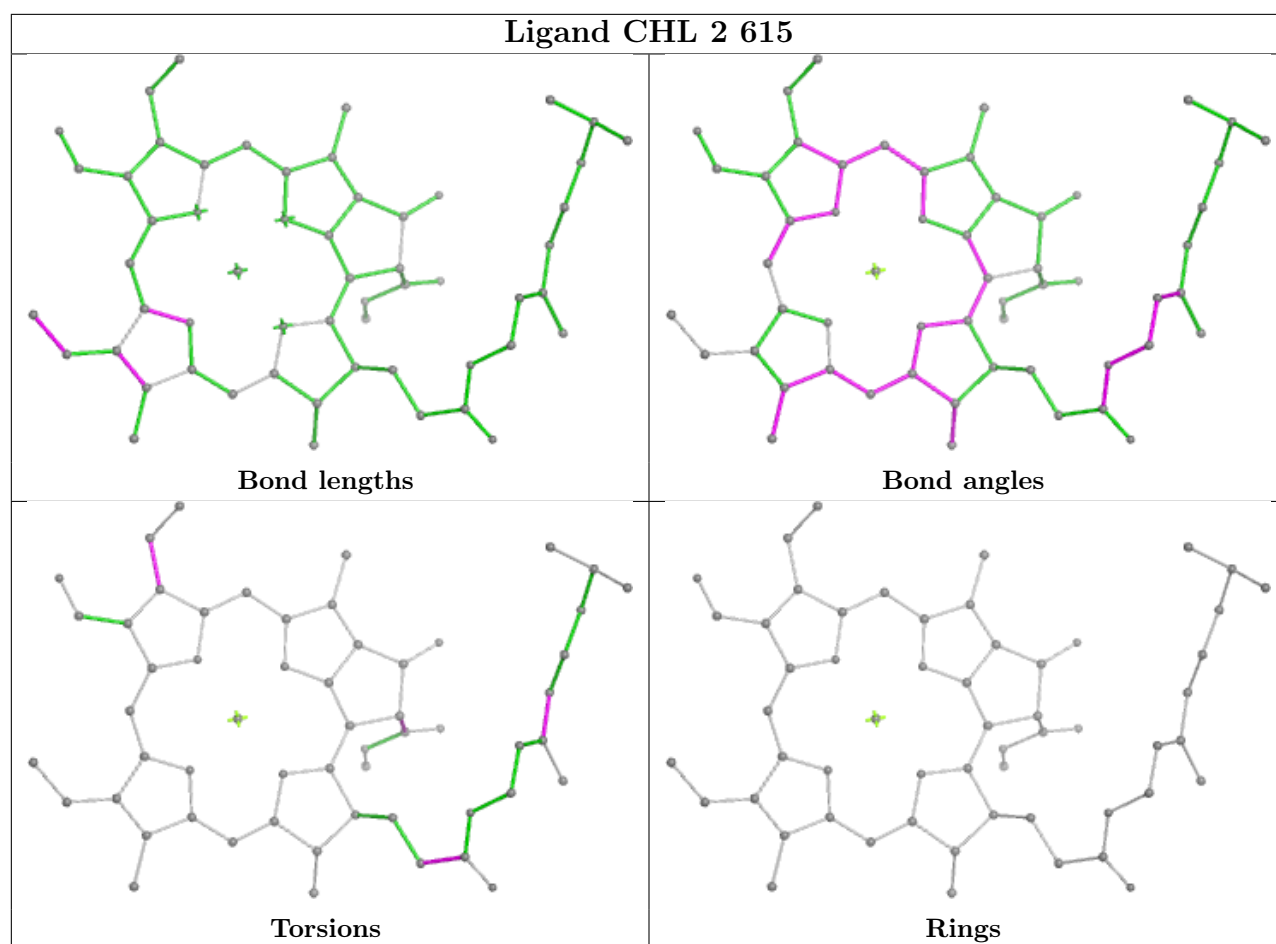
Ligand CHL 4 615

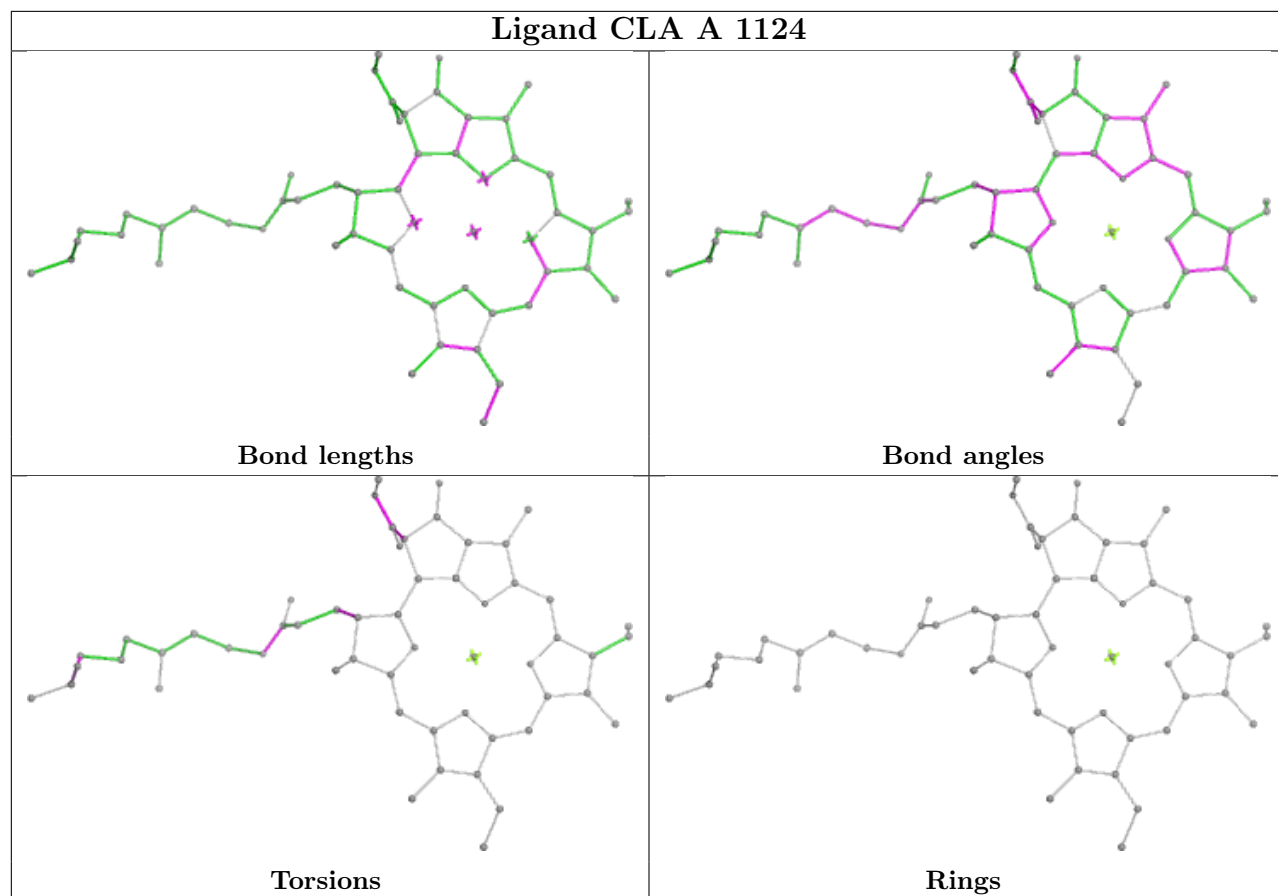




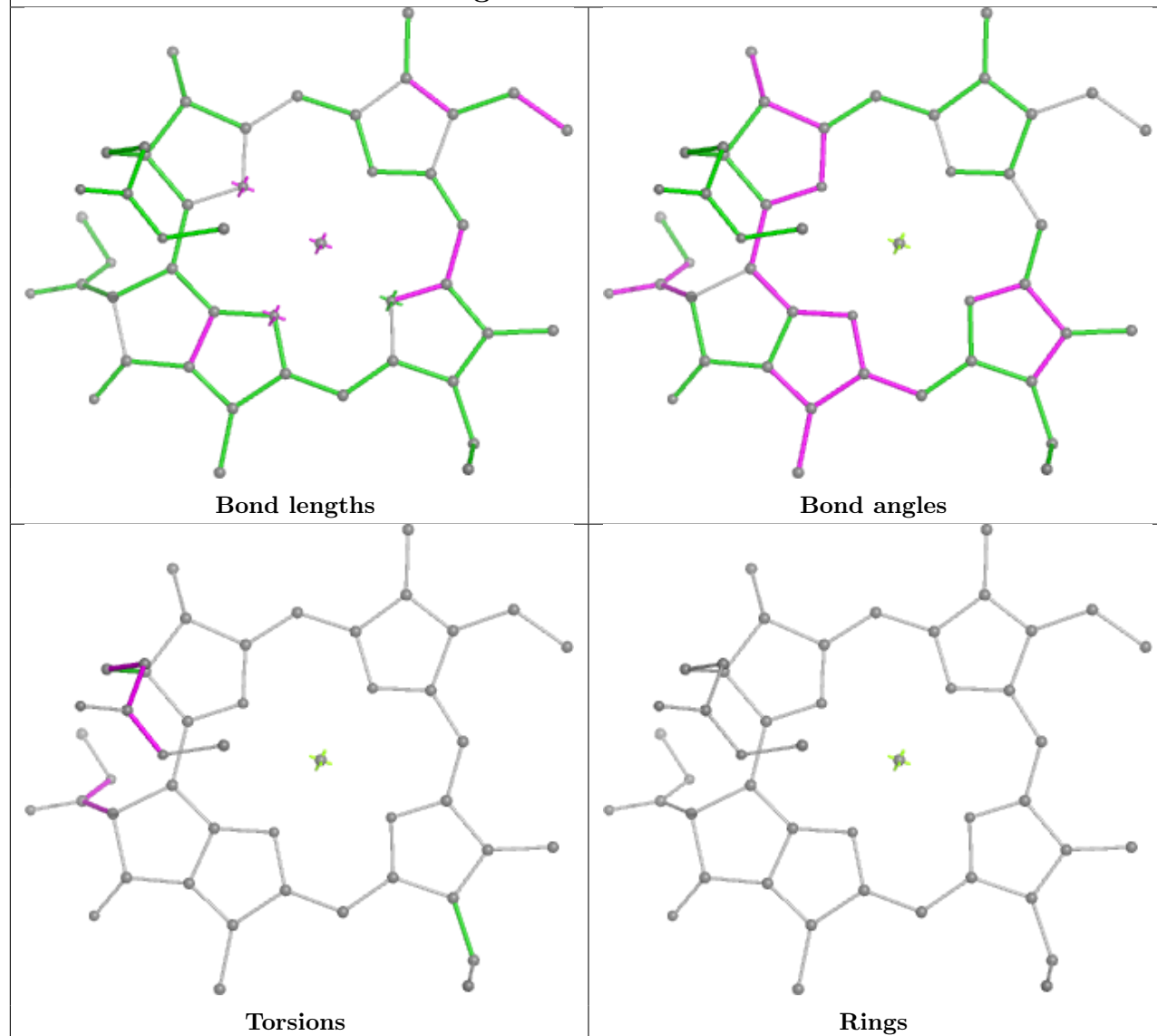




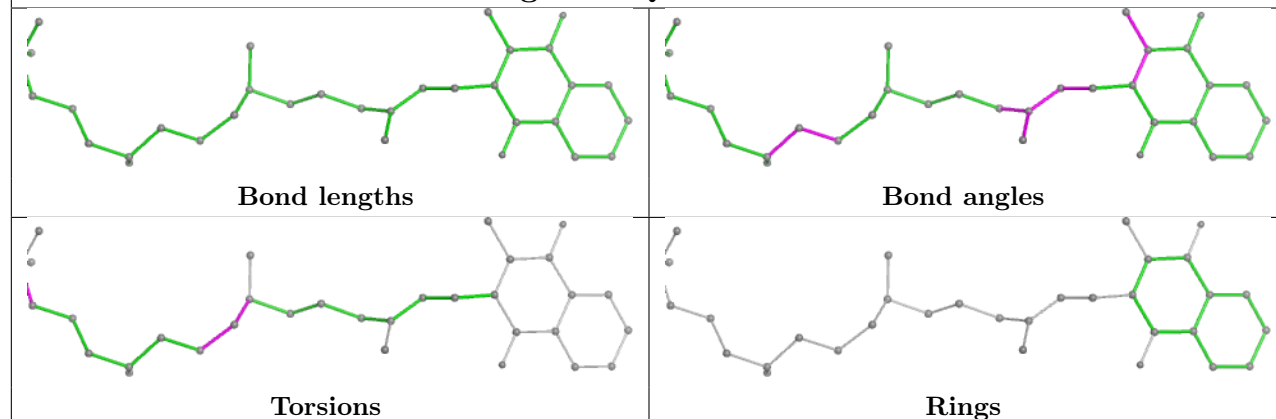


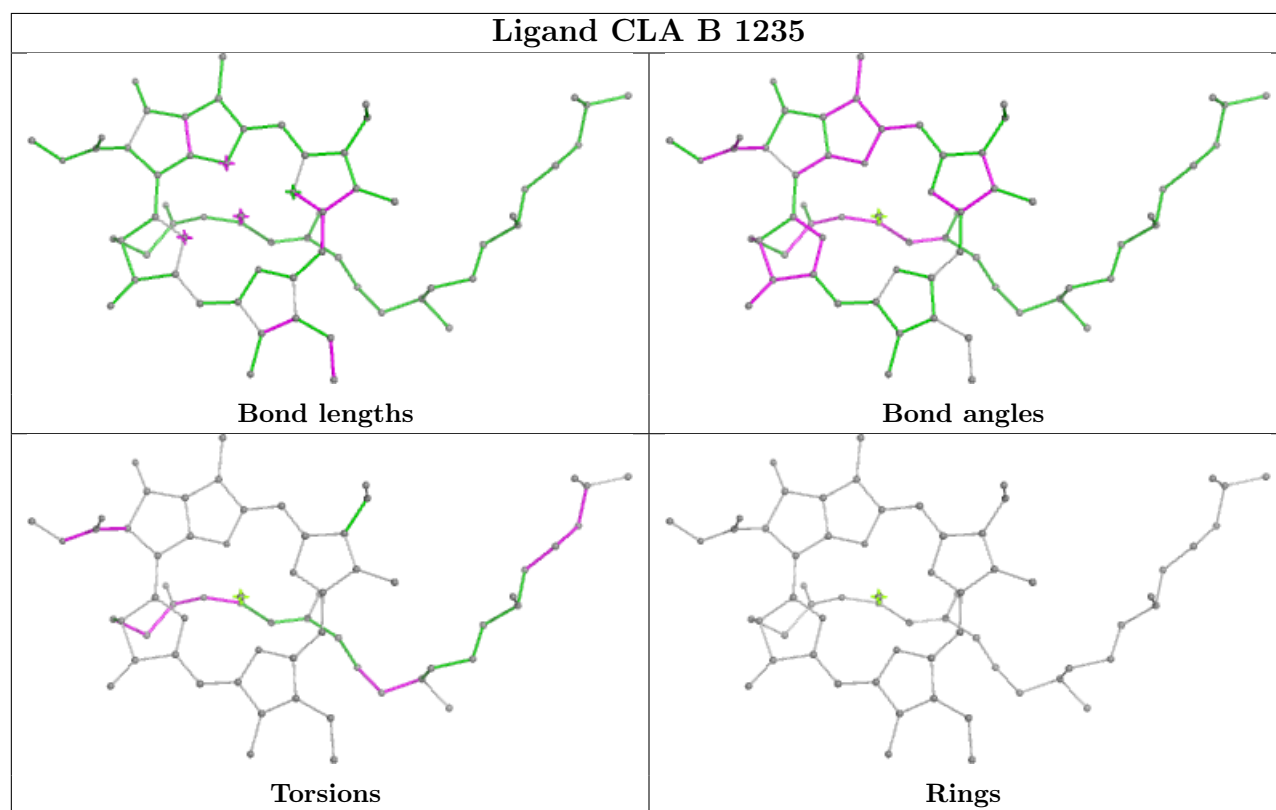
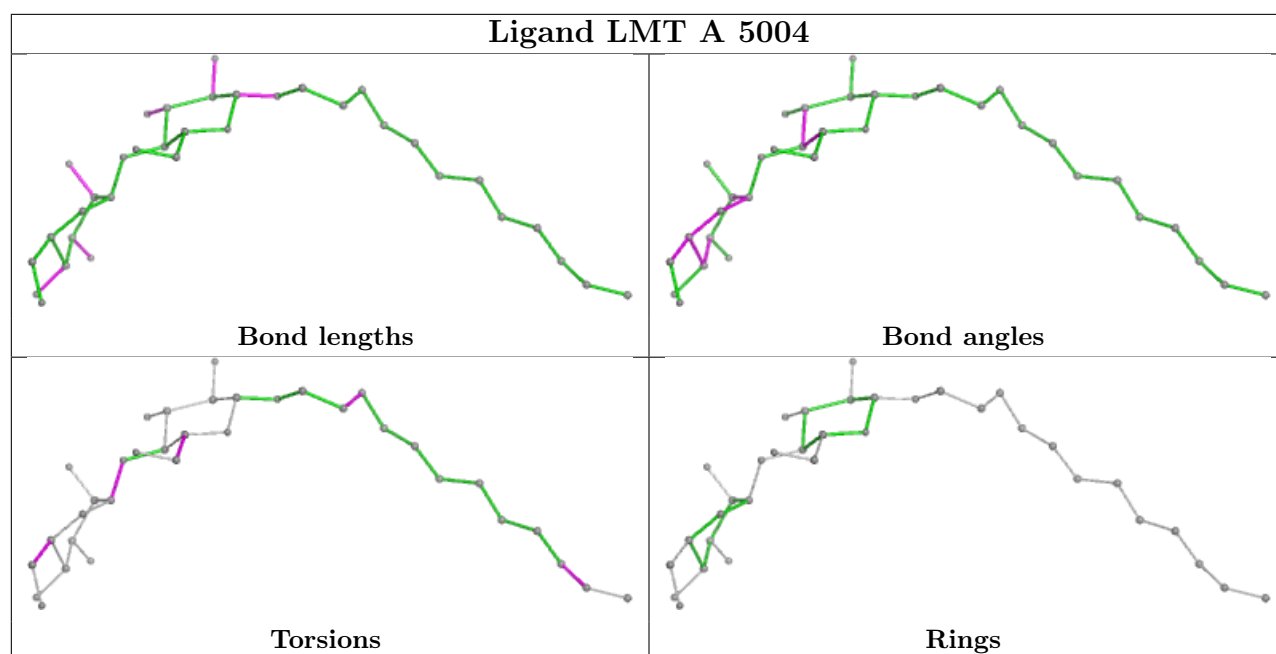


Ligand CLA A 1114

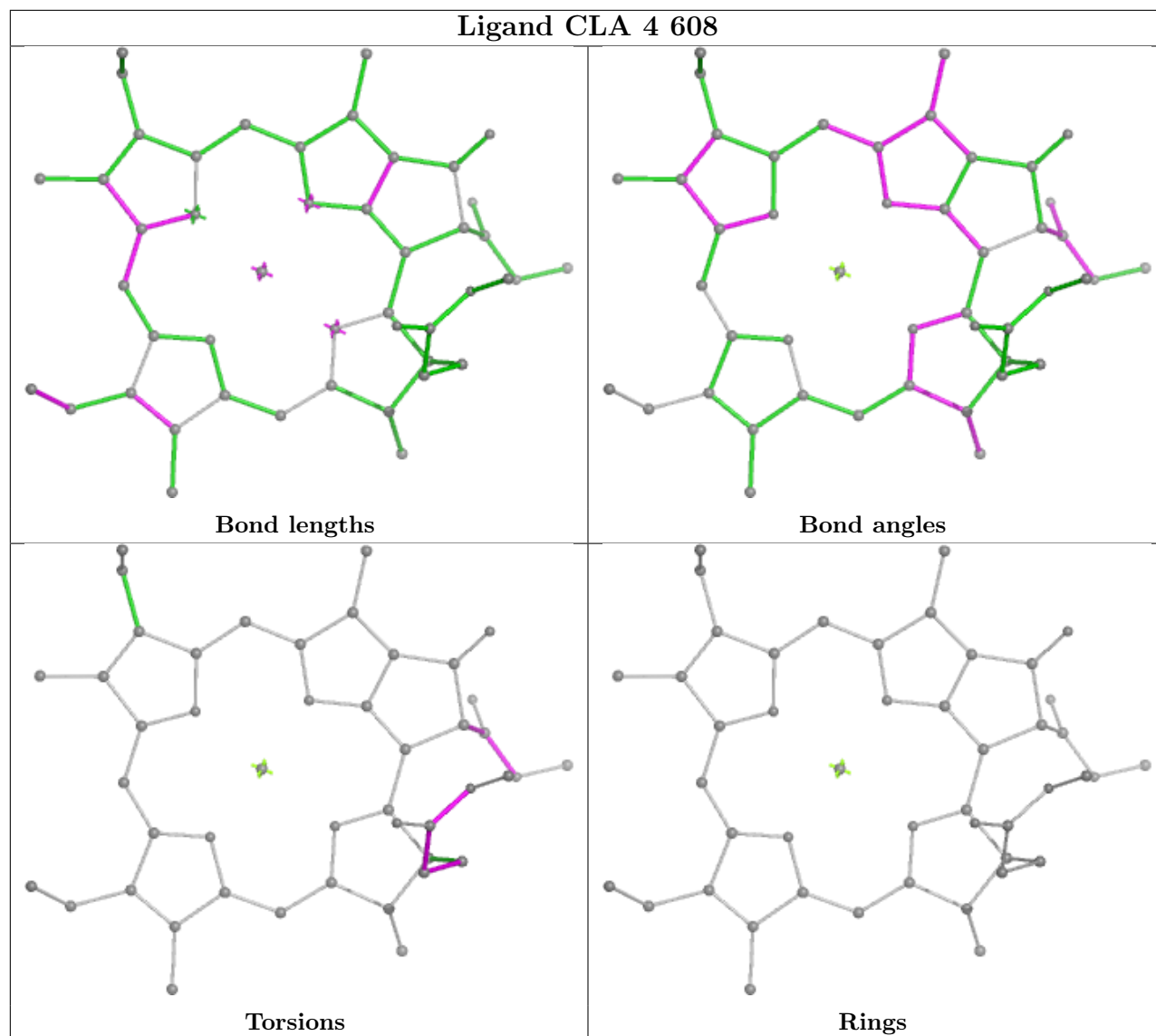


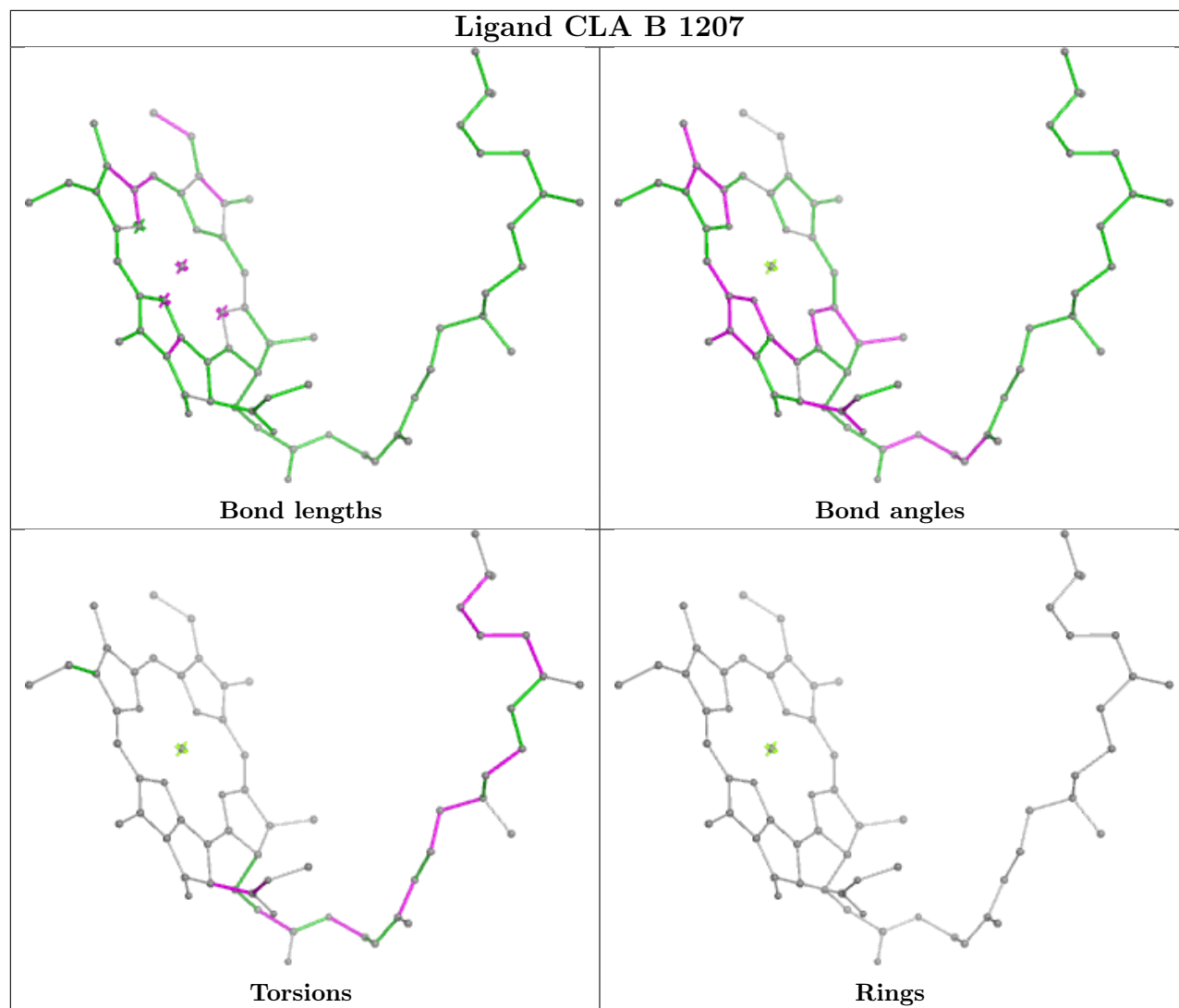
Ligand PQN A 2001

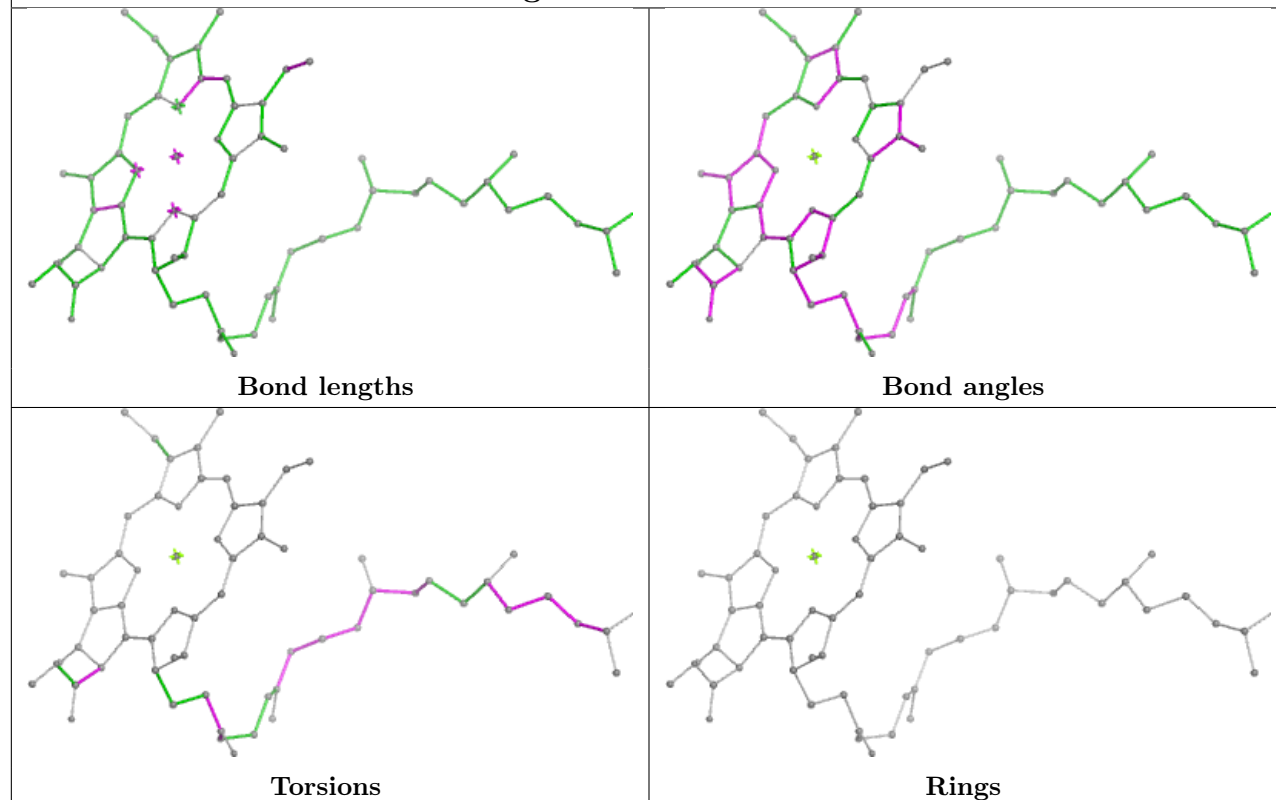
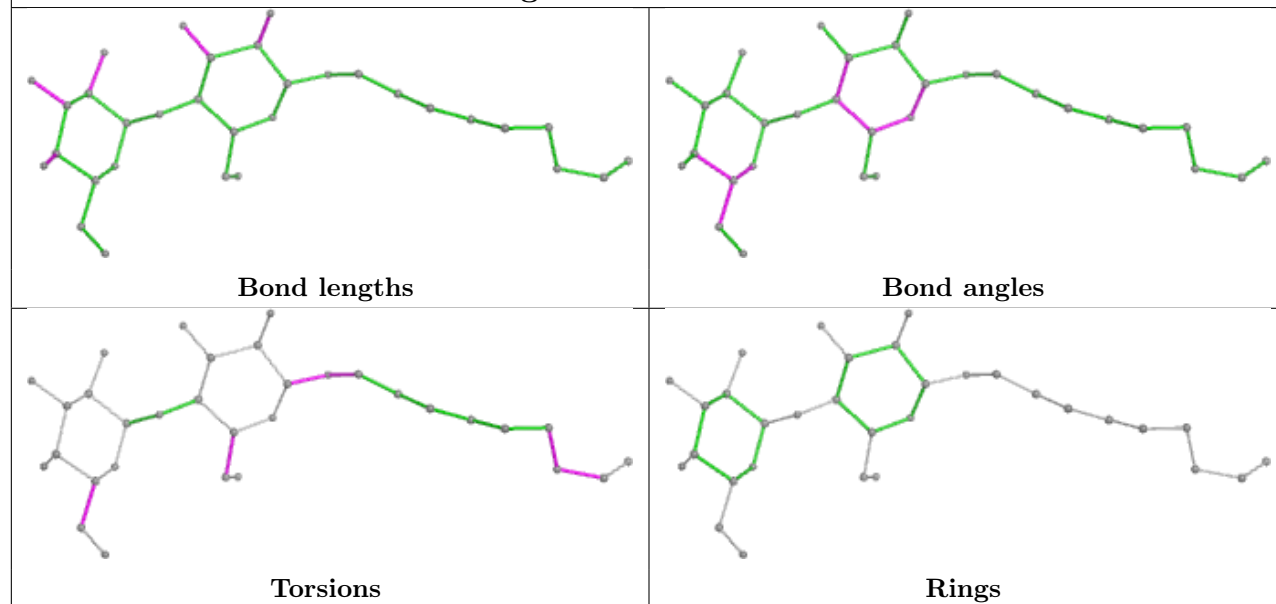


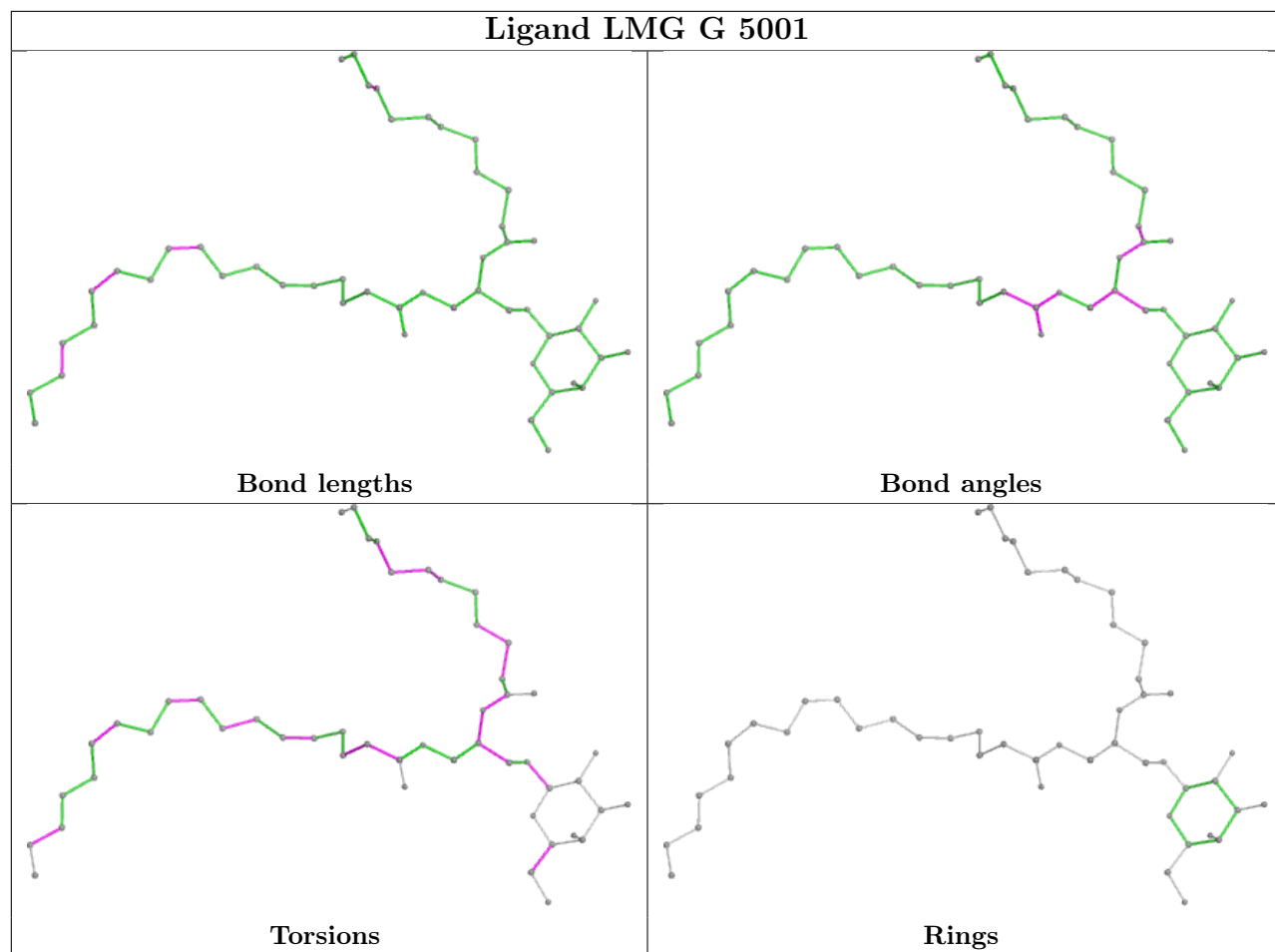


Ligand CLA 4 608

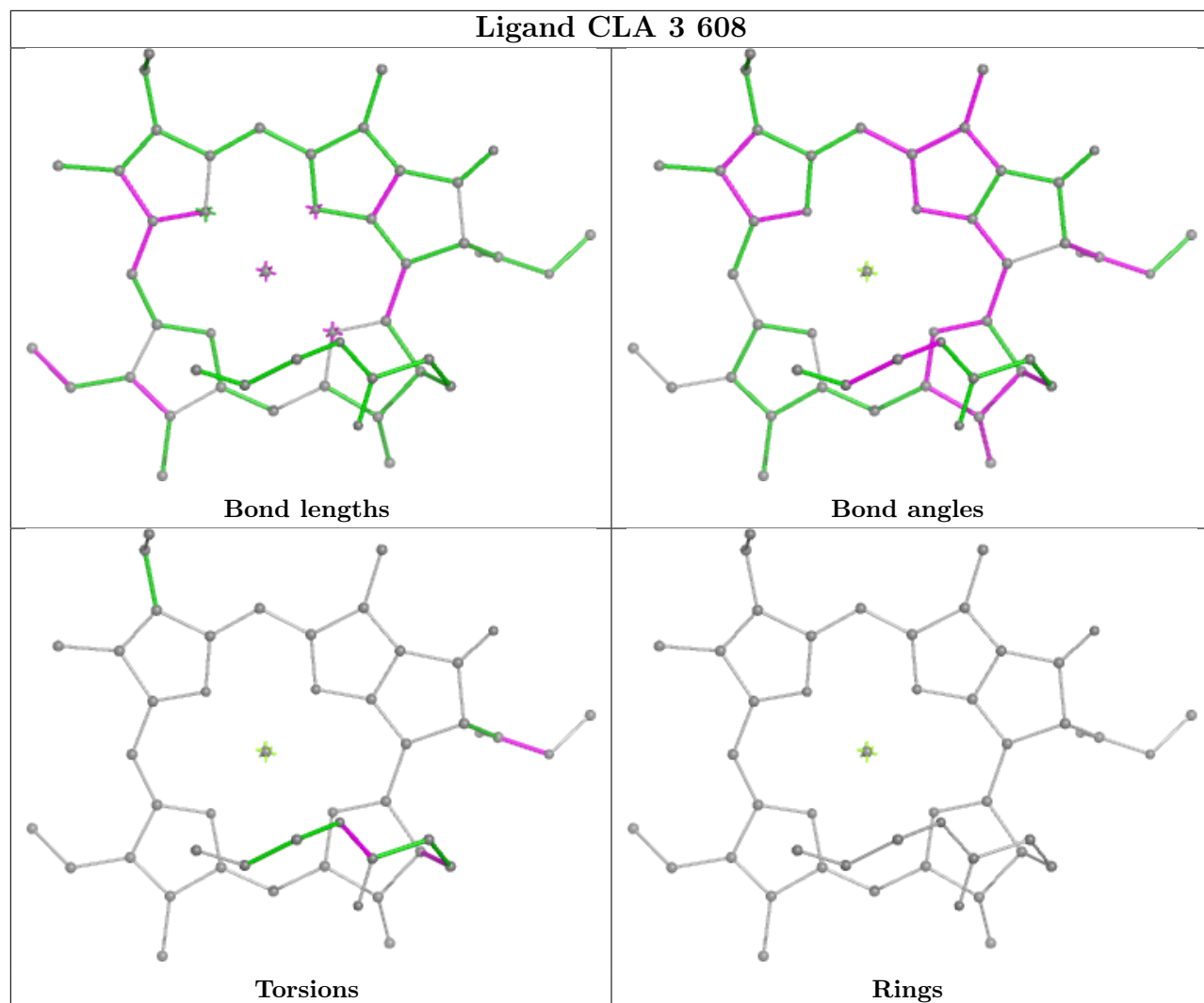


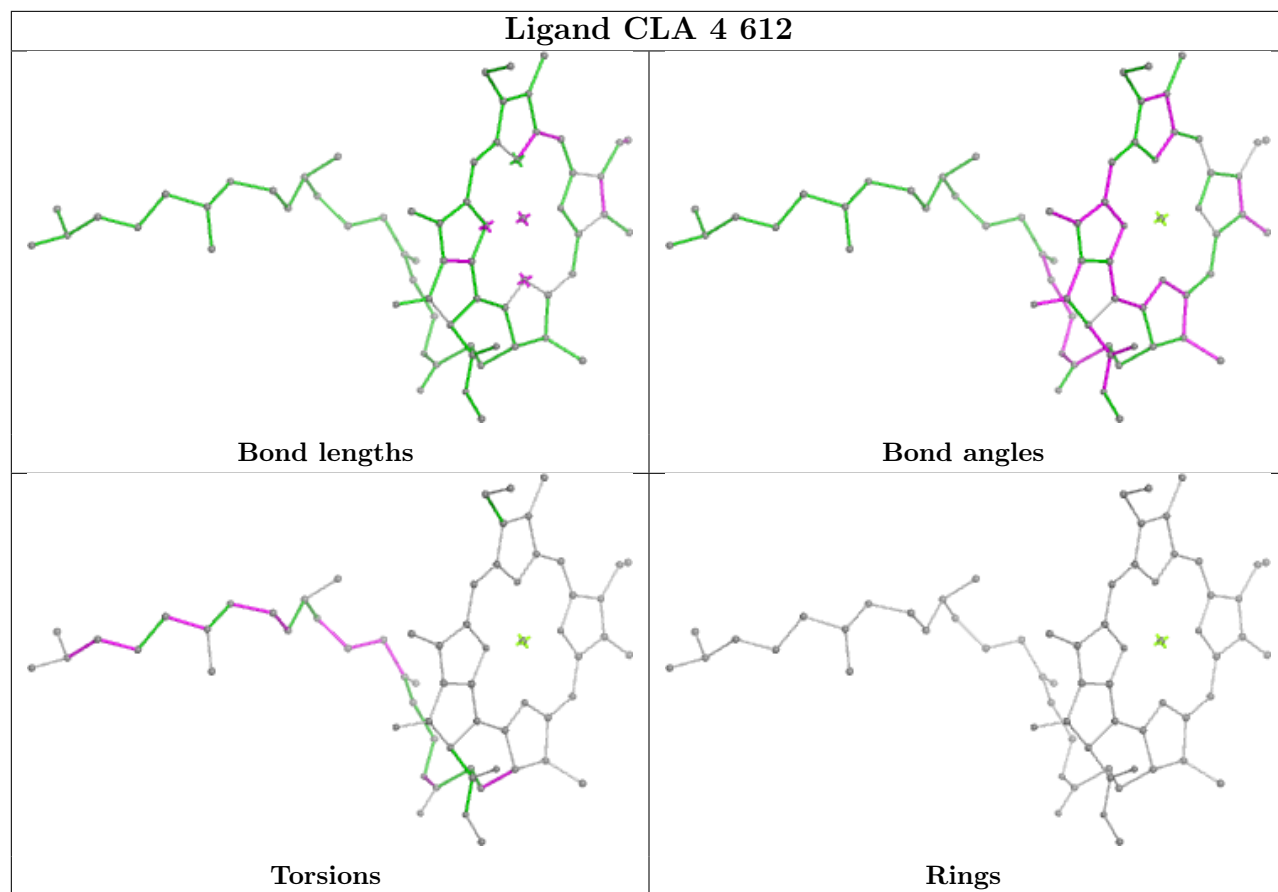


Ligand CLA B 1211**Ligand LMT B 5006**

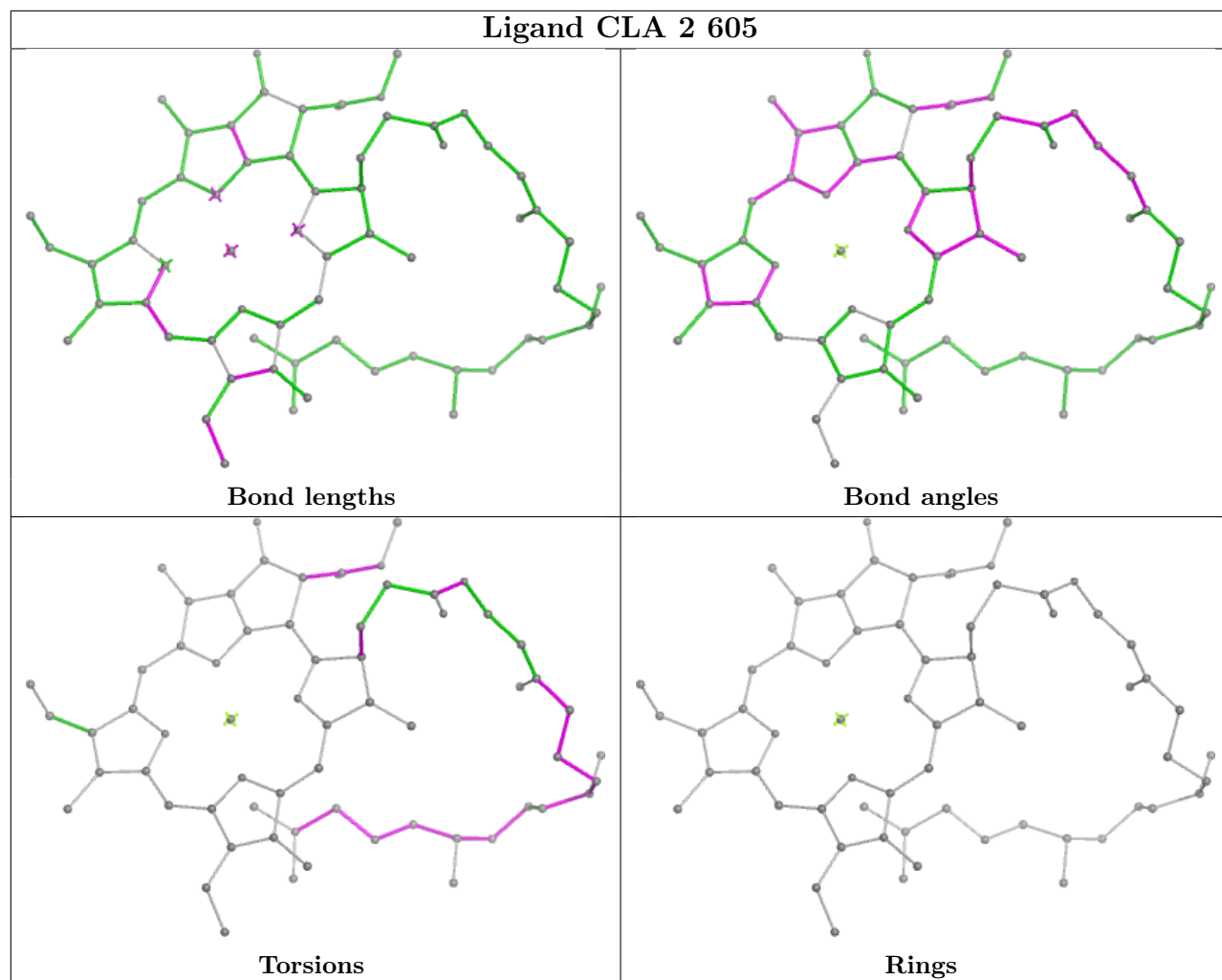


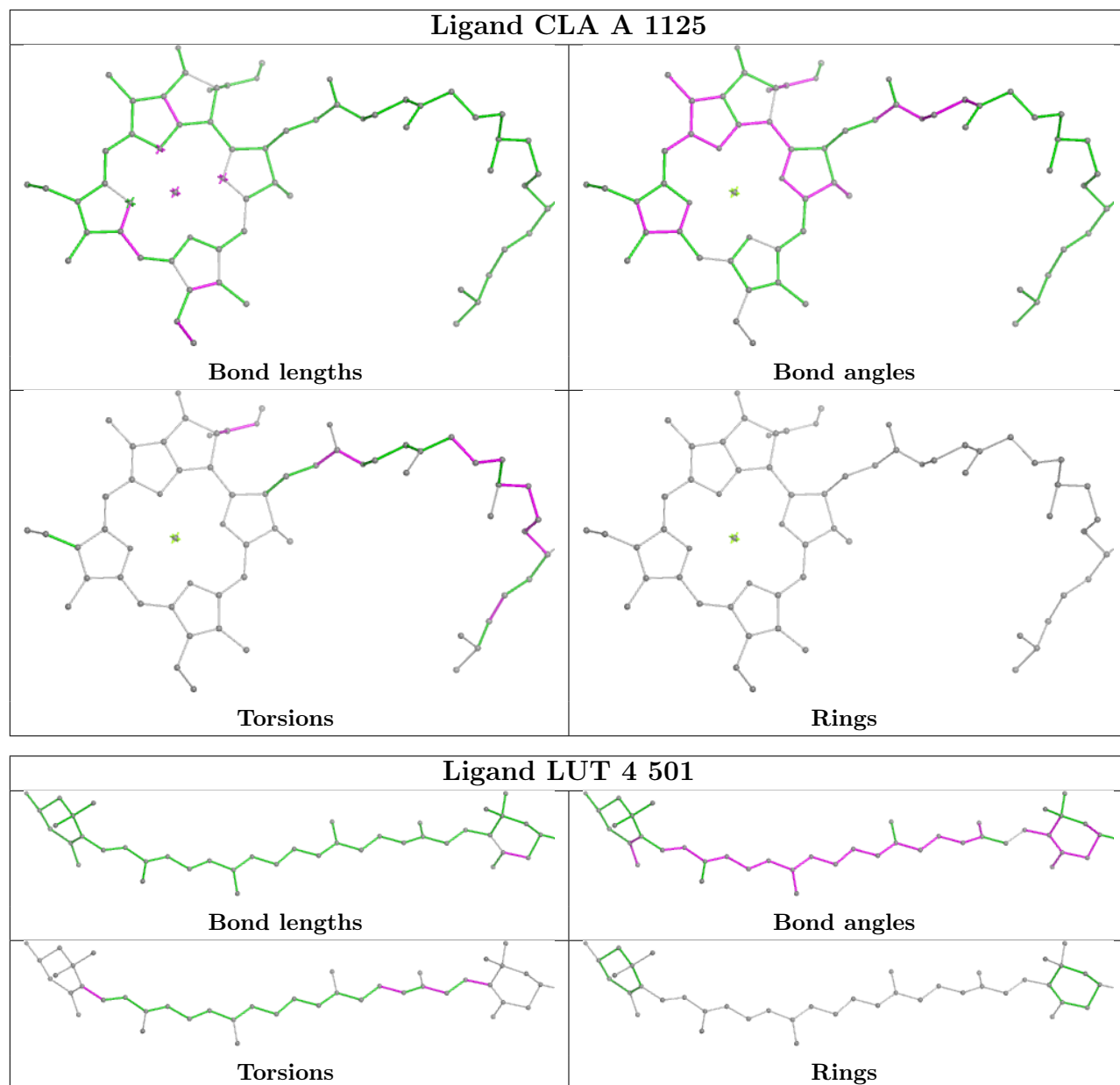
Ligand CLA 3 608

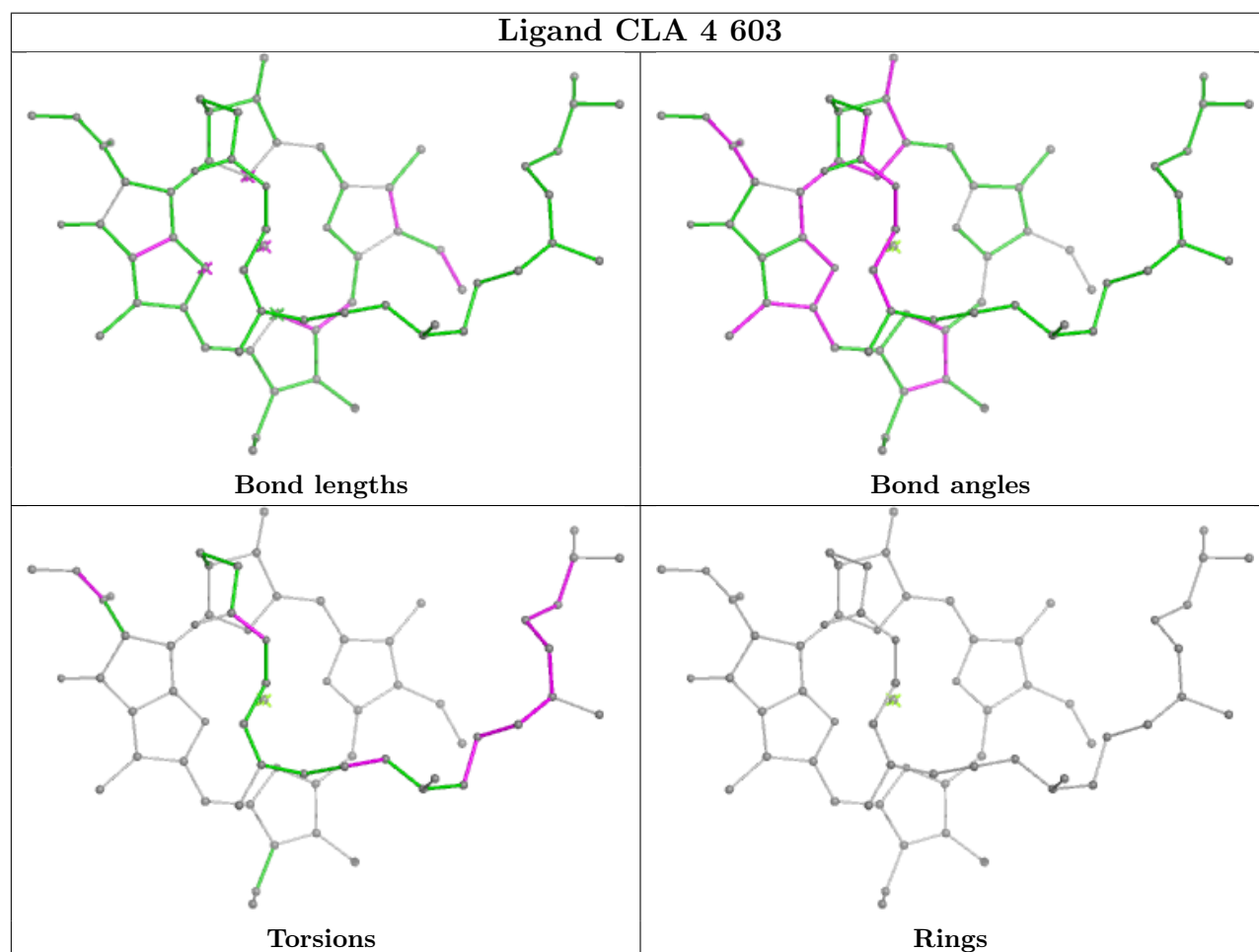
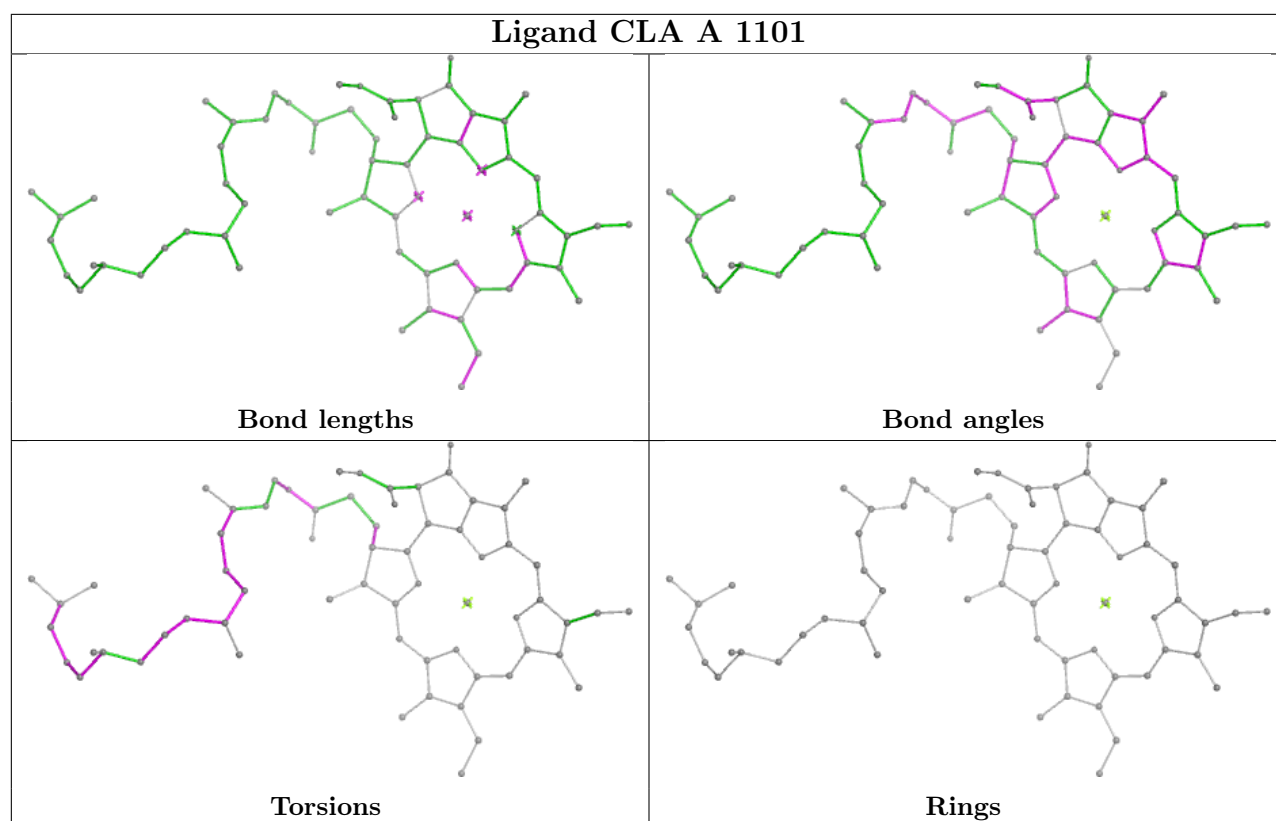


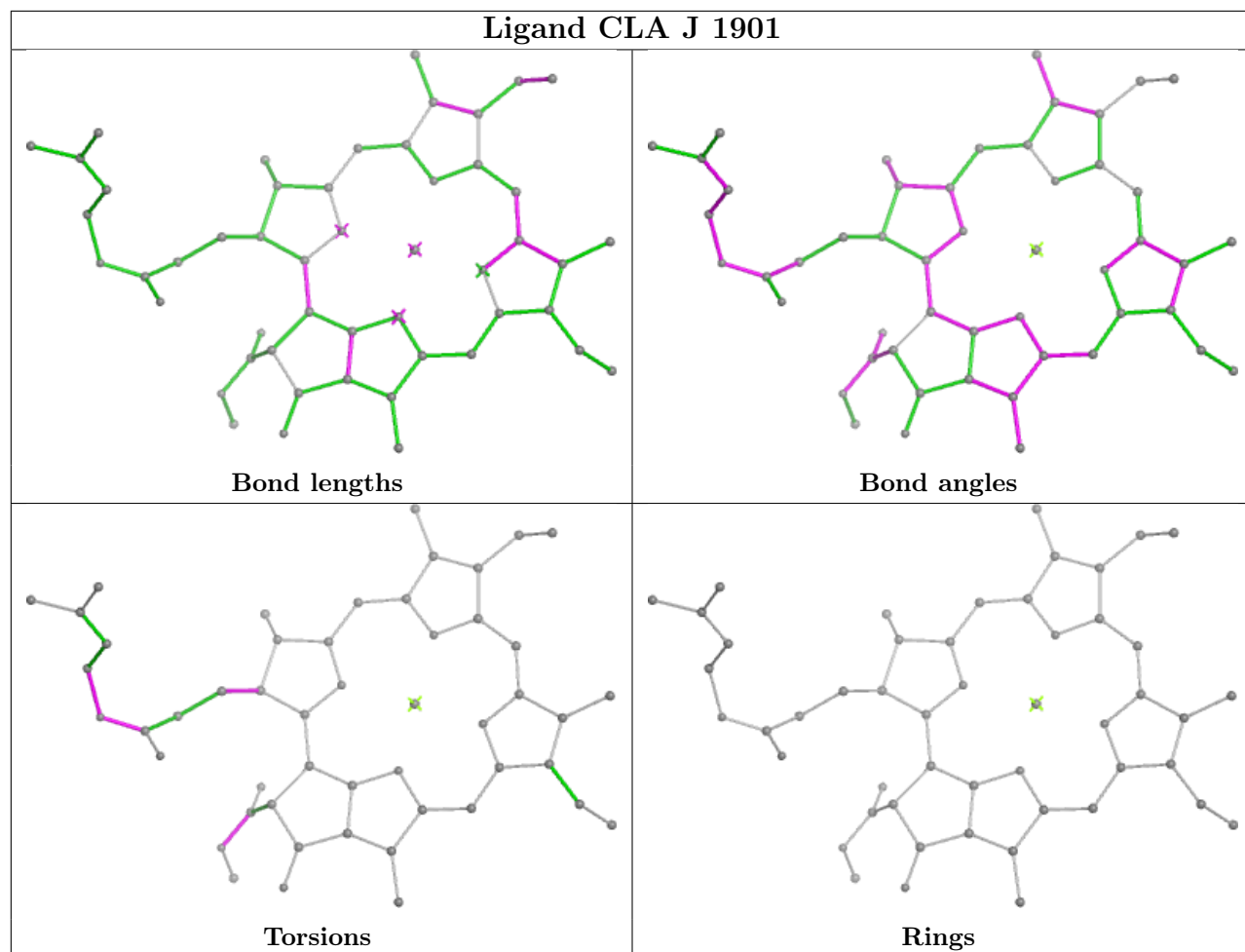


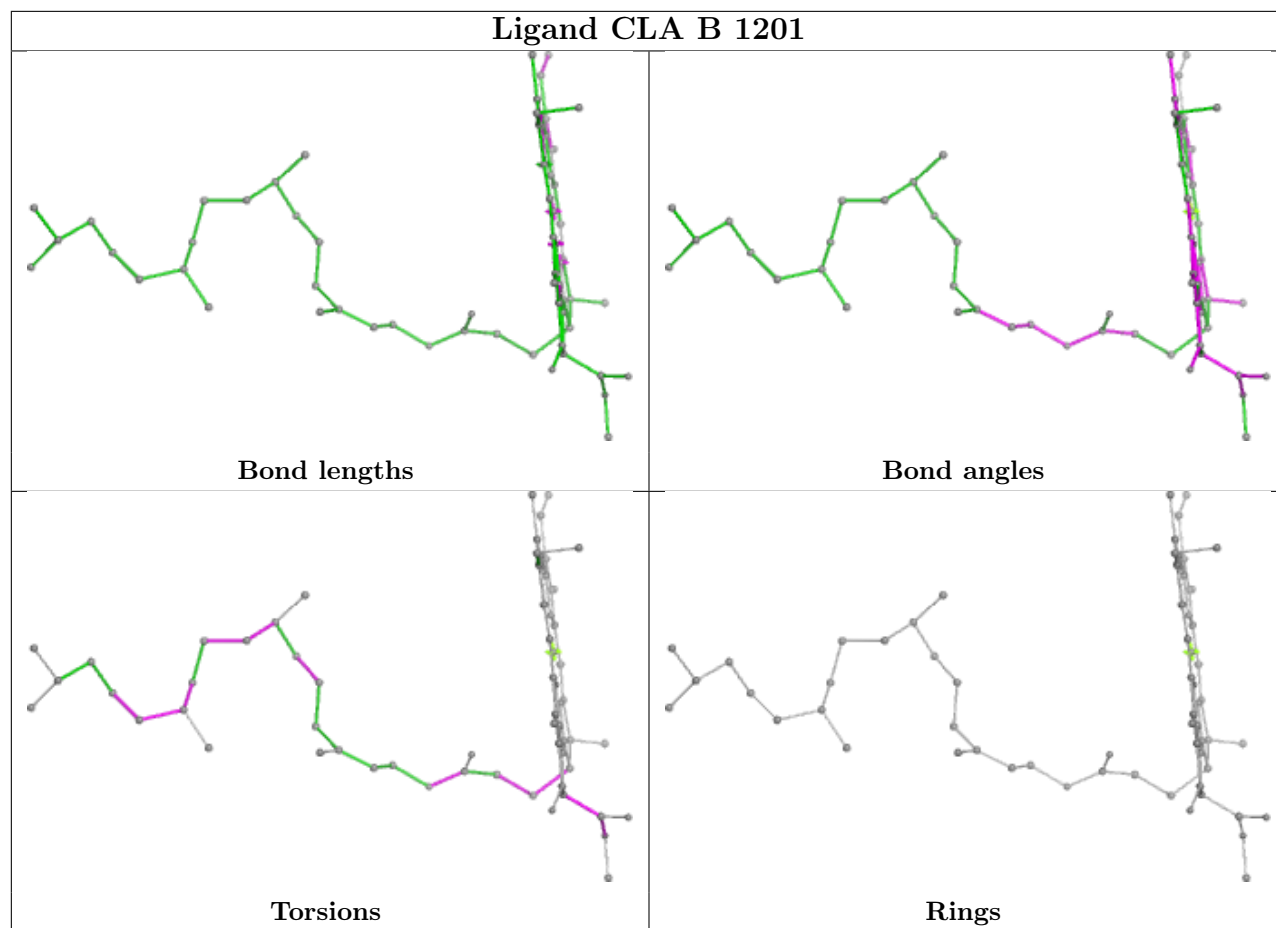
Ligand CLA 2 605



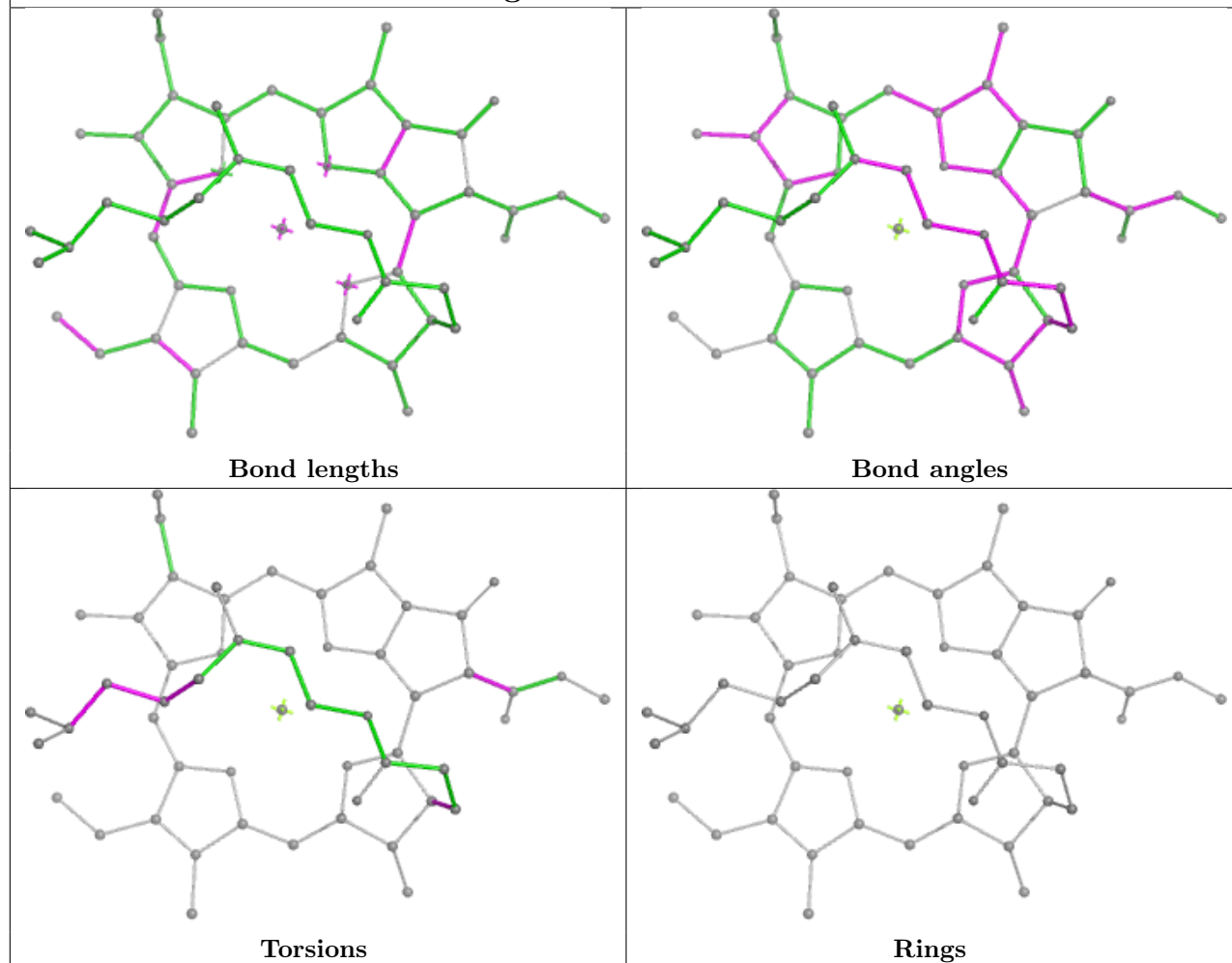




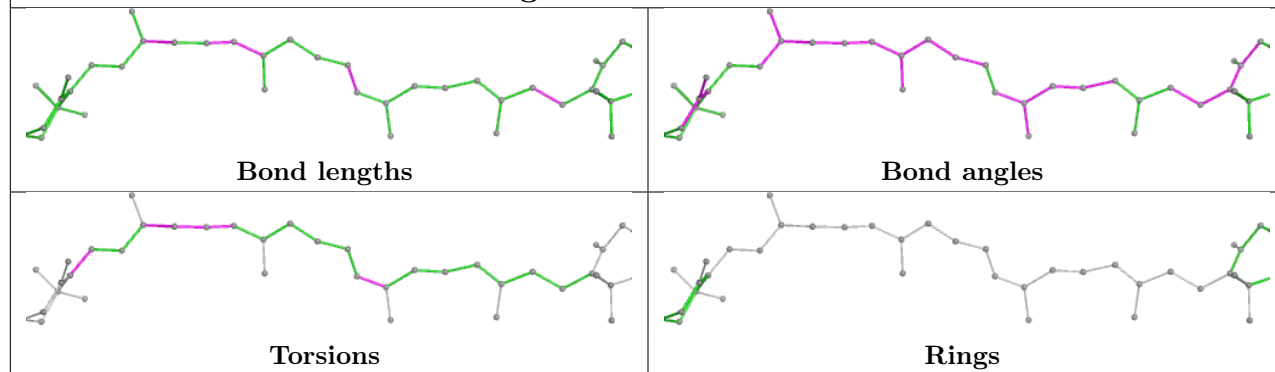


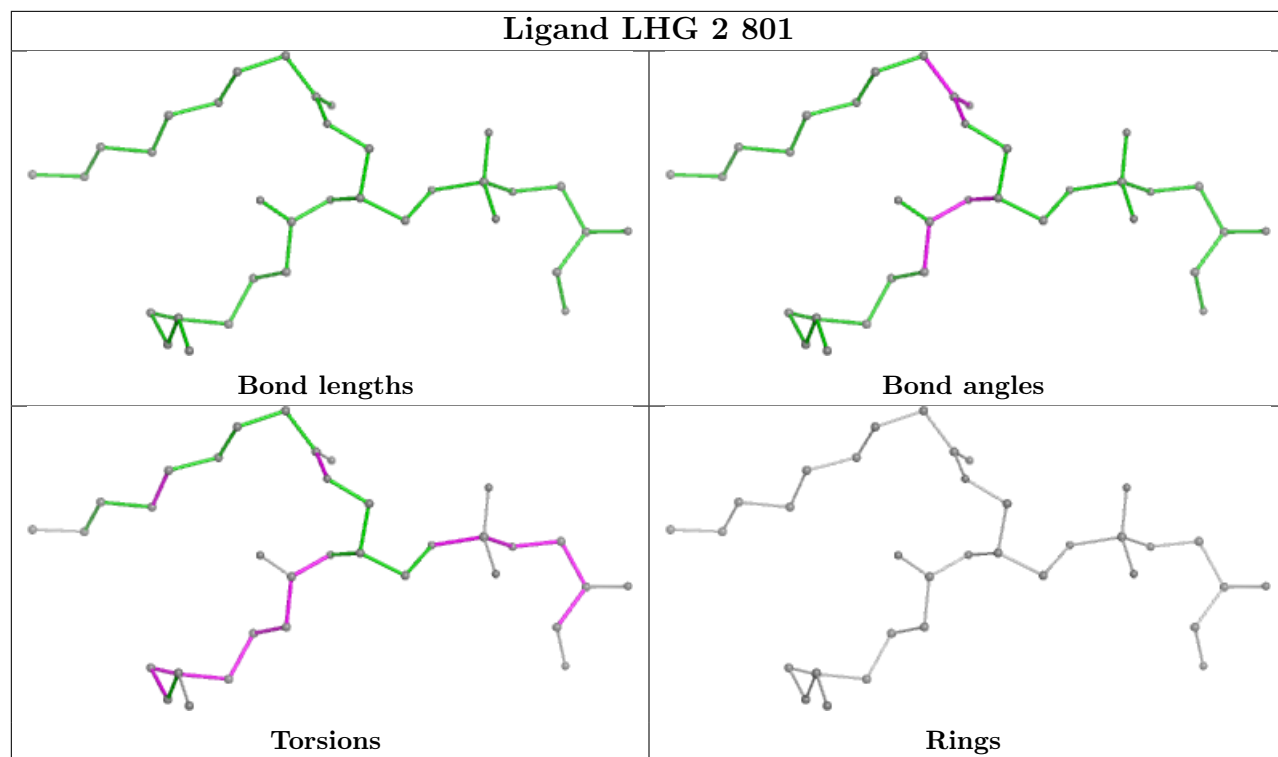


Ligand CLA A 1110

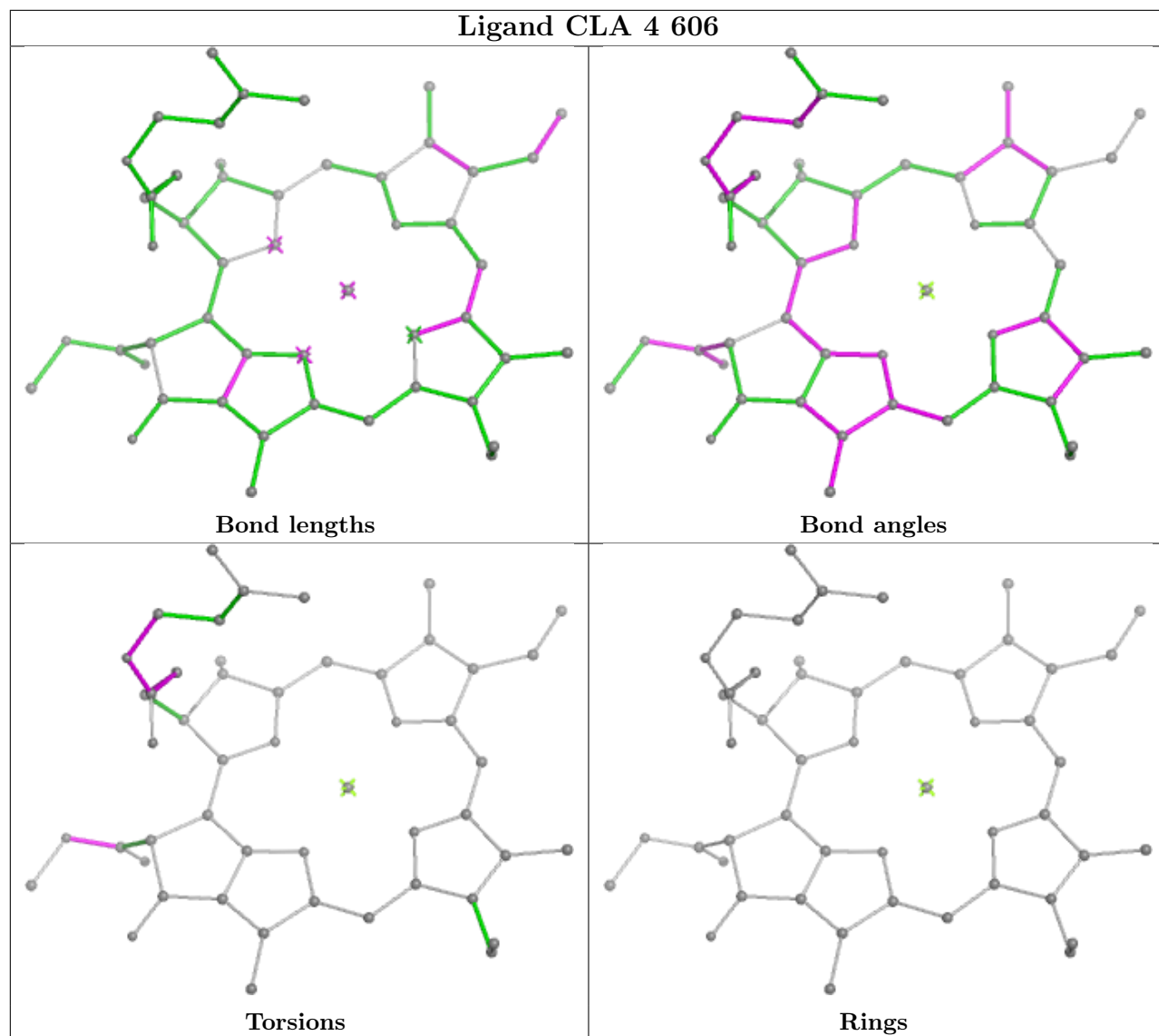


Ligand BCR A 4017

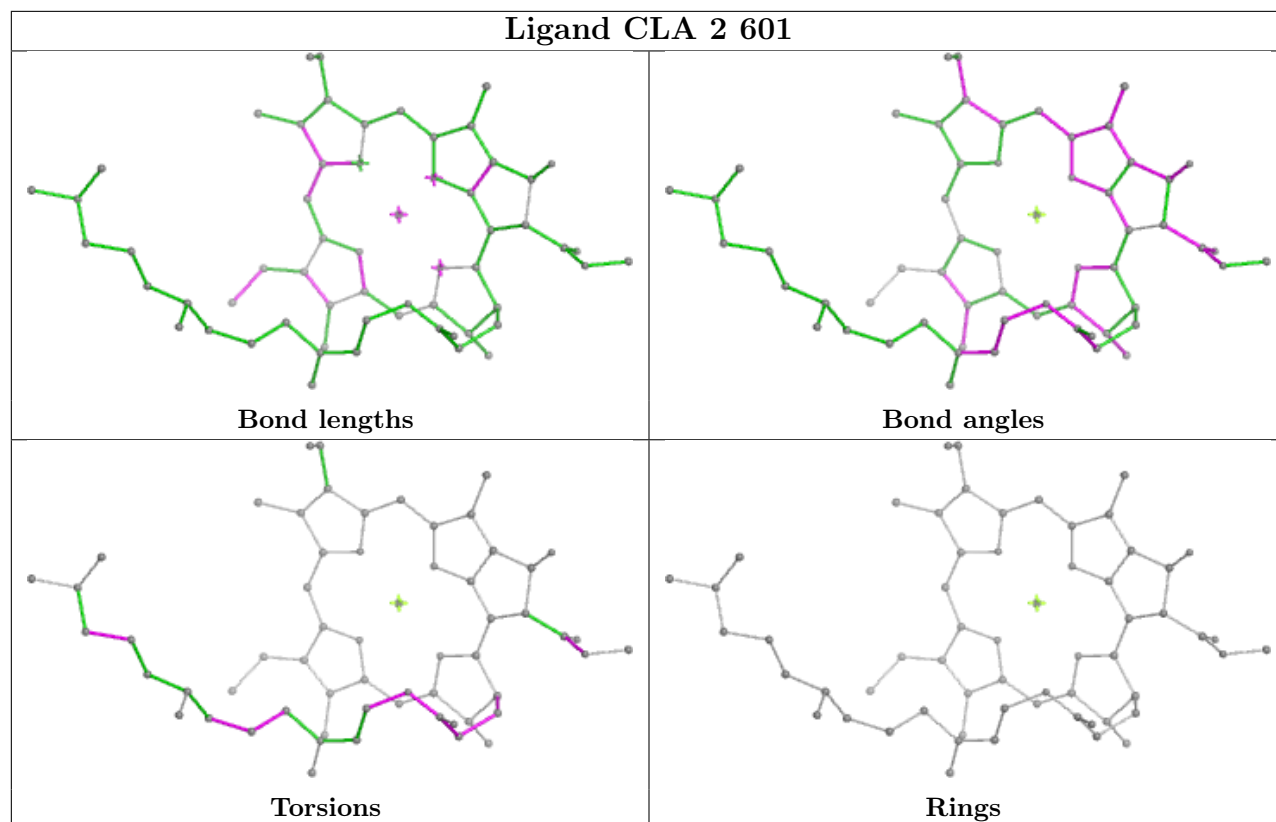




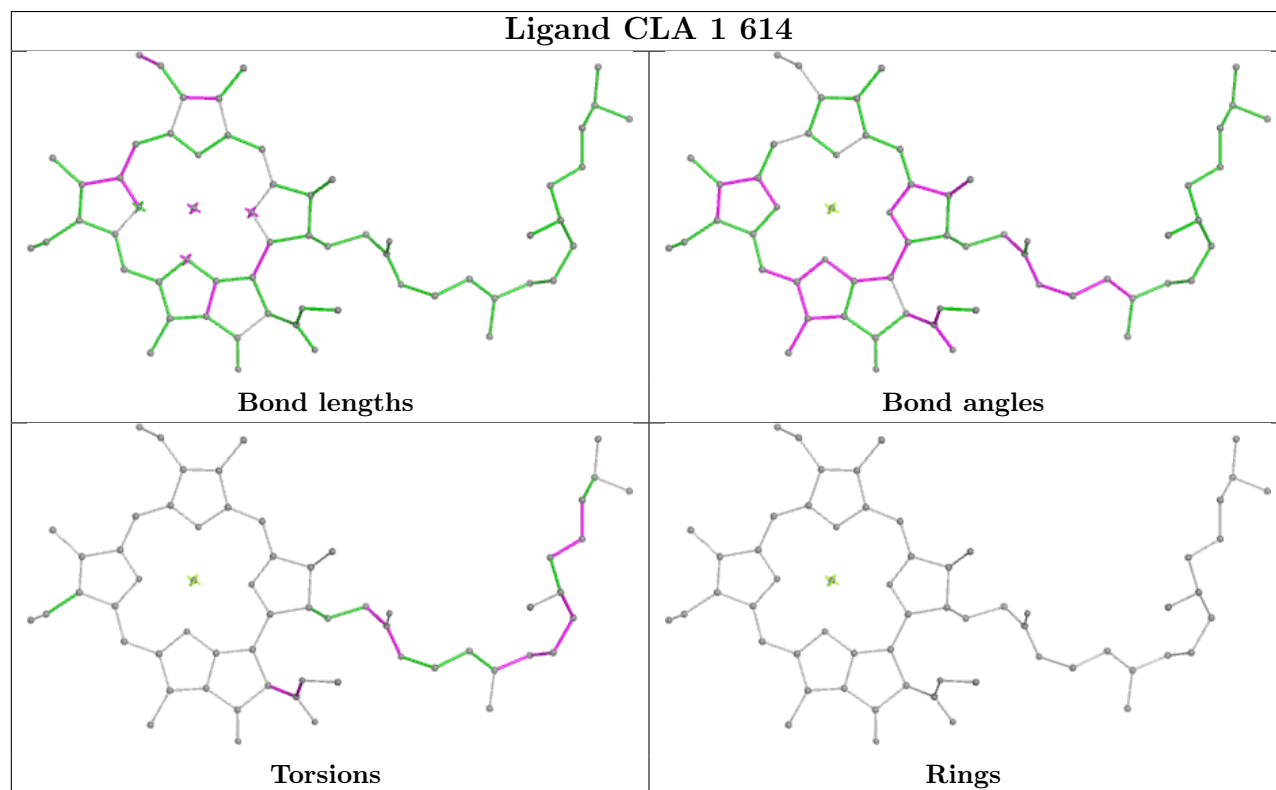
Ligand CLA 4 606

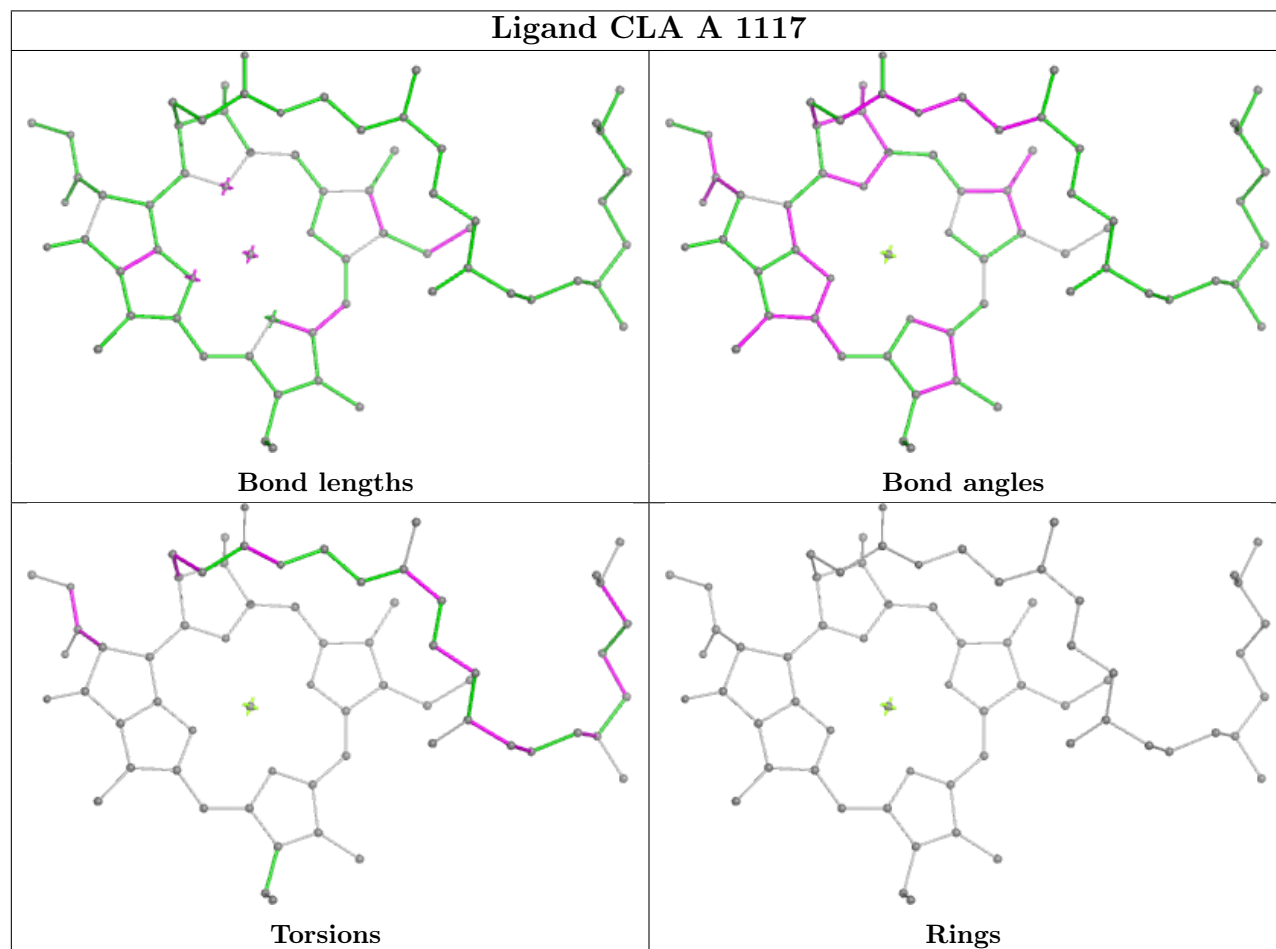
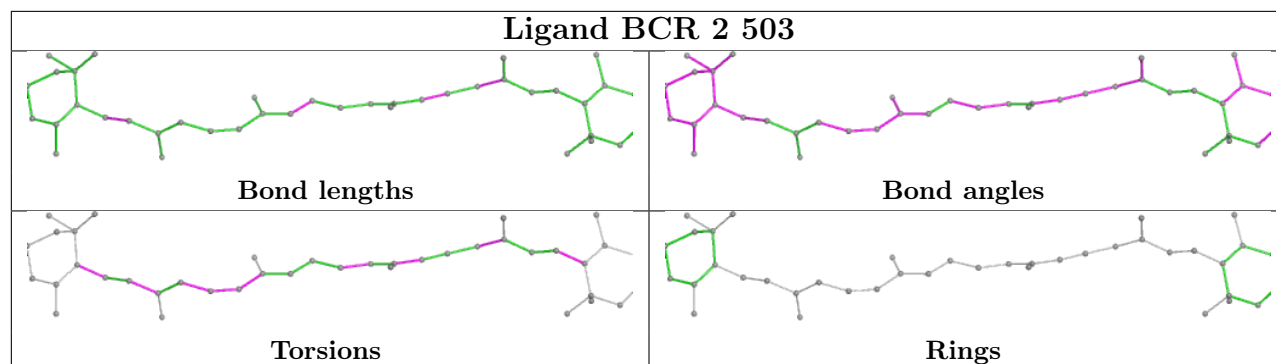


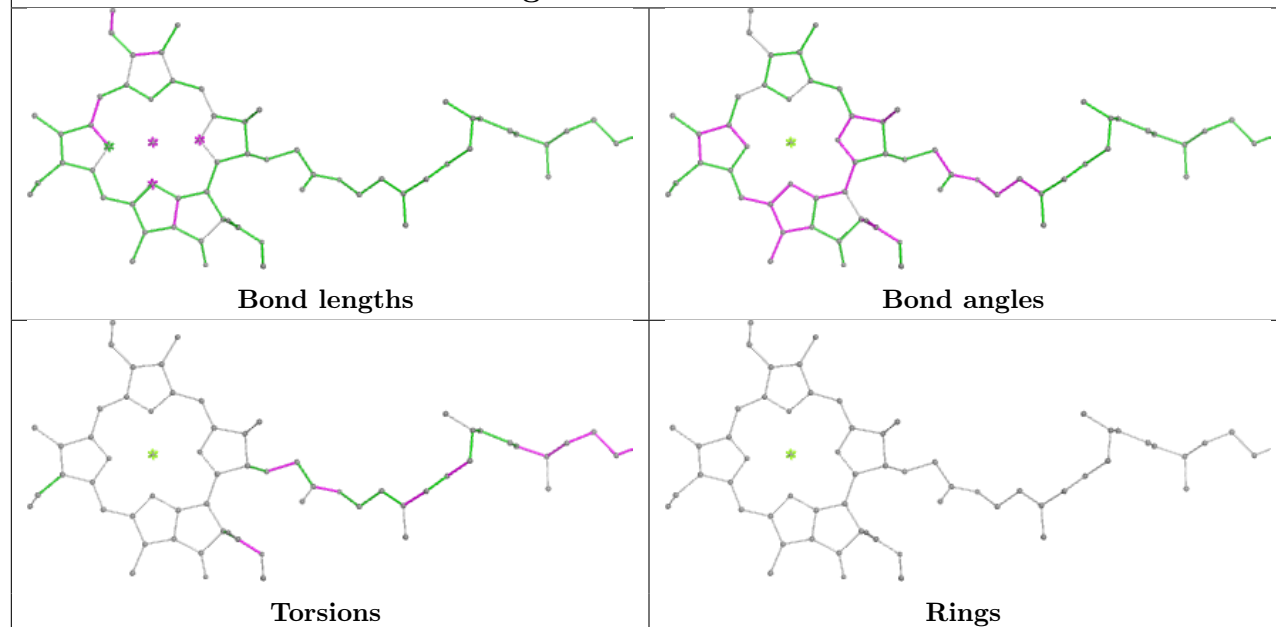
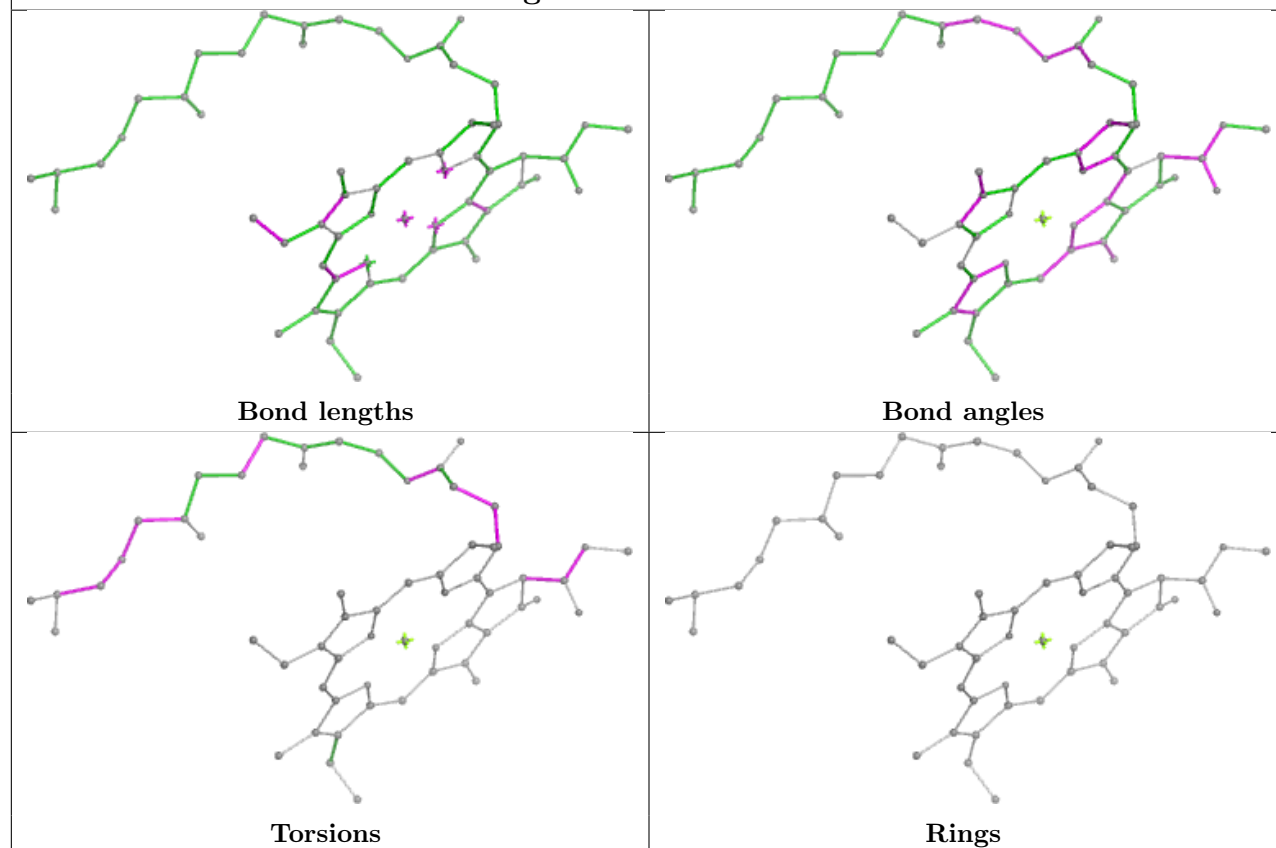
Ligand CLA 2 601

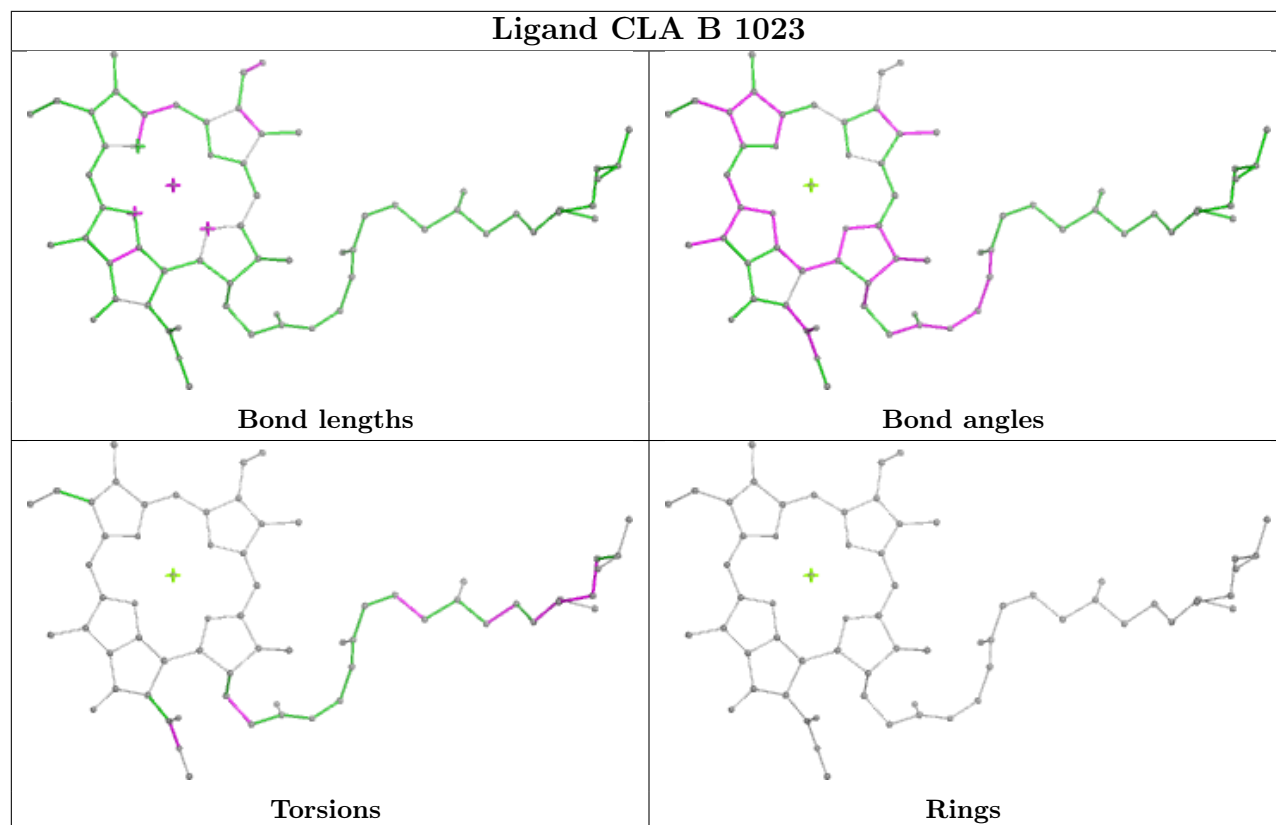


Ligand CLA 1 614

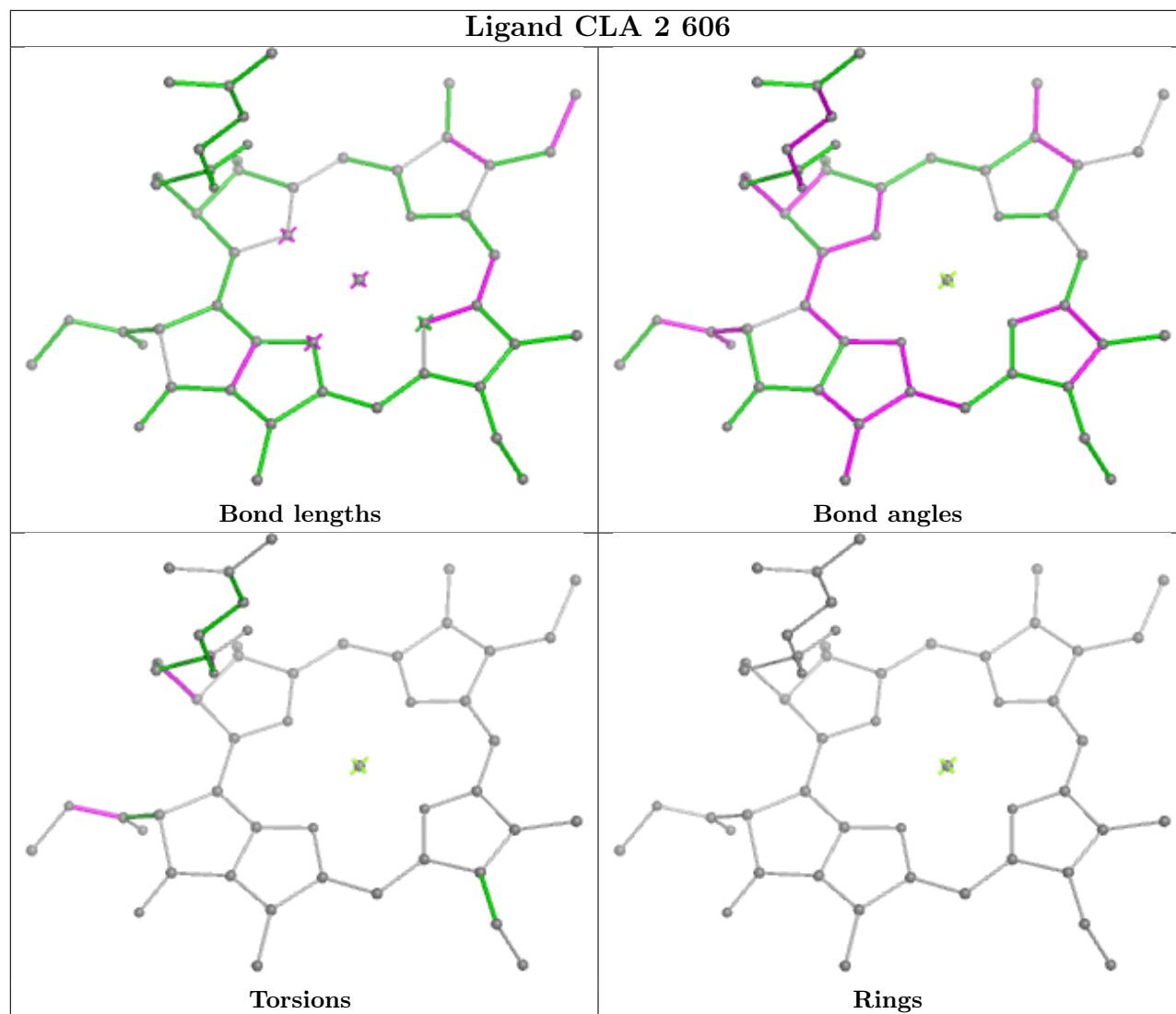




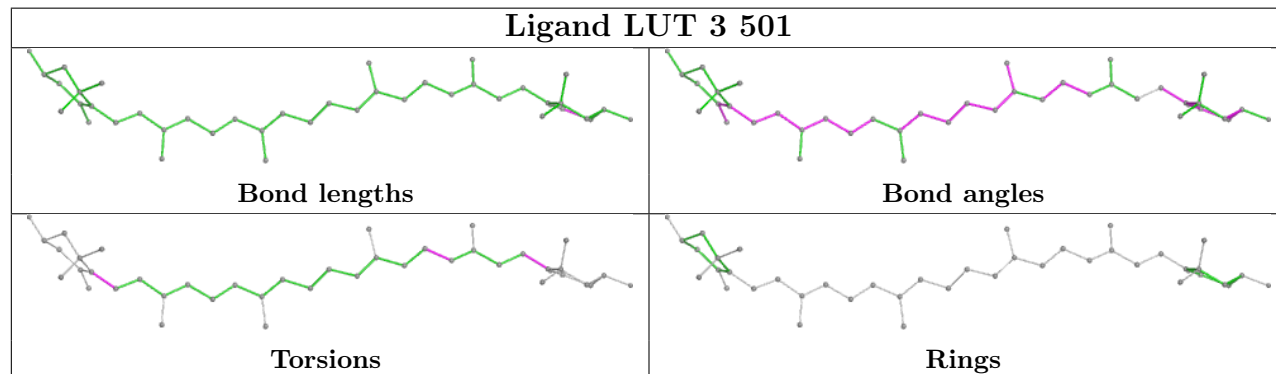
Ligand CLA A 1131**Ligand CLA B 1228**

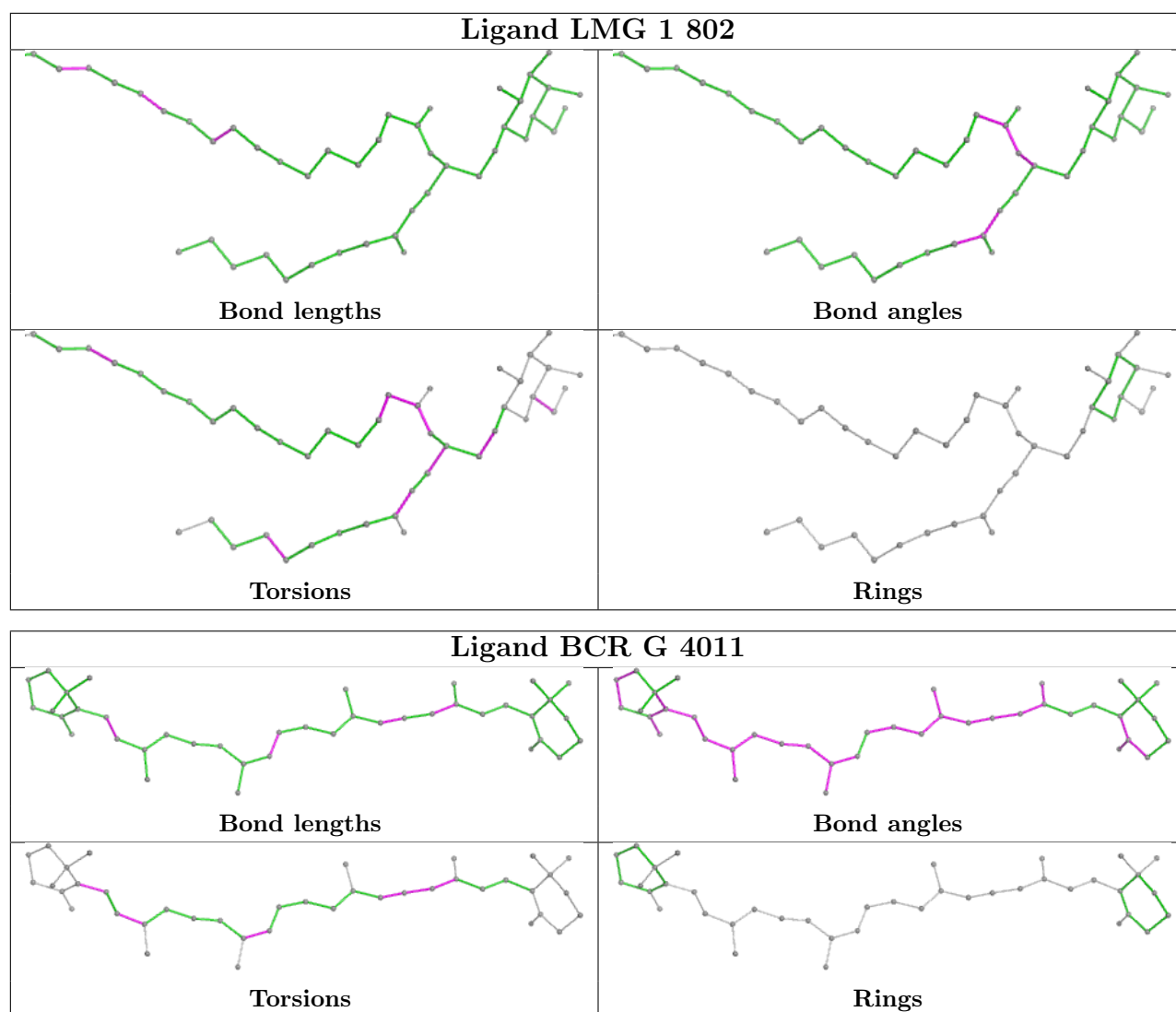


Ligand CLA 2 606

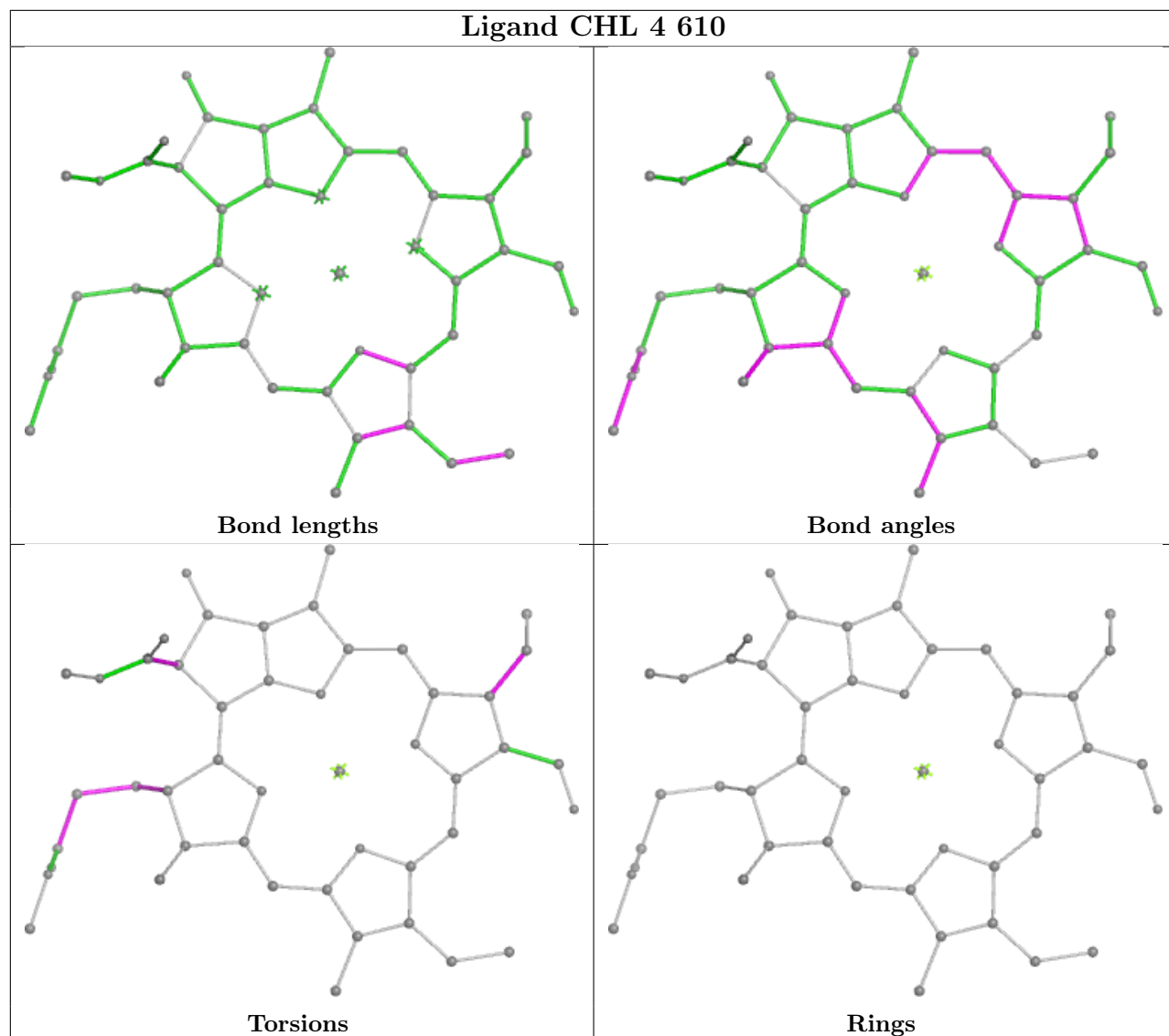


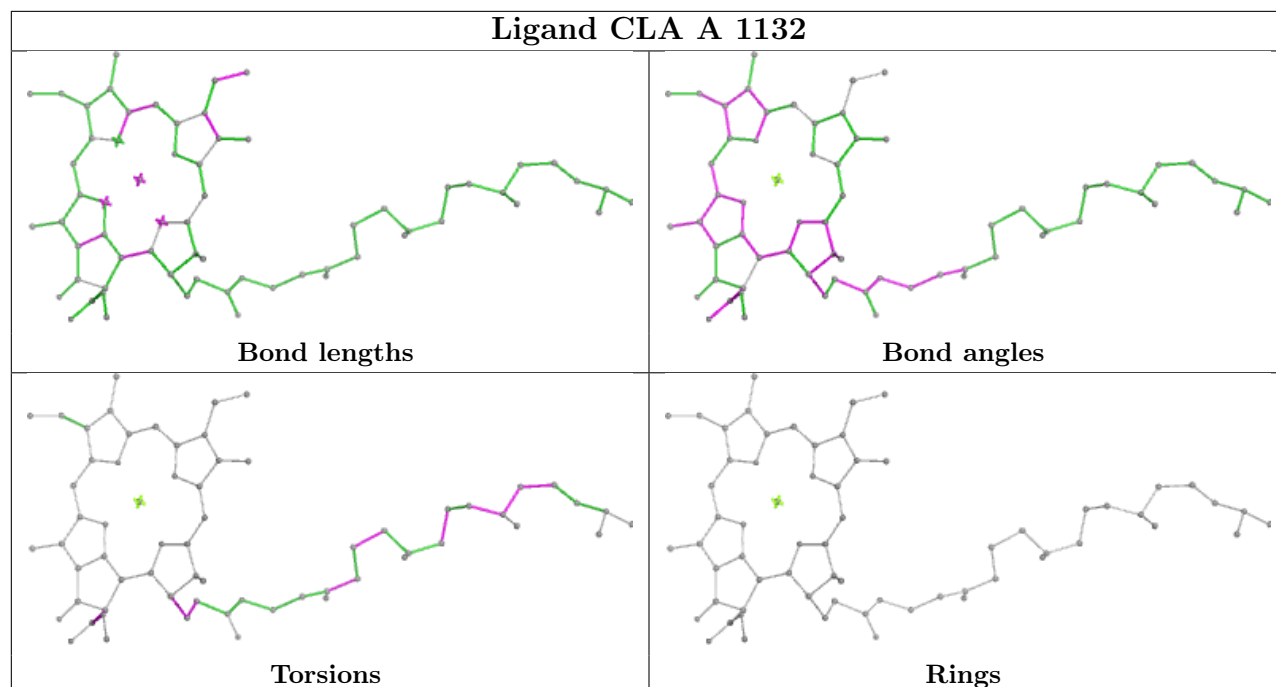
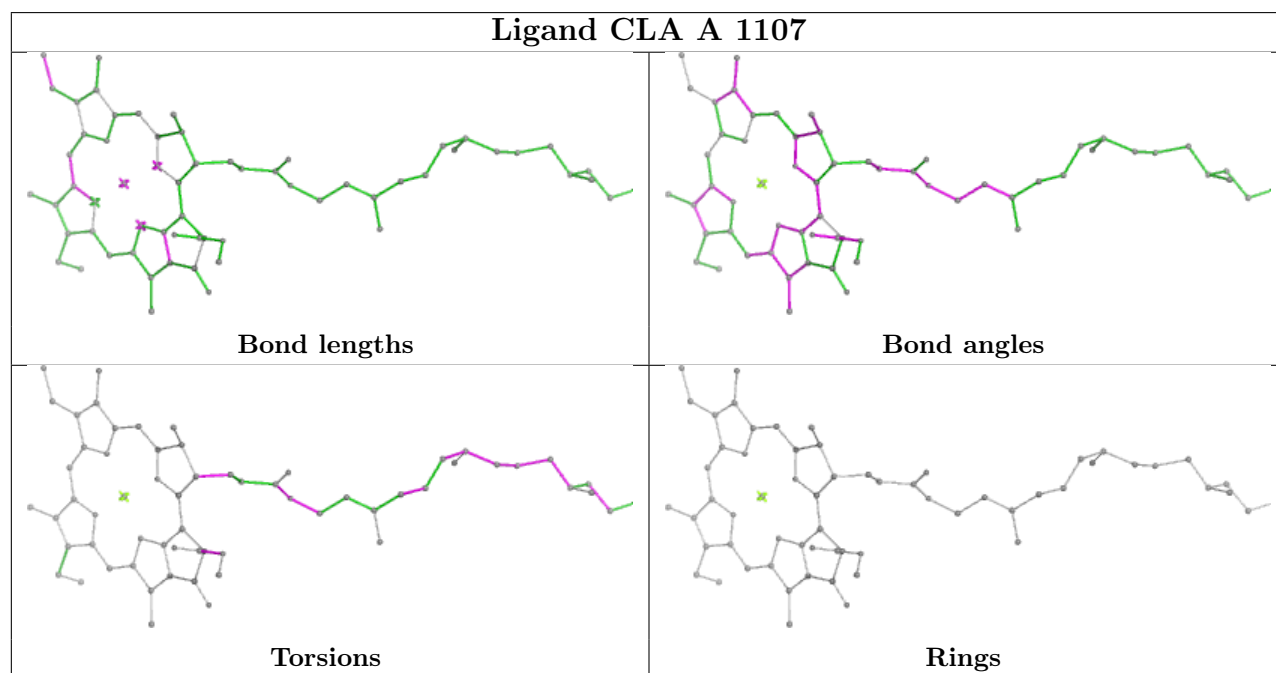
Ligand LUT 3 501



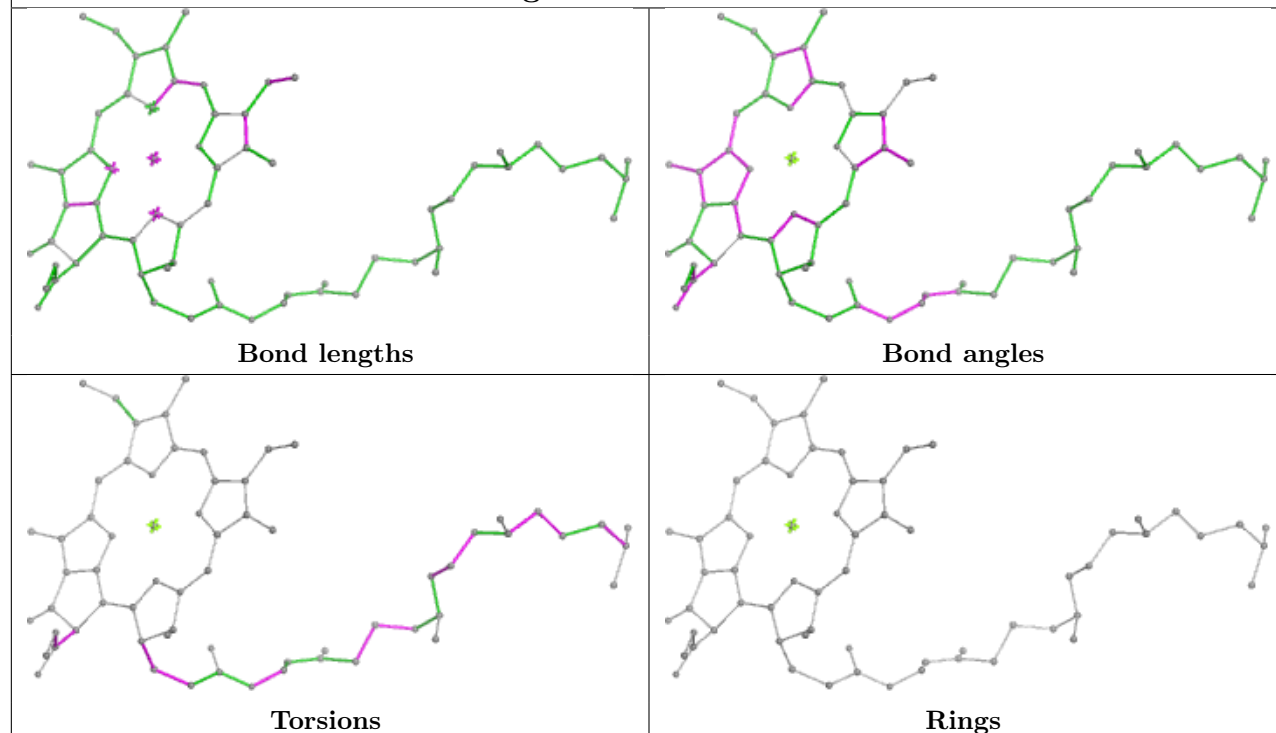


Ligand CHL 4 610

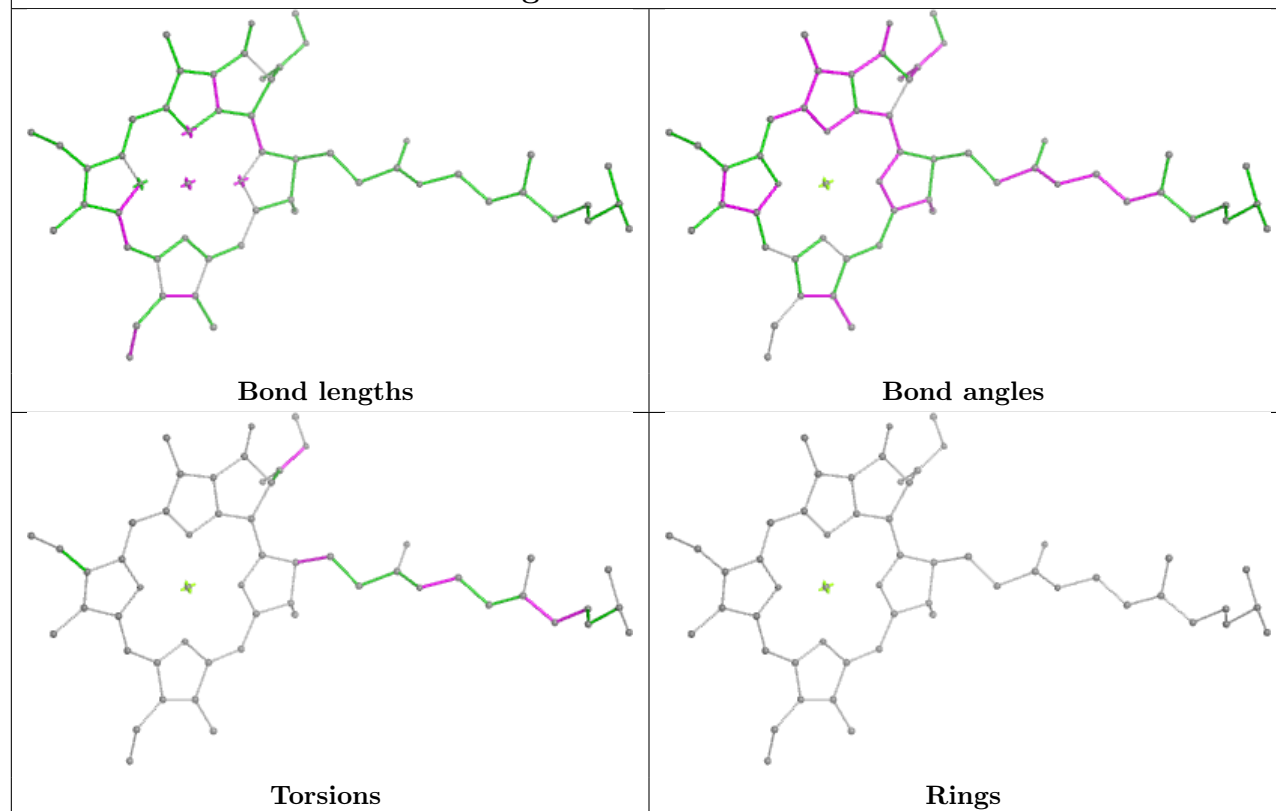


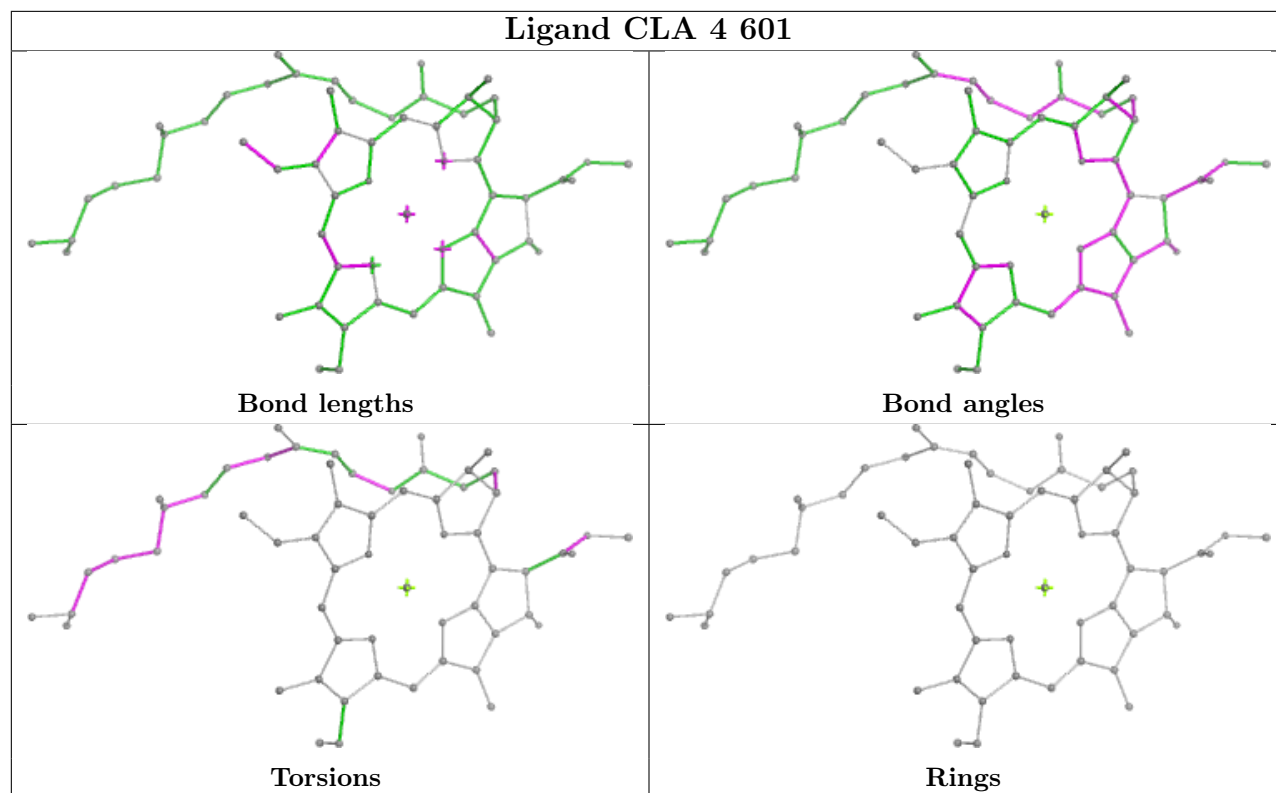
Ligand CLA A 1132**Ligand CLA A 1107**

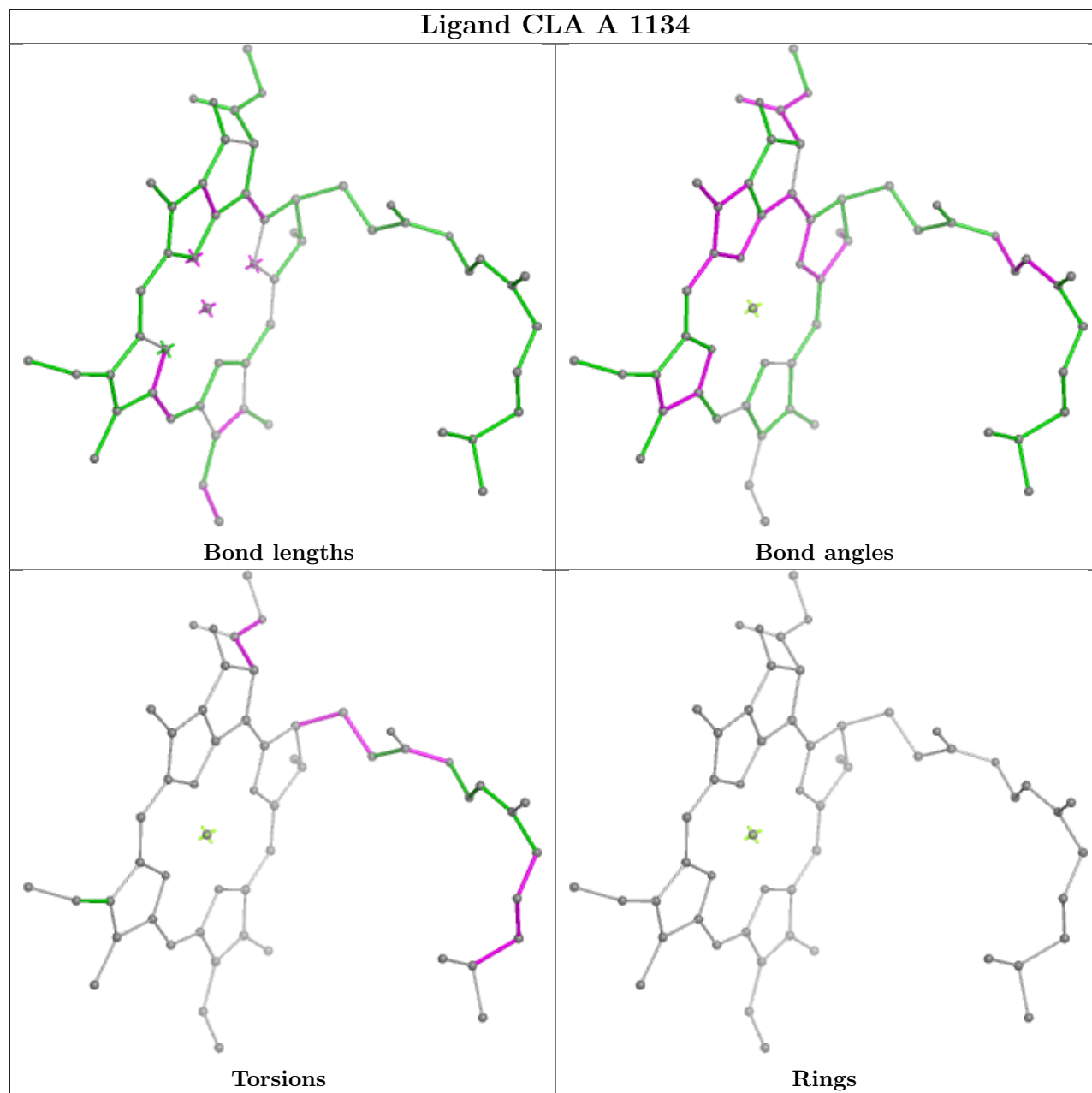
Ligand CLA A 1106

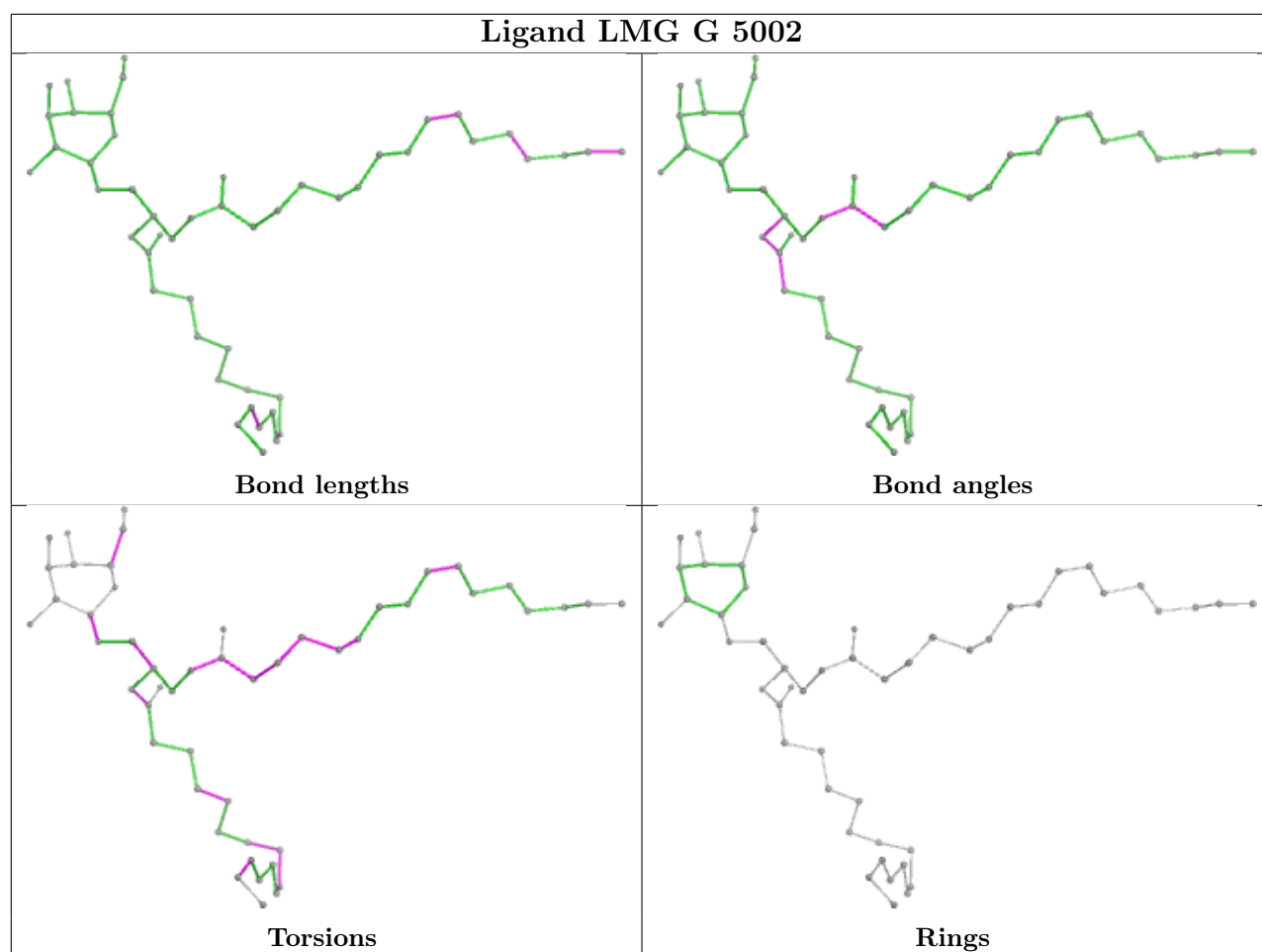


Ligand CLA G 1601

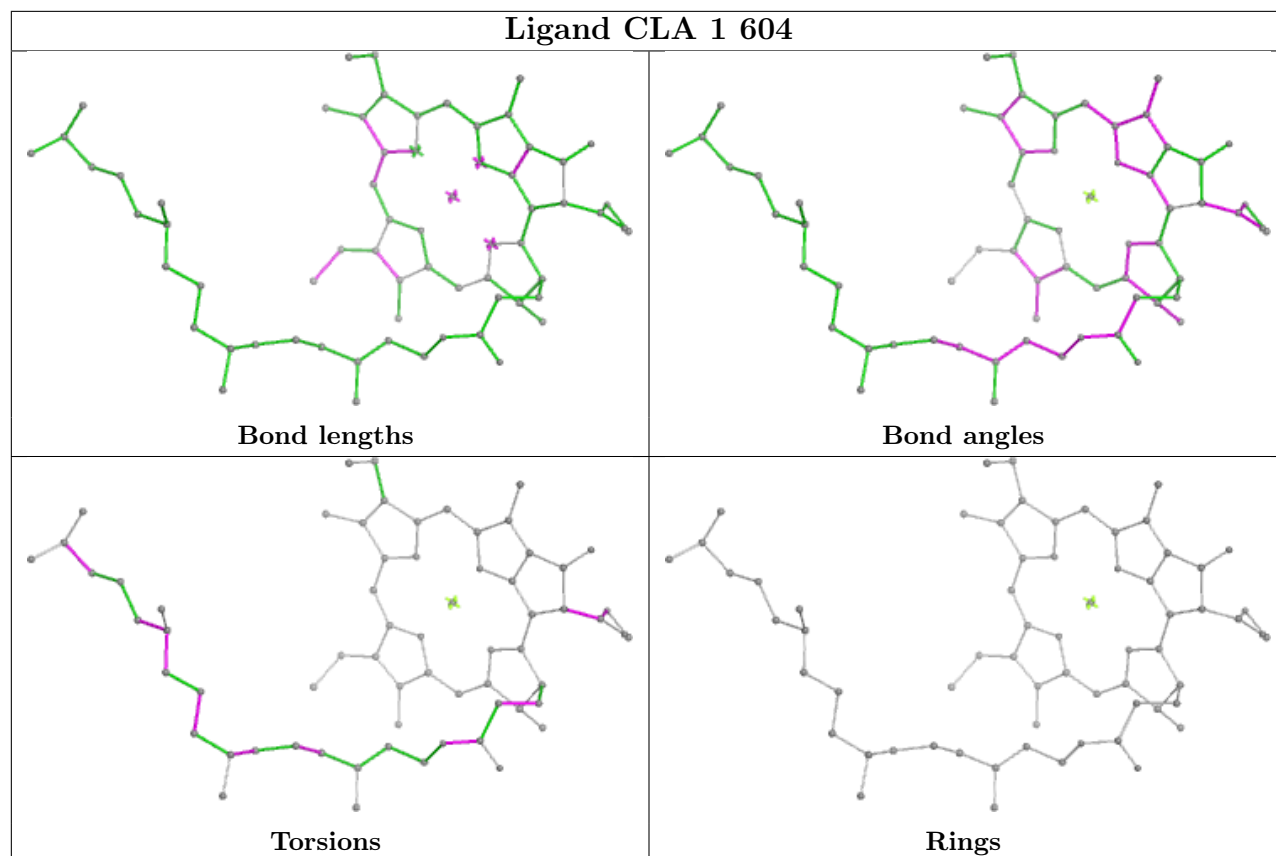




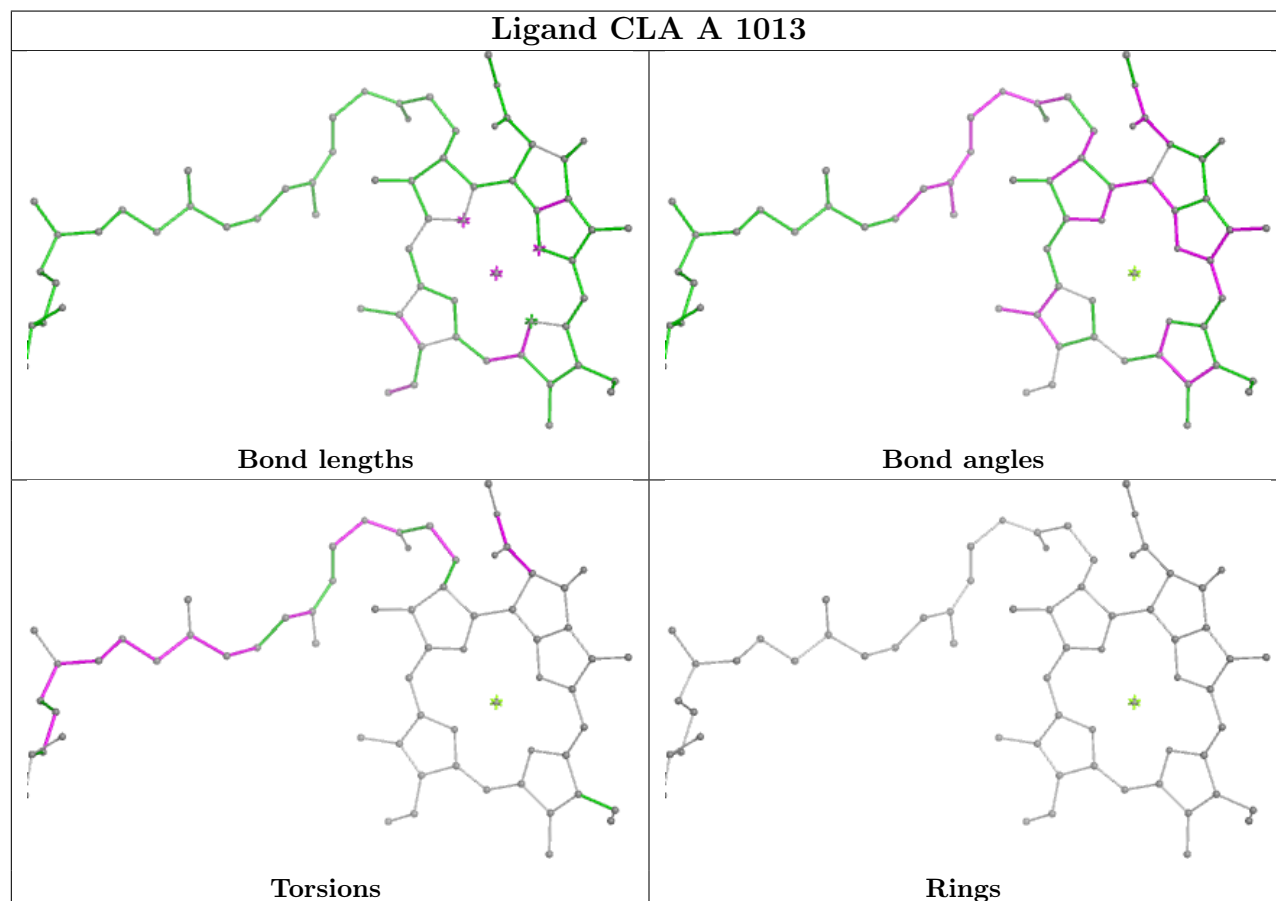


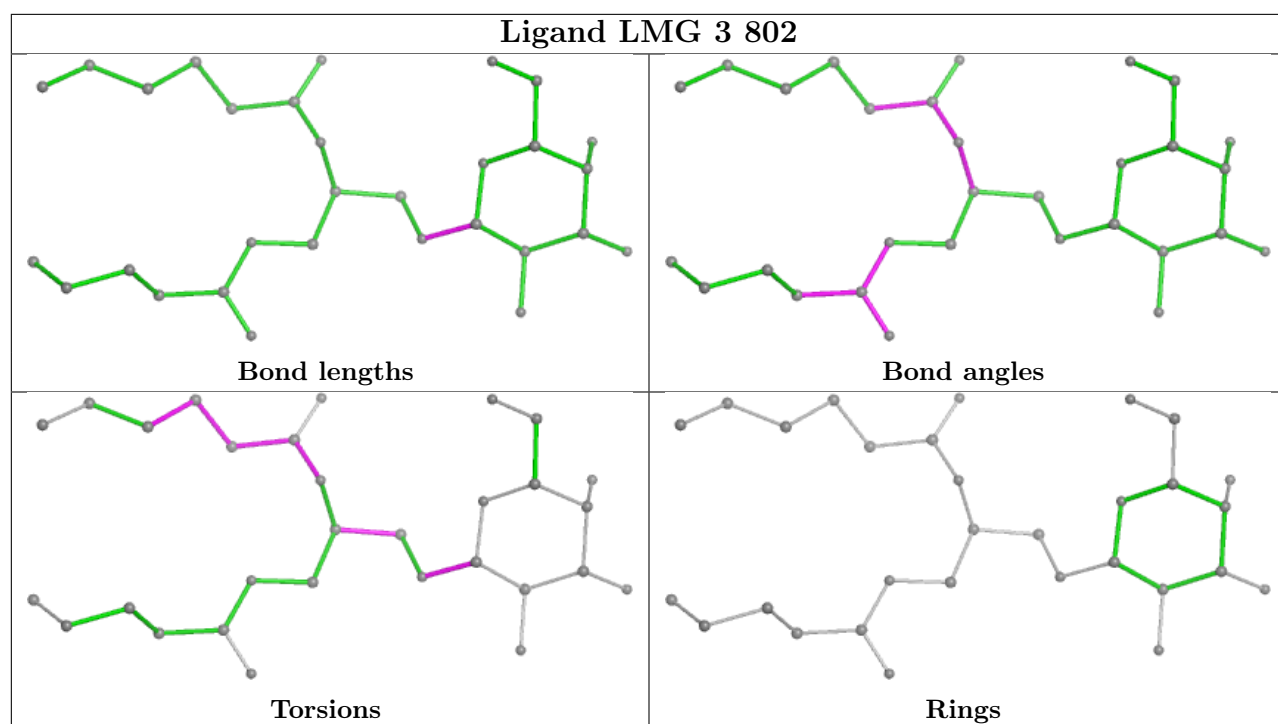


Ligand CLA 1 604

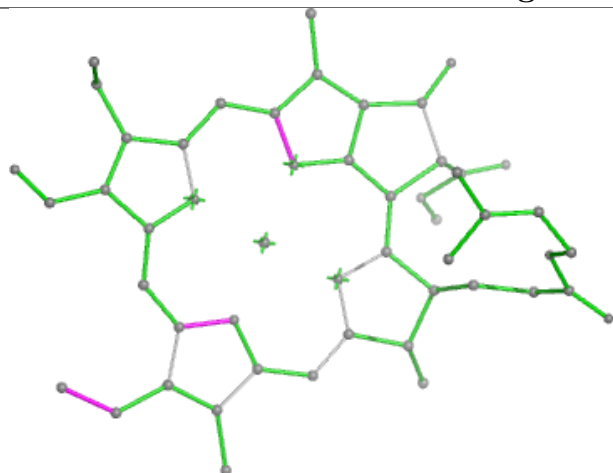


Ligand CLA A 1013

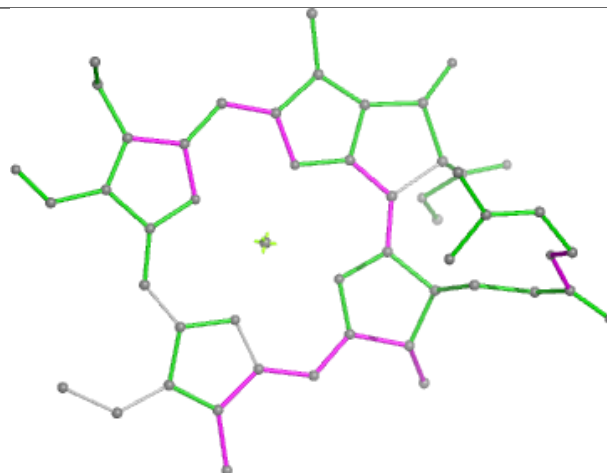




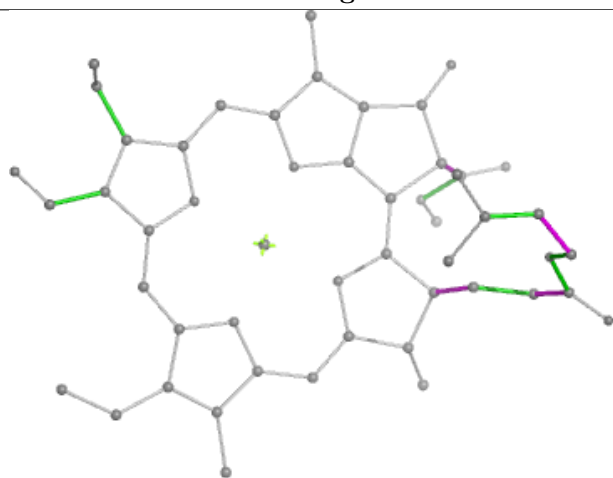
Ligand CHL 3 607



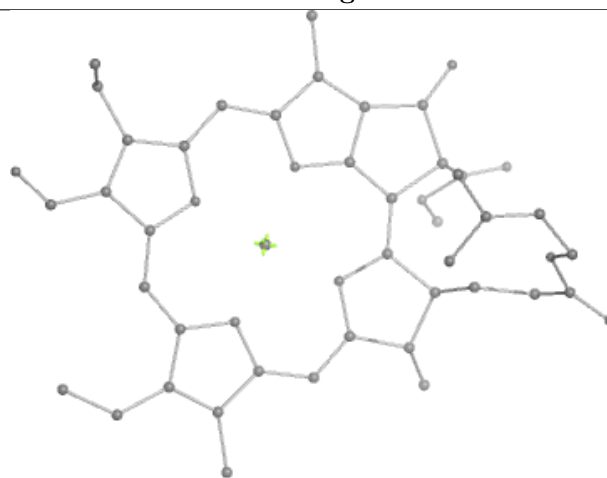
Bond lengths



Bond angles

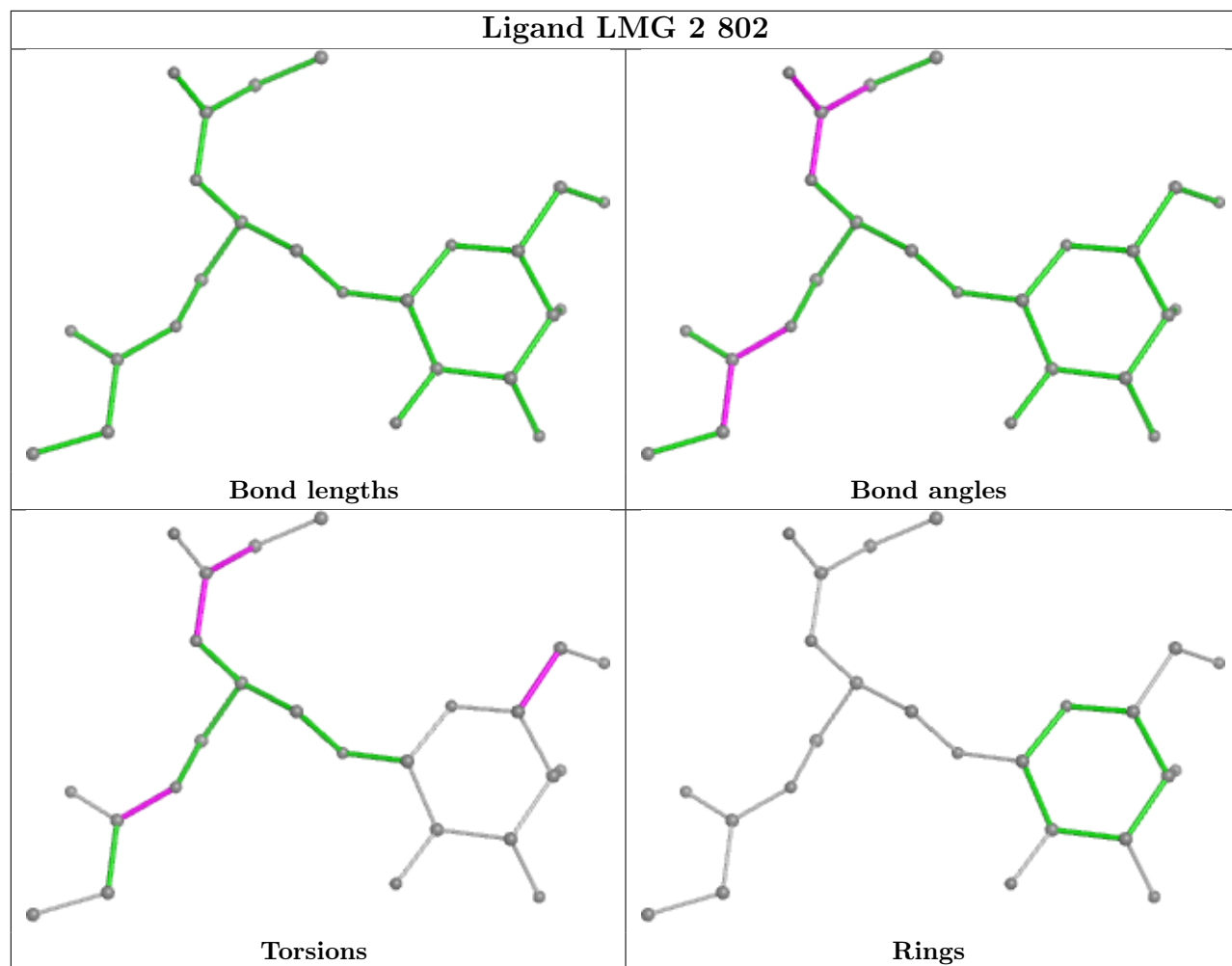


Torsions

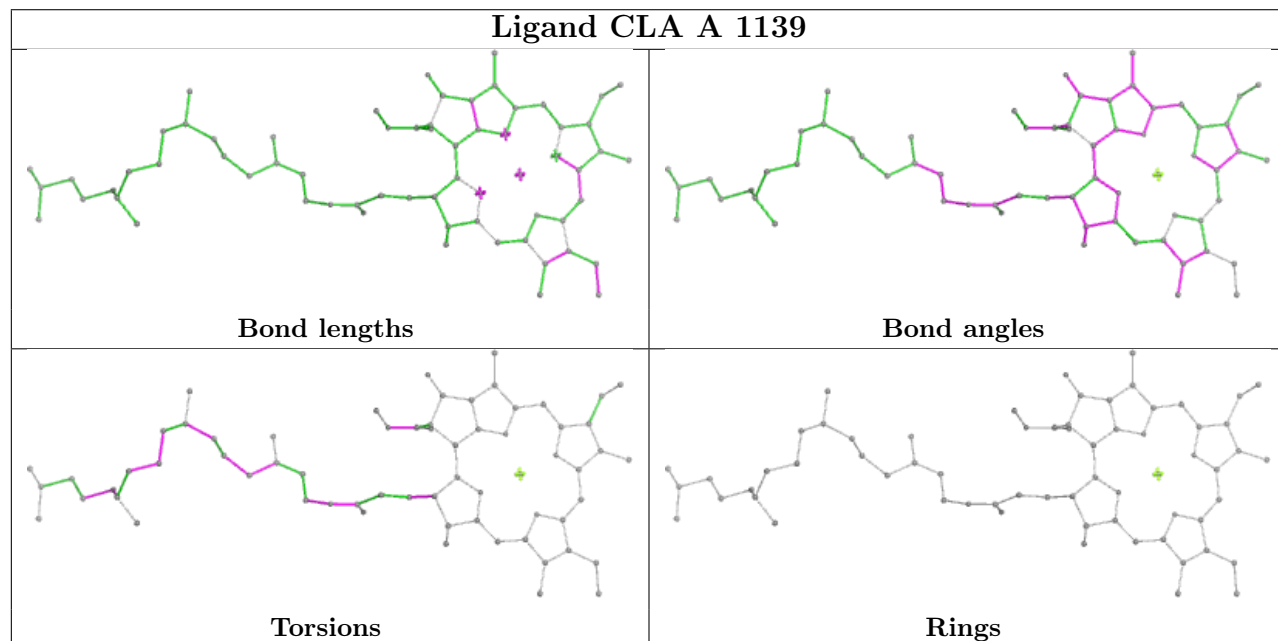


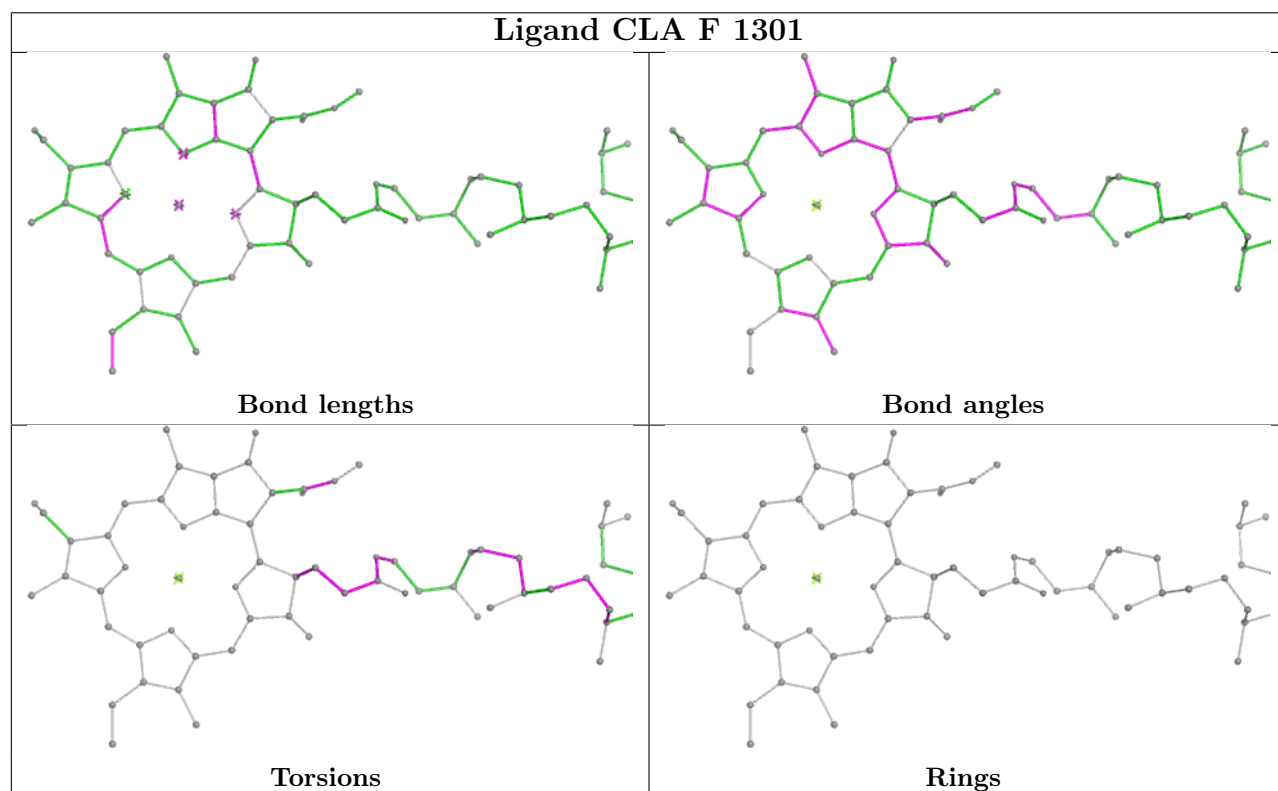
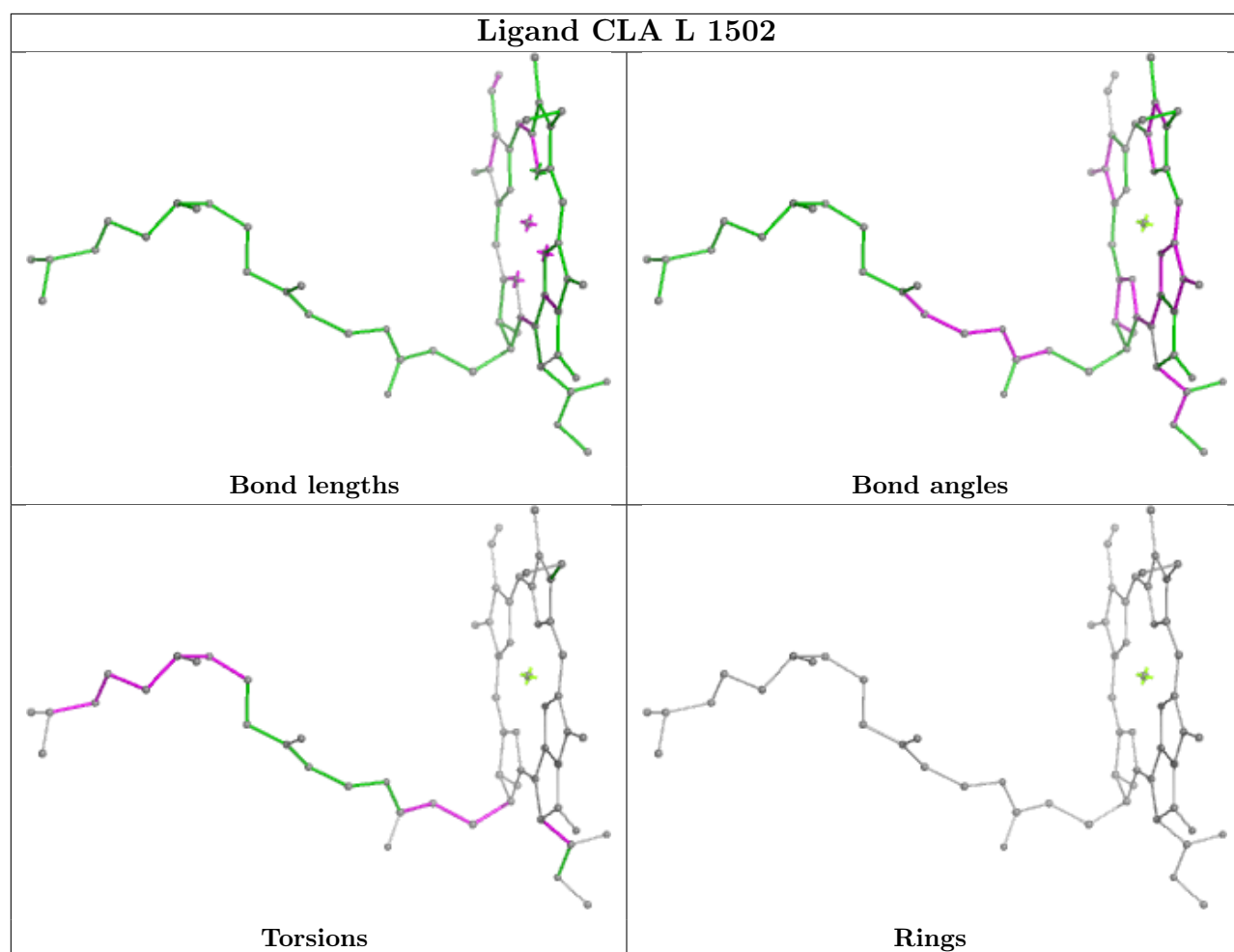
Rings

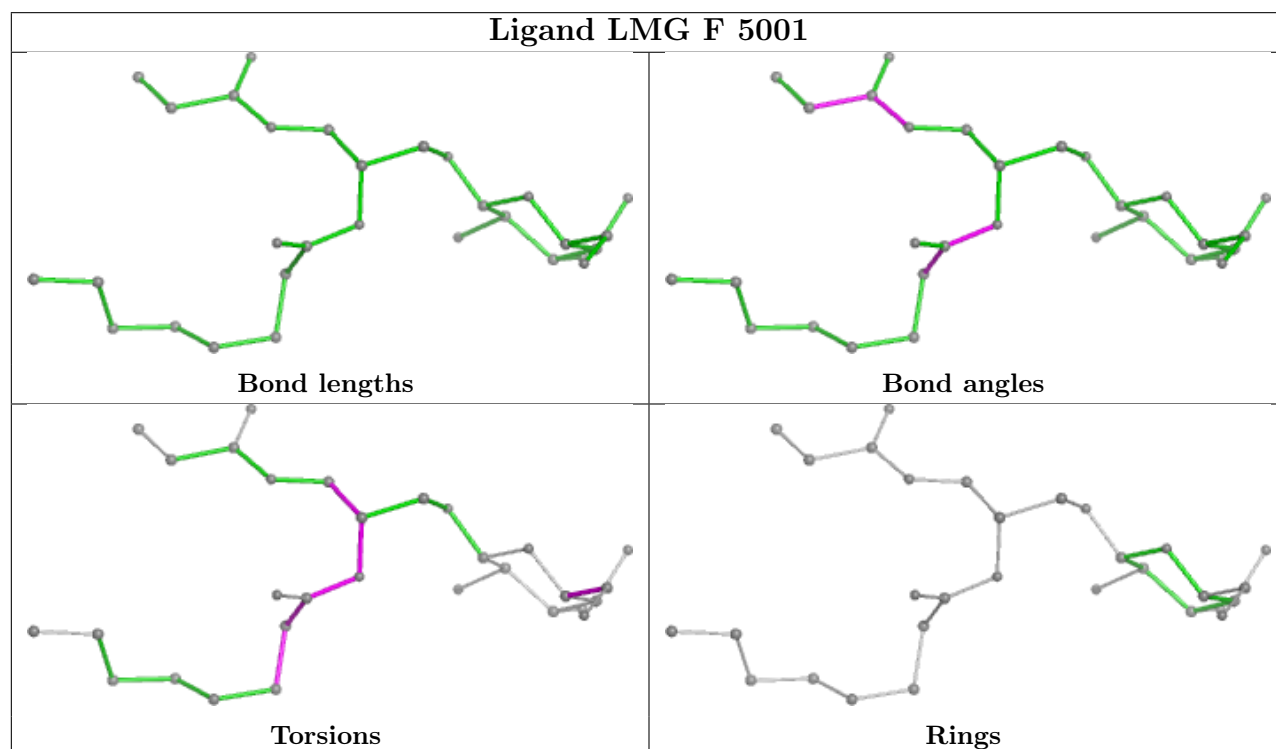
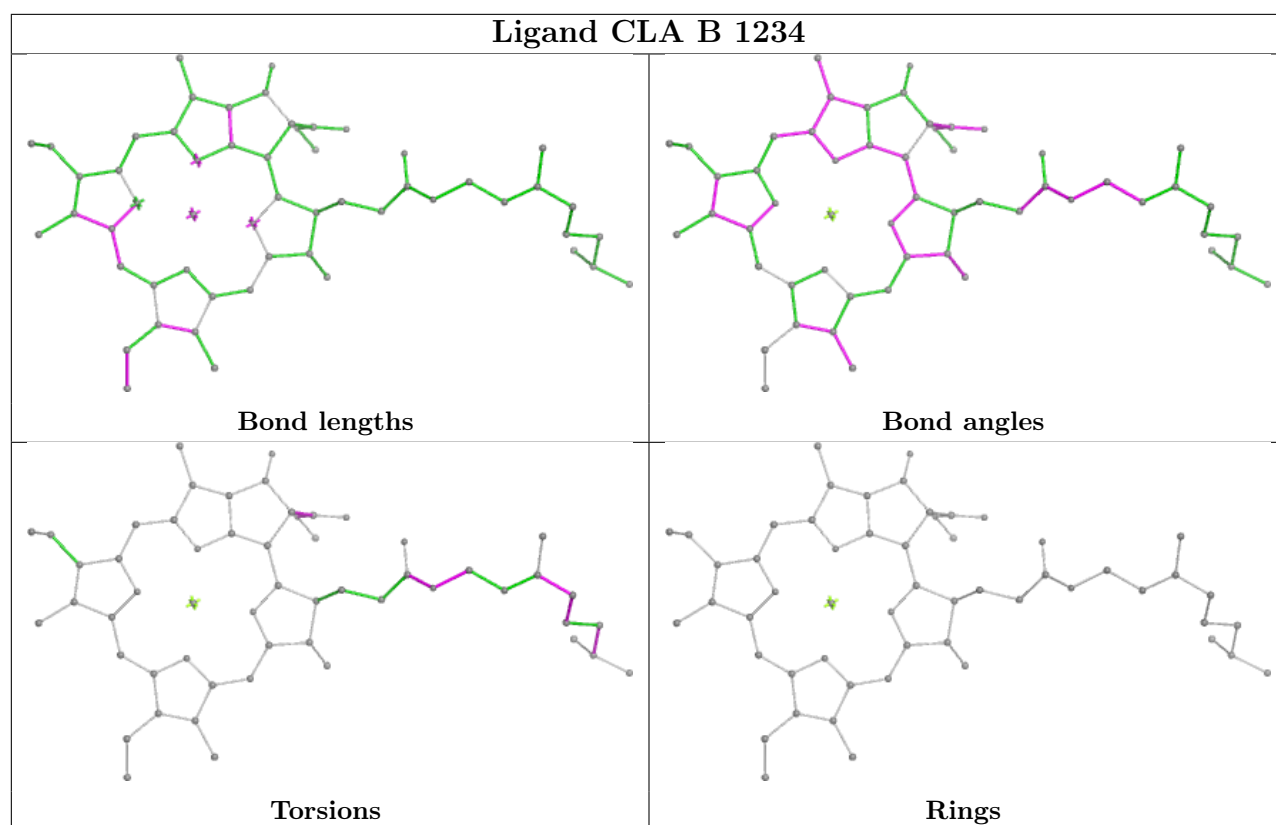
Ligand LMG 2 802

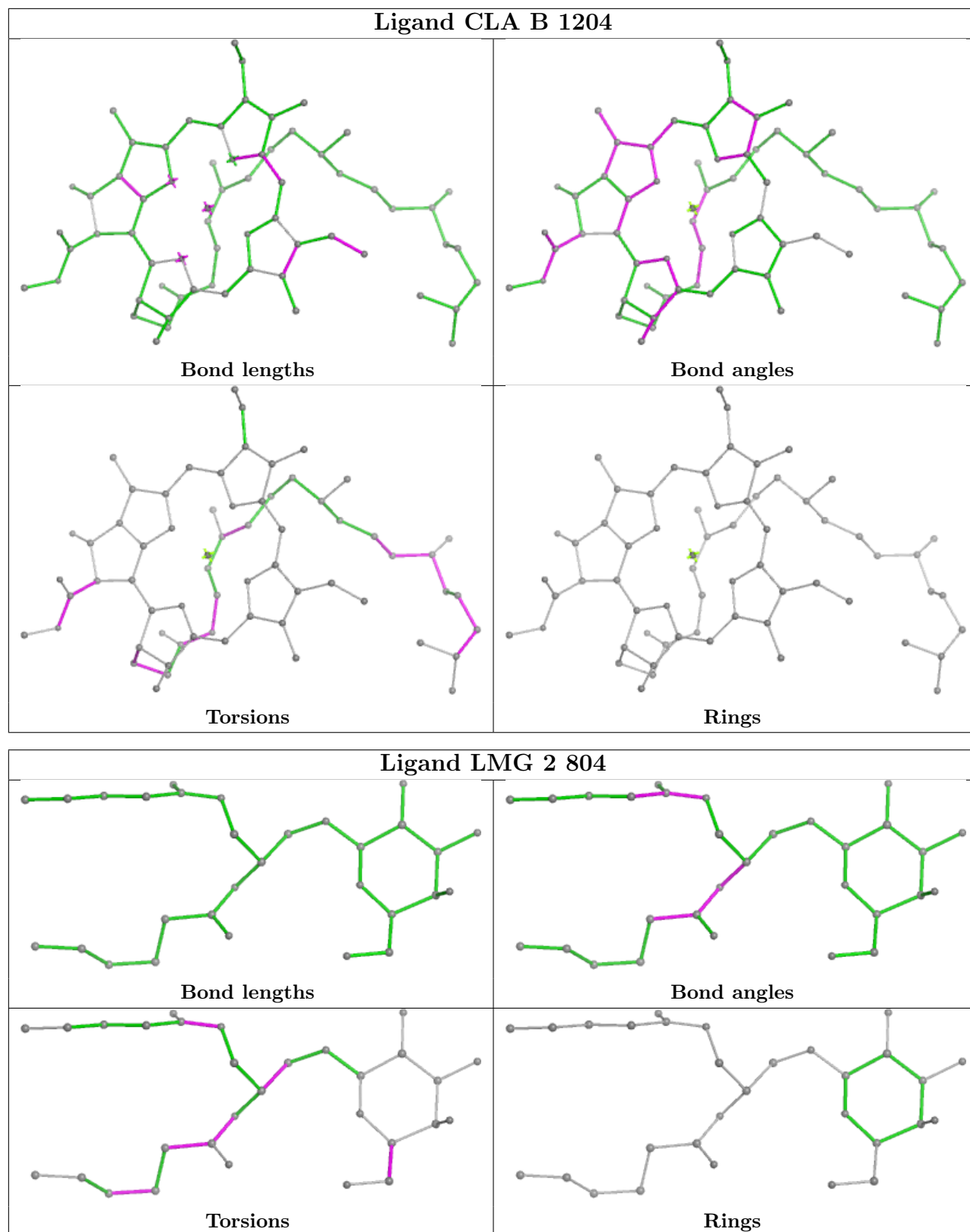


Ligand CLA A 1139

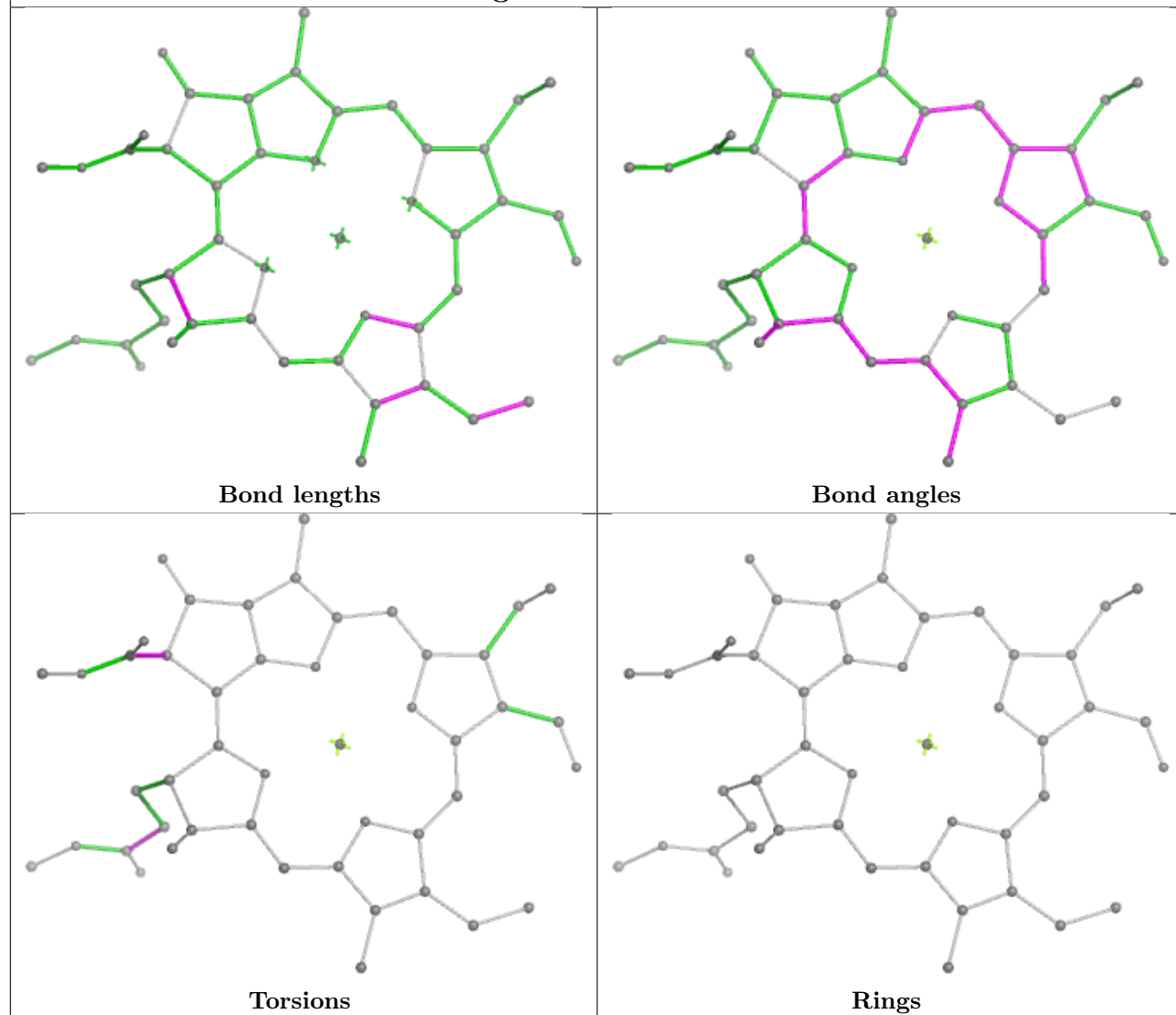




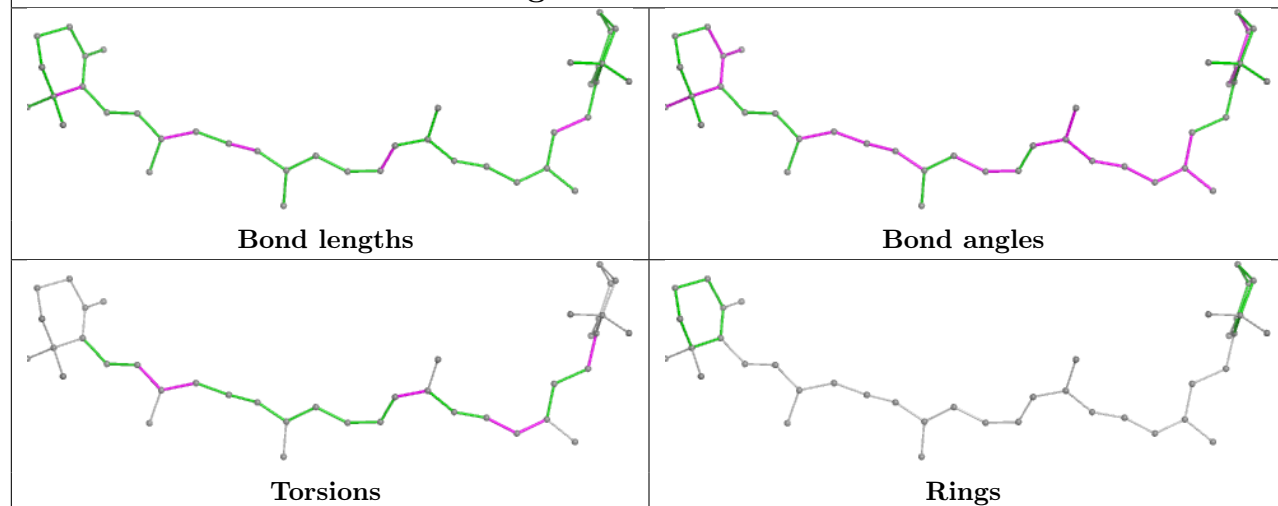


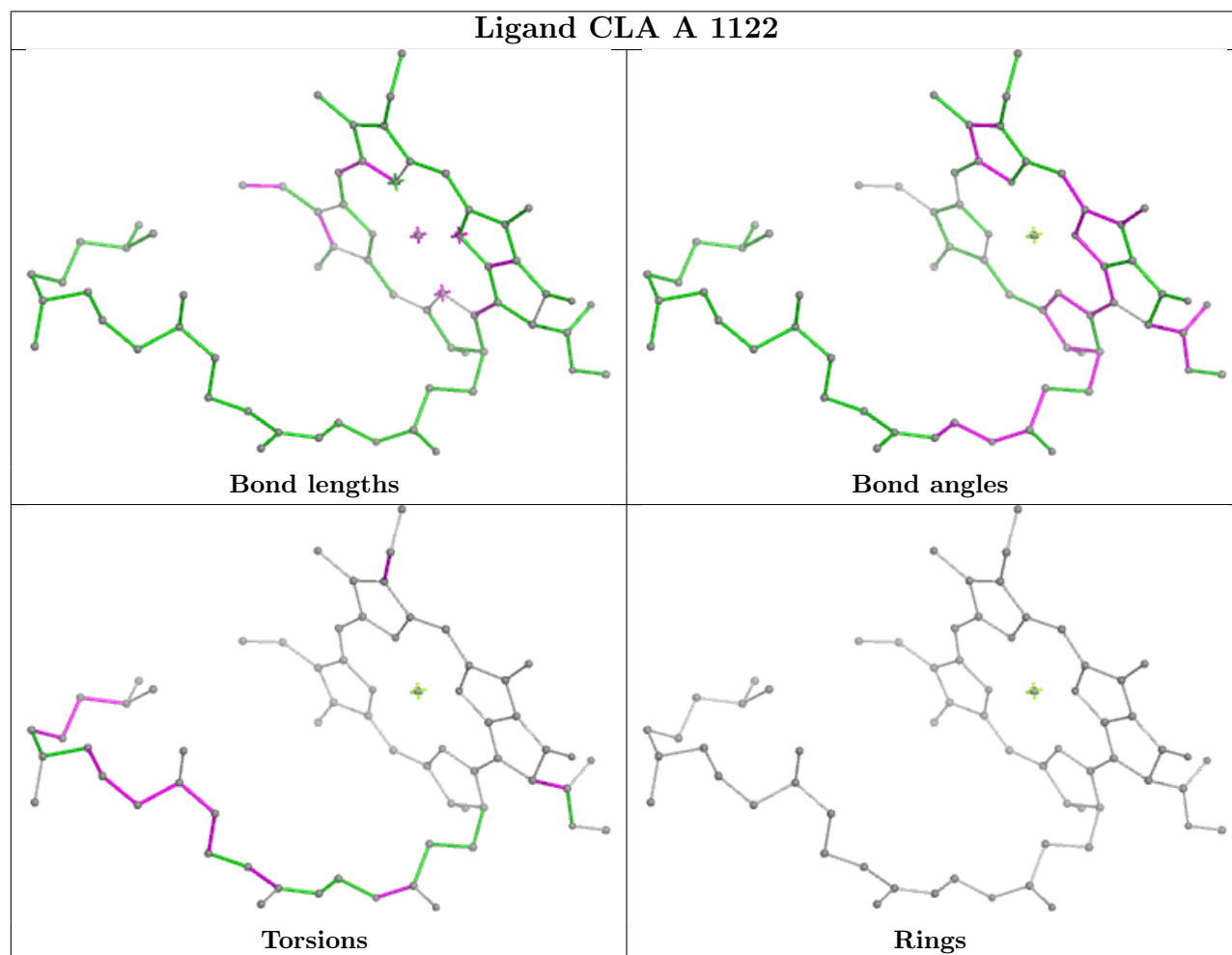
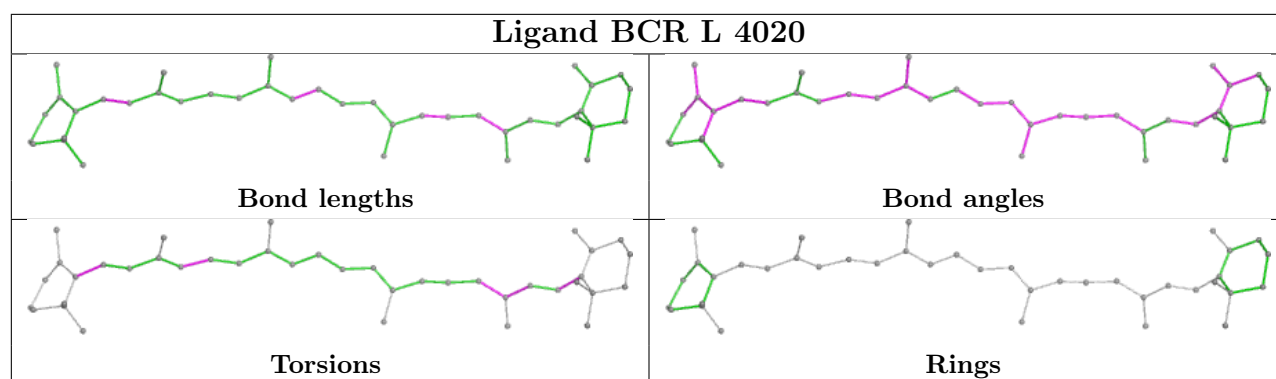


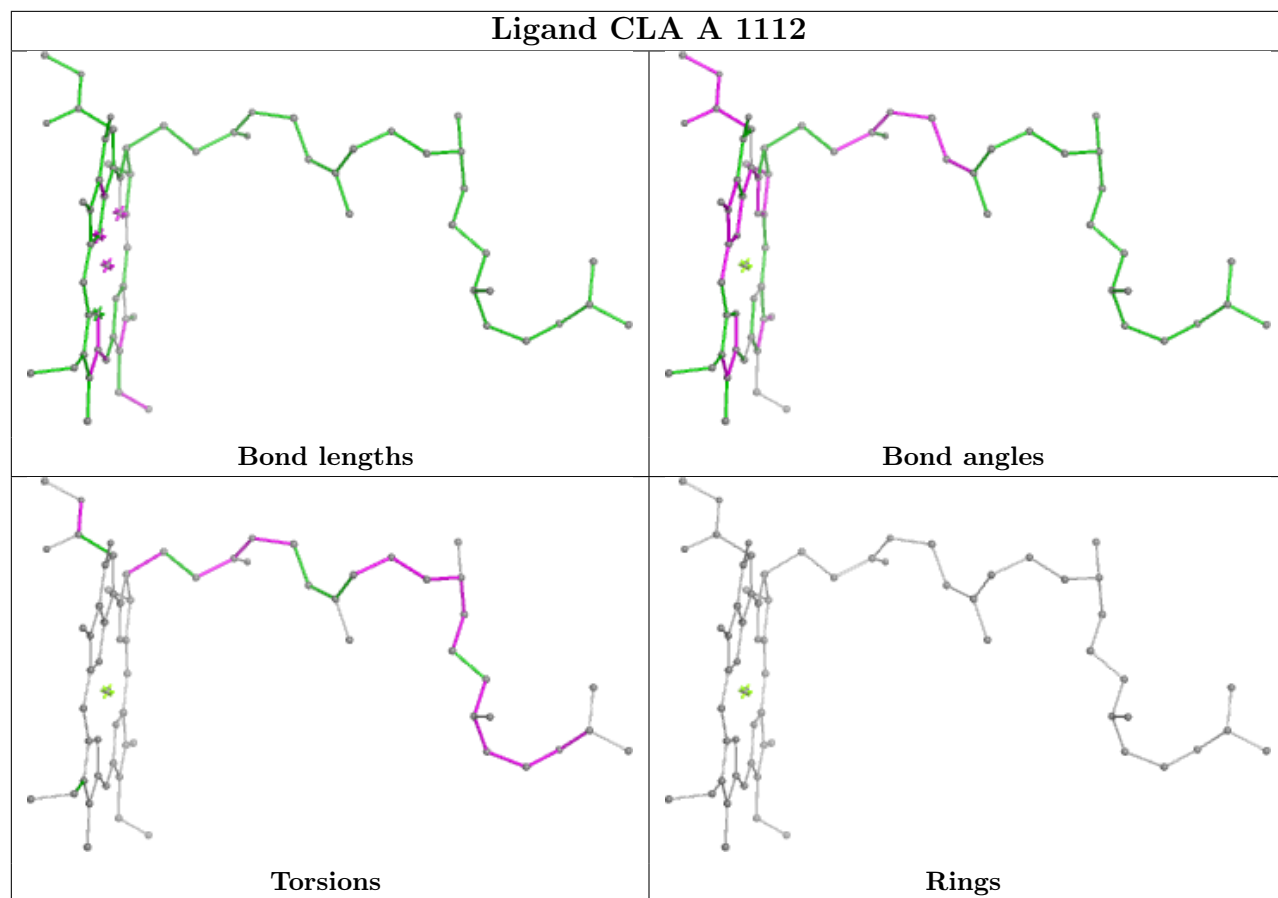
Ligand CHL 1 610

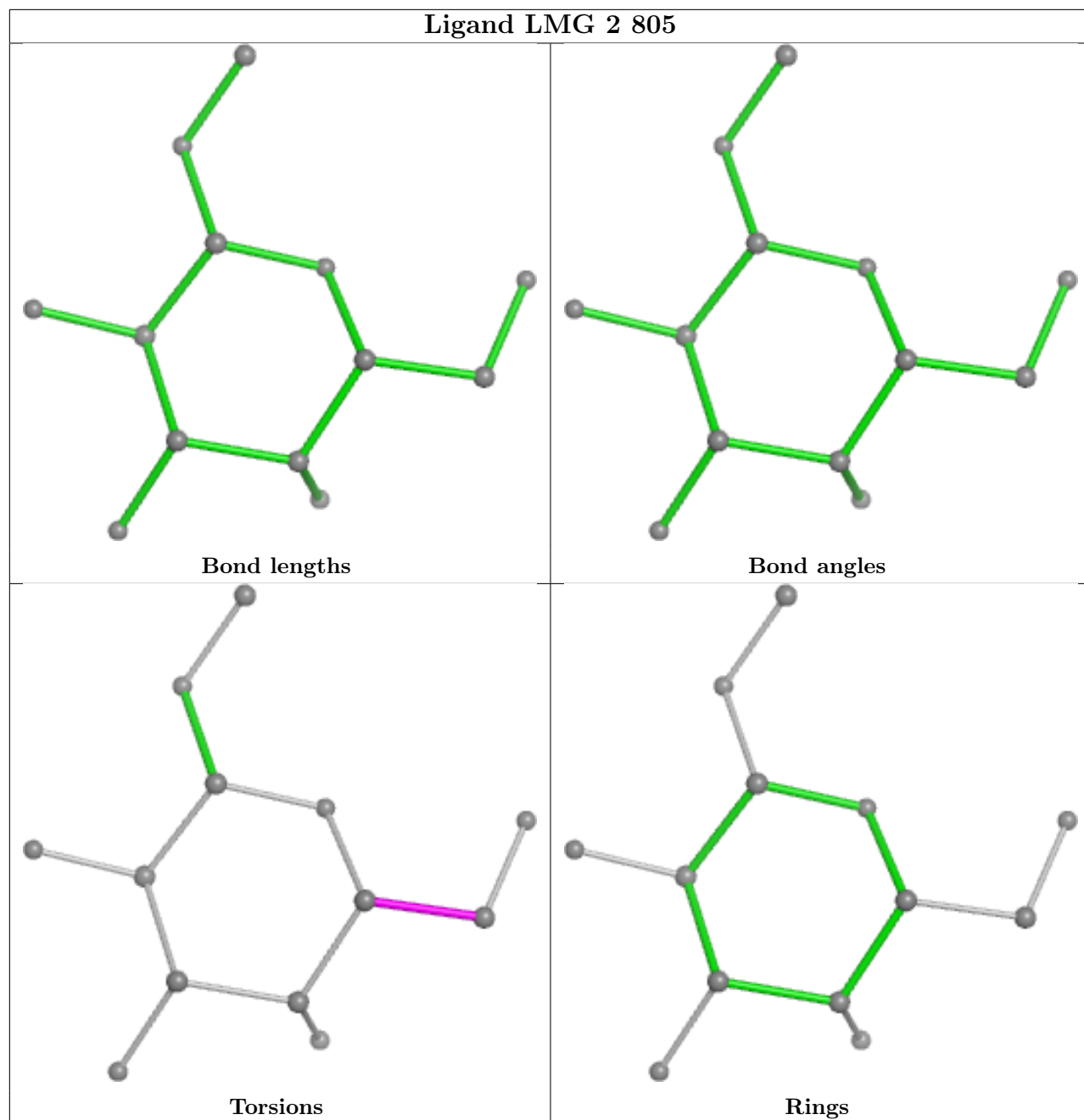


Ligand BCR I 4020

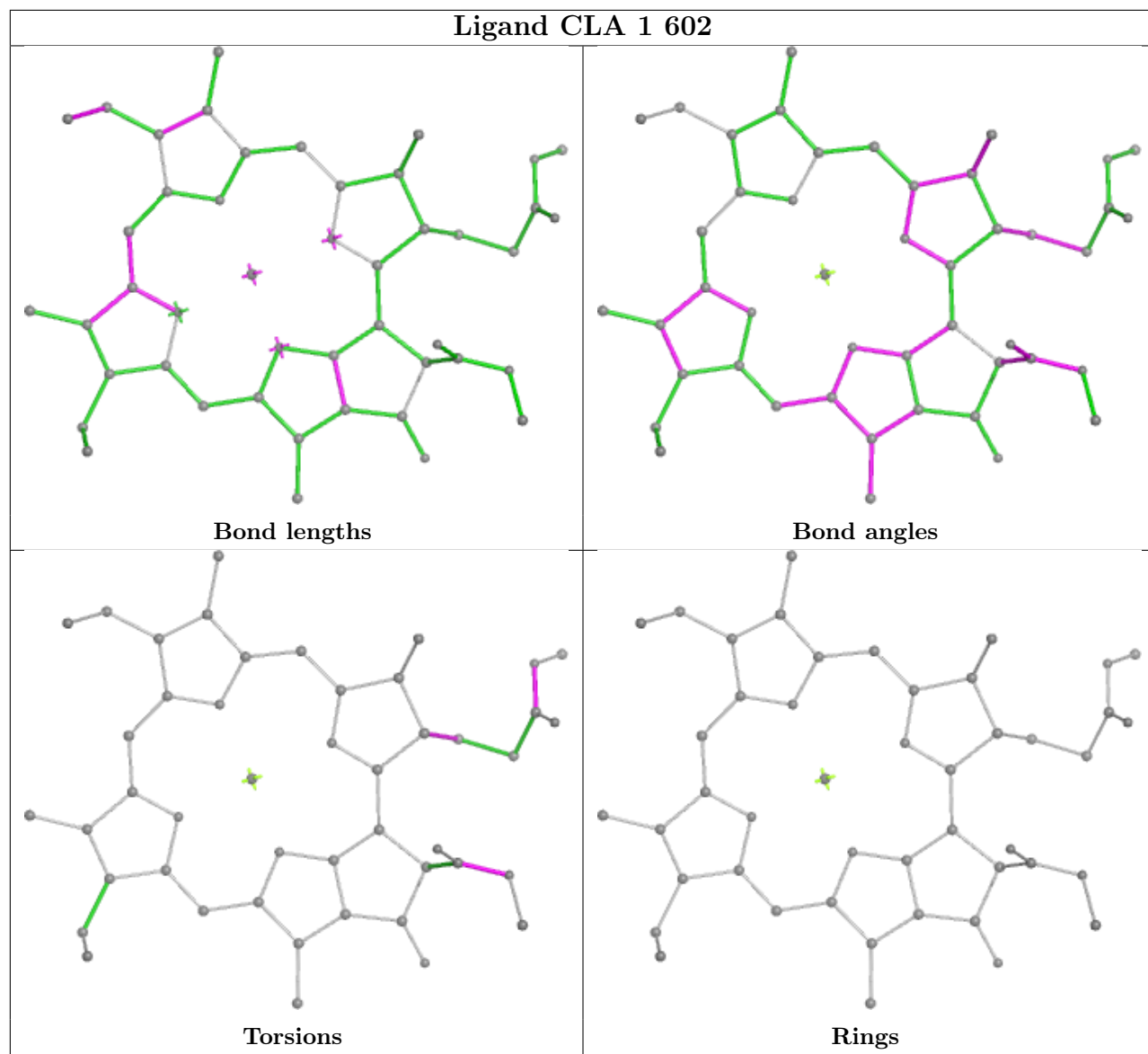


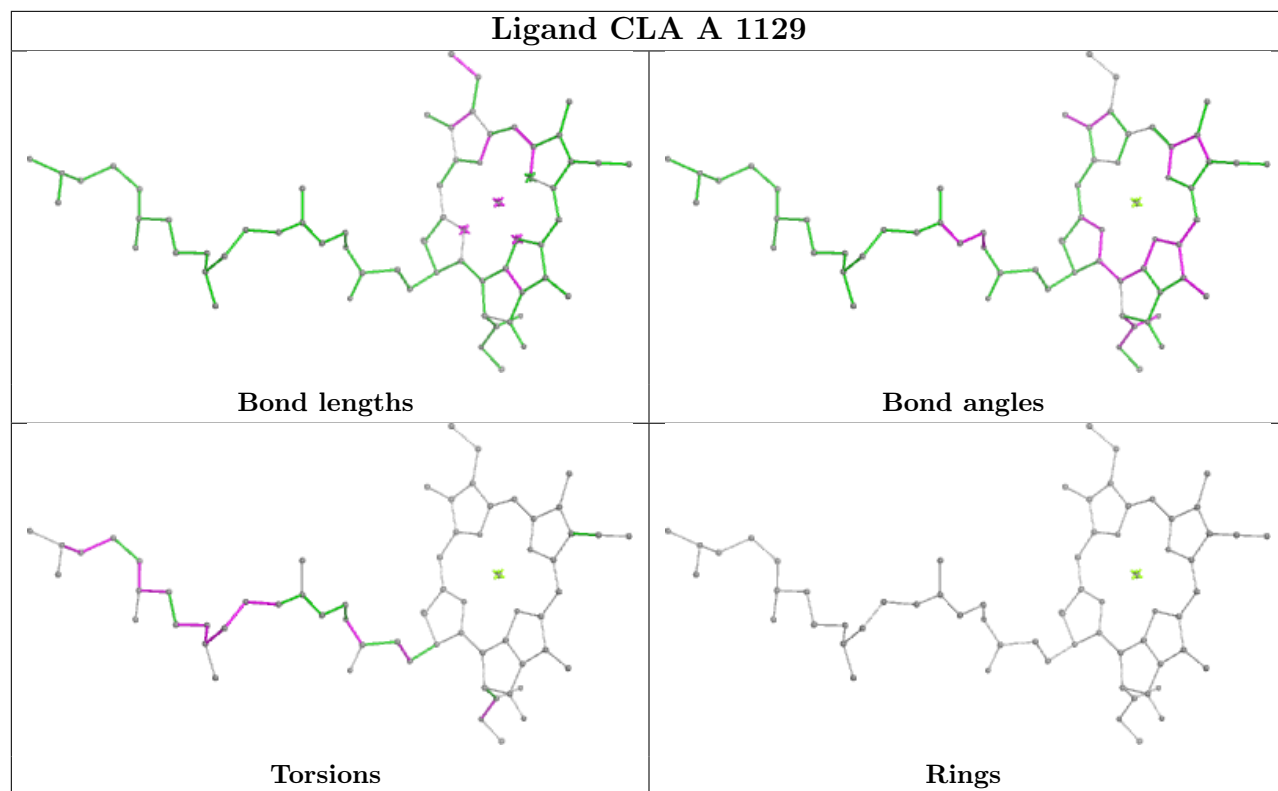




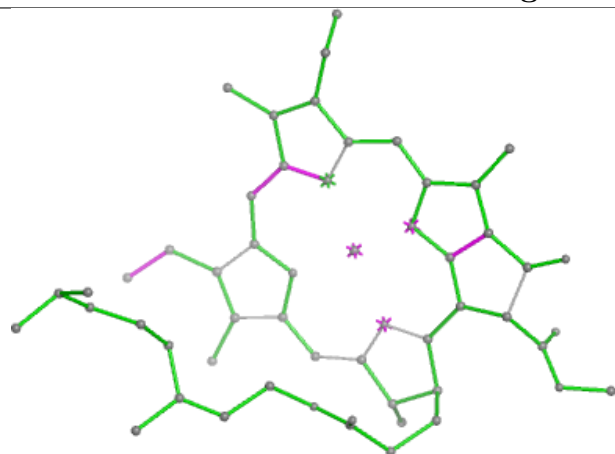


Ligand CLA 1 602

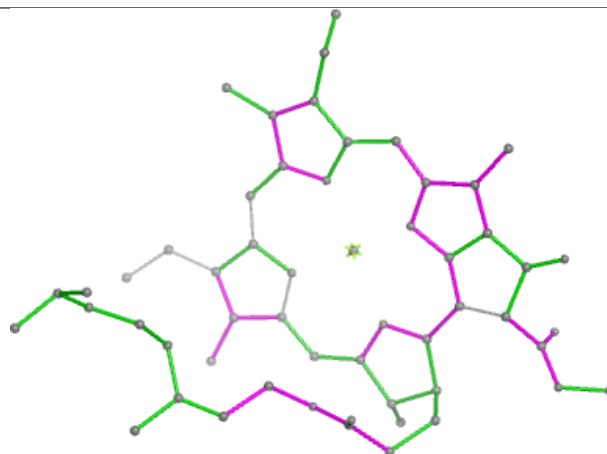




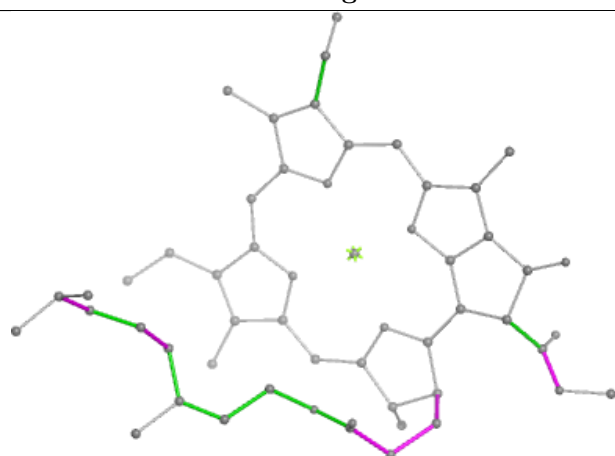
Ligand CLA 3 601



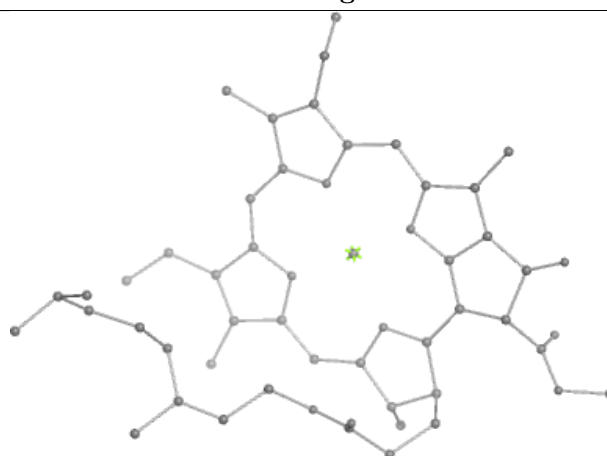
Bond lengths



Bond angles

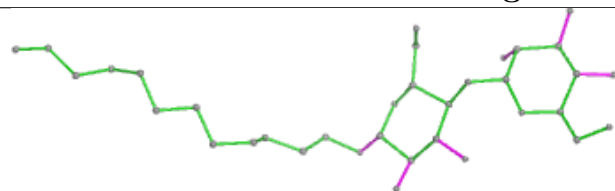


Torsions

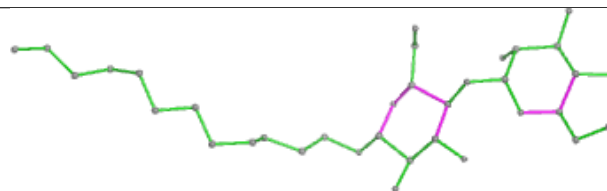


Rings

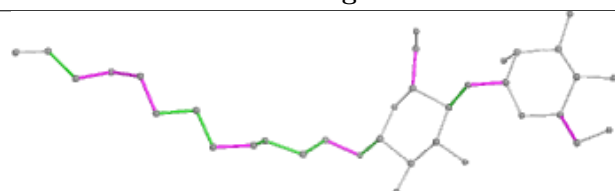
Ligand LMT G 5004



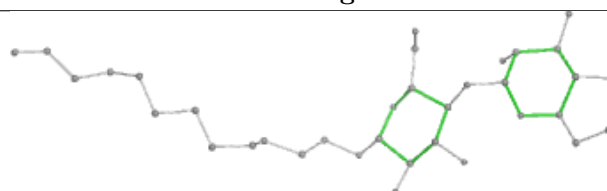
Bond lengths



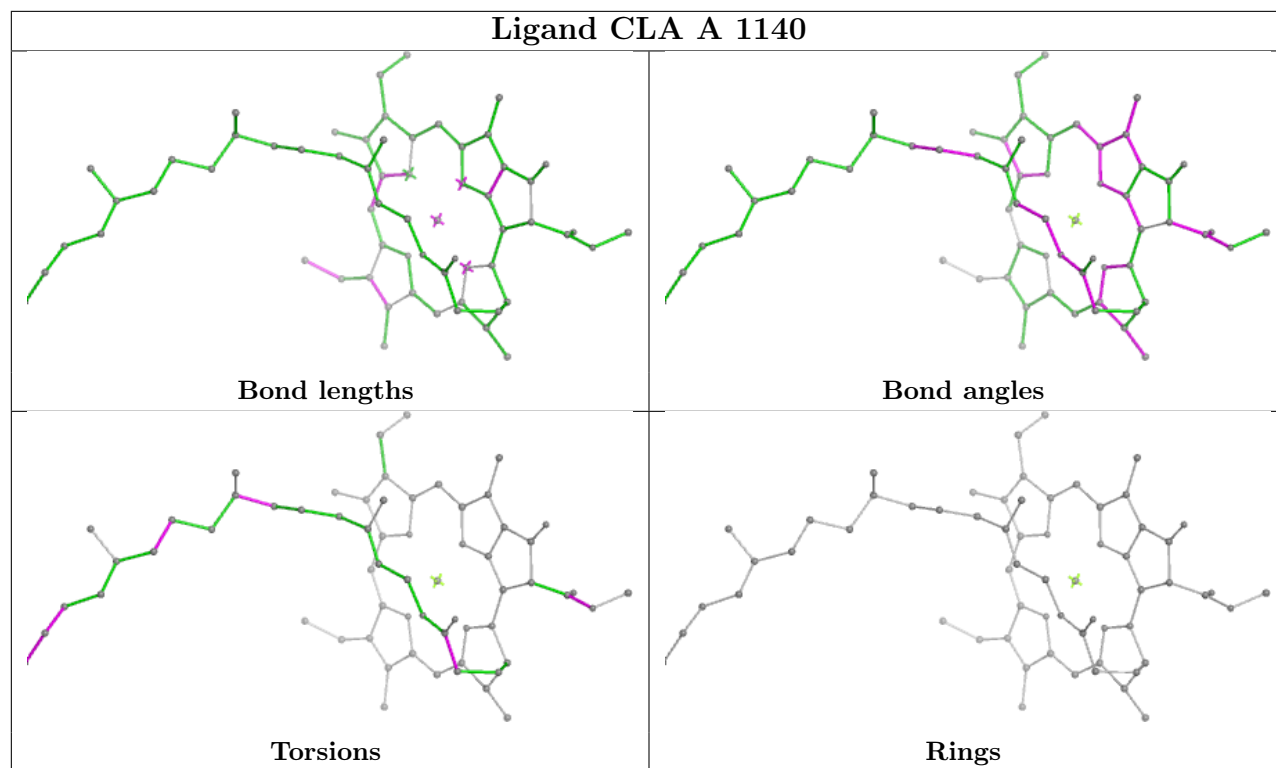
Bond angles



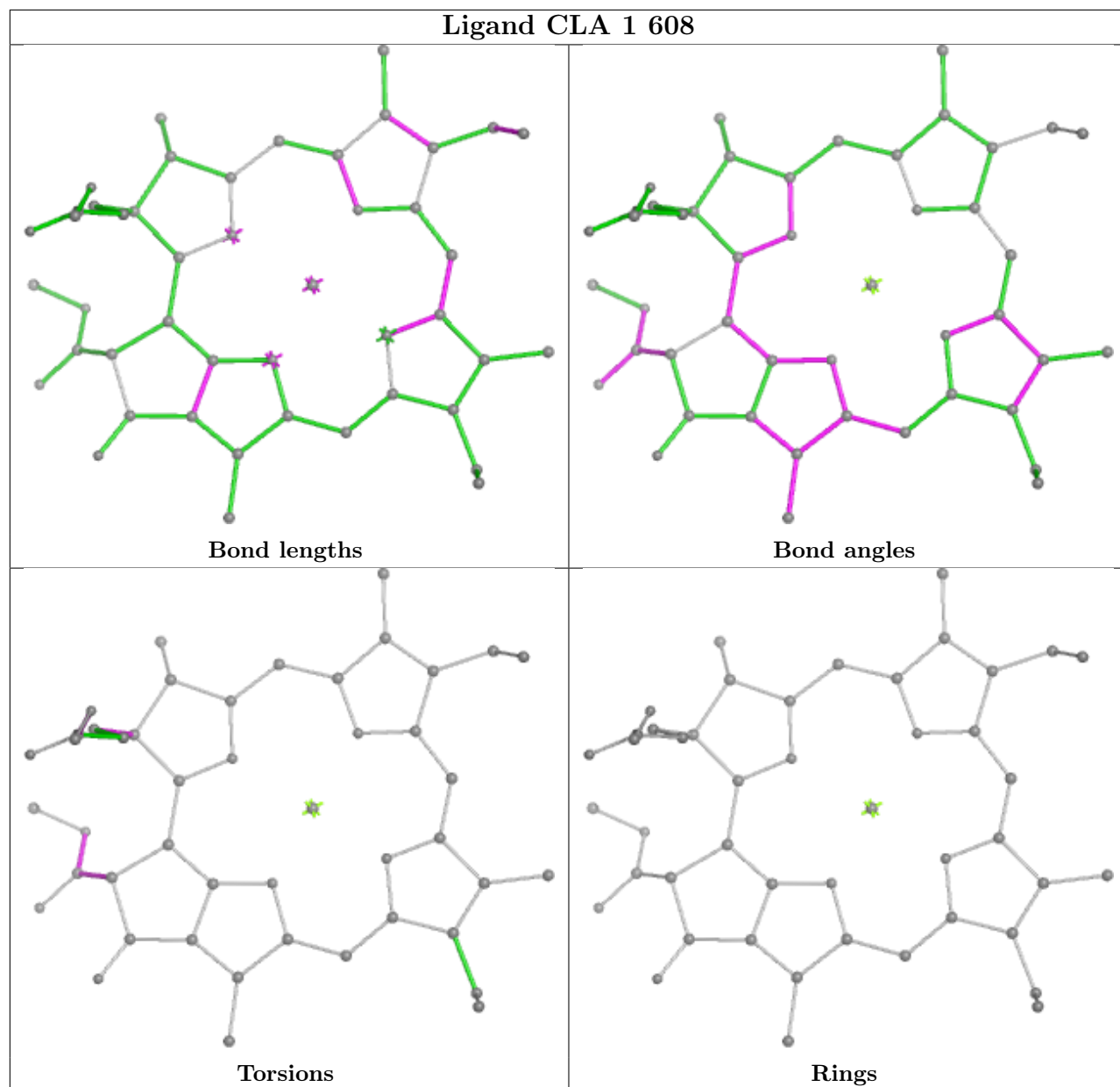
Torsions

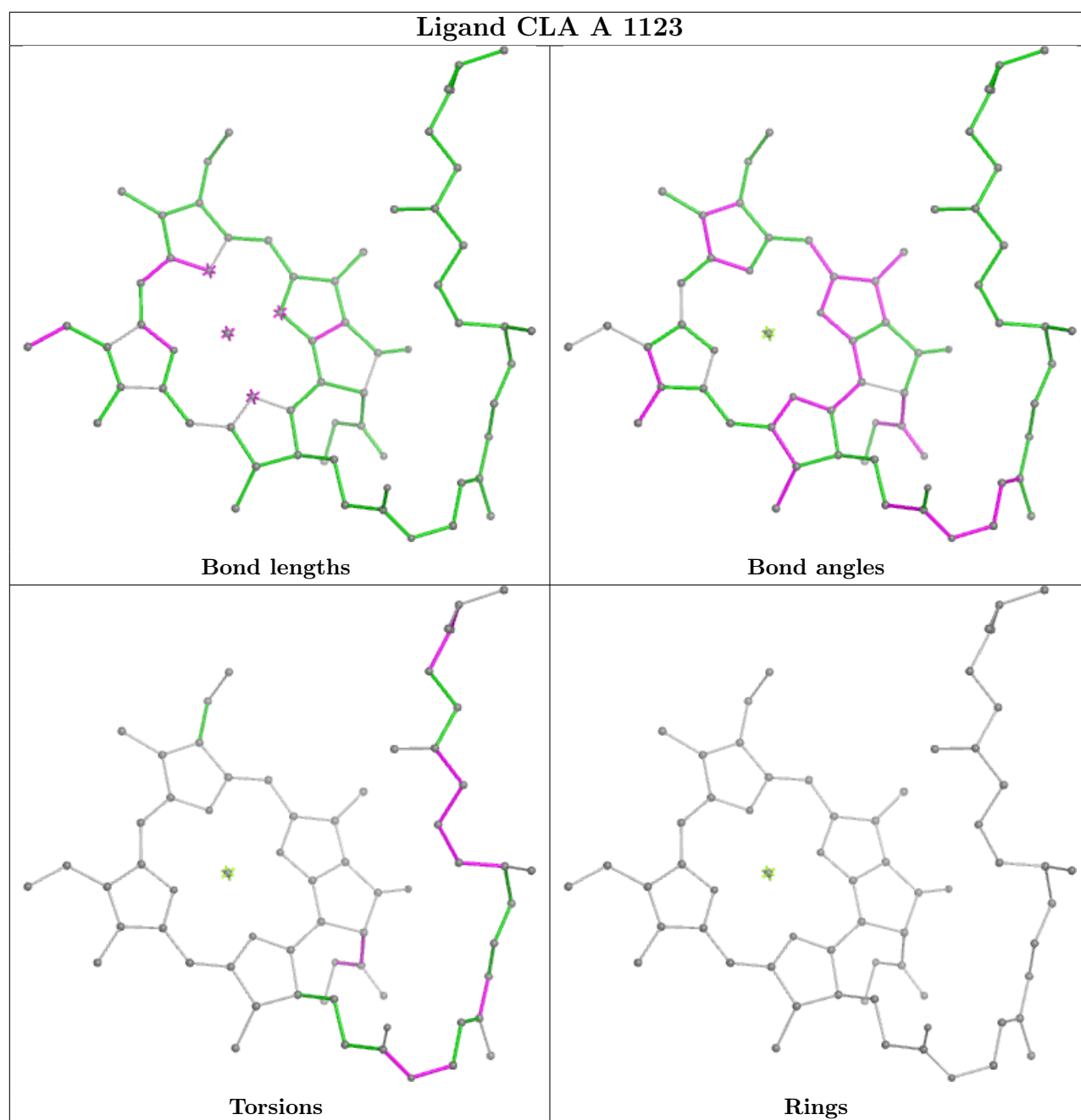


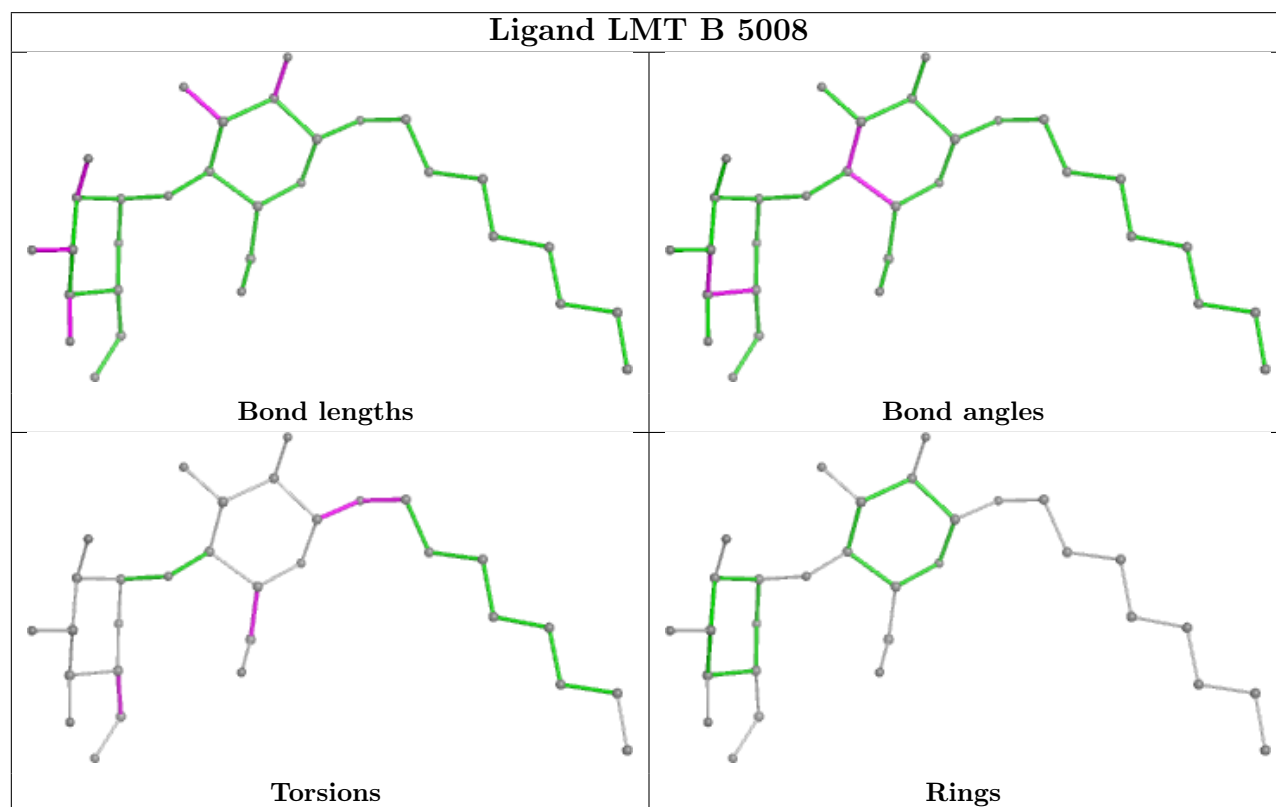
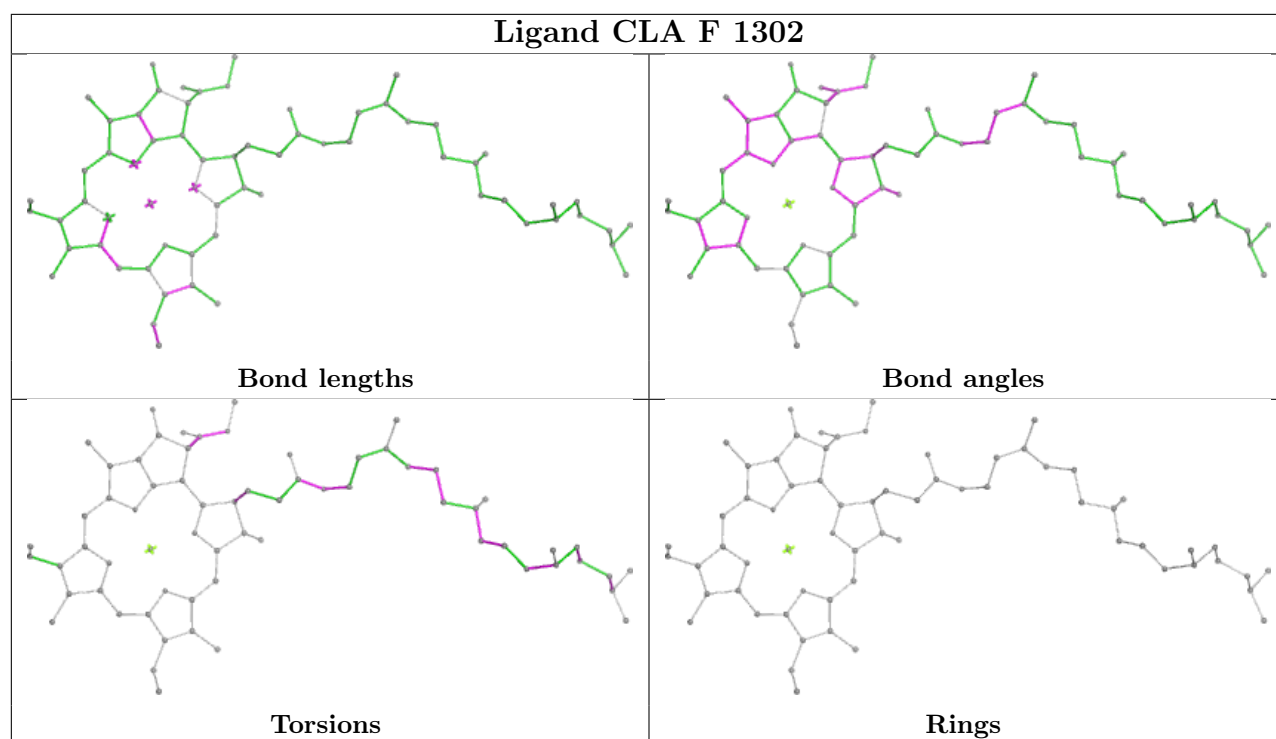
Rings

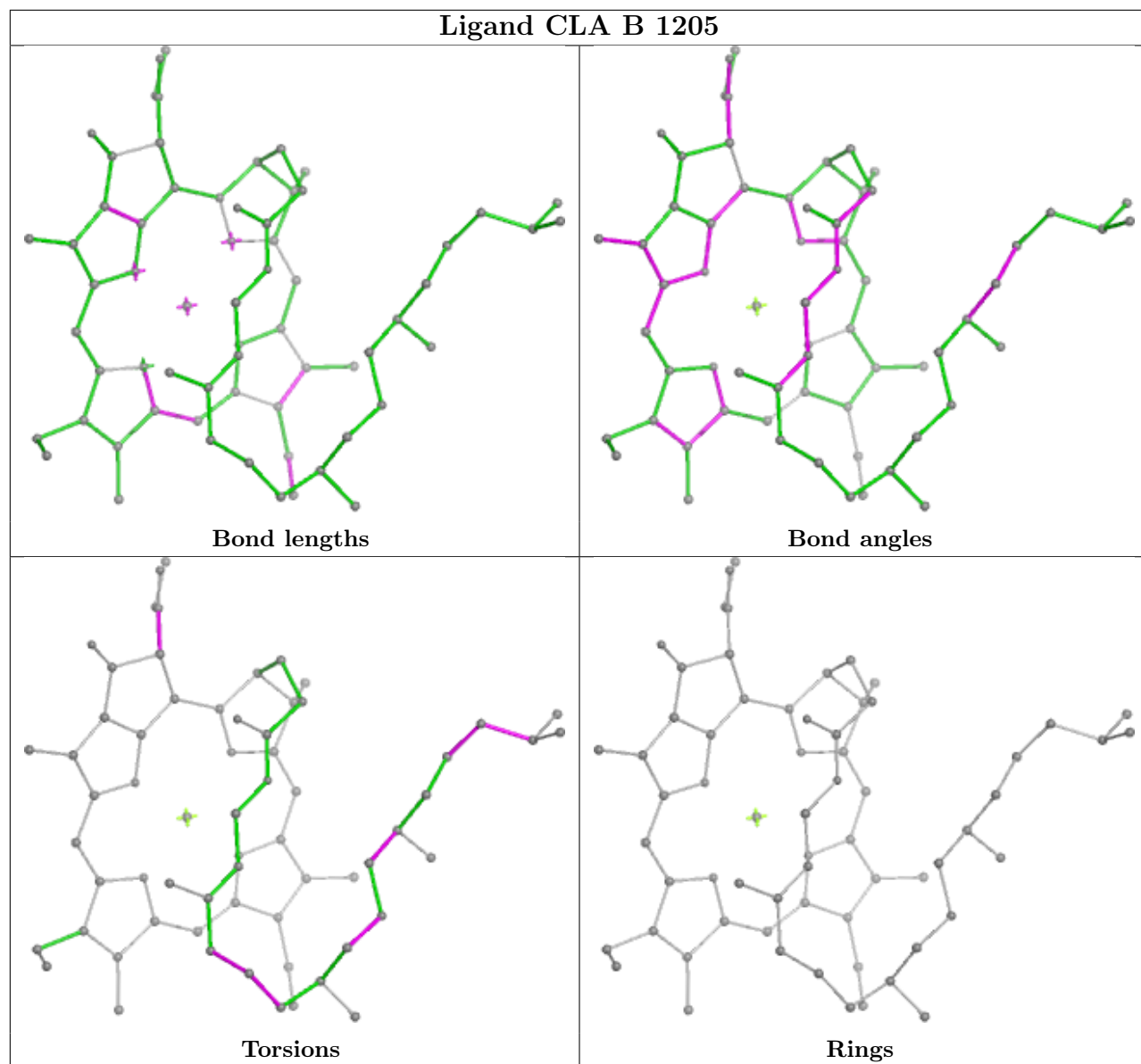


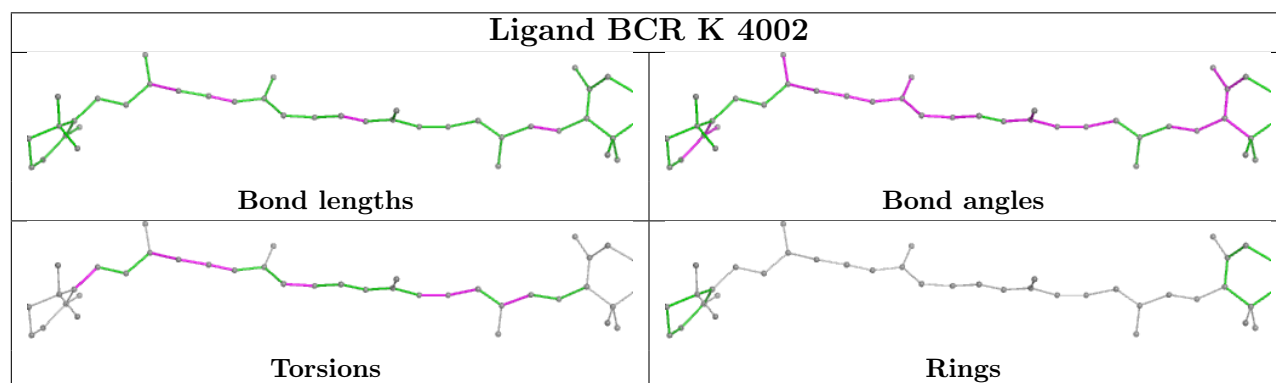
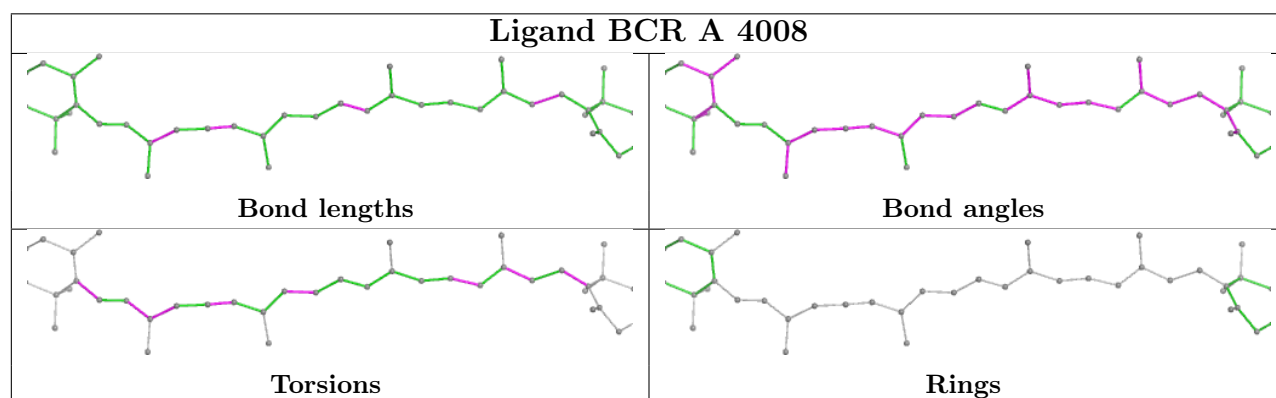
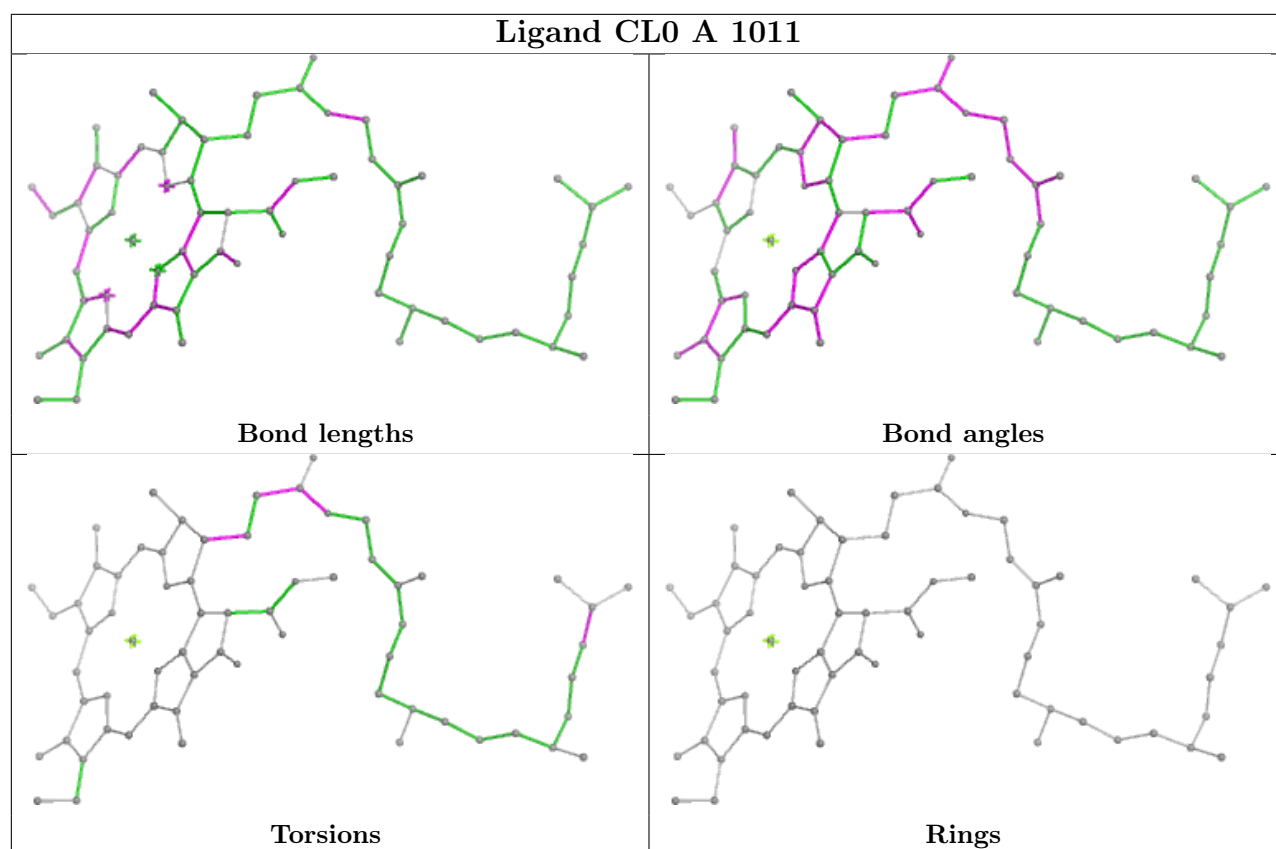
Ligand CLA 1 608

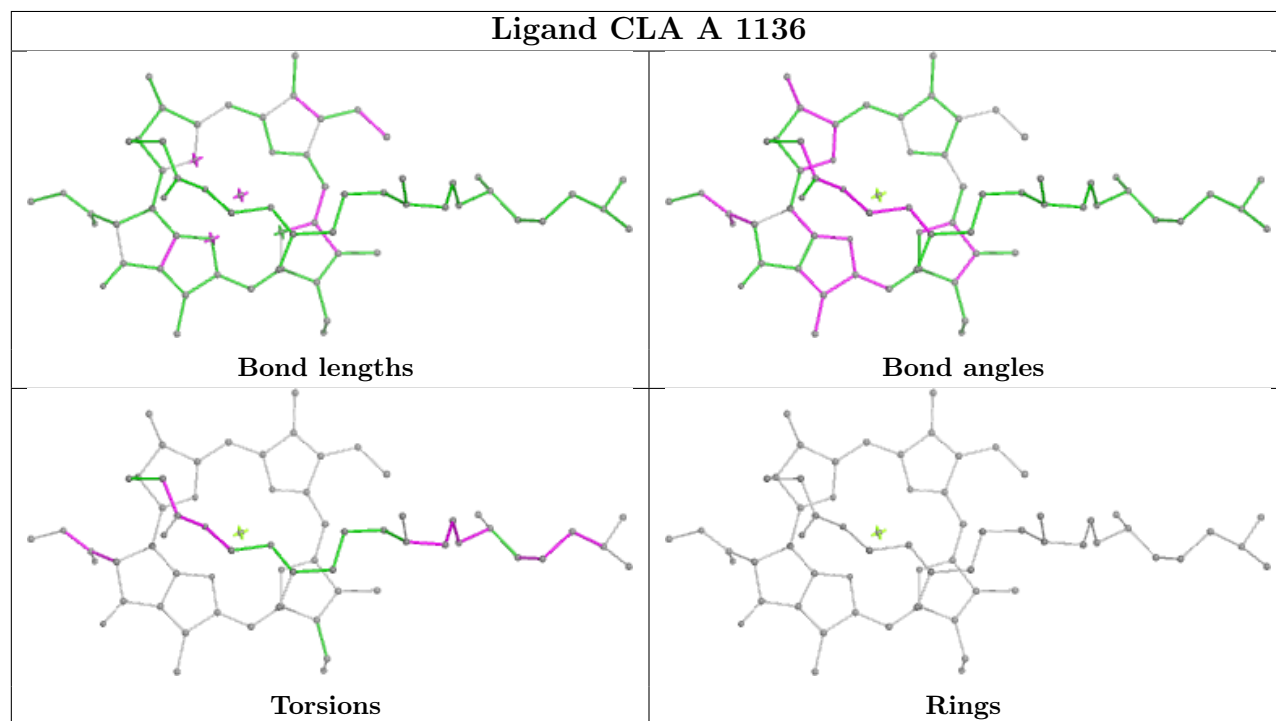
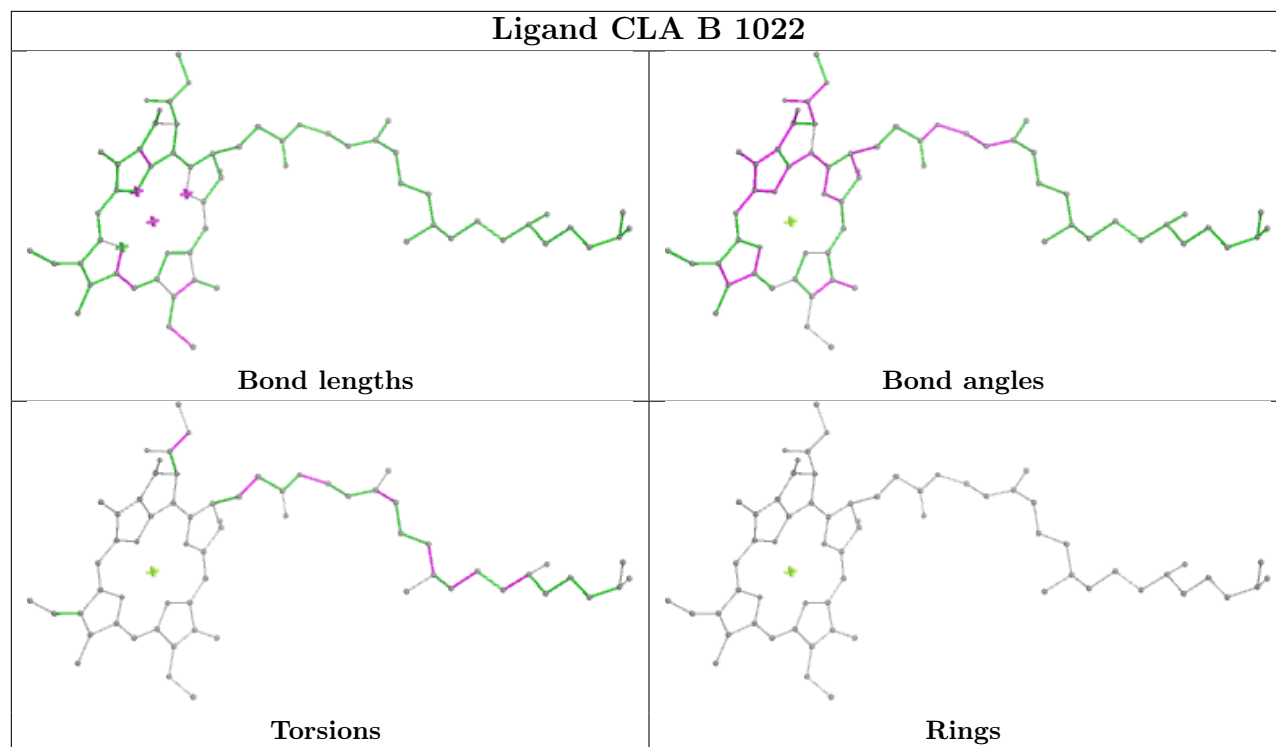


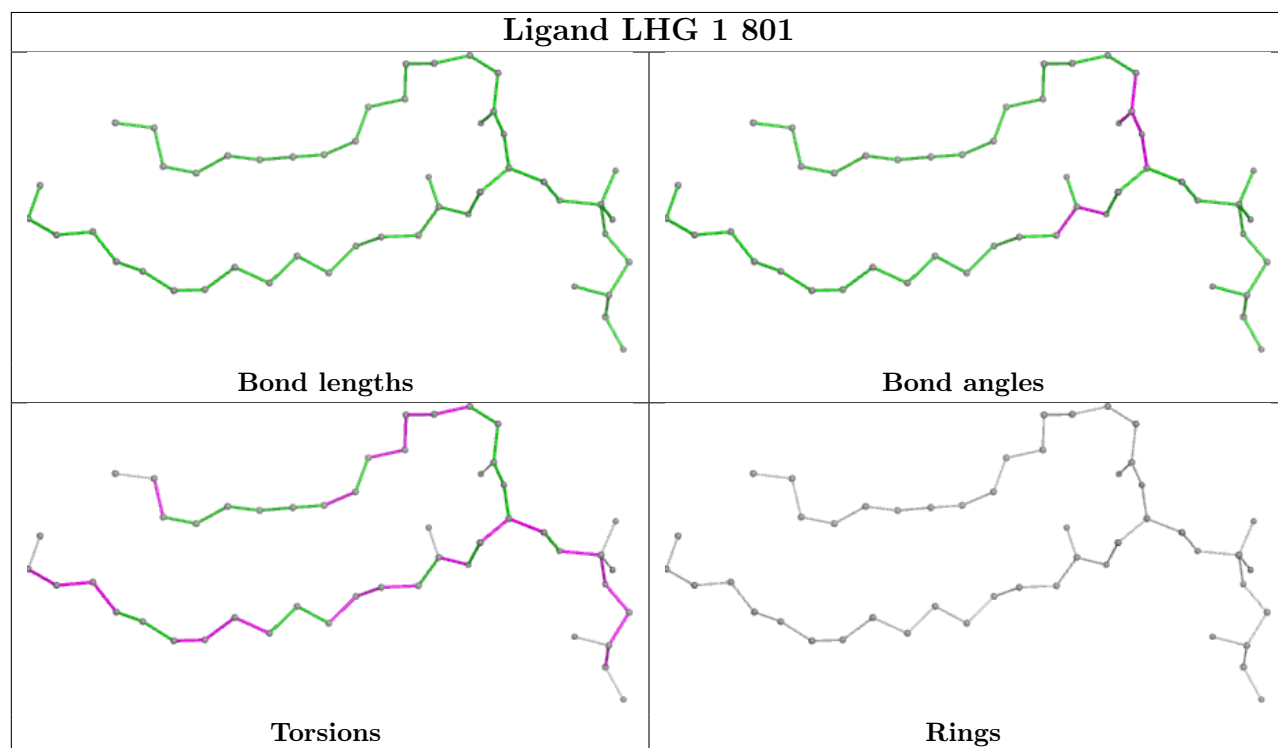
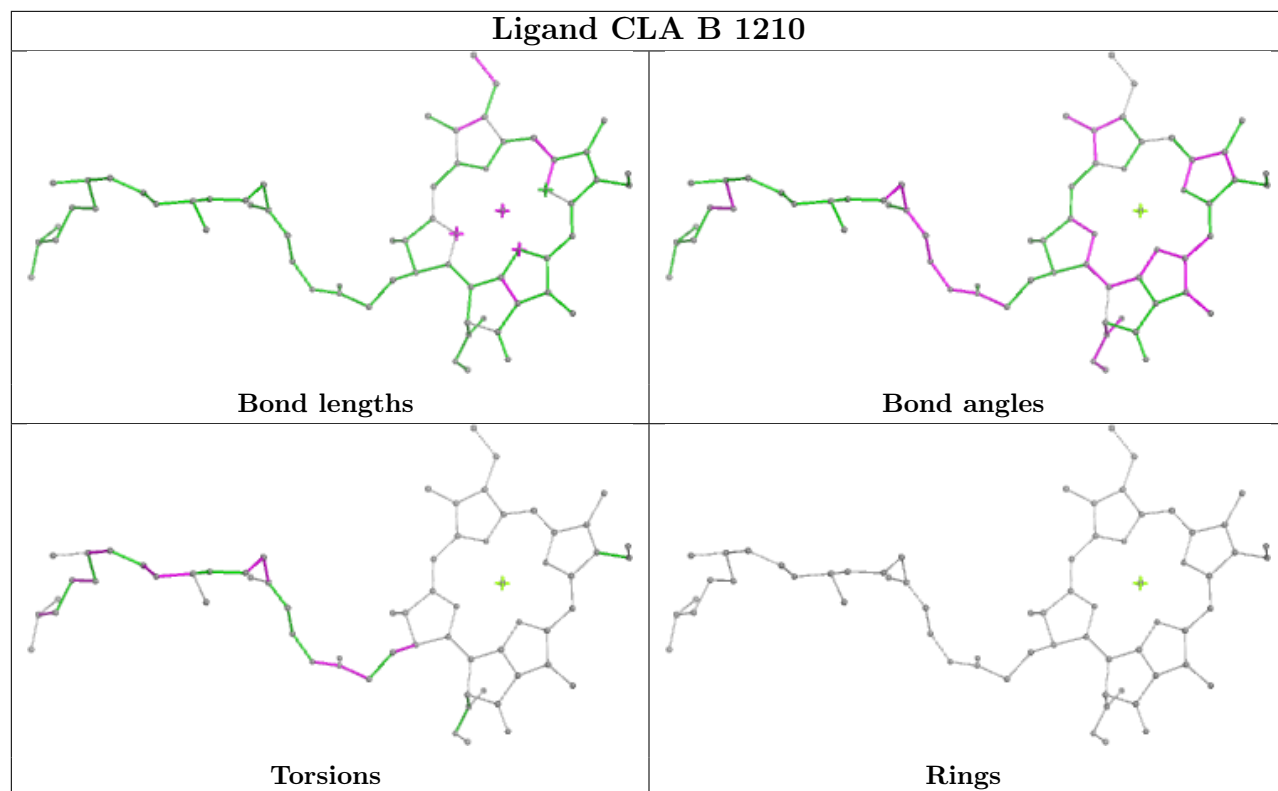




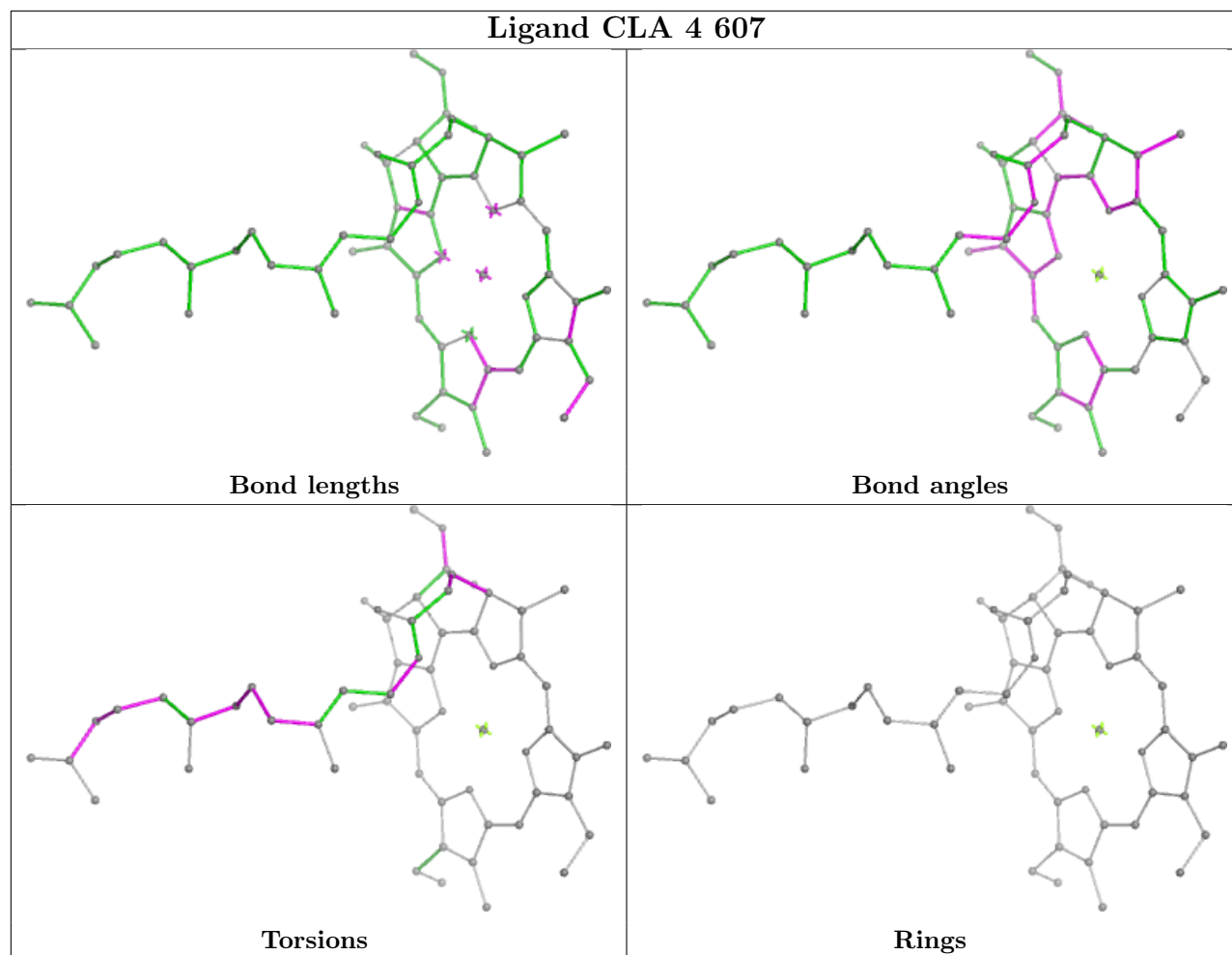




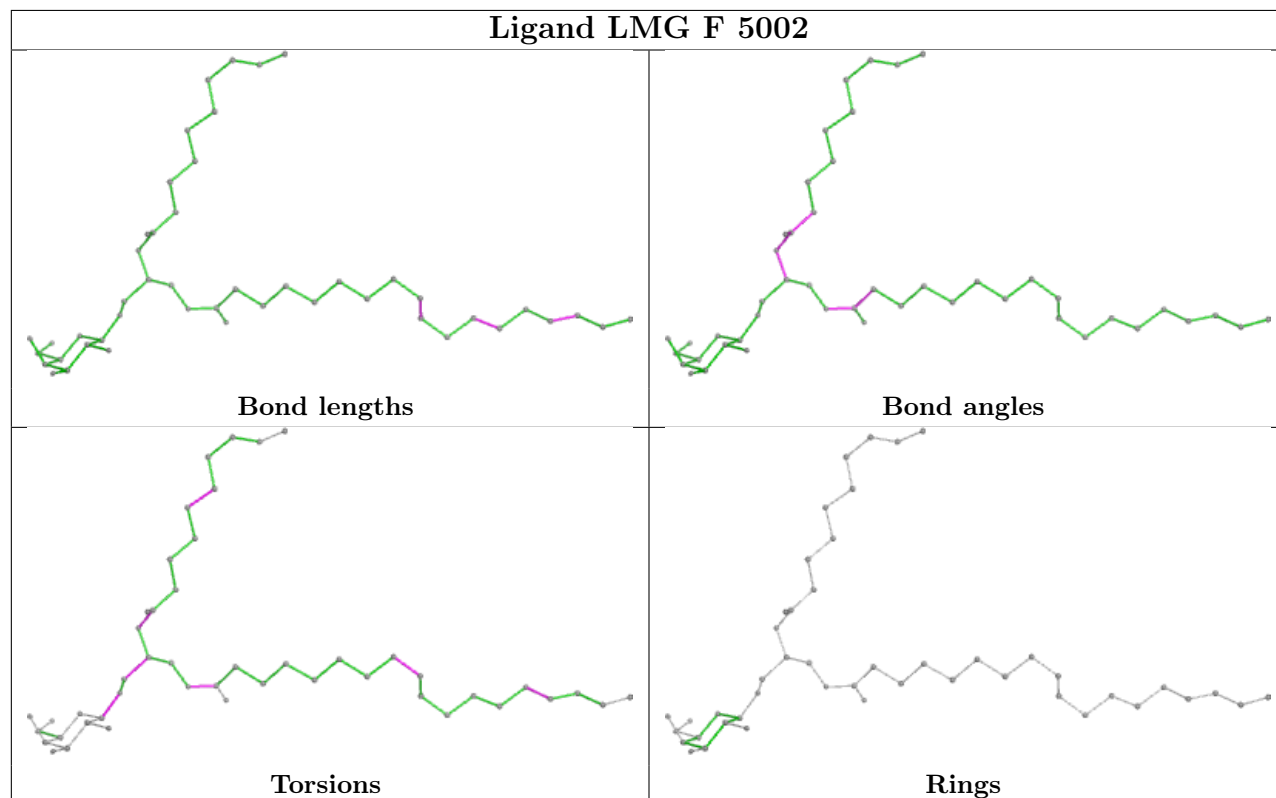


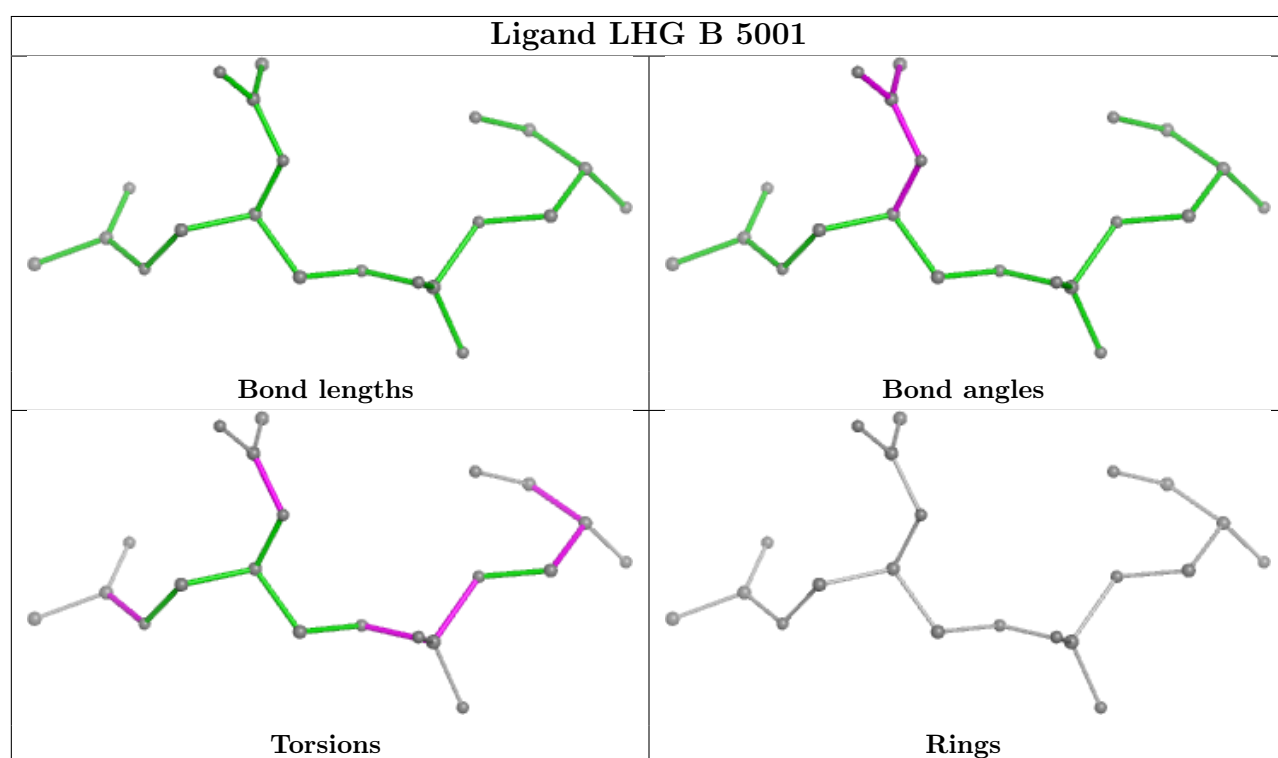
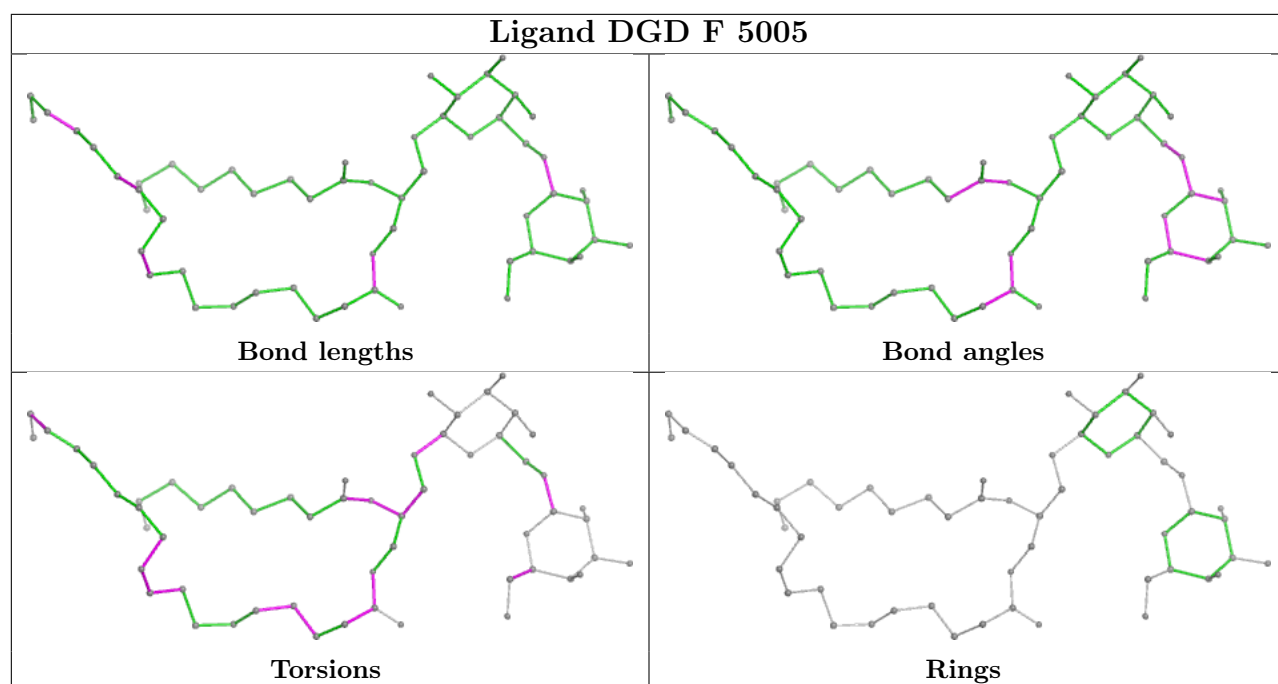


Ligand CLA 4 607

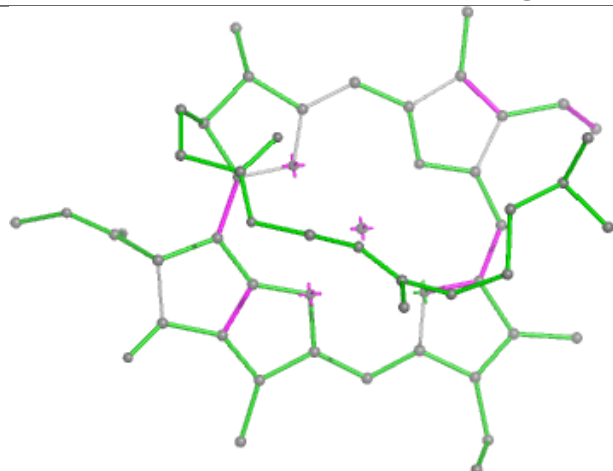


Ligand LMG F 5002

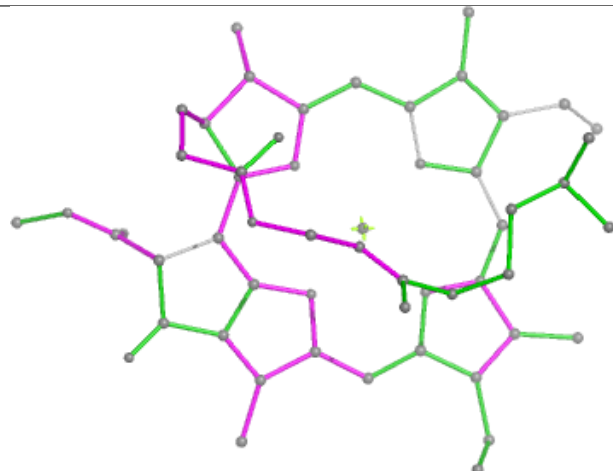




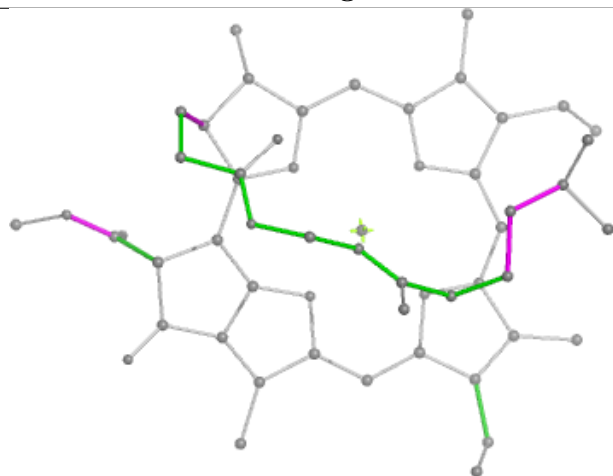
Ligand CLA 1 603



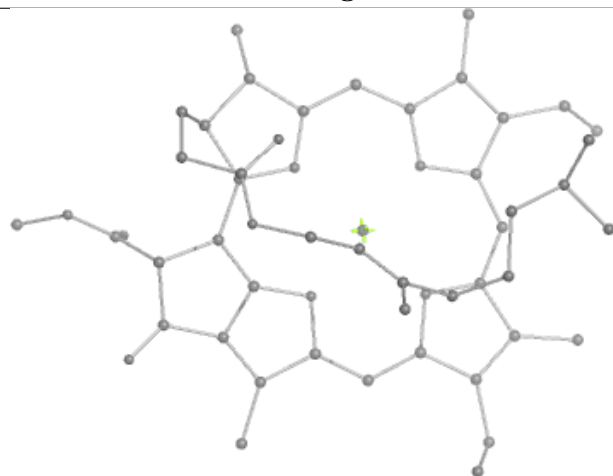
Bond lengths



Bond angles

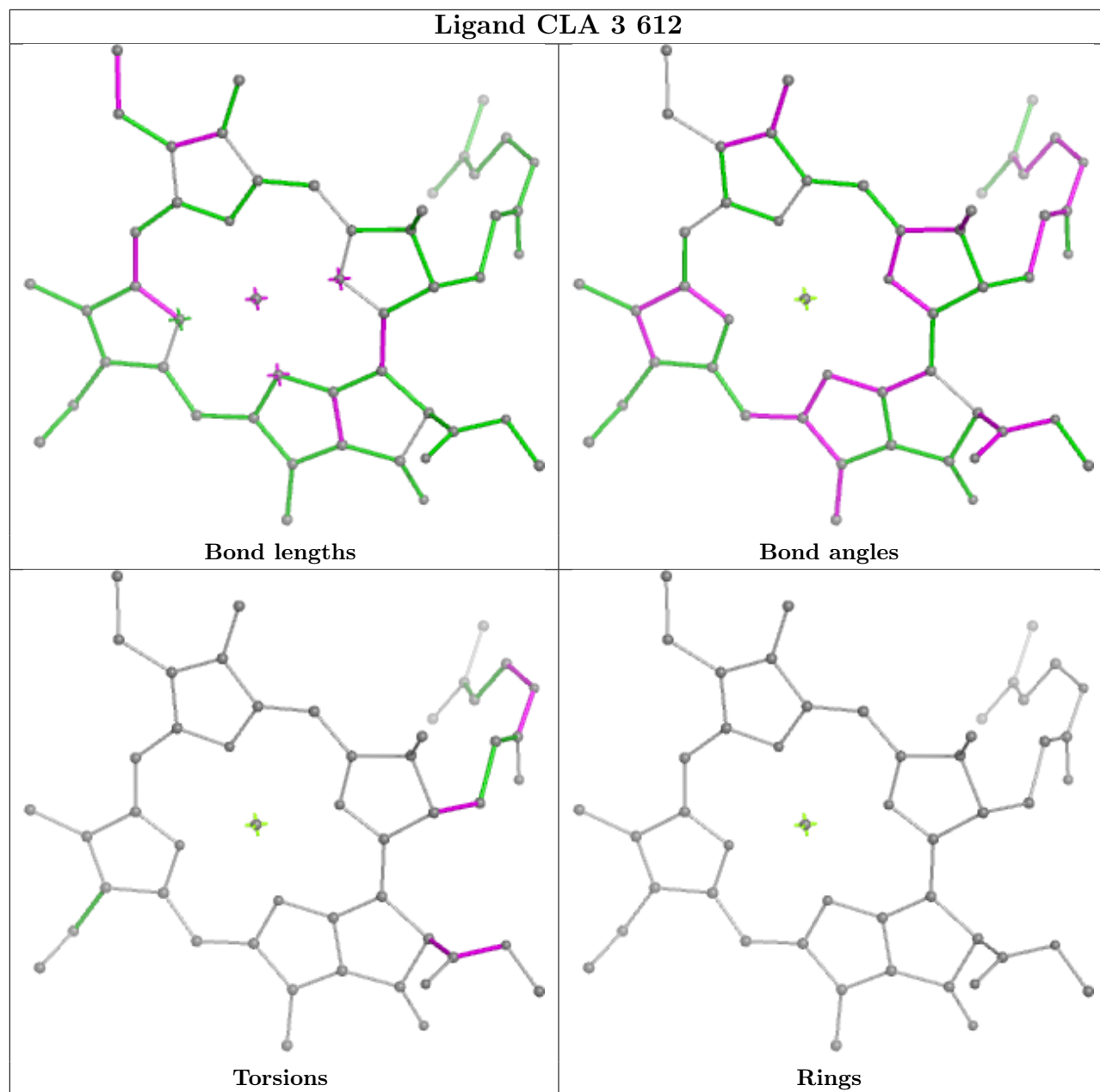


Torsions

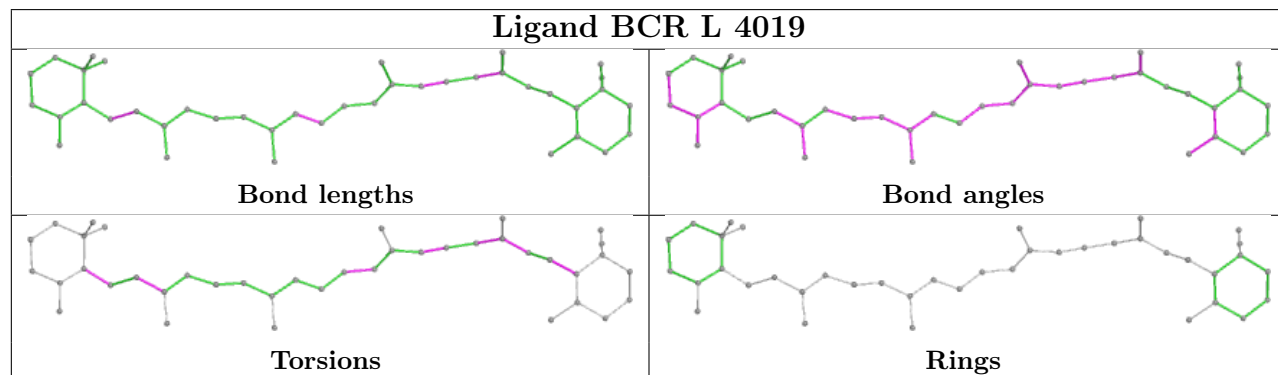


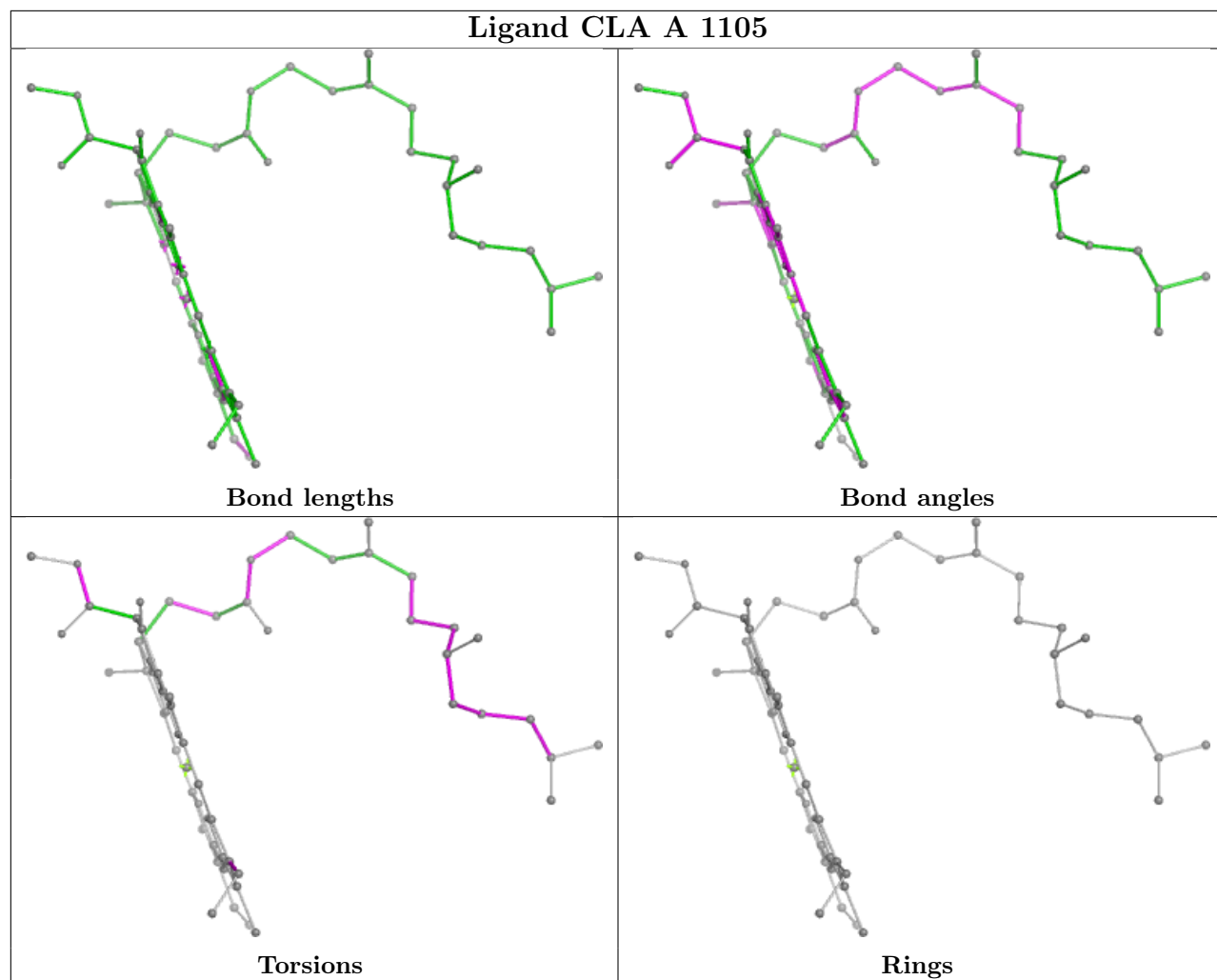
Rings

Ligand CLA 3 612

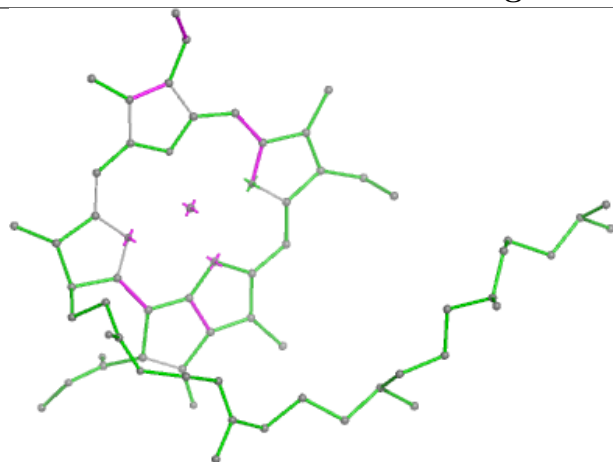


Ligand BCR L 4019

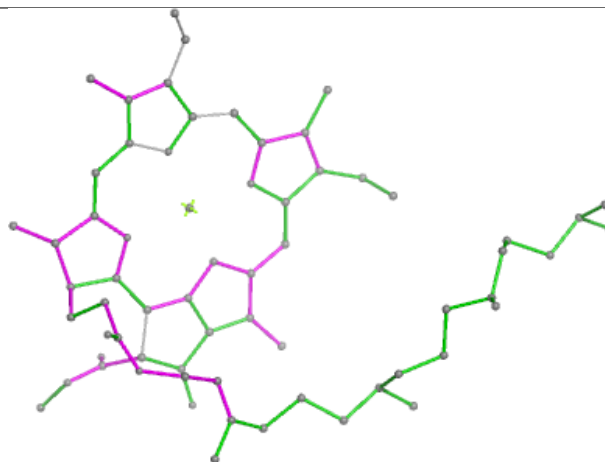




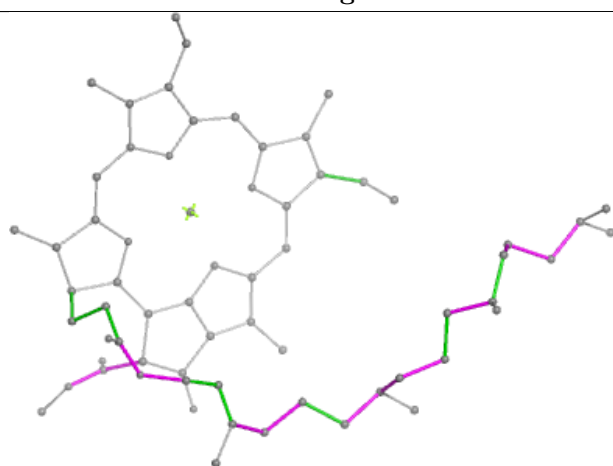
Ligand CLA A 1127



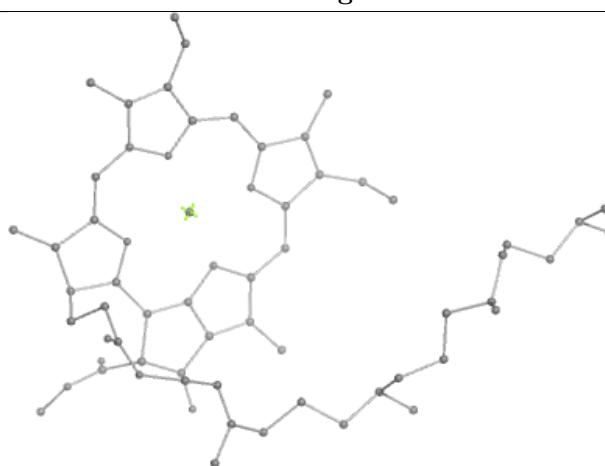
Bond lengths



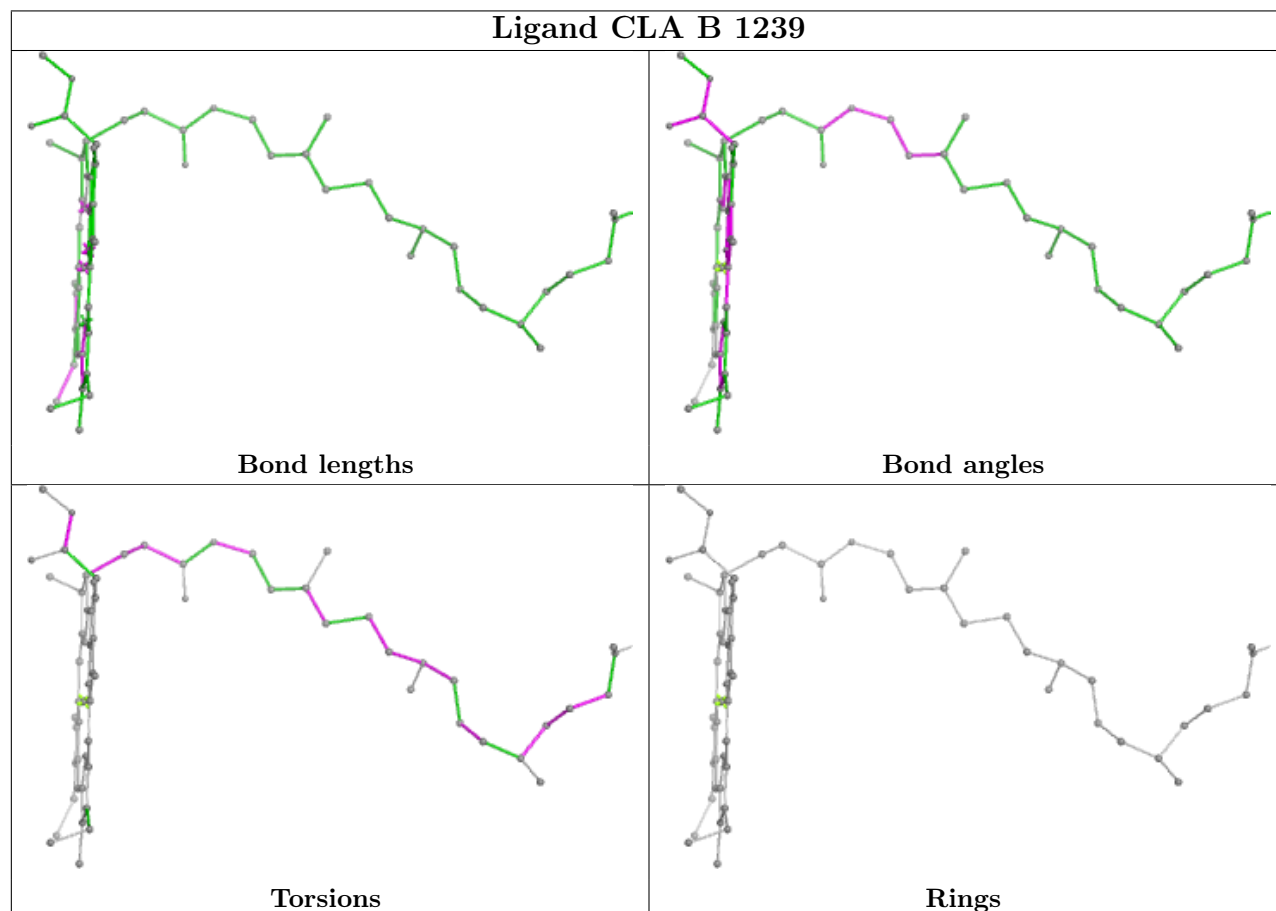
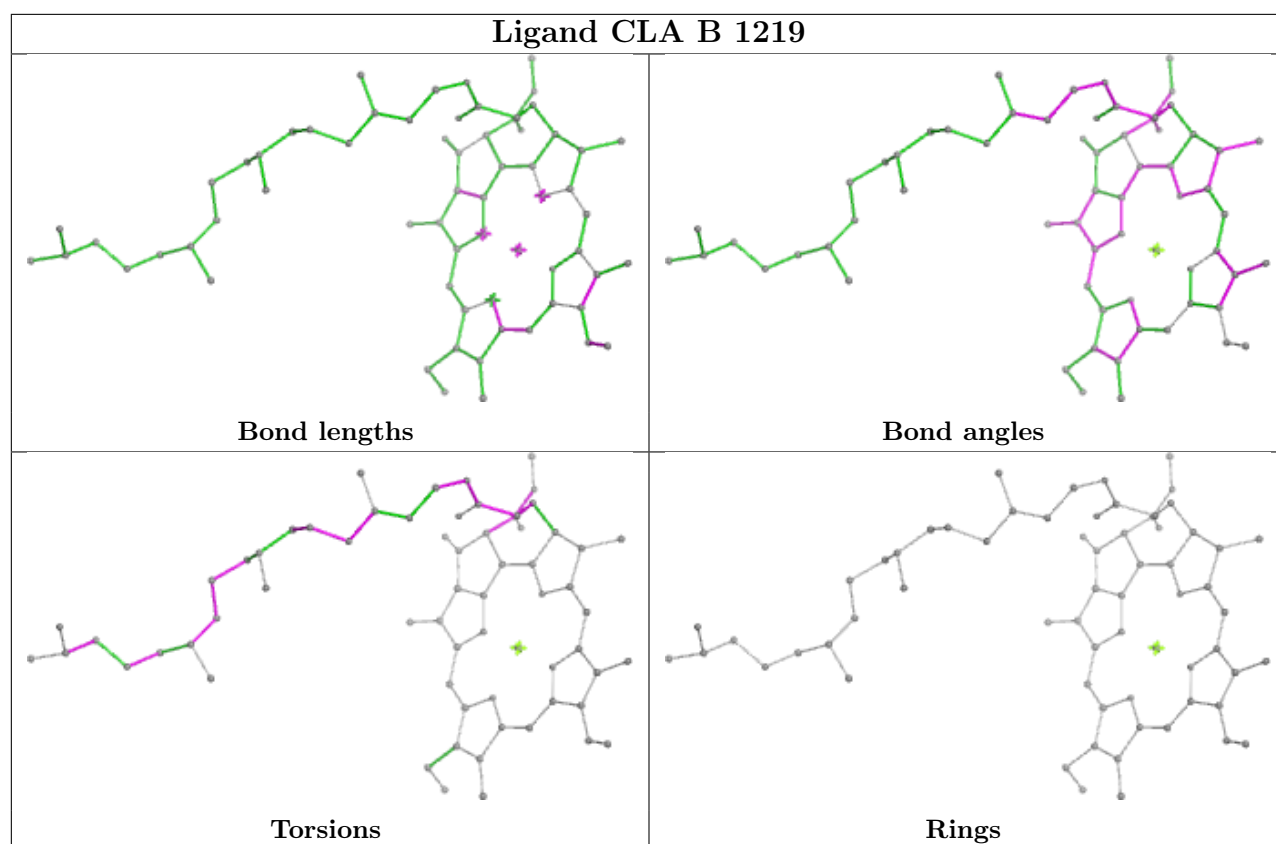
Bond angles

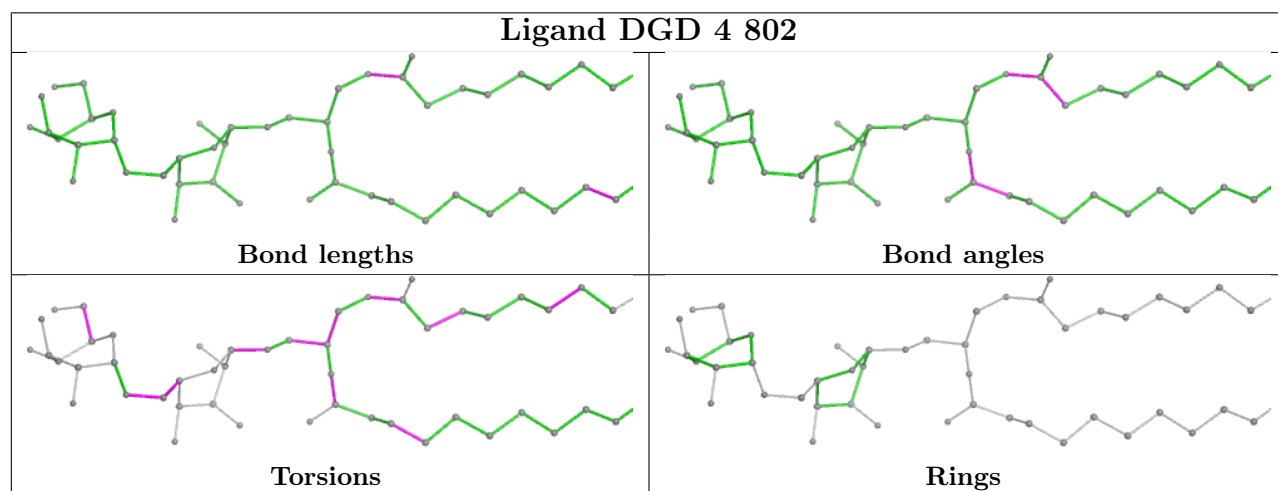
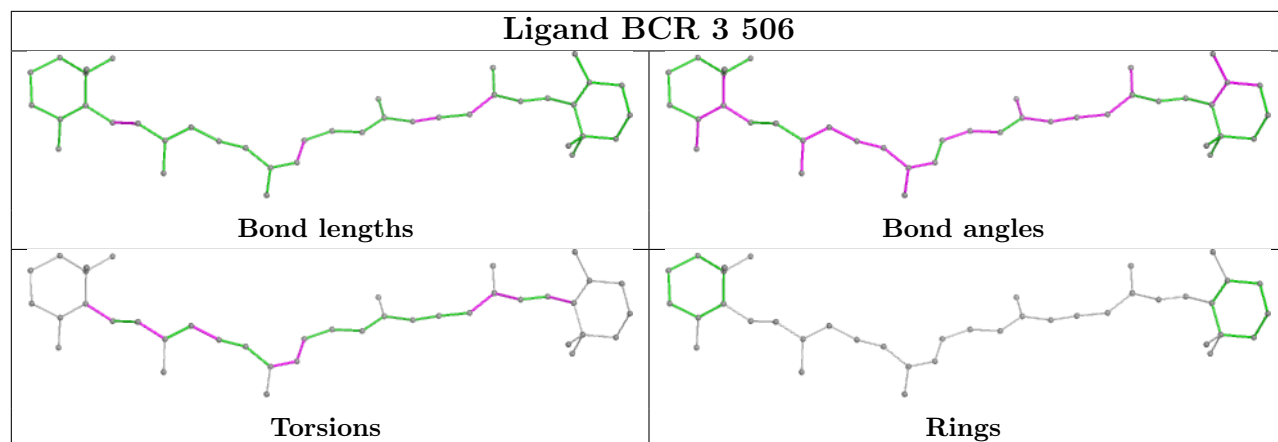


Torsions

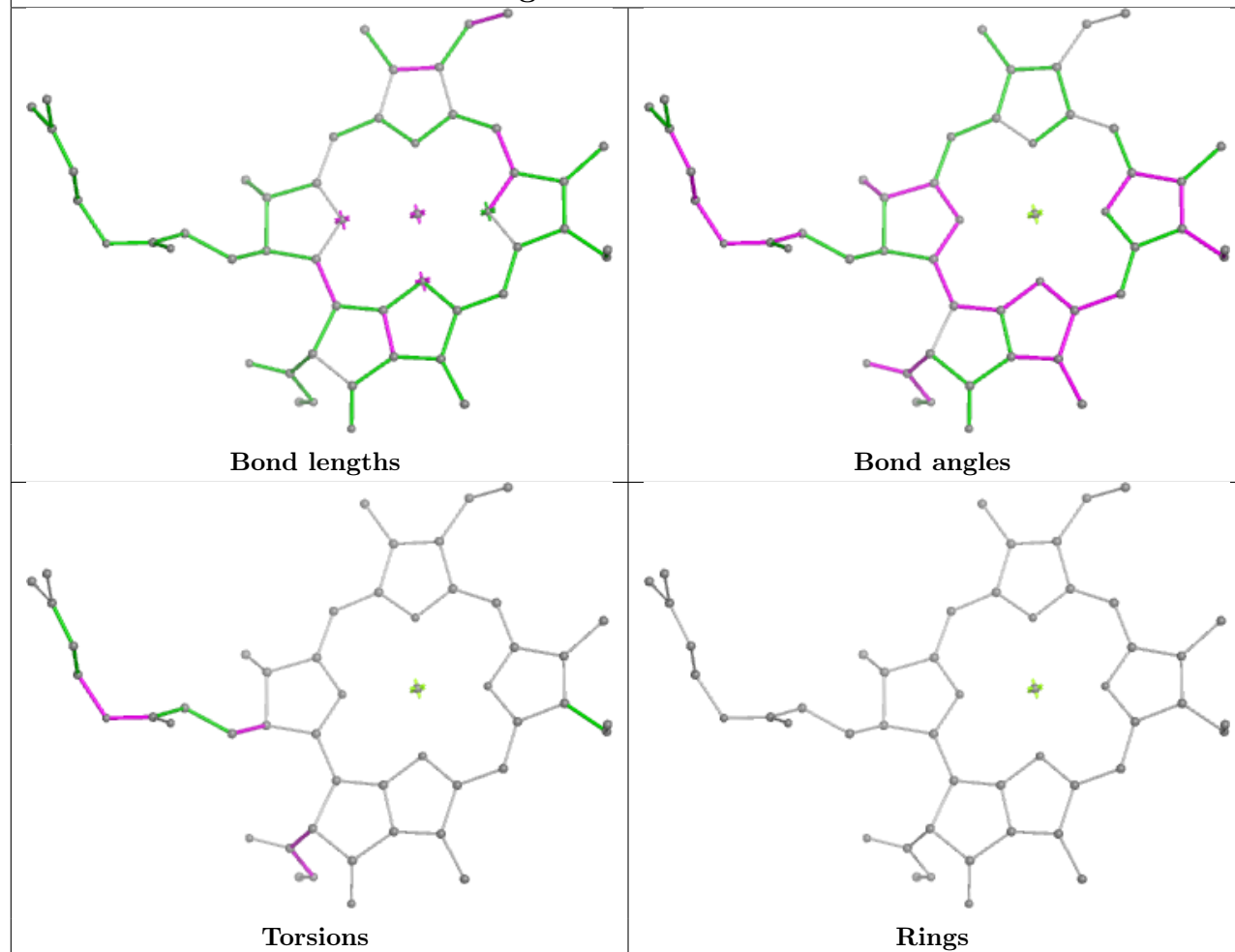


Rings

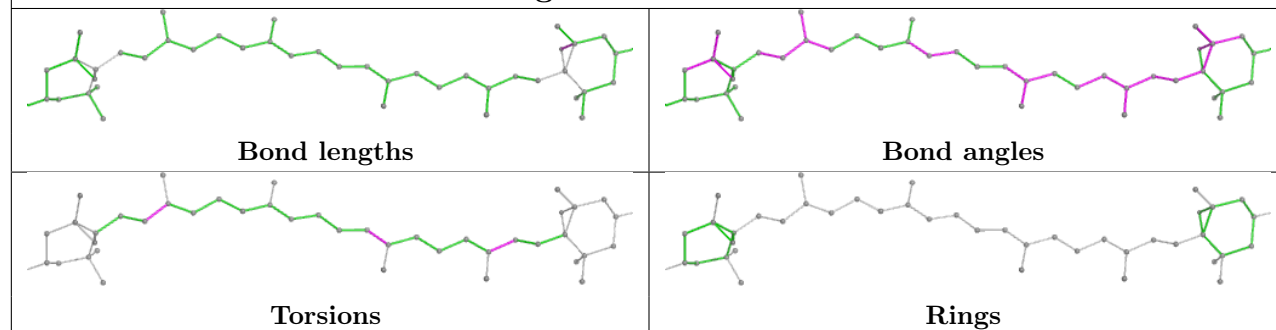


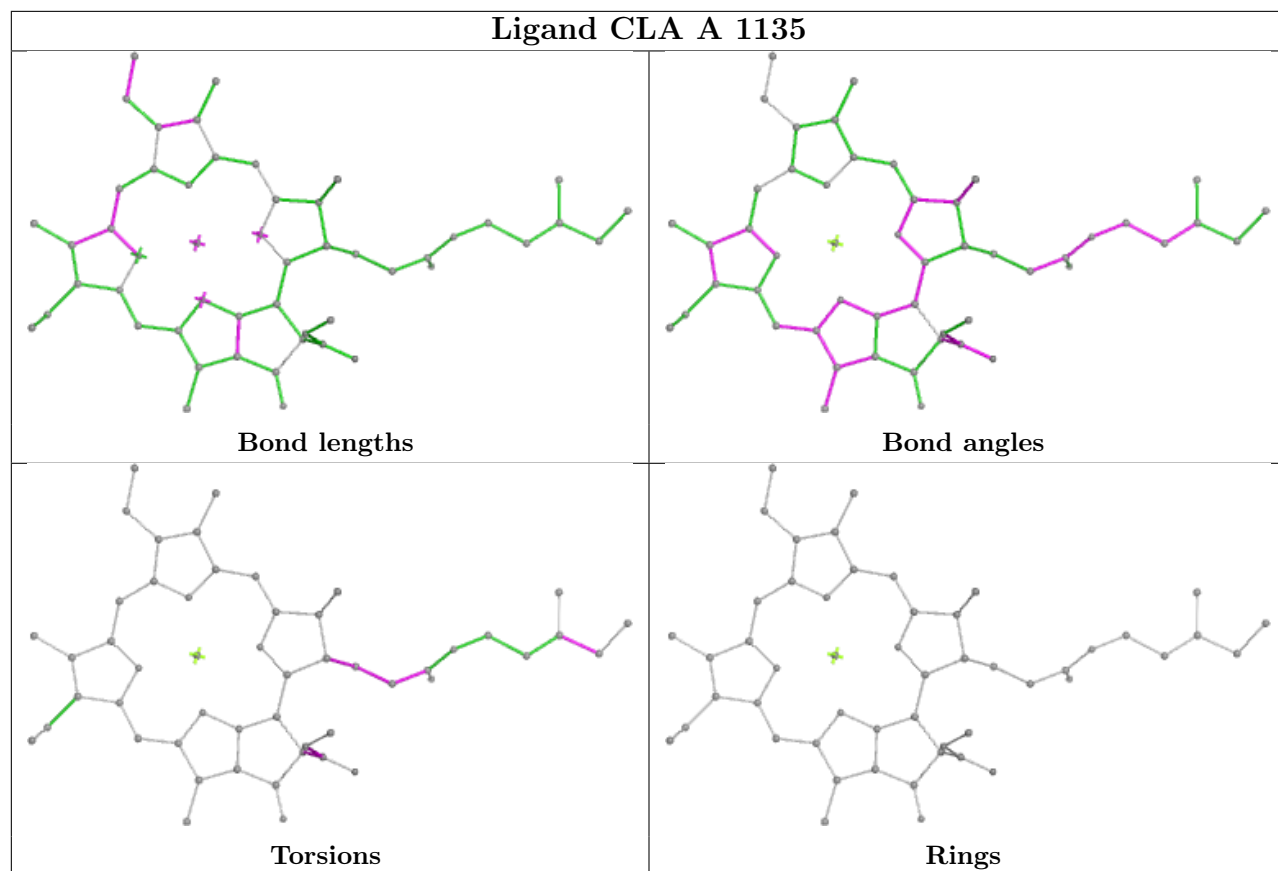


Ligand CLA 4 609

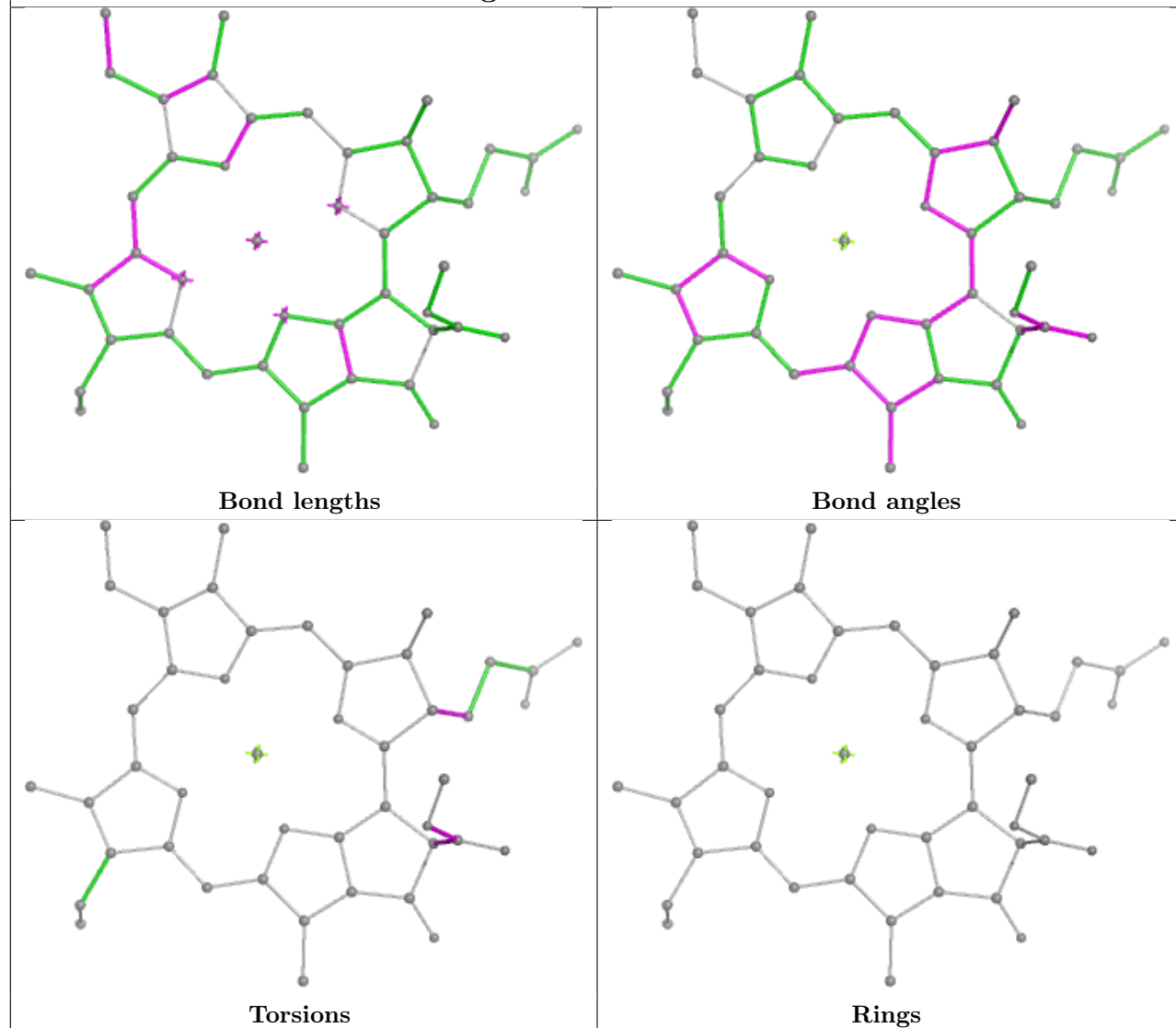


Ligand XAT 4 502

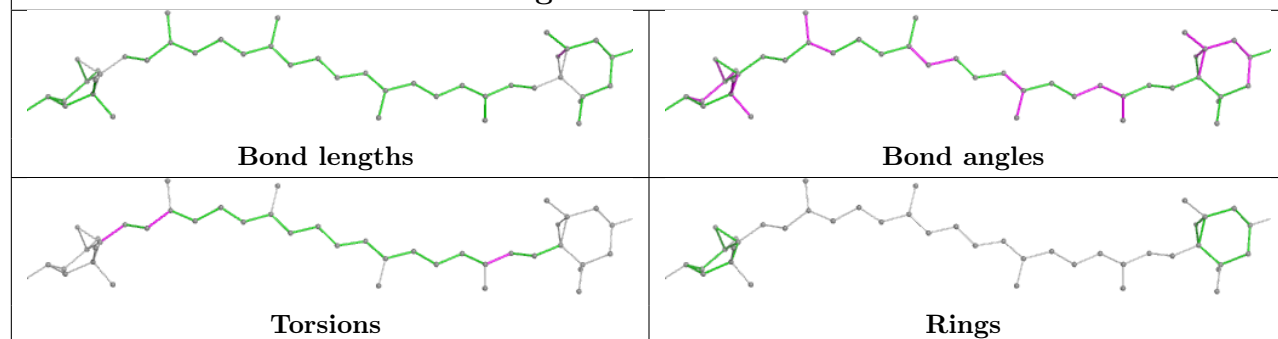


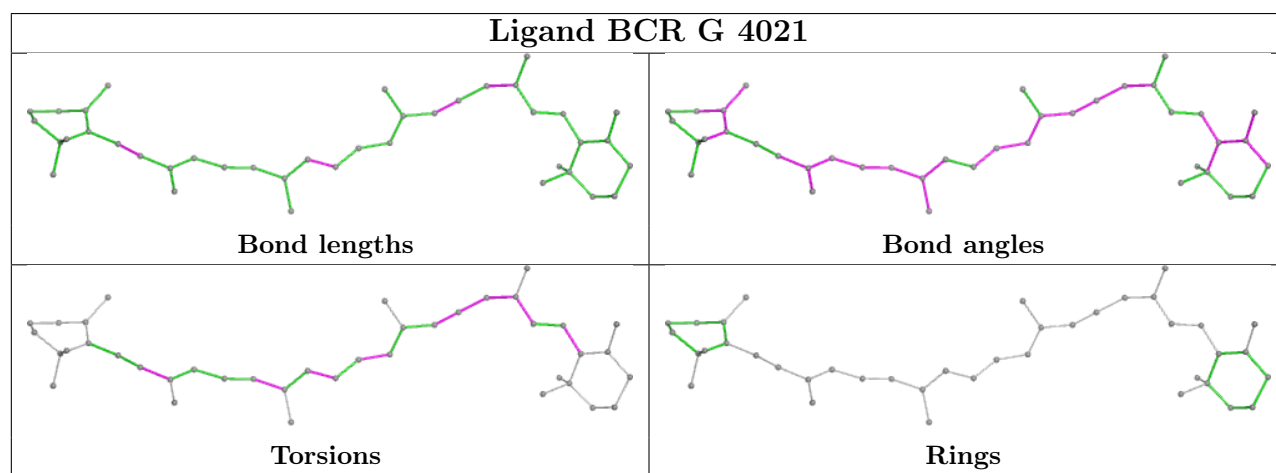
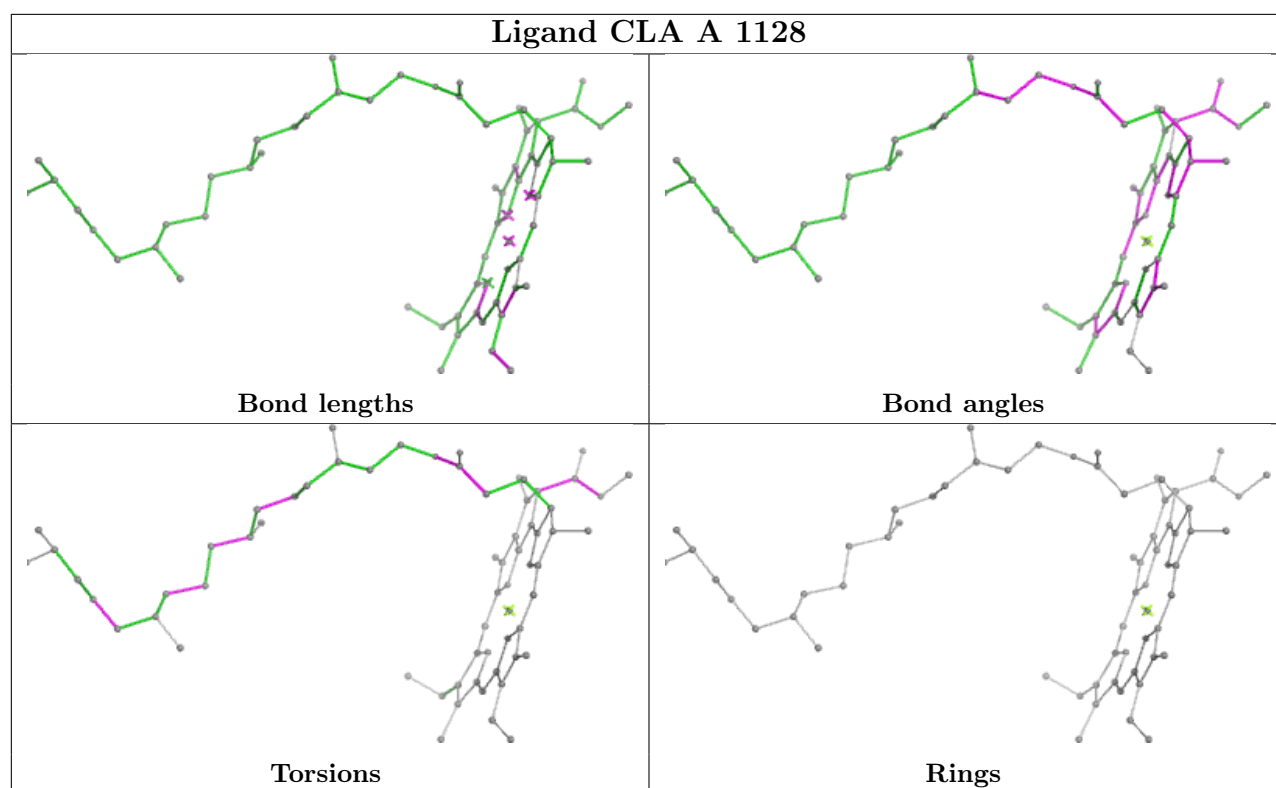


Ligand CLA K 1401

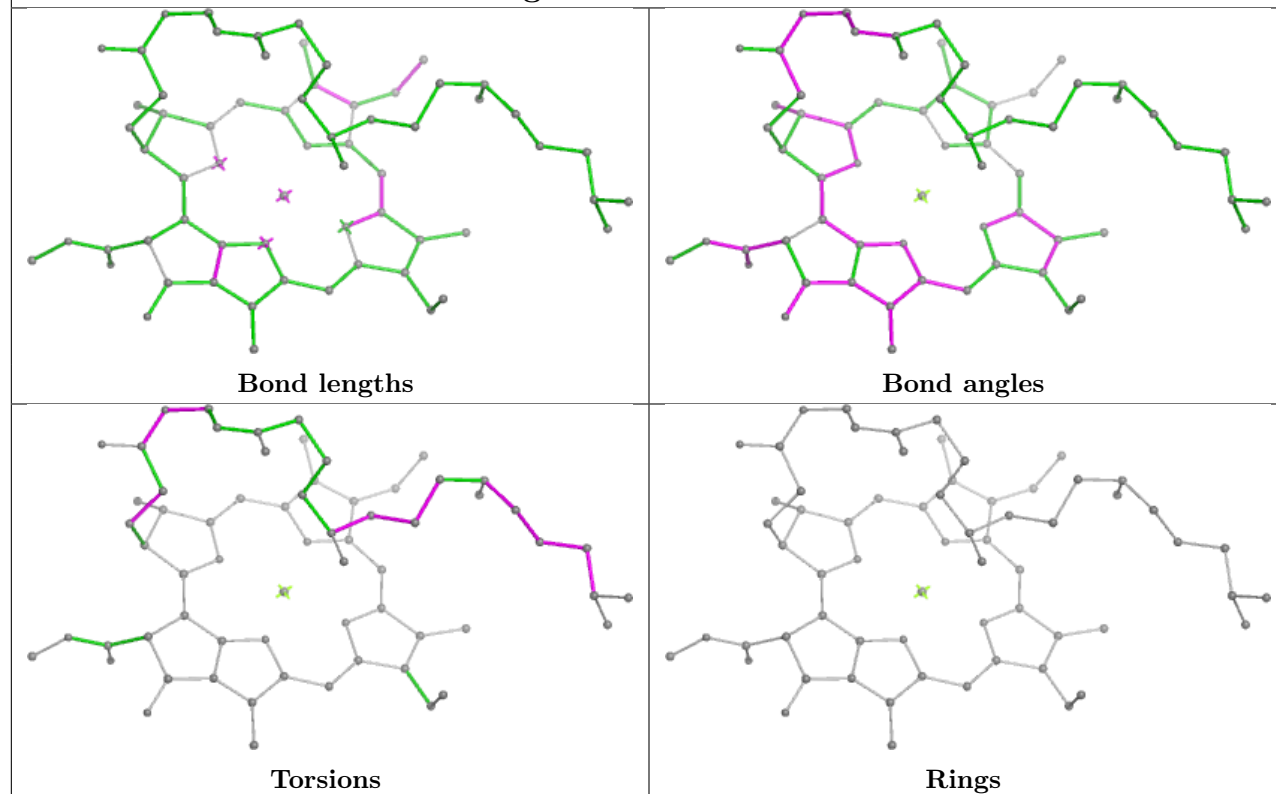


Ligand XAT 2 502

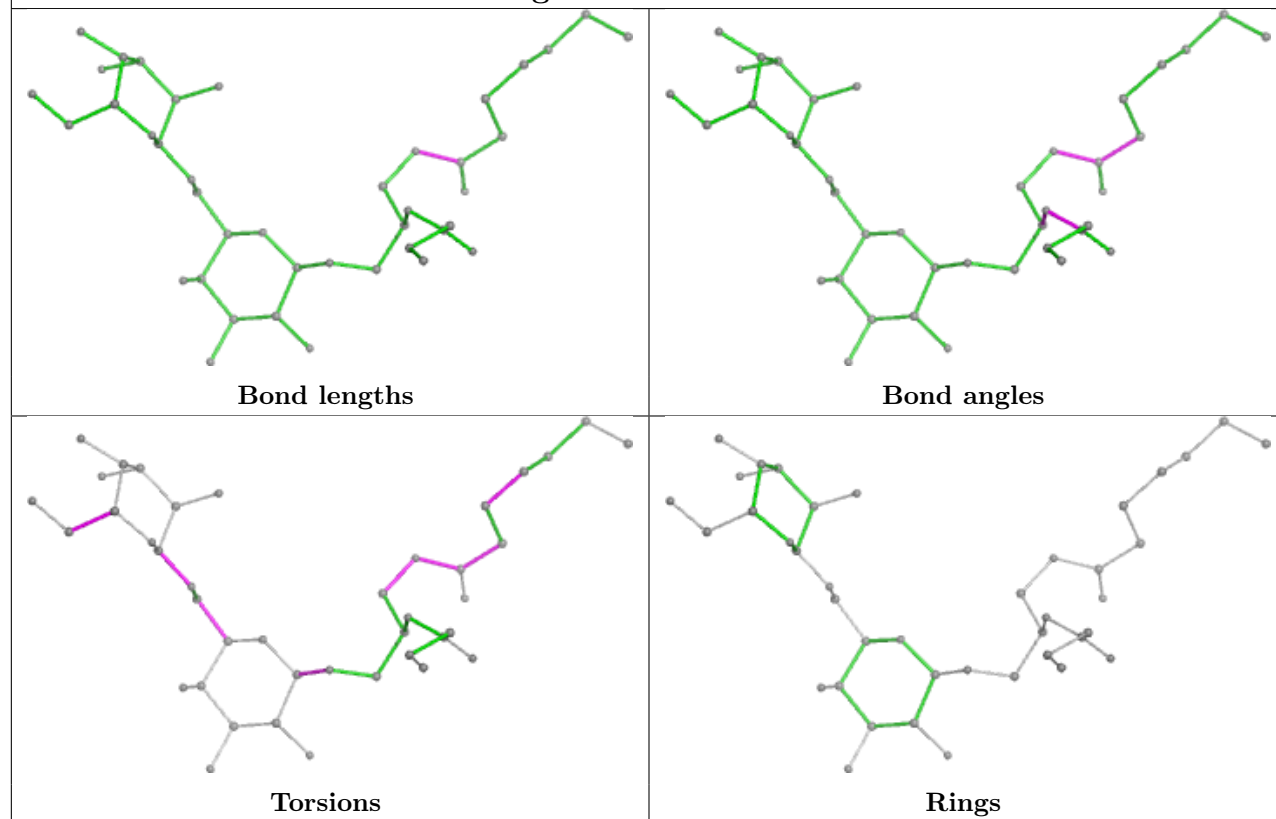


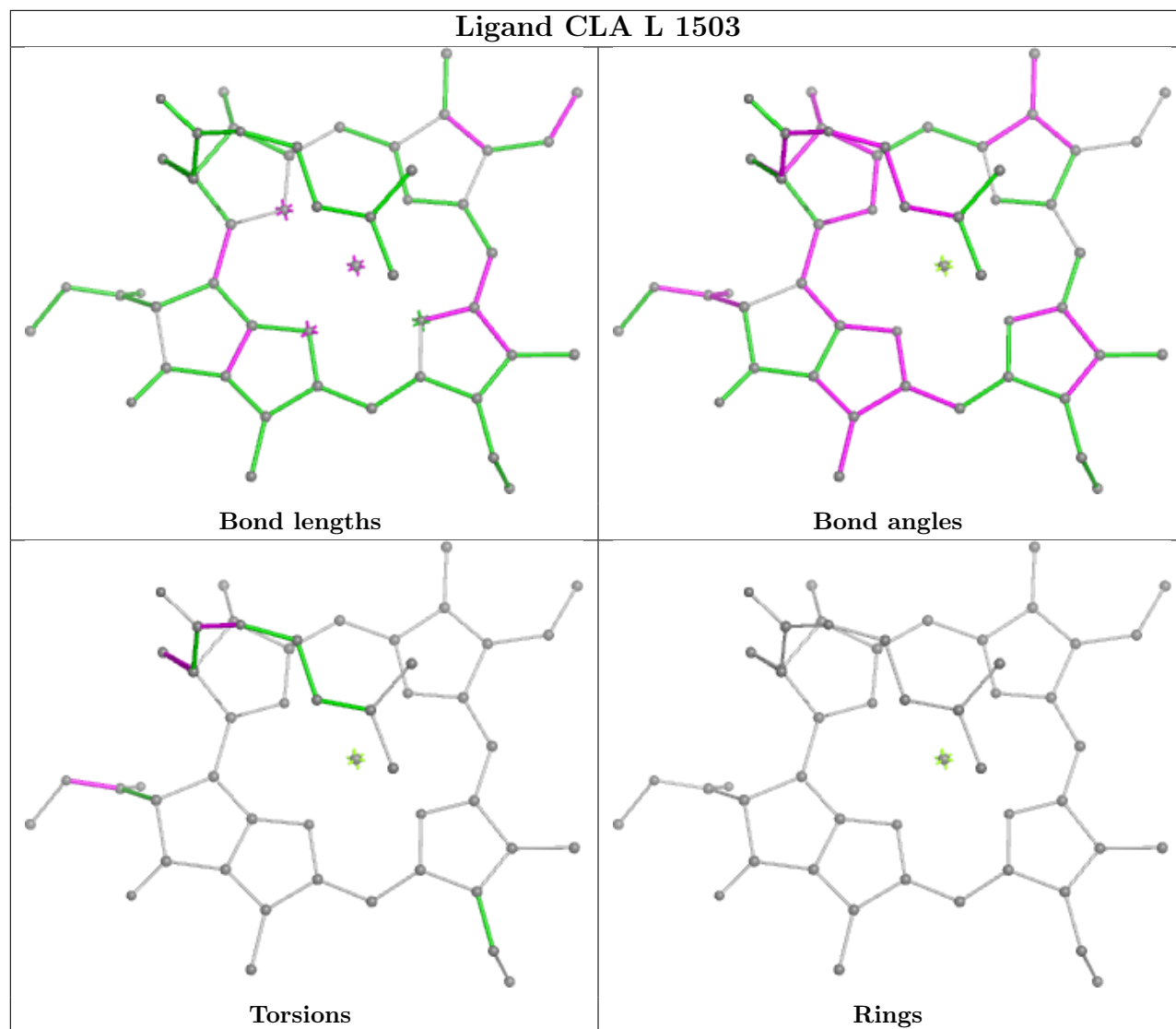


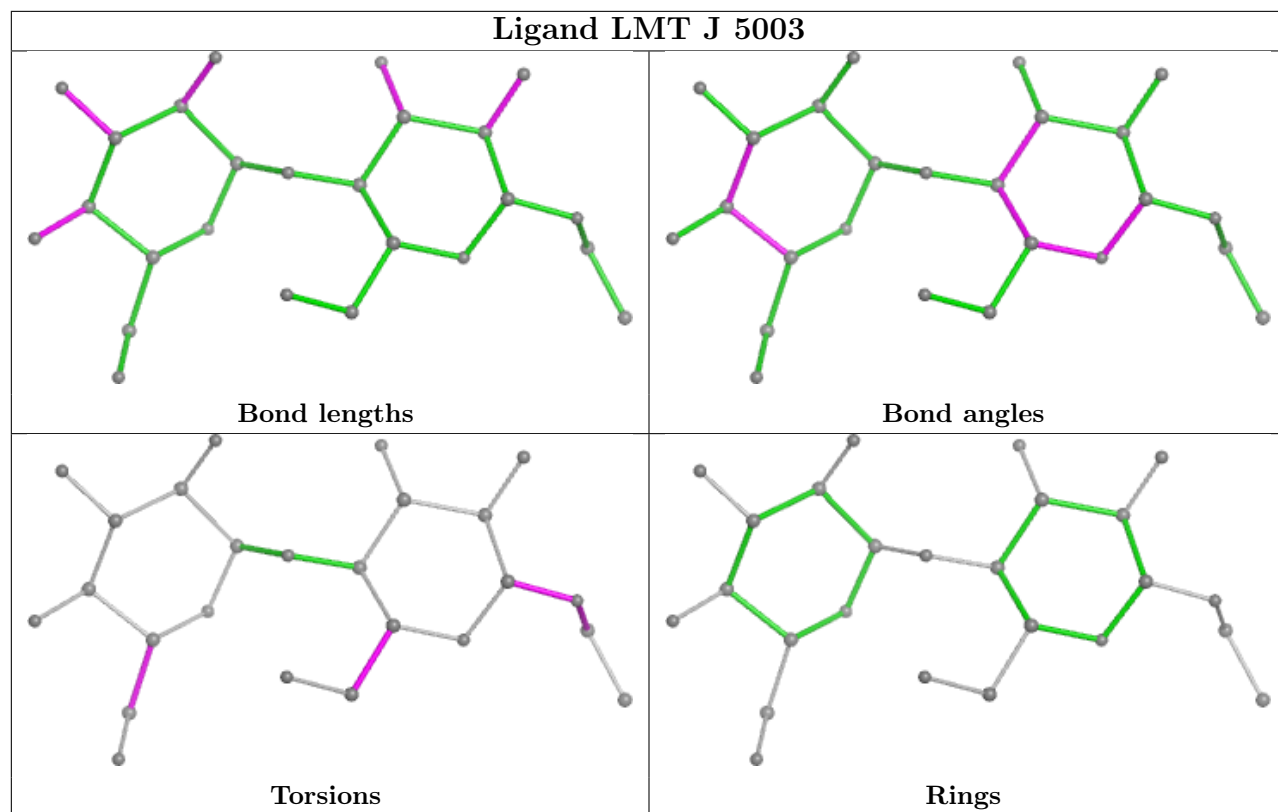
Ligand CLA B 1214



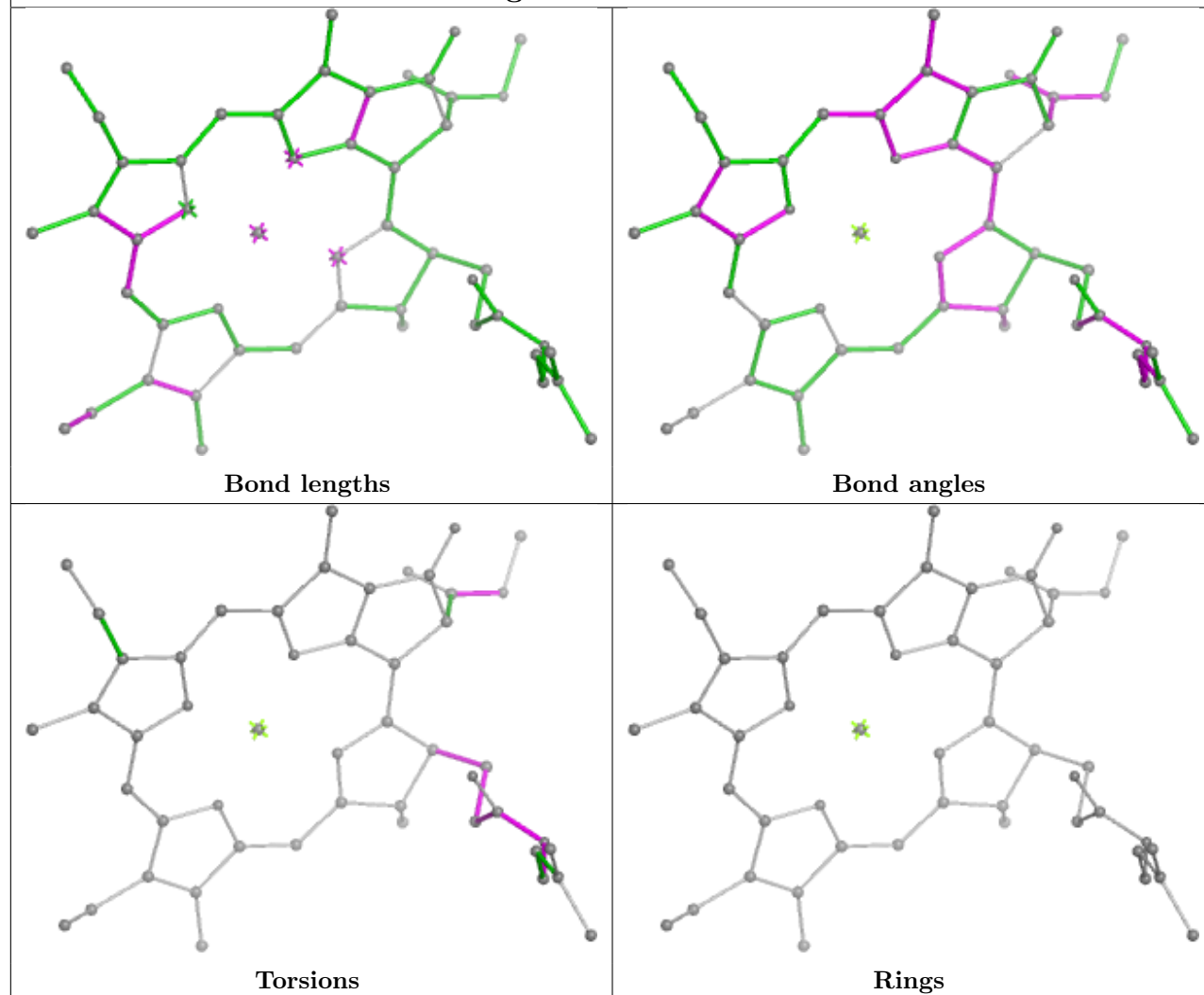
Ligand DGD 1 803



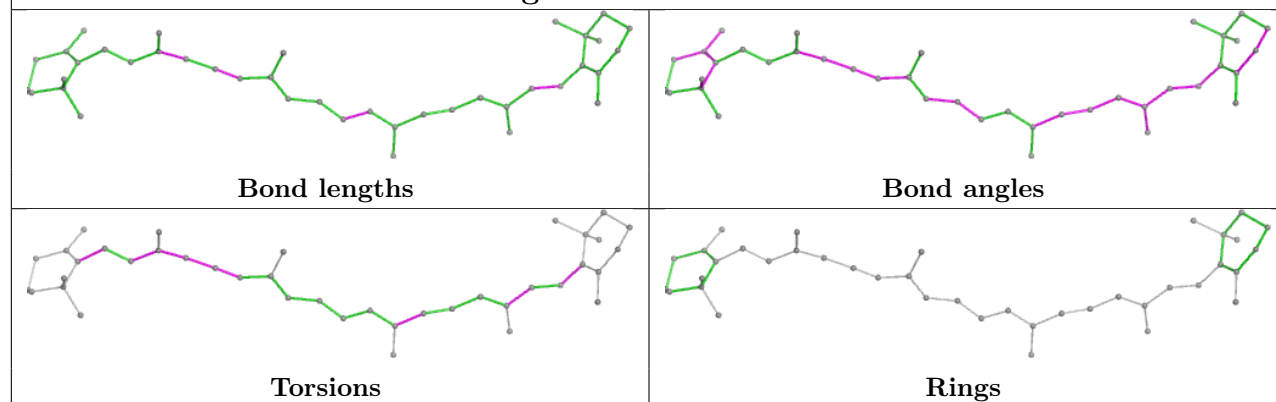


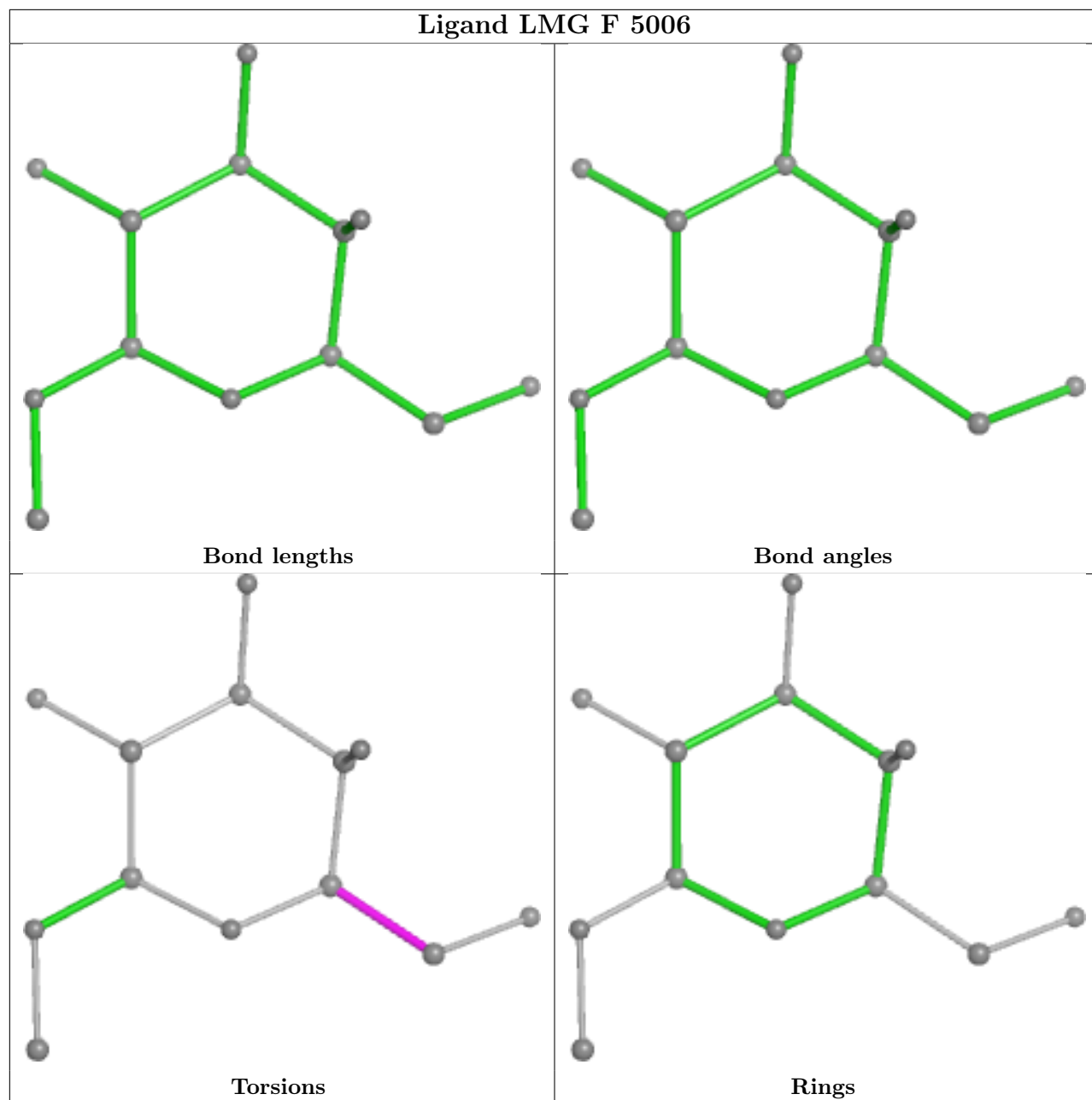


Ligand CLA 2 608

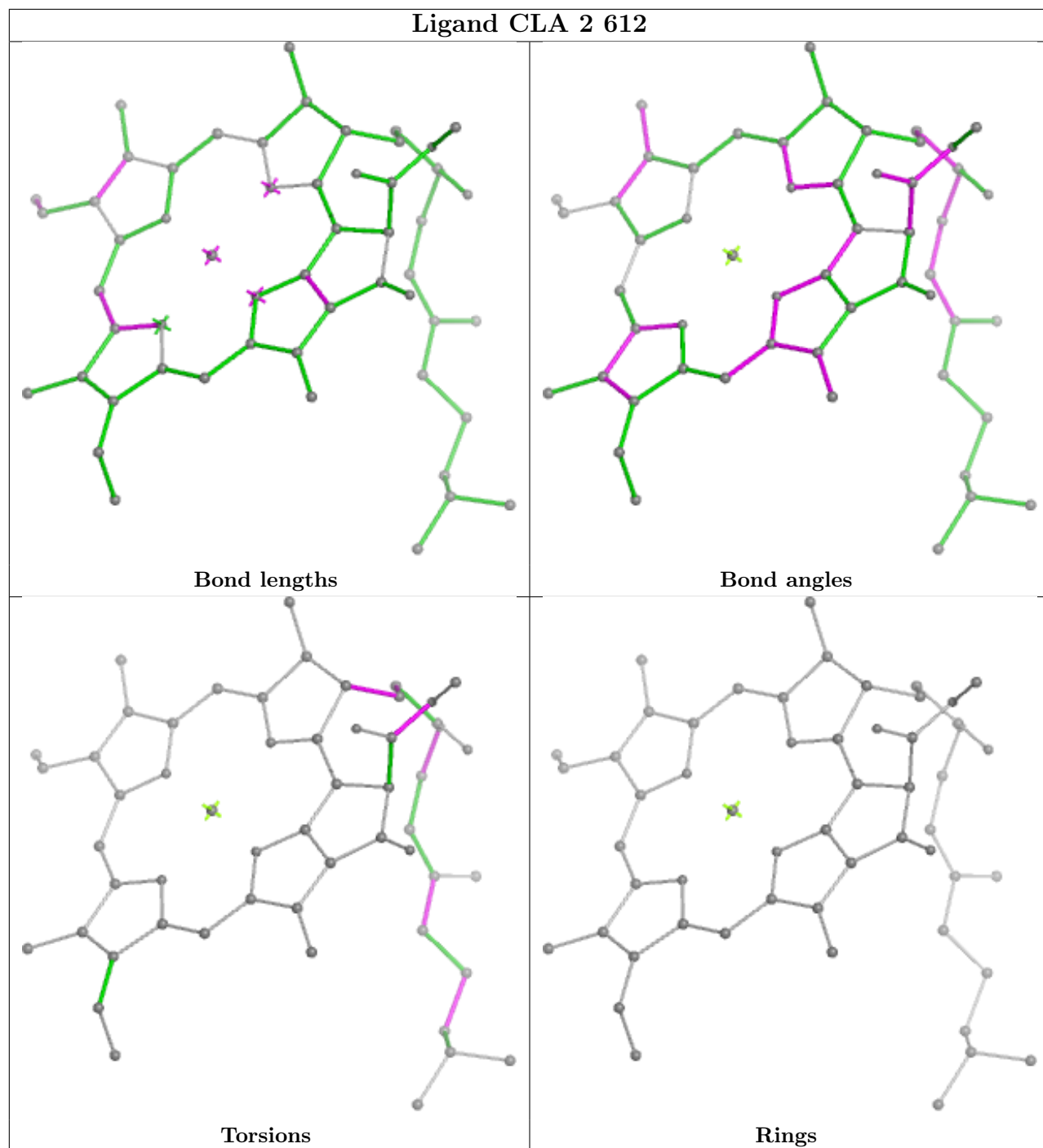


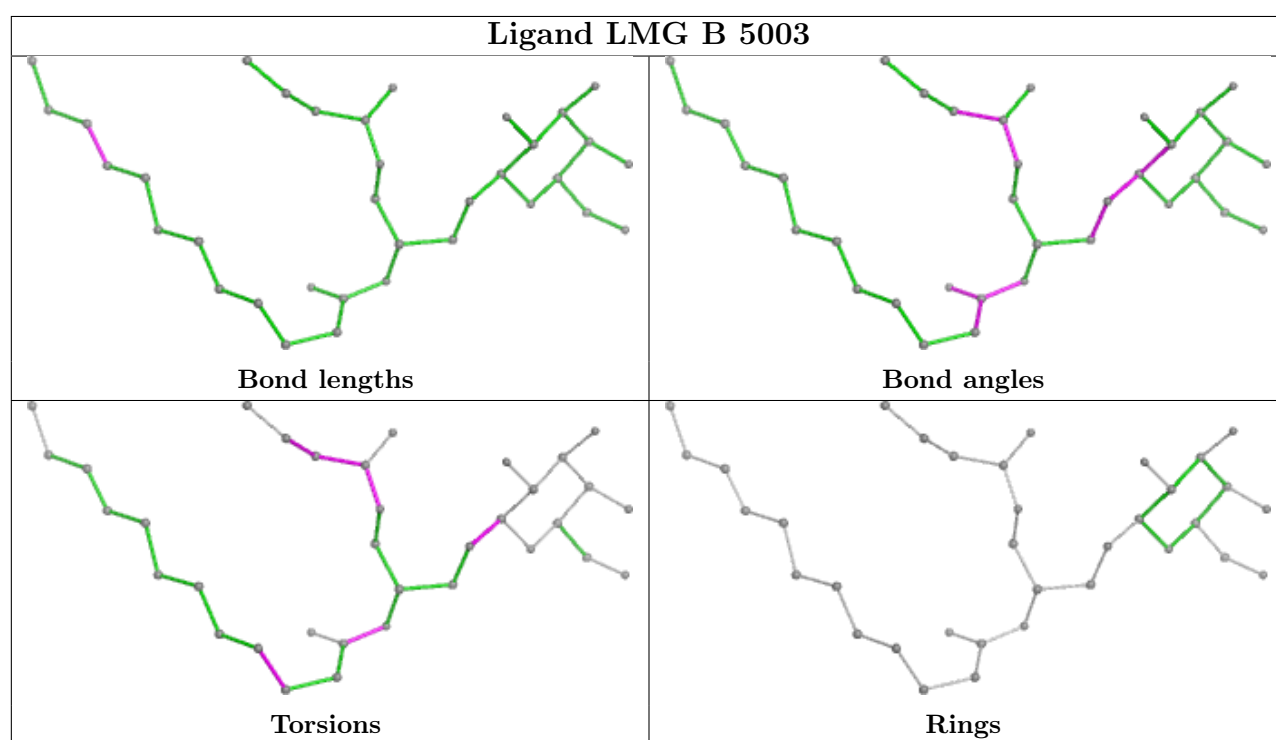
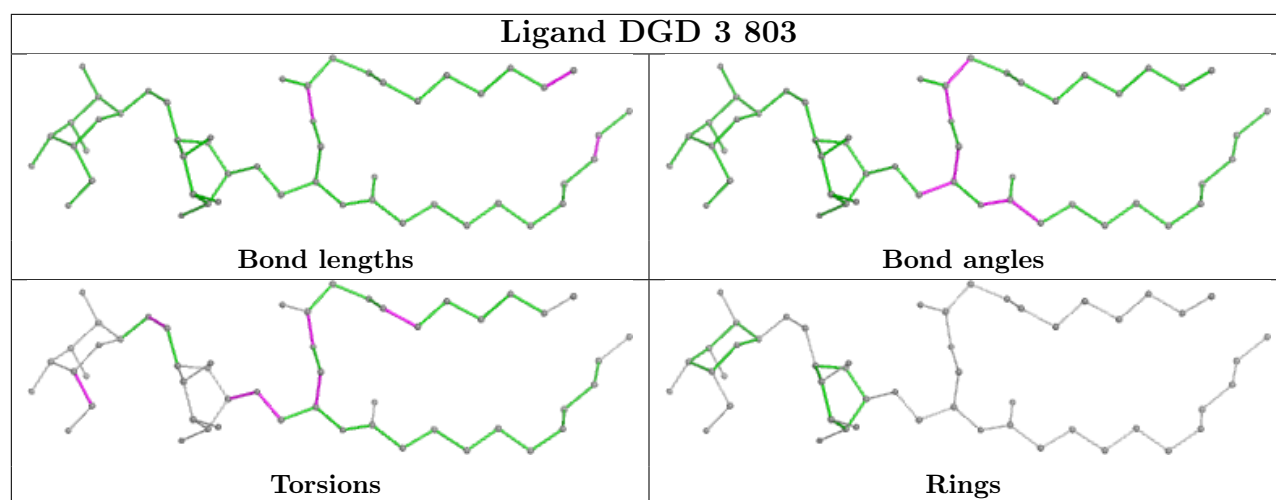
Ligand BCR B 4010

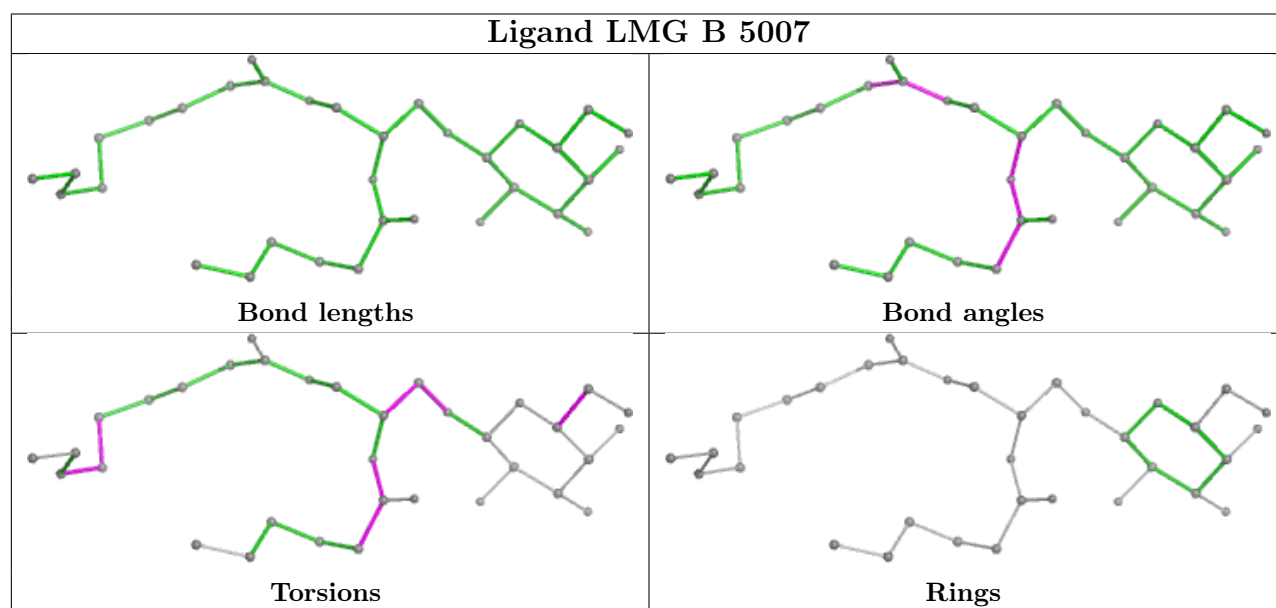
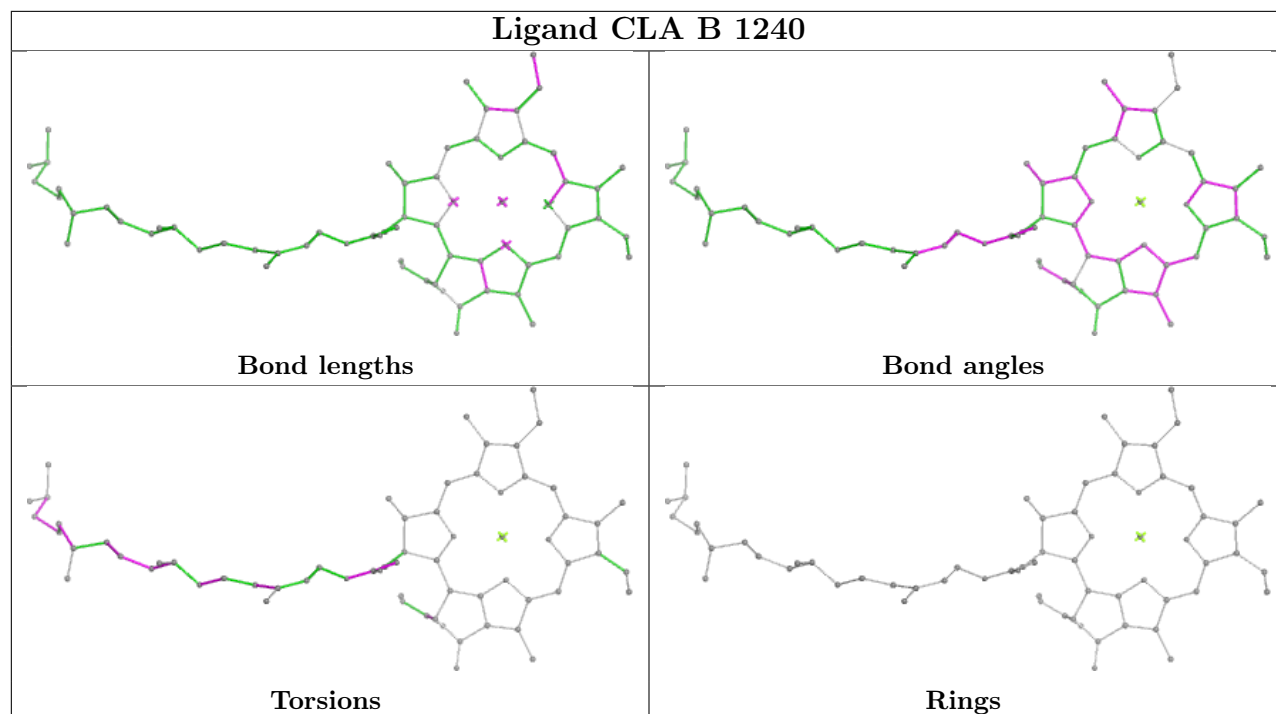


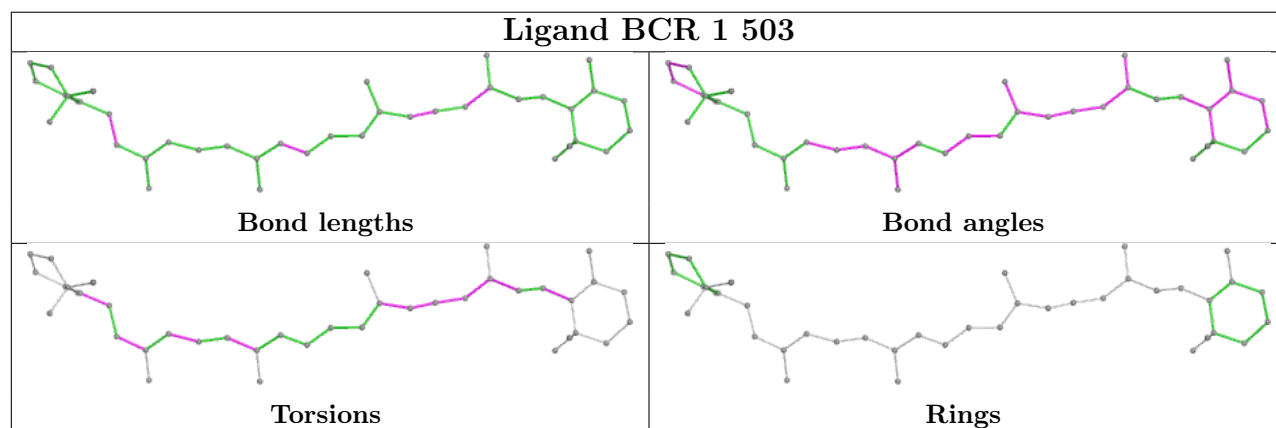
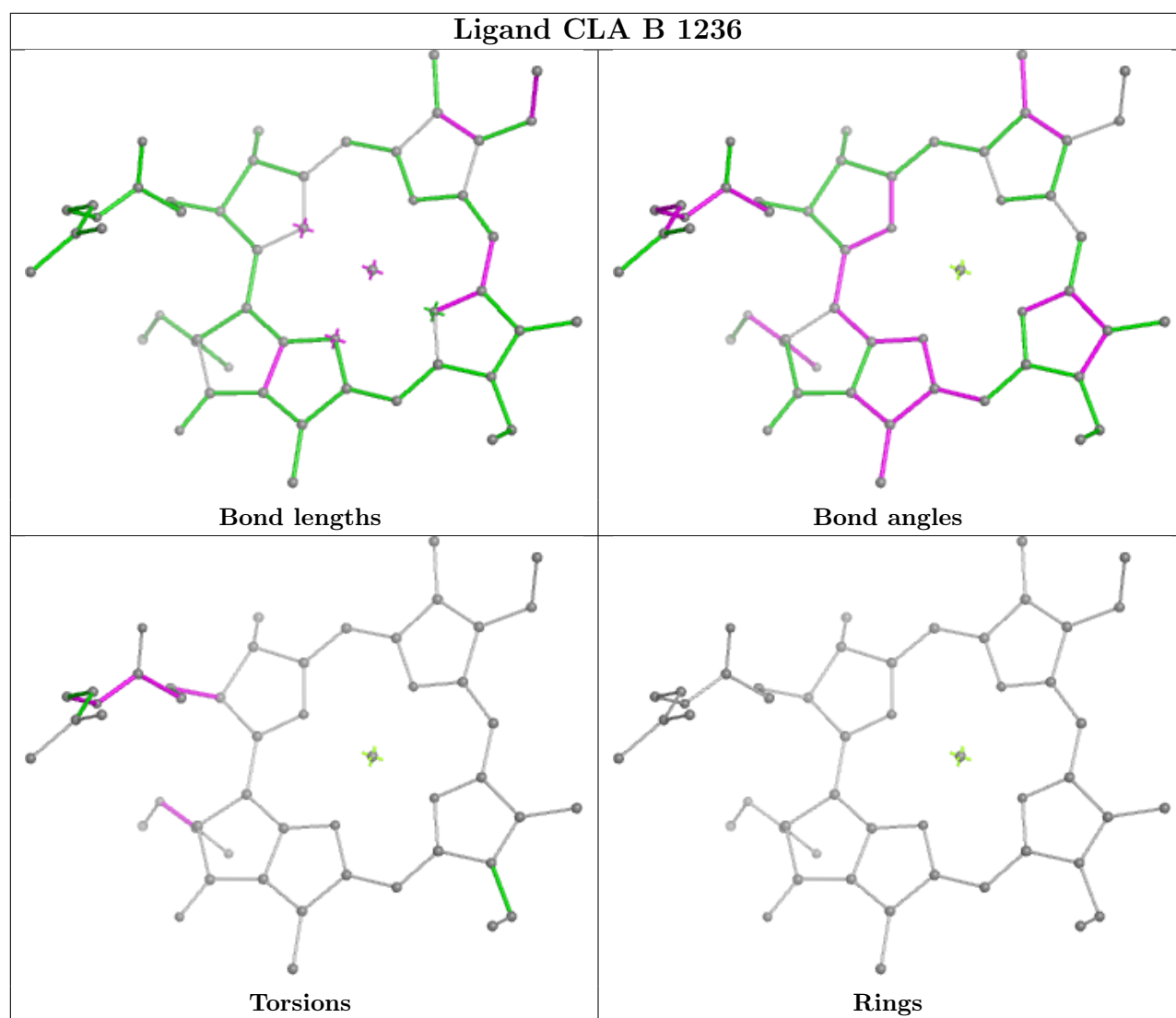


Ligand CLA 2 612

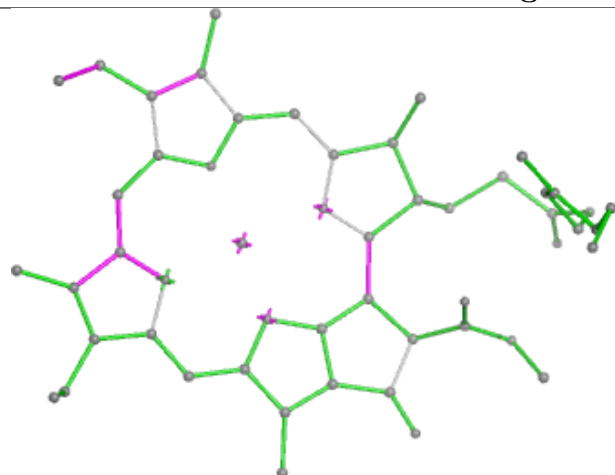




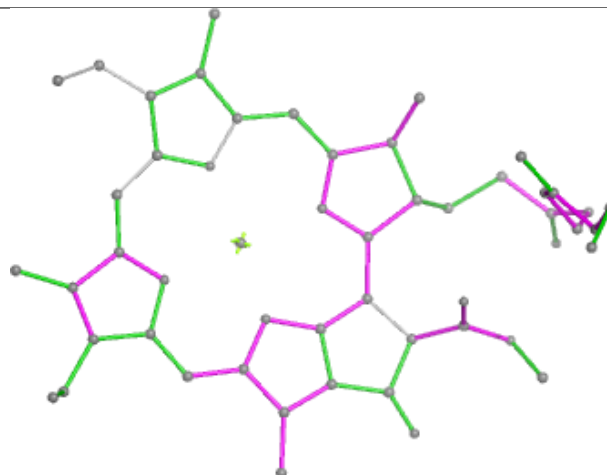




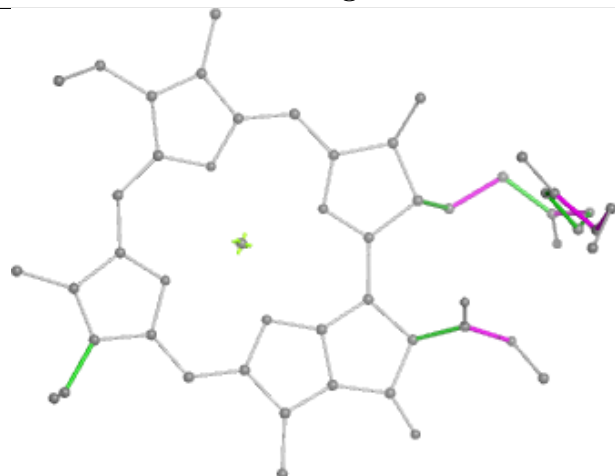
Ligand CLA 2 602



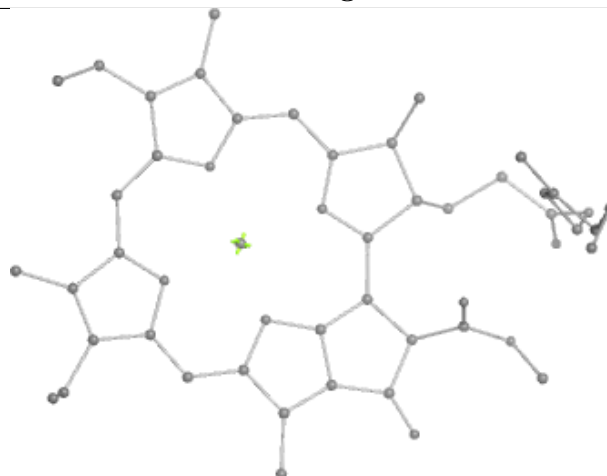
Bond lengths



Bond angles

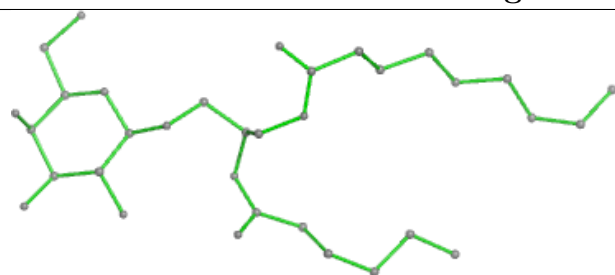


Torsions

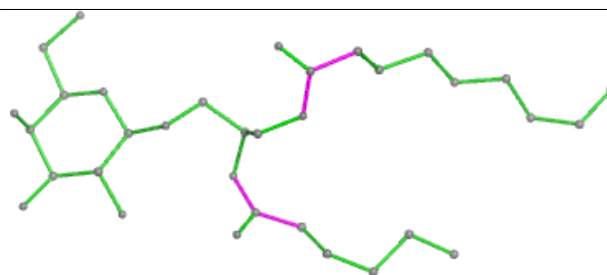


Rings

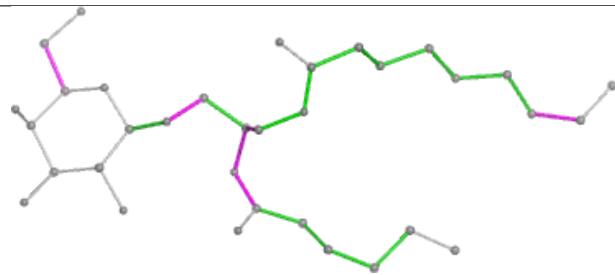
Ligand LMG F 5004



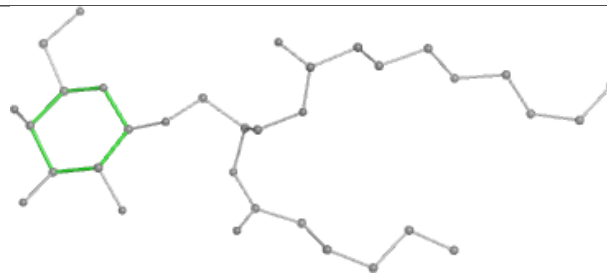
Bond lengths



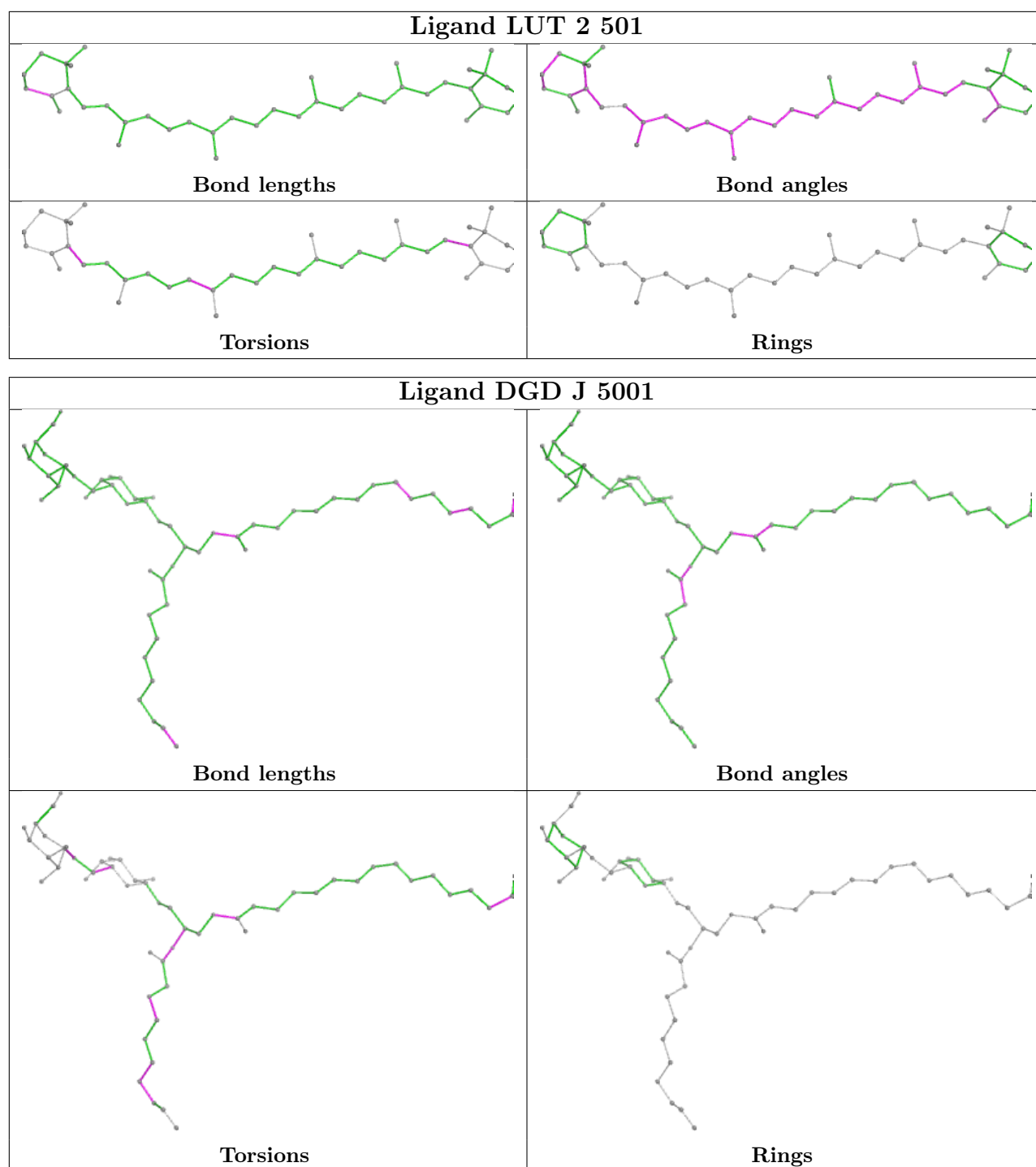
Bond angles

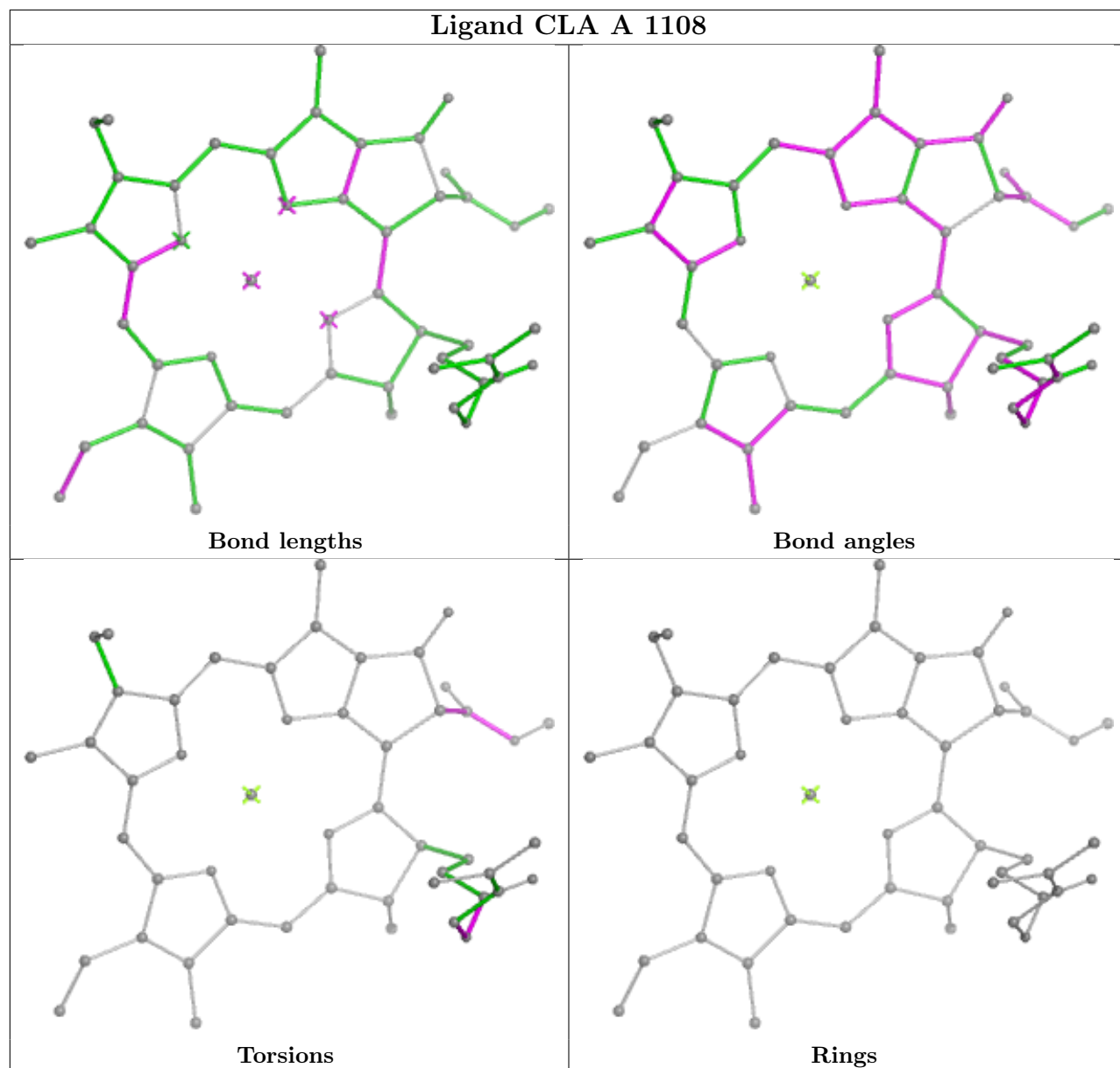


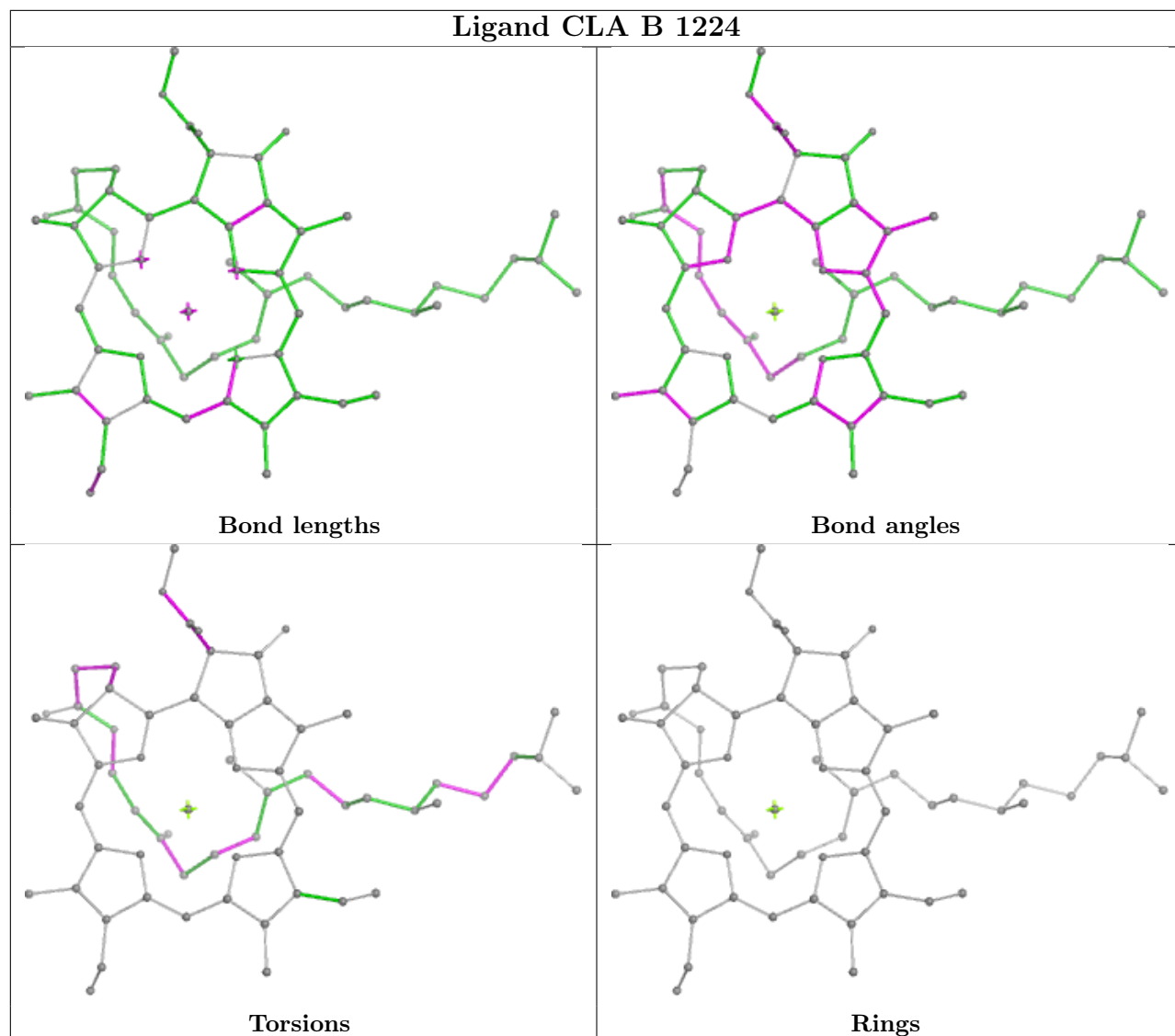
Torsions



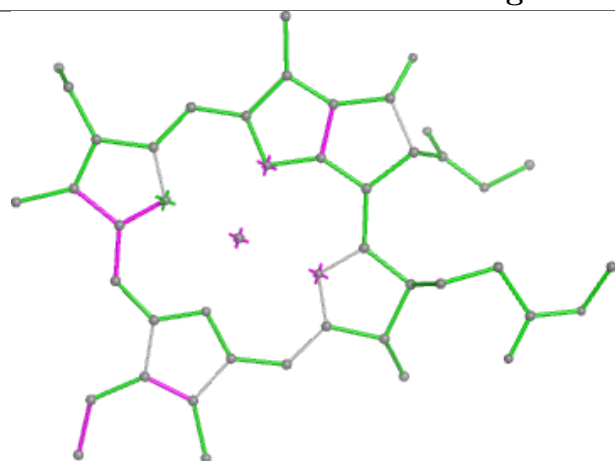
Rings



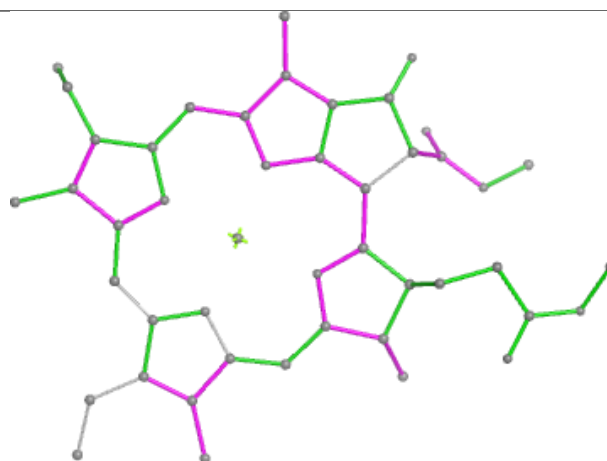




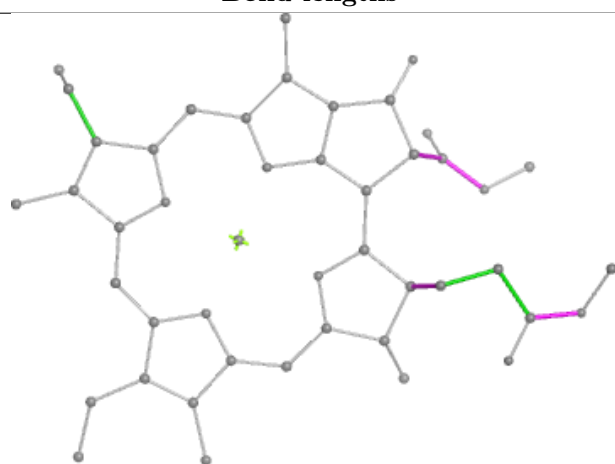
Ligand CLA G 1602



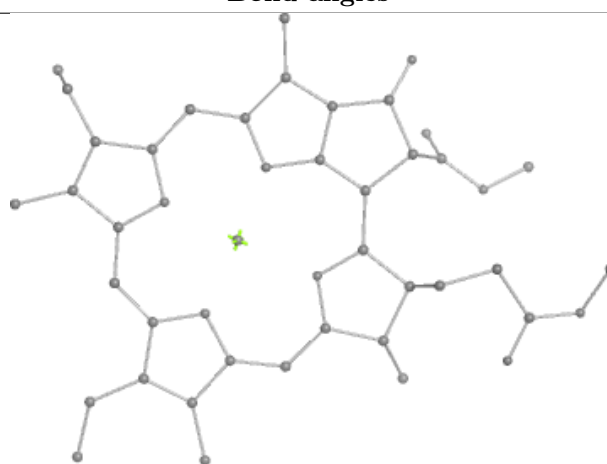
Bond lengths



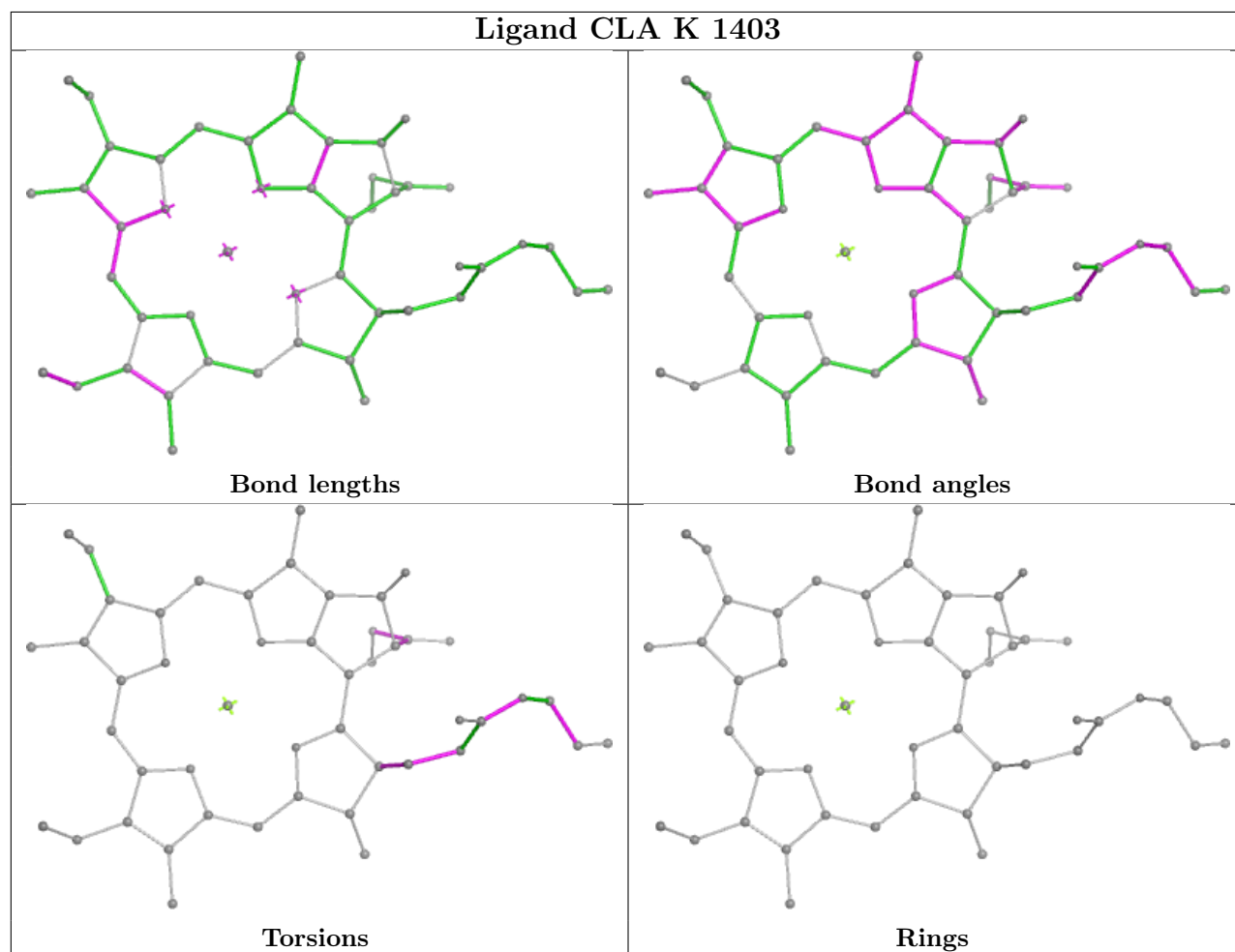
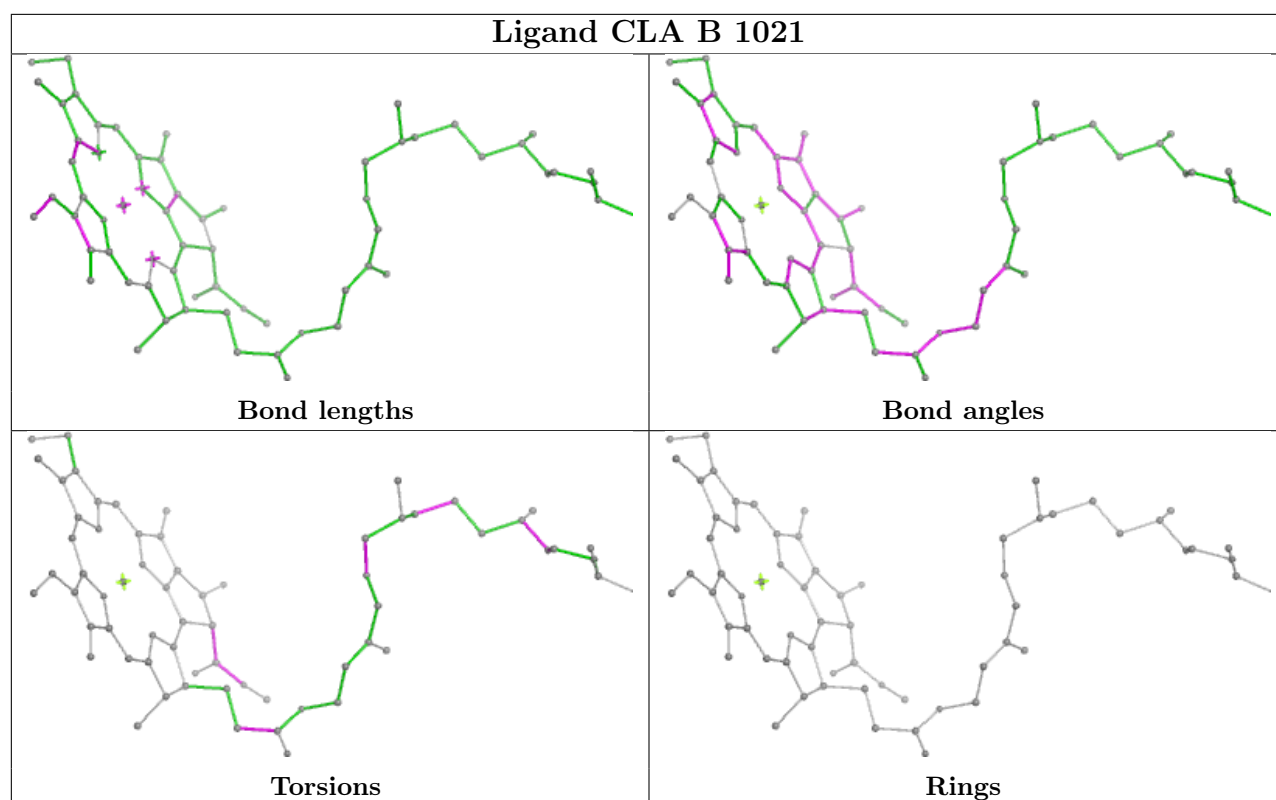
Bond angles

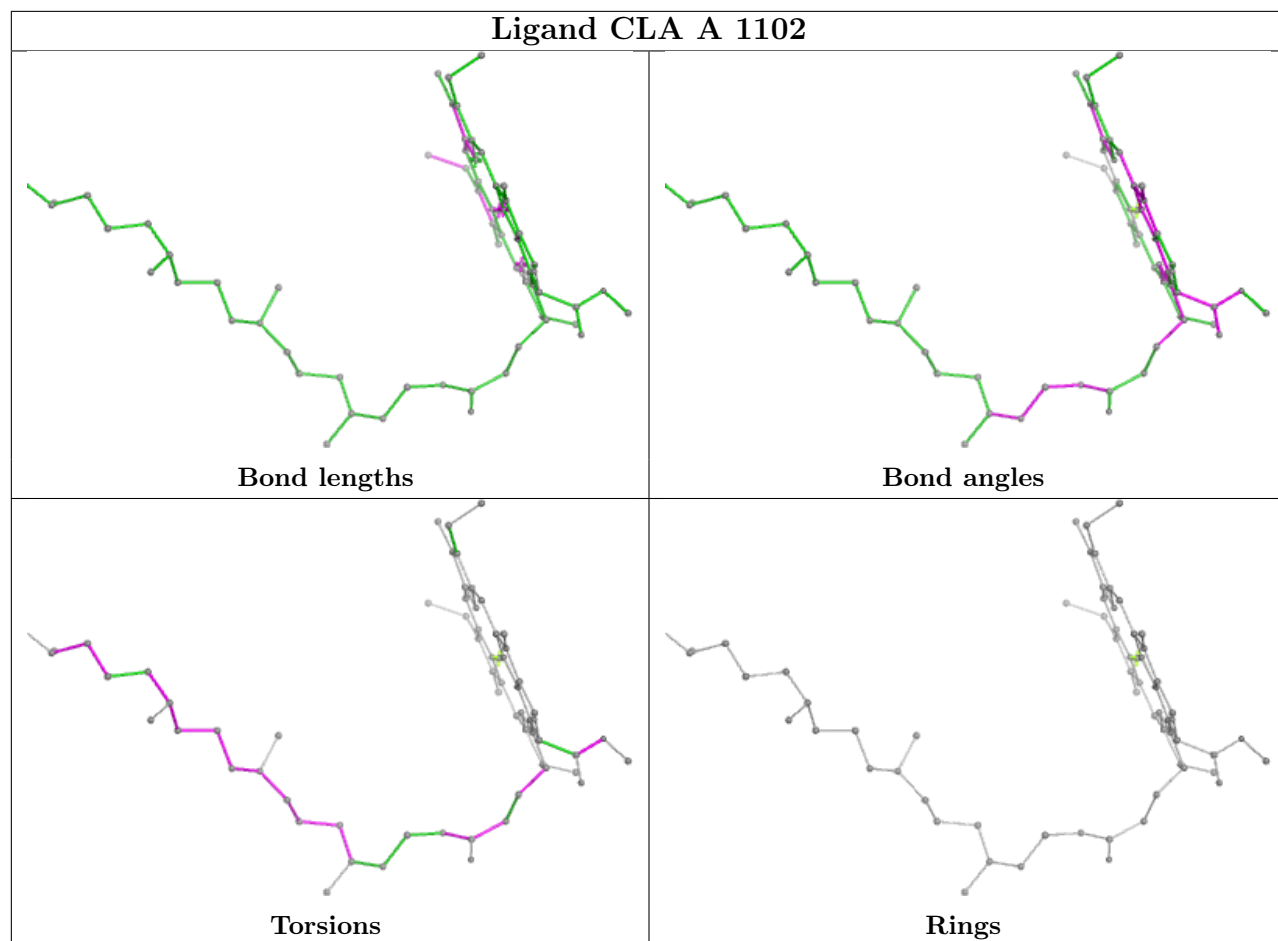


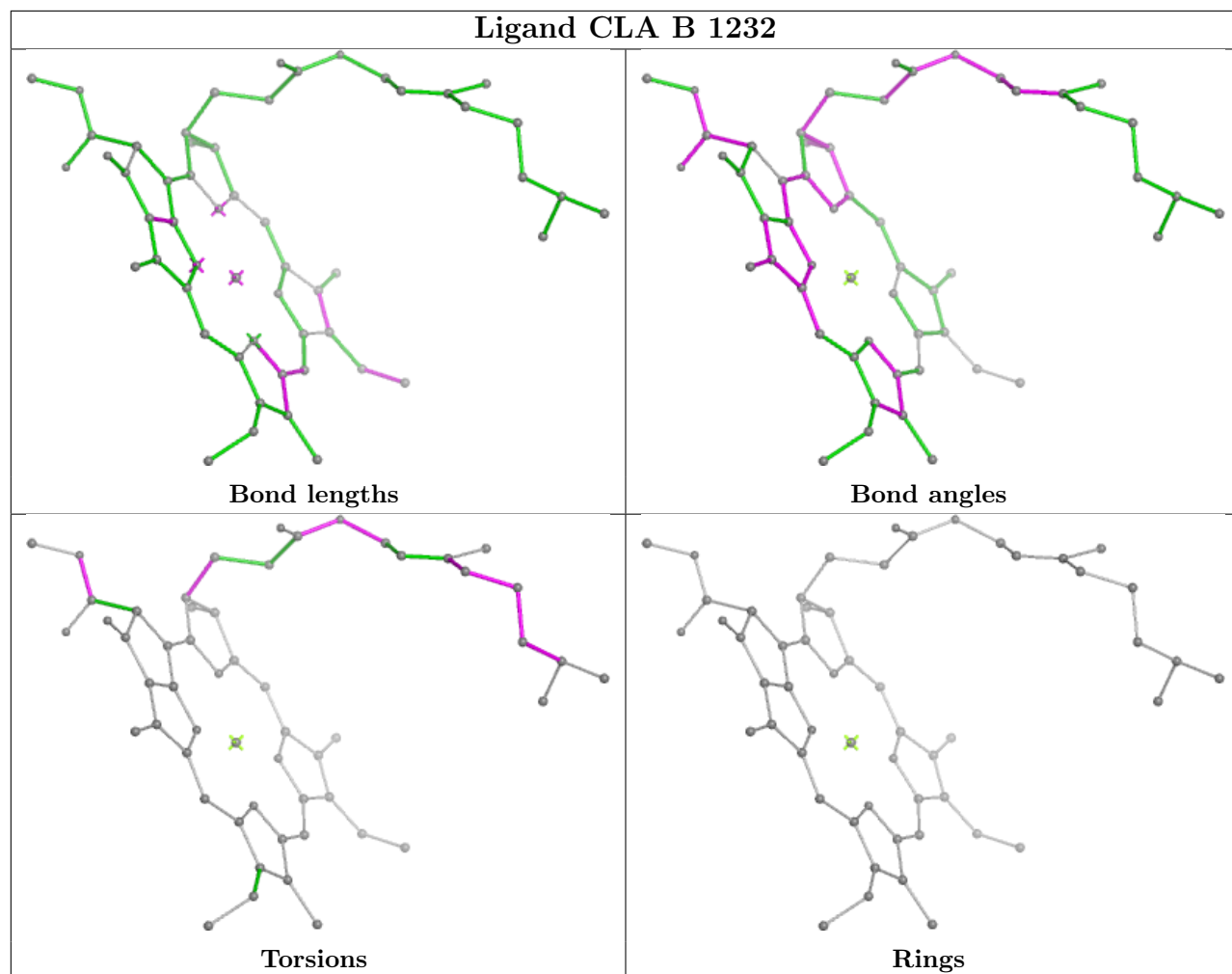
Torsions



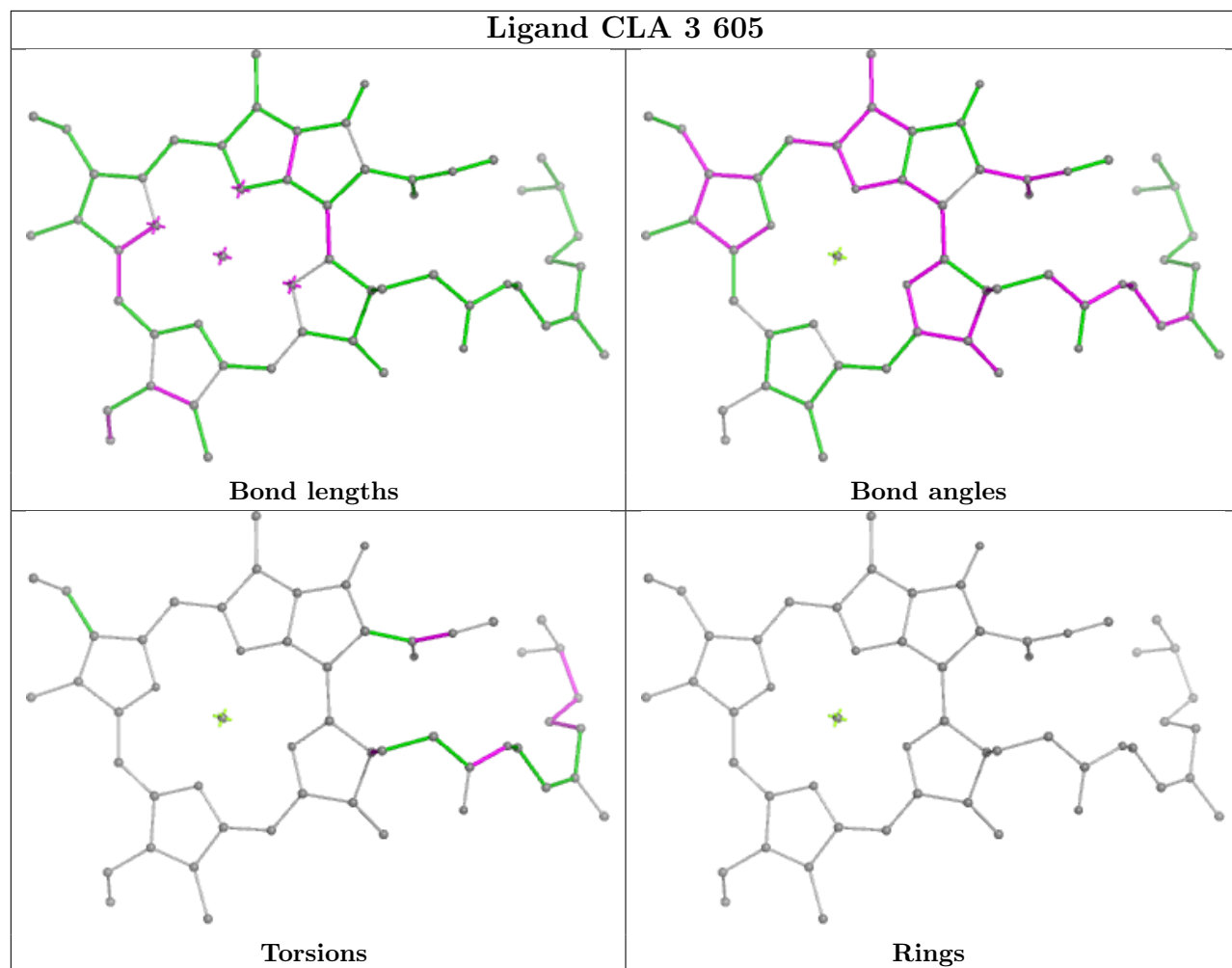
Rings



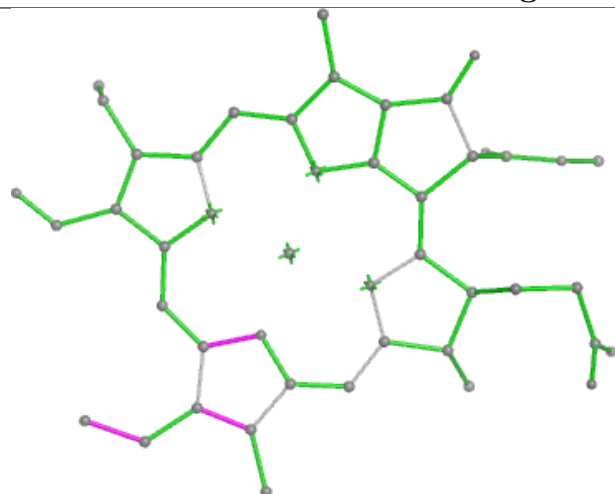




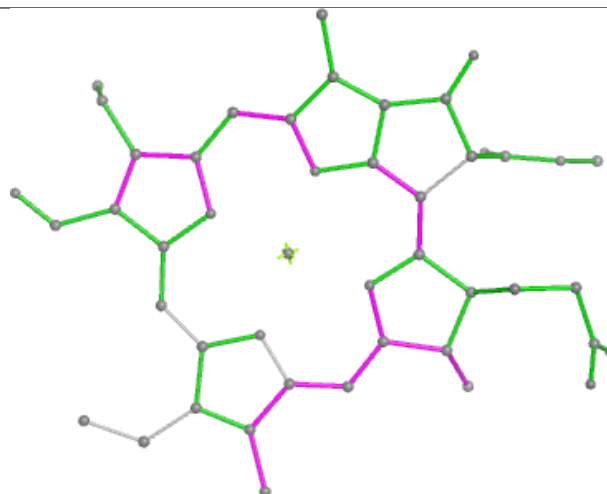
Ligand CLA 3 605



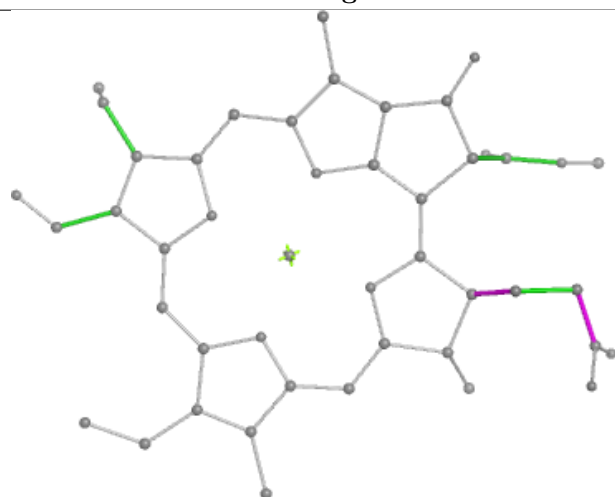
Ligand CHL 2 613



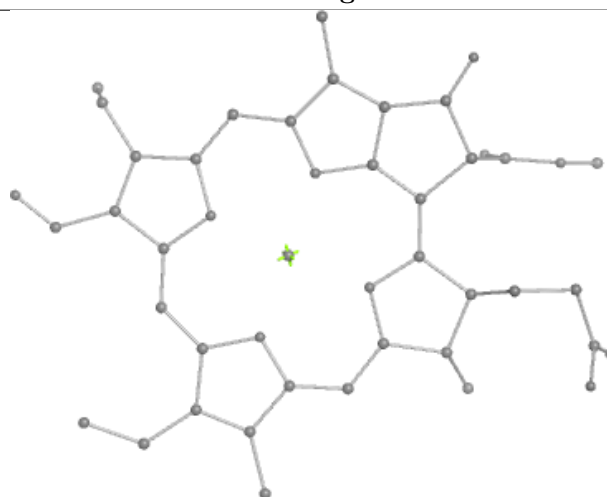
Bond lengths



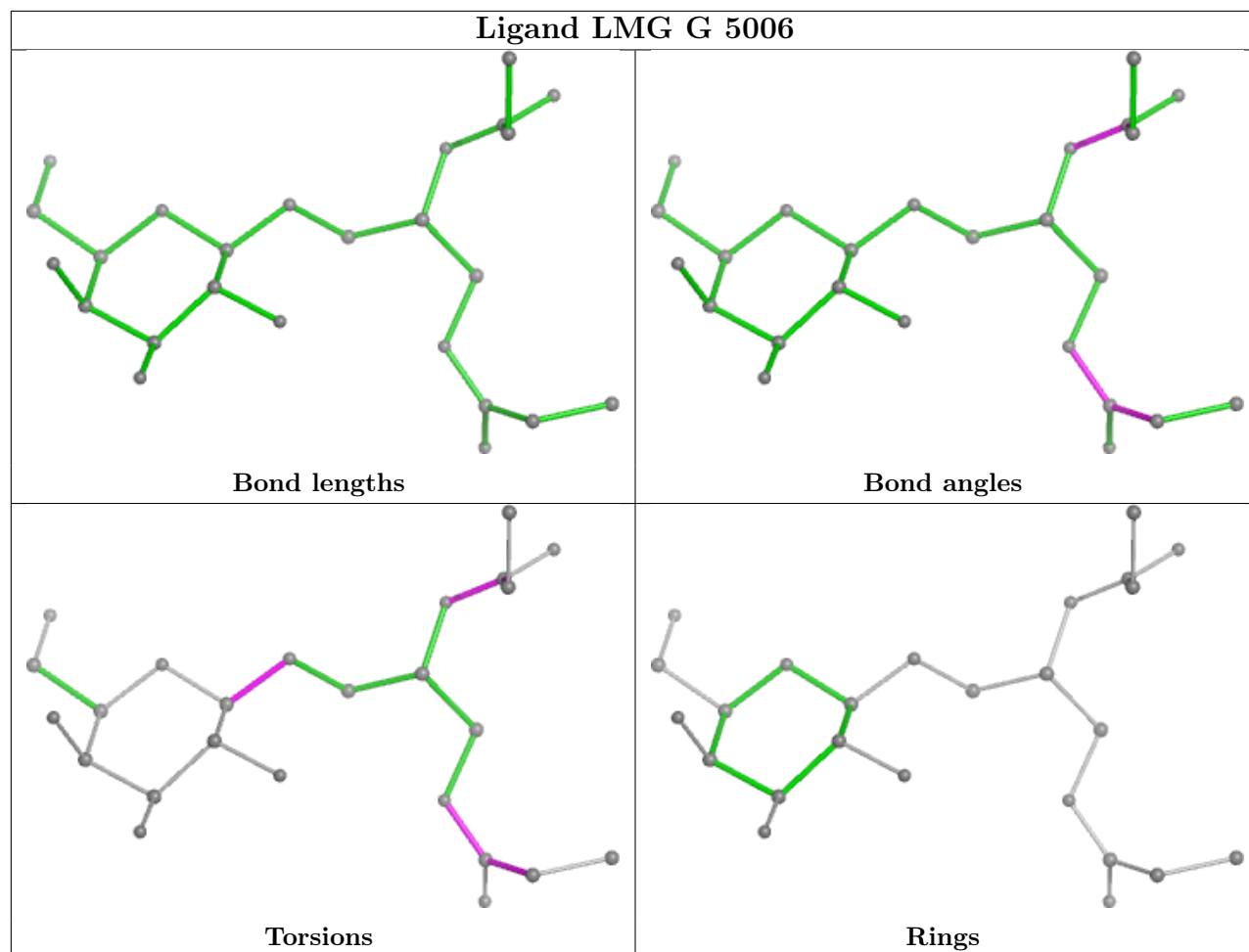
Bond angles



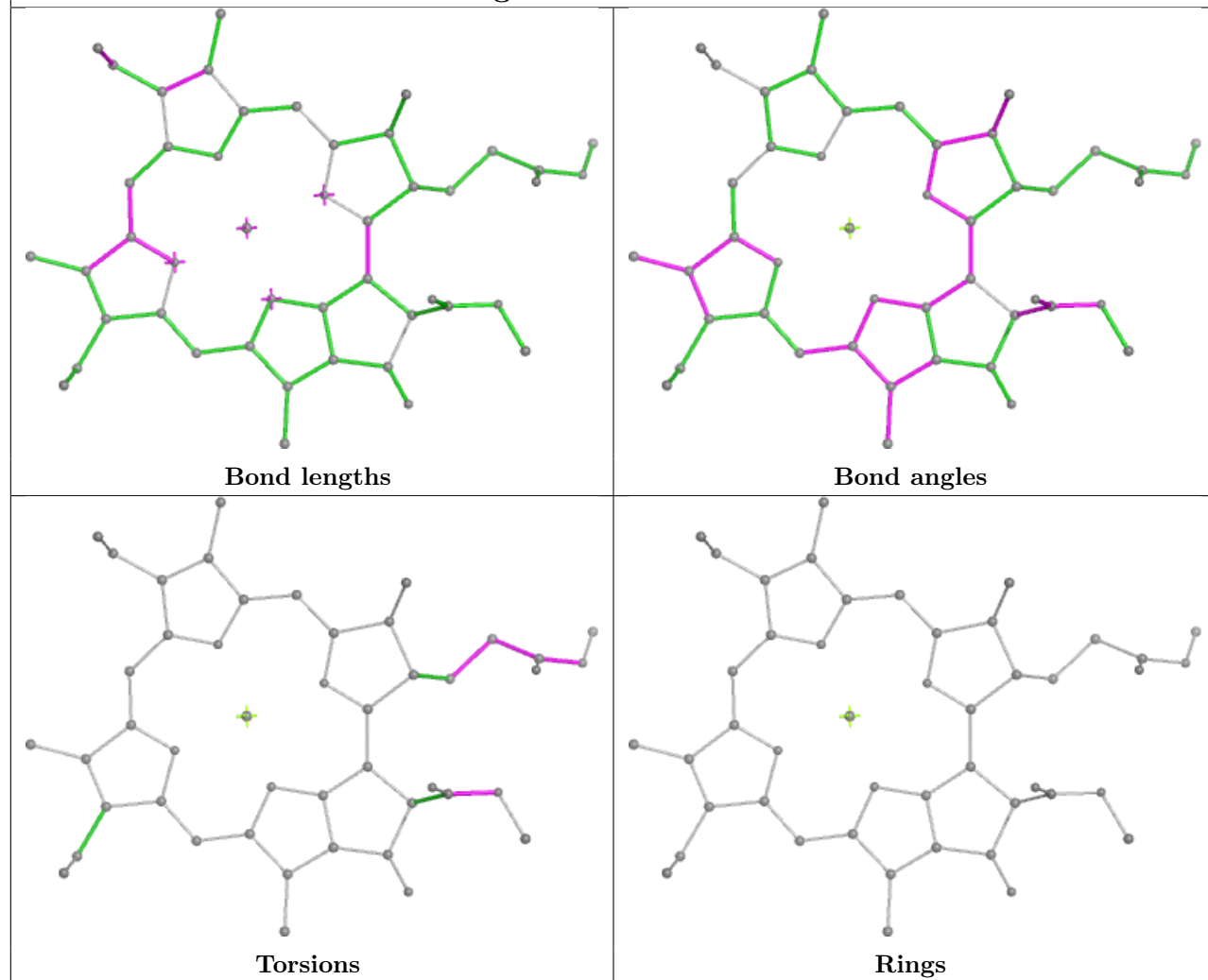
Torsions



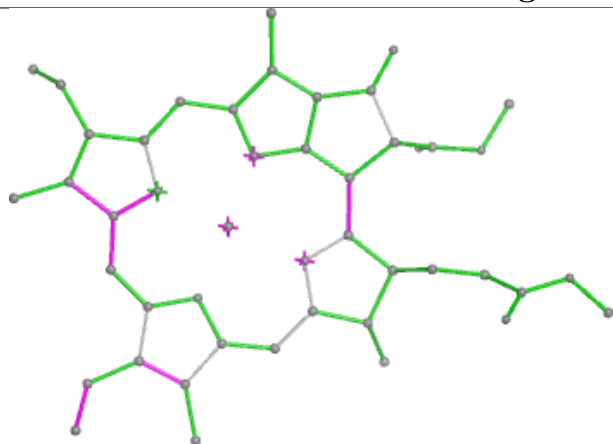
Rings



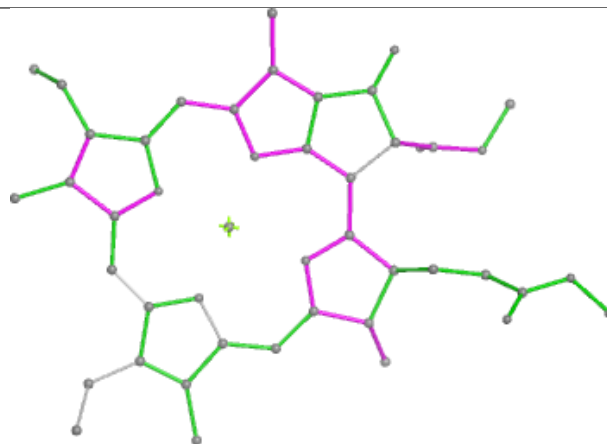
Ligand CLA K 1404



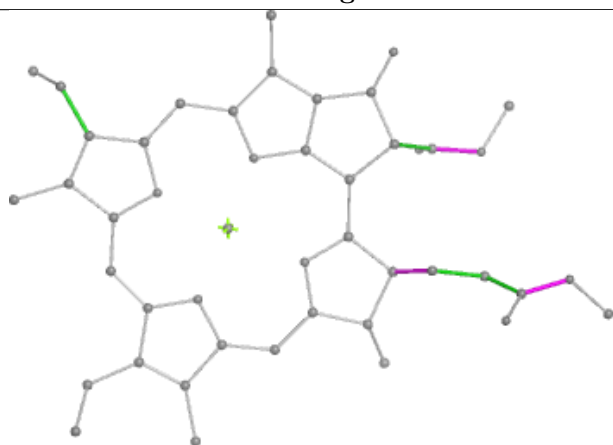
Ligand CLA 3 613



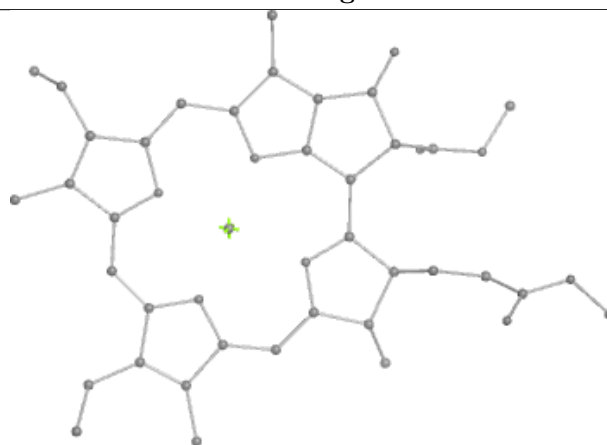
Bond lengths



Bond angles

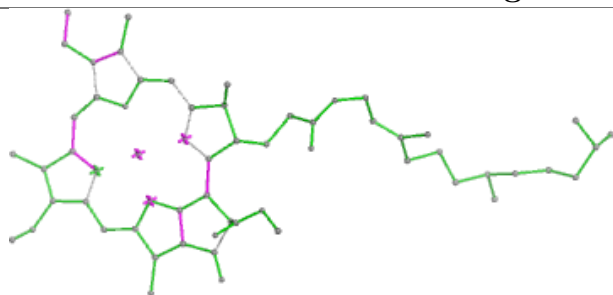


Torsions

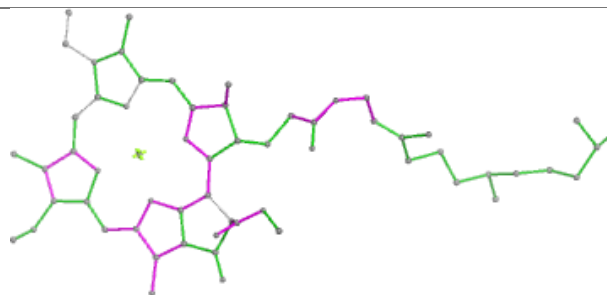


Rings

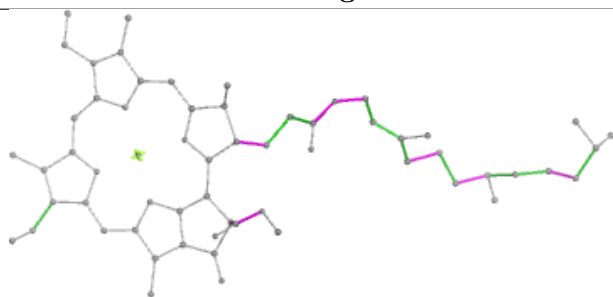
Ligand CLA G 1701



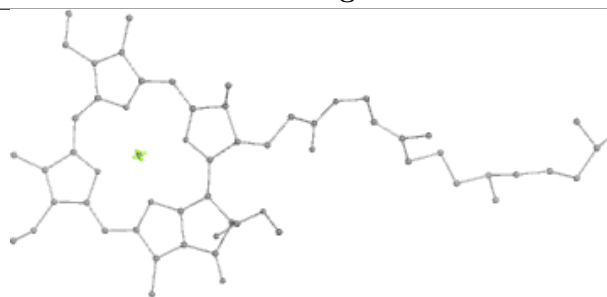
Bond lengths



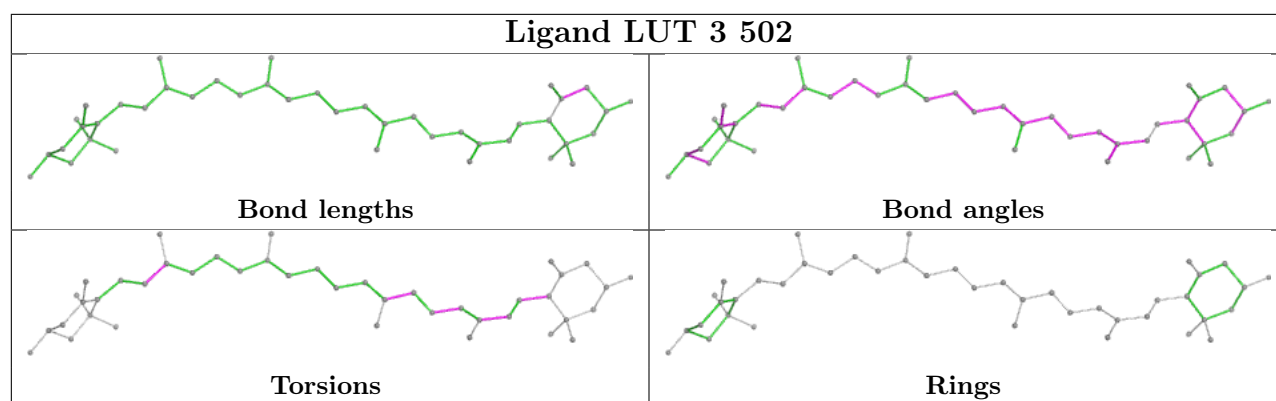
Bond angles



Torsions



Rings



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Map visualisation

This section contains visualisations of the EMDB entry EMD-10746. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

6.1 Orthogonal projections

This section was not generated.

6.2 Central slices

This section was not generated.

6.3 Largest variance slices

This section was not generated.

6.4 Orthogonal standard-deviation projections (False-color)

This section was not generated.

6.5 Orthogonal surface views

This section was not generated.

6.6 Mask visualisation

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

7 Map analysis ⓘ

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

7.1 Map-value distribution ⓘ

This section was not generated.

7.2 Volume estimate versus contour level ⓘ

This section was not generated.

7.3 Rotationally averaged power spectrum ⓘ

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

8 Fourier-Shell correlation

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

9 Map-model fit

This section was not generated.