



Full wwPDB EM Validation Report ⓘ

Mar 29, 2026 – 11:25 PM UTC

PDB ID : 6ZOO / pdb_00006zoo
EMDB ID : EMD-11326
Title : Photosystem I reduced Plastocyanin Complex
Authors : Nelson, N.; Caspy, I.; Shkolnisky, Y.
Deposited on : 2020-07-07
Resolution : 2.74 Å(reported)
Based on initial model : 6YEZ

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

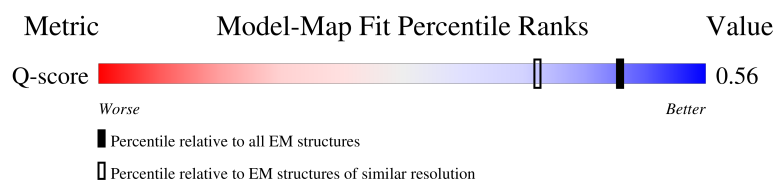
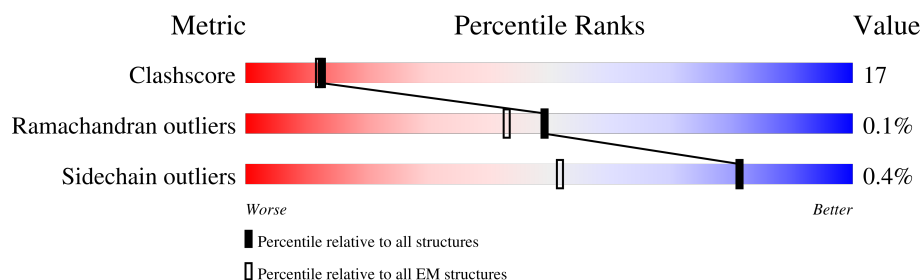
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance

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

The reported resolution of this entry is 2.74 Å.

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



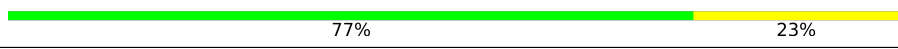
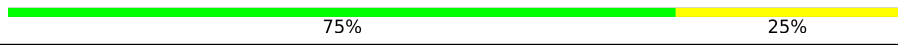
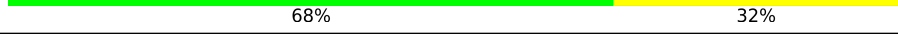
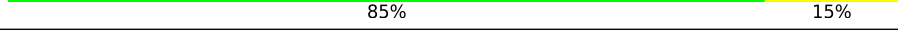
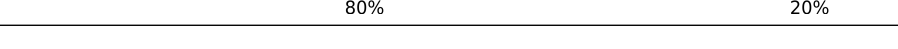
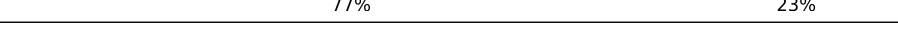
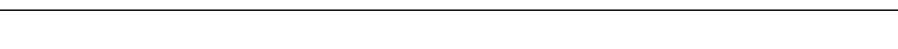
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	10492 (2.24 - 3.24)

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

Mol	Chain	Length	Quality of chain
1	A	743	
2	B	733	
3	C	80	
4	D	143	

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Mol	Chain	Length	Quality of chain
5	E	66	
6	F	154	
7	G	97	
8	H	93	
9	I	31	
10	J	42	
11	K	81	
12	L	159	
13	1	193	
14	2	208	
15	3	221	
16	4	198	
17	P	99	

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
1	SNK	A	636	X	-	-	-
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	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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	-	-	-
19	CLA	3	603	X	-	-	-
19	CLA	3	605	X	-	-	-
19	CLA	3	606	X	-	-	-
19	CLA	3	607	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	605	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	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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	-	-	-
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	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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	-	-	-
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	H	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	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	CLA	L	1501	X	-	-	-
19	CLA	L	1502	X	-	-	-
19	CLA	L	1503	X	-	-	-
28	LUT	1	501	X	-	-	-
28	LUT	1	502	X	-	-	-
28	LUT	2	501	X	-	-	-
28	LUT	3	501	X	-	-	-
28	LUT	3	502	X	-	-	-
28	LUT	4	501	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	-	-	-
29	CHL	2	613	X	-	-	-
29	CHL	2	615	X	-	-	-
29	CHL	3	604	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 [i](#)

There are 33 unique types of molecules in this entry. The entry contains 38497 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
			5866	3843	998	1005	20		

- 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		

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	69	GLY	-	insertion	UNP E1C9K8
D	70	PHE	-	insertion	UNP E1C9K8
D	71	THR	-	insertion	UNP E1C9K8
D	72	PRO	-	insertion	UNP E1C9K8
D	73	PRO	-	insertion	UNP E1C9K8
D	106	GLU	ASP	conflict	UNP E1C9K8
D	161	SER	ASN	conflict	UNP E1C9K8
D	180	PRO	ALA	conflict	UNP E1C9K8
D	187	VAL	GLN	conflict	UNP E1C9K8

- Molecule 5 is a protein called Putative uncharacterized protein.

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

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	64	PRO	-	insertion	UNP E1C9K6
E	65	PRO	-	insertion	UNP E1C9K6
E	79	GLN	LYS	conflict	UNP E1C9K6
E	125	VAL	ILE	conflict	UNP E1C9K6
E	126	GLU	VAL	conflict	UNP E1C9K6
E	129	LYS	GLU	conflict	UNP E1C9K6

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

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

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	80	ALA	SER	conflict	UNP A0A0M3KL12
F	87	ASP	GLU	conflict	UNP A0A0M3KL12
F	108	LEU	ILE	conflict	UNP A0A0M3KL12
F	111	PRO	ALA	conflict	UNP A0A0M3KL12
F	134	GLY	ALA	conflict	UNP A0A0M3KL12
F	188	ASP	GLU	conflict	UNP A0A0M3KL12
F	204	THR	SER	conflict	UNP A0A0M3KL12
F	205	GLY	ARG	conflict	UNP A0A0M3KL12

- Molecule 7 is a protein called photosystem I reaction center.

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

There are 13 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	106	THR	SER	conflict	UNP A0A0M3KL13

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Chain	Residue	Modelled	Actual	Comment	Reference
G	112	VAL	ALA	conflict	UNP A0A0M3KL13
G	113	SER	GLY	conflict	UNP A0A0M3KL13
G	114	LEU	VAL	conflict	UNP A0A0M3KL13
G	115	LEU	SER	conflict	UNP A0A0M3KL13
G	118	ASN	-	insertion	UNP A0A0M3KL13
G	119	ASP	-	insertion	UNP A0A0M3KL13
G	120	PRO	-	insertion	UNP A0A0M3KL13
G	121	VAL	-	insertion	UNP A0A0M3KL13
G	122	GLY	ALA	conflict	UNP A0A0M3KL13
G	123	PHE	ALA	conflict	UNP A0A0M3KL13
G	124	ASN	ALA	conflict	UNP A0A0M3KL13
G	125	ILE	LEU	conflict	UNP A0A0M3KL13

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

Mol	Chain	Residues	Atoms				AltConf	Trace
8	H	93	Total	C	N	O	0	0
			712	466	112	134		

- 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 domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	159	Total	C	N	O	S	0	0
			1197	788	191	217	1		

- Molecule 13 is a protein called Chlorophyll a-b binding protein 6, chloroplastic.

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

There are 19 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	40	ASP	HIS	conflict	UNP Q01667
1	45	GLN	GLU	conflict	UNP Q01667
1	49	SER	ALA	conflict	UNP Q01667
1	65	ARG	GLY	conflict	UNP Q01667
1	71	GLU	ALA	conflict	UNP Q01667
1	76	PHE	TYR	conflict	UNP Q01667
1	102	LEU	TYR	conflict	UNP Q01667
1	136	VAL	ALA	conflict	UNP Q01667
1	141	SER	ALA	conflict	UNP Q01667
1	177	PHE	LEU	conflict	UNP Q01667
1	178	HIS	GLU	conflict	UNP Q01667
1	180	TYR	LEU	conflict	UNP Q01667
1	182	ILE	VAL	conflict	UNP Q01667
1	185	VAL	ILE	conflict	UNP Q01667
1	198	ILE	PHE	conflict	UNP Q01667
1	225	THR	ASN	conflict	UNP Q01667
1	228	ASN	ASP	conflict	UNP Q01667
1	229	VAL	ILE	conflict	UNP Q01667
1	230	LEU	VAL	conflict	UNP Q01667

- 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		

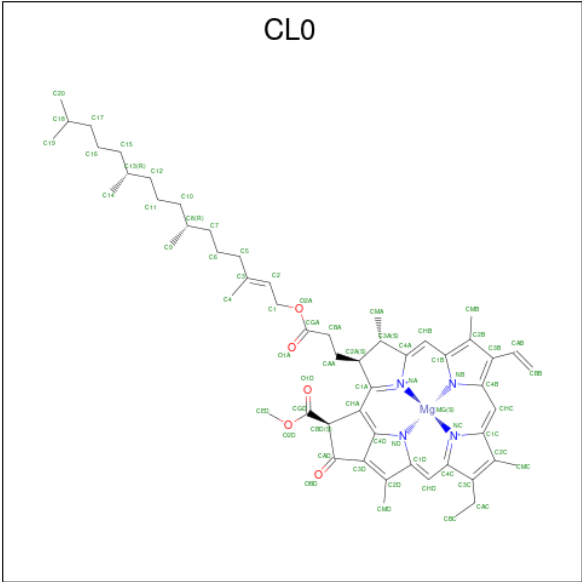
There are 3 discrepancies between the modelled and reference sequences:

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 Plastocyanin, chloroplastic.

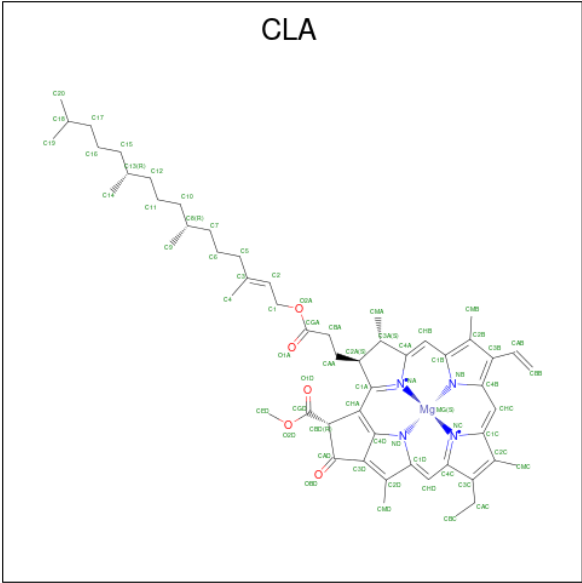
Mol	Chain	Residues	Atoms					AltConf	Trace
17	P	99	Total	C	N	O	S	0	0
			728	460	115	150	3		

- 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: C₅₅H₇₂MgN₄O₅).



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 65	C 55	Mg 1	N 4	O 5	0
19	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	A	1	Total 60	C 50	Mg 1	N 4	O 5	0
19	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
19	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	A	1	Total 46	C 36	Mg 1	N 4	O 5	0
19	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	A	1	Total 56	C 46	Mg 1	N 4	O 5	0
19	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	A	1	Total 50	C 40	Mg 1	N 4	O 5	0
19	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	A	1	Total 60	C 50	Mg 1	N 4	O 5	0
19	A	1	Total 60	C 50	Mg 1	N 4	O 5	0
19	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
19	A	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
19	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
19	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
19	A	1	Total 51	C 41	Mg 1	N 4	O 5	0
19	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	A	1	Total 60	C 50	Mg 1	N 4	O 5	0
19	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	A	1	Total 50	C 40	Mg 1	N 4	O 5	0
19	A	1	Total 45	C 35	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

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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	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
			58	48	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
			55	45	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
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			50	40	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	F	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	F	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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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	H	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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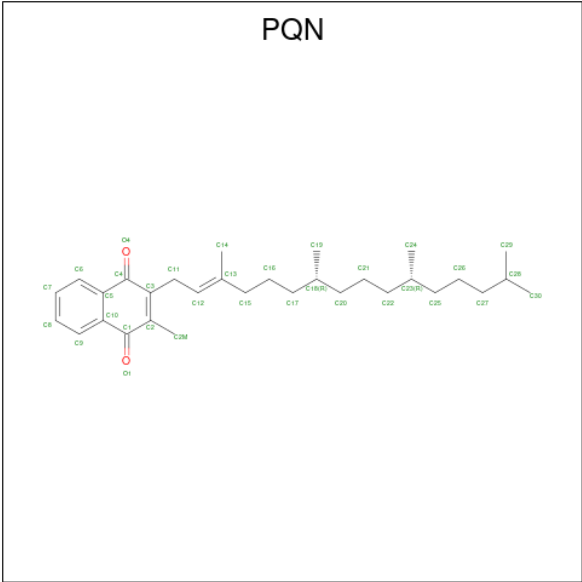
Mol	Chain	Residues	Atoms					AltConf
19	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
19	1	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
19	2	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
19	2	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
19	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	2	1	Total	C	Mg	N	O	0
			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
			55	45	1	4	5	
19	2	1	Total	C	Mg	N	O	0
			50	40	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
			52	42	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	

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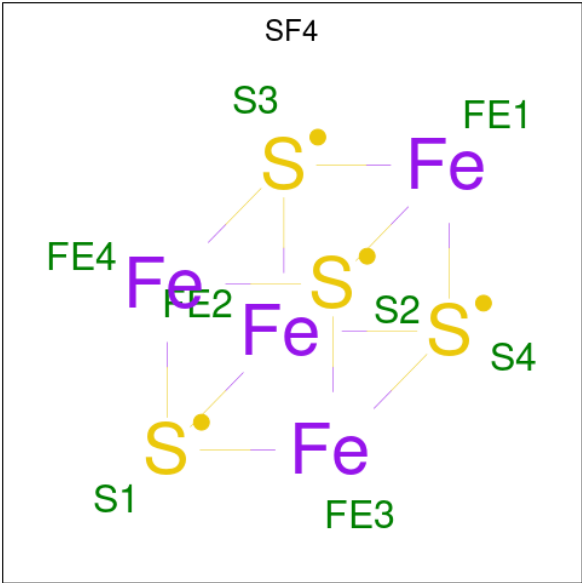
Mol	Chain	Residues	Atoms					AltConf
19	3	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
19	3	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
19	4	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
19	4	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
19	4	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
19	4	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
19	4	1	Total	C	Mg	N	O	0
			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
			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: C₃₁H₄₆O₂).



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: Fe₄S₄).



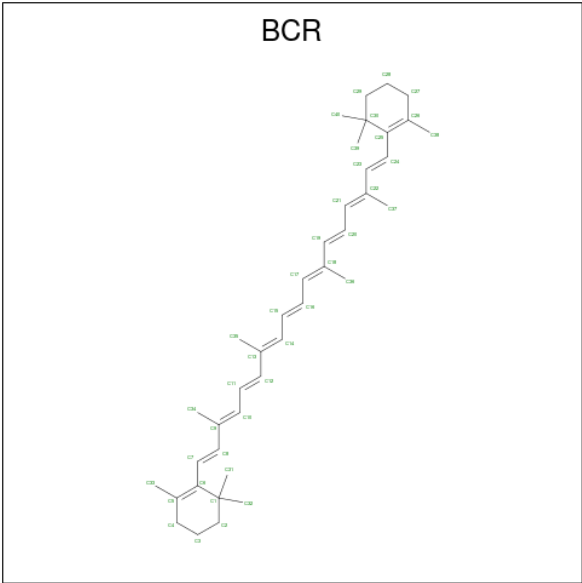
Mol	Chain	Residues	Atoms			AltConf
21	A	1	Total	Fe	S	0
			8	4	4	
21	C	1	Total	Fe	S	0
			8	4	4	

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

- Molecule 22 is BETA-CAROTENE (CCD ID: BCR) (formula: C₄₀H₅₆).



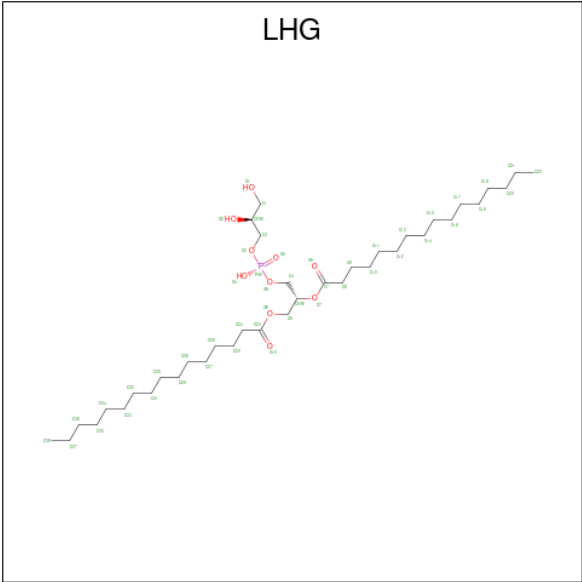
Mol	Chain	Residues	Atoms		AltConf
22	A	1	Total	C	0
			40	40	
22	A	1	Total	C	0
			40	40	
22	A	1	Total	C	0
			40	40	
22	A	1	Total	C	0
			40	40	
22	A	1	Total	C	0
			40	40	
22	A	1	Total	C	0
			40	40	
22	B	1	Total	C	0
			40	40	
22	B	1	Total	C	0
			40	40	
22	B	1	Total	C	0
			40	40	
22	B	1	Total	C	0
			40	40	

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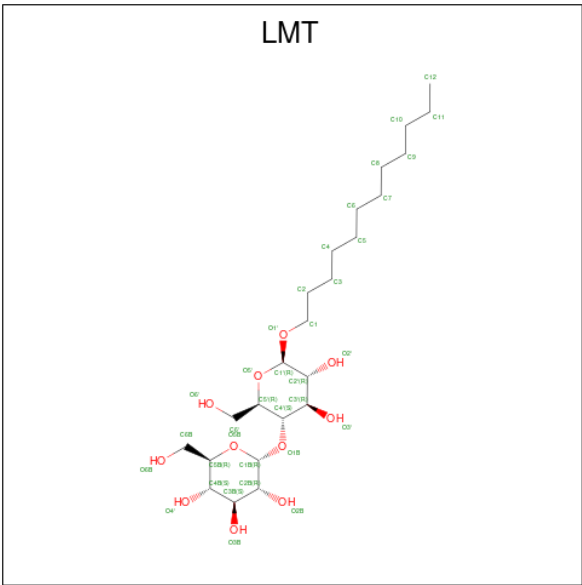
Mol	Chain	Residues	Atoms	AltConf
22	B	1	Total C 40 40	0
22	F	1	Total C 40 40	0
22	F	1	Total C 40 40	0
22	G	1	Total C 40 40	0
22	H	1	Total C 40 40	0
22	I	1	Total C 40 40	0
22	I	1	Total C 40 40	0
22	J	1	Total C 40 40	0
22	K	1	Total C 40 40	0
22	K	1	Total C 40 40	0
22	L	1	Total C 40 40	0
22	L	1	Total C 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: $C_{38}H_{75}O_{10}P$).



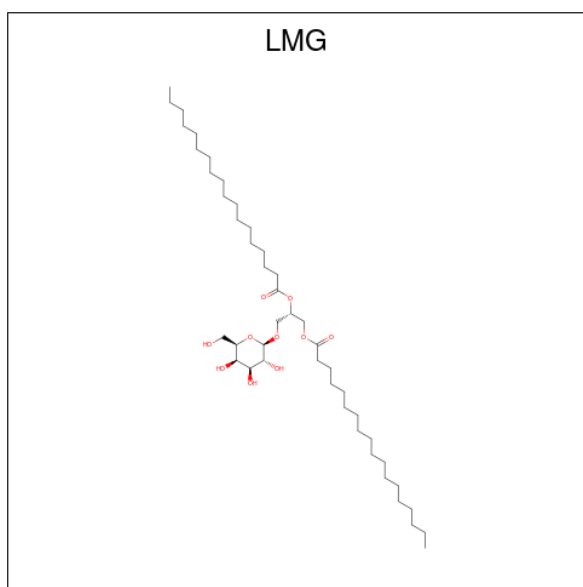
Mol	Chain	Residues	Atoms				AltConf
23	A	1	Total	C	O	P	0
			40	29	10	1	
23	A	1	Total	C	O	P	0
			49	38	10	1	
23	B	1	Total	C	O	P	0
			21	10	10	1	
23	B	1	Total	C	O	P	0
			49	38	10	1	
23	1	1	Total	C	O	P	0
			49	38	10	1	
23	2	1	Total	C	O	P	0
			35	24	10	1	
23	3	1	Total	C	O	P	0
			17	8	8	1	
23	4	1	Total	C	O	P	0
			35	24	10	1	

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



Mol	Chain	Residues	Atoms			AltConf
24	A	1	Total	C	O	0
			35	24	11	
24	B	1	Total	C	O	0
			31	20	11	
24	B	1	Total	C	O	0
			32	21	11	
24	G	1	Total	C	O	0
			35	24	11	
24	G	1	Total	C	O	0
			31	20	11	
24	2	1	Total	C	O	0
			35	24	11	

- Molecule 25 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: C₄₅H₈₆O₁₀).



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
			25	15	10	
25	G	1	Total	C	O	0
			49	39	10	
25	G	1	Total	C	O	0
			50	40	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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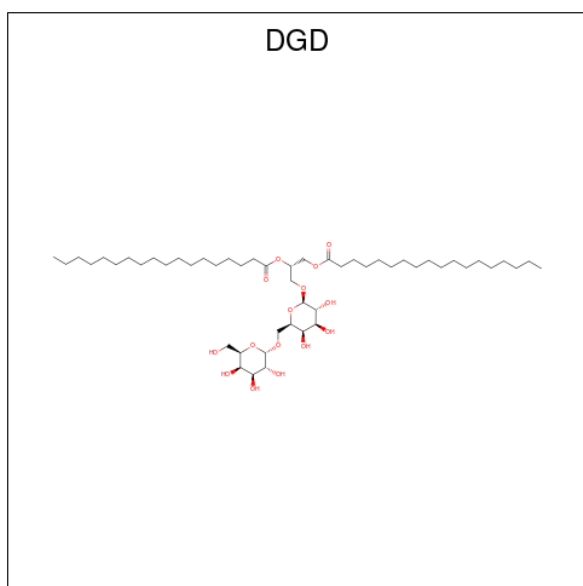
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Mol	Chain	Residues	Atoms			AltConf
25	2	1	Total	C	O	0
			36	26	10	
25	2	1	Total	C	O	0
			30	20	10	
25	2	1	Total	C	O	0
			30	20	10	
25	2	1	Total	C	O	0
			13	7	6	
25	3	1	Total	C	O	0
			30	20	10	

- 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).



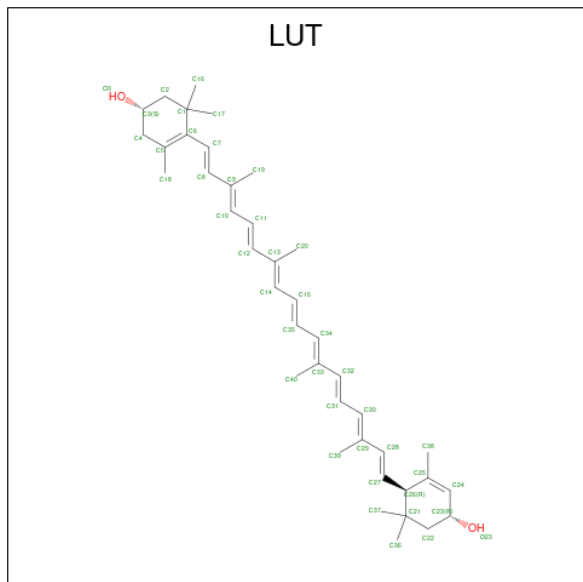
Mol	Chain	Residues	Atoms			AltConf
27	B	1	Total	C	O	0
			61	46	15	
27	F	1	Total	C	O	0
			57	42	15	

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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
			50	35	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).



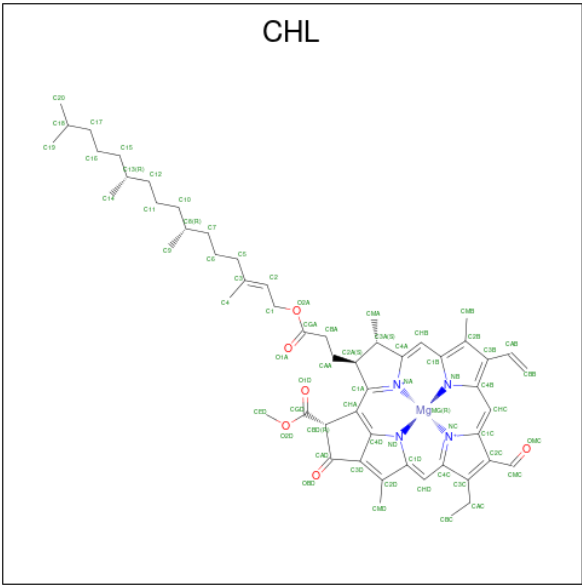
Mol	Chain	Residues	Atoms			AltConf
28	J	1	Total	C	O	0
			42	40	2	
28	1	1	Total	C	O	0
			42	40	2	
28	1	1	Total	C	O	0
			42	40	2	
28	2	1	Total	C	O	0
			42	40	2	
28	3	1	Total	C	O	0
			42	40	2	
28	3	1	Total	C	O	0
			42	40	2	

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Mol	Chain	Residues	Atoms			AltConf
28	4	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).



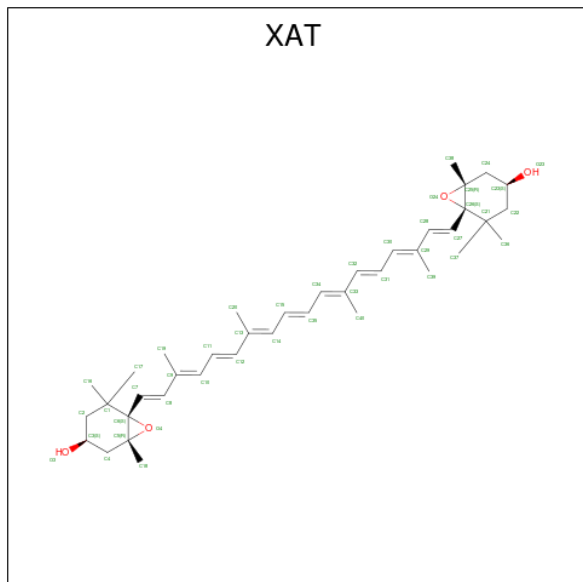
Mol	Chain	Residues	Atoms						AltConf
29	1	1	Total	C	Mg	N	O	0	
			56	45	1	4	6		
29	1	1	Total	C	Mg	N	O	0	
			47	36	1	4	6		
29	1	1	Total	C	Mg	N	O	0	
			61	50	1	4	6		
29	2	1	Total	C	Mg	N	O	0	
			56	45	1	4	6		
29	2	1	Total	C	Mg	N	O	0	
			48	37	1	4	6		
29	2	1	Total	C	Mg	N	O	0	
			46	35	1	4	6		
29	2	1	Total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

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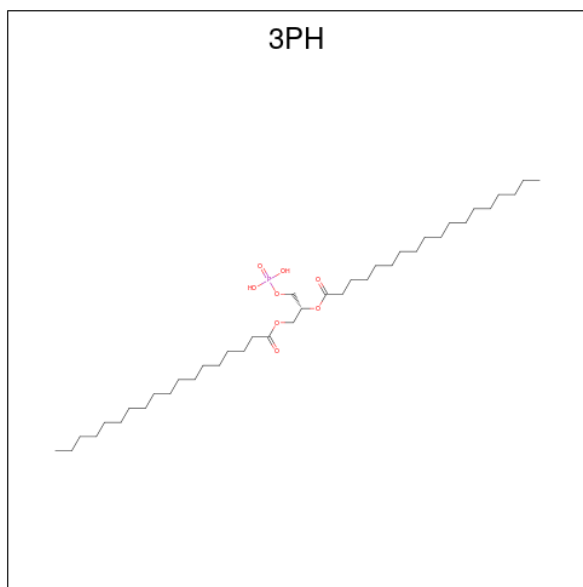
Mol	Chain	Residues	Atoms					AltConf
29	3	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
29	4	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
29	4	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
29	4	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
29	4	1	Total	C	Mg	N	O	0
			43	34	1	4	4	

- 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 1,2-DIACYL-GLYCEROL-3-SN-PHOSPHATE (CCD ID: 3PH) (formula: C₃₉H₇₇O₈P).



Mol	Chain	Residues	Atoms				AltConf
31	2	1	Total	C	O	P	0
			33	24	8	1	

- Molecule 32 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		AltConf
32	P	1	Total	Cu	0
			1	1	

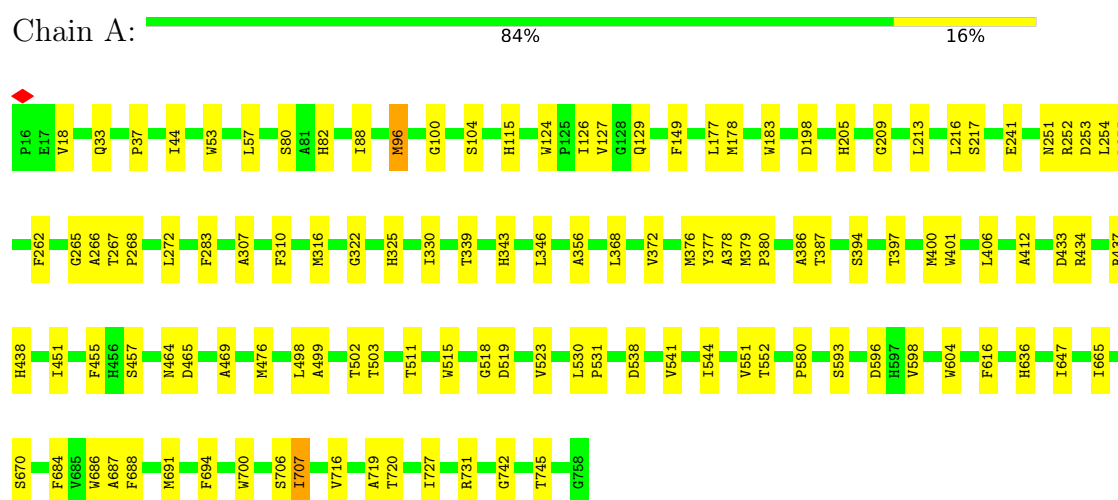
- Molecule 33 is water.

Mol	Chain	Residues	Atoms		AltConf
33	B	2	Total	O	0
			2	2	

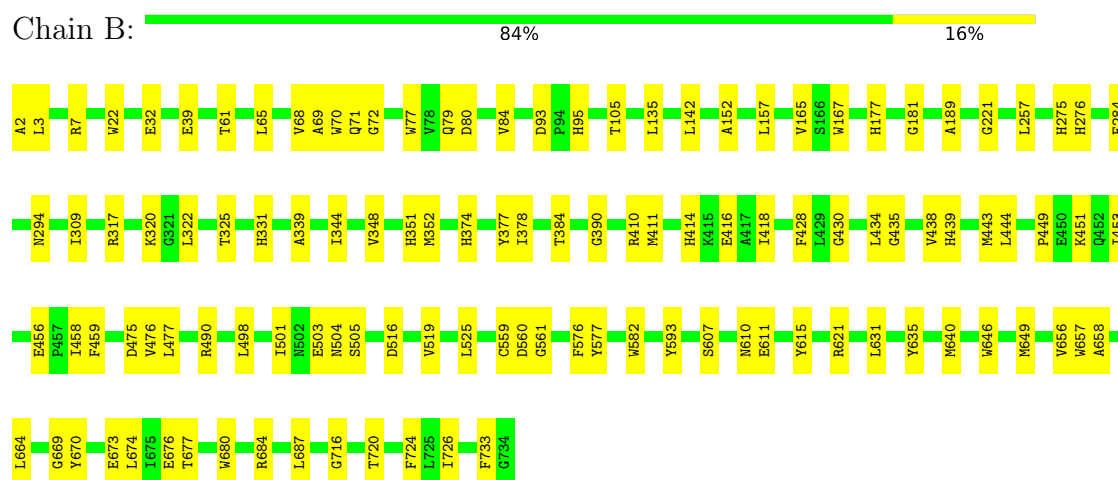
3 Residue-property plots

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

- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

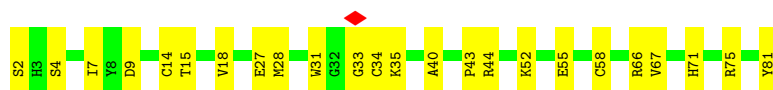


- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

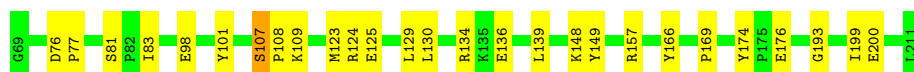
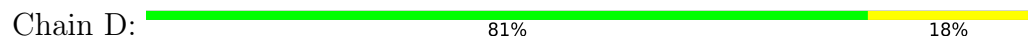


- Molecule 3: Photosystem I iron-sulfur center

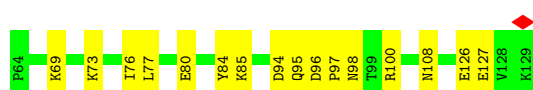
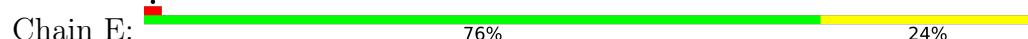




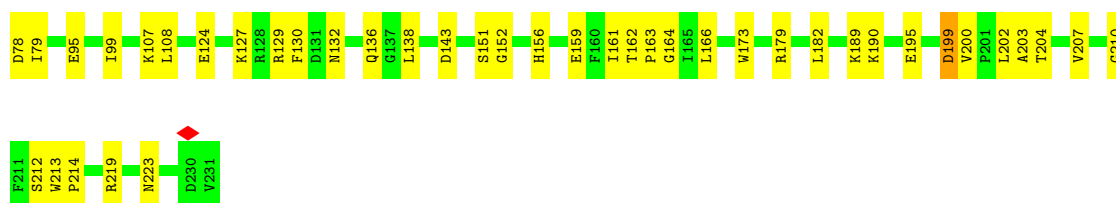
- Molecule 4: PsaD



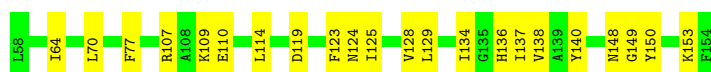
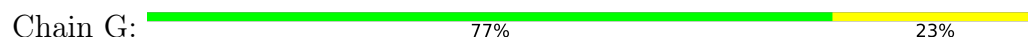
- Molecule 5: Putative uncharacterized protein



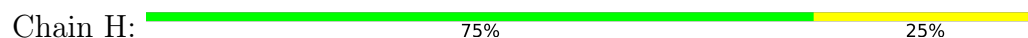
- Molecule 6: Photosystem I reaction center subunit III



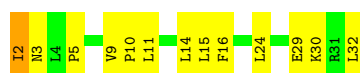
- Molecule 7: photosystem I reaction center



- Molecule 8: Photosystem I reaction center subunit VI,Photosystem I reaction center subunit VI



- Molecule 9: Photosystem I reaction center subunit VIII



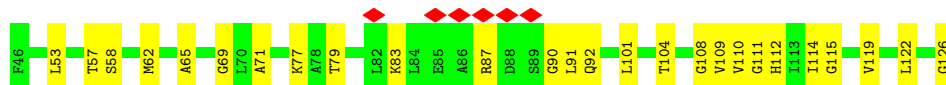
- Molecule 10: Photosystem I reaction center subunit IX

Chain J:  83% 17%



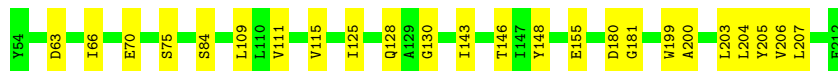
- Molecule 11: Photosystem I reaction center subunit X psaK

Chain K:  7% 68% 32%



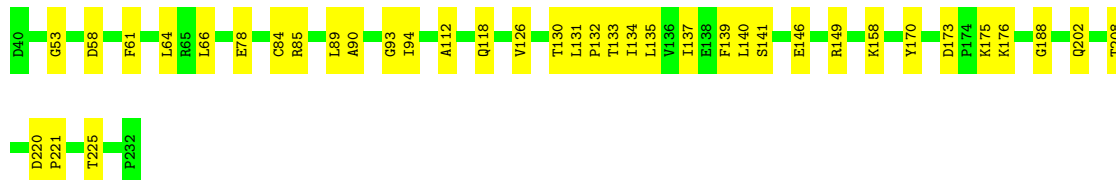
- Molecule 12: PsaL domain-containing protein

Chain L:  85% 15%



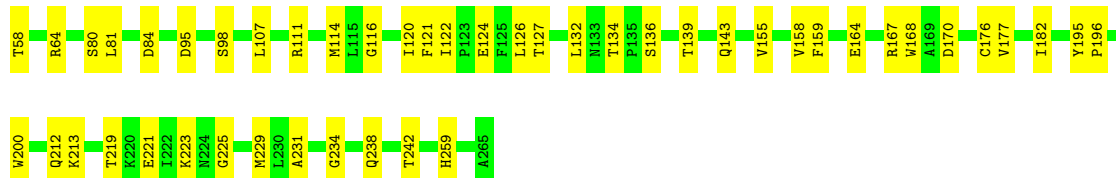
- Molecule 13: Chlorophyll a-b binding protein 6, chloroplastic

Chain 1:  80% 20%



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

Chain 2:  77% 23%



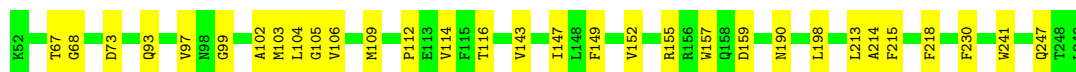
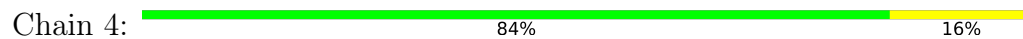
- Molecule 15: Chlorophyll a-b binding protein 3, chloroplastic

Chain 3:  67% 33%





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



- Molecule 17: Plastocyanin, chloroplastic



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	104127	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 ($e^-/\text{\AA}^2$)	40.8	Depositor
Minimum defocus (nm)	300	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	130000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.176	Depositor
Minimum map value	-0.074	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.0125	Depositor
Map size ($\text{\AA}$)	392.4, 392.4, 392.4	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.308, 1.308, 1.308	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: DGD, SNK, XAT, LHG, LMT, CA, SF4, BCR, LMG, CU, PQN, 3PH, CHL, LUT, CLA, CL0

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.15	0/6033	0.31	0/8228
2	B	0.15	0/6069	0.32	0/8286
3	C	0.13	0/625	0.34	0/846
4	D	0.14	0/1163	0.31	0/1572
5	E	0.14	0/540	0.31	0/734
6	F	0.14	0/1234	0.35	0/1670
7	G	0.13	0/776	0.31	0/1054
8	H	0.13	0/733	0.32	0/995
9	I	0.17	0/246	0.39	0/335
10	J	0.15	0/349	0.27	0/476
11	K	0.14	0/576	0.30	0/779
12	L	0.12	0/1232	0.29	0/1684
13	1	0.16	0/1558	0.35	0/2125
14	2	0.15	0/1679	0.33	0/2302
15	3	0.19	0/1760	0.40	0/2390
16	4	0.14	0/1608	0.32	0/2191
17	P	0.87	3/743 (0.4%)	1.15	9/1009 (0.9%)
All	All	0.21	3/26924 (0.0%)	0.38	9/36676 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	1	0
15	3	0	1
All	All	1	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	P	16	PRO	N-CA	12.99	1.69	1.47
17	P	15	VAL	C-N	5.79	1.45	1.34
17	P	15	VAL	N-CA	5.15	1.50	1.46

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	P	47	PRO	N-CA-C	8.25	124.32	110.95
17	P	16	PRO	CA-N-CD	-7.58	100.89	111.50
17	P	15	VAL	N-CA-C	7.55	115.62	108.15
17	P	47	PRO	CB-CA-C	-6.33	103.48	111.71
17	P	51	ASP	CA-C-N	-5.70	110.83	120.58
17	P	51	ASP	C-N-CA	-5.70	110.83	120.58
17	P	20	GLU	CB-CG-CD	5.69	122.28	112.60
17	P	15	VAL	CB-CA-C	5.21	116.03	111.08
17	P	57	MET	N-CA-C	-5.01	103.88	110.39

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	636	SNK	CA

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
15	3	86	PRO	Peptide

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	5866	0	5705	125	0
2	B	5857	0	5653	121	0
3	C	612	0	591	27	0
4	D	1132	0	1141	43	0
5	E	528	0	528	18	0
6	F	1206	0	1231	36	0
7	G	757	0	743	31	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	H	712	0	701	35	0
9	I	240	0	264	26	0
10	J	338	0	345	12	0
11	K	569	0	596	40	0
12	L	1197	0	1197	36	0
13	1	1508	0	1489	38	0
14	2	1620	0	1557	70	0
15	3	1706	0	1661	102	0
16	4	1559	0	1527	32	0
17	P	728	0	699	61	0
18	A	65	0	72	2	0
19	1	608	0	564	28	0
19	2	522	0	501	38	0
19	3	630	0	539	42	0
19	4	631	0	600	40	0
19	A	2643	0	2752	137	0
19	B	2610	0	2750	146	0
19	F	130	0	144	2	0
19	G	166	0	152	8	0
19	H	60	0	59	3	0
19	J	50	0	38	2	0
19	K	199	0	159	9	0
19	L	160	0	137	11	0
20	A	33	0	46	2	0
20	B	33	0	46	1	0
21	A	8	0	0	0	0
21	C	16	0	0	2	0
22	1	80	0	103	9	0
22	2	40	0	51	8	0
22	3	80	0	105	25	0
22	A	240	0	311	41	0
22	B	200	0	261	44	0
22	F	80	0	104	13	0
22	G	40	0	52	8	0
22	H	40	0	52	10	0
22	I	80	0	104	10	0
22	J	40	0	52	9	0
22	K	80	0	104	25	0
22	L	80	0	104	17	0
23	1	49	0	74	0	0
23	2	35	0	40	0	0
23	3	17	0	12	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	4	35	0	40	0	0
23	A	89	0	127	1	0
23	B	70	0	86	0	0
24	2	35	0	45	0	0
24	A	35	0	45	0	0
24	B	63	0	70	2	0
24	G	66	0	79	3	0
25	1	46	0	65	0	0
25	2	134	0	133	0	0
25	3	30	0	30	0	0
25	A	50	0	73	2	0
25	B	102	0	114	0	0
25	F	160	0	188	1	0
25	G	124	0	161	2	0
26	A	1	0	0	0	0
26	B	1	0	0	0	0
27	1	41	0	40	0	0
27	3	51	0	60	0	0
27	4	50	0	58	1	0
27	B	61	0	83	0	0
27	F	57	0	75	1	0
27	G	47	0	52	1	0
27	J	58	0	77	0	0
28	1	84	0	110	17	0
28	2	42	0	55	11	0
28	3	84	0	110	24	0
28	4	84	0	110	23	0
28	J	42	0	55	12	0
29	1	164	0	135	5	0
29	2	272	0	225	19	0
29	3	113	0	99	6	0
29	4	202	0	152	6	0
30	2	44	0	56	4	0
30	4	44	0	56	2	0
31	2	33	0	39	0	0
32	P	1	0	0	0	0
33	B	2	0	0	0	0
All	All	38497	0	38619	1298	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 17.

All (1298) 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)
1:A:377:TYR:OH	19:A:1135:CLA:HBC3	1.26	1.35
17:P:16:PRO:CA	17:P:16:PRO:N	1.69	1.32
1:A:178:MET:HE1	19:A:1108:CLA:CMC	1.69	1.22
12:L:204:LEU:HD21	19:L:1503:CLA:HED1	1.26	1.14
1:A:178:MET:HE2	1:A:178:MET:HA	1.29	1.14
17:P:55:ILE:HG22	17:P:72:VAL:CG2	1.78	1.13
5:E:96:ASP:OD2	5:E:97:PRO:O	1.69	1.11
8:H:103:LEU:HB3	12:L:143:ILE:HD11	1.27	1.10
8:H:120:GLY:HA2	8:H:126:LYS:NZ	1.66	1.10
8:H:120:GLY:HA2	8:H:126:LYS:HZ2	1.00	1.10
17:P:1:VAL:HG21	17:P:19:LEU:HD11	1.29	1.10
11:K:110:VAL:HG21	22:K:4001:BCR:H383	1.29	1.09
19:A:1113:CLA:CAA	15:3:273:LYS:HE3	1.85	1.06
15:3:236:LEU:HD13	29:3:604:CHL:OMC	1.56	1.05
7:G:148:ASN:HD21	7:G:150:TYR:HB3	1.22	1.02
6:F:129:ARG:HD3	10:J:35:ASP:OD2	1.58	1.01
1:A:377:TYR:OH	19:A:1135:CLA:CBC	2.09	1.01
19:A:1113:CLA:HAA1	15:3:273:LYS:HE3	1.02	1.01
1:A:178:MET:HE1	19:A:1108:CLA:HMC3	1.45	0.98
16:4:102:ALA:O	16:4:106:VAL:HG22	1.62	0.97
14:2:177:VAL:HG23	29:2:611:CHL:OMC	1.64	0.97
22:K:4001:BCR:HC31	15:3:273:LYS:HZ1	1.29	0.97
12:L:155:GLU:OE2	12:L:155:GLU:N	1.97	0.97
11:K:58:SER:HB2	11:K:114:ILE:HD11	1.44	0.97
8:H:51:LYS:HG3	8:H:52:SER:H	1.30	0.96
17:P:55:ILE:HG22	17:P:72:VAL:HG23	1.47	0.96
11:K:91:LEU:HD11	15:3:59:PHE:HE1	1.31	0.95
1:A:251:ASN:OD1	1:A:253:ASP:OD1	1.81	0.95
11:K:110:VAL:CG2	22:K:4001:BCR:H383	1.97	0.95
15:3:188:LEU:CD1	22:3:503:BCR:H342	1.97	0.95
1:A:251:ASN:OD1	1:A:254:LEU:HD13	1.67	0.95
19:A:1122:CLA:HHC	19:A:1122:CLA:HBB1	1.50	0.94
16:4:105:GLY:O	16:4:109:MET:HG3	1.68	0.93
6:F:78:ASP:OD2	6:F:79:ILE:HD12	1.68	0.93
19:B:1239:CLA:HHC	19:B:1239:CLA:HBB1	1.52	0.92
4:D:107:SER:HB2	4:D:123:MET:HE3	1.49	0.91
22:L:4020:BCR:HC8	22:L:4020:BCR:H331	1.51	0.91
19:1:603:CLA:HHC	19:1:603:CLA:HBB1	1.53	0.90
11:K:91:LEU:HD11	15:3:59:PHE:CE1	2.06	0.90
19:2:603:CLA:HHC	19:2:603:CLA:HBB1	1.54	0.89
17:P:51:ASP:OD2	17:P:54:LYS:HG3	1.72	0.89
13:1:130:THR:HG22	13:1:132:PRO:HD2	1.55	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:4:109:MET:HE1	16:4:215:PHE:HD1	1.36	0.89
1:A:178:MET:HE2	1:A:178:MET:CA	2.01	0.89
19:3:603:CLA:HHC	19:3:603:CLA:HBB1	1.53	0.89
16:4:99:GLY:O	16:4:103:MET:HG3	1.72	0.89
19:4:603:CLA:HHC	19:4:603:CLA:HBB1	1.55	0.89
19:B:1208:CLA:HHC	19:B:1208:CLA:HBB1	1.52	0.89
19:J:1901:CLA:HHC	19:J:1901:CLA:HBB1	1.55	0.88
14:2:259:HIS:HA	15:3:153:ASP:OD1	1.73	0.88
19:B:1207:CLA:H191	9:I:15:LEU:CD1	2.03	0.87
12:L:204:LEU:CD2	19:L:1503:CLA:HED1	2.04	0.87
19:B:1207:CLA:H191	9:I:15:LEU:HD12	1.54	0.87
22:K:4001:BCR:HC31	15:3:273:LYS:NZ	1.89	0.87
1:A:377:TYR:CZ	19:A:1135:CLA:HBC3	2.08	0.87
15:3:188:LEU:HD12	22:3:503:BCR:H342	1.55	0.87
28:4:501:LUT:H373	19:4:601:CLA:H12	1.58	0.86
14:2:114:MET:HE2	19:2:601:CLA:HMC2	1.57	0.86
4:D:109:LYS:HA	4:D:125:GLU:OE2	1.74	0.86
2:B:344:ILE:HD11	19:B:1225:CLA:HBC1	1.57	0.86
14:2:223:LYS:HZ1	19:2:607:CLA:C4D	1.89	0.86
8:H:103:LEU:HD13	12:L:143:ILE:HD13	1.58	0.85
19:A:1117:CLA:HMB1	19:A:1117:CLA:HBB1	1.58	0.85
7:G:148:ASN:OD1	7:G:150:TYR:N	2.08	0.85
1:A:401:TRP:CD1	19:A:1126:CLA:HAB	2.12	0.85
4:D:107:SER:CB	4:D:123:MET:HE3	2.06	0.85
17:P:19:LEU:HD23	17:P:96:VAL:CG2	2.06	0.85
1:A:178:MET:CE	19:A:1108:CLA:CMC	2.54	0.85
19:A:1140:CLA:HHC	19:A:1140:CLA:HBB1	1.57	0.85
22:F:4014:BCR:H331	22:F:4014:BCR:HC8	1.58	0.85
11:K:77:LYS:CD	11:K:87:ARG:NH1	2.39	0.85
15:3:229:LYS:HE2	19:3:607:CLA:HED1	1.59	0.85
14:2:223:LYS:NZ	19:2:607:CLA:C4D	2.40	0.85
2:B:559:CYS:SG	2:B:561:GLY:N	2.50	0.84
3:C:75:ARG:NH1	4:D:157:ARG:CZ	2.39	0.84
11:K:53:LEU:O	11:K:57:THR:HG22	1.77	0.84
19:B:1219:CLA:HBB1	19:B:1219:CLA:HMB1	1.60	0.84
8:H:126:LYS:HD2	8:H:126:LYS:C	2.02	0.84
11:K:77:LYS:HE3	11:K:87:ARG:NH1	1.91	0.84
19:A:1114:CLA:HHC	19:A:1114:CLA:HBB1	1.58	0.84
2:B:475:ASP:O	2:B:475:ASP:OD2	1.96	0.83
2:B:344:ILE:CD1	19:B:1225:CLA:HBC1	2.08	0.83
19:F:1301:CLA:HBB1	19:F:1301:CLA:HMB1	1.59	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:3:186:TYR:HA	15:3:191:GLU:OE2	1.78	0.83
7:G:148:ASN:ND2	7:G:150:TYR:HB3	1.91	0.83
15:3:94:GLU:OE1	15:3:97:TRP:N	2.11	0.83
16:4:112:PRO:O	16:4:116:THR:HG22	1.78	0.83
30:2:502:XAT:H8	30:2:502:XAT:H181	1.59	0.83
2:B:7:ARG:HH12	9:I:32:LEU:HD23	1.44	0.82
14:2:114:MET:CE	19:2:601:CLA:HHC	2.08	0.82
13:1:149:ARG:NH2	29:1:612:CHL:O1D	2.13	0.82
8:H:108:GLY:HA3	9:I:15:LEU:HD21	1.62	0.82
19:A:1113:CLA:HAA1	15:3:273:LYS:CE	1.99	0.82
11:K:62:MET:HE2	11:K:110:VAL:HG11	1.60	0.81
3:C:75:ARG:HH11	4:D:157:ARG:NH1	1.79	0.81
28:3:501:LUT:H373	19:3:601:CLA:H12	1.63	0.81
19:4:617:CLA:HBB1	19:4:617:CLA:HMB1	1.62	0.81
14:2:223:LYS:NZ	19:2:607:CLA:C3D	2.45	0.80
19:A:1109:CLA:HBB1	19:A:1109:CLA:HHC	1.64	0.80
14:2:114:MET:HE3	19:2:601:CLA:HHC	1.64	0.80
4:D:98:GLU:HA	4:D:98:GLU:OE2	1.80	0.80
19:L:1503:CLA:HBB1	19:L:1503:CLA:HMB1	1.63	0.80
1:A:377:TYR:CZ	19:A:1135:CLA:CBC	2.65	0.80
19:A:1111:CLA:HBB1	19:A:1111:CLA:HMB3	1.64	0.80
2:B:658:ALA:HB3	19:B:1023:CLA:HBB2	1.64	0.79
6:F:199:ASP:OD2	6:F:202:LEU:CB	2.30	0.79
19:B:1230:CLA:HBB1	19:B:1230:CLA:HMB3	1.64	0.79
22:A:4002:BCR:H331	22:A:4002:BCR:HC8	1.63	0.79
19:B:1206:CLA:HBB1	19:B:1206:CLA:HMB3	1.64	0.79
19:B:1220:CLA:HAB	19:B:1227:CLA:HMD2	1.65	0.79
22:H:4021:BCR:C38	12:L:203:LEU:HD21	2.13	0.79
22:A:4017:BCR:H331	22:A:4017:BCR:HC8	1.63	0.79
4:D:124:ARG:HH11	4:D:124:ARG:HG2	1.46	0.79
11:K:77:LYS:CE	11:K:87:ARG:NH1	2.46	0.79
8:H:120:GLY:CA	8:H:126:LYS:NZ	2.46	0.79
7:G:148:ASN:HD22	19:G:1603:CLA:HED2	1.48	0.79
10:J:16:THR:HG21	28:J:4013:LUT:C37	2.13	0.78
19:K:1402:CLA:HHC	19:K:1402:CLA:HBB1	1.66	0.78
1:A:57:LEU:HD21	19:A:1101:CLA:HBC2	1.65	0.78
1:A:178:MET:HA	1:A:178:MET:CE	2.12	0.78
19:A:1135:CLA:HMB1	19:A:1135:CLA:HBB1	1.64	0.78
17:P:26:THR:HG22	17:P:73:LYS:HG2	1.64	0.78
1:A:100:GLY:O	1:A:104:SER:OG	2.01	0.78
19:A:1119:CLA:H111	22:A:4007:BCR:H10C	1.66	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:73:LYS:O	5:E:127:GLU:OE1	2.02	0.77
4:D:139:LEU:HD13	4:D:139:LEU:O	1.85	0.77
8:H:103:LEU:HB3	12:L:143:ILE:CD1	2.11	0.77
2:B:7:ARG:NH1	9:I:32:LEU:HD23	2.00	0.77
1:A:322:GLY:O	11:K:87:ARG:NH2	2.17	0.77
3:C:7:ILE:HD12	3:C:40:ALA:HB3	1.67	0.76
2:B:79:GLN:OE1	2:B:79:GLN:HA	1.83	0.76
6:F:199:ASP:OD2	6:F:202:LEU:HB3	1.85	0.76
28:4:505:LUT:H8	28:4:505:LUT:H171	1.65	0.76
19:4:606:CLA:HBB1	19:4:606:CLA:HMB3	1.67	0.76
1:A:178:MET:HE1	19:A:1108:CLA:HMC1	1.64	0.76
9:I:2:ILE:HD12	9:I:3:ASN:N	2.01	0.75
4:D:107:SER:HB2	4:D:123:MET:CE	2.16	0.75
22:H:4021:BCR:H321	22:H:4021:BCR:HC8	1.68	0.75
3:C:75:ARG:NH1	4:D:157:ARG:NH1	2.34	0.75
19:A:1134:CLA:HHC	19:A:1134:CLA:HBB1	1.67	0.75
14:2:58:THR:OG1	14:2:80:SER:OG	1.66	0.75
7:G:148:ASN:OD1	7:G:149:GLY:N	2.20	0.75
1:A:593:SER:OG	1:A:596:ASP:OD1	2.05	0.74
19:B:1223:CLA:HBB1	19:B:1223:CLA:HMB3	1.67	0.74
12:L:70:GLU:HG3	12:L:75:SER:OG	1.88	0.74
19:3:602:CLA:HHC	19:3:602:CLA:HBB1	1.69	0.74
14:2:114:MET:HE2	19:2:601:CLA:CMC	2.18	0.74
4:D:169:PRO:HG3	4:D:174:TYR:CE1	2.23	0.74
17:P:19:LEU:HD23	17:P:96:VAL:HG23	1.68	0.74
6:F:95:GLU:HG2	6:F:130:PHE:CG	2.22	0.73
1:A:691:MET:HE3	19:A:1013:CLA:NA	2.03	0.73
19:B:1021:CLA:HBB1	19:B:1021:CLA:HMB1	1.70	0.73
19:B:1207:CLA:HHC	19:B:1207:CLA:HBB1	1.70	0.73
22:B:4005:BCR:H331	22:B:4005:BCR:HC8	1.70	0.73
19:A:1012:CLA:HAB	2:B:582:TRP:CH2	2.23	0.73
14:2:136:SER:OG	14:2:139:THR:OG1	2.07	0.73
19:3:608:CLA:HHC	19:3:608:CLA:HBB1	1.69	0.73
17:P:1:VAL:CG2	17:P:19:LEU:HD11	2.16	0.73
1:A:604:TRP:CH2	19:B:1022:CLA:HAB	2.23	0.73
22:B:4006:BCR:H321	22:B:4006:BCR:HC8	1.71	0.73
5:E:69:LYS:H	5:E:69:LYS:HD2	1.53	0.73
22:1:503:BCR:HC8	22:1:503:BCR:H321	1.69	0.73
2:B:503:GLU:OE1	2:B:505:SER:N	2.21	0.73
8:H:126:LYS:HD2	8:H:127:LYS:N	2.02	0.73
19:B:1215:CLA:HMB1	19:B:1215:CLA:HBB1	1.69	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:356:ALA:HB1	22:A:4007:BCR:H313	1.69	0.73
22:A:4003:BCR:H383	22:A:4003:BCR:H23C	1.69	0.73
17:P:46:ILE:HG13	17:P:47:PRO:HD2	1.71	0.73
7:G:107:ARG:NE	24:G:5004:LMT:O6'	2.22	0.72
22:3:506:BCR:H321	22:3:506:BCR:HC8	1.69	0.72
13:1:90:ALA:HB2	28:1:502:LUT:H392	1.71	0.72
19:1:606:CLA:HBB1	19:1:606:CLA:HMB3	1.68	0.72
2:B:61:THR:HG23	2:B:142:LEU:HD13	1.71	0.72
22:K:4001:BCR:HC8	22:K:4001:BCR:H321	1.69	0.72
16:4:109:MET:HE1	16:4:215:PHE:CD1	2.23	0.72
19:4:604:CLA:HBB1	19:4:604:CLA:HMB1	1.72	0.72
1:A:178:MET:CE	19:A:1108:CLA:HMC1	2.17	0.72
22:1:503:BCR:H403	22:1:503:BCR:H23C	1.72	0.72
19:A:1120:CLA:HMB1	19:A:1120:CLA:HBB1	1.72	0.72
22:H:4021:BCR:H383	12:L:203:LEU:HD21	1.72	0.72
13:1:89:LEU:HD22	19:1:601:CLA:HAC2	1.71	0.72
19:1:608:CLA:HHC	19:1:608:CLA:HBB1	1.72	0.72
19:B:1229:CLA:HBB1	19:B:1229:CLA:HMB1	1.72	0.71
14:2:223:LYS:HZ3	19:2:607:CLA:C3D	2.00	0.71
13:1:133:THR:O	13:1:137:ILE:HD12	1.90	0.71
17:P:76:ALA:HB3	17:P:80:TYR:OH	1.90	0.71
12:L:206:VAL:C	12:L:207:LEU:HD23	2.16	0.71
17:P:19:LEU:HD23	17:P:96:VAL:HG21	1.72	0.71
22:B:4009:BCR:H23C	22:B:4009:BCR:H403	1.72	0.71
7:G:124:ASN:O	7:G:128:VAL:HG13	1.89	0.71
28:4:501:LUT:H191	19:4:602:CLA:HMC2	1.73	0.71
2:B:65:LEU:HD11	22:B:4006:BCR:H292	1.71	0.71
15:3:117:ILE:HD12	15:3:252:PRO:HG2	1.73	0.71
22:A:4003:BCR:H321	22:A:4003:BCR:HC8	1.73	0.70
14:2:114:MET:HE1	19:2:601:CLA:CHC	2.20	0.70
28:J:4013:LUT:H181	28:J:4013:LUT:H8	1.74	0.70
17:P:55:ILE:HG22	17:P:72:VAL:HG21	1.72	0.70
2:B:284:PHE:HE1	19:B:1216:CLA:HAB	1.57	0.70
8:H:103:LEU:CB	12:L:143:ILE:HD11	2.15	0.70
19:A:1121:CLA:HHC	19:A:1121:CLA:HBB1	1.72	0.70
19:A:1122:CLA:H43	22:A:4008:BCR:H351	1.71	0.70
7:G:123:PHE:CE2	7:G:128:VAL:HG12	2.27	0.70
17:P:19:LEU:HB3	17:P:96:VAL:HG23	1.73	0.70
1:A:511:THR:HG21	19:A:1125:CLA:HAB	1.73	0.70
19:4:602:CLA:HHC	19:4:602:CLA:HBB1	1.74	0.70
15:3:174:GLN:HB3	15:3:182:MET:HE3	1.74	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:251:ASN:CG	1:A:253:ASP:OD1	2.34	0.69
15:3:188:LEU:HD11	22:3:503:BCR:H342	1.73	0.69
19:A:1110:CLA:HHC	19:A:1110:CLA:HBB1	1.75	0.69
19:A:1112:CLA:C1B	22:A:4002:BCR:H10C	2.22	0.69
12:L:199:TRP:CD2	22:L:4020:BCR:H10C	2.27	0.69
19:B:1229:CLA:O2A	22:F:4014:BCR:H362	1.93	0.69
19:3:613:CLA:HBB1	19:3:613:CLA:HMB3	1.75	0.69
19:B:1236:CLA:H43	22:B:4010:BCR:H10C	1.72	0.69
14:2:114:MET:CE	19:2:601:CLA:CHC	2.71	0.69
14:2:229:MET:HE1	19:2:604:CLA:HAB	1.74	0.69
19:A:1128:CLA:HBB1	19:A:1128:CLA:HMB3	1.75	0.68
13:1:53:GLY:N	13:1:58:ASP:OD2	2.26	0.68
1:A:596:ASP:OD2	1:A:731:ARG:NH1	2.26	0.68
22:B:4004:BCR:H403	22:B:4004:BCR:H23C	1.75	0.68
8:H:111:LEU:HD21	9:I:14:LEU:HD12	1.76	0.68
22:A:4011:BCR:HC8	22:A:4011:BCR:H331	1.75	0.68
19:B:1234:CLA:HMB1	19:B:1234:CLA:HBB1	1.74	0.68
19:B:1231:CLA:C4C	19:B:1232:CLA:HAB	2.24	0.68
22:K:4001:BCR:H382	22:K:4001:BCR:H23C	1.75	0.68
19:4:604:CLA:H3A	19:4:604:CLA:O1A	1.94	0.68
22:F:4014:BCR:H383	22:F:4014:BCR:H23C	1.76	0.68
4:D:76:ASP:OD2	4:D:77:PRO:O	2.12	0.68
22:H:4021:BCR:H382	22:H:4021:BCR:H23C	1.76	0.68
22:B:4010:BCR:H321	22:B:4010:BCR:HC8	1.74	0.68
4:D:134:ARG:NH2	4:D:136:GLU:OE1	2.27	0.68
22:1:504:BCR:H403	22:1:504:BCR:H23C	1.76	0.68
8:H:126:LYS:C	8:H:126:LYS:CD	2.66	0.67
2:B:475:ASP:OD2	2:B:475:ASP:C	2.36	0.67
4:D:129:LEU:C	4:D:129:LEU:HD23	2.19	0.67
15:3:94:GLU:CD	15:3:96:ARG:H	2.02	0.67
22:3:503:BCR:H321	22:3:503:BCR:HC8	1.74	0.67
12:L:204:LEU:HD21	19:L:1503:CLA:CED	2.16	0.67
1:A:310:PHE:HE1	19:A:1119:CLA:HAB	1.59	0.67
1:A:476:MET:CE	1:A:647:ILE:HD12	2.24	0.67
3:C:18:VAL:CG2	3:C:28:MET:HE3	2.24	0.67
1:A:465:ASP:OD1	2:B:635:TYR:OH	2.04	0.67
19:A:1138:CLA:HAB	19:A:1138:CLA:H111	1.76	0.67
19:A:1101:CLA:HMB3	19:A:1101:CLA:HBB1	1.77	0.67
11:K:77:LYS:CD	11:K:87:ARG:CZ	2.74	0.66
5:E:127:GLU:OE1	5:E:127:GLU:HA	1.94	0.66
7:G:64:ILE:HD11	7:G:140:TYR:CE2	2.31	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:112:HIS:HD2	22:K:4002:BCR:H353	1.61	0.66
19:A:1102:CLA:HAB	19:A:1104:CLA:CAD	2.26	0.66
2:B:658:ALA:CB	19:B:1023:CLA:HBB2	2.25	0.66
19:B:1231:CLA:HMB1	19:B:1231:CLA:HBB1	1.76	0.66
28:1:501:LUT:C28	28:1:501:LUT:H381	2.25	0.66
2:B:656:VAL:HG22	19:B:1239:CLA:HMB2	1.77	0.66
16:4:67:THR:HG22	16:4:67:THR:O	1.96	0.66
2:B:577:TYR:OH	2:B:664:LEU:HD22	1.96	0.66
7:G:119:ASP:OD1	7:G:123:PHE:HB3	1.96	0.66
13:1:85:ARG:HB3	19:1:601:CLA:HBC3	1.77	0.66
16:4:114:VAL:HG12	16:4:230:PHE:CD1	2.29	0.66
1:A:469:ALA:O	2:B:640:MET:HE3	1.96	0.66
15:3:262:ASP:CG	15:3:263:PRO:HD2	2.21	0.66
17:P:26:THR:HB	17:P:73:LYS:HA	1.78	0.66
1:A:684:PHE:CG	22:A:4011:BCR:H363	2.30	0.65
11:K:77:LYS:HD3	11:K:87:ARG:NH1	2.11	0.65
14:2:158:VAL:HG13	14:2:159:PHE:HD2	1.61	0.65
28:3:501:LUT:H371	28:3:501:LUT:H28	1.77	0.65
22:J:4012:BCR:H382	22:J:4012:BCR:H23C	1.76	0.65
1:A:310:PHE:CE1	19:A:1119:CLA:HAB	2.31	0.65
22:G:4011:BCR:H403	22:G:4011:BCR:H23C	1.78	0.65
11:K:77:LYS:HD3	11:K:87:ARG:CZ	2.27	0.65
1:A:400:MET:HE1	19:A:1124:CLA:HMD1	1.77	0.65
2:B:451:LYS:HD3	10:J:35:ASP:OD2	1.95	0.64
9:I:2:ILE:HD12	9:I:3:ASN:H	1.61	0.64
11:K:77:LYS:HD3	11:K:87:ARG:HD3	1.80	0.64
22:K:4001:BCR:C3	15:3:273:LYS:NZ	2.60	0.64
12:L:204:LEU:O	12:L:206:VAL:N	2.31	0.64
19:B:1217:CLA:HHC	19:B:1217:CLA:HBB1	1.79	0.64
13:1:94:ILE:HD11	28:1:502:LUT:H373	1.80	0.64
1:A:124:TRP:HB3	28:J:4013:LUT:H183	1.79	0.64
2:B:669:GLY:O	2:B:673:GLU:HG3	1.98	0.64
22:1:503:BCR:H362	16:4:152:VAL:HG21	1.79	0.64
28:4:501:LUT:H371	28:4:501:LUT:H28	1.78	0.64
14:2:200:TRP:CE2	29:2:615:CHL:C1D	2.81	0.64
8:H:51:LYS:HG3	8:H:52:SER:N	2.04	0.64
13:1:173:ASP:C	13:1:173:ASP:OD1	2.40	0.64
19:1:614:CLA:HHC	19:1:614:CLA:HBB1	1.80	0.64
14:2:200:TRP:CH2	29:2:615:CHL:C1C	2.81	0.64
29:3:604:CHL:H93	29:3:604:CHL:H52	1.80	0.64
19:3:612:CLA:HBB1	19:3:612:CLA:HMB3	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:P:80:TYR:HB2	17:P:96:VAL:HG12	1.80	0.64
11:K:77:LYS:HE3	11:K:87:ARG:HH12	1.62	0.64
6:F:199:ASP:OD2	6:F:202:LEU:HB2	1.98	0.64
14:2:223:LYS:HZ3	19:2:607:CLA:CAD	2.12	0.63
1:A:498:LEU:O	1:A:502:THR:OG1	2.16	0.63
19:B:1205:CLA:HAB	19:B:1206:CLA:O1A	1.98	0.63
2:B:390:GLY:HA2	22:B:4010:BCR:H393	1.80	0.63
3:C:75:ARG:HH12	4:D:157:ARG:CZ	2.11	0.63
13:1:58:ASP:C	13:1:58:ASP:OD1	2.40	0.63
29:2:610:CHL:HBB1	29:2:610:CHL:HMB1	1.81	0.63
16:4:103:MET:HE3	19:4:601:CLA:HMC3	1.79	0.63
1:A:96:MET:HG3	1:A:149:PHE:CZ	2.34	0.63
22:K:4001:BCR:C3	15:3:273:LYS:HZ1	2.09	0.63
28:4:505:LUT:H371	28:4:505:LUT:H28	1.81	0.63
22:H:4021:BCR:H381	12:L:203:LEU:HD21	1.80	0.62
19:A:1137:CLA:HHC	19:A:1137:CLA:HBB1	1.81	0.62
22:I:4020:BCR:H23C	22:I:4020:BCR:H392	1.79	0.62
1:A:183:TRP:HB2	19:A:1109:CLA:HMC2	1.80	0.62
10:J:12:PRO:O	10:J:16:THR:HG22	1.98	0.62
14:2:177:VAL:CG2	29:2:611:CHL:OMC	2.45	0.62
15:3:110:MET:SD	19:3:601:CLA:HAB	2.40	0.62
17:P:55:ILE:CG2	17:P:72:VAL:CG2	2.69	0.62
8:H:78:TYR:OH	19:L:1501:CLA:O1D	2.07	0.62
7:G:70:LEU:HD21	13:1:140:LEU:HD11	1.80	0.62
22:3:503:BCR:H373	19:3:613:CLA:H3A	1.81	0.62
7:G:125:ILE:O	7:G:128:VAL:HG22	2.00	0.62
19:B:1202:CLA:HHC	19:B:1202:CLA:HBB1	1.82	0.62
22:I:4018:BCR:HC8	22:I:4018:BCR:H321	1.82	0.62
19:3:610:CLA:HMB1	19:3:610:CLA:HBB1	1.80	0.62
19:B:1223:CLA:HBB1	19:B:1223:CLA:CMB	2.30	0.62
11:K:91:LEU:CD1	15:3:59:PHE:HE1	2.07	0.62
13:1:78:GLU:OE1	13:1:158:LYS:HG2	1.99	0.62
22:3:503:BCR:H19C	22:3:506:BCR:H342	1.81	0.62
22:3:503:BCR:H402	19:3:606:CLA:C1B	2.30	0.62
14:2:196:PRO:HB3	29:2:611:CHL:HBC2	1.81	0.61
15:3:74:GLY:H	15:3:225:LEU:CD2	2.13	0.61
11:K:62:MET:HE2	11:K:110:VAL:CG1	2.28	0.61
19:K:1403:CLA:HHC	19:K:1403:CLA:HBB1	1.82	0.61
1:A:241:GLU:N	1:A:241:GLU:OE1	2.33	0.61
15:3:152:ALA:HB3	15:3:157:LEU:HG	1.82	0.61
2:B:559:CYS:SG	2:B:560:ASP:N	2.74	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:2:503:BCR:H311	22:2:503:BCR:HC8	1.83	0.61
3:C:14:CYS:O	3:C:15:THR:OG1	2.11	0.61
22:L:4019:BCR:HC8	22:L:4019:BCR:H331	1.82	0.61
7:G:138:VAL:HG23	25:G:5002:LMG:H212	1.82	0.61
1:A:205:HIS:O	1:A:209:GLY:N	2.33	0.61
2:B:344:ILE:HD11	19:B:1225:CLA:CBC	2.30	0.61
4:D:81:SER:O	4:D:124:ARG:HD2	2.01	0.61
14:2:170:ASP:OD2	29:2:611:CHL:HBC1	2.00	0.61
1:A:124:TRP:CB	28:J:4013:LUT:H183	2.31	0.60
10:J:16:THR:HG21	28:J:4013:LUT:H372	1.82	0.60
28:J:4013:LUT:H28	28:J:4013:LUT:H361	1.83	0.60
8:H:48:TYR:CE2	8:H:54:TYR:HA	2.36	0.60
14:2:168:TRP:CD2	19:2:612:CLA:HMA2	2.37	0.60
15:3:94:GLU:OE1	15:3:94:GLU:C	2.44	0.60
16:4:106:VAL:HA	16:4:109:MET:HE3	1.82	0.60
6:F:179:ARG:HD2	22:F:4016:BCR:H401	1.83	0.60
12:L:204:LEU:HB2	12:L:205:TYR:CD2	2.37	0.60
2:B:411:MET:HE2	22:B:4009:BCR:H393	1.83	0.60
19:A:1107:CLA:HBB1	19:A:1107:CLA:HMB3	1.82	0.60
5:E:96:ASP:OD2	5:E:96:ASP:C	2.42	0.60
14:2:95:ASP:HB3	14:2:98:SER:HB3	1.83	0.60
15:3:94:GLU:OE2	15:3:96:ARG:N	2.29	0.60
19:3:607:CLA:HHC	19:3:607:CLA:HBB1	1.82	0.60
29:4:610:CHL:HBC3	29:4:610:CHL:HHH	1.82	0.60
8:H:108:GLY:CA	9:I:15:LEU:HD11	2.32	0.60
7:G:148:ASN:OD1	7:G:148:ASN:C	2.44	0.60
13:1:173:ASP:OD1	13:1:175:LYS:HG3	2.01	0.60
22:A:4017:BCR:H331	22:A:4017:BCR:C8	2.31	0.60
2:B:430:GLY:HA2	2:B:525:LEU:HD22	1.83	0.60
13:1:61:PHE:CZ	28:1:502:LUT:H162	2.37	0.60
15:3:185:GLN:O	15:3:191:GLU:HG2	2.02	0.60
22:A:4011:BCR:H23C	22:A:4011:BCR:H382	1.83	0.60
3:C:18:VAL:HG21	3:C:28:MET:HE3	1.83	0.59
17:P:59:GLU:O	17:P:59:GLU:HG2	2.01	0.59
27:F:5005:DGD:HB82	27:F:5005:DGD:HAT2	1.84	0.59
28:1:501:LUT:H381	28:1:501:LUT:H28	1.83	0.59
1:A:316:MET:HG3	19:A:1121:CLA:C3C	2.32	0.59
19:A:1125:CLA:HMB1	19:A:1125:CLA:HBB1	1.83	0.59
22:A:4008:BCR:H382	22:A:4008:BCR:H23C	1.84	0.59
5:E:95:GLN:HA	5:E:95:GLN:NE2	2.18	0.59
28:J:4013:LUT:H361	28:J:4013:LUT:C28	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:3:117:ILE:CD1	15:3:252:PRO:HG2	2.32	0.59
15:3:269:LEU:C	15:3:269:LEU:HD23	2.27	0.59
16:4:247:GLN:OE1	16:4:247:GLN:N	2.34	0.59
1:A:687:ALA:HB3	19:A:1013:CLA:HBB2	1.84	0.59
19:B:1203:CLA:HMB1	19:B:1203:CLA:HBB1	1.85	0.59
8:H:120:GLY:CA	8:H:126:LYS:HZ2	1.94	0.59
4:D:174:TYR:HB3	4:D:176:GLU:OE1	2.03	0.59
2:B:607:SER:O	2:B:611:GLU:OE1	2.21	0.59
11:K:110:VAL:O	11:K:114:ILE:HG23	2.02	0.59
15:3:94:GLU:CD	15:3:96:ARG:N	2.60	0.59
19:A:1112:CLA:NB	22:A:4002:BCR:H10C	2.17	0.59
19:B:1022:CLA:OBD	19:B:1021:CLA:HMB3	2.03	0.59
8:H:72:SER:OG	12:L:84:SER:O	2.21	0.59
13:1:220:ASP:OD1	13:1:220:ASP:O	2.21	0.59
29:3:604:CHL:HMB3	29:3:604:CHL:HBB1	1.84	0.59
16:4:93:GLN:O	16:4:97:VAL:HG23	2.02	0.59
2:B:444:LEU:HD12	2:B:615:TYR:CG	2.38	0.58
19:B:1205:CLA:HHC	19:B:1205:CLA:HBB1	1.84	0.58
19:B:1223:CLA:C4B	19:B:1231:CLA:HMA3	2.33	0.58
19:A:1110:CLA:C1A	19:A:1110:CLA:CGA	2.81	0.58
7:G:148:ASN:ND2	19:G:1603:CLA:HED2	2.15	0.58
16:4:106:VAL:HG12	16:4:218:PHE:CE2	2.39	0.58
14:2:132:LEU:CD1	14:2:134:THR:HG23	2.32	0.58
15:3:94:GLU:OE2	15:3:96:ARG:HB2	2.02	0.58
17:P:1:VAL:HG21	17:P:19:LEU:CD1	2.20	0.58
28:1:501:LUT:H362	19:1:611:CLA:C4	2.33	0.58
4:D:124:ARG:HG2	4:D:124:ARG:NH1	2.14	0.58
14:2:81:LEU:HD22	14:2:81:LEU:H	1.68	0.58
22:2:503:BCR:H23C	22:2:503:BCR:H402	1.85	0.58
17:P:16:PRO:N	17:P:16:PRO:C	2.57	0.58
19:A:1114:CLA:HHC	19:A:1114:CLA:CBB	2.32	0.58
2:B:7:ARG:NH1	9:I:32:LEU:CD2	2.66	0.58
19:A:1111:CLA:HBB1	19:A:1111:CLA:CMB	2.33	0.58
22:I:4018:BCR:H382	22:I:4018:BCR:H23C	1.85	0.58
12:L:155:GLU:H	12:L:155:GLU:CD	2.04	0.58
19:B:1209:CLA:HBB1	19:B:1209:CLA:HMB1	1.86	0.58
24:G:5004:LMT:O3'	24:G:5004:LMT:O5B	2.21	0.58
19:4:604:CLA:H3A	19:4:604:CLA:CGA	2.34	0.58
2:B:390:GLY:CA	22:B:4010:BCR:H393	2.33	0.57
8:H:108:GLY:HA2	9:I:15:LEU:HD11	1.86	0.57
11:K:112:HIS:CD2	22:K:4002:BCR:H353	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:1:502:LUT:H371	28:1:502:LUT:H28	1.86	0.57
14:2:158:VAL:HG13	14:2:159:PHE:CD2	2.39	0.57
1:A:283:PHE:CE2	19:A:1116:CLA:HBB1	2.40	0.57
1:A:686:TRP:CE3	18:A:1011:CL0:H6	2.39	0.57
22:J:4012:BCR:H321	22:J:4012:BCR:HC8	1.86	0.57
14:2:116:GLY:O	14:2:120:ILE:HG13	2.04	0.57
25:A:5006:LMG:H211	25:A:5006:LMG:H171	1.86	0.57
30:2:502:XAT:H171	19:2:606:CLA:HMB2	1.85	0.57
1:A:251:ASN:ND2	1:A:253:ASP:OD1	2.37	0.57
2:B:65:LEU:HD11	22:B:4006:BCR:C29	2.34	0.57
5:E:127:GLU:OE1	5:E:127:GLU:CA	2.51	0.57
19:2:608:CLA:HHC	19:2:608:CLA:HBB1	1.85	0.57
2:B:657:TRP:CD2	19:B:1021:CLA:HMA2	2.40	0.57
10:J:16:THR:HG21	28:J:4013:LUT:H371	1.87	0.57
15:3:235:MET:HG3	28:3:502:LUT:C34	2.34	0.57
19:B:1221:CLA:HMB1	19:B:1221:CLA:HBB1	1.86	0.57
28:3:502:LUT:H381	28:3:502:LUT:H28	1.87	0.57
1:A:216:LEU:HD11	22:K:4001:BCR:H10C	1.86	0.57
1:A:252:ARG:NH1	1:A:262:PHE:O	2.38	0.57
19:B:1231:CLA:CHD	19:B:1232:CLA:HAB	2.33	0.57
22:F:4016:BCR:H331	22:F:4016:BCR:HC8	1.85	0.57
1:A:476:MET:HE2	1:A:647:ILE:HD12	1.85	0.57
3:C:27:GLU:O	3:C:28:MET:HE2	2.05	0.57
4:D:109:LYS:CA	4:D:125:GLU:OE2	2.51	0.57
8:H:48:TYR:HE2	8:H:54:TYR:HA	1.70	0.57
15:3:188:LEU:HD12	22:3:503:BCR:C34	2.31	0.57
4:D:169:PRO:HG3	4:D:174:TYR:HE1	1.70	0.57
17:P:58:PRO:C	17:P:60:GLU:H	2.11	0.57
2:B:444:LEU:HD21	2:B:449:PRO:HB3	1.86	0.56
3:C:55:GLU:OE1	3:C:67:VAL:N	2.36	0.56
15:3:256:LEU:HD22	28:3:501:LUT:H172	1.85	0.56
17:P:46:ILE:CG1	17:P:47:PRO:HD2	2.33	0.56
1:A:511:THR:HG23	19:A:1116:CLA:O1A	2.05	0.56
2:B:444:LEU:CD2	2:B:449:PRO:HB3	2.35	0.56
22:B:4005:BCR:H382	22:B:4005:BCR:H23C	1.86	0.56
6:F:143:ASP:OD2	6:F:143:ASP:N	2.35	0.56
22:H:4021:BCR:H321	22:H:4021:BCR:C8	2.36	0.56
19:2:602:CLA:HHC	19:2:602:CLA:HBB1	1.87	0.56
19:3:603:CLA:HHC	19:3:603:CLA:CBB	2.31	0.56
1:A:376:MET:HE1	19:A:1127:CLA:O1D	2.05	0.56
1:A:688:PHE:HZ	19:A:1140:CLA:HBC2	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:B:1239:CLA:HHC	19:B:1239:CLA:CBB	2.31	0.56
19:1:603:CLA:HHC	19:1:603:CLA:CBB	2.32	0.56
28:4:501:LUT:H373	19:4:601:CLA:C1	2.33	0.56
19:4:603:CLA:HHC	19:4:603:CLA:CBB	2.34	0.56
19:A:1013:CLA:HMB1	19:A:1013:CLA:HBB1	1.88	0.56
19:A:1104:CLA:H151	19:A:1127:CLA:HBB2	1.86	0.56
19:B:1236:CLA:HBB1	19:B:1236:CLA:HMB1	1.85	0.56
19:B:1229:CLA:HBB1	19:B:1229:CLA:CMB	2.34	0.56
14:2:139:THR:O	14:2:143:GLN:NE2	2.35	0.56
19:3:608:CLA:HHC	19:3:608:CLA:CBB	2.35	0.56
1:A:216:LEU:CD1	22:K:4001:BCR:H10C	2.35	0.56
19:A:1139:CLA:O1D	6:F:195:GLU:HG2	2.05	0.56
14:2:229:MET:HE1	19:2:604:CLA:CAB	2.36	0.56
15:3:187:PHE:CE2	22:3:503:BCR:H343	2.40	0.56
28:3:502:LUT:C8	28:3:502:LUT:H181	2.36	0.56
28:4:501:LUT:H371	19:4:601:CLA:H71	1.88	0.56
19:B:1222:CLA:HMB1	19:B:1222:CLA:HBB1	1.87	0.56
1:A:434:ARG:O	1:A:438:HIS:ND1	2.38	0.56
19:A:1138:CLA:HBB1	19:A:1138:CLA:HMB1	1.87	0.56
2:B:22:TRP:HE1	19:B:1238:CLA:HBB1	1.71	0.56
28:3:502:LUT:H161	19:3:613:CLA:HAB	1.88	0.56
2:B:476:VAL:HG12	2:B:477:LEU:H	1.71	0.55
19:B:1220:CLA:HMD3	19:B:1221:CLA:HAB	1.87	0.55
15:3:166:GLY:CA	19:3:612:CLA:CBB	2.84	0.55
28:3:502:LUT:H381	28:3:502:LUT:C28	2.35	0.55
22:B:4006:BCR:H321	22:B:4006:BCR:C8	2.36	0.55
8:H:108:GLY:HA2	9:I:15:LEU:CD1	2.36	0.55
15:3:120:GLU:CD	15:3:253:TYR:HB3	2.32	0.55
15:3:266:ASN:OD1	15:3:267:ASN:N	2.39	0.55
19:A:1134:CLA:HHC	19:A:1134:CLA:CBB	2.37	0.55
19:B:1206:CLA:HBB1	19:B:1206:CLA:CMB	2.34	0.55
17:P:1:VAL:HG11	17:P:19:LEU:HD21	1.89	0.55
1:A:37:PRO:HA	19:A:1101:CLA:HBC1	1.89	0.55
19:A:1135:CLA:HBB1	19:A:1135:CLA:CMB	2.35	0.55
15:3:94:GLU:CD	15:3:94:GLU:C	2.75	0.55
19:B:1205:CLA:C1A	19:B:1205:CLA:CGA	2.85	0.55
22:B:4010:BCR:H383	22:B:4010:BCR:H23C	1.87	0.55
10:J:26:LEU:CB	22:J:4012:BCR:H343	2.37	0.55
28:3:501:LUT:C30	22:3:506:BCR:H363	2.37	0.55
15:3:117:ILE:CD1	15:3:252:PRO:HB2	2.37	0.55
7:G:77:PHE:CE2	19:G:1602:CLA:HAB	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:3:229:LYS:HE2	19:3:607:CLA:CED	2.33	0.55
30:4:502:XAT:H183	19:4:606:CLA:C2B	2.36	0.55
19:4:607:CLA:HHC	19:4:607:CLA:HBB1	1.89	0.55
1:A:178:MET:CA	1:A:178:MET:CE	2.78	0.55
19:A:1109:CLA:H192	28:J:4013:LUT:H381	1.87	0.55
19:A:1122:CLA:HHC	19:A:1122:CLA:CBB	2.30	0.55
22:K:4002:BCR:H321	22:K:4002:BCR:HC8	1.89	0.55
19:A:1112:CLA:HMB1	19:A:1112:CLA:HBB1	1.89	0.54
19:B:1023:CLA:HMA3	19:B:1023:CLA:H2	1.88	0.54
4:D:193:GLY:HA3	5:E:80:GLU:OE2	2.06	0.54
11:K:58:SER:HB2	11:K:114:ILE:CD1	2.29	0.54
17:P:38:ASN:OD1	17:P:39:VAL:N	2.40	0.54
3:C:55:GLU:OE1	3:C:66:ARG:HA	2.07	0.54
9:I:14:LEU:CD2	22:I:4018:BCR:H351	2.37	0.54
19:1:608:CLA:HHC	19:1:608:CLA:CBB	2.37	0.54
19:1:611:CLA:HMB3	19:1:611:CLA:HBB1	1.90	0.54
19:B:1208:CLA:HHC	19:B:1208:CLA:CBB	2.33	0.54
28:J:4013:LUT:H8	28:J:4013:LUT:C18	2.37	0.54
1:A:552:THR:HG21	19:A:1124:CLA:HBC3	1.88	0.54
13:1:133:THR:C	13:1:137:ILE:HD12	2.32	0.54
22:3:506:BCR:H321	22:3:506:BCR:C8	2.36	0.54
17:P:21:VAL:HG22	17:P:22:SER:N	2.23	0.54
1:A:377:TYR:HH	19:A:1135:CLA:CBC	2.14	0.54
19:K:1402:CLA:HHC	19:K:1402:CLA:CBB	2.36	0.54
19:A:1127:CLA:HBB1	19:A:1127:CLA:HMB1	1.90	0.54
11:K:115:GLY:O	11:K:119:VAL:HG12	2.08	0.54
12:L:206:VAL:O	12:L:207:LEU:HD23	2.06	0.54
14:2:107:LEU:HD22	14:2:111:ARG:NH1	2.23	0.54
22:A:4002:BCR:H382	22:A:4002:BCR:H23C	1.89	0.54
2:B:39:GLU:HG2	2:B:165:VAL:HG11	1.89	0.54
22:B:4009:BCR:H403	22:B:4009:BCR:C23	2.36	0.54
14:2:121:PHE:CD1	28:2:501:LUT:H373	2.42	0.54
2:B:221:GLY:O	24:B:5008:LMT:O2B	2.21	0.54
2:B:317:ARG:NH2	2:B:320:LYS:HD2	2.23	0.54
2:B:320:LYS:HB2	2:B:320:LYS:NZ	2.22	0.54
22:L:4019:BCR:H392	22:L:4019:BCR:H23C	1.90	0.54
14:2:219:THR:HG22	14:2:223:LYS:HD2	1.88	0.54
15:3:153:ASP:O	15:3:154:ASN:HB3	2.08	0.54
28:1:501:LUT:H8	28:1:501:LUT:H171	1.90	0.54
1:A:380:PRO:HG2	1:A:386:ALA:HB2	1.90	0.53
22:A:4007:BCR:H23C	22:A:4007:BCR:H382	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:109:LYS:HD3	7:G:110:GLU:O	2.08	0.53
15:3:59:PHE:O	15:3:59:PHE:CD1	2.61	0.53
19:A:1138:CLA:HAA2	19:B:1228:CLA:HMB2	1.91	0.53
6:F:124:GLU:OE2	6:F:124:GLU:HA	2.08	0.53
7:G:148:ASN:CG	7:G:150:TYR:H	2.10	0.53
28:3:501:LUT:H371	19:3:601:CLA:H61	1.89	0.53
1:A:707:ILE:HD13	1:A:707:ILE:N	2.23	0.53
6:F:189:LYS:HD2	6:F:190:LYS:HG2	1.89	0.53
22:3:503:BCR:H321	22:3:503:BCR:C8	2.37	0.53
19:3:606:CLA:HMA2	19:3:613:CLA:C3C	2.38	0.53
2:B:428:PHE:CE1	19:B:1235:CLA:HAB	2.44	0.53
13:1:133:THR:O	13:1:134:ILE:C	2.50	0.53
15:3:94:GLU:OE2	15:3:96:ARG:CB	2.56	0.53
19:4:601:CLA:HMB1	19:4:601:CLA:HBB1	1.90	0.53
2:B:93:ASP:OD1	2:B:95:HIS:ND1	2.42	0.53
3:C:2:SER:N	3:C:71:HIS:O	2.41	0.53
4:D:83:ILE:CD1	4:D:124:ARG:NH2	2.72	0.53
14:2:225:GLY:O	14:2:229:MET:HG3	2.09	0.53
19:2:607:CLA:HBB1	22:3:503:BCR:HC41	1.91	0.53
1:A:272:LEU:CD1	11:K:119:VAL:HG11	2.38	0.53
8:H:108:GLY:CA	9:I:15:LEU:HD21	2.38	0.53
22:K:4001:BCR:H321	22:K:4001:BCR:C8	2.36	0.53
19:2:603:CLA:HHC	19:2:603:CLA:CBB	2.34	0.53
16:4:67:THR:O	16:4:67:THR:CG2	2.57	0.53
2:B:257:LEU:HD22	19:B:1214:CLA:HBB1	1.91	0.53
19:B:1203:CLA:HBB1	19:B:1203:CLA:CMB	2.39	0.53
16:4:241:TRP:CZ3	19:4:608:CLA:HMA2	2.44	0.53
1:A:451:ILE:HD11	22:A:4017:BCR:H402	1.90	0.52
29:1:610:CHL:HBB2	19:1:613:CLA:HBB2	1.90	0.52
19:3:602:CLA:HHC	19:3:602:CLA:CBB	2.37	0.52
1:A:387:THR:HG21	1:A:523:VAL:HB	1.90	0.52
11:K:111:GLY:O	11:K:114:ILE:HG13	2.09	0.52
29:1:609:CHL:HED1	16:4:155:ARG:HA	1.91	0.52
14:2:182:ILE:CD1	19:4:607:CLA:HAB	2.39	0.52
17:P:51:ASP:OD2	17:P:54:LYS:CG	2.51	0.52
2:B:142:LEU:CD1	22:B:4006:BCR:H402	2.39	0.52
19:B:1219:CLA:HMB1	19:B:1219:CLA:CBB	2.37	0.52
19:B:1232:CLA:O1A	19:G:1603:CLA:HHB	2.10	0.52
19:1:603:CLA:CGA	19:1:603:CLA:C1A	2.88	0.52
19:B:1234:CLA:HBB1	19:B:1234:CLA:CMB	2.39	0.52
19:B:1216:CLA:HMB1	19:B:1216:CLA:HBB1	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:B:1227:CLA:H122	19:B:1227:CLA:H202	1.92	0.52
19:K:1403:CLA:HHC	19:K:1403:CLA:CBB	2.39	0.52
13:1:141:SER:HB2	22:1:504:BCR:H363	1.91	0.52
17:P:21:VAL:HG22	17:P:22:SER:O	2.10	0.52
1:A:272:LEU:HD13	11:K:119:VAL:HG11	1.91	0.52
1:A:476:MET:CE	1:A:647:ILE:CD1	2.87	0.52
28:4:501:LUT:C19	19:4:602:CLA:HMC2	2.40	0.52
22:B:4010:BCR:H321	22:B:4010:BCR:C8	2.39	0.52
22:L:4020:BCR:H331	22:L:4020:BCR:C8	2.29	0.52
22:1:503:BCR:H321	22:1:503:BCR:C8	2.38	0.52
15:3:94:GLU:OE1	15:3:96:ARG:N	2.43	0.52
19:A:1120:CLA:HBB1	19:A:1120:CLA:CMB	2.40	0.52
10:J:26:LEU:HB3	22:J:4012:BCR:H343	1.92	0.52
13:1:53:GLY:CA	13:1:58:ASP:OD2	2.58	0.52
15:3:93:ILE:O	15:3:93:ILE:HG22	2.10	0.52
19:4:606:CLA:HBB1	19:4:606:CLA:CMB	2.38	0.52
14:2:200:TRP:HE1	29:2:615:CHL:C4D	2.22	0.51
15:3:225:LEU:HD13	15:3:225:LEU:O	2.09	0.51
28:3:501:LUT:H191	19:3:602:CLA:HMC3	1.92	0.51
19:B:1228:CLA:HMB3	19:B:1228:CLA:HBB1	1.93	0.51
22:K:4002:BCR:HC8	22:K:4002:BCR:H311	1.91	0.51
1:A:217:SER:OG	22:A:4002:BCR:H16C	2.11	0.51
4:D:169:PRO:HG3	4:D:174:TYR:CD1	2.44	0.51
8:H:120:GLY:CA	8:H:126:LYS:HZ1	2.22	0.51
22:3:506:BCR:H403	22:3:506:BCR:H23C	1.91	0.51
19:3:610:CLA:HBB1	19:3:610:CLA:CMB	2.40	0.51
1:A:670:SER:HB3	17:P:60:GLU:OE2	2.09	0.51
19:B:1215:CLA:CGA	19:B:1215:CLA:H3A	2.40	0.51
19:B:1220:CLA:HAB	19:B:1227:CLA:CMD	2.38	0.51
19:B:1226:CLA:HMB3	19:B:1226:CLA:HBB1	1.92	0.51
22:B:4004:BCR:H403	22:B:4004:BCR:C23	2.41	0.51
4:D:199:ILE:HG23	4:D:200:GLU:OE1	2.11	0.51
7:G:64:ILE:HD11	7:G:140:TYR:CZ	2.46	0.51
19:3:607:CLA:HHC	19:3:607:CLA:CBB	2.40	0.51
17:P:51:ASP:OD2	17:P:51:ASP:C	2.53	0.51
18:A:1011:CL0:H13	19:A:1012:CLA:OBD	2.10	0.51
19:A:1131:CLA:HBB1	19:A:1132:CLA:H2	1.92	0.51
2:B:411:MET:CE	22:B:4009:BCR:H393	2.40	0.51
12:L:63:ASP:OD2	12:L:66:ILE:HG12	2.10	0.51
9:I:30:LYS:NZ	9:I:32:LEU:HD12	2.25	0.51
13:1:53:GLY:HA2	13:1:58:ASP:OD2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:2:502:XAT:H28	19:2:604:CLA:H71	1.93	0.51
17:P:74:LEU:HD22	17:P:80:TYR:CE2	2.46	0.51
1:A:457:SER:OG	1:A:544:ILE:HD13	2.10	0.51
19:A:1112:CLA:HBB1	19:A:1112:CLA:CMB	2.40	0.51
4:D:139:LEU:HD13	4:D:139:LEU:C	2.36	0.51
28:J:4013:LUT:H28	28:J:4013:LUT:H371	1.92	0.51
14:2:114:MET:CE	19:2:601:CLA:CMC	2.87	0.51
14:2:200:TRP:CE2	29:2:615:CHL:ND	2.75	0.51
28:2:501:LUT:H28	28:2:501:LUT:H361	1.93	0.51
4:D:108:PRO:O	4:D:125:GLU:OE2	2.29	0.51
15:3:248:THR:HG22	15:3:250:VAL:HG22	1.92	0.51
19:4:604:CLA:HBB1	19:4:604:CLA:CMB	2.41	0.51
2:B:444:LEU:CD1	2:B:615:TYR:CD1	2.94	0.51
13:1:220:ASP:OD1	13:1:220:ASP:C	2.53	0.51
19:A:1106:CLA:HBB1	19:A:1106:CLA:HMB3	1.93	0.50
22:A:4017:BCR:H343	19:B:1022:CLA:H202	1.93	0.50
19:A:1101:CLA:HBB1	19:A:1101:CLA:CMB	2.40	0.50
2:B:687:LEU:HD12	19:L:1502:CLA:H11	1.93	0.50
19:J:1901:CLA:HHC	19:J:1901:CLA:CBB	2.33	0.50
13:1:89:LEU:HD22	19:1:601:CLA:CBC	2.41	0.50
1:A:283:PHE:CD2	19:A:1116:CLA:HBB1	2.46	0.50
19:A:1109:CLA:HHC	19:A:1109:CLA:CBB	2.39	0.50
19:A:1110:CLA:HHC	19:A:1110:CLA:CBB	2.41	0.50
19:B:1218:CLA:HHC	19:B:1218:CLA:HBB1	1.94	0.50
6:F:162:THR:CG2	6:F:163:PRO:HD3	2.41	0.50
13:1:89:LEU:HD22	19:1:601:CLA:CAC	2.39	0.50
13:1:146:GLU:OE1	13:1:149:ARG:NH1	2.44	0.50
28:1:502:LUT:H193	19:1:604:CLA:H13	1.93	0.50
1:A:88:ILE:HG13	19:A:1102:CLA:HBB1	1.92	0.50
2:B:716:GLY:O	2:B:720:THR:HG22	2.12	0.50
2:B:189:ALA:HB1	19:B:1211:CLA:HAB	1.92	0.50
24:G:5004:LMT:O6B	24:G:5004:LMT:O4'	2.16	0.50
17:P:58:PRO:C	17:P:60:GLU:N	2.69	0.50
2:B:142:LEU:HD11	22:B:4006:BCR:H402	1.93	0.50
19:B:1218:CLA:C1D	22:B:4004:BCR:H402	2.41	0.50
22:B:4004:BCR:H392	7:G:134:ILE:HD11	1.93	0.50
9:I:16:PHE:C	9:I:16:PHE:CD2	2.90	0.50
11:K:109:VAL:HG13	22:K:4002:BCR:H343	1.92	0.50
1:A:720:THR:HG23	1:A:720:THR:O	2.11	0.50
19:B:1202:CLA:HHC	19:B:1202:CLA:CBB	2.41	0.50
1:A:126:ILE:HG23	1:A:127:VAL:N	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:203:ALA:O	6:F:207:VAL:HG13	2.12	0.50
12:L:180:ASP:OD1	12:L:181:GLY:N	2.45	0.50
15:3:63:GLN:HG3	15:3:64:SER:N	2.25	0.50
19:4:607:CLA:HHC	19:4:607:CLA:CBB	2.41	0.50
2:B:351:HIS:ND1	19:B:1214:CLA:OBD	2.43	0.50
1:A:406:LEU:HD21	19:A:1104:CLA:H142	1.94	0.50
19:A:1117:CLA:HBB1	19:A:1117:CLA:CMB	2.38	0.50
19:A:1136:CLA:HBB1	19:A:1136:CLA:HHC	1.94	0.50
19:A:1138:CLA:H72	20:A:2001:PQN:H293	1.93	0.50
19:B:1231:CLA:HBB1	19:B:1231:CLA:CMB	2.41	0.50
6:F:166:LEU:HD23	22:F:4014:BCR:H391	1.94	0.50
17:P:19:LEU:HD21	17:P:27:ILE:HD13	1.93	0.49
2:B:476:VAL:HG12	2:B:477:LEU:N	2.27	0.49
8:H:103:LEU:CB	12:L:143:ILE:CD1	2.84	0.49
22:J:4012:BCR:HC8	22:J:4012:BCR:H311	1.94	0.49
15:3:94:GLU:OE1	15:3:94:GLU:O	2.30	0.49
15:3:199:ASN:OD1	15:3:202:TYR:HD2	1.95	0.49
16:4:190:ASN:OD1	28:4:501:LUT:O23	2.15	0.49
19:A:1139:CLA:HBB1	19:A:1139:CLA:HMB1	1.94	0.49
22:A:4011:BCR:H391	19:B:1229:CLA:HMA1	1.93	0.49
2:B:105:THR:HG23	2:B:105:THR:O	2.12	0.49
22:B:4005:BCR:H331	22:B:4005:BCR:C8	2.37	0.49
8:H:103:LEU:HD13	12:L:143:ILE:CD1	2.38	0.49
11:K:122:LEU:O	11:K:126:GLY:N	2.36	0.49
14:2:212:GLN:NE2	14:2:213:LYS:HA	2.28	0.49
2:B:32:GLU:OE1	2:B:331:HIS:NE2	2.45	0.49
13:1:118:GLN:NE2	13:1:126:VAL:O	2.45	0.49
1:A:691:MET:HG3	19:A:1013:CLA:NC	2.28	0.49
2:B:384:THR:HG22	2:B:576:PHE:CE1	2.47	0.49
2:B:443:MET:CE	2:B:451:LYS:CE	2.90	0.49
2:B:676:GLU:HG3	3:C:81:TYR:HE1	1.77	0.49
3:C:55:GLU:OE2	3:C:66:ARG:NH1	2.46	0.49
5:E:126:GLU:OE1	5:E:127:GLU:O	2.30	0.49
14:2:231:ALA:HB2	28:2:501:LUT:H392	1.95	0.49
15:3:173:PHE:HB2	19:3:612:CLA:CMA	2.42	0.49
2:B:670:TYR:OH	19:B:1023:CLA:OBD	2.28	0.49
19:B:1211:CLA:H3A	22:B:4006:BCR:H392	1.95	0.49
19:B:1236:CLA:HBB1	19:B:1236:CLA:CMB	2.42	0.49
3:C:27:GLU:OE1	3:C:43:PRO:CG	2.61	0.49
3:C:27:GLU:OE1	3:C:44:ARG:NH2	2.46	0.49
4:D:81:SER:O	4:D:124:ARG:NE	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:24:LEU:HB3	22:L:4019:BCR:H333	1.95	0.49
14:2:124:GLU:HA	14:2:127:THR:HG22	1.93	0.49
15:3:262:ASP:OD1	15:3:263:PRO:N	2.45	0.49
17:P:26:THR:CB	17:P:73:LYS:HA	2.43	0.49
17:P:38:ASN:HB2	17:P:62:LEU:HD23	1.95	0.49
4:D:129:LEU:HD23	4:D:130:LEU:N	2.27	0.49
4:D:174:TYR:CB	4:D:176:GLU:OE1	2.61	0.49
15:3:255:ASN:O	15:3:258:ASP:OD1	2.31	0.49
15:3:274:PHE:HD1	15:3:275:HIS:N	2.10	0.49
16:4:68:GLY:N	16:4:73:ASP:OD2	2.43	0.49
19:4:602:CLA:HHC	19:4:602:CLA:CBB	2.41	0.49
3:C:28:MET:HE2	3:C:40:ALA:HA	1.94	0.49
6:F:219:ARG:O	6:F:223:ASN:ND2	2.46	0.49
19:K:1401:CLA:HMB1	19:K:1401:CLA:HBB1	1.95	0.49
22:2:503:BCR:H23C	22:2:503:BCR:C40	2.43	0.49
19:A:1110:CLA:HMC3	22:A:4003:BCR:H343	1.95	0.49
19:B:1205:CLA:HHC	19:B:1205:CLA:CBB	2.43	0.49
13:1:53:GLY:HA2	13:1:58:ASP:CG	2.37	0.49
13:1:173:ASP:HB3	13:1:176:LYS:HE3	1.94	0.49
28:1:501:LUT:H171	28:1:501:LUT:C8	2.42	0.49
14:2:121:PHE:CE1	28:2:501:LUT:H373	2.48	0.49
16:4:149:PHE:HA	16:4:152:VAL:HG22	1.94	0.49
12:L:207:LEU:HD23	12:L:207:LEU:N	2.28	0.48
13:1:133:THR:OG1	13:1:134:ILE:N	2.45	0.48
14:2:182:ILE:HD12	19:4:607:CLA:HAB	1.93	0.48
15:3:192:LYS:HD2	15:3:193:GLY:N	2.28	0.48
19:B:1206:CLA:H91	19:B:1239:CLA:H12	1.95	0.48
28:3:502:LUT:H24	29:3:604:CHL:H2	1.94	0.48
1:A:684:PHE:CD2	22:A:4011:BCR:H363	2.48	0.48
2:B:410:ARG:O	2:B:414:HIS:ND1	2.45	0.48
4:D:148:LYS:HB3	4:D:149:TYR:CD1	2.48	0.48
15:3:236:LEU:CD1	29:3:604:CHL:OMC	2.44	0.48
19:B:1213:CLA:HMB1	19:B:1213:CLA:HBB1	1.96	0.48
14:2:114:MET:SD	14:2:225:GLY:HA2	2.54	0.48
28:2:501:LUT:H28	28:2:501:LUT:H371	1.95	0.48
4:D:81:SER:O	4:D:124:ARG:CD	2.60	0.48
8:H:68:ASP:OD2	8:H:68:ASP:N	2.47	0.48
19:2:608:CLA:HHC	19:2:608:CLA:CBB	2.43	0.48
1:A:379:MET:HG2	1:A:379:MET:O	2.13	0.48
22:A:4002:BCR:H291	19:K:1401:CLA:HAB	1.96	0.48
19:B:1206:CLA:H62	22:I:4018:BCR:H373	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:83:ILE:HD13	4:D:124:ARG:NH2	2.29	0.48
22:G:4011:BCR:H393	22:G:4011:BCR:H271	1.96	0.48
11:K:108:GLY:O	11:K:112:HIS:CD2	2.67	0.48
28:1:502:LUT:H28	28:1:502:LUT:H361	1.95	0.48
1:A:511:THR:HG21	19:A:1125:CLA:CAB	2.41	0.48
19:A:1121:CLA:HHC	19:A:1121:CLA:CBB	2.40	0.48
3:C:35:LYS:NZ	5:E:94:ASP:OD2	2.40	0.48
4:D:83:ILE:HD11	4:D:124:ARG:CZ	2.44	0.48
19:1:614:CLA:HHC	19:1:614:CLA:CBB	2.44	0.48
15:3:262:ASP:OD1	15:3:263:PRO:HD2	2.14	0.48
28:3:501:LUT:C31	22:3:506:BCR:H363	2.44	0.48
17:P:84:CYS:CB	17:P:92:MET:HE2	2.36	0.48
19:A:1137:CLA:HHC	19:A:1137:CLA:CBB	2.42	0.48
19:B:1221:CLA:HBB1	19:B:1221:CLA:CMB	2.43	0.48
11:K:77:LYS:HD2	11:K:87:ARG:CZ	2.42	0.48
12:L:115:VAL:HG11	12:L:205:TYR:OH	2.13	0.48
19:1:605:CLA:H43	19:1:605:CLA:HED3	1.96	0.48
15:3:120:GLU:OE2	15:3:253:TYR:HB3	2.13	0.48
15:3:225:LEU:HD13	15:3:225:LEU:C	2.38	0.48
19:A:1125:CLA:C3B	19:A:1133:CLA:HMA2	2.43	0.48
19:2:604:CLA:HBB1	19:2:604:CLA:HMB1	1.95	0.48
16:4:213:LEU:CD2	19:4:604:CLA:HMC1	2.44	0.48
19:B:1201:CLA:HBB1	19:B:1202:CLA:CMB	2.44	0.48
12:L:111:VAL:HG21	12:L:200:ALA:HB3	1.96	0.48
15:3:153:ASP:OD2	15:3:156:THR:CG2	2.61	0.48
19:4:608:CLA:HHC	19:4:608:CLA:HBB1	1.96	0.48
28:4:501:LUT:C8	28:4:501:LUT:H181	2.44	0.48
17:P:1:VAL:CG1	17:P:19:LEU:HD21	2.44	0.48
22:A:4003:BCR:HC8	22:A:4003:BCR:C32	2.42	0.47
10:J:27:ILE:HG13	22:J:4012:BCR:H341	1.95	0.47
2:B:607:SER:O	2:B:610:ASN:N	2.47	0.47
5:E:84:TYR:CE2	5:E:85:LYS:HD2	2.49	0.47
22:I:4018:BCR:HC8	22:I:4018:BCR:C32	2.44	0.47
19:1:611:CLA:HBB1	19:1:611:CLA:CMB	2.44	0.47
19:A:1141:CLA:O1A	25:A:5006:LMG:H372	2.14	0.47
22:A:4011:BCR:HC8	22:A:4011:BCR:C33	2.42	0.47
2:B:70:TRP:CE3	2:B:71:GLN:NE2	2.82	0.47
2:B:443:MET:HE1	2:B:451:LYS:CE	2.44	0.47
19:B:1227:CLA:HBA2	19:B:1240:CLA:H41	1.96	0.47
24:B:5008:LMT:O6B	24:B:5008:LMT:O4'	2.28	0.47
6:F:138:LEU:HD21	10:J:38:THR:HG21	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:3:120:GLU:OE2	15:3:253:TYR:N	2.45	0.47
28:3:501:LUT:H402	19:3:601:CLA:HMC1	1.96	0.47
1:A:178:MET:HE2	1:A:178:MET:N	2.28	0.47
19:A:1013:CLA:HBB1	19:A:1013:CLA:CMB	2.44	0.47
22:A:4011:BCR:H391	19:B:1229:CLA:CMA	2.44	0.47
19:B:1217:CLA:HHC	19:B:1217:CLA:CBB	2.43	0.47
19:B:1219:CLA:HBB2	22:B:4009:BCR:H343	1.96	0.47
22:L:4019:BCR:HC8	22:L:4019:BCR:C33	2.44	0.47
14:2:159:PHE:CD2	14:2:159:PHE:N	2.83	0.47
14:2:200:TRP:HE1	29:2:615:CHL:C3D	2.26	0.47
22:2:503:BCR:H17C	29:2:611:CHL:HMB3	1.95	0.47
15:3:217:GLU:O	15:3:217:GLU:OE2	2.32	0.47
1:A:44:ILE:HG23	1:A:53:TRP:NE1	2.30	0.47
2:B:374:HIS:CE1	2:B:378:ILE:HD12	2.50	0.47
11:K:114:ILE:HD12	11:K:114:ILE:C	2.39	0.47
13:1:78:GLU:CD	13:1:158:LYS:HG2	2.39	0.47
15:3:225:LEU:CD1	19:3:607:CLA:CED	2.93	0.47
16:4:214:ALA:CB	28:4:501:LUT:H10	2.45	0.47
17:P:27:ILE:CD1	17:P:96:VAL:HG21	2.45	0.47
2:B:458:ILE:HG21	6:F:151:SER:HB3	1.96	0.47
2:B:503:GLU:CD	2:B:504:ASN:N	2.72	0.47
9:I:30:LYS:HZ2	9:I:32:LEU:HD12	1.78	0.47
12:L:115:VAL:HG22	12:L:130:GLY:HA3	1.96	0.47
28:1:501:LUT:H28	28:1:501:LUT:C38	2.44	0.47
14:2:212:GLN:NE2	14:2:213:LYS:N	2.63	0.47
15:3:274:PHE:HD1	15:3:275:HIS:H	1.60	0.47
22:3:506:BCR:H15C	22:3:506:BCR:H351	1.63	0.47
19:A:1111:CLA:HMB3	19:A:1111:CLA:CBB	2.41	0.47
22:A:4002:BCR:H331	22:A:4002:BCR:C8	2.36	0.47
2:B:80:ASP:O	2:B:84:VAL:HG12	2.15	0.47
2:B:443:MET:HE2	2:B:451:LYS:HB2	1.96	0.47
11:K:79:THR:OG1	11:K:83:LYS:O	2.33	0.47
22:K:4002:BCR:H321	22:K:4002:BCR:C8	2.45	0.47
22:3:506:BCR:H10C	29:3:611:CHL:HBA1	1.96	0.47
16:4:105:GLY:HA2	30:4:502:XAT:H181	1.96	0.47
16:4:157:TRP:CD2	19:4:617:CLA:HBC1	2.50	0.47
17:P:19:LEU:CB	17:P:96:VAL:HG23	2.43	0.47
17:P:19:LEU:CD2	17:P:96:VAL:HG23	2.40	0.47
17:P:21:VAL:HG13	17:P:98:VAL:HG12	1.95	0.47
1:A:378:ALA:HB1	19:A:1125:CLA:HMC2	1.95	0.47
1:A:433:ASP:OD2	1:A:437:ARG:NH1	2.43	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:551:VAL:HG11	1:A:604:TRP:CZ2	2.49	0.47
1:A:604:TRP:HH2	19:B:1022:CLA:HAB	1.77	0.47
19:A:1104:CLA:C15	19:A:1127:CLA:HBB2	2.44	0.47
19:B:1023:CLA:H143	22:I:4018:BCR:H323	1.97	0.47
22:B:4005:BCR:H351	22:B:4005:BCR:H15C	1.72	0.47
22:I:4018:BCR:H343	22:I:4020:BCR:H343	1.96	0.47
19:1:606:CLA:HBB1	19:1:606:CLA:CMB	2.39	0.47
22:1:503:BCR:H351	22:1:503:BCR:H15C	1.68	0.47
14:2:195:TYR:HB3	19:2:601:CLA:HED3	1.97	0.47
1:A:530:LEU:HD12	1:A:531:PRO:O	2.15	0.47
19:A:1108:CLA:HBB1	19:A:1108:CLA:HMB3	1.96	0.47
19:B:1021:CLA:HMB1	19:B:1021:CLA:CBB	2.42	0.47
3:C:18:VAL:HG23	3:C:28:MET:HE3	1.93	0.47
14:2:223:LYS:HZ1	19:2:607:CLA:C3D	2.14	0.47
14:2:223:LYS:NZ	19:2:607:CLA:CHA	2.78	0.47
1:A:255:LEU:HD13	1:A:262:PHE:CZ	2.50	0.47
1:A:691:MET:HE2	1:A:700:TRP:CH2	2.50	0.47
19:A:1140:CLA:HHC	19:A:1140:CLA:CBB	2.37	0.47
3:C:9:ASP:OD2	5:E:100:ARG:HD2	2.14	0.47
3:C:52:LYS:N	21:C:3002:SF4:S1	2.81	0.46
5:E:96:ASP:OD2	5:E:97:PRO:N	2.48	0.46
6:F:95:GLU:HG2	6:F:130:PHE:CD2	2.50	0.46
12:L:199:TRP:CE2	22:L:4020:BCR:H10C	2.50	0.46
14:2:200:TRP:NE1	29:2:615:CHL:C3D	2.78	0.46
15:3:174:GLN:CB	15:3:182:MET:HE3	2.43	0.46
1:A:616:PHE:HD2	19:A:1135:CLA:HBC2	1.80	0.46
2:B:377:TYR:CD2	19:B:1224:CLA:HAB	2.50	0.46
2:B:439:HIS:CE1	2:B:453:ILE:HG13	2.51	0.46
2:B:443:MET:CE	2:B:451:LYS:HE3	2.46	0.46
19:B:1207:CLA:HHC	19:B:1207:CLA:CBB	2.42	0.46
19:B:1204:CLA:H61	19:B:1204:CLA:H41	1.67	0.46
12:L:206:VAL:HG12	12:L:207:LEU:HD23	1.97	0.46
19:L:1501:CLA:HAA2	22:L:4020:BCR:H352	1.97	0.46
28:2:501:LUT:H361	28:2:501:LUT:C28	2.45	0.46
1:A:251:ASN:HD21	1:A:253:ASP:CG	2.23	0.46
19:B:1210:CLA:HMB1	19:B:1210:CLA:HBB1	1.96	0.46
19:B:1204:CLA:HED2	9:I:5:PRO:HB3	1.97	0.46
28:1:501:LUT:H362	19:1:611:CLA:H41	1.97	0.46
14:2:159:PHE:HD2	14:2:159:PHE:N	2.13	0.46
17:P:1:VAL:HG13	17:P:27:ILE:HG23	1.96	0.46
15:3:59:PHE:O	15:3:59:PHE:CG	2.67	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:3:81:LEU:CD2	28:3:502:LUT:H221	2.46	0.46
1:A:719:ALA:HB3	6:F:195:GLU:OE1	2.16	0.46
2:B:490:ARG:HB3	7:G:153:LYS:NZ	2.30	0.46
22:H:4021:BCR:H383	12:L:203:LEU:CD2	2.43	0.46
22:3:503:BCR:HC8	22:3:503:BCR:H311	1.96	0.46
19:B:1209:CLA:HBB1	19:B:1209:CLA:CMB	2.45	0.46
19:B:1220:CLA:HMD3	19:B:1221:CLA:HHC	1.97	0.46
19:B:1222:CLA:H141	19:B:1236:CLA:CBC	2.45	0.46
22:I:4018:BCR:H331	22:I:4020:BCR:H341	1.98	0.46
22:J:4012:BCR:H15C	22:J:4012:BCR:H351	1.69	0.46
22:3:503:BCR:H351	22:3:503:BCR:H15C	1.67	0.46
1:A:80:SER:OG	19:A:1109:CLA:HHD	2.15	0.46
19:B:1222:CLA:HBB1	19:B:1222:CLA:CMB	2.46	0.46
4:D:101:TYR:OH	4:D:157:ARG:NH1	2.46	0.46
30:2:502:XAT:C17	19:2:606:CLA:HMB2	2.45	0.46
1:A:33:GLN:OE1	1:A:33:GLN:N	2.47	0.46
19:B:1238:CLA:HED2	12:L:148:TYR:CD2	2.51	0.46
22:B:4004:BCR:HC8	22:B:4004:BCR:H331	1.97	0.46
19:K:1401:CLA:HBB1	19:K:1401:CLA:CMB	2.46	0.46
22:L:4019:BCR:H331	22:L:4019:BCR:C8	2.45	0.46
15:3:59:PHE:CD1	15:3:59:PHE:C	2.94	0.46
1:A:96:MET:HE1	19:A:1106:CLA:HBA2	1.98	0.46
19:B:1235:CLA:C1A	19:B:1235:CLA:CGA	2.94	0.46
22:3:503:BCR:H382	22:3:503:BCR:H23C	1.98	0.46
17:P:98:VAL:HG23	17:P:98:VAL:O	2.16	0.46
19:B:1232:CLA:O1A	19:G:1603:CLA:HMB1	2.16	0.46
19:G:1603:CLA:H42	25:G:5002:LMG:H222	1.98	0.46
12:L:199:TRP:NE1	12:L:203:LEU:HD22	2.31	0.46
28:1:502:LUT:H361	28:1:502:LUT:C28	2.46	0.46
19:2:608:CLA:O2A	15:3:160:LEU:HD13	2.15	0.46
29:2:609:CHL:H41	29:2:609:CHL:H71	1.98	0.46
15:3:74:GLY:H	15:3:225:LEU:HD22	1.81	0.46
14:2:238:GLN:OE1	28:2:501:LUT:H24	2.16	0.45
15:3:55:ARG:NH1	15:3:69:ASP:O	2.50	0.45
15:3:235:MET:HG3	28:3:502:LUT:C35	2.45	0.45
19:4:608:CLA:HHC	19:4:608:CLA:CBB	2.45	0.45
5:E:98:ASN:OD1	5:E:98:ASN:C	2.59	0.45
22:F:4014:BCR:H383	22:F:4014:BCR:C23	2.46	0.45
22:F:4016:BCR:H351	22:F:4016:BCR:H15C	1.81	0.45
11:K:69:GLY:O	11:K:71:ALA:N	2.50	0.45
11:K:109:VAL:HG11	22:K:4001:BCR:C20	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:L:1503:CLA:HBB1	19:L:1503:CLA:CMB	2.42	0.45
28:2:501:LUT:H191	19:2:601:CLA:H13	1.98	0.45
15:3:166:GLY:HA2	19:3:612:CLA:CBB	2.46	0.45
17:P:42:ASP:O	17:P:43:GLU:CB	2.64	0.45
1:A:213:LEU:HD21	22:A:4003:BCR:H342	1.99	0.45
1:A:464:ASN:HB3	1:A:476:MET:HE3	1.99	0.45
2:B:39:GLU:CG	2:B:165:VAL:HG11	2.46	0.45
2:B:443:MET:CE	2:B:451:LYS:HE2	2.46	0.45
6:F:95:GLU:CG	6:F:130:PHE:CG	2.94	0.45
19:H:1701:CLA:NB	22:H:4021:BCR:H362	2.31	0.45
13:1:170:TYR:HB2	19:1:601:CLA:CGA	2.46	0.45
14:2:107:LEU:HB3	14:2:111:ARG:NH1	2.32	0.45
19:2:604:CLA:HHD	29:2:609:CHL:HBB2	1.98	0.45
15:3:247:VAL:HG21	19:3:603:CLA:HMD2	1.97	0.45
28:4:501:LUT:H161	19:4:603:CLA:HMB2	1.97	0.45
19:A:1104:CLA:H42	19:A:1128:CLA:NC	2.32	0.45
1:A:100:GLY:C	1:A:104:SER:HG	2.14	0.45
1:A:511:THR:CG2	19:A:1125:CLA:HAB	2.45	0.45
19:A:1125:CLA:HBB1	19:A:1125:CLA:CMB	2.47	0.45
2:B:2:ALA:C	2:B:3:LEU:HG	2.42	0.45
2:B:152:ALA:HB2	19:B:1208:CLA:HBC2	1.98	0.45
6:F:136:GLN:HE21	10:J:40:PRO:HG3	1.82	0.45
12:L:155:GLU:N	12:L:155:GLU:CD	2.71	0.45
19:4:612:CLA:H93	19:4:612:CLA:C5	2.47	0.45
1:A:82:HIS:HB3	19:A:1111:CLA:HED3	1.99	0.45
19:A:1106:CLA:HBB1	19:A:1106:CLA:CMB	2.47	0.45
22:A:4008:BCR:H382	22:A:4008:BCR:C23	2.47	0.45
22:L:4020:BCR:H392	22:L:4020:BCR:H23C	1.97	0.45
19:2:602:CLA:HHC	19:2:602:CLA:CBB	2.46	0.45
15:3:258:ASP:OD1	15:3:259:HIS:N	2.50	0.45
19:A:1107:CLA:HBB1	19:A:1107:CLA:CMB	2.45	0.45
19:A:1127:CLA:HBB1	19:A:1127:CLA:CMB	2.46	0.45
2:B:456:GLU:O	2:B:458:ILE:N	2.48	0.45
22:F:4014:BCR:H331	22:F:4014:BCR:C8	2.33	0.45
28:2:501:LUT:H383	19:2:603:CLA:C4B	2.47	0.45
15:3:81:LEU:HD22	28:3:502:LUT:H221	1.99	0.45
22:3:503:BCR:H402	19:3:606:CLA:NB	2.32	0.45
28:4:501:LUT:H35	28:4:501:LUT:H401	1.76	0.45
2:B:516:ASP:OD1	2:B:593:TYR:OH	2.27	0.45
2:B:631:LEU:HD22	2:B:724:PHE:HA	1.98	0.45
19:1:606:CLA:HMA3	19:1:613:CLA:C3C	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:B:1223:CLA:HMB3	19:B:1223:CLA:CBB	2.40	0.45
19:B:1235:CLA:C4	19:F:1302:CLA:HBB1	2.47	0.45
4:D:76:ASP:OD2	4:D:76:ASP:C	2.60	0.45
19:3:613:CLA:HBB1	19:3:613:CLA:CMB	2.46	0.45
2:B:374:HIS:HD2	19:B:1224:CLA:NA	2.15	0.45
2:B:476:VAL:O	2:B:477:LEU:C	2.60	0.45
22:B:4004:BCR:HC8	22:B:4004:BCR:C33	2.47	0.45
22:B:4009:BCR:H351	22:B:4009:BCR:H15C	1.84	0.45
22:F:4016:BCR:H382	22:F:4016:BCR:H23C	1.99	0.45
11:K:77:LYS:HD3	11:K:87:ARG:CD	2.44	0.45
22:L:4019:BCR:H351	22:L:4019:BCR:H15C	1.72	0.45
29:2:609:CHL:H41	29:2:609:CHL:C7	2.46	0.45
28:3:501:LUT:H402	19:3:601:CLA:CMC	2.47	0.45
19:A:1130:CLA:HBB1	19:A:1130:CLA:CMB	2.46	0.44
2:B:498:LEU:HA	2:B:501:ILE:HG22	1.99	0.44
19:B:1225:CLA:CMB	19:B:1225:CLA:HBB1	2.47	0.44
29:4:611:CHL:H42	29:4:613:CHL:H93	1.98	0.44
1:A:213:LEU:HD21	22:A:4003:BCR:C34	2.47	0.44
2:B:351:HIS:HB3	19:B:1214:CLA:HED2	1.98	0.44
2:B:68:VAL:O	2:B:72:GLY:HA3	2.17	0.44
22:F:4016:BCR:H331	22:F:4016:BCR:C8	2.44	0.44
9:I:11:LEU:HD12	9:I:11:LEU:HA	1.86	0.44
9:I:24:LEU:HD13	22:L:4019:BCR:C33	2.47	0.44
10:J:26:LEU:HB2	22:J:4012:BCR:H343	1.99	0.44
12:L:109:LEU:HD11	19:L:1502:CLA:HMB2	1.99	0.44
16:4:114:VAL:HG12	16:4:230:PHE:CG	2.53	0.44
19:4:606:CLA:HMA3	29:4:613:CHL:C2C	2.47	0.44
2:B:189:ALA:CB	19:B:1211:CLA:HAB	2.48	0.44
2:B:352:MET:SD	19:B:1215:CLA:CGA	3.04	0.44
19:B:1210:CLA:HBB1	19:B:1210:CLA:CMB	2.47	0.44
19:B:1234:CLA:HMB1	19:B:1234:CLA:CBB	2.46	0.44
4:D:129:LEU:C	4:D:129:LEU:CD2	2.88	0.44
6:F:200:VAL:O	6:F:204:THR:HG23	2.18	0.44
22:F:4016:BCR:HC8	22:F:4016:BCR:C33	2.47	0.44
19:G:1603:CLA:H142	13:1:135:LEU:HD11	2.00	0.44
22:K:4001:BCR:H351	22:K:4001:BCR:H15C	1.80	0.44
22:K:4002:BCR:H351	22:K:4002:BCR:H15C	1.83	0.44
14:2:212:GLN:NE2	14:2:213:LYS:CA	2.80	0.44
17:P:21:VAL:CG2	17:P:22:SER:N	2.80	0.44
17:P:27:ILE:HD11	17:P:74:LEU:HD12	1.99	0.44
19:A:1136:CLA:HHC	19:A:1136:CLA:CBB	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:607:SER:C	2:B:611:GLU:OE1	2.60	0.44
19:B:1211:CLA:H161	22:B:4005:BCR:H363	1.99	0.44
4:D:83:ILE:HD11	4:D:124:ARG:NH2	2.33	0.44
13:1:202:GLN:NE2	13:1:208:THR:O	2.50	0.44
19:A:1128:CLA:HBB1	19:A:1128:CLA:CMB	2.46	0.44
19:B:1213:CLA:HBA1	7:G:148:ASN:HB2	1.99	0.44
11:K:92:GLN:C	11:K:92:GLN:OE1	2.61	0.44
14:2:200:TRP:NE1	29:2:615:CHL:C4D	2.80	0.44
17:P:26:THR:HG22	17:P:73:LYS:CG	2.43	0.44
19:A:1121:CLA:H142	19:K:1402:CLA:HBC1	1.99	0.44
2:B:322:LEU:HA	2:B:325:THR:HG22	2.00	0.44
19:B:1216:CLA:HBB1	19:B:1216:CLA:CMB	2.47	0.44
3:C:7:ILE:HD12	3:C:40:ALA:CB	2.45	0.44
9:I:9:VAL:HB	9:I:10:PRO:HD3	1.98	0.44
14:2:155:VAL:O	14:2:159:PHE:CD2	2.71	0.44
14:2:177:VAL:HG23	14:2:177:VAL:O	2.18	0.44
15:3:235:MET:CG	28:3:502:LUT:C34	2.95	0.44
17:P:19:LEU:CD2	17:P:27:ILE:HD13	2.47	0.44
1:A:394:SER:HB3	19:A:1126:CLA:HMA1	2.00	0.44
19:B:1234:CLA:HMB2	19:B:1236:CLA:HED1	1.99	0.44
22:B:4004:BCR:H392	7:G:134:ILE:CD1	2.47	0.44
4:D:166:TYR:OH	4:D:169:PRO:O	2.20	0.44
19:H:1701:CLA:C4B	22:H:4021:BCR:H362	2.48	0.44
14:2:111:ARG:NH2	14:2:221:GLU:OE2	2.50	0.44
15:3:162:MET:HE3	19:3:612:CLA:HAB	2.00	0.44
15:3:225:LEU:HD11	19:3:607:CLA:CED	2.48	0.44
19:4:617:CLA:HBB1	19:4:617:CLA:CMB	2.41	0.44
17:P:38:ASN:OD1	17:P:38:ASN:C	2.61	0.44
2:B:352:MET:SD	19:B:1215:CLA:O1A	2.76	0.44
7:G:70:LEU:HD23	27:G:5003:DGD:HB61	2.00	0.44
22:G:4011:BCR:H351	22:G:4011:BCR:H15C	1.71	0.44
9:I:24:LEU:HD13	22:L:4019:BCR:H333	1.99	0.44
19:3:603:CLA:H41	19:3:603:CLA:H62	1.72	0.44
1:A:518:GLY:O	1:A:519:ASP:C	2.61	0.43
2:B:443:MET:HE2	2:B:451:LYS:CB	2.48	0.43
6:F:156:HIS:ND1	6:F:159:GLU:OE2	2.51	0.43
15:3:86:PRO:HG2	15:3:87:GLU:H	1.83	0.43
16:4:104:LEU:HB3	19:4:606:CLA:HAB	1.99	0.43
19:A:1117:CLA:HMB1	19:A:1117:CLA:CBB	2.40	0.43
19:A:1130:CLA:HBB1	19:A:1130:CLA:HMB1	2.00	0.43
22:B:4009:BCR:H402	22:B:4010:BCR:H21C	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:79:ASN:HD21	19:H:1701:CLA:CMD	2.31	0.43
8:H:83:SER:HB3	8:H:87:GLU:OE2	2.17	0.43
15:3:153:ASP:O	15:3:154:ASN:CB	2.65	0.43
15:3:262:ASP:OD1	15:3:263:PRO:CD	2.66	0.43
28:4:505:LUT:H371	28:4:505:LUT:C28	2.45	0.43
2:B:344:ILE:CD1	19:B:1225:CLA:CBC	2.89	0.43
2:B:477:LEU:HD21	19:B:1232:CLA:HBC2	1.99	0.43
19:B:1211:CLA:H3A	22:B:4006:BCR:C39	2.47	0.43
14:2:122:ILE:O	14:2:126:LEU:HB2	2.17	0.43
28:3:502:LUT:C8	28:3:502:LUT:C18	2.93	0.43
2:B:444:LEU:HD12	2:B:615:TYR:CD1	2.53	0.43
19:B:1210:CLA:CMA	22:B:4005:BCR:H362	2.48	0.43
19:B:1226:CLA:H193	19:B:1239:CLA:HMA2	2.01	0.43
15:3:74:GLY:N	15:3:225:LEU:HD22	2.33	0.43
19:3:617:CLA:HMA2	19:3:617:CLA:H2	2.01	0.43
17:P:9:ASP:OD2	17:P:9:ASP:N	2.51	0.43
2:B:167:TRP:CZ2	19:B:1208:CLA:HMA1	2.53	0.43
19:B:1205:CLA:HMB1	19:B:1206:CLA:O1A	2.18	0.43
28:1:501:LUT:H31	28:1:501:LUT:H391	1.79	0.43
15:3:270:THR:HG22	15:3:270:THR:O	2.18	0.43
16:4:159:ASP:OD1	29:4:611:CHL:HBC1	2.19	0.43
17:P:58:PRO:O	17:P:60:GLU:N	2.52	0.43
19:A:1104:CLA:HMA2	19:A:1128:CLA:C3B	2.48	0.43
19:A:1106:CLA:H191	19:A:1101:CLA:HMA3	1.99	0.43
19:B:1237:CLA:H112	19:B:1237:CLA:H151	1.92	0.43
25:F:5002:LMG:H151	25:F:5002:LMG:H182	1.95	0.43
7:G:136:HIS:HB2	22:G:4011:BCR:H21C	1.99	0.43
22:G:4011:BCR:H393	22:G:4011:BCR:C27	2.48	0.43
29:1:610:CHL:CBB	19:1:613:CLA:HBB2	2.49	0.43
15:3:237:ALA:HB1	28:3:501:LUT:H8	1.99	0.43
17:P:35:PHE:HB2	17:P:36:PRO:HA	2.01	0.43
17:P:61:ASP:OD1	17:P:62:LEU:N	2.52	0.43
1:A:530:LEU:HD12	1:A:530:LEU:C	2.44	0.43
19:G:1601:CLA:CBB	22:G:4011:BCR:H363	2.48	0.43
13:1:221:PRO:O	13:1:225:THR:HG23	2.19	0.43
28:2:501:LUT:H15	28:2:501:LUT:H201	1.73	0.43
15:3:91:GLY:C	15:3:93:ILE:H	2.26	0.43
15:3:117:ILE:CD1	15:3:252:PRO:CG	2.96	0.43
19:4:603:CLA:H193	19:4:607:CLA:HAC2	2.01	0.43
19:4:606:CLA:HMB3	19:4:606:CLA:CBB	2.44	0.43
2:B:459:PHE:HB3	19:B:1234:CLA:H42	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:B:4009:BCR:C33	22:B:4009:BCR:HC8	2.49	0.43
6:F:173:TRP:CD1	6:F:210:GLY:HA3	2.54	0.43
22:H:4021:BCR:H351	22:H:4021:BCR:H15C	1.76	0.43
9:I:29:GLU:O	9:I:30:LYS:HB3	2.19	0.43
22:L:4019:BCR:H382	19:L:1502:CLA:HAC2	2.01	0.43
22:1:504:BCR:H403	22:1:504:BCR:C23	2.47	0.43
15:3:85:ASP:O	15:3:88:GLY:O	2.36	0.43
29:4:615:CHL:HMA3	29:4:615:CHL:CBA	2.48	0.43
17:P:51:ASP:CG	17:P:54:LYS:HG3	2.43	0.43
1:A:267:THR:OG1	1:A:268:PRO:HD3	2.18	0.43
22:A:4017:BCR:HC42	2:B:649:MET:HE2	2.00	0.43
2:B:275:HIS:HB3	19:B:1214:CLA:HMB2	2.01	0.43
8:H:51:LYS:CG	8:H:52:SER:N	2.77	0.43
12:L:125:ILE:HA	12:L:128:GLN:OE1	2.17	0.43
14:2:164:GLU:OE1	14:2:167:ARG:NH2	2.41	0.43
15:3:86:PRO:CG	15:3:87:GLU:H	2.31	0.43
22:A:4011:BCR:H15C	22:A:4011:BCR:H351	1.89	0.43
22:B:4006:BCR:H392	22:B:4006:BCR:H23C	2.01	0.43
22:3:506:BCR:H24C	22:3:506:BCR:H371	1.95	0.43
1:A:377:TYR:CD2	1:A:377:TYR:C	2.97	0.42
1:A:706:SER:HA	2:B:416:GLU:HG2	2.00	0.42
19:A:1106:CLA:H101	22:J:4012:BCR:H372	2.01	0.42
2:B:339:ALA:HB2	22:B:4010:BCR:C37	2.49	0.42
2:B:435:GLY:HA3	19:B:1230:CLA:HAB	2.01	0.42
19:B:1211:CLA:HMA3	22:B:4006:BCR:H393	2.01	0.42
19:B:1213:CLA:C1A	19:B:1213:CLA:CGA	2.97	0.42
19:B:1226:CLA:HBB1	19:B:1226:CLA:CMB	2.49	0.42
5:E:108:ASN:OD1	5:E:108:ASN:N	2.50	0.42
1:A:325:HIS:HB3	1:A:330:ILE:HD11	2.01	0.42
2:B:475:ASP:O	2:B:475:ASP:CG	2.56	0.42
14:2:200:TRP:NE1	29:2:615:CHL:C2D	2.82	0.42
22:2:503:BCR:H17C	29:2:611:CHL:CMB	2.49	0.42
15:3:178:LYS:HE3	15:3:178:LYS:HB3	1.86	0.42
17:P:55:ILE:CG2	17:P:72:VAL:HG21	2.43	0.42
1:A:18:VAL:HG22	1:A:198:ASP:OD2	2.19	0.42
19:A:1139:CLA:HMD2	6:F:182:LEU:HD11	2.01	0.42
2:B:443:MET:HE2	2:B:451:LYS:HE3	2.01	0.42
19:2:604:CLA:HBB1	19:2:604:CLA:CMB	2.49	0.42
1:A:339:THR:HG23	23:A:5001:LHG:O4	2.19	0.42
19:B:1218:CLA:HHC	19:B:1218:CLA:CBB	2.49	0.42
8:H:125:ILE:HG23	8:H:126:LYS:N	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:I:4020:BCR:H351	22:I:4020:BCR:H15C	1.87	0.42
28:4:505:LUT:H31	28:4:505:LUT:H391	1.65	0.42
22:A:4011:BCR:H321	22:A:4011:BCR:HC7	1.81	0.42
19:A:1113:CLA:C4B	22:K:4001:BCR:H323	2.49	0.42
2:B:77:TRP:HA	2:B:84:VAL:HG11	2.02	0.42
2:B:177:HIS:O	2:B:181:GLY:N	2.52	0.42
19:B:1022:CLA:C19	19:B:1207:CLA:HBB1	2.50	0.42
6:F:212:SER:C	6:F:214:PRO:HD2	2.44	0.42
8:H:100:LEU:HB2	12:L:146:THR:HG21	2.01	0.42
11:K:65:ALA:O	11:K:69:GLY:O	2.38	0.42
13:1:84:CYS:HB3	13:1:188:GLY:HA3	2.01	0.42
22:3:503:BCR:H281	19:3:614:CLA:HBB1	2.00	0.42
1:A:368:LEU:O	1:A:372:VAL:HG23	2.19	0.42
1:A:397:THR:HG22	19:A:1126:CLA:CAB	2.50	0.42
1:A:499:ALA:HA	1:A:503:THR:HG22	2.02	0.42
19:A:1141:CLA:HMB1	19:A:1141:CLA:HBB1	2.01	0.42
22:B:4009:BCR:HC8	22:B:4009:BCR:H331	2.01	0.42
7:G:148:ASN:ND2	7:G:150:TYR:CB	2.73	0.42
14:2:176:CYS:SG	14:2:177:VAL:HG13	2.59	0.42
16:4:198:LEU:C	16:4:198:LEU:HD23	2.45	0.42
17:P:59:GLU:O	17:P:59:GLU:CG	2.68	0.42
19:B:1203:CLA:H93	19:B:1203:CLA:H61	1.93	0.42
19:B:1219:CLA:H201	7:G:137:ILE:HG21	2.01	0.42
14:2:64:ARG:NE	14:2:84:ASP:OD1	2.53	0.42
15:3:265:ASN:HA	15:3:269:LEU:HD13	2.02	0.42
19:3:610:CLA:H91	19:3:610:CLA:H111	1.86	0.42
28:4:505:LUT:H181	28:4:505:LUT:H7	1.69	0.42
17:P:25:GLU:OE1	17:P:25:GLU:HA	2.20	0.42
1:A:684:PHE:HB2	19:A:1012:CLA:O1A	2.19	0.42
2:B:157:LEU:HD23	2:B:157:LEU:HA	1.78	0.42
2:B:276:HIS:HB2	19:B:1214:CLA:C1B	2.49	0.42
6:F:99:ILE:HD11	6:F:127:LYS:HG2	2.01	0.42
6:F:162:THR:N	6:F:163:PRO:CD	2.83	0.42
14:2:238:GLN:O	14:2:242:THR:OG1	2.36	0.42
15:3:143:PRO:N	15:3:144:PRO:CD	2.83	0.42
28:3:502:LUT:H28	28:3:502:LUT:C38	2.48	0.42
19:3:605:CLA:HED2	19:3:612:CLA:O1A	2.20	0.42
28:4:501:LUT:H382	19:4:601:CLA:ND	2.34	0.42
19:4:601:CLA:HBB1	19:4:601:CLA:CMB	2.49	0.42
17:P:42:ASP:O	17:P:43:GLU:HB3	2.19	0.42
19:A:1104:CLA:H42	19:A:1128:CLA:C4C	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:B:1211:CLA:HBB1	19:B:1211:CLA:CMB	2.49	0.42
22:B:4010:BCR:H15C	22:B:4010:BCR:H351	1.78	0.42
4:D:107:SER:HB3	4:D:123:MET:HE3	1.98	0.42
6:F:152:GLY:HA2	6:F:161:ILE:HD11	2.02	0.42
1:A:694:PHE:HB2	19:A:1013:CLA:HBC2	2.02	0.42
22:A:4017:BCR:HC8	22:A:4017:BCR:C33	2.43	0.42
19:L:1503:CLA:HMB1	19:L:1503:CLA:CBB	2.44	0.42
14:2:114:MET:HE3	19:2:601:CLA:HAB	2.02	0.42
22:2:503:BCR:H392	22:2:503:BCR:H282	1.47	0.42
27:4:802:DGD:O5E	27:4:802:DGD:O4E	2.33	0.42
1:A:580:PRO:HB3	1:A:727:ILE:HB	2.02	0.41
22:A:4002:BCR:H391	19:K:1401:CLA:HMC3	2.01	0.41
22:3:503:BCR:H331	22:3:503:BCR:HC7	1.75	0.41
22:A:4017:BCR:H382	22:A:4017:BCR:H23C	2.01	0.41
2:B:503:GLU:CD	2:B:503:GLU:C	2.88	0.41
2:B:646:TRP:CZ2	2:B:726:ILE:HG21	2.55	0.41
6:F:189:LYS:O	6:F:189:LYS:HD3	2.20	0.41
14:2:234:GLY:HA2	19:2:603:CLA:C3C	2.50	0.41
15:3:218:LYS:O	15:3:219:SER:C	2.63	0.41
17:P:20:GLU:HG3	17:P:97:THR:CG2	2.50	0.41
17:P:27:ILE:HD11	17:P:74:LEU:CD1	2.50	0.41
1:A:343:HIS:HA	1:A:346:LEU:HD12	2.01	0.41
3:C:9:ASP:OD2	5:E:100:ARG:CD	2.69	0.41
22:K:4001:BCR:HC7	22:K:4001:BCR:H331	1.77	0.41
28:1:501:LUT:H362	19:1:611:CLA:H43	2.01	0.41
22:2:503:BCR:H311	22:2:503:BCR:C8	2.49	0.41
19:2:605:CLA:H141	19:2:605:CLA:H161	1.92	0.41
16:4:143:VAL:O	16:4:147:ILE:HG12	2.21	0.41
1:A:126:ILE:HG22	1:A:129:GLN:NE2	2.36	0.41
1:A:742:GLY:O	1:A:745:THR:HG22	2.21	0.41
19:A:1122:CLA:H61	19:A:1122:CLA:H41	1.98	0.41
19:A:1126:CLA:C1A	19:A:1126:CLA:CGA	2.99	0.41
19:A:1138:CLA:HBC1	20:A:2001:PQN:H201	2.01	0.41
22:A:4011:BCR:H331	22:A:4011:BCR:C8	2.41	0.41
2:B:680:TRP:CE2	2:B:684:ARG:HG3	2.55	0.41
5:E:69:LYS:HD2	5:E:69:LYS:N	2.28	0.41
22:1:503:BCR:HC7	22:1:503:BCR:H331	1.85	0.41
28:4:501:LUT:H27	28:4:501:LUT:H381	1.82	0.41
29:4:610:CHL:CBB	29:4:613:CHL:HBB2	2.51	0.41
1:A:412:ALA:HA	1:A:598:VAL:HG21	2.03	0.41
1:A:455:PHE:O	19:A:1132:CLA:HBB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:A:1115:CLA:CMB	19:A:1115:CLA:HBB1	2.51	0.41
22:B:4010:BCR:H383	22:B:4010:BCR:C23	2.49	0.41
19:B:1229:CLA:HMB1	19:B:1229:CLA:CBB	2.45	0.41
3:C:31:TRP:HZ3	3:C:34:CYS:SG	2.42	0.41
4:D:149:TYR:CD1	4:D:149:TYR:N	2.89	0.41
4:D:199:ILE:CG2	4:D:200:GLU:OE1	2.69	0.41
6:F:107:LYS:HD2	6:F:108:LEU:N	2.36	0.41
7:G:114:LEU:HD23	7:G:114:LEU:H	1.86	0.41
13:1:90:ALA:O	13:1:93:GLY:N	2.54	0.41
28:1:501:LUT:H15	28:1:501:LUT:H201	1.93	0.41
15:3:122:LEU:HB2	15:3:128:ILE:HD13	2.02	0.41
15:3:172:ARG:NH2	19:3:612:CLA:O1D	2.50	0.41
1:A:265:GLY:O	1:A:266:ALA:HB3	2.20	0.41
19:A:1109:CLA:H62	19:A:1109:CLA:H41	1.69	0.41
19:B:1225:CLA:HBA2	19:B:1225:CLA:H3A	1.95	0.41
19:B:1231:CLA:H142	19:B:1232:CLA:H71	2.02	0.41
22:B:4004:BCR:H331	22:B:4004:BCR:C8	2.50	0.41
4:D:139:LEU:C	4:D:139:LEU:CD1	2.94	0.41
8:H:130:GLN:O	8:H:131:LEU:HD12	2.21	0.41
11:K:101:LEU:O	11:K:104:THR:HG22	2.20	0.41
19:1:601:CLA:HBB1	19:1:601:CLA:CMB	2.51	0.41
29:1:610:CHL:HBC3	19:1:613:CLA:CBC	2.51	0.41
19:3:605:CLA:OBD	19:3:612:CLA:O1A	2.38	0.41
16:4:73:ASP:OD1	16:4:73:ASP:C	2.63	0.41
28:4:501:LUT:H31	28:4:501:LUT:H391	1.86	0.41
1:A:216:LEU:HB2	1:A:307:ALA:HB1	2.03	0.41
19:A:1122:CLA:HMD2	19:A:1123:CLA:HAB	2.03	0.41
19:B:1203:CLA:HMA2	19:B:1226:CLA:C4B	2.50	0.41
22:B:4009:BCR:H331	22:B:4009:BCR:C8	2.51	0.41
3:C:31:TRP:HZ3	3:C:34:CYS:HG	1.69	0.41
22:F:4014:BCR:HC7	22:F:4014:BCR:H321	1.86	0.41
8:H:57:LEU:HD13	8:H:60:LEU:HD21	2.02	0.41
22:L:4020:BCR:H15C	22:L:4020:BCR:H351	1.83	0.41
14:2:81:LEU:HD22	14:2:81:LEU:N	2.34	0.41
28:2:501:LUT:H27	28:2:501:LUT:H381	1.89	0.41
19:A:1013:CLA:HMA3	19:A:1013:CLA:C2	2.50	0.41
22:A:4008:BCR:C33	22:A:4008:BCR:HC8	2.51	0.41
2:B:434:LEU:O	2:B:438:VAL:HG23	2.21	0.41
2:B:503:GLU:OE1	2:B:504:ASN:N	2.54	0.41
19:B:1213:CLA:HBB1	19:B:1213:CLA:CMB	2.51	0.41
19:B:1238:CLA:HMA1	9:I:29:GLU:OE2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:B:1229:CLA:HBC3	6:F:164:GLY:HA2	2.02	0.41
19:B:1229:CLA:HBC3	6:F:164:GLY:CA	2.51	0.41
5:E:76:ILE:O	5:E:77:LEU:HD12	2.20	0.41
6:F:210:GLY:O	6:F:213:TRP:HD1	2.03	0.41
11:K:90:GLY:O	15:3:62:LYS:NZ	2.53	0.41
28:4:501:LUT:H191	28:4:501:LUT:H11	1.93	0.41
19:A:1101:CLA:H143	28:J:4013:LUT:C34	2.51	0.41
2:B:348:VAL:O	2:B:352:MET:HG2	2.21	0.41
2:B:516:ASP:HA	2:B:519:VAL:HG12	2.03	0.41
6:F:213:TRP:CG	6:F:214:PRO:HD3	2.56	0.41
22:G:4011:BCR:C33	22:G:4011:BCR:HC8	2.51	0.41
11:K:109:VAL:HG22	22:K:4002:BCR:H341	2.02	0.41
22:K:4001:BCR:H24C	22:K:4001:BCR:H371	1.98	0.41
13:1:64:LEU:HD23	13:1:66:LEU:HD21	2.03	0.41
19:1:605:CLA:H41	19:1:605:CLA:H62	1.94	0.41
15:3:117:ILE:HD11	15:3:252:PRO:HB2	2.03	0.41
19:4:601:CLA:H62	19:4:602:CLA:HMA2	2.03	0.41
1:A:356:ALA:CB	22:A:4007:BCR:H313	2.45	0.41
1:A:665:ILE:HD12	2:B:621:ARG:HG3	2.02	0.41
19:A:1125:CLA:HMB3	19:A:1133:CLA:H43	2.02	0.41
2:B:733:PHE:O	8:H:138:ARG:NE	2.49	0.41
14:2:132:LEU:HD11	14:2:134:THR:HG23	2.01	0.41
16:4:214:ALA:HB1	28:4:501:LUT:H8	2.03	0.41
2:B:284:PHE:CE1	19:B:1216:CLA:HAB	2.46	0.40
22:K:4002:BCR:HC7	22:K:4002:BCR:H331	1.68	0.40
22:L:4020:BCR:H403	22:L:4020:BCR:C23	2.51	0.40
15:3:229:LYS:NZ	23:3:801:LHG:O5	2.52	0.40
17:P:28:VAL:O	17:P:28:VAL:CG2	2.69	0.40
19:A:1128:CLA:H162	19:A:1140:CLA:HMA3	2.02	0.40
22:A:4007:BCR:C33	22:A:4007:BCR:HC8	2.52	0.40
2:B:69:ALA:HB2	2:B:135:LEU:HB2	2.03	0.40
2:B:674:LEU:O	2:B:677:THR:HG22	2.20	0.40
22:B:4006:BCR:HC7	22:B:4006:BCR:H331	1.84	0.40
13:1:112:ALA:HB1	13:1:131:LEU:HD12	2.03	0.40
17:P:38:ASN:OD1	17:P:40:VAL:HG23	2.21	0.40
19:A:1102:CLA:H11	19:A:1109:CLA:H92	2.02	0.40
19:A:1119:CLA:HBB1	19:A:1119:CLA:CMB	2.51	0.40
22:A:4017:BCR:C27	20:B:2002:PQN:H142	2.51	0.40
2:B:309:ILE:HG23	2:B:309:ILE:O	2.22	0.40
2:B:490:ARG:HB3	7:G:153:LYS:HZ2	1.86	0.40
3:C:31:TRP:CZ2	3:C:33:GLY:HA3	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:2:200:TRP:CZ2	29:2:615:CHL:C1D	2.98	0.40
28:3:501:LUT:H31	28:3:501:LUT:H391	1.87	0.40
28:3:501:LUT:H381	28:3:501:LUT:H27	1.67	0.40
28:4:501:LUT:H181	28:4:501:LUT:H8	2.02	0.40
28:4:501:LUT:H30	19:4:601:CLA:H93	2.04	0.40
1:A:255:LEU:HD13	1:A:262:PHE:CE1	2.57	0.40
1:A:515:TRP:CH2	19:A:1125:CLA:HBC2	2.56	0.40
19:A:1132:CLA:HAC1	19:B:1206:CLA:HBB2	2.03	0.40
19:B:1207:CLA:C19	9:I:15:LEU:CD1	2.88	0.40
19:B:1218:CLA:H201	13:1:139:PHE:HA	2.04	0.40
4:D:176:GLU:CD	4:D:176:GLU:H	2.29	0.40
22:2:503:BCR:H383	19:2:606:CLA:CAB	2.51	0.40
15:3:274:PHE:CD1	15:3:275:HIS:N	2.89	0.40
1:A:177:LEU:HD22	19:A:1108:CLA:HBC1	2.02	0.40
1:A:538:ASP:HA	1:A:541:VAL:HG12	2.04	0.40
1:A:716:VAL:O	1:A:716:VAL:HG22	2.21	0.40
2:B:294:ASN:O	7:G:110:GLU:HG3	2.22	0.40
2:B:418:ILE:HG23	19:B:1236:CLA:HBB2	2.03	0.40
19:B:1225:CLA:HBB1	19:B:1225:CLA:HMB1	2.04	0.40
3:C:58:CYS:HA	21:C:3003:SF4:S2	2.62	0.40
6:F:95:GLU:C	6:F:95:GLU:OE2	2.64	0.40
7:G:129:LEU:HA	22:G:4011:BCR:H362	2.03	0.40
19:1:607:CLA:HBB1	19:1:607:CLA:HMB3	2.03	0.40
15:3:107:ARG:HB3	19:3:601:CLA:HBC3	2.04	0.40
19:3:610:CLA:HMB1	19:3:610:CLA:CBB	2.49	0.40
16:4:103:MET:HE3	19:4:601:CLA:CMC	2.49	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	739/743 (100%)	710 (96%)	29 (4%)	0	100	100
2	B	731/733 (100%)	698 (96%)	33 (4%)	0	100	100
3	C	78/80 (98%)	72 (92%)	6 (8%)	0	100	100
4	D	141/143 (99%)	134 (95%)	6 (4%)	1 (1%)	18	32
5	E	64/66 (97%)	59 (92%)	5 (8%)	0	100	100
6	F	152/154 (99%)	149 (98%)	3 (2%)	0	100	100
7	G	95/97 (98%)	94 (99%)	1 (1%)	0	100	100
8	H	91/93 (98%)	86 (94%)	5 (6%)	0	100	100
9	I	29/31 (94%)	26 (90%)	3 (10%)	0	100	100
10	J	40/42 (95%)	40 (100%)	0	0	100	100
11	K	79/81 (98%)	72 (91%)	7 (9%)	0	100	100
12	L	157/159 (99%)	147 (94%)	10 (6%)	0	100	100
13	1	191/193 (99%)	182 (95%)	9 (5%)	0	100	100
14	2	206/208 (99%)	194 (94%)	12 (6%)	0	100	100
15	3	219/221 (99%)	202 (92%)	15 (7%)	2 (1%)	14	26
16	4	196/198 (99%)	183 (93%)	13 (7%)	0	100	100
17	P	97/99 (98%)	87 (90%)	9 (9%)	1 (1%)	12	22
All	All	3305/3341 (99%)	3135 (95%)	166 (5%)	4 (0%)	49	69

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
15	3	86	PRO
15	3	87	GLU
4	D	107	SER
17	P	50	VAL

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	602/602 (100%)	600 (100%)	2 (0%)	86	92
2	B	598/598 (100%)	598 (100%)	0	100	100
3	C	69/69 (100%)	68 (99%)	1 (1%)	59	74
4	D	122/122 (100%)	122 (100%)	0	100	100
5	E	58/58 (100%)	58 (100%)	0	100	100
6	F	125/126 (99%)	123 (98%)	2 (2%)	55	72
7	G	82/82 (100%)	82 (100%)	0	100	100
8	H	75/75 (100%)	75 (100%)	0	100	100
9	I	27/27 (100%)	26 (96%)	1 (4%)	30	52
10	J	35/35 (100%)	35 (100%)	0	100	100
11	K	59/59 (100%)	59 (100%)	0	100	100
12	L	126/126 (100%)	126 (100%)	0	100	100
13	1	158/158 (100%)	158 (100%)	0	100	100
14	2	167/167 (100%)	167 (100%)	0	100	100
15	3	171/172 (99%)	171 (100%)	0	100	100
16	4	164/164 (100%)	164 (100%)	0	100	100
17	P	79/79 (100%)	75 (95%)	4 (5%)	21	39
All	All	2717/2719 (100%)	2707 (100%)	10 (0%)	81	90

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	96	MET
1	A	707	ILE
3	C	4	SER
6	F	132	ASN
6	F	199	ASP
9	I	2	ILE
17	P	1	VAL
17	P	15	VAL
17	P	27	ILE
17	P	28	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	62	HIS
1	A	251	ASN
1	A	301	HIS
1	A	543	HIS
1	A	574	ASN
1	A	712	ASN
2	B	89	HIS
2	B	585	ASN
2	B	627	ASN
5	E	114	ASN
6	F	90	GLN
6	F	223	ASN
8	H	79	ASN
11	K	112	HIS
13	1	223	HIS
14	2	212	GLN
14	2	224	ASN
14	2	249	ASN
15	3	185	GLN
15	3	199	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	SNK	A	636	1	11,14,15	1.27	2 (18%)	8,18,20	2.10	4 (50%)
1	SNK	A	115	1	11,14,15	1.38	2 (18%)	8,18,20	2.11	3 (37%)

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
1	SNK	A	636	1	1/1/2/3	6/8/10/12	0/1/1/1
1	SNK	A	115	1	-	5/8/10/12	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	115	SNK	CE1-ND1	2.68	1.39	1.35
1	A	636	SNK	CE1-ND1	2.47	1.39	1.35
1	A	636	SNK	C02-S04	2.31	1.85	1.77
1	A	115	SNK	C02-S04	2.28	1.85	1.77

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	115	SNK	CE1-NE2-CD2	3.46	106.04	103.50
1	A	636	SNK	CE1-NE2-CD2	3.34	105.96	103.50
1	A	115	SNK	ND1-CE1-NE2	-2.65	109.91	112.98
1	A	115	SNK	C01-C02-S04	2.60	122.95	112.63
1	A	636	SNK	C01-C02-S04	2.58	122.85	112.63
1	A	636	SNK	ND1-CE1-NE2	-2.48	110.10	112.98
1	A	636	SNK	CG-CD2-S04	2.44	128.63	125.80

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	636	SNK	CA

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	115	SNK	CG-CD2-S04-C02
1	A	115	SNK	C01-C02-S04-CD2
1	A	115	SNK	O03-C02-S04-CD2
1	A	636	SNK	O-C-CA-CB
1	A	636	SNK	CG-CD2-S04-C02
1	A	115	SNK	CA-CB-CG-ND1
1	A	115	SNK	C-CA-CB-CG
1	A	636	SNK	C-CA-CB-CG

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Mol	Chain	Res	Type	Atoms
1	A	636	SNK	C01-C02-S04-CD2
1	A	636	SNK	N-CA-CB-CG
1	A	636	SNK	O03-C02-S04-CD2

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 243 ligands modelled in this entry, 3 are monoatomic - leaving 240 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
25	LMG	F	5002	-	47,47,55	1.09	4 (8%)	55,55,63	1.12	4 (7%)
22	BCR	J	4012	-	41,41,41	1.58	4 (9%)	56,56,56	4.72	17 (30%)
18	CL0	A	1011	-	58,73,73	3.20	17 (29%)	60,113,113	2.50	15 (25%)
19	CLA	1	608	-	50,54,73	1.58	7 (14%)	59,90,113	2.07	11 (18%)
22	BCR	L	4020	-	41,41,41	1.59	4 (9%)	56,56,56	4.62	18 (32%)
19	CLA	B	1209	-	50,54,73	1.58	7 (14%)	59,90,113	2.00	12 (20%)
22	BCR	B	4010	-	41,41,41	1.58	4 (9%)	56,56,56	4.64	20 (35%)
19	CLA	2	608	-	54,58,73	1.53	6 (11%)	64,95,113	2.08	17 (26%)
25	LMG	B	5003	-	35,35,55	0.80	1 (2%)	43,43,63	1.16	4 (9%)
25	LMG	2	804	-	30,30,55	0.54	0	38,38,63	1.09	2 (5%)
20	PQN	B	2002	-	34,34,34	0.42	0	43,45,45	1.15	3 (6%)
19	CLA	4	606	-	54,58,73	1.52	5 (9%)	64,95,113	2.00	13 (20%)
29	CHL	2	613	-	40,54,74	1.62	8 (20%)	34,90,114	2.16	8 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	CHL	2	615	-	50,64,74	1.48	8 (16%)	46,102,114	1.92	12 (26%)
19	CLA	1	613	-	49,53,73	1.62	8 (16%)	58,89,113	2.03	11 (18%)
22	BCR	B	4004	-	41,41,41	1.61	4 (9%)	56,56,56	4.97	17 (30%)
19	CLA	B	1235	-	69,73,73	1.35	8 (11%)	82,113,113	1.84	14 (17%)
19	CLA	A	1118	-	54,58,73	1.52	6 (11%)	64,95,113	2.04	14 (21%)
22	BCR	A	4002	-	41,41,41	1.62	4 (9%)	56,56,56	4.46	22 (39%)
24	LMT	B	5008	-	32,32,36	1.20	5 (15%)	43,43,47	1.00	3 (6%)
21	SF4	C	3002	3	0,12,12	-	-	-		
19	CLA	B	1228	-	64,68,73	1.42	7 (10%)	76,107,113	1.87	15 (19%)
22	BCR	A	4011	-	41,41,41	1.58	4 (9%)	56,56,56	4.60	21 (37%)
19	CLA	A	1121	-	64,68,73	1.40	7 (10%)	76,107,113	1.93	16 (21%)
19	CLA	A	1108	-	54,58,73	1.53	6 (11%)	64,95,113	2.02	13 (20%)
23	LHG	A	5001	-	39,39,48	0.43	0	42,45,54	1.03	2 (4%)
22	BCR	F	4014	-	41,41,41	1.60	4 (9%)	56,56,56	4.63	19 (33%)
19	CLA	B	1203	2	69,73,73	1.35	6 (8%)	82,113,113	1.78	13 (15%)
19	CLA	A	1125	-	69,73,73	1.36	7 (10%)	82,113,113	1.86	15 (18%)
19	CLA	B	1240	23	69,73,73	1.36	7 (10%)	82,113,113	1.81	15 (18%)
19	CLA	A	1119	-	69,73,73	1.37	6 (8%)	82,113,113	1.85	15 (18%)
25	LMG	2	803	-	36,36,55	0.73	2 (5%)	44,44,63	1.08	2 (4%)
19	CLA	A	1133	-	69,73,73	1.35	7 (10%)	82,113,113	1.75	13 (15%)
19	CLA	F	1302	6	69,73,73	1.36	6 (8%)	82,113,113	1.83	16 (19%)
19	CLA	L	1502	-	64,68,73	1.40	7 (10%)	76,107,113	1.95	17 (22%)
19	CLA	3	617	-	64,68,73	1.40	6 (9%)	76,107,113	1.91	15 (19%)
22	BCR	A	4017	-	41,41,41	1.60	4 (9%)	56,56,56	5.08	20 (35%)
19	CLA	1	602	13	50,54,73	1.57	6 (12%)	59,90,113	1.96	12 (20%)
19	CLA	B	1232	-	59,63,73	1.47	7 (11%)	70,101,113	1.93	13 (18%)
27	DGD	B	5005	-	62,62,67	1.21	6 (9%)	76,76,81	1.01	3 (3%)
28	LUT	4	505	-	42,43,43	2.38	1 (2%)	51,60,60	2.37	19 (37%)
29	CHL	3	611	-	41,55,74	1.72	8 (19%)	35,91,114	2.09	10 (28%)
19	CLA	B	1221	-	69,73,73	1.36	7 (10%)	82,113,113	1.86	14 (17%)
19	CLA	2	602	-	56,60,73	1.49	6 (10%)	65,97,113	2.01	19 (29%)
28	LUT	3	502	-	42,43,43	2.33	1 (2%)	51,60,60	1.78	16 (31%)
19	CLA	B	1211	-	69,73,73	1.33	6 (8%)	82,113,113	1.79	16 (19%)
25	LMG	2	805	-	30,30,55	0.56	0	38,38,63	1.09	3 (7%)
19	CLA	A	1139	-	69,73,73	1.37	7 (10%)	82,113,113	1.84	17 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	CLA	B	1237	-	69,73,73	1.36	7 (10%)	82,113,113	1.78	13 (15%)
21	SF4	C	3003	3	0,12,12	-	-	-		
25	LMG	F	5001	-	30,30,55	0.53	0	38,38,63	1.07	2 (5%)
19	CLA	A	1104	-	69,73,73	1.34	7 (10%)	82,113,113	1.83	16 (19%)
19	CLA	B	1213	-	64,68,73	1.40	7 (10%)	76,107,113	1.86	14 (18%)
19	CLA	4	604	16	64,68,73	1.40	6 (9%)	76,107,113	1.93	15 (19%)
22	BCR	H	4021	-	41,41,41	1.59	4 (9%)	56,56,56	4.73	19 (33%)
27	DGD	4	802	-	51,51,67	0.95	2 (3%)	65,65,81	0.99	4 (6%)
22	BCR	A	4003	-	41,41,41	1.59	4 (9%)	56,56,56	4.59	22 (39%)
22	BCR	I	4018	-	41,41,41	1.61	5 (12%)	56,56,56	4.60	25 (44%)
19	CLA	4	601	16	64,68,73	1.42	7 (10%)	76,107,113	1.90	16 (21%)
19	CLA	4	617	-	69,73,73	1.33	6 (8%)	82,113,113	1.86	17 (20%)
25	LMG	1	802	-	46,46,55	1.04	3 (6%)	54,54,63	1.02	2 (3%)
19	CLA	B	1217	-	50,54,73	1.57	6 (12%)	59,90,113	2.00	11 (18%)
19	CLA	G	1601	-	59,63,73	1.47	6 (10%)	70,101,113	1.95	15 (21%)
19	CLA	3	606	-	54,58,73	1.51	6 (11%)	64,95,113	2.02	14 (21%)
19	CLA	B	1208	-	64,68,73	1.40	6 (9%)	76,107,113	1.84	14 (18%)
25	LMG	3	802	-	30,30,55	0.56	0	38,38,63	1.10	3 (7%)
22	BCR	1	504	-	41,41,41	1.61	4 (9%)	56,56,56	4.81	19 (33%)
25	LMG	B	5004	-	33,33,55	0.53	0	41,41,63	1.23	5 (12%)
19	CLA	K	1404	-	50,54,73	1.58	7 (14%)	59,90,113	1.99	11 (18%)
27	DGD	G	5003	-	48,48,67	0.89	2 (4%)	62,62,81	0.98	3 (4%)
19	CLA	1	614	13	64,68,73	1.40	7 (10%)	76,107,113	1.85	14 (18%)
19	CLA	B	1231	-	64,68,73	1.40	6 (9%)	76,107,113	1.88	15 (19%)
20	PQN	A	2001	-	34,34,34	0.38	0	43,45,45	1.15	3 (6%)
19	CLA	3	610	15	69,73,73	1.35	6 (8%)	82,113,113	1.81	15 (18%)
25	LMG	F	5006	-	13,13,55	0.58	0	18,18,63	0.71	0
21	SF4	A	3001	2,1	0,12,12	-	-	-		
19	CLA	B	1227	-	69,73,73	1.34	6 (8%)	82,113,113	1.86	16 (19%)
19	CLA	G	1602	7	50,54,73	1.59	7 (14%)	59,90,113	2.06	13 (22%)
19	CLA	A	1013	-	69,73,73	1.34	7 (10%)	82,113,113	1.77	15 (18%)
19	CLA	4	612	16	69,73,73	1.36	7 (10%)	82,113,113	1.79	14 (17%)
19	CLA	A	1132	-	69,73,73	1.35	6 (8%)	82,113,113	1.85	16 (19%)
19	CLA	B	1220	-	59,63,73	1.46	7 (11%)	70,101,113	1.91	14 (20%)
19	CLA	B	1223	-	69,73,73	1.36	8 (11%)	82,113,113	1.88	17 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	LMT	2	808	-	36,36,36	1.12	5 (13%)	47,47,47	0.97	2 (4%)
19	CLA	3	605	-	59,63,73	1.48	8 (13%)	70,101,113	2.00	17 (24%)
25	LMG	A	5006	-	50,50,55	1.18	5 (10%)	58,58,63	1.06	3 (5%)
19	CLA	A	1135	-	55,59,73	1.51	6 (10%)	64,96,113	2.05	14 (21%)
19	CLA	A	1113	-	49,53,73	1.60	7 (14%)	58,89,113	2.00	13 (22%)
19	CLA	B	1023	-	69,73,73	1.37	5 (7%)	82,113,113	1.70	13 (15%)
24	LMT	G	5005	-	32,32,36	1.18	4 (12%)	43,43,47	0.97	2 (4%)
19	CLA	A	1105	-	64,68,73	1.41	6 (9%)	76,107,113	1.86	13 (17%)
19	CLA	B	1222	33	69,73,73	1.34	7 (10%)	82,113,113	1.85	16 (19%)
19	CLA	K	1402	-	64,68,73	1.40	6 (9%)	76,107,113	1.90	14 (18%)
28	LUT	1	502	-	42,43,43	2.41	1 (2%)	51,60,60	2.05	14 (27%)
19	CLA	1	606	-	54,58,73	1.52	6 (11%)	64,95,113	2.01	15 (23%)
19	CLA	B	1234	-	59,63,73	1.46	5 (8%)	70,101,113	1.95	13 (18%)
19	CLA	2	601	14	64,68,73	1.42	7 (10%)	76,107,113	1.93	17 (22%)
27	DGD	F	5005	-	58,58,67	1.14	6 (10%)	72,72,81	1.04	5 (6%)
19	CLA	A	1130	-	59,63,73	1.47	7 (11%)	70,101,113	1.92	14 (20%)
19	CLA	A	1107	1	69,73,73	1.36	6 (8%)	82,113,113	1.81	15 (18%)
19	CLA	1	607	-	50,54,73	1.58	7 (14%)	59,90,113	2.04	10 (16%)
19	CLA	3	601	15	59,63,73	1.48	7 (11%)	70,101,113	1.91	14 (20%)
19	CLA	A	1122	-	69,73,73	1.35	7 (10%)	82,113,113	1.87	15 (18%)
25	LMG	F	5003	-	36,36,55	0.79	1 (2%)	44,44,63	1.03	2 (4%)
25	LMG	F	5004	-	34,34,55	0.50	0	42,42,63	1.10	3 (7%)
19	CLA	3	608	-	52,56,73	1.55	7 (13%)	61,92,113	2.06	13 (21%)
19	CLA	2	607	-	64,68,73	1.40	7 (10%)	76,107,113	2.00	17 (22%)
19	CLA	A	1012	-	69,73,73	1.36	7 (10%)	82,113,113	1.81	15 (18%)
19	CLA	A	1136	-	69,73,73	1.35	7 (10%)	82,113,113	1.82	14 (17%)
22	BCR	B	4009	-	41,41,41	1.58	4 (9%)	56,56,56	4.36	21 (37%)
19	CLA	A	1111	-	69,73,73	1.34	7 (10%)	82,113,113	1.79	13 (15%)
19	CLA	A	1120	-	64,68,73	1.41	6 (9%)	76,107,113	1.85	14 (18%)
22	BCR	A	4007	-	41,41,41	1.62	4 (9%)	56,56,56	4.76	20 (35%)
22	BCR	B	4005	-	41,41,41	1.56	4 (9%)	56,56,56	4.56	17 (30%)
24	LMT	G	5004	-	36,36,36	1.12	5 (13%)	47,47,47	0.98	2 (4%)
28	LUT	1	501	-	42,43,43	2.39	1 (2%)	51,60,60	2.10	20 (39%)
19	CLA	A	1114	-	50,54,73	1.57	7 (14%)	59,90,113	2.10	12 (20%)
19	CLA	B	1212	-	59,63,73	1.46	8 (13%)	70,101,113	2.00	16 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	CLA	G	1603	-	69,73,73	1.36	6 (8%)	82,113,113	1.81	14 (17%)
28	LUT	2	501	-	42,43,43	2.40	1 (2%)	51,60,60	2.14	18 (35%)
29	CHL	4	611	-	45,59,74	1.64	9 (20%)	40,96,114	2.00	11 (27%)
19	CLA	B	1224	-	69,73,73	1.36	7 (10%)	82,113,113	1.85	14 (17%)
22	BCR	3	503	-	41,41,41	1.59	5 (12%)	56,56,56	4.46	18 (32%)
19	CLA	A	1141	-	64,68,73	1.40	7 (10%)	76,107,113	1.88	15 (19%)
19	CLA	A	1106	1	69,73,73	1.34	7 (10%)	82,113,113	1.87	16 (19%)
19	CLA	L	1503	-	54,58,73	1.53	7 (12%)	64,95,113	2.06	18 (28%)
19	CLA	B	1238	33	69,73,73	1.35	5 (7%)	82,113,113	1.84	12 (14%)
22	BCR	1	503	-	41,41,41	1.58	4 (9%)	56,56,56	4.83	22 (39%)
19	CLA	B	1218	-	69,73,73	1.35	7 (10%)	82,113,113	1.85	16 (19%)
25	LMG	B	5007	-	34,34,55	0.51	0	42,42,63	1.08	2 (4%)
29	CHL	1	612	13	55,69,74	1.43	8 (14%)	52,108,114	1.80	10 (19%)
28	LUT	J	4013	-	42,43,43	2.40	1 (2%)	51,60,60	2.00	13 (25%)
19	CLA	B	1206	2	69,73,73	1.35	6 (8%)	82,113,113	1.83	13 (15%)
22	BCR	F	4016	-	41,41,41	1.57	4 (9%)	56,56,56	4.48	17 (30%)
23	LHG	2	801	-	34,34,48	0.46	0	37,40,54	1.11	3 (8%)
22	BCR	K	4002	-	41,41,41	1.56	4 (9%)	56,56,56	4.58	21 (37%)
19	CLA	J	1901	10	54,58,73	1.53	7 (12%)	64,95,113	1.99	14 (21%)
19	CLA	1	601	13	69,73,73	1.38	7 (10%)	82,113,113	1.79	14 (17%)
19	CLA	A	1117	-	69,73,73	1.35	6 (8%)	82,113,113	1.82	15 (18%)
19	CLA	2	603	14	69,73,73	1.34	6 (8%)	82,113,113	1.83	15 (18%)
22	BCR	I	4020	-	41,41,41	1.61	4 (9%)	56,56,56	4.58	20 (35%)
19	CLA	4	605	-	64,68,73	1.42	8 (12%)	76,107,113	1.91	16 (21%)
22	BCR	L	4019	-	41,41,41	1.61	4 (9%)	56,56,56	4.75	20 (35%)
25	LMG	2	802	-	25,25,55	0.57	0	33,33,63	1.23	3 (9%)
29	CHL	2	611	-	42,56,74	1.68	9 (21%)	36,92,114	2.06	10 (27%)
19	CLA	A	1109	-	69,73,73	1.35	7 (10%)	82,113,113	1.89	17 (20%)
29	CHL	1	609	13	50,64,74	1.69	8 (16%)	46,102,114	1.84	9 (19%)
29	CHL	4	610	-	41,55,74	1.82	10 (24%)	35,91,114	2.03	11 (31%)
25	LMG	G	5002	-	50,50,55	1.18	5 (10%)	58,58,63	1.18	4 (6%)
19	CLA	B	1226	-	69,73,73	1.36	6 (8%)	82,113,113	1.84	14 (17%)
19	CLA	3	603	-	59,63,73	1.45	6 (10%)	70,101,113	2.07	18 (25%)
19	CLA	A	1124	-	59,63,73	1.48	7 (11%)	70,101,113	1.90	14 (20%)
19	CLA	A	1134	1	59,63,73	1.45	6 (10%)	70,101,113	1.93	14 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	CLA	2	604	14	69,73,73	1.36	6 (8%)	82,113,113	1.84	15 (18%)
19	CLA	B	1202	-	69,73,73	1.32	6 (8%)	82,113,113	1.92	17 (20%)
23	LHG	B	5001	19	20,20,48	0.59	0	23,26,54	1.53	3 (13%)
19	CLA	A	1101	-	69,73,73	1.35	7 (10%)	82,113,113	1.84	15 (18%)
19	CLA	B	1230	-	62,66,73	1.43	6 (9%)	73,104,113	1.96	17 (23%)
19	CLA	1	605	-	69,73,73	1.36	6 (8%)	82,113,113	1.89	15 (18%)
19	CLA	4	607	-	64,68,73	1.40	7 (10%)	76,107,113	1.89	14 (18%)
19	CLA	B	1204	-	69,73,73	1.36	7 (10%)	82,113,113	1.83	16 (19%)
19	CLA	B	1214	-	69,73,73	1.36	7 (10%)	82,113,113	1.85	16 (19%)
22	BCR	K	4001	-	41,41,41	1.59	5 (12%)	56,56,56	4.75	16 (28%)
19	CLA	3	613	-	50,54,73	1.60	7 (14%)	59,90,113	2.05	12 (20%)
19	CLA	A	1138	-	69,73,73	1.35	7 (10%)	82,113,113	1.78	13 (15%)
25	LMG	G	5001	-	49,49,55	1.14	4 (8%)	57,57,63	1.22	4 (7%)
22	BCR	A	4008	-	41,41,41	1.59	5 (12%)	56,56,56	4.60	25 (44%)
27	DGD	J	5001	-	59,59,67	1.16	6 (10%)	73,73,81	1.01	2 (2%)
19	CLA	2	612	-	59,63,73	1.45	7 (11%)	70,101,113	1.90	13 (18%)
30	XAT	2	502	-	41,47,47	0.71	1 (2%)	54,74,74	1.99	14 (25%)
31	3PH	2	807	-	32,32,47	1.04	4 (12%)	35,37,52	1.20	2 (5%)
29	CHL	4	613	-	55,69,74	1.59	10 (18%)	52,108,114	1.76	10 (19%)
29	CHL	4	615	16	37,51,74	1.66	8 (21%)	30,86,114	2.28	10 (33%)
30	XAT	4	502	-	41,47,47	0.69	1 (2%)	54,74,74	1.76	15 (27%)
19	CLA	B	1205	-	69,73,73	1.34	6 (8%)	82,113,113	1.87	14 (17%)
22	BCR	3	506	-	41,41,41	1.59	4 (9%)	56,56,56	4.66	21 (37%)
19	CLA	2	606	-	54,58,73	1.54	6 (11%)	64,95,113	2.00	14 (21%)
19	CLA	3	607	-	56,60,73	1.50	6 (10%)	65,97,113	2.02	15 (23%)
19	CLA	A	1127	-	69,73,73	1.36	6 (8%)	82,113,113	1.72	15 (18%)
19	CLA	K	1401	-	49,53,73	1.60	7 (14%)	58,89,113	2.07	11 (18%)
19	CLA	4	603	-	69,73,73	1.34	7 (10%)	82,113,113	1.89	15 (18%)
27	DGD	3	803	-	52,52,67	0.94	3 (5%)	66,66,81	1.07	3 (4%)
19	CLA	A	1126	-	69,73,73	1.38	6 (8%)	82,113,113	1.87	16 (19%)
19	CLA	B	1021	-	69,73,73	1.35	7 (10%)	82,113,113	1.88	15 (18%)
22	BCR	G	4011	-	41,41,41	1.63	4 (9%)	56,56,56	4.63	21 (37%)
19	CLA	4	608	-	50,54,73	1.57	7 (14%)	59,90,113	2.04	14 (23%)
27	DGD	1	803	-	42,42,67	0.88	1 (2%)	56,56,81	1.01	2 (3%)
19	CLA	B	1225	-	69,73,73	1.35	6 (8%)	82,113,113	1.79	14 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	CLA	B	1201	-	69,73,73	1.35	7 (10%)	82,113,113	1.78	15 (18%)
19	CLA	A	1103	-	69,73,73	1.33	6 (8%)	82,113,113	1.84	13 (15%)
19	CLA	B	1210	-	69,73,73	1.36	8 (11%)	82,113,113	1.86	16 (19%)
28	LUT	3	501	-	42,43,43	2.44	1 (2%)	51,60,60	2.08	16 (31%)
19	CLA	A	1102	-	69,73,73	1.35	7 (10%)	82,113,113	1.92	16 (19%)
19	CLA	B	1219	-	69,73,73	1.35	8 (11%)	82,113,113	1.86	13 (15%)
19	CLA	H	1701	-	64,68,73	1.40	6 (9%)	76,107,113	1.82	13 (17%)
19	CLA	4	602	-	54,58,73	1.52	7 (12%)	64,95,113	2.02	16 (25%)
24	LMT	B	5006	-	33,33,36	1.17	5 (15%)	44,44,47	0.93	2 (4%)
19	CLA	A	1112	-	69,73,73	1.36	6 (8%)	82,113,113	1.84	16 (19%)
19	CLA	2	605	-	69,73,73	1.35	8 (11%)	82,113,113	1.82	14 (17%)
19	CLA	A	1128	-	69,73,73	1.35	8 (11%)	82,113,113	1.80	15 (18%)
19	CLA	1	603	-	59,63,73	1.46	6 (10%)	70,101,113	2.00	16 (22%)
19	CLA	A	1140	-	69,73,73	1.33	7 (10%)	82,113,113	1.83	16 (19%)
19	CLA	K	1403	-	52,56,73	1.56	7 (13%)	61,92,113	2.14	15 (24%)
19	CLA	B	1215	-	69,73,73	1.34	6 (8%)	82,113,113	1.87	14 (17%)
19	CLA	B	1207	-	69,73,73	1.34	8 (11%)	82,113,113	1.78	16 (19%)
22	BCR	2	503	-	41,41,41	1.66	5 (12%)	56,56,56	5.63	27 (48%)
29	CHL	1	610	13	41,55,74	1.70	8 (19%)	35,91,114	2.10	10 (28%)
19	CLA	B	1022	-	69,73,73	1.35	7 (10%)	82,113,113	1.83	17 (20%)
19	CLA	B	1216	-	69,73,73	1.36	6 (8%)	82,113,113	1.77	14 (17%)
19	CLA	B	1229	-	69,73,73	1.35	6 (8%)	82,113,113	1.84	16 (19%)
23	LHG	1	801	-	48,48,48	0.40	0	51,54,54	0.98	2 (3%)
19	CLA	1	611	-	69,73,73	1.36	6 (8%)	82,113,113	1.78	13 (15%)
19	CLA	B	1236	-	54,58,73	1.52	6 (11%)	64,95,113	2.06	17 (26%)
19	CLA	A	1123	-	69,73,73	1.36	6 (8%)	82,113,113	1.84	12 (14%)
24	LMT	A	5004	-	36,36,36	1.13	5 (13%)	47,47,47	1.02	2 (4%)
23	LHG	A	5002	-	48,48,48	0.40	0	51,54,54	1.12	4 (7%)
19	CLA	L	1501	12	54,58,73	1.52	7 (12%)	64,95,113	2.07	16 (25%)
19	CLA	A	1116	-	60,64,73	1.46	8 (13%)	71,102,113	2.03	16 (22%)
23	LHG	4	801	-	34,34,48	0.47	0	37,40,54	1.20	3 (8%)
25	LMG	2	806	-	13,13,55	0.55	0	18,18,63	0.57	0
19	CLA	B	1239	-	69,73,73	1.35	6 (8%)	82,113,113	1.86	16 (19%)
19	CLA	A	1131	-	69,73,73	1.35	7 (10%)	82,113,113	1.77	14 (17%)
25	LMG	G	5006	-	25,25,55	0.59	0	33,33,63	1.08	3 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	BCR	B	4006	-	41,41,41	1.58	4 (9%)	56,56,56	4.54	28 (50%)
23	LHG	B	5002	-	48,48,48	0.40	0	51,54,54	1.05	4 (7%)
28	LUT	4	501	-	42,43,43	2.35	1 (2%)	51,60,60	2.14	17 (33%)
19	CLA	A	1129	-	69,73,73	1.36	7 (10%)	82,113,113	1.92	17 (20%)
19	CLA	4	609	16	54,58,73	1.53	7 (12%)	64,95,113	2.00	14 (21%)
19	CLA	F	1301	-	69,73,73	1.36	7 (10%)	82,113,113	1.78	13 (15%)
19	CLA	A	1115	-	69,73,73	1.36	7 (10%)	82,113,113	1.80	15 (18%)
29	CHL	2	609	14	60,74,74	1.43	8 (13%)	58,114,114	1.63	10 (17%)
19	CLA	1	604	13	69,73,73	1.36	7 (10%)	82,113,113	1.81	14 (17%)
19	CLA	3	612	15	54,58,73	1.52	7 (12%)	64,95,113	2.03	14 (21%)
19	CLA	3	614	-	46,50,73	1.65	6 (13%)	53,85,113	2.13	11 (20%)
29	CHL	3	604	15	60,74,74	1.35	9 (15%)	58,114,114	1.70	12 (20%)
23	LHG	3	801	-	16,16,48	0.88	1 (6%)	17,20,54	0.69	0
29	CHL	2	610	-	50,64,74	1.35	8 (16%)	46,102,114	1.89	11 (23%)
19	CLA	A	1110	-	59,63,73	1.45	6 (10%)	70,101,113	1.99	14 (20%)
19	CLA	3	602	-	56,60,73	1.50	7 (12%)	65,97,113	2.02	16 (24%)
19	CLA	A	1137	-	69,73,73	1.34	7 (10%)	82,113,113	1.84	14 (17%)

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
25	LMG	F	5002	-	-	11/42/62/70	0/1/1/1
22	BCR	J	4012	-	-	6/29/63/63	0/2/2/2
18	CL0	A	1011	-	3/3/20/25	9/37/135/135	-
19	CLA	1	608	-	1/1/11/20	7/17/93/115	-
22	BCR	L	4020	-	-	7/29/63/63	0/2/2/2
19	CLA	B	1209	-	1/1/11/20	4/17/93/115	-
22	BCR	B	4010	-	-	8/29/63/63	0/2/2/2
19	CLA	2	608	-	1/1/12/20	7/21/97/115	-
25	LMG	B	5003	-	-	8/30/50/70	0/1/1/1
25	LMG	2	804	-	-	5/25/45/70	0/1/1/1
20	PQN	B	2002	-	-	5/23/43/43	0/2/2/2
19	CLA	4	606	-	1/1/12/20	5/21/97/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CHL	2	613	-	3/3/16/26	4/15/113/137	-
29	CHL	2	615	-	4/4/18/26	5/27/125/137	-
19	CLA	1	613	-	1/1/11/20	4/15/91/115	-
22	BCR	B	4004	-	-	10/29/63/63	0/2/2/2
19	CLA	B	1235	-	1/1/15/20	11/39/115/115	-
19	CLA	A	1118	-	1/1/12/20	6/21/97/115	-
22	BCR	A	4002	-	-	7/29/63/63	0/2/2/2
24	LMT	B	5008	-	-	8/17/57/61	0/2/2/2
21	SF4	C	3002	3	-	-	0/6/5/5
19	CLA	B	1228	-	1/1/14/20	11/33/109/115	-
22	BCR	A	4011	-	-	8/29/63/63	0/2/2/2
19	CLA	A	1121	-	1/1/14/20	15/33/109/115	-
19	CLA	A	1108	-	1/1/12/20	6/21/97/115	-
23	LHG	A	5001	-	-	26/44/44/53	-
22	BCR	F	4014	-	-	8/29/63/63	0/2/2/2
19	CLA	B	1203	2	1/1/15/20	12/39/115/115	-
19	CLA	A	1125	-	1/1/15/20	13/39/115/115	-
19	CLA	B	1240	23	1/1/15/20	17/39/115/115	-
19	CLA	A	1119	-	1/1/15/20	18/39/115/115	-
25	LMG	2	803	-	-	12/31/51/70	0/1/1/1
19	CLA	A	1133	-	1/1/15/20	18/39/115/115	-
19	CLA	F	1302	6	1/1/15/20	11/39/115/115	-
19	CLA	L	1502	-	1/1/14/20	11/33/109/115	-
19	CLA	3	617	-	1/1/14/20	19/33/109/115	-
29	CHL	3	611	-	3/3/16/26	0/17/115/137	-
19	CLA	1	602	13	1/1/11/20	6/17/93/115	-
19	CLA	B	1232	-	1/1/13/20	13/27/103/115	-
22	BCR	A	4017	-	-	9/29/63/63	0/2/2/2
27	DGD	B	5005	-	-	19/50/90/95	0/2/2/2
28	LUT	4	505	-	-	3/29/67/67	0/2/2/2
19	CLA	B	1221	-	1/1/15/20	18/39/115/115	-
19	CLA	2	602	-	1/1/12/20	7/24/100/115	-
28	LUT	3	502	-	1/1/12/27	2/29/67/67	0/2/2/2
19	CLA	B	1211	-	1/1/15/20	16/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	LMG	2	805	-	-	6/25/45/70	0/1/1/1
19	CLA	A	1139	-	1/1/15/20	14/39/115/115	-
19	CLA	B	1237	-	1/1/15/20	16/39/115/115	-
21	SF4	C	3003	3	-	-	0/6/5/5
25	LMG	F	5001	-	-	4/25/45/70	0/1/1/1
19	CLA	A	1104	-	1/1/15/20	15/39/115/115	-
19	CLA	B	1213	-	1/1/14/20	8/33/109/115	-
19	CLA	4	604	16	1/1/14/20	7/33/109/115	-
22	BCR	H	4021	-	-	8/29/63/63	0/2/2/2
27	DGD	4	802	-	-	16/39/79/95	0/2/2/2
22	BCR	A	4003	-	-	6/29/63/63	0/2/2/2
22	BCR	I	4018	-	-	7/29/63/63	0/2/2/2
19	CLA	4	601	16	1/1/14/20	13/33/109/115	-
19	CLA	4	617	-	1/1/15/20	15/39/115/115	-
25	LMG	1	802	-	-	4/41/61/70	0/1/1/1
19	CLA	B	1217	-	1/1/11/20	7/17/93/115	-
19	CLA	G	1601	-	1/1/13/20	10/27/103/115	-
19	CLA	3	606	-	1/1/12/20	10/21/97/115	-
19	CLA	B	1208	-	1/1/14/20	14/33/109/115	-
25	LMG	3	802	-	-	6/25/45/70	0/1/1/1
22	BCR	1	504	-	-	9/29/63/63	0/2/2/2
25	LMG	B	5004	-	-	10/28/48/70	0/1/1/1
19	CLA	K	1404	-	1/1/11/20	7/17/93/115	-
27	DGD	G	5003	-	-	11/36/76/95	0/2/2/2
19	CLA	1	614	13	1/1/14/20	16/33/109/115	-
19	CLA	B	1231	-	1/1/14/20	6/33/109/115	-
20	PQN	A	2001	-	-	7/23/43/43	0/2/2/2
19	CLA	3	610	15	1/1/15/20	18/39/115/115	-
25	LMG	F	5006	-	-	1/4/24/70	0/1/1/1
21	SF4	A	3001	2,1	-	-	0/6/5/5
19	CLA	B	1227	-	1/1/15/20	15/39/115/115	-
19	CLA	G	1602	7	1/1/11/20	7/17/93/115	-
19	CLA	A	1013	-	1/1/15/20	12/39/115/115	-
19	CLA	4	612	16	1/1/15/20	13/39/115/115	-
19	CLA	A	1132	-	1/1/15/20	17/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	B	1220	-	1/1/13/20	7/27/103/115	-
19	CLA	B	1223	-	1/1/15/20	11/39/115/115	-
24	LMT	2	808	-	-	4/21/61/61	0/2/2/2
19	CLA	3	605	-	1/1/13/20	9/27/103/115	-
25	LMG	A	5006	-	-	11/45/65/70	0/1/1/1
19	CLA	A	1135	-	1/1/12/20	10/23/99/115	-
19	CLA	A	1113	-	1/1/11/20	6/15/91/115	-
19	CLA	B	1023	-	1/1/15/20	16/39/115/115	-
24	LMT	G	5005	-	-	5/17/57/61	0/2/2/2
19	CLA	A	1105	-	1/1/14/20	13/33/109/115	-
19	CLA	B	1222	33	1/1/15/20	18/39/115/115	-
19	CLA	K	1402	-	1/1/14/20	16/33/109/115	-
28	LUT	1	502	-	1/1/12/27	5/29/67/67	0/2/2/2
19	CLA	1	606	-	1/1/12/20	5/21/97/115	-
19	CLA	B	1234	-	1/1/13/20	7/27/103/115	-
19	CLA	2	601	14	1/1/14/20	9/33/109/115	-
27	DGD	F	5005	-	-	15/46/86/95	0/2/2/2
19	CLA	A	1130	-	1/1/13/20	4/27/103/115	-
19	CLA	A	1107	1	1/1/15/20	14/39/115/115	-
19	CLA	1	607	-	1/1/11/20	7/17/93/115	-
19	CLA	3	601	15	1/1/13/20	10/27/103/115	-
19	CLA	A	1122	-	1/1/15/20	15/39/115/115	-
25	LMG	F	5003	-	-	11/31/51/70	0/1/1/1
25	LMG	F	5004	-	-	8/29/49/70	0/1/1/1
19	CLA	3	608	-	1/1/11/20	6/19/95/115	-
19	CLA	2	607	-	1/1/14/20	18/33/109/115	-
19	CLA	A	1012	-	1/1/15/20	10/39/115/115	-
19	CLA	A	1136	-	1/1/15/20	18/39/115/115	-
22	BCR	B	4009	-	-	8/29/63/63	0/2/2/2
19	CLA	A	1111	-	1/1/15/20	14/39/115/115	-
19	CLA	A	1120	-	1/1/14/20	14/33/109/115	-
22	BCR	A	4007	-	-	10/29/63/63	0/2/2/2
22	BCR	B	4005	-	-	10/29/63/63	0/2/2/2
24	LMT	G	5004	-	-	10/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	LUT	1	501	-	1/1/12/27	4/29/67/67	0/2/2/2
19	CLA	A	1114	-	1/1/11/20	9/17/93/115	-
19	CLA	B	1212	-	1/1/13/20	12/27/103/115	-
19	CLA	G	1603	-	1/1/15/20	9/39/115/115	-
28	LUT	2	501	-	1/1/12/27	6/29/67/67	0/2/2/2
29	CHL	4	611	-	3/3/17/26	1/21/119/137	-
19	CLA	B	1224	-	1/1/15/20	16/39/115/115	-
22	BCR	3	503	-	-	10/29/63/63	0/2/2/2
19	CLA	A	1141	-	1/1/14/20	13/33/109/115	-
19	CLA	A	1106	1	1/1/15/20	15/39/115/115	-
19	CLA	L	1503	-	1/1/12/20	6/21/97/115	-
19	CLA	B	1238	33	1/1/15/20	12/39/115/115	-
29	CHL	1	612	13	4/4/19/26	6/33/131/137	-
19	CLA	B	1218	-	1/1/15/20	7/39/115/115	-
22	BCR	1	503	-	-	6/29/63/63	0/2/2/2
25	LMG	B	5007	-	-	10/29/49/70	0/1/1/1
28	LUT	J	4013	-	1/1/12/27	4/29/67/67	0/2/2/2
19	CLA	B	1206	2	1/1/15/20	16/39/115/115	-
22	BCR	F	4016	-	-	10/29/63/63	0/2/2/2
23	LHG	2	801	-	-	18/39/39/53	-
22	BCR	K	4002	-	-	5/29/63/63	0/2/2/2
19	CLA	J	1901	10	1/1/12/20	7/21/97/115	-
19	CLA	1	601	13	1/1/15/20	15/39/115/115	-
19	CLA	A	1117	-	1/1/15/20	13/39/115/115	-
19	CLA	2	603	14	1/1/15/20	13/39/115/115	-
22	BCR	I	4020	-	-	14/29/63/63	0/2/2/2
19	CLA	4	605	-	1/1/14/20	10/33/109/115	-
22	BCR	L	4019	-	-	6/29/63/63	0/2/2/2
25	LMG	2	802	-	-	4/20/40/70	0/1/1/1
29	CHL	2	611	-	3/3/16/26	2/18/116/137	-
19	CLA	A	1109	-	1/1/15/20	18/39/115/115	-
29	CHL	1	609	13	4/4/18/26	3/27/125/137	-
29	CHL	4	610	-	3/3/16/26	4/17/115/137	-
25	LMG	G	5002	-	-	17/45/65/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	B	1226	-	1/1/15/20	16/39/115/115	-
19	CLA	3	603	-	1/1/13/20	12/27/103/115	-
19	CLA	A	1124	-	1/1/13/20	8/27/103/115	-
19	CLA	A	1134	1	1/1/13/20	8/27/103/115	-
19	CLA	2	604	14	1/1/15/20	16/39/115/115	-
19	CLA	B	1202	-	1/1/15/20	17/39/115/115	-
23	LHG	B	5001	19	-	9/23/23/53	-
19	CLA	A	1101	-	1/1/15/20	14/39/115/115	-
19	CLA	B	1230	-	1/1/13/20	15/31/107/115	-
19	CLA	1	605	-	1/1/15/20	16/39/115/115	-
19	CLA	4	607	-	1/1/14/20	11/33/109/115	-
19	CLA	B	1204	-	1/1/15/20	16/39/115/115	-
19	CLA	B	1214	-	1/1/15/20	14/39/115/115	-
30	XAT	2	502	-	2/2/12/26	7/31/93/93	0/4/4/4
19	CLA	3	613	-	1/1/11/20	6/17/93/115	-
19	CLA	A	1138	-	1/1/15/20	15/39/115/115	-
22	BCR	K	4001	-	-	6/29/63/63	0/2/2/2
22	BCR	A	4008	-	-	10/29/63/63	0/2/2/2
25	LMG	G	5001	-	-	16/44/64/70	0/1/1/1
19	CLA	2	612	-	1/1/13/20	8/27/103/115	-
27	DGD	J	5001	-	-	11/47/87/95	0/2/2/2
31	3PH	2	807	-	-	16/34/34/49	-
29	CHL	4	613	-	4/4/19/26	8/33/131/137	-
29	CHL	4	615	16	4/4/15/26	0/12/110/137	-
30	XAT	4	502	-	2/2/12/26	2/31/93/93	0/4/4/4
19	CLA	B	1205	-	1/1/15/20	13/39/115/115	-
22	BCR	3	506	-	-	5/29/63/63	0/2/2/2
19	CLA	2	606	-	1/1/12/20	6/21/97/115	-
19	CLA	3	607	-	1/1/12/20	7/24/100/115	-
19	CLA	A	1127	-	1/1/15/20	14/39/115/115	-
19	CLA	K	1401	-	1/1/11/20	9/15/91/115	-
19	CLA	4	603	-	1/1/15/20	13/39/115/115	-
27	DGD	3	803	-	-	8/40/80/95	0/2/2/2
19	CLA	A	1126	-	1/1/15/20	13/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	B	1021	-	1/1/15/20	5/39/115/115	-
22	BCR	G	4011	-	-	7/29/63/63	0/2/2/2
19	CLA	4	608	-	1/1/11/20	5/17/93/115	-
27	DGD	1	803	-	-	14/30/70/95	0/2/2/2
19	CLA	B	1225	-	1/1/15/20	13/39/115/115	-
19	CLA	B	1201	-	1/1/15/20	13/39/115/115	-
19	CLA	A	1103	-	1/1/15/20	15/39/115/115	-
19	CLA	B	1210	-	1/1/15/20	9/39/115/115	-
28	LUT	3	501	-	1/1/12/27	6/29/67/67	0/2/2/2
19	CLA	A	1102	-	1/1/15/20	21/39/115/115	-
19	CLA	B	1219	-	1/1/15/20	14/39/115/115	-
19	CLA	H	1701	-	1/1/14/20	12/33/109/115	-
19	CLA	4	602	-	1/1/12/20	5/21/97/115	-
24	LMT	B	5006	-	-	4/18/58/61	0/2/2/2
19	CLA	A	1112	-	1/1/15/20	18/39/115/115	-
19	CLA	2	605	-	1/1/15/20	17/39/115/115	-
19	CLA	A	1128	-	1/1/15/20	16/39/115/115	-
19	CLA	1	603	-	1/1/13/20	8/27/103/115	-
19	CLA	A	1140	-	1/1/15/20	7/39/115/115	-
19	CLA	K	1403	-	1/1/11/20	10/19/95/115	-
19	CLA	B	1215	-	1/1/15/20	12/39/115/115	-
19	CLA	B	1207	-	1/1/15/20	13/39/115/115	-
22	BCR	2	503	-	-	13/29/63/63	0/2/2/2
29	CHL	1	610	13	3/3/16/26	3/17/115/137	-
19	CLA	B	1022	-	1/1/15/20	10/39/115/115	-
19	CLA	B	1216	-	1/1/15/20	10/39/115/115	-
19	CLA	B	1229	-	1/1/15/20	13/39/115/115	-
23	LHG	1	801	-	-	29/53/53/53	-
19	CLA	1	611	-	1/1/15/20	14/39/115/115	-
19	CLA	B	1236	-	1/1/12/20	8/21/97/115	-
19	CLA	A	1123	-	1/1/15/20	13/39/115/115	-
24	LMT	A	5004	-	-	7/21/61/61	0/2/2/2
23	LHG	A	5002	-	-	27/53/53/53	-
19	CLA	L	1501	12	1/1/12/20	7/21/97/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	A	1116	-	1/1/13/20	12/29/105/115	-
23	LHG	4	801	-	-	21/39/39/53	-
25	LMG	2	806	-	-	1/4/24/70	0/1/1/1
19	CLA	B	1239	-	1/1/15/20	9/39/115/115	-
19	CLA	A	1131	-	1/1/15/20	17/39/115/115	-
25	LMG	G	5006	-	-	11/20/40/70	0/1/1/1
22	BCR	B	4006	-	-	3/29/63/63	0/2/2/2
23	LHG	B	5002	-	-	27/53/53/53	-
28	LUT	4	501	-	1/1/12/27	7/29/67/67	0/2/2/2
19	CLA	A	1129	-	1/1/15/20	11/39/115/115	-
19	CLA	4	609	16	1/1/12/20	11/21/97/115	-
19	CLA	F	1301	-	1/1/15/20	17/39/115/115	-
19	CLA	A	1115	-	1/1/15/20	9/39/115/115	-
29	CHL	2	609	14	4/4/20/26	4/39/137/137	-
19	CLA	1	604	13	1/1/15/20	15/39/115/115	-
19	CLA	3	612	15	1/1/12/20	6/21/97/115	-
19	CLA	3	614	-	1/1/10/20	3/12/88/115	-
29	CHL	3	604	15	4/4/20/26	8/39/137/137	-
23	LHG	3	801	-	-	12/19/19/53	-
29	CHL	2	610	-	4/4/18/26	5/27/125/137	-
19	CLA	A	1110	-	1/1/13/20	8/27/103/115	-
19	CLA	3	602	-	1/1/12/20	8/24/100/115	-
19	CLA	A	1137	-	1/1/15/20	17/39/115/115	-

All (1286) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	3	501	LUT	C24-C25	15.01	1.51	1.33
28	1	502	LUT	C24-C25	14.94	1.50	1.33
28	2	501	LUT	C24-C25	14.83	1.50	1.33
28	J	4013	LUT	C24-C25	14.80	1.50	1.33
28	1	501	LUT	C24-C25	14.75	1.50	1.33
28	4	505	LUT	C24-C25	14.54	1.50	1.33
28	4	501	LUT	C24-C25	14.43	1.50	1.33
28	3	502	LUT	C24-C25	14.42	1.50	1.33
18	A	1011	CL0	C1A-CHA	9.55	1.50	1.40
18	A	1011	CL0	C1D-C2D	8.89	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	1011	CL0	C1B-C2B	8.86	1.49	1.39
18	A	1011	CL0	C3B-C4B	7.08	1.48	1.41
29	4	613	CHL	C3B-C4B	6.82	1.48	1.41
29	1	609	CHL	C3A-C2A	-6.74	1.48	1.54
19	K	1403	CLA	MG-NA	6.33	2.21	2.06
19	3	605	CLA	MG-NA	6.33	2.21	2.06
19	G	1602	CLA	MG-NA	6.30	2.21	2.06
19	A	1126	CLA	MG-NA	6.29	2.21	2.06
19	3	608	CLA	MG-NA	6.29	2.21	2.06
19	K	1404	CLA	MG-NA	6.28	2.21	2.06
19	A	1115	CLA	MG-NA	6.26	2.21	2.06
19	K	1402	CLA	MG-NA	6.25	2.21	2.06
19	1	602	CLA	MG-NA	6.25	2.21	2.06
19	1	613	CLA	MG-NA	6.25	2.21	2.06
19	A	1116	CLA	MG-NA	6.24	2.21	2.06
19	3	607	CLA	MG-NA	6.24	2.21	2.06
19	J	1901	CLA	MG-NA	6.23	2.21	2.06
19	G	1603	CLA	MG-NA	6.23	2.21	2.06
19	A	1130	CLA	MG-NA	6.23	2.21	2.06
19	1	603	CLA	MG-NA	6.23	2.21	2.06
19	2	602	CLA	MG-NA	6.23	2.21	2.06
19	2	607	CLA	MG-NA	6.22	2.21	2.06
19	4	609	CLA	MG-NA	6.22	2.21	2.06
19	1	607	CLA	MG-NA	6.21	2.21	2.06
19	A	1123	CLA	MG-NA	6.21	2.21	2.06
19	1	614	CLA	MG-NA	6.21	2.21	2.06
19	3	601	CLA	MG-NA	6.21	2.21	2.06
29	4	611	CHL	C3B-C4B	6.21	1.47	1.41
19	A	1107	CLA	MG-NA	6.20	2.21	2.06
19	A	1112	CLA	MG-NA	6.20	2.21	2.06
19	B	1228	CLA	MG-NA	6.20	2.21	2.06
19	B	1223	CLA	MG-NA	6.20	2.21	2.06
19	B	1207	CLA	MG-NA	6.19	2.21	2.06
19	B	1204	CLA	MG-NA	6.19	2.21	2.06
19	2	606	CLA	MG-NA	6.19	2.21	2.06
19	A	1139	CLA	MG-NA	6.19	2.21	2.06
19	2	605	CLA	MG-NA	6.18	2.21	2.06
19	4	605	CLA	MG-NA	6.18	2.21	2.06
19	B	1214	CLA	MG-NA	6.18	2.21	2.06
19	A	1113	CLA	MG-NA	6.18	2.21	2.06
19	3	614	CLA	MG-NA	6.18	2.20	2.06
19	4	603	CLA	MG-NA	6.18	2.20	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	3	613	CLA	MG-NA	6.18	2.20	2.06
19	B	1213	CLA	MG-NA	6.17	2.20	2.06
19	B	1232	CLA	MG-NA	6.17	2.20	2.06
19	A	1105	CLA	MG-NA	6.17	2.20	2.06
19	4	601	CLA	MG-NA	6.17	2.20	2.06
19	A	1101	CLA	MG-NA	6.17	2.20	2.06
19	3	603	CLA	MG-NA	6.17	2.20	2.06
19	A	1114	CLA	MG-NA	6.17	2.20	2.06
19	A	1012	CLA	MG-NA	6.16	2.20	2.06
19	G	1601	CLA	MG-NA	6.16	2.20	2.06
19	A	1120	CLA	MG-NA	6.16	2.20	2.06
19	B	1217	CLA	MG-NA	6.15	2.20	2.06
19	A	1118	CLA	MG-NA	6.15	2.20	2.06
19	B	1234	CLA	MG-NA	6.15	2.20	2.06
19	B	1239	CLA	MG-NA	6.15	2.20	2.06
19	1	608	CLA	MG-NA	6.15	2.20	2.06
19	K	1401	CLA	MG-NA	6.15	2.20	2.06
19	1	611	CLA	MG-NA	6.15	2.20	2.06
19	B	1221	CLA	MG-NA	6.15	2.20	2.06
19	A	1129	CLA	MG-NA	6.15	2.20	2.06
19	3	617	CLA	MG-NA	6.15	2.20	2.06
19	B	1023	CLA	MG-NA	6.14	2.20	2.06
19	F	1301	CLA	MG-NA	6.14	2.20	2.06
19	B	1224	CLA	MG-NA	6.14	2.20	2.06
19	A	1131	CLA	MG-NA	6.14	2.20	2.06
19	3	602	CLA	MG-NA	6.14	2.20	2.06
19	A	1121	CLA	MG-NA	6.13	2.20	2.06
19	2	604	CLA	MG-NA	6.13	2.20	2.06
19	A	1136	CLA	MG-NA	6.13	2.20	2.06
19	2	601	CLA	MG-NA	6.13	2.20	2.06
19	B	1206	CLA	MG-NA	6.13	2.20	2.06
19	A	1134	CLA	MG-NA	6.13	2.20	2.06
19	F	1302	CLA	MG-NA	6.12	2.20	2.06
19	2	603	CLA	MG-NA	6.12	2.20	2.06
29	2	613	CHL	C3B-C4B	6.12	1.47	1.41
19	B	1209	CLA	MG-NA	6.12	2.20	2.06
19	B	1210	CLA	MG-NA	6.11	2.20	2.06
19	4	607	CLA	MG-NA	6.11	2.20	2.06
19	L	1502	CLA	MG-NA	6.11	2.20	2.06
19	B	1238	CLA	MG-NA	6.11	2.20	2.06
19	B	1201	CLA	MG-NA	6.11	2.20	2.06
19	3	610	CLA	MG-NA	6.11	2.20	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	H	1701	CLA	MG-NA	6.11	2.20	2.06
19	2	608	CLA	MG-NA	6.11	2.20	2.06
19	A	1135	CLA	MG-NA	6.11	2.20	2.06
19	B	1218	CLA	MG-NA	6.11	2.20	2.06
19	4	606	CLA	MG-NA	6.11	2.20	2.06
19	A	1119	CLA	MG-NA	6.11	2.20	2.06
19	A	1137	CLA	MG-NA	6.11	2.20	2.06
19	1	606	CLA	MG-NA	6.11	2.20	2.06
19	L	1501	CLA	MG-NA	6.10	2.20	2.06
19	A	1141	CLA	MG-NA	6.10	2.20	2.06
19	B	1203	CLA	MG-NA	6.10	2.20	2.06
19	4	608	CLA	MG-NA	6.10	2.20	2.06
19	B	1208	CLA	MG-NA	6.10	2.20	2.06
19	B	1219	CLA	MG-NA	6.10	2.20	2.06
19	A	1104	CLA	MG-NA	6.10	2.20	2.06
19	B	1227	CLA	MG-NA	6.10	2.20	2.06
19	1	605	CLA	MG-NA	6.10	2.20	2.06
19	A	1127	CLA	MG-NA	6.09	2.20	2.06
19	B	1240	CLA	MG-NA	6.09	2.20	2.06
29	3	611	CHL	C3B-C4B	6.09	1.47	1.41
19	A	1109	CLA	MG-NA	6.09	2.20	2.06
19	B	1212	CLA	MG-NA	6.09	2.20	2.06
19	4	602	CLA	MG-NA	6.08	2.20	2.06
29	2	615	CHL	C3B-C4B	6.08	1.47	1.41
19	B	1230	CLA	MG-NA	6.08	2.20	2.06
19	B	1229	CLA	MG-NA	6.08	2.20	2.06
19	A	1110	CLA	MG-NA	6.07	2.20	2.06
19	4	612	CLA	MG-NA	6.07	2.20	2.06
19	A	1124	CLA	MG-NA	6.07	2.20	2.06
19	B	1022	CLA	MG-NA	6.07	2.20	2.06
19	L	1503	CLA	MG-NA	6.07	2.20	2.06
19	A	1133	CLA	MG-NA	6.06	2.20	2.06
19	A	1132	CLA	MG-NA	6.06	2.20	2.06
19	B	1225	CLA	MG-NA	6.06	2.20	2.06
19	B	1226	CLA	MG-NA	6.06	2.20	2.06
19	A	1138	CLA	MG-NA	6.06	2.20	2.06
19	A	1125	CLA	MG-NA	6.05	2.20	2.06
19	1	601	CLA	MG-NA	6.05	2.20	2.06
29	1	610	CHL	C3B-C4B	6.05	1.47	1.41
19	A	1103	CLA	MG-NA	6.05	2.20	2.06
19	1	604	CLA	MG-NA	6.05	2.20	2.06
19	B	1220	CLA	MG-NA	6.05	2.20	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	1111	CLA	MG-NA	6.05	2.20	2.06
19	A	1122	CLA	MG-NA	6.04	2.20	2.06
19	A	1128	CLA	MG-NA	6.04	2.20	2.06
19	B	1236	CLA	MG-NA	6.04	2.20	2.06
19	4	604	CLA	MG-NA	6.03	2.20	2.06
19	B	1237	CLA	MG-NA	6.03	2.20	2.06
22	H	4021	BCR	C24-C23	6.02	1.51	1.33
19	A	1140	CLA	MG-NA	6.01	2.20	2.06
19	3	612	CLA	MG-NA	6.01	2.20	2.06
19	A	1102	CLA	MG-NA	6.01	2.20	2.06
19	3	606	CLA	MG-NA	6.00	2.20	2.06
19	A	1117	CLA	MG-NA	6.00	2.20	2.06
19	B	1235	CLA	MG-NA	6.00	2.20	2.06
19	B	1231	CLA	MG-NA	5.99	2.20	2.06
19	4	617	CLA	MG-NA	5.99	2.20	2.06
29	4	615	CHL	C3B-C4B	5.99	1.47	1.41
22	A	4002	BCR	C24-C23	5.97	1.50	1.33
19	A	1013	CLA	MG-NA	5.97	2.20	2.06
19	A	1108	CLA	MG-NA	5.97	2.20	2.06
19	2	612	CLA	MG-NA	5.96	2.20	2.06
22	I	4020	BCR	C24-C23	5.96	1.50	1.33
19	B	1216	CLA	MG-NA	5.96	2.20	2.06
19	B	1021	CLA	MG-NA	5.96	2.20	2.06
22	L	4019	BCR	C24-C23	5.95	1.50	1.33
22	K	4001	BCR	C24-C23	5.95	1.50	1.33
19	B	1205	CLA	MG-NA	5.94	2.20	2.06
22	A	4007	BCR	C24-C23	5.93	1.50	1.33
22	J	4012	BCR	C24-C23	5.92	1.50	1.33
22	G	4011	BCR	C24-C23	5.92	1.50	1.33
19	B	1202	CLA	MG-NA	5.92	2.20	2.06
29	4	610	CHL	C3B-C4B	5.91	1.47	1.41
29	4	610	CHL	C3A-C2A	-5.88	1.49	1.54
22	1	503	BCR	C24-C23	5.87	1.50	1.33
19	B	1222	CLA	MG-NA	5.87	2.20	2.06
22	1	504	BCR	C24-C23	5.86	1.50	1.33
22	A	4017	BCR	C24-C23	5.86	1.50	1.33
19	A	1106	CLA	MG-NA	5.86	2.20	2.06
22	B	4004	BCR	C24-C23	5.85	1.50	1.33
22	3	506	BCR	C24-C23	5.83	1.50	1.33
19	B	1215	CLA	MG-NA	5.83	2.20	2.06
22	B	4005	BCR	C24-C23	5.82	1.50	1.33
22	F	4014	BCR	C24-C23	5.81	1.50	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	3	503	BCR	C24-C23	5.79	1.50	1.33
22	K	4002	BCR	C24-C23	5.79	1.50	1.33
22	I	4018	BCR	C24-C23	5.79	1.50	1.33
29	1	612	CHL	C3B-C4B	5.77	1.47	1.41
22	L	4020	BCR	C24-C23	5.77	1.50	1.33
22	A	4003	BCR	C24-C23	5.76	1.50	1.33
22	B	4010	BCR	C24-C23	5.73	1.50	1.33
29	1	609	CHL	C3B-C4B	5.72	1.47	1.41
29	2	609	CHL	C3A-C2A	-5.71	1.49	1.54
19	B	1211	CLA	MG-NA	5.69	2.19	2.06
22	A	4008	BCR	C24-C23	5.68	1.50	1.33
22	A	4011	BCR	C24-C23	5.62	1.49	1.33
22	F	4016	BCR	C24-C23	5.61	1.49	1.33
22	B	4006	BCR	C24-C23	5.57	1.49	1.33
22	B	4009	BCR	C24-C23	5.56	1.49	1.33
22	2	503	BCR	C24-C23	5.53	1.49	1.33
29	2	611	CHL	C3B-C4B	5.46	1.46	1.41
22	A	4008	BCR	C11-C12	-5.40	1.20	1.34
18	A	1011	CL0	O2A-C1	5.39	1.60	1.46
22	K	4001	BCR	C11-C12	-5.38	1.20	1.34
22	I	4018	BCR	C11-C12	-5.37	1.20	1.34
22	B	4009	BCR	C11-C12	-5.35	1.20	1.34
18	A	1011	CL0	CHC-C4B	5.32	1.48	1.39
22	3	503	BCR	C11-C12	-5.30	1.20	1.34
22	B	4010	BCR	C11-C12	-5.30	1.20	1.34
22	G	4011	BCR	C11-C12	-5.29	1.20	1.34
22	A	4011	BCR	C11-C12	-5.29	1.20	1.34
22	2	503	BCR	C11-C12	-5.28	1.20	1.34
22	B	4006	BCR	C11-C12	-5.24	1.21	1.34
22	F	4016	BCR	C11-C12	-5.23	1.21	1.34
29	2	609	CHL	C3B-C4B	5.23	1.46	1.41
22	L	4019	BCR	C11-C12	-5.23	1.21	1.34
22	F	4014	BCR	C11-C12	-5.21	1.21	1.34
22	A	4017	BCR	C11-C12	-5.19	1.21	1.34
22	A	4003	BCR	C11-C12	-5.18	1.21	1.34
22	L	4020	BCR	C11-C12	-5.18	1.21	1.34
22	1	503	BCR	C11-C12	-5.17	1.21	1.34
18	A	1011	CL0	CHB-C1B	5.15	1.48	1.39
22	A	4007	BCR	C11-C12	-5.15	1.21	1.34
29	4	613	CHL	C3A-C2A	-5.15	1.50	1.54
22	B	4005	BCR	C11-C12	-5.12	1.21	1.34
22	1	504	BCR	C11-C12	-5.10	1.21	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	H	4021	BCR	C11-C12	-5.09	1.21	1.34
22	J	4012	BCR	C11-C12	-5.09	1.21	1.34
22	I	4020	BCR	C11-C12	-5.06	1.21	1.34
22	3	506	BCR	C11-C12	-5.05	1.21	1.34
22	B	4004	BCR	C11-C12	-5.05	1.21	1.34
22	A	4002	BCR	C11-C12	-5.04	1.21	1.34
22	K	4002	BCR	C11-C12	-5.01	1.21	1.34
18	A	1011	CL0	CHD-C1D	5.00	1.47	1.39
18	A	1011	CL0	O2D-CGD	4.98	1.45	1.33
29	3	604	CHL	C3B-C4B	4.98	1.46	1.41
18	A	1011	CL0	OBD-CAD	4.94	1.28	1.22
18	A	1011	CL0	CHD-C4C	4.81	1.48	1.39
18	A	1011	CL0	CHC-C1C	4.65	1.48	1.39
18	A	1011	CL0	C3D-C4D	-4.64	1.34	1.41
29	2	611	CHL	C3A-C2A	-4.64	1.50	1.54
22	2	503	BCR	C16-C17	-4.61	1.28	1.43
18	A	1011	CL0	C3D-C2D	4.53	1.47	1.39
29	2	610	CHL	C3B-C4B	4.52	1.45	1.41
29	3	611	CHL	C3A-C2A	-4.51	1.50	1.54
29	4	611	CHL	C3A-C2A	-4.47	1.50	1.54
19	B	1201	CLA	CBB-CAB	4.44	1.51	1.30
19	3	612	CLA	CBB-CAB	4.43	1.51	1.30
19	H	1701	CLA	CBB-CAB	4.42	1.51	1.30
19	3	602	CLA	CBB-CAB	4.41	1.51	1.30
19	2	612	CLA	CBB-CAB	4.41	1.51	1.30
19	G	1602	CLA	CBB-CAB	4.41	1.51	1.30
18	A	1011	CL0	C3B-C2B	4.40	1.46	1.40
19	G	1603	CLA	CBB-CAB	4.40	1.51	1.30
19	B	1228	CLA	CBB-CAB	4.40	1.51	1.30
19	K	1403	CLA	CBB-CAB	4.40	1.51	1.30
19	3	610	CLA	CBB-CAB	4.39	1.51	1.30
19	1	608	CLA	CBB-CAB	4.39	1.51	1.30
19	2	608	CLA	CBB-CAB	4.39	1.51	1.30
19	4	602	CLA	CBB-CAB	4.39	1.51	1.30
19	K	1401	CLA	CBB-CAB	4.39	1.51	1.30
19	L	1501	CLA	CBB-CAB	4.39	1.51	1.30
19	3	607	CLA	CBB-CAB	4.39	1.51	1.30
19	A	1141	CLA	CBB-CAB	4.39	1.51	1.30
19	B	1222	CLA	CBB-CAB	4.39	1.51	1.30
19	4	608	CLA	CBB-CAB	4.39	1.51	1.30
19	L	1503	CLA	CBB-CAB	4.39	1.51	1.30
19	F	1301	CLA	CBB-CAB	4.39	1.51	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	1127	CLA	CBB-CAB	4.38	1.51	1.30
19	K	1404	CLA	CBB-CAB	4.38	1.51	1.30
19	A	1012	CLA	CBB-CAB	4.38	1.51	1.30
19	B	1235	CLA	CBB-CAB	4.38	1.51	1.30
19	3	606	CLA	CBB-CAB	4.38	1.51	1.30
19	B	1221	CLA	CBB-CAB	4.38	1.51	1.30
19	B	1239	CLA	CBB-CAB	4.38	1.51	1.30
19	B	1212	CLA	CBB-CAB	4.38	1.51	1.30
19	G	1601	CLA	CBB-CAB	4.38	1.51	1.30
19	1	604	CLA	CBB-CAB	4.37	1.51	1.30
19	A	1103	CLA	CBB-CAB	4.37	1.51	1.30
19	A	1126	CLA	CBB-CAB	4.37	1.51	1.30
19	F	1302	CLA	CBB-CAB	4.37	1.51	1.30
19	B	1237	CLA	CBB-CAB	4.37	1.51	1.30
19	L	1502	CLA	CBB-CAB	4.37	1.51	1.30
19	B	1219	CLA	CBB-CAB	4.37	1.51	1.30
19	4	617	CLA	CBB-CAB	4.37	1.51	1.30
19	4	607	CLA	CBB-CAB	4.37	1.51	1.30
19	A	1125	CLA	CBB-CAB	4.37	1.51	1.30
19	2	602	CLA	CBB-CAB	4.37	1.51	1.30
19	3	601	CLA	CBB-CAB	4.37	1.51	1.30
19	3	608	CLA	CBB-CAB	4.37	1.51	1.30
19	B	1227	CLA	CBB-CAB	4.37	1.51	1.30
19	B	1213	CLA	CBB-CAB	4.37	1.51	1.30
19	B	1230	CLA	CBB-CAB	4.37	1.51	1.30
19	A	1121	CLA	CBB-CAB	4.37	1.51	1.30
19	A	1116	CLA	CBB-CAB	4.37	1.51	1.30
19	A	1130	CLA	CBB-CAB	4.37	1.51	1.30
19	J	1901	CLA	CBB-CAB	4.37	1.51	1.30
19	4	603	CLA	CBB-CAB	4.37	1.51	1.30
19	A	1105	CLA	CBB-CAB	4.37	1.51	1.30
19	4	601	CLA	CBB-CAB	4.37	1.51	1.30
19	A	1101	CLA	CBB-CAB	4.37	1.51	1.30
19	A	1104	CLA	CBB-CAB	4.36	1.51	1.30
19	1	607	CLA	CBB-CAB	4.36	1.51	1.30
19	1	605	CLA	CBB-CAB	4.36	1.51	1.30
19	1	602	CLA	CBB-CAB	4.36	1.51	1.30
19	A	1131	CLA	CBB-CAB	4.36	1.51	1.30
19	1	611	CLA	CBB-CAB	4.36	1.51	1.30
19	A	1111	CLA	CBB-CAB	4.36	1.51	1.30
19	3	603	CLA	CBB-CAB	4.36	1.51	1.30
19	B	1225	CLA	CBB-CAB	4.36	1.51	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	4	606	CLA	CBB-CAB	4.36	1.51	1.30
19	2	606	CLA	CBB-CAB	4.36	1.51	1.30
19	B	1223	CLA	CBB-CAB	4.36	1.51	1.30
19	A	1132	CLA	CBB-CAB	4.35	1.51	1.30
19	B	1224	CLA	CBB-CAB	4.35	1.51	1.30
19	2	604	CLA	CBB-CAB	4.35	1.51	1.30
19	B	1209	CLA	CBB-CAB	4.35	1.51	1.30
19	B	1210	CLA	CBB-CAB	4.35	1.51	1.30
19	3	605	CLA	CBB-CAB	4.35	1.51	1.30
19	A	1113	CLA	CBB-CAB	4.35	1.51	1.30
19	B	1215	CLA	CBB-CAB	4.35	1.51	1.30
27	F	5005	DGD	O1G-C1A	4.35	1.46	1.33
19	A	1118	CLA	CBB-CAB	4.35	1.51	1.30
19	A	1107	CLA	CBB-CAB	4.35	1.51	1.30
19	1	601	CLA	CBB-CAB	4.35	1.51	1.30
19	A	1119	CLA	CBB-CAB	4.35	1.51	1.30
19	A	1109	CLA	CBB-CAB	4.35	1.51	1.30
19	A	1134	CLA	CBB-CAB	4.35	1.51	1.30
19	2	601	CLA	CBB-CAB	4.35	1.51	1.30
19	B	1205	CLA	CBB-CAB	4.35	1.51	1.30
19	A	1102	CLA	CBB-CAB	4.35	1.51	1.30
19	A	1124	CLA	CBB-CAB	4.35	1.51	1.30
27	G	5003	DGD	O1G-C1A	4.35	1.46	1.33
19	A	1128	CLA	CBB-CAB	4.35	1.51	1.30
19	A	1114	CLA	CBB-CAB	4.35	1.51	1.30
19	4	604	CLA	CBB-CAB	4.35	1.51	1.30
19	B	1218	CLA	CBB-CAB	4.34	1.51	1.30
19	2	603	CLA	CBB-CAB	4.34	1.51	1.30
19	A	1123	CLA	CBB-CAB	4.34	1.51	1.30
19	B	1022	CLA	CBB-CAB	4.34	1.51	1.30
19	B	1232	CLA	CBB-CAB	4.34	1.51	1.30
19	A	1013	CLA	CBB-CAB	4.34	1.51	1.30
19	B	1211	CLA	CBB-CAB	4.34	1.51	1.30
19	2	605	CLA	CBB-CAB	4.34	1.51	1.30
19	A	1133	CLA	CBB-CAB	4.34	1.51	1.30
19	B	1217	CLA	CBB-CAB	4.34	1.51	1.30
19	1	606	CLA	CBB-CAB	4.34	1.51	1.30
19	B	1208	CLA	CBB-CAB	4.34	1.51	1.30
19	B	1220	CLA	CBB-CAB	4.33	1.51	1.30
19	A	1120	CLA	CBB-CAB	4.33	1.51	1.30
19	A	1136	CLA	CBB-CAB	4.33	1.51	1.30
19	B	1238	CLA	CBB-CAB	4.33	1.51	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	4	605	CLA	CBB-CAB	4.33	1.51	1.30
19	B	1234	CLA	CBB-CAB	4.33	1.51	1.30
19	4	609	CLA	CBB-CAB	4.33	1.51	1.30
19	A	1106	CLA	CBB-CAB	4.33	1.51	1.30
19	B	1226	CLA	CBB-CAB	4.32	1.51	1.30
19	K	1402	CLA	CBB-CAB	4.32	1.51	1.30
19	B	1202	CLA	CBB-CAB	4.32	1.51	1.30
19	A	1140	CLA	CBB-CAB	4.32	1.51	1.30
29	1	612	CHL	C3A-C2A	-4.31	1.51	1.54
19	4	612	CLA	CBB-CAB	4.31	1.51	1.30
19	A	1137	CLA	CBB-CAB	4.31	1.51	1.30
19	1	614	CLA	CBB-CAB	4.31	1.51	1.30
19	1	613	CLA	CBB-CAB	4.31	1.51	1.30
19	B	1240	CLA	CBB-CAB	4.31	1.51	1.30
19	B	1021	CLA	CBB-CAB	4.31	1.51	1.30
19	B	1231	CLA	CBB-CAB	4.30	1.51	1.30
19	A	1115	CLA	CBB-CAB	4.30	1.51	1.30
19	B	1214	CLA	CBB-CAB	4.30	1.51	1.30
19	A	1117	CLA	CBB-CAB	4.30	1.51	1.30
19	A	1110	CLA	CBB-CAB	4.30	1.51	1.30
19	B	1023	CLA	CBB-CAB	4.30	1.51	1.30
19	A	1108	CLA	CBB-CAB	4.29	1.51	1.30
19	A	1129	CLA	CBB-CAB	4.29	1.51	1.30
19	B	1236	CLA	CBB-CAB	4.29	1.51	1.30
19	B	1206	CLA	CBB-CAB	4.29	1.51	1.30
22	A	4007	BCR	C16-C17	-4.29	1.29	1.43
19	2	607	CLA	CBB-CAB	4.28	1.51	1.30
19	B	1204	CLA	CBB-CAB	4.28	1.51	1.30
19	B	1229	CLA	CBB-CAB	4.28	1.51	1.30
22	G	4011	BCR	C16-C17	-4.28	1.29	1.43
19	B	1203	CLA	CBB-CAB	4.28	1.50	1.30
27	1	803	DGD	O1G-C1A	4.27	1.45	1.33
19	A	1138	CLA	CBB-CAB	4.27	1.50	1.30
19	1	603	CLA	CBB-CAB	4.27	1.50	1.30
22	A	4017	BCR	C16-C17	-4.27	1.29	1.43
19	3	614	CLA	CBB-CAB	4.26	1.50	1.30
19	A	1135	CLA	CBB-CAB	4.26	1.50	1.30
27	4	802	DGD	O1G-C1A	4.25	1.45	1.33
19	B	1216	CLA	CBB-CAB	4.24	1.50	1.30
19	3	613	CLA	CBB-CAB	4.24	1.50	1.30
19	3	617	CLA	CBB-CAB	4.24	1.50	1.30
22	B	4004	BCR	C10-C9	4.23	1.45	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	J	5001	DGD	O1G-C1A	4.23	1.45	1.33
27	B	5005	DGD	O1G-C1A	4.23	1.45	1.33
19	A	1112	CLA	CBB-CAB	4.22	1.50	1.30
19	B	1207	CLA	CBB-CAB	4.22	1.50	1.30
27	3	803	DGD	O1G-C1A	4.22	1.45	1.33
22	1	504	BCR	C16-C17	-4.22	1.30	1.43
19	A	1124	CLA	MG-ND	-4.22	1.97	2.05
22	A	4002	BCR	C16-C17	-4.21	1.30	1.43
19	A	1139	CLA	CBB-CAB	4.21	1.50	1.30
22	H	4021	BCR	C10-C9	4.19	1.45	1.35
22	B	4004	BCR	C16-C17	-4.19	1.30	1.43
29	1	610	CHL	C3A-C2A	-4.18	1.51	1.54
19	4	605	CLA	MG-ND	-4.17	1.97	2.05
22	I	4018	BCR	C16-C17	-4.17	1.30	1.43
19	A	1122	CLA	CBB-CAB	4.16	1.50	1.30
29	3	604	CHL	C3A-C2A	-4.14	1.51	1.54
19	A	1012	CLA	MG-ND	-4.13	1.97	2.05
22	A	4003	BCR	C16-C17	-4.13	1.30	1.43
22	3	506	BCR	C16-C17	-4.13	1.30	1.43
22	1	503	BCR	C10-C9	4.12	1.45	1.35
22	3	506	BCR	C10-C9	4.12	1.45	1.35
22	I	4020	BCR	C16-C17	-4.12	1.30	1.43
22	1	504	BCR	C10-C9	4.09	1.45	1.35
22	I	4020	BCR	C10-C9	4.09	1.45	1.35
19	A	1116	CLA	MG-ND	-4.09	1.97	2.05
19	B	1021	CLA	MG-ND	-4.09	1.97	2.05
22	B	4009	BCR	C16-C17	-4.09	1.30	1.43
19	B	1226	CLA	MG-ND	-4.08	1.97	2.05
19	B	1022	CLA	MG-ND	-4.08	1.97	2.05
19	3	605	CLA	MG-ND	-4.08	1.97	2.05
19	A	1126	CLA	MG-ND	-4.07	1.97	2.05
19	B	1224	CLA	MG-ND	-4.07	1.97	2.05
19	A	1108	CLA	MG-ND	-4.06	1.97	2.05
19	B	1023	CLA	MG-ND	-4.05	1.97	2.05
19	A	1119	CLA	MG-ND	-4.05	1.97	2.05
22	J	4012	BCR	C10-C9	4.04	1.45	1.35
22	A	4008	BCR	C16-C17	-4.04	1.30	1.43
19	B	1203	CLA	MG-ND	-4.04	1.97	2.05
19	1	604	CLA	MG-ND	-4.04	1.97	2.05
19	A	1112	CLA	MG-ND	-4.04	1.97	2.05
19	A	1139	CLA	MG-ND	-4.03	1.97	2.05
19	A	1131	CLA	MG-ND	-4.03	1.97	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	1127	CLA	MG-ND	-4.03	1.97	2.05
19	B	1206	CLA	MG-ND	-4.03	1.97	2.05
19	B	1221	CLA	MG-ND	-4.03	1.97	2.05
22	A	4011	BCR	C16-C17	-4.03	1.30	1.43
22	B	4006	BCR	C16-C17	-4.02	1.30	1.43
19	B	1216	CLA	MG-ND	-4.02	1.97	2.05
19	B	1220	CLA	MG-ND	-4.02	1.97	2.05
19	B	1223	CLA	MG-ND	-4.01	1.97	2.05
19	3	613	CLA	MG-ND	-4.01	1.97	2.05
22	2	503	BCR	C10-C9	4.01	1.45	1.35
19	A	1129	CLA	MG-ND	-4.01	1.97	2.05
19	B	1204	CLA	MG-ND	-4.01	1.97	2.05
22	L	4019	BCR	C10-C9	4.01	1.45	1.35
19	A	1128	CLA	MG-ND	-4.01	1.97	2.05
19	B	1234	CLA	MG-ND	-4.00	1.97	2.05
22	A	4002	BCR	C10-C9	4.00	1.45	1.35
19	4	612	CLA	MG-ND	-4.00	1.97	2.05
19	1	613	CLA	MG-ND	-4.00	1.97	2.05
19	1	601	CLA	MG-ND	-4.00	1.97	2.05
19	B	1237	CLA	MG-ND	-4.00	1.97	2.05
22	K	4002	BCR	C10-C9	3.99	1.45	1.35
19	B	1205	CLA	MG-ND	-3.99	1.97	2.05
19	G	1601	CLA	MG-ND	-3.99	1.97	2.05
22	F	4014	BCR	C10-C9	3.98	1.45	1.35
19	A	1123	CLA	MG-ND	-3.98	1.97	2.05
19	A	1122	CLA	MG-ND	-3.98	1.97	2.05
19	2	601	CLA	MG-ND	-3.98	1.97	2.05
19	B	1231	CLA	MG-ND	-3.98	1.97	2.05
19	B	1228	CLA	MG-ND	-3.97	1.97	2.05
19	B	1213	CLA	MG-ND	-3.97	1.97	2.05
22	G	4011	BCR	C10-C9	3.97	1.45	1.35
19	B	1210	CLA	MG-ND	-3.97	1.97	2.05
19	B	1219	CLA	MG-ND	-3.97	1.97	2.05
22	L	4020	BCR	C16-C17	-3.97	1.30	1.43
19	B	1212	CLA	MG-ND	-3.97	1.97	2.05
19	B	1222	CLA	MG-ND	-3.96	1.97	2.05
19	A	1107	CLA	MG-ND	-3.96	1.97	2.05
22	F	4014	BCR	C16-C17	-3.96	1.30	1.43
19	B	1232	CLA	MG-ND	-3.96	1.97	2.05
19	4	609	CLA	MG-ND	-3.96	1.97	2.05
19	2	606	CLA	MG-ND	-3.96	1.97	2.05
22	A	4007	BCR	C10-C9	3.96	1.44	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	K	4002	BCR	C16-C17	-3.95	1.30	1.43
19	B	1235	CLA	MG-ND	-3.95	1.98	2.05
19	B	1236	CLA	MG-ND	-3.95	1.98	2.05
19	3	614	CLA	MG-ND	-3.95	1.98	2.05
19	F	1301	CLA	MG-ND	-3.94	1.98	2.05
19	B	1214	CLA	MG-ND	-3.94	1.98	2.05
19	3	617	CLA	MG-ND	-3.94	1.98	2.05
19	A	1102	CLA	MG-ND	-3.94	1.98	2.05
19	A	1105	CLA	MG-ND	-3.94	1.98	2.05
19	A	1130	CLA	MG-ND	-3.94	1.98	2.05
19	2	605	CLA	MG-ND	-3.94	1.98	2.05
19	F	1302	CLA	MG-ND	-3.93	1.98	2.05
19	A	1115	CLA	MG-ND	-3.93	1.98	2.05
22	3	503	BCR	C16-C17	-3.93	1.31	1.43
19	A	1133	CLA	MG-ND	-3.93	1.98	2.05
19	B	1211	CLA	MG-ND	-3.92	1.98	2.05
19	A	1135	CLA	MG-ND	-3.92	1.98	2.05
19	B	1240	CLA	MG-ND	-3.92	1.98	2.05
19	A	1132	CLA	MG-ND	-3.92	1.98	2.05
19	B	1217	CLA	MG-ND	-3.92	1.98	2.05
19	G	1602	CLA	MG-ND	-3.92	1.98	2.05
19	3	601	CLA	MG-ND	-3.92	1.98	2.05
22	F	4016	BCR	C16-C17	-3.92	1.31	1.43
22	F	4016	BCR	C10-C9	3.91	1.44	1.35
19	L	1502	CLA	MG-ND	-3.91	1.98	2.05
19	1	608	CLA	MG-ND	-3.91	1.98	2.05
19	B	1230	CLA	MG-ND	-3.91	1.98	2.05
19	A	1013	CLA	MG-ND	-3.91	1.98	2.05
19	A	1117	CLA	MG-ND	-3.91	1.98	2.05
19	A	1113	CLA	MG-ND	-3.91	1.98	2.05
19	B	1227	CLA	MG-ND	-3.91	1.98	2.05
19	A	1138	CLA	MG-ND	-3.90	1.98	2.05
19	L	1501	CLA	MG-ND	-3.90	1.98	2.05
19	B	1215	CLA	MG-ND	-3.90	1.98	2.05
19	1	605	CLA	MG-ND	-3.90	1.98	2.05
19	2	604	CLA	MG-ND	-3.90	1.98	2.05
19	B	1238	CLA	MG-ND	-3.90	1.98	2.05
22	B	4005	BCR	C10-C9	3.90	1.44	1.35
22	J	4012	BCR	C16-C17	-3.90	1.31	1.43
19	A	1125	CLA	MG-ND	-3.90	1.98	2.05
19	2	607	CLA	MG-ND	-3.90	1.98	2.05
19	1	603	CLA	MG-ND	-3.89	1.98	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	1137	CLA	MG-ND	-3.89	1.98	2.05
19	B	1207	CLA	MG-ND	-3.89	1.98	2.05
19	3	610	CLA	MG-ND	-3.88	1.98	2.05
19	A	1118	CLA	MG-ND	-3.88	1.98	2.05
19	B	1225	CLA	MG-ND	-3.88	1.98	2.05
19	3	606	CLA	MG-ND	-3.88	1.98	2.05
22	B	4010	BCR	C16-C17	-3.88	1.31	1.43
19	B	1229	CLA	MG-ND	-3.88	1.98	2.05
19	1	607	CLA	MG-ND	-3.88	1.98	2.05
19	4	602	CLA	MG-ND	-3.88	1.98	2.05
22	3	503	BCR	C10-C9	3.88	1.44	1.35
19	G	1603	CLA	MG-ND	-3.88	1.98	2.05
19	A	1141	CLA	MG-ND	-3.88	1.98	2.05
19	1	611	CLA	MG-ND	-3.88	1.98	2.05
19	4	604	CLA	MG-ND	-3.88	1.98	2.05
19	A	1134	CLA	MG-ND	-3.87	1.98	2.05
19	K	1404	CLA	MG-ND	-3.87	1.98	2.05
19	B	1209	CLA	MG-ND	-3.87	1.98	2.05
19	1	602	CLA	MG-ND	-3.87	1.98	2.05
19	A	1103	CLA	MG-ND	-3.87	1.98	2.05
19	A	1110	CLA	MG-ND	-3.87	1.98	2.05
22	B	4006	BCR	C10-C9	3.87	1.44	1.35
19	4	601	CLA	MG-ND	-3.87	1.98	2.05
19	A	1111	CLA	MG-ND	-3.87	1.98	2.05
19	A	1104	CLA	MG-ND	-3.86	1.98	2.05
19	A	1120	CLA	MG-ND	-3.86	1.98	2.05
19	A	1101	CLA	MG-ND	-3.86	1.98	2.05
19	4	606	CLA	MG-ND	-3.86	1.98	2.05
19	B	1218	CLA	MG-ND	-3.86	1.98	2.05
19	K	1401	CLA	MG-ND	-3.86	1.98	2.05
19	B	1208	CLA	MG-ND	-3.85	1.98	2.05
22	B	4010	BCR	C10-C9	3.85	1.44	1.35
19	A	1106	CLA	MG-ND	-3.85	1.98	2.05
19	A	1136	CLA	MG-ND	-3.85	1.98	2.05
19	H	1701	CLA	MG-ND	-3.85	1.98	2.05
22	L	4020	BCR	C10-C9	3.85	1.44	1.35
19	B	1239	CLA	MG-ND	-3.84	1.98	2.05
22	A	4003	BCR	C10-C9	3.84	1.44	1.35
19	B	1201	CLA	MG-ND	-3.84	1.98	2.05
19	3	612	CLA	MG-ND	-3.84	1.98	2.05
22	L	4019	BCR	C16-C17	-3.83	1.31	1.43
19	1	606	CLA	MG-ND	-3.83	1.98	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	3	608	CLA	MG-ND	-3.83	1.98	2.05
19	L	1503	CLA	MG-ND	-3.83	1.98	2.05
19	3	602	CLA	MG-ND	-3.83	1.98	2.05
19	4	607	CLA	MG-ND	-3.82	1.98	2.05
19	A	1114	CLA	MG-ND	-3.82	1.98	2.05
19	4	608	CLA	MG-ND	-3.82	1.98	2.05
19	2	608	CLA	MG-ND	-3.82	1.98	2.05
19	3	603	CLA	MG-ND	-3.82	1.98	2.05
19	2	602	CLA	MG-ND	-3.82	1.98	2.05
22	K	4001	BCR	C16-C17	-3.82	1.31	1.43
19	A	1140	CLA	MG-ND	-3.82	1.98	2.05
19	K	1402	CLA	MG-ND	-3.81	1.98	2.05
19	4	603	CLA	MG-ND	-3.81	1.98	2.05
19	4	617	CLA	MG-ND	-3.80	1.98	2.05
19	J	1901	CLA	MG-ND	-3.78	1.98	2.05
19	A	1121	CLA	MG-ND	-3.77	1.98	2.05
22	B	4009	BCR	C10-C9	3.77	1.44	1.35
19	A	1109	CLA	MG-ND	-3.77	1.98	2.05
19	2	603	CLA	MG-ND	-3.76	1.98	2.05
19	2	612	CLA	MG-ND	-3.76	1.98	2.05
19	3	607	CLA	MG-ND	-3.76	1.98	2.05
19	1	614	CLA	MG-ND	-3.75	1.98	2.05
27	J	5001	DGD	CAA-C9A	-3.74	1.33	1.51
27	J	5001	DGD	CDA-CCA	-3.74	1.33	1.51
22	1	503	BCR	C16-C17	-3.74	1.31	1.43
25	1	802	LMG	C19-C18	-3.74	1.33	1.51
22	A	4011	BCR	C10-C9	3.74	1.44	1.35
22	B	4005	BCR	C16-C17	-3.74	1.31	1.43
27	B	5005	DGD	CDB-CCB	-3.73	1.33	1.51
25	1	802	LMG	C22-C21	-3.73	1.33	1.51
19	B	1202	CLA	MG-ND	-3.73	1.98	2.05
22	K	4001	BCR	C10-C9	3.72	1.44	1.35
22	H	4021	BCR	C16-C17	-3.72	1.31	1.43
25	G	5001	LMG	C43-C42	-3.72	1.33	1.51
27	B	5005	DGD	CAB-C9B	-3.71	1.33	1.51
25	B	5003	LMG	C19-C18	-3.71	1.33	1.51
25	F	5002	LMG	C40-C39	-3.71	1.33	1.51
25	F	5002	LMG	C43-C42	-3.71	1.33	1.51
25	1	802	LMG	C25-C24	-3.71	1.33	1.51
19	K	1403	CLA	MG-ND	-3.71	1.98	2.05
27	B	5005	DGD	CGB-CFB	-3.70	1.33	1.51
27	F	5005	DGD	CDA-CCA	-3.70	1.33	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	G	5001	LMG	C19-C18	-3.70	1.33	1.51
25	A	5006	LMG	C37-C36	-3.70	1.33	1.51
27	4	802	DGD	CAB-C9B	-3.70	1.33	1.51
25	A	5006	LMG	C22-C21	-3.69	1.33	1.51
25	A	5006	LMG	C25-C24	-3.69	1.33	1.51
27	F	5005	DGD	CGA-CFA	-3.69	1.33	1.51
25	G	5002	LMG	C22-C21	-3.69	1.33	1.51
25	F	5003	LMG	C37-C36	-3.68	1.33	1.51
25	G	5002	LMG	C40-C39	-3.68	1.33	1.51
22	A	4017	BCR	C10-C9	3.68	1.44	1.35
22	A	4008	BCR	C10-C9	3.68	1.44	1.35
27	J	5001	DGD	CGA-CFA	-3.68	1.33	1.51
25	G	5002	LMG	C37-C36	-3.67	1.33	1.51
25	F	5002	LMG	C37-C36	-3.67	1.33	1.51
27	F	5005	DGD	CAA-C9A	-3.65	1.33	1.51
27	B	5005	DGD	CAA-C9A	-3.63	1.33	1.51
25	G	5001	LMG	C37-C36	-3.63	1.33	1.51
25	A	5006	LMG	C19-C18	-3.63	1.33	1.51
25	G	5001	LMG	C40-C39	-3.63	1.33	1.51
29	2	615	CHL	CBB-CAB	3.62	1.52	1.29
29	4	610	CHL	CBB-CAB	3.59	1.51	1.29
29	1	612	CHL	CBB-CAB	3.59	1.51	1.29
29	2	610	CHL	CBB-CAB	3.58	1.51	1.29
29	1	610	CHL	CBB-CAB	3.58	1.51	1.29
29	2	609	CHL	CBB-CAB	3.58	1.51	1.29
29	3	604	CHL	CBB-CAB	3.58	1.51	1.29
29	4	615	CHL	CBB-CAB	3.57	1.51	1.29
25	G	5002	LMG	C19-C18	-3.57	1.34	1.51
29	2	613	CHL	CBB-CAB	3.55	1.51	1.29
29	3	611	CHL	CBB-CAB	3.48	1.51	1.29
19	A	1108	CLA	C1C-NC	-3.48	1.32	1.37
29	2	611	CHL	CBB-CAB	3.47	1.51	1.29
29	1	609	CHL	CBB-CAB	3.45	1.51	1.29
19	1	601	CLA	C1C-NC	-3.45	1.32	1.37
29	3	611	CHL	C1A-CHA	-3.43	1.36	1.40
29	4	611	CHL	CBB-CAB	3.40	1.50	1.29
22	I	4018	BCR	C10-C9	3.40	1.43	1.35
19	B	1205	CLA	C1C-NC	-3.39	1.32	1.37
29	2	610	CHL	C3A-C2A	-3.38	1.51	1.54
29	2	611	CHL	C1A-CHA	-3.37	1.36	1.40
29	4	613	CHL	CBB-CAB	3.32	1.50	1.29
29	1	609	CHL	C1A-CHA	-3.32	1.36	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B	1226	CLA	C1C-NC	-3.31	1.32	1.37
19	A	1110	CLA	C1C-NC	-3.30	1.32	1.37
19	A	1124	CLA	C1C-NC	-3.29	1.32	1.37
19	B	1210	CLA	C1C-NC	-3.29	1.32	1.37
19	A	1128	CLA	C1C-NC	-3.29	1.32	1.37
19	K	1401	CLA	C1C-NC	-3.28	1.32	1.37
19	A	1139	CLA	C1C-NC	-3.27	1.32	1.37
19	4	604	CLA	C1C-NC	-3.26	1.32	1.37
19	B	1211	CLA	C1C-NC	-3.25	1.32	1.37
29	2	615	CHL	C1A-CHA	-3.25	1.36	1.40
19	B	1239	CLA	C1C-NC	-3.24	1.32	1.37
19	A	1138	CLA	C1C-NC	-3.24	1.32	1.37
19	1	604	CLA	C1C-NC	-3.24	1.32	1.37
19	3	613	CLA	C1C-NC	-3.23	1.32	1.37
19	B	1222	CLA	C1C-NC	-3.22	1.32	1.37
19	A	1129	CLA	C1C-NC	-3.21	1.32	1.37
19	B	1231	CLA	C1C-NC	-3.21	1.32	1.37
19	A	1122	CLA	C1C-NC	-3.20	1.32	1.37
19	2	604	CLA	C1C-NC	-3.20	1.32	1.37
29	2	615	CHL	C3A-C2A	-3.20	1.52	1.54
19	2	606	CLA	C1C-NC	-3.20	1.32	1.37
19	B	1204	CLA	C1C-NC	-3.19	1.32	1.37
19	B	1219	CLA	C1C-NC	-3.19	1.32	1.37
19	B	1234	CLA	C1C-NC	-3.19	1.32	1.37
19	2	601	CLA	C1C-NC	-3.19	1.32	1.37
29	1	610	CHL	C1A-CHA	-3.19	1.36	1.40
19	1	613	CLA	C1C-NC	-3.18	1.32	1.37
19	4	612	CLA	C1C-NC	-3.18	1.32	1.37
19	A	1105	CLA	C1C-NC	-3.18	1.32	1.37
19	A	1117	CLA	C1C-NC	-3.18	1.32	1.37
19	A	1135	CLA	C1C-NC	-3.18	1.32	1.37
19	B	1237	CLA	C1C-NC	-3.18	1.32	1.37
19	B	1238	CLA	C1C-NC	-3.18	1.32	1.37
19	F	1302	CLA	C1C-NC	-3.18	1.32	1.37
19	4	603	CLA	C1C-NC	-3.17	1.32	1.37
19	B	1230	CLA	C1C-NC	-3.17	1.32	1.37
19	A	1106	CLA	C1C-NC	-3.16	1.32	1.37
19	B	1209	CLA	C1C-NC	-3.16	1.32	1.37
19	1	605	CLA	C1C-NC	-3.16	1.32	1.37
19	2	608	CLA	C1C-NC	-3.16	1.32	1.37
19	B	1229	CLA	C1C-NC	-3.15	1.32	1.37
19	4	608	CLA	C1C-NC	-3.15	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B	1206	CLA	C1C-NC	-3.15	1.32	1.37
19	4	605	CLA	C1C-NC	-3.15	1.32	1.37
19	A	1111	CLA	C1C-NC	-3.15	1.32	1.37
19	B	1215	CLA	C1C-NC	-3.15	1.32	1.37
19	3	603	CLA	C1C-NC	-3.15	1.32	1.37
19	B	1236	CLA	C1C-NC	-3.15	1.32	1.37
19	1	608	CLA	C1C-NC	-3.15	1.32	1.37
19	4	602	CLA	C1C-NC	-3.14	1.32	1.37
19	A	1114	CLA	C1C-NC	-3.14	1.32	1.37
19	B	1021	CLA	C1C-NC	-3.14	1.32	1.37
19	A	1126	CLA	C1C-NC	-3.14	1.32	1.37
19	A	1136	CLA	C1C-NC	-3.14	1.32	1.37
19	A	1109	CLA	C1C-NC	-3.14	1.32	1.37
19	B	1240	CLA	C1C-NC	-3.14	1.32	1.37
18	A	1011	CL0	CHB-C4A	-3.14	1.34	1.38
19	B	1225	CLA	C1C-NC	-3.13	1.33	1.37
19	A	1112	CLA	C1C-NC	-3.13	1.33	1.37
19	3	601	CLA	C1C-NC	-3.13	1.33	1.37
19	B	1023	CLA	C1C-NC	-3.13	1.33	1.37
19	A	1133	CLA	C1C-NC	-3.13	1.33	1.37
19	1	611	CLA	C1C-NC	-3.12	1.33	1.37
19	B	1228	CLA	C1C-NC	-3.12	1.33	1.37
19	2	601	CLA	C4B-NB	-3.12	1.33	1.37
19	A	1121	CLA	C1C-NC	-3.12	1.33	1.37
19	3	614	CLA	C1C-NC	-3.12	1.33	1.37
19	A	1120	CLA	C1C-NC	-3.12	1.33	1.37
19	B	1216	CLA	C1C-NC	-3.12	1.33	1.37
19	A	1118	CLA	C1C-NC	-3.11	1.33	1.37
19	F	1301	CLA	C1C-NC	-3.11	1.33	1.37
19	A	1113	CLA	C1C-NC	-3.11	1.33	1.37
19	B	1213	CLA	C1C-NC	-3.11	1.33	1.37
19	B	1232	CLA	C1C-NC	-3.11	1.33	1.37
19	B	1218	CLA	C1C-NC	-3.10	1.33	1.37
19	B	1203	CLA	C1C-NC	-3.10	1.33	1.37
19	4	601	CLA	C1C-NC	-3.10	1.33	1.37
19	B	1220	CLA	C1C-NC	-3.10	1.33	1.37
19	3	606	CLA	C1C-NC	-3.10	1.33	1.37
19	A	1013	CLA	C1C-NC	-3.10	1.33	1.37
19	A	1123	CLA	C1C-NC	-3.10	1.33	1.37
19	3	612	CLA	C1C-NC	-3.10	1.33	1.37
19	B	1212	CLA	C1C-NC	-3.10	1.33	1.37
19	A	1107	CLA	C1C-NC	-3.09	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	2	613	CHL	C3A-C2A	-3.09	1.52	1.54
19	B	1208	CLA	C1C-NC	-3.09	1.33	1.37
19	H	1701	CLA	C1C-NC	-3.09	1.33	1.37
19	A	1119	CLA	C1C-NC	-3.09	1.33	1.37
19	A	1127	CLA	C1C-NC	-3.09	1.33	1.37
19	B	1235	CLA	C1C-NC	-3.09	1.33	1.37
19	3	608	CLA	C1C-NC	-3.09	1.33	1.37
19	B	1227	CLA	C1C-NC	-3.09	1.33	1.37
19	B	1202	CLA	C1C-NC	-3.08	1.33	1.37
19	B	1224	CLA	C1C-NC	-3.08	1.33	1.37
19	L	1503	CLA	C1C-NC	-3.08	1.33	1.37
19	B	1207	CLA	C1C-NC	-3.08	1.33	1.37
19	2	603	CLA	C1C-NC	-3.08	1.33	1.37
19	A	1141	CLA	C1C-NC	-3.08	1.33	1.37
19	A	1130	CLA	C1C-NC	-3.07	1.33	1.37
19	A	1125	CLA	C1C-NC	-3.07	1.33	1.37
19	2	612	CLA	C1C-NC	-3.07	1.33	1.37
19	G	1601	CLA	C1C-NC	-3.07	1.33	1.37
19	A	1115	CLA	C1C-NC	-3.07	1.33	1.37
19	A	1137	CLA	C1C-NC	-3.07	1.33	1.37
19	4	617	CLA	C1C-NC	-3.07	1.33	1.37
19	4	606	CLA	C1C-NC	-3.07	1.33	1.37
19	A	1103	CLA	C1C-NC	-3.06	1.33	1.37
19	3	602	CLA	C1C-NC	-3.06	1.33	1.37
29	3	604	CHL	C1A-CHA	-3.06	1.36	1.40
19	A	1140	CLA	C1C-NC	-3.06	1.33	1.37
19	A	1132	CLA	C1C-NC	-3.06	1.33	1.37
19	1	606	CLA	C1C-NC	-3.06	1.33	1.37
19	A	1012	CLA	C1C-NC	-3.05	1.33	1.37
19	L	1501	CLA	C1C-NC	-3.05	1.33	1.37
19	L	1502	CLA	C1C-NC	-3.04	1.33	1.37
19	4	607	CLA	C1C-NC	-3.04	1.33	1.37
19	3	605	CLA	C1C-NC	-3.04	1.33	1.37
19	A	1101	CLA	C1C-NC	-3.04	1.33	1.37
19	B	1223	CLA	C1C-NC	-3.04	1.33	1.37
19	B	1214	CLA	C1C-NC	-3.04	1.33	1.37
19	3	607	CLA	C1C-NC	-3.03	1.33	1.37
19	A	1104	CLA	C1C-NC	-3.03	1.33	1.37
19	A	1102	CLA	C1C-NC	-3.02	1.33	1.37
19	3	617	CLA	C1C-NC	-3.02	1.33	1.37
19	B	1201	CLA	C1C-NC	-3.01	1.33	1.37
19	1	603	CLA	C1C-NC	-3.01	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	2	602	CLA	C1C-NC	-3.01	1.33	1.37
19	2	605	CLA	C1C-NC	-3.00	1.33	1.37
19	A	1116	CLA	C1C-NC	-3.00	1.33	1.37
19	B	1221	CLA	C1C-NC	-3.00	1.33	1.37
19	K	1402	CLA	C1C-NC	-2.99	1.33	1.37
19	J	1901	CLA	C1C-NC	-2.99	1.33	1.37
19	G	1603	CLA	C1C-NC	-2.99	1.33	1.37
19	4	609	CLA	C1C-NC	-2.99	1.33	1.37
19	B	1217	CLA	C1C-NC	-2.99	1.33	1.37
19	1	601	CLA	C4B-NB	-2.99	1.33	1.37
19	G	1602	CLA	C1C-NC	-2.98	1.33	1.37
19	K	1403	CLA	C1C-NC	-2.98	1.33	1.37
19	A	1134	CLA	C1C-NC	-2.98	1.33	1.37
19	1	607	CLA	C1C-NC	-2.98	1.33	1.37
29	4	611	CHL	CHB-C4A	-2.97	1.35	1.38
19	1	602	CLA	C1C-NC	-2.97	1.33	1.37
19	2	607	CLA	C1C-NC	-2.97	1.33	1.37
19	B	1022	CLA	C1C-NC	-2.97	1.33	1.37
19	A	1131	CLA	C1C-NC	-2.96	1.33	1.37
19	3	610	CLA	C1C-NC	-2.96	1.33	1.37
29	1	612	CHL	C1A-CHA	-2.96	1.36	1.40
19	3	613	CLA	C4B-NB	-2.96	1.34	1.37
25	2	803	LMG	C19-C18	-2.95	1.33	1.51
27	3	803	DGD	CAB-C9B	-2.94	1.33	1.51
19	B	1023	CLA	C4B-NB	-2.94	1.34	1.37
19	1	614	CLA	C1C-NC	-2.94	1.33	1.37
29	4	610	CHL	C1A-CHA	-2.94	1.36	1.40
19	A	1139	CLA	C4B-NB	-2.93	1.34	1.37
19	B	1224	CLA	C4B-NB	-2.92	1.34	1.37
29	4	613	CHL	CHB-C4A	-2.92	1.35	1.38
19	A	1125	CLA	C4B-NB	-2.92	1.34	1.37
19	A	1126	CLA	C4B-NB	-2.91	1.34	1.37
29	4	610	CHL	CHB-C4A	-2.91	1.35	1.38
19	B	1216	CLA	C4B-NB	-2.91	1.34	1.37
19	K	1404	CLA	C1C-NC	-2.90	1.33	1.37
19	A	1108	CLA	C4B-NB	-2.90	1.34	1.37
19	B	1215	CLA	C4B-NB	-2.90	1.34	1.37
19	A	1124	CLA	C4B-NB	-2.90	1.34	1.37
19	A	1129	CLA	C4B-NB	-2.90	1.34	1.37
29	2	610	CHL	C1A-CHA	-2.89	1.36	1.40
19	A	1106	CLA	C4B-NB	-2.87	1.34	1.37
29	2	610	CHL	C1B-C2B	2.86	1.42	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B	1210	CLA	C4B-NB	-2.86	1.34	1.37
29	3	604	CHL	CHB-C4A	-2.86	1.35	1.38
29	4	611	CHL	C1D-C2D	2.85	1.42	1.39
29	2	609	CHL	C1B-C2B	2.85	1.42	1.39
19	3	614	CLA	C4B-NB	-2.84	1.34	1.37
19	B	1229	CLA	C4B-NB	-2.84	1.34	1.37
29	2	611	CHL	CHB-C4A	-2.84	1.35	1.38
29	3	611	CHL	CHB-C4A	-2.83	1.35	1.38
29	1	610	CHL	C1B-C2B	2.83	1.42	1.39
29	4	615	CHL	C3A-C2A	-2.83	1.52	1.54
29	2	613	CHL	C1D-C2D	2.82	1.42	1.39
29	1	609	CHL	CHB-C4A	-2.82	1.35	1.38
19	B	1240	CLA	C4B-NB	-2.82	1.34	1.37
19	A	1117	CLA	C4B-NB	-2.81	1.34	1.37
19	4	604	CLA	C4B-NB	-2.81	1.34	1.37
29	2	611	CHL	C1D-C2D	2.80	1.42	1.39
29	4	613	CHL	C1D-C2D	2.80	1.42	1.39
19	B	1231	CLA	C4B-NB	-2.80	1.34	1.37
29	1	609	CHL	C1D-C2D	2.80	1.42	1.39
29	1	610	CHL	C1D-C2D	2.79	1.42	1.39
19	1	605	CLA	C4B-NB	-2.79	1.34	1.37
29	3	604	CHL	C1D-C2D	2.78	1.42	1.39
19	B	1236	CLA	C4B-NB	-2.78	1.34	1.37
29	4	611	CHL	C1A-CHA	-2.78	1.36	1.40
19	F	1302	CLA	C4B-NB	-2.77	1.34	1.37
19	A	1112	CLA	C4B-NB	-2.77	1.34	1.37
29	1	612	CHL	C1B-C2B	2.77	1.42	1.39
19	A	1113	CLA	C4B-NB	-2.77	1.34	1.37
19	A	1135	CLA	C4B-NB	-2.77	1.34	1.37
30	4	502	XAT	O24-C25	-2.77	1.42	1.46
19	B	1214	CLA	C4B-NB	-2.76	1.34	1.37
19	2	604	CLA	C4B-NB	-2.76	1.34	1.37
29	2	615	CHL	C1D-C2D	2.76	1.42	1.39
19	B	1203	CLA	C4B-NB	-2.75	1.34	1.37
29	4	615	CHL	C1B-C2B	2.75	1.42	1.39
29	3	611	CHL	C1D-C2D	2.75	1.42	1.39
19	A	1138	CLA	C4B-NB	-2.75	1.34	1.37
29	4	615	CHL	C1D-C2D	2.75	1.42	1.39
19	B	1222	CLA	C4B-NB	-2.75	1.34	1.37
29	2	610	CHL	C1D-C2D	2.75	1.42	1.39
19	B	1211	CLA	C4B-NB	-2.75	1.34	1.37
19	B	1234	CLA	C4B-NB	-2.74	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B	1022	CLA	C4B-NB	-2.74	1.34	1.37
19	B	1204	CLA	C4B-NB	-2.74	1.34	1.37
29	2	609	CHL	C1D-C2D	2.73	1.42	1.39
19	A	1013	CLA	C4B-NB	-2.73	1.34	1.37
19	3	601	CLA	C4B-NB	-2.73	1.34	1.37
29	3	604	CHL	C1B-C2B	2.73	1.42	1.39
19	1	613	CLA	C4B-NB	-2.73	1.34	1.37
29	2	611	CHL	C1B-C2B	2.72	1.42	1.39
19	B	1238	CLA	C4B-NB	-2.72	1.34	1.37
29	4	611	CHL	C1B-C2B	2.71	1.42	1.39
29	2	613	CHL	C1B-C2B	2.71	1.42	1.39
19	B	1228	CLA	C4B-NB	-2.71	1.34	1.37
19	B	1021	CLA	C4B-NB	-2.71	1.34	1.37
19	K	1401	CLA	C4B-NB	-2.71	1.34	1.37
29	1	610	CHL	CHB-C4A	-2.71	1.35	1.38
19	B	1235	CLA	C4B-NB	-2.71	1.34	1.37
19	4	612	CLA	C4B-NB	-2.71	1.34	1.37
29	1	612	CHL	CHB-C4A	-2.70	1.35	1.38
29	2	615	CHL	C1B-C2B	2.70	1.42	1.39
29	1	609	CHL	C1B-C2B	2.70	1.42	1.39
19	4	601	CLA	C4B-NB	-2.70	1.34	1.37
19	A	1119	CLA	C4B-NB	-2.69	1.34	1.37
29	2	609	CHL	CHB-C4A	-2.69	1.35	1.38
19	2	606	CLA	C4B-NB	-2.69	1.34	1.37
19	3	617	CLA	C4B-NB	-2.69	1.34	1.37
29	3	611	CHL	C1B-C2B	2.69	1.42	1.39
19	3	612	CLA	C4B-NB	-2.69	1.34	1.37
29	4	610	CHL	C1D-C2D	2.69	1.42	1.39
29	4	615	CHL	CHB-C4A	-2.68	1.35	1.38
19	1	604	CLA	C4B-NB	-2.68	1.34	1.37
19	B	1212	CLA	C4B-NB	-2.68	1.34	1.37
19	B	1225	CLA	C4B-NB	-2.68	1.34	1.37
19	A	1111	CLA	C4B-NB	-2.68	1.34	1.37
19	A	1120	CLA	C4B-NB	-2.68	1.34	1.37
19	G	1601	CLA	C4B-NB	-2.68	1.34	1.37
19	A	1130	CLA	C4B-NB	-2.67	1.34	1.37
29	4	610	CHL	C1B-C2B	2.67	1.42	1.39
19	B	1221	CLA	C4B-NB	-2.67	1.34	1.37
29	4	613	CHL	C1B-C2B	2.67	1.42	1.39
19	B	1206	CLA	C4B-NB	-2.67	1.34	1.37
19	A	1103	CLA	C4B-NB	-2.67	1.34	1.37
19	B	1226	CLA	C4B-NB	-2.67	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	1127	CLA	C4B-NB	-2.67	1.34	1.37
19	A	1101	CLA	C4B-NB	-2.66	1.34	1.37
29	2	615	CHL	CHB-C4A	-2.66	1.35	1.38
29	2	613	CHL	CHB-C4A	-2.66	1.35	1.38
29	4	613	CHL	C1A-CHA	-2.66	1.37	1.40
19	B	1209	CLA	C4B-NB	-2.66	1.34	1.37
19	A	1128	CLA	C4B-NB	-2.66	1.34	1.37
29	2	610	CHL	CHB-C4A	-2.65	1.35	1.38
19	A	1102	CLA	C4B-NB	-2.65	1.34	1.37
19	B	1230	CLA	C4B-NB	-2.65	1.34	1.37
19	A	1012	CLA	C4B-NB	-2.65	1.34	1.37
19	A	1115	CLA	C4B-NB	-2.65	1.34	1.37
19	1	607	CLA	C4B-NB	-2.64	1.34	1.37
19	B	1232	CLA	C4B-NB	-2.63	1.34	1.37
19	A	1105	CLA	C4B-NB	-2.63	1.34	1.37
19	A	1133	CLA	C4B-NB	-2.63	1.34	1.37
19	A	1141	CLA	C4B-NB	-2.63	1.34	1.37
19	4	606	CLA	C4B-NB	-2.63	1.34	1.37
19	B	1213	CLA	C4B-NB	-2.62	1.34	1.37
29	1	612	CHL	C1D-C2D	2.62	1.42	1.39
19	G	1602	CLA	C4B-NB	-2.62	1.34	1.37
19	H	1701	CLA	C4B-NB	-2.61	1.34	1.37
19	A	1107	CLA	C4B-NB	-2.61	1.34	1.37
19	2	612	CLA	C4B-NB	-2.60	1.34	1.37
19	3	610	CLA	C4B-NB	-2.60	1.34	1.37
19	F	1301	CLA	C4B-NB	-2.60	1.34	1.37
19	A	1132	CLA	C4B-NB	-2.60	1.34	1.37
19	3	606	CLA	C4B-NB	-2.60	1.34	1.37
31	2	807	3PH	O21-C2	-2.60	1.40	1.46
19	B	1220	CLA	C4B-NB	-2.59	1.34	1.37
24	G	5004	LMT	O3'-C3'	-2.58	1.36	1.43
19	4	605	CLA	C4B-NB	-2.58	1.34	1.37
30	2	502	XAT	O24-C25	-2.57	1.42	1.46
24	B	5008	LMT	O3'-C3'	-2.57	1.36	1.43
19	2	605	CLA	C4B-NB	-2.57	1.34	1.37
24	G	5005	LMT	O3'-C3'	-2.57	1.36	1.43
19	1	611	CLA	C4B-NB	-2.57	1.34	1.37
19	B	1237	CLA	C4B-NB	-2.56	1.34	1.37
19	1	606	CLA	C4B-NB	-2.55	1.34	1.37
19	L	1503	CLA	C4B-NB	-2.55	1.34	1.37
24	B	5006	LMT	O3'-C3'	-2.54	1.36	1.43
19	3	605	CLA	C4B-NB	-2.54	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	1123	CLA	C4B-NB	-2.54	1.34	1.37
19	A	1118	CLA	C4B-NB	-2.53	1.34	1.37
19	4	617	CLA	C4B-NB	-2.53	1.34	1.37
24	2	808	LMT	O3'-C3'	-2.53	1.36	1.43
19	4	609	CLA	C4B-NB	-2.53	1.34	1.37
24	A	5004	LMT	O3'-C3'	-2.53	1.36	1.43
19	L	1501	CLA	C4B-NB	-2.53	1.34	1.37
19	A	1116	CLA	C4B-NB	-2.52	1.34	1.37
19	A	1104	CLA	C4B-NB	-2.51	1.34	1.37
19	L	1502	CLA	C4B-NB	-2.51	1.34	1.37
19	B	1223	CLA	C4B-NB	-2.51	1.34	1.37
19	4	607	CLA	C4B-NB	-2.49	1.34	1.37
19	B	1219	CLA	C4B-NB	-2.48	1.34	1.37
19	3	602	CLA	C4B-NB	-2.46	1.34	1.37
19	G	1603	CLA	C4B-NB	-2.46	1.34	1.37
19	B	1227	CLA	C4B-NB	-2.46	1.34	1.37
19	B	1201	CLA	C4B-NB	-2.44	1.34	1.37
19	B	1205	CLA	C4B-NB	-2.43	1.34	1.37
19	B	1202	CLA	C4B-NB	-2.42	1.34	1.37
29	4	611	CHL	C3B-C2B	-2.42	1.37	1.40
29	4	615	CHL	C1A-CHA	-2.41	1.37	1.40
19	K	1404	CLA	C4B-NB	-2.40	1.34	1.37
19	3	607	CLA	C4B-NB	-2.40	1.34	1.37
31	2	807	3PH	O31-C31	2.40	1.40	1.33
25	F	5002	LMG	C19-C18	-2.39	1.33	1.50
29	3	604	CHL	C2C-C3C	2.39	1.38	1.36
19	4	608	CLA	C4B-NB	-2.38	1.34	1.37
27	J	5001	DGD	CAB-C9B	-2.38	1.33	1.50
19	A	1122	CLA	C4B-NB	-2.38	1.34	1.37
19	1	602	CLA	C4B-NB	-2.38	1.34	1.37
27	3	803	DGD	CAA-C9A	-2.38	1.33	1.50
19	A	1136	CLA	C4B-NB	-2.38	1.34	1.37
25	G	5002	LMG	C43-C42	-2.38	1.33	1.50
27	G	5003	DGD	CAB-C9B	-2.38	1.33	1.50
25	A	5006	LMG	C40-C39	-2.37	1.33	1.50
19	A	1131	CLA	C4B-NB	-2.37	1.34	1.37
27	B	5005	DGD	CDA-CCA	-2.36	1.33	1.50
19	1	608	CLA	C4B-NB	-2.36	1.34	1.37
19	A	1110	CLA	C4B-NB	-2.36	1.34	1.37
19	1	603	CLA	C4B-NB	-2.35	1.34	1.37
29	2	611	CHL	C3B-C2B	-2.35	1.37	1.40
19	2	607	CLA	C4B-NB	-2.35	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	2	609	CHL	C1A-CHA	-2.35	1.37	1.40
22	I	4018	BCR	C12-C13	-2.34	1.40	1.46
19	K	1403	CLA	C4B-NB	-2.32	1.34	1.37
19	K	1402	CLA	C4B-NB	-2.32	1.34	1.37
29	4	613	CHL	C2C-C3C	2.32	1.38	1.36
19	B	1239	CLA	C4B-NB	-2.31	1.34	1.37
19	3	608	CLA	C4B-NB	-2.31	1.34	1.37
19	4	602	CLA	C4B-NB	-2.30	1.34	1.37
19	2	608	CLA	C4B-NB	-2.29	1.34	1.37
19	B	1218	CLA	C4B-NB	-2.29	1.34	1.37
19	2	603	CLA	C4B-NB	-2.29	1.34	1.37
19	B	1217	CLA	C4B-NB	-2.29	1.34	1.37
23	3	801	LHG	O7-C7	-2.28	1.34	1.42
19	A	1114	CLA	C4B-NB	-2.28	1.34	1.37
29	1	609	CHL	C3B-C2B	-2.27	1.37	1.40
19	A	1125	CLA	C1C-C2C	2.27	1.49	1.44
19	A	1137	CLA	C4B-NB	-2.26	1.34	1.37
29	4	610	CHL	C2C-C3C	2.26	1.38	1.36
24	B	5008	LMT	O3B-C3B	-2.25	1.37	1.43
19	A	1121	CLA	C4B-NB	-2.24	1.34	1.37
19	A	1134	CLA	C4B-NB	-2.24	1.34	1.37
24	2	808	LMT	O2B-C2B	-2.24	1.37	1.43
19	B	1201	CLA	C1C-C2C	2.23	1.49	1.44
19	3	603	CLA	C4B-NB	-2.23	1.34	1.37
24	A	5004	LMT	O3B-C3B	-2.23	1.37	1.43
19	A	1109	CLA	C4B-NB	-2.23	1.34	1.37
19	J	1901	CLA	C4B-NB	-2.23	1.34	1.37
24	B	5006	LMT	O2'-C2'	-2.22	1.37	1.43
24	B	5006	LMT	O3B-C3B	-2.22	1.37	1.43
19	A	1102	CLA	C1C-C2C	2.22	1.49	1.44
19	B	1208	CLA	C4B-NB	-2.22	1.34	1.37
19	A	1122	CLA	C1C-C2C	2.22	1.49	1.44
24	B	5008	LMT	O2B-C2B	-2.22	1.37	1.43
19	2	602	CLA	C4B-NB	-2.22	1.34	1.37
19	1	614	CLA	C4B-NB	-2.22	1.34	1.37
24	2	808	LMT	O3B-C3B	-2.22	1.37	1.43
19	A	1141	CLA	C1C-C2C	2.21	1.49	1.44
29	1	612	CHL	CHA-CBD	2.21	1.54	1.51
24	G	5005	LMT	O3B-C3B	-2.20	1.37	1.43
22	2	503	BCR	C30-C25	2.20	1.56	1.53
24	A	5004	LMT	O2B-C2B	-2.20	1.37	1.43
19	A	1104	CLA	C1C-C2C	2.20	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	4	605	CLA	C3D-C4D	-2.20	1.39	1.44
24	G	5005	LMT	O2B-C2B	-2.20	1.37	1.43
19	J	1901	CLA	C1C-C2C	2.19	1.49	1.44
31	2	807	3PH	O31-C3	-2.19	1.40	1.45
24	B	5006	LMT	O2B-C2B	-2.19	1.37	1.43
19	4	607	CLA	C1C-C2C	2.19	1.49	1.44
19	B	1223	CLA	C1C-C2C	2.19	1.49	1.44
29	2	613	CHL	C1A-CHA	-2.19	1.37	1.40
31	2	807	3PH	O21-C21	2.18	1.40	1.34
19	B	1207	CLA	C4B-NB	-2.18	1.35	1.37
24	G	5004	LMT	O3B-C3B	-2.18	1.37	1.43
19	A	1121	CLA	C1C-C2C	2.18	1.48	1.44
19	A	1140	CLA	C1C-C2C	2.18	1.48	1.44
24	G	5004	LMT	O2'-C2'	-2.17	1.37	1.43
19	3	602	CLA	C1C-C2C	2.17	1.48	1.44
19	A	1137	CLA	C1C-C2C	2.17	1.48	1.44
19	4	605	CLA	C1C-C2C	2.17	1.48	1.44
19	2	602	CLA	C1C-C2C	2.17	1.48	1.44
19	B	1208	CLA	C1C-C2C	2.17	1.48	1.44
29	1	610	CHL	CHA-CBD	2.17	1.54	1.51
19	1	614	CLA	C1C-C2C	2.16	1.48	1.44
19	2	601	CLA	C1C-C2C	2.16	1.48	1.44
19	B	1223	CLA	C3D-C4D	-2.16	1.39	1.44
19	1	601	CLA	C1C-C2C	2.15	1.48	1.44
24	A	5004	LMT	O2'-C2'	-2.15	1.37	1.43
19	2	601	CLA	C1A-CHA	2.15	1.52	1.43
19	2	603	CLA	C1C-C2C	2.15	1.48	1.44
19	L	1503	CLA	C1C-C2C	2.15	1.48	1.44
27	J	5001	DGD	O5D-C1E	2.14	1.43	1.40
24	B	5008	LMT	O2'-C2'	-2.14	1.37	1.43
19	4	603	CLA	C4B-NB	-2.14	1.35	1.37
29	2	613	CHL	CHA-CBD	2.14	1.54	1.51
27	F	5005	DGD	O3G-C1D	2.14	1.43	1.40
19	A	1012	CLA	C1A-CHA	2.14	1.51	1.43
19	1	611	CLA	C1C-C2C	2.14	1.48	1.44
19	B	1207	CLA	C1C-C2C	2.14	1.48	1.44
29	2	611	CHL	CHA-CBD	2.14	1.54	1.51
19	B	1221	CLA	C1A-CHA	2.14	1.51	1.43
19	3	612	CLA	C1C-C2C	2.13	1.48	1.44
29	4	615	CHL	CHA-CBD	2.13	1.54	1.51
25	2	803	LMG	O1-C1	2.13	1.43	1.40
19	G	1601	CLA	C1A-CHA	2.13	1.51	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B	1220	CLA	C1C-C2C	2.12	1.48	1.44
19	G	1602	CLA	C1C-C2C	2.12	1.48	1.44
19	3	601	CLA	C1C-C2C	2.12	1.48	1.44
24	2	808	LMT	O2'-C2'	-2.12	1.37	1.43
24	A	5004	LMT	O1'-C1'	-2.12	1.36	1.40
24	G	5005	LMT	O2'-C2'	-2.12	1.37	1.43
19	2	607	CLA	C1A-CHA	2.12	1.51	1.43
19	B	1206	CLA	C1A-CHA	2.12	1.51	1.43
24	G	5004	LMT	O2B-C2B	-2.12	1.37	1.43
29	4	610	CHL	CHA-CBD	2.12	1.54	1.51
19	K	1404	CLA	C1C-C2C	2.11	1.48	1.44
19	A	1134	CLA	C1A-CHA	2.11	1.51	1.43
29	2	610	CHL	CHA-CBD	2.11	1.54	1.51
19	B	1222	CLA	C1A-CHA	2.11	1.51	1.43
29	4	613	CHL	CHA-CBD	2.11	1.54	1.51
19	B	1232	CLA	C1A-CHA	2.11	1.51	1.43
19	1	602	CLA	C1C-C2C	2.11	1.48	1.44
19	L	1502	CLA	C1A-CHA	2.11	1.51	1.43
19	B	1228	CLA	C1A-CHA	2.11	1.51	1.43
19	B	1209	CLA	C3D-C4D	-2.10	1.39	1.44
19	A	1140	CLA	C4B-NB	-2.10	1.35	1.37
19	B	1211	CLA	C3D-C4D	-2.10	1.39	1.44
19	K	1404	CLA	C1A-CHA	2.10	1.51	1.43
19	4	602	CLA	C1A-CHA	2.10	1.51	1.43
19	1	613	CLA	C1C-C2C	2.10	1.48	1.44
19	2	608	CLA	C1C-C2C	2.10	1.48	1.44
24	G	5004	LMT	O1'-C1'	-2.10	1.36	1.40
19	2	607	CLA	C1C-C2C	2.10	1.48	1.44
29	2	615	CHL	CHA-CBD	2.10	1.54	1.51
19	B	1235	CLA	C1C-C2C	2.10	1.48	1.44
29	4	611	CHL	CHA-CBD	2.09	1.54	1.51
19	A	1106	CLA	C1C-C2C	2.09	1.48	1.44
29	4	613	CHL	C3B-C2B	-2.09	1.37	1.40
19	B	1224	CLA	C1A-CHA	2.09	1.51	1.43
19	A	1127	CLA	C3D-C4D	-2.09	1.39	1.44
29	2	609	CHL	CHA-CBD	2.09	1.54	1.51
19	A	1102	CLA	C1A-CHA	2.09	1.51	1.43
19	A	1103	CLA	C1A-CHA	2.09	1.51	1.43
19	1	603	CLA	C1A-CHA	2.09	1.51	1.43
19	A	1131	CLA	C1C-C2C	2.09	1.48	1.44
19	B	1213	CLA	C1A-CHA	2.09	1.51	1.43
19	A	1136	CLA	C1A-CHA	2.08	1.51	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	4	608	CLA	C1C-C2C	2.08	1.48	1.44
19	4	609	CLA	C1C-C2C	2.08	1.48	1.44
19	B	1232	CLA	C1C-C2C	2.08	1.48	1.44
19	B	1215	CLA	C3D-C4D	-2.08	1.39	1.44
19	A	1130	CLA	C1C-C2C	2.08	1.48	1.44
19	B	1212	CLA	C1C-C2C	2.08	1.48	1.44
19	B	1205	CLA	C3D-C4D	-2.08	1.39	1.44
19	1	605	CLA	C3D-C4D	-2.08	1.39	1.44
19	A	1129	CLA	C1A-CHA	2.08	1.51	1.43
19	A	1115	CLA	C1C-C2C	2.08	1.48	1.44
19	K	1402	CLA	C1C-C2C	2.08	1.48	1.44
19	A	1132	CLA	C3D-C4D	-2.08	1.39	1.44
19	L	1502	CLA	C1C-C2C	2.07	1.48	1.44
19	3	605	CLA	C1C-C2C	2.07	1.48	1.44
19	A	1012	CLA	C1C-C2C	2.07	1.48	1.44
19	A	1119	CLA	C3D-C4D	-2.07	1.39	1.44
19	B	1236	CLA	C3D-C4D	-2.07	1.39	1.44
19	3	608	CLA	C1C-C2C	2.07	1.48	1.44
19	A	1109	CLA	C1A-CHA	2.07	1.51	1.43
19	A	1116	CLA	C1C-C2C	2.07	1.48	1.44
19	2	612	CLA	C3D-C4D	-2.07	1.39	1.44
19	3	605	CLA	C1A-CHA	2.07	1.51	1.43
29	3	611	CHL	CHA-CBD	2.07	1.54	1.51
19	B	1225	CLA	C1A-CHA	2.07	1.51	1.43
19	B	1221	CLA	C1C-C2C	2.07	1.48	1.44
19	A	1121	CLA	C1A-CHA	2.07	1.51	1.43
19	B	1022	CLA	C3D-C4D	-2.07	1.39	1.44
19	B	1218	CLA	C1C-C2C	2.07	1.48	1.44
29	3	604	CHL	CHA-CBD	2.07	1.54	1.51
19	A	1116	CLA	C1A-CHA	2.07	1.51	1.43
19	A	1116	CLA	C3D-C4D	-2.07	1.39	1.44
19	B	1203	CLA	C3D-C4D	-2.06	1.39	1.44
19	4	604	CLA	C3D-C4D	-2.06	1.39	1.44
19	A	1138	CLA	C1C-C2C	2.06	1.48	1.44
19	2	604	CLA	C1C-C2C	2.06	1.48	1.44
19	3	612	CLA	C1A-CHA	2.06	1.51	1.43
19	4	609	CLA	C1A-CHA	2.06	1.51	1.43
19	3	607	CLA	C1C-C2C	2.06	1.48	1.44
19	F	1302	CLA	C1A-CHA	2.06	1.51	1.43
22	K	4001	BCR	C12-C13	-2.06	1.41	1.46
19	A	1133	CLA	C3D-C4D	-2.06	1.39	1.44
19	2	612	CLA	CHD-C1D	2.06	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B	1217	CLA	C1C-C2C	2.06	1.48	1.44
19	B	1213	CLA	C1C-C2C	2.06	1.48	1.44
19	A	1013	CLA	C3D-C4D	-2.06	1.39	1.44
19	A	1128	CLA	C3D-C4D	-2.05	1.39	1.44
19	B	1231	CLA	C3D-C4D	-2.05	1.39	1.44
19	L	1501	CLA	C3D-C4D	-2.05	1.39	1.44
19	A	1114	CLA	C1A-CHA	2.05	1.51	1.43
19	2	605	CLA	C1A-CHA	2.05	1.51	1.43
19	4	601	CLA	C3D-C4D	-2.05	1.39	1.44
19	4	603	CLA	C1C-C2C	2.05	1.48	1.44
27	F	5005	DGD	O5D-C1E	2.05	1.43	1.40
19	F	1301	CLA	C1C-C2C	2.05	1.48	1.44
19	A	1101	CLA	C1C-C2C	2.05	1.48	1.44
19	A	1130	CLA	C1A-CHA	2.05	1.51	1.43
19	3	605	CLA	C3D-C4D	-2.05	1.39	1.44
19	B	1222	CLA	C3D-C4D	-2.05	1.39	1.44
19	3	601	CLA	C1A-CHA	2.05	1.51	1.43
19	B	1237	CLA	C1C-C2C	2.05	1.48	1.44
19	B	1219	CLA	C1C-C2C	2.05	1.48	1.44
19	B	1223	CLA	C1A-CHA	2.05	1.51	1.43
19	A	1108	CLA	C3D-C4D	-2.05	1.39	1.44
19	1	608	CLA	C1C-C2C	2.05	1.48	1.44
19	A	1138	CLA	C1A-CHA	2.05	1.51	1.43
19	2	606	CLA	C1A-CHA	2.05	1.51	1.43
19	B	1204	CLA	C3D-C4D	-2.05	1.39	1.44
19	A	1123	CLA	C1A-CHA	2.05	1.51	1.43
19	A	1111	CLA	C3D-C4D	-2.05	1.39	1.44
19	B	1220	CLA	C3D-C4D	-2.05	1.39	1.44
19	A	1133	CLA	C1C-C2C	2.05	1.48	1.44
19	B	1214	CLA	C1A-CHA	2.05	1.51	1.43
19	A	1124	CLA	C1A-CHA	2.05	1.51	1.43
19	1	604	CLA	C3D-C4D	-2.05	1.39	1.44
19	B	1237	CLA	C3D-C4D	-2.05	1.39	1.44
19	B	1226	CLA	C3D-C4D	-2.04	1.39	1.44
19	A	1114	CLA	C1C-C2C	2.04	1.48	1.44
19	A	1136	CLA	C1C-C2C	2.04	1.48	1.44
19	4	605	CLA	C1A-CHA	2.04	1.51	1.43
24	B	5008	LMT	O4'-C4B	-2.04	1.37	1.43
19	B	1216	CLA	C3D-C4D	-2.04	1.39	1.44
19	B	1022	CLA	C1C-C2C	2.04	1.48	1.44
19	B	1240	CLA	C1C-C2C	2.04	1.48	1.44
19	A	1139	CLA	C1A-CHA	2.04	1.51	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	4	617	CLA	C1C-C2C	2.04	1.48	1.44
19	B	1235	CLA	C1A-CHA	2.04	1.51	1.43
19	4	603	CLA	C1A-CHA	2.04	1.51	1.43
19	A	1137	CLA	C3D-C4D	-2.04	1.39	1.44
19	B	1021	CLA	C3D-C4D	-2.04	1.39	1.44
19	3	613	CLA	C3D-C4D	-2.04	1.39	1.44
19	A	1111	CLA	C1A-CHA	2.04	1.51	1.43
19	K	1401	CLA	CHD-C1D	2.04	1.42	1.38
19	1	613	CLA	C3D-C4D	-2.04	1.39	1.44
19	A	1126	CLA	C1A-CHA	2.04	1.51	1.43
19	A	1118	CLA	C1A-CHA	2.04	1.51	1.43
29	4	610	CHL	C3B-C2B	-2.04	1.37	1.40
19	3	603	CLA	C1A-CHA	2.04	1.51	1.43
19	A	1120	CLA	C3D-C4D	-2.03	1.39	1.44
19	B	1219	CLA	C1A-CHA	2.03	1.51	1.43
19	B	1239	CLA	C3D-C4D	-2.03	1.39	1.44
19	A	1124	CLA	C1C-C2C	2.03	1.48	1.44
19	B	1209	CLA	C1C-C2C	2.03	1.48	1.44
19	A	1128	CLA	C1A-CHA	2.03	1.51	1.43
19	3	614	CLA	C1A-CHA	2.03	1.51	1.43
19	1	613	CLA	C1A-CHA	2.03	1.51	1.43
19	H	1701	CLA	C1C-C2C	2.03	1.48	1.44
19	A	1101	CLA	C1A-CHA	2.03	1.51	1.43
19	2	605	CLA	C3D-C4D	-2.03	1.39	1.44
19	K	1403	CLA	C1C-C2C	2.03	1.48	1.44
19	B	1212	CLA	C3D-C4D	-2.03	1.39	1.44
22	3	503	BCR	C12-C13	-2.03	1.41	1.46
19	F	1301	CLA	C1A-CHA	2.03	1.51	1.43
19	4	612	CLA	C3D-C4D	-2.03	1.39	1.44
19	A	1106	CLA	C3D-C4D	-2.03	1.39	1.44
19	J	1901	CLA	C1A-CHA	2.03	1.51	1.43
19	A	1129	CLA	C1C-C2C	2.03	1.48	1.44
19	B	1207	CLA	C1A-CHA	2.03	1.51	1.43
19	B	1210	CLA	C1A-CHA	2.03	1.51	1.43
18	A	1011	CL0	C3A-C2A	-2.02	1.53	1.54
19	A	1112	CLA	C3D-C4D	-2.02	1.39	1.44
19	L	1503	CLA	C3D-C4D	-2.02	1.39	1.44
19	K	1403	CLA	C3D-C4D	-2.02	1.39	1.44
19	A	1115	CLA	C1A-CHA	2.02	1.51	1.43
19	3	617	CLA	C1A-CHA	2.02	1.51	1.43
19	A	1013	CLA	C1C-C2C	2.02	1.48	1.44
19	A	1122	CLA	C3D-C4D	-2.02	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B	1235	CLA	C3D-C4D	-2.02	1.39	1.44
19	A	1141	CLA	C1A-CHA	2.02	1.51	1.43
19	B	1021	CLA	C1A-CHA	2.02	1.51	1.43
19	B	1214	CLA	C3D-C4D	-2.02	1.39	1.44
19	B	1212	CLA	C1A-CHA	2.02	1.51	1.43
19	A	1105	CLA	C1A-CHA	2.02	1.51	1.43
19	A	1104	CLA	C1A-CHA	2.02	1.51	1.43
19	B	1210	CLA	C3D-C4D	-2.02	1.39	1.44
19	G	1603	CLA	C1C-C2C	2.02	1.48	1.44
19	3	606	CLA	C3D-C4D	-2.02	1.39	1.44
19	A	1107	CLA	C1C-C2C	2.02	1.48	1.44
19	L	1501	CLA	C1C-C2C	2.02	1.48	1.44
19	B	1224	CLA	C3D-C4D	-2.02	1.39	1.44
19	B	1218	CLA	C3D-C4D	-2.02	1.39	1.44
19	B	1228	CLA	C1C-C2C	2.02	1.48	1.44
19	B	1230	CLA	C3D-C4D	-2.02	1.39	1.44
19	4	612	CLA	CHD-C1D	2.02	1.42	1.38
19	A	1109	CLA	C3D-C4D	-2.02	1.39	1.44
24	B	5006	LMT	O1'-C1'	-2.01	1.36	1.40
19	4	608	CLA	C3D-C4D	-2.01	1.39	1.44
19	1	607	CLA	C1A-CHA	2.01	1.51	1.43
19	4	607	CLA	C1A-CHA	2.01	1.51	1.43
19	4	602	CLA	C1C-C2C	2.01	1.48	1.44
19	A	1128	CLA	CHD-C1D	2.01	1.42	1.38
19	3	608	CLA	C1A-CHA	2.01	1.51	1.43
19	3	610	CLA	C1A-CHA	2.01	1.51	1.43
19	A	1113	CLA	C1A-CHA	2.01	1.51	1.43
19	A	1135	CLA	C3D-C4D	-2.01	1.39	1.44
19	A	1140	CLA	C3D-C4D	-2.01	1.39	1.44
19	B	1227	CLA	C3D-C4D	-2.01	1.39	1.44
19	A	1139	CLA	C1C-C2C	2.01	1.48	1.44
19	1	604	CLA	C1C-C2C	2.01	1.48	1.44
19	A	1131	CLA	C3D-C4D	-2.01	1.39	1.44
24	2	808	LMT	O1'-C1'	-2.01	1.36	1.40
19	B	1202	CLA	C1A-CHA	2.01	1.51	1.43
19	1	606	CLA	C1A-CHA	2.01	1.51	1.43
19	3	602	CLA	C1A-CHA	2.01	1.51	1.43
19	B	1240	CLA	C1A-CHA	2.01	1.51	1.43
19	3	613	CLA	C1A-CHA	2.01	1.51	1.43
19	A	1113	CLA	CHD-C1D	2.01	1.42	1.38
19	B	1204	CLA	C1A-CHA	2.01	1.51	1.43
19	K	1401	CLA	C1A-CHA	2.01	1.51	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	1125	CLA	C3D-C4D	-2.00	1.39	1.44
19	A	1110	CLA	C3D-C4D	-2.00	1.39	1.44
19	1	608	CLA	C3D-C4D	-2.00	1.39	1.44
19	1	601	CLA	C3D-C4D	-2.00	1.39	1.44
19	4	601	CLA	C1C-C2C	2.00	1.48	1.44
19	B	1201	CLA	C1A-CHA	2.00	1.51	1.43
19	B	1229	CLA	C3D-C4D	-2.00	1.39	1.44
22	A	4008	BCR	C12-C13	-2.00	1.41	1.46
19	B	1210	CLA	CHD-C1D	2.00	1.42	1.38
19	1	614	CLA	C1A-CHA	2.00	1.51	1.43
19	B	1219	CLA	C3D-C4D	-2.00	1.39	1.44
19	G	1602	CLA	C1A-CHA	2.00	1.51	1.43
19	A	1117	CLA	C3D-C4D	-2.00	1.39	1.44
19	1	607	CLA	C1C-C2C	2.00	1.48	1.44
19	2	605	CLA	C1C-C2C	2.00	1.48	1.44
19	B	1207	CLA	C3D-C4D	-2.00	1.39	1.44

All (3059) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	K	4001	BCR	C10-C11-C12	19.60	180.00	123.20
22	I	4018	BCR	C10-C11-C12	19.51	179.74	123.20
22	B	4005	BCR	C10-C11-C12	19.42	179.47	123.20
22	A	4017	BCR	C10-C11-C12	19.39	179.37	123.20
22	1	504	BCR	C10-C11-C12	19.20	178.82	123.20
22	B	4009	BCR	C10-C11-C12	19.09	178.53	123.20
22	H	4021	BCR	C10-C11-C12	19.07	178.45	123.20
22	F	4016	BCR	C10-C11-C12	19.07	178.44	123.20
22	F	4014	BCR	C10-C11-C12	19.06	178.41	123.20
22	A	4003	BCR	C10-C11-C12	19.05	178.40	123.20
22	A	4008	BCR	C10-C11-C12	19.03	178.35	123.20
22	J	4012	BCR	C10-C11-C12	19.03	178.35	123.20
22	B	4004	BCR	C10-C11-C12	19.00	178.27	123.20
22	L	4020	BCR	C10-C11-C12	19.00	178.26	123.20
22	B	4010	BCR	C10-C11-C12	19.00	178.26	123.20
22	K	4002	BCR	C10-C11-C12	19.00	178.26	123.20
22	2	503	BCR	C10-C11-C12	18.93	178.04	123.20
22	I	4020	BCR	C10-C11-C12	18.85	177.81	123.20
22	3	503	BCR	C10-C11-C12	18.82	177.73	123.20
22	G	4011	BCR	C10-C11-C12	18.82	177.73	123.20
22	3	506	BCR	C10-C11-C12	18.71	177.42	123.20
22	1	503	BCR	C10-C11-C12	18.70	177.39	123.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	4007	BCR	C10-C11-C12	18.70	177.38	123.20
22	L	4019	BCR	C10-C11-C12	18.65	177.24	123.20
22	A	4017	BCR	C16-C15-C14	18.06	160.47	123.52
22	B	4006	BCR	C10-C11-C12	17.95	175.22	123.20
22	A	4002	BCR	C10-C11-C12	17.88	175.02	123.20
22	A	4011	BCR	C10-C11-C12	17.81	174.81	123.20
22	2	503	BCR	C16-C15-C14	16.83	157.96	123.52
22	B	4004	BCR	C16-C15-C14	16.72	157.73	123.52
22	1	504	BCR	C16-C15-C14	15.52	155.27	123.52
22	B	4010	BCR	C21-C20-C19	15.28	167.47	123.20
22	A	4017	BCR	C21-C20-C19	15.25	167.37	123.20
22	1	503	BCR	C11-C10-C9	14.98	148.29	127.28
22	A	4002	BCR	C21-C20-C19	14.89	166.34	123.20
22	K	4001	BCR	C21-C20-C19	14.81	166.11	123.20
22	A	4007	BCR	C16-C15-C14	14.54	153.28	123.52
22	A	4007	BCR	C21-C20-C19	14.52	165.27	123.20
22	L	4019	BCR	C11-C10-C9	14.51	147.63	127.28
22	3	506	BCR	C21-C20-C19	14.31	164.65	123.20
22	A	4003	BCR	C21-C20-C19	14.29	164.61	123.20
22	2	503	BCR	C11-C10-C9	14.28	147.30	127.28
22	B	4004	BCR	C21-C20-C19	14.26	164.51	123.20
22	A	4008	BCR	C21-C20-C19	14.25	164.48	123.20
22	J	4012	BCR	C21-C20-C19	14.06	163.93	123.20
22	L	4020	BCR	C21-C20-C19	13.94	163.60	123.20
22	3	506	BCR	C16-C15-C14	13.86	151.88	123.52
22	G	4011	BCR	C21-C20-C19	13.62	162.67	123.20
22	2	503	BCR	C29-C30-C25	-13.57	90.72	110.44
22	H	4021	BCR	C21-C20-C19	13.54	162.44	123.20
22	L	4019	BCR	C21-C20-C19	13.43	162.12	123.20
22	K	4001	BCR	C16-C15-C14	13.39	150.92	123.52
22	G	4011	BCR	C16-C15-C14	13.37	150.88	123.52
22	3	503	BCR	C21-C20-C19	13.27	161.65	123.20
22	1	504	BCR	C21-C20-C19	13.27	161.65	123.20
22	3	503	BCR	C16-C15-C14	13.27	150.67	123.52
22	B	4004	BCR	C11-C10-C9	13.13	145.69	127.28
22	B	4010	BCR	C16-C15-C14	13.07	150.27	123.52
22	I	4020	BCR	C16-C15-C14	13.00	150.11	123.52
22	2	503	BCR	C21-C20-C19	12.95	160.72	123.20
22	I	4018	BCR	C16-C15-C14	12.81	149.73	123.52
22	A	4011	BCR	C11-C12-C13	12.78	161.41	126.36
22	1	503	BCR	C16-C15-C14	12.76	149.64	123.52
22	F	4014	BCR	C21-C20-C19	12.76	160.16	123.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	K	4002	BCR	C21-C20-C19	12.72	160.05	123.20
22	I	4018	BCR	C21-C20-C19	12.70	159.99	123.20
22	B	4006	BCR	C11-C12-C13	12.65	161.06	126.36
22	I	4020	BCR	C21-C20-C19	12.65	159.85	123.20
22	B	4005	BCR	C21-C20-C19	12.60	159.70	123.20
22	1	503	BCR	C21-C20-C19	12.52	159.47	123.20
22	K	4001	BCR	C11-C10-C9	12.52	144.83	127.28
22	B	4005	BCR	C16-C15-C14	12.48	149.06	123.52
22	2	503	BCR	C20-C19-C18	12.46	160.54	126.36
22	B	4009	BCR	C16-C15-C14	12.41	148.91	123.52
22	L	4019	BCR	C16-C15-C14	12.40	148.90	123.52
22	H	4021	BCR	C16-C15-C14	12.30	148.69	123.52
22	F	4016	BCR	C16-C15-C14	12.24	148.56	123.52
22	F	4016	BCR	C21-C20-C19	12.24	158.66	123.20
22	J	4012	BCR	C11-C10-C9	12.17	144.34	127.28
22	J	4012	BCR	C16-C15-C14	12.15	148.38	123.52
22	B	4006	BCR	C11-C10-C9	12.12	144.28	127.28
22	B	4009	BCR	C21-C20-C19	11.90	157.67	123.20
22	A	4011	BCR	C11-C10-C9	11.88	143.94	127.28
22	A	4003	BCR	C11-C12-C13	11.72	158.49	126.36
22	K	4002	BCR	C11-C12-C13	11.69	158.43	126.36
22	K	4002	BCR	C20-C19-C18	11.68	158.38	126.36
22	F	4014	BCR	C11-C10-C9	11.66	143.62	127.28
22	1	503	BCR	C20-C19-C18	11.61	158.20	126.36
22	L	4020	BCR	C11-C10-C9	11.61	143.56	127.28
22	B	4005	BCR	C20-C19-C18	11.58	158.10	126.36
22	A	4007	BCR	C11-C10-C9	11.49	143.39	127.28
22	H	4021	BCR	C11-C10-C9	11.47	143.36	127.28
22	1	504	BCR	C20-C19-C18	11.39	157.59	126.36
22	F	4014	BCR	C16-C15-C14	11.38	146.81	123.52
22	F	4014	BCR	C20-C19-C18	11.33	157.43	126.36
22	K	4002	BCR	C16-C15-C14	11.33	146.70	123.52
22	A	4011	BCR	C21-C20-C19	11.32	156.01	123.20
22	2	503	BCR	C40-C30-C25	11.32	128.00	110.24
22	L	4019	BCR	C20-C19-C18	11.32	157.41	126.36
22	I	4020	BCR	C20-C19-C18	11.30	157.35	126.36
22	H	4021	BCR	C20-C19-C18	11.28	157.31	126.36
22	L	4020	BCR	C16-C15-C14	11.27	146.58	123.52
22	L	4020	BCR	C20-C19-C18	11.17	157.00	126.36
18	A	1011	CL0	C1B-CHB-C4A	11.13	128.48	121.32
22	H	4021	BCR	C11-C12-C13	11.10	156.80	126.36
22	F	4014	BCR	C11-C12-C13	10.98	156.48	126.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	I	4020	BCR	C11-C10-C9	10.97	142.66	127.28
22	A	4008	BCR	C16-C15-C14	10.90	145.83	123.52
22	B	4005	BCR	C11-C12-C13	10.90	156.25	126.36
22	F	4016	BCR	C11-C10-C9	10.89	142.55	127.28
22	3	506	BCR	C20-C19-C18	10.89	156.22	126.36
22	G	4011	BCR	C20-C19-C18	10.88	156.21	126.36
22	J	4012	BCR	C20-C19-C18	10.86	156.15	126.36
22	A	4007	BCR	C20-C19-C18	10.83	156.06	126.36
22	A	4003	BCR	C16-C15-C14	10.74	145.49	123.52
22	A	4002	BCR	C16-C15-C14	10.71	145.43	123.52
22	A	4011	BCR	C16-C15-C14	10.63	145.26	123.52
22	F	4016	BCR	C11-C12-C13	10.54	155.26	126.36
22	A	4011	BCR	C20-C19-C18	10.51	155.19	126.36
22	A	4008	BCR	C20-C19-C18	10.49	155.13	126.36
22	K	4001	BCR	C20-C19-C18	10.45	155.01	126.36
22	3	503	BCR	C11-C12-C13	10.43	154.95	126.36
22	A	4008	BCR	C11-C10-C9	10.42	141.89	127.28
22	A	4017	BCR	C11-C12-C13	10.42	154.93	126.36
22	J	4012	BCR	C11-C12-C13	10.40	154.87	126.36
22	1	504	BCR	C11-C12-C13	10.39	154.85	126.36
22	A	4003	BCR	C20-C19-C18	10.31	154.65	126.36
22	B	4010	BCR	C20-C19-C18	10.25	154.47	126.36
22	B	4009	BCR	C11-C12-C13	10.25	154.46	126.36
22	3	503	BCR	C11-C10-C9	10.23	141.62	127.28
22	B	4004	BCR	C20-C19-C18	10.21	154.36	126.36
22	A	4002	BCR	C20-C19-C18	10.14	154.16	126.36
22	A	4002	BCR	C11-C12-C13	10.11	154.07	126.36
22	L	4020	BCR	C11-C12-C13	10.02	153.83	126.36
22	A	4017	BCR	C20-C19-C18	10.01	153.82	126.36
22	1	504	BCR	C11-C10-C9	9.95	141.24	127.28
22	A	4008	BCR	C11-C12-C13	9.86	153.40	126.36
19	4	603	CLA	C4A-NA-C1A	9.71	111.11	106.68
19	3	603	CLA	C4A-NA-C1A	9.69	111.10	106.68
22	B	4005	BCR	C11-C10-C9	9.63	140.79	127.28
22	B	4006	BCR	C16-C15-C14	9.60	143.16	123.52
19	2	601	CLA	C4A-NA-C1A	9.57	111.04	106.68
22	B	4010	BCR	C11-C10-C9	9.56	140.69	127.28
22	G	4011	BCR	C11-C12-C13	9.54	152.52	126.36
19	B	1021	CLA	C4A-NA-C1A	9.53	111.03	106.68
22	B	4010	BCR	C11-C12-C13	9.49	152.40	126.36
19	A	1110	CLA	C4A-NA-C1A	9.48	111.00	106.68
19	B	1202	CLA	C4A-NA-C1A	9.47	111.00	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	F	4016	BCR	C20-C19-C18	9.45	152.29	126.36
19	B	1219	CLA	C4A-NA-C1A	9.45	110.99	106.68
19	A	1114	CLA	C4A-NA-C1A	9.43	110.98	106.68
19	A	1129	CLA	C4A-NA-C1A	9.42	110.97	106.68
22	K	4002	BCR	C11-C10-C9	9.41	140.48	127.28
19	B	1222	CLA	C4A-NA-C1A	9.41	110.97	106.68
22	K	4001	BCR	C11-C12-C13	9.40	152.15	126.36
22	B	4009	BCR	C11-C10-C9	9.40	140.47	127.28
19	B	1235	CLA	C4A-NA-C1A	9.40	110.97	106.68
19	A	1123	CLA	C4A-NA-C1A	9.39	110.96	106.68
19	A	1103	CLA	C4A-NA-C1A	9.37	110.95	106.68
19	B	1206	CLA	C4A-NA-C1A	9.36	110.95	106.68
19	B	1205	CLA	C4A-NA-C1A	9.34	110.94	106.68
22	I	4020	BCR	C11-C12-C13	9.33	151.95	126.36
22	B	4004	BCR	C11-C12-C13	9.31	151.90	126.36
19	L	1502	CLA	C4A-NA-C1A	9.31	110.93	106.68
19	3	612	CLA	C4A-NA-C1A	9.31	110.92	106.68
19	A	1109	CLA	C4A-NA-C1A	9.30	110.92	106.68
22	B	4006	BCR	C21-C20-C19	9.30	150.15	123.20
19	A	1121	CLA	C4A-NA-C1A	9.30	110.92	106.68
19	4	617	CLA	C4A-NA-C1A	9.29	110.92	106.68
19	1	607	CLA	C4A-NA-C1A	9.27	110.91	106.68
19	4	602	CLA	C4A-NA-C1A	9.27	110.91	106.68
22	L	4019	BCR	C11-C12-C13	9.26	151.75	126.36
19	A	1108	CLA	C4A-NA-C1A	9.25	110.90	106.68
19	B	1238	CLA	C4A-NA-C1A	9.23	110.89	106.68
19	A	1102	CLA	C4A-NA-C1A	9.21	110.88	106.68
19	2	603	CLA	C4A-NA-C1A	9.21	110.88	106.68
19	3	606	CLA	C4A-NA-C1A	9.19	110.87	106.68
19	3	614	CLA	C4A-NA-C1A	9.19	110.87	106.68
22	A	4007	BCR	C11-C12-C13	9.18	151.54	126.36
19	F	1302	CLA	C4A-NA-C1A	9.18	110.87	106.68
19	B	1221	CLA	C4A-NA-C1A	9.18	110.86	106.68
19	B	1224	CLA	C4A-NA-C1A	9.17	110.86	106.68
19	B	1213	CLA	C4A-NA-C1A	9.16	110.86	106.68
22	I	4018	BCR	C20-C19-C18	9.16	151.47	126.36
19	3	613	CLA	C4A-NA-C1A	9.15	110.85	106.68
19	A	1111	CLA	C4A-NA-C1A	9.15	110.85	106.68
22	3	506	BCR	C11-C10-C9	9.14	140.10	127.28
19	A	1125	CLA	C4A-NA-C1A	9.14	110.85	106.68
19	1	603	CLA	C4A-NA-C1A	9.13	110.84	106.68
22	2	503	BCR	C11-C12-C13	9.13	151.39	126.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	1135	CLA	C4A-NA-C1A	9.09	110.83	106.68
19	B	1228	CLA	C4A-NA-C1A	9.08	110.82	106.68
19	B	1239	CLA	C4A-NA-C1A	9.08	110.82	106.68
19	B	1212	CLA	C4A-NA-C1A	9.08	110.82	106.68
19	B	1214	CLA	C4A-NA-C1A	9.08	110.82	106.68
22	1	503	BCR	C11-C12-C13	9.08	151.25	126.36
19	2	607	CLA	C4A-NA-C1A	9.06	110.81	106.68
19	A	1118	CLA	C4A-NA-C1A	9.04	110.81	106.68
19	G	1601	CLA	C4A-NA-C1A	9.02	110.79	106.68
19	4	607	CLA	C4A-NA-C1A	9.02	110.79	106.68
19	H	1701	CLA	C4A-NA-C1A	9.02	110.79	106.68
19	A	1012	CLA	C4A-NA-C1A	9.01	110.79	106.68
19	A	1117	CLA	C4A-NA-C1A	9.01	110.79	106.68
19	B	1232	CLA	C4A-NA-C1A	9.00	110.78	106.68
22	I	4018	BCR	C11-C12-C13	9.00	151.03	126.36
19	3	602	CLA	C4A-NA-C1A	8.99	110.78	106.68
19	3	608	CLA	C4A-NA-C1A	8.99	110.78	106.68
19	1	613	CLA	C4A-NA-C1A	8.98	110.78	106.68
19	A	1140	CLA	C4A-NA-C1A	8.97	110.77	106.68
19	B	1240	CLA	C4A-NA-C1A	8.97	110.77	106.68
19	A	1141	CLA	C4A-NA-C1A	8.97	110.77	106.68
19	A	1128	CLA	C4A-NA-C1A	8.95	110.76	106.68
19	2	608	CLA	C4A-NA-C1A	8.95	110.76	106.68
19	4	604	CLA	C4A-NA-C1A	8.95	110.76	106.68
19	A	1139	CLA	C4A-NA-C1A	8.94	110.76	106.68
19	A	1106	CLA	C4A-NA-C1A	8.94	110.76	106.68
22	B	4009	BCR	C20-C19-C18	8.93	150.86	126.36
19	B	1234	CLA	C4A-NA-C1A	8.93	110.75	106.68
19	A	1124	CLA	C4A-NA-C1A	8.92	110.75	106.68
19	J	1901	CLA	C4A-NA-C1A	8.92	110.75	106.68
19	1	608	CLA	C4A-NA-C1A	8.92	110.75	106.68
19	3	605	CLA	C4A-NA-C1A	8.92	110.75	106.68
19	1	605	CLA	C4A-NA-C1A	8.92	110.75	106.68
19	K	1401	CLA	C4A-NA-C1A	8.92	110.75	106.68
19	2	605	CLA	C4A-NA-C1A	8.91	110.75	106.68
19	2	606	CLA	C4A-NA-C1A	8.89	110.74	106.68
19	B	1201	CLA	C4A-NA-C1A	8.89	110.74	106.68
19	B	1231	CLA	C4A-NA-C1A	8.89	110.74	106.68
19	G	1602	CLA	C4A-NA-C1A	8.88	110.73	106.68
18	A	1011	CL0	O2D-CGD-CBD	8.88	120.70	110.95
19	1	606	CLA	C4A-NA-C1A	8.88	110.73	106.68
19	A	1134	CLA	C4A-NA-C1A	8.87	110.73	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	1215	CLA	C4A-NA-C1A	8.86	110.72	106.68
22	3	506	BCR	C11-C12-C13	8.86	150.65	126.36
19	A	1105	CLA	C4A-NA-C1A	8.84	110.71	106.68
19	B	1236	CLA	C4A-NA-C1A	8.83	110.71	106.68
19	B	1211	CLA	C4A-NA-C1A	8.83	110.71	106.68
19	B	1225	CLA	C4A-NA-C1A	8.83	110.71	106.68
19	4	612	CLA	C4A-NA-C1A	8.82	110.70	106.68
19	B	1229	CLA	C4A-NA-C1A	8.82	110.70	106.68
19	L	1501	CLA	C4A-NA-C1A	8.81	110.70	106.68
19	3	617	CLA	C4A-NA-C1A	8.81	110.70	106.68
19	K	1402	CLA	C4A-NA-C1A	8.81	110.70	106.68
19	4	609	CLA	C4A-NA-C1A	8.80	110.70	106.68
19	A	1013	CLA	C4A-NA-C1A	8.80	110.69	106.68
19	K	1403	CLA	C4A-NA-C1A	8.80	110.69	106.68
19	B	1223	CLA	C4A-NA-C1A	8.79	110.69	106.68
19	A	1138	CLA	C4A-NA-C1A	8.79	110.69	106.68
19	4	601	CLA	C4A-NA-C1A	8.78	110.69	106.68
19	4	608	CLA	C4A-NA-C1A	8.77	110.68	106.68
19	A	1107	CLA	C4A-NA-C1A	8.77	110.68	106.68
19	4	605	CLA	C4A-NA-C1A	8.75	110.67	106.68
19	A	1104	CLA	C4A-NA-C1A	8.75	110.67	106.68
22	A	4003	BCR	C11-C10-C9	8.74	139.53	127.28
19	1	601	CLA	C4A-NA-C1A	8.73	110.66	106.68
19	3	610	CLA	C4A-NA-C1A	8.73	110.66	106.68
19	B	1204	CLA	C4A-NA-C1A	8.72	110.66	106.68
19	1	611	CLA	C4A-NA-C1A	8.72	110.66	106.68
19	B	1022	CLA	C4A-NA-C1A	8.71	110.66	106.68
19	B	1203	CLA	C4A-NA-C1A	8.71	110.66	106.68
19	B	1237	CLA	C4A-NA-C1A	8.71	110.65	106.68
19	A	1101	CLA	C4A-NA-C1A	8.70	110.65	106.68
19	B	1210	CLA	C4A-NA-C1A	8.70	110.65	106.68
19	A	1136	CLA	C4A-NA-C1A	8.70	110.65	106.68
19	A	1122	CLA	C4A-NA-C1A	8.70	110.65	106.68
19	F	1301	CLA	C4A-NA-C1A	8.69	110.64	106.68
19	A	1126	CLA	C4A-NA-C1A	8.69	110.64	106.68
19	1	604	CLA	C4A-NA-C1A	8.68	110.64	106.68
19	2	604	CLA	C4A-NA-C1A	8.68	110.64	106.68
19	3	601	CLA	C4A-NA-C1A	8.68	110.64	106.68
19	B	1226	CLA	C4A-NA-C1A	8.68	110.64	106.68
19	A	1112	CLA	C4A-NA-C1A	8.67	110.63	106.68
19	A	1137	CLA	C4A-NA-C1A	8.66	110.63	106.68
19	B	1217	CLA	C4A-NA-C1A	8.62	110.61	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	1115	CLA	C4A-NA-C1A	8.62	110.61	106.68
19	3	607	CLA	C4A-NA-C1A	8.60	110.60	106.68
19	A	1120	CLA	C4A-NA-C1A	8.56	110.59	106.68
19	B	1227	CLA	C4A-NA-C1A	8.56	110.59	106.68
19	B	1218	CLA	C4A-NA-C1A	8.56	110.58	106.68
19	1	602	CLA	C4A-NA-C1A	8.55	110.58	106.68
19	G	1603	CLA	C4A-NA-C1A	8.55	110.58	106.68
19	A	1130	CLA	C4A-NA-C1A	8.55	110.58	106.68
28	4	505	LUT	C21-C26-C27	8.52	122.62	112.83
19	B	1209	CLA	C4A-NA-C1A	8.52	110.56	106.68
19	K	1404	CLA	C4A-NA-C1A	8.52	110.56	106.68
19	1	614	CLA	C4A-NA-C1A	8.49	110.55	106.68
19	4	606	CLA	C4A-NA-C1A	8.48	110.55	106.68
19	B	1208	CLA	C4A-NA-C1A	8.46	110.54	106.68
19	A	1119	CLA	C4A-NA-C1A	8.45	110.54	106.68
19	A	1132	CLA	C4A-NA-C1A	8.40	110.51	106.68
19	A	1131	CLA	C4A-NA-C1A	8.39	110.51	106.68
19	L	1503	CLA	C4A-NA-C1A	8.39	110.51	106.68
19	B	1216	CLA	C4A-NA-C1A	8.39	110.50	106.68
19	A	1133	CLA	C4A-NA-C1A	8.36	110.49	106.68
19	2	612	CLA	C4A-NA-C1A	8.34	110.48	106.68
22	G	4011	BCR	C11-C10-C9	8.32	138.95	127.28
19	2	602	CLA	C4A-NA-C1A	8.31	110.47	106.68
19	B	1230	CLA	C4A-NA-C1A	8.28	110.45	106.68
19	A	1113	CLA	C4A-NA-C1A	8.24	110.44	106.68
19	A	1116	CLA	C4A-NA-C1A	8.20	110.42	106.68
19	B	1023	CLA	C4A-NA-C1A	8.17	110.41	106.68
22	I	4018	BCR	C11-C10-C9	8.00	138.49	127.28
19	A	1127	CLA	C4A-NA-C1A	7.95	110.31	106.68
19	B	1207	CLA	C4A-NA-C1A	7.94	110.30	106.68
22	B	4006	BCR	C20-C19-C18	7.93	148.10	126.36
29	2	613	CHL	C1B-CHB-C4A	7.89	126.40	121.32
28	3	501	LUT	C21-C26-C27	7.88	121.89	112.83
19	B	1220	CLA	C4A-NA-C1A	7.87	110.27	106.68
22	A	4017	BCR	C11-C10-C9	7.80	138.22	127.28
22	3	503	BCR	C20-C19-C18	7.76	147.65	126.36
29	1	612	CHL	C1B-CHB-C4A	7.63	126.23	121.32
22	A	4017	BCR	C15-C14-C13	-7.62	116.60	127.28
28	4	501	LUT	C21-C26-C27	7.59	121.55	112.83
28	1	502	LUT	C21-C26-C27	7.46	121.41	112.83
29	4	613	CHL	C1B-CHB-C4A	7.41	126.09	121.32
28	J	4013	LUT	C21-C26-C27	7.22	121.13	112.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	2	501	LUT	C21-C26-C27	7.19	121.09	112.83
29	1	610	CHL	C1B-CHB-C4A	6.77	125.68	121.32
22	B	4006	BCR	C19-C18-C17	6.73	129.59	119.01
22	A	4002	BCR	C11-C10-C9	6.71	136.69	127.28
29	2	610	CHL	C1B-CHB-C4A	6.66	125.61	121.32
19	K	1403	CLA	CMD-C2D-C1D	6.65	136.44	124.73
30	2	502	XAT	O4-C5-C18	-6.60	107.67	115.05
29	4	611	CHL	C1B-CHB-C4A	6.55	125.54	121.32
29	2	611	CHL	C1B-CHB-C4A	6.49	125.50	121.32
22	B	4004	BCR	C15-C14-C13	-6.43	118.27	127.28
29	4	615	CHL	C1B-CHB-C4A	6.42	125.45	121.32
19	A	1102	CLA	O2D-CGD-CBD	6.42	122.46	111.23
29	2	615	CHL	C1B-CHB-C4A	6.34	125.40	121.32
29	2	609	CHL	C1B-CHB-C4A	6.29	125.37	121.32
19	B	1226	CLA	O2D-CGD-CBD	6.24	122.14	111.23
19	A	1101	CLA	O2D-CGD-CBD	6.16	122.00	111.23
22	2	503	BCR	C40-C30-C29	-6.15	85.33	108.95
29	3	611	CHL	C1B-CHB-C4A	6.09	125.24	121.32
30	2	502	XAT	O4-C5-C4	-6.08	107.79	113.49
19	B	1218	CLA	O2D-CGD-CBD	6.07	121.85	111.23
19	A	1137	CLA	O2D-CGD-CBD	6.06	121.83	111.23
22	F	4014	BCR	C28-C27-C26	-6.02	103.32	114.06
19	A	1129	CLA	O2D-CGD-CBD	6.02	121.75	111.23
19	B	1205	CLA	O2D-CGD-CBD	5.98	121.68	111.23
28	3	502	LUT	C8-C7-C6	-5.96	111.09	127.00
19	A	1132	CLA	CMD-C2D-C1D	5.95	135.20	124.73
19	1	608	CLA	O2D-CGD-CBD	5.91	121.56	111.23
19	B	1221	CLA	O2D-CGD-CBD	5.91	121.56	111.23
19	B	1223	CLA	O2D-CGD-CBD	5.91	121.55	111.23
19	B	1227	CLA	O2D-CGD-CBD	5.89	121.52	111.23
19	4	608	CLA	CMD-C2D-C1D	5.87	135.06	124.73
19	B	1222	CLA	O2D-CGD-CBD	5.87	121.49	111.23
19	K	1401	CLA	CMD-C2D-C1D	5.86	135.05	124.73
19	A	1122	CLA	CMD-C2D-C1D	5.83	135.00	124.73
19	2	607	CLA	O2D-CGD-CBD	5.82	121.40	111.23
19	B	1212	CLA	O2D-CGD-CBD	5.80	121.37	111.23
19	L	1502	CLA	O2D-CGD-CBD	5.80	121.37	111.23
22	1	503	BCR	C30-C25-C26	-5.79	114.73	122.64
19	A	1109	CLA	CMD-C2D-C1D	5.78	134.91	124.73
19	A	1106	CLA	O2D-CGD-CBD	5.78	121.33	111.23
19	A	1128	CLA	O2D-CGD-CBD	5.77	121.31	111.23
19	L	1503	CLA	CMD-C2D-C1D	5.77	134.88	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	2	608	CLA	CMD-C2D-C1D	5.76	134.87	124.73
19	A	1116	CLA	O2D-CGD-CBD	5.74	121.27	111.23
19	4	601	CLA	CMD-C2D-C1D	5.73	134.82	124.73
19	3	605	CLA	O2D-CGD-CBD	5.73	121.24	111.23
19	4	605	CLA	CMD-C2D-C1D	5.72	134.80	124.73
22	G	4011	BCR	C30-C25-C26	-5.71	114.84	122.64
22	1	504	BCR	C15-C14-C13	-5.68	119.31	127.28
19	L	1501	CLA	O2D-CGD-CBD	5.68	121.17	111.23
19	B	1236	CLA	O2D-CGD-CBD	5.68	121.16	111.23
19	1	605	CLA	CMD-C2D-C1D	5.67	134.72	124.73
19	A	1132	CLA	O2D-CGD-CBD	5.67	121.14	111.23
19	B	1229	CLA	O2D-CGD-CBD	5.66	121.12	111.23
19	3	602	CLA	O2D-CGD-CBD	5.64	121.09	111.23
19	B	1209	CLA	CMD-C2D-C1D	5.63	134.65	124.73
19	B	1223	CLA	CMD-C2D-C1D	5.63	134.64	124.73
19	B	1217	CLA	O2D-CGD-CBD	5.62	121.06	111.23
19	G	1602	CLA	O2D-CGD-CBD	5.61	121.04	111.23
19	1	608	CLA	CMD-C2D-C1D	5.61	134.61	124.73
19	B	1224	CLA	CMD-C2D-C1D	5.60	134.59	124.73
19	B	1210	CLA	O2D-CGD-CBD	5.60	121.02	111.23
19	B	1224	CLA	O2D-CGD-CBD	5.59	121.00	111.23
19	1	614	CLA	CMD-C2D-C1D	5.58	134.55	124.73
19	2	607	CLA	CMD-C2D-C1D	5.58	134.55	124.73
19	4	617	CLA	O2D-CGD-CBD	5.57	120.97	111.23
29	1	609	CHL	C1B-CHB-C4A	5.57	124.91	121.32
19	A	1112	CLA	O2D-CGD-CBD	5.57	120.96	111.23
19	A	1140	CLA	O2D-CGD-CBD	5.56	120.95	111.23
19	B	1227	CLA	CMD-C2D-C1D	5.55	134.50	124.73
19	B	1202	CLA	CMD-C2D-C1D	5.55	134.50	124.73
19	B	1229	CLA	CMD-C2D-C1D	5.55	134.50	124.73
19	1	603	CLA	CMD-C2D-C1D	5.54	134.48	124.73
19	L	1501	CLA	CMD-C2D-C1D	5.54	134.48	124.73
19	B	1230	CLA	CMD-C2D-C1D	5.54	134.48	124.73
19	A	1115	CLA	O2D-CGD-CBD	5.53	120.90	111.23
19	B	1215	CLA	CMD-C2D-C1D	5.53	134.47	124.73
29	3	604	CHL	C1B-CHB-C4A	5.53	124.88	121.32
19	A	1114	CLA	CMD-C2D-C1D	5.53	134.47	124.73
19	B	1021	CLA	O2D-CGD-CBD	5.53	120.89	111.23
19	A	1118	CLA	O2D-CGD-CBD	5.52	120.88	111.23
19	A	1131	CLA	O2D-CGD-CBD	5.52	120.88	111.23
19	B	1204	CLA	O2D-CGD-CBD	5.51	120.87	111.23
19	A	1111	CLA	CMD-C2D-C1D	5.51	134.43	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	1105	CLA	O2D-CGD-CBD	5.50	120.85	111.23
19	B	1209	CLA	O2D-CGD-CBD	5.50	120.84	111.23
19	A	1119	CLA	CMD-C2D-C1D	5.50	134.41	124.73
19	A	1012	CLA	O2D-CGD-CBD	5.49	120.83	111.23
19	3	607	CLA	CMD-C2D-C1D	5.49	134.40	124.73
19	B	1218	CLA	CMD-C2D-C1D	5.49	134.39	124.73
19	B	1238	CLA	CMD-C2D-C1D	5.49	134.39	124.73
19	A	1137	CLA	CMD-C2D-C1D	5.49	134.39	124.73
19	A	1113	CLA	CMD-C2D-C1D	5.48	134.38	124.73
19	2	612	CLA	CMD-C2D-C1D	5.48	134.38	124.73
19	B	1022	CLA	O2D-CGD-CBD	5.48	120.81	111.23
19	A	1126	CLA	O2D-CGD-CBD	5.48	120.81	111.23
19	3	603	CLA	CMD-C2D-C1D	5.48	134.37	124.73
19	A	1130	CLA	O2D-CGD-CBD	5.48	120.80	111.23
19	2	605	CLA	CMD-C2D-C1D	5.47	134.37	124.73
19	B	1208	CLA	CMD-C2D-C1D	5.47	134.35	124.73
19	A	1120	CLA	CMD-C2D-C1D	5.47	134.35	124.73
19	4	604	CLA	CMD-C2D-C1D	5.46	134.35	124.73
19	B	1228	CLA	O2D-CGD-CBD	5.46	120.78	111.23
19	B	1236	CLA	CMD-C2D-C1D	5.46	134.35	124.73
19	4	607	CLA	O2D-CGD-CBD	5.46	120.77	111.23
19	A	1102	CLA	CMD-C2D-C1D	5.46	134.34	124.73
19	G	1602	CLA	CMD-C2D-C1D	5.46	134.34	124.73
19	A	1136	CLA	CMD-C2D-C1D	5.46	134.34	124.73
19	A	1130	CLA	CMD-C2D-C1D	5.46	134.34	124.73
19	3	608	CLA	CMD-C2D-C1D	5.44	134.31	124.73
19	A	1134	CLA	O2D-CGD-CBD	5.44	120.75	111.23
19	A	1106	CLA	CMD-C2D-C1D	5.44	134.31	124.73
19	3	617	CLA	O2D-CGD-CBD	5.44	120.74	111.23
19	L	1502	CLA	CMD-C2D-C1D	5.44	134.31	124.73
19	1	606	CLA	CMD-C2D-C1D	5.44	134.31	124.73
19	B	1211	CLA	O2D-CGD-CBD	5.44	120.74	111.23
19	A	1103	CLA	CMD-C2D-C1D	5.44	134.30	124.73
19	1	604	CLA	CMD-C2D-C1D	5.43	134.29	124.73
19	3	606	CLA	CMD-C2D-C1D	5.43	134.28	124.73
19	J	1901	CLA	CMD-C2D-C1D	5.42	134.28	124.73
19	G	1603	CLA	O2D-CGD-CBD	5.42	120.71	111.23
19	A	1101	CLA	CMD-C2D-C1D	5.42	134.27	124.73
19	B	1239	CLA	CMD-C2D-C1D	5.42	134.27	124.73
19	A	1126	CLA	CMD-C2D-C1D	5.42	134.26	124.73
19	B	1201	CLA	CMD-C2D-C1D	5.41	134.26	124.73
19	K	1402	CLA	CMD-C2D-C1D	5.41	134.26	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	1230	CLA	O2D-CGD-CBD	5.41	120.69	111.23
19	3	610	CLA	CMD-C2D-C1D	5.40	134.24	124.73
19	A	1134	CLA	CMD-C2D-C1D	5.39	134.22	124.73
22	J	4012	BCR	C30-C25-C26	-5.39	115.27	122.64
19	B	1231	CLA	CMD-C2D-C1D	5.39	134.22	124.73
19	3	617	CLA	CMD-C2D-C1D	5.39	134.22	124.73
19	A	1114	CLA	O2D-CGD-CBD	5.39	120.65	111.23
19	4	609	CLA	CMD-C2D-C1D	5.38	134.21	124.73
28	1	501	LUT	C18-C5-C6	-5.38	118.61	124.48
19	4	603	CLA	CMD-C2D-C1D	5.38	134.21	124.73
19	4	606	CLA	CMD-C2D-C1D	5.38	134.21	124.73
19	1	611	CLA	CMD-C2D-C1D	5.38	134.20	124.73
19	A	1105	CLA	CMD-C2D-C1D	5.38	134.20	124.73
19	3	613	CLA	CMD-C2D-C1D	5.38	134.20	124.73
19	B	1214	CLA	CMD-C2D-C1D	5.38	134.20	124.73
19	2	604	CLA	CMD-C2D-C1D	5.38	134.19	124.73
19	G	1603	CLA	CMD-C2D-C1D	5.37	134.19	124.73
19	A	1129	CLA	CMD-C2D-C1D	5.37	134.19	124.73
19	1	614	CLA	O2D-CGD-CBD	5.37	120.62	111.23
19	1	613	CLA	CMD-C2D-C1D	5.37	134.18	124.73
19	A	1103	CLA	O2D-CGD-CBD	5.37	120.61	111.23
19	A	1123	CLA	CMD-C2D-C1D	5.36	134.16	124.73
18	A	1011	CL0	O2A-CGA-O1A	-5.35	110.24	123.63
19	B	1210	CLA	CMD-C2D-C1D	5.35	134.15	124.73
19	3	602	CLA	CMD-C2D-C1D	5.35	134.15	124.73
30	4	502	XAT	O4-C5-C18	-5.35	109.07	115.05
19	A	1119	CLA	O2D-CGD-CBD	5.35	120.58	111.23
19	A	1113	CLA	O2D-CGD-CBD	5.35	120.58	111.23
19	A	1116	CLA	CMD-C2D-C1D	5.35	134.14	124.73
19	B	1232	CLA	CMD-C2D-C1D	5.35	134.14	124.73
19	A	1104	CLA	O2D-CGD-CBD	5.34	120.57	111.23
19	B	1021	CLA	CMD-C2D-C1D	5.34	134.14	124.73
19	B	1235	CLA	CMD-C2D-C1D	5.34	134.14	124.73
19	A	1141	CLA	CMD-C2D-C1D	5.34	134.13	124.73
19	H	1701	CLA	CMD-C2D-C1D	5.34	134.13	124.73
19	K	1404	CLA	CMD-C2D-C1D	5.33	134.12	124.73
19	3	605	CLA	CMD-C2D-C1D	5.33	134.12	124.73
19	B	1239	CLA	O2D-CGD-CBD	5.33	120.55	111.23
19	3	614	CLA	CMD-C2D-C1D	5.33	134.11	124.73
19	1	602	CLA	CMD-C2D-C1D	5.33	134.11	124.73
19	2	604	CLA	O2D-CGD-CBD	5.32	120.54	111.23
19	A	1135	CLA	O2D-CGD-CBD	5.32	120.53	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	1213	CLA	O2D-CGD-CBD	5.32	120.53	111.23
19	B	1235	CLA	O2D-CGD-CBD	5.32	120.53	111.23
19	3	610	CLA	O2D-CGD-CBD	5.32	120.53	111.23
19	A	1123	CLA	O2D-CGD-CBD	5.32	120.52	111.23
19	A	1124	CLA	O2D-CGD-CBD	5.31	120.52	111.23
19	A	1140	CLA	CMD-C2D-C1D	5.31	134.08	124.73
19	B	1203	CLA	CMD-C2D-C1D	5.31	134.07	124.73
19	A	1108	CLA	CMD-C2D-C1D	5.30	134.07	124.73
29	4	610	CHL	C1C-CHC-C4B	5.30	135.04	116.07
19	B	1219	CLA	CMD-C2D-C1D	5.30	134.06	124.73
19	A	1133	CLA	CMD-C2D-C1D	5.30	134.06	124.73
19	A	1136	CLA	O2D-CGD-CBD	5.29	120.48	111.23
19	B	1213	CLA	CMD-C2D-C1D	5.29	134.05	124.73
19	B	1216	CLA	O2D-CGD-CBD	5.29	120.48	111.23
19	B	1207	CLA	O2D-CGD-CBD	5.29	120.48	111.23
19	A	1117	CLA	CMD-C2D-C1D	5.29	134.04	124.73
19	B	1226	CLA	CMD-C2D-C1D	5.28	134.03	124.73
19	B	1228	CLA	CMD-C2D-C1D	5.28	134.03	124.73
19	G	1601	CLA	O2D-CGD-CBD	5.28	120.46	111.23
19	A	1125	CLA	CMD-C2D-C1D	5.28	134.02	124.73
19	1	606	CLA	O2D-CGD-CBD	5.28	120.45	111.23
19	2	608	CLA	O2D-CGD-CBD	5.28	120.45	111.23
19	1	607	CLA	O2D-CGD-CBD	5.27	120.45	111.23
19	3	603	CLA	O2D-CGD-CBD	5.27	120.45	111.23
19	B	1202	CLA	O2D-CGD-CBD	5.27	120.44	111.23
19	B	1215	CLA	O2D-CGD-CBD	5.27	120.44	111.23
19	2	605	CLA	O2D-CGD-CBD	5.27	120.44	111.23
19	A	1139	CLA	CMD-C2D-C1D	5.27	134.00	124.73
19	4	608	CLA	O2D-CGD-CBD	5.26	120.43	111.23
19	A	1112	CLA	CMD-C2D-C1D	5.26	134.00	124.73
19	F	1301	CLA	CMD-C2D-C1D	5.26	134.00	124.73
19	B	1220	CLA	CMD-C2D-C1D	5.26	133.99	124.73
19	A	1110	CLA	CMD-C2D-C1D	5.26	133.99	124.73
19	A	1127	CLA	O2D-CGD-CBD	5.26	120.42	111.23
19	B	1225	CLA	CMD-C2D-C1D	5.25	133.98	124.73
19	B	1214	CLA	O2D-CGD-CBD	5.25	120.41	111.23
19	3	607	CLA	O2D-CGD-CBD	5.25	120.41	111.23
19	A	1118	CLA	CMD-C2D-C1D	5.25	133.97	124.73
19	B	1211	CLA	CMD-C2D-C1D	5.24	133.96	124.73
19	3	601	CLA	CMD-C2D-C1D	5.24	133.96	124.73
19	2	602	CLA	CMD-C2D-C1D	5.24	133.96	124.73
19	A	1121	CLA	CMD-C2D-C1D	5.24	133.95	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	1237	CLA	O2D-CGD-CBD	5.23	120.38	111.23
19	4	601	CLA	O2D-CGD-CBD	5.23	120.38	111.23
19	A	1104	CLA	CMD-C2D-C1D	5.23	133.94	124.73
19	2	606	CLA	CMD-C2D-C1D	5.23	133.93	124.73
19	F	1302	CLA	CMD-C2D-C1D	5.22	133.93	124.73
19	B	1240	CLA	CMD-C2D-C1D	5.22	133.92	124.73
19	B	1207	CLA	CMD-C2D-C1D	5.22	133.92	124.73
19	2	602	CLA	O2D-CGD-CBD	5.22	120.36	111.23
19	B	1212	CLA	CMD-C2D-C1D	5.22	133.92	124.73
19	B	1208	CLA	O2D-CGD-CBD	5.22	120.35	111.23
19	4	607	CLA	CMD-C2D-C1D	5.22	133.91	124.73
19	K	1402	CLA	O2D-CGD-CBD	5.21	120.34	111.23
19	A	1107	CLA	O2D-CGD-CBD	5.21	120.34	111.23
19	B	1217	CLA	CMD-C2D-C1D	5.21	133.90	124.73
19	1	604	CLA	O2D-CGD-CBD	5.21	120.33	111.23
19	A	1135	CLA	CMD-C2D-C1D	5.21	133.90	124.73
19	1	607	CLA	CMD-C2D-C1D	5.20	133.89	124.73
23	B	5001	LHG	O7-C7-C8	5.20	120.36	111.09
22	H	4021	BCR	C27-C26-C25	-5.20	115.68	122.70
19	A	1117	CLA	O2D-CGD-CBD	5.20	120.32	111.23
19	B	1234	CLA	CMD-C2D-C1D	5.19	133.87	124.73
19	K	1401	CLA	O2D-CGD-CBD	5.19	120.30	111.23
19	A	1125	CLA	O2D-CGD-CBD	5.19	120.30	111.23
19	B	1222	CLA	CMD-C2D-C1D	5.18	133.86	124.73
19	G	1601	CLA	CMD-C2D-C1D	5.18	133.85	124.73
19	B	1234	CLA	O2D-CGD-CBD	5.18	120.28	111.23
19	3	612	CLA	CMD-C2D-C1D	5.18	133.84	124.73
19	3	606	CLA	O2D-CGD-CBD	5.18	120.28	111.23
22	A	4002	BCR	C19-C18-C17	5.17	127.14	119.01
19	B	1240	CLA	O2D-CGD-CBD	5.17	120.27	111.23
19	B	1237	CLA	CMD-C2D-C1D	5.17	133.83	124.73
19	2	601	CLA	CMD-C2D-C1D	5.17	133.83	124.73
19	1	611	CLA	O2D-CGD-CBD	5.16	120.26	111.23
19	B	1206	CLA	O2D-CGD-CBD	5.16	120.25	111.23
19	A	1120	CLA	O2D-CGD-CBD	5.16	120.25	111.23
29	1	609	CHL	C1C-CHC-C4B	5.16	134.52	116.07
19	B	1203	CLA	O2D-CGD-CBD	5.15	120.24	111.23
19	F	1302	CLA	O2D-CGD-CBD	5.15	120.24	111.23
19	4	602	CLA	CMD-C2D-C1D	5.15	133.79	124.73
19	4	609	CLA	O2D-CGD-CBD	5.14	120.22	111.23
19	3	608	CLA	O2D-CGD-CBD	5.14	120.22	111.23
19	A	1127	CLA	CMD-C2D-C1D	5.14	133.78	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	2	603	CLA	CMD-C2D-C1D	5.14	133.78	124.73
22	H	4021	BCR	C30-C25-C26	-5.14	115.62	122.64
19	B	1221	CLA	CMD-C2D-C1D	5.13	133.77	124.73
19	B	1204	CLA	CMD-C2D-C1D	5.13	133.77	124.73
19	B	1231	CLA	O2D-CGD-CBD	5.13	120.19	111.23
19	4	603	CLA	O2D-CGD-CBD	5.11	120.17	111.23
19	4	612	CLA	O2D-CGD-CBD	5.11	120.16	111.23
19	A	1110	CLA	O2D-CGD-CBD	5.11	120.16	111.23
19	F	1301	CLA	O2D-CGD-CBD	5.10	120.15	111.23
19	A	1139	CLA	O2D-CGD-CBD	5.10	120.14	111.23
19	A	1138	CLA	CMD-C2D-C1D	5.10	133.71	124.73
19	1	602	CLA	O2D-CGD-CBD	5.10	120.14	111.23
19	4	606	CLA	O2D-CGD-CBD	5.09	120.13	111.23
19	4	617	CLA	CMD-C2D-C1D	5.09	133.69	124.73
19	3	612	CLA	O2D-CGD-CBD	5.08	120.12	111.23
19	A	1128	CLA	CMD-C2D-C1D	5.08	133.68	124.73
19	B	1206	CLA	CMD-C2D-C1D	5.08	133.67	124.73
19	4	602	CLA	O2D-CGD-CBD	5.08	120.11	111.23
22	I	4018	BCR	C1-C6-C7	5.07	129.41	115.65
19	A	1115	CLA	CMD-C2D-C1D	5.06	133.65	124.73
19	B	1022	CLA	CMD-C2D-C1D	5.06	133.63	124.73
19	A	1111	CLA	O2D-CGD-CBD	5.05	120.06	111.23
19	B	1225	CLA	O2D-CGD-CBD	5.05	120.06	111.23
19	K	1404	CLA	O2D-CGD-CBD	5.05	120.06	111.23
19	B	1201	CLA	O2D-CGD-CBD	5.03	120.03	111.23
29	3	611	CHL	C1C-CHC-C4B	5.02	134.05	116.07
19	3	601	CLA	O2D-CGD-CBD	5.02	120.00	111.23
19	A	1133	CLA	O2D-CGD-CBD	5.02	120.00	111.23
28	J	4013	LUT	C1-C6-C5	-5.01	115.79	122.64
19	B	1232	CLA	O2D-CGD-CBD	5.01	119.99	111.23
19	A	1107	CLA	CMD-C2D-C1D	5.01	133.55	124.73
19	A	1141	CLA	O2D-CGD-CBD	5.01	119.98	111.23
19	B	1219	CLA	O2D-CGD-CBD	5.01	119.98	111.23
19	2	612	CLA	O2D-CGD-CBD	5.01	119.98	111.23
19	3	614	CLA	O2D-CGD-CBD	5.00	119.97	111.23
19	4	604	CLA	O2D-CGD-CBD	5.00	119.96	111.23
19	A	1108	CLA	O2D-CGD-CBD	4.99	119.96	111.23
19	1	613	CLA	O2D-CGD-CBD	4.99	119.96	111.23
19	B	1220	CLA	O2D-CGD-CBD	4.99	119.96	111.23
29	3	604	CHL	C1C-CHC-C4B	4.99	133.92	116.07
29	2	615	CHL	C1C-CHC-C4B	4.98	133.89	116.07
29	2	609	CHL	C1C-CHC-C4B	4.98	133.88	116.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	1131	CLA	CMD-C2D-C1D	4.98	133.49	124.73
29	1	610	CHL	C1C-CHC-C4B	4.98	133.87	116.07
28	4	505	LUT	C31-C30-C29	-4.97	120.30	127.28
29	4	615	CHL	C1C-CHC-C4B	4.97	133.87	116.07
19	1	601	CLA	CMD-C2D-C1D	4.97	133.48	124.73
19	4	612	CLA	CMD-C2D-C1D	4.97	133.48	124.73
19	B	1216	CLA	CMD-C2D-C1D	4.96	133.46	124.73
19	1	605	CLA	O2D-CGD-CBD	4.95	119.89	111.23
22	B	4006	BCR	C27-C26-C25	-4.95	116.02	122.70
19	B	1023	CLA	CMD-C2D-C1D	4.94	133.43	124.73
22	A	4002	BCR	C30-C25-C26	-4.93	115.89	122.64
19	A	1013	CLA	CMD-C2D-C1D	4.93	133.41	124.73
29	2	611	CHL	C1C-CHC-C4B	4.93	133.69	116.07
19	A	1109	CLA	O2D-CGD-CBD	4.91	119.81	111.23
29	4	611	CHL	C1C-CHC-C4B	4.90	133.61	116.07
19	H	1701	CLA	O2D-CGD-CBD	4.90	119.79	111.23
19	3	613	CLA	O2D-CGD-CBD	4.90	119.79	111.23
22	A	4017	BCR	C19-C18-C17	4.90	126.71	119.01
19	1	603	CLA	O2D-CGD-CBD	4.89	119.78	111.23
19	2	603	CLA	O2D-CGD-CBD	4.87	119.74	111.23
29	1	612	CHL	C1C-CHC-C4B	4.86	133.46	116.07
22	B	4006	BCR	C30-C25-C26	-4.86	116.00	122.64
19	A	1121	CLA	O2D-CGD-CBD	4.85	119.71	111.23
19	K	1403	CLA	O2D-CGD-CBD	4.85	119.71	111.23
19	A	1013	CLA	O2D-CGD-CBD	4.85	119.70	111.23
28	4	505	LUT	C7-C8-C9	-4.84	119.07	126.23
19	B	1238	CLA	O2D-CGD-CBD	4.84	119.69	111.23
22	G	4011	BCR	C30-C25-C24	4.83	128.76	115.65
29	4	613	CHL	C1C-CHC-C4B	4.83	133.34	116.07
19	2	606	CLA	O2D-CGD-CBD	4.83	119.67	111.23
29	2	610	CHL	C1C-CHC-C4B	4.80	133.26	116.07
19	A	1012	CLA	CMD-C2D-C1D	4.80	133.18	124.73
19	A	1122	CLA	O2D-CGD-CBD	4.80	119.62	111.23
19	L	1503	CLA	O2D-CGD-CBD	4.80	119.61	111.23
19	A	1138	CLA	O2D-CGD-CBD	4.79	119.61	111.23
22	K	4002	BCR	C30-C25-C26	-4.79	116.10	122.64
22	A	4017	BCR	C34-C9-C10	-4.78	115.07	122.82
29	2	613	CHL	C1C-CHC-C4B	4.78	133.17	116.07
18	A	1011	CL0	O2A-CGA-CBA	4.78	126.39	111.83
29	4	610	CHL	C1B-CHB-C4A	4.76	124.39	121.32
25	G	5001	LMG	O7-C10-C11	4.76	121.78	111.48
19	1	601	CLA	O2D-CGD-CBD	4.76	119.55	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	2	601	CLA	O2D-CGD-CBD	4.73	119.50	111.23
22	J	4012	BCR	C27-C26-C25	-4.71	116.35	122.70
22	A	4007	BCR	C30-C25-C26	-4.70	116.21	122.64
19	B	1205	CLA	CMD-C2D-C1D	4.70	133.01	124.73
27	B	5005	DGD	O2G-C1B-C2B	4.66	121.57	111.48
19	B	1023	CLA	O2D-CGD-CBD	4.66	119.37	111.23
22	A	4011	BCR	C30-C25-C26	-4.62	116.32	122.64
22	I	4018	BCR	C34-C9-C10	-4.61	115.34	122.82
22	A	4017	BCR	C30-C25-C26	-4.61	116.33	122.64
22	B	4010	BCR	C23-C22-C21	4.60	126.25	119.01
19	J	1901	CLA	O2D-CGD-CBD	4.60	119.27	111.23
22	A	4011	BCR	C27-C26-C25	-4.58	116.52	122.70
22	2	503	BCR	C33-C5-C6	-4.53	119.54	124.48
22	L	4019	BCR	C28-C27-C26	-4.53	105.98	114.06
22	3	506	BCR	C30-C25-C26	-4.53	116.45	122.64
27	3	803	DGD	O2G-C1B-C2B	4.51	121.24	111.48
22	A	4002	BCR	C34-C9-C10	-4.51	115.51	122.82
25	G	5002	LMG	O7-C10-C11	4.51	121.24	111.48
23	A	5002	LHG	O7-C7-C8	4.50	121.22	111.48
22	1	503	BCR	C30-C25-C24	4.49	127.83	115.65
28	4	501	LUT	C7-C8-C9	-4.47	119.62	126.23
22	A	4002	BCR	C27-C26-C25	-4.46	116.68	122.70
22	B	4006	BCR	C30-C25-C24	4.45	127.72	115.65
19	4	605	CLA	O2D-CGD-CBD	4.45	119.00	111.23
22	I	4018	BCR	C1-C6-C5	-4.44	116.57	122.64
30	2	502	XAT	C38-C25-C24	4.42	119.21	114.24
19	A	1124	CLA	CMD-C2D-C1D	4.41	132.49	124.73
22	A	4007	BCR	C27-C26-C25	-4.38	116.78	122.70
22	F	4016	BCR	C30-C25-C26	-4.35	116.69	122.64
25	F	5004	LMG	O7-C10-C11	4.33	120.85	111.48
25	F	5002	LMG	O7-C10-C11	4.33	120.84	111.48
22	L	4020	BCR	C27-C26-C25	-4.32	116.86	122.70
22	A	4003	BCR	C19-C18-C17	4.32	125.80	119.01
30	4	502	XAT	C18-C5-C4	4.30	119.07	114.24
22	A	4017	BCR	C27-C26-C25	-4.28	116.92	122.70
27	F	5005	DGD	O2G-C1B-C2B	4.27	120.72	111.48
25	B	5003	LMG	O7-C10-C11	4.24	120.66	111.48
22	I	4018	BCR	C30-C25-C26	-4.24	116.84	122.64
22	F	4016	BCR	C27-C26-C25	-4.23	116.99	122.70
31	2	807	3PH	O21-C21-C22	4.23	120.63	111.48
22	B	4004	BCR	C30-C25-C26	-4.22	116.88	122.64
22	3	506	BCR	C27-C26-C25	-4.20	117.03	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	4005	BCR	C30-C25-C26	-4.19	116.91	122.64
30	2	502	XAT	C19-C9-C8	4.19	124.49	118.09
22	3	503	BCR	C30-C25-C26	-4.15	116.97	122.64
27	4	802	DGD	O2G-C1B-C2B	4.14	120.44	111.48
23	4	801	LHG	O7-C7-C8	4.13	120.41	111.48
22	A	4008	BCR	C30-C25-C26	-4.11	117.02	122.64
27	G	5003	DGD	O2G-C1B-C2B	4.09	120.33	111.48
22	A	4011	BCR	C4-C5-C6	-4.09	117.18	122.70
29	1	612	CHL	C3D-C4D-CHA	4.08	114.74	108.54
29	2	615	CHL	CHA-C1A-C2A	-4.07	123.75	133.31
22	B	4006	BCR	C12-C13-C14	-4.06	112.62	119.01
29	4	610	CHL	C3D-C4D-CHA	4.06	114.71	108.54
19	B	1220	CLA	C1-C2-C3	-4.05	119.55	126.20
29	2	610	CHL	C3D-C4D-CHA	4.05	114.70	108.54
19	A	1110	CLA	O2A-C1-C2	4.04	123.65	108.11
22	I	4020	BCR	C19-C18-C17	4.02	125.34	119.01
22	A	4003	BCR	C1-C6-C7	4.01	126.53	115.65
29	1	609	CHL	C1A-CHA-C4D	4.01	125.67	118.98
25	1	802	LMG	O7-C10-C11	4.01	120.15	111.48
29	2	609	CHL	C3D-C4D-CHA	4.00	114.62	108.54
23	B	5002	LHG	O7-C7-C8	4.00	120.13	111.48
22	A	4011	BCR	C12-C13-C14	-3.99	112.73	119.01
27	1	803	DGD	O2G-C1B-C2B	3.99	120.10	111.48
28	1	501	LUT	C38-C25-C24	-3.99	113.93	123.36
22	I	4018	BCR	C27-C26-C25	-3.98	117.32	122.70
23	A	5001	LHG	O7-C7-C8	3.97	120.07	111.48
22	B	4010	BCR	C33-C5-C6	-3.97	120.16	124.48
22	K	4001	BCR	C27-C26-C25	-3.97	117.35	122.70
28	2	501	LUT	C15-C14-C13	-3.96	121.72	127.28
29	3	604	CHL	CHA-C1A-C2A	-3.95	124.03	133.31
25	B	5007	LMG	O7-C10-C11	3.95	120.03	111.48
29	4	611	CHL	C3D-C4D-CHA	3.95	114.54	108.54
25	B	5004	LMG	O7-C10-C11	3.95	120.02	111.48
29	3	604	CHL	C3D-C4D-CHA	3.94	114.54	108.54
29	2	613	CHL	C3D-C4D-CHA	3.94	114.53	108.54
25	2	804	LMG	O7-C10-C11	3.93	119.99	111.48
19	B	1202	CLA	C1-C2-C3	-3.93	119.75	126.20
29	4	615	CHL	C3D-C4D-CHA	3.93	114.52	108.54
25	2	805	LMG	O7-C10-C11	3.93	119.98	111.48
25	2	803	LMG	O7-C10-C11	3.93	119.97	111.48
29	4	613	CHL	C3D-C4D-CHA	3.92	114.50	108.54
29	2	610	CHL	CHA-C1A-C2A	-3.92	124.11	133.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	L	4020	BCR	C19-C18-C17	3.92	125.17	119.01
28	4	505	LUT	C37-C21-C36	3.91	113.57	107.87
29	3	611	CHL	CHA-C1A-C2A	-3.90	124.16	133.31
29	2	615	CHL	C3D-C4D-CHA	3.90	114.46	108.54
25	F	5003	LMG	O7-C10-C11	3.89	119.91	111.48
29	2	611	CHL	C3D-C4D-CHA	3.89	114.45	108.54
18	A	1011	CL0	CHA-C1A-C2A	-3.88	124.19	133.31
22	L	4020	BCR	C30-C25-C26	-3.87	117.35	122.64
30	4	502	XAT	C38-C25-C24	3.87	118.58	114.24
28	1	501	LUT	C26-C27-C28	-3.86	118.58	124.58
23	2	801	LHG	O7-C7-C8	3.85	119.82	111.48
28	4	501	LUT	C35-C34-C33	-3.85	121.88	127.28
29	1	609	CHL	C3D-C4D-CHA	3.85	114.39	108.54
29	1	610	CHL	C3D-C4D-CHA	3.84	114.38	108.54
22	K	4001	BCR	C30-C25-C26	-3.84	117.38	122.64
29	4	615	CHL	CHA-C1A-C2A	-3.84	124.29	133.31
29	3	611	CHL	C3D-C4D-CHA	3.84	114.37	108.54
28	2	501	LUT	C7-C8-C9	-3.83	120.57	126.23
22	F	4014	BCR	C27-C26-C25	-3.83	117.53	122.70
22	I	4018	BCR	C32-C1-C6	3.81	116.22	110.24
27	J	5001	DGD	O2G-C1B-C2B	3.80	119.71	111.48
19	L	1501	CLA	C1-C2-C3	-3.80	120.62	126.76
29	4	610	CHL	CHA-C1A-C2A	-3.79	124.40	133.31
19	A	1126	CLA	C1-C2-C3	-3.79	119.98	126.20
23	1	801	LHG	O7-C7-C8	3.79	119.69	111.48
22	I	4018	BCR	C12-C13-C14	3.79	124.97	119.01
22	2	503	BCR	C39-C30-C25	3.78	116.17	110.24
29	1	609	CHL	CHA-C1A-C2A	-3.77	124.45	133.31
29	1	610	CHL	CHA-C1A-C2A	-3.77	124.45	133.31
22	A	4011	BCR	C19-C18-C17	-3.76	113.10	119.01
22	A	4008	BCR	C1-C6-C5	-3.75	117.51	122.64
22	A	4007	BCR	C15-C14-C13	-3.74	122.03	127.28
19	3	612	CLA	C1-C2-C3	-3.74	120.71	126.76
22	A	4008	BCR	C4-C5-C6	-3.74	117.65	122.70
25	3	802	LMG	O7-C10-C11	3.73	119.56	111.48
22	B	4005	BCR	C27-C26-C25	-3.73	117.66	122.70
22	2	503	BCR	C24-C25-C26	-3.73	112.96	121.56
25	A	5006	LMG	O7-C10-C11	3.73	119.54	111.48
19	A	1125	CLA	C1-C2-C3	-3.72	120.10	126.20
19	L	1503	CLA	C1-C2-C3	-3.72	120.75	126.76
22	3	506	BCR	C15-C14-C13	-3.72	122.07	127.28
25	2	802	LMG	O7-C10-C11	3.71	124.58	110.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	4006	BCR	C39-C30-C25	3.71	116.06	110.24
19	A	1119	CLA	C1-C2-C3	-3.71	120.12	126.20
19	B	1215	CLA	C1-C2-C3	-3.71	120.12	126.20
28	1	501	LUT	C31-C30-C29	-3.70	122.08	127.28
29	2	611	CHL	CHA-C1A-C2A	-3.70	124.61	133.31
29	3	604	CHL	C1A-CHA-C4D	3.70	125.15	118.98
19	A	1122	CLA	C3B-C4B-NB	-3.69	107.23	110.53
19	A	1119	CLA	O2A-C1-C2	3.69	122.32	108.11
22	A	4002	BCR	C36-C18-C17	-3.68	116.85	122.82
19	A	1116	CLA	C1-C2-C3	-3.68	120.16	126.20
29	3	611	CHL	C1A-CHA-C4D	3.68	125.12	118.98
22	B	4004	BCR	C27-C26-C25	-3.66	117.76	122.70
22	K	4001	BCR	C19-C18-C17	3.66	124.77	119.01
29	2	615	CHL	C1A-CHA-C4D	3.65	125.07	118.98
28	4	501	LUT	C37-C21-C26	3.65	115.07	109.55
19	B	1210	CLA	C1-C2-C3	-3.65	120.22	126.20
19	4	604	CLA	C1-C2-C3	-3.64	120.23	126.20
22	K	4002	BCR	C34-C9-C10	-3.64	116.92	122.82
22	L	4019	BCR	C27-C26-C25	-3.64	117.79	122.70
22	G	4011	BCR	C19-C18-C17	3.63	124.71	119.01
28	3	501	LUT	C37-C21-C26	3.62	115.04	109.55
28	2	501	LUT	C38-C25-C24	-3.62	114.78	123.36
25	F	5001	LMG	O7-C10-C11	3.62	119.32	111.48
22	B	4010	BCR	C37-C22-C21	-3.62	116.95	122.82
22	J	4012	BCR	C19-C18-C17	3.62	124.70	119.01
22	A	4008	BCR	C19-C18-C17	3.61	124.69	119.01
19	4	601	CLA	O2A-C1-C2	3.61	122.00	108.11
22	2	503	BCR	C39-C30-C29	-3.59	95.18	108.95
22	I	4018	BCR	C4-C5-C6	-3.59	117.86	122.70
19	A	1109	CLA	O2A-C1-C2	3.58	121.89	108.11
28	4	505	LUT	C16-C1-C6	-3.58	104.63	110.24
22	3	506	BCR	C30-C25-C24	3.57	125.34	115.65
28	3	501	LUT	C7-C8-C9	-3.57	120.95	126.23
19	B	1207	CLA	C3B-C4B-NB	-3.57	107.35	110.53
19	L	1502	CLA	O2A-C1-C2	3.56	121.82	108.11
22	G	4011	BCR	C40-C30-C25	3.55	115.80	110.24
22	I	4020	BCR	C39-C30-C25	3.53	115.78	110.24
19	L	1502	CLA	C1-C2-C3	-3.53	120.42	126.20
29	4	610	CHL	C1A-CHA-C4D	3.53	124.87	118.98
19	A	1121	CLA	O2A-C1-C2	3.52	121.67	108.11
22	B	4006	BCR	C35-C13-C12	3.52	123.46	118.09
22	A	4007	BCR	C19-C18-C17	3.51	124.52	119.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	4011	BCR	C35-C13-C12	3.50	123.44	118.09
29	3	604	CHL	C1-O2A-CGA	3.50	125.12	116.65
19	3	606	CLA	C1-C2-C3	-3.49	121.11	126.76
28	3	501	LUT	C38-C25-C24	-3.49	115.10	123.36
28	2	501	LUT	C27-C28-C29	-3.48	118.83	126.32
29	2	609	CHL	CHA-C1A-C2A	-3.48	125.13	133.31
22	3	503	BCR	C15-C14-C13	-3.48	122.39	127.28
22	3	506	BCR	C19-C18-C17	3.48	124.48	119.01
22	A	4003	BCR	C32-C1-C6	3.48	115.70	110.24
22	1	504	BCR	C30-C25-C24	3.48	125.08	115.65
20	A	2001	PQN	C11-C12-C13	-3.47	120.85	126.83
19	B	1212	CLA	C1-C2-C3	-3.47	120.52	126.20
22	1	504	BCR	C30-C25-C26	-3.46	117.90	122.64
29	4	611	CHL	C1A-CHA-C4D	3.46	124.76	118.98
29	4	615	CHL	C1A-CHA-C4D	3.45	124.74	118.98
19	A	1108	CLA	C1-C2-C3	-3.45	121.18	126.76
22	B	4006	BCR	C36-C18-C17	-3.45	117.23	122.82
19	B	1023	CLA	O2A-C1-C2	3.44	121.36	108.11
19	B	1215	CLA	O2A-C1-C2	3.44	121.35	108.11
19	B	1220	CLA	C3B-C4B-NB	-3.44	107.46	110.53
19	4	605	CLA	C3B-C4B-NB	-3.44	107.46	110.53
19	A	1137	CLA	C3B-C4B-NB	-3.44	107.46	110.53
22	H	4021	BCR	C19-C18-C17	3.43	124.41	119.01
22	A	4008	BCR	C27-C26-C25	-3.43	118.06	122.70
29	4	611	CHL	CHA-C1A-C2A	-3.43	125.25	133.31
22	J	4012	BCR	C34-C9-C8	3.43	123.33	118.09
22	A	4003	BCR	C1-C6-C5	-3.43	117.95	122.64
19	B	1205	CLA	C1-C2-C3	-3.43	120.58	126.20
22	1	503	BCR	C34-C9-C10	-3.43	117.27	122.82
19	2	607	CLA	O2A-CGA-CBA	3.42	122.27	111.83
29	1	612	CHL	CHA-C1A-C2A	-3.41	125.29	133.31
19	4	606	CLA	C1-C2-C3	-3.41	121.24	126.76
22	A	4011	BCR	C1-C6-C5	-3.41	117.98	122.64
19	2	608	CLA	C1-C2-C3	-3.40	121.26	126.76
28	1	501	LUT	C22-C23-C24	-3.40	106.14	111.18
19	4	602	CLA	C1-C2-C3	-3.39	121.28	126.76
19	1	605	CLA	C4-C3-C5	3.38	121.10	115.23
28	4	501	LUT	C31-C30-C29	-3.38	122.53	127.28
19	A	1140	CLA	C3B-C4B-NB	-3.38	107.52	110.53
28	1	502	LUT	C22-C23-C24	-3.37	106.18	111.18
18	A	1011	CL0	C1C-CHC-C4B	3.37	128.13	116.07
19	2	607	CLA	C1-O2A-CGA	3.36	124.79	116.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	4005	BCR	C34-C9-C10	-3.35	117.39	122.82
19	G	1601	CLA	O2A-C1-C2	3.34	120.97	108.11
28	4	505	LUT	C17-C1-C6	3.34	115.47	110.24
19	B	1218	CLA	C3B-C4B-NB	-3.33	107.55	110.53
19	B	1216	CLA	O2A-C1-C2	3.33	120.94	108.11
28	1	502	LUT	C37-C21-C36	3.33	112.72	107.87
20	A	2001	PQN	C14-C13-C15	3.33	121.00	115.23
29	2	611	CHL	C1A-CHA-C4D	3.33	124.53	118.98
19	A	1116	CLA	C3B-C4B-NB	-3.32	107.56	110.53
28	3	501	LUT	C35-C34-C33	-3.32	122.62	127.28
19	1	605	CLA	C4-C3-C2	-3.32	115.10	123.63
19	B	1219	CLA	C1-C2-C3	-3.32	120.75	126.20
28	1	502	LUT	C7-C8-C9	-3.32	121.33	126.23
29	4	613	CHL	CHA-C1A-C2A	-3.31	125.53	133.31
19	B	1217	CLA	C3B-C4B-NB	-3.31	107.58	110.53
19	2	602	CLA	C4-C3-C5	3.31	120.97	115.23
22	I	4020	BCR	C23-C24-C25	-3.31	118.17	127.00
28	3	501	LUT	C31-C30-C29	-3.30	122.64	127.28
28	4	505	LUT	C11-C10-C9	-3.30	122.65	127.28
22	A	4003	BCR	C34-C9-C10	-3.30	117.47	122.82
29	2	613	CHL	CHA-C1A-C2A	-3.30	125.56	133.31
28	J	4013	LUT	C35-C34-C33	-3.30	122.65	127.28
19	2	602	CLA	C3B-C4B-NB	-3.30	107.59	110.53
19	A	1106	CLA	CAA-C2A-C1A	-3.30	101.17	111.97
28	2	501	LUT	C1-C6-C5	-3.30	118.13	122.64
20	B	2002	PQN	C11-C12-C13	-3.30	121.15	126.83
22	3	503	BCR	C23-C24-C25	-3.29	118.20	127.00
22	G	4011	BCR	C34-C9-C10	-3.29	117.48	122.82
19	2	606	CLA	C1-C2-C3	-3.29	121.44	126.76
25	G	5002	LMG	C8-O7-C10	-3.29	109.92	117.80
22	G	4011	BCR	C27-C26-C25	-3.29	118.26	122.70
22	A	4011	BCR	C3-C4-C5	-3.29	108.19	114.06
19	A	1116	CLA	O2A-C1-C2	3.28	120.74	108.11
19	B	1230	CLA	C1-C2-C3	-3.28	120.82	126.20
19	1	602	CLA	C3B-C4B-NB	-3.28	107.60	110.53
19	B	1220	CLA	O2A-C1-C2	3.28	120.71	108.11
19	A	1102	CLA	O2A-C1-C2	3.27	120.71	108.11
22	I	4018	BCR	C7-C6-C5	-3.27	114.02	121.56
19	1	614	CLA	C3B-C4B-NB	-3.27	107.61	110.53
19	A	1121	CLA	C3B-C4B-NB	-3.27	107.61	110.53
19	A	1136	CLA	C3B-C4B-NB	-3.27	107.61	110.53
22	A	4017	BCR	C8-C9-C10	3.27	124.15	119.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	1228	CLA	O2A-C1-C2	3.27	120.69	108.11
20	B	2002	PQN	C14-C13-C15	3.27	120.90	115.23
22	1	503	BCR	C27-C26-C25	-3.27	118.29	122.70
19	B	1231	CLA	C1-C2-C3	-3.27	120.84	126.20
19	J	1901	CLA	C1-C2-C3	-3.26	121.48	126.76
19	B	1208	CLA	C3B-C4B-NB	-3.26	107.62	110.53
28	4	501	LUT	C38-C25-C24	-3.26	115.64	123.36
19	B	1215	CLA	O2A-CGA-CBA	3.26	121.78	111.83
22	A	4002	BCR	C32-C1-C6	-3.26	105.13	110.24
29	2	609	CHL	C1A-CHA-C4D	3.26	124.41	118.98
19	B	1022	CLA	C3B-C4B-NB	-3.25	107.63	110.53
22	I	4020	BCR	C1-C6-C5	-3.25	118.19	122.64
22	I	4018	BCR	C31-C1-C6	-3.25	105.15	110.24
19	A	1131	CLA	C3B-C4B-NB	-3.25	107.63	110.53
19	K	1403	CLA	CMD-C2D-C3D	-3.24	120.26	127.69
29	1	610	CHL	C1A-CHA-C4D	3.24	124.38	118.98
22	B	4006	BCR	C36-C18-C19	-3.23	113.15	118.09
29	1	609	CHL	C1-O2A-CGA	3.23	124.47	116.65
19	A	1129	CLA	O2A-C1-C2	3.23	120.55	108.11
28	3	502	LUT	C38-C25-C24	-3.23	115.72	123.36
22	G	4011	BCR	C15-C14-C13	-3.22	122.76	127.28
19	A	1132	CLA	C3B-C4B-NB	-3.22	107.65	110.53
28	4	501	LUT	C22-C23-C24	-3.22	106.40	111.18
29	2	610	CHL	C1A-CHA-C4D	3.22	124.35	118.98
19	3	608	CLA	CMA-C3A-C4A	3.21	120.41	111.77
19	B	1234	CLA	C1-C2-C3	-3.21	120.93	126.20
19	A	1135	CLA	O2A-C1-C2	3.21	120.46	108.11
22	A	4017	BCR	C36-C18-C17	-3.21	117.62	122.82
22	3	506	BCR	C34-C9-C10	-3.21	117.62	122.82
19	A	1110	CLA	C1-C2-C3	-3.21	120.94	126.20
19	A	1129	CLA	C1-C2-C3	-3.20	120.95	126.20
29	4	611	CHL	C3C-C4C-NC	-3.20	106.82	114.65
22	1	503	BCR	C37-C22-C23	3.20	122.98	118.09
28	3	501	LUT	C11-C10-C9	-3.20	122.79	127.28
19	4	605	CLA	C1-C2-C3	-3.20	120.95	126.20
19	1	603	CLA	C3B-C4B-NB	-3.20	107.67	110.53
19	A	1122	CLA	O2A-C1-C2	3.20	120.41	108.11
19	B	1239	CLA	O2A-C1-C2	3.20	120.41	108.11
22	1	504	BCR	C1-C6-C5	-3.19	118.28	122.64
19	B	1226	CLA	O2A-C1-C2	3.19	120.37	108.11
19	2	603	CLA	CMA-C3A-C4A	3.18	120.33	111.77
19	K	1402	CLA	CMA-C3A-C4A	3.18	120.32	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	1234	CLA	O2A-C1-C2	3.18	120.34	108.11
19	2	604	CLA	O2A-C1-C2	3.18	120.33	108.11
22	L	4020	BCR	C31-C1-C6	-3.17	105.26	110.24
19	B	1223	CLA	C1-C2-C3	-3.17	121.00	126.20
19	K	1404	CLA	C3B-C4B-NB	-3.17	107.70	110.53
28	1	501	LUT	C39-C29-C28	3.17	122.93	118.09
19	2	603	CLA	C3B-C4B-NB	-3.17	107.70	110.53
19	B	1230	CLA	O2A-C1-C2	3.16	120.28	108.11
22	1	503	BCR	C15-C14-C13	-3.16	122.84	127.28
19	B	1225	CLA	O2A-C1-C2	3.16	120.27	108.11
19	3	613	CLA	C2C-C1C-NC	3.16	113.30	109.98
29	4	613	CHL	C1A-CHA-C4D	3.16	124.25	118.98
28	4	505	LUT	C39-C29-C30	-3.16	117.70	122.82
28	1	502	LUT	C40-C33-C32	3.16	122.91	118.09
19	L	1501	CLA	O2A-C1-C2	3.16	120.26	108.11
22	L	4020	BCR	C36-C18-C17	-3.16	117.70	122.82
27	F	5005	DGD	O1G-C1A-C2A	3.16	121.45	111.83
19	3	603	CLA	O2A-C1-C2	3.15	120.24	108.11
19	1	601	CLA	C4-C3-C5	3.15	120.70	115.23
19	3	603	CLA	CMA-C3A-C4A	3.15	120.25	111.77
19	B	1219	CLA	O2A-C1-C2	3.15	120.22	108.11
28	2	501	LUT	C20-C13-C12	3.15	122.89	118.09
19	B	1212	CLA	O2A-C1-C2	3.15	120.21	108.11
19	4	609	CLA	C1-C2-C3	-3.15	121.67	126.76
19	3	607	CLA	CMA-C3A-C4A	3.14	120.22	111.77
19	B	1232	CLA	O2A-C1-C2	3.14	120.20	108.11
19	B	1223	CLA	C3B-C4B-NB	-3.14	107.72	110.53
22	L	4020	BCR	C34-C9-C10	-3.14	117.73	122.82
22	A	4002	BCR	C28-C27-C26	-3.14	108.45	114.06
22	A	4017	BCR	C16-C17-C18	3.14	131.68	127.28
19	A	1107	CLA	C1-C2-C3	-3.14	121.05	126.20
19	K	1402	CLA	C1-C2-C3	-3.14	121.06	126.20
19	A	1139	CLA	O2A-C1-C2	3.14	120.17	108.11
22	F	4014	BCR	C37-C22-C23	3.13	122.88	118.09
19	A	1118	CLA	C1-C2-C3	-3.13	121.69	126.76
19	A	1138	CLA	C3B-C4B-NB	-3.13	107.73	110.53
19	A	1104	CLA	C3B-C4B-NB	-3.13	107.73	110.53
29	4	615	CHL	CMA-C3A-C4A	3.13	121.35	114.61
19	A	1107	CLA	O2A-C1-C2	3.13	120.15	108.11
30	4	502	XAT	O24-C25-C38	-3.13	111.56	115.05
22	B	4009	BCR	C30-C25-C24	3.12	124.12	115.65
19	B	1202	CLA	O2A-C1-C2	3.12	120.10	108.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	2	607	CLA	C3B-C4B-NB	-3.11	107.75	110.53
19	4	602	CLA	O2A-C1-C2	3.11	120.09	108.11
19	2	608	CLA	O2A-C1-C2	3.11	120.08	108.11
19	K	1402	CLA	C3B-C4B-NB	-3.11	107.75	110.53
28	2	501	LUT	C22-C23-C24	-3.11	106.57	111.18
19	B	1205	CLA	O2A-C1-C2	3.11	120.06	108.11
19	2	607	CLA	O2A-C1-C2	3.11	120.06	108.11
19	B	1221	CLA	O2A-C1-C2	3.10	120.05	108.11
22	K	4002	BCR	C35-C13-C12	3.10	122.83	118.09
19	J	1901	CLA	C3B-C4B-NB	-3.10	107.76	110.53
19	2	601	CLA	O2A-C1-C2	3.10	120.03	108.11
29	1	612	CHL	C3C-C4C-NC	-3.10	107.08	114.65
19	3	605	CLA	O2A-C1-C2	3.10	120.03	108.11
19	G	1603	CLA	CMA-C3A-C4A	3.10	120.10	111.77
28	1	501	LUT	C37-C21-C26	-3.09	104.86	109.55
19	2	608	CLA	CMA-C3A-C4A	3.09	120.09	111.77
19	A	1134	CLA	C3B-C4B-NB	-3.09	107.77	110.53
19	B	1210	CLA	O2A-C1-C2	3.09	120.01	108.11
19	K	1403	CLA	CMA-C3A-C4A	3.09	120.08	111.77
25	B	5004	LMG	O8-C28-C29	3.09	121.26	111.83
19	A	1136	CLA	C1-C2-C3	-3.09	121.14	126.20
19	B	1205	CLA	C3B-C4B-NB	-3.09	107.77	110.53
19	B	1238	CLA	CMA-C3A-C4A	3.09	120.08	111.77
23	B	5001	LHG	C5-O7-C7	-3.09	112.40	117.85
19	4	603	CLA	CMA-C3A-C4A	3.09	120.06	111.77
19	A	1116	CLA	O2A-CGA-CBA	3.08	121.23	111.83
19	B	1227	CLA	O2A-C1-C2	3.08	119.97	108.11
25	2	802	LMG	O8-C28-C29	3.08	120.50	111.15
19	A	1109	CLA	C3B-C4B-NB	-3.08	107.78	110.53
22	J	4012	BCR	C34-C9-C10	-3.08	117.83	122.82
19	B	1204	CLA	C3B-C4B-NB	-3.08	107.78	110.53
23	4	801	LHG	O8-C23-C24	3.08	121.22	111.83
19	A	1127	CLA	O2A-C1-C2	3.07	119.94	108.11
19	B	1231	CLA	O2A-C1-C2	3.07	119.94	108.11
28	J	4013	LUT	C40-C33-C32	3.07	122.78	118.09
19	B	1224	CLA	O2A-CGA-CBA	3.07	121.20	111.83
29	2	610	CHL	C3C-C4C-NC	-3.07	107.14	114.65
19	A	1131	CLA	O2A-C1-C2	3.07	119.92	108.11
19	A	1116	CLA	C4-C3-C5	3.07	120.56	115.23
22	B	4004	BCR	C30-C25-C24	3.07	123.97	115.65
19	2	601	CLA	O2A-CGA-CBA	3.07	121.19	111.83
29	2	613	CHL	C1A-CHA-C4D	3.06	124.09	118.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	3	502	LUT	C20-C13-C12	3.06	122.77	118.09
29	1	609	CHL	C3C-C4C-NC	-3.06	107.17	114.65
25	G	5001	LMG	O8-C28-C29	3.06	121.17	111.83
22	2	503	BCR	C15-C14-C13	-3.06	122.98	127.28
23	A	5002	LHG	O8-C23-C24	3.06	121.17	111.83
22	A	4008	BCR	C3-C4-C5	-3.06	108.60	114.06
30	4	502	XAT	C15-C14-C13	-3.06	122.99	127.28
19	1	606	CLA	O2A-C1-C2	3.06	119.88	108.11
19	4	606	CLA	O2A-C1-C2	3.06	119.88	108.11
19	A	1121	CLA	CMA-C3A-C4A	3.06	119.99	111.77
19	2	608	CLA	C3B-C4B-NB	-3.05	107.80	110.53
19	A	1012	CLA	C3B-C4B-NB	-3.05	107.81	110.53
28	4	501	LUT	C27-C28-C29	-3.05	119.76	126.32
19	1	603	CLA	O2A-C1-C2	3.05	119.84	108.11
19	A	1132	CLA	O2A-C1-C2	3.05	119.83	108.11
19	K	1403	CLA	O2A-C1-C2	3.04	119.61	109.44
28	1	502	LUT	C3-C4-C5	-3.04	104.62	112.18
28	1	502	LUT	C39-C29-C28	3.04	122.73	118.09
22	A	4011	BCR	C31-C1-C6	-3.04	105.48	110.24
19	B	1235	CLA	C1-C2-C3	-3.04	121.22	126.20
19	A	1128	CLA	O2A-C1-C2	3.03	119.78	108.11
22	L	4019	BCR	C34-C9-C10	-3.03	117.90	122.82
29	1	610	CHL	C3C-C4C-NC	-3.03	107.24	114.65
27	J	5001	DGD	O1G-C1A-C2A	3.03	121.07	111.83
19	B	1211	CLA	O2A-C1-C2	3.03	119.76	108.11
29	2	615	CHL	C3C-C4C-NC	-3.03	107.25	114.65
22	K	4002	BCR	C23-C24-C25	-3.03	118.92	127.00
19	A	1104	CLA	O2A-C1-C2	3.03	119.75	108.11
19	3	608	CLA	O2A-C1-C2	3.03	119.56	109.44
18	A	1011	CL0	O2A-C1-C2	3.02	119.75	108.11
22	B	4004	BCR	C37-C22-C23	3.02	122.71	118.09
22	L	4019	BCR	C19-C18-C17	3.02	123.77	119.01
19	A	1141	CLA	O2A-C1-C2	3.02	119.73	108.11
19	2	607	CLA	CMA-C3A-C4A	3.02	119.89	111.77
19	4	603	CLA	O2A-C1-C2	3.02	119.73	108.11
28	4	505	LUT	C1-C6-C7	3.02	123.84	115.65
22	I	4018	BCR	C3-C4-C5	-3.02	108.67	114.06
19	3	601	CLA	O2A-C1-C2	3.02	119.72	108.11
19	4	609	CLA	C3B-C4B-NB	-3.02	107.84	110.53
28	1	502	LUT	C28-C29-C30	-3.02	114.27	119.01
28	4	505	LUT	C15-C35-C34	-3.01	117.35	123.52
19	A	1102	CLA	C3B-C4B-NB	-3.01	107.84	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	3	614	CLA	C2C-C1C-NC	3.01	113.14	109.98
19	B	1237	CLA	C3B-C4B-NB	-3.01	107.84	110.53
22	B	4009	BCR	C37-C22-C23	3.01	122.68	118.09
28	4	501	LUT	C11-C10-C9	-3.01	123.06	127.28
29	2	611	CHL	C3C-C4C-NC	-3.01	107.30	114.65
22	B	4010	BCR	C19-C18-C17	3.01	123.74	119.01
19	3	607	CLA	C3B-C4B-NB	-3.01	107.85	110.53
29	4	610	CHL	C3C-C4C-NC	-3.00	107.31	114.65
19	3	610	CLA	O2A-C1-C2	3.00	119.66	108.11
19	A	1114	CLA	CMA-C3A-C4A	3.00	119.83	111.77
19	L	1503	CLA	O2A-C1-C2	3.00	119.65	108.11
22	F	4016	BCR	C28-C27-C26	-3.00	108.71	114.06
22	I	4020	BCR	C16-C17-C18	3.00	131.48	127.28
19	B	1219	CLA	CMA-C3A-C4A	3.00	119.82	111.77
19	A	1123	CLA	CMA-C3A-C4A	2.99	119.82	111.77
19	A	1105	CLA	O2A-C1-C2	2.99	119.63	108.11
19	4	608	CLA	C3B-C4B-NB	-2.99	107.86	110.53
29	3	611	CHL	C3C-C4C-NC	-2.99	107.34	114.65
19	B	1222	CLA	O2A-C1-C2	2.99	119.61	108.11
19	A	1101	CLA	C1-C2-C3	-2.99	121.30	126.20
19	A	1117	CLA	C1-C2-C3	-2.98	121.31	126.20
19	2	605	CLA	O2A-C1-C2	2.98	119.58	108.11
29	2	615	CHL	C1-O2A-CGA	2.98	123.87	116.65
19	A	1102	CLA	O2D-CGD-O1D	-2.98	118.04	123.85
22	A	4008	BCR	C12-C13-C14	-2.98	114.32	119.01
19	L	1503	CLA	O2A-CGA-CBA	2.98	120.92	111.83
19	4	604	CLA	O2A-C1-C2	2.98	119.57	108.11
22	1	503	BCR	C40-C30-C25	2.97	114.91	110.24
19	B	1238	CLA	O2A-C1-C2	2.97	119.55	108.11
19	A	1115	CLA	O2A-C1-C2	2.97	119.55	108.11
19	B	1201	CLA	C3B-C4B-NB	-2.97	107.88	110.53
19	B	1236	CLA	O2A-C1-C2	2.97	119.54	108.11
19	2	602	CLA	O2A-C1-C2	2.97	119.54	108.11
29	2	613	CHL	C3C-C4C-NC	-2.97	107.39	114.65
29	2	609	CHL	C3C-C4C-NC	-2.97	107.39	114.65
19	2	603	CLA	O2A-C1-C2	2.97	119.53	108.11
22	1	504	BCR	C19-C18-C17	2.97	123.67	119.01
19	A	1124	CLA	C3B-C4B-NB	-2.97	107.88	110.53
25	F	5001	LMG	O8-C28-C29	2.96	120.14	111.15
29	4	611	CHL	C1-C2-C3	-2.96	121.97	126.76
19	K	1402	CLA	O2A-C1-C2	2.96	119.50	108.11
22	3	503	BCR	C28-C27-C26	-2.96	108.78	114.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	4	505	LUT	C39-C29-C28	2.96	122.61	118.09
22	B	4009	BCR	C38-C26-C25	-2.96	121.26	124.48
19	A	1119	CLA	C3B-C4B-NB	-2.96	107.89	110.53
19	B	1225	CLA	C1-O2A-CGA	2.95	123.80	116.65
19	3	613	CLA	C1C-C2C-C3C	-2.95	103.87	106.98
19	L	1502	CLA	C3B-C4B-NB	-2.95	107.89	110.53
22	K	4002	BCR	C28-C27-C26	-2.95	108.79	114.06
19	B	1202	CLA	C3B-C4B-NB	-2.95	107.90	110.53
19	3	612	CLA	O2A-C1-C2	2.95	119.45	108.11
28	J	4013	LUT	C15-C14-C13	-2.95	123.15	127.28
19	A	1136	CLA	O2A-C1-C2	2.95	119.44	108.11
19	L	1501	CLA	C3B-C4B-NB	-2.94	107.90	110.53
22	3	503	BCR	C27-C26-C25	-2.94	118.73	122.70
19	1	613	CLA	CMA-C3A-C4A	2.94	119.68	111.77
19	B	1234	CLA	O2A-CGA-CBA	2.94	120.81	111.83
19	B	1021	CLA	C1C-C2C-C3C	-2.94	103.89	106.98
19	4	607	CLA	CMA-C3A-C4A	2.94	119.68	111.77
19	B	1232	CLA	C3B-C4B-NB	-2.94	107.91	110.53
19	4	602	CLA	C3B-C4B-NB	-2.94	107.91	110.53
29	1	612	CHL	C1-O2A-CGA	2.94	123.76	116.65
25	G	5006	LMG	O8-C28-C29	2.94	120.07	111.15
19	B	1229	CLA	O2A-CGA-CBA	2.94	120.79	111.83
19	1	601	CLA	O2A-C1-C2	2.94	119.41	108.11
23	B	5002	LHG	C5-O7-C7	-2.93	110.77	117.80
19	A	1130	CLA	O2A-C1-C2	2.93	119.40	108.11
19	B	1223	CLA	O2D-CGD-O1D	-2.93	118.14	123.85
19	A	1135	CLA	C1-C2-C3	-2.93	121.39	126.20
29	4	615	CHL	C3C-C4C-NC	-2.93	107.48	114.65
19	B	1214	CLA	O2A-C1-C2	2.93	119.39	108.11
19	3	608	CLA	C3B-C4B-NB	-2.93	107.91	110.53
19	A	1126	CLA	C3B-C4B-NB	-2.93	107.92	110.53
22	K	4002	BCR	C27-C26-C25	-2.93	118.75	122.70
19	3	605	CLA	C3B-C4B-NB	-2.92	107.92	110.53
25	B	5003	LMG	O8-C28-C29	2.92	120.75	111.83
19	B	1213	CLA	O2A-C1-C2	2.92	119.36	108.11
19	A	1141	CLA	C1-C2-C3	-2.92	121.41	126.20
24	A	5004	LMT	C3'-C4'-C5'	-2.92	104.45	110.93
19	A	1125	CLA	O2A-C1-C2	2.92	119.36	108.11
19	A	1104	CLA	C1-C2-C3	-2.92	121.41	126.20
19	A	1118	CLA	O2A-C1-C2	2.92	119.35	108.11
19	A	1106	CLA	O2A-C1-C2	2.92	119.35	108.11
19	1	603	CLA	CMA-C3A-C4A	2.92	119.62	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	H	4021	BCR	C38-C26-C25	2.92	127.67	124.48
19	B	1239	CLA	C3B-C4B-NB	-2.92	107.92	110.53
19	2	606	CLA	C2C-C1C-NC	2.92	113.05	109.98
19	B	1216	CLA	C3B-C4B-NB	-2.92	107.93	110.53
19	A	1013	CLA	O2A-C1-C2	2.92	119.33	108.11
19	A	1139	CLA	C2C-C1C-NC	2.91	113.04	109.98
19	B	1204	CLA	O2A-C1-C2	2.91	119.32	108.11
19	1	607	CLA	CMA-C3A-C4A	2.91	119.60	111.77
22	B	4006	BCR	C38-C26-C27	2.91	119.80	113.60
19	A	1103	CLA	O2A-C1-C2	2.91	119.31	108.11
22	B	4009	BCR	C34-C9-C10	-2.91	118.10	122.82
19	4	604	CLA	CMA-C3A-C4A	2.91	119.59	111.77
19	3	603	CLA	C3B-C4B-NB	-2.91	107.93	110.53
19	A	1101	CLA	O2D-CGD-O1D	-2.91	118.19	123.85
19	A	1133	CLA	O2A-C1-C2	2.91	119.30	108.11
28	J	4013	LUT	C18-C5-C6	2.91	127.65	124.48
19	1	604	CLA	C3B-C4B-NB	-2.90	107.94	110.53
22	K	4001	BCR	C36-C18-C17	-2.90	118.12	122.82
25	2	802	LMG	O7-C10-O9	-2.90	116.92	123.70
28	2	501	LUT	C15-C35-C34	-2.90	117.59	123.52
25	1	802	LMG	O8-C28-C29	2.90	120.67	111.83
30	4	502	XAT	C26-C27-C28	-2.90	119.87	125.99
19	B	1227	CLA	C3B-C4B-NB	-2.90	107.94	110.53
28	1	502	LUT	C38-C25-C24	-2.90	116.51	123.36
28	4	505	LUT	C27-C28-C29	-2.89	120.10	126.32
19	A	1129	CLA	O2D-CGD-O1D	-2.89	118.22	123.85
19	1	614	CLA	O2A-C1-C2	2.89	119.24	108.11
19	3	607	CLA	O2A-C1-C2	2.89	119.23	108.11
22	3	506	BCR	C28-C27-C26	-2.89	108.90	114.06
19	B	1203	CLA	O2A-C1-C2	2.89	119.23	108.11
22	A	4002	BCR	C34-C9-C8	2.89	122.50	118.09
19	2	612	CLA	O2A-C1-C2	2.89	119.22	108.11
19	A	1112	CLA	C2C-C1C-NC	2.89	113.02	109.98
19	3	602	CLA	O2A-C1-C2	2.89	119.22	108.11
19	G	1603	CLA	O2A-C1-C2	2.89	119.22	108.11
19	B	1236	CLA	C2C-C1C-NC	2.89	113.01	109.98
19	4	607	CLA	O2A-C1-C2	2.89	119.21	108.11
19	A	1140	CLA	O2A-C1-C2	2.88	119.20	108.11
23	4	801	LHG	C5-O7-C7	-2.88	110.90	117.80
19	1	608	CLA	C3B-C4B-NB	-2.88	107.96	110.53
19	B	1201	CLA	O2A-C1-C2	2.88	119.20	108.11
19	B	1022	CLA	O2A-C1-C2	2.88	119.19	108.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	3	617	CLA	C3B-C4B-NB	-2.88	107.96	110.53
19	G	1602	CLA	C3B-C4B-NB	-2.88	107.96	110.53
22	I	4020	BCR	C34-C9-C10	-2.88	118.15	122.82
19	3	617	CLA	C1-C2-C3	-2.88	121.48	126.20
19	B	1208	CLA	O2A-C1-C2	2.88	119.18	108.11
22	A	4003	BCR	C36-C18-C17	-2.88	118.16	122.82
19	B	1236	CLA	C1C-C2C-C3C	-2.88	103.96	106.98
19	4	617	CLA	C1C-C2C-C3C	-2.88	103.96	106.98
22	3	506	BCR	C16-C17-C18	2.87	131.31	127.28
19	A	1115	CLA	C3B-C4B-NB	-2.87	107.96	110.53
19	B	1207	CLA	O2A-C1-C2	2.87	119.16	108.11
19	3	610	CLA	C1-C2-C3	-2.87	121.50	126.20
27	4	802	DGD	O1G-C1A-C2A	2.87	120.58	111.83
19	2	603	CLA	O2A-CGA-CBA	2.87	120.58	111.83
19	B	1206	CLA	C1-C2-C3	-2.87	121.50	126.20
19	B	1021	CLA	O2A-C1-C2	2.87	119.14	108.11
19	A	1114	CLA	C3B-C4B-NB	-2.86	107.97	110.53
19	A	1133	CLA	C3B-C4B-NB	-2.86	107.97	110.53
19	A	1110	CLA	C3B-C4B-NB	-2.86	107.97	110.53
22	I	4020	BCR	C23-C22-C21	2.86	123.51	119.01
22	L	4020	BCR	C30-C25-C24	2.86	123.41	115.65
22	B	4004	BCR	C3-C4-C5	-2.86	108.96	114.06
19	B	1224	CLA	O2A-C1-C2	2.86	119.11	108.11
19	A	1137	CLA	O2D-CGD-O1D	-2.86	118.29	123.85
19	L	1503	CLA	C3B-C4B-NB	-2.86	107.98	110.53
19	4	607	CLA	C3B-C4B-NB	-2.86	107.98	110.53
30	2	502	XAT	C31-C30-C29	-2.85	123.28	127.28
22	B	4006	BCR	C23-C22-C21	-2.85	114.52	119.01
19	A	1137	CLA	O2A-C1-C2	2.85	119.09	108.11
19	4	617	CLA	O2A-C1-C2	2.85	119.08	108.11
22	F	4016	BCR	C3-C4-C5	-2.85	108.97	114.06
19	4	609	CLA	O2A-C1-C2	2.85	119.08	108.11
19	A	1013	CLA	C3B-C4B-NB	-2.85	107.99	110.53
19	A	1101	CLA	O2A-C1-C2	2.85	119.07	108.11
19	A	1120	CLA	O2A-C1-C2	2.85	119.07	108.11
22	G	4011	BCR	C16-C17-C18	2.85	131.27	127.28
28	1	501	LUT	C1-C6-C7	2.85	123.37	115.65
29	4	613	CHL	C3C-C4C-NC	-2.84	107.70	114.65
19	B	1203	CLA	C3B-C4B-NB	-2.84	107.99	110.53
19	2	605	CLA	C1C-C2C-C3C	-2.84	103.99	106.98
28	1	501	LUT	C20-C13-C12	2.84	122.43	118.09
25	F	5002	LMG	C8-O7-C10	-2.84	111.00	117.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	1130	CLA	C3B-C4B-NB	-2.84	108.00	110.53
22	I	4020	BCR	C4-C5-C6	-2.84	118.87	122.70
29	1	612	CHL	C1A-CHA-C4D	2.84	123.71	118.98
19	A	1135	CLA	C3B-C4B-NB	-2.83	108.00	110.53
19	B	1237	CLA	O2A-C1-C2	2.83	119.01	108.11
28	4	505	LUT	C15-C14-C13	-2.83	123.31	127.28
19	1	601	CLA	C1-O2A-CGA	2.83	123.50	116.65
22	G	4011	BCR	C3-C4-C5	-2.83	109.01	114.06
19	A	1129	CLA	C3B-C4B-NB	-2.83	108.01	110.53
19	4	603	CLA	C3B-C4B-NB	-2.83	108.01	110.53
22	A	4003	BCR	C35-C13-C12	2.83	122.40	118.09
19	K	1403	CLA	C3B-C4B-NB	-2.83	108.01	110.53
19	F	1301	CLA	O2A-C1-C2	2.82	118.98	108.11
19	B	1219	CLA	C3B-C4B-NB	-2.82	108.01	110.53
19	B	1221	CLA	C3B-C4B-NB	-2.82	108.01	110.53
19	3	617	CLA	CMB-C2B-C1B	2.82	129.72	125.42
19	B	1206	CLA	O2A-C1-C2	2.82	118.97	108.11
22	1	504	BCR	C34-C9-C10	-2.82	118.25	122.82
22	L	4019	BCR	C15-C14-C13	-2.82	123.32	127.28
30	2	502	XAT	O24-C25-C24	2.82	116.13	113.49
22	I	4018	BCR	C33-C5-C4	2.82	119.61	113.60
19	A	1101	CLA	C3B-C4B-NB	-2.82	108.01	110.53
25	G	5001	LMG	C9-C8-C7	-2.82	105.21	111.78
19	A	1129	CLA	C2C-C1C-NC	2.82	112.94	109.98
19	4	605	CLA	O2A-C1-C2	2.82	118.95	108.11
22	F	4016	BCR	C38-C26-C27	2.81	119.60	113.60
28	2	501	LUT	C31-C30-C29	-2.81	123.33	127.28
19	A	1112	CLA	C3B-C4B-NB	-2.81	108.02	110.53
25	B	5007	LMG	O8-C28-C29	2.81	120.41	111.83
22	J	4012	BCR	C28-C27-C26	-2.81	109.04	114.06
19	A	1124	CLA	O2A-C1-C2	2.81	118.93	108.11
22	G	4011	BCR	C28-C27-C26	-2.81	109.04	114.06
19	B	1230	CLA	C4-C3-C5	2.81	120.11	115.23
27	B	5005	DGD	O1G-C1A-C2A	2.81	120.41	111.83
19	A	1121	CLA	C1-O2A-CGA	2.81	123.45	116.65
19	B	1226	CLA	O2D-CGD-O1D	-2.81	118.38	123.85
19	2	604	CLA	C1-C2-C3	-2.81	121.60	126.20
19	A	1127	CLA	C3B-C4B-NB	-2.81	108.02	110.53
19	A	1121	CLA	O2A-CGA-CBA	2.81	120.39	111.83
19	1	605	CLA	C1C-C2C-C3C	-2.81	104.03	106.98
29	3	604	CHL	C3C-C4C-NC	-2.80	107.80	114.65
19	A	1113	CLA	C3B-C4B-NB	-2.80	108.03	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	L	4020	BCR	C34-C9-C8	2.80	122.37	118.09
19	3	602	CLA	C3B-C4B-NB	-2.80	108.03	110.53
19	A	1139	CLA	C1C-C2C-C3C	-2.80	104.03	106.98
19	A	1108	CLA	O2A-C1-C2	2.80	118.87	108.11
19	B	1229	CLA	C3B-C4B-NB	-2.80	108.03	110.53
19	2	605	CLA	C3B-C4B-NB	-2.80	108.03	110.53
22	L	4019	BCR	C3-C4-C5	-2.80	109.07	114.06
19	A	1105	CLA	C3B-C4B-NB	-2.79	108.03	110.53
22	A	4007	BCR	C3-C4-C5	-2.79	109.07	114.06
19	3	606	CLA	O2A-C1-C2	2.79	118.86	108.11
22	K	4001	BCR	C15-C14-C13	-2.79	123.37	127.28
19	K	1403	CLA	C2C-C1C-NC	2.79	112.91	109.98
19	4	604	CLA	C1C-C2C-C3C	-2.79	104.05	106.98
19	A	1117	CLA	O2A-C1-C2	2.79	118.84	108.11
19	B	1207	CLA	C5-C3-C2	2.79	127.42	121.17
22	L	4019	BCR	C37-C22-C23	2.79	122.34	118.09
19	B	1235	CLA	O2A-CGA-CBA	2.78	120.32	111.83
19	H	1701	CLA	O2A-C1-C2	2.78	118.82	108.11
22	K	4002	BCR	C8-C9-C10	2.78	123.39	119.01
19	B	1209	CLA	O2D-CGD-O1D	-2.78	118.43	123.85
22	A	4003	BCR	C31-C1-C6	-2.78	105.88	110.24
19	J	1901	CLA	CMA-C3A-C4A	2.78	119.25	111.77
19	1	605	CLA	O2A-C1-C2	2.78	118.80	108.11
19	3	617	CLA	O2A-C1-C2	2.78	118.80	108.11
19	4	612	CLA	O2A-C1-C2	2.78	118.79	108.11
19	1	611	CLA	C3B-C4B-NB	-2.78	108.05	110.53
19	B	1205	CLA	O2D-CGD-O1D	-2.77	118.45	123.85
19	J	1901	CLA	O2A-C1-C2	2.77	118.78	108.11
19	B	1211	CLA	C3B-C4B-NB	-2.77	108.06	110.53
19	1	608	CLA	O2D-CGD-O1D	-2.77	118.45	123.85
19	A	1122	CLA	CMA-C3A-C4A	2.77	119.22	111.77
22	B	4010	BCR	C28-C27-C26	-2.77	109.11	114.06
19	A	1128	CLA	O2D-CGD-O1D	-2.77	118.46	123.85
19	A	1112	CLA	O2A-C1-C2	2.77	118.77	108.11
22	A	4017	BCR	C28-C27-C26	-2.77	109.12	114.06
19	4	603	CLA	C1C-C2C-C3C	-2.77	104.07	106.98
19	F	1302	CLA	C1C-C2C-C3C	-2.77	104.07	106.98
19	A	1128	CLA	C1-C2-C3	-2.77	121.67	126.20
19	A	1126	CLA	O2A-C1-C2	2.77	118.75	108.11
19	A	1138	CLA	O2A-C1-C2	2.76	118.75	108.11
19	G	1602	CLA	CMA-C3A-C4A	2.76	119.20	111.77
19	4	612	CLA	C3B-C4B-NB	-2.76	108.06	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	1103	CLA	O2D-CGD-O1D	-2.76	118.47	123.85
19	A	1141	CLA	C3B-C4B-NB	-2.76	108.07	110.53
19	1	601	CLA	C3B-C4B-NB	-2.76	108.07	110.53
27	1	803	DGD	O1G-C1A-C2A	2.76	120.24	111.83
19	2	604	CLA	C1C-C2C-C3C	-2.76	104.08	106.98
23	2	801	LHG	O8-C23-C24	2.75	120.23	111.83
19	2	607	CLA	O2D-CGD-O1D	-2.75	118.49	123.85
19	4	617	CLA	C3B-C4B-NB	-2.75	108.07	110.53
18	A	1011	CL0	O2D-CGD-O1D	-2.75	118.49	123.85
19	B	1214	CLA	C3B-C4B-NB	-2.75	108.08	110.53
19	B	1221	CLA	O2D-CGD-O1D	-2.75	118.50	123.85
19	B	1212	CLA	C3B-C4B-NB	-2.75	108.08	110.53
19	A	1125	CLA	CMA-C3A-C4A	2.75	119.16	111.77
19	4	609	CLA	O2D-CGD-O1D	-2.75	118.50	123.85
19	A	1125	CLA	C3B-C4B-NB	-2.75	108.08	110.53
19	2	601	CLA	C1-C2-C3	-2.75	121.70	126.20
22	A	4007	BCR	C28-C27-C26	-2.75	109.16	114.06
28	3	502	LUT	C7-C8-C9	-2.75	122.17	126.23
22	B	4006	BCR	C29-C30-C25	-2.74	106.45	110.44
19	2	603	CLA	C1-C2-C3	-2.74	121.70	126.20
19	A	1138	CLA	C1C-C2C-C3C	-2.74	104.10	106.98
19	1	613	CLA	C2C-C1C-NC	2.74	112.86	109.98
29	2	609	CHL	C4D-CHA-CBD	-2.74	106.20	108.97
19	B	1215	CLA	C3B-C4B-NB	-2.74	108.08	110.53
19	B	1225	CLA	C3B-C4B-NB	-2.74	108.08	110.53
19	2	606	CLA	O2A-C1-C2	2.74	118.65	108.11
19	2	606	CLA	C1C-C2C-C3C	-2.74	104.10	106.98
19	3	601	CLA	C3B-C4B-NB	-2.74	108.09	110.53
22	I	4018	BCR	C15-C14-C13	-2.74	123.44	127.28
19	B	1236	CLA	C1-C2-C3	-2.74	122.34	126.76
19	3	614	CLA	C1C-C2C-C3C	-2.73	104.10	106.98
22	J	4012	BCR	C36-C18-C17	-2.73	118.39	122.82
19	3	605	CLA	O2D-CGD-O1D	-2.73	118.53	123.85
19	B	1207	CLA	O2D-CGD-O1D	-2.73	118.53	123.85
22	J	4012	BCR	C15-C14-C13	-2.73	123.44	127.28
19	B	1225	CLA	CBA-CAA-C2A	2.73	121.92	113.79
22	L	4019	BCR	C37-C22-C21	-2.73	118.39	122.82
18	A	1011	CL0	CBC-CAC-C3C	-2.73	108.97	112.87
28	3	502	LUT	C19-C9-C8	2.73	122.26	118.09
19	1	611	CLA	O2A-C1-C2	2.73	118.61	108.11
19	4	617	CLA	C1D-ND-C4D	-2.73	104.40	106.31
19	A	1120	CLA	C2C-C1C-NC	2.73	112.85	109.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	F	1302	CLA	O2A-C1-C2	2.73	118.61	108.11
19	4	605	CLA	OBD-CAD-C3D	-2.73	122.05	128.42
19	B	1227	CLA	C1-C2-C3	-2.73	121.73	126.20
19	B	1223	CLA	O2A-C1-C2	2.73	118.59	108.11
19	F	1301	CLA	C3B-C4B-NB	-2.72	108.10	110.53
19	K	1401	CLA	C2C-C1C-NC	2.72	112.84	109.98
22	B	4005	BCR	C19-C18-C17	2.72	123.29	119.01
19	A	1132	CLA	CMD-C2D-C3D	-2.72	121.45	127.69
29	2	615	CHL	CMA-C3A-C4A	2.72	120.47	114.61
19	A	1129	CLA	C1C-C2C-C3C	-2.72	104.12	106.98
19	B	1209	CLA	C3B-C4B-NB	-2.72	108.10	110.53
19	A	1119	CLA	C1-O2A-CGA	2.72	123.23	116.65
19	A	1106	CLA	O2D-CGD-O1D	-2.72	118.56	123.85
22	H	4021	BCR	C33-C5-C6	-2.71	121.52	124.48
29	2	613	CHL	C4D-CHA-CBD	-2.71	106.23	108.97
25	A	5006	LMG	O8-C28-C29	2.71	120.11	111.83
19	A	1106	CLA	C3B-C4B-NB	-2.71	108.11	110.53
19	B	1240	CLA	C3B-C4B-NB	-2.71	108.11	110.53
19	B	1205	CLA	O2A-CGA-CBA	2.71	120.10	111.83
19	3	603	CLA	C1C-C2C-C3C	-2.71	104.13	106.98
27	G	5003	DGD	O1G-C1A-C2A	2.71	120.09	111.83
19	A	1118	CLA	O2D-CGD-O1D	-2.71	118.58	123.85
19	B	1235	CLA	C3B-C4B-NB	-2.71	108.11	110.53
22	1	504	BCR	C16-C17-C18	2.71	131.07	127.28
19	B	1217	CLA	O2D-CGD-O1D	-2.70	118.59	123.85
19	A	1109	CLA	C1-O2A-CGA	2.70	123.19	116.65
19	B	1202	CLA	C1C-C2C-C3C	-2.70	104.14	106.98
22	F	4014	BCR	C19-C18-C17	2.70	123.26	119.01
19	L	1503	CLA	C1-O2A-CGA	2.70	123.19	116.65
22	I	4018	BCR	C16-C17-C18	2.70	131.07	127.28
19	1	604	CLA	O2A-C1-C2	2.70	118.50	108.11
22	I	4020	BCR	C36-C18-C17	-2.70	118.44	122.82
22	I	4020	BCR	C37-C22-C21	-2.70	118.44	122.82
19	B	1230	CLA	C3B-C4B-NB	-2.70	108.12	110.53
28	3	501	LUT	C27-C28-C29	-2.70	120.52	126.32
22	B	4005	BCR	C15-C14-C13	-2.70	123.50	127.28
19	B	1240	CLA	O2A-C1-C2	2.70	118.48	108.11
19	3	603	CLA	C2C-C1C-NC	2.70	112.81	109.98
19	A	1140	CLA	O2D-CGD-O1D	-2.69	118.60	123.85
19	A	1112	CLA	C1C-C2C-C3C	-2.69	104.15	106.98
29	3	604	CHL	C1-C2-C3	-2.69	121.78	126.20
19	4	605	CLA	C1C-C2C-C3C	-2.69	104.15	106.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	1238	CLA	C3B-C4B-NB	-2.69	108.13	110.53
19	B	1236	CLA	O2D-CGD-O1D	-2.69	118.61	123.85
19	A	1111	CLA	C3B-C4B-NB	-2.69	108.13	110.53
19	B	1210	CLA	C2C-C1C-NC	2.69	112.81	109.98
19	A	1102	CLA	O2A-CGA-CBA	2.69	120.04	111.83
19	B	1227	CLA	O2D-CGD-O1D	-2.69	118.61	123.85
19	A	1104	CLA	C1C-C2C-C3C	-2.69	104.15	106.98
22	A	4011	BCR	C39-C30-C25	-2.69	106.03	110.24
19	B	1226	CLA	C1C-C2C-C3C	-2.69	104.15	106.98
29	4	613	CHL	C1-O2A-CGA	2.69	123.15	116.65
19	A	1012	CLA	O2A-C1-C2	2.69	118.45	108.11
19	B	1206	CLA	C3B-C4B-NB	-2.69	108.13	110.53
22	A	4002	BCR	C7-C6-C5	2.69	127.74	121.56
19	1	605	CLA	C2C-C1C-NC	2.68	112.80	109.98
19	4	612	CLA	C2C-C1C-NC	2.68	112.80	109.98
19	A	1135	CLA	C1C-C2C-C3C	-2.68	104.16	106.98
22	A	4007	BCR	C16-C17-C18	2.68	131.04	127.28
22	3	506	BCR	C38-C26-C27	2.68	119.32	113.60
25	2	804	LMG	O8-C28-C29	2.68	120.01	111.83
19	B	1204	CLA	C2C-C1C-NC	2.68	112.80	109.98
19	B	1023	CLA	C3B-C4B-NB	-2.68	108.14	110.53
19	1	606	CLA	C1-C2-C3	-2.68	122.43	126.76
19	A	1105	CLA	O2D-CGD-O1D	-2.68	118.63	123.85
19	4	605	CLA	CHA-C4D-ND	2.68	138.08	132.55
22	I	4020	BCR	C34-C9-C8	2.68	122.18	118.09
19	G	1603	CLA	O2D-CGD-O1D	-2.68	118.64	123.85
25	3	802	LMG	O8-C28-C29	2.68	119.99	111.83
19	B	1227	CLA	C1C-C2C-C3C	-2.68	104.17	106.98
29	2	610	CHL	C1-O2A-CGA	2.67	123.12	116.65
19	A	1107	CLA	C3B-C4B-NB	-2.67	108.14	110.53
19	3	603	CLA	C1-O2A-CGA	2.67	123.12	116.65
19	B	1235	CLA	O2A-C1-C2	2.67	118.40	108.11
23	A	5002	LHG	C5-O7-C7	-2.67	111.40	117.80
19	B	1202	CLA	O2D-CGD-O1D	-2.67	118.64	123.85
22	J	4012	BCR	C33-C5-C6	-2.67	121.57	124.48
19	A	1114	CLA	C1C-C2C-C3C	-2.67	104.17	106.98
19	B	1210	CLA	O2D-CGD-O1D	-2.67	118.65	123.85
28	2	501	LUT	C37-C21-C36	2.67	111.76	107.87
19	3	612	CLA	C1C-C2C-C3C	-2.67	104.17	106.98
28	2	501	LUT	C40-C33-C32	2.67	122.16	118.09
22	A	4008	BCR	C37-C22-C23	2.67	122.16	118.09
19	A	1132	CLA	C1C-C2C-C3C	-2.67	104.18	106.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	F	4016	BCR	C31-C1-C6	-2.67	106.06	110.24
19	3	617	CLA	C2C-C1C-NC	2.66	112.78	109.98
19	4	608	CLA	CMD-C2D-C3D	-2.66	121.59	127.69
19	A	1120	CLA	C1C-C2C-C3C	-2.66	104.18	106.98
19	A	1123	CLA	C2C-C1C-NC	2.66	112.77	109.98
19	K	1402	CLA	O2A-CGA-CBA	2.66	119.94	111.83
19	4	606	CLA	C3B-C4B-NB	-2.66	108.16	110.53
19	A	1116	CLA	O2D-CGD-O1D	-2.66	118.68	123.85
24	B	5008	LMT	C3'-C4'-C5'	-2.66	105.04	110.93
19	B	1216	CLA	C1-O2A-CGA	2.66	123.08	116.65
23	1	801	LHG	O8-C23-C24	2.65	119.93	111.83
22	I	4018	BCR	C34-C9-C8	2.65	122.14	118.09
28	1	502	LUT	C30-C31-C32	-2.65	115.51	123.20
19	1	605	CLA	C3B-C4B-NB	-2.65	108.16	110.53
22	B	4006	BCR	C3-C4-C5	-2.65	109.32	114.06
22	L	4019	BCR	C30-C25-C24	2.65	122.84	115.65
19	B	1214	CLA	C2C-C1C-NC	2.65	112.77	109.98
19	B	1226	CLA	C2C-C1C-NC	2.65	112.77	109.98
19	A	1138	CLA	C1-C2-C3	-2.65	121.85	126.20
19	A	1132	CLA	O2D-CGD-O1D	-2.65	118.69	123.85
19	B	1222	CLA	O2D-CGD-O1D	-2.65	118.69	123.85
22	2	503	BCR	C1-C6-C7	2.65	122.84	115.65
19	A	1118	CLA	C3B-C4B-NB	-2.65	108.17	110.53
19	1	613	CLA	C3B-C4B-NB	-2.65	108.17	110.53
22	1	504	BCR	C36-C18-C17	-2.65	118.52	122.82
19	A	1135	CLA	C2C-C1C-NC	2.65	112.76	109.98
24	2	808	LMT	C3'-C4'-C5'	-2.65	105.06	110.93
25	F	5003	LMG	O8-C28-C29	2.65	119.91	111.83
19	A	1107	CLA	C2C-C1C-NC	2.65	112.76	109.98
23	B	5002	LHG	O8-C23-C24	2.65	119.91	111.83
22	G	4011	BCR	C36-C18-C17	-2.64	118.53	122.82
22	A	4008	BCR	C35-C13-C12	2.64	122.12	118.09
19	4	601	CLA	O2A-CGA-CBA	2.64	119.89	111.83
19	B	1212	CLA	O2D-CGD-O1D	-2.64	118.71	123.85
19	3	605	CLA	CHA-C4D-ND	2.64	138.00	132.55
19	B	1223	CLA	CHA-C4D-ND	2.64	138.00	132.55
19	A	1107	CLA	C1C-C2C-C3C	-2.64	104.20	106.98
19	K	1401	CLA	CMD-C2D-C3D	-2.64	121.64	127.69
22	I	4018	BCR	C35-C13-C14	-2.64	118.54	122.82
22	B	4010	BCR	C1-C6-C7	2.64	122.81	115.65
19	B	1021	CLA	C2C-C1C-NC	2.64	112.75	109.98
28	1	501	LUT	C7-C8-C9	-2.64	122.33	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	2	612	CLA	C1C-C2C-C3C	-2.64	104.21	106.98
19	2	604	CLA	C2C-C1C-NC	2.64	112.75	109.98
19	4	612	CLA	C1C-C2C-C3C	-2.64	104.21	106.98
19	L	1501	CLA	O2D-CGD-O1D	-2.64	118.72	123.85
19	A	1114	CLA	C2C-C1C-NC	2.64	112.75	109.98
25	G	5006	LMG	O7-C10-C11	2.63	120.61	110.93
19	B	1218	CLA	C1-C2-C3	-2.63	121.88	126.20
19	G	1603	CLA	C3B-C4B-NB	-2.63	108.18	110.53
19	A	1013	CLA	O2D-CGD-O1D	-2.63	118.72	123.85
19	A	1112	CLA	O2D-CGD-O1D	-2.63	118.72	123.85
19	B	1206	CLA	C1C-C2C-C3C	-2.63	104.21	106.98
28	2	501	LUT	C39-C29-C28	2.63	122.11	118.09
19	A	1122	CLA	O2A-CGA-CBA	2.63	119.86	111.83
19	B	1236	CLA	C3B-C4B-NB	-2.63	108.18	110.53
19	A	1134	CLA	O2A-C1-C2	2.63	118.23	108.11
22	A	4003	BCR	C7-C6-C5	-2.63	115.50	121.56
28	3	501	LUT	C17-C1-C6	-2.63	106.12	110.24
19	B	1229	CLA	O2D-CGD-O1D	-2.63	118.73	123.85
19	3	603	CLA	O2A-CGA-CBA	2.63	119.85	111.83
19	B	1214	CLA	C1C-C2C-C3C	-2.63	104.22	106.98
22	A	4003	BCR	C37-C22-C21	-2.63	118.56	122.82
22	G	4011	BCR	C4-C5-C6	-2.63	119.16	122.70
19	A	1141	CLA	C1C-C2C-C3C	-2.62	104.22	106.98
19	A	1105	CLA	C2C-C1C-NC	2.62	112.74	109.98
22	B	4010	BCR	C34-C9-C8	2.62	122.09	118.09
19	B	1218	CLA	O1D-CGD-CBD	-2.62	119.35	124.52
19	G	1601	CLA	C1-C2-C3	-2.62	121.91	126.20
19	B	1234	CLA	C2C-C1C-NC	2.62	112.73	109.98
19	B	1210	CLA	C6-C5-C3	-2.62	107.09	113.47
19	A	1117	CLA	C3B-C4B-NB	-2.62	108.19	110.53
22	A	4007	BCR	C33-C5-C6	-2.62	121.63	124.48
19	B	1204	CLA	O2D-CGD-O1D	-2.62	118.76	123.85
27	3	803	DGD	O1G-C1A-C2A	2.61	119.81	111.83
22	F	4014	BCR	C34-C9-C10	-2.61	118.58	122.82
19	F	1302	CLA	C2C-C1C-NC	2.61	112.73	109.98
19	B	1211	CLA	O2D-CGD-O1D	-2.61	118.76	123.85
28	1	501	LUT	C35-C34-C33	-2.61	123.61	127.28
19	4	604	CLA	C2C-C1C-NC	2.61	112.72	109.98
19	B	1229	CLA	C1C-C2C-C3C	-2.61	104.23	106.98
19	A	1130	CLA	O2D-CGD-O1D	-2.61	118.77	123.85
22	A	4003	BCR	C37-C22-C23	2.61	122.07	118.09
19	3	605	CLA	C2C-C1C-NC	2.61	112.72	109.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	1123	CLA	O2A-C1-C2	2.61	118.14	108.11
19	B	1204	CLA	C1C-C2C-C3C	-2.61	104.24	106.98
19	G	1602	CLA	O2D-CGD-O1D	-2.61	118.78	123.85
19	1	611	CLA	C1C-C2C-C3C	-2.61	104.24	106.98
30	4	502	XAT	O24-C26-C27	-2.61	109.41	116.88
29	3	604	CHL	CMA-C3A-C4A	2.61	120.22	114.61
19	A	1122	CLA	CMD-C2D-C3D	-2.60	121.72	127.69
19	A	1123	CLA	C3B-C4B-NB	-2.60	108.20	110.53
19	4	607	CLA	C1C-C2C-C3C	-2.60	104.24	106.98
19	L	1502	CLA	O2D-CGD-O1D	-2.60	118.78	123.85
19	2	612	CLA	C3B-C4B-NB	-2.60	108.21	110.53
22	A	4007	BCR	C36-C18-C17	-2.60	118.60	122.82
19	A	1110	CLA	O2D-CGD-O1D	-2.60	118.78	123.85
19	3	602	CLA	O2D-CGD-O1D	-2.60	118.79	123.85
19	B	1231	CLA	C1C-C2C-C3C	-2.60	104.25	106.98
19	B	1206	CLA	C2C-C1C-NC	2.60	112.71	109.98
19	B	1237	CLA	O2A-CGA-CBA	2.60	119.76	111.83
19	G	1601	CLA	C3B-C4B-NB	-2.60	108.21	110.53
22	B	4010	BCR	C34-C9-C10	-2.60	118.60	122.82
19	A	1131	CLA	O2D-CGD-O1D	-2.60	118.79	123.85
22	A	4008	BCR	C23-C24-C25	-2.60	120.06	127.00
19	B	1231	CLA	C2C-C1C-NC	2.60	112.71	109.98
22	A	4008	BCR	C28-C27-C26	-2.60	109.42	114.06
19	3	612	CLA	C3B-C4B-NB	-2.60	108.21	110.53
19	B	1223	CLA	OBD-CAD-C3D	-2.60	122.35	128.42
19	1	604	CLA	O2A-CGA-CBA	2.60	119.75	111.83
30	4	502	XAT	C19-C9-C8	2.60	122.05	118.09
19	B	1239	CLA	O2D-CGD-O1D	-2.60	118.80	123.85
19	A	1117	CLA	C1C-C2C-C3C	-2.60	104.25	106.98
19	A	1104	CLA	O2D-CGD-O1D	-2.60	118.80	123.85
23	A	5001	LHG	O8-C23-C24	2.59	119.75	111.83
22	B	4010	BCR	C15-C14-C13	-2.59	123.64	127.28
19	3	607	CLA	O2D-CGD-O1D	-2.59	118.80	123.85
19	B	1218	CLA	O2D-CGD-O1D	-2.59	118.80	123.85
19	B	1218	CLA	O2A-C1-C2	2.59	118.09	108.11
25	F	5002	LMG	O8-C28-C29	2.59	119.74	111.83
19	A	1118	CLA	C2C-C1C-NC	2.59	112.70	109.98
18	A	1011	CL0	O1D-CGD-CBD	-2.59	120.79	124.72
19	B	1206	CLA	O2D-CGD-O1D	-2.59	118.80	123.85
28	J	4013	LUT	C20-C13-C12	2.59	122.05	118.09
19	B	1229	CLA	C2C-C1C-NC	2.59	112.70	109.98
19	2	605	CLA	C2C-C1C-NC	2.59	112.70	109.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	1134	CLA	O2D-CGD-O1D	-2.59	118.81	123.85
19	A	1114	CLA	O2D-CGD-O1D	-2.59	118.81	123.85
19	3	610	CLA	C3B-C4B-NB	-2.59	108.22	110.53
19	B	1228	CLA	O2D-CGD-O1D	-2.59	118.81	123.85
19	B	1237	CLA	C1C-C2C-C3C	-2.59	104.26	106.98
19	1	613	CLA	C1C-C2C-C3C	-2.59	104.26	106.98
19	A	1130	CLA	C1C-C2C-C3C	-2.59	104.26	106.98
19	B	1224	CLA	C1C-C2C-C3C	-2.59	104.26	106.98
28	4	505	LUT	C22-C23-C24	-2.59	107.34	111.18
19	B	1232	CLA	C1C-C2C-C3C	-2.59	104.26	106.98
19	B	1216	CLA	C1C-C2C-C3C	-2.58	104.26	106.98
22	H	4021	BCR	C36-C18-C17	-2.58	118.63	122.82
19	G	1603	CLA	C1C-C2C-C3C	-2.58	104.26	106.98
19	A	1012	CLA	C2C-C1C-NC	2.58	112.69	109.98
25	F	5004	LMG	O8-C28-C29	2.58	119.71	111.83
19	B	1212	CLA	C1C-C2C-C3C	-2.58	104.27	106.98
30	2	502	XAT	C38-C25-C26	-2.58	118.06	122.30
19	B	1210	CLA	O2A-CGA-CBA	2.58	119.70	111.83
22	1	504	BCR	C3-C4-C5	-2.58	109.46	114.06
19	B	1215	CLA	O2D-CGD-O1D	-2.58	118.83	123.85
19	A	1131	CLA	C1-C2-C3	-2.58	121.97	126.20
19	B	1224	CLA	O2D-CGD-O1D	-2.58	118.83	123.85
19	B	1239	CLA	C1C-C2C-C3C	-2.58	104.27	106.98
22	A	4003	BCR	C8-C9-C10	2.58	123.06	119.01
25	A	5006	LMG	C8-O7-C10	-2.58	111.63	117.80
22	H	4021	BCR	C3-C4-C5	-2.57	109.47	114.06
19	A	1125	CLA	O2D-CGD-O1D	-2.57	118.84	123.85
22	B	4006	BCR	C28-C27-C26	-2.57	109.47	114.06
19	B	1213	CLA	O2D-CGD-O1D	-2.57	118.84	123.85
19	B	1232	CLA	C2C-C1C-NC	2.57	112.68	109.98
19	A	1135	CLA	O2D-CGD-O1D	-2.57	118.85	123.85
19	B	1021	CLA	CHA-C4D-ND	2.57	137.85	132.55
19	A	1115	CLA	O2D-CGD-O1D	-2.57	118.85	123.85
19	4	617	CLA	O2D-CGD-O1D	-2.57	118.85	123.85
19	A	1124	CLA	CMA-C3A-C4A	2.57	118.67	111.77
22	2	503	BCR	C30-C25-C26	2.57	126.14	122.64
22	A	4011	BCR	C28-C27-C26	-2.57	109.48	114.06
19	3	605	CLA	C1C-C2C-C3C	-2.56	104.28	106.98
19	A	1107	CLA	O2D-CGD-O1D	-2.56	118.86	123.85
28	3	502	LUT	C35-C15-C14	-2.56	118.28	123.52
19	K	1403	CLA	C1C-C2C-C3C	-2.56	104.28	106.98
19	2	605	CLA	O2D-CGD-O1D	-2.56	118.86	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	1136	CLA	O2D-CGD-O1D	-2.56	118.86	123.85
19	F	1301	CLA	C1C-C2C-C3C	-2.56	104.29	106.98
19	A	1127	CLA	O2D-CGD-O1D	-2.56	118.87	123.85
19	B	1021	CLA	O1D-CGD-CBD	-2.56	119.47	124.52
19	B	1022	CLA	C1C-C2C-C3C	-2.56	104.29	106.98
25	G	5002	LMG	O8-C28-C29	2.56	119.63	111.83
19	B	1224	CLA	C3B-C4B-NB	-2.56	108.25	110.53
29	4	613	CHL	C4D-CHA-CBD	-2.56	106.39	108.97
19	A	1012	CLA	O2A-CGA-CBA	2.56	119.63	111.83
19	A	1140	CLA	O2A-CGA-CBA	2.56	119.63	111.83
19	A	1132	CLA	C1-C2-C3	-2.55	122.01	126.20
19	B	1226	CLA	O1D-CGD-CBD	-2.55	119.48	124.52
28	J	4013	LUT	C38-C25-C24	-2.55	117.31	123.36
19	B	1239	CLA	C2C-C1C-NC	2.55	112.67	109.98
19	A	1123	CLA	C1C-C2C-C3C	-2.55	104.30	106.98
19	1	601	CLA	C2C-C1C-NC	2.55	112.66	109.98
19	2	608	CLA	CMD-C2D-C3D	-2.55	121.84	127.69
19	L	1501	CLA	C1C-C2C-C3C	-2.55	104.30	106.98
19	1	614	CLA	O2D-CGD-O1D	-2.55	118.89	123.85
28	1	502	LUT	C15-C35-C34	-2.55	118.30	123.52
22	L	4020	BCR	C29-C30-C25	-2.55	106.74	110.44
19	3	601	CLA	C1C-C2C-C3C	-2.55	104.30	106.98
19	B	1238	CLA	O2A-CGA-CBA	2.55	119.61	111.83
19	A	1115	CLA	C1-C2-C3	-2.55	122.02	126.20
19	B	1235	CLA	C1C-C2C-C3C	-2.55	104.30	106.98
19	A	1120	CLA	C3B-C4B-NB	-2.55	108.26	110.53
19	A	1012	CLA	C1C-C2C-C3C	-2.55	104.30	106.98
19	B	1203	CLA	C1C-C2C-C3C	-2.55	104.30	106.98
19	A	1123	CLA	O2D-CGD-O1D	-2.55	118.89	123.85
19	A	1102	CLA	O1D-CGD-CBD	-2.55	119.50	124.52
19	A	1117	CLA	O2A-CGA-CBA	2.55	119.59	111.83
29	4	610	CHL	CMA-C3A-C4A	2.54	120.09	114.61
19	3	608	CLA	C2C-C1C-NC	2.54	112.65	109.98
19	B	1022	CLA	O2D-CGD-O1D	-2.54	118.90	123.85
29	2	610	CHL	CMA-C3A-C4A	2.54	120.09	114.61
22	B	4004	BCR	C4-C5-C6	-2.54	119.27	122.70
29	4	615	CHL	C4D-CHA-CBD	-2.54	106.41	108.97
19	1	607	CLA	C1C-C2C-C3C	-2.54	104.31	106.98
19	4	601	CLA	C2C-C1C-NC	2.54	112.65	109.98
24	G	5004	LMT	C3'-C4'-C5'	-2.54	105.30	110.93
22	I	4020	BCR	C3-C4-C5	-2.54	109.53	114.06
19	A	1105	CLA	C1C-C2C-C3C	-2.54	104.31	106.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	1128	CLA	C1C-C2C-C3C	-2.54	104.31	106.98
29	1	609	CHL	C4D-CHA-CBD	-2.54	106.41	108.97
19	B	1214	CLA	O2A-CGA-CBA	2.54	119.57	111.83
19	1	607	CLA	C2C-C1C-NC	2.54	112.65	109.98
19	A	1119	CLA	C2C-C1C-NC	2.54	112.64	109.98
19	B	1240	CLA	C2C-C1C-NC	2.54	112.64	109.98
19	1	606	CLA	C3B-C4B-NB	-2.54	108.27	110.53
19	B	1223	CLA	C1C-C2C-C3C	-2.53	104.31	106.98
22	3	506	BCR	C3-C4-C5	-2.53	109.54	114.06
19	B	1203	CLA	O2D-CGD-O1D	-2.53	118.92	123.85
19	4	603	CLA	C2C-C1C-NC	2.53	112.64	109.98
19	3	612	CLA	O2A-CGA-CBA	2.53	119.56	111.83
19	H	1701	CLA	C1C-C2C-C3C	-2.53	104.32	106.98
19	2	601	CLA	C1C-C2C-C3C	-2.53	104.32	106.98
19	B	1231	CLA	C3B-C4B-NB	-2.53	108.27	110.53
19	B	1240	CLA	O2D-CGD-O1D	-2.53	118.92	123.85
19	A	1103	CLA	C1C-C2C-C3C	-2.53	104.32	106.98
19	1	601	CLA	C1C-C2C-C3C	-2.53	104.32	106.98
19	B	1234	CLA	C3B-C4B-NB	-2.53	108.27	110.53
22	B	4009	BCR	C30-C25-C26	-2.53	119.18	122.64
19	A	1012	CLA	CHA-C4D-ND	2.53	137.77	132.55
19	G	1601	CLA	C1C-C2C-C3C	-2.53	104.32	106.98
19	1	603	CLA	C2C-C1C-NC	2.53	112.64	109.98
19	B	1237	CLA	O2D-CGD-O1D	-2.53	118.93	123.85
25	2	803	LMG	O8-C28-C29	2.53	119.54	111.83
19	B	1235	CLA	O2D-CGD-O1D	-2.53	118.93	123.85
22	A	4008	BCR	C37-C22-C21	-2.53	118.72	122.82
19	A	1125	CLA	C1C-C2C-C3C	-2.53	104.32	106.98
19	1	606	CLA	C2C-C1C-NC	2.52	112.63	109.98
28	4	501	LUT	C39-C29-C28	2.52	121.94	118.09
19	B	1021	CLA	C1-C2-C3	-2.52	122.06	126.20
19	2	605	CLA	C1-C2-C3	-2.52	122.06	126.20
19	1	603	CLA	C1C-C2C-C3C	-2.52	104.33	106.98
19	2	612	CLA	O2D-CGD-O1D	-2.52	118.94	123.85
19	1	606	CLA	C1C-C2C-C3C	-2.52	104.33	106.98
28	3	502	LUT	C10-C11-C12	-2.52	115.90	123.20
19	A	1131	CLA	C1C-C2C-C3C	-2.52	104.33	106.98
19	A	1109	CLA	CMD-C2D-C3D	-2.52	121.91	127.69
19	1	608	CLA	C1C-C2C-C3C	-2.52	104.33	106.98
19	H	1701	CLA	C3B-C4B-NB	-2.52	108.28	110.53
19	2	606	CLA	C3B-C4B-NB	-2.52	108.28	110.53
28	4	505	LUT	C7-C6-C5	-2.52	115.76	121.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	1230	CLA	O2A-CGA-CBA	2.52	119.51	111.83
19	B	1220	CLA	O2D-CGD-O1D	-2.52	118.95	123.85
19	1	607	CLA	O2D-CGD-O1D	-2.52	118.95	123.85
19	A	1111	CLA	O2D-CGD-O1D	-2.52	118.95	123.85
19	2	607	CLA	CHA-C4D-ND	2.52	137.74	132.55
19	B	1021	CLA	C6-C5-C3	-2.52	107.34	113.47
19	A	1117	CLA	O2D-CGD-O1D	-2.52	118.95	123.85
19	B	1226	CLA	C3B-C4B-NB	-2.51	108.28	110.53
19	B	1023	CLA	C1-O2A-CGA	2.51	122.74	116.65
19	K	1403	CLA	CHA-C4D-ND	2.51	137.74	132.55
19	B	1216	CLA	C2C-C1C-NC	2.51	112.62	109.98
19	B	1221	CLA	O2A-CGA-CBA	2.51	119.50	111.83
19	L	1503	CLA	C1C-C2C-C3C	-2.51	104.34	106.98
19	B	1225	CLA	O2D-CGD-O1D	-2.51	118.95	123.85
19	F	1301	CLA	C2C-C1C-NC	2.51	112.62	109.98
22	2	503	BCR	C34-C9-C10	-2.51	118.74	122.82
19	3	610	CLA	O2D-CGD-O1D	-2.51	118.96	123.85
22	A	4002	BCR	C38-C26-C27	2.51	118.95	113.60
19	B	1234	CLA	C1C-C2C-C3C	-2.51	104.34	106.98
19	4	612	CLA	O2A-CGA-CBA	2.51	119.49	111.83
22	1	503	BCR	C19-C18-C17	2.51	122.96	119.01
19	4	603	CLA	C5-C3-C2	2.51	126.80	121.17
22	2	503	BCR	C40-C30-C39	2.51	115.82	108.63
22	K	4002	BCR	C36-C18-C17	-2.51	118.75	122.82
19	L	1503	CLA	C1D-ND-C4D	-2.51	104.55	106.31
22	K	4002	BCR	C12-C13-C14	-2.51	115.06	119.01
19	A	1118	CLA	C1C-C2C-C3C	-2.51	104.34	106.98
19	A	1113	CLA	C1C-C2C-C3C	-2.51	104.34	106.98
19	G	1601	CLA	C2C-C1C-NC	2.51	112.62	109.98
19	B	1211	CLA	C1C-C2C-C3C	-2.51	104.34	106.98
19	B	1238	CLA	C1C-C2C-C3C	-2.51	104.34	106.98
29	3	611	CHL	CMA-C3A-C4A	2.51	120.01	114.61
19	A	1122	CLA	CHD-C1D-ND	-2.51	121.28	124.80
19	3	607	CLA	C1-C2-C3	-2.51	122.09	126.20
19	1	608	CLA	C2C-C1C-NC	2.51	112.61	109.98
19	1	603	CLA	CHA-C4D-ND	2.51	137.72	132.55
19	B	1230	CLA	O2D-CGD-O1D	-2.51	118.97	123.85
19	A	1115	CLA	C1C-C2C-C3C	-2.50	104.35	106.98
19	G	1601	CLA	O2D-CGD-O1D	-2.50	118.97	123.85
19	A	1126	CLA	C6-C5-C3	-2.50	107.37	113.47
19	B	1221	CLA	C1C-C2C-C3C	-2.50	104.35	106.98
19	3	607	CLA	C1C-C2C-C3C	-2.50	104.35	106.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	3	607	CLA	C2C-C1C-NC	2.50	112.61	109.98
19	2	608	CLA	C1-O2A-CGA	2.50	122.71	116.65
22	A	4003	BCR	C30-C25-C26	-2.50	119.22	122.64
19	L	1503	CLA	CMD-C2D-C3D	-2.50	121.95	127.69
19	3	617	CLA	CHA-C4D-ND	2.50	137.71	132.55
19	A	1117	CLA	C2C-C1C-NC	2.50	112.61	109.98
28	3	501	LUT	C22-C23-C24	-2.50	107.47	111.18
19	B	1209	CLA	C1C-C2C-C3C	-2.50	104.35	106.98
19	A	1126	CLA	O2D-CGD-O1D	-2.50	118.98	123.85
19	A	1138	CLA	C2C-C1C-NC	2.50	112.61	109.98
19	2	608	CLA	O2D-CGD-O1D	-2.50	118.98	123.85
19	3	617	CLA	O2D-CGD-O1D	-2.50	118.98	123.85
19	1	608	CLA	CHA-C4D-ND	2.50	137.70	132.55
19	K	1402	CLA	O2D-CGD-O1D	-2.50	118.99	123.85
19	B	1215	CLA	C1C-C2C-C3C	-2.50	104.35	106.98
19	A	1126	CLA	C2C-C1C-NC	2.50	112.61	109.98
19	B	1222	CLA	C3B-C4B-NB	-2.50	108.30	110.53
19	B	1208	CLA	O2D-CGD-O1D	-2.50	118.99	123.85
19	B	1234	CLA	O2D-CGD-O1D	-2.50	118.99	123.85
22	L	4019	BCR	C29-C30-C25	2.50	114.06	110.44
19	A	1136	CLA	C1C-C2C-C3C	-2.49	104.36	106.98
19	2	604	CLA	O2D-CGD-O1D	-2.49	118.99	123.85
19	4	601	CLA	CMD-C2D-C3D	-2.49	121.97	127.69
28	1	502	LUT	C35-C34-C33	-2.49	123.78	127.28
19	A	1127	CLA	O2A-CGA-CBA	2.49	119.44	111.83
19	A	1121	CLA	C1D-ND-C4D	-2.49	104.56	106.31
19	B	1209	CLA	CMD-C2D-C3D	-2.49	121.97	127.69
28	4	501	LUT	C40-C33-C32	2.49	121.90	118.09
19	B	1216	CLA	O2D-CGD-O1D	-2.49	119.00	123.85
19	3	601	CLA	C2C-C1C-NC	2.49	112.60	109.98
28	1	501	LUT	C37-C21-C36	2.49	111.50	107.87
22	B	4009	BCR	C3-C4-C5	-2.49	109.61	114.06
19	A	1124	CLA	C2C-C1C-NC	2.49	112.60	109.98
19	A	1103	CLA	C3B-C4B-NB	-2.49	108.31	110.53
19	4	609	CLA	C2C-C1C-NC	2.49	112.60	109.98
19	A	1129	CLA	O2A-CGA-CBA	2.49	119.43	111.83
19	L	1503	CLA	CMA-C3A-C4A	2.49	118.47	111.77
22	H	4021	BCR	C1-C6-C7	2.49	122.40	115.65
19	A	1120	CLA	O2D-CGD-O1D	-2.49	119.00	123.85
29	2	611	CHL	CMA-C3A-C4A	2.49	119.97	114.61
19	K	1404	CLA	C2C-C1C-NC	2.49	112.59	109.98
22	1	504	BCR	C37-C22-C21	-2.49	118.79	122.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	1021	CLA	C3B-C4B-NB	-2.49	108.31	110.53
19	B	1213	CLA	C3B-C4B-NB	-2.48	108.31	110.53
19	A	1133	CLA	C1C-C2C-C3C	-2.48	104.37	106.98
19	G	1602	CLA	C1C-C2C-C3C	-2.48	104.37	106.98
19	B	1232	CLA	C1-C2-C3	-2.48	122.13	126.20
28	2	501	LUT	C20-C13-C14	-2.48	118.80	122.82
19	3	606	CLA	C1C-C2C-C3C	-2.48	104.37	106.98
19	B	1219	CLA	C1C-C2C-C3C	-2.48	104.37	106.98
19	3	617	CLA	C1C-C2C-C3C	-2.48	104.37	106.98
19	B	1223	CLA	O2A-CGA-CBA	2.48	119.39	111.83
19	1	606	CLA	O2D-CGD-O1D	-2.48	119.02	123.85
19	B	1224	CLA	C2C-C1C-NC	2.48	112.59	109.98
19	B	1022	CLA	C1-C2-C3	-2.48	122.14	126.20
19	1	611	CLA	O2D-CGD-O1D	-2.48	119.03	123.85
19	B	1214	CLA	CHA-C4D-ND	2.48	137.66	132.55
19	3	610	CLA	C1C-C2C-C3C	-2.48	104.38	106.98
19	4	612	CLA	O2D-CGD-O1D	-2.48	119.03	123.85
19	A	1124	CLA	O2A-CGA-CBA	2.48	119.39	111.83
19	A	1121	CLA	C2D-C1D-ND	2.48	112.58	110.13
19	A	1106	CLA	C1C-C2C-C3C	-2.47	104.38	106.98
19	A	1113	CLA	O2D-CGD-O1D	-2.47	119.03	123.85
19	A	1013	CLA	C1C-C2C-C3C	-2.47	104.38	106.98
19	A	1122	CLA	C1C-C2C-C3C	-2.47	104.38	106.98
19	L	1503	CLA	O2D-CGD-O1D	-2.47	119.04	123.85
28	3	501	LUT	C37-C21-C22	-2.47	104.80	109.41
19	A	1134	CLA	C1C-C2C-C3C	-2.47	104.38	106.98
19	1	604	CLA	C1C-C2C-C3C	-2.47	104.38	106.98
19	A	1119	CLA	O2D-CGD-O1D	-2.47	119.04	123.85
19	3	606	CLA	C3B-C4B-NB	-2.47	108.33	110.53
19	B	1224	CLA	CHA-C4D-ND	2.47	137.65	132.55
19	4	609	CLA	C1C-C2C-C3C	-2.47	104.38	106.98
28	3	502	LUT	C35-C34-C33	-2.47	123.82	127.28
19	B	1231	CLA	O2D-CGD-O1D	-2.47	119.04	123.85
28	J	4013	LUT	C27-C28-C29	-2.47	121.02	126.32
19	1	605	CLA	CMD-C2D-C3D	-2.47	122.03	127.69
19	A	1132	CLA	CHA-C4D-ND	2.47	137.64	132.55
19	A	1119	CLA	C1C-C2C-C3C	-2.47	104.39	106.98
19	B	1225	CLA	C2C-C1C-NC	2.47	112.57	109.98
19	A	1119	CLA	CMD-C2D-C3D	-2.47	122.03	127.69
19	L	1501	CLA	CMA-C3A-C4A	2.46	118.40	111.77
19	3	608	CLA	C1C-C2C-C3C	-2.46	104.39	106.98
19	B	1217	CLA	C1C-C2C-C3C	-2.46	104.39	106.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	3	506	BCR	C1-C6-C7	2.46	122.33	115.65
22	J	4012	BCR	C38-C26-C25	2.46	127.17	124.48
19	A	1122	CLA	C1-C2-C3	-2.46	122.16	126.20
22	B	4006	BCR	C37-C22-C23	2.46	121.85	118.09
19	4	604	CLA	O2A-CGA-CBA	2.46	119.34	111.83
19	4	608	CLA	C1C-C2C-C3C	-2.46	104.39	106.98
22	A	4011	BCR	C34-C9-C10	-2.46	118.83	122.82
19	B	1214	CLA	C1-C2-C3	-2.46	122.17	126.20
19	J	1901	CLA	C2C-C1C-NC	2.46	112.56	109.98
29	3	604	CHL	C4D-CHA-CBD	-2.46	106.49	108.97
19	2	602	CLA	C1C-C2C-C3C	-2.46	104.39	106.98
19	4	606	CLA	C1C-C2C-C3C	-2.46	104.39	106.98
29	1	612	CHL	C4D-CHA-CBD	-2.46	106.49	108.97
19	2	605	CLA	CHA-C4D-ND	2.46	137.62	132.55
22	K	4002	BCR	C19-C18-C17	2.46	122.87	119.01
19	B	1222	CLA	CHA-C4D-ND	2.46	137.62	132.55
27	4	802	DGD	O3G-C1D-C2D	2.46	112.00	108.27
19	1	604	CLA	O2D-CGD-O1D	-2.46	119.07	123.85
19	A	1134	CLA	CHA-C4D-ND	2.46	137.62	132.55
19	4	603	CLA	C1-O2A-CGA	2.46	122.59	116.65
19	B	1220	CLA	O2A-CGA-CBA	2.46	119.32	111.83
28	3	501	LUT	C3-C4-C5	-2.46	106.06	112.18
22	F	4016	BCR	C34-C9-C10	-2.45	118.84	122.82
19	4	608	CLA	O2D-CGD-O1D	-2.45	119.07	123.85
19	K	1401	CLA	O2D-CGD-O1D	-2.45	119.07	123.85
19	B	1022	CLA	CHA-C4D-ND	2.45	137.61	132.55
22	B	4010	BCR	C3-C4-C5	-2.45	109.68	114.06
22	3	506	BCR	C36-C18-C17	-2.45	118.85	122.82
19	3	613	CLA	CMA-C3A-C4A	2.45	118.36	111.77
19	4	601	CLA	C1C-C2C-C3C	-2.45	104.40	106.98
19	4	609	CLA	CHA-C4D-ND	2.45	137.60	132.55
19	B	1219	CLA	C2C-C1C-NC	2.45	112.56	109.98
19	1	607	CLA	C3B-C4B-NB	-2.45	108.34	110.53
19	A	1012	CLA	C1-C2-C3	-2.45	122.19	126.20
19	3	602	CLA	C1-C2-C3	-2.45	122.19	126.20
22	2	503	BCR	C34-C9-C8	2.45	121.83	118.09
19	3	606	CLA	O2D-CGD-O1D	-2.45	119.08	123.85
19	A	1136	CLA	C1-O2A-CGA	2.45	122.57	116.65
19	B	1208	CLA	C1C-C2C-C3C	-2.45	104.41	106.98
19	K	1404	CLA	C1C-C2C-C3C	-2.45	104.41	106.98
19	2	608	CLA	C1C-C2C-C3C	-2.45	104.41	106.98
22	I	4020	BCR	C33-C5-C4	2.44	118.81	113.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	1119	CLA	CHA-C4D-ND	2.44	137.59	132.55
19	1	602	CLA	C1C-C2C-C3C	-2.44	104.41	106.98
19	A	1116	CLA	C1C-C2C-C3C	-2.44	104.41	106.98
19	B	1240	CLA	C1C-C2C-C3C	-2.44	104.41	106.98
19	A	1012	CLA	O2D-CGD-O1D	-2.44	119.09	123.85
25	2	805	LMG	O8-C28-C29	2.44	119.28	111.83
19	A	1102	CLA	CHA-C4D-ND	2.44	137.59	132.55
19	4	601	CLA	C3B-C4B-NB	-2.44	108.35	110.53
29	4	610	CHL	C4D-CHA-CBD	-2.44	106.50	108.97
19	A	1113	CLA	C2C-C1C-NC	2.44	112.55	109.98
19	B	1234	CLA	CHA-C4D-ND	2.44	137.59	132.55
19	B	1230	CLA	C1C-C2C-C3C	-2.44	104.41	106.98
19	K	1402	CLA	C1C-C2C-C3C	-2.44	104.41	106.98
19	B	1206	CLA	CHA-C4D-ND	2.44	137.58	132.55
19	F	1301	CLA	O2D-CGD-O1D	-2.44	119.10	123.85
19	A	1116	CLA	CHA-C4D-ND	2.44	137.58	132.55
19	B	1201	CLA	C1C-C2C-C3C	-2.44	104.41	106.98
19	B	1238	CLA	O2D-CGD-O1D	-2.44	119.10	123.85
19	4	606	CLA	C2C-C1C-NC	2.44	112.54	109.98
19	4	603	CLA	O2D-CGD-O1D	-2.44	119.10	123.85
19	2	603	CLA	C1D-ND-C4D	-2.44	104.60	106.31
19	K	1401	CLA	CHA-C4D-ND	2.44	137.58	132.55
19	B	1228	CLA	C1C-C2C-C3C	-2.44	104.42	106.98
19	3	612	CLA	O2D-CGD-O1D	-2.44	119.10	123.85
19	B	1023	CLA	C2C-C1C-NC	2.44	112.54	109.98
30	2	502	XAT	C15-C14-C13	-2.44	123.86	127.28
19	A	1110	CLA	O2A-CGA-CBA	2.44	119.26	111.83
29	4	611	CHL	C4D-CHA-CBD	-2.44	106.51	108.97
19	A	1130	CLA	C2C-C1C-NC	2.44	112.54	109.98
19	2	602	CLA	O2D-CGD-O1D	-2.44	119.11	123.85
19	B	1203	CLA	CHA-C4D-ND	2.44	137.57	132.55
19	J	1901	CLA	C1C-C2C-C3C	-2.43	104.42	106.98
22	3	503	BCR	C34-C9-C10	-2.43	118.87	122.82
18	A	1011	CL0	CMC-C2C-C1C	2.43	129.11	124.73
22	1	504	BCR	C4-C5-C6	-2.43	119.42	122.70
19	1	605	CLA	CHA-C4D-ND	2.43	137.57	132.55
28	J	4013	LUT	C37-C21-C36	2.43	111.41	107.87
19	B	1219	CLA	O2D-CGD-O1D	-2.43	119.12	123.85
19	F	1301	CLA	CHA-C4D-ND	2.43	137.56	132.55
19	B	1224	CLA	CMD-C2D-C3D	-2.43	122.11	127.69
19	K	1403	CLA	CHD-C1D-ND	-2.43	121.38	124.80
28	4	501	LUT	C35-C15-C14	-2.43	118.55	123.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	G	1603	CLA	C2C-C1C-NC	2.43	112.53	109.98
19	B	1212	CLA	C2C-C1C-NC	2.43	112.53	109.98
27	F	5005	DGD	O3G-C1D-C2D	2.43	111.96	108.27
19	A	1124	CLA	C1-C2-C3	-2.43	122.22	126.20
28	3	502	LUT	C15-C14-C13	-2.43	123.87	127.28
19	A	1115	CLA	C2C-C1C-NC	2.43	112.53	109.98
19	3	601	CLA	C1-O2A-CGA	2.43	122.53	116.65
31	2	807	3PH	O31-C31-C32	2.43	119.23	111.83
19	A	1104	CLA	CHA-C4D-ND	2.43	137.55	132.55
19	A	1137	CLA	C1C-C2C-C3C	-2.43	104.43	106.98
19	B	1023	CLA	C1C-C2C-C3C	-2.43	104.43	106.98
19	B	1237	CLA	C2C-C1C-NC	2.42	112.53	109.98
19	B	1238	CLA	C2C-C1C-NC	2.42	112.53	109.98
19	4	601	CLA	O1D-CGD-CBD	-2.42	119.74	124.52
19	A	1103	CLA	CHA-C4D-ND	2.42	137.55	132.55
19	A	1141	CLA	CMA-C3A-C4A	2.42	118.29	111.77
19	1	614	CLA	CHA-C4D-ND	2.42	137.55	132.55
28	4	505	LUT	C35-C34-C33	-2.42	123.88	127.28
19	K	1403	CLA	O2D-CGD-O1D	-2.42	119.13	123.85
19	4	606	CLA	O2A-CGA-CBA	2.42	119.22	111.83
19	F	1302	CLA	C5-C3-C2	2.42	126.61	121.17
19	L	1501	CLA	CMD-C2D-C3D	-2.42	122.14	127.69
19	B	1201	CLA	O2D-CGD-O1D	-2.42	119.14	123.85
19	A	1119	CLA	C7-C6-C5	-2.42	106.81	113.26
19	3	603	CLA	O2D-CGD-O1D	-2.42	119.14	123.85
19	4	606	CLA	O2D-CGD-O1D	-2.42	119.14	123.85
19	A	1141	CLA	O2A-CGA-CBA	2.42	119.22	111.83
19	A	1118	CLA	CHA-C4D-ND	2.42	137.54	132.55
19	2	604	CLA	C3B-C4B-NB	-2.42	108.37	110.53
19	1	614	CLA	CMD-C2D-C3D	-2.42	122.14	127.69
19	A	1126	CLA	C1C-C2C-C3C	-2.42	104.44	106.98
19	3	602	CLA	C1C-C2C-C3C	-2.42	104.44	106.98
19	B	1220	CLA	CHA-C4D-ND	2.42	137.54	132.55
19	A	1108	CLA	C3B-C4B-NB	-2.42	108.37	110.53
19	1	611	CLA	C2C-C1C-NC	2.42	112.52	109.98
22	2	503	BCR	C16-C17-C18	2.42	130.67	127.28
19	1	602	CLA	O2D-CGD-O1D	-2.42	119.14	123.85
19	B	1237	CLA	CHA-C4D-ND	2.42	137.53	132.55
19	1	603	CLA	CMD-C2D-C3D	-2.42	122.15	127.69
19	B	1221	CLA	CHA-C4D-ND	2.42	137.53	132.55
19	1	602	CLA	CHA-C4D-ND	2.42	137.53	132.55
19	4	617	CLA	C2D-C1D-ND	2.42	112.52	110.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	K	1404	CLA	CHA-C4D-ND	2.42	137.53	132.55
19	G	1602	CLA	C2C-C1C-NC	2.42	112.52	109.98
19	A	1125	CLA	C1D-ND-C4D	-2.41	104.62	106.31
19	A	1129	CLA	CHA-C4D-ND	2.41	137.53	132.55
19	1	613	CLA	CHA-C4D-ND	2.41	137.53	132.55
28	1	501	LUT	C8-C7-C6	-2.41	120.55	127.00
19	B	1226	CLA	C1-C2-C3	-2.41	122.24	126.20
19	B	1214	CLA	O2D-CGD-O1D	-2.41	119.15	123.85
19	B	1023	CLA	O2D-CGD-O1D	-2.41	119.15	123.85
19	1	607	CLA	CHA-C4D-ND	2.41	137.53	132.55
19	K	1402	CLA	C2C-C1C-NC	2.41	112.52	109.98
19	A	1113	CLA	CHA-C4D-ND	2.41	137.52	132.55
19	B	1207	CLA	CHA-C4D-ND	2.41	137.52	132.55
19	3	613	CLA	CHA-C4D-ND	2.41	137.52	132.55
19	A	1141	CLA	C2C-C1C-NC	2.41	112.51	109.98
19	H	1701	CLA	C2C-C1C-NC	2.41	112.51	109.98
22	A	4017	BCR	C39-C30-C25	-2.41	106.46	110.24
19	2	612	CLA	CMD-C2D-C3D	-2.41	122.16	127.69
29	2	610	CHL	C4D-CHA-CBD	-2.41	106.54	108.97
19	K	1404	CLA	CMA-C3A-C4A	2.41	118.25	111.77
29	2	615	CHL	C1-C2-C3	-2.41	122.25	126.20
19	A	1112	CLA	CHA-C4D-ND	2.41	137.52	132.55
19	2	602	CLA	C1-C2-C3	-2.41	122.25	126.20
19	1	611	CLA	CMA-C3A-C4A	2.41	118.25	111.77
19	B	1226	CLA	O2A-CGA-CBA	2.41	119.18	111.83
19	B	1239	CLA	CAA-C2A-C3A	2.41	119.51	113.00
19	B	1232	CLA	CHA-C4D-ND	2.41	137.52	132.55
19	3	602	CLA	O2A-CGA-CBA	2.41	119.18	111.83
19	B	1225	CLA	CHA-C4D-ND	2.41	137.52	132.55
19	A	1109	CLA	CHD-C1D-ND	-2.41	121.42	124.80
19	2	603	CLA	C1C-C2C-C3C	-2.41	104.45	106.98
22	A	4007	BCR	C38-C26-C27	2.41	118.73	113.60
28	4	505	LUT	C40-C33-C32	2.41	121.76	118.09
19	A	1127	CLA	C1C-C2C-C3C	-2.41	104.45	106.98
19	4	604	CLA	C3B-C4B-NB	-2.41	108.38	110.53
28	3	502	LUT	C12-C13-C14	-2.41	115.23	119.01
19	A	1114	CLA	CHA-C4D-ND	2.40	137.51	132.55
19	B	1230	CLA	CMD-C2D-C3D	-2.40	122.18	127.69
19	A	1137	CLA	O2A-CGA-CBA	2.40	119.16	111.83
19	A	1113	CLA	CMD-C2D-C3D	-2.40	122.18	127.69
19	A	1123	CLA	CHA-C4D-ND	2.40	137.51	132.55
19	B	1213	CLA	CHA-C4D-ND	2.40	137.51	132.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	4	601	CLA	C5-C3-C2	2.40	126.56	121.17
19	B	1206	CLA	O2A-CGA-CBA	2.40	119.16	111.83
22	B	4006	BCR	C33-C5-C6	-2.40	121.86	124.48
19	B	1213	CLA	C1C-C2C-C3C	-2.40	104.45	106.98
19	A	1106	CLA	C1-C2-C3	-2.40	122.26	126.20
22	A	4008	BCR	C33-C5-C4	2.40	118.71	113.60
19	B	1022	CLA	C2C-C1C-NC	2.40	112.50	109.98
19	2	601	CLA	C2C-C1C-NC	2.40	112.50	109.98
19	3	608	CLA	CHA-C4D-ND	2.40	137.50	132.55
19	2	607	CLA	C1C-C2C-C3C	-2.40	104.46	106.98
19	A	1137	CLA	CHA-C4D-ND	2.40	137.50	132.55
19	B	1221	CLA	C2C-C1C-NC	2.40	112.50	109.98
19	A	1120	CLA	CHA-C4D-ND	2.40	137.50	132.55
19	1	604	CLA	C2C-C1C-NC	2.40	112.50	109.98
27	B	5005	DGD	O2G-C1B-O1B	-2.40	118.11	123.70
22	F	4014	BCR	C31-C1-C6	-2.40	106.49	110.24
19	B	1203	CLA	C2C-C1C-NC	2.39	112.50	109.98
19	4	608	CLA	C2C-C1C-NC	2.39	112.50	109.98
19	A	1102	CLA	C1C-C2C-C3C	-2.39	104.46	106.98
19	G	1601	CLA	CHA-C4D-ND	2.39	137.49	132.55
19	1	614	CLA	C1-C2-C3	-2.39	122.28	126.20
19	A	1141	CLA	O2D-CGD-O1D	-2.39	119.19	123.85
19	3	603	CLA	CMB-C2B-C1B	2.39	129.06	125.42
28	1	501	LUT	C15-C14-C13	-2.39	123.92	127.28
19	A	1131	CLA	CHA-C4D-ND	2.39	137.48	132.55
22	2	503	BCR	C33-C5-C4	2.39	118.69	113.60
19	J	1901	CLA	CHA-C4D-ND	2.39	137.48	132.55
19	B	1202	CLA	C1D-ND-C4D	-2.39	104.64	106.31
19	B	1229	CLA	CMD-C2D-C3D	-2.39	122.21	127.69
19	B	1225	CLA	C1C-C2C-C3C	-2.39	104.47	106.98
19	A	1107	CLA	O2A-CGA-CBA	2.39	119.12	111.83
19	4	608	CLA	CHA-C4D-ND	2.39	137.48	132.55
19	A	1130	CLA	CHA-C4D-ND	2.39	137.48	132.55
19	A	1101	CLA	O1D-CGD-CBD	-2.39	119.81	124.52
19	B	1222	CLA	O1D-CGD-CBD	-2.39	119.81	124.52
19	A	1115	CLA	CMA-C3A-C4A	2.39	118.19	111.77
19	B	1230	CLA	CHA-C4D-ND	2.39	137.47	132.55
19	1	608	CLA	CMD-C2D-C3D	-2.39	122.22	127.69
19	A	1109	CLA	O2A-CGA-CBA	2.39	119.11	111.83
22	K	4002	BCR	C30-C25-C24	2.39	122.12	115.65
19	B	1227	CLA	CHA-C4D-ND	2.39	137.47	132.55
22	3	506	BCR	C33-C5-C6	-2.39	121.88	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	1215	CLA	CMD-C2D-C3D	-2.39	122.22	127.69
19	3	617	CLA	O2A-CGA-CBA	2.38	119.11	111.83
19	3	608	CLA	O2D-CGD-O1D	-2.38	119.21	123.85
22	B	4009	BCR	C24-C25-C26	-2.38	116.06	121.56
19	B	1228	CLA	CHA-C4D-ND	2.38	137.47	132.55
19	F	1302	CLA	O2D-CGD-O1D	-2.38	119.21	123.85
22	A	4008	BCR	C36-C18-C17	-2.38	118.96	122.82
19	4	602	CLA	O2D-CGD-O1D	-2.38	119.21	123.85
19	B	1227	CLA	C2C-C1C-NC	2.38	112.48	109.98
19	3	612	CLA	CHA-C4D-ND	2.38	137.46	132.55
19	A	1135	CLA	CMA-C3A-C4A	2.38	118.17	111.77
19	B	1229	CLA	CHA-C4D-ND	2.38	137.46	132.55
19	4	609	CLA	CMA-C3A-C4A	2.38	118.17	111.77
19	4	601	CLA	CHA-C4D-ND	2.38	137.46	132.55
19	A	1123	CLA	O2A-CGA-CBA	2.38	119.09	111.83
22	1	503	BCR	C1-C6-C7	2.38	122.10	115.65
19	A	1120	CLA	CMD-C2D-C3D	-2.38	122.23	127.69
19	B	1208	CLA	CHA-C4D-ND	2.38	137.45	132.55
19	B	1218	CLA	C1C-C2C-C3C	-2.38	104.48	106.98
19	A	1013	CLA	C1-C2-C3	-2.38	122.31	126.20
19	1	606	CLA	CHA-C4D-ND	2.38	137.45	132.55
19	A	1128	CLA	C2C-C1C-NC	2.38	112.48	109.98
22	B	4006	BCR	C24-C25-C26	-2.38	116.08	121.56
19	B	1227	CLA	CMD-C2D-C3D	-2.38	122.24	127.69
19	2	606	CLA	CHA-C4D-ND	2.37	137.45	132.55
19	3	610	CLA	C2C-C1C-NC	2.37	112.47	109.98
19	B	1204	CLA	CHA-C4D-ND	2.37	137.45	132.55
19	B	1215	CLA	CHA-C4D-ND	2.37	137.44	132.55
19	B	1218	CLA	C1D-ND-C4D	-2.37	104.65	106.31
22	A	4002	BCR	C39-C30-C25	-2.37	106.52	110.24
19	A	1134	CLA	C2C-C1C-NC	2.37	112.47	109.98
19	4	602	CLA	CHA-C4D-ND	2.37	137.44	132.55
22	F	4016	BCR	C4-C5-C6	-2.37	119.50	122.70
19	F	1301	CLA	CMA-C3A-C4A	2.37	118.15	111.77
22	L	4020	BCR	C23-C24-C25	-2.37	120.66	127.00
25	B	5004	LMG	C8-O7-C10	-2.37	112.12	117.80
19	B	1213	CLA	C2C-C1C-NC	2.37	112.47	109.98
19	B	1023	CLA	CHA-C4D-ND	2.37	137.44	132.55
19	B	1226	CLA	CHA-C4D-ND	2.37	137.44	132.55
19	A	1133	CLA	O2D-CGD-O1D	-2.37	119.24	123.85
19	1	606	CLA	O2A-CGA-CBA	2.37	119.06	111.83
19	A	1122	CLA	C1-O2A-CGA	2.37	122.38	116.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	4002	BCR	C12-C13-C14	-2.37	115.28	119.01
19	A	1139	CLA	C3B-C4B-NB	-2.37	108.42	110.53
28	1	501	LUT	C18-C5-C4	2.37	118.78	114.42
19	A	1120	CLA	CMA-C3A-C4A	2.37	118.14	111.77
19	L	1502	CLA	O1D-CGD-CBD	-2.37	119.85	124.52
19	B	1209	CLA	C2C-C1C-NC	2.37	112.47	109.98
19	A	1121	CLA	C1C-C2C-C3C	-2.37	104.49	106.98
19	A	1139	CLA	CHA-C4D-ND	2.37	137.43	132.55
24	G	5005	LMT	C3'-C4'-C5'	-2.37	105.69	110.93
19	A	1105	CLA	CMA-C3A-C4A	2.37	118.13	111.77
19	B	1217	CLA	CHA-C4D-ND	2.36	137.43	132.55
19	A	1013	CLA	O2A-CGA-CBA	2.36	119.05	111.83
19	K	1402	CLA	CHA-C4D-ND	2.36	137.43	132.55
19	B	1210	CLA	C3B-C4B-NB	-2.36	108.42	110.53
19	A	1111	CLA	CHA-C4D-ND	2.36	137.43	132.55
19	G	1601	CLA	O2A-CGA-CBA	2.36	119.04	111.83
30	4	502	XAT	C31-C30-C29	-2.36	123.96	127.28
19	K	1404	CLA	O2D-CGD-O1D	-2.36	119.25	123.85
19	B	1208	CLA	CMD-C2D-C3D	-2.36	122.27	127.69
19	3	613	CLA	O2D-CGD-O1D	-2.36	119.25	123.85
28	1	501	LUT	C1-C6-C5	-2.36	119.41	122.64
19	2	607	CLA	C2C-C1C-NC	2.36	112.46	109.98
19	B	1220	CLA	C1C-C2C-C3C	-2.36	104.50	106.98
19	4	607	CLA	O2D-CGD-O1D	-2.36	119.25	123.85
22	1	503	BCR	C8-C9-C10	2.36	122.72	119.01
19	B	1210	CLA	CAC-C3C-C4C	2.36	127.86	124.79
19	A	1132	CLA	C2C-C1C-NC	2.36	112.46	109.98
19	B	1227	CLA	O1D-CGD-CBD	-2.36	119.86	124.52
19	B	1238	CLA	CHA-C4D-ND	2.36	137.42	132.55
19	4	612	CLA	CHA-C4D-ND	2.36	137.41	132.55
19	2	608	CLA	CHA-C4D-ND	2.36	137.41	132.55
19	B	1202	CLA	O2A-CGA-CBA	2.36	119.02	111.83
19	A	1139	CLA	CMA-C3A-C4A	2.36	118.11	111.77
19	A	1109	CLA	O2D-CGD-O1D	-2.36	119.26	123.85
19	B	1205	CLA	O1D-CGD-CBD	-2.36	119.87	124.52
19	F	1302	CLA	CMA-C3A-C4A	2.36	118.11	111.77
19	A	1122	CLA	O2D-CGD-O1D	-2.36	119.26	123.85
19	A	1105	CLA	O2A-CGA-CBA	2.36	119.02	111.83
19	H	1701	CLA	CHA-C4D-ND	2.36	137.41	132.55
19	A	1101	CLA	CHA-C4D-ND	2.36	137.41	132.55
19	3	610	CLA	CHA-C4D-ND	2.36	137.41	132.55
19	3	603	CLA	CHA-C4D-ND	2.36	137.41	132.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	1139	CLA	CHC-C4B-NB	2.36	127.58	124.05
19	B	1212	CLA	CHA-C4D-ND	2.35	137.41	132.55
19	2	603	CLA	O2D-CGD-O1D	-2.35	119.27	123.85
19	2	604	CLA	O2A-CGA-CBA	2.35	119.01	111.83
19	G	1603	CLA	CHA-C4D-ND	2.35	137.40	132.55
19	A	1118	CLA	O2A-CGA-CBA	2.35	119.01	111.83
19	2	606	CLA	O2D-CGD-O1D	-2.35	119.27	123.85
19	A	1124	CLA	O2D-CGD-O1D	-2.35	119.27	123.85
19	1	613	CLA	O2D-CGD-O1D	-2.35	119.27	123.85
19	B	1219	CLA	CHA-C4D-ND	2.35	137.40	132.55
19	A	1111	CLA	C2C-C1C-NC	2.35	112.45	109.98
22	B	4010	BCR	C7-C6-C5	-2.35	116.14	121.56
19	B	1210	CLA	CHA-C4D-ND	2.35	137.40	132.55
19	B	1211	CLA	CHA-C4D-ND	2.35	137.40	132.55
19	2	612	CLA	C2C-C1C-NC	2.35	112.45	109.98
19	B	1209	CLA	CHA-C4D-ND	2.35	137.40	132.55
19	L	1503	CLA	CHD-C1D-ND	-2.35	121.50	124.80
19	3	614	CLA	C3B-C4B-NB	-2.35	108.43	110.53
19	A	1113	CLA	CMA-C3A-C4A	2.35	118.09	111.77
19	A	1137	CLA	O1D-CGD-CBD	-2.35	119.88	124.52
19	G	1602	CLA	CHA-C4D-ND	2.35	137.40	132.55
19	K	1403	CLA	O2A-CGA-CBA	2.35	119.00	111.83
19	B	1231	CLA	CHA-C4D-ND	2.35	137.40	132.55
19	2	602	CLA	O2A-CGA-CBA	2.35	119.00	111.83
19	3	608	CLA	CMD-C2D-C3D	-2.35	122.30	127.69
19	3	614	CLA	CMA-C3A-C4A	2.35	118.09	111.77
29	3	611	CHL	C4D-CHA-CBD	-2.35	106.60	108.97
19	3	607	CLA	CHA-C4D-ND	2.35	137.39	132.55
19	1	605	CLA	O2D-CGD-O1D	-2.35	119.28	123.85
19	2	602	CLA	CHA-C4D-ND	2.35	137.39	132.55
19	A	1111	CLA	CMD-C2D-C3D	-2.35	122.31	127.69
22	A	4003	BCR	C27-C26-C25	-2.35	119.53	122.70
28	1	501	LUT	C35-C15-C14	-2.34	118.72	123.52
19	3	606	CLA	C2C-C1C-NC	2.34	112.44	109.98
19	A	1106	CLA	CMD-C2D-C3D	-2.34	122.31	127.69
19	2	607	CLA	CMD-C2D-C3D	-2.34	122.31	127.69
19	1	603	CLA	CAA-C2A-C3A	-2.34	106.67	113.00
19	4	607	CLA	CHA-C4D-ND	2.34	137.38	132.55
19	3	605	CLA	C1-C2-C3	-2.34	122.36	126.20
22	1	503	BCR	C28-C27-C26	-2.34	109.88	114.06
19	4	604	CLA	CMD-C2D-C3D	-2.34	122.32	127.69
19	A	1107	CLA	CHA-C4D-ND	2.34	137.38	132.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	1127	CLA	CHA-C4D-ND	2.34	137.38	132.55
29	1	610	CHL	CMA-C3A-C4A	2.34	119.65	114.61
19	B	1235	CLA	CHA-C4D-ND	2.34	137.38	132.55
19	B	1239	CLA	CHA-C4D-ND	2.34	137.38	132.55
19	4	601	CLA	C4-C3-C2	-2.34	117.62	123.63
19	B	1231	CLA	CMD-C2D-C3D	-2.34	122.33	127.69
19	2	602	CLA	CMA-C3A-C4A	2.34	118.06	111.77
19	A	1128	CLA	CHA-C4D-ND	2.34	137.37	132.55
19	A	1141	CLA	CHA-C4D-ND	2.34	137.37	132.55
19	B	1236	CLA	CHA-C4D-ND	2.34	137.37	132.55
19	4	606	CLA	CHA-C4D-ND	2.34	137.37	132.55
19	A	1110	CLA	CHA-C4D-ND	2.34	137.37	132.55
22	2	503	BCR	C28-C27-C26	-2.34	109.89	114.06
19	G	1603	CLA	C5-C3-C2	2.34	126.41	121.17
19	A	1105	CLA	CHA-C4D-ND	2.34	137.37	132.55
19	3	602	CLA	CHA-C4D-ND	2.33	137.37	132.55
19	A	1103	CLA	C2C-C1C-NC	2.33	112.43	109.98
19	K	1401	CLA	C3B-C4B-NB	-2.33	108.45	110.53
19	A	1114	CLA	CMD-C2D-C3D	-2.33	122.34	127.69
19	A	1124	CLA	C1C-C2C-C3C	-2.33	104.53	106.98
19	2	602	CLA	C4-C3-C2	-2.33	117.64	123.63
19	1	602	CLA	CMA-C3A-C4A	2.33	118.04	111.77
19	F	1302	CLA	CHA-C4D-ND	2.33	137.36	132.55
19	A	1137	CLA	C1-C2-C3	-2.33	122.38	126.20
19	B	1202	CLA	CHA-C4D-ND	2.33	137.36	132.55
19	A	1115	CLA	CHA-C4D-ND	2.33	137.36	132.55
19	3	614	CLA	O2D-CGD-O1D	-2.33	119.31	123.85
19	A	1122	CLA	CHA-C4D-ND	2.33	137.36	132.55
24	B	5006	LMT	C1'-O5'-C5'	-2.33	109.17	113.72
19	3	607	CLA	CMD-C2D-C3D	-2.33	122.35	127.69
19	B	1212	CLA	O1D-CGD-CBD	-2.33	119.93	124.52
19	2	604	CLA	CHA-C4D-ND	2.33	137.35	132.55
30	2	502	XAT	C19-C9-C10	-2.33	119.05	122.82
22	B	4005	BCR	C31-C1-C6	-2.33	106.59	110.24
19	A	1126	CLA	CHA-C4D-ND	2.33	137.35	132.55
19	A	1135	CLA	CHA-C4D-ND	2.33	137.35	132.55
19	4	604	CLA	C1D-ND-C4D	-2.33	104.68	106.31
19	B	1237	CLA	CMA-C3A-C4A	2.33	118.03	111.77
19	A	1128	CLA	C3B-C4B-NB	-2.33	108.45	110.53
19	B	1021	CLA	CHA-C1A-NA	-2.33	121.12	126.39
19	B	1238	CLA	CMD-C2D-C3D	-2.32	122.36	127.69
19	A	1108	CLA	O2D-CGD-O1D	-2.32	119.33	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	1136	CLA	CHA-C4D-ND	2.32	137.34	132.55
19	4	604	CLA	CHA-C4D-ND	2.32	137.34	132.55
19	A	1136	CLA	C2C-C1C-NC	2.32	112.42	109.98
19	B	1228	CLA	C2C-C1C-NC	2.32	112.42	109.98
19	4	607	CLA	C2C-C1C-NC	2.32	112.42	109.98
19	A	1116	CLA	CMD-C2D-C3D	-2.32	122.37	127.69
19	B	1221	CLA	O1D-CGD-CBD	-2.32	119.94	124.52
19	1	614	CLA	C1C-C2C-C3C	-2.32	104.54	106.98
19	K	1401	CLA	CMA-C3A-C4A	2.32	118.01	111.77
19	L	1502	CLA	C1-O2A-CGA	2.32	122.27	116.65
19	3	606	CLA	CHA-C4D-ND	2.32	137.34	132.55
19	3	614	CLA	CHA-C4D-ND	2.32	137.34	132.55
19	L	1502	CLA	CHA-C4D-ND	2.32	137.33	132.55
19	3	603	CLA	CMD-C2D-C3D	-2.32	122.37	127.69
22	K	4001	BCR	C28-C27-C26	-2.32	109.92	114.06
19	A	1106	CLA	CHA-C4D-ND	2.32	137.33	132.55
19	B	1223	CLA	C2C-C1C-NC	2.32	112.42	109.98
19	2	608	CLA	C2C-C1C-NC	2.32	112.42	109.98
19	B	1201	CLA	CHA-C4D-ND	2.32	137.33	132.55
19	4	617	CLA	C2C-C1C-NC	2.32	112.41	109.98
19	B	1223	CLA	CMD-C2D-C3D	-2.32	122.38	127.69
19	2	603	CLA	CHA-C4D-ND	2.31	137.32	132.55
19	A	1112	CLA	CMA-C3A-C4A	2.31	117.99	111.77
19	B	1213	CLA	O2A-CGA-CBA	2.31	118.89	111.83
19	L	1501	CLA	CHA-C4D-ND	2.31	137.32	132.55
19	2	612	CLA	CHA-C4D-ND	2.31	137.32	132.55
19	A	1132	CLA	C1-O2A-CGA	2.31	122.25	116.65
19	A	1140	CLA	C1D-ND-C4D	-2.31	104.69	106.31
28	4	505	LUT	C18-C5-C6	-2.31	121.96	124.48
19	B	1212	CLA	CMA-C3A-C4A	2.31	117.98	111.77
19	1	606	CLA	CMD-C2D-C3D	-2.31	122.39	127.69
19	A	1137	CLA	CMD-C2D-C3D	-2.31	122.39	127.69
19	4	606	CLA	CMD-C2D-C3D	-2.31	122.39	127.69
19	A	1109	CLA	CHA-C4D-ND	2.31	137.31	132.55
19	B	1216	CLA	CHA-C4D-ND	2.31	137.31	132.55
19	A	1131	CLA	C2C-C1C-NC	2.31	112.41	109.98
19	B	1230	CLA	C2C-C1C-NC	2.31	112.41	109.98
19	B	1216	CLA	C1-C2-C3	-2.31	122.42	126.20
19	B	1209	CLA	CMA-C3A-C4A	2.31	117.98	111.77
19	A	1121	CLA	O2D-CGD-O1D	-2.31	119.36	123.85
19	A	1125	CLA	CHA-C4D-ND	2.31	137.31	132.55
19	B	1229	CLA	CAA-CBA-CGA	-2.31	106.66	113.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	H	1701	CLA	O2D-CGD-O1D	-2.31	119.36	123.85
19	B	1228	CLA	C1-C2-C3	-2.31	122.42	126.20
19	4	603	CLA	CHA-C4D-ND	2.31	137.31	132.55
22	A	4007	BCR	C34-C9-C10	-2.31	119.08	122.82
19	A	1124	CLA	CHA-C4D-ND	2.30	137.30	132.55
19	L	1501	CLA	C2C-C1C-NC	2.30	112.40	109.98
19	J	1901	CLA	O2A-CGA-CBA	2.30	118.86	111.83
19	B	1202	CLA	CMD-C2D-C3D	-2.30	122.41	127.69
19	4	604	CLA	O2D-CGD-O1D	-2.30	119.36	123.85
19	4	607	CLA	O1D-CGD-CBD	-2.30	119.97	124.52
19	B	1205	CLA	CHA-C4D-ND	2.30	137.30	132.55
19	3	606	CLA	CMD-C2D-C3D	-2.30	122.41	127.69
19	1	602	CLA	C2C-C1C-NC	2.30	112.40	109.98
29	2	611	CHL	C4D-CHA-CBD	-2.30	106.65	108.97
19	3	613	CLA	CMD-C2D-C3D	-2.30	122.41	127.69
19	A	1121	CLA	CHA-C4D-ND	2.30	137.30	132.55
19	A	1136	CLA	CMD-C2D-C3D	-2.30	122.41	127.69
19	B	1232	CLA	O2D-CGD-O1D	-2.30	119.37	123.85
19	1	611	CLA	CHA-C4D-ND	2.30	137.29	132.55
22	1	504	BCR	C33-C5-C4	2.30	118.50	113.60
19	A	1125	CLA	C2C-C1C-NC	2.30	112.40	109.98
19	A	1138	CLA	O2D-CGD-O1D	-2.30	119.38	123.85
19	1	608	CLA	O1D-CGD-CBD	-2.30	119.99	124.52
19	B	1214	CLA	CMD-C2D-C3D	-2.30	122.42	127.69
19	A	1108	CLA	CHA-C4D-ND	2.30	137.29	132.55
19	2	606	CLA	CMA-C3A-C4A	2.30	117.95	111.77
19	A	1122	CLA	C2C-C1C-NC	2.30	112.39	109.98
19	B	1228	CLA	C3B-C4B-NB	-2.30	108.48	110.53
19	B	1236	CLA	CMD-C2D-C3D	-2.30	122.42	127.69
19	1	601	CLA	CHA-C4D-ND	2.30	137.28	132.55
19	B	1211	CLA	CMD-C2D-C3D	-2.30	122.42	127.69
19	A	1105	CLA	CMD-C2D-C3D	-2.29	122.43	127.69
19	B	1235	CLA	C2C-C1C-NC	2.29	112.39	109.98
19	4	612	CLA	CMA-C3A-C4A	2.29	117.94	111.77
22	3	503	BCR	C37-C22-C23	2.29	121.59	118.09
19	3	610	CLA	CMD-C2D-C3D	-2.29	122.43	127.69
19	A	1138	CLA	CHA-C4D-ND	2.29	137.28	132.55
30	2	502	XAT	C17-C1-C16	2.29	110.70	107.37
22	A	4011	BCR	C2-C1-C6	2.29	113.77	110.44
19	B	1225	CLA	C1-C2-C3	-2.29	122.44	126.20
28	3	502	LUT	C27-C28-C29	-2.29	121.39	126.32
29	4	610	CHL	C1-O2A-CGA	2.29	123.41	116.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	1232	CLA	O2A-CGA-CBA	2.29	118.82	111.83
29	4	613	CHL	C4C-CHD-C1D	2.29	124.27	116.07
19	A	1013	CLA	CHA-C4D-ND	2.29	137.27	132.55
19	B	1210	CLA	C1C-C2C-C3C	-2.29	104.57	106.98
22	L	4020	BCR	C38-C26-C27	2.29	118.48	113.60
22	A	4003	BCR	C28-C27-C26	-2.29	109.97	114.06
19	3	601	CLA	CHA-C4D-ND	2.29	137.27	132.55
19	A	1139	CLA	O2A-CGA-CBA	2.29	118.81	111.83
28	2	501	LUT	C11-C10-C9	-2.29	124.07	127.28
24	B	5006	LMT	C3'-C4'-C5'	-2.29	105.86	110.93
24	G	5004	LMT	C1'-O5'-C5'	-2.29	109.25	113.72
19	2	605	CLA	CMD-C2D-C3D	-2.29	122.44	127.69
19	A	1111	CLA	C1C-C2C-C3C	-2.29	104.58	106.98
22	1	504	BCR	C33-C5-C6	-2.29	121.99	124.48
24	A	5004	LMT	C1'-O5'-C5'	-2.29	109.25	113.72
30	2	502	XAT	C35-C15-C14	-2.29	118.84	123.52
19	4	605	CLA	CHA-C1A-NA	-2.29	121.21	126.39
19	A	1126	CLA	O2A-CGA-CBA	2.29	118.80	111.83
19	A	1139	CLA	C4-C3-C2	-2.29	117.76	123.63
19	B	1208	CLA	C1-C2-C3	-2.29	122.45	126.20
19	B	1217	CLA	C2C-C1C-NC	2.29	112.38	109.98
22	3	503	BCR	C37-C22-C21	-2.28	119.11	122.82
19	A	1133	CLA	CHA-C4D-ND	2.28	137.26	132.55
28	3	501	LUT	C35-C15-C14	-2.28	118.85	123.52
19	G	1602	CLA	CMD-C2D-C3D	-2.28	122.45	127.69
19	A	1012	CLA	CHA-C1A-NA	-2.28	121.22	126.39
19	J	1901	CLA	CMD-C2D-C3D	-2.28	122.46	127.69
19	4	605	CLA	CMD-C2D-C3D	-2.28	122.46	127.69
19	1	614	CLA	O2A-CGA-CBA	2.28	118.79	111.83
19	A	1132	CLA	CHD-C1D-ND	-2.28	121.59	124.80
19	B	1202	CLA	C2C-C1C-NC	2.28	112.38	109.98
22	A	4008	BCR	C34-C9-C8	2.28	121.57	118.09
19	B	1226	CLA	CMD-C2D-C3D	-2.28	122.46	127.69
29	2	613	CHL	C4C-CHD-C1D	2.28	124.23	116.07
22	A	4017	BCR	C38-C26-C27	2.28	118.46	113.60
22	B	4005	BCR	C23-C24-C25	-2.28	120.91	127.00
19	F	1302	CLA	C3B-C4B-NB	-2.28	108.50	110.53
19	A	1126	CLA	CMD-C2D-C3D	-2.28	122.46	127.69
19	B	1023	CLA	O2A-CGA-CBA	2.28	118.78	111.83
19	2	602	CLA	C2C-C1C-NC	2.28	112.38	109.98
19	B	1021	CLA	CMD-C2D-C3D	-2.28	122.47	127.69
19	4	605	CLA	C3D-C2D-C1D	-2.28	102.72	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	2	612	CLA	O2A-CGA-CBA	2.28	118.78	111.83
22	B	4005	BCR	C28-C27-C26	-2.28	110.00	114.06
19	A	1129	CLA	O1D-CGD-CBD	-2.28	120.03	124.52
19	A	1117	CLA	CHA-C4D-ND	2.28	137.24	132.55
19	B	1226	CLA	CMA-C3A-C4A	2.27	117.89	111.77
19	4	604	CLA	C6-C5-C3	-2.27	107.93	113.47
19	A	1140	CLA	CHA-C4D-ND	2.27	137.24	132.55
22	B	4004	BCR	C36-C18-C19	2.27	121.56	118.09
19	3	617	CLA	CMD-C2D-C3D	-2.27	122.48	127.69
22	H	4021	BCR	C28-C27-C26	-2.27	110.00	114.06
24	G	5005	LMT	C1'-O5'-C5'	-2.27	109.28	113.72
29	1	612	CHL	C4C-CHD-C1D	2.27	124.20	116.07
19	B	1239	CLA	CMA-C3A-C4A	2.27	117.88	111.77
19	B	1210	CLA	CMD-C2D-C3D	-2.27	122.48	127.69
19	A	1116	CLA	O1D-CGD-CBD	-2.27	120.04	124.52
19	B	1218	CLA	CMA-C3A-C4A	2.27	117.87	111.77
19	A	1138	CLA	C1-O2A-CGA	2.27	122.14	116.65
19	A	1120	CLA	O2A-CGA-CBA	2.27	118.75	111.83
19	A	1112	CLA	O2A-CGA-CBA	2.27	118.75	111.83
22	2	503	BCR	C1-C6-C5	-2.27	119.54	122.64
19	2	601	CLA	CHA-C4D-ND	2.27	137.23	132.55
19	A	1101	CLA	CMD-C2D-C3D	-2.27	122.49	127.69
19	B	1220	CLA	CMD-C2D-C3D	-2.27	122.49	127.69
22	B	4009	BCR	C37-C22-C21	-2.27	119.14	122.82
22	K	4001	BCR	C34-C9-C8	2.27	121.55	118.09
19	B	1218	CLA	CMD-C2D-C3D	-2.27	122.49	127.69
19	B	1218	CLA	CHA-C4D-ND	2.27	137.22	132.55
19	1	603	CLA	O2D-CGD-O1D	-2.27	119.44	123.85
19	A	1116	CLA	C2C-C1C-NC	2.27	112.36	109.98
22	K	4002	BCR	C40-C30-C25	2.26	113.79	110.24
19	B	1219	CLA	O2A-CGA-CBA	2.26	118.74	111.83
19	A	1118	CLA	CMA-C3A-C4A	2.26	117.86	111.77
19	B	1229	CLA	O2A-C1-C2	2.26	116.82	108.11
22	I	4018	BCR	C28-C27-C26	-2.26	110.02	114.06
19	A	1012	CLA	O1D-CGD-CBD	-2.26	120.06	124.52
22	L	4019	BCR	C4-C5-C6	-2.26	119.65	122.70
19	A	1130	CLA	CMD-C2D-C3D	-2.26	122.50	127.69
19	K	1402	CLA	CMD-C2D-C3D	-2.26	122.50	127.69
19	B	1240	CLA	CHA-C4D-ND	2.26	137.22	132.55
19	A	1107	CLA	C1-O2A-CGA	2.26	122.13	116.65
19	A	1109	CLA	CBA-CAA-C2A	2.26	120.52	113.79
19	G	1603	CLA	CMD-C2D-C3D	-2.26	122.50	127.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	K	4001	BCR	C33-C5-C6	-2.26	122.02	124.48
22	B	4004	BCR	C31-C1-C6	-2.26	106.70	110.24
20	B	2002	PQN	C2M-C2-C3	-2.26	120.74	124.45
22	F	4014	BCR	C7-C6-C5	2.26	126.76	121.56
19	G	1601	CLA	CHA-C1A-NA	-2.26	121.28	126.39
19	B	1239	CLA	CMD-C2D-C3D	-2.26	122.52	127.69
19	B	1211	CLA	O2A-CGA-CBA	2.26	118.71	111.83
25	3	802	LMG	C8-O7-C10	-2.25	112.40	117.80
19	A	1127	CLA	C2C-C1C-NC	2.25	112.35	109.98
22	J	4012	BCR	C1-C6-C7	2.25	121.76	115.65
19	B	1204	CLA	C4-C3-C2	-2.25	117.84	123.63
19	B	1228	CLA	C1-O2A-CGA	2.25	122.10	116.65
22	B	4010	BCR	C27-C26-C25	-2.25	119.66	122.70
19	1	611	CLA	CMD-C2D-C3D	-2.25	122.52	127.69
19	A	1127	CLA	CMA-C3A-C4A	2.25	117.83	111.77
19	A	1109	CLA	C1C-C2C-C3C	-2.25	104.61	106.98
22	H	4021	BCR	C34-C9-C10	-2.25	119.17	122.82
19	4	617	CLA	O2A-CGA-CBA	2.25	118.70	111.83
22	A	4017	BCR	C35-C13-C14	-2.25	119.17	122.82
19	A	1134	CLA	CMD-C2D-C3D	-2.25	122.54	127.69
19	A	1102	CLA	C4-C3-C2	-2.25	117.86	123.63
19	A	1102	CLA	CMD-C2D-C3D	-2.25	122.54	127.69
19	A	1101	CLA	C2C-C1C-NC	2.25	112.34	109.98
19	1	604	CLA	CMD-C2D-C3D	-2.24	122.54	127.69
29	2	611	CHL	C1-O2A-CGA	2.24	123.05	116.67
19	A	1133	CLA	CMD-C2D-C3D	-2.24	122.54	127.69
19	B	1201	CLA	CMD-C2D-C3D	-2.24	122.54	127.69
22	A	4007	BCR	C34-C9-C8	2.24	121.52	118.09
22	L	4019	BCR	C36-C18-C17	-2.24	119.18	122.82
22	G	4011	BCR	C24-C25-C26	-2.24	116.39	121.56
19	B	1218	CLA	CHD-C1D-ND	-2.24	121.65	124.80
19	A	1139	CLA	O1D-CGD-CBD	-2.24	120.10	124.52
19	A	1101	CLA	C1C-C2C-C3C	-2.24	104.62	106.98
19	4	602	CLA	C1D-ND-C4D	-2.24	104.74	106.31
19	2	604	CLA	CMD-C2D-C3D	-2.24	122.55	127.69
19	F	1302	CLA	O2A-CGA-CBA	2.24	118.67	111.83
19	B	1227	CLA	O2A-CGA-CBA	2.24	118.67	111.83
22	H	4021	BCR	C34-C9-C8	2.24	121.51	118.09
30	2	502	XAT	O4-C6-C7	-2.24	110.46	116.88
19	A	1140	CLA	C1C-C2C-C3C	-2.24	104.62	106.98
19	B	1216	CLA	O2A-CGA-CBA	2.24	118.66	111.83
19	2	612	CLA	CHD-C1D-ND	-2.24	121.65	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	3	614	CLA	CMD-C2D-C3D	-2.24	122.56	127.69
19	1	613	CLA	CMD-C2D-C3D	-2.24	122.56	127.69
19	1	604	CLA	C1-O2A-CGA	2.24	122.07	116.65
19	3	613	CLA	C3B-C4B-NB	-2.24	108.53	110.53
19	2	608	CLA	O2A-CGA-CBA	2.24	118.66	111.83
19	A	1117	CLA	CMD-C2D-C3D	-2.24	122.56	127.69
19	F	1301	CLA	O2A-CGA-CBA	2.24	118.65	111.83
19	G	1603	CLA	O2A-CGA-CBA	2.24	118.65	111.83
19	A	1106	CLA	O1D-CGD-CBD	-2.24	120.11	124.52
19	L	1501	CLA	O1D-CGD-CBD	-2.24	120.11	124.52
19	4	603	CLA	C1D-ND-C4D	-2.23	104.74	106.31
19	2	607	CLA	O1D-CGD-CBD	-2.23	120.11	124.52
27	G	5003	DGD	C2G-O2G-C1B	-2.23	112.45	117.80
19	B	1235	CLA	CMD-C2D-C3D	-2.23	122.57	127.69
19	4	603	CLA	CMD-C2D-C3D	-2.23	122.57	127.69
22	B	4009	BCR	C34-C9-C8	2.23	121.50	118.09
19	1	602	CLA	CMD-C2D-C3D	-2.23	122.57	127.69
19	1	601	CLA	C4B-CHC-C1C	2.23	131.50	126.25
19	3	614	CLA	CHC-C4B-NB	2.23	127.40	124.05
19	A	1112	CLA	CMD-C2D-C3D	-2.23	122.57	127.69
22	A	4011	BCR	C36-C18-C19	2.23	121.50	118.09
19	1	606	CLA	CMA-C3A-C4A	2.23	117.77	111.77
19	H	1701	CLA	CMD-C2D-C3D	-2.23	122.57	127.69
19	A	1110	CLA	CMD-C2D-C3D	-2.23	122.58	127.69
19	4	602	CLA	CMA-C3A-C4A	2.23	117.77	111.77
22	A	4008	BCR	C34-C9-C10	-2.23	119.20	122.82
19	1	605	CLA	CMA-C3A-C4A	2.23	117.77	111.77
19	1	603	CLA	C1-O2A-CGA	2.23	122.04	116.65
29	2	615	CHL	C4D-CHA-CBD	-2.23	106.72	108.97
19	B	1021	CLA	O2A-CGA-CBA	2.23	118.63	111.83
23	2	801	LHG	C5-O7-C7	-2.23	112.47	117.80
19	B	1239	CLA	CMB-C2B-C1B	2.23	128.81	125.42
22	2	503	BCR	C38-C26-C25	-2.23	122.05	124.48
19	3	602	CLA	O1D-CGD-CBD	-2.23	120.13	124.52
19	B	1201	CLA	C1-C2-C3	-2.23	122.55	126.20
19	B	1205	CLA	C6-C5-C3	-2.23	108.05	113.47
19	B	1225	CLA	CMD-C2D-C3D	-2.23	122.58	127.69
22	A	4008	BCR	C31-C1-C6	-2.23	106.75	110.24
19	B	1227	CLA	CMA-C3A-C4A	2.22	117.75	111.77
19	A	1108	CLA	CMA-C3A-C4A	2.22	117.75	111.77
19	B	1211	CLA	CHD-C1D-ND	-2.22	121.67	124.80
19	J	1901	CLA	O2D-CGD-O1D	-2.22	119.52	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	L	1502	CLA	C1C-C2C-C3C	-2.22	104.65	106.98
19	B	1229	CLA	O1D-CGD-CBD	-2.22	120.14	124.52
19	2	602	CLA	C1D-ND-C4D	-2.22	104.76	106.31
22	3	506	BCR	C23-C22-C21	2.22	122.50	119.01
19	G	1601	CLA	CMA-C3A-C4A	2.22	117.73	111.77
19	B	1222	CLA	C1-O2A-CGA	2.22	122.02	116.65
22	B	4004	BCR	C35-C13-C14	-2.21	119.23	122.82
19	1	604	CLA	CHA-C4D-ND	2.21	137.12	132.55
19	A	1128	CLA	O2A-CGA-CBA	2.21	118.59	111.83
22	1	503	BCR	C3-C4-C5	-2.21	110.11	114.06
19	3	601	CLA	O2A-CGA-CBA	2.21	118.58	111.83
19	B	1224	CLA	O1D-CGD-CBD	-2.21	120.15	124.52
29	2	610	CHL	C4C-CHD-C1D	2.21	123.98	116.07
19	1	604	CLA	C1D-ND-C4D	-2.21	104.76	106.31
22	3	503	BCR	C34-C9-C8	2.21	121.47	118.09
19	B	1232	CLA	CMD-C2D-C3D	-2.21	122.62	127.69
28	4	501	LUT	C37-C21-C36	2.21	111.09	107.87
29	1	610	CHL	C4C-CHD-C1D	2.21	123.97	116.07
19	K	1403	CLA	C1D-ND-C4D	-2.21	104.76	106.31
19	B	1237	CLA	CMD-C2D-C3D	-2.21	122.62	127.69
19	A	1136	CLA	O2A-CGA-CBA	2.21	118.57	111.83
19	B	1205	CLA	C2C-C1C-NC	2.21	112.30	109.98
30	4	502	XAT	C35-C15-C14	-2.21	119.00	123.52
19	B	1240	CLA	C1-C2-C3	-2.21	122.58	126.20
19	A	1106	CLA	C1D-ND-C4D	-2.21	104.76	106.31
23	A	5002	LHG	O7-C7-O9	-2.21	118.54	123.70
19	L	1502	CLA	CMD-C2D-C3D	-2.21	122.63	127.69
19	A	1108	CLA	C2C-C1C-NC	2.21	112.30	109.98
19	B	1208	CLA	C2C-C1C-NC	2.21	112.30	109.98
19	A	1140	CLA	C1-O2A-CGA	2.21	121.99	116.65
19	2	601	CLA	C3B-C4B-NB	-2.21	108.56	110.53
19	A	1136	CLA	CMA-C3A-C4A	2.21	117.70	111.77
19	A	1132	CLA	O1D-CGD-CBD	-2.20	120.17	124.52
18	A	1011	CL0	CMB-C2B-C3B	2.20	129.09	124.68
19	A	1118	CLA	CMD-C2D-C3D	-2.20	122.64	127.69
19	4	617	CLA	O1D-CGD-CBD	-2.20	120.17	124.52
22	B	4005	BCR	C37-C22-C23	2.20	121.45	118.09
19	A	1129	CLA	CMD-C2D-C3D	-2.20	122.64	127.69
19	3	605	CLA	CMD-C2D-C3D	-2.20	122.64	127.69
29	1	610	CHL	C4D-CHA-CBD	-2.20	106.75	108.97
19	3	610	CLA	O2A-CGA-CBA	2.20	118.54	111.83
19	3	610	CLA	CMA-C3A-C4A	2.20	117.69	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	G	1602	CLA	O1D-CGD-CBD	-2.20	120.18	124.52
19	3	605	CLA	C1-O2A-CGA	2.20	121.97	116.65
22	K	4002	BCR	C33-C5-C6	-2.20	122.08	124.48
19	B	1222	CLA	C1C-C2C-C3C	-2.20	104.67	106.98
19	B	1022	CLA	OBD-CAD-C3D	-2.20	123.28	128.42
19	B	1023	CLA	CHD-C1D-ND	-2.20	121.71	124.80
19	A	1108	CLA	O2A-CGA-CBA	2.20	118.53	111.83
28	1	501	LUT	C21-C26-C27	2.20	115.35	112.83
19	3	612	CLA	C2C-C1C-NC	2.20	112.29	109.98
22	I	4018	BCR	C8-C9-C10	2.20	122.46	119.01
29	4	611	CHL	C1-O2A-CGA	2.19	121.96	116.65
22	H	4021	BCR	C31-C1-C6	-2.19	106.80	110.24
19	B	1215	CLA	C2C-C1C-NC	2.19	112.28	109.98
19	A	1123	CLA	CMD-C2D-C3D	-2.19	122.66	127.69
19	B	1022	CLA	O2A-CGA-CBA	2.19	118.52	111.83
19	A	1133	CLA	CHD-C1D-ND	-2.19	121.72	124.80
19	B	1204	CLA	CMA-C3A-C4A	2.19	117.66	111.77
19	A	1013	CLA	C1-O2A-CGA	2.19	121.95	116.65
19	A	1102	CLA	CAA-C2A-C1A	-2.19	104.80	111.97
27	F	5005	DGD	O2G-C1B-O1B	-2.19	118.58	123.70
19	3	601	CLA	O1D-CGD-CBD	-2.19	120.20	124.52
19	A	1107	CLA	CMA-C3A-C4A	2.19	117.65	111.77
19	A	1126	CLA	O1D-CGD-CBD	-2.19	120.21	124.52
22	B	4006	BCR	C31-C1-C6	-2.19	106.81	110.24
28	3	501	LUT	C18-C5-C6	-2.19	122.10	124.48
22	A	4003	BCR	C12-C13-C14	-2.19	115.57	119.01
19	K	1404	CLA	CHA-C1A-NA	-2.19	121.44	126.39
19	4	602	CLA	C1C-C2C-C3C	-2.18	104.68	106.98
19	4	609	CLA	CMD-C2D-C3D	-2.18	122.68	127.69
19	3	602	CLA	CMD-C2D-C3D	-2.18	122.68	127.69
19	B	1229	CLA	CMA-C3A-C4A	2.18	117.64	111.77
19	K	1404	CLA	CMD-C2D-C3D	-2.18	122.68	127.69
19	B	1231	CLA	O2A-CGA-CBA	2.18	118.49	111.83
22	2	503	BCR	C23-C24-C25	-2.18	121.17	127.00
19	A	1140	CLA	CMD-C2D-C3D	-2.18	122.68	127.69
19	B	1213	CLA	CMD-C2D-C3D	-2.18	122.68	127.69
19	A	1124	CLA	O1D-CGD-CBD	-2.18	120.21	124.52
28	2	501	LUT	C30-C31-C32	-2.18	116.88	123.20
19	A	1103	CLA	CMD-C2D-C3D	-2.18	122.69	127.69
19	B	1217	CLA	CMA-C3A-C4A	2.18	117.64	111.77
30	2	502	XAT	C26-C27-C28	-2.18	121.38	125.99
19	3	602	CLA	C2C-C1C-NC	2.18	112.27	109.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	4	605	CLA	C2C-C1C-NC	2.18	112.27	109.98
19	4	602	CLA	C2C-C1C-NC	2.18	112.27	109.98
19	B	1213	CLA	C1-C2-C3	-2.18	122.63	126.20
19	B	1213	CLA	CMA-C3A-C4A	2.18	117.63	111.77
19	A	1133	CLA	C1-O2A-CGA	2.18	121.92	116.65
30	4	502	XAT	C6-C7-C8	-2.18	121.39	125.99
29	4	611	CHL	C4C-CHD-C1D	2.18	123.86	116.07
19	3	601	CLA	CHA-C1A-NA	-2.18	121.46	126.39
19	1	603	CLA	CHA-C1A-NA	-2.18	121.46	126.39
19	4	609	CLA	O2A-CGA-CBA	2.18	118.47	111.83
19	A	1127	CLA	CMD-C2D-C3D	-2.18	122.70	127.69
19	A	1013	CLA	C1D-ND-C4D	-2.18	104.78	106.31
24	2	808	LMT	C1'-O5'-C5'	-2.18	109.47	113.72
19	B	1236	CLA	CMA-C3A-C4A	2.17	117.62	111.77
19	A	1128	CLA	O1D-CGD-CBD	-2.17	120.23	124.52
19	3	605	CLA	O1D-CGD-CBD	-2.17	120.23	124.52
19	B	1208	CLA	CMA-C3A-C4A	2.17	117.62	111.77
19	B	1236	CLA	O1D-CGD-CBD	-2.17	120.23	124.52
22	A	4017	BCR	C12-C13-C14	2.17	122.43	119.01
19	2	603	CLA	C2C-C1C-NC	2.17	112.26	109.98
19	B	1225	CLA	CHA-C1A-NA	-2.17	121.48	126.39
25	F	5004	LMG	O7-C10-O9	-2.17	118.63	123.70
22	F	4016	BCR	C23-C24-C25	-2.17	121.20	127.00
22	L	4019	BCR	C24-C25-C26	-2.17	116.56	121.56
30	4	502	XAT	C7-C8-C9	-2.17	122.16	125.53
19	4	608	CLA	C1D-ND-C4D	-2.17	104.79	106.31
28	J	4013	LUT	C36-C21-C26	-2.17	106.26	109.55
19	B	1021	CLA	O2D-CGD-O1D	-2.17	119.63	123.85
19	4	605	CLA	C2D-C1D-ND	2.17	112.27	110.13
23	B	5002	LHG	O7-C7-O9	-2.17	118.64	123.70
19	B	1222	CLA	CMA-C3A-C4A	2.17	117.60	111.77
19	3	617	CLA	CHA-C1A-NA	-2.17	121.48	126.39
19	4	602	CLA	C1-O2A-CGA	2.17	121.90	116.65
22	B	4004	BCR	C16-C17-C18	2.17	130.32	127.28
19	A	1115	CLA	O1D-CGD-CBD	-2.17	120.24	124.52
22	3	503	BCR	C39-C30-C25	-2.17	106.84	110.24
19	A	1125	CLA	C2D-C1D-ND	2.17	112.27	110.13
19	2	605	CLA	CHA-C1A-NA	-2.17	121.49	126.39
22	A	4008	BCR	C38-C26-C27	2.17	118.21	113.60
22	K	4002	BCR	C2-C3-C4	-2.17	106.52	111.28
19	1	607	CLA	CMD-C2D-C3D	-2.17	122.72	127.69
22	F	4014	BCR	C12-C13-C14	-2.17	115.60	119.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	1112	CLA	CHA-C1A-NA	-2.17	121.49	126.39
19	A	1133	CLA	C2C-C1C-NC	2.17	112.26	109.98
19	A	1137	CLA	C2C-C1C-NC	2.17	112.26	109.98
22	3	503	BCR	C16-C17-C18	2.16	130.31	127.28
25	G	5001	LMG	O7-C10-O9	-2.16	118.65	123.70
22	G	4011	BCR	C37-C22-C21	-2.16	119.31	122.82
28	4	501	LUT	C36-C21-C26	-2.16	106.27	109.55
30	4	502	XAT	C17-C1-C16	2.16	110.51	107.37
19	B	1211	CLA	C1-C2-C3	-2.16	122.66	126.20
19	A	1109	CLA	CMA-C3A-C4A	2.16	117.58	111.77
19	B	1201	CLA	C1D-ND-C4D	-2.16	104.80	106.31
19	B	1236	CLA	O2A-CGA-CBA	2.16	118.42	111.83
19	B	1214	CLA	CMA-C3A-C4A	2.16	117.58	111.77
19	A	1125	CLA	O2A-CGA-CBA	2.16	118.42	111.83
28	1	502	LUT	C15-C14-C13	-2.16	124.25	127.28
29	2	609	CHL	C4C-CHD-C1D	2.16	123.80	116.07
19	A	1104	CLA	C2C-C1C-NC	2.16	112.25	109.98
19	B	1211	CLA	C2C-C1C-NC	2.16	112.25	109.98
19	B	1222	CLA	C2C-C1C-NC	2.16	112.25	109.98
19	B	1209	CLA	C1D-ND-C4D	-2.16	104.80	106.31
19	1	604	CLA	CHD-C1D-ND	-2.16	121.77	124.80
19	A	1109	CLA	C1D-ND-C4D	-2.15	104.80	106.31
19	4	605	CLA	O2D-CGD-O1D	-2.15	119.65	123.85
19	B	1210	CLA	CHA-C1A-NA	-2.15	121.51	126.39
19	2	606	CLA	CMD-C2D-C3D	-2.15	122.75	127.69
19	B	1220	CLA	CHA-C1A-NA	-2.15	121.51	126.39
19	3	605	CLA	CHA-C1A-NA	-2.15	121.51	126.39
19	A	1141	CLA	CMD-C2D-C3D	-2.15	122.75	127.69
19	B	1221	CLA	C5-C3-C2	2.15	126.00	121.17
19	3	617	CLA	O1D-CGD-CBD	-2.15	120.27	124.52
19	A	1139	CLA	CMD-C2D-C3D	-2.15	122.75	127.69
19	B	1205	CLA	CMA-C3A-C4A	2.15	117.56	111.77
19	K	1401	CLA	CAC-C3C-C4C	2.15	127.59	124.79
22	B	4006	BCR	C1-C6-C7	2.15	121.49	115.65
28	J	4013	LUT	C40-C33-C34	-2.15	119.33	122.82
19	3	602	CLA	C1D-ND-C4D	-2.15	104.80	106.31
19	F	1301	CLA	CMD-C2D-C3D	-2.15	122.76	127.69
19	B	1022	CLA	CHA-C1A-NA	-2.15	121.52	126.39
27	3	803	DGD	C2G-O2G-C1B	-2.15	112.65	117.80
22	A	4007	BCR	C1-C6-C5	-2.15	119.70	122.64
19	A	1109	CLA	C4-C3-C2	-2.15	118.11	123.63
19	B	1219	CLA	CMD-C2D-C3D	-2.15	122.76	127.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	1228	CLA	CMD-C2D-C3D	-2.15	122.76	127.69
22	F	4014	BCR	C29-C30-C25	2.15	113.56	110.44
19	4	617	CLA	CHA-C4D-ND	2.15	136.98	132.55
19	B	1207	CLA	CHA-C1A-NA	-2.15	121.53	126.39
22	1	503	BCR	C33-C5-C6	-2.15	122.14	124.48
19	B	1202	CLA	C2D-C1D-ND	2.15	112.25	110.13
22	B	4009	BCR	C29-C28-C27	2.15	116.00	111.28
19	L	1503	CLA	C2C-C1C-NC	2.15	112.24	109.98
19	4	612	CLA	C1-C2-C3	-2.15	122.68	126.20
19	2	605	CLA	O2A-CGA-CBA	2.15	118.38	111.83
19	1	614	CLA	C1D-ND-C4D	-2.14	104.81	106.31
19	1	601	CLA	O2D-CGD-O1D	-2.14	119.67	123.85
19	K	1401	CLA	C1C-C2C-C3C	-2.14	104.72	106.98
19	A	1104	CLA	C1D-ND-C4D	-2.14	104.81	106.31
19	B	1230	CLA	CHD-C1D-ND	-2.14	121.79	124.80
19	1	614	CLA	C2C-C1C-NC	2.14	112.23	109.98
19	B	1239	CLA	C1D-ND-C4D	-2.14	104.81	106.31
19	B	1022	CLA	O1D-CGD-CBD	-2.14	120.29	124.52
19	2	608	CLA	CHD-C1D-ND	-2.14	121.79	124.80
19	A	1121	CLA	C3D-C2D-C1D	-2.14	102.91	105.83
19	L	1503	CLA	CHA-C4D-ND	2.14	136.97	132.55
19	3	612	CLA	CHA-C1A-NA	-2.14	121.54	126.39
19	1	601	CLA	O2A-CGA-CBA	2.14	118.36	111.83
19	1	608	CLA	CMA-C3A-C4A	2.14	117.52	111.77
19	B	1234	CLA	CMD-C2D-C3D	-2.14	122.78	127.69
19	2	607	CLA	C1-C2-C3	-2.14	122.69	126.20
19	4	601	CLA	CMA-C3A-C4A	2.14	117.52	111.77
19	A	1121	CLA	C1-C2-C3	-2.14	122.69	126.20
19	A	1102	CLA	CMA-C3A-C4A	2.14	117.52	111.77
19	A	1104	CLA	C2D-C1D-ND	2.14	112.24	110.13
19	B	1223	CLA	O1D-CGD-CBD	-2.14	120.30	124.52
19	L	1501	CLA	C1D-ND-C4D	-2.14	104.81	106.31
19	3	607	CLA	O2A-CGA-CBA	2.14	118.35	111.83
25	B	5003	LMG	C8-O7-C10	-2.14	112.69	117.80
19	B	1207	CLA	C1D-ND-C4D	-2.13	104.81	106.31
22	K	4002	BCR	C39-C30-C25	-2.13	106.90	110.24
19	B	1211	CLA	C1D-ND-C4D	-2.13	104.81	106.31
19	L	1501	CLA	CHD-C1D-ND	-2.13	121.80	124.80
19	2	603	CLA	C2D-C1D-ND	2.13	112.24	110.13
29	2	611	CHL	C4C-CHD-C1D	2.13	123.70	116.07
19	B	1240	CLA	C4-C3-C2	-2.13	118.15	123.63
19	3	601	CLA	CMD-C2D-C3D	-2.13	122.80	127.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	4	502	XAT	O4-C5-C4	-2.13	111.49	113.49
19	3	603	CLA	C1-C2-C3	-2.13	122.70	126.20
22	B	4006	BCR	C34-C9-C8	2.13	121.34	118.09
19	F	1301	CLA	CHA-C1A-NA	-2.13	121.57	126.39
19	A	1112	CLA	O1D-CGD-CBD	-2.13	120.32	124.52
19	A	1138	CLA	O2A-CGA-CBA	2.13	118.33	111.83
19	4	617	CLA	CHD-C1D-ND	-2.13	121.81	124.80
19	2	608	CLA	C1D-ND-C4D	-2.13	104.82	106.31
19	L	1502	CLA	C1D-ND-C4D	-2.13	104.82	106.31
19	B	1220	CLA	C2C-C1C-NC	2.13	112.22	109.98
19	4	602	CLA	O2A-CGA-CBA	2.13	118.32	111.83
19	B	1210	CLA	O1D-CGD-CBD	-2.13	120.32	124.52
19	4	602	CLA	C2D-C1D-ND	2.13	112.23	110.13
29	3	611	CHL	C4C-CHD-C1D	2.13	123.67	116.07
22	A	4017	BCR	C23-C24-C25	-2.13	121.32	127.00
22	B	4009	BCR	C29-C30-C25	-2.13	107.35	110.44
19	A	1013	CLA	CHD-C1D-ND	-2.13	121.81	124.80
28	3	501	LUT	C36-C21-C26	-2.13	106.33	109.55
19	L	1501	CLA	O2A-CGA-CBA	2.12	118.31	111.83
19	B	1203	CLA	CMD-C2D-C3D	-2.12	122.82	127.69
19	2	607	CLA	CAA-CBA-CGA	-2.12	107.18	113.21
19	A	1012	CLA	OBD-CAD-C3D	-2.12	123.45	128.42
19	B	1203	CLA	O2A-CGA-CBA	2.12	118.31	111.83
19	B	1212	CLA	C1D-ND-C4D	-2.12	104.82	106.31
19	A	1131	CLA	O1D-CGD-CBD	-2.12	120.33	124.52
19	L	1502	CLA	C2C-C1C-NC	2.12	112.21	109.98
19	A	1104	CLA	O2A-CGA-CBA	2.12	118.31	111.83
19	A	1126	CLA	CHA-C1A-NA	-2.12	121.59	126.39
19	B	1228	CLA	O2A-CGA-CBA	2.12	118.30	111.83
28	1	501	LUT	C10-C11-C12	-2.12	117.05	123.20
28	4	501	LUT	C40-C33-C34	-2.12	119.38	122.82
19	A	1131	CLA	CHA-C1A-NA	-2.12	121.59	126.39
19	B	1203	CLA	CHA-C1A-NA	-2.12	121.59	126.39
22	A	4008	BCR	C29-C30-C25	-2.12	107.36	110.44
19	B	1218	CLA	C2D-C1D-ND	2.12	112.22	110.13
19	L	1502	CLA	CMA-C3A-C4A	2.12	117.47	111.77
19	B	1230	CLA	O1D-CGD-CBD	-2.12	120.34	124.52
25	B	5003	LMG	O7-C10-O9	-2.12	118.75	123.70
22	F	4014	BCR	C23-C24-C25	-2.12	121.34	127.00
19	B	1224	CLA	CHD-C1D-ND	-2.12	121.82	124.80
22	B	4009	BCR	C12-C13-C14	-2.12	115.68	119.01
19	L	1503	CLA	C4D-CHA-C1A	2.12	123.77	121.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	1218	CLA	C2C-C1C-NC	2.12	112.20	109.98
19	B	1240	CLA	CMD-C2D-C3D	-2.12	122.84	127.69
19	B	1240	CLA	CMA-C3A-C4A	2.12	117.46	111.77
19	B	1231	CLA	C6-C5-C3	-2.12	108.31	113.47
24	B	5008	LMT	C1'-O5'-C5'	-2.12	109.59	113.72
19	A	1108	CLA	CMD-C2D-C3D	-2.12	122.84	127.69
19	A	1129	CLA	C1-O2A-CGA	2.11	121.77	116.65
18	A	1011	CL0	C4C-C3C-C2C	-2.11	105.02	113.37
19	2	605	CLA	CMA-C3A-C4A	2.11	117.45	111.77
19	B	1234	CLA	CHA-C1A-NA	-2.11	121.61	126.39
28	3	502	LUT	C15-C35-C34	-2.11	119.20	123.52
19	4	617	CLA	C4-C3-C2	-2.11	118.20	123.63
19	B	1217	CLA	O1D-CGD-CBD	-2.11	120.35	124.52
19	B	1239	CLA	O2A-CGA-CBA	2.11	118.27	111.83
19	B	1236	CLA	CHD-C1D-ND	-2.11	121.83	124.80
29	4	610	CHL	C4C-CHD-C1D	2.11	123.62	116.07
19	2	602	CLA	CMD-C2D-C3D	-2.11	122.85	127.69
19	A	1113	CLA	CHA-C1A-NA	-2.11	121.61	126.39
19	B	1232	CLA	CMA-C3A-C4A	2.11	117.44	111.77
28	4	505	LUT	C36-C21-C26	-2.11	106.35	109.55
29	3	604	CHL	C4C-CHD-C1D	2.11	123.61	116.07
19	1	611	CLA	C1-C2-C3	-2.11	122.74	126.20
19	B	1217	CLA	CMD-C2D-C3D	-2.11	122.86	127.69
19	B	1205	CLA	C1C-C2C-C3C	-2.11	104.76	106.98
19	A	1101	CLA	O2A-CGA-CBA	2.11	118.26	111.83
22	1	503	BCR	C31-C1-C6	-2.11	106.94	110.24
22	F	4014	BCR	C30-C25-C26	-2.11	119.76	122.64
29	4	615	CHL	C4C-CHD-C1D	2.11	123.60	116.07
19	B	1204	CLA	O1D-CGD-CBD	-2.11	120.36	124.52
22	B	4006	BCR	C34-C9-C10	-2.11	119.41	122.82
19	B	1207	CLA	CMA-C3A-C4A	2.11	117.43	111.77
19	A	1129	CLA	CHD-C1D-ND	-2.10	121.84	124.80
19	A	1101	CLA	CHA-C1A-NA	-2.10	121.63	126.39
19	A	1110	CLA	C2C-C1C-NC	2.10	112.19	109.98
19	B	1227	CLA	C1-O2A-CGA	2.10	121.74	116.65
19	4	608	CLA	CMA-C3A-C4A	2.10	117.43	111.77
19	B	1212	CLA	CMD-C2D-C3D	-2.10	122.86	127.69
19	K	1403	CLA	CHA-C1A-NA	-2.10	121.63	126.39
19	4	607	CLA	CMD-C2D-C3D	-2.10	122.87	127.69
19	4	603	CLA	CMB-C2B-C1B	2.10	128.62	125.42
19	3	610	CLA	CAA-C2A-C3A	2.10	118.68	113.00
19	A	1104	CLA	CHA-C1A-NA	-2.10	121.63	126.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	1202	CLA	CHD-C1D-ND	-2.10	121.84	124.80
19	A	1130	CLA	C1-C2-C3	-2.10	122.75	126.20
29	2	610	CHL	CMD-C2D-C3D	2.10	128.88	124.68
19	B	1209	CLA	CHD-C1D-ND	-2.10	121.84	124.80
19	4	617	CLA	CMA-C3A-C4A	2.10	117.42	111.77
22	A	4002	BCR	C15-C16-C17	2.10	127.82	123.52
19	B	1222	CLA	CAA-C2A-C1A	-2.10	105.09	111.97
19	4	607	CLA	C1D-ND-C4D	-2.10	104.84	106.31
19	B	1223	CLA	CHA-C1A-NA	-2.10	121.63	126.39
19	B	1201	CLA	O2A-CGA-CBA	2.10	118.24	111.83
19	A	1119	CLA	O1D-CGD-CBD	-2.10	120.38	124.52
19	A	1114	CLA	C1D-ND-C4D	-2.10	104.84	106.31
19	B	1207	CLA	CMD-C2D-C3D	-2.10	122.88	127.69
19	A	1139	CLA	O2D-CGD-O1D	-2.10	119.76	123.85
19	A	1125	CLA	CMD-C2D-C3D	-2.10	122.88	127.69
19	A	1128	CLA	CMD-C2D-C3D	-2.10	122.88	127.69
19	3	605	CLA	OBD-CAD-C3D	-2.10	123.51	128.42
19	B	1204	CLA	C1-C2-C3	-2.10	122.76	126.20
19	B	1223	CLA	CMA-C3A-C4A	2.10	117.41	111.77
29	1	610	CHL	C1-O2A-CGA	2.10	122.78	116.07
25	G	5006	LMG	C8-O7-C10	-2.10	112.78	117.80
19	3	603	CLA	C4-C3-C5	2.10	118.87	115.23
19	4	608	CLA	CHD-C1D-ND	-2.10	121.85	124.80
19	1	602	CLA	C1D-ND-C4D	-2.10	104.84	106.31
19	A	1113	CLA	O1D-CGD-CBD	-2.09	120.39	124.52
19	4	605	CLA	CMA-C3A-C4A	2.09	117.40	111.77
28	2	501	LUT	C18-C5-C6	-2.09	122.20	124.48
19	3	603	CLA	C1D-ND-C4D	-2.09	104.84	106.31
19	A	1129	CLA	CHC-C4B-NB	2.09	127.19	124.05
19	1	605	CLA	C6-C5-C3	2.09	118.56	113.47
19	F	1302	CLA	CMD-C2D-C3D	-2.09	122.90	127.69
19	B	1223	CLA	C3D-C2D-C1D	-2.09	102.98	105.83
19	A	1106	CLA	C2C-C1C-NC	2.09	112.18	109.98
19	3	607	CLA	CHD-C1D-ND	-2.09	121.86	124.80
19	A	1103	CLA	C2D-C1D-ND	2.09	112.19	110.13
19	A	1120	CLA	C1-C2-C3	-2.09	122.77	126.20
19	B	1216	CLA	CMD-C2D-C3D	-2.09	122.90	127.69
22	B	4010	BCR	C16-C17-C18	2.09	130.21	127.28
22	K	4001	BCR	C1-C6-C7	2.09	121.31	115.65
19	A	1133	CLA	C1D-ND-C4D	-2.09	104.85	106.31
19	K	1402	CLA	C1D-ND-C4D	-2.09	104.85	106.31
19	A	1121	CLA	C2C-C1C-NC	2.09	112.17	109.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	1203	CLA	C1D-ND-C4D	-2.09	104.85	106.31
19	A	1116	CLA	CHA-C1A-NA	-2.09	121.67	126.39
19	G	1602	CLA	CHA-C1A-NA	-2.09	121.67	126.39
19	B	1230	CLA	CMA-C3A-C4A	2.09	117.38	111.77
19	3	601	CLA	O2D-CGD-O1D	-2.09	119.79	123.85
19	B	1204	CLA	C4-C3-C5	2.08	118.85	115.23
19	B	1240	CLA	C4-C3-C5	2.08	118.85	115.23
19	4	607	CLA	O2A-CGA-CBA	2.08	118.19	111.83
19	B	1228	CLA	O1D-CGD-CBD	-2.08	120.41	124.52
19	B	1208	CLA	CHD-C1D-ND	-2.08	121.87	124.80
19	A	1130	CLA	CHA-C1A-NA	-2.08	121.67	126.39
29	2	615	CHL	CMD-C2D-C3D	2.08	128.84	124.68
22	L	4020	BCR	C7-C6-C5	2.08	126.35	121.56
19	A	1139	CLA	CHA-C1A-NA	-2.08	121.68	126.39
19	3	602	CLA	CMA-C3A-C4A	2.08	117.37	111.77
19	3	605	CLA	CMA-C3A-C4A	2.08	117.37	111.77
19	B	1212	CLA	O2A-CGA-CBA	2.08	118.18	111.83
19	3	606	CLA	CMA-C3A-C4A	2.08	117.37	111.77
19	B	1221	CLA	CHA-C1A-NA	-2.08	121.68	126.39
19	A	1134	CLA	C1-C2-C3	-2.08	122.79	126.20
19	A	1135	CLA	CMD-C2D-C3D	-2.08	122.92	127.69
19	3	603	CLA	O1D-CGD-CBD	-2.08	120.42	124.52
19	B	1023	CLA	CHA-C1A-NA	-2.08	121.68	126.39
19	2	606	CLA	CHA-C1A-NA	-2.08	121.69	126.39
19	A	1111	CLA	C1D-ND-C4D	-2.08	104.85	106.31
19	A	1127	CLA	C1-C2-C3	-2.08	122.79	126.20
19	A	1106	CLA	CMA-C3A-C4A	2.08	117.36	111.77
19	A	1115	CLA	O2A-CGA-CBA	2.08	118.17	111.83
22	2	503	BCR	C32-C1-C31	2.08	114.58	108.63
19	B	1214	CLA	O1D-CGD-CBD	-2.08	120.42	124.52
22	F	4014	BCR	C34-C9-C8	2.08	121.26	118.09
22	A	4007	BCR	C33-C5-C4	2.07	118.02	113.60
22	A	4011	BCR	C37-C22-C23	2.07	121.26	118.09
20	A	2001	PQN	C2M-C2-C3	-2.07	121.04	124.45
19	A	1130	CLA	O1D-CGD-CBD	-2.07	120.43	124.52
19	3	613	CLA	CHC-C4B-NB	2.07	127.16	124.05
19	3	605	CLA	O2A-CGA-CBA	2.07	118.15	111.83
19	B	1220	CLA	CMA-C3A-C4A	2.07	117.34	111.77
22	G	4011	BCR	C1-C6-C5	-2.07	119.80	122.64
22	F	4016	BCR	C2-C1-C6	2.07	113.45	110.44
25	G	5002	LMG	O7-C10-O9	-2.07	118.86	123.70
19	2	601	CLA	CHA-C1A-NA	-2.07	121.70	126.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	L	1502	CLA	C2D-C1D-ND	2.07	112.18	110.13
19	B	1224	CLA	CHA-C1A-NA	-2.07	121.70	126.39
29	3	611	CHL	C1-O2A-CGA	2.07	122.70	116.07
19	A	1117	CLA	CHD-C1D-ND	-2.07	121.89	124.80
19	B	1206	CLA	CHA-C1A-NA	-2.07	121.70	126.39
19	A	1140	CLA	O1D-CGD-CBD	-2.07	120.44	124.52
19	B	1229	CLA	C1D-ND-C4D	-2.07	104.86	106.31
19	H	1701	CLA	C1D-ND-C4D	-2.07	104.86	106.31
22	A	4002	BCR	C37-C22-C21	-2.07	119.46	122.82
19	1	613	CLA	CHA-C1A-NA	-2.07	121.71	126.39
28	2	501	LUT	O23-C23-C22	2.07	113.72	110.06
19	A	1013	CLA	C2C-C1C-NC	2.07	112.15	109.98
19	A	1124	CLA	CHA-C1A-NA	-2.07	121.71	126.39
19	B	1227	CLA	CHD-C1D-ND	-2.07	121.89	124.80
22	A	4002	BCR	C1-C6-C7	-2.07	110.05	115.65
19	2	601	CLA	CMA-C3A-C4A	2.07	117.33	111.77
19	3	612	CLA	CMD-C2D-C3D	-2.07	122.95	127.69
19	B	1201	CLA	C2C-C1C-NC	2.07	112.15	109.98
29	1	612	CHL	CMD-C2D-C3D	2.07	128.81	124.68
19	A	1103	CLA	C3D-C2D-C1D	-2.07	103.01	105.83
19	1	603	CLA	C1-C2-C3	-2.07	122.81	126.20
19	B	1240	CLA	C1D-ND-C4D	-2.07	104.86	106.31
19	A	1132	CLA	O2A-CGA-CBA	2.06	118.13	111.83
19	A	1127	CLA	CHD-C1D-ND	-2.06	121.90	124.80
19	B	1214	CLA	CBB-CAB-C3B	-2.06	117.21	127.53
19	A	1112	CLA	CHC-C4B-NB	2.06	127.14	124.05
19	A	1101	CLA	C1D-ND-C4D	-2.06	104.86	106.31
29	4	615	CHL	CMD-C2D-C3D	2.06	128.81	124.68
19	A	1134	CLA	O1D-CGD-CBD	-2.06	120.45	124.52
19	B	1228	CLA	CMA-C3A-C4A	2.06	117.32	111.77
19	A	1140	CLA	CHD-C1D-ND	-2.06	121.90	124.80
22	B	4005	BCR	C16-C17-C18	2.06	130.17	127.28
22	B	4009	BCR	C23-C24-C25	-2.06	121.49	127.00
19	A	1110	CLA	C1D-ND-C4D	-2.06	104.87	106.31
19	B	1236	CLA	C1D-ND-C4D	-2.06	104.87	106.31
19	4	612	CLA	CMD-C2D-C3D	-2.06	122.96	127.69
19	2	604	CLA	C1-O2A-CGA	2.06	121.64	116.65
19	2	602	CLA	CHA-C1A-NA	-2.06	121.72	126.39
19	4	609	CLA	CHA-C1A-NA	-2.06	121.73	126.39
28	1	502	LUT	C32-C33-C34	-2.06	115.77	119.01
19	A	1103	CLA	O2A-CGA-CBA	2.06	118.11	111.83
19	B	1201	CLA	CHD-C1D-ND	-2.06	121.91	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	1102	CLA	C2C-C1C-NC	2.06	112.14	109.98
19	A	1117	CLA	CMA-C3A-C4A	2.06	117.30	111.77
19	A	1115	CLA	CHA-C1A-NA	-2.06	121.73	126.39
19	A	1113	CLA	CHD-C1D-ND	-2.06	121.91	124.80
22	2	503	BCR	C29-C28-C27	-2.06	106.76	111.28
19	A	1102	CLA	CHD-C1D-ND	-2.06	121.91	124.80
25	F	5002	LMG	O7-C10-O9	-2.06	118.90	123.70
22	1	503	BCR	C16-C17-C18	2.06	130.16	127.28
19	B	1201	CLA	CMA-C3A-C4A	2.06	117.30	111.77
19	2	601	CLA	C1D-ND-C4D	-2.06	104.87	106.31
25	B	5004	LMG	O6-C5-C6	2.05	111.53	106.44
19	B	1222	CLA	CMD-C2D-C3D	-2.05	122.98	127.69
19	2	602	CLA	C2D-C1D-ND	2.05	112.16	110.13
19	B	1239	CLA	C1-C2-C3	-2.05	122.83	126.20
19	A	1129	CLA	CHA-C1A-NA	-2.05	121.74	126.39
19	2	604	CLA	O1D-CGD-CBD	-2.05	120.47	124.52
28	4	501	LUT	C18-C5-C6	-2.05	122.25	124.48
19	B	1230	CLA	CAA-C2A-C1A	-2.05	105.25	111.97
19	B	1215	CLA	C1D-ND-C4D	-2.05	104.87	106.31
19	A	1112	CLA	C1-C2-C3	-2.05	122.84	126.20
19	B	1213	CLA	CHA-C1A-NA	-2.05	121.75	126.39
19	A	1115	CLA	CMD-C2D-C3D	-2.05	122.99	127.69
19	G	1601	CLA	CMD-C2D-C3D	-2.05	122.99	127.69
19	2	601	CLA	CMD-C2D-C3D	-2.05	122.99	127.69
19	A	1141	CLA	C1D-ND-C4D	-2.05	104.87	106.31
19	A	1109	CLA	C2C-C1C-NC	2.05	112.13	109.98
19	B	1237	CLA	C1-O2A-CGA	2.05	121.61	116.65
19	A	1107	CLA	CHA-C1A-NA	-2.05	121.75	126.39
19	A	1138	CLA	CMD-C2D-C3D	-2.05	122.99	127.69
19	3	606	CLA	C1D-ND-C4D	-2.05	104.88	106.31
29	1	609	CHL	CMD-C2D-C3D	2.05	128.78	124.68
22	I	4018	BCR	C38-C26-C27	2.05	117.96	113.60
19	A	1130	CLA	C1-O2A-CGA	2.05	121.61	116.65
19	A	1111	CLA	CHD-C1D-ND	-2.05	121.92	124.80
19	A	1139	CLA	C1-O2A-CGA	2.05	121.61	116.65
19	A	1110	CLA	CMA-C3A-C4A	2.05	117.27	111.77
19	2	601	CLA	O2D-CGD-O1D	-2.05	119.86	123.85
28	1	501	LUT	C8-C9-C10	-2.05	115.79	119.01
19	A	1131	CLA	CMD-C2D-C3D	-2.05	123.00	127.69
19	2	607	CLA	CHA-C1A-NA	-2.05	121.76	126.39
22	A	4002	BCR	C23-C24-C25	-2.05	121.53	127.00
19	4	617	CLA	C3D-C2D-C1D	-2.04	103.04	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	4	602	CLA	CMD-C2D-C3D	-2.04	123.00	127.69
19	B	1235	CLA	C1D-ND-C4D	-2.04	104.88	106.31
19	A	1134	CLA	CHA-C1A-NA	-2.04	121.76	126.39
29	4	610	CHL	CMD-C2D-C3D	2.04	128.77	124.68
22	H	4021	BCR	C15-C14-C13	-2.04	124.41	127.28
19	A	1117	CLA	C1D-ND-C4D	-2.04	104.88	106.31
19	A	1132	CLA	CMA-C3A-C4A	2.04	117.26	111.77
28	3	502	LUT	C8-C9-C10	-2.04	115.80	119.01
19	B	1207	CLA	C2D-C1D-ND	2.04	112.15	110.13
29	3	604	CHL	CMD-C2D-C3D	2.04	128.76	124.68
19	B	1236	CLA	C1-O2A-CGA	2.04	121.59	116.65
28	4	501	LUT	C11-C12-C13	-2.04	120.77	126.36
27	F	5005	DGD	C2G-O2G-C1B	-2.04	112.91	117.80
22	I	4020	BCR	C33-C5-C6	-2.04	122.26	124.48
19	A	1137	CLA	C1D-ND-C4D	-2.04	104.88	106.31
19	A	1104	CLA	C3D-C2D-C1D	-2.04	103.05	105.83
19	1	603	CLA	CBA-CAA-C2A	2.04	119.86	113.79
19	F	1302	CLA	CHA-C1A-NA	-2.04	121.77	126.39
19	B	1211	CLA	C1-O2A-CGA	2.04	121.59	116.65
22	B	4006	BCR	C20-C21-C22	2.04	130.14	127.28
19	1	614	CLA	O1D-CGD-CBD	-2.04	120.50	124.52
28	3	502	LUT	C31-C30-C29	-2.04	124.42	127.28
30	4	502	XAT	C24-C23-C22	-2.04	106.98	110.79
29	2	615	CHL	C4C-CHD-C1D	2.04	123.36	116.07
22	3	503	BCR	C2-C3-C4	-2.04	106.79	111.28
19	B	1231	CLA	CHA-C1A-NA	-2.04	121.77	126.39
19	4	608	CLA	O1D-CGD-CBD	-2.04	120.50	124.52
22	B	4009	BCR	C1-C6-C5	-2.04	119.85	122.64
19	4	601	CLA	CHD-C1D-ND	-2.04	121.93	124.80
18	A	1011	CL0	C1-C2-C3	-2.04	122.86	126.20
19	A	1135	CLA	O2A-CGA-CBA	2.04	118.05	111.83
19	A	1104	CLA	CMD-C2D-C3D	-2.04	123.02	127.69
19	3	613	CLA	CHA-C1A-NA	-2.04	121.78	126.39
19	A	1111	CLA	O2A-C1-C2	2.04	115.94	108.11
22	3	506	BCR	C7-C6-C5	-2.04	116.86	121.56
19	B	1211	CLA	O1D-CGD-CBD	-2.04	120.50	124.52
19	G	1603	CLA	CHA-C1A-NA	-2.04	121.78	126.39
19	B	1206	CLA	CMD-C2D-C3D	-2.04	123.02	127.69
19	4	601	CLA	O2D-CGD-O1D	-2.04	119.89	123.85
23	B	5001	LHG	O7-C7-O9	-2.04	119.06	122.99
19	L	1503	CLA	CHA-C1A-NA	-2.03	121.78	126.39
19	A	1140	CLA	C2D-C1D-ND	2.03	112.14	110.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	1116	CLA	C4-C3-C2	-2.03	118.41	123.63
22	L	4019	BCR	C31-C1-C6	-2.03	107.06	110.24
19	3	602	CLA	CHD-C1D-ND	-2.03	121.94	124.80
22	F	4016	BCR	C19-C18-C17	-2.03	115.81	119.01
19	H	1701	CLA	CMA-C3A-C4A	2.03	117.23	111.77
19	1	605	CLA	O2A-CGA-CBA	2.03	118.03	111.83
19	B	1204	CLA	CMD-C2D-C3D	-2.03	123.03	127.69
19	4	606	CLA	CMA-C3A-C4A	2.03	117.23	111.77
19	L	1502	CLA	C3D-C2D-C1D	-2.03	103.06	105.83
19	A	1135	CLA	C1-O2A-CGA	2.03	121.57	116.65
29	2	609	CHL	C1-C2-C3	-2.03	122.87	126.20
19	A	1126	CLA	CHD-C1D-ND	-2.03	121.95	124.80
19	B	1215	CLA	CHD-C1D-ND	-2.03	121.95	124.80
19	3	610	CLA	O1D-CGD-CBD	-2.03	120.52	124.52
19	A	1140	CLA	C1-C2-C3	-2.03	122.87	126.20
19	A	1110	CLA	C1C-C2C-C3C	-2.03	104.85	106.98
19	A	1105	CLA	O1D-CGD-CBD	-2.03	120.52	124.52
19	2	601	CLA	CBA-CAA-C2A	2.03	119.83	113.79
19	B	1214	CLA	CHA-C1A-NA	-2.03	121.80	126.39
19	B	1216	CLA	O1D-CGD-CBD	-2.03	120.52	124.52
19	1	606	CLA	O1D-CGD-CBD	-2.03	120.52	124.52
29	2	609	CHL	CMD-C2D-C3D	2.03	128.73	124.68
22	B	4009	BCR	C16-C17-C18	2.03	130.12	127.28
19	B	1208	CLA	C1-O2A-CGA	2.03	121.55	116.65
19	2	604	CLA	CHA-C1A-NA	-2.03	121.81	126.39
30	2	502	XAT	C10-C11-C12	-2.03	117.33	123.20
27	4	802	DGD	C2G-O2G-C1B	-2.02	112.95	117.80
19	2	603	CLA	CMD-C2D-C3D	-2.02	123.05	127.69
19	1	601	CLA	CHA-C1A-NA	-2.02	121.81	126.39
19	B	1221	CLA	CMD-C2D-C3D	-2.02	123.05	127.69
28	3	502	LUT	C11-C10-C9	-2.02	124.44	127.28
19	A	1119	CLA	CHA-C1A-NA	-2.02	121.81	126.39
19	3	608	CLA	CHA-C1A-NA	-2.02	121.81	126.39
22	K	4001	BCR	C31-C1-C6	-2.02	107.07	110.24
19	A	1127	CLA	C1-O2A-CGA	2.02	121.54	116.65
19	B	1202	CLA	C5-C3-C2	2.02	125.70	121.17
19	A	1134	CLA	O2A-CGA-CBA	2.02	118.00	111.83
19	2	606	CLA	CHC-C4B-NB	2.02	127.08	124.05
25	2	805	LMG	C8-O7-C10	-2.02	112.96	117.80
19	F	1302	CLA	C1D-ND-C4D	-2.02	104.89	106.31
19	G	1602	CLA	C1D-ND-C4D	-2.02	104.89	106.31
19	1	606	CLA	C1D-ND-C4D	-2.02	104.89	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	1207	CLA	O2A-CGA-CBA	2.02	118.00	111.83
19	B	1022	CLA	CHD-C1D-ND	-2.02	121.96	124.80
19	B	1229	CLA	CHD-C1D-ND	-2.02	121.96	124.80
19	A	1013	CLA	CMD-C2D-C3D	-2.02	123.06	127.69
19	3	607	CLA	C1D-ND-C4D	-2.02	104.89	106.31
19	A	1118	CLA	O1D-CGD-CBD	-2.02	120.53	124.52
19	2	602	CLA	O1D-CGD-CBD	-2.02	120.53	124.52
19	B	1235	CLA	O1D-CGD-CBD	-2.02	120.54	124.52
19	A	1128	CLA	CMA-C3A-C4A	2.02	117.20	111.77
19	1	602	CLA	CHA-C1A-NA	-2.02	121.83	126.39
19	A	1131	CLA	CHD-C1D-ND	-2.02	121.97	124.80
22	B	4010	BCR	C33-C5-C4	2.02	117.89	113.60
19	B	1207	CLA	C1-O2A-CGA	2.02	121.53	116.65
19	B	1204	CLA	CHA-C1A-NA	-2.02	121.83	126.39
19	A	1111	CLA	O2A-CGA-CBA	2.02	117.98	111.83
19	A	1141	CLA	C2D-C1D-ND	2.01	112.12	110.13
18	A	1011	CL0	C1A-CHA-C4D	2.01	122.34	118.98
19	A	1106	CLA	CHD-C1D-ND	-2.01	121.97	124.80
19	B	1222	CLA	O2A-CGA-CBA	2.01	117.98	111.83
19	A	1120	CLA	CHD-C1D-ND	-2.01	121.97	124.80
19	A	1114	CLA	O1D-CGD-CBD	-2.01	120.55	124.52
19	B	1222	CLA	CHA-C1A-NA	-2.01	121.83	126.39
19	F	1302	CLA	O1D-CGD-CBD	-2.01	120.55	124.52
28	J	4013	LUT	C35-C15-C14	-2.01	119.40	123.52
19	A	1107	CLA	CMD-C2D-C3D	-2.01	123.08	127.69
19	H	1701	CLA	CHA-C1A-NA	-2.01	121.84	126.39
19	A	1108	CLA	C3D-C2D-C1D	-2.01	103.09	105.83
19	2	601	CLA	C2D-C1D-ND	2.01	112.12	110.13
19	3	612	CLA	CHD-C1D-ND	-2.01	121.97	124.80
22	1	503	BCR	C7-C6-C5	-2.01	116.92	121.56
19	2	612	CLA	C1D-ND-C4D	-2.01	104.90	106.31
19	B	1212	CLA	C2D-C1D-ND	2.01	112.11	110.13
28	3	502	LUT	C22-C23-C24	-2.01	108.20	111.18
22	F	4014	BCR	C2-C3-C4	-2.01	106.86	111.28
19	4	608	CLA	O2A-CGA-CBA	2.01	119.73	112.14
28	3	501	LUT	C11-C12-C13	-2.01	120.86	126.36
19	A	1128	CLA	CHD-C1D-ND	-2.01	121.98	124.80
19	B	1231	CLA	CHD-C1D-ND	-2.01	121.98	124.80
19	2	608	CLA	O1D-CGD-CBD	-2.01	120.56	124.52
29	4	613	CHL	CMD-C2D-C3D	2.01	128.69	124.68
24	B	5008	LMT	C3B-C4B-C5B	-2.01	106.60	110.23
19	4	612	CLA	CHA-C1A-NA	-2.01	121.85	126.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	4005	BCR	C8-C9-C10	2.01	122.16	119.01
19	1	611	CLA	CHD-C1D-ND	-2.00	121.98	124.80
19	3	606	CLA	CHD-C1D-ND	-2.00	121.98	124.80
29	4	611	CHL	CMD-C2D-C3D	2.00	128.69	124.68
19	G	1601	CLA	O1D-CGD-CBD	-2.00	120.56	124.52
19	B	1202	CLA	C3D-C2D-C1D	-2.00	103.10	105.83
19	B	1022	CLA	CMD-C2D-C3D	-2.00	123.10	127.69
19	B	1207	CLA	C4-C3-C2	-2.00	118.48	123.63
25	B	5004	LMG	O8-C28-O10	-2.00	118.62	123.63
19	3	608	CLA	O1D-CGD-CBD	-2.00	120.57	124.52
19	A	1012	CLA	CMA-C3A-C4A	2.00	117.15	111.77
19	J	1901	CLA	CHA-C1A-NA	-2.00	121.86	126.39
19	B	1022	CLA	C6-C5-C3	-2.00	108.60	113.47

All (206) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
18	A	1011	CL0	NC
18	A	1011	CL0	NA
18	A	1011	CL0	ND
19	A	1012	CLA	ND
19	A	1013	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	1109	CLA	ND
19	A	1110	CLA	ND
19	A	1111	CLA	ND
19	A	1112	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
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

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Mol	Chain	Res	Type	Atom
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	A	1101	CLA	ND
19	A	1108	CLA	ND
19	A	1113	CLA	ND
19	B	1022	CLA	ND
19	B	1237	CLA	ND
19	B	1021	CLA	ND
19	B	1023	CLA	ND
19	B	1201	CLA	ND
19	B	1202	CLA	ND
19	B	1203	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
19	B	1217	CLA	ND
19	B	1218	CLA	ND

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Mol	Chain	Res	Type	Atom
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	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	1238	CLA	ND
19	B	1239	CLA	ND
19	B	1229	CLA	ND
19	B	1204	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	H	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
19	1	606	CLA	ND
19	1	607	CLA	ND

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Mol	Chain	Res	Type	Atom
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	612	CLA	ND
19	2	608	CLA	ND
19	3	601	CLA	ND
19	3	602	CLA	ND
19	3	603	CLA	ND
19	3	605	CLA	ND
19	3	606	CLA	ND
19	3	607	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	608	CLA	ND
19	4	609	CLA	ND
19	4	601	CLA	ND
19	4	602	CLA	ND
19	4	603	CLA	ND
19	4	604	CLA	ND
19	4	605	CLA	ND
19	4	606	CLA	ND
19	4	607	CLA	ND
19	4	612	CLA	ND
19	4	617	CLA	ND
28	J	4013	LUT	C26
28	1	501	LUT	C26
28	1	502	LUT	C26
28	2	501	LUT	C26
28	3	501	LUT	C26
28	3	502	LUT	C26

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Mol	Chain	Res	Type	Atom
28	4	501	LUT	C26
29	1	609	CHL	NC
29	1	609	CHL	NA
29	1	609	CHL	ND
29	1	609	CHL	C8
29	1	610	CHL	NC
29	1	610	CHL	NA
29	1	610	CHL	ND
29	1	612	CHL	NC
29	1	612	CHL	NA
29	1	612	CHL	ND
29	1	612	CHL	C8
29	2	610	CHL	NC
29	2	610	CHL	NA
29	2	610	CHL	ND
29	2	610	CHL	C8
29	2	611	CHL	NC
29	2	611	CHL	NA
29	2	611	CHL	ND
29	2	613	CHL	NC
29	2	613	CHL	NA
29	2	613	CHL	ND
29	2	615	CHL	NC
29	2	615	CHL	NA
29	2	615	CHL	ND
29	2	615	CHL	C8
29	2	609	CHL	NC
29	2	609	CHL	NA
29	2	609	CHL	ND
29	2	609	CHL	C8
29	3	604	CHL	NC
29	3	604	CHL	NA
29	3	604	CHL	ND
29	3	604	CHL	C8
29	3	611	CHL	NC
29	3	611	CHL	NA
29	3	611	CHL	ND
29	4	610	CHL	NC
29	4	610	CHL	NA
29	4	610	CHL	ND
29	4	611	CHL	NC
29	4	611	CHL	NA

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Mol	Chain	Res	Type	Atom
29	4	611	CHL	ND
29	4	613	CHL	NC
29	4	613	CHL	NA
29	4	613	CHL	ND
29	4	613	CHL	C8
29	4	615	CHL	NC
29	4	615	CHL	NA
29	4	615	CHL	C3A
29	4	615	CHL	ND
30	2	502	XAT	C6
30	2	502	XAT	C5
30	4	502	XAT	C26
30	4	502	XAT	C5

All (2450) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
18	A	1011	CL0	C3A-C2A-CAA-CBA
19	A	1012	CLA	CBD-CGD-O2D-CED
19	A	1013	CLA	C2-C1-O2A-CGA
19	A	1013	CLA	CBD-CGD-O2D-CED
19	A	1102	CLA	CHA-CBD-CGD-O1D
19	A	1102	CLA	CHA-CBD-CGD-O2D
19	A	1103	CLA	C2-C1-O2A-CGA
19	A	1103	CLA	CAD-CBD-CGD-O1D
19	A	1103	CLA	CAD-CBD-CGD-O2D
19	A	1104	CLA	CBD-CGD-O2D-CED
19	A	1105	CLA	C2-C1-O2A-CGA
19	A	1106	CLA	C1A-C2A-CAA-CBA
19	A	1106	CLA	C3A-C2A-CAA-CBA
19	A	1106	CLA	CHA-CBD-CGD-O1D
19	A	1106	CLA	CHA-CBD-CGD-O2D
19	A	1107	CLA	CBD-CGD-O2D-CED
19	A	1109	CLA	C1A-C2A-CAA-CBA
19	A	1110	CLA	C1A-C2A-CAA-CBA
19	A	1112	CLA	C2-C1-O2A-CGA
19	A	1114	CLA	CBA-CGA-O2A-C1
19	A	1114	CLA	CHA-CBD-CGD-O1D
19	A	1114	CLA	CHA-CBD-CGD-O2D
19	A	1115	CLA	CBD-CGD-O2D-CED
19	A	1116	CLA	C3A-C2A-CAA-CBA
19	A	1116	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
19	A	1117	CLA	CBD-CGD-O2D-CED
19	A	1119	CLA	C2-C1-O2A-CGA
19	A	1119	CLA	CBD-CGD-O2D-CED
19	A	1120	CLA	CBD-CGD-O2D-CED
19	A	1121	CLA	C1A-C2A-CAA-CBA
19	A	1122	CLA	CBD-CGD-O2D-CED
19	A	1123	CLA	C2-C1-O2A-CGA
19	A	1125	CLA	C1A-C2A-CAA-CBA
19	A	1126	CLA	C6-C7-C8-C9
19	A	1127	CLA	CBD-CGD-O2D-CED
19	A	1128	CLA	CHA-CBD-CGD-O1D
19	A	1128	CLA	CHA-CBD-CGD-O2D
19	A	1131	CLA	C2B-C3B-CAB-CBB
19	A	1131	CLA	C4B-C3B-CAB-CBB
19	A	1131	CLA	CBD-CGD-O2D-CED
19	A	1132	CLA	CHA-CBD-CGD-O1D
19	A	1132	CLA	CHA-CBD-CGD-O2D
19	A	1133	CLA	CBD-CGD-O2D-CED
19	A	1137	CLA	CHA-CBD-CGD-O1D
19	A	1137	CLA	CHA-CBD-CGD-O2D
19	A	1108	CLA	CBD-CGD-O2D-CED
19	A	1113	CLA	CBD-CGD-O2D-CED
19	B	1237	CLA	C14-C13-C15-C16
19	B	1023	CLA	C2-C1-O2A-CGA
19	B	1023	CLA	CBD-CGD-O2D-CED
19	B	1201	CLA	CBD-CGD-O2D-CED
19	B	1202	CLA	C3A-C2A-CAA-CBA
19	B	1202	CLA	CAD-CBD-CGD-O1D
19	B	1202	CLA	CAD-CBD-CGD-O2D
19	B	1205	CLA	CHA-CBD-CGD-O1D
19	B	1205	CLA	CHA-CBD-CGD-O2D
19	B	1205	CLA	C11-C12-C13-C14
19	B	1207	CLA	C2-C1-O2A-CGA
19	B	1207	CLA	CAD-CBD-CGD-O1D
19	B	1207	CLA	CAD-CBD-CGD-O2D
19	B	1207	CLA	CBD-CGD-O2D-CED
19	B	1208	CLA	CBD-CGD-O2D-CED
19	B	1212	CLA	CHA-CBD-CGD-O1D
19	B	1212	CLA	CHA-CBD-CGD-O2D
19	B	1213	CLA	CBD-CGD-O2D-CED
19	B	1217	CLA	CHA-CBD-CGD-O1D
19	B	1217	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
19	B	1222	CLA	C1A-C2A-CAA-CBA
19	B	1222	CLA	C3A-C2A-CAA-CBA
19	B	1222	CLA	CHA-CBD-CGD-O1D
19	B	1222	CLA	CHA-CBD-CGD-O2D
19	B	1223	CLA	C1A-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	1225	CLA	CBD-CGD-O2D-CED
19	B	1226	CLA	C11-C12-C13-C14
19	B	1227	CLA	CBD-CGD-O2D-CED
19	B	1228	CLA	CBD-CGD-O2D-CED
19	B	1230	CLA	C1A-C2A-CAA-CBA
19	B	1230	CLA	C3A-C2A-CAA-CBA
19	B	1230	CLA	CHA-CBD-CGD-O1D
19	B	1230	CLA	CHA-CBD-CGD-O2D
19	B	1230	CLA	C2-C3-C5-C6
19	B	1230	CLA	C4-C3-C5-C6
19	B	1232	CLA	C2B-C3B-CAB-CBB
19	B	1232	CLA	C4B-C3B-CAB-CBB
19	B	1234	CLA	CBD-CGD-O2D-CED
19	B	1239	CLA	C1A-C2A-CAA-CBA
19	B	1239	CLA	C3A-C2A-CAA-CBA
19	B	1239	CLA	CBD-CGD-O2D-CED
19	B	1229	CLA	C2-C1-O2A-CGA
19	B	1204	CLA	CBD-CGD-O2D-CED
19	F	1301	CLA	CBD-CGD-O2D-CED
19	F	1302	CLA	C2-C1-O2A-CGA
19	F	1302	CLA	CBD-CGD-O2D-CED
19	G	1601	CLA	CBD-CGD-O2D-CED
19	G	1602	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	CHA-CBD-CGD-O1D
19	K	1401	CLA	CHA-CBD-CGD-O2D
19	K	1403	CLA	O1A-CGA-O2A-C1
19	K	1403	CLA	CBD-CGD-O2D-CED
19	K	1404	CLA	CBA-CGA-O2A-C1
19	L	1501	CLA	C2-C1-O2A-CGA
19	L	1503	CLA	CBA-CGA-O2A-C1
19	L	1503	CLA	O1A-CGA-O2A-C1
19	L	1503	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
19	1	602	CLA	CBA-CGA-O2A-C1
19	1	602	CLA	O1A-CGA-O2A-C1
19	1	603	CLA	C1A-C2A-CAA-CBA
19	1	605	CLA	CHA-CBD-CGD-O1D
19	1	605	CLA	CHA-CBD-CGD-O2D
19	1	605	CLA	C4-C3-C5-C6
19	1	606	CLA	CBD-CGD-O2D-CED
19	1	608	CLA	CBD-CGD-O2D-CED
19	1	611	CLA	CBD-CGD-O2D-CED
19	1	614	CLA	CHA-CBD-CGD-O1D
19	1	614	CLA	CHA-CBD-CGD-O2D
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	601	CLA	CBD-CGD-O2D-CED
19	2	604	CLA	C3A-C2A-CAA-CBA
19	2	604	CLA	CHA-CBD-CGD-O1D
19	2	604	CLA	CHA-CBD-CGD-O2D
19	2	605	CLA	C1A-C2A-CAA-CBA
19	2	607	CLA	CBA-CGA-O2A-C1
19	2	607	CLA	O1A-CGA-O2A-C1
19	2	607	CLA	C2B-C3B-CAB-CBB
19	2	607	CLA	C4B-C3B-CAB-CBB
19	2	607	CLA	CHA-CBD-CGD-O2D
19	2	607	CLA	CBD-CGD-O2D-CED
19	2	607	CLA	C6-C7-C8-C9
19	2	612	CLA	C1A-C2A-CAA-CBA
19	2	612	CLA	C3A-C2A-CAA-CBA
19	2	608	CLA	CBD-CGD-O2D-CED
19	3	601	CLA	C1A-C2A-CAA-CBA
19	3	601	CLA	C3A-C2A-CAA-CBA
19	3	606	CLA	CBD-CGD-O2D-CED
19	3	607	CLA	CBD-CGD-O2D-CED
19	3	607	CLA	C3-C5-C6-C7
19	3	610	CLA	C3A-C2A-CAA-CBA
19	3	610	CLA	CBD-CGD-O2D-CED
19	3	612	CLA	C2-C1-O2A-CGA
19	3	613	CLA	CBA-CGA-O2A-C1
19	3	613	CLA	O1A-CGA-O2A-C1
19	3	614	CLA	C1A-C2A-CAA-CBA
19	3	617	CLA	CHA-CBD-CGD-O1D
19	3	617	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
19	4	608	CLA	CBD-CGD-O2D-CED
19	4	609	CLA	CAD-CBD-CGD-O1D
19	4	609	CLA	CAD-CBD-CGD-O2D
19	4	603	CLA	CBD-CGD-O2D-CED
19	4	603	CLA	C6-C7-C8-C9
19	4	605	CLA	C1A-C2A-CAA-CBA
19	4	605	CLA	C3A-C2A-CAA-CBA
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	612	CLA	O1A-CGA-O2A-C1
19	4	612	CLA	C2-C1-O2A-CGA
19	4	612	CLA	CBD-CGD-O2D-CED
19	4	617	CLA	C2-C1-O2A-CGA
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	C23-C24-C25-C26
22	A	4003	BCR	C11-C10-C9-C8
22	A	4003	BCR	C11-C10-C9-C34
22	A	4003	BCR	C10-C11-C12-C13
22	A	4007	BCR	C11-C10-C9-C8
22	A	4007	BCR	C11-C10-C9-C34
22	A	4007	BCR	C10-C11-C12-C13
22	A	4007	BCR	C23-C24-C25-C26
22	A	4008	BCR	C1-C6-C7-C8
22	A	4008	BCR	C5-C6-C7-C8
22	A	4008	BCR	C11-C10-C9-C8
22	A	4008	BCR	C11-C10-C9-C34
22	A	4008	BCR	C9-C10-C11-C12
22	A	4008	BCR	C10-C11-C12-C13
22	A	4008	BCR	C11-C12-C13-C14
22	A	4008	BCR	C11-C12-C13-C35
22	A	4011	BCR	C5-C6-C7-C8
22	A	4011	BCR	C11-C10-C9-C8
22	A	4011	BCR	C11-C10-C9-C34
22	A	4011	BCR	C23-C24-C25-C26
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	C5-C6-C7-C8
22	B	4004	BCR	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
22	B	4004	BCR	C11-C10-C9-C34
22	B	4004	BCR	C10-C11-C12-C13
22	B	4005	BCR	C5-C6-C7-C8
22	B	4005	BCR	C11-C10-C9-C8
22	B	4005	BCR	C11-C10-C9-C34
22	B	4005	BCR	C10-C11-C12-C13
22	B	4005	BCR	C11-C12-C13-C14
22	B	4005	BCR	C11-C12-C13-C35
22	B	4005	BCR	C23-C24-C25-C26
22	B	4005	BCR	C23-C24-C25-C30
22	B	4009	BCR	C5-C6-C7-C8
22	B	4009	BCR	C11-C10-C9-C8
22	B	4009	BCR	C11-C10-C9-C34
22	B	4009	BCR	C9-C10-C11-C12
22	B	4009	BCR	C10-C11-C12-C13
22	B	4010	BCR	C11-C10-C9-C8
22	B	4010	BCR	C11-C10-C9-C34
22	B	4010	BCR	C9-C10-C11-C12
22	B	4010	BCR	C10-C11-C12-C13
22	B	4010	BCR	C17-C18-C19-C20
22	F	4014	BCR	C1-C6-C7-C8
22	F	4014	BCR	C5-C6-C7-C8
22	F	4014	BCR	C11-C10-C9-C8
22	F	4014	BCR	C11-C10-C9-C34
22	F	4014	BCR	C10-C11-C12-C13
22	F	4014	BCR	C23-C24-C25-C26
22	F	4016	BCR	C1-C6-C7-C8
22	F	4016	BCR	C5-C6-C7-C8
22	F	4016	BCR	C11-C10-C9-C8
22	F	4016	BCR	C11-C10-C9-C34
22	F	4016	BCR	C9-C10-C11-C12
22	F	4016	BCR	C10-C11-C12-C13
22	F	4016	BCR	C23-C24-C25-C26
22	G	4011	BCR	C5-C6-C7-C8
22	G	4011	BCR	C11-C10-C9-C8
22	G	4011	BCR	C11-C10-C9-C34
22	H	4021	BCR	C11-C10-C9-C8
22	H	4021	BCR	C11-C10-C9-C34
22	H	4021	BCR	C10-C11-C12-C13
22	H	4021	BCR	C11-C12-C13-C14
22	H	4021	BCR	C23-C24-C25-C26
22	H	4021	BCR	C23-C24-C25-C30

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Mol	Chain	Res	Type	Atoms
22	I	4020	BCR	C5-C6-C7-C8
22	I	4020	BCR	C11-C10-C9-C8
22	I	4020	BCR	C11-C10-C9-C34
22	I	4020	BCR	C9-C10-C11-C12
22	I	4020	BCR	C10-C11-C12-C13
22	I	4020	BCR	C11-C12-C13-C14
22	I	4020	BCR	C23-C24-C25-C26
22	J	4012	BCR	C11-C10-C9-C8
22	J	4012	BCR	C11-C10-C9-C34
22	J	4012	BCR	C10-C11-C12-C13
22	J	4012	BCR	C23-C24-C25-C26
22	J	4012	BCR	C23-C24-C25-C30
22	K	4001	BCR	C11-C10-C9-C8
22	K	4001	BCR	C11-C10-C9-C34
22	K	4001	BCR	C23-C24-C25-C26
22	K	4001	BCR	C23-C24-C25-C30
22	K	4002	BCR	C11-C10-C9-C8
22	K	4002	BCR	C11-C10-C9-C34
22	L	4019	BCR	C1-C6-C7-C8
22	L	4019	BCR	C5-C6-C7-C8
22	L	4019	BCR	C11-C10-C9-C8
22	L	4019	BCR	C11-C10-C9-C34
22	L	4019	BCR	C9-C10-C11-C12
22	L	4019	BCR	C10-C11-C12-C13
22	L	4020	BCR	C5-C6-C7-C8
22	L	4020	BCR	C11-C10-C9-C8
22	L	4020	BCR	C11-C10-C9-C34
22	L	4020	BCR	C10-C11-C12-C13
22	1	504	BCR	C5-C6-C7-C8
22	1	504	BCR	C11-C10-C9-C8
22	1	504	BCR	C11-C10-C9-C34
22	1	504	BCR	C11-C12-C13-C14
22	1	504	BCR	C11-C12-C13-C35
22	1	503	BCR	C10-C11-C12-C13
22	1	503	BCR	C11-C12-C13-C14
22	2	503	BCR	C11-C10-C9-C8
22	2	503	BCR	C11-C10-C9-C34
22	2	503	BCR	C10-C11-C12-C13
22	2	503	BCR	C11-C12-C13-C14
22	2	503	BCR	C11-C12-C13-C35
22	2	503	BCR	C18-C19-C20-C21
22	3	503	BCR	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
22	3	503	BCR	C11-C10-C9-C34
22	3	503	BCR	C10-C11-C12-C13
22	3	503	BCR	C11-C12-C13-C14
22	3	503	BCR	C11-C12-C13-C35
22	3	503	BCR	C17-C18-C19-C20
22	3	506	BCR	C11-C10-C9-C8
22	3	506	BCR	C11-C10-C9-C34
23	A	5001	LHG	O1-C1-C2-C3
23	A	5001	LHG	C3-O3-P-O6
23	A	5001	LHG	C4-O6-P-O3
23	A	5001	LHG	C4-O6-P-O4
23	A	5001	LHG	C4-O6-P-O5
23	A	5002	LHG	O2-C2-C3-O3
23	A	5002	LHG	C3-O3-P-O6
23	A	5002	LHG	C4-O6-P-O3
23	A	5002	LHG	O7-C5-C6-O8
23	B	5001	LHG	C3-O3-P-O4
23	B	5001	LHG	C3-O3-P-O6
23	B	5001	LHG	C4-O6-P-O3
23	B	5001	LHG	C4-O6-P-O5
23	B	5001	LHG	C8-C7-O7-C5
23	B	5002	LHG	C3-O3-P-O4
23	B	5002	LHG	C3-O3-P-O5
23	B	5002	LHG	C3-O3-P-O6
23	B	5002	LHG	C4-O6-P-O3
23	B	5002	LHG	C4-O6-P-O5
23	B	5002	LHG	C8-C7-O7-C5
23	1	801	LHG	O2-C2-C3-O3
23	1	801	LHG	C3-O3-P-O6
23	1	801	LHG	C4-O6-P-O5
23	2	801	LHG	C3-O3-P-O4
23	2	801	LHG	C3-O3-P-O6
23	2	801	LHG	C4-O6-P-O3
23	2	801	LHG	C8-C7-O7-C5
23	3	801	LHG	C3-O3-P-O5
23	4	801	LHG	O1-C1-C2-O2
23	4	801	LHG	O1-C1-C2-C3
23	4	801	LHG	C3-O3-P-O5
23	4	801	LHG	C4-O6-P-O3
23	4	801	LHG	C4-O6-P-O5
23	4	801	LHG	O7-C5-C6-O8
23	4	801	LHG	C8-C7-O7-C5

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Mol	Chain	Res	Type	Atoms
24	G	5005	LMT	O5'-C1'-O1'-C1
24	G	5005	LMT	C2-C1-O1'-C1'
25	A	5006	LMG	C2-C1-O1-C7
25	A	5006	LMG	O6-C1-O1-C7
25	A	5006	LMG	C11-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	O9-C10-O7-C8
25	F	5004	LMG	C11-C10-O7-C8
25	G	5006	LMG	C11-C10-O7-C8
25	G	5001	LMG	C11-C10-O7-C8
25	G	5002	LMG	C11-C10-O7-C8
25	2	802	LMG	O9-C10-O7-C8
25	2	802	LMG	C11-C10-O7-C8
25	2	805	LMG	C2-C1-O1-C7
25	2	805	LMG	O6-C1-O1-C7
25	3	802	LMG	C11-C10-O7-C8
27	B	5005	DGD	O1B-C1B-O2G-C2G
27	F	5005	DGD	O1B-C1B-O2G-C2G
27	F	5005	DGD	C2E-C1E-O5D-C6D
27	F	5005	DGD	O6E-C1E-O5D-C6D
27	J	5001	DGD	C2B-C1B-O2G-C2G
27	J	5001	DGD	O6E-C1E-O5D-C6D
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	4	802	DGD	C2B-C1B-O2G-C2G
27	4	802	DGD	O6D-C1D-O3G-C3G
28	J	4013	LUT	C21-C26-C27-C28
28	J	4013	LUT	C25-C26-C27-C28
28	1	501	LUT	C21-C26-C27-C28
28	1	501	LUT	C25-C26-C27-C28
28	1	502	LUT	C21-C26-C27-C28
28	1	502	LUT	C25-C26-C27-C28
28	2	501	LUT	C21-C26-C27-C28
28	2	501	LUT	C25-C26-C27-C28
28	2	501	LUT	C27-C28-C29-C30
28	3	501	LUT	C21-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
28	3	501	LUT	C25-C26-C27-C28
28	3	501	LUT	C27-C28-C29-C30
28	3	502	LUT	C21-C26-C27-C28
28	3	502	LUT	C25-C26-C27-C28
28	4	505	LUT	C21-C26-C27-C28
28	4	505	LUT	C25-C26-C27-C28
28	4	501	LUT	C21-C26-C27-C28
28	4	501	LUT	C25-C26-C27-C28
28	4	501	LUT	C27-C28-C29-C30
29	1	610	CHL	C4C-C3C-CAC-CBC
29	1	612	CHL	CHA-CBD-CGD-O1D
29	1	612	CHL	CHA-CBD-CGD-O2D
29	2	609	CHL	CAD-CBD-CGD-O1D
29	2	609	CHL	CAD-CBD-CGD-O2D
29	4	610	CHL	C4C-C3C-CAC-CBC
30	2	502	XAT	C5-C6-C7-C8
30	2	502	XAT	O4-C6-C7-C8
30	2	502	XAT	C11-C12-C13-C14
31	2	807	3PH	C1-O11-P-O13
31	2	807	3PH	C1-O11-P-O14
31	2	807	3PH	C1-O11-P-O12
19	A	1126	CLA	O1D-CGD-O2D-CED
19	B	1021	CLA	O1D-CGD-O2D-CED
19	B	1201	CLA	O1D-CGD-O2D-CED
19	B	1219	CLA	O1D-CGD-O2D-CED
19	2	606	CLA	O1D-CGD-O2D-CED
19	3	608	CLA	O1D-CGD-O2D-CED
19	A	1104	CLA	O1D-CGD-O2D-CED
19	A	1121	CLA	O1D-CGD-O2D-CED
19	A	1139	CLA	O1D-CGD-O2D-CED
19	1	603	CLA	O1D-CGD-O2D-CED
19	2	603	CLA	O1D-CGD-O2D-CED
19	3	601	CLA	O1D-CGD-O2D-CED
19	3	605	CLA	O1D-CGD-O2D-CED
19	3	613	CLA	O1D-CGD-O2D-CED
19	3	614	CLA	O1D-CGD-O2D-CED
23	B	5001	LHG	O9-C7-O7-C5
19	A	1103	CLA	CBD-CGD-O2D-CED
19	A	1105	CLA	CBD-CGD-O2D-CED
19	A	1111	CLA	CBD-CGD-O2D-CED
19	A	1112	CLA	CBD-CGD-O2D-CED
19	A	1121	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
19	A	1126	CLA	CBD-CGD-O2D-CED
19	A	1130	CLA	CBD-CGD-O2D-CED
19	A	1134	CLA	CBD-CGD-O2D-CED
19	A	1138	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	1237	CLA	CBD-CGD-O2D-CED
19	B	1021	CLA	CBD-CGD-O2D-CED
19	B	1203	CLA	CBD-CGD-O2D-CED
19	B	1206	CLA	CBD-CGD-O2D-CED
19	B	1209	CLA	CBD-CGD-O2D-CED
19	B	1214	CLA	CBD-CGD-O2D-CED
19	B	1215	CLA	CBD-CGD-O2D-CED
19	B	1216	CLA	CBD-CGD-O2D-CED
19	B	1219	CLA	CBD-CGD-O2D-CED
19	B	1220	CLA	CBD-CGD-O2D-CED
19	B	1231	CLA	CBD-CGD-O2D-CED
19	B	1232	CLA	CBD-CGD-O2D-CED
19	B	1236	CLA	CBD-CGD-O2D-CED
19	B	1238	CLA	CBD-CGD-O2D-CED
19	G	1603	CLA	CBD-CGD-O2D-CED
19	H	1701	CLA	CBD-CGD-O2D-CED
19	J	1901	CLA	CBD-CGD-O2D-CED
19	K	1402	CLA	CBD-CGD-O2D-CED
19	K	1404	CLA	CBD-CGD-O2D-CED
19	L	1501	CLA	CBD-CGD-O2D-CED
19	L	1502	CLA	CBD-CGD-O2D-CED
19	1	601	CLA	CBD-CGD-O2D-CED
19	1	602	CLA	CBD-CGD-O2D-CED
19	1	603	CLA	CBD-CGD-O2D-CED
19	1	613	CLA	CBD-CGD-O2D-CED
19	2	602	CLA	CBD-CGD-O2D-CED
19	2	603	CLA	CBD-CGD-O2D-CED
19	2	605	CLA	CBD-CGD-O2D-CED
19	2	606	CLA	CBD-CGD-O2D-CED
19	3	601	CLA	CBD-CGD-O2D-CED
19	3	602	CLA	CBD-CGD-O2D-CED
19	3	603	CLA	CBD-CGD-O2D-CED
19	3	605	CLA	CBD-CGD-O2D-CED
19	3	608	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
19	3	612	CLA	CBD-CGD-O2D-CED
19	3	613	CLA	CBD-CGD-O2D-CED
19	3	614	CLA	CBD-CGD-O2D-CED
19	4	601	CLA	CBD-CGD-O2D-CED
19	4	604	CLA	CBD-CGD-O2D-CED
19	4	606	CLA	CBD-CGD-O2D-CED
24	G	5004	LMT	O5B-C1B-O1B-C4'
19	A	1127	CLA	O1A-CGA-O2A-C1
19	A	1129	CLA	O1A-CGA-O2A-C1
19	B	1237	CLA	O1A-CGA-O2A-C1
19	B	1219	CLA	O1A-CGA-O2A-C1
19	F	1302	CLA	O1A-CGA-O2A-C1
19	G	1603	CLA	O1A-CGA-O2A-C1
19	4	609	CLA	O1A-CGA-O2A-C1
25	2	803	LMG	O10-C28-O8-C9
19	A	1114	CLA	O1A-CGA-O2A-C1
19	G	1602	CLA	O1A-CGA-O2A-C1
19	K	1404	CLA	O1A-CGA-O2A-C1
19	G	1602	CLA	CBA-CGA-O2A-C1
19	A	1111	CLA	O1D-CGD-O2D-CED
19	A	1141	CLA	O1D-CGD-O2D-CED
19	B	1203	CLA	O1D-CGD-O2D-CED
19	B	1206	CLA	O1D-CGD-O2D-CED
19	B	1238	CLA	O1D-CGD-O2D-CED
19	H	1701	CLA	O1D-CGD-O2D-CED
19	J	1901	CLA	O1D-CGD-O2D-CED
19	K	1404	CLA	O1D-CGD-O2D-CED
19	1	601	CLA	O1D-CGD-O2D-CED
19	1	613	CLA	O1D-CGD-O2D-CED
19	2	602	CLA	O1D-CGD-O2D-CED
19	3	603	CLA	O1D-CGD-O2D-CED
19	3	612	CLA	O1D-CGD-O2D-CED
19	4	601	CLA	O1D-CGD-O2D-CED
19	F	1302	CLA	CBA-CGA-O2A-C1
19	2	612	CLA	CBA-CGA-O2A-C1
19	4	609	CLA	CBA-CGA-O2A-C1
25	F	5003	LMG	C29-C28-O8-C9
25	2	803	LMG	C29-C28-O8-C9
19	A	1121	CLA	O1A-CGA-O2A-C1
19	A	1122	CLA	O1A-CGA-O2A-C1
19	A	1126	CLA	O1A-CGA-O2A-C1
19	A	1108	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
19	B	1214	CLA	O1A-CGA-O2A-C1
19	B	1222	CLA	O1A-CGA-O2A-C1
19	B	1227	CLA	O1A-CGA-O2A-C1
19	B	1232	CLA	O1A-CGA-O2A-C1
19	J	1901	CLA	O1A-CGA-O2A-C1
19	1	606	CLA	O1A-CGA-O2A-C1
19	2	603	CLA	O1A-CGA-O2A-C1
19	2	612	CLA	O1A-CGA-O2A-C1
19	3	602	CLA	O1A-CGA-O2A-C1
19	3	607	CLA	O1A-CGA-O2A-C1
19	4	605	CLA	O1A-CGA-O2A-C1
19	4	606	CLA	O1A-CGA-O2A-C1
19	4	607	CLA	O1A-CGA-O2A-C1
25	B	5003	LMG	O10-C28-O8-C9
25	F	5002	LMG	O10-C28-O8-C9
25	F	5003	LMG	O10-C28-O8-C9
25	G	5006	LMG	O10-C28-O8-C9
25	G	5002	LMG	O10-C28-O8-C9
19	A	1107	CLA	O1D-CGD-O2D-CED
19	A	1119	CLA	O1D-CGD-O2D-CED
19	A	1120	CLA	O1D-CGD-O2D-CED
19	A	1108	CLA	O1D-CGD-O2D-CED
19	A	1113	CLA	O1D-CGD-O2D-CED
19	B	1023	CLA	O1D-CGD-O2D-CED
19	B	1208	CLA	O1D-CGD-O2D-CED
19	B	1213	CLA	O1D-CGD-O2D-CED
19	B	1232	CLA	O1D-CGD-O2D-CED
19	F	1302	CLA	O1D-CGD-O2D-CED
19	G	1602	CLA	O1D-CGD-O2D-CED
19	L	1503	CLA	O1D-CGD-O2D-CED
19	1	602	CLA	O1D-CGD-O2D-CED
19	1	606	CLA	O1D-CGD-O2D-CED
19	1	611	CLA	O1D-CGD-O2D-CED
19	3	606	CLA	O1D-CGD-O2D-CED
19	3	607	CLA	O1D-CGD-O2D-CED
19	4	603	CLA	O1D-CGD-O2D-CED
19	4	606	CLA	O1D-CGD-O2D-CED
19	A	1012	CLA	O1D-CGD-O2D-CED
19	A	1013	CLA	O1D-CGD-O2D-CED
19	A	1115	CLA	O1D-CGD-O2D-CED
19	A	1116	CLA	O1D-CGD-O2D-CED
19	A	1122	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
19	A	1127	CLA	O1D-CGD-O2D-CED
19	A	1133	CLA	O1D-CGD-O2D-CED
19	B	1207	CLA	O1D-CGD-O2D-CED
19	B	1224	CLA	O1D-CGD-O2D-CED
19	B	1228	CLA	O1D-CGD-O2D-CED
19	B	1234	CLA	O1D-CGD-O2D-CED
19	B	1204	CLA	O1D-CGD-O2D-CED
19	F	1301	CLA	O1D-CGD-O2D-CED
19	G	1601	CLA	O1D-CGD-O2D-CED
19	K	1403	CLA	O1D-CGD-O2D-CED
19	2	601	CLA	O1D-CGD-O2D-CED
19	4	608	CLA	O1D-CGD-O2D-CED
19	A	1110	CLA	CBD-CGD-O2D-CED
19	A	1118	CLA	CBD-CGD-O2D-CED
19	2	612	CLA	CBD-CGD-O2D-CED
23	B	5002	LHG	O9-C7-O7-C5
23	2	801	LHG	O9-C7-O7-C5
23	4	801	LHG	O9-C7-O7-C5
25	A	5006	LMG	O9-C10-O7-C8
25	B	5003	LMG	O9-C10-O7-C8
25	G	5006	LMG	O9-C10-O7-C8
25	G	5001	LMG	O9-C10-O7-C8
25	G	5002	LMG	O9-C10-O7-C8
27	J	5001	DGD	O1B-C1B-O2G-C2G
27	4	802	DGD	O1B-C1B-O2G-C2G
19	B	1225	CLA	O1D-CGD-O2D-CED
19	4	608	CLA	CBA-CGA-O2A-C1
19	B	1217	CLA	O1A-CGA-O2A-C1
19	1	608	CLA	O1A-CGA-O2A-C1
19	4	608	CLA	O1A-CGA-O2A-C1
19	A	1012	CLA	C3-C5-C6-C7
19	A	1105	CLA	C3-C5-C6-C7
19	A	1107	CLA	C3-C5-C6-C7
19	A	1112	CLA	C3-C5-C6-C7
19	A	1134	CLA	C3-C5-C6-C7
19	A	1137	CLA	C3-C5-C6-C7
19	B	1203	CLA	C3-C5-C6-C7
19	B	1219	CLA	C3-C5-C6-C7
19	B	1223	CLA	C3-C5-C6-C7
19	B	1226	CLA	C3-C5-C6-C7
19	B	1228	CLA	C3-C5-C6-C7
19	F	1302	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
19	2	603	CLA	C3-C5-C6-C7
19	2	604	CLA	C3-C5-C6-C7
19	3	601	CLA	C3-C5-C6-C7
19	3	603	CLA	C3-C5-C6-C7
19	3	610	CLA	C3-C5-C6-C7
19	4	601	CLA	C3-C5-C6-C7
29	4	613	CHL	C3-C5-C6-C7
19	B	1216	CLA	O1D-CGD-O2D-CED
19	1	608	CLA	O1D-CGD-O2D-CED
19	4	612	CLA	O1D-CGD-O2D-CED
19	A	1122	CLA	CBA-CGA-O2A-C1
19	A	1127	CLA	CBA-CGA-O2A-C1
19	A	1129	CLA	CBA-CGA-O2A-C1
19	B	1237	CLA	CBA-CGA-O2A-C1
19	B	1201	CLA	CBA-CGA-O2A-C1
19	B	1208	CLA	CBA-CGA-O2A-C1
19	B	1214	CLA	CBA-CGA-O2A-C1
19	B	1219	CLA	CBA-CGA-O2A-C1
19	B	1222	CLA	CBA-CGA-O2A-C1
19	B	1232	CLA	CBA-CGA-O2A-C1
19	G	1603	CLA	CBA-CGA-O2A-C1
19	J	1901	CLA	CBA-CGA-O2A-C1
19	K	1402	CLA	CBA-CGA-O2A-C1
19	K	1403	CLA	CBA-CGA-O2A-C1
19	1	606	CLA	CBA-CGA-O2A-C1
19	3	602	CLA	CBA-CGA-O2A-C1
19	3	603	CLA	CBA-CGA-O2A-C1
19	3	606	CLA	CBA-CGA-O2A-C1
19	3	610	CLA	CBA-CGA-O2A-C1
19	4	606	CLA	CBA-CGA-O2A-C1
19	4	612	CLA	CBA-CGA-O2A-C1
25	B	5003	LMG	C29-C28-O8-C9
25	F	5002	LMG	C29-C28-O8-C9
25	G	5006	LMG	C29-C28-O8-C9
25	G	5002	LMG	C29-C28-O8-C9
27	3	803	DGD	C2A-C1A-O1G-C1G
19	A	1109	CLA	CBD-CGD-O2D-CED
19	A	1125	CLA	CBD-CGD-O2D-CED
19	A	1128	CLA	CBD-CGD-O2D-CED
19	A	1129	CLA	CBD-CGD-O2D-CED
19	A	1132	CLA	CBD-CGD-O2D-CED
19	A	1135	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
19	A	1136	CLA	CBD-CGD-O2D-CED
19	A	1137	CLA	CBD-CGD-O2D-CED
19	B	1212	CLA	CBD-CGD-O2D-CED
19	B	1222	CLA	CBD-CGD-O2D-CED
19	B	1235	CLA	CBD-CGD-O2D-CED
19	B	1229	CLA	CBD-CGD-O2D-CED
19	4	602	CLA	CBD-CGD-O2D-CED
19	4	605	CLA	CBD-CGD-O2D-CED
27	B	5005	DGD	C2B-C1B-O2G-C2G
27	F	5005	DGD	C2B-C1B-O2G-C2G
19	A	1117	CLA	O1D-CGD-O2D-CED
19	A	1131	CLA	O1D-CGD-O2D-CED
19	B	1022	CLA	O1D-CGD-O2D-CED
19	B	1227	CLA	O1D-CGD-O2D-CED
19	B	1239	CLA	O1D-CGD-O2D-CED
19	L	1502	CLA	O1D-CGD-O2D-CED
19	2	607	CLA	O1D-CGD-O2D-CED
19	2	608	CLA	O1D-CGD-O2D-CED
19	3	610	CLA	O1D-CGD-O2D-CED
19	4	604	CLA	O1D-CGD-O2D-CED
19	4	607	CLA	O1D-CGD-O2D-CED
19	A	1109	CLA	C4-C3-C5-C6
19	A	1116	CLA	C4-C3-C5-C6
19	A	1122	CLA	C4-C3-C5-C6
19	A	1139	CLA	C4-C3-C5-C6
19	B	1204	CLA	C4-C3-C5-C6
19	G	1601	CLA	C4-C3-C5-C6
19	2	602	CLA	C4-C3-C5-C6
19	3	603	CLA	C4-C3-C5-C6
19	A	1109	CLA	C2-C3-C5-C6
19	A	1122	CLA	C2-C3-C5-C6
19	A	1139	CLA	C2-C3-C5-C6
19	B	1204	CLA	C2-C3-C5-C6
19	G	1601	CLA	C2-C3-C5-C6
19	1	605	CLA	C2-C3-C5-C6
19	2	602	CLA	C2-C3-C5-C6
19	3	603	CLA	C2-C3-C5-C6
19	1	608	CLA	CBA-CGA-O2A-C1
19	3	617	CLA	CBD-CGD-O2D-CED
19	A	1110	CLA	C2A-CAA-CBA-CGA
19	A	1129	CLA	C2A-CAA-CBA-CGA
19	B	1230	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
19	A	1102	CLA	C3-C5-C6-C7
19	A	1106	CLA	C3-C5-C6-C7
19	A	1110	CLA	C3-C5-C6-C7
19	B	1205	CLA	C3-C5-C6-C7
19	B	1207	CLA	C3-C5-C6-C7
19	1	611	CLA	C3-C5-C6-C7
19	A	1104	CLA	CBA-CGA-O2A-C1
19	A	1109	CLA	CBA-CGA-O2A-C1
19	A	1121	CLA	CBA-CGA-O2A-C1
19	A	1126	CLA	CBA-CGA-O2A-C1
19	A	1130	CLA	CBA-CGA-O2A-C1
19	A	1108	CLA	CBA-CGA-O2A-C1
19	B	1206	CLA	CBA-CGA-O2A-C1
19	B	1227	CLA	CBA-CGA-O2A-C1
19	B	1230	CLA	CBA-CGA-O2A-C1
19	B	1231	CLA	CBA-CGA-O2A-C1
19	2	603	CLA	CBA-CGA-O2A-C1
19	2	605	CLA	CBA-CGA-O2A-C1
19	2	608	CLA	CBA-CGA-O2A-C1
19	3	607	CLA	CBA-CGA-O2A-C1
19	3	612	CLA	CBA-CGA-O2A-C1
19	4	605	CLA	CBA-CGA-O2A-C1
19	4	607	CLA	CBA-CGA-O2A-C1
25	2	804	LMG	C29-C28-O8-C9
27	G	5003	DGD	C2A-C1A-O1G-C1G
25	A	5006	LMG	C17-C18-C19-C20
25	G	5001	LMG	C38-C39-C40-C41
27	F	5005	DGD	C8A-C9A-CAA-CBA
29	4	610	CHL	C2C-C3C-CAC-CBC
19	K	1401	CLA	CBD-CGD-O2D-CED
24	A	5004	LMT	O5B-C5B-C6B-O6B
24	A	5004	LMT	C4B-C5B-C6B-O6B
22	B	4004	BCR	C19-C20-C21-C22
22	H	4021	BCR	C9-C10-C11-C12
22	J	4012	BCR	C9-C10-C11-C12
22	2	503	BCR	C13-C14-C15-C16
19	A	1104	CLA	O1A-CGA-O2A-C1
19	A	1109	CLA	O1A-CGA-O2A-C1
19	B	1201	CLA	O1A-CGA-O2A-C1
19	B	1208	CLA	O1A-CGA-O2A-C1
19	2	606	CLA	O1A-CGA-O2A-C1
19	2	608	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
19	3	603	CLA	O1A-CGA-O2A-C1
19	3	610	CLA	O1A-CGA-O2A-C1
25	B	5004	LMG	O10-C28-O8-C9
25	F	5002	LMG	O9-C10-O7-C8
25	3	802	LMG	O9-C10-O7-C8
19	B	1217	CLA	CBA-CGA-O2A-C1
25	G	5002	LMG	C17-C18-C19-C20
25	G	5002	LMG	C35-C36-C37-C38
27	B	5005	DGD	C8A-C9A-CAA-CBA
19	A	1103	CLA	O1D-CGD-O2D-CED
19	A	1130	CLA	O1D-CGD-O2D-CED
19	B	1237	CLA	O1D-CGD-O2D-CED
19	B	1209	CLA	O1D-CGD-O2D-CED
19	B	1215	CLA	O1D-CGD-O2D-CED
19	2	605	CLA	O1D-CGD-O2D-CED
19	A	1102	CLA	CBD-CGD-O2D-CED
19	A	1106	CLA	CBD-CGD-O2D-CED
19	A	1114	CLA	CBD-CGD-O2D-CED
19	A	1101	CLA	CBD-CGD-O2D-CED
19	B	1217	CLA	CBD-CGD-O2D-CED
19	1	614	CLA	CBD-CGD-O2D-CED
25	G	5001	LMG	C35-C36-C37-C38
23	A	5001	LHG	O2-C2-C3-O3
19	A	1105	CLA	O1D-CGD-O2D-CED
19	A	1140	CLA	O1D-CGD-O2D-CED
19	B	1214	CLA	O1D-CGD-O2D-CED
19	B	1220	CLA	O1D-CGD-O2D-CED
19	B	1236	CLA	O1D-CGD-O2D-CED
19	G	1603	CLA	O1D-CGD-O2D-CED
19	K	1402	CLA	O1D-CGD-O2D-CED
19	3	602	CLA	O1D-CGD-O2D-CED
19	A	1013	CLA	CBA-CGA-O2A-C1
19	A	1119	CLA	CBA-CGA-O2A-C1
19	A	1134	CLA	CBA-CGA-O2A-C1
19	B	1202	CLA	CBA-CGA-O2A-C1
19	B	1211	CLA	CBA-CGA-O2A-C1
19	B	1220	CLA	CBA-CGA-O2A-C1
19	2	606	CLA	CBA-CGA-O2A-C1
24	A	5004	LMT	O5'-C5'-C6'-O6'
24	G	5004	LMT	O5'-C5'-C6'-O6'
24	2	808	LMT	O5'-C5'-C6'-O6'
19	K	1402	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
19	3	606	CLA	O1A-CGA-O2A-C1
27	3	803	DGD	O1A-C1A-O1G-C1G
24	B	5008	LMT	C4B-C5B-C6B-O6B
19	A	1134	CLA	O1D-CGD-O2D-CED
19	B	1231	CLA	O1D-CGD-O2D-CED
19	L	1501	CLA	O1D-CGD-O2D-CED
19	B	1205	CLA	CBD-CGD-O2D-CED
23	A	5002	LHG	C8-C7-O7-C5
19	1	607	CLA	CBA-CGA-O2A-C1
19	B	1231	CLA	O1A-CGA-O2A-C1
19	2	605	CLA	O1A-CGA-O2A-C1
24	B	5008	LMT	O5'-C5'-C6'-O6'
24	B	5006	LMT	C4B-C5B-C6B-O6B
19	A	1138	CLA	O1D-CGD-O2D-CED
19	B	1202	CLA	CBD-CGD-O2D-CED
19	1	604	CLA	CBD-CGD-O2D-CED
19	1	605	CLA	CBD-CGD-O2D-CED
19	A	1101	CLA	CBA-CGA-O2A-C1
25	B	5004	LMG	C29-C28-O8-C9
19	A	1104	CLA	C4-C3-C5-C6
19	A	1133	CLA	C4-C3-C5-C6
19	1	601	CLA	C4-C3-C5-C6
19	A	1133	CLA	C2-C3-C5-C6
19	B	1232	CLA	C2-C3-C5-C6
19	1	601	CLA	C2-C3-C5-C6
29	2	609	CHL	C2-C3-C5-C6
19	A	1013	CLA	O1A-CGA-O2A-C1
19	A	1134	CLA	O1A-CGA-O2A-C1
19	B	1206	CLA	O1A-CGA-O2A-C1
19	B	1220	CLA	O1A-CGA-O2A-C1
19	3	612	CLA	O1A-CGA-O2A-C1
25	2	804	LMG	O10-C28-O8-C9
27	G	5003	DGD	O1A-C1A-O1G-C1G
24	B	5008	LMT	O5B-C5B-C6B-O6B
24	B	5006	LMT	O5B-C5B-C6B-O6B
19	2	604	CLA	CBD-CGD-O2D-CED
19	4	617	CLA	CBD-CGD-O2D-CED
19	A	1102	CLA	C2A-CAA-CBA-CGA
19	B	1217	CLA	C2A-CAA-CBA-CGA
19	L	1502	CLA	C2A-CAA-CBA-CGA
29	1	610	CHL	C2A-CAA-CBA-CGA
19	A	1119	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
19	A	1130	CLA	O1A-CGA-O2A-C1
19	B	1202	CLA	O1A-CGA-O2A-C1
19	B	1211	CLA	O1A-CGA-O2A-C1
25	G	5006	LMG	O6-C1-O1-C7
27	B	5005	DGD	O6D-C1D-O3G-C3G
27	3	803	DGD	O6E-C1E-O5D-C6D
24	G	5004	LMT	O5B-C5B-C6B-O6B
19	A	1118	CLA	O1D-CGD-O2D-CED
19	2	612	CLA	O1D-CGD-O2D-CED
19	A	1105	CLA	CBA-CGA-O2A-C1
19	1	604	CLA	CBA-CGA-O2A-C1
19	B	1230	CLA	CBD-CGD-O2D-CED
19	1	607	CLA	CBD-CGD-O2D-CED
19	4	609	CLA	CBD-CGD-O2D-CED
19	A	1101	CLA	O1A-CGA-O2A-C1
19	1	604	CLA	O1A-CGA-O2A-C1
19	A	1110	CLA	O1D-CGD-O2D-CED
19	A	1112	CLA	O1D-CGD-O2D-CED
23	A	5001	LHG	C13-C14-C15-C16
19	A	1123	CLA	CBD-CGD-O2D-CED
25	2	804	LMG	C11-C10-O7-C8
19	1	605	CLA	C3-C5-C6-C7
22	1	503	BCR	C9-C10-C11-C12
23	A	5002	LHG	C1-C2-C3-O3
23	B	5001	LHG	C1-C2-C3-O3
23	B	5002	LHG	C1-C2-C3-O3
23	1	801	LHG	C1-C2-C3-O3
23	2	801	LHG	C1-C2-C3-O3
18	A	1011	CL0	CBA-CGA-O2A-C1
19	A	1103	CLA	CBA-CGA-O2A-C1
19	A	1112	CLA	CBA-CGA-O2A-C1
19	A	1116	CLA	CBA-CGA-O2A-C1
19	A	1124	CLA	CBA-CGA-O2A-C1
19	B	1235	CLA	CBA-CGA-O2A-C1
19	B	1229	CLA	CBA-CGA-O2A-C1
19	1	614	CLA	CBA-CGA-O2A-C1
19	2	604	CLA	CBA-CGA-O2A-C1
19	3	605	CLA	CBA-CGA-O2A-C1
19	4	602	CLA	CBA-CGA-O2A-C1
19	4	617	CLA	CBA-CGA-O2A-C1
27	4	802	DGD	C2A-C1A-O1G-C1G
24	2	808	LMT	C4'-C5'-C6'-O6'

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Mol	Chain	Res	Type	Atoms
19	A	1105	CLA	O1A-CGA-O2A-C1
19	B	1232	CLA	C4-C3-C5-C6
19	B	1240	CLA	C4-C3-C5-C6
29	2	609	CHL	C4-C3-C5-C6
19	A	1116	CLA	C2-C3-C5-C6
19	B	1240	CLA	C2-C3-C5-C6
19	B	1226	CLA	CBD-CGD-O2D-CED
19	A	1115	CLA	C11-C10-C8-C9
19	A	1119	CLA	C11-C10-C8-C9
19	A	1120	CLA	C11-C10-C8-C9
19	A	1123	CLA	C11-C12-C13-C14
19	A	1125	CLA	C6-C7-C8-C9
19	A	1137	CLA	C6-C7-C8-C9
19	B	1203	CLA	C6-C7-C8-C9
19	B	1206	CLA	C14-C13-C15-C16
19	B	1208	CLA	C11-C10-C8-C9
19	B	1214	CLA	C11-C10-C8-C9
19	B	1216	CLA	C14-C13-C15-C16
19	B	1219	CLA	C6-C7-C8-C9
19	B	1222	CLA	C6-C7-C8-C9
19	B	1240	CLA	C11-C10-C8-C9
19	B	1240	CLA	C14-C13-C15-C16
19	H	1701	CLA	C11-C10-C8-C9
19	L	1502	CLA	C6-C7-C8-C9
19	2	604	CLA	C6-C7-C8-C9
19	2	605	CLA	C11-C10-C8-C9
19	2	605	CLA	C14-C13-C15-C16
19	4	612	CLA	C14-C13-C15-C16
19	A	1125	CLA	O1D-CGD-O2D-CED
19	A	1129	CLA	O1D-CGD-O2D-CED
19	A	1137	CLA	O1D-CGD-O2D-CED
19	B	1229	CLA	O1D-CGD-O2D-CED
25	G	5006	LMG	C2-C1-O1-C7
27	B	5005	DGD	C2D-C1D-O3G-C3G
27	1	803	DGD	C2D-C1D-O3G-C3G
19	A	1132	CLA	O1D-CGD-O2D-CED
19	A	1116	CLA	O1A-CGA-O2A-C1
19	2	604	CLA	O1A-CGA-O2A-C1
27	4	802	DGD	O1A-C1A-O1G-C1G
19	B	1222	CLA	O1D-CGD-O2D-CED
19	4	605	CLA	O1D-CGD-O2D-CED
22	H	4021	BCR	C11-C12-C13-C35

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Mol	Chain	Res	Type	Atoms
22	I	4020	BCR	C11-C12-C13-C35
22	1	503	BCR	C11-C12-C13-C35
22	2	503	BCR	C36-C18-C19-C20
22	3	503	BCR	C36-C18-C19-C20
30	2	502	XAT	C11-C12-C13-C20
19	A	1126	CLA	C2A-CAA-CBA-CGA
19	B	1212	CLA	O1D-CGD-O2D-CED
19	1	607	CLA	O1A-CGA-O2A-C1
19	A	1112	CLA	O1A-CGA-O2A-C1
19	A	1124	CLA	O1A-CGA-O2A-C1
19	B	1229	CLA	O1A-CGA-O2A-C1
19	3	605	CLA	O1A-CGA-O2A-C1
19	4	617	CLA	O1A-CGA-O2A-C1
23	A	5002	LHG	O9-C7-O7-C5
25	G	5002	LMG	O1-C7-C8-O7
27	F	5005	DGD	O2G-C2G-C3G-O3G
19	A	1123	CLA	CBA-CGA-O2A-C1
19	B	1228	CLA	CBA-CGA-O2A-C1
19	B	1240	CLA	CBA-CGA-O2A-C1
27	J	5001	DGD	C2A-C1A-O1G-C1G
19	A	1106	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	1133	CLA	C2-C1-O2A-CGA
19	A	1135	CLA	C2-C1-O2A-CGA
19	A	1137	CLA	C2-C1-O2A-CGA
19	B	1022	CLA	C2-C1-O2A-CGA
19	B	1237	CLA	C2-C1-O2A-CGA
19	B	1203	CLA	C2-C1-O2A-CGA
19	B	1206	CLA	C2-C1-O2A-CGA
19	B	1212	CLA	C2-C1-O2A-CGA
19	B	1214	CLA	C2-C1-O2A-CGA
19	B	1219	CLA	C2-C1-O2A-CGA
19	B	1220	CLA	C2-C1-O2A-CGA
19	B	1221	CLA	C2-C1-O2A-CGA
19	B	1236	CLA	C2-C1-O2A-CGA
19	B	1238	CLA	C2-C1-O2A-CGA
19	F	1301	CLA	C2-C1-O2A-CGA
19	J	1901	CLA	C2-C1-O2A-CGA
19	K	1403	CLA	C2-C1-O2A-CGA
19	1	611	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
19	1	614	CLA	C2-C1-O2A-CGA
19	2	601	CLA	C2-C1-O2A-CGA
19	2	612	CLA	C2-C1-O2A-CGA
19	4	609	CLA	C2-C1-O2A-CGA
19	4	601	CLA	C2-C1-O2A-CGA
19	4	606	CLA	C2-C1-O2A-CGA
29	3	604	CHL	C2-C1-O2A-CGA
18	A	1011	CL0	O1A-CGA-O2A-C1
19	A	1109	CLA	O1D-CGD-O2D-CED
19	A	1128	CLA	O1D-CGD-O2D-CED
19	A	1136	CLA	O1D-CGD-O2D-CED
19	A	1107	CLA	C10-C11-C12-C13
19	A	1117	CLA	C8-C10-C11-C12
19	A	1124	CLA	C5-C6-C7-C8
19	A	1138	CLA	C8-C10-C11-C12
19	A	1101	CLA	C8-C10-C11-C12
19	B	1228	CLA	C8-C10-C11-C12
19	B	1231	CLA	C8-C10-C11-C12
19	B	1238	CLA	C5-C6-C7-C8
19	2	612	CLA	C5-C6-C7-C8
19	4	612	CLA	C10-C11-C12-C13
19	4	617	CLA	C5-C6-C7-C8
23	1	801	LHG	O1-C1-C2-O2
19	B	1235	CLA	O1D-CGD-O2D-CED
19	B	1237	CLA	C11-C12-C13-C15
19	B	1204	CLA	C6-C7-C8-C10
25	G	5002	LMG	O6-C5-C6-O5
23	A	5002	LHG	C7-C8-C9-C10
23	B	5002	LHG	C23-C24-C25-C26
22	K	4001	BCR	C9-C10-C11-C12
25	2	804	LMG	O9-C10-O7-C8
19	4	602	CLA	O1D-CGD-O2D-CED
19	B	1206	CLA	C3-C5-C6-C7
19	B	1229	CLA	C3-C5-C6-C7
19	F	1301	CLA	C3-C5-C6-C7
19	A	1122	CLA	C10-C11-C12-C13
19	2	603	CLA	C10-C11-C12-C13
19	3	610	CLA	C8-C10-C11-C12
19	A	1102	CLA	C5-C6-C7-C8
19	A	1109	CLA	C10-C11-C12-C13
19	B	1205	CLA	C15-C16-C17-C18
19	B	1240	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
19	F	1301	CLA	C8-C10-C11-C12
19	1	611	CLA	C8-C10-C11-C12
19	2	605	CLA	C5-C6-C7-C8
19	4	603	CLA	C8-C10-C11-C12
19	4	607	CLA	C5-C6-C7-C8
19	A	1105	CLA	C2A-CAA-CBA-CGA
19	A	1114	CLA	C2A-CAA-CBA-CGA
19	A	1121	CLA	C2A-CAA-CBA-CGA
19	A	1141	CLA	C2A-CAA-CBA-CGA
19	B	1214	CLA	C2A-CAA-CBA-CGA
29	3	604	CHL	C2A-CAA-CBA-CGA
19	A	1104	CLA	C8-C10-C11-C12
19	A	1111	CLA	C10-C11-C12-C13
19	A	1132	CLA	C10-C11-C12-C13
19	B	1023	CLA	C13-C15-C16-C17
19	B	1023	CLA	C15-C16-C17-C18
19	B	1218	CLA	C8-C10-C11-C12
19	B	1223	CLA	C13-C15-C16-C17
19	B	1230	CLA	C5-C6-C7-C8
23	2	801	LHG	C7-C8-C9-C10
25	F	5003	LMG	C10-C11-C12-C13
19	A	1135	CLA	O1D-CGD-O2D-CED
19	A	1103	CLA	O1A-CGA-O2A-C1
19	B	1235	CLA	O1A-CGA-O2A-C1
19	1	614	CLA	O1A-CGA-O2A-C1
18	A	1011	CL0	CBD-CGD-O2D-CED
24	B	5008	LMT	O5'-C1'-O1'-C1
19	A	1123	CLA	C15-C16-C17-C18
19	A	1127	CLA	C8-C10-C11-C12
19	A	1127	CLA	C15-C16-C17-C18
19	A	1131	CLA	C5-C6-C7-C8
19	A	1132	CLA	C13-C15-C16-C17
19	B	1021	CLA	C13-C15-C16-C17
19	B	1205	CLA	C8-C10-C11-C12
19	B	1219	CLA	C8-C10-C11-C12
19	B	1228	CLA	C10-C11-C12-C13
19	3	610	CLA	C13-C15-C16-C17
19	4	601	CLA	C5-C6-C7-C8
23	B	5001	LHG	O2-C2-C3-O3
23	B	5002	LHG	O2-C2-C3-O3
23	2	801	LHG	O2-C2-C3-O3
23	4	801	LHG	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
19	K	1401	CLA	O1D-CGD-O2D-CED
19	B	1212	CLA	CBA-CGA-O2A-C1
19	2	601	CLA	CBA-CGA-O2A-C1
19	B	1221	CLA	CBD-CGD-O2D-CED
19	4	602	CLA	O1A-CGA-O2A-C1
24	A	5004	LMT	C4'-C5'-C6'-O6'
24	G	5004	LMT	C4B-C5B-C6B-O6B
23	4	801	LHG	C23-C24-C25-C26
25	B	5004	LMG	C10-C11-C12-C13
19	A	1117	CLA	C5-C6-C7-C8
19	B	1227	CLA	C15-C16-C17-C18
19	2	603	CLA	C15-C16-C17-C18
19	B	1217	CLA	O1D-CGD-O2D-CED
19	A	1106	CLA	O1D-CGD-O2D-CED
19	A	1114	CLA	O1D-CGD-O2D-CED
19	A	1131	CLA	C15-C16-C17-C18
19	B	1207	CLA	C8-C10-C11-C12
19	B	1213	CLA	C8-C10-C11-C12
19	B	1222	CLA	C8-C10-C11-C12
19	4	617	CLA	C15-C16-C17-C18
19	A	1123	CLA	O1A-CGA-O2A-C1
27	J	5001	DGD	O1A-C1A-O1G-C1G
19	A	1104	CLA	C2-C3-C5-C6
24	G	5004	LMT	C4'-C5'-C6'-O6'
23	A	5001	LHG	C23-C24-C25-C26
25	3	802	LMG	C10-C11-C12-C13
19	A	1101	CLA	O1D-CGD-O2D-CED
19	1	614	CLA	O1D-CGD-O2D-CED
19	3	617	CLA	O1D-CGD-O2D-CED
19	A	1133	CLA	C5-C6-C7-C8
19	A	1138	CLA	C5-C6-C7-C8
19	B	1201	CLA	C5-C6-C7-C8
19	B	1211	CLA	C5-C6-C7-C8
19	G	1603	CLA	C10-C11-C12-C13
19	4	605	CLA	C8-C10-C11-C12
19	A	1107	CLA	CBA-CGA-O2A-C1
19	A	1118	CLA	CBA-CGA-O2A-C1
27	B	5005	DGD	C2A-C1A-O1G-C1G
19	B	1228	CLA	O1A-CGA-O2A-C1
19	B	1240	CLA	O1A-CGA-O2A-C1
24	G	5004	LMT	C2B-C1B-O1B-C4'
19	H	1701	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
19	B	1219	CLA	C5-C6-C7-C8
23	A	5001	LHG	C1-C2-C3-O3
23	4	801	LHG	C1-C2-C3-O3
19	A	1135	CLA	C2A-CAA-CBA-CGA
19	B	1237	CLA	C2A-CAA-CBA-CGA
19	A	1102	CLA	O1D-CGD-O2D-CED
19	B	1023	CLA	CBA-CGA-O2A-C1
19	B	1204	CLA	CBA-CGA-O2A-C1
19	A	1102	CLA	C10-C11-C12-C13
19	A	1111	CLA	C13-C15-C16-C17
19	A	1112	CLA	C15-C16-C17-C18
19	A	1115	CLA	C13-C15-C16-C17
19	A	1129	CLA	C13-C15-C16-C17
19	A	1101	CLA	C5-C6-C7-C8
19	B	1201	CLA	C8-C10-C11-C12
19	B	1218	CLA	C5-C6-C7-C8
19	B	1220	CLA	C5-C6-C7-C8
19	B	1240	CLA	C10-C11-C12-C13
19	1	611	CLA	C13-C15-C16-C17
19	2	603	CLA	C5-C6-C7-C8
19	2	607	CLA	C8-C10-C11-C12
19	B	1222	CLA	C3-C5-C6-C7
19	A	1119	CLA	C13-C15-C16-C17
19	B	1237	CLA	C15-C16-C17-C18
19	B	1202	CLA	C13-C15-C16-C17
19	B	1203	CLA	C5-C6-C7-C8
19	F	1302	CLA	C5-C6-C7-C8
19	4	605	CLA	C5-C6-C7-C8
19	A	1120	CLA	CBA-CGA-O2A-C1
19	L	1501	CLA	CBA-CGA-O2A-C1
19	1	605	CLA	O1D-CGD-O2D-CED
19	B	1202	CLA	C15-C16-C17-C18
19	B	1240	CLA	C15-C16-C17-C18
19	4	601	CLA	C8-C10-C11-C12
25	F	5001	LMG	C11-C10-O7-C8
19	B	1211	CLA	C14-C13-C15-C16
25	F	5001	LMG	O9-C10-O7-C8
24	B	5008	LMT	C2'-C1'-O1'-C1
24	B	5006	LMT	C2'-C1'-O1'-C1
24	G	5005	LMT	C2'-C1'-O1'-C1
25	F	5002	LMG	C2-C1-O1-C7
27	G	5003	DGD	C2D-C1D-O3G-C3G

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Mol	Chain	Res	Type	Atoms
27	J	5001	DGD	C2E-C1E-O5D-C6D
23	B	5002	LHG	C7-C8-C9-C10
19	B	1205	CLA	O1D-CGD-O2D-CED
23	3	801	LHG	O2-C2-C3-O3
19	B	1226	CLA	CBA-CGA-O2A-C1
19	B	1236	CLA	CBA-CGA-O2A-C1
19	A	1102	CLA	C16-C17-C18-C19
19	B	1223	CLA	C16-C17-C18-C20
22	B	4006	BCR	C11-C10-C9-C34
22	1	503	BCR	C11-C10-C9-C34
19	A	1121	CLA	C8-C10-C11-C12
19	B	1229	CLA	C15-C16-C17-C18
22	B	4010	BCR	C36-C18-C19-C20
28	2	501	LUT	C27-C28-C29-C39
28	3	501	LUT	C27-C28-C29-C39
28	4	501	LUT	C27-C28-C29-C39
22	B	4010	BCR	C21-C22-C23-C24
19	A	1107	CLA	O1A-CGA-O2A-C1
27	B	5005	DGD	O1A-C1A-O1G-C1G
19	A	1119	CLA	C2A-CAA-CBA-CGA
19	A	1140	CLA	C2A-CAA-CBA-CGA
19	1	603	CLA	C2A-CAA-CBA-CGA
19	3	603	CLA	C2A-CAA-CBA-CGA
19	A	1107	CLA	C13-C15-C16-C17
19	A	1120	CLA	C5-C6-C7-C8
23	1	801	LHG	O1-C1-C2-C3
23	2	801	LHG	O1-C1-C2-C3
22	A	4003	BCR	C9-C10-C11-C12
19	A	1012	CLA	C16-C17-C18-C19
19	A	1107	CLA	C16-C17-C18-C19
19	A	1127	CLA	C16-C17-C18-C20
19	A	1137	CLA	C16-C17-C18-C20
19	B	1207	CLA	C16-C17-C18-C20
19	B	1222	CLA	C16-C17-C18-C20
19	B	1240	CLA	C16-C17-C18-C20
19	2	607	CLA	C11-C12-C13-C14
19	3	603	CLA	C6-C7-C8-C10
19	B	1202	CLA	O1D-CGD-O2D-CED
19	4	617	CLA	O1D-CGD-O2D-CED
19	B	1023	CLA	O1A-CGA-O2A-C1
19	B	1204	CLA	O1A-CGA-O2A-C1
19	A	1129	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
19	K	1402	CLA	C3-C5-C6-C7
19	3	617	CLA	C3-C5-C6-C7
19	A	1117	CLA	C13-C15-C16-C17
19	L	1502	CLA	C10-C11-C12-C13
22	B	4006	BCR	C11-C10-C9-C8
22	I	4018	BCR	C11-C10-C9-C8
22	1	503	BCR	C11-C10-C9-C8
24	B	5006	LMT	O5'-C1'-O1'-C1
27	G	5003	DGD	O6D-C1D-O3G-C3G
23	A	5001	LHG	C8-C7-O7-C5
23	1	801	LHG	C8-C7-O7-C5
25	B	5007	LMG	C11-C10-O7-C8
19	1	604	CLA	O1D-CGD-O2D-CED
19	2	604	CLA	O1D-CGD-O2D-CED
19	A	1141	CLA	CBA-CGA-O2A-C1
19	1	601	CLA	C8-C10-C11-C12
19	A	1107	CLA	C2-C1-O2A-CGA
19	A	1116	CLA	C2-C1-O2A-CGA
19	A	1131	CLA	C2-C1-O2A-CGA
19	A	1134	CLA	C2-C1-O2A-CGA
19	A	1101	CLA	C2-C1-O2A-CGA
19	A	1108	CLA	C2-C1-O2A-CGA
19	B	1211	CLA	C2-C1-O2A-CGA
19	B	1213	CLA	C2-C1-O2A-CGA
19	B	1223	CLA	C2-C1-O2A-CGA
19	B	1230	CLA	C2-C1-O2A-CGA
19	G	1603	CLA	C2-C1-O2A-CGA
19	H	1701	CLA	C2-C1-O2A-CGA
19	1	605	CLA	C2-C1-O2A-CGA
19	1	606	CLA	C2-C1-O2A-CGA
19	2	602	CLA	C2-C1-O2A-CGA
19	2	604	CLA	C2-C1-O2A-CGA
19	3	602	CLA	C2-C1-O2A-CGA
19	3	606	CLA	C2-C1-O2A-CGA
19	3	610	CLA	C2-C1-O2A-CGA
19	3	617	CLA	C2-C1-O2A-CGA
19	A	1110	CLA	C6-C7-C8-C9
19	A	1111	CLA	C16-C17-C18-C20
19	A	1101	CLA	C16-C17-C18-C19
19	B	1207	CLA	C16-C17-C18-C19
19	B	1222	CLA	C16-C17-C18-C19
19	B	1223	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
19	B	1240	CLA	C16-C17-C18-C19
19	2	607	CLA	C11-C12-C13-C15
19	A	1109	CLA	C13-C15-C16-C17
19	A	1136	CLA	C10-C11-C12-C13
19	B	1216	CLA	C8-C10-C11-C12
20	B	2002	PQN	C25-C26-C27-C28
19	4	609	CLA	O1D-CGD-O2D-CED
23	1	801	LHG	C30-C31-C32-C33
19	B	1211	CLA	CBD-CGD-O2D-CED
19	1	607	CLA	O1D-CGD-O2D-CED
19	B	1218	CLA	C15-C16-C17-C18
23	A	5002	LHG	C34-C35-C36-C37
25	B	5007	LMG	O9-C10-O7-C8
23	A	5001	LHG	O1-C1-C2-O2
19	B	1231	CLA	C5-C6-C7-C8
19	B	1214	CLA	C4B-C3B-CAB-CBB
19	K	1404	CLA	C4B-C3B-CAB-CBB
23	A	5002	LHG	C23-C24-C25-C26
19	A	1107	CLA	C16-C17-C18-C20
19	A	1127	CLA	C16-C17-C18-C19
19	A	1137	CLA	C16-C17-C18-C19
19	B	1021	CLA	C16-C17-C18-C20
19	3	603	CLA	C6-C7-C8-C9
19	3	610	CLA	C16-C17-C18-C19
19	3	610	CLA	C16-C17-C18-C20
19	A	1118	CLA	O1A-CGA-O2A-C1
19	2	601	CLA	O1A-CGA-O2A-C1
19	B	1239	CLA	C2A-CAA-CBA-CGA
19	K	1402	CLA	C2A-CAA-CBA-CGA
23	1	801	LHG	C24-C25-C26-C27
19	A	1111	CLA	C15-C16-C17-C18
19	A	1139	CLA	C5-C6-C7-C8
19	B	1215	CLA	C15-C16-C17-C18
19	B	1224	CLA	C13-C15-C16-C17
19	B	1225	CLA	C13-C15-C16-C17
19	1	605	CLA	C13-C15-C16-C17
25	2	805	LMG	C11-C10-O7-C8
19	A	1105	CLA	C2C-C3C-CAC-CBC
19	A	1132	CLA	C11-C10-C8-C7
19	B	1237	CLA	C6-C7-C8-C10
19	B	1203	CLA	C11-C12-C13-C15
19	3	610	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
19	3	617	CLA	C11-C10-C8-C7
19	A	1140	CLA	CBA-CGA-O2A-C1
19	B	1214	CLA	C10-C11-C12-C13
19	B	1221	CLA	C10-C11-C12-C13
23	A	5001	LHG	C11-C12-C13-C14
25	G	5002	LMG	C16-C17-C18-C19
19	B	1212	CLA	O1A-CGA-O2A-C1
19	B	1236	CLA	O1A-CGA-O2A-C1
24	B	5008	LMT	C4'-C5'-C6'-O6'
19	A	1109	CLA	C3-C5-C6-C7
19	A	1102	CLA	C4-C3-C5-C6
19	A	1103	CLA	C3A-C2A-CAA-CBA
19	A	1104	CLA	C3A-C2A-CAA-CBA
19	A	1110	CLA	C3A-C2A-CAA-CBA
19	A	1121	CLA	C3A-C2A-CAA-CBA
19	A	1125	CLA	C3A-C2A-CAA-CBA
19	A	1135	CLA	C3A-C2A-CAA-CBA
19	A	1101	CLA	C3A-C2A-CAA-CBA
19	B	1221	CLA	C3A-C2A-CAA-CBA
19	B	1223	CLA	C3A-C2A-CAA-CBA
19	G	1602	CLA	C3A-C2A-CAA-CBA
19	J	1901	CLA	C3A-C2A-CAA-CBA
19	K	1403	CLA	C3A-C2A-CAA-CBA
19	1	602	CLA	C3A-C2A-CAA-CBA
19	1	603	CLA	C3A-C2A-CAA-CBA
19	2	605	CLA	C3A-C2A-CAA-CBA
19	3	605	CLA	C3A-C2A-CAA-CBA
19	3	617	CLA	C3A-C2A-CAA-CBA
19	4	617	CLA	C3A-C2A-CAA-CBA
19	B	1230	CLA	O1D-CGD-O2D-CED
19	B	1211	CLA	C15-C16-C17-C18
19	B	1214	CLA	C15-C16-C17-C18
19	A	1012	CLA	C16-C17-C18-C20
19	A	1111	CLA	C16-C17-C18-C19
19	A	1125	CLA	C16-C17-C18-C20
19	B	1021	CLA	C16-C17-C18-C19
19	G	1601	CLA	C6-C7-C8-C9
19	3	601	CLA	C6-C7-C8-C10
19	A	1120	CLA	O1A-CGA-O2A-C1
19	K	1401	CLA	C2C-C3C-CAC-CBC
23	1	801	LHG	C28-C29-C30-C31
19	A	1128	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
19	B	1234	CLA	CBA-CGA-O2A-C1
19	4	604	CLA	CBA-CGA-O2A-C1
27	1	803	DGD	C2A-C1A-O1G-C1G
19	A	1132	CLA	C3-C5-C6-C7
19	K	1402	CLA	C8-C10-C11-C12
19	B	1226	CLA	O1A-CGA-O2A-C1
19	L	1501	CLA	O1A-CGA-O2A-C1
19	B	1224	CLA	C8-C10-C11-C12
27	F	5005	DGD	C3A-C4A-C5A-C6A
19	A	1110	CLA	C6-C7-C8-C10
19	A	1134	CLA	C6-C7-C8-C10
22	A	4002	BCR	C5-C6-C7-C8
22	A	4002	BCR	C23-C24-C25-C30
22	A	4003	BCR	C23-C24-C25-C26
22	A	4003	BCR	C23-C24-C25-C30
22	A	4007	BCR	C1-C6-C7-C8
22	A	4007	BCR	C5-C6-C7-C8
22	A	4007	BCR	C23-C24-C25-C30
22	A	4008	BCR	C23-C24-C25-C26
22	A	4011	BCR	C1-C6-C7-C8
22	A	4011	BCR	C23-C24-C25-C30
22	A	4017	BCR	C1-C6-C7-C8
22	A	4017	BCR	C5-C6-C7-C8
22	A	4017	BCR	C23-C24-C25-C26
22	B	4004	BCR	C1-C6-C7-C8
22	B	4005	BCR	C1-C6-C7-C8
22	B	4009	BCR	C1-C6-C7-C8
22	B	4009	BCR	C23-C24-C25-C26
22	F	4014	BCR	C23-C24-C25-C30
22	F	4016	BCR	C23-C24-C25-C30
22	G	4011	BCR	C1-C6-C7-C8
22	I	4018	BCR	C23-C24-C25-C26
22	I	4018	BCR	C23-C24-C25-C30
22	I	4020	BCR	C1-C6-C7-C8
22	I	4020	BCR	C23-C24-C25-C30
22	L	4020	BCR	C1-C6-C7-C8
22	1	504	BCR	C1-C6-C7-C8
22	2	503	BCR	C23-C24-C25-C26
28	J	4013	LUT	C5-C6-C7-C8
28	1	502	LUT	C1-C6-C7-C8
28	1	502	LUT	C5-C6-C7-C8
28	2	501	LUT	C1-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
28	2	501	LUT	C5-C6-C7-C8
28	3	501	LUT	C5-C6-C7-C8
28	4	501	LUT	C5-C6-C7-C8
23	1	801	LHG	C13-C14-C15-C16
25	2	803	LMG	C11-C10-O7-C8
31	2	807	3PH	C22-C21-O21-C2
19	B	1218	CLA	CBA-CGA-O2A-C1
19	H	1701	CLA	CBA-CGA-O2A-C1
23	4	801	LHG	C11-C12-C13-C14
19	A	1123	CLA	O1D-CGD-O2D-CED
19	2	603	CLA	C2A-CAA-CBA-CGA
19	B	1237	CLA	C8-C10-C11-C12
23	B	5002	LHG	C11-C12-C13-C14
19	A	1141	CLA	O1A-CGA-O2A-C1
19	4	604	CLA	O1A-CGA-O2A-C1
23	A	5001	LHG	O9-C7-O7-C5
23	1	801	LHG	O9-C7-O7-C5
25	2	803	LMG	O9-C10-O7-C8
19	4	617	CLA	C4-C3-C5-C6
22	B	4004	BCR	C18-C19-C20-C21
19	A	1102	CLA	C2-C3-C5-C6
19	B	1206	CLA	C2-C3-C5-C6
19	4	617	CLA	C2-C3-C5-C6
23	A	5002	LHG	C11-C12-C13-C14
19	B	1215	CLA	CBA-CGA-O2A-C1
19	F	1301	CLA	CBA-CGA-O2A-C1
25	2	802	LMG	C29-C28-O8-C9
19	1	604	CLA	C3-C5-C6-C7
19	B	1221	CLA	C14-C13-C15-C16
19	B	1239	CLA	C11-C10-C8-C9
25	G	5002	LMG	O6-C1-O1-C7
25	B	5004	LMG	C2-C1-O1-C7
25	2	803	LMG	C2-C1-O1-C7
27	1	803	DGD	C2E-C1E-O5D-C6D
19	B	1229	CLA	C5-C6-C7-C8
19	B	1204	CLA	C13-C15-C16-C17
27	1	803	DGD	O6D-C5D-C6D-O5D
22	B	4004	BCR	C9-C10-C11-C12
22	B	4005	BCR	C9-C10-C11-C12
22	L	4020	BCR	C9-C10-C11-C12
25	F	5003	LMG	C11-C10-O7-C8
23	1	801	LHG	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
27	F	5005	DGD	C1A-C2A-C3A-C4A
23	A	5002	LHG	C28-C29-C30-C31
25	F	5003	LMG	O9-C10-O7-C8
25	2	805	LMG	O9-C10-O7-C8
19	4	612	CLA	C2C-C3C-CAC-CBC
19	A	1140	CLA	O1A-CGA-O2A-C1
19	A	1125	CLA	C5-C6-C7-C8
19	B	1215	CLA	C3-C5-C6-C7
19	3	605	CLA	C3-C5-C6-C7
25	B	5007	LMG	C8-C7-O1-C1
19	B	1201	CLA	C2A-CAA-CBA-CGA
19	3	602	CLA	C3-C5-C6-C7
19	G	1601	CLA	C6-C7-C8-C10
19	A	1117	CLA	C4-C3-C5-C6
19	A	1136	CLA	C4-C3-C5-C6
19	B	1206	CLA	C4-C3-C5-C6
19	B	1234	CLA	C4-C3-C5-C6
29	1	609	CHL	C4-C3-C5-C6
19	A	1117	CLA	C2-C3-C5-C6
19	A	1128	CLA	O1A-CGA-O2A-C1
19	F	1301	CLA	O1A-CGA-O2A-C1
19	A	1112	CLA	C5-C6-C7-C8
19	A	1112	CLA	C13-C15-C16-C17
19	A	1122	CLA	C13-C15-C16-C17
31	2	807	3PH	O22-C21-O21-C2
25	B	5007	LMG	O6-C5-C6-O5
25	F	5006	LMG	O6-C5-C6-O5
27	1	803	DGD	C2G-C1G-O1G-C1A
19	B	1226	CLA	C15-C16-C17-C18
19	B	1235	CLA	C15-C16-C17-C18
19	1	601	CLA	C15-C16-C17-C18
19	A	1102	CLA	C16-C17-C18-C20
19	A	1124	CLA	C6-C7-C8-C9
19	B	1234	CLA	O1A-CGA-O2A-C1
27	1	803	DGD	O1A-C1A-O1G-C1G
25	G	5002	LMG	C10-C11-C12-C13
19	A	1109	CLA	C8-C10-C11-C12
19	B	1210	CLA	C10-C11-C12-C13
19	4	601	CLA	C10-C11-C12-C13
23	B	5002	LHG	C31-C32-C33-C34
19	A	1128	CLA	C3-C5-C6-C7
19	A	1138	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
19	B	1212	CLA	C3-C5-C6-C7
19	A	1123	CLA	C5-C6-C7-C8
19	B	1211	CLA	C13-C15-C16-C17
27	F	5005	DGD	O6E-C5E-C6E-O5E
19	A	1012	CLA	C2-C1-O2A-CGA
19	A	1128	CLA	C2-C1-O2A-CGA
19	B	1227	CLA	C2-C1-O2A-CGA
19	4	607	CLA	C2-C1-O2A-CGA
25	A	5006	LMG	O6-C5-C6-O5
27	4	802	DGD	O6E-C5E-C6E-O5E
19	B	1216	CLA	C16-C17-C18-C19
19	B	1201	CLA	C13-C15-C16-C17
23	4	801	LHG	C2-C3-O3-P
19	B	1226	CLA	O1D-CGD-O2D-CED
19	B	1238	CLA	C3-C5-C6-C7
29	1	609	CHL	C2-C3-C5-C6
23	3	801	LHG	C1-C2-C3-O3
19	L	1501	CLA	C2A-CAA-CBA-CGA
25	G	5001	LMG	C29-C28-O8-C9
25	2	806	LMG	O6-C5-C6-O5
23	B	5002	LHG	C34-C35-C36-C37
23	2	801	LHG	O1-C1-C2-O2
19	H	1701	CLA	O1A-CGA-O2A-C1
19	A	1103	CLA	C1A-C2A-CAA-CBA
19	A	1104	CLA	C1A-C2A-CAA-CBA
19	A	1107	CLA	C1A-C2A-CAA-CBA
19	A	1112	CLA	C1A-C2A-CAA-CBA
19	A	1116	CLA	C1A-C2A-CAA-CBA
19	A	1120	CLA	C1A-C2A-CAA-CBA
19	A	1133	CLA	C1A-C2A-CAA-CBA
19	A	1135	CLA	C1A-C2A-CAA-CBA
19	A	1137	CLA	C1A-C2A-CAA-CBA
19	A	1141	CLA	C1A-C2A-CAA-CBA
19	A	1101	CLA	C1A-C2A-CAA-CBA
19	A	1108	CLA	C1A-C2A-CAA-CBA
19	B	1202	CLA	C1A-C2A-CAA-CBA
19	B	1208	CLA	C1A-C2A-CAA-CBA
19	B	1218	CLA	C1A-C2A-CAA-CBA
19	B	1221	CLA	C1A-C2A-CAA-CBA
19	B	1224	CLA	C1A-C2A-CAA-CBA
19	G	1602	CLA	C1A-C2A-CAA-CBA
19	J	1901	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
19	K	1403	CLA	C1A-C2A-CAA-CBA
19	L	1503	CLA	C1A-C2A-CAA-CBA
19	1	602	CLA	C1A-C2A-CAA-CBA
19	2	604	CLA	C1A-C2A-CAA-CBA
19	2	606	CLA	C1A-C2A-CAA-CBA
19	3	605	CLA	C1A-C2A-CAA-CBA
19	3	606	CLA	C1A-C2A-CAA-CBA
19	3	608	CLA	C1A-C2A-CAA-CBA
19	3	610	CLA	C1A-C2A-CAA-CBA
19	3	617	CLA	C1A-C2A-CAA-CBA
19	4	601	CLA	C1A-C2A-CAA-CBA
19	4	617	CLA	C1A-C2A-CAA-CBA
18	A	1011	CL0	O1D-CGD-O2D-CED
19	2	603	CLA	C13-C15-C16-C17
24	A	5004	LMT	C1-C2-C3-C4
19	B	1218	CLA	O1A-CGA-O2A-C1
25	2	802	LMG	O10-C28-O8-C9
24	A	5004	LMT	C2B-C1B-O1B-C4'
23	B	5002	LHG	O6-C4-C5-C6
19	A	1104	CLA	C11-C12-C13-C15
19	A	1112	CLA	C11-C12-C13-C15
19	A	1117	CLA	C11-C10-C8-C7
19	A	1119	CLA	C12-C13-C15-C16
19	A	1123	CLA	C11-C10-C8-C7
19	A	1136	CLA	C11-C10-C8-C7
19	A	1136	CLA	C12-C13-C15-C16
19	A	1137	CLA	C6-C7-C8-C10
19	A	1139	CLA	C6-C7-C8-C10
19	B	1237	CLA	C12-C13-C15-C16
19	B	1023	CLA	C11-C12-C13-C15
19	B	1206	CLA	C12-C13-C15-C16
19	B	1214	CLA	C11-C10-C8-C7
19	B	1215	CLA	C12-C13-C15-C16
19	B	1226	CLA	C6-C7-C8-C10
19	B	1226	CLA	C11-C12-C13-C15
19	B	1229	CLA	C12-C13-C15-C16
19	F	1302	CLA	C11-C10-C8-C7
19	1	601	CLA	C12-C13-C15-C16
19	2	605	CLA	C11-C10-C8-C7
20	B	2002	PQN	C17-C18-C20-C21
29	3	604	CHL	C11-C12-C13-C15
29	4	613	CHL	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
19	B	1205	CLA	C16-C17-C18-C20
19	A	1126	CLA	C15-C16-C17-C18
19	B	1206	CLA	C8-C10-C11-C12
19	B	1207	CLA	C5-C6-C7-C8
19	4	617	CLA	C2A-CAA-CBA-CGA
19	A	1103	CLA	C6-C7-C8-C9
19	A	1104	CLA	C11-C12-C13-C14
19	A	1106	CLA	C11-C12-C13-C14
19	A	1123	CLA	C11-C10-C8-C9
19	A	1139	CLA	C6-C7-C8-C9
19	B	1203	CLA	C11-C12-C13-C14
19	B	1229	CLA	C14-C13-C15-C16
19	F	1301	CLA	C6-C7-C8-C9
19	F	1302	CLA	C11-C10-C8-C9
19	2	604	CLA	C11-C10-C8-C9
19	2	605	CLA	C11-C12-C13-C14
29	3	604	CHL	C11-C12-C13-C14
25	2	803	LMG	O6-C5-C6-O5
19	A	1125	CLA	CBA-CGA-O2A-C1
19	B	1224	CLA	CBA-CGA-O2A-C1
19	B	1221	CLA	O1D-CGD-O2D-CED
19	A	1137	CLA	C10-C11-C12-C13
19	B	1215	CLA	C8-C10-C11-C12
19	B	1224	CLA	C10-C11-C12-C13
27	B	5005	DGD	O6E-C5E-C6E-O5E
23	A	5002	LHG	C4-C5-C6-O8
25	F	5004	LMG	C7-C8-C9-O8
25	G	5002	LMG	O1-C7-C8-C9
27	F	5005	DGD	C1G-C2G-C3G-O3G
25	B	5004	LMG	O6-C5-C6-O5
19	1	614	CLA	C8-C10-C11-C12
19	2	602	CLA	CBA-CGA-O2A-C1
25	1	802	LMG	O6-C5-C6-O5
19	A	1124	CLA	C6-C7-C8-C10
19	B	1219	CLA	C16-C17-C18-C20
27	B	5005	DGD	CCB-CDB-CEB-CFB
25	G	5001	LMG	O6-C5-C6-O5
22	I	4018	BCR	C11-C10-C9-C34
29	2	610	CHL	CHA-CBD-CGD-O1D
29	2	610	CHL	CHA-CBD-CGD-O2D
19	H	1701	CLA	C10-C11-C12-C13
24	G	5005	LMT	O5B-C5B-C6B-O6B

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Mol	Chain	Res	Type	Atoms
19	A	1119	CLA	C4-C3-C5-C6
19	A	1119	CLA	C2-C3-C5-C6
19	A	1136	CLA	C2-C3-C5-C6
19	B	1234	CLA	C2-C3-C5-C6
19	A	1136	CLA	C8-C10-C11-C12
19	B	1219	CLA	C13-C15-C16-C17
19	2	604	CLA	C15-C16-C17-C18
23	1	801	LHG	C11-C10-C9-C8
19	1	604	CLA	C16-C17-C18-C19
27	1	803	DGD	O6E-C5E-C6E-O5E
27	3	803	DGD	O6E-C5E-C6E-O5E
22	G	4011	BCR	C10-C11-C12-C13
22	I	4018	BCR	C10-C11-C12-C13
22	2	503	BCR	C9-C10-C11-C12
22	3	503	BCR	C9-C10-C11-C12
19	A	1101	CLA	C16-C17-C18-C20
19	B	1205	CLA	C16-C17-C18-C19
25	G	5001	LMG	O10-C28-O8-C9
19	B	1211	CLA	C3-C5-C6-C7
27	1	803	DGD	C4D-C5D-C6D-O5D
19	A	1138	CLA	CBA-CGA-O2A-C1
19	L	1502	CLA	CBA-CGA-O2A-C1
19	1	601	CLA	CBA-CGA-O2A-C1
19	B	1229	CLA	C2-C3-C5-C6
23	2	801	LHG	C25-C26-C27-C28
19	A	1122	CLA	C16-C17-C18-C20
25	B	5003	LMG	C12-C13-C14-C15
25	2	804	LMG	C10-C11-C12-C13
23	B	5002	LHG	O7-C5-C6-O8
23	A	5002	LHG	C25-C26-C27-C28
19	B	1216	CLA	CBA-CGA-O2A-C1
19	A	1129	CLA	C2-C1-O2A-CGA
19	B	1224	CLA	O1A-CGA-O2A-C1
19	H	1701	CLA	C8-C10-C11-C12
23	A	5002	LHG	C13-C14-C15-C16
27	G	5003	DGD	C2B-C1B-O2G-C2G
24	A	5004	LMT	O5B-C1B-O1B-C4'
23	1	801	LHG	C25-C26-C27-C28
19	A	1133	CLA	C13-C15-C16-C17
19	B	1215	CLA	O1A-CGA-O2A-C1
19	A	1109	CLA	C15-C16-C17-C18
19	A	1139	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
19	B	1206	CLA	C5-C6-C7-C8
19	B	1212	CLA	C5-C6-C7-C8
19	B	1232	CLA	C5-C6-C7-C8
19	A	1119	CLA	C16-C17-C18-C20
19	A	1121	CLA	C11-C12-C13-C15
19	B	1023	CLA	C16-C17-C18-C19
19	B	1229	CLA	C4-C3-C5-C6
27	4	802	DGD	C2B-C3B-C4B-C5B
19	3	608	CLA	CBA-CGA-O2A-C1
19	A	1013	CLA	C10-C11-C12-C13
24	B	5008	LMT	C2-C1-O1'-C1'
24	G	5004	LMT	C2-C1-O1'-C1'
19	A	1103	CLA	C11-C12-C13-C14
19	A	1112	CLA	C11-C12-C13-C14
19	A	1117	CLA	C11-C10-C8-C9
19	A	1122	CLA	C11-C10-C8-C9
19	A	1132	CLA	C11-C10-C8-C9
19	A	1136	CLA	C11-C12-C13-C14
19	A	1136	CLA	C14-C13-C15-C16
19	A	1139	CLA	C11-C12-C13-C14
19	B	1023	CLA	C11-C12-C13-C14
19	B	1215	CLA	C14-C13-C15-C16
19	B	1226	CLA	C6-C7-C8-C9
19	B	1227	CLA	C11-C12-C13-C14
19	1	601	CLA	C14-C13-C15-C16
19	3	610	CLA	C11-C12-C13-C14
19	3	617	CLA	C11-C10-C8-C9
29	4	613	CHL	C11-C10-C8-C9
19	A	1131	CLA	C8-C10-C11-C12
19	B	1214	CLA	C8-C10-C11-C12
19	A	1132	CLA	C4B-C3B-CAB-CBB
19	B	1227	CLA	C4B-C3B-CAB-CBB
19	B	1204	CLA	C4B-C3B-CAB-CBB
31	2	807	3PH	O21-C21-C22-C23
19	A	1104	CLA	C5-C6-C7-C8
19	2	607	CLA	C10-C11-C12-C13
25	3	802	LMG	C2-C1-O1-C7
27	F	5005	DGD	C2D-C1D-O3G-C3G
27	3	803	DGD	C2D-C1D-O3G-C3G
27	4	802	DGD	C2D-C1D-O3G-C3G
19	A	1122	CLA	C15-C16-C17-C18
19	A	1116	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
19	A	1103	CLA	C6-C7-C8-C10
19	A	1103	CLA	C11-C12-C13-C15
19	A	1106	CLA	C11-C12-C13-C15
19	A	1123	CLA	C11-C12-C13-C15
19	A	1125	CLA	C6-C7-C8-C10
19	A	1127	CLA	C11-C12-C13-C15
19	A	1132	CLA	C11-C12-C13-C15
19	A	1136	CLA	C11-C12-C13-C15
19	A	1137	CLA	C11-C12-C13-C15
19	A	1139	CLA	C11-C10-C8-C7
19	B	1205	CLA	C11-C12-C13-C15
19	B	1222	CLA	C6-C7-C8-C10
19	B	1227	CLA	C11-C12-C13-C15
19	B	1239	CLA	C6-C7-C8-C10
19	1	604	CLA	C11-C12-C13-C15
19	1	614	CLA	C6-C7-C8-C10
19	2	604	CLA	C11-C10-C8-C7
19	2	605	CLA	C11-C12-C13-C15
19	2	605	CLA	C12-C13-C15-C16
19	4	603	CLA	C6-C7-C8-C10
25	2	805	LMG	C11-C12-C13-C14
23	A	5002	LHG	C11-C10-C9-C8
19	1	611	CLA	C5-C6-C7-C8
19	A	1115	CLA	C16-C17-C18-C19
25	G	5001	LMG	C31-C32-C33-C34
19	A	1109	CLA	C3A-C2A-CAA-CBA
19	A	1131	CLA	C3A-C2A-CAA-CBA
19	A	1101	CLA	C4-C3-C5-C6
19	B	1224	CLA	C3A-C2A-CAA-CBA
19	G	1601	CLA	C3A-C2A-CAA-CBA
19	3	610	CLA	C4-C3-C5-C6
19	4	609	CLA	C3A-C2A-CAA-CBA
29	2	615	CHL	C3A-C2A-CAA-CBA
29	2	615	CHL	C4-C3-C5-C6
19	B	1225	CLA	C15-C16-C17-C18
19	B	1226	CLA	C8-C10-C11-C12
23	A	5001	LHG	C26-C27-C28-C29
19	A	1125	CLA	O1A-CGA-O2A-C1
19	1	601	CLA	O1A-CGA-O2A-C1
19	2	602	CLA	O1A-CGA-O2A-C1
19	B	1216	CLA	C10-C11-C12-C13
19	3	606	CLA	C2C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
22	A	4002	BCR	C9-C10-C11-C12
22	A	4007	BCR	C9-C10-C11-C12
22	2	503	BCR	C15-C16-C17-C18
19	A	1126	CLA	C3-C5-C6-C7
30	4	502	XAT	C27-C28-C29-C39
19	B	1228	CLA	C2A-CAA-CBA-CGA
23	A	5002	LHG	C31-C32-C33-C34
23	3	801	LHG	C4-C5-C6-O8
23	4	801	LHG	C4-C5-C6-O8
25	F	5002	LMG	O1-C7-C8-C9
25	G	5001	LMG	O1-C7-C8-C9
31	2	807	3PH	C1-C2-C3-O31
19	B	1208	CLA	C11-C12-C13-C14
19	B	1219	CLA	C16-C17-C18-C19
19	A	1112	CLA	C8-C10-C11-C12
19	A	1137	CLA	C13-C15-C16-C17
19	B	1227	CLA	C13-C15-C16-C17
19	K	1402	CLA	C5-C6-C7-C8
23	1	801	LHG	C29-C30-C31-C32
18	A	1011	CL0	C1A-C2A-CAA-CBA
23	1	801	LHG	C35-C36-C37-C38
19	A	1121	CLA	C10-C11-C12-C13
19	A	1129	CLA	C5-C6-C7-C8
19	3	610	CLA	C2-C3-C5-C6
29	2	615	CHL	C2-C3-C5-C6
19	B	1204	CLA	C3-C5-C6-C7
19	1	614	CLA	C3-C5-C6-C7
19	B	1235	CLA	C13-C15-C16-C17
19	B	1208	CLA	C11-C12-C13-C15
19	1	604	CLA	C16-C17-C18-C20
23	B	5002	LHG	O6-C4-C5-O7
23	1	801	LHG	O6-C4-C5-O7
19	A	1138	CLA	O1A-CGA-O2A-C1
19	B	1211	CLA	O1D-CGD-O2D-CED
22	A	4017	BCR	C23-C24-C25-C30
22	B	4010	BCR	C23-C24-C25-C26
22	K	4002	BCR	C23-C24-C25-C26
22	2	503	BCR	C23-C24-C25-C30
22	3	503	BCR	C23-C24-C25-C26
28	1	501	LUT	C5-C6-C7-C8
23	1	801	LHG	C2-C3-O3-P
19	F	1301	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
23	1	801	LHG	C16-C17-C18-C19
23	2	801	LHG	C11-C12-C13-C14
19	A	1121	CLA	C11-C12-C13-C14
19	A	1122	CLA	C16-C17-C18-C19
19	A	1134	CLA	C6-C7-C8-C9
19	A	1140	CLA	C16-C17-C18-C20
19	3	601	CLA	C6-C7-C8-C9
19	B	1240	CLA	CAA-CBA-CGA-O2A
23	1	801	LHG	O7-C5-C6-O8
25	F	5004	LMG	O7-C8-C9-O8
27	G	5003	DGD	O1G-C1G-C2G-O2G
27	4	802	DGD	O2G-C2G-C3G-O3G
31	2	807	3PH	O21-C2-C3-O31
19	A	1105	CLA	C4C-C3C-CAC-CBC
23	A	5002	LHG	C27-C28-C29-C30
23	B	5002	LHG	C13-C14-C15-C16
19	G	1603	CLA	C15-C16-C17-C18
19	A	1119	CLA	C16-C17-C18-C19
19	A	1125	CLA	C16-C17-C18-C19
19	B	1023	CLA	C16-C17-C18-C20
31	2	807	3PH	C25-C26-C27-C28
19	L	1502	CLA	O1A-CGA-O2A-C1
19	A	1119	CLA	C14-C13-C15-C16
19	A	1127	CLA	C11-C12-C13-C14
19	A	1128	CLA	C11-C10-C8-C9
19	A	1137	CLA	C11-C12-C13-C14
19	A	1139	CLA	C11-C10-C8-C9
19	A	1141	CLA	C6-C7-C8-C9
19	B	1239	CLA	C6-C7-C8-C9
19	1	604	CLA	C11-C12-C13-C14
19	4	604	CLA	C11-C10-C8-C9
19	A	1133	CLA	C15-C16-C17-C18
19	B	1227	CLA	C5-C6-C7-C8
19	3	617	CLA	C2C-C3C-CAC-CBC
25	A	5006	LMG	C34-C35-C36-C37
19	A	1140	CLA	C16-C17-C18-C19
19	B	1216	CLA	C16-C17-C18-C20
25	G	5001	LMG	C2-C1-O1-C7
19	A	1106	CLA	C5-C6-C7-C8
19	4	601	CLA	O1A-CGA-O2A-C1
19	1	604	CLA	C10-C11-C12-C13
23	3	801	LHG	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
19	A	1133	CLA	CBA-CGA-O2A-C1
19	A	1101	CLA	C2-C3-C5-C6
18	A	1011	CL0	C16-C17-C18-C19
19	A	1115	CLA	C16-C17-C18-C20
22	2	503	BCR	C16-C17-C18-C36
19	A	1012	CLA	CBA-CGA-O2A-C1
19	A	1137	CLA	CBA-CGA-O2A-C1
19	4	601	CLA	CBA-CGA-O2A-C1
19	B	1221	CLA	C5-C6-C7-C8
23	1	801	LHG	O6-C4-C5-C6
19	A	1013	CLA	C6-C7-C8-C10
19	A	1119	CLA	C11-C12-C13-C15
19	A	1120	CLA	C11-C10-C8-C7
19	A	1126	CLA	C6-C7-C8-C10
19	A	1128	CLA	C11-C10-C8-C7
19	A	1131	CLA	C12-C13-C15-C16
19	A	1133	CLA	C11-C12-C13-C15
19	B	1206	CLA	C11-C10-C8-C7
19	B	1216	CLA	C12-C13-C15-C16
19	B	1223	CLA	C12-C13-C15-C16
19	B	1235	CLA	C6-C7-C8-C10
19	1	604	CLA	C6-C7-C8-C10
19	1	605	CLA	C6-C7-C8-C10
19	1	605	CLA	C11-C12-C13-C15
19	2	607	CLA	C11-C10-C8-C7
19	4	612	CLA	C12-C13-C15-C16
20	A	2001	PQN	C21-C22-C23-C25
19	B	1225	CLA	C3-C5-C6-C7
19	A	1122	CLA	C5-C6-C7-C8
19	A	1131	CLA	C13-C15-C16-C17
19	B	1221	CLA	C15-C16-C17-C18
19	K	1402	CLA	C10-C11-C12-C13
19	1	614	CLA	C5-C6-C7-C8
22	3	503	BCR	C21-C22-C23-C24
19	B	1203	CLA	CBA-CGA-O2A-C1
25	G	5002	LMG	C8-C7-O1-C1
19	A	1128	CLA	C5-C6-C7-C8
19	A	1101	CLA	C10-C11-C12-C13
19	B	1239	CLA	C15-C16-C17-C18
19	B	1023	CLA	C2A-CAA-CBA-CGA
19	B	1224	CLA	C2A-CAA-CBA-CGA
19	B	1238	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
19	H	1701	CLA	C2A-CAA-CBA-CGA
19	1	604	CLA	C2A-CAA-CBA-CGA
19	A	1104	CLA	C16-C17-C18-C19
27	G	5003	DGD	O1B-C1B-O2G-C2G
19	A	1123	CLA	C4-C3-C5-C6
19	B	1224	CLA	C4-C3-C5-C6
27	B	5005	DGD	C2G-C1G-O1G-C1A
19	B	1230	CLA	C3-C5-C6-C7
19	A	1117	CLA	CBA-CGA-O2A-C1
23	1	801	LHG	C33-C34-C35-C36
19	B	1202	CLA	C10-C11-C12-C13
19	A	1133	CLA	O1A-CGA-O2A-C1
19	3	608	CLA	O1A-CGA-O2A-C1
19	F	1302	CLA	C10-C11-C12-C13
23	A	5001	LHG	C16-C17-C18-C19
19	A	1137	CLA	O1A-CGA-O2A-C1
19	B	1216	CLA	O1A-CGA-O2A-C1
19	B	1210	CLA	CBA-CGA-O2A-C1
19	B	1238	CLA	CBA-CGA-O2A-C1
19	A	1012	CLA	C15-C16-C17-C18
25	G	5002	LMG	C14-C15-C16-C17
23	1	801	LHG	C4-C5-C6-O8
23	A	5001	LHG	C7-C8-C9-C10
19	A	1136	CLA	C16-C17-C18-C20
19	B	1203	CLA	O1A-CGA-O2A-C1
31	2	807	3PH	C24-C25-C26-C27
19	B	1204	CLA	C5-C6-C7-C8
19	1	603	CLA	C5-C6-C7-C8
19	A	1127	CLA	C3-C5-C6-C7
19	2	605	CLA	C3-C5-C6-C7
23	3	801	LHG	O7-C5-C6-O8
25	B	5007	LMG	O7-C8-C9-O8
25	F	5002	LMG	O1-C7-C8-O7
29	1	610	CHL	C2C-C3C-CAC-CBC
19	A	1013	CLA	C6-C7-C8-C9
19	A	1119	CLA	C11-C12-C13-C14
19	B	1206	CLA	C11-C10-C8-C9
29	3	604	CHL	C14-C13-C15-C16
24	G	5004	LMT	C6-C7-C8-C9
23	2	801	LHG	C26-C27-C28-C29
27	J	5001	DGD	C6A-C7A-C8A-C9A
19	A	1117	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
23	A	5001	LHG	C15-C16-C17-C18
19	A	1109	CLA	C2-C1-O2A-CGA
19	A	1115	CLA	C2-C1-O2A-CGA
19	A	1122	CLA	C2-C1-O2A-CGA
19	A	1139	CLA	C2-C1-O2A-CGA
19	A	1141	CLA	C2-C1-O2A-CGA
19	2	608	CLA	C2-C1-O2A-CGA
19	3	608	CLA	C2-C1-O2A-CGA
19	A	1105	CLA	C11-C12-C13-C15
19	B	1201	CLA	C10-C11-C12-C13
19	4	612	CLA	C4C-C3C-CAC-CBC
19	B	1023	CLA	C2C-C3C-CAC-CBC
25	G	5001	LMG	C33-C34-C35-C36
19	A	1128	CLA	C10-C11-C12-C13
19	2	604	CLA	C10-C11-C12-C13
19	2	605	CLA	C13-C15-C16-C17
19	B	1221	CLA	C16-C17-C18-C19
19	4	601	CLA	C11-C12-C13-C15
19	B	1210	CLA	O1A-CGA-O2A-C1
29	2	610	CHL	C4C-C3C-CAC-CBC
19	A	1126	CLA	C16-C17-C18-C20
19	4	603	CLA	C13-C15-C16-C17
19	A	1132	CLA	C1A-C2A-CAA-CBA
19	B	1211	CLA	C1A-C2A-CAA-CBA
19	K	1402	CLA	C1A-C2A-CAA-CBA
19	3	617	CLA	C4B-C3B-CAB-CBB
19	4	609	CLA	C1A-C2A-CAA-CBA
19	B	1214	CLA	C13-C15-C16-C17
23	4	801	LHG	C28-C29-C30-C31
23	B	5002	LHG	C25-C26-C27-C28
25	2	803	LMG	C11-C12-C13-C14
19	A	1139	CLA	C13-C15-C16-C17
23	A	5001	LHG	O6-C4-C5-C6
23	3	801	LHG	O6-C4-C5-C6
19	A	1135	CLA	C2-C3-C5-C6
19	B	1237	CLA	C13-C15-C16-C17
19	A	1102	CLA	C6-C7-C8-C10
19	A	1109	CLA	C11-C12-C13-C15
19	A	1119	CLA	C11-C10-C8-C7
19	A	1141	CLA	C6-C7-C8-C10
19	B	1023	CLA	C11-C10-C8-C7
19	B	1223	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
19	B	1226	CLA	C12-C13-C15-C16
19	B	1228	CLA	C6-C7-C8-C10
19	1	611	CLA	C12-C13-C15-C16
19	4	604	CLA	C11-C10-C8-C7
19	4	607	CLA	C6-C7-C8-C10
19	A	1136	CLA	CBA-CGA-O2A-C1
27	B	5005	DGD	C6B-C7B-C8B-C9B
25	G	5002	LMG	C4-C5-C6-O5
23	B	5002	LHG	C19-C20-C21-C22
27	4	802	DGD	C2G-C1G-O1G-C1A
19	A	1012	CLA	O1A-CGA-O2A-C1
23	A	5001	LHG	C17-C18-C19-C20
23	4	801	LHG	C11-C10-C9-C8
25	1	802	LMG	C30-C31-C32-C33
23	A	5001	LHG	O6-C4-C5-O7
23	A	5002	LHG	O6-C4-C5-O7
23	3	801	LHG	O6-C4-C5-O7
29	2	613	CHL	C2A-CAA-CBA-CGA
19	A	1131	CLA	C14-C13-C15-C16
19	A	1132	CLA	C11-C12-C13-C14
19	A	1133	CLA	C11-C12-C13-C14
19	B	1223	CLA	C14-C13-C15-C16
19	B	1235	CLA	C6-C7-C8-C9
19	B	1204	CLA	C6-C7-C8-C9
19	1	604	CLA	C6-C7-C8-C9
19	2	607	CLA	C11-C10-C8-C9
20	A	2001	PQN	C21-C22-C23-C24
19	A	1136	CLA	O1A-CGA-O2A-C1
19	A	1138	CLA	C13-C15-C16-C17
19	2	601	CLA	C10-C11-C12-C13
23	1	801	LHG	C34-C35-C36-C37
25	B	5003	LMG	C11-C12-C13-C14
19	A	1119	CLA	C3-C5-C6-C7
19	K	1401	CLA	C4C-C3C-CAC-CBC
25	G	5001	LMG	O1-C7-C8-O7
27	B	5005	DGD	O2G-C2G-C3G-O3G
19	A	1116	CLA	C5-C6-C7-C8
25	G	5002	LMG	C32-C33-C34-C35
23	B	5002	LHG	C4-C5-C6-O8
25	F	5003	LMG	O1-C7-C8-C9
25	2	803	LMG	O1-C7-C8-C9
27	B	5005	DGD	C1G-C2G-C3G-O3G

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Mol	Chain	Res	Type	Atoms
27	4	802	DGD	O1G-C1G-C2G-C3G
19	B	1226	CLA	C10-C11-C12-C13
19	A	1123	CLA	C2-C3-C5-C6
19	A	1115	CLA	C3-C5-C6-C7
23	2	801	LHG	C28-C29-C30-C31
19	3	606	CLA	CAD-CBD-CGD-O2D
19	A	1117	CLA	C16-C17-C18-C20
19	B	1022	CLA	C16-C17-C18-C20
19	B	1232	CLA	C3-C5-C6-C7
19	A	1138	CLA	C2A-CAA-CBA-CGA
19	B	1238	CLA	O1A-CGA-O2A-C1
19	2	608	CLA	C2C-C3C-CAC-CBC
19	B	1226	CLA	C13-C15-C16-C17
19	B	1211	CLA	CHA-CBD-CGD-O1D
19	B	1211	CLA	CHA-CBD-CGD-O2D
19	B	1221	CLA	CHA-CBD-CGD-O1D
19	B	1221	CLA	CHA-CBD-CGD-O2D
19	K	1403	CLA	CHA-CBD-CGD-O1D
19	K	1403	CLA	CHA-CBD-CGD-O2D
19	1	604	CLA	CHA-CBD-CGD-O1D
19	1	604	CLA	CHA-CBD-CGD-O2D
19	1	608	CLA	CHA-CBD-CGD-O1D
19	1	608	CLA	CHA-CBD-CGD-O2D
19	2	607	CLA	CHA-CBD-CGD-O1D
19	3	606	CLA	CAD-CBD-CGD-O1D
19	4	605	CLA	CHA-CBD-CGD-O1D
23	A	5001	LHG	C3-O3-P-O5
23	A	5002	LHG	C3-O3-P-O5
23	A	5002	LHG	C4-O6-P-O5
23	1	801	LHG	C3-O3-P-O5
23	2	801	LHG	C4-O6-P-O5
23	3	801	LHG	C4-O6-P-O5
29	2	613	CHL	CHA-CBD-CGD-O2D
29	4	613	CHL	CHA-CBD-CGD-O1D
29	4	613	CHL	CHA-CBD-CGD-O2D
19	B	1214	CLA	C2B-C3B-CAB-CBB
19	K	1404	CLA	C2B-C3B-CAB-CBB
28	J	4013	LUT	C1-C6-C7-C8
19	B	1224	CLA	C2-C3-C5-C6
23	4	801	LHG	C26-C27-C28-C29
23	A	5001	LHG	C2-C3-O3-P
23	A	5002	LHG	C2-C3-O3-P

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Mol	Chain	Res	Type	Atoms
23	3	801	LHG	C2-C3-O3-P
30	2	502	XAT	C27-C28-C29-C39
25	F	5002	LMG	C16-C17-C18-C19
19	A	1102	CLA	C8-C10-C11-C12
27	F	5005	DGD	C1B-C2B-C3B-C4B
25	F	5001	LMG	C9-C8-O7-C10
25	G	5006	LMG	C9-C8-O7-C10
25	G	5001	LMG	C7-C8-O7-C10
25	2	803	LMG	C7-C8-O7-C10
27	B	5005	DGD	C1G-C2G-O2G-C1B
27	J	5001	DGD	C1G-C2G-O2G-C1B
25	A	5006	LMG	C32-C33-C34-C35
22	B	4006	BCR	C18-C19-C20-C21
22	K	4001	BCR	C10-C11-C12-C13
22	K	4002	BCR	C18-C19-C20-C21
18	A	1011	CL0	C16-C17-C18-C20
19	A	1104	CLA	C16-C17-C18-C20
19	A	1105	CLA	C11-C12-C13-C14
19	A	1141	CLA	C11-C12-C13-C14
19	F	1301	CLA	C5-C6-C7-C8
23	A	5002	LHG	O6-C4-C5-C6
19	1	605	CLA	C11-C12-C13-C14
19	1	611	CLA	C14-C13-C15-C16
19	3	610	CLA	C11-C10-C8-C9
19	A	1112	CLA	C11-C10-C8-C7
19	2	604	CLA	C6-C7-C8-C10
22	A	4017	BCR	C16-C17-C18-C19
22	G	4011	BCR	C16-C17-C18-C19
25	F	5004	LMG	O6-C1-O1-C7
19	B	1221	CLA	C16-C17-C18-C20
19	1	614	CLA	C11-C12-C13-C14
29	2	615	CHL	CAA-CBA-CGA-O2A
27	J	5001	DGD	CDA-CEA-CFA-CGA
19	4	612	CLA	C13-C15-C16-C17
19	B	1224	CLA	CAA-CBA-CGA-O2A
19	4	601	CLA	C11-C12-C13-C14
23	B	5002	LHG	C35-C36-C37-C38
31	2	807	3PH	C22-C23-C24-C25
25	F	5003	LMG	O1-C7-C8-O7
18	A	1011	CL0	CAA-CBA-CGA-O2A
22	F	4014	BCR	C9-C10-C11-C12
19	1	601	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
19	B	1215	CLA	CAA-CBA-CGA-O2A
19	3	606	CLA	C4C-C3C-CAC-CBC
19	A	1124	CLA	C2-C1-O2A-CGA
19	B	1240	CLA	C2-C1-O2A-CGA
19	2	605	CLA	C2-C1-O2A-CGA
19	3	607	CLA	C2-C1-O2A-CGA
19	A	1131	CLA	C16-C17-C18-C20
19	B	1209	CLA	CAA-CBA-CGA-O2A
25	1	802	LMG	O7-C10-C11-C12
27	1	803	DGD	O1G-C1A-C2A-C3A
30	4	502	XAT	C27-C28-C29-C30
31	2	807	3PH	C32-C31-O31-C3
25	B	5004	LMG	C28-C29-C30-C31
19	4	608	CLA	CAA-CBA-CGA-O2A
25	F	5003	LMG	C8-C7-O1-C1
25	1	802	LMG	C8-C7-O1-C1
27	3	803	DGD	C5D-C6D-O5D-C1E
19	B	1219	CLA	C2A-CAA-CBA-CGA
19	B	1238	CLA	C16-C17-C18-C20
29	4	613	CHL	C11-C12-C13-C15
19	A	1103	CLA	C4-C3-C5-C6
19	B	1221	CLA	C4-C3-C5-C6
19	3	617	CLA	C5-C6-C7-C8
24	G	5004	LMT	C5'-C4'-O1B-C1B
25	G	5006	LMG	O8-C28-C29-C30
19	A	1129	CLA	C16-C17-C18-C19
24	G	5005	LMT	C1-C2-C3-C4
19	B	1023	CLA	C11-C10-C8-C9
19	B	1201	CLA	C11-C12-C13-C14
19	B	1208	CLA	C6-C7-C8-C9
19	B	1223	CLA	C6-C7-C8-C9
19	F	1301	CLA	C11-C12-C13-C14
19	4	603	CLA	C11-C12-C13-C14
19	A	1124	CLA	C2C-C3C-CAC-CBC
19	4	609	CLA	C4B-C3B-CAB-CBB
19	B	1235	CLA	C16-C17-C18-C19
19	3	617	CLA	CBA-CGA-O2A-C1
19	A	1111	CLA	C8-C10-C11-C12
23	A	5002	LHG	C35-C36-C37-C38
19	A	1121	CLA	C4-C3-C5-C6
19	3	617	CLA	C4-C3-C5-C6
29	1	612	CHL	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
25	F	5004	LMG	C2-C1-O1-C7
19	A	1133	CLA	C10-C11-C12-C13
19	A	1113	CLA	CAA-CBA-CGA-O2A
19	3	617	CLA	O1A-CGA-O2A-C1
31	2	807	3PH	O32-C31-O31-C3
23	A	5001	LHG	C11-C10-C9-C8
25	2	803	LMG	O7-C10-C11-C12
19	A	1106	CLA	C12-C13-C15-C16
19	B	1208	CLA	C6-C7-C8-C10
19	B	1221	CLA	C6-C7-C8-C10
19	L	1502	CLA	C6-C7-C8-C10
20	B	2002	PQN	C21-C22-C23-C25
19	A	1141	CLA	C10-C11-C12-C13
19	B	1224	CLA	C15-C16-C17-C18
19	A	1102	CLA	C3A-C2A-CAA-CBA
19	F	1301	CLA	C3A-C2A-CAA-CBA
19	H	1701	CLA	C3A-C2A-CAA-CBA
19	4	617	CLA	C13-C15-C16-C17
19	B	1213	CLA	C2A-CAA-CBA-CGA
22	A	4007	BCR	C16-C17-C18-C36
22	A	4011	BCR	C16-C17-C18-C36
22	A	4017	BCR	C16-C17-C18-C36
22	B	4004	BCR	C16-C17-C18-C36
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	3	506	BCR	C16-C17-C18-C36
25	B	5007	LMG	O6-C1-O1-C7
24	2	808	LMT	C11-C10-C9-C8
19	1	614	CLA	C10-C11-C12-C13
19	L	1503	CLA	C2-C1-O2A-CGA
19	2	603	CLA	C2-C1-O2A-CGA
19	4	602	CLA	C2-C1-O2A-CGA
22	1	504	BCR	C19-C20-C21-C22
20	B	2002	PQN	C15-C16-C17-C18
19	A	1135	CLA	C4-C3-C5-C6
23	B	5002	LHG	C11-C10-C9-C8
19	A	1113	CLA	CAA-CBA-CGA-O1A
19	3	610	CLA	C15-C16-C17-C18
31	2	807	3PH	O22-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
19	A	1106	CLA	C14-C13-C15-C16
19	A	1107	CLA	C11-C10-C8-C9
19	A	1112	CLA	C14-C13-C15-C16
19	A	1133	CLA	C11-C10-C8-C9
19	B	1210	CLA	C6-C7-C8-C9
19	B	1218	CLA	C14-C13-C15-C16
19	B	1221	CLA	C6-C7-C8-C9
19	G	1603	CLA	C14-C13-C15-C16
19	2	601	CLA	C11-C10-C8-C9
19	4	604	CLA	C6-C7-C8-C9
20	B	2002	PQN	C21-C22-C23-C24
19	A	1105	CLA	C8-C10-C11-C12
19	B	1204	CLA	C15-C16-C17-C18
19	1	605	CLA	C5-C6-C7-C8
25	F	5003	LMG	C9-C8-O7-C10
27	B	5005	DGD	C3G-C2G-O2G-C1B
19	A	1139	CLA	C15-C16-C17-C18
19	B	1210	CLA	C3-C5-C6-C7
19	A	1138	CLA	C4-C3-C5-C6
19	A	1141	CLA	C11-C12-C13-C15
29	2	613	CHL	CAA-CBA-CGA-O1A
19	A	1013	CLA	C2A-CAA-CBA-CGA
19	A	1102	CLA	C1A-C2A-CAA-CBA
19	A	1128	CLA	C1A-C2A-CAA-CBA
19	A	1131	CLA	C1A-C2A-CAA-CBA
19	B	1209	CLA	C1A-C2A-CAA-CBA
19	B	1210	CLA	C1A-C2A-CAA-CBA
19	B	1212	CLA	C1A-C2A-CAA-CBA
19	B	1236	CLA	C1A-C2A-CAA-CBA
19	F	1301	CLA	C1A-C2A-CAA-CBA
19	G	1601	CLA	C1A-C2A-CAA-CBA
19	1	608	CLA	C1A-C2A-CAA-CBA
19	3	613	CLA	C1A-C2A-CAA-CBA
22	A	4007	BCR	C16-C17-C18-C19
22	A	4011	BCR	C16-C17-C18-C19
22	B	4004	BCR	C16-C17-C18-C19
22	F	4016	BCR	C16-C17-C18-C19
22	I	4018	BCR	C12-C13-C14-C15
22	I	4020	BCR	C20-C21-C22-C23
22	1	504	BCR	C16-C17-C18-C19
19	2	608	CLA	C4C-C3C-CAC-CBC
19	B	1212	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
19	2	605	CLA	C16-C17-C18-C19
19	4	605	CLA	C11-C12-C13-C15
25	B	5003	LMG	O6-C1-O1-C7
19	A	1132	CLA	C2B-C3B-CAB-CBB
19	B	1227	CLA	C2B-C3B-CAB-CBB
19	3	617	CLA	C2B-C3B-CAB-CBB
22	B	4009	BCR	C23-C24-C25-C30
19	A	1111	CLA	CBA-CGA-O2A-C1
19	A	1105	CLA	C4-C3-C5-C6
19	A	1112	CLA	C4-C3-C5-C6
19	B	1222	CLA	C4-C3-C5-C6
19	1	611	CLA	C4-C3-C5-C6
19	A	1111	CLA	O1A-CGA-O2A-C1
19	A	1103	CLA	C2-C3-C5-C6
29	1	612	CHL	C2-C3-C5-C6
19	A	1115	CLA	C11-C10-C8-C7
19	A	1121	CLA	C11-C10-C8-C7
19	B	1201	CLA	C11-C12-C13-C15
19	B	1225	CLA	C6-C7-C8-C10
19	F	1301	CLA	C11-C12-C13-C15
19	4	603	CLA	C11-C12-C13-C15
23	B	5001	LHG	C24-C23-O8-C6
19	1	601	CLA	C2A-CAA-CBA-CGA
19	1	607	CLA	C2A-CAA-CBA-CGA
23	A	5001	LHG	O7-C5-C6-O8
23	3	801	LHG	C4-C5-O7-C7
23	3	801	LHG	C6-C5-O7-C7
25	G	5001	LMG	C36-C37-C38-C39
19	4	612	CLA	C3-C5-C6-C7
19	A	1117	CLA	C16-C17-C18-C19
19	1	613	CLA	CAA-CBA-CGA-O2A
19	F	1301	CLA	C4-C3-C5-C6
19	3	605	CLA	C4-C3-C5-C6
19	A	1112	CLA	C2-C3-C5-C6
19	A	1121	CLA	C2-C3-C5-C6
19	F	1301	CLA	C2-C3-C5-C6
19	3	617	CLA	C2-C3-C5-C6
23	B	5002	LHG	C28-C29-C30-C31
19	B	1224	CLA	C2-C1-O2A-CGA
19	A	1141	CLA	C5-C6-C7-C8
29	2	613	CHL	CAA-CBA-CGA-O2A
19	B	1232	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
19	A	1102	CLA	C11-C10-C8-C9
19	B	1225	CLA	C14-C13-C15-C16
19	1	611	CLA	C11-C10-C8-C9
20	A	2001	PQN	C19-C18-C20-C21
19	A	1132	CLA	O1A-CGA-O2A-C1
27	B	5005	DGD	C5A-C6A-C7A-C8A
19	B	1208	CLA	C4-C3-C5-C6
19	B	1211	CLA	C4-C3-C5-C6
19	A	1138	CLA	C2-C3-C5-C6
19	1	601	CLA	C16-C17-C18-C19
19	A	1132	CLA	C5-C6-C7-C8
19	B	1237	CLA	C10-C11-C12-C13
19	B	1225	CLA	C5-C6-C7-C8
24	G	5004	LMT	C7-C8-C9-C10
27	4	802	DGD	C1G-C2G-C3G-O3G
19	3	605	CLA	C2A-CAA-CBA-CGA
19	B	1220	CLA	CAA-CBA-CGA-O2A
23	4	801	LHG	O6-C4-C5-O7
19	B	1202	CLA	C4-C3-C5-C6
19	K	1402	CLA	C4-C3-C5-C6
19	1	601	CLA	C2C-C3C-CAC-CBC
19	A	1131	CLA	C16-C17-C18-C19
19	A	1136	CLA	C16-C17-C18-C19
19	B	1022	CLA	C16-C17-C18-C19
19	B	1022	CLA	C4B-C3B-CAB-CBB
19	L	1501	CLA	C4B-C3B-CAB-CBB
19	1	613	CLA	CAA-CBA-CGA-O1A
24	B	5008	LMT	O1'-C1-C2-C3
19	4	603	CLA	O1A-CGA-O2A-C1
22	1	504	BCR	C16-C17-C18-C36
29	2	611	CHL	CHA-CBD-CGD-O2D
29	2	615	CHL	CHA-CBD-CGD-O2D
29	4	610	CHL	CHA-CBD-CGD-O1D
29	4	610	CHL	CHA-CBD-CGD-O2D
19	1	601	CLA	C4C-C3C-CAC-CBC
23	1	801	LHG	C26-C27-C28-C29
19	A	1120	CLA	C11-C12-C13-C14
27	F	5005	DGD	O1G-C1G-C2G-O2G
19	B	1208	CLA	C2-C3-C5-C6
19	B	1211	CLA	C2-C3-C5-C6
25	2	803	LMG	O6-C1-O1-C7
19	A	1013	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
19	B	1203	CLA	C6-C7-C8-C10
19	B	1225	CLA	C12-C13-C15-C16
19	B	1240	CLA	C11-C10-C8-C7
19	B	1240	CLA	C12-C13-C15-C16
19	1	611	CLA	C11-C10-C8-C7
19	B	1213	CLA	O1A-CGA-O2A-C1
23	A	5002	LHG	C29-C30-C31-C32
19	B	1240	CLA	CAA-CBA-CGA-O1A
19	A	1102	CLA	C11-C12-C13-C14
19	A	1138	CLA	C11-C10-C8-C9
19	B	1230	CLA	C11-C10-C8-C9
19	B	1204	CLA	C14-C13-C15-C16
19	4	603	CLA	C14-C13-C15-C16
25	G	5006	LMG	O10-C28-C29-C30
19	A	1124	CLA	C2A-CAA-CBA-CGA
19	2	607	CLA	C2-C1-O2A-CGA
29	4	613	CHL	C2-C1-O2A-CGA
23	2	801	LHG	C9-C10-C11-C12
29	1	612	CHL	C11-C12-C13-C14
24	2	808	LMT	C1-C2-C3-C4
19	G	1603	CLA	C8-C10-C11-C12
19	A	1126	CLA	C3A-C2A-CAA-CBA
19	A	1113	CLA	C3A-C2A-CAA-CBA
19	B	1210	CLA	C3A-C2A-CAA-CBA
19	B	1210	CLA	C4-C3-C5-C6
19	3	612	CLA	C3A-C2A-CAA-CBA
19	3	613	CLA	C3A-C2A-CAA-CBA
29	2	611	CHL	C3A-C2A-CAA-CBA
19	B	1221	CLA	CAA-CBA-CGA-O2A
23	4	801	LHG	O8-C23-C24-C25
29	4	613	CHL	C11-C12-C13-C14
19	B	1219	CLA	O2A-C1-C2-C3
25	F	5003	LMG	C7-C8-O7-C10
25	F	5004	LMG	C7-C8-O7-C10
25	F	5004	LMG	C9-C8-O7-C10
27	G	5003	DGD	C1G-C2G-O2G-C1B
25	B	5007	LMG	C10-C11-C12-C13
23	A	5001	LHG	C25-C26-C27-C28
19	B	1224	CLA	C5-C6-C7-C8
19	B	1222	CLA	C13-C15-C16-C17
31	2	807	3PH	C33-C34-C35-C36
22	I	4020	BCR	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
22	3	506	BCR	C16-C17-C18-C19
19	A	1132	CLA	CBA-CGA-O2A-C1
19	B	1213	CLA	CBA-CGA-O2A-C1
25	B	5007	LMG	C7-C8-C9-O8
27	G	5003	DGD	O1G-C1G-C2G-C3G
19	A	1127	CLA	C13-C15-C16-C17
19	B	1238	CLA	C16-C17-C18-C19
23	A	5001	LHG	C19-C20-C21-C22
19	A	1118	CLA	C2A-CAA-CBA-CGA
29	1	609	CHL	C2A-CAA-CBA-CGA
29	4	611	CHL	C2A-CAA-CBA-CGA
19	A	1129	CLA	C16-C17-C18-C20
19	A	1102	CLA	CAA-CBA-CGA-O2A
19	B	1236	CLA	CAA-CBA-CGA-O2A
19	B	1238	CLA	CAA-CBA-CGA-O2A
25	B	5007	LMG	O7-C10-C11-C12
27	F	5005	DGD	O1G-C1A-C2A-C3A
27	J	5001	DGD	O1G-C1G-C2G-O2G
27	3	803	DGD	O2G-C2G-C3G-O3G
19	A	1102	CLA	C6-C7-C8-C9
19	A	1106	CLA	C11-C10-C8-C9
19	A	1107	CLA	C11-C12-C13-C14
19	A	1109	CLA	C11-C12-C13-C14
19	B	1226	CLA	C14-C13-C15-C16
19	B	1228	CLA	C6-C7-C8-C9
19	K	1402	CLA	C6-C7-C8-C9
19	1	605	CLA	C6-C7-C8-C9
19	B	1212	CLA	C6-C7-C8-C9
19	B	1232	CLA	C6-C7-C8-C10
19	A	1125	CLA	CAA-CBA-CGA-O2A
19	A	1131	CLA	CAA-CBA-CGA-O2A
19	A	1136	CLA	CAA-CBA-CGA-O2A
19	1	614	CLA	CAA-CBA-CGA-O2A
29	2	610	CHL	CAA-CBA-CGA-O2A
30	2	502	XAT	C27-C28-C29-C30
19	3	603	CLA	CAA-CBA-CGA-O2A
19	A	1122	CLA	C2A-CAA-CBA-CGA
19	3	601	CLA	C2A-CAA-CBA-CGA
19	A	1111	CLA	C6-C7-C8-C10
19	A	1120	CLA	C6-C7-C8-C10
19	B	1201	CLA	C12-C13-C15-C16
19	B	1208	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
19	B	1227	CLA	C11-C10-C8-C7
19	B	1230	CLA	C11-C10-C8-C7
19	B	1204	CLA	C12-C13-C15-C16
19	1	611	CLA	C6-C7-C8-C10
19	2	607	CLA	C6-C7-C8-C10
19	4	603	CLA	C12-C13-C15-C16
20	A	2001	PQN	C17-C18-C20-C21
29	3	604	CHL	C12-C13-C15-C16
19	A	1128	CLA	C2B-C3B-CAB-CBB
19	B	1022	CLA	C2B-C3B-CAB-CBB
19	B	1228	CLA	C2B-C3B-CAB-CBB
19	B	1204	CLA	C2B-C3B-CAB-CBB
19	4	609	CLA	C2B-C3B-CAB-CBB
22	A	4008	BCR	C23-C24-C25-C30
22	L	4020	BCR	C23-C24-C25-C26
25	G	5006	LMG	O7-C10-C11-C12
28	1	501	LUT	C1-C6-C7-C8
28	3	501	LUT	C1-C6-C7-C8
28	4	501	LUT	C1-C6-C7-C8
19	B	1202	CLA	CAA-CBA-CGA-O2A
19	B	1201	CLA	C2-C1-O2A-CGA
27	B	5005	DGD	C4A-C5A-C6A-C7A
19	A	1138	CLA	CAA-CBA-CGA-O2A
23	B	5002	LHG	C14-C15-C16-C17
19	4	603	CLA	CBA-CGA-O2A-C1
19	B	1202	CLA	C2-C3-C5-C6
19	1	611	CLA	C2-C3-C5-C6
19	1	603	CLA	O1A-CGA-O2A-C1
19	A	1106	CLA	C2A-CAA-CBA-CGA
19	B	1208	CLA	C2A-CAA-CBA-CGA
19	B	1235	CLA	CAA-CBA-CGA-O2A
19	1	605	CLA	CAA-CBA-CGA-O2A
25	A	5006	LMG	O7-C10-C11-C12
25	G	5001	LMG	O8-C28-C29-C30
25	3	802	LMG	O7-C10-C11-C12
27	1	803	DGD	C4A-C5A-C6A-C7A
19	1	607	CLA	CAA-CBA-CGA-O2A
23	2	801	LHG	O8-C23-C24-C25
27	G	5003	DGD	O2G-C1B-C2B-C3B
25	F	5002	LMG	C15-C16-C17-C18
19	L	1502	CLA	C8-C10-C11-C12
19	B	1221	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
19	B	1222	CLA	C2-C3-C5-C6
23	B	5002	LHG	C16-C17-C18-C19
25	B	5004	LMG	C29-C30-C31-C32
19	B	1023	CLA	C3-C5-C6-C7
29	1	612	CHL	C2A-CAA-CBA-CGA
19	A	1128	CLA	CAA-CBA-CGA-O2A
19	A	1107	CLA	C6-C7-C8-C9
19	B	1225	CLA	C6-C7-C8-C9
19	4	603	CLA	C10-C11-C12-C13
27	J	5001	DGD	O1G-C1G-C2G-C3G
19	A	1116	CLA	C4B-C3B-CAB-CBB
19	A	1126	CLA	C1A-C2A-CAA-CBA
19	A	1113	CLA	C1A-C2A-CAA-CBA
19	B	1213	CLA	C1A-C2A-CAA-CBA
19	B	1215	CLA	C1A-C2A-CAA-CBA
19	B	1229	CLA	C1A-C2A-CAA-CBA
19	B	1240	CLA	C1A-C2A-CAA-CBA
19	H	1701	CLA	C1A-C2A-CAA-CBA
23	B	5002	LHG	C27-C28-C29-C30
19	B	1205	CLA	C4-C3-C5-C6
19	2	603	CLA	C4-C3-C5-C6
19	A	1127	CLA	CAA-CBA-CGA-O2A
19	3	601	CLA	CAA-CBA-CGA-O2A
23	A	5002	LHG	O7-C7-C8-C9
27	4	802	DGD	O1G-C1A-C2A-C3A
22	3	506	BCR	C11-C12-C13-C14
28	1	502	LUT	C27-C28-C29-C30
28	4	501	LUT	C11-C12-C13-C14
22	K	4002	BCR	C15-C16-C17-C18
19	A	1013	CLA	C16-C17-C18-C20
19	A	1111	CLA	CAA-CBA-CGA-O2A
19	B	1237	CLA	CAA-CBA-CGA-O2A
19	3	602	CLA	CAA-CBA-CGA-O2A
25	B	5003	LMG	O8-C28-C29-C30
27	1	803	DGD	O2G-C1B-C2B-C3B
29	3	604	CHL	CAA-CBA-CGA-O2A
19	G	1602	CLA	C2A-CAA-CBA-CGA
19	F	1302	CLA	C13-C15-C16-C17
19	B	1206	CLA	C16-C17-C18-C19
19	A	1114	CLA	CAA-CBA-CGA-O2A
19	A	1120	CLA	CAA-CBA-CGA-O2A
19	B	1207	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
19	G	1601	CLA	CAA-CBA-CGA-O2A
27	B	5005	DGD	C3A-C4A-C5A-C6A
19	A	1120	CLA	C8-C10-C11-C12
19	B	1234	CLA	C2-C1-O2A-CGA
19	K	1402	CLA	CAA-CBA-CGA-O2A
19	3	607	CLA	CAA-CBA-CGA-O2A
19	A	1104	CLA	C6-C7-C8-C10
19	A	1133	CLA	C12-C13-C15-C16
19	B	1202	CLA	C12-C13-C15-C16
19	B	1222	CLA	C11-C12-C13-C15
19	K	1402	CLA	C6-C7-C8-C10
19	F	1301	CLA	C2C-C3C-CAC-CBC
19	L	1502	CLA	C5-C6-C7-C8
19	B	1215	CLA	C2A-CAA-CBA-CGA
19	B	1225	CLA	C2A-CAA-CBA-CGA
19	A	1012	CLA	C13-C15-C16-C17
19	A	1138	CLA	C16-C17-C18-C20
25	F	5003	LMG	C30-C31-C32-C33
20	A	2001	PQN	C3-C11-C12-C13
19	A	1111	CLA	C4-C3-C5-C6
19	2	606	CLA	C3A-C2A-CAA-CBA
23	1	801	LHG	C19-C20-C21-C22
19	2	603	CLA	CAA-CBA-CGA-O2A
25	2	805	LMG	O7-C10-C11-C12
23	4	801	LHG	C25-C26-C27-C28
19	B	1236	CLA	CAA-CBA-CGA-O1A
19	3	603	CLA	CAA-CBA-CGA-O1A
19	A	1112	CLA	CAA-CBA-CGA-O2A
19	A	1136	CLA	CAA-CBA-CGA-O1A
19	1	614	CLA	CAA-CBA-CGA-O1A
27	F	5005	DGD	O1A-C1A-C2A-C3A
19	B	1210	CLA	C13-C15-C16-C17
19	B	1232	CLA	C2A-CAA-CBA-CGA
19	B	1022	CLA	CBA-CGA-O2A-C1
19	1	603	CLA	CBA-CGA-O2A-C1
19	A	1013	CLA	C11-C12-C13-C14
19	A	1121	CLA	C11-C10-C8-C9
19	A	1133	CLA	C14-C13-C15-C16
19	A	1136	CLA	C11-C10-C8-C9
19	B	1202	CLA	C14-C13-C15-C16
19	B	1227	CLA	C11-C10-C8-C9
19	4	607	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
19	4	617	CLA	C11-C12-C13-C14
19	B	1235	CLA	CAA-CBA-CGA-O1A
25	B	5007	LMG	O9-C10-C11-C12
25	G	5001	LMG	O10-C28-C29-C30
19	A	1133	CLA	C8-C10-C11-C12
20	A	2001	PQN	C18-C20-C21-C22
19	4	617	CLA	C10-C11-C12-C13
19	B	1202	CLA	CAA-CBA-CGA-O1A
19	1	605	CLA	CAA-CBA-CGA-O1A
19	1	607	CLA	CAA-CBA-CGA-O1A
19	3	601	CLA	CAA-CBA-CGA-O1A
19	4	607	CLA	CAA-CBA-CGA-O2A
30	2	502	XAT	C1-C6-C7-C8
19	A	1131	CLA	CAA-CBA-CGA-O1A
19	A	1138	CLA	CAA-CBA-CGA-O1A
23	1	801	LHG	C31-C32-C33-C34
27	4	802	DGD	O2G-C1B-C2B-C3B
28	4	505	LUT	C7-C8-C9-C10
25	G	5006	LMG	O9-C10-C11-C12
19	A	1102	CLA	CAA-CBA-CGA-O1A
19	A	1120	CLA	CAA-CBA-CGA-O1A
19	A	1125	CLA	CAA-CBA-CGA-O1A
19	A	1127	CLA	CAA-CBA-CGA-O1A
19	A	1128	CLA	CAA-CBA-CGA-O1A
19	B	1238	CLA	CAA-CBA-CGA-O1A
19	G	1601	CLA	CAA-CBA-CGA-O1A
19	K	1402	CLA	CAA-CBA-CGA-O1A
19	3	602	CLA	CAA-CBA-CGA-O1A
25	A	5006	LMG	O9-C10-C11-C12
27	1	803	DGD	C2G-C3G-O3G-C1D
25	2	803	LMG	O1-C7-C8-O7
27	4	802	DGD	O1A-C1A-C2A-C3A
29	2	610	CHL	CAA-CBA-CGA-O1A
19	A	1111	CLA	CAA-CBA-CGA-O1A
19	B	1207	CLA	C13-C15-C16-C17
19	3	617	CLA	CAA-CBA-CGA-O2A
23	A	5002	LHG	O8-C23-C24-C25
19	K	1402	CLA	C2-C3-C5-C6
23	2	801	LHG	O10-C23-C24-C25
27	G	5003	DGD	O1B-C1B-C2B-C3B
19	A	1135	CLA	CAD-CBD-CGD-O2D
19	B	1203	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
19	B	1226	CLA	CAD-CBD-CGD-O2D
19	K	1403	CLA	CAD-CBD-CGD-O2D
19	L	1502	CLA	CAA-CBA-CGA-O2A
19	K	1401	CLA	CAA-CBA-CGA-O2A
25	A	5006	LMG	C8-C9-O8-C28
19	B	1207	CLA	CAA-CBA-CGA-O1A
25	G	5002	LMG	C13-C14-C15-C16
23	4	801	LHG	O6-C4-C5-C6
31	2	807	3PH	O11-C1-C2-C3
27	4	802	DGD	C9B-CAB-CBB-CCB
25	3	802	LMG	O9-C10-C11-C12
29	3	604	CHL	CAA-CBA-CGA-O1A
19	B	1211	CLA	CAA-CBA-CGA-O2A
19	4	612	CLA	C16-C17-C18-C20
27	B	5005	DGD	C6A-C7A-C8A-C9A
19	B	1022	CLA	C8-C10-C11-C12
19	B	1022	CLA	O1A-CGA-O2A-C1
19	2	607	CLA	C2C-C3C-CAC-CBC
19	A	1109	CLA	CAA-CBA-CGA-O2A
19	A	1135	CLA	CAA-CBA-CGA-O2A
19	B	1205	CLA	CAA-CBA-CGA-O2A
19	B	1206	CLA	CAA-CBA-CGA-O2A
19	K	1404	CLA	CAA-CBA-CGA-O2A
19	4	601	CLA	CAA-CBA-CGA-O2A
20	A	2001	PQN	C20-C21-C22-C23
19	A	1114	CLA	CAA-CBA-CGA-O1A
19	B	1227	CLA	C8-C10-C11-C12
25	F	5002	LMG	C14-C15-C16-C17
25	F	5001	LMG	O7-C10-C11-C12
19	A	1109	CLA	CAA-CBA-CGA-O1A
19	B	1237	CLA	CAA-CBA-CGA-O1A

There are no ring outliers.

198 monomers are involved in 753 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	F	5002	LMG	1	0
22	J	4012	BCR	9	0
18	A	1011	CL0	2	0
19	1	608	CLA	2	0
22	L	4020	BCR	8	0
19	B	1209	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	B	4010	BCR	10	0
19	2	608	CLA	3	0
20	B	2002	PQN	1	0
19	4	606	CLA	6	0
29	2	615	CHL	9	0
19	1	613	CLA	4	0
22	B	4004	BCR	8	0
19	B	1235	CLA	3	0
22	A	4002	BCR	8	0
24	B	5008	LMT	2	0
21	C	3002	SF4	1	0
19	B	1228	CLA	2	0
22	A	4011	BCR	10	0
19	A	1121	CLA	4	0
19	A	1108	CLA	7	0
23	A	5001	LHG	1	0
22	F	4014	BCR	7	0
19	B	1203	CLA	4	0
19	A	1125	CLA	9	0
19	B	1240	CLA	1	0
19	A	1119	CLA	4	0
19	A	1133	CLA	2	0
19	F	1302	CLA	1	0
19	L	1502	CLA	3	0
19	3	617	CLA	1	0
22	A	4017	BCR	8	0
19	B	1232	CLA	6	0
28	4	505	LUT	5	0
29	3	611	CHL	1	0
19	B	1221	CLA	4	0
19	2	602	CLA	2	0
28	3	502	LUT	12	0
19	B	1211	CLA	7	0
19	A	1139	CLA	3	0
19	B	1237	CLA	1	0
21	C	3003	SF4	1	0
19	A	1104	CLA	7	0
19	B	1213	CLA	4	0
19	4	604	CLA	5	0
22	H	4021	BCR	10	0
27	4	802	DGD	1	0
22	A	4003	BCR	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	I	4018	BCR	8	0
19	4	601	CLA	10	0
19	4	617	CLA	3	0
19	B	1217	CLA	2	0
19	G	1601	CLA	1	0
19	3	606	CLA	3	0
19	B	1208	CLA	4	0
22	1	504	BCR	3	0
27	G	5003	DGD	1	0
19	1	614	CLA	2	0
19	B	1231	CLA	6	0
20	A	2001	PQN	2	0
19	3	610	CLA	4	0
19	B	1227	CLA	4	0
19	G	1602	CLA	1	0
19	A	1013	CLA	7	0
19	4	612	CLA	1	0
19	A	1132	CLA	3	0
19	B	1220	CLA	4	0
19	B	1223	CLA	4	0
19	3	605	CLA	2	0
25	A	5006	LMG	2	0
19	A	1135	CLA	8	0
19	A	1113	CLA	4	0
19	B	1023	CLA	5	0
19	B	1222	CLA	3	0
19	K	1402	CLA	3	0
28	1	502	LUT	7	0
19	1	606	CLA	3	0
19	B	1234	CLA	5	0
19	2	601	CLA	10	0
27	F	5005	DGD	1	0
19	A	1130	CLA	2	0
19	A	1107	CLA	2	0
19	1	607	CLA	1	0
19	3	601	CLA	6	0
19	A	1122	CLA	5	0
19	3	608	CLA	2	0
19	2	607	CLA	8	0
19	A	1012	CLA	3	0
19	A	1136	CLA	2	0
22	B	4009	BCR	10	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	A	1111	CLA	4	0
19	A	1120	CLA	2	0
22	A	4007	BCR	5	0
22	B	4005	BCR	6	0
24	G	5004	LMT	3	0
28	1	501	LUT	10	0
19	A	1114	CLA	2	0
19	G	1603	CLA	6	0
28	2	501	LUT	11	0
29	4	611	CHL	2	0
19	B	1224	CLA	2	0
22	3	503	BCR	17	0
19	A	1141	CLA	2	0
19	A	1106	CLA	5	0
19	L	1503	CLA	6	0
19	B	1238	CLA	3	0
22	1	503	BCR	6	0
19	B	1218	CLA	4	0
29	1	612	CHL	1	0
28	J	4013	LUT	12	0
19	B	1206	CLA	7	0
22	F	4016	BCR	6	0
22	K	4002	BCR	9	0
19	J	1901	CLA	2	0
19	1	601	CLA	6	0
19	A	1117	CLA	3	0
19	2	603	CLA	4	0
22	I	4020	BCR	4	0
22	L	4019	BCR	9	0
29	2	611	CHL	6	0
19	A	1109	CLA	7	0
29	1	609	CHL	1	0
29	4	610	CHL	2	0
25	G	5002	LMG	2	0
19	B	1226	CLA	4	0
19	3	603	CLA	4	0
19	A	1124	CLA	2	0
19	A	1134	CLA	2	0
19	2	604	CLA	6	0
19	B	1202	CLA	3	0
19	A	1101	CLA	6	0
19	B	1230	CLA	2	0

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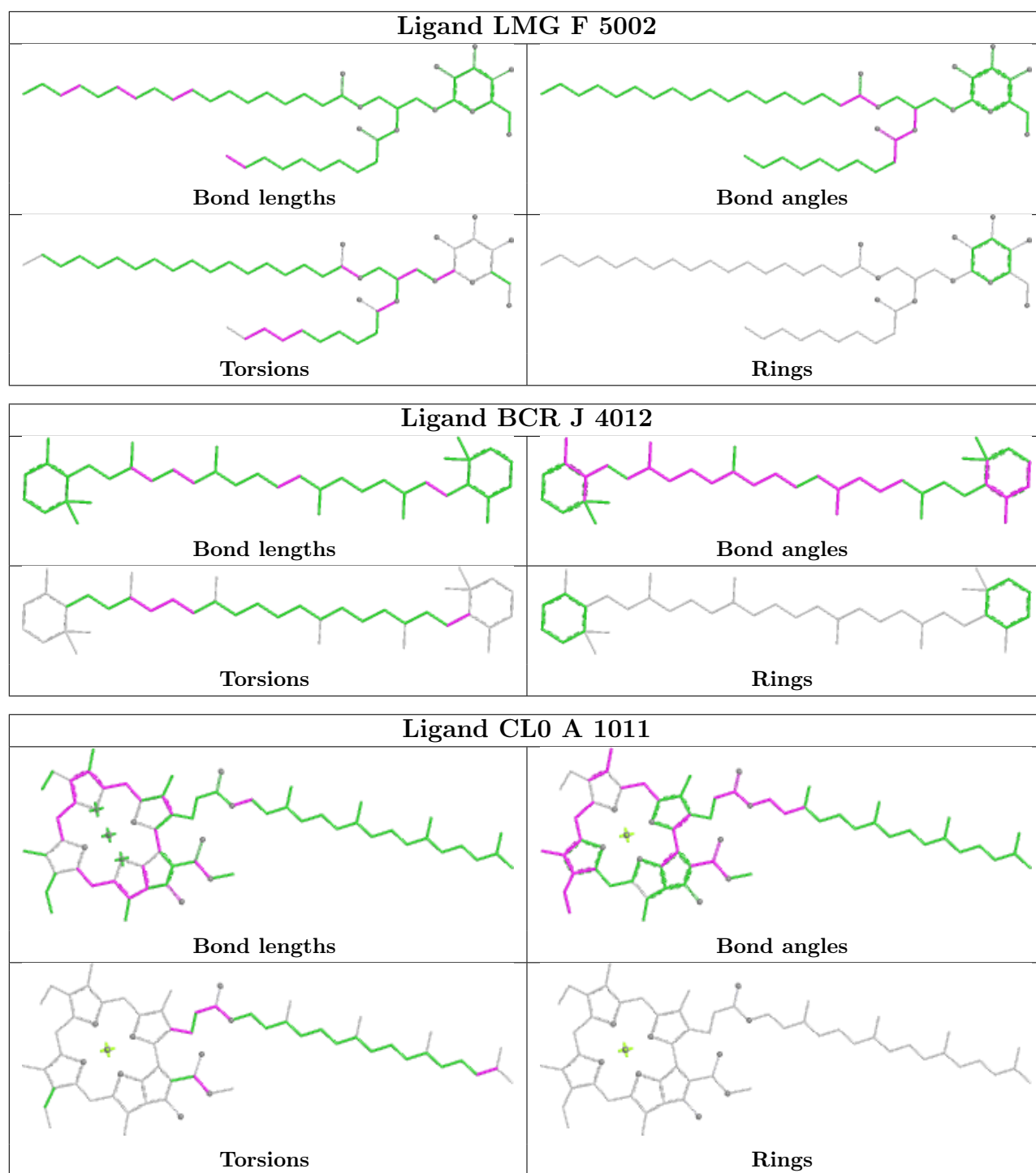
Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	1	605	CLA	2	0
19	4	607	CLA	5	0
19	B	1204	CLA	2	0
19	B	1214	CLA	5	0
22	K	4001	BCR	16	0
19	3	613	CLA	5	0
19	A	1138	CLA	5	0
22	A	4008	BCR	4	0
19	2	612	CLA	1	0
30	2	502	XAT	4	0
29	4	613	CHL	3	0
29	4	615	CHL	1	0
30	4	502	XAT	2	0
19	B	1205	CLA	5	0
22	3	506	BCR	9	0
19	2	606	CLA	3	0
19	3	607	CLA	6	0
19	A	1127	CLA	5	0
19	K	1401	CLA	4	0
19	4	603	CLA	4	0
19	A	1126	CLA	4	0
19	B	1021	CLA	4	0
22	G	4011	BCR	8	0
19	4	608	CLA	3	0
19	B	1225	CLA	7	0
19	B	1201	CLA	1	0
19	B	1210	CLA	3	0
28	3	501	LUT	12	0
19	A	1102	CLA	3	0
19	B	1219	CLA	4	0
19	H	1701	CLA	3	0
19	4	602	CLA	5	0
19	A	1112	CLA	4	0
19	2	605	CLA	1	0
19	A	1128	CLA	6	0
19	1	603	CLA	3	0
19	A	1140	CLA	4	0
19	K	1403	CLA	2	0
19	B	1215	CLA	4	0
19	B	1207	CLA	6	0
22	2	503	BCR	8	0
29	1	610	CHL	3	0

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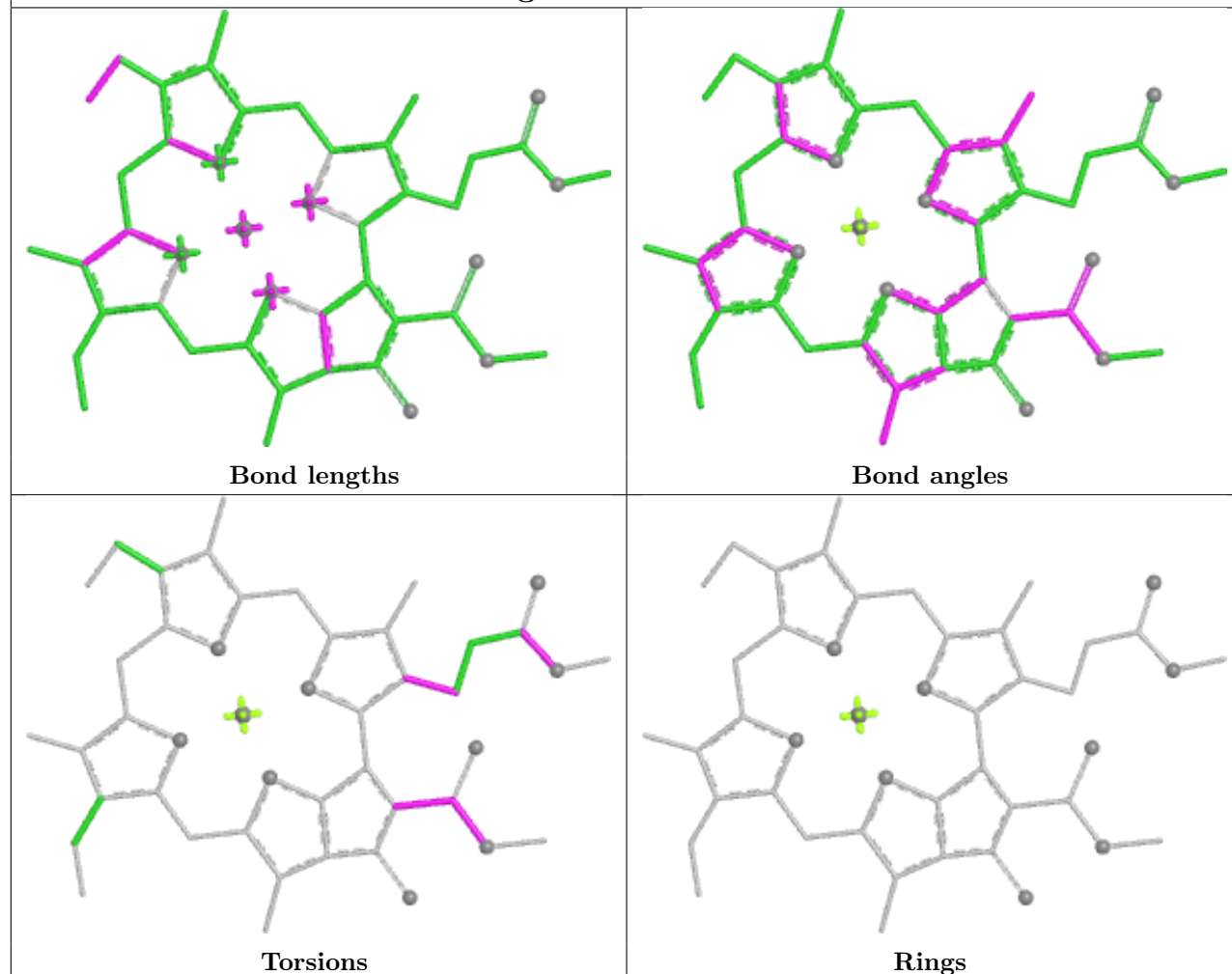
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	B	1022	CLA	5	0
19	B	1216	CLA	4	0
19	B	1229	CLA	8	0
19	1	611	CLA	5	0
19	B	1236	CLA	6	0
19	A	1123	CLA	1	0
19	L	1501	CLA	2	0
19	A	1116	CLA	3	0
19	B	1239	CLA	5	0
19	A	1131	CLA	1	0
22	B	4006	BCR	11	0
28	4	501	LUT	18	0
19	F	1301	CLA	1	0
19	A	1115	CLA	1	0
29	2	609	CHL	3	0
19	1	604	CLA	1	0
19	3	612	CLA	8	0
19	3	614	CLA	1	0
29	3	604	CHL	5	0
23	3	801	LHG	1	0
29	2	610	CHL	1	0
19	A	1110	CLA	4	0
19	3	602	CLA	3	0
19	A	1137	CLA	2	0

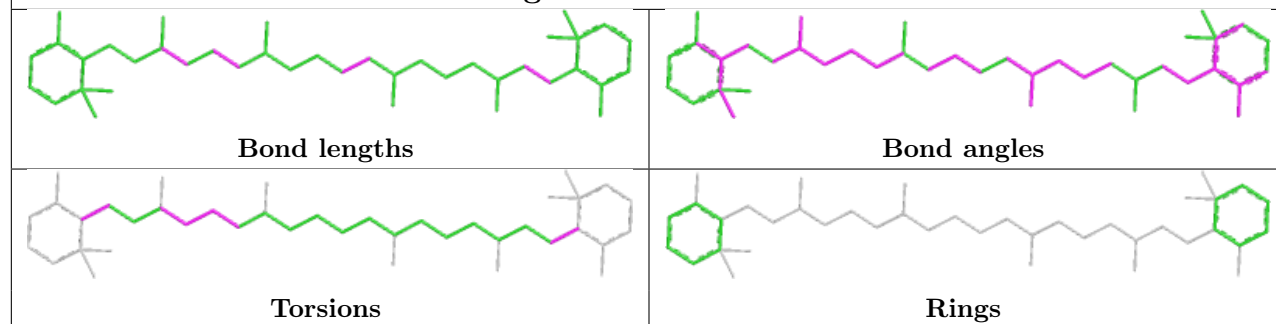
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

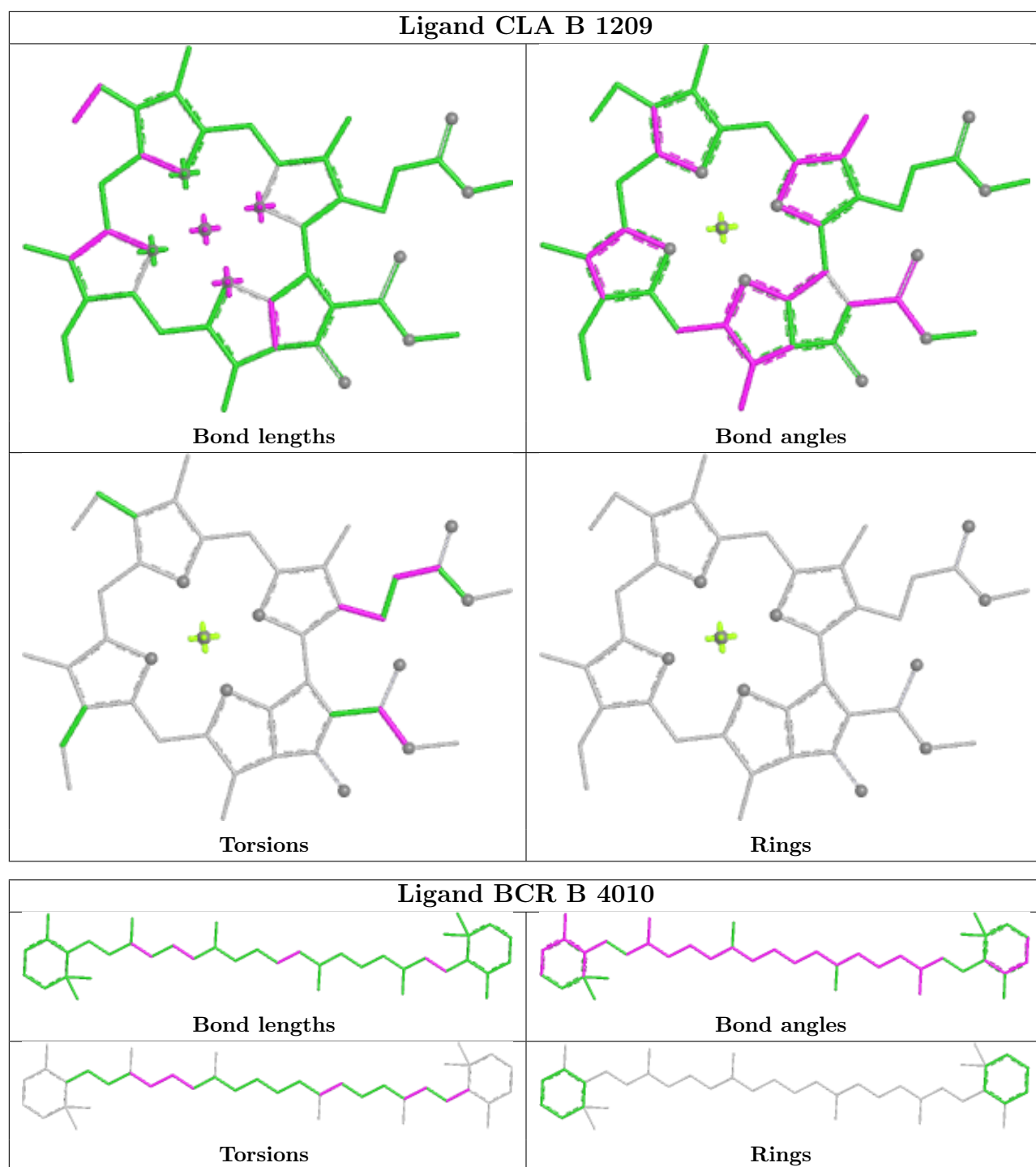


Ligand CLA 1 608

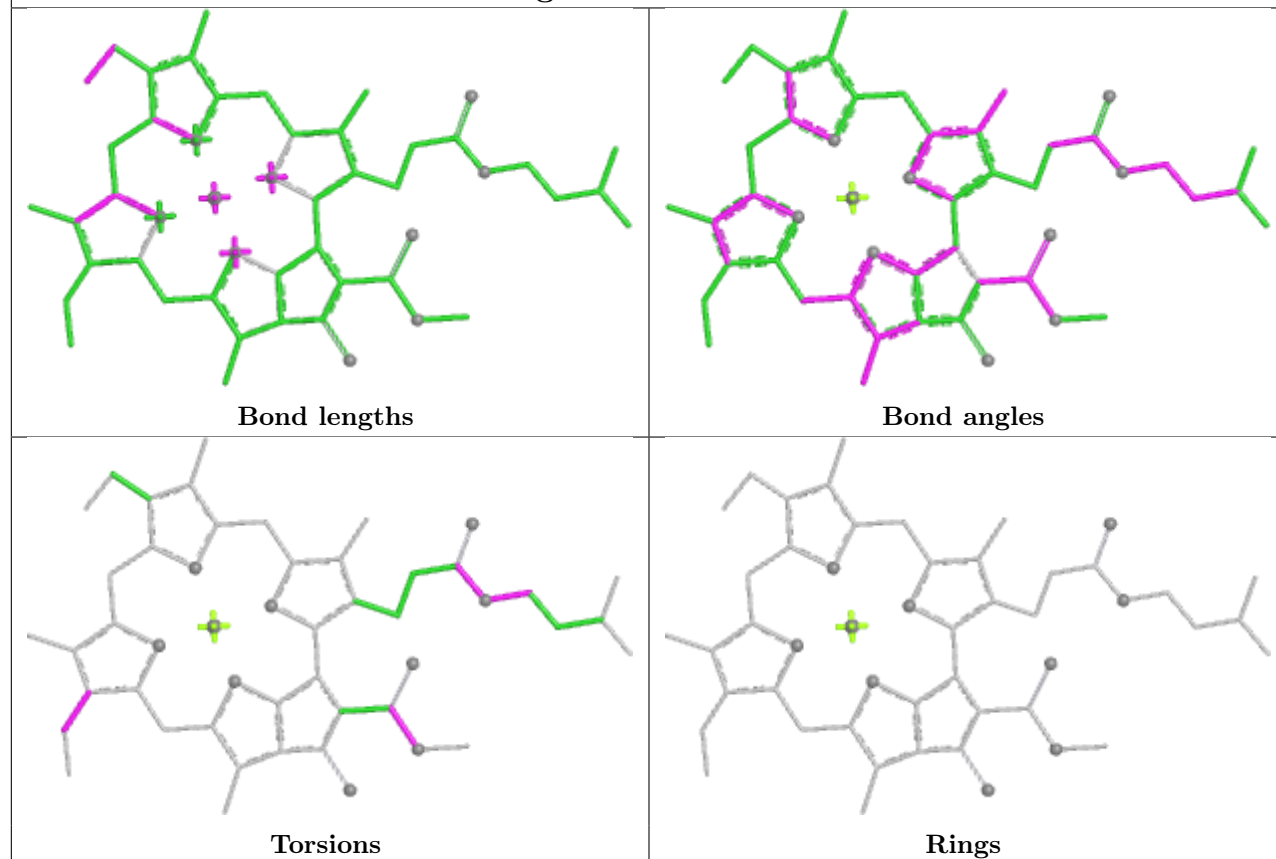


Ligand BCR L 4020

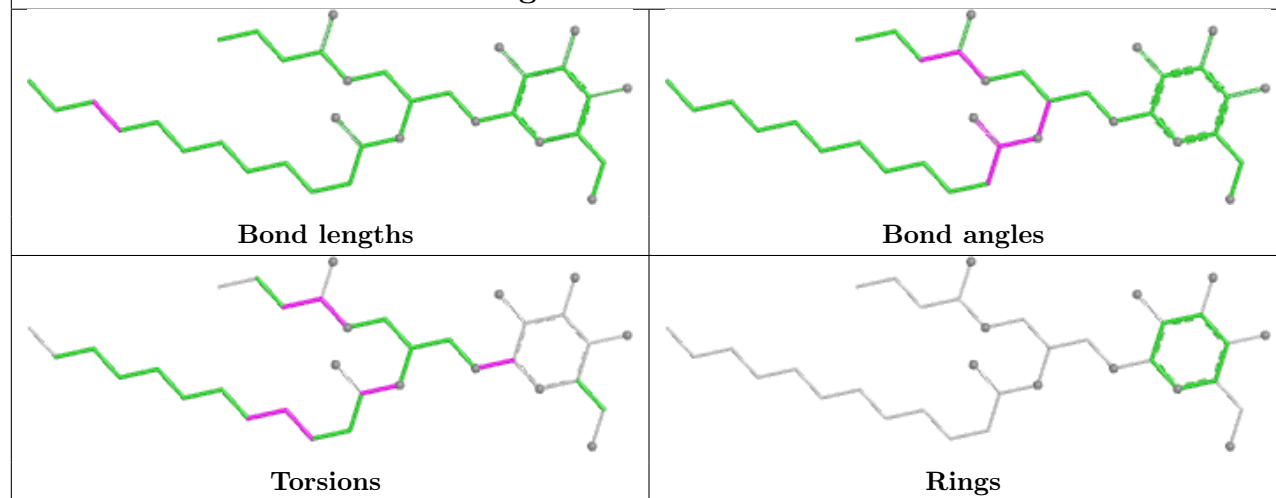


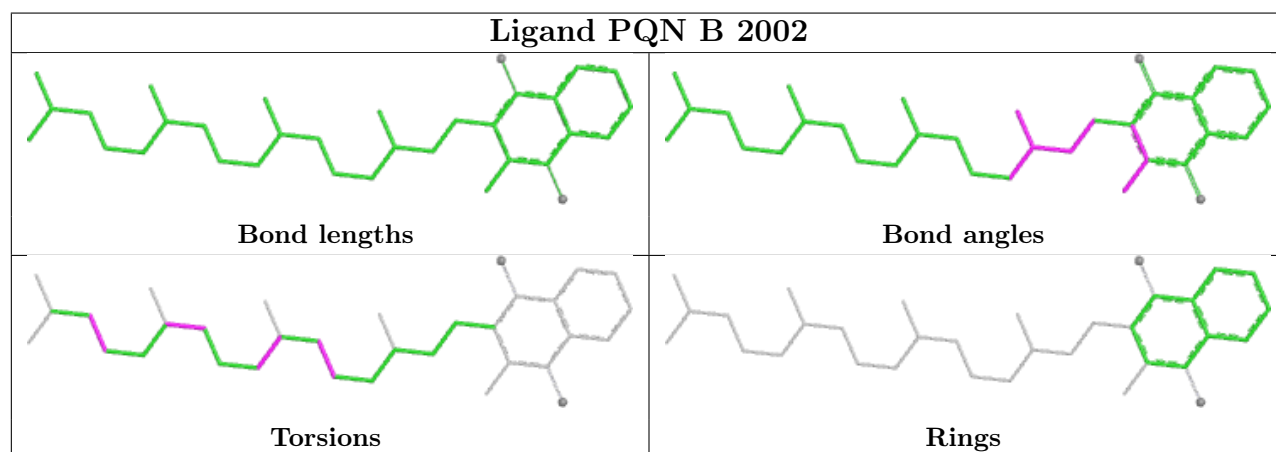
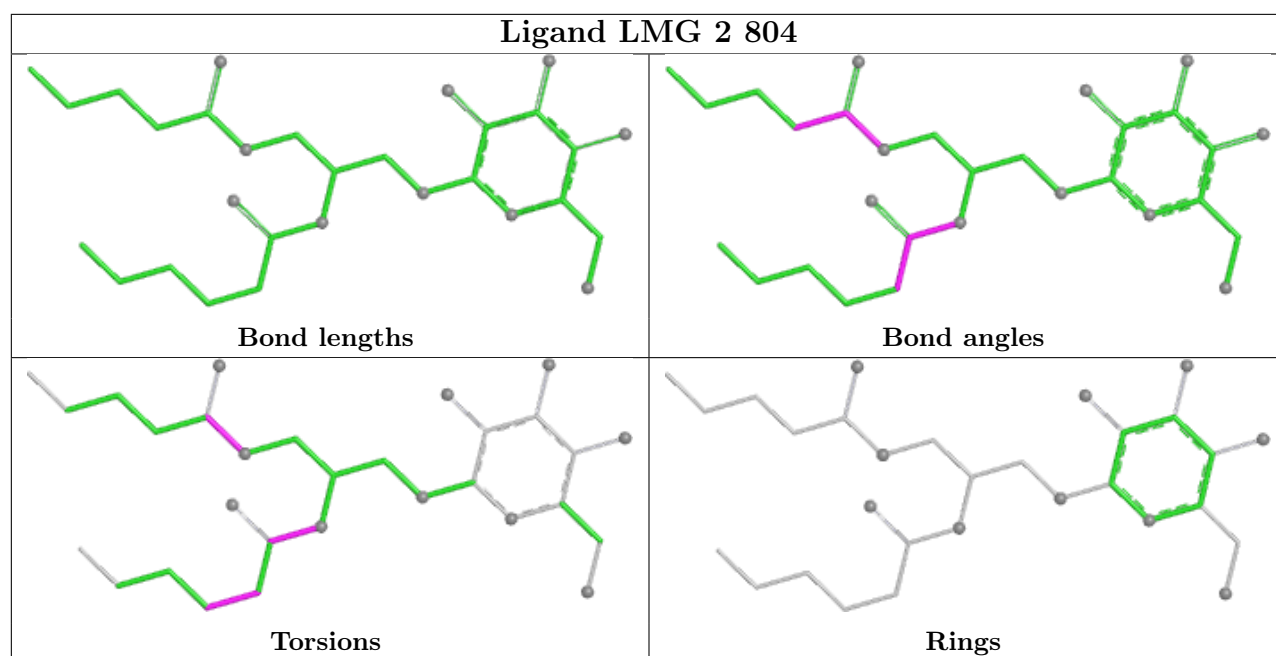


Ligand CLA 2 608

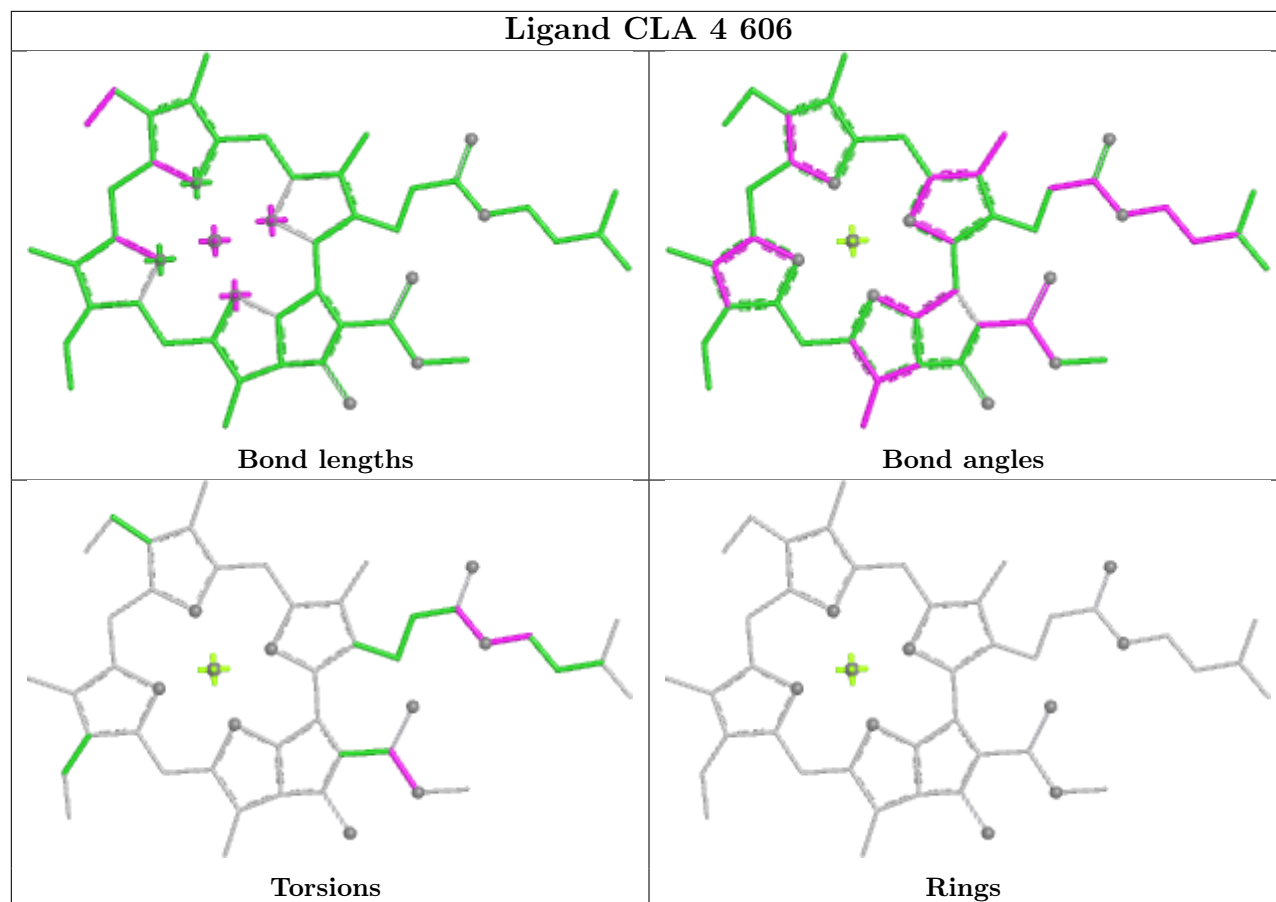


Ligand LMG B 5003

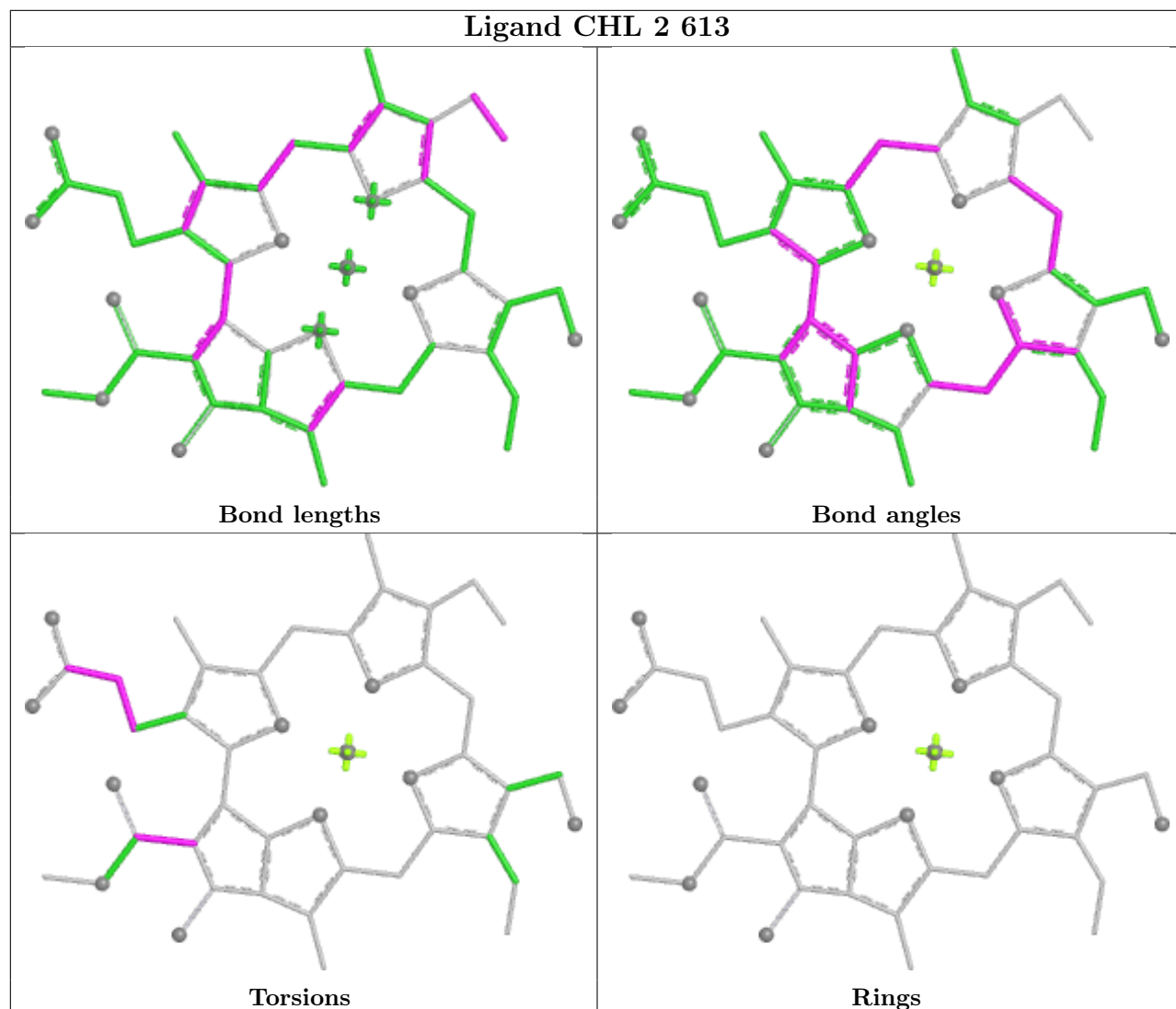


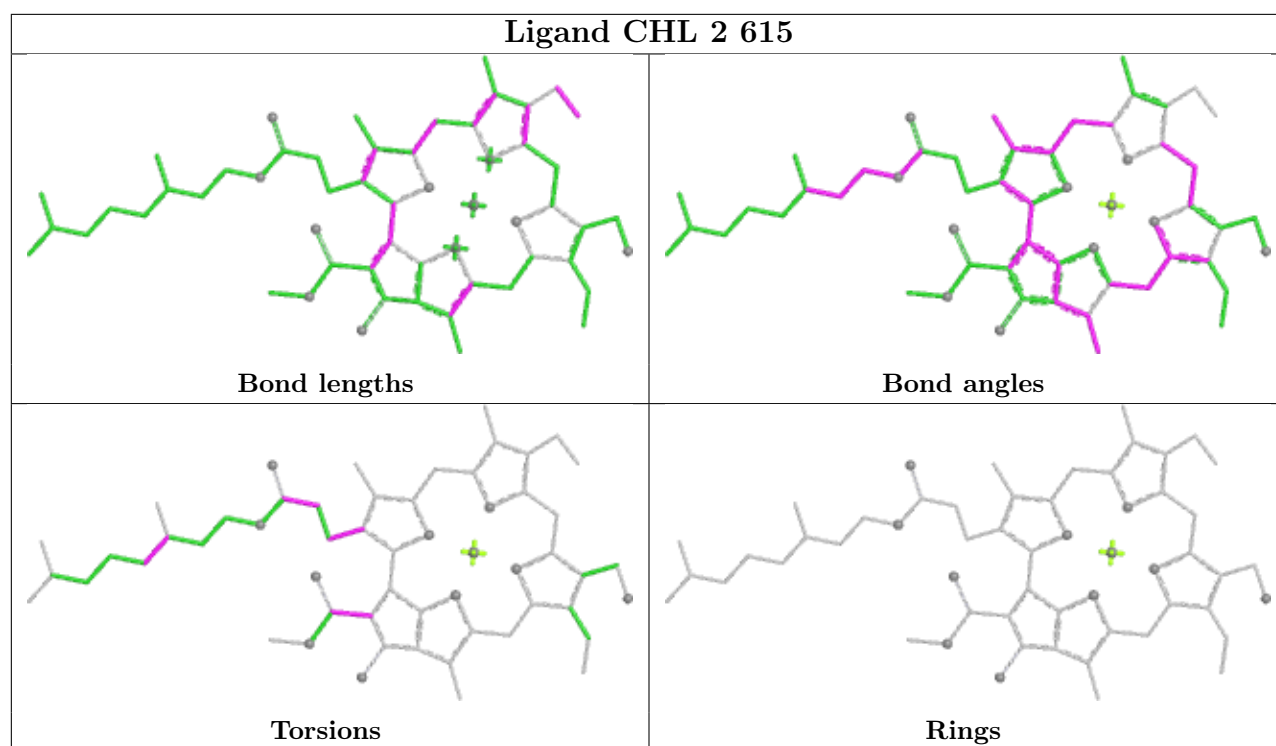


Ligand CLA 4 606

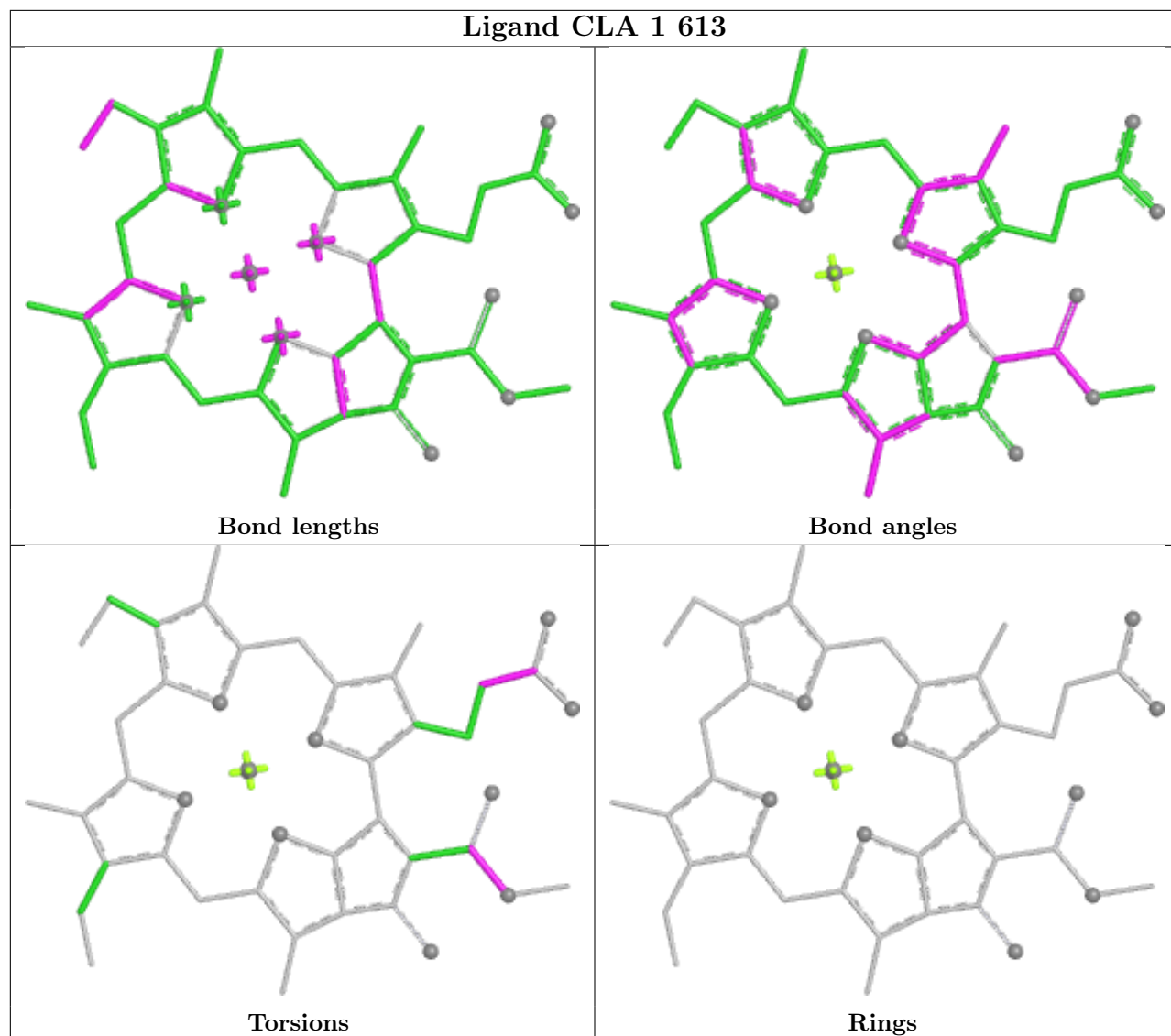


Ligand CHL 2 613

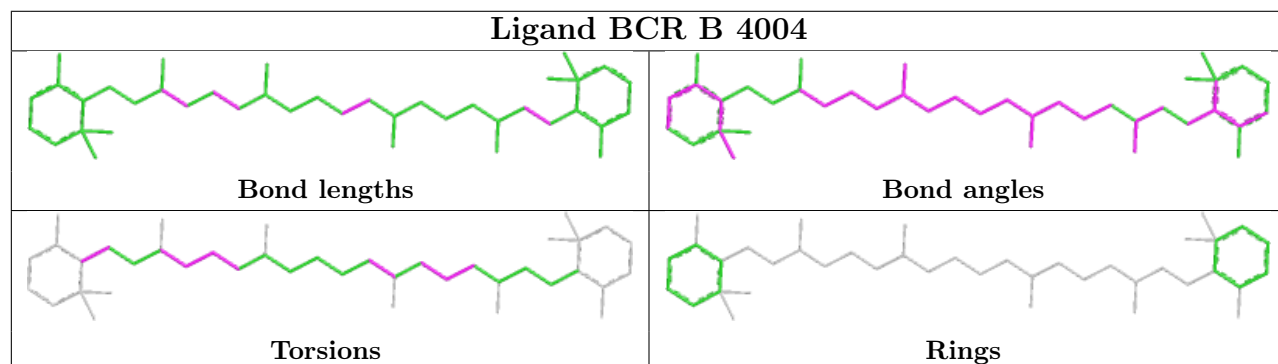


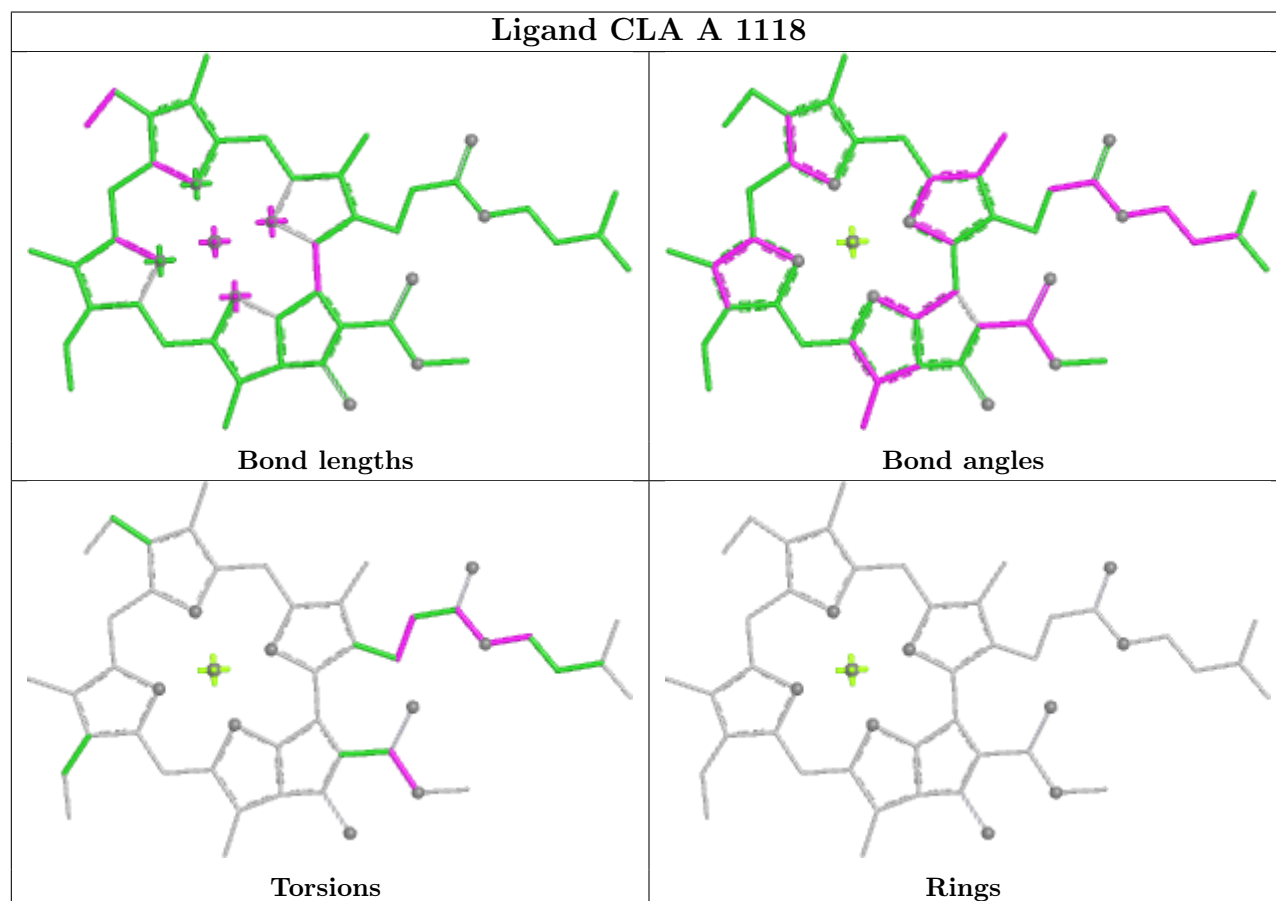
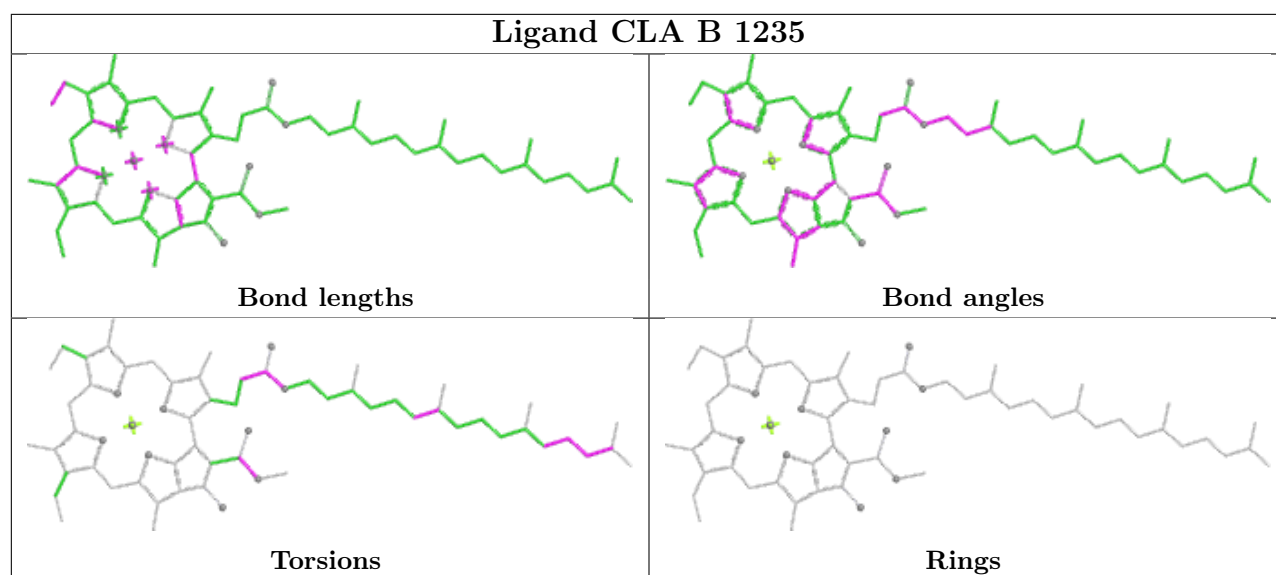


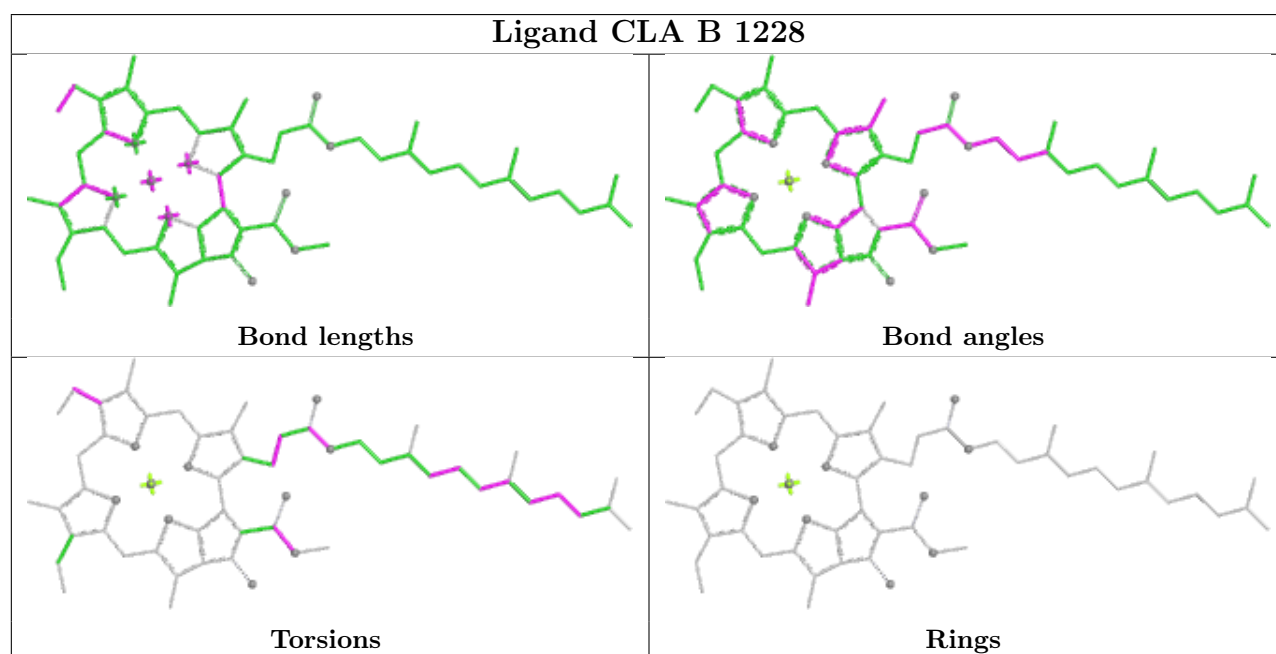
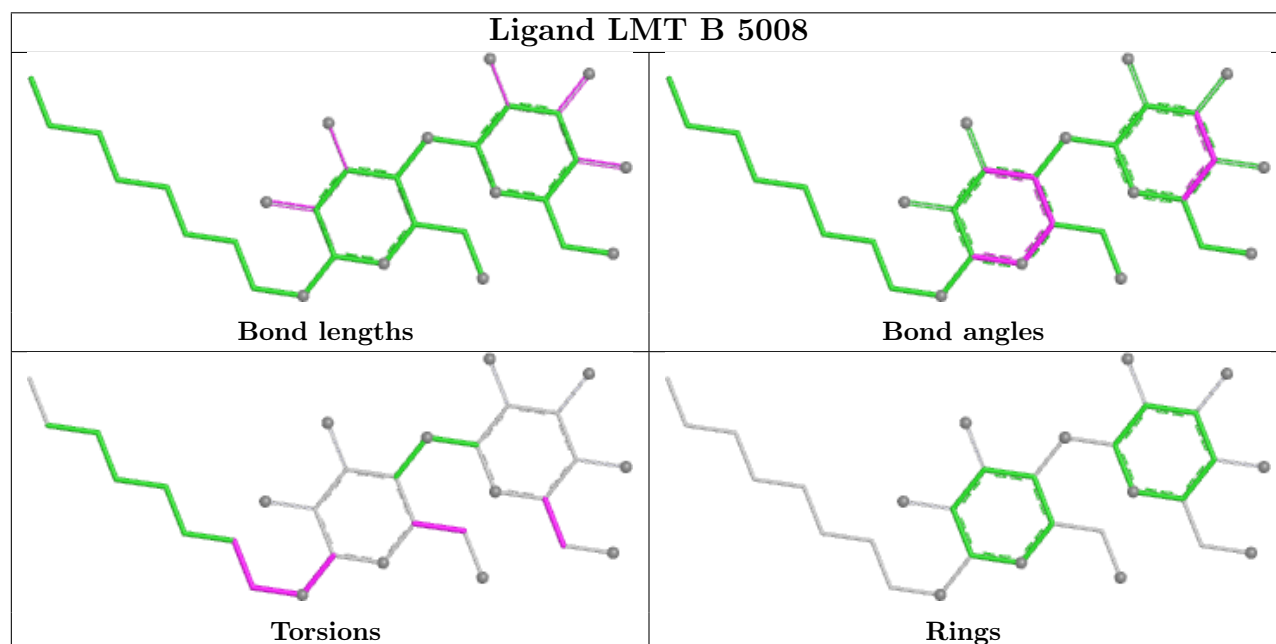
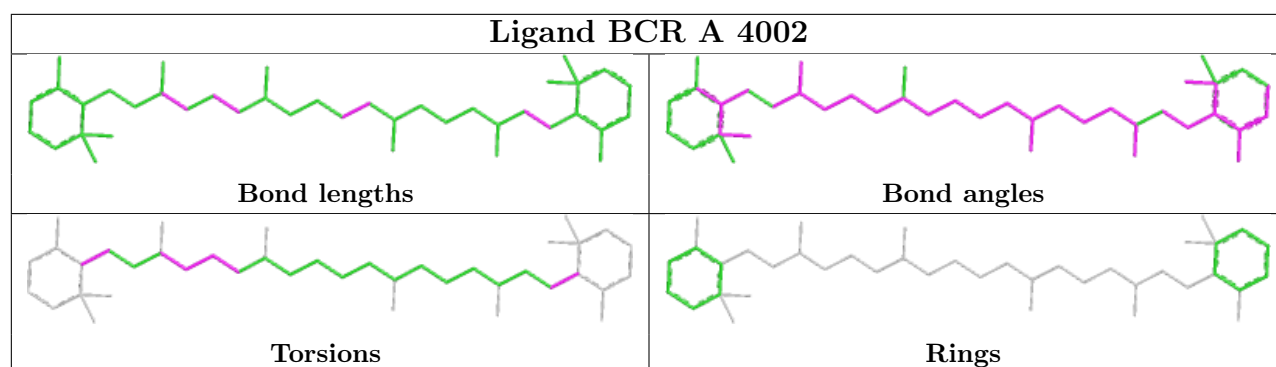
Ligand CLA 1 613

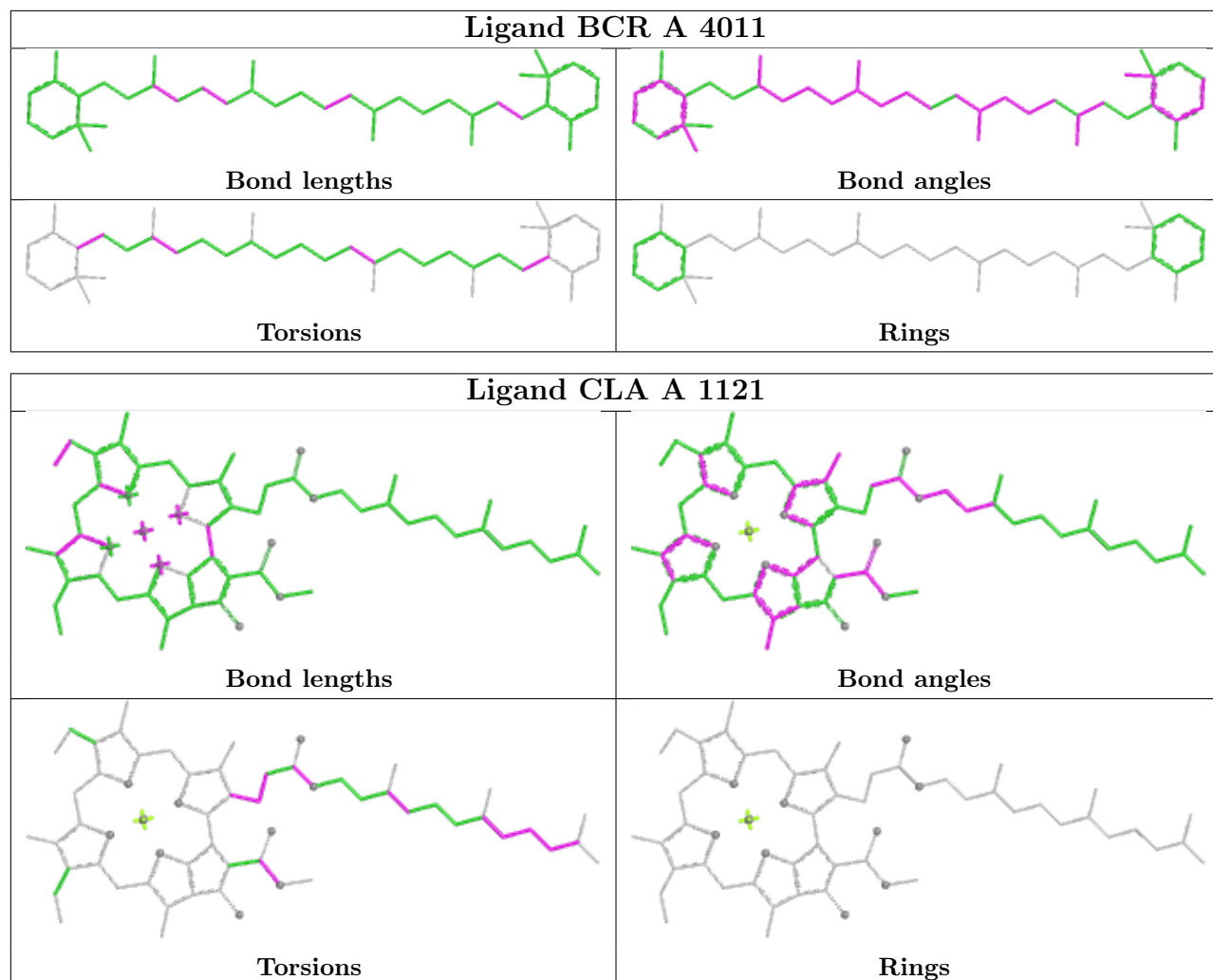


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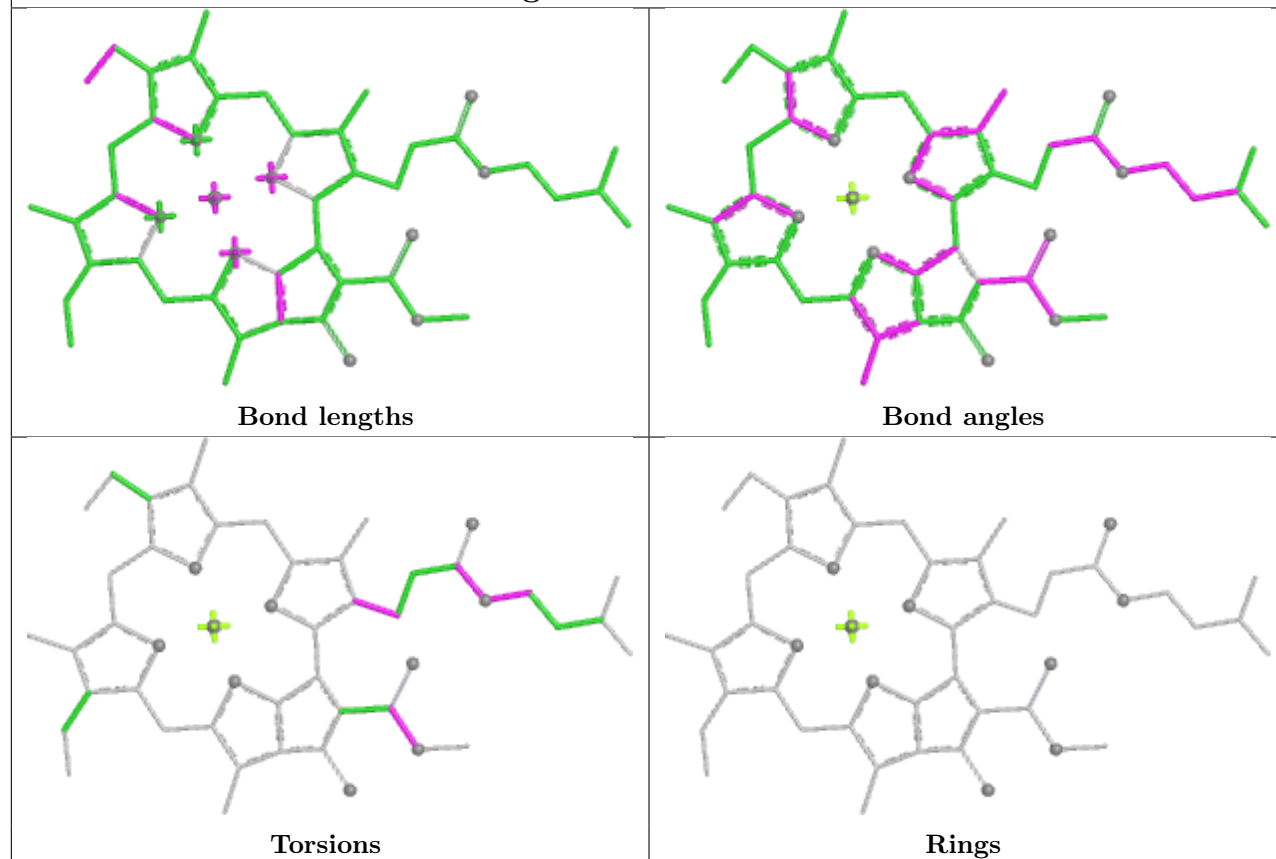




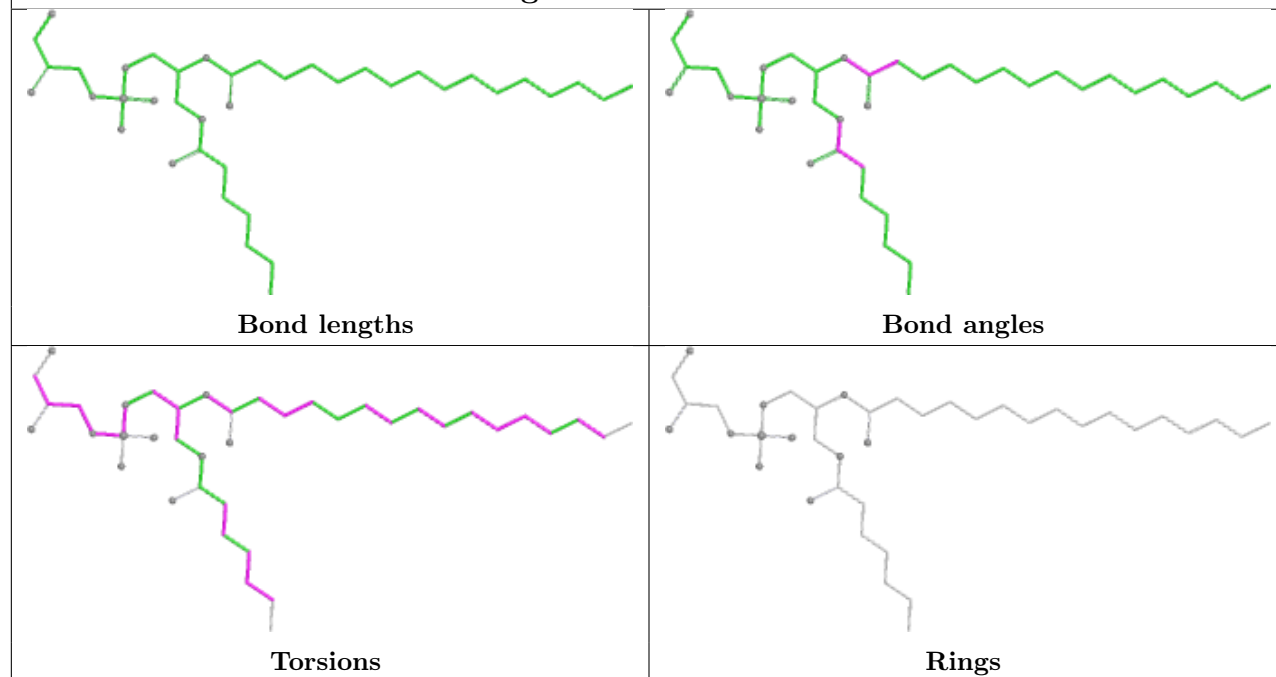


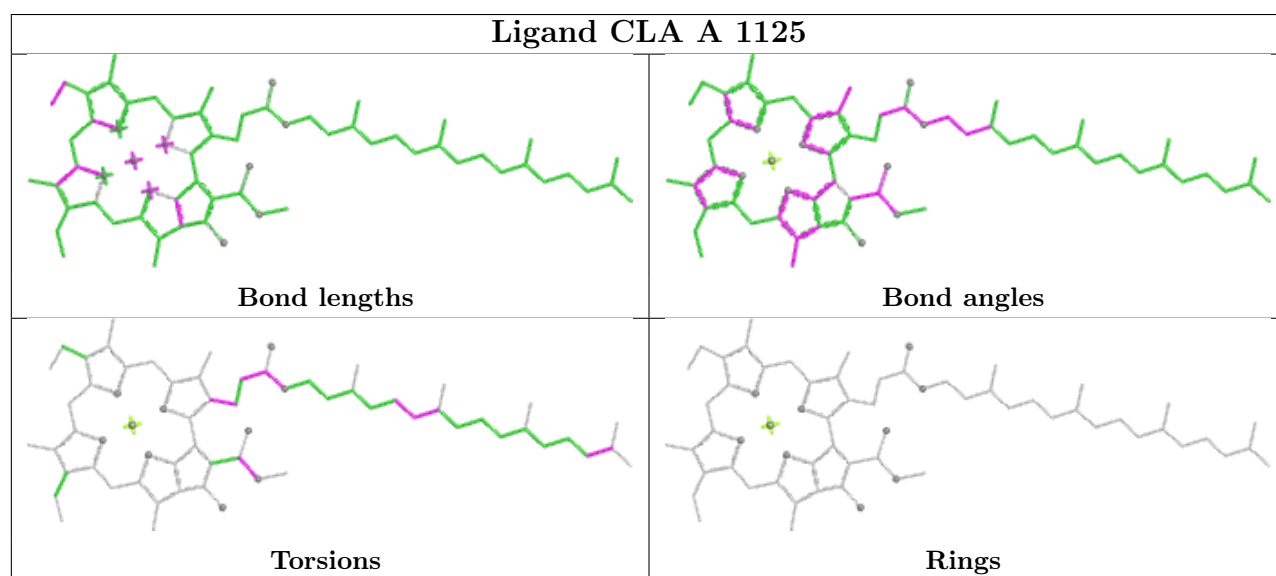
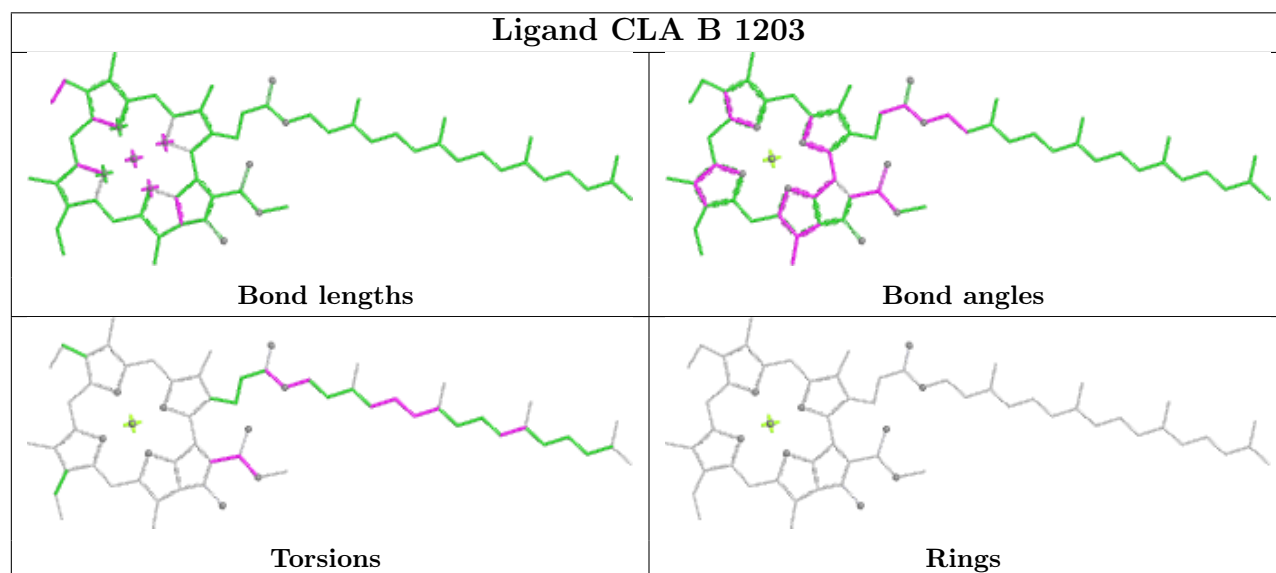
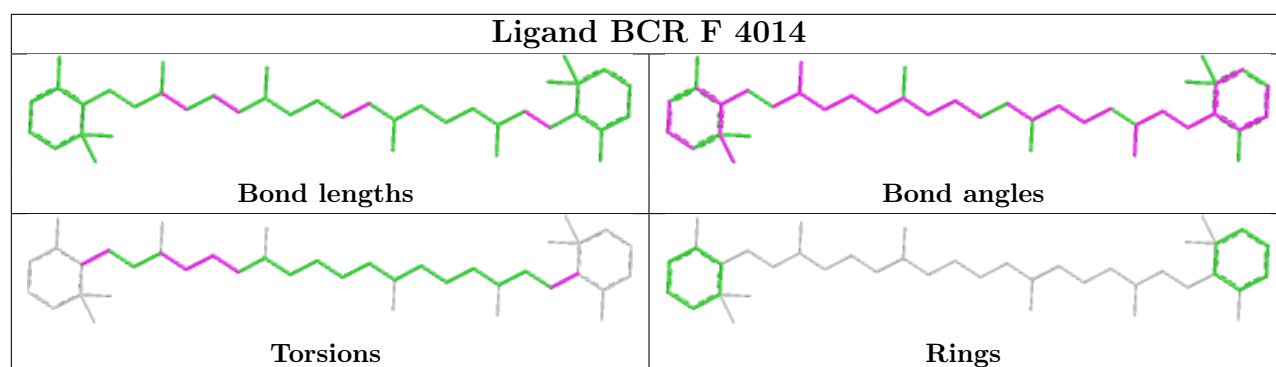


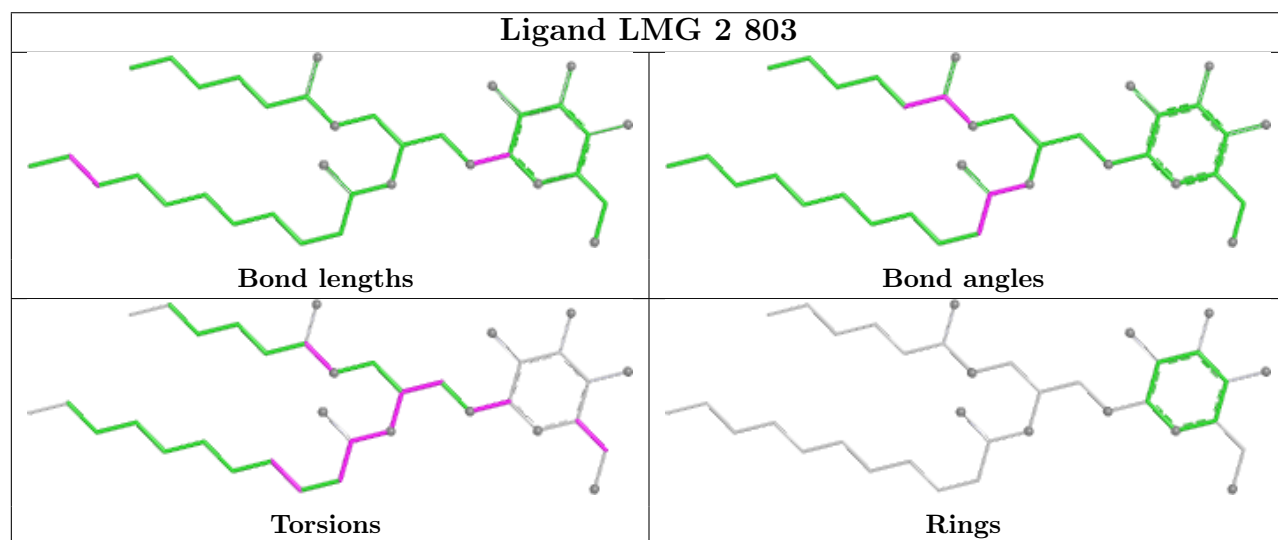
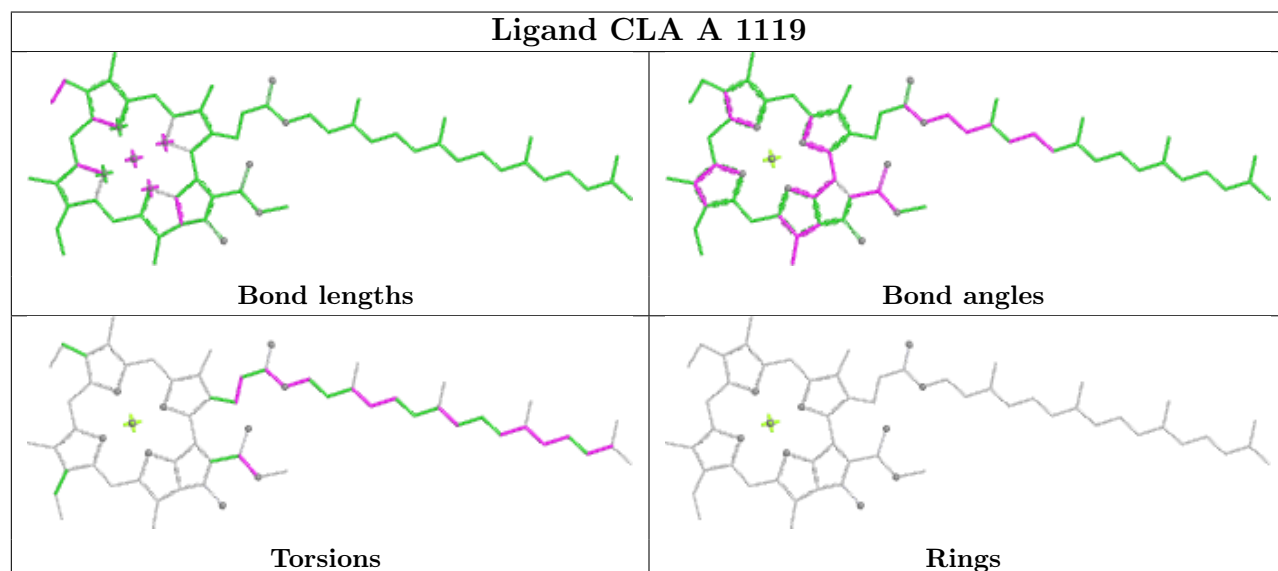
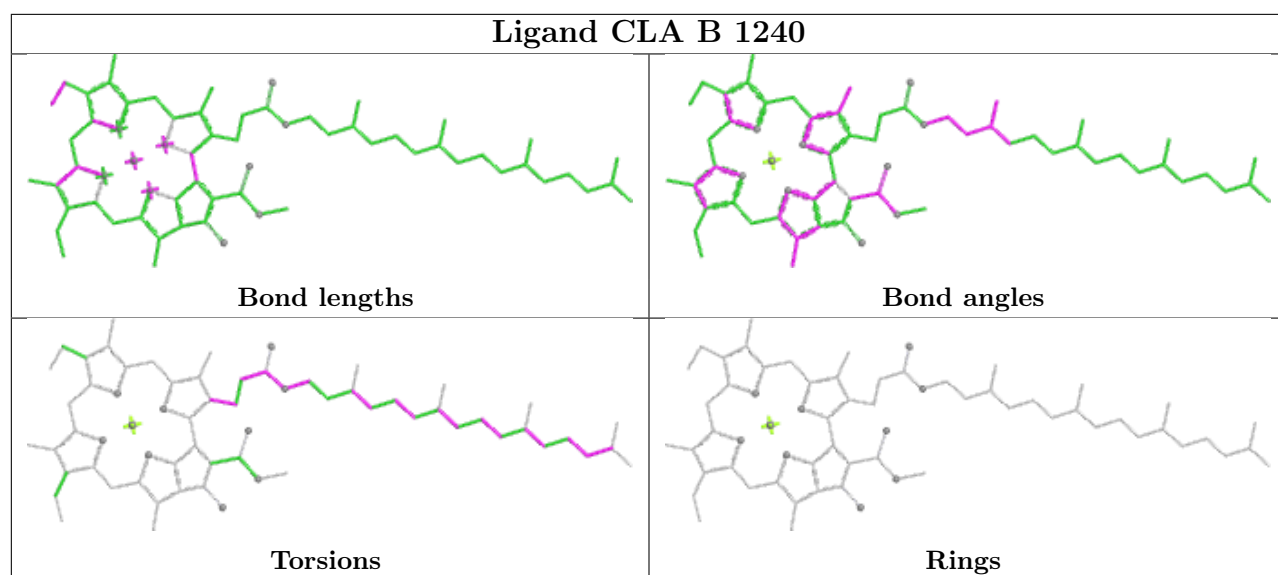
Ligand CLA A 1108

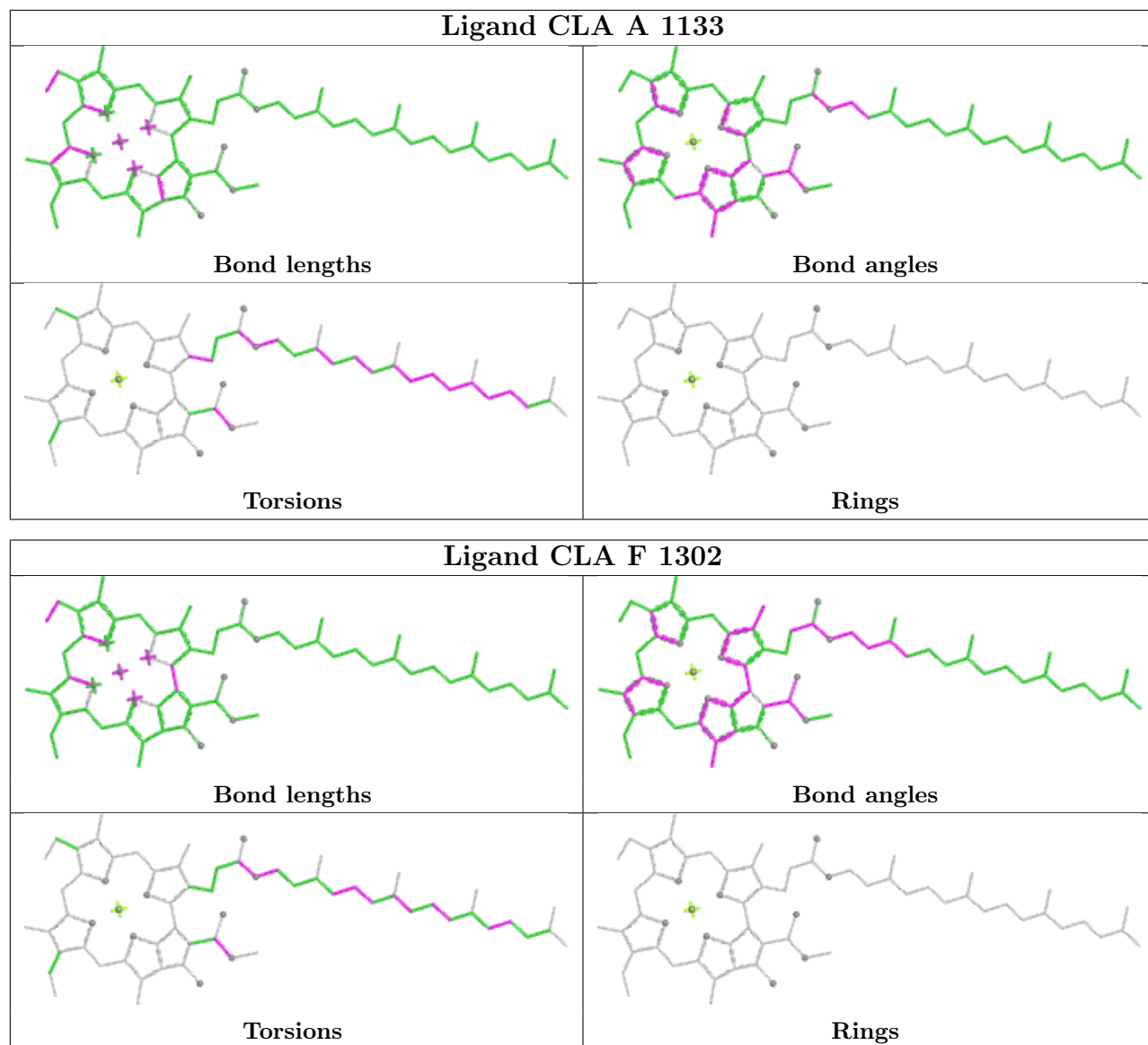


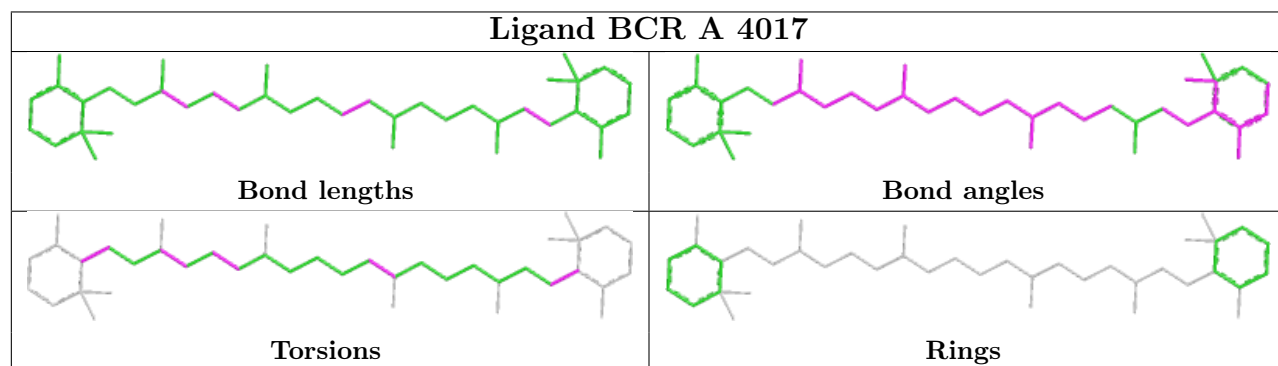
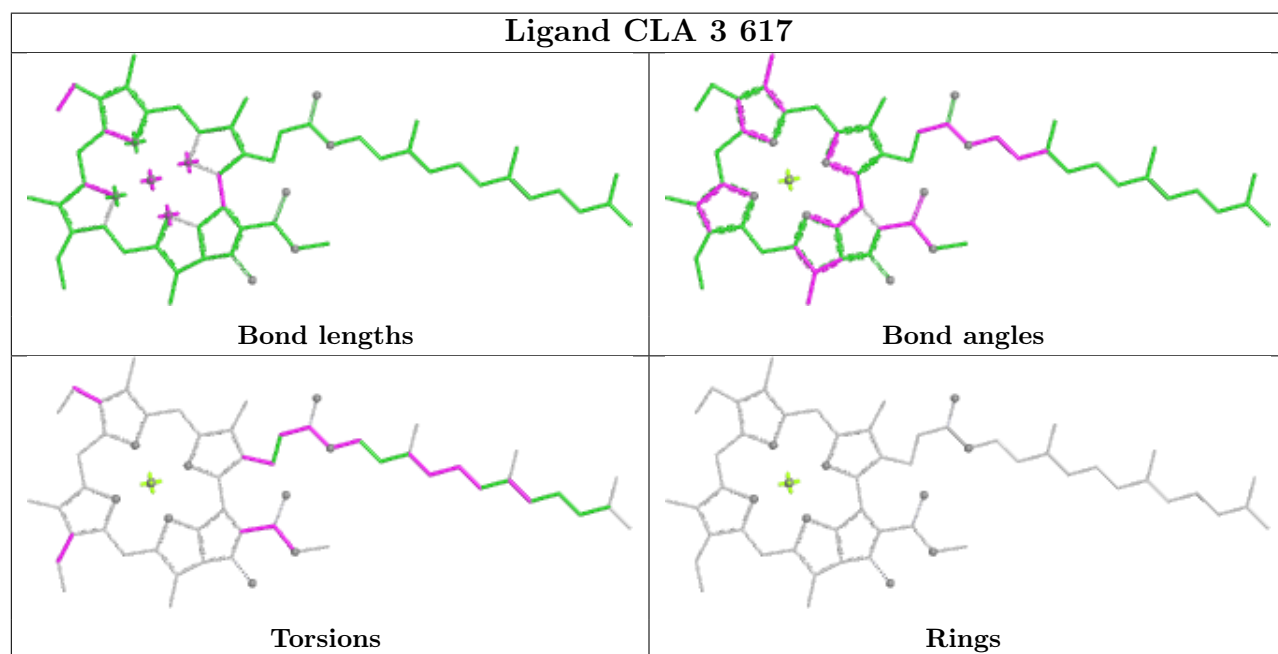
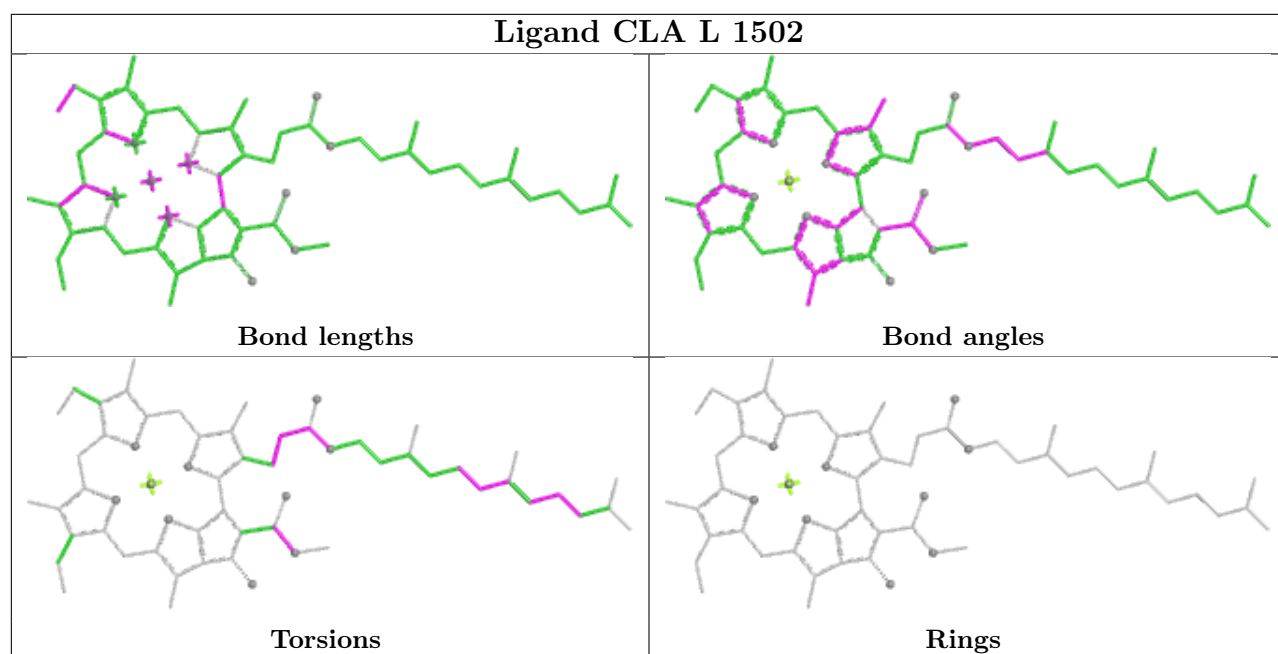
Ligand LHG A 5001



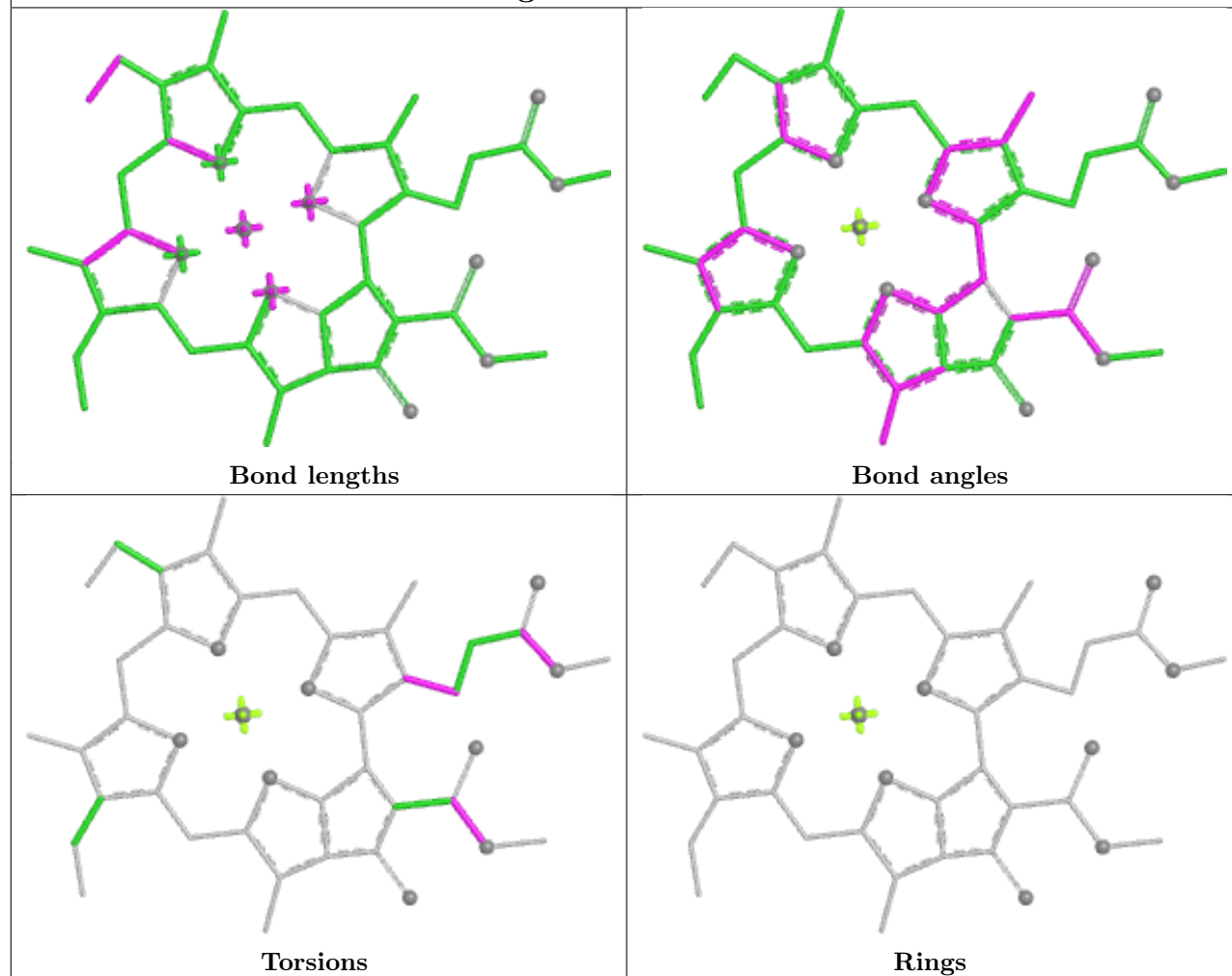


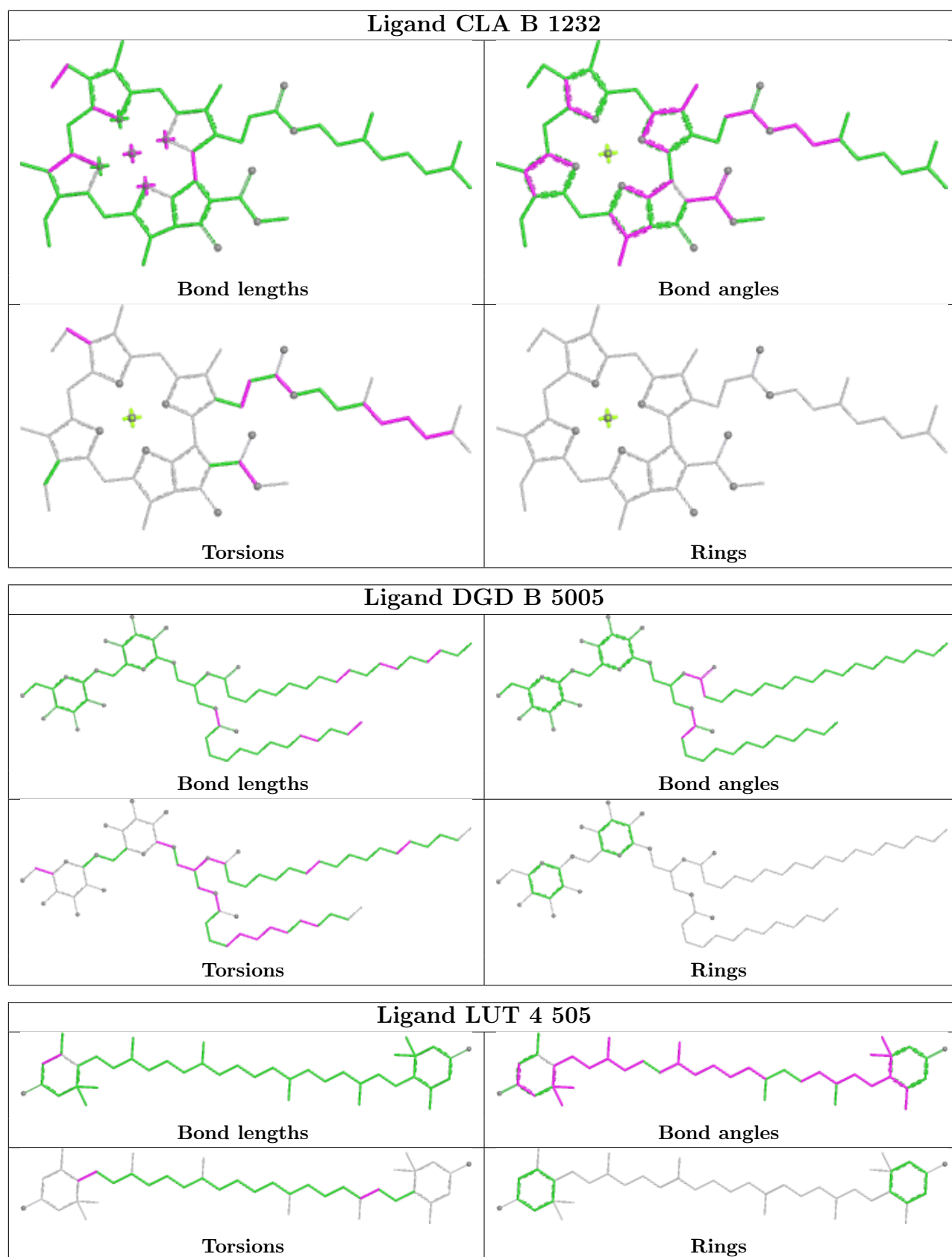




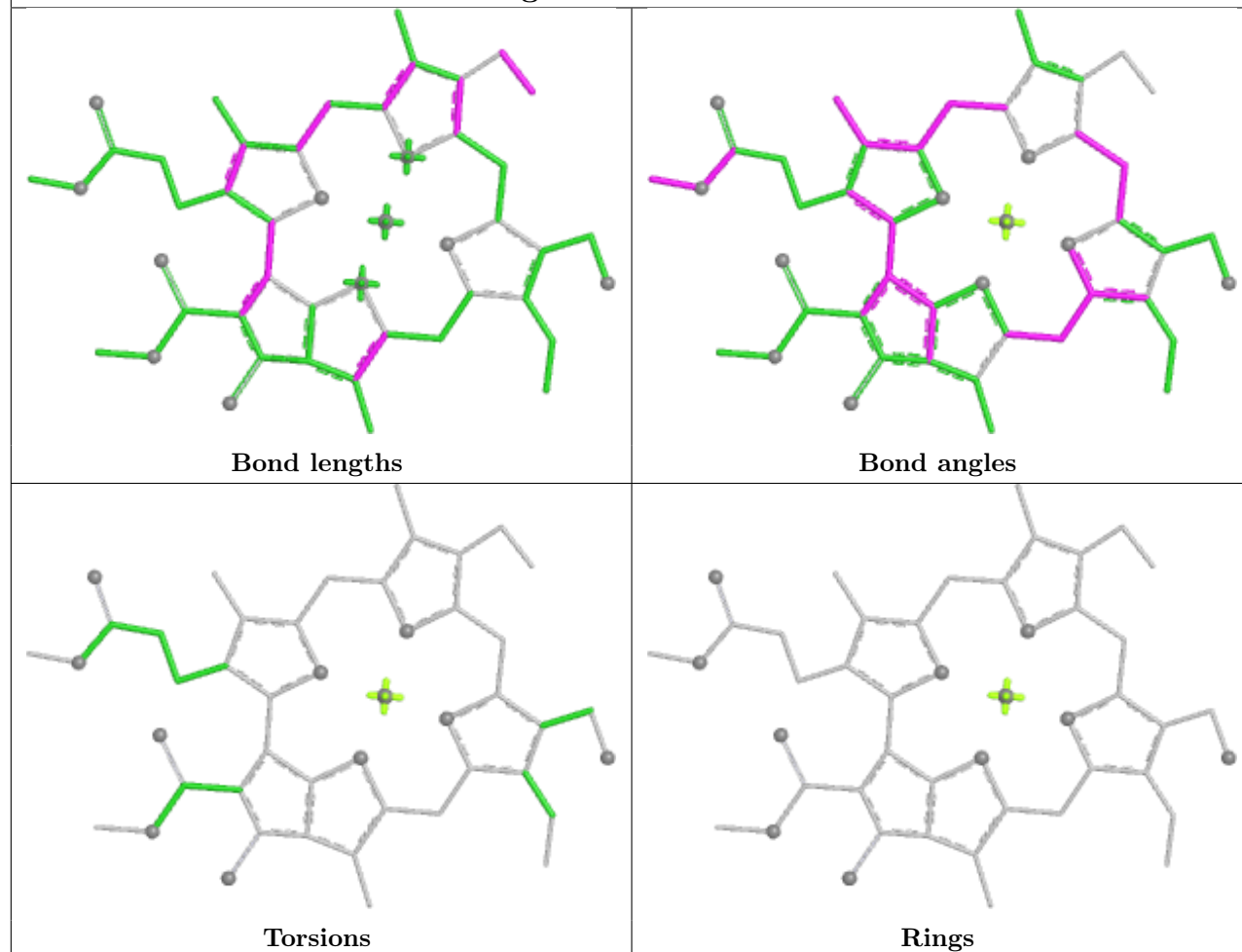


Ligand CLA 1 602

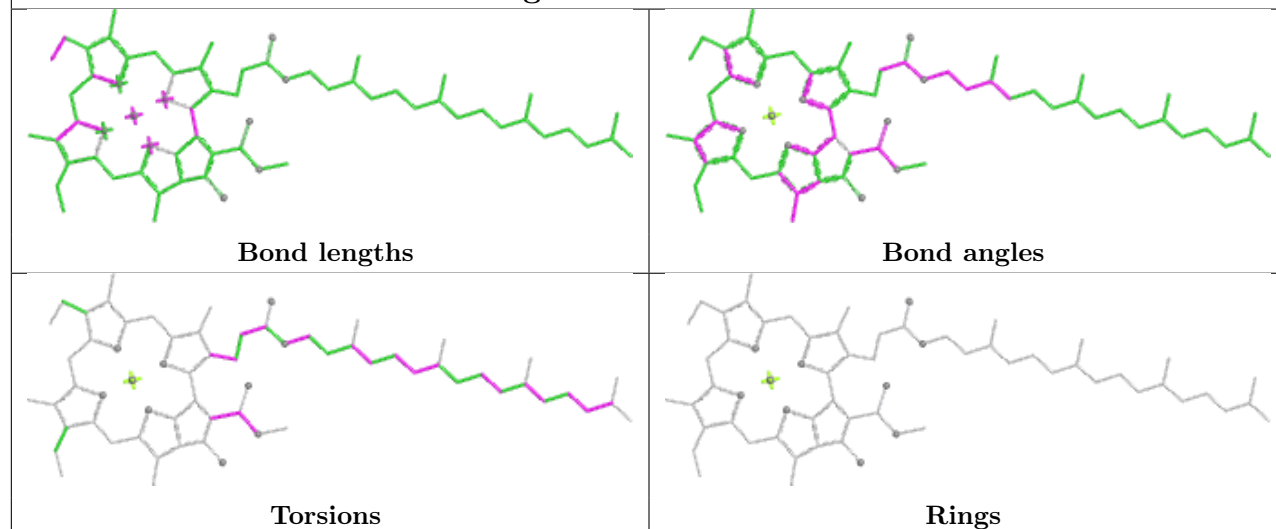


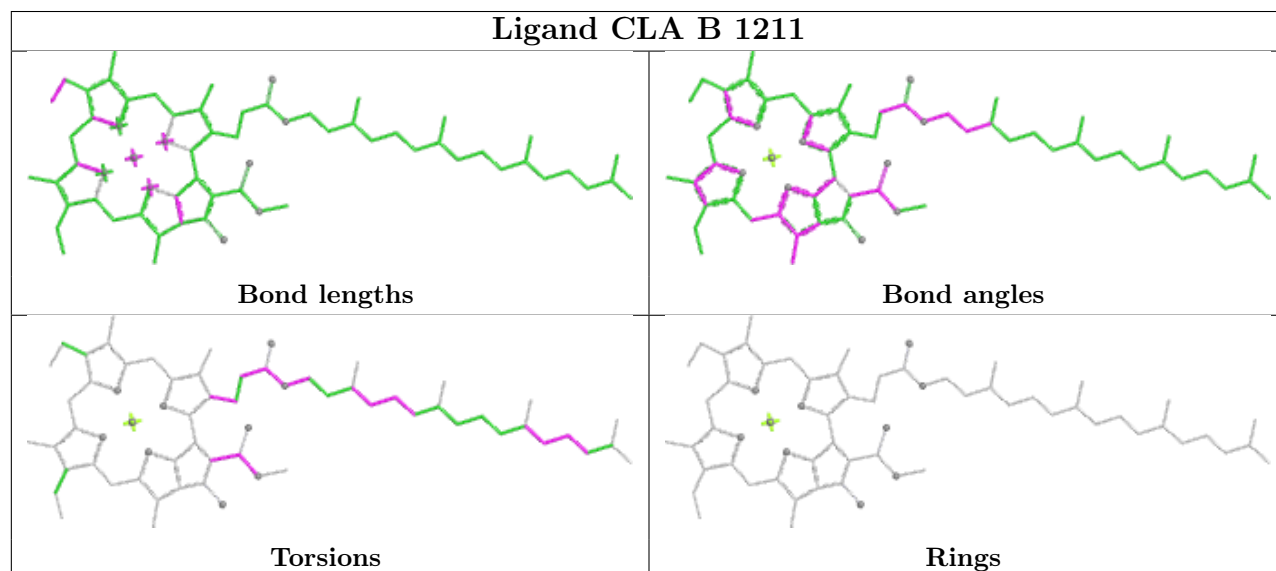
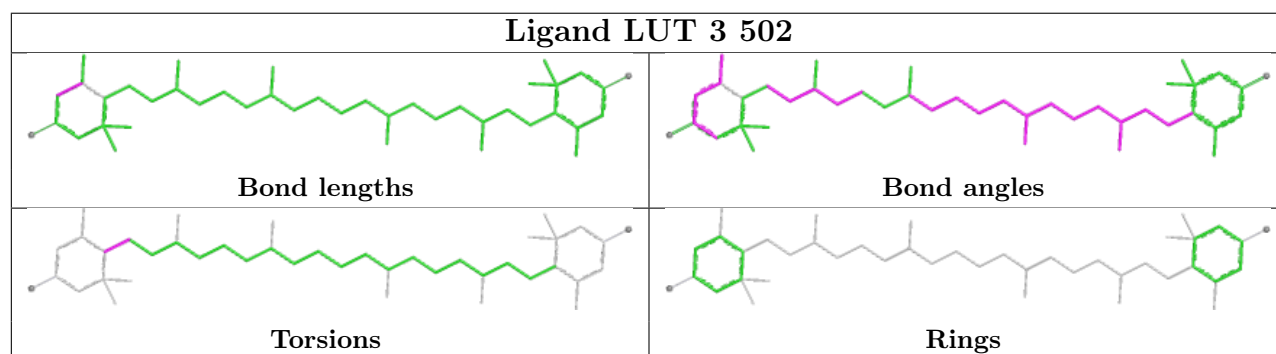
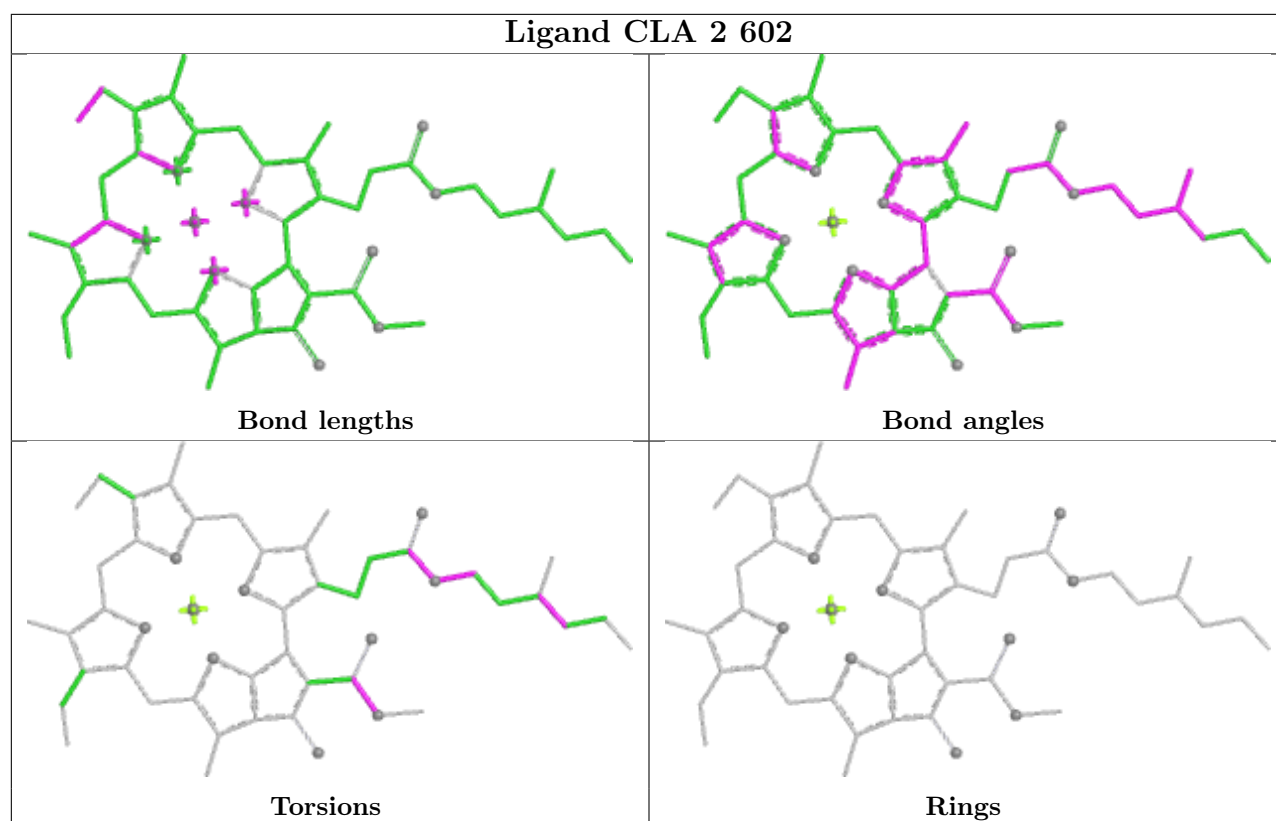


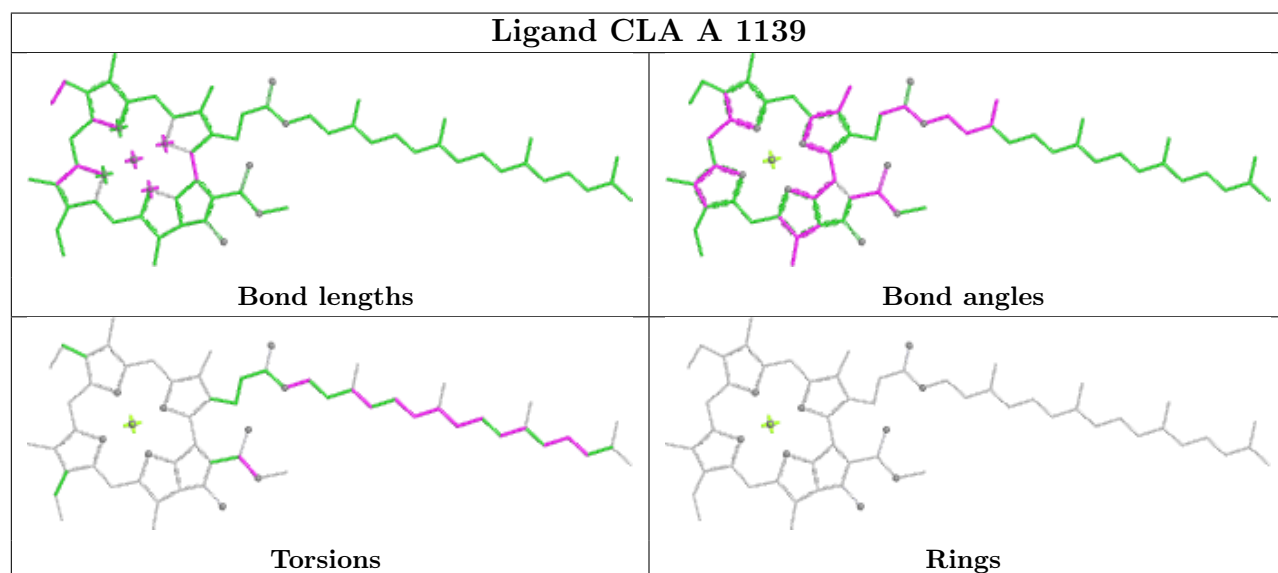
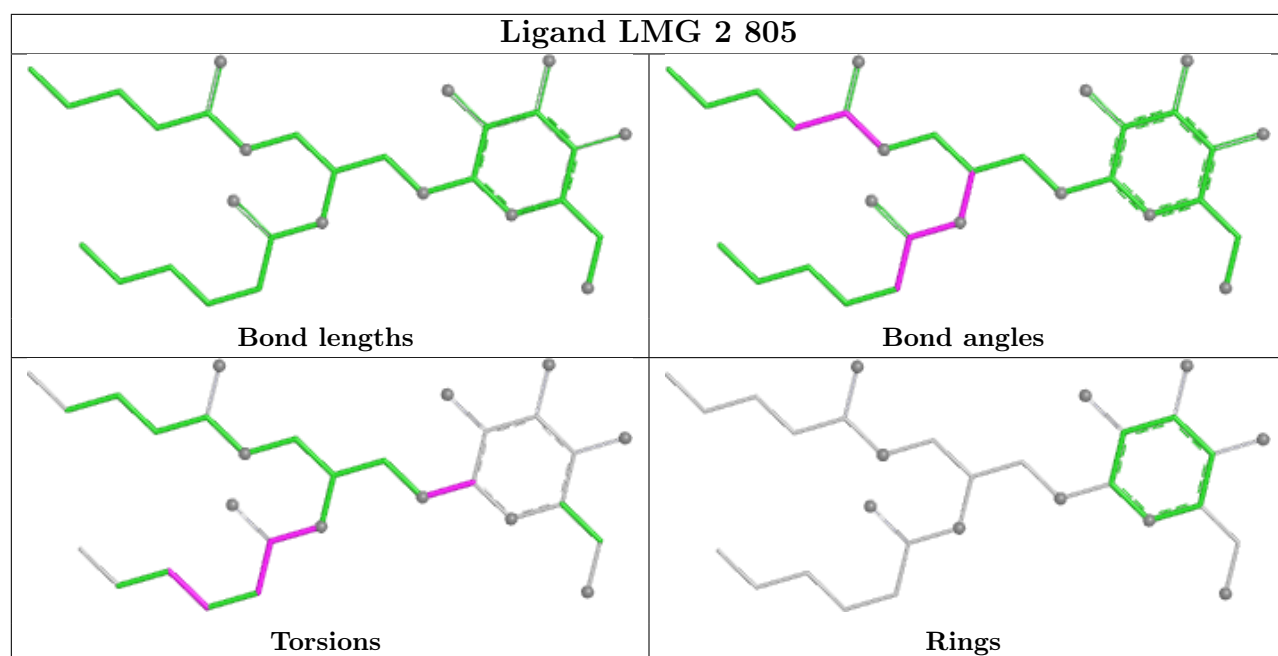
Ligand CHL 3 611

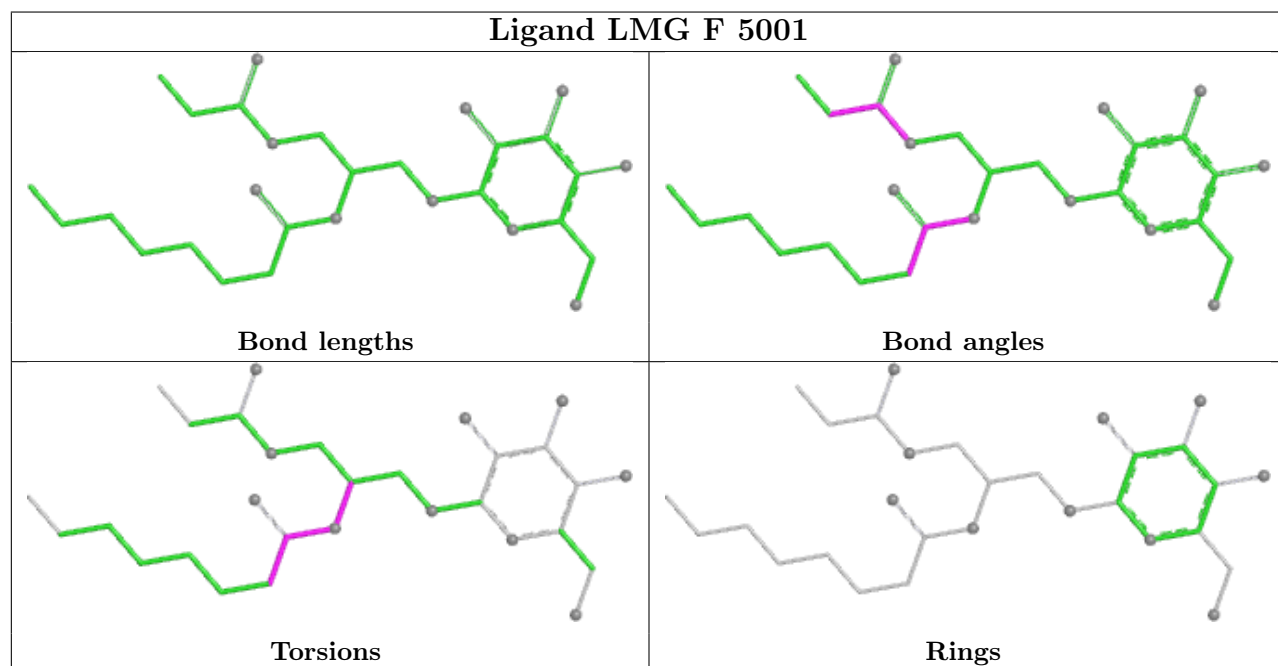
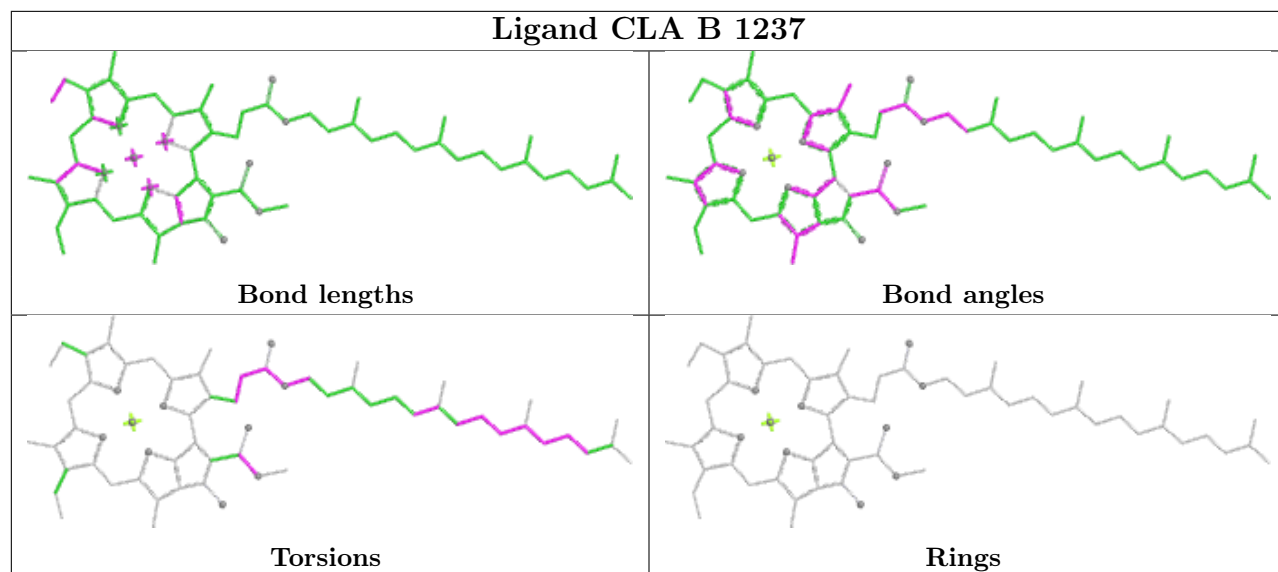


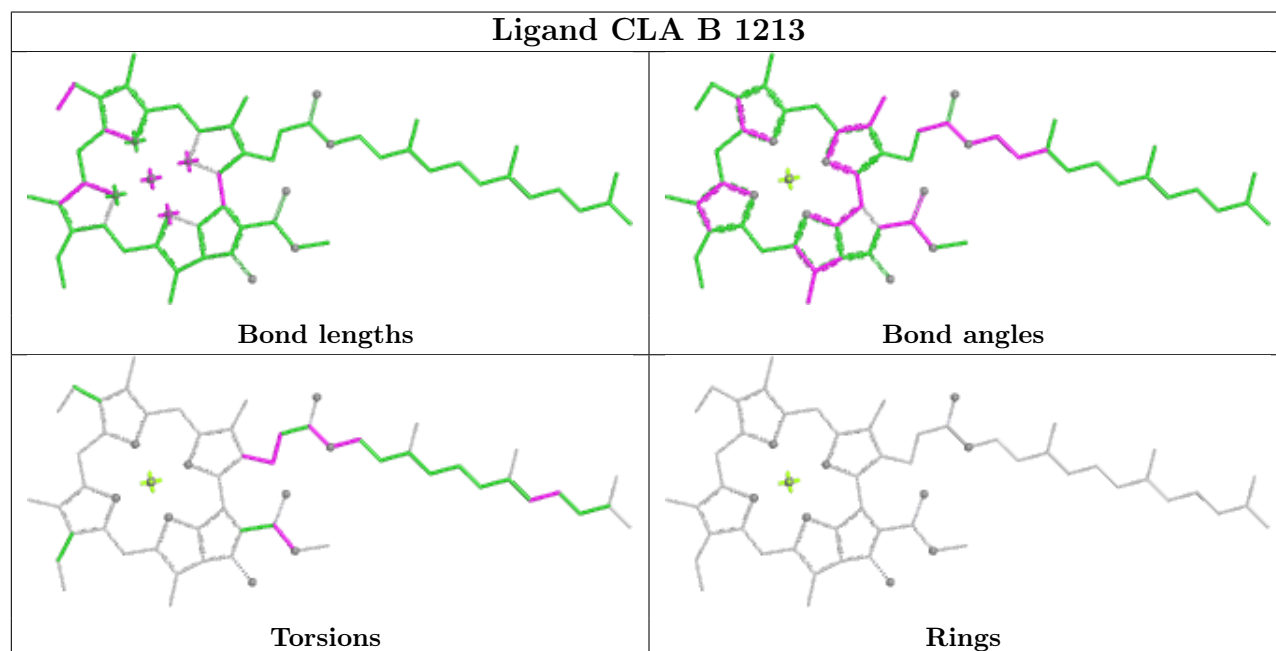
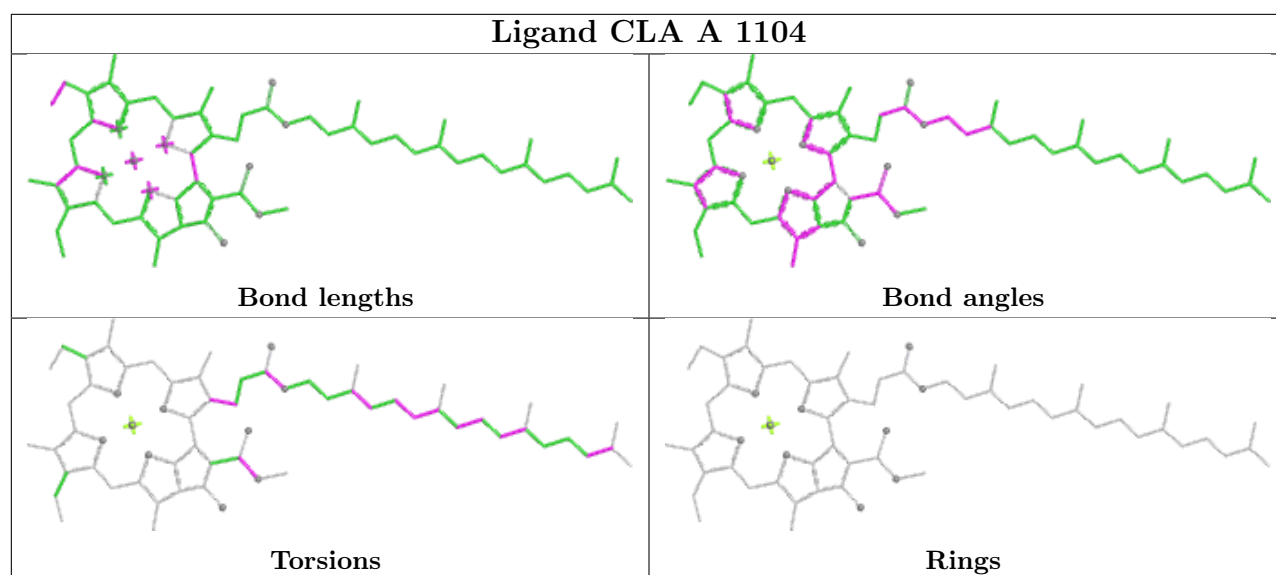
Ligand CLA B 1221

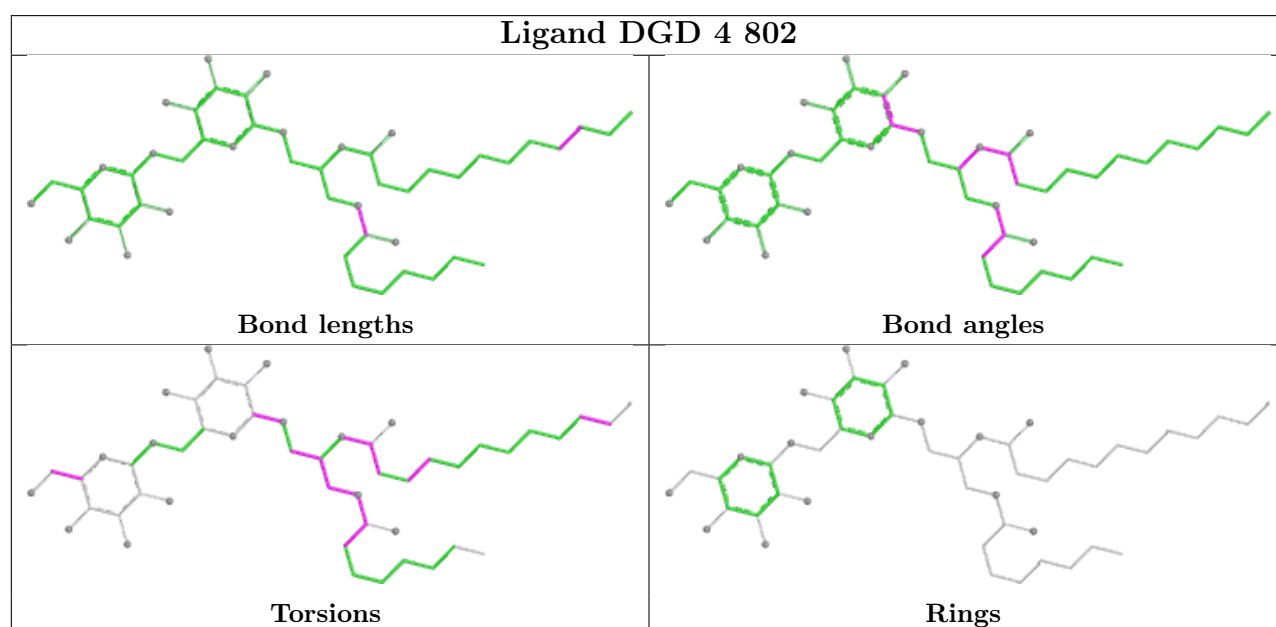
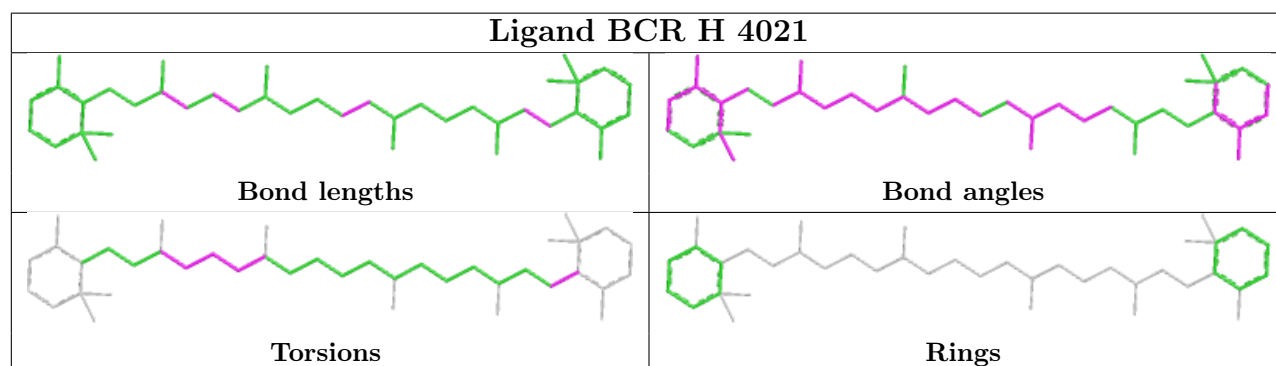
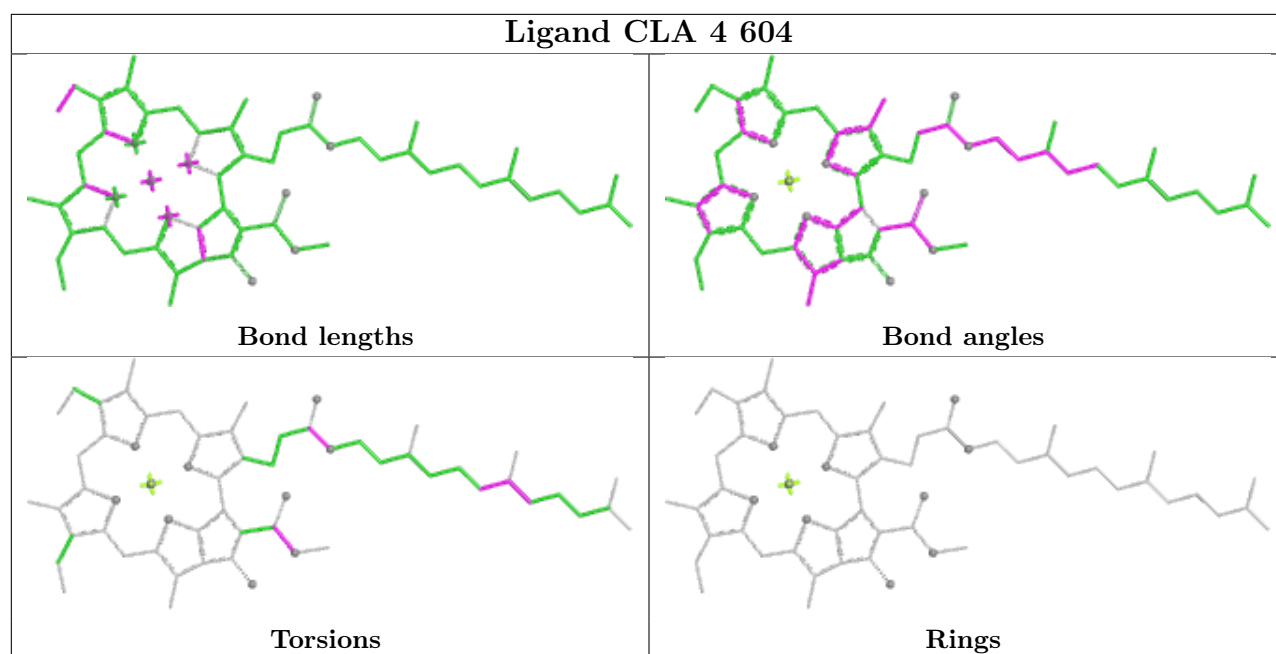


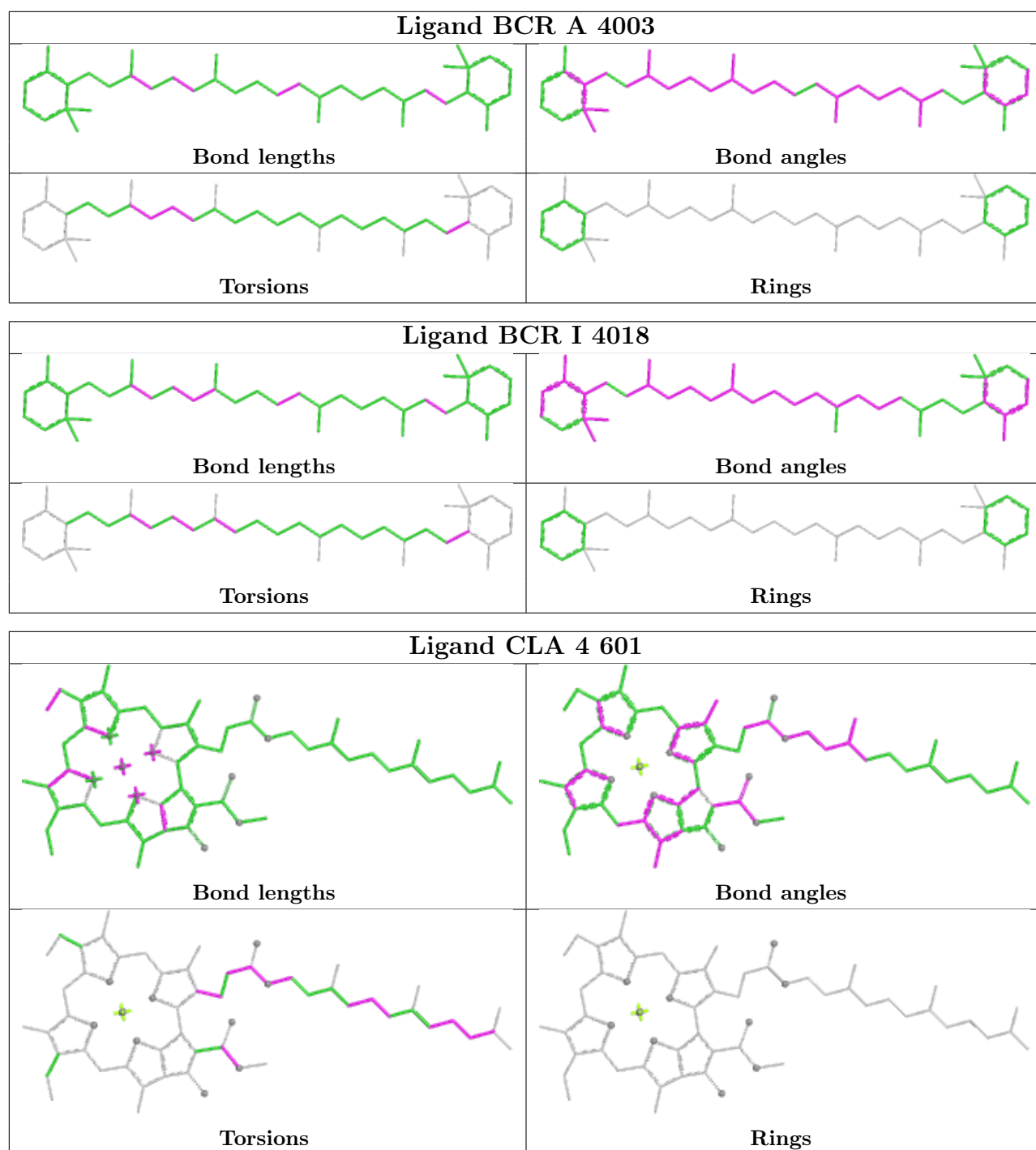


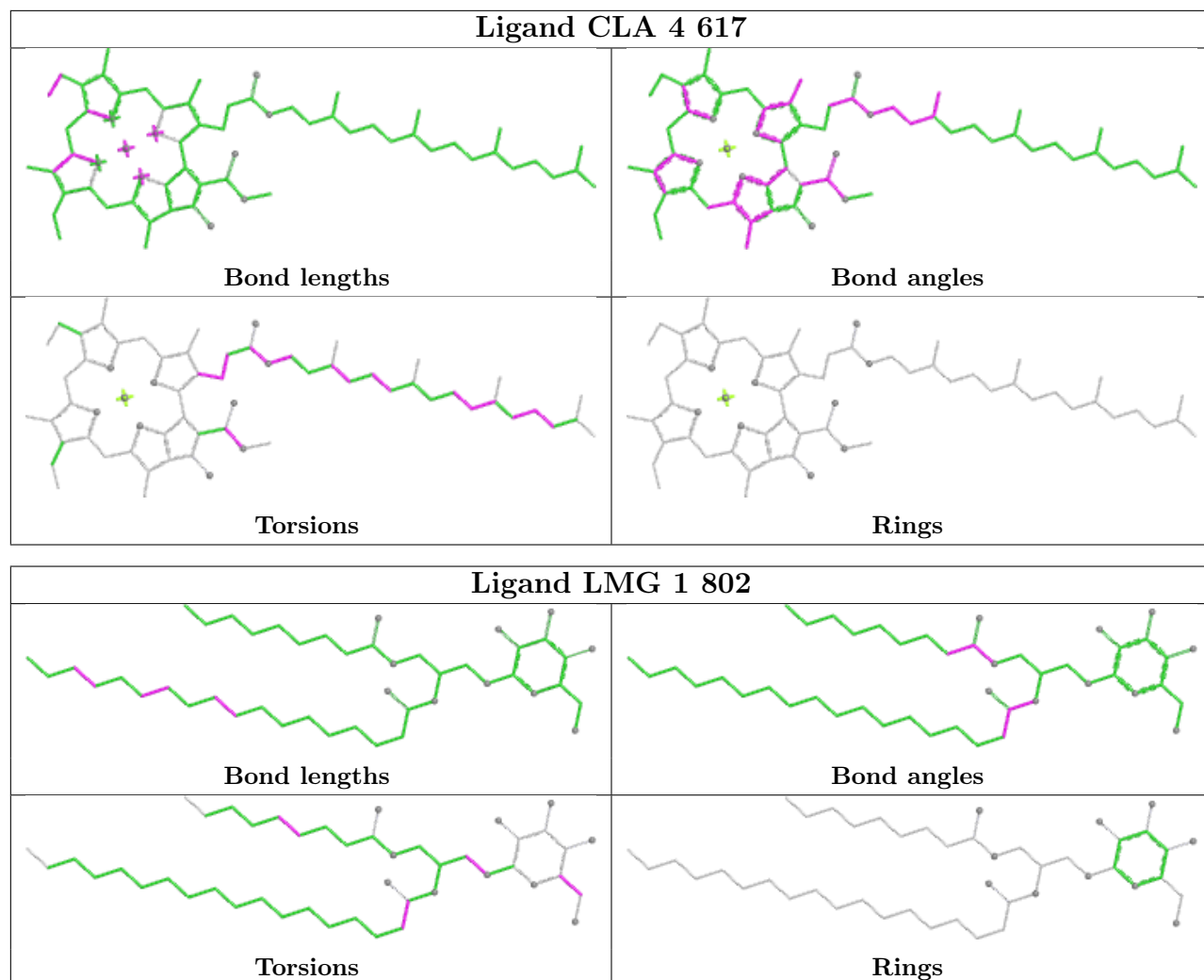


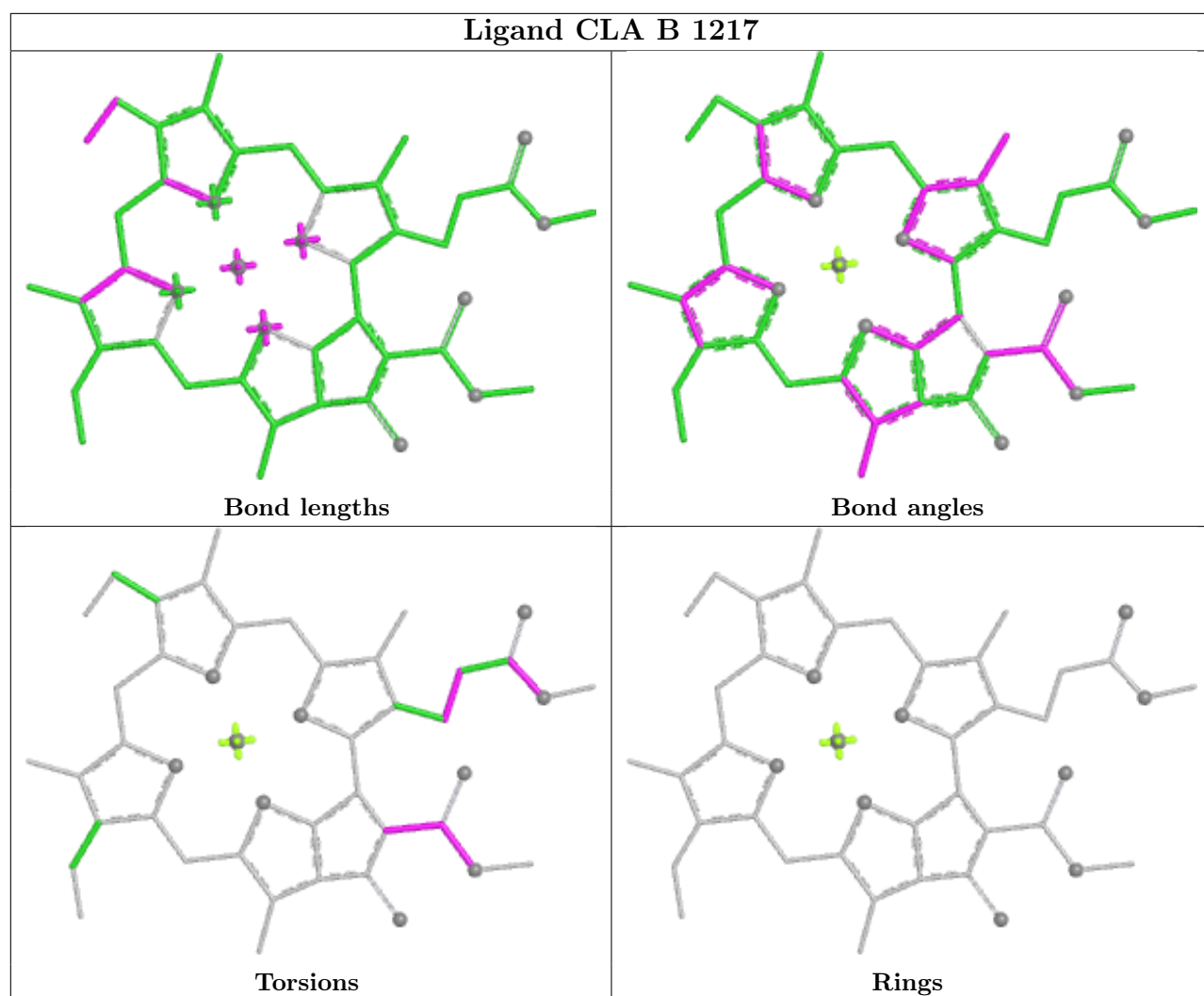


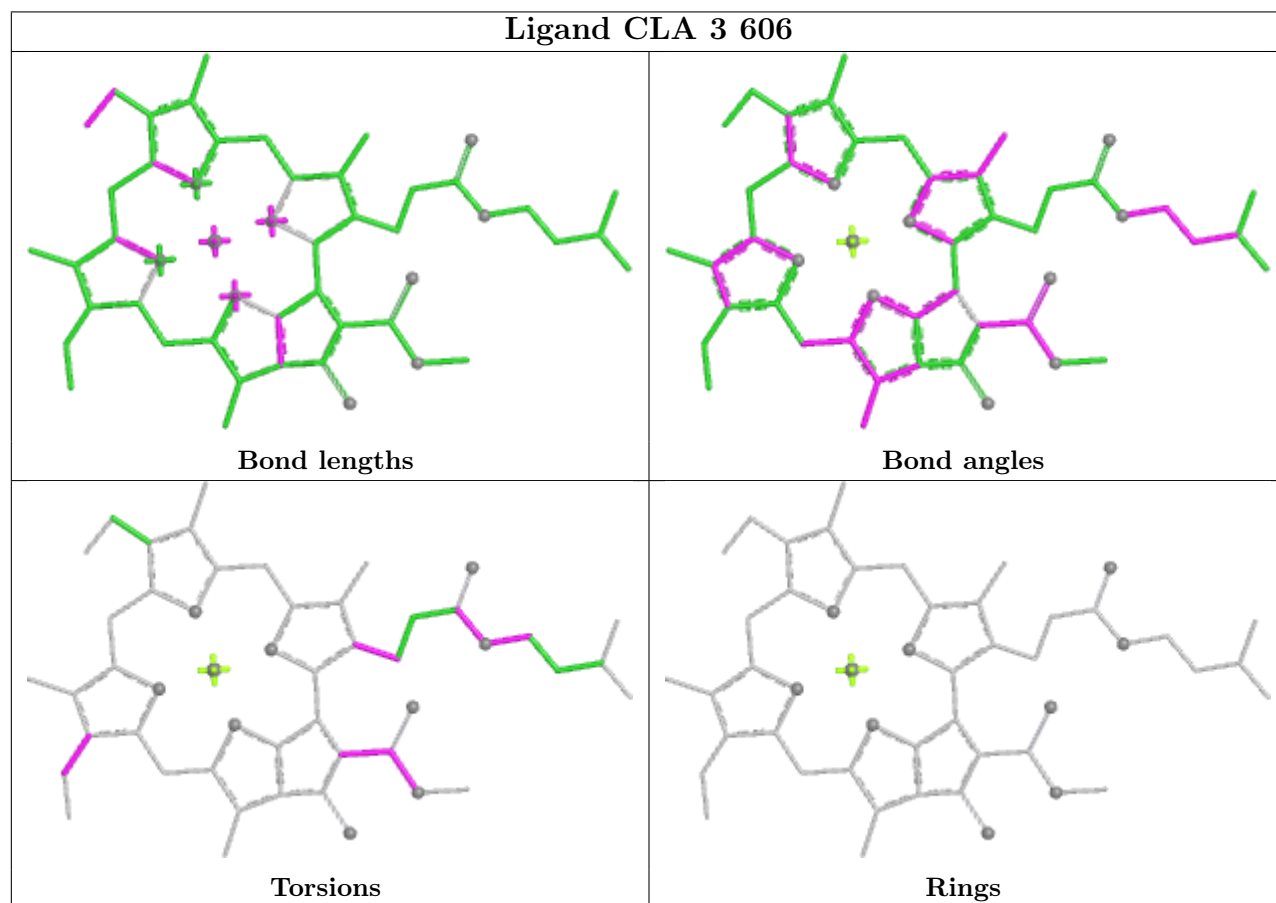
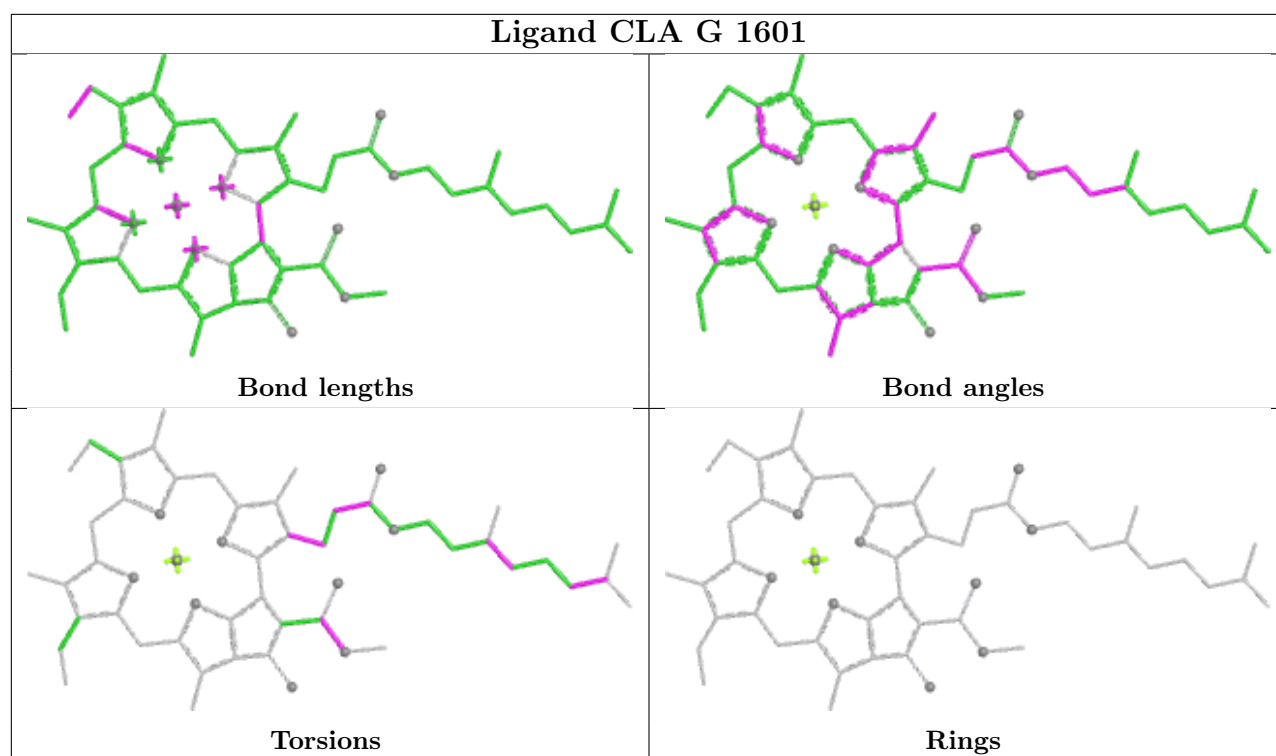


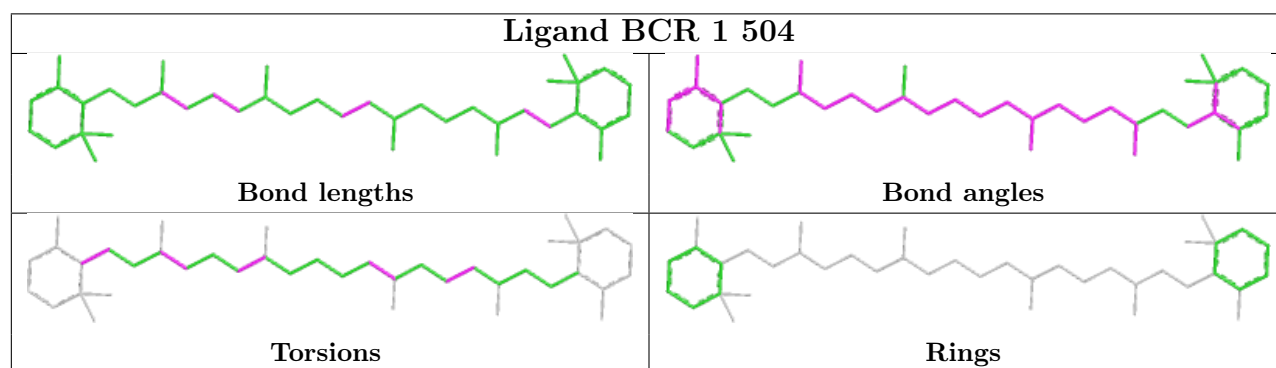
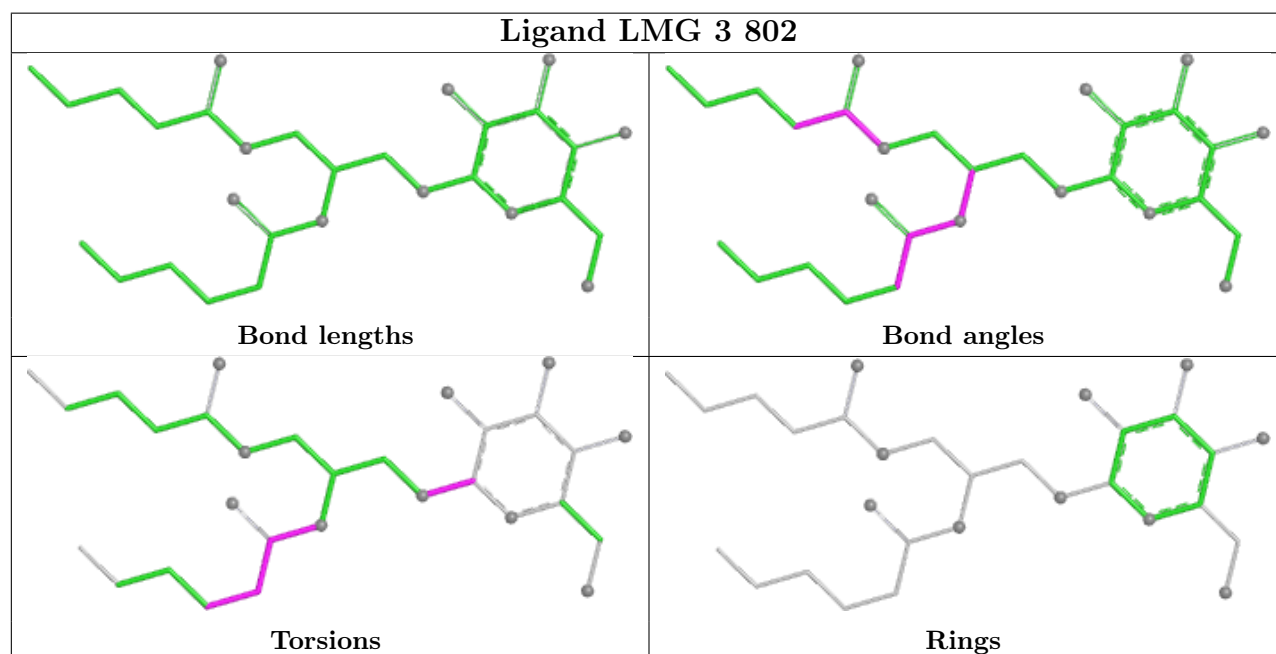
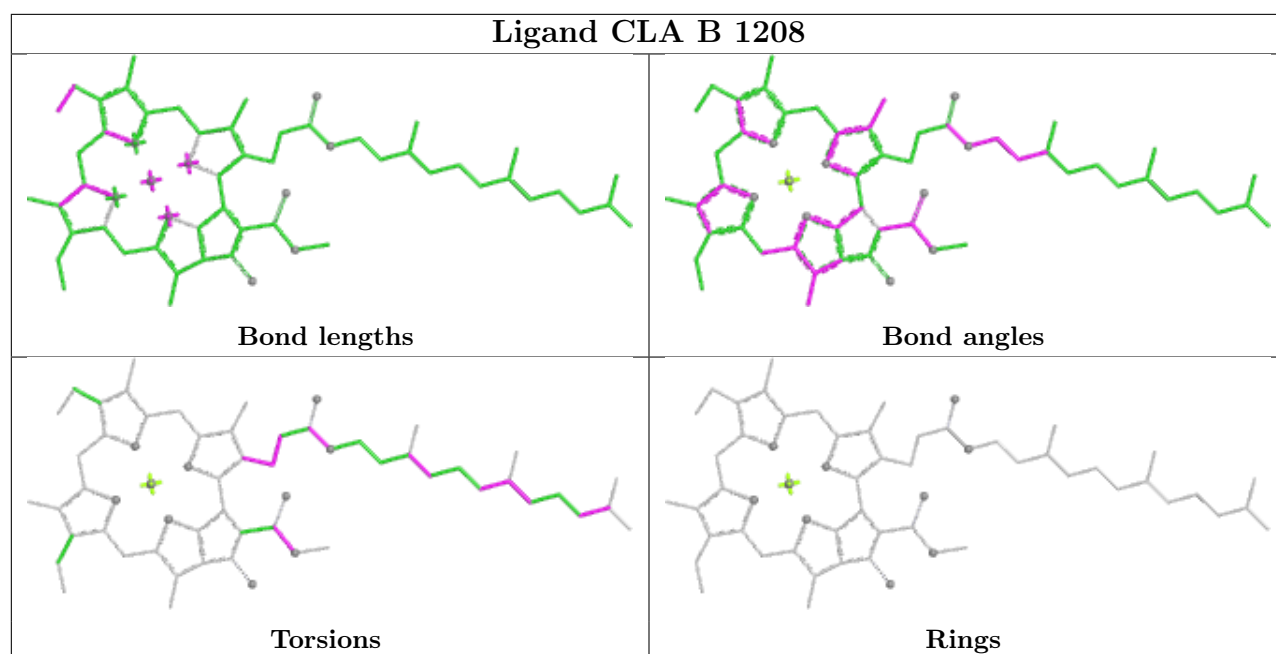


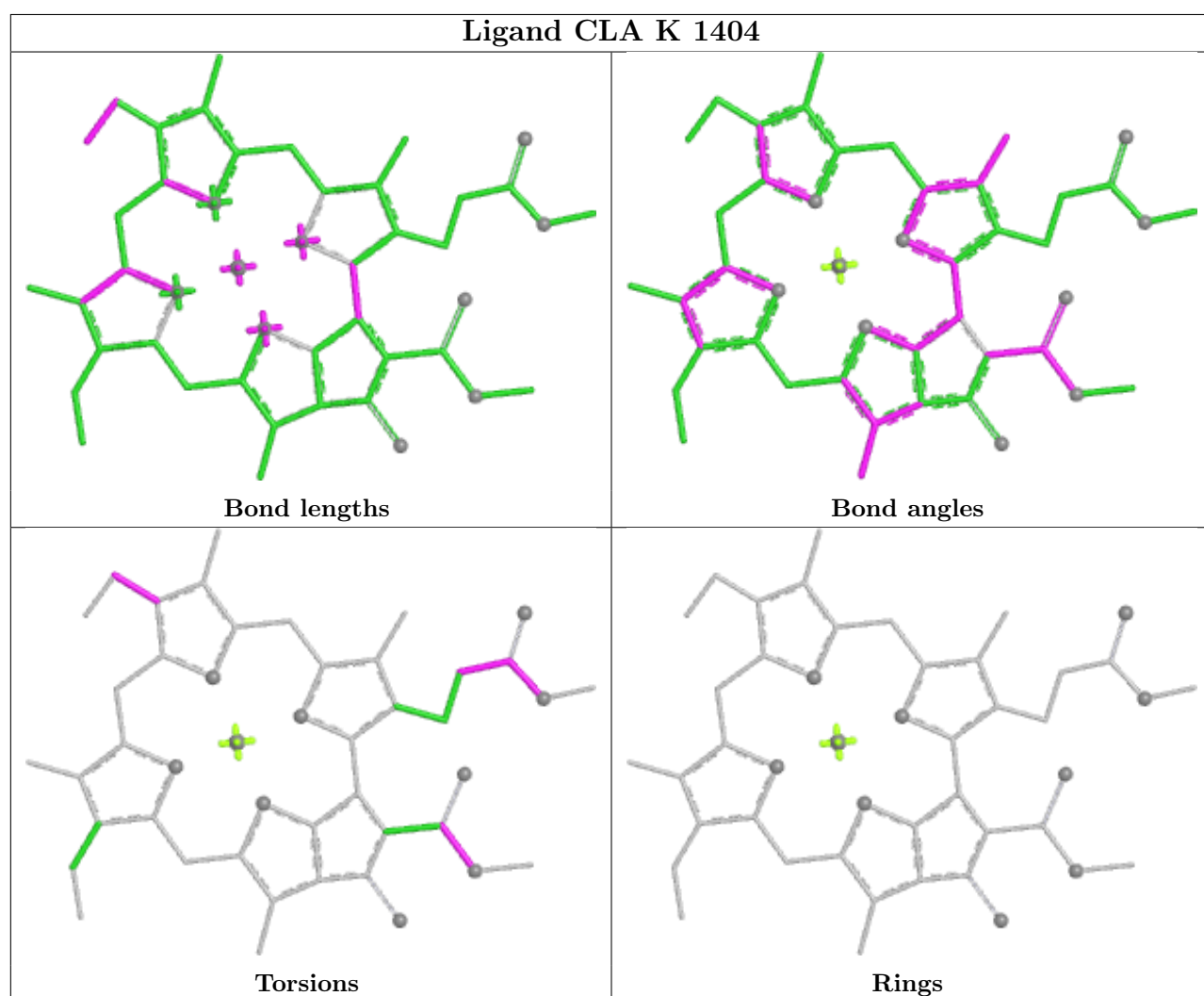
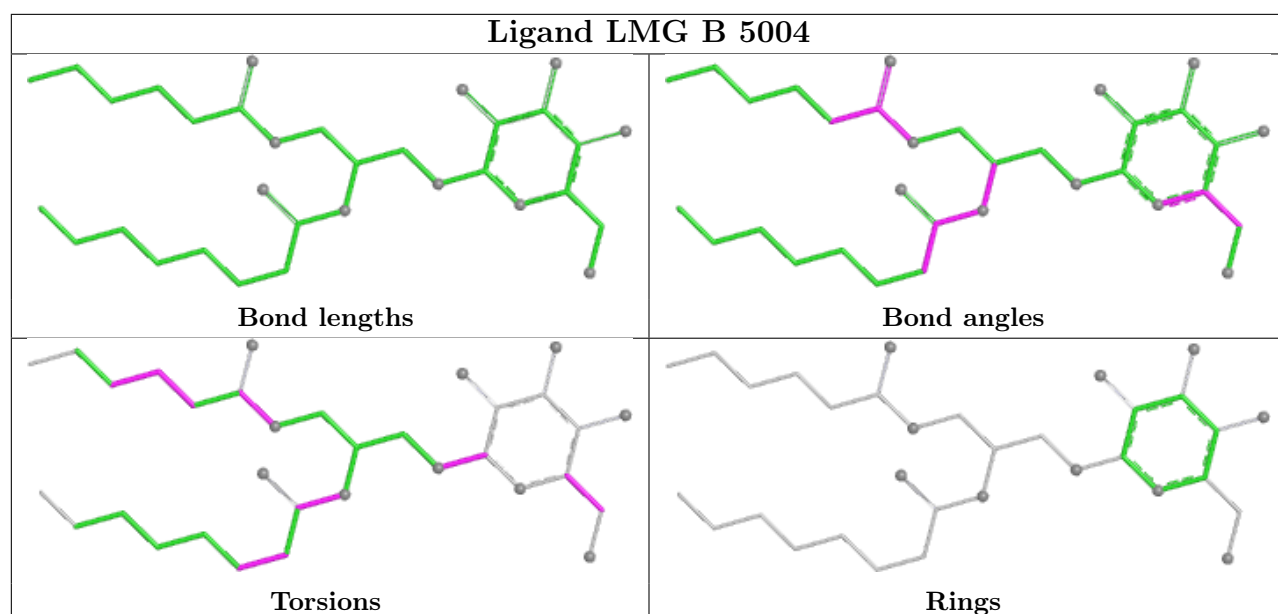


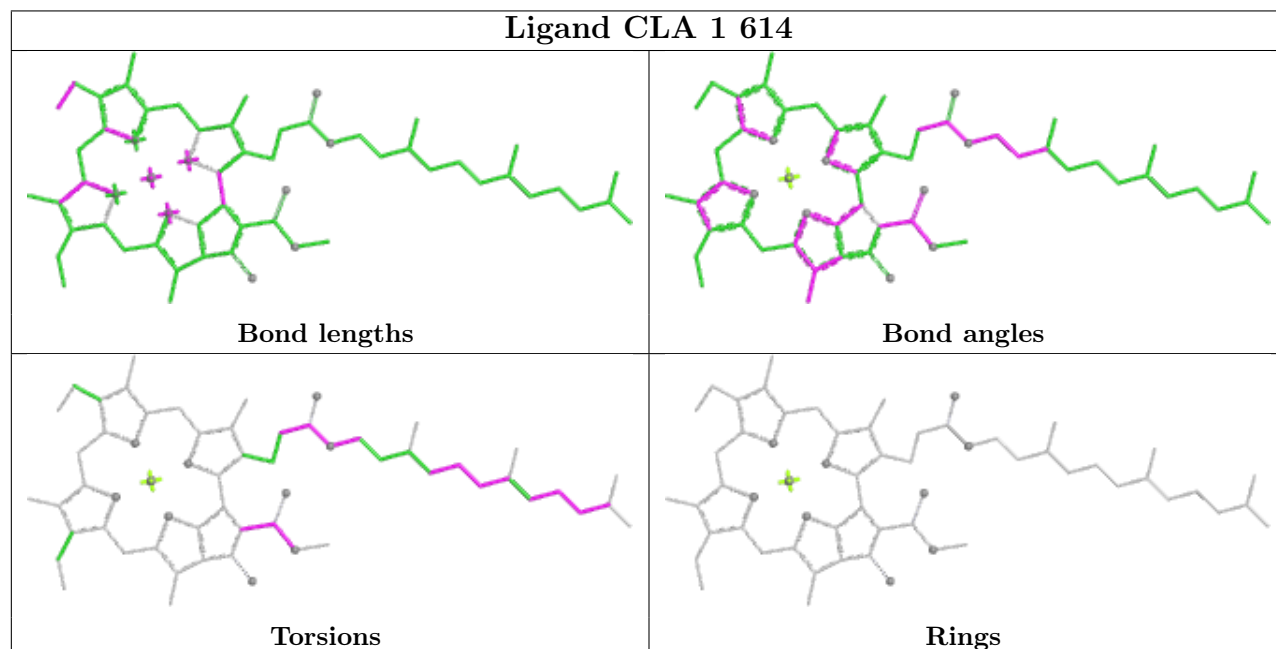
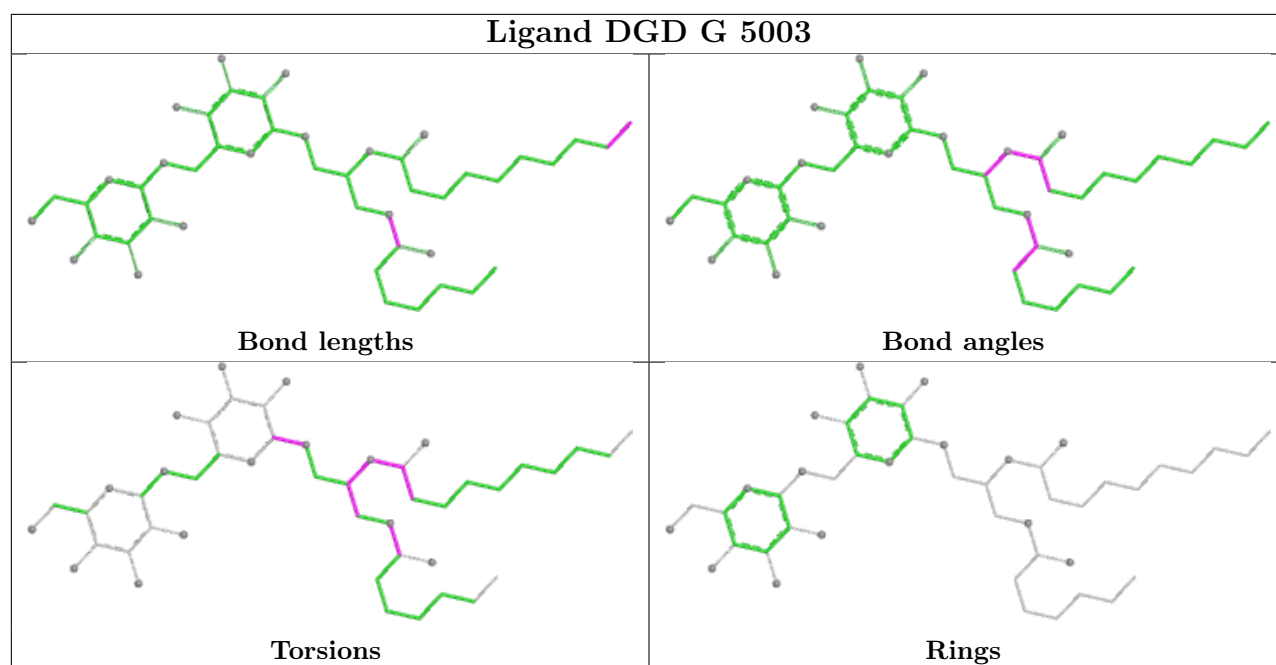


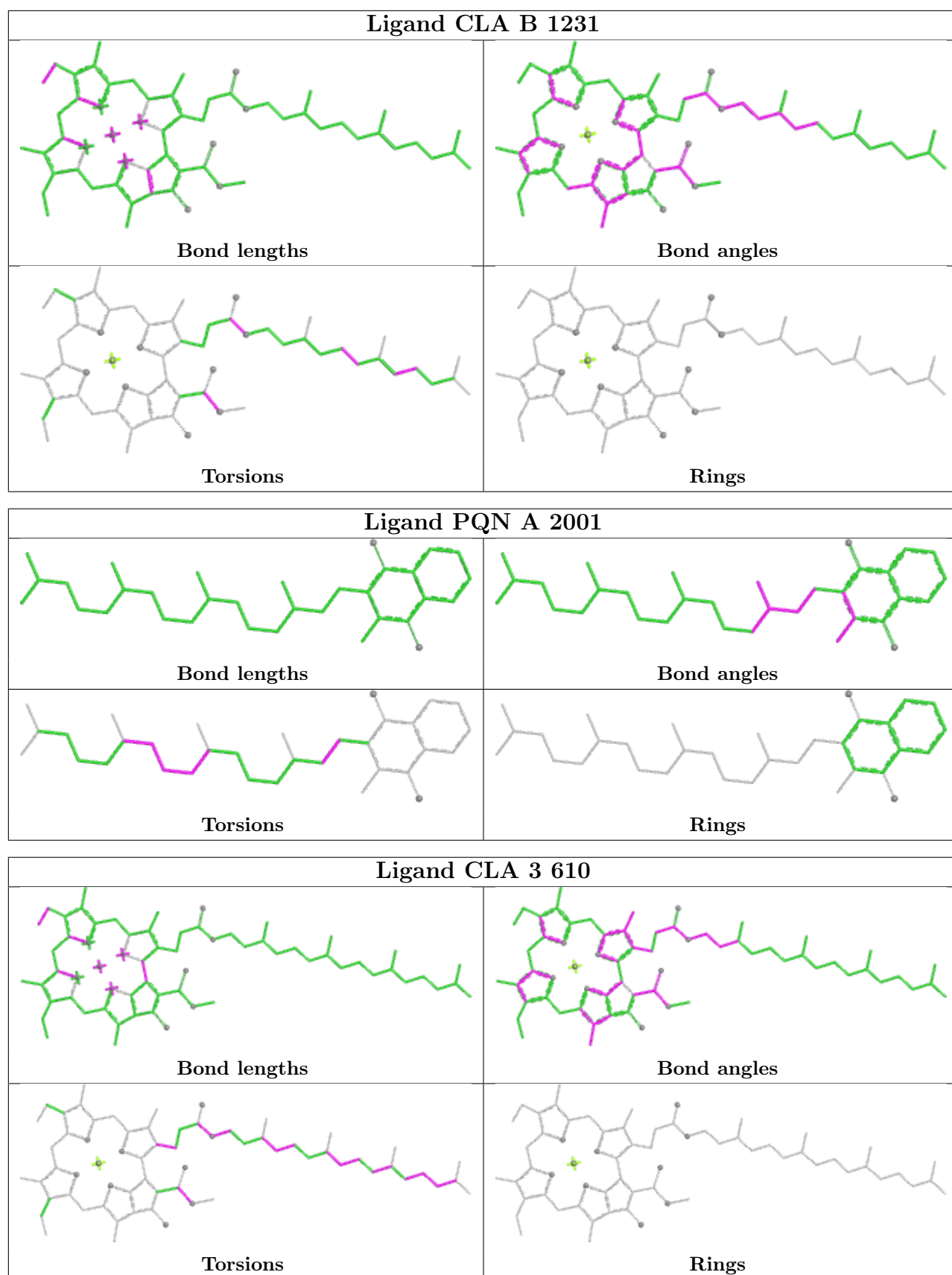


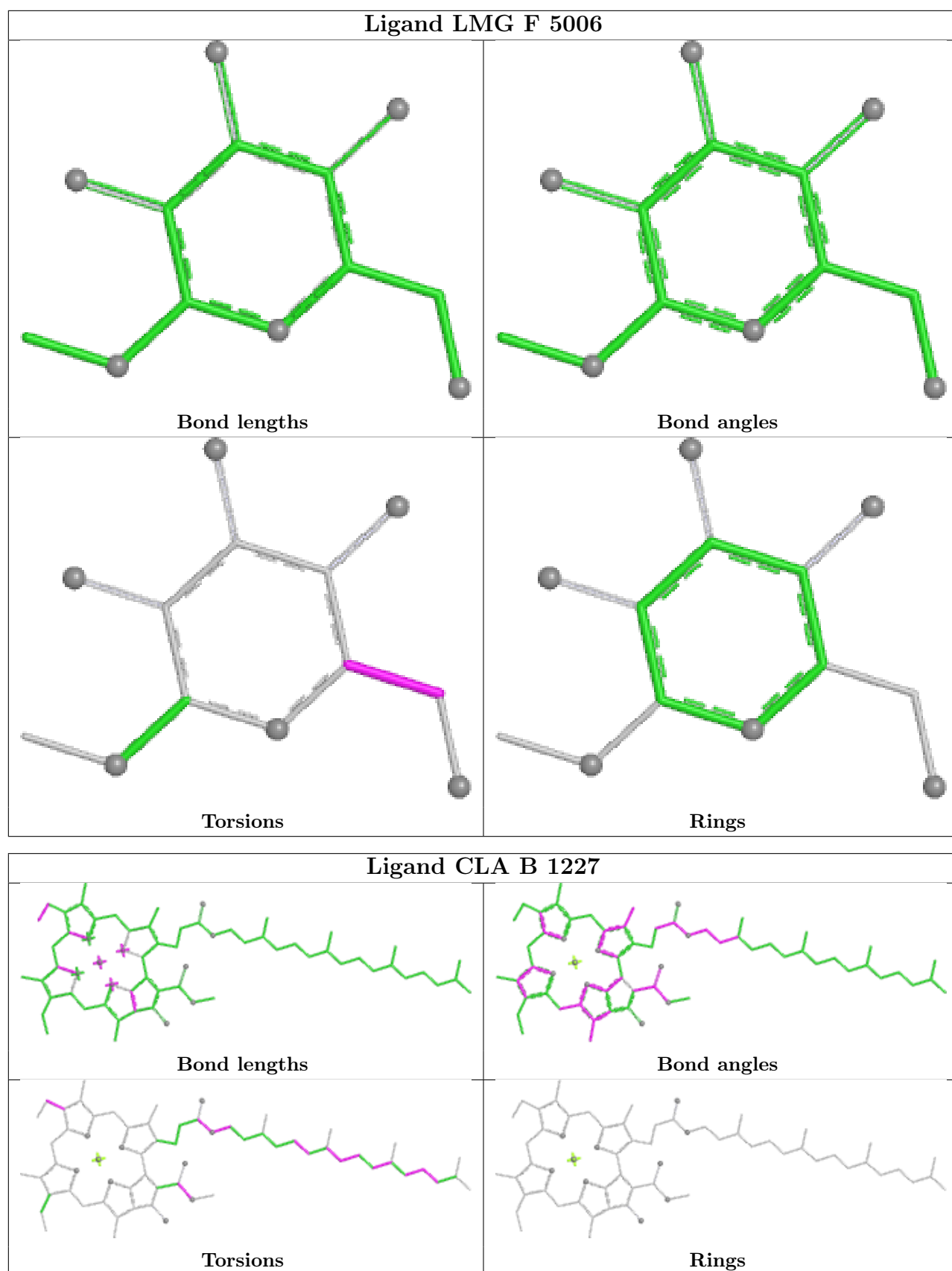




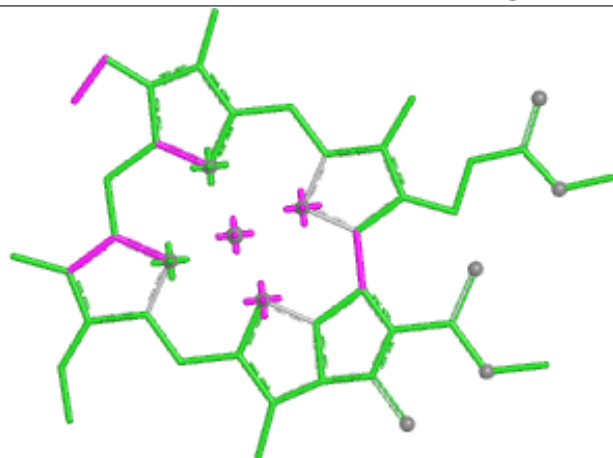




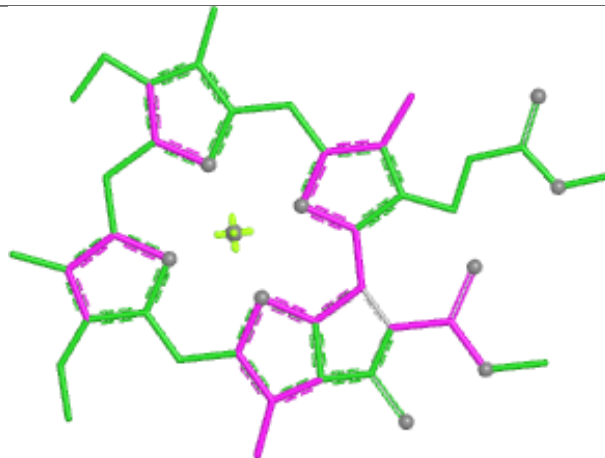




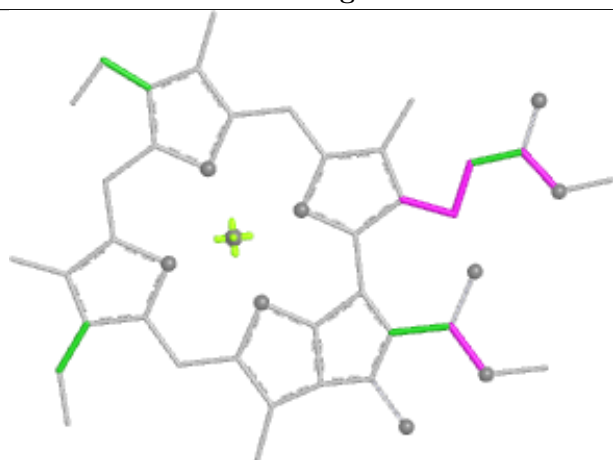
Ligand CLA G 1602



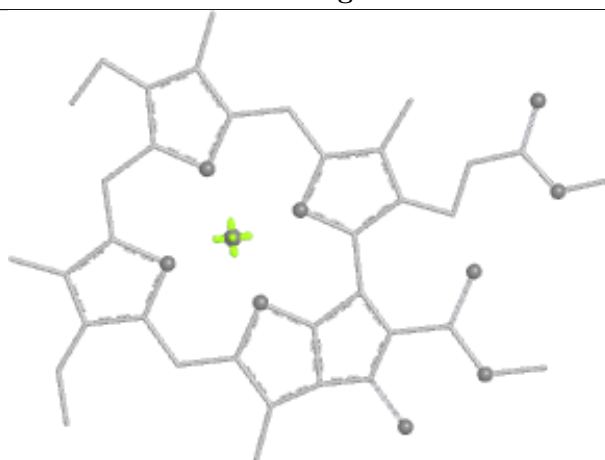
Bond lengths



Bond angles

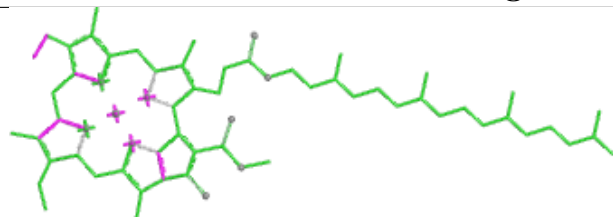


Torsions

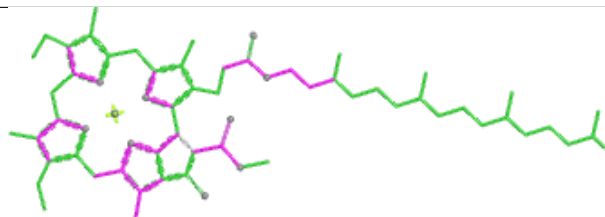


Rings

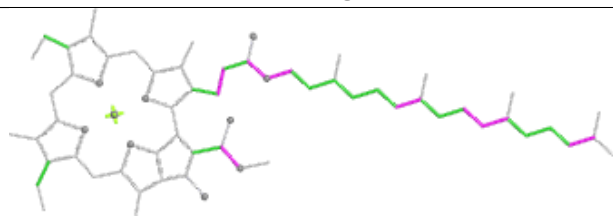
Ligand CLA A 1013



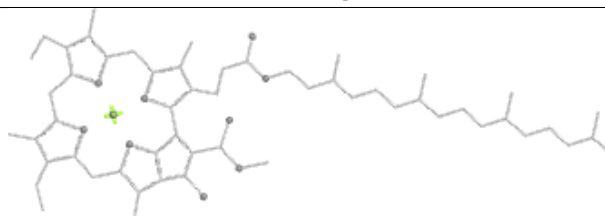
Bond lengths



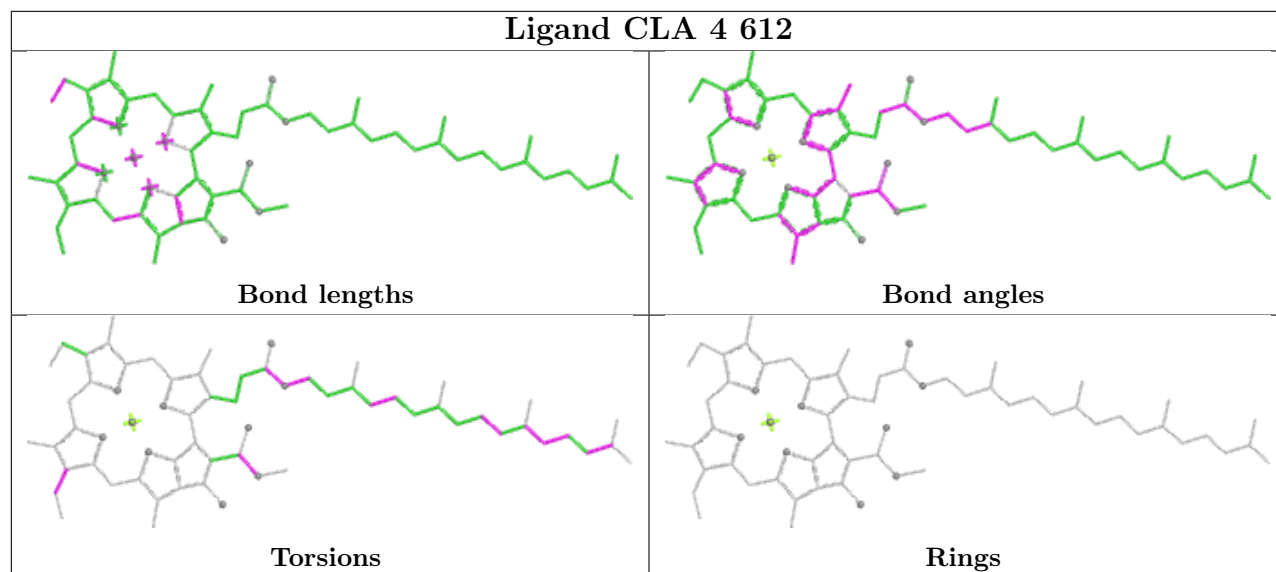
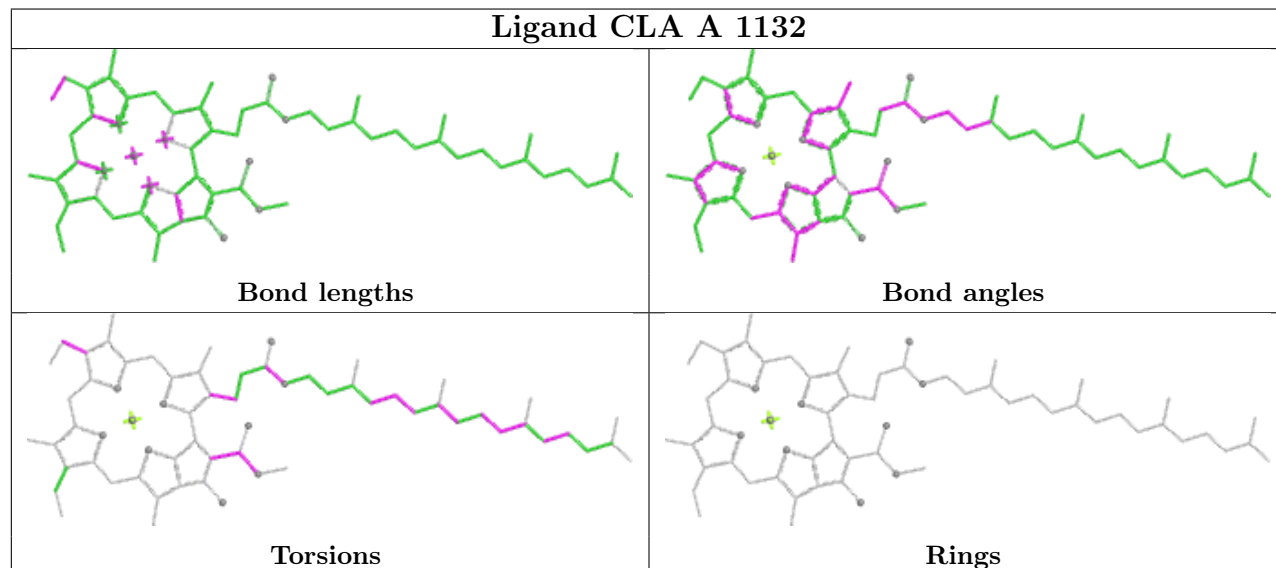
Bond angles

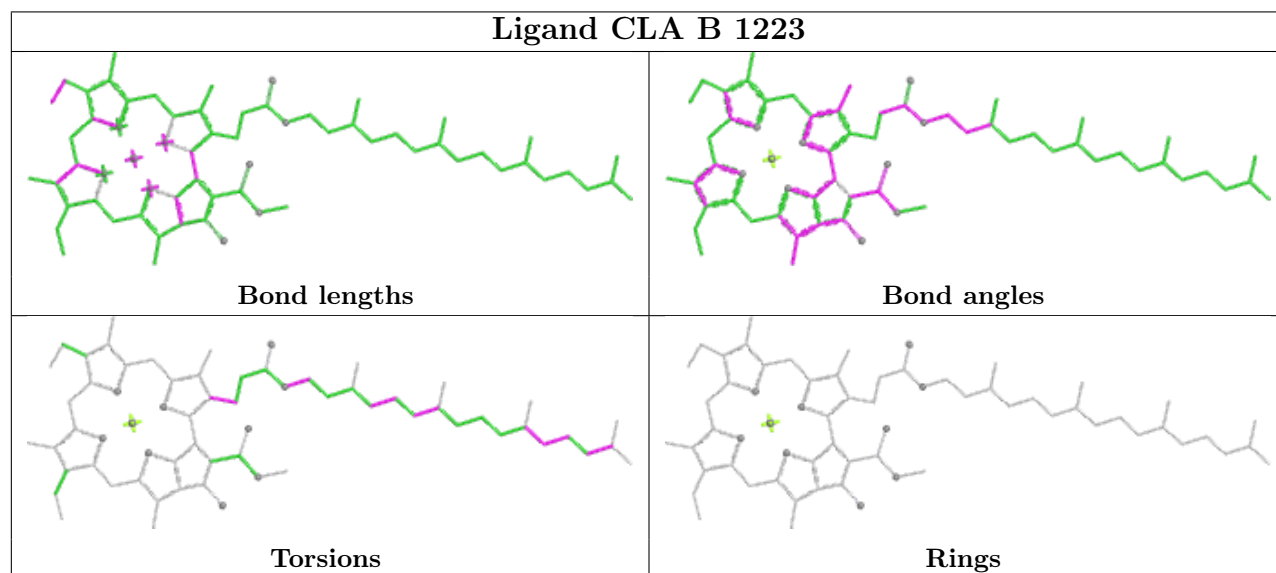
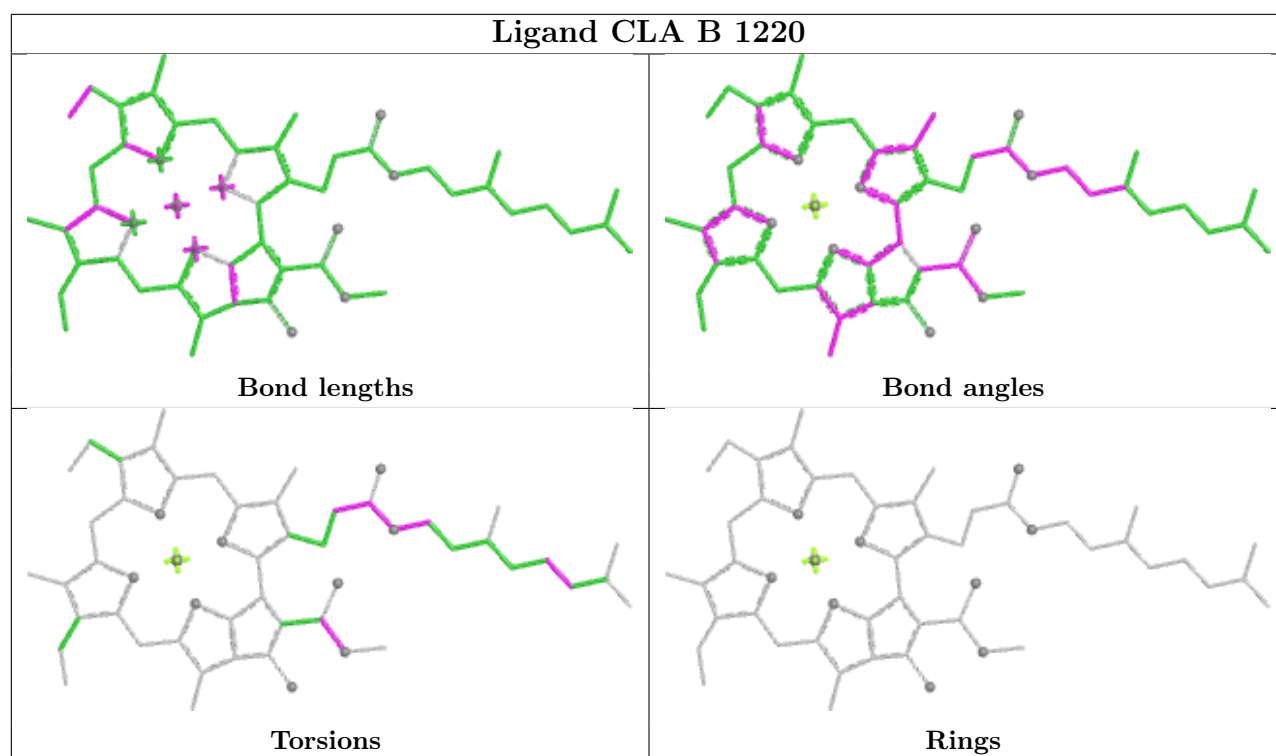


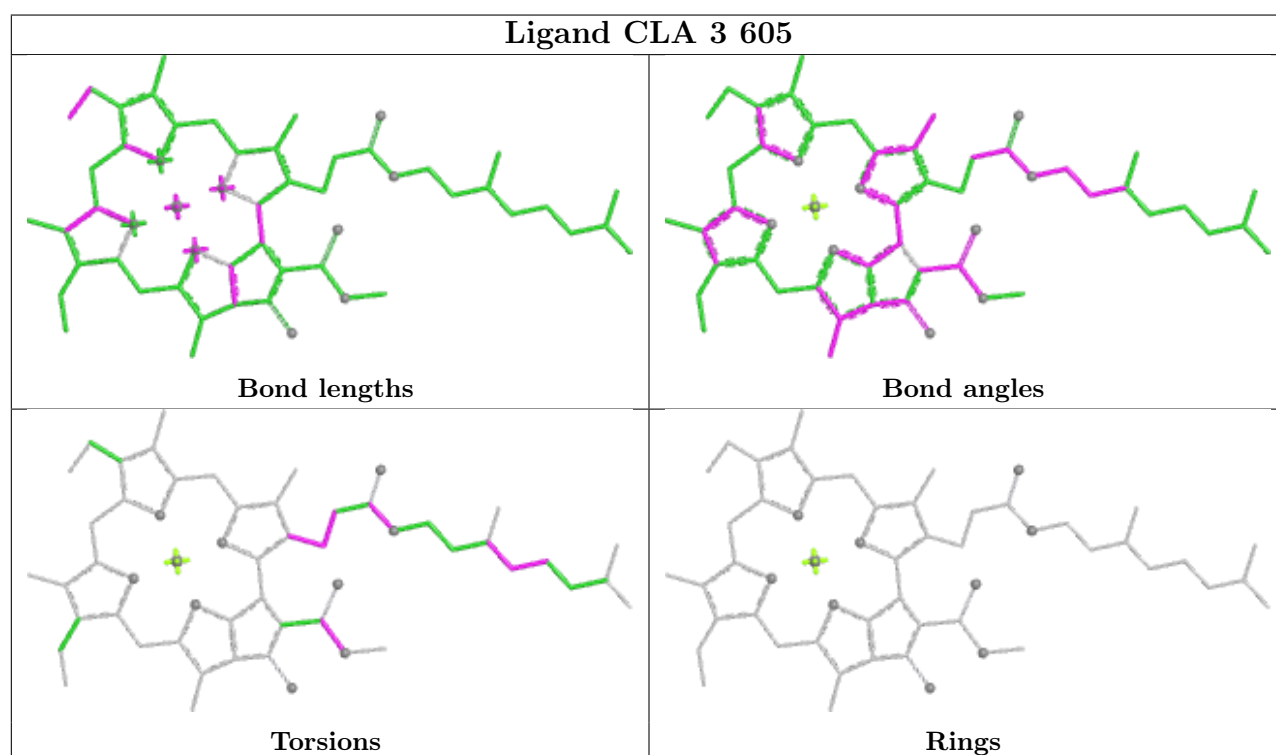
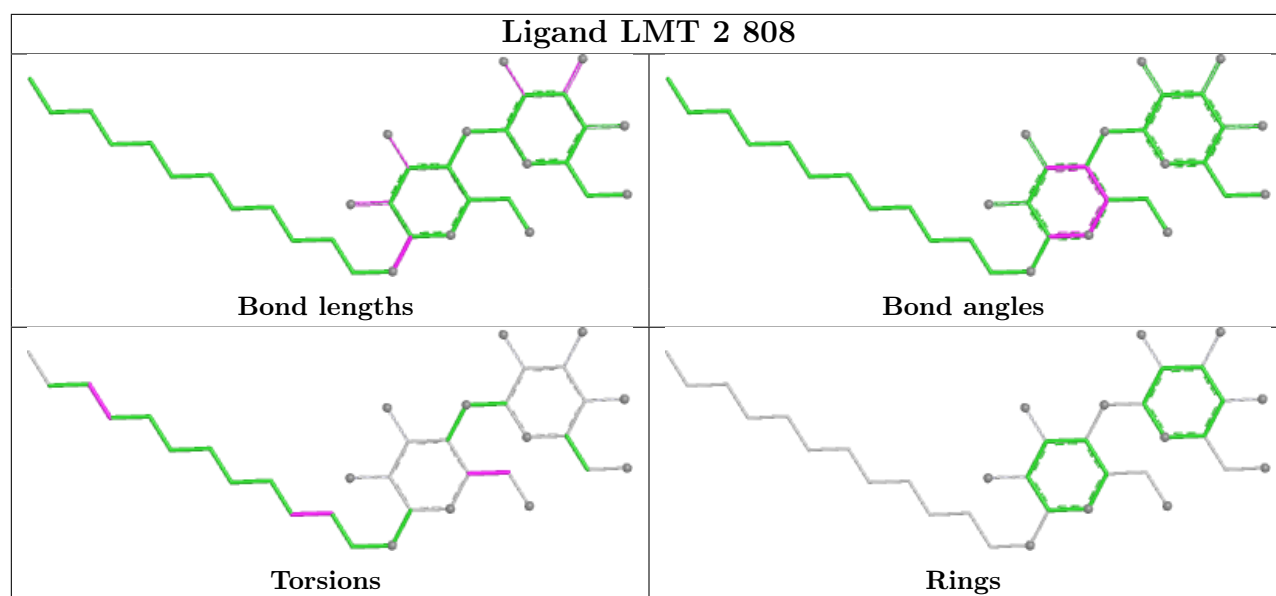
Torsions

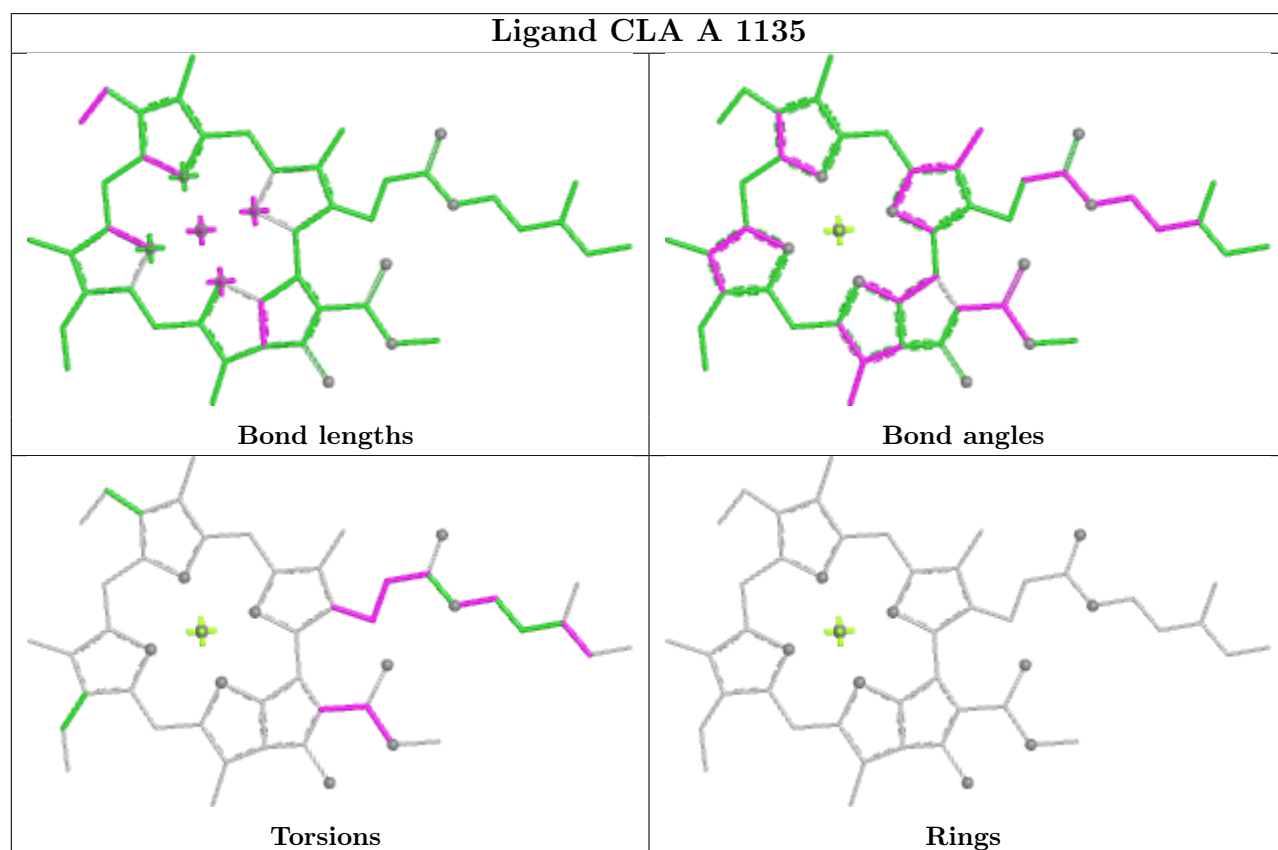
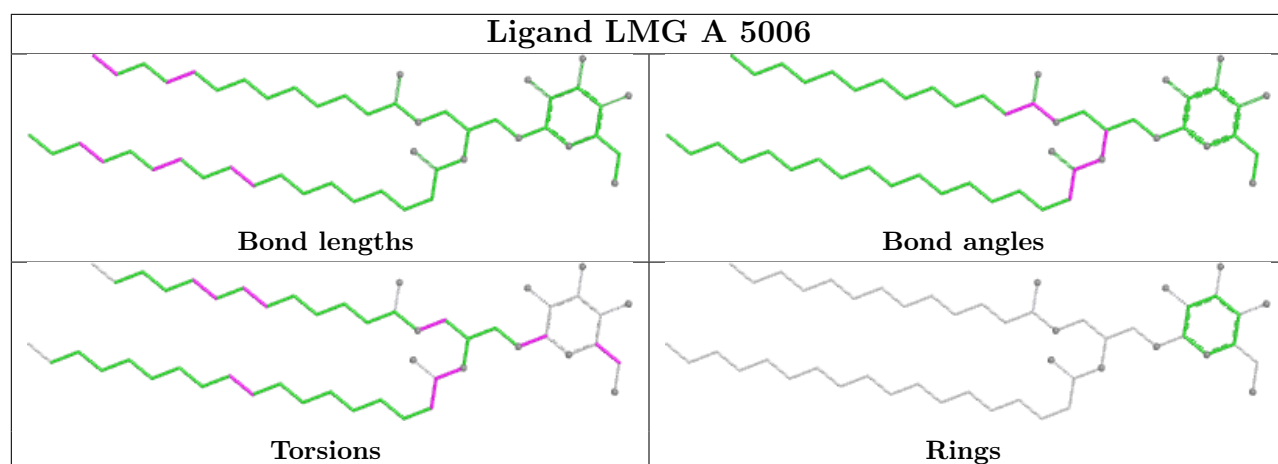


Rings

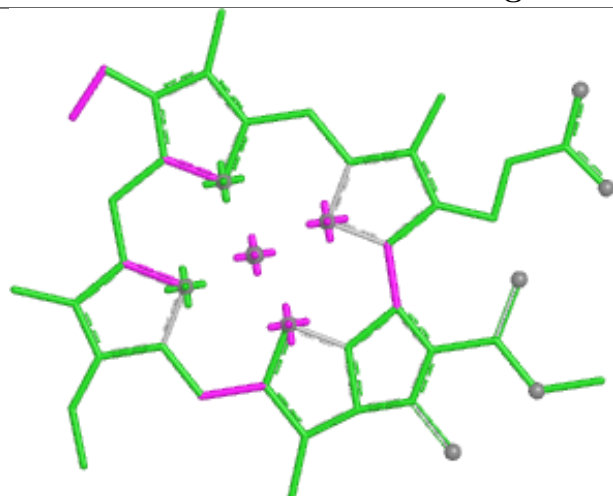
Ligand CLA 4 612**Ligand CLA A 1132**



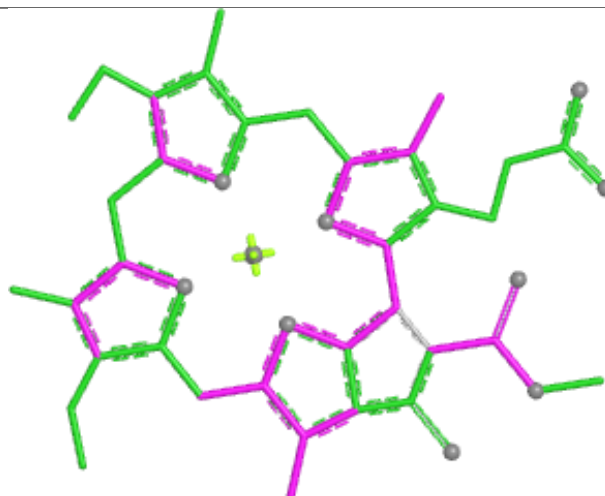




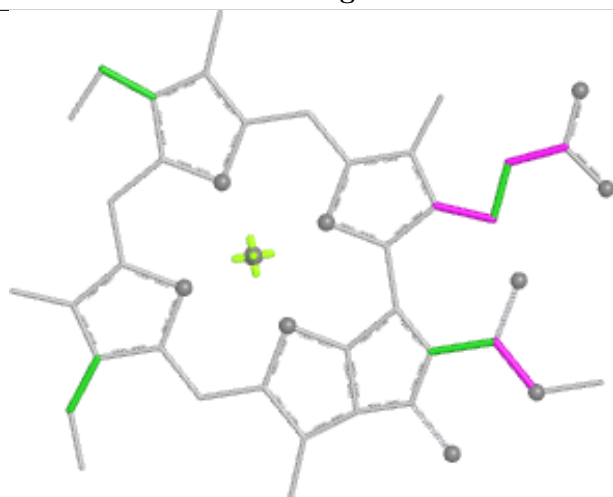
Ligand CLA A 1113



Bond lengths



Bond angles

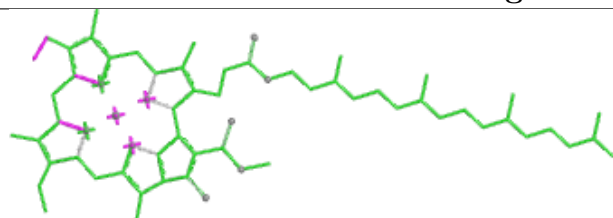


Torsions

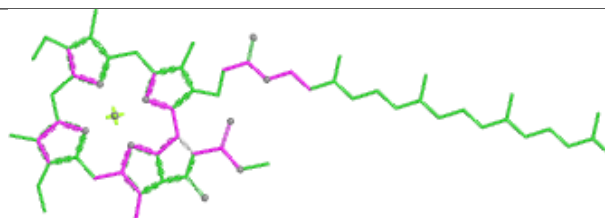


Rings

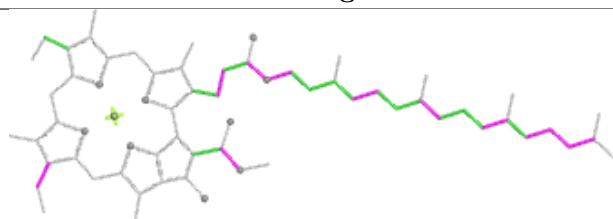
Ligand CLA B 1023



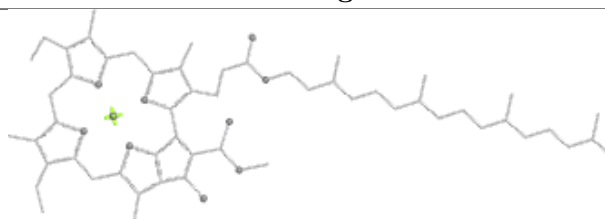
Bond lengths



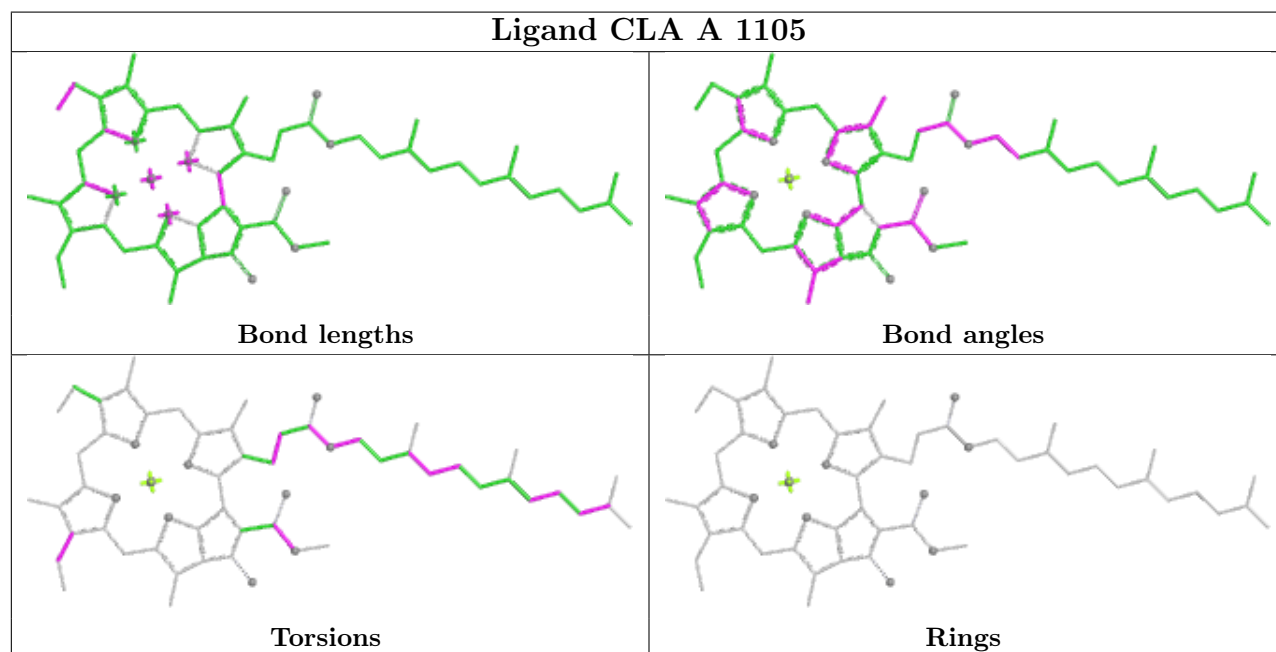
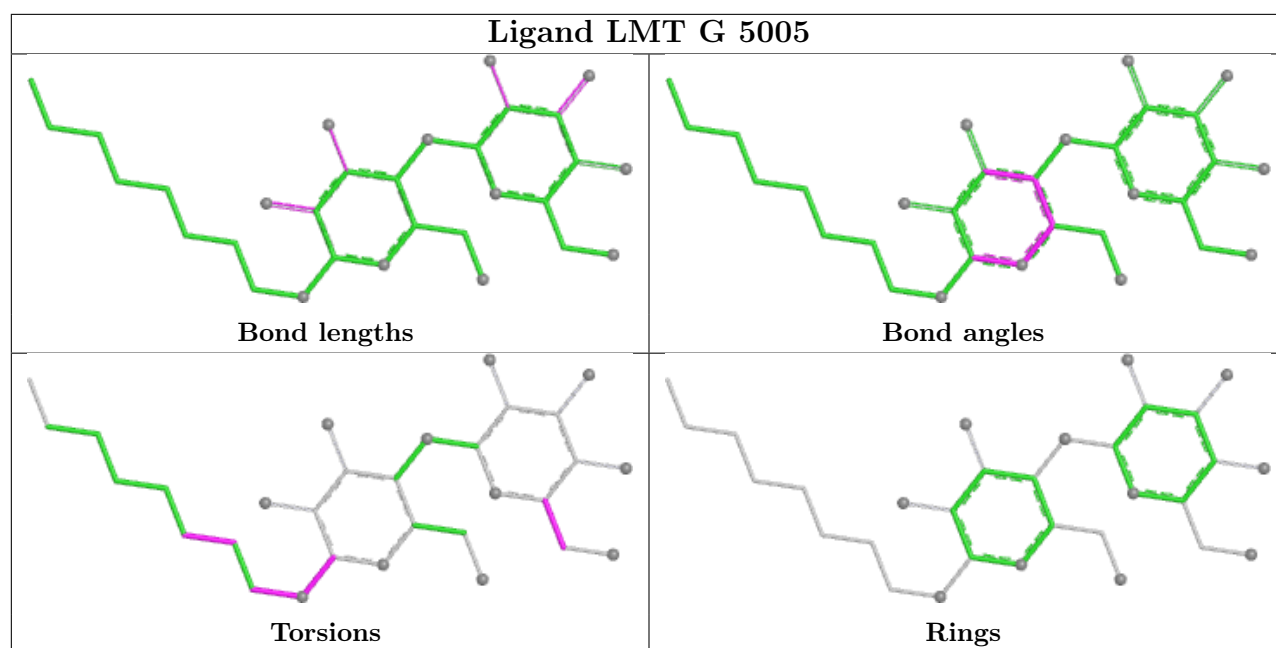
Bond angles

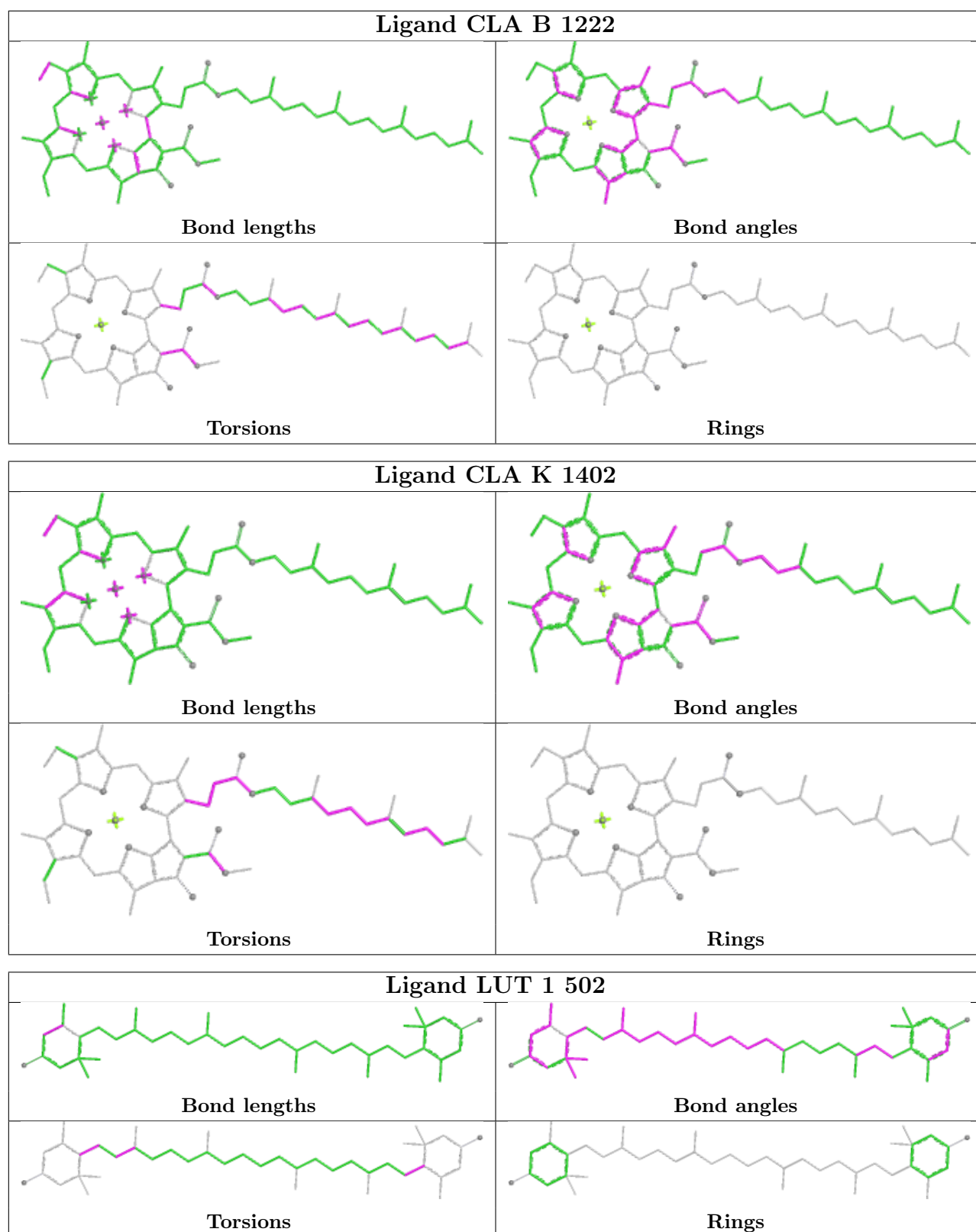


Torsions

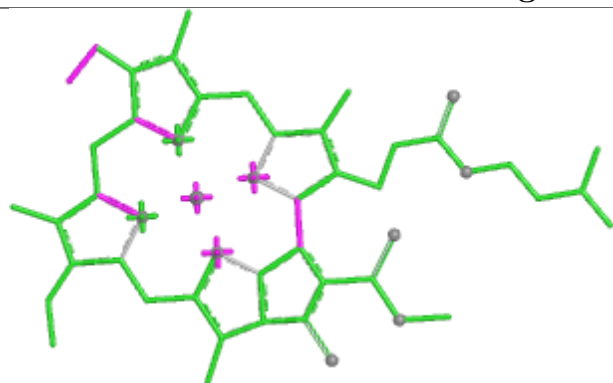


Rings

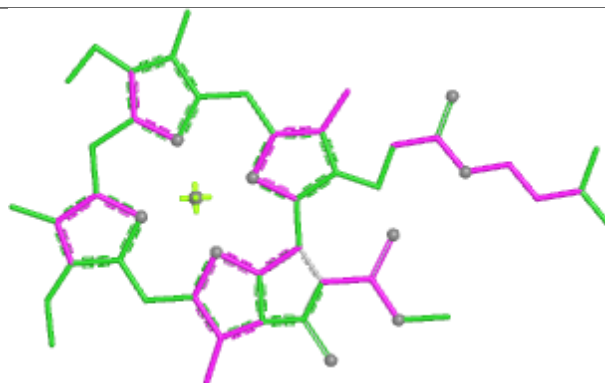




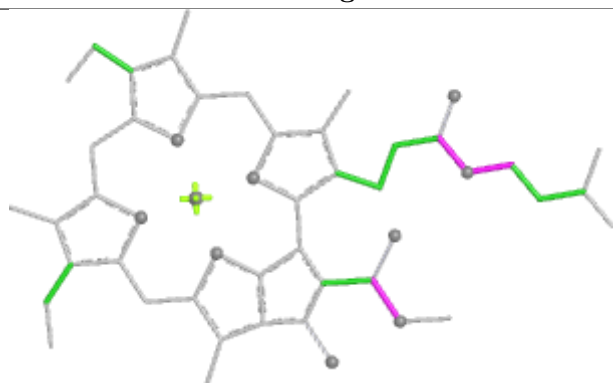
Ligand CLA 1 606



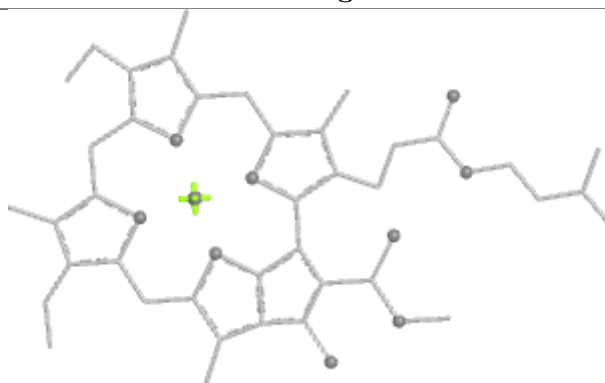
Bond lengths



Bond angles

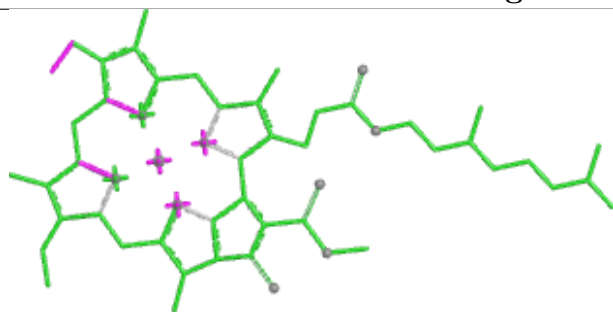


Torsions

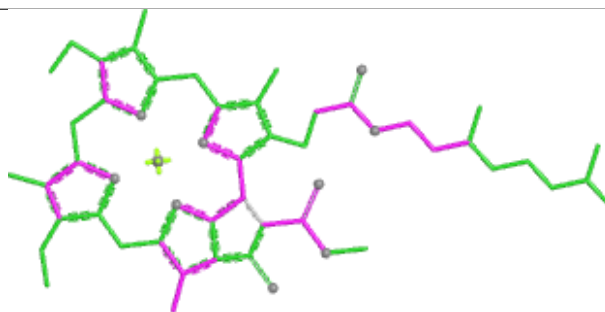


Rings

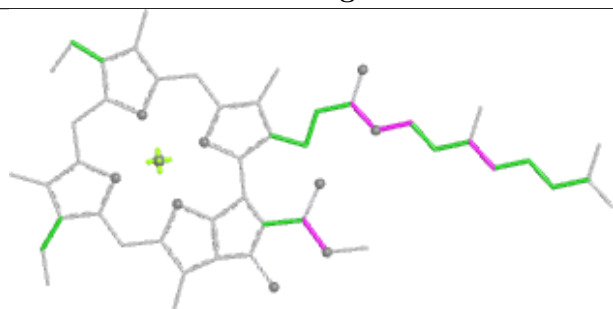
Ligand CLA B 1234



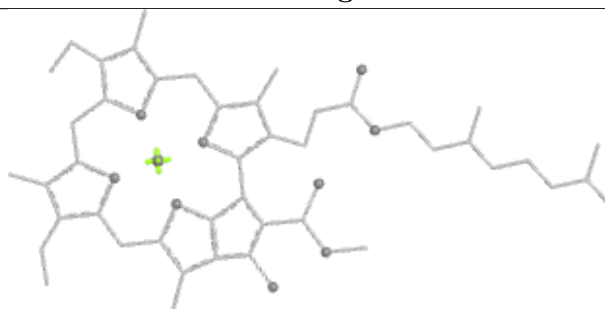
Bond lengths



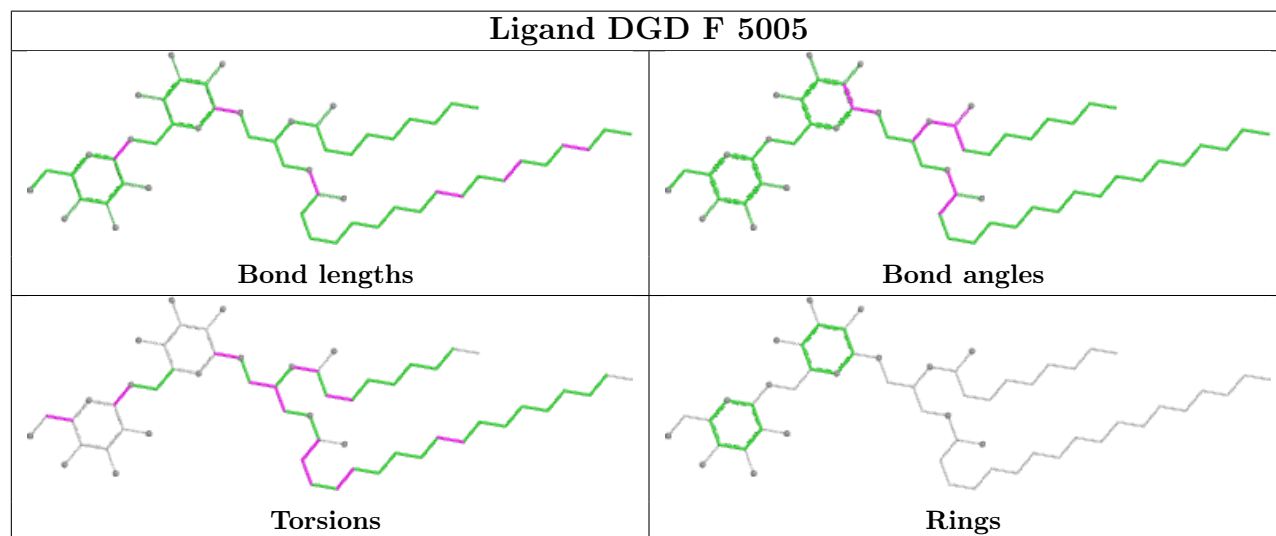
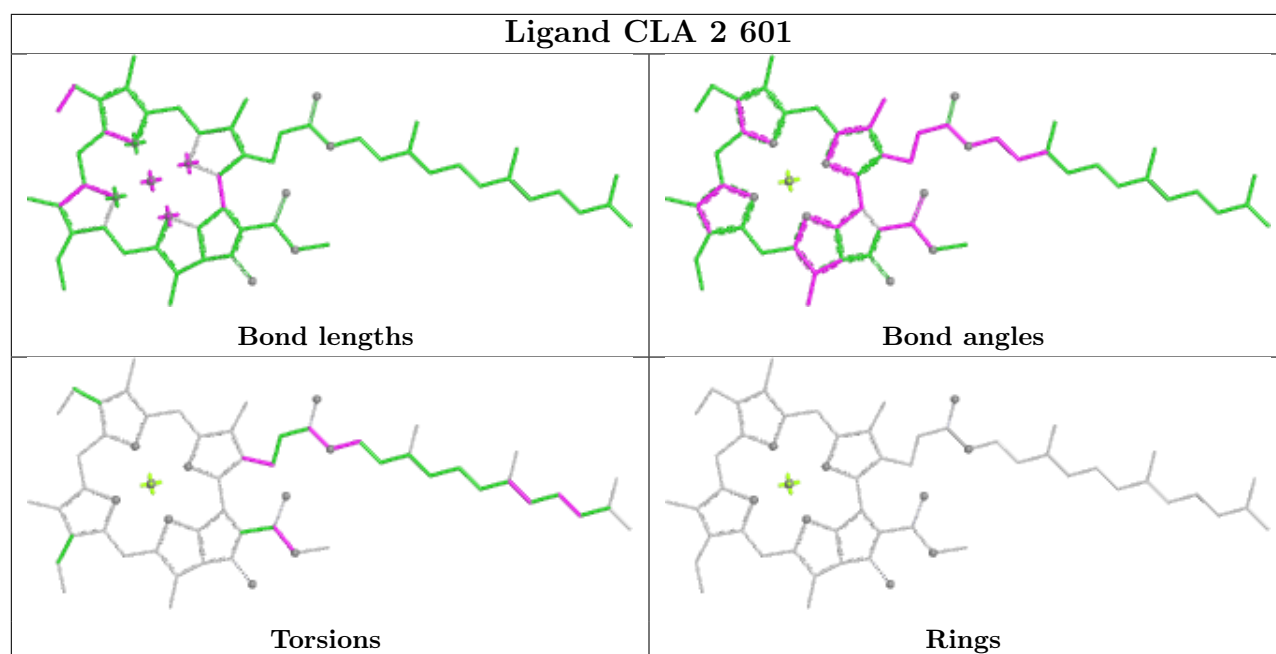
Bond angles

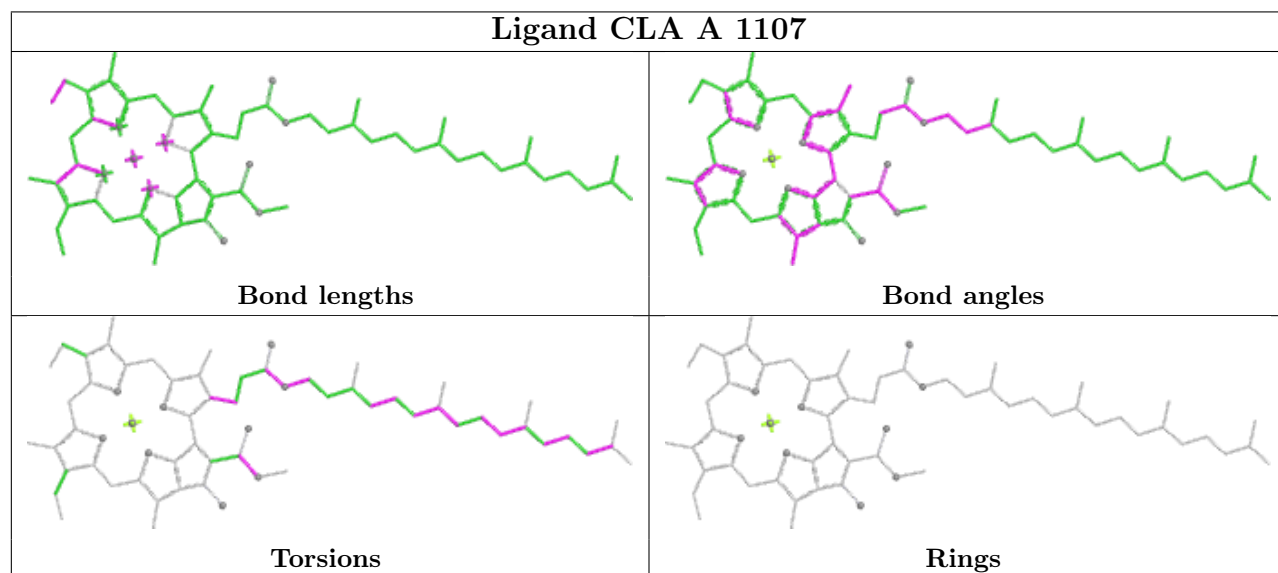
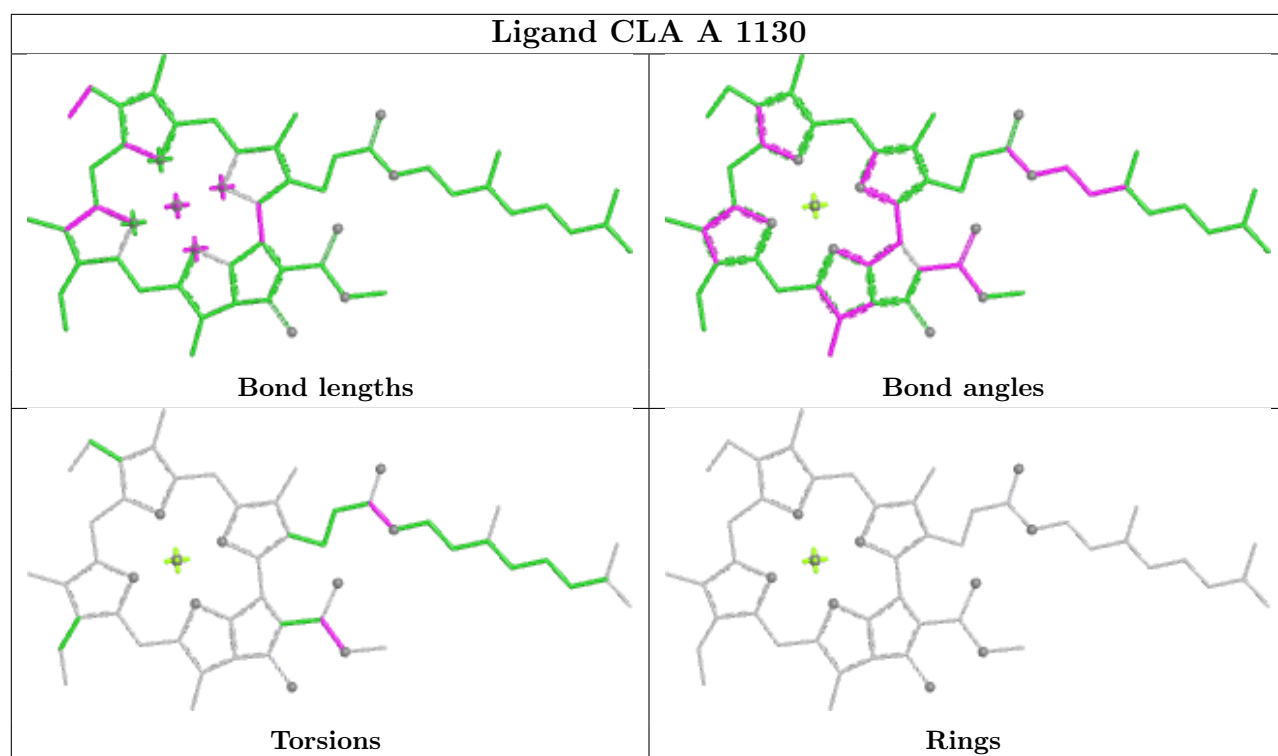


Torsions

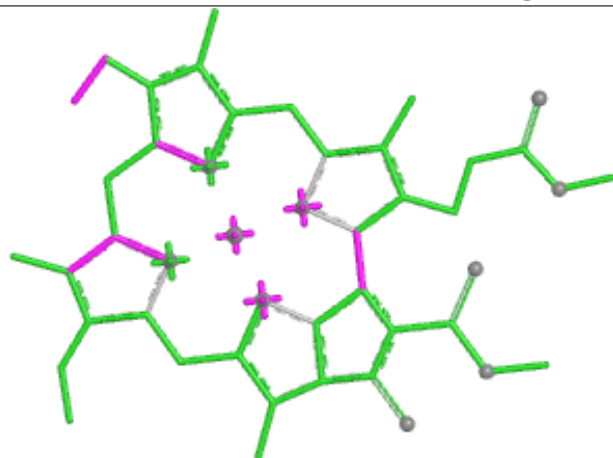


Rings

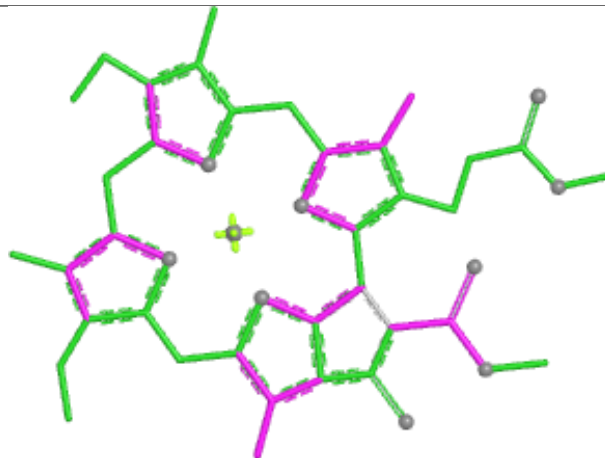




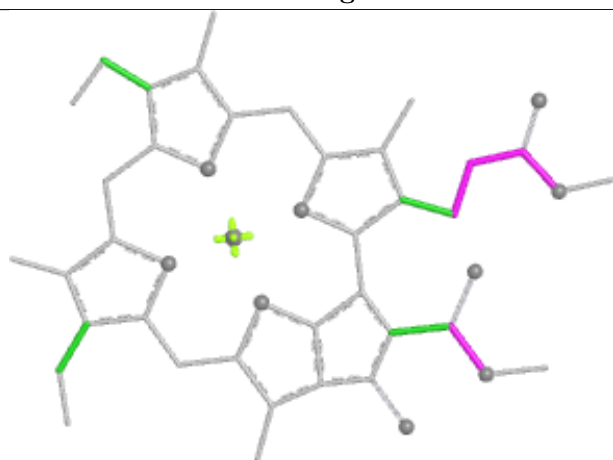
Ligand CLA 1 607



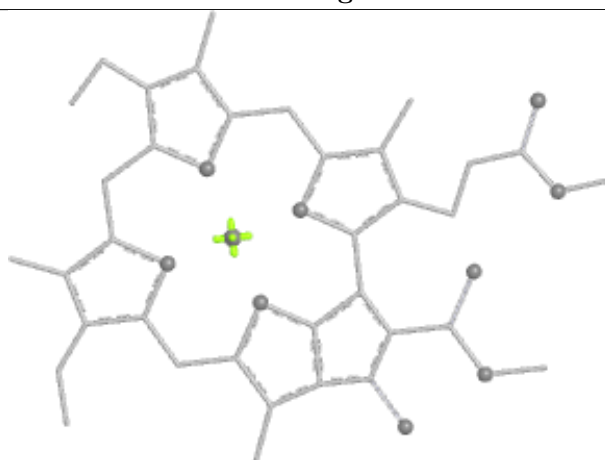
Bond lengths



Bond angles

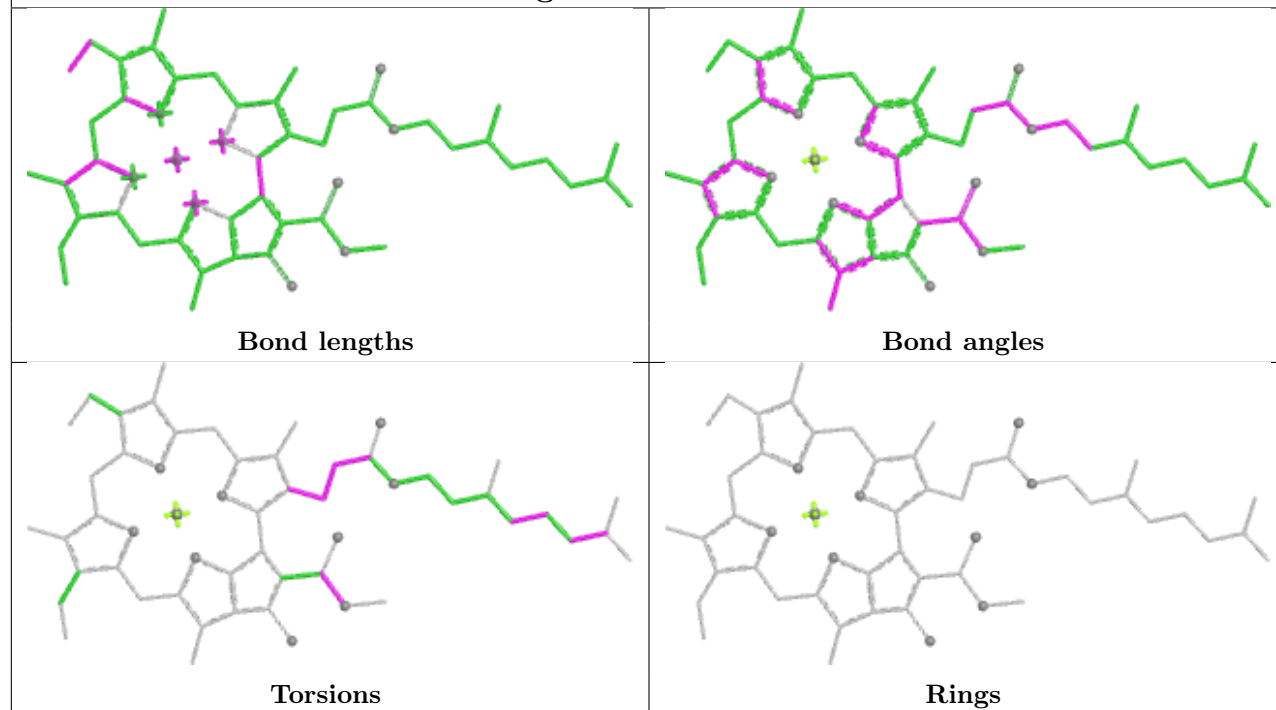


Torsions

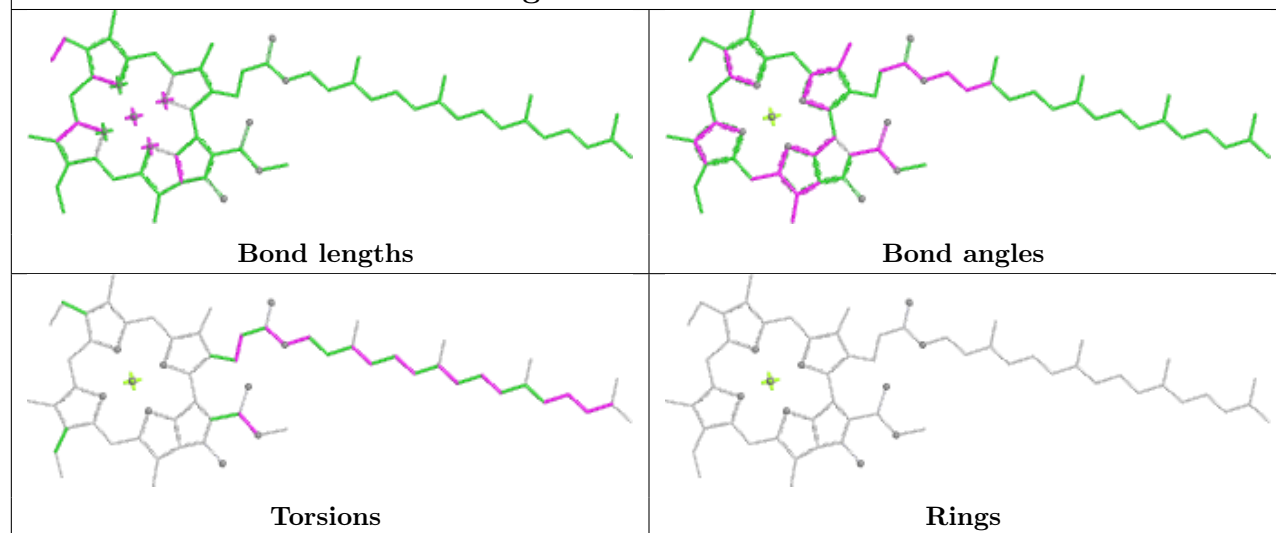


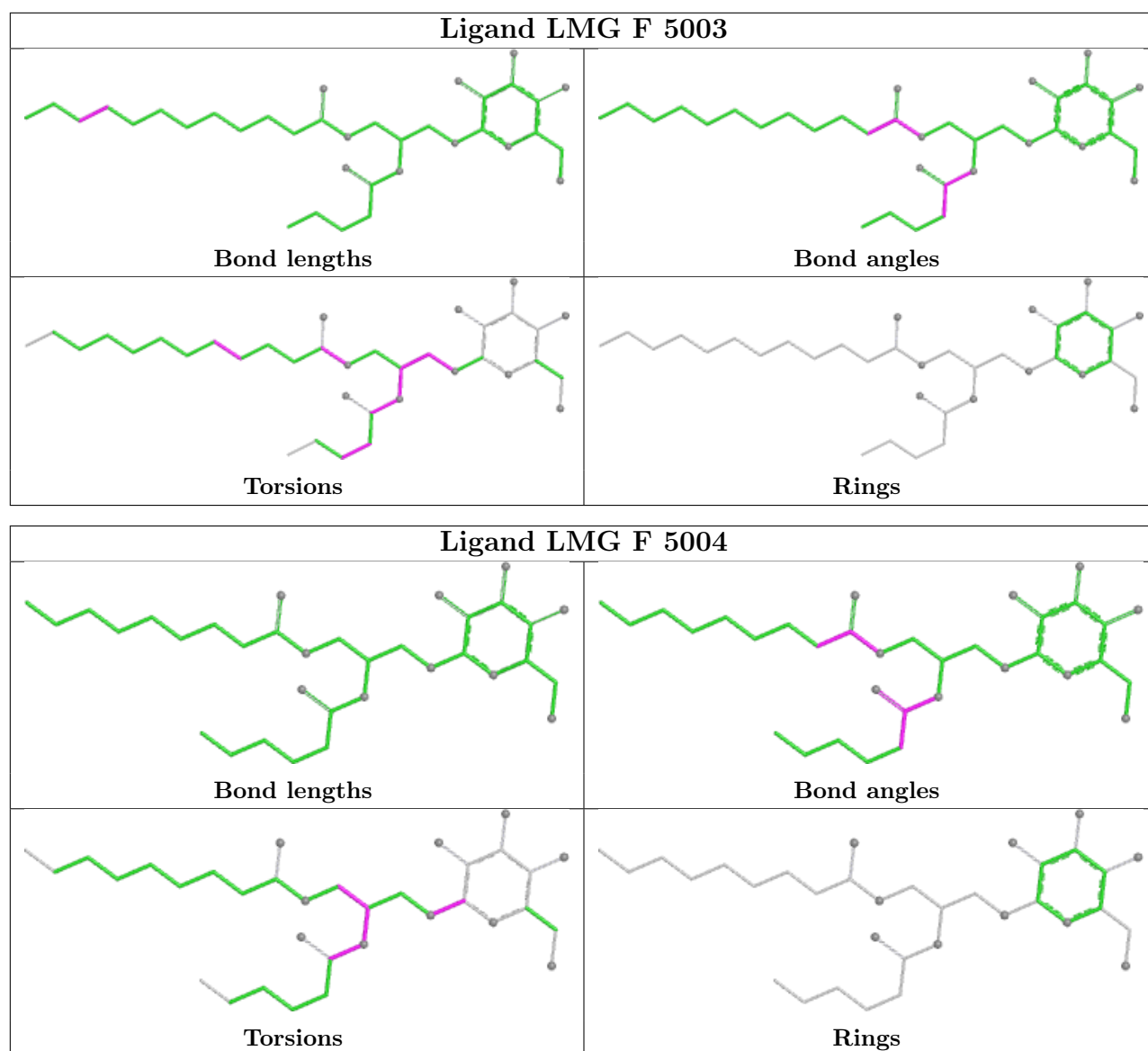
Rings

Ligand CLA 3 601

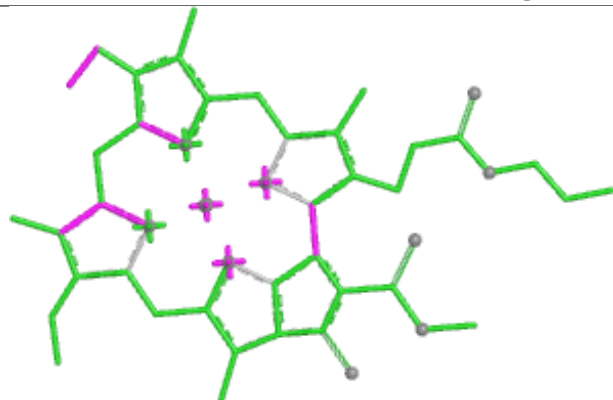


Ligand CLA A 1122

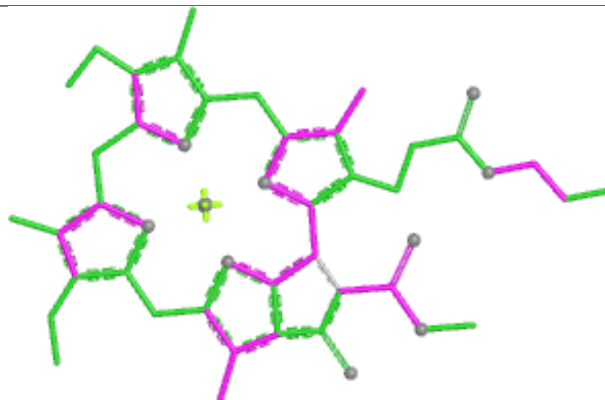




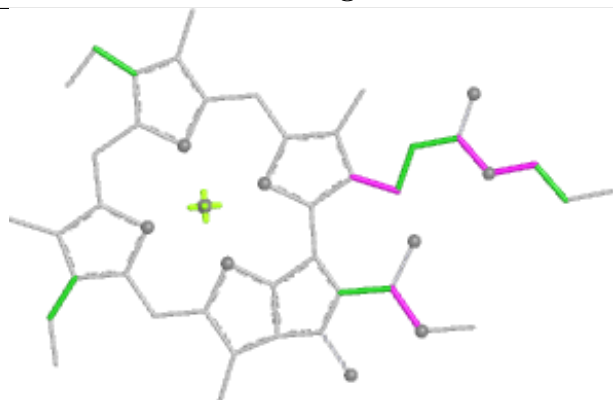
Ligand CLA 3 608



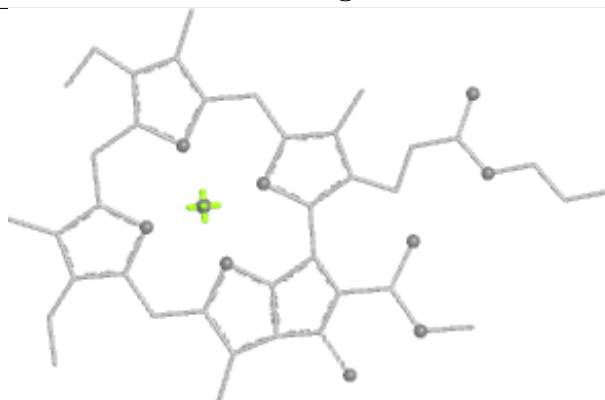
Bond lengths



Bond angles

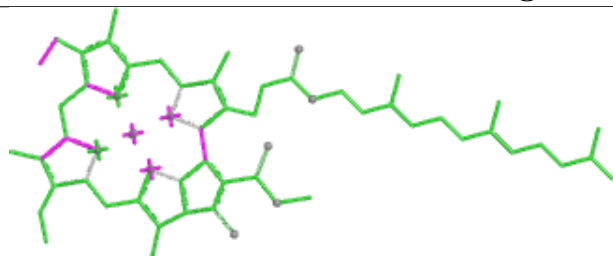


Torsions

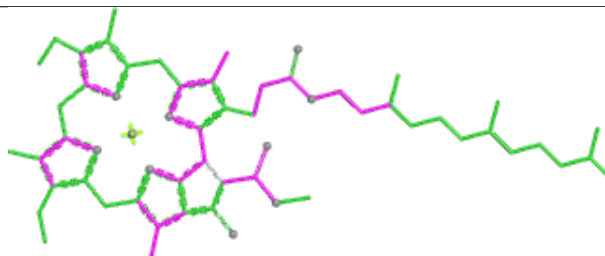


Rings

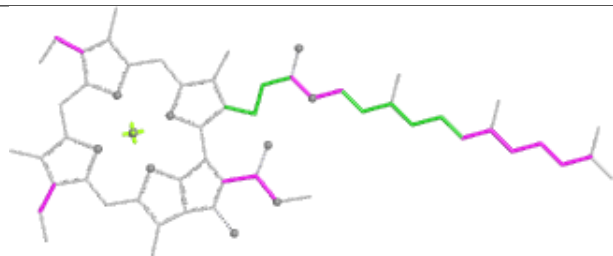
Ligand CLA 2 607



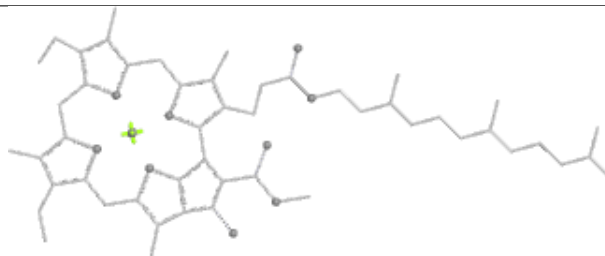
Bond lengths



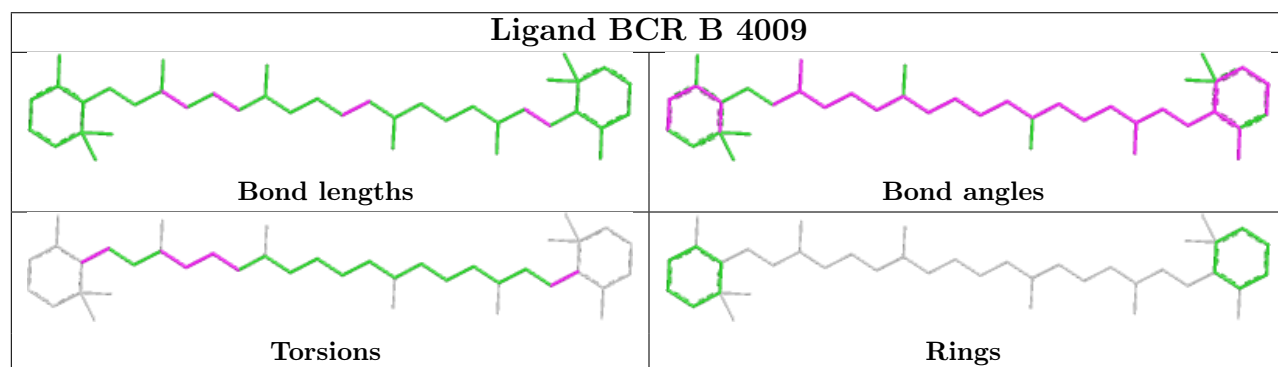
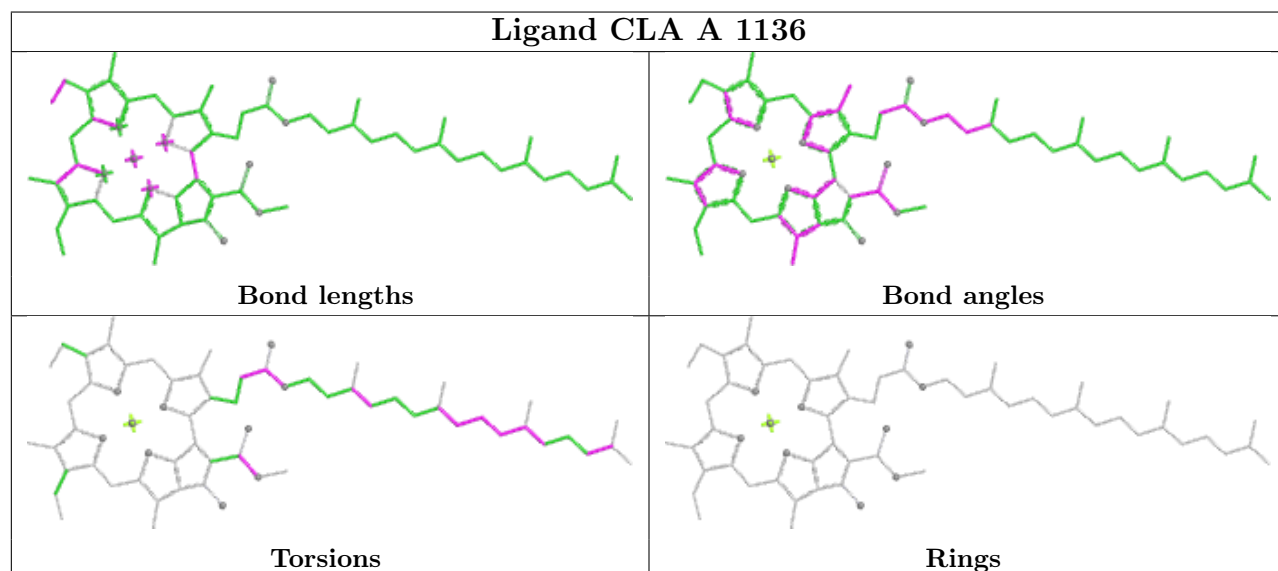
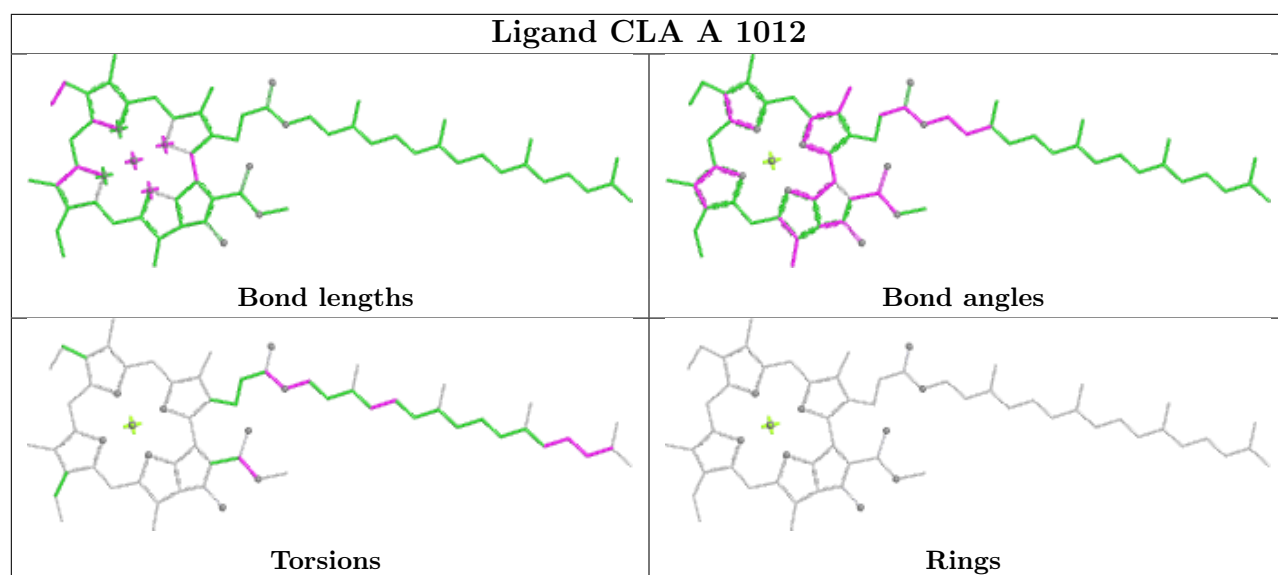
Bond angles

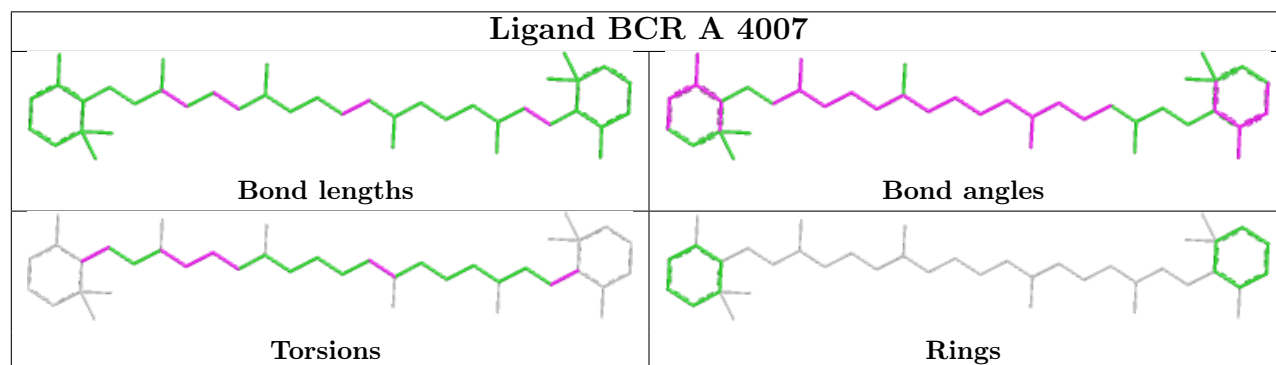
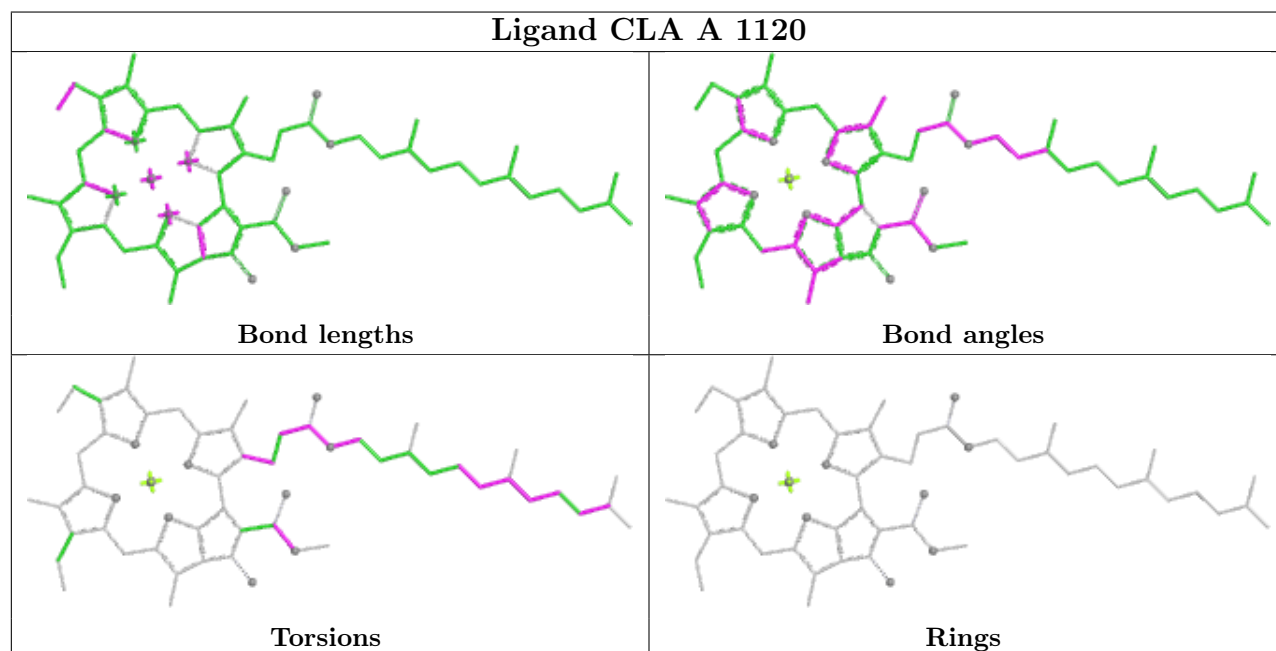
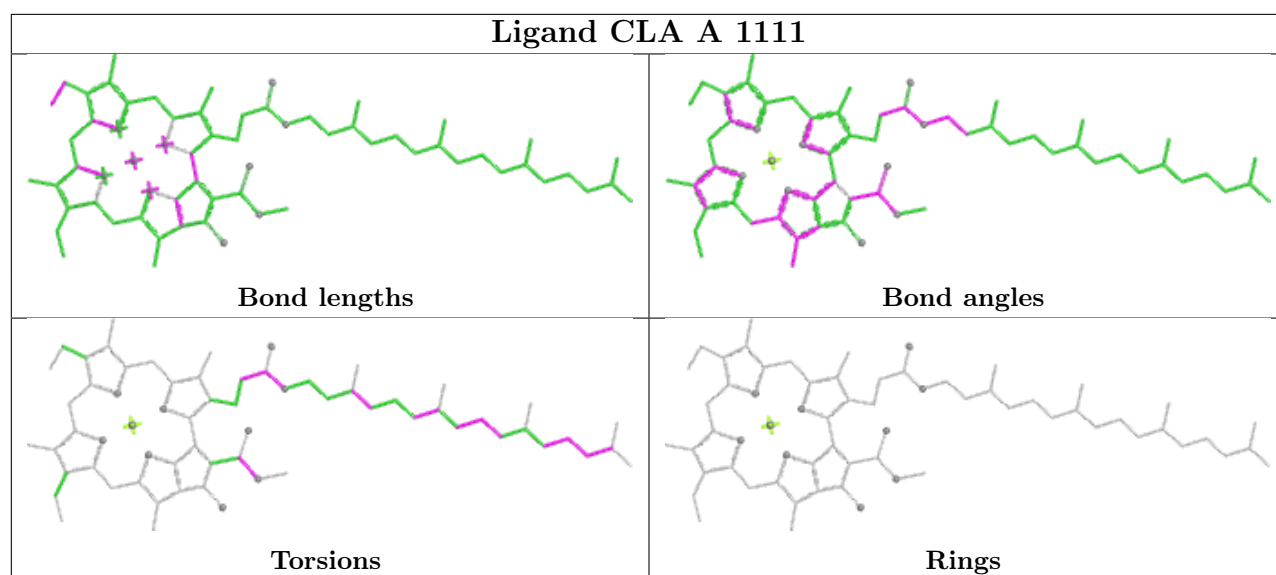


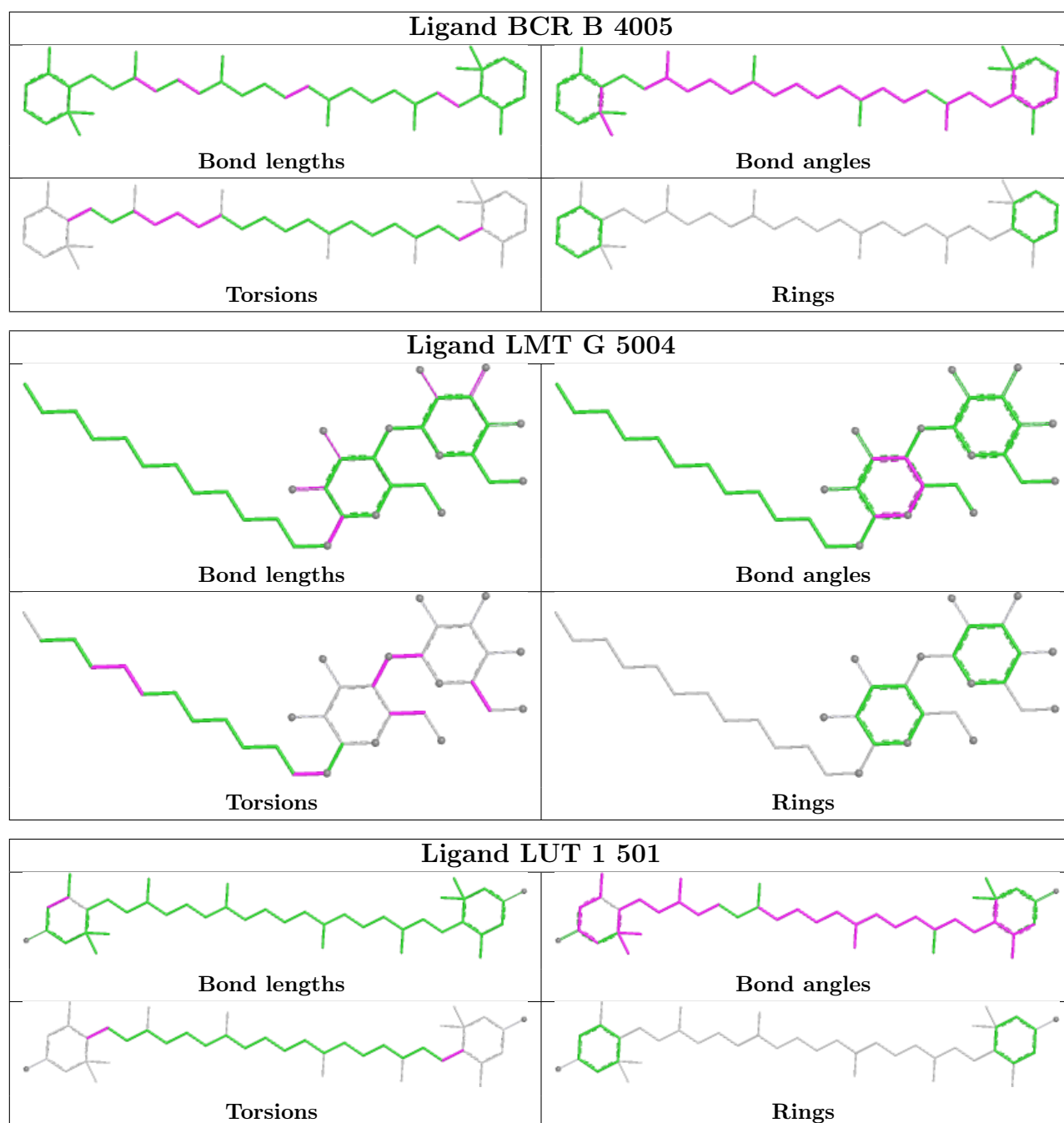
Torsions



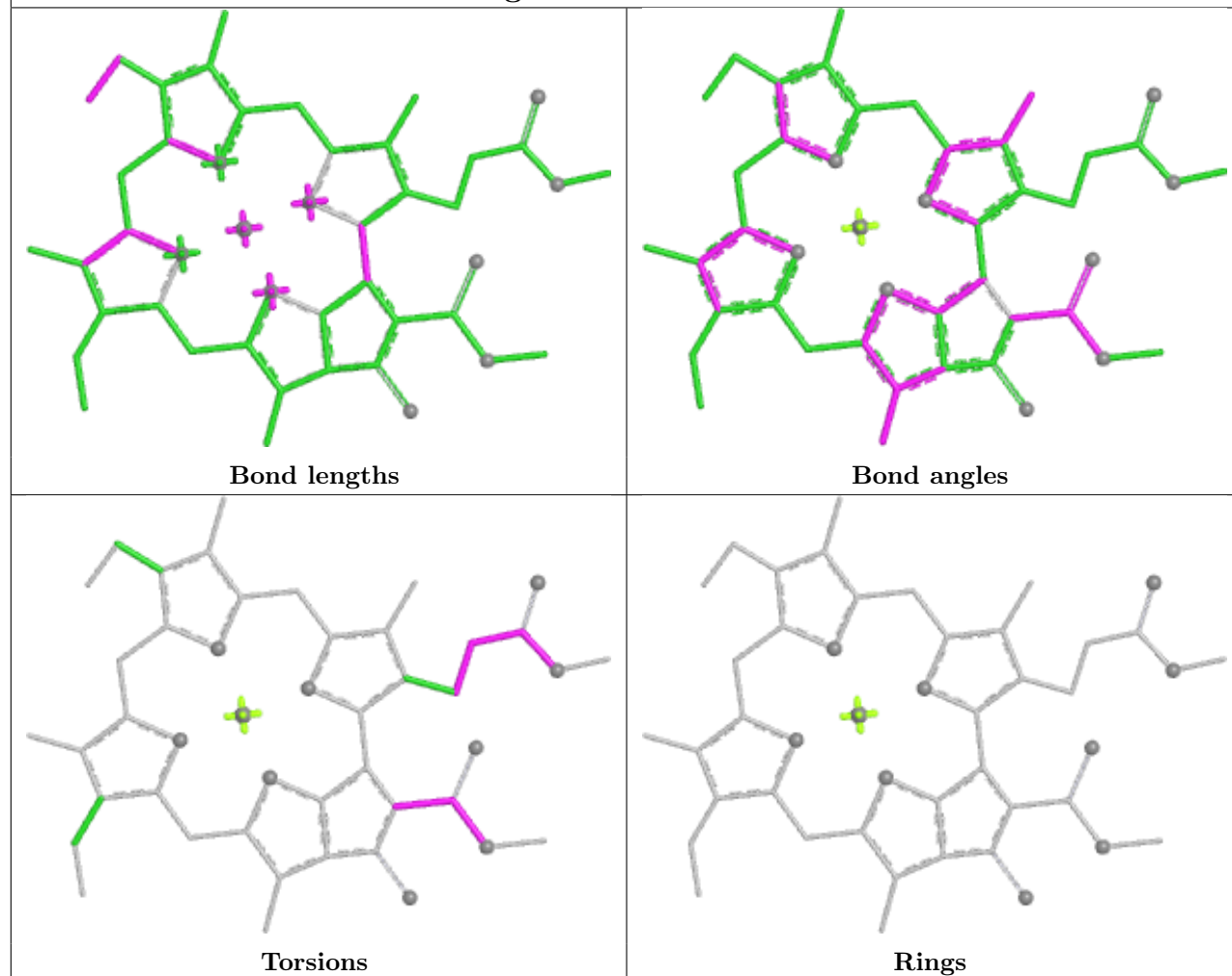
Rings

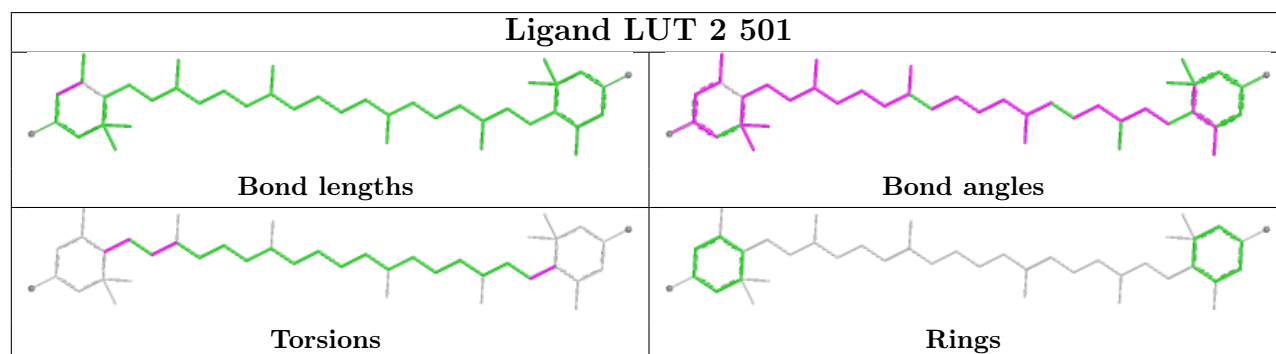
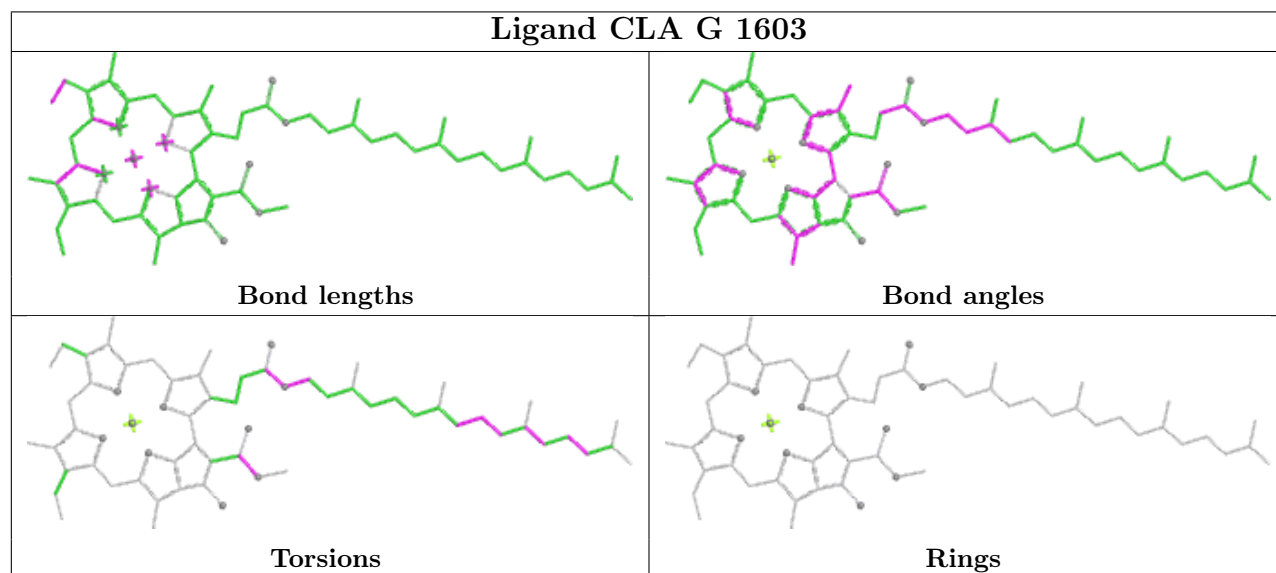
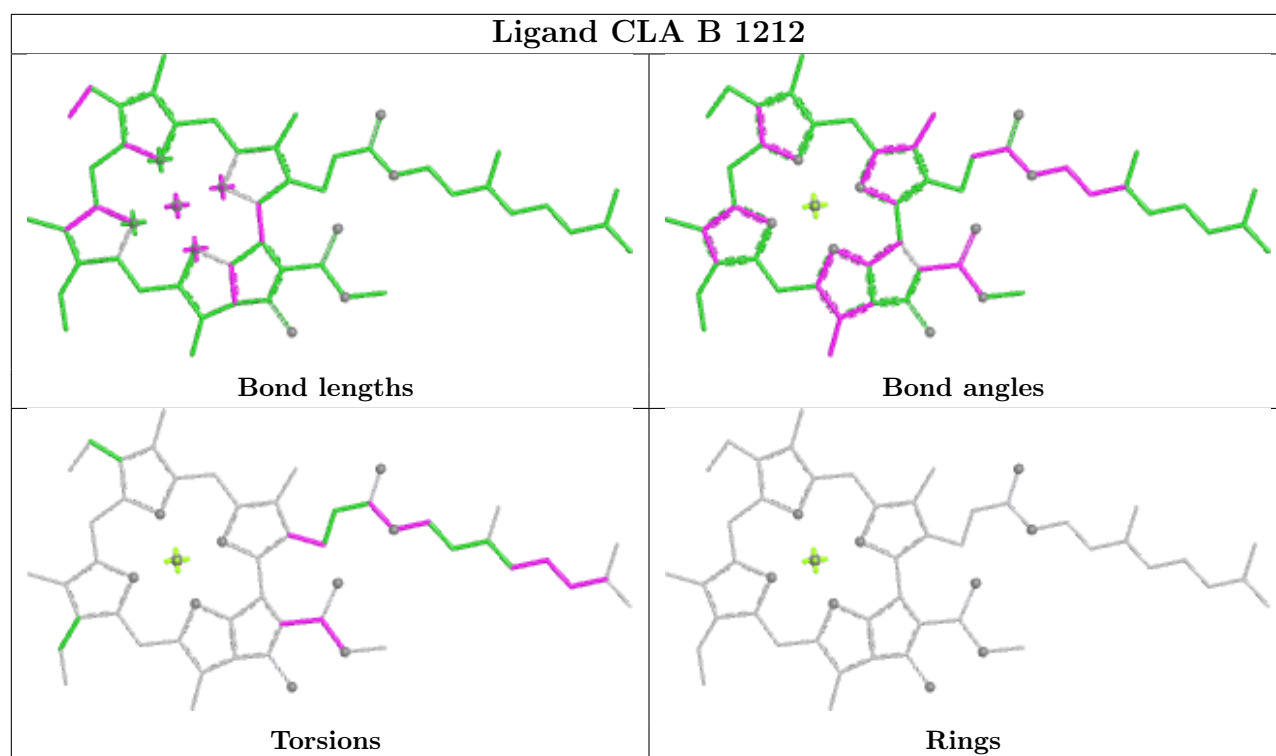




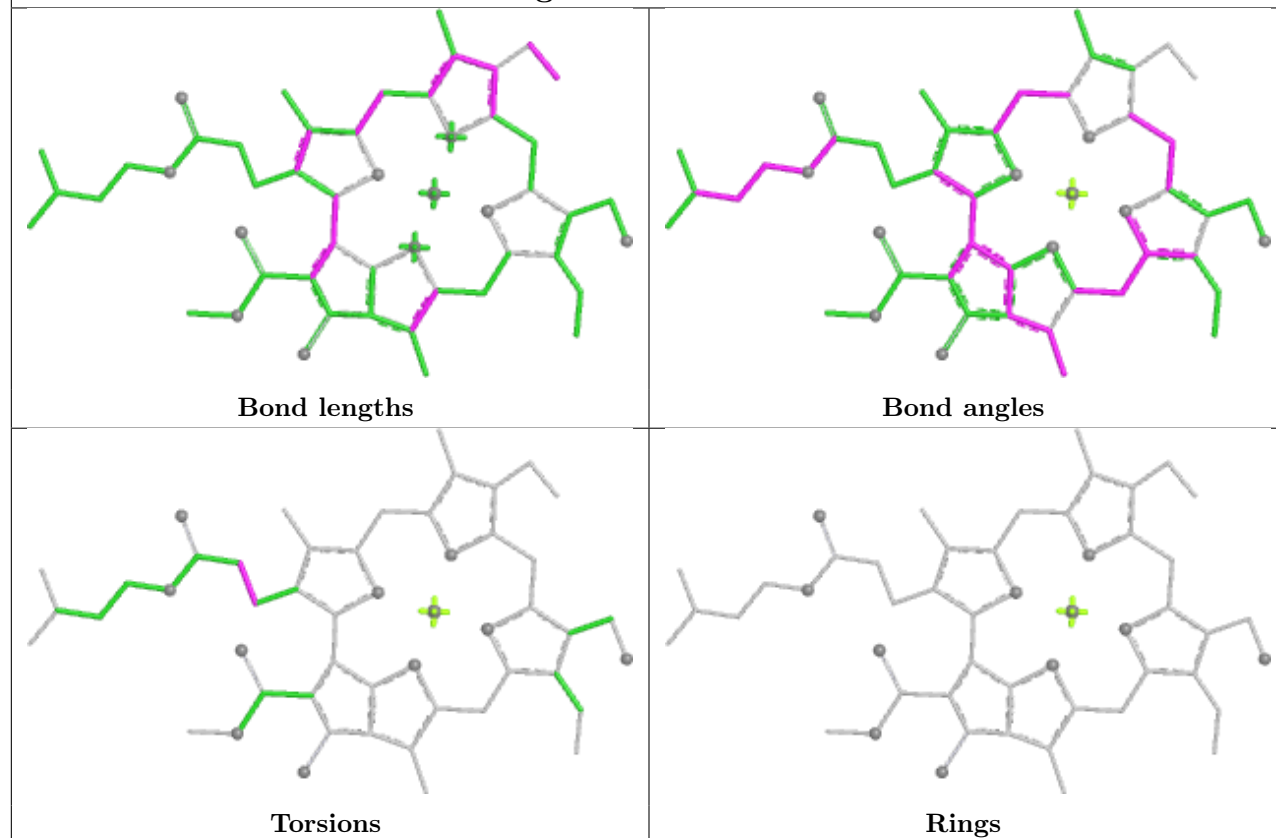


Ligand CLA A 1114

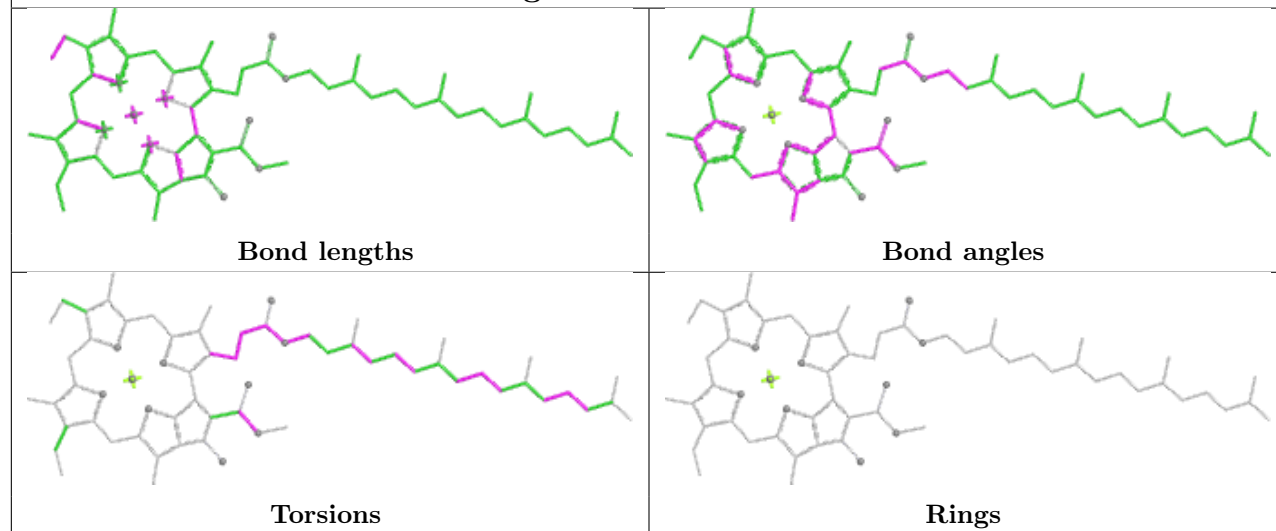


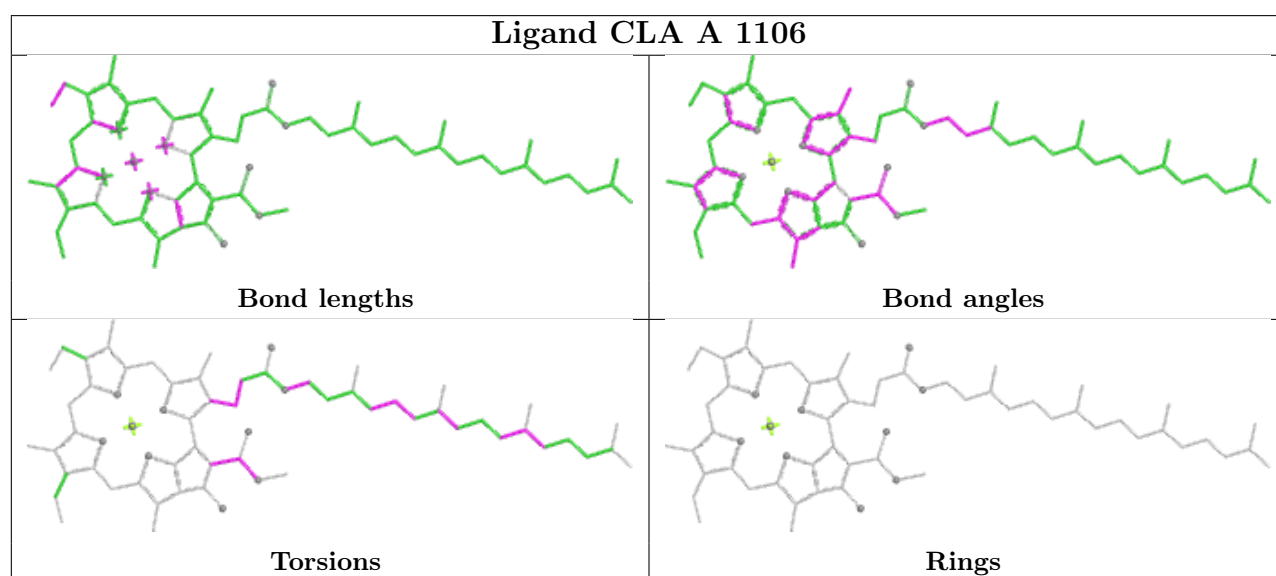
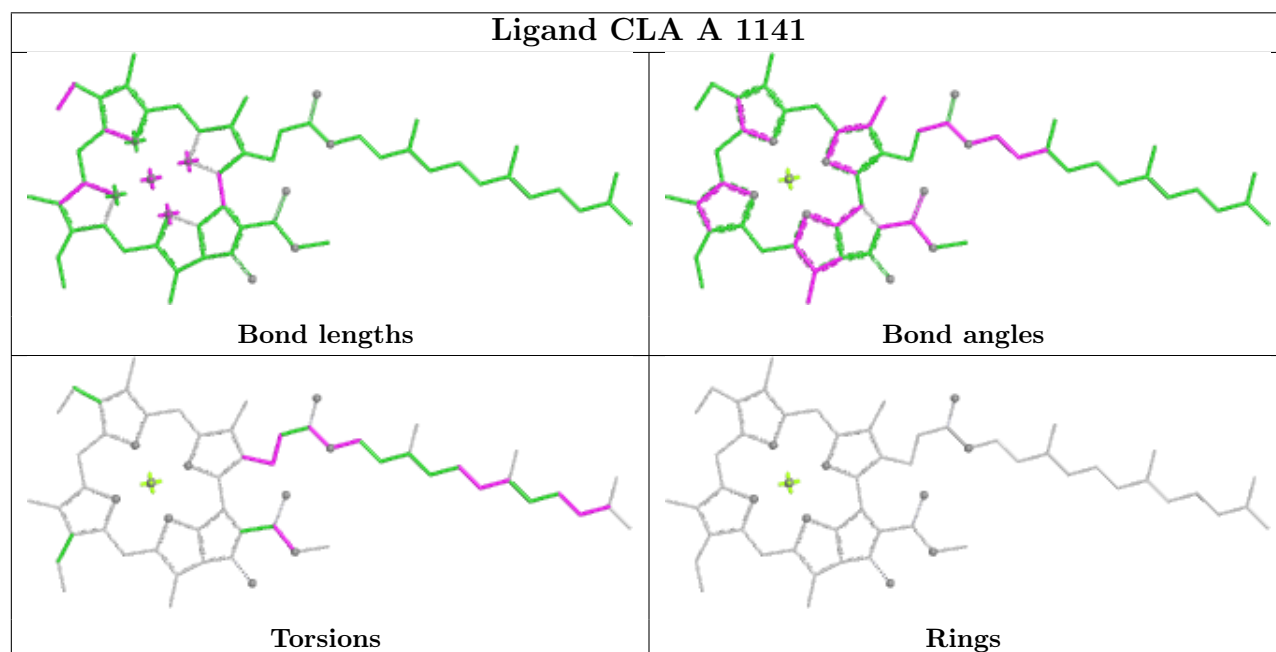
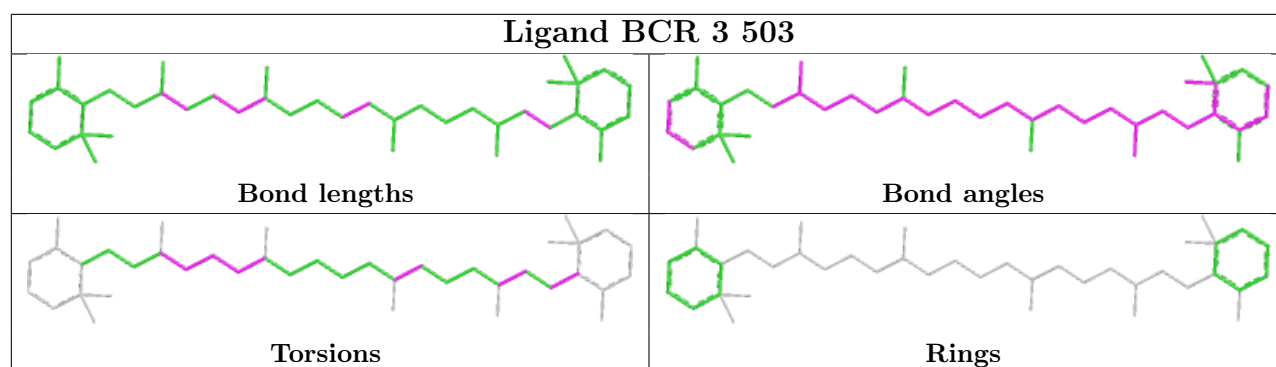


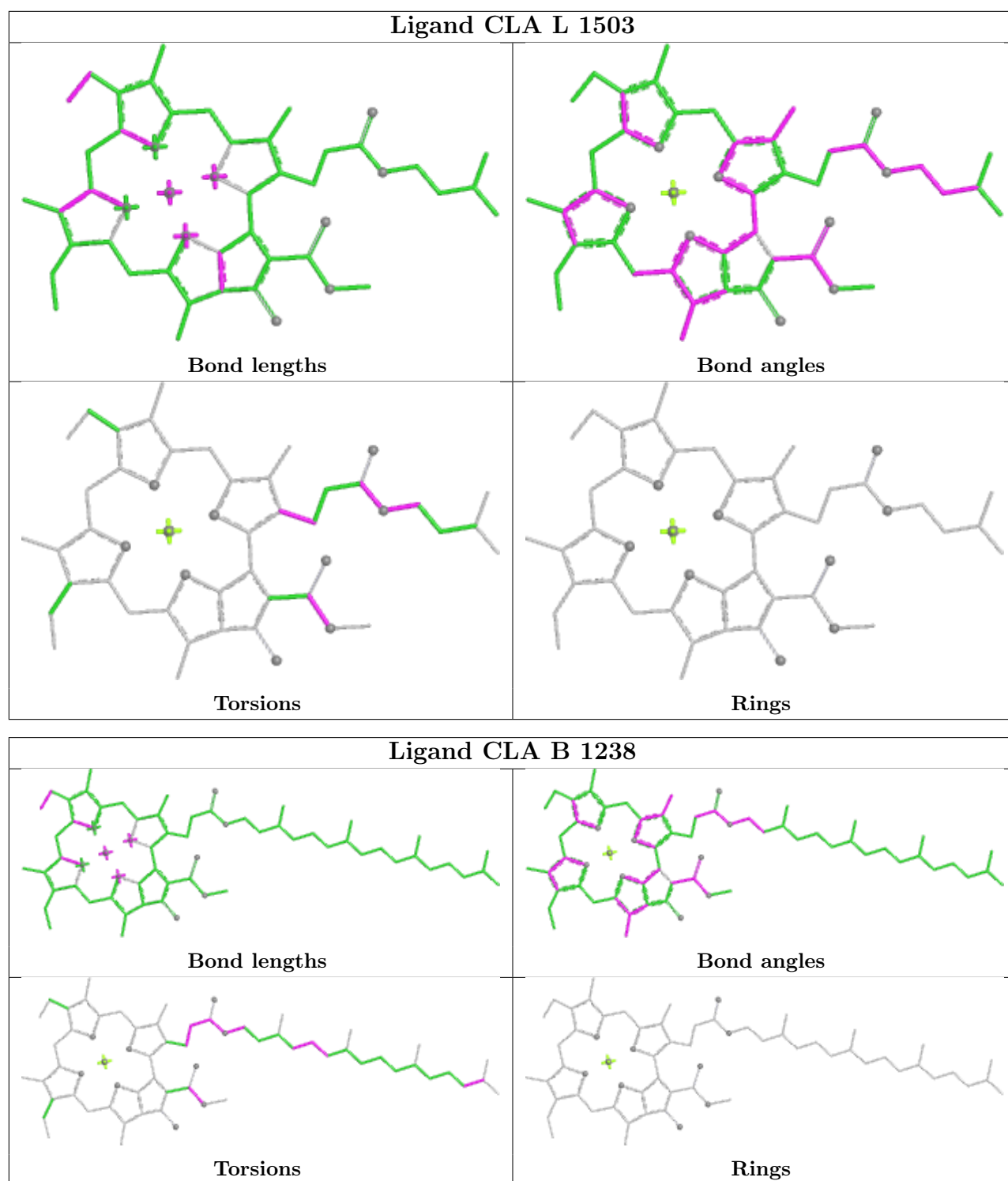
Ligand CHL 4 611

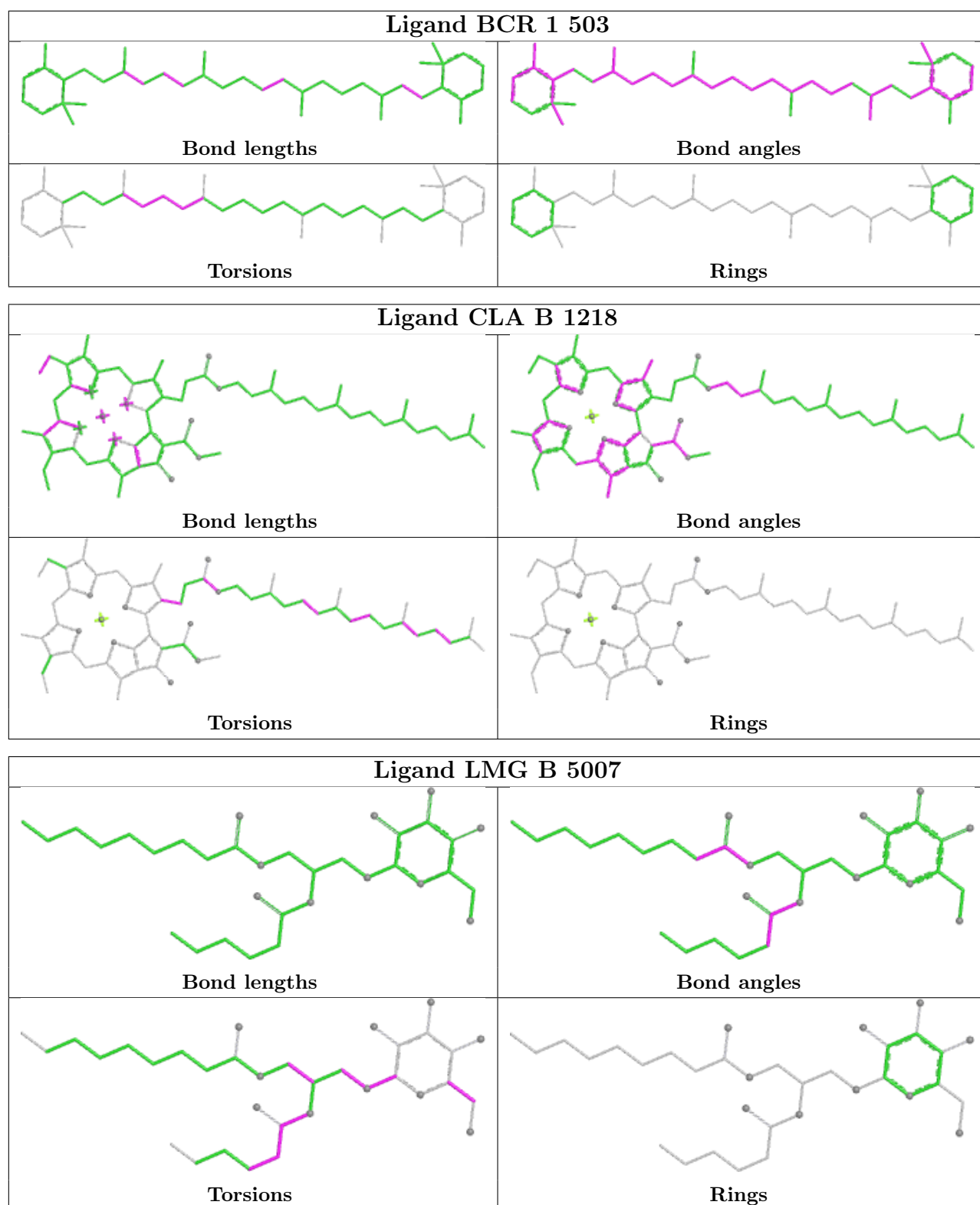


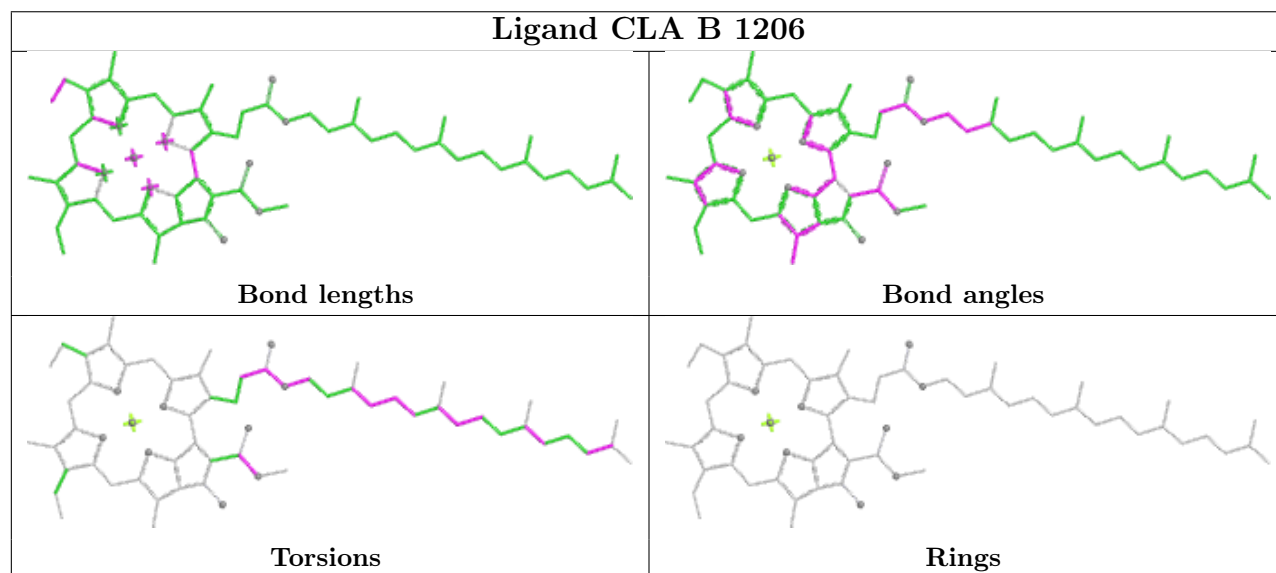
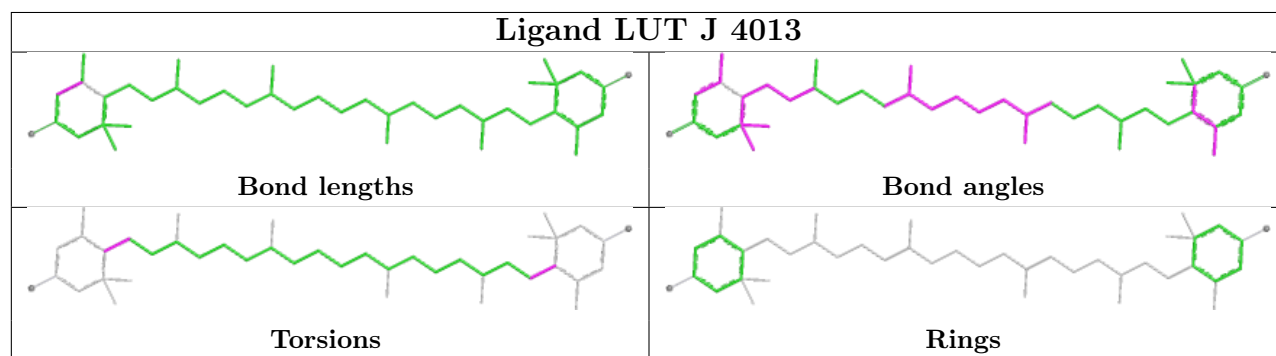
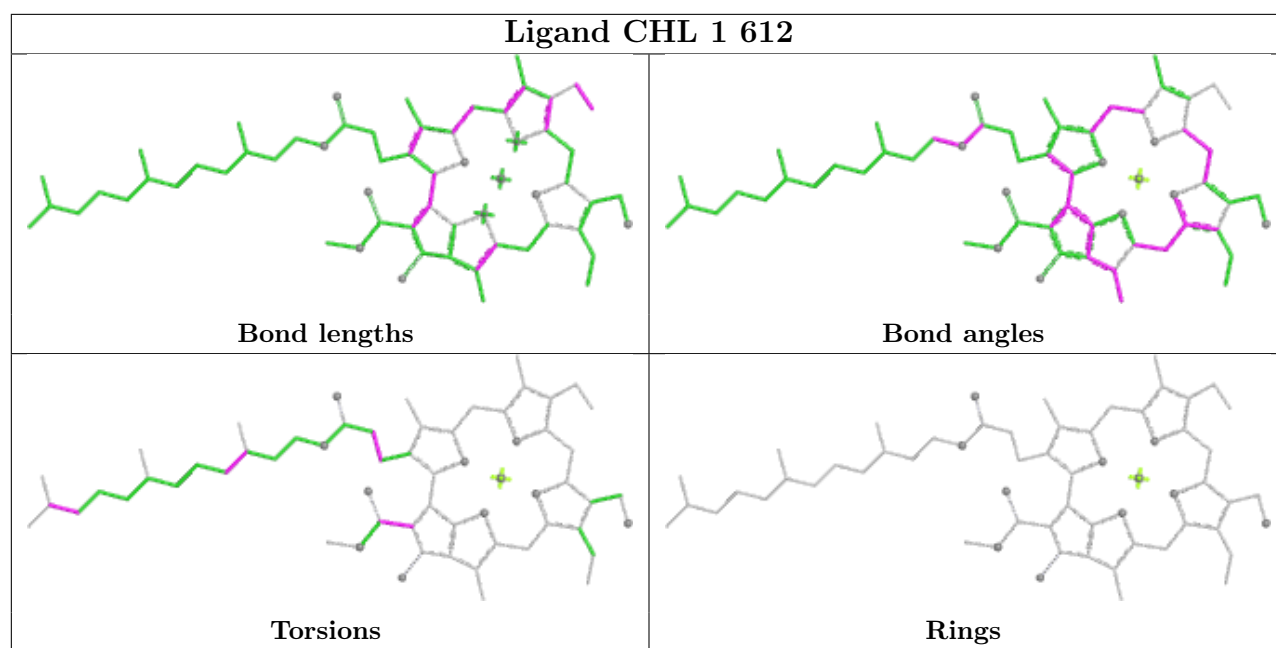
Ligand CLA B 1224

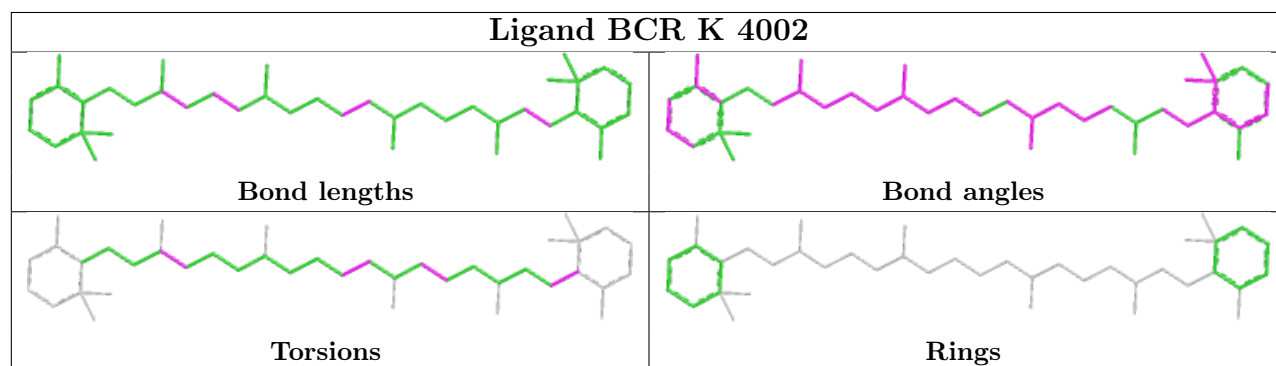
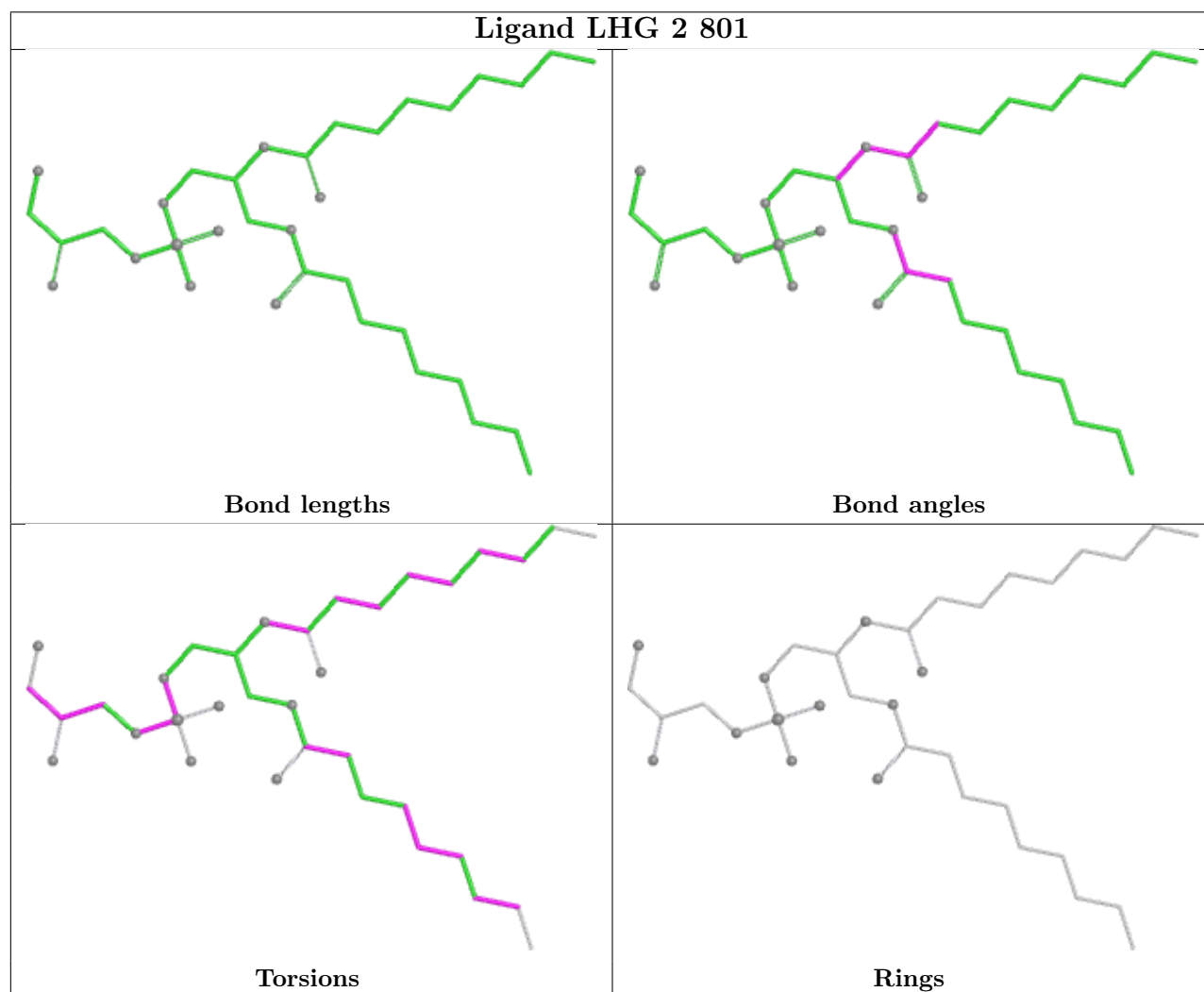
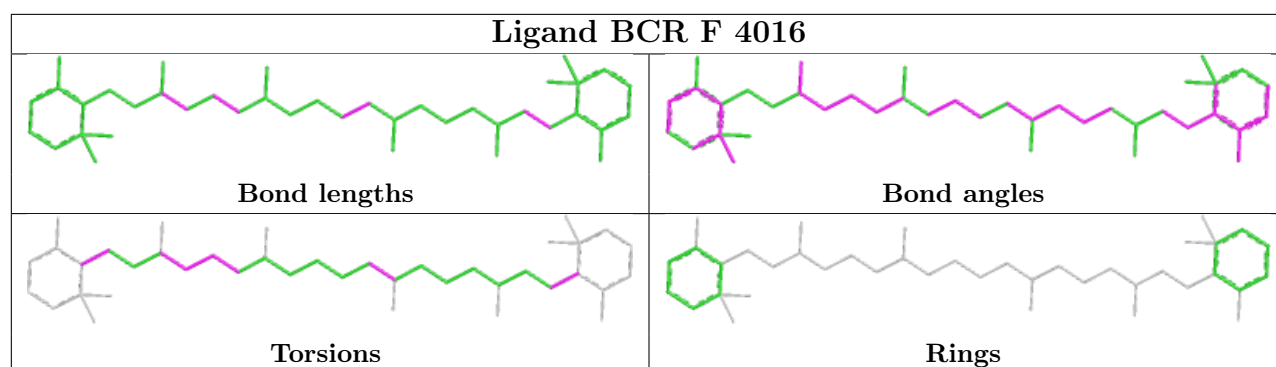


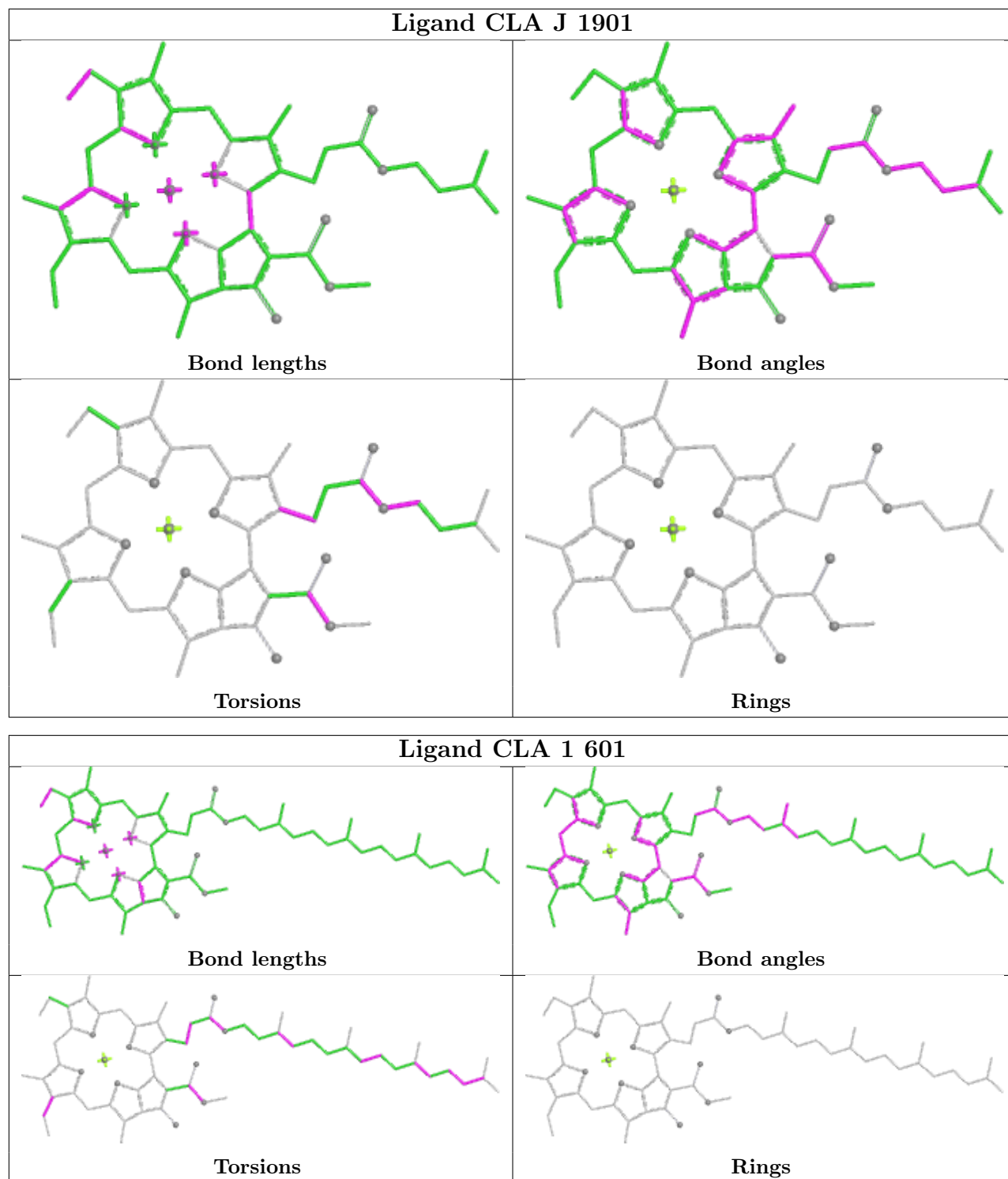


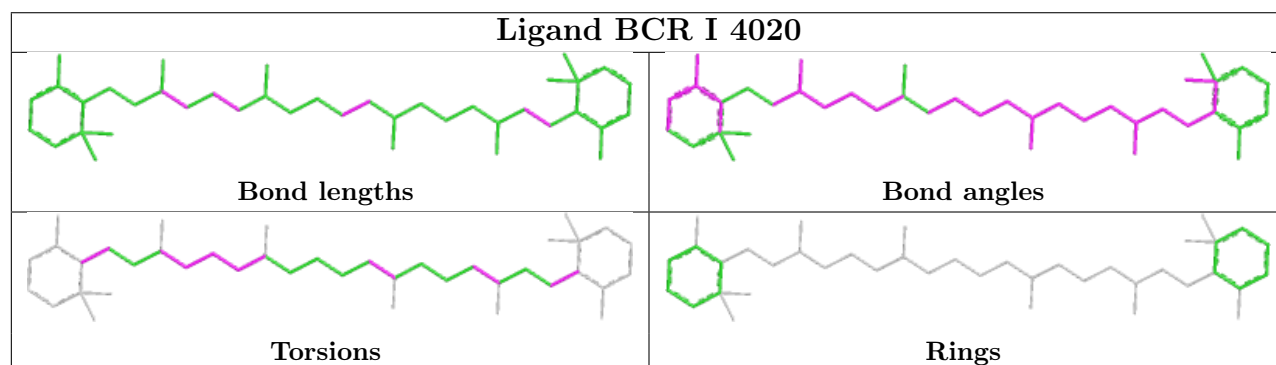
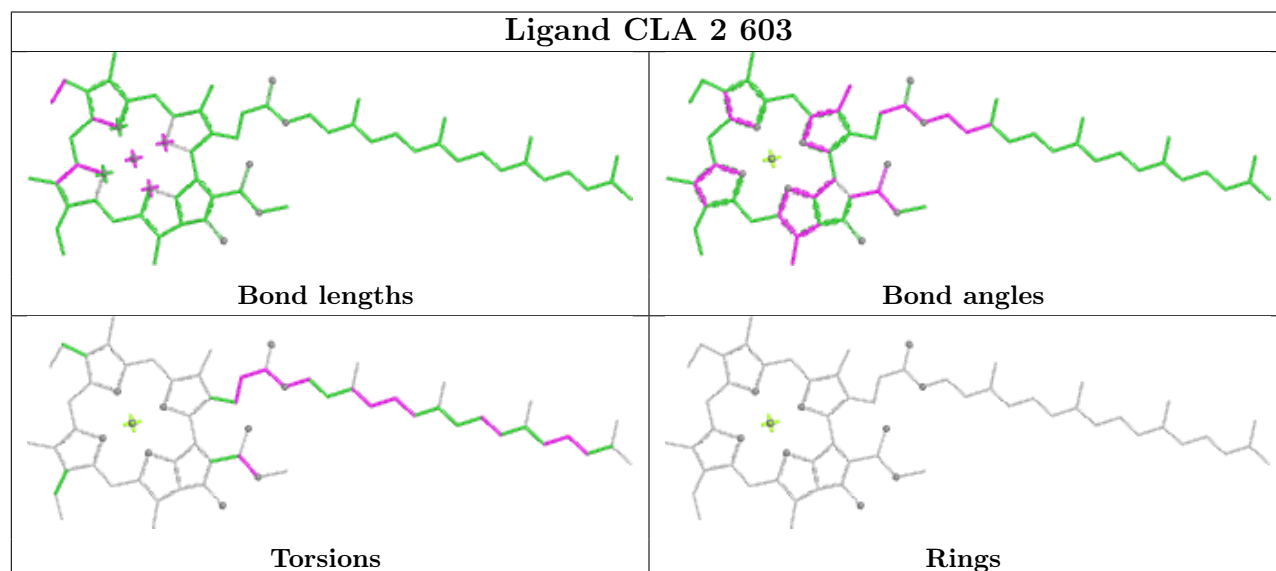
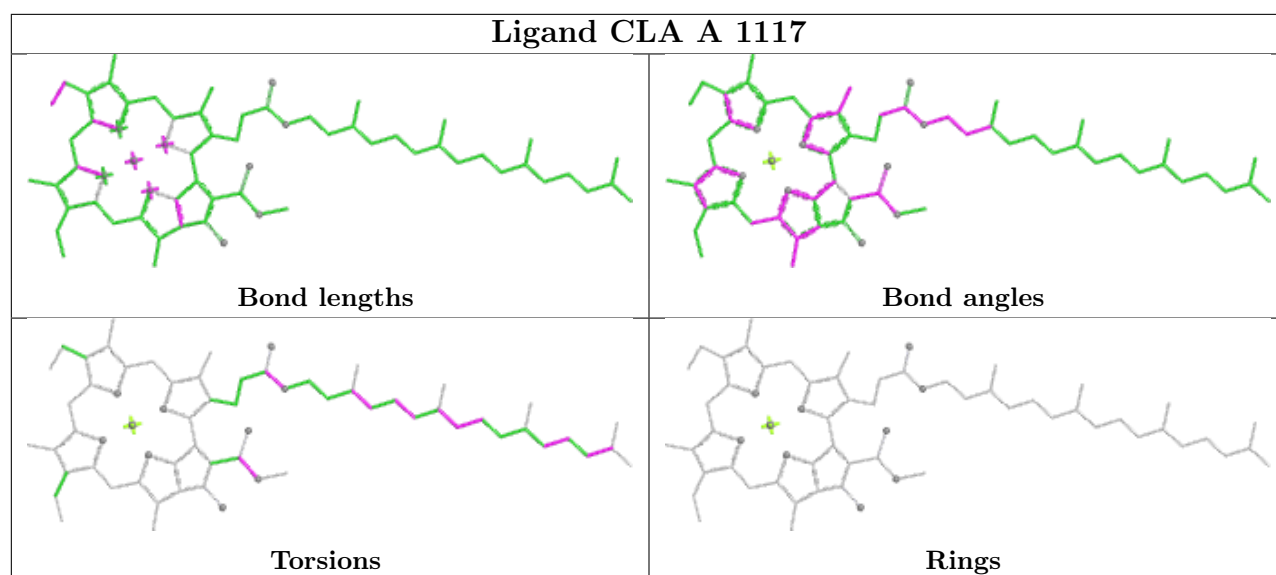


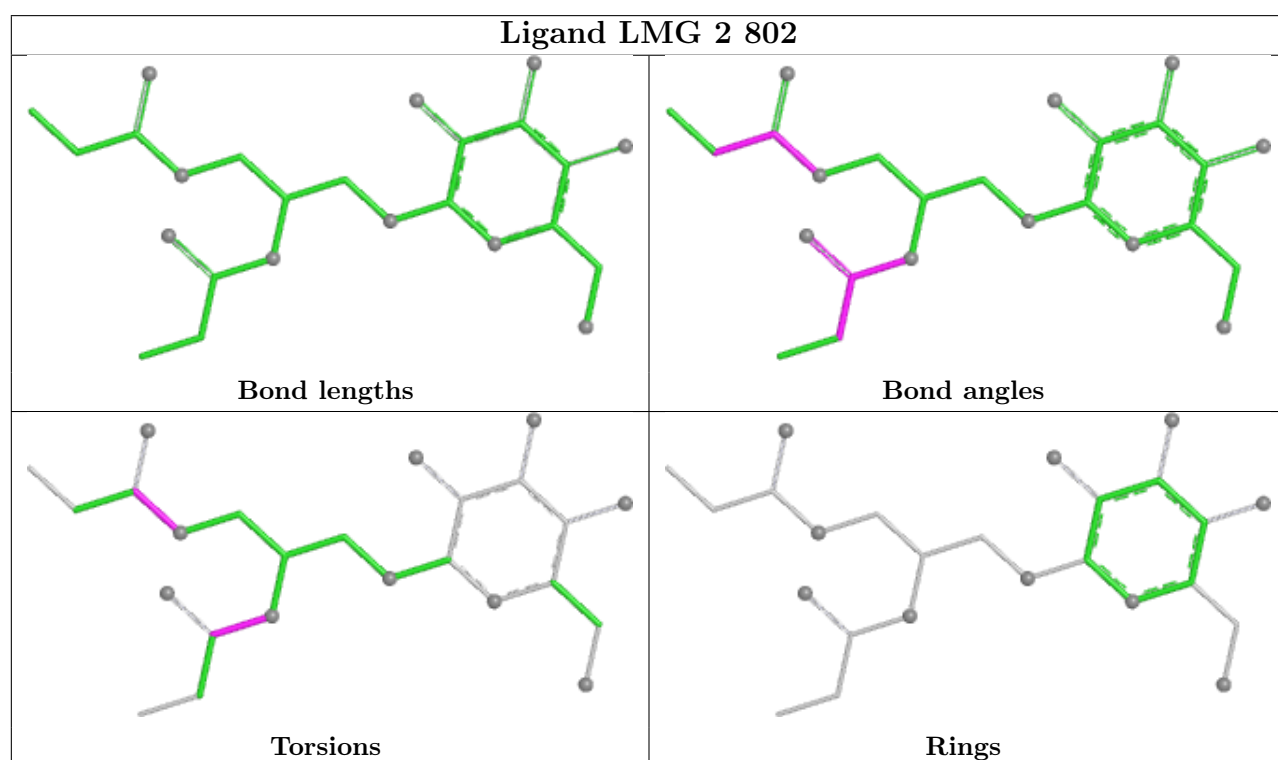
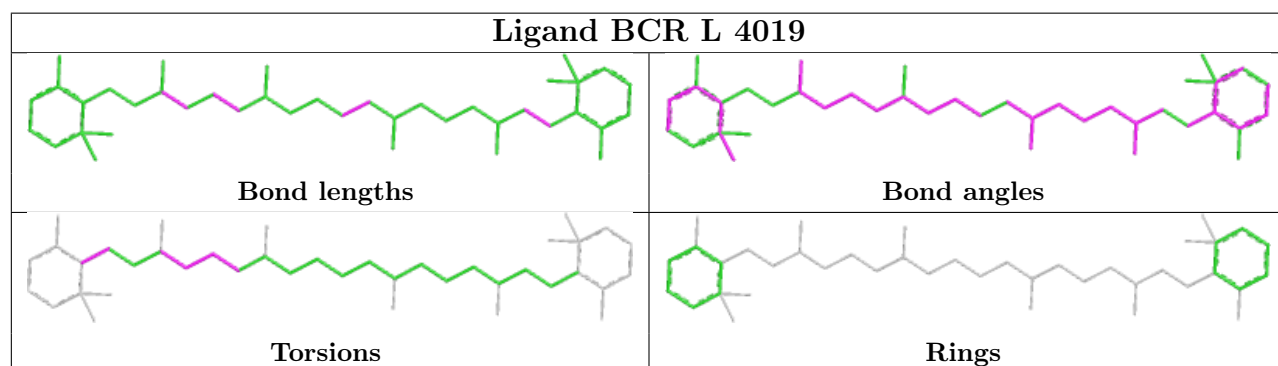
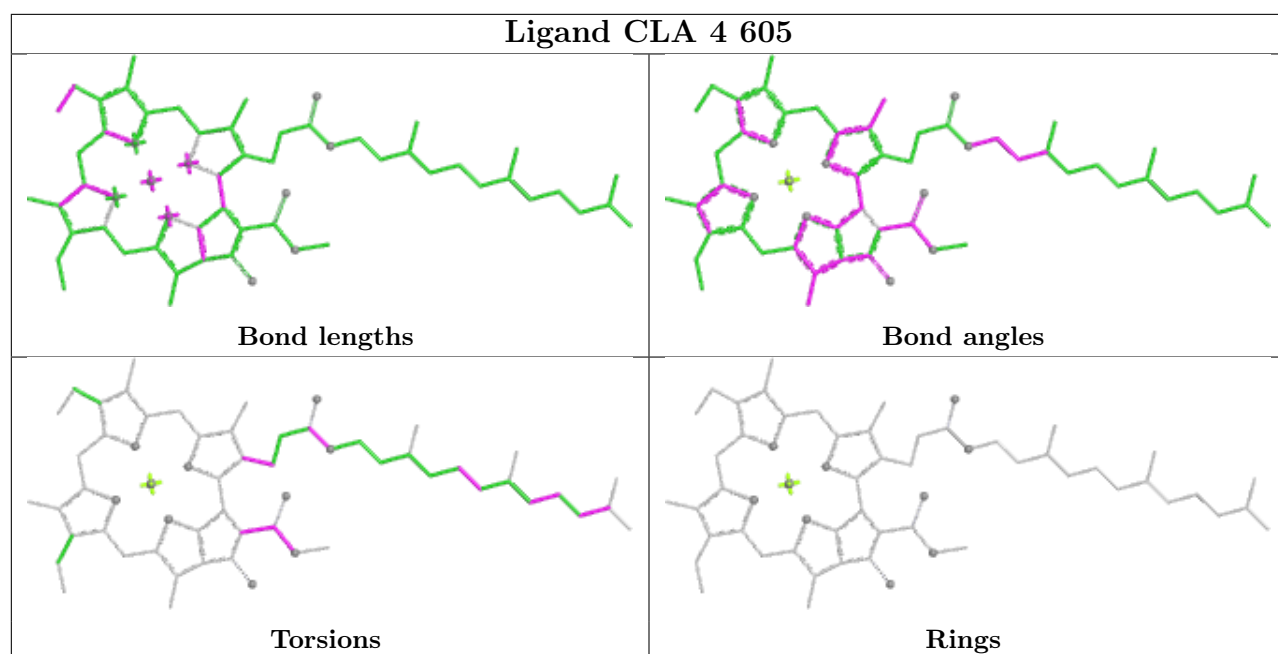




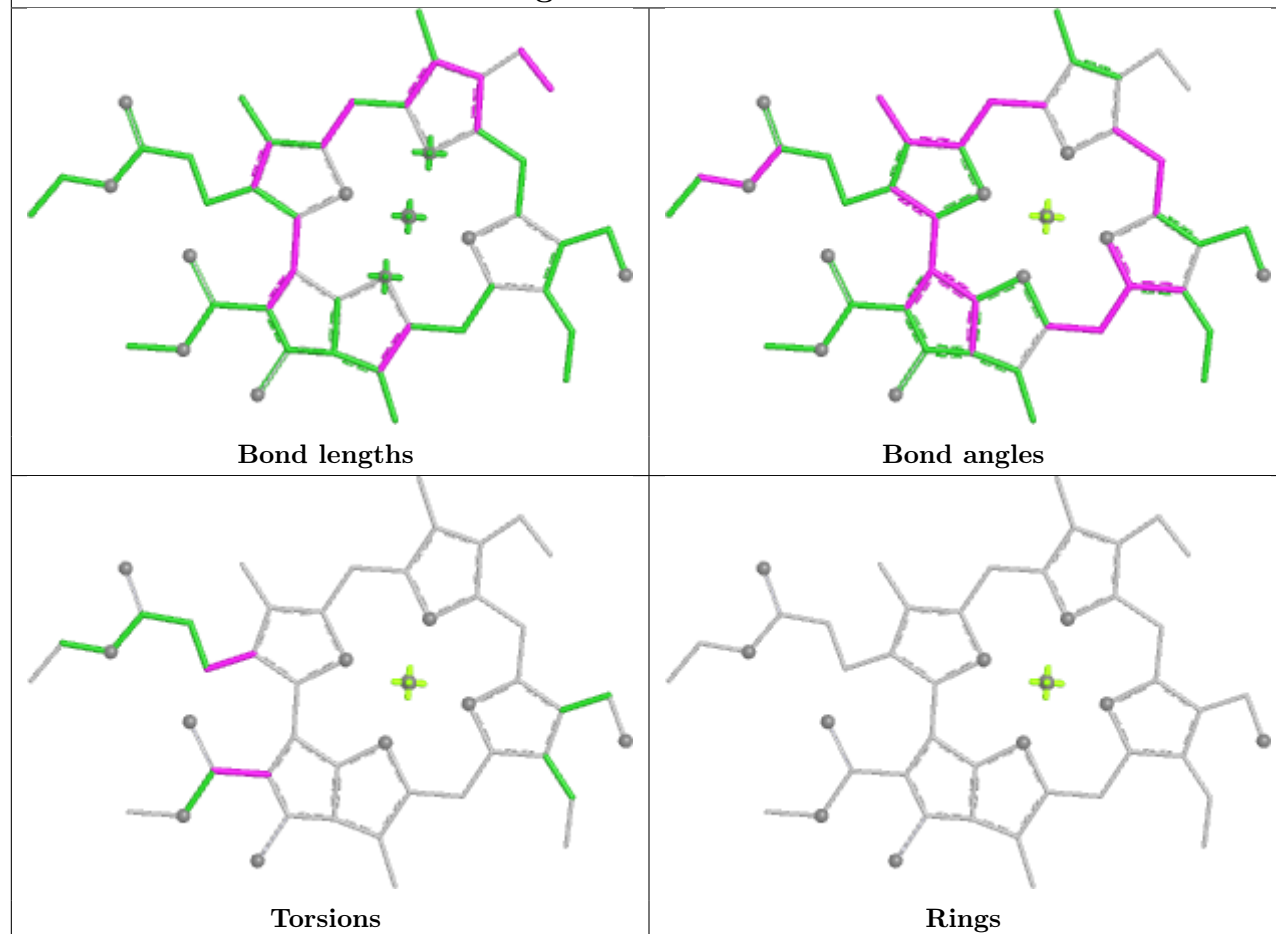




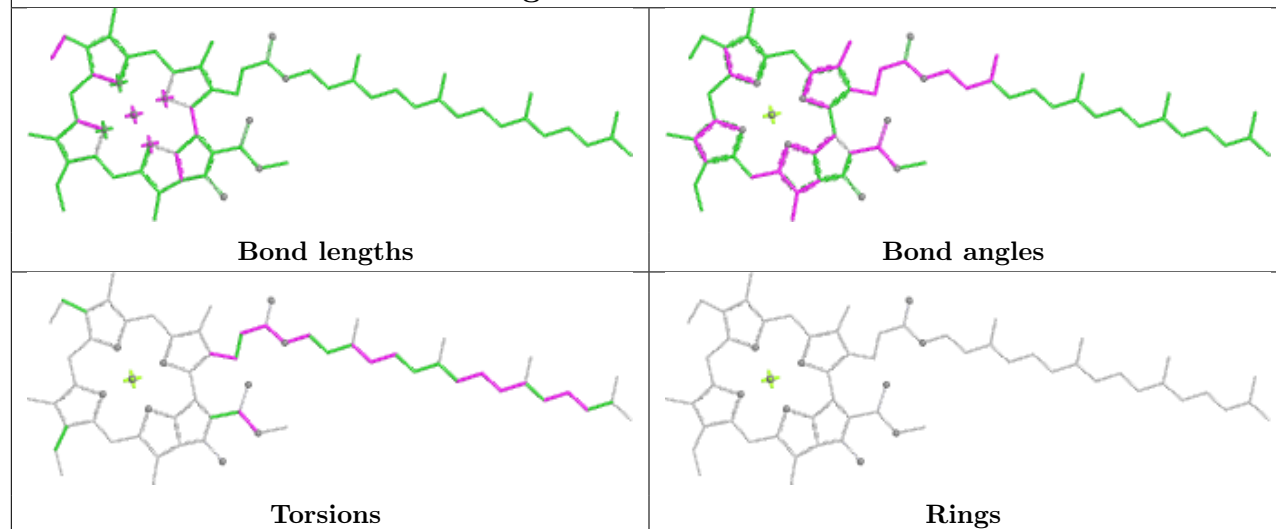




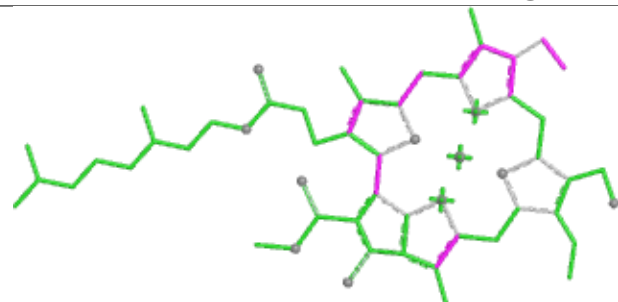
Ligand CHL 2 611



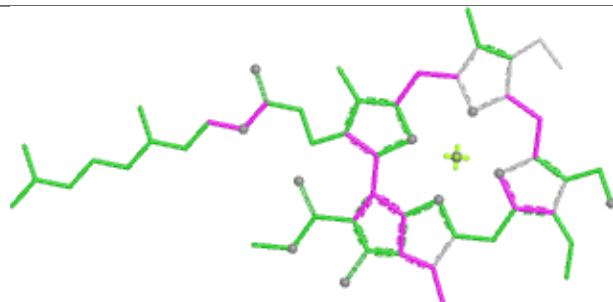
Ligand CLA A 1109



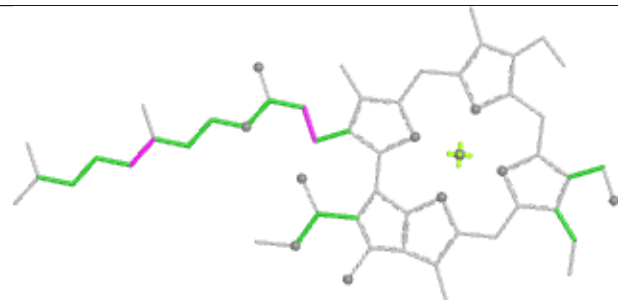
Ligand CHL 1 609



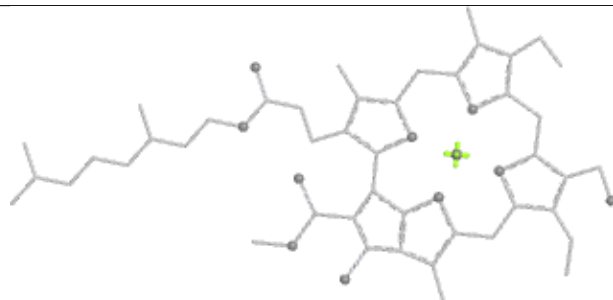
Bond lengths



Bond angles

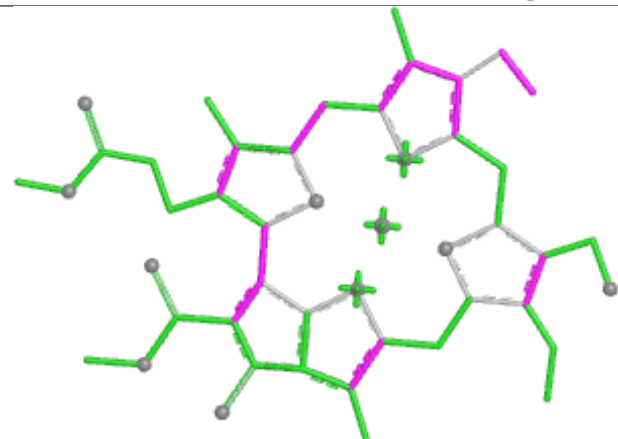


Torsions

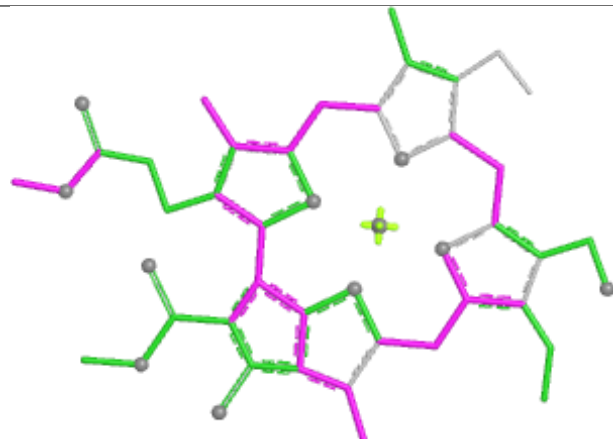


Rings

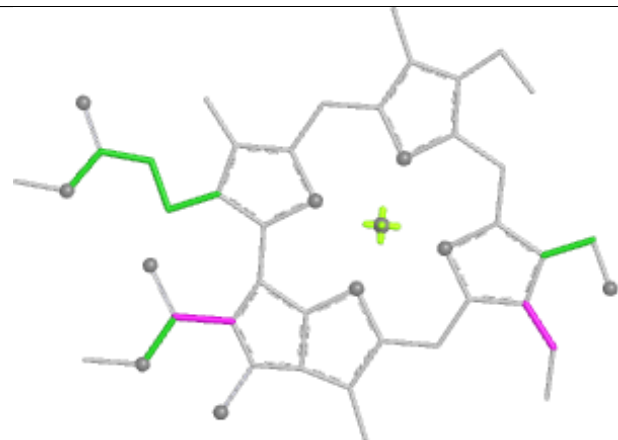
Ligand CHL 4 610



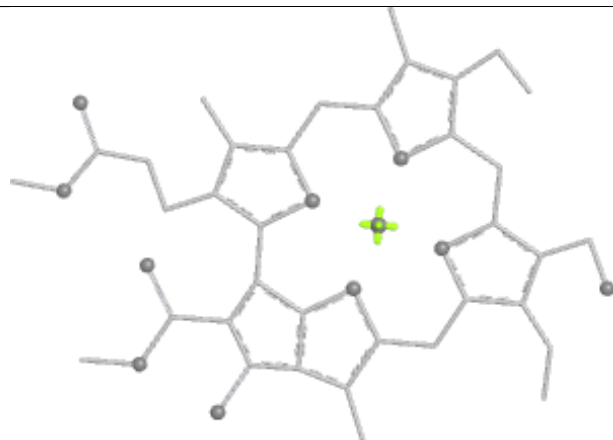
Bond lengths



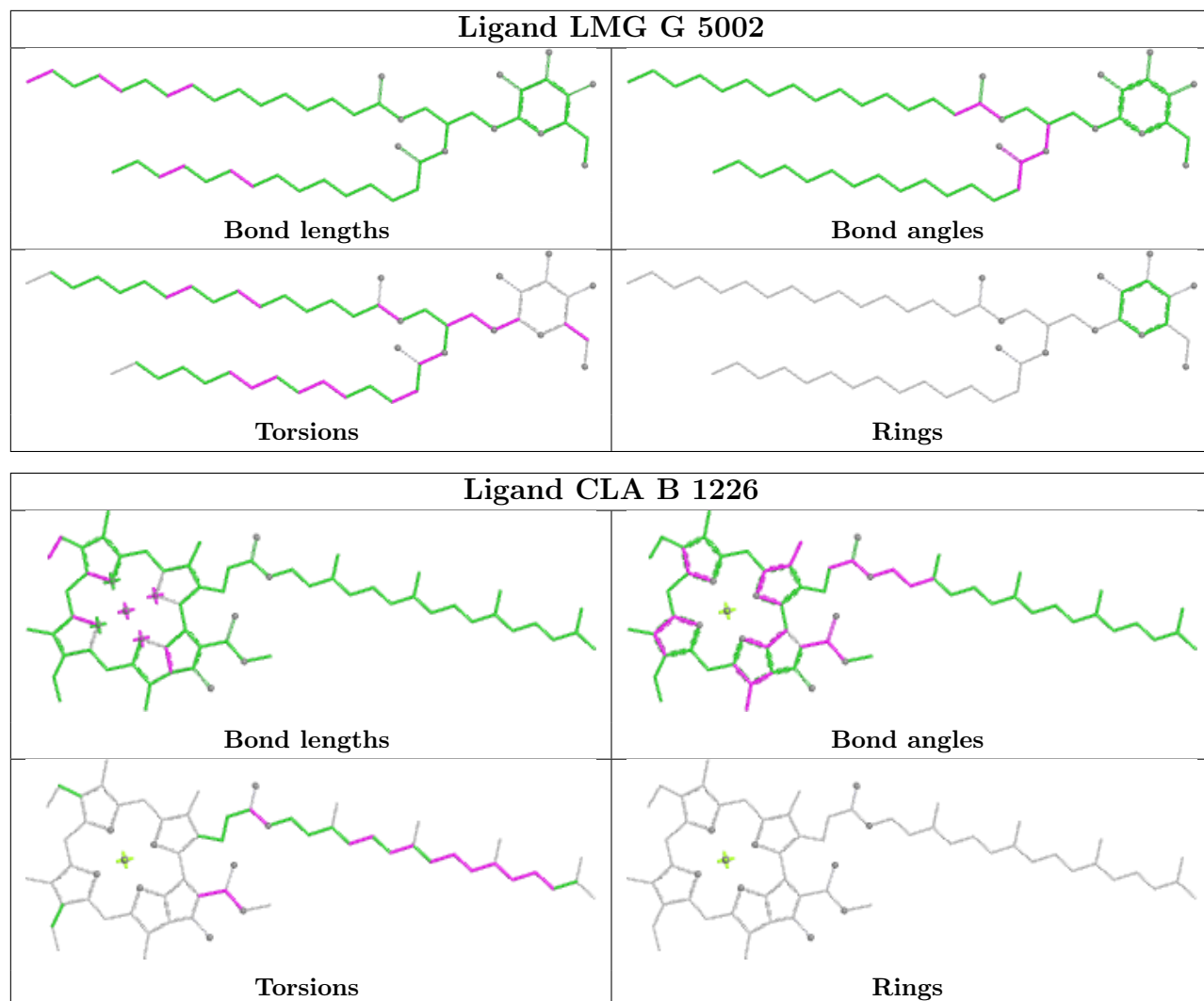
Bond angles



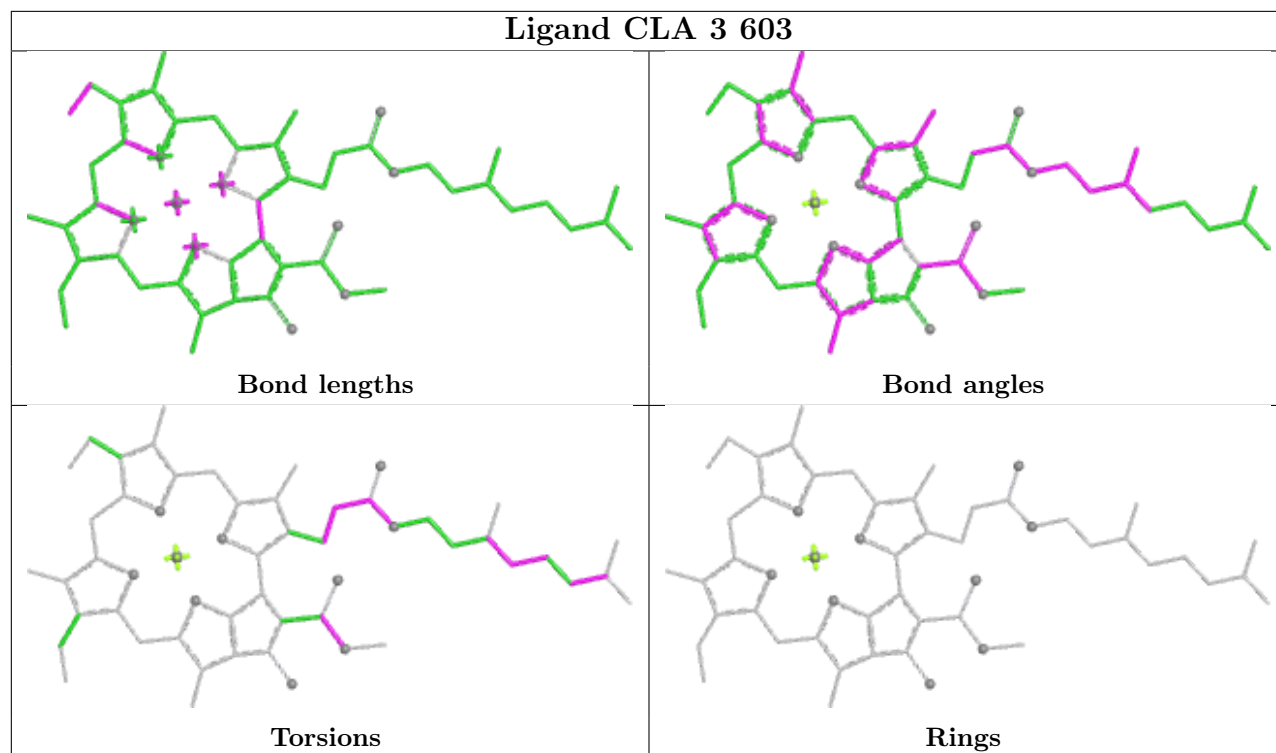
Torsions



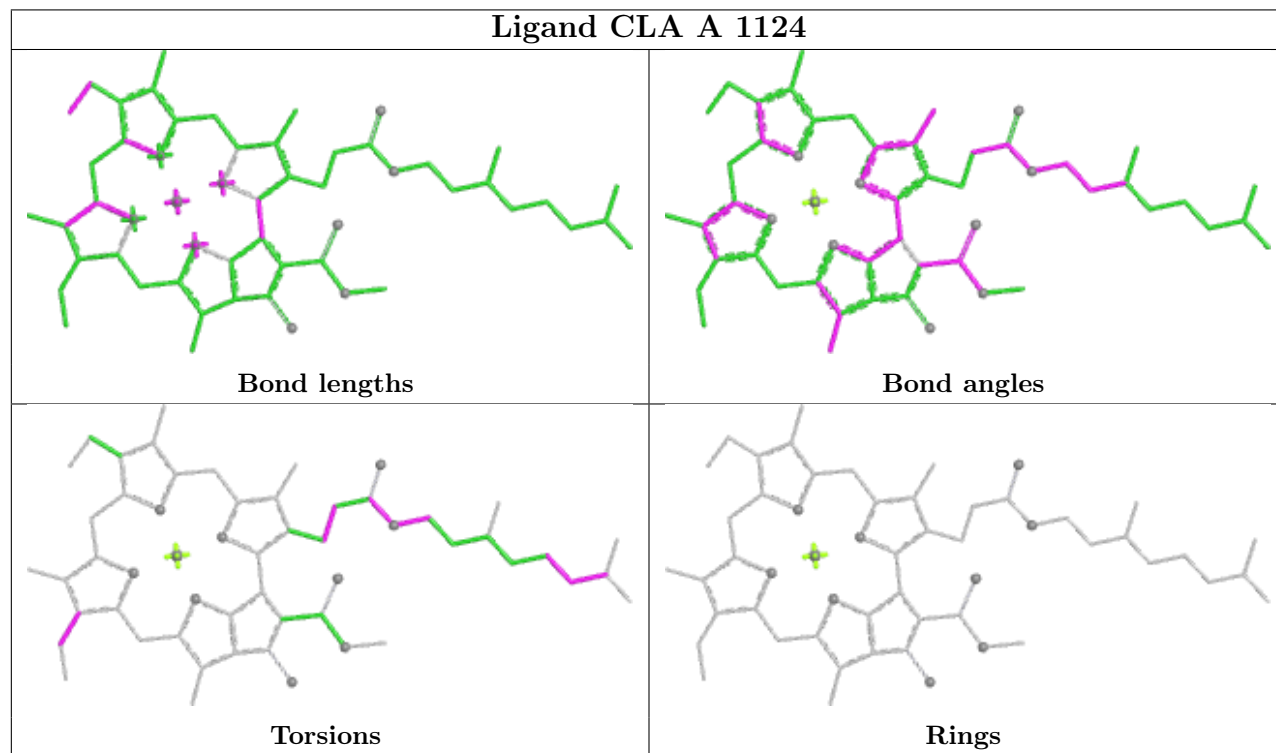
Rings

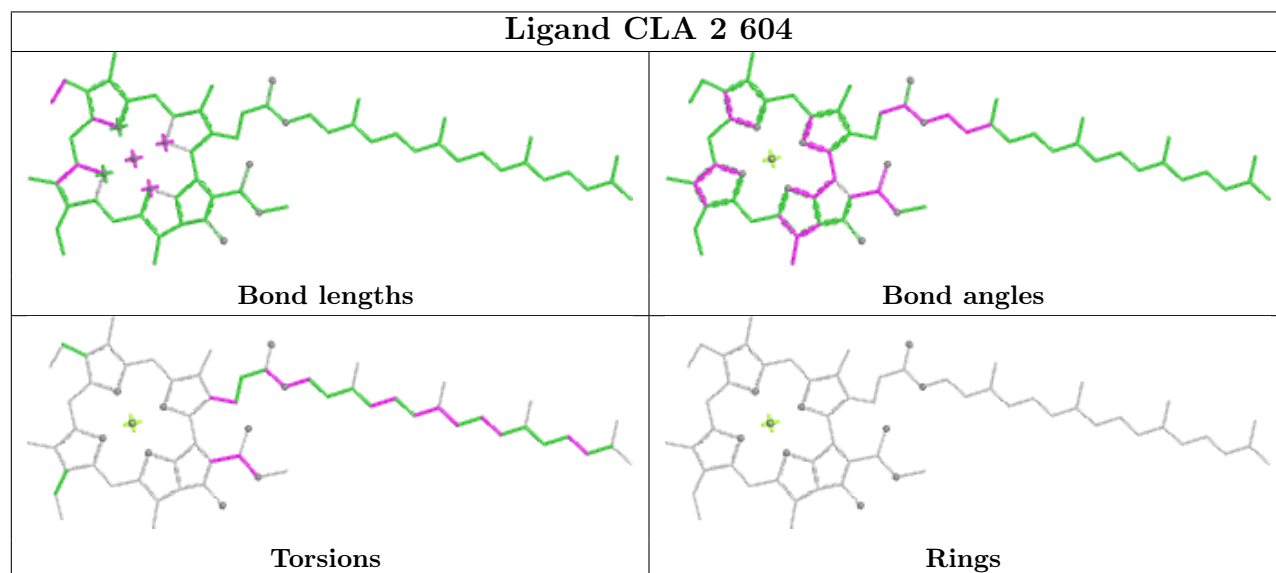
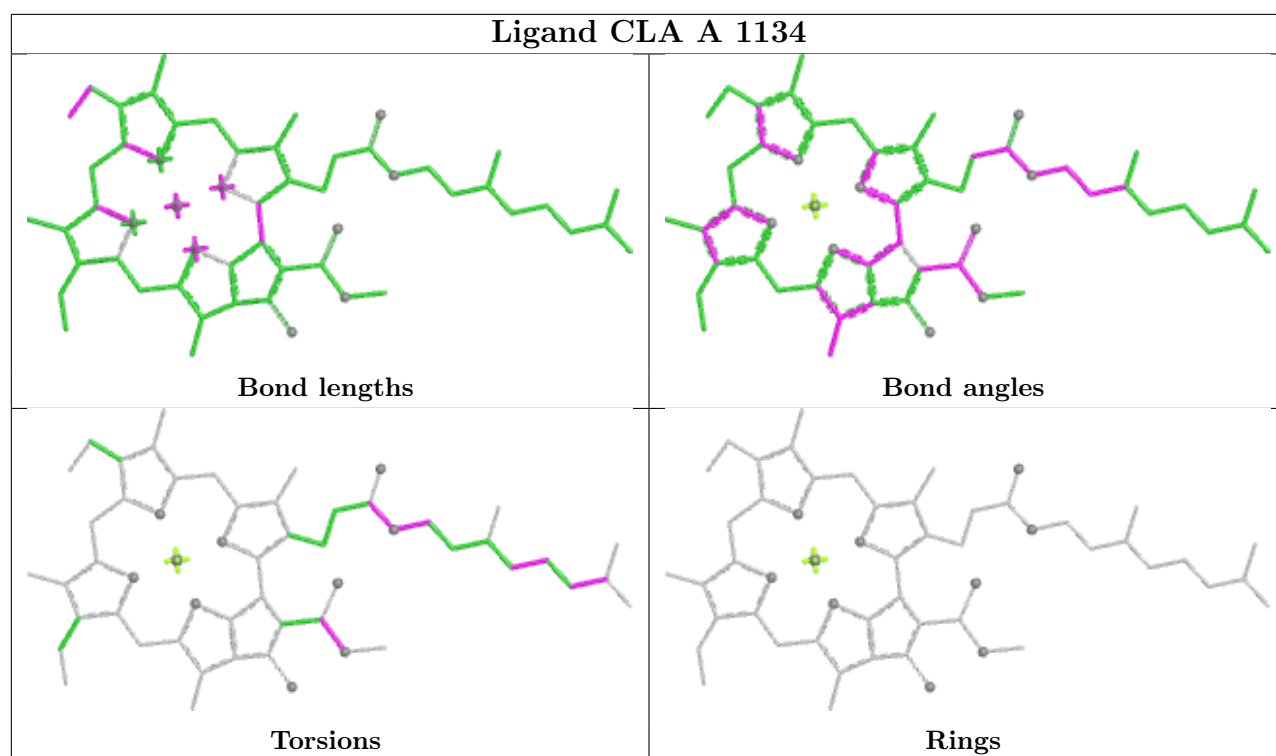


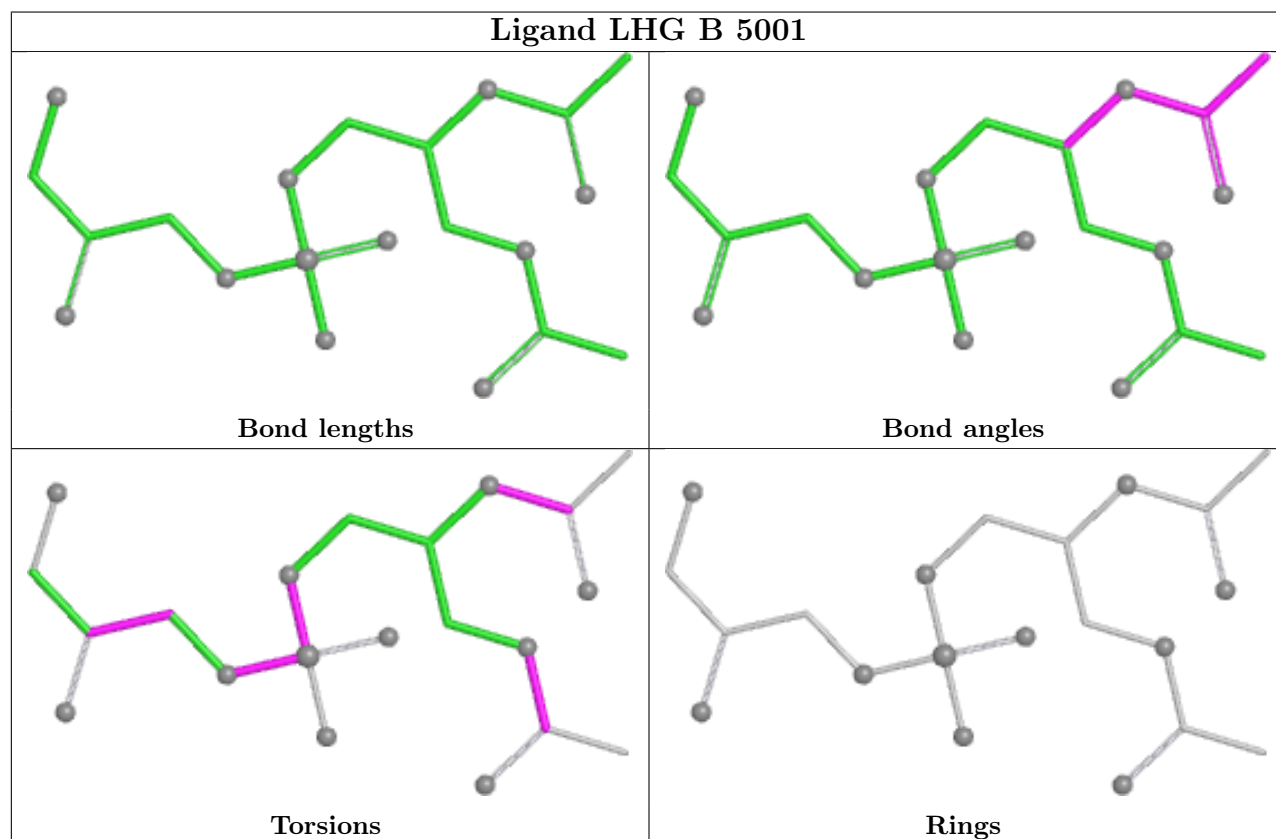
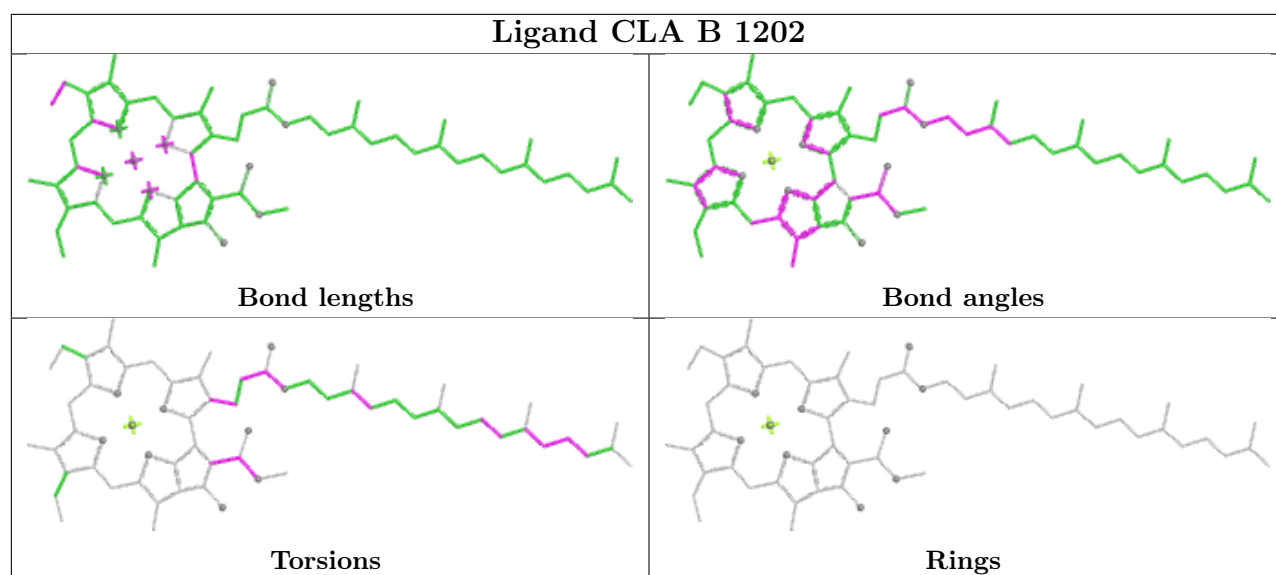
Ligand CLA 3 603

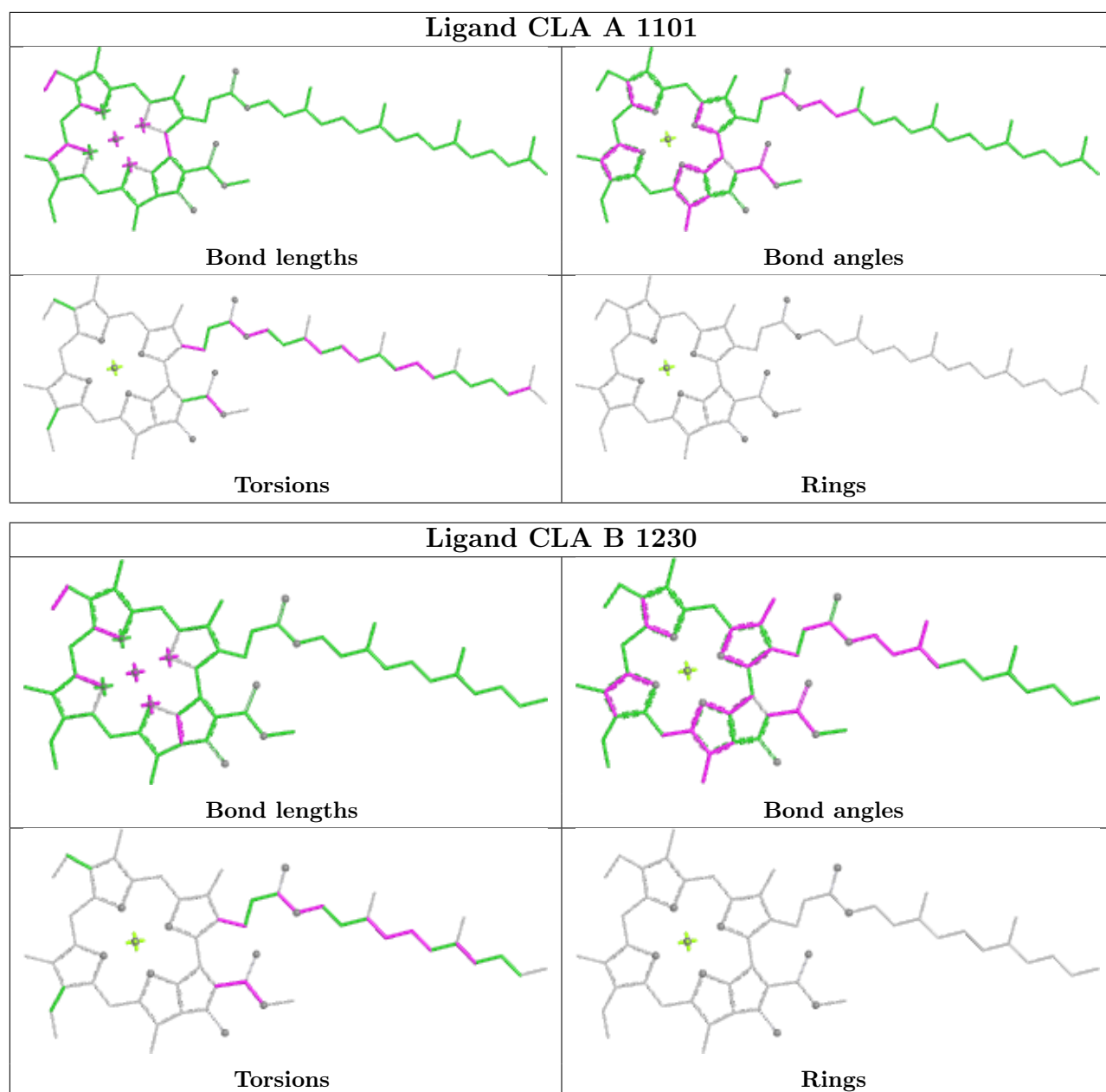


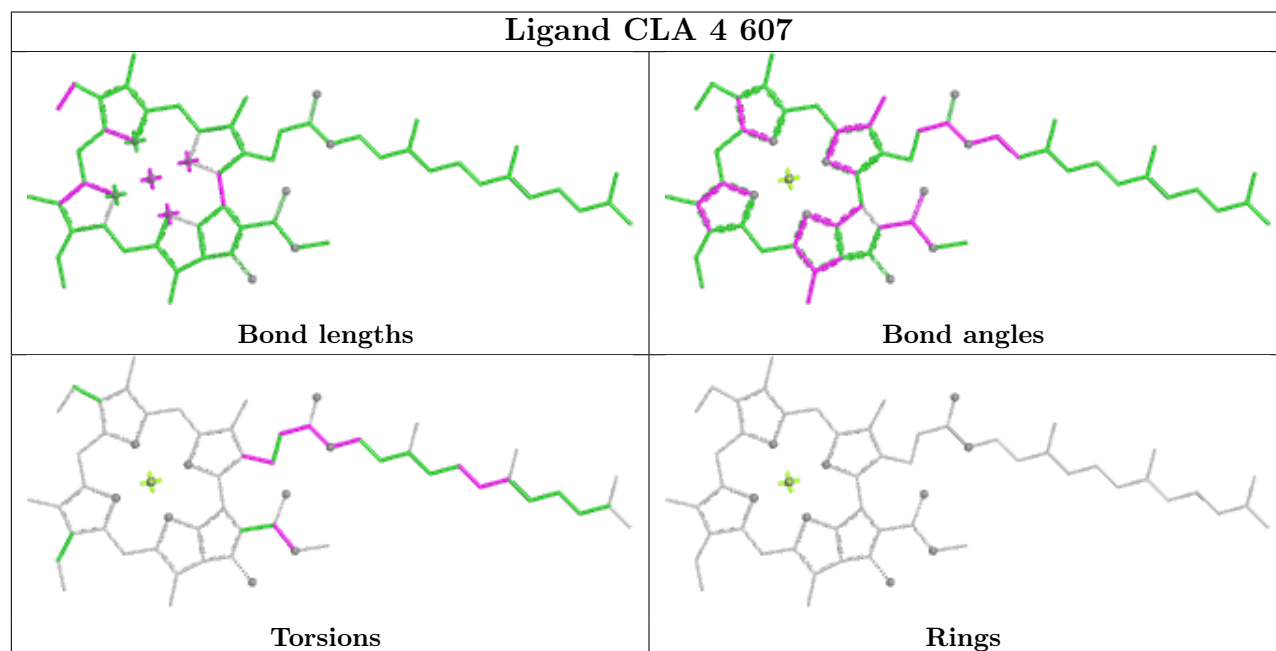
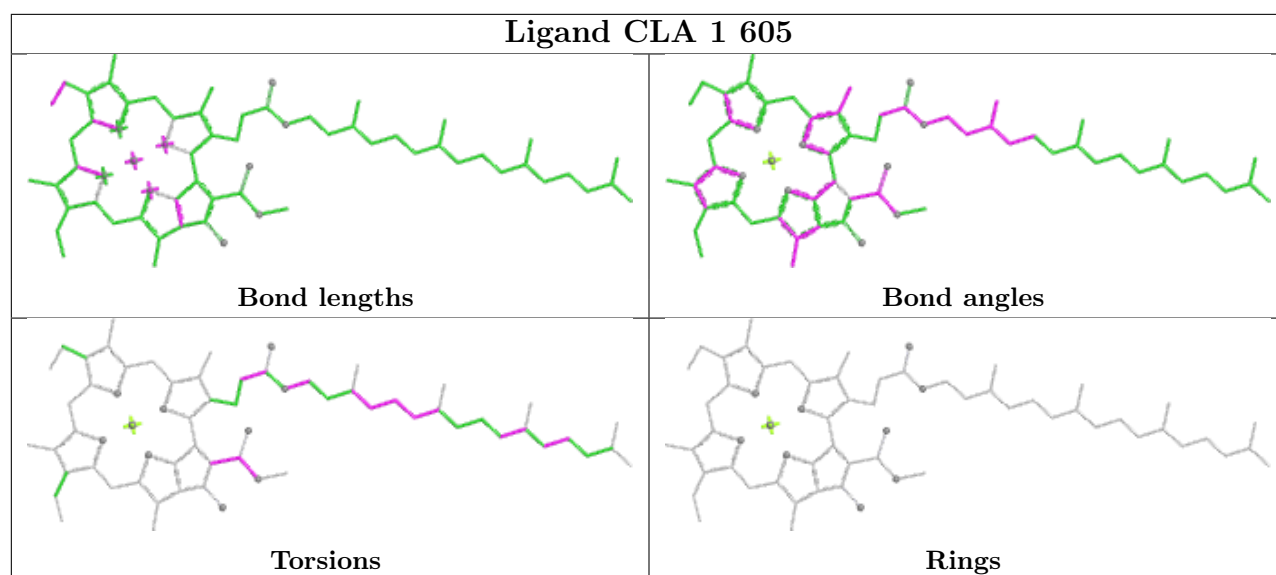
Ligand CLA A 1124

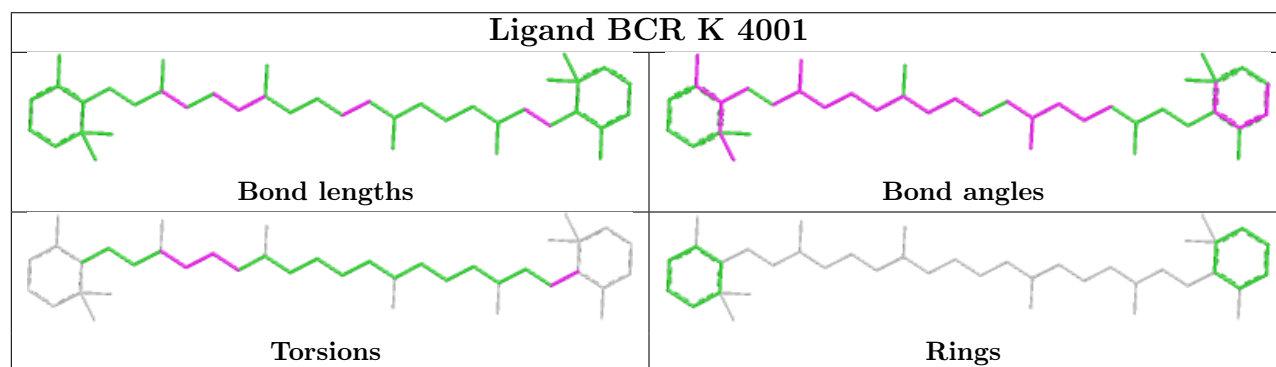
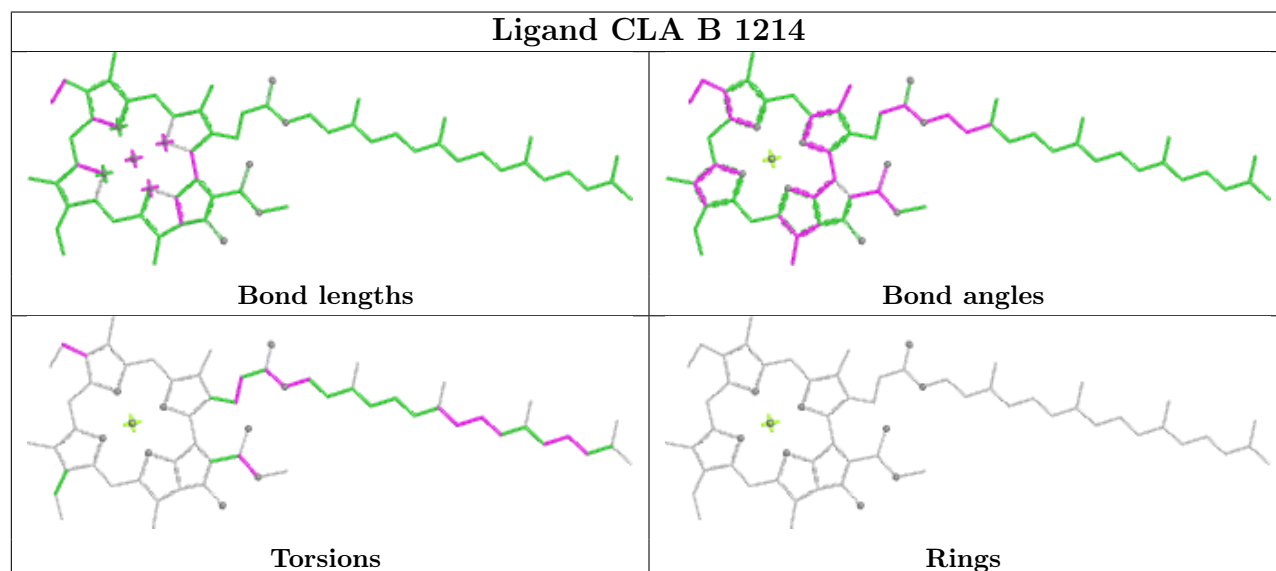
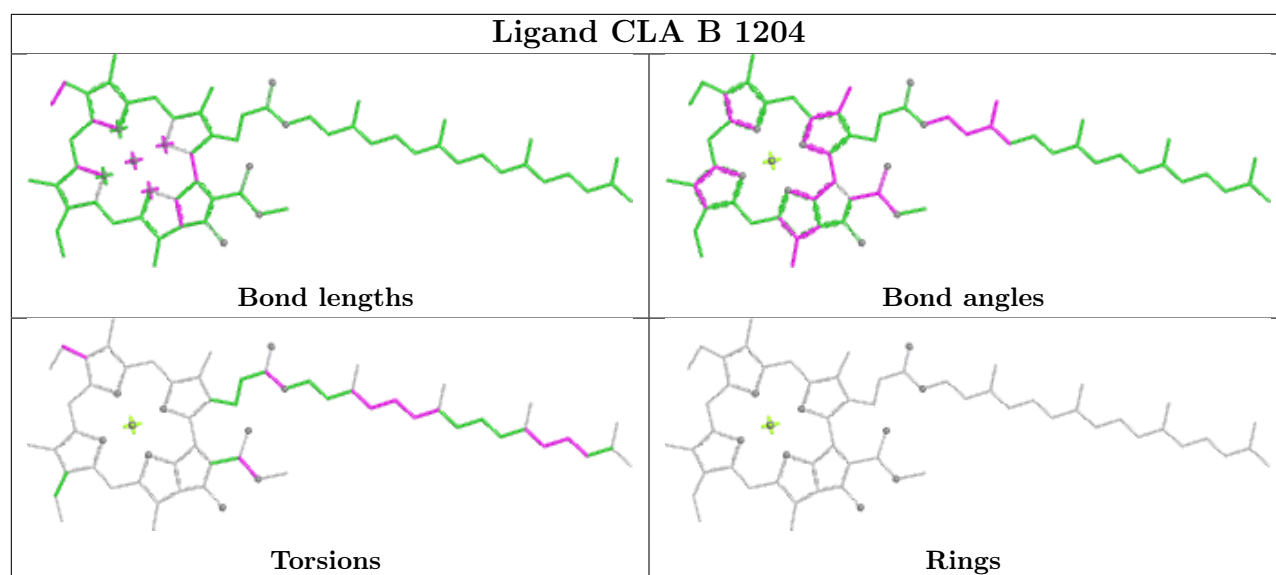




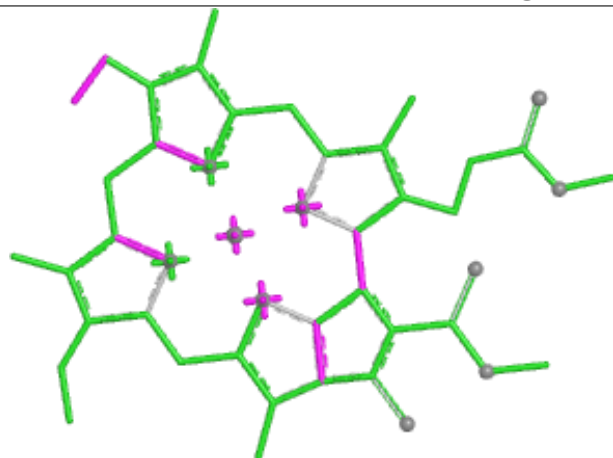




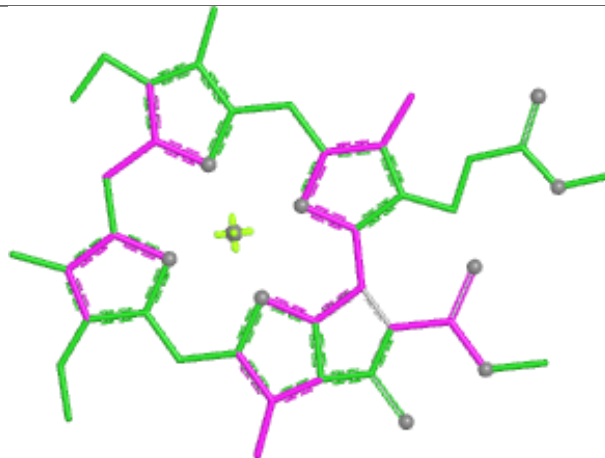




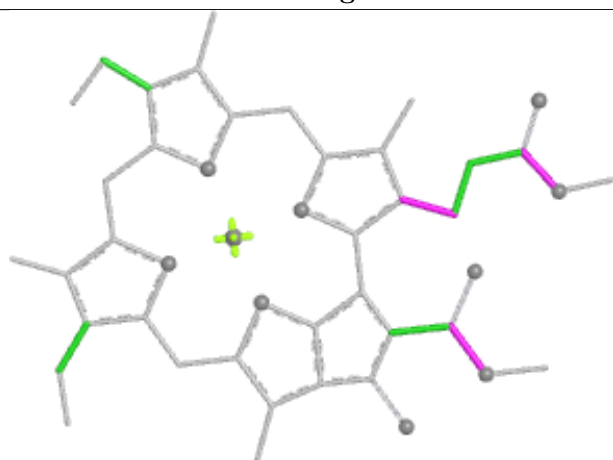
Ligand CLA 3 613



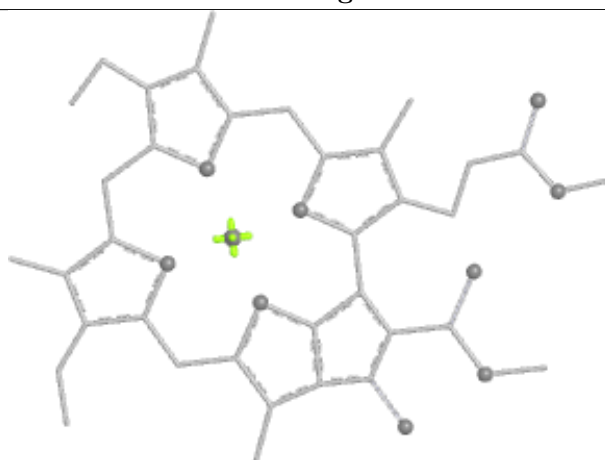
Bond lengths



Bond angles

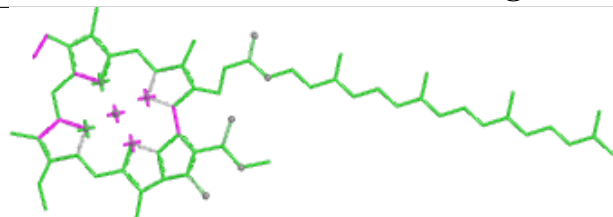


Torsions

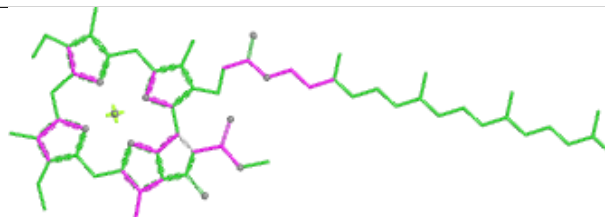


Rings

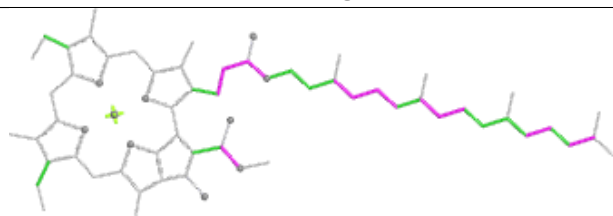
Ligand CLA A 1138



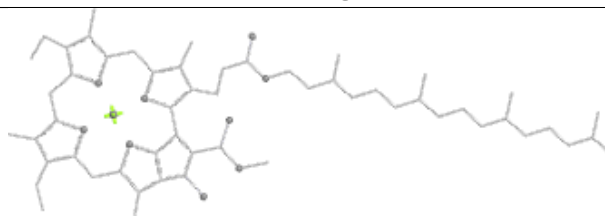
Bond lengths



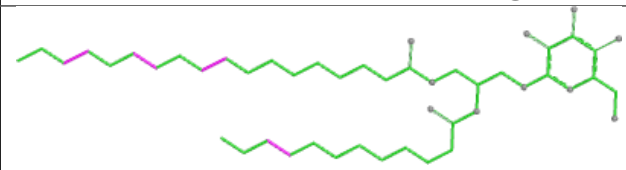
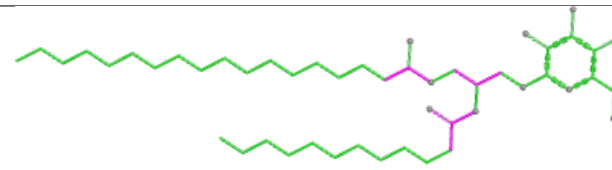
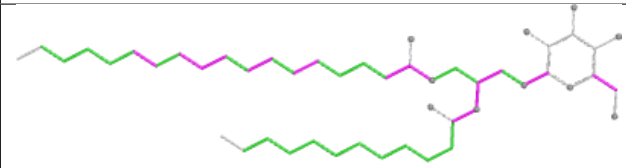
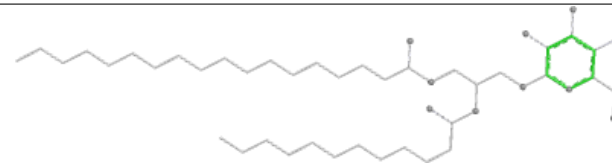
Bond angles

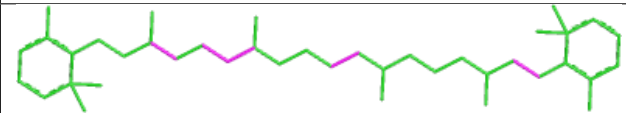
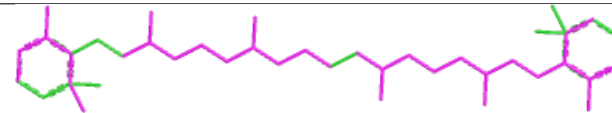
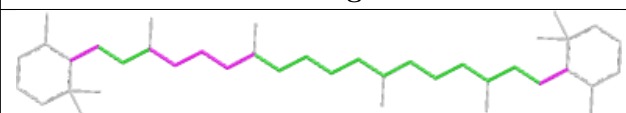
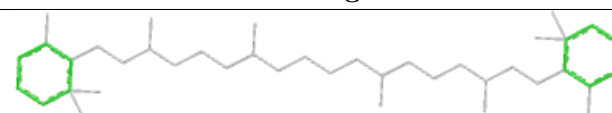


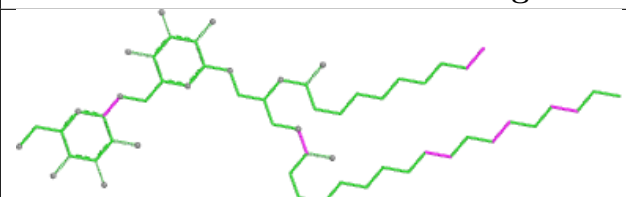
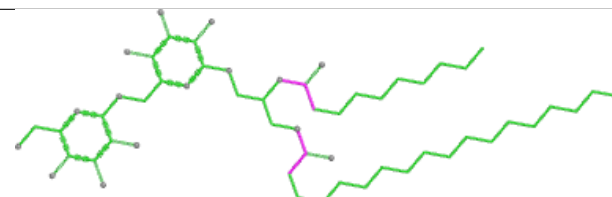
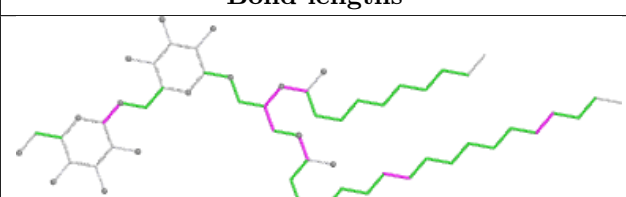
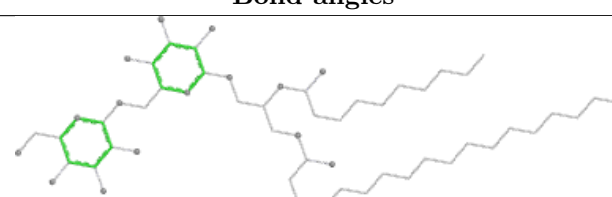
Torsions

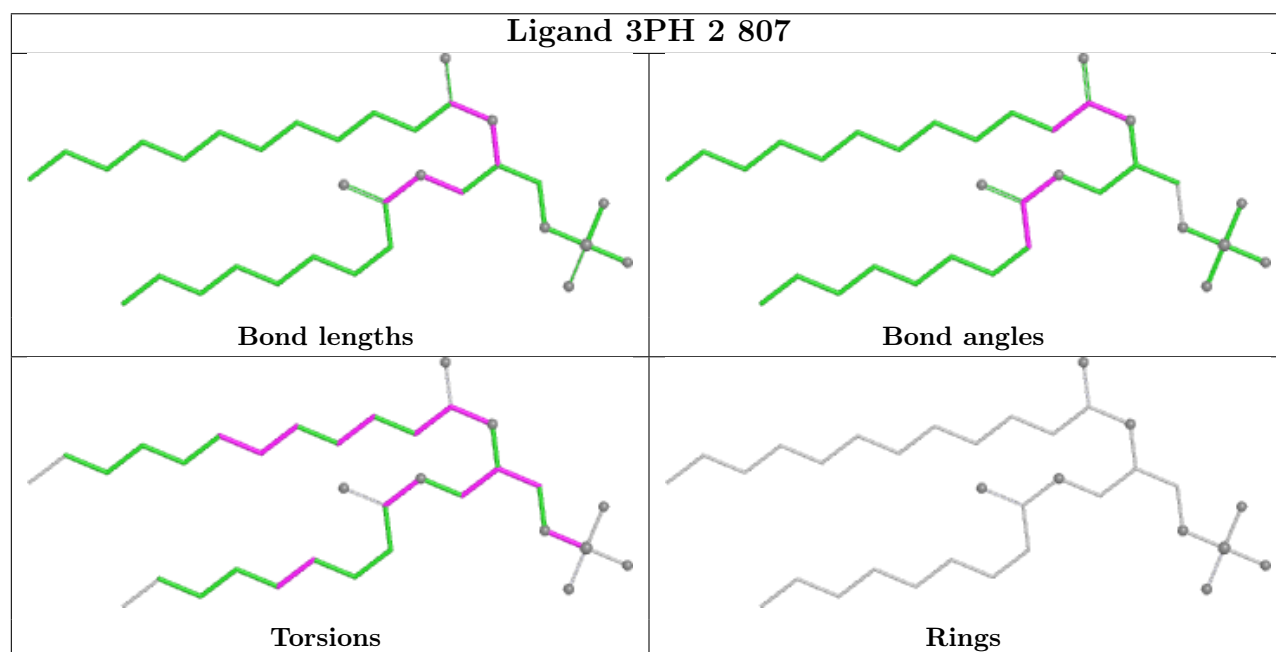
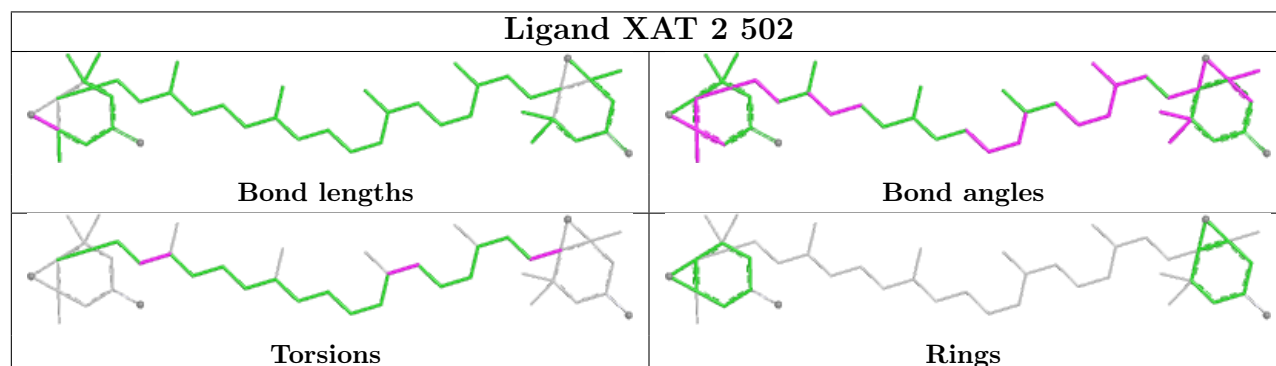
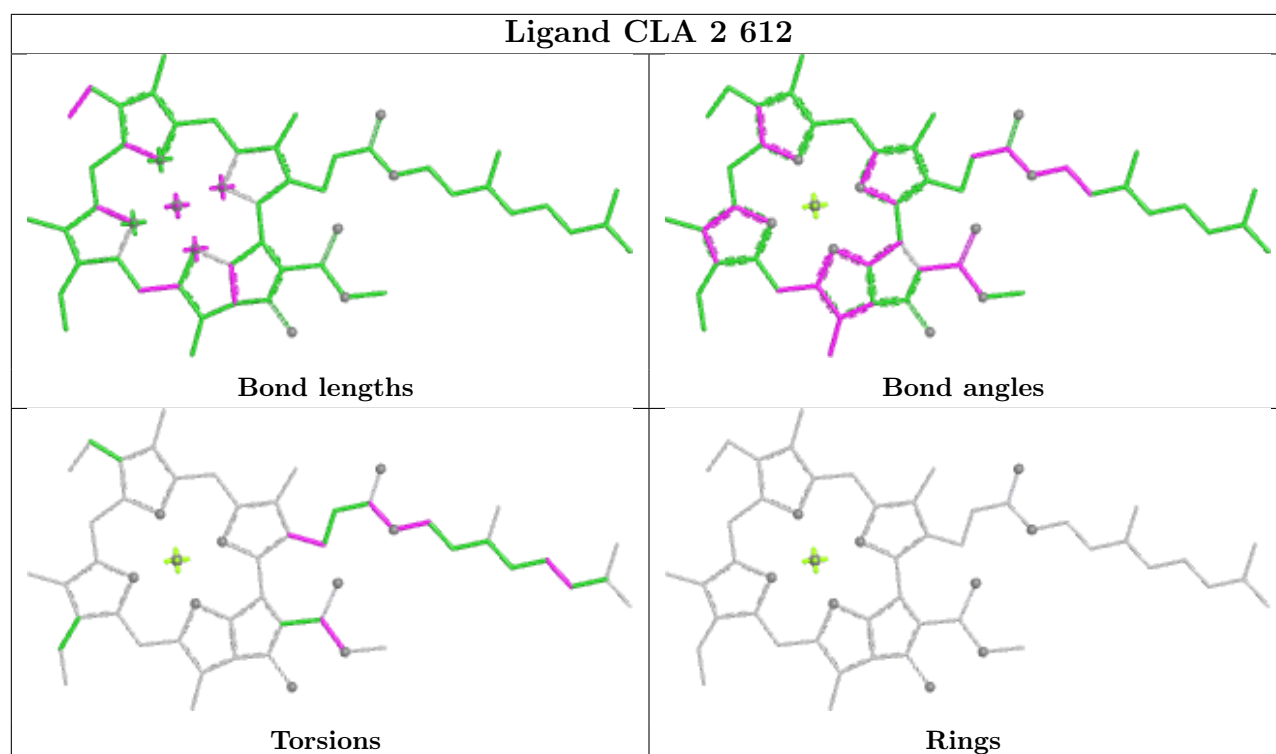


Rings

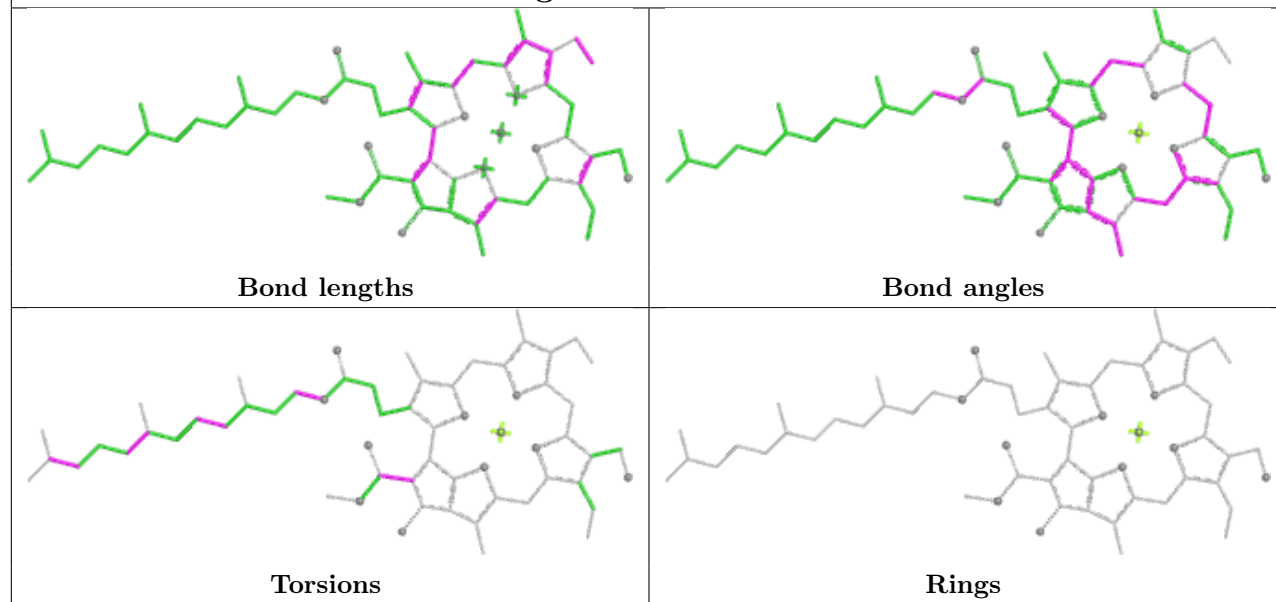
Ligand LMG G 5001	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCR A 4008	
 Bond lengths	 Bond angles
 Torsions	 Rings

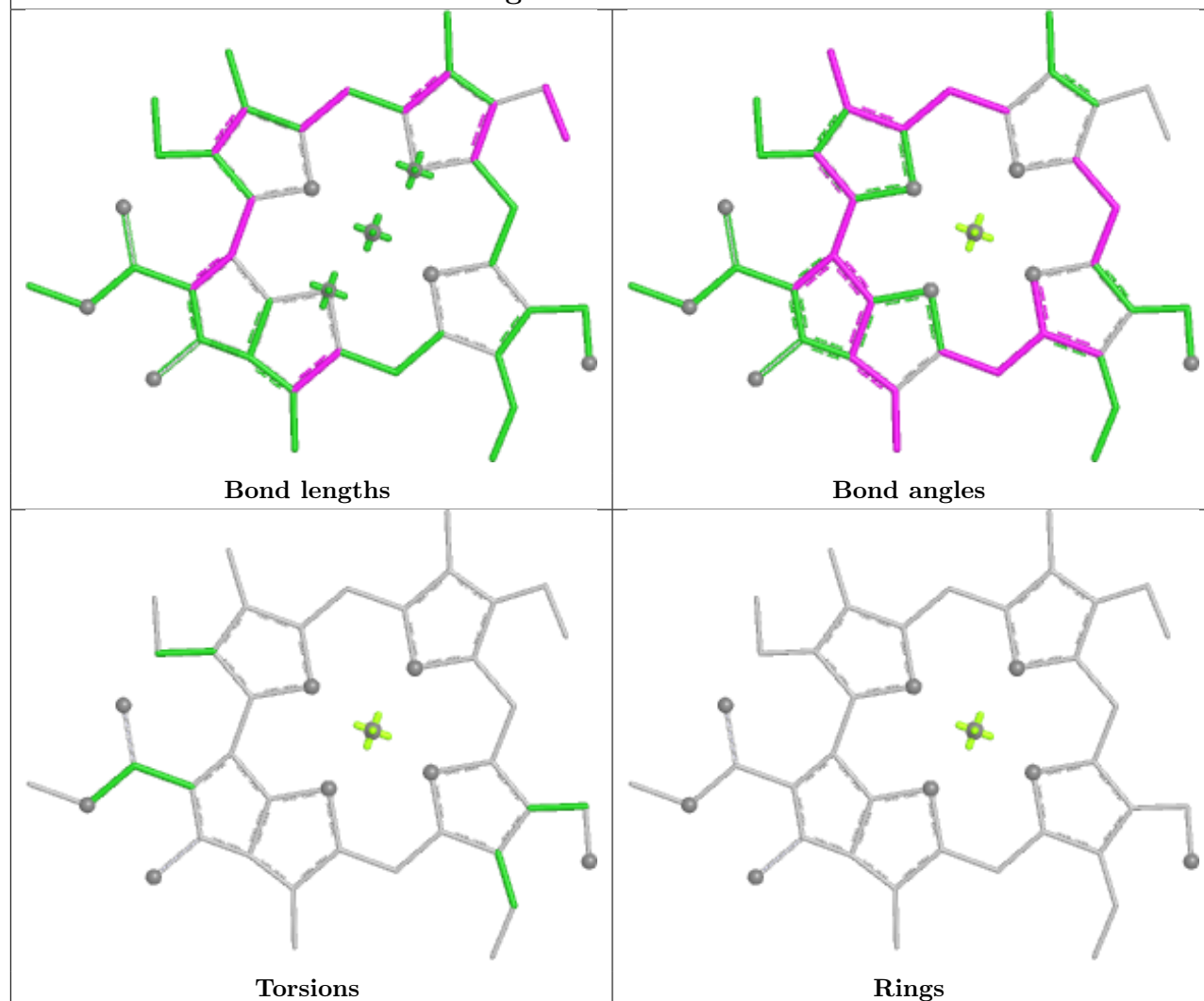
Ligand DGD J 5001	
 Bond lengths	 Bond angles
 Torsions	 Rings

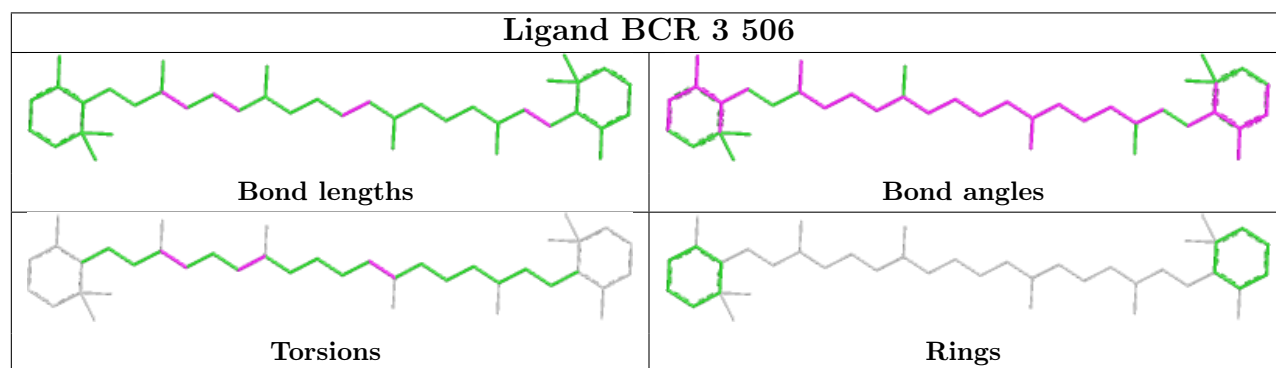
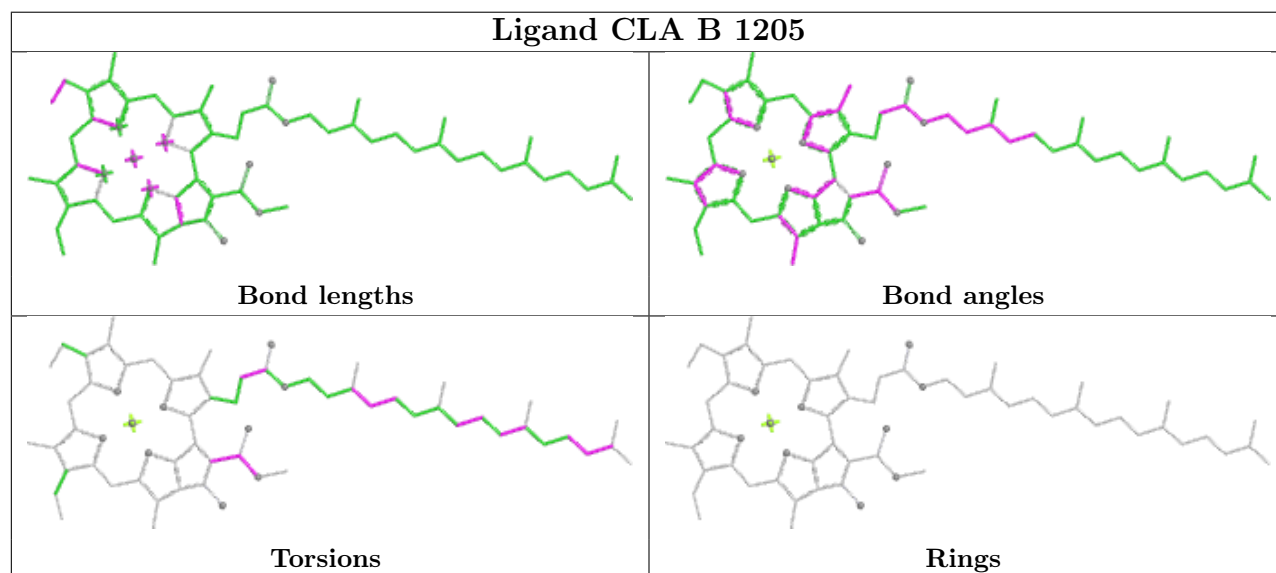
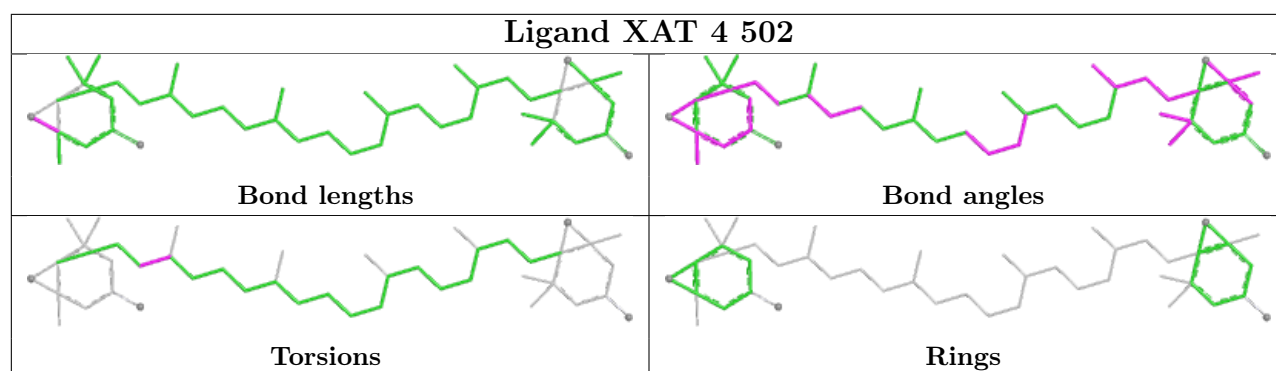


Ligand CHL 4 613

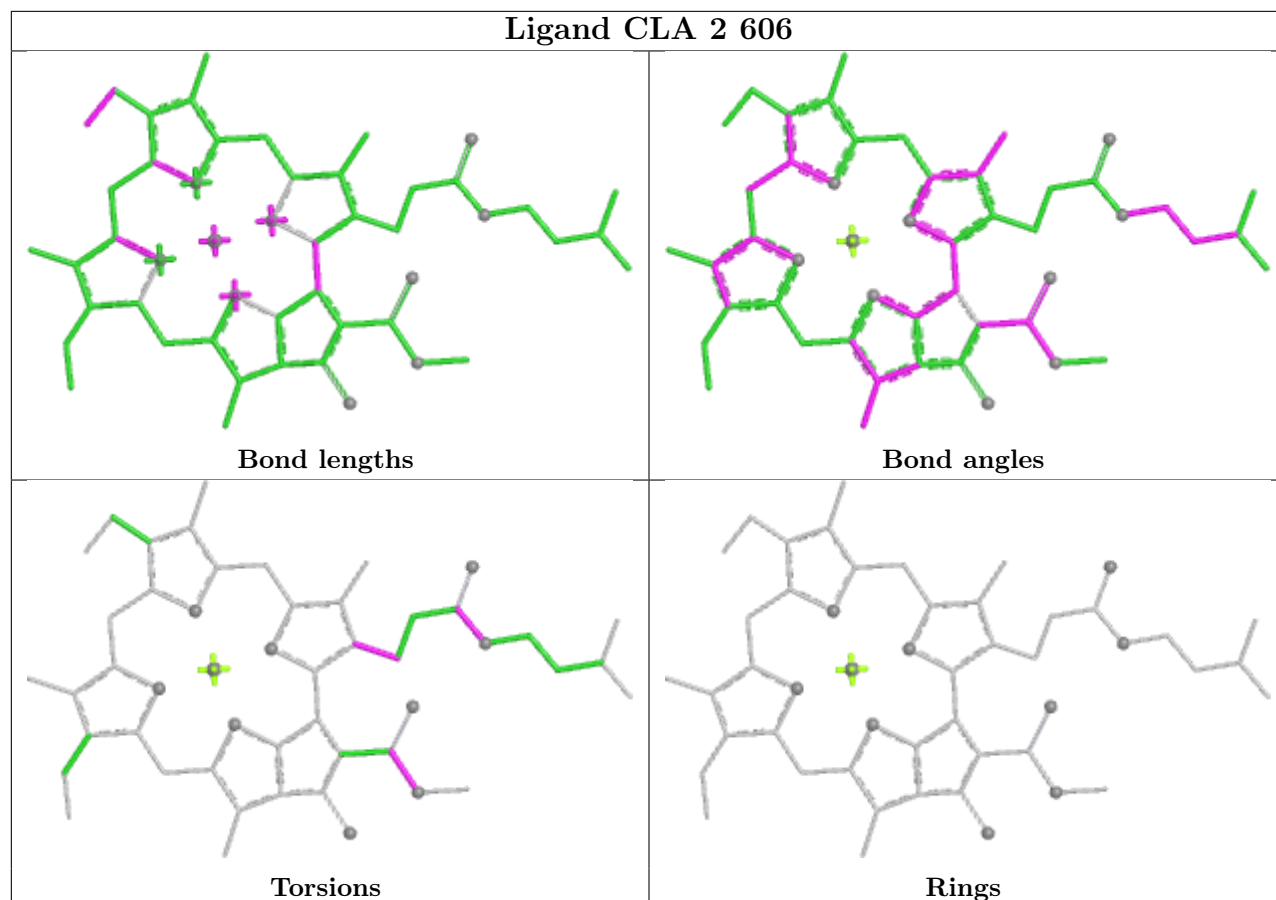


Ligand CHL 4 615

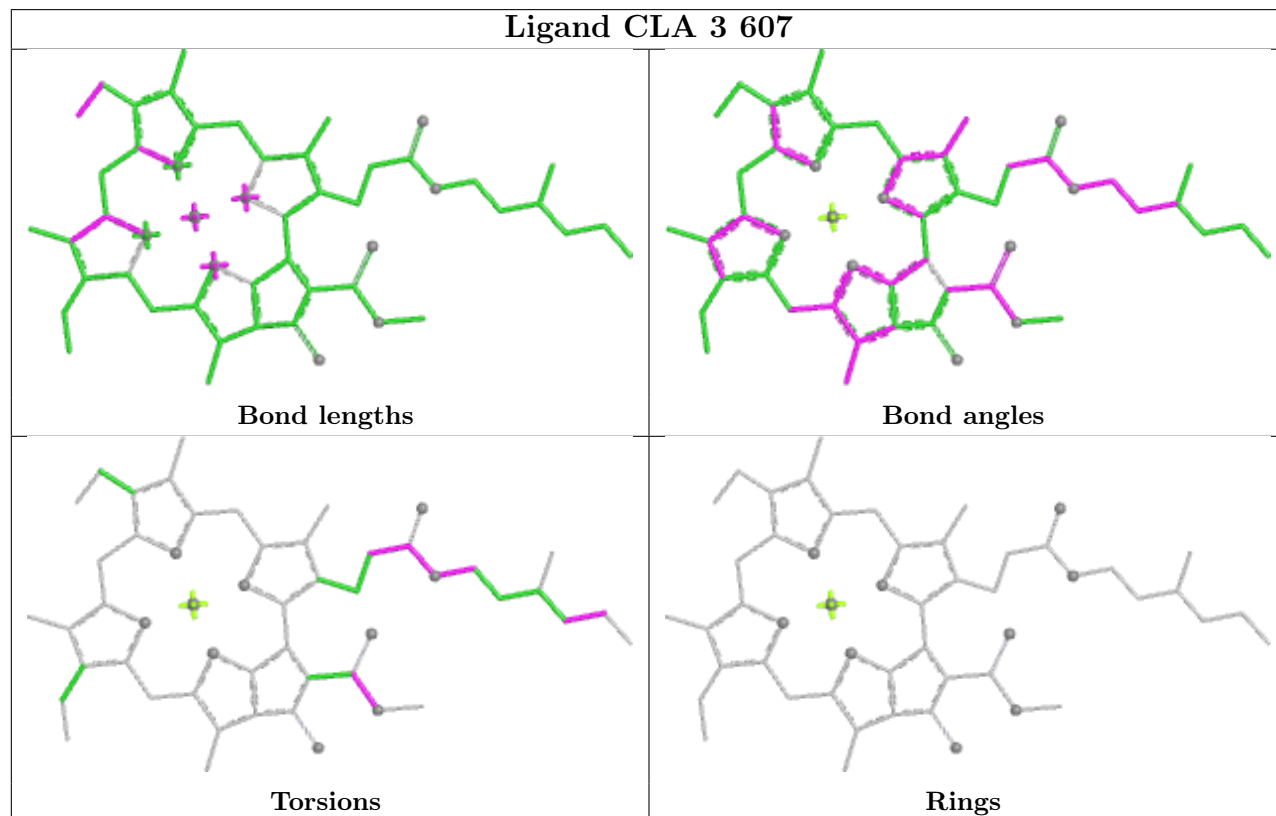


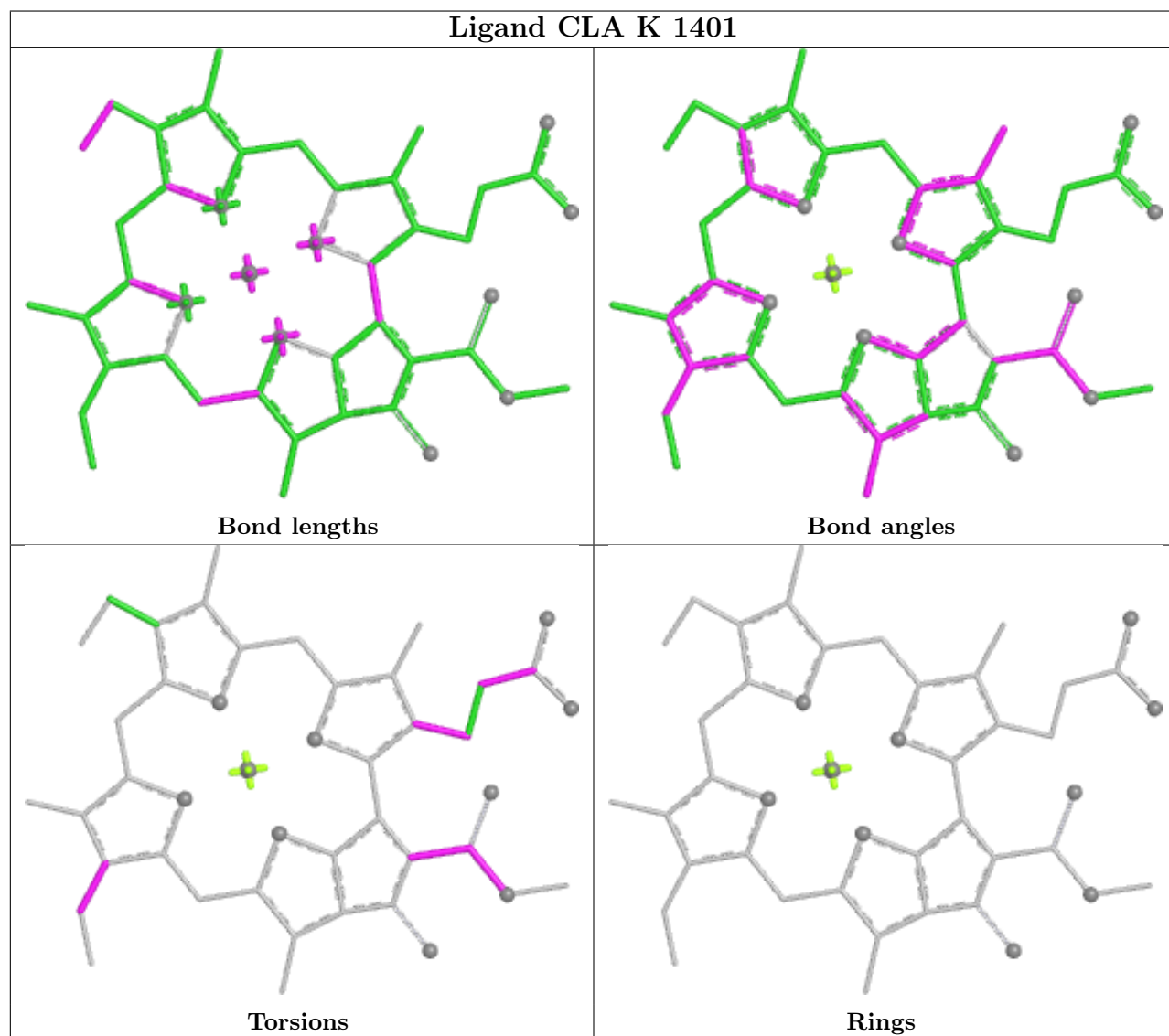
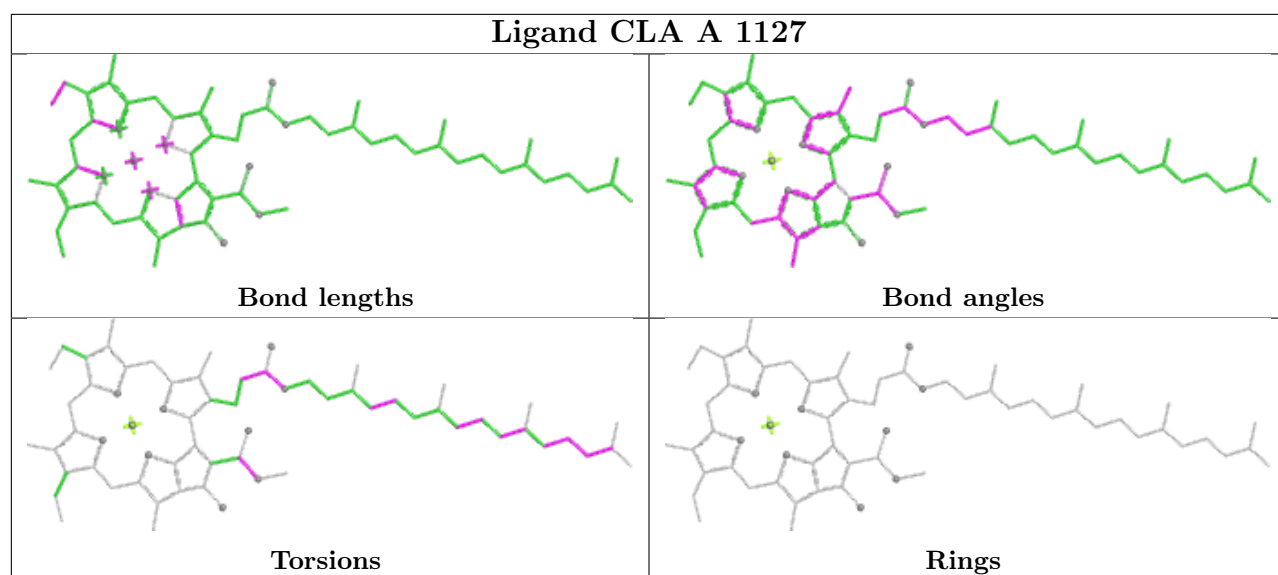


Ligand CLA 2 606

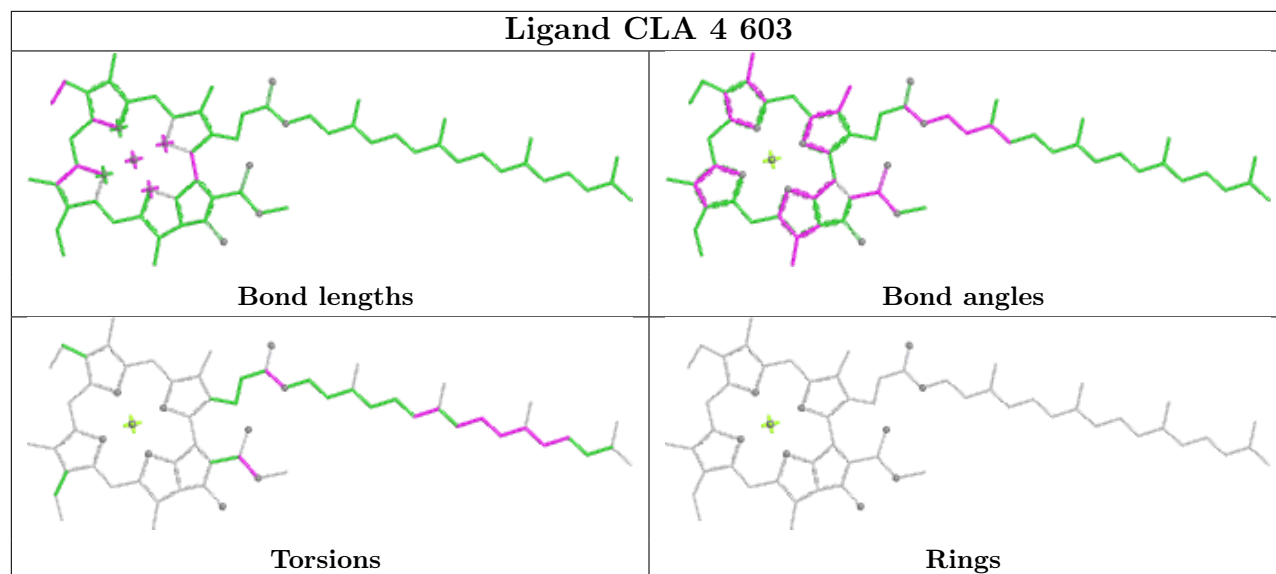


Ligand CLA 3 607

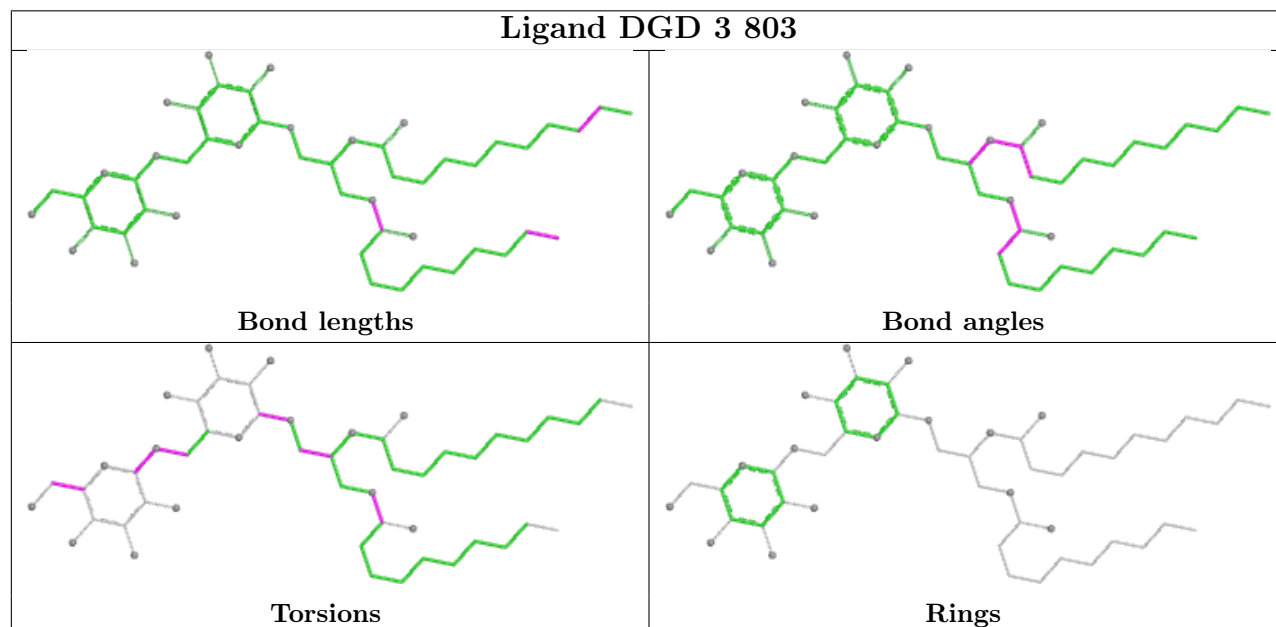




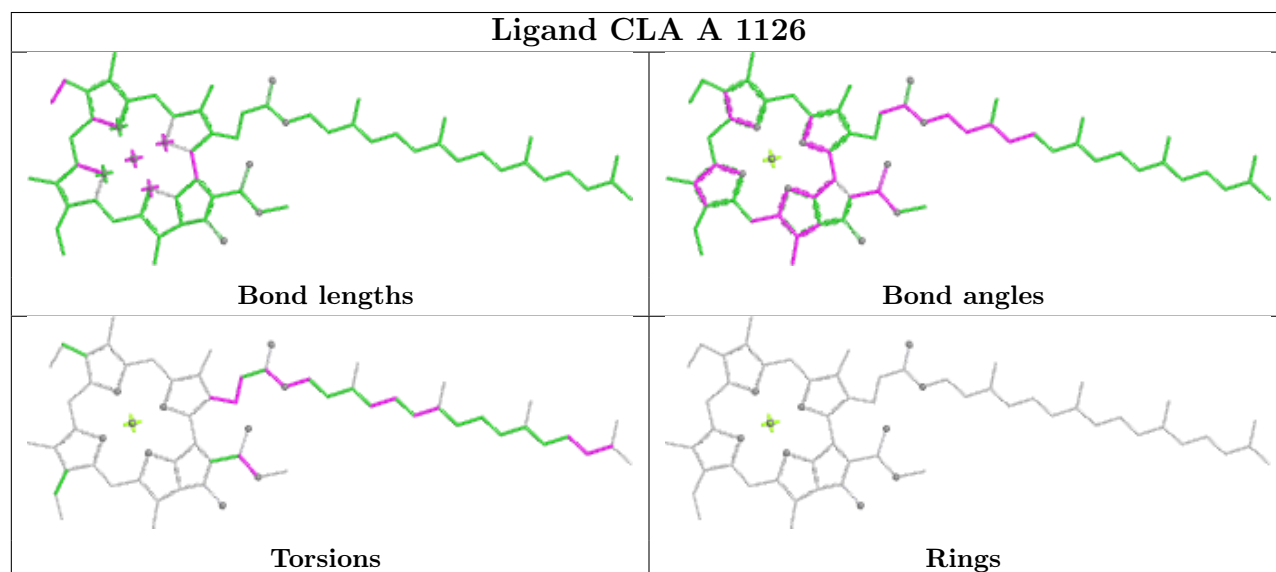
Ligand CLA 4 603

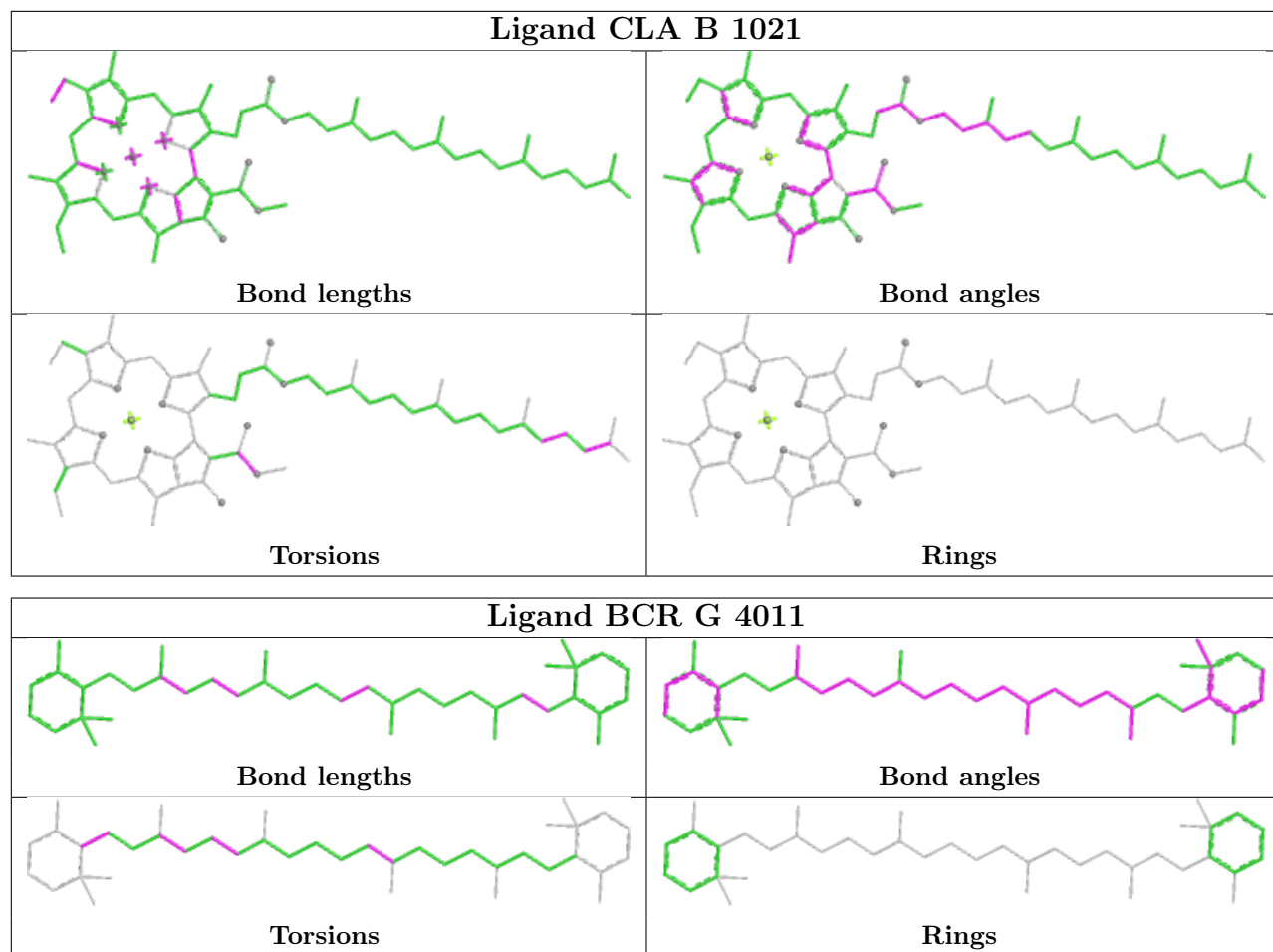


Ligand DGD 3 803

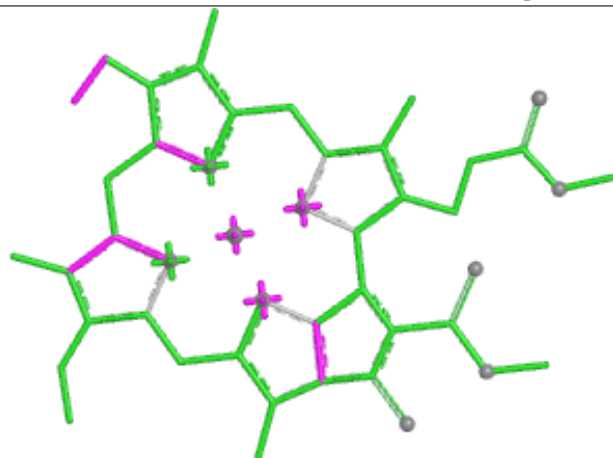


Ligand CLA A 1126

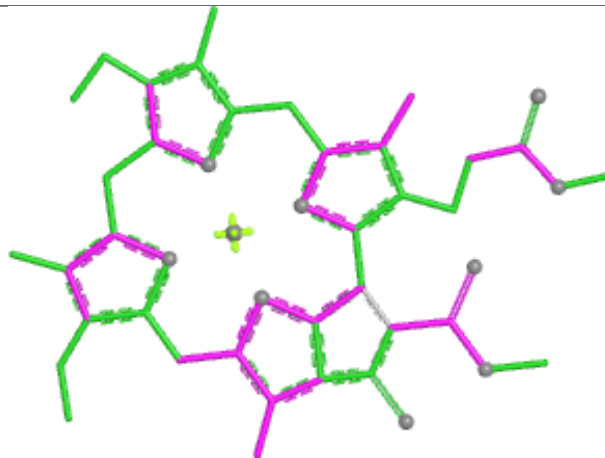




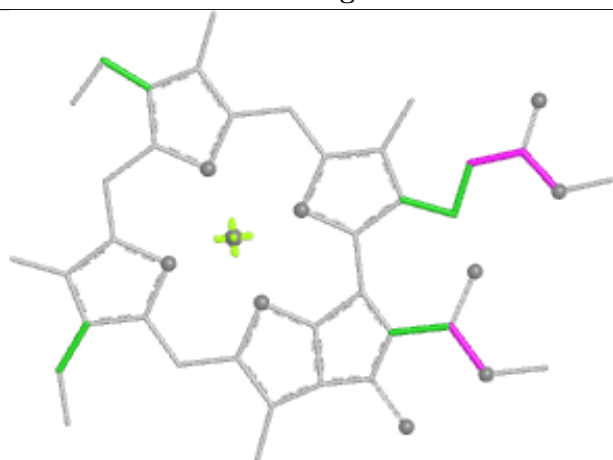
Ligand CLA 4 608



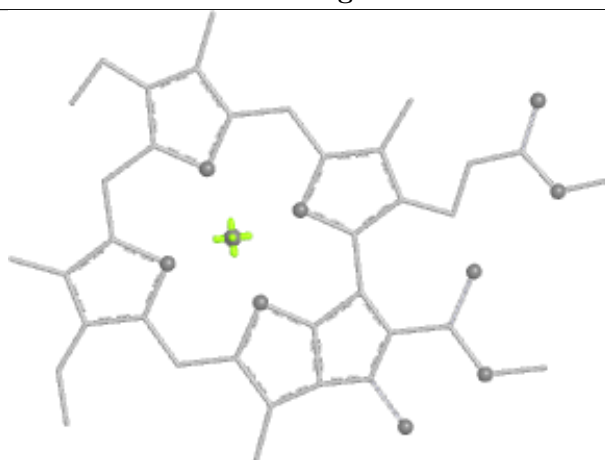
Bond lengths



Bond angles

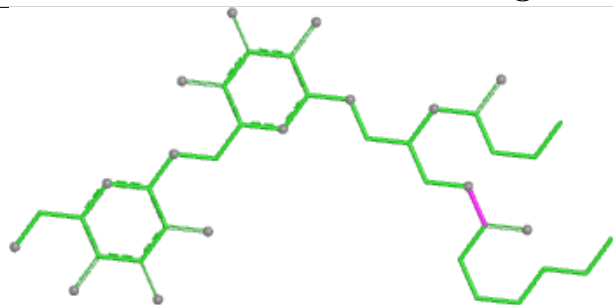


Torsions

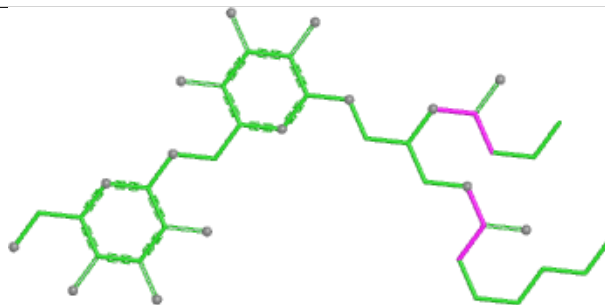


Rings

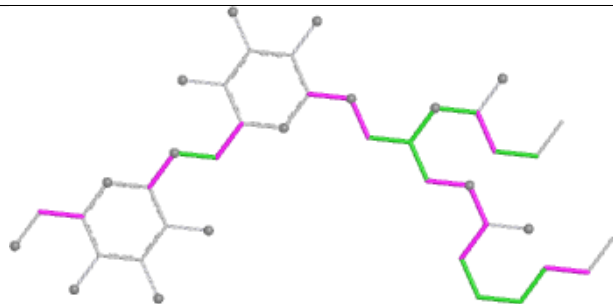
Ligand DGD 1 803



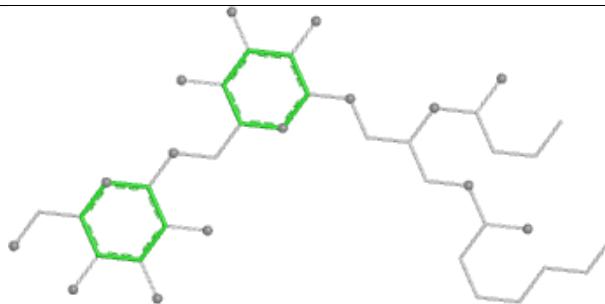
Bond lengths



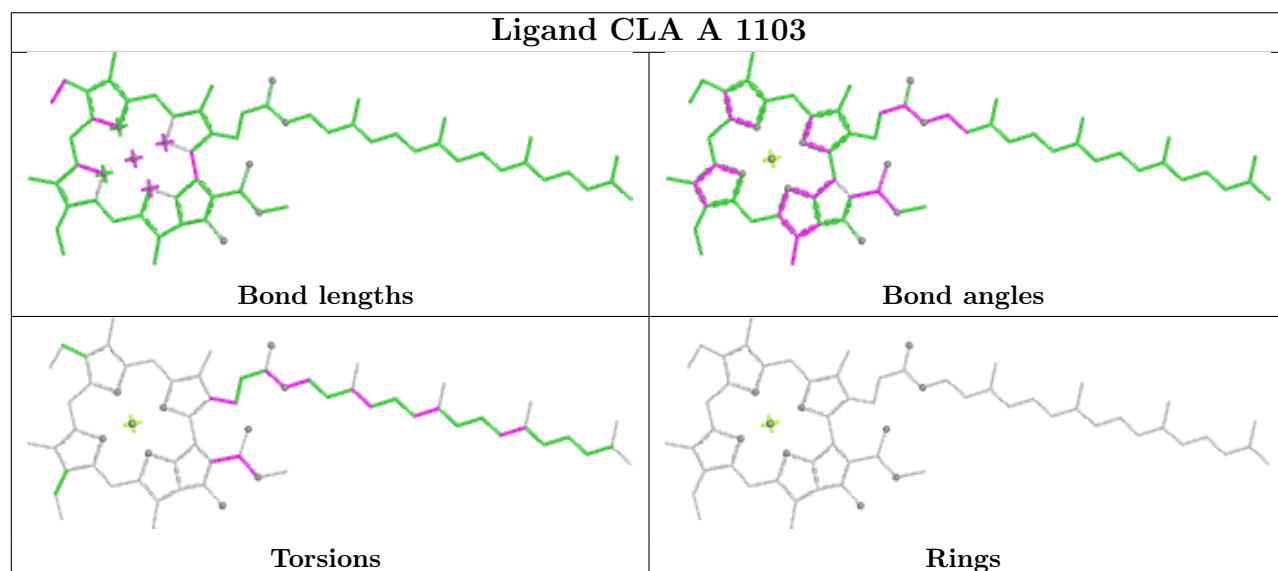
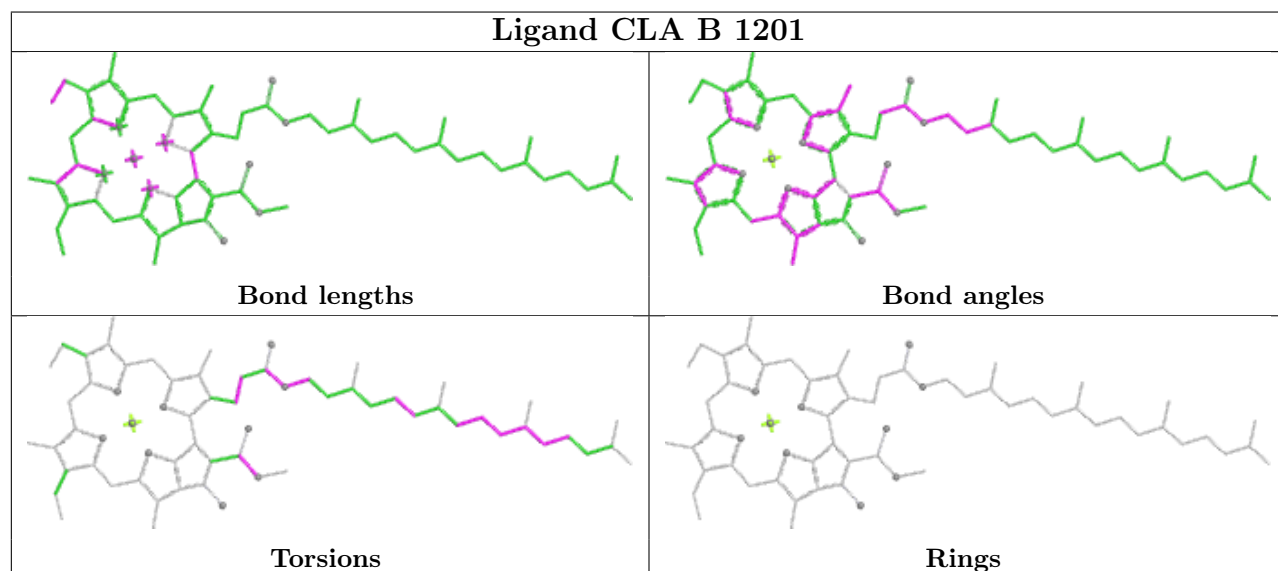
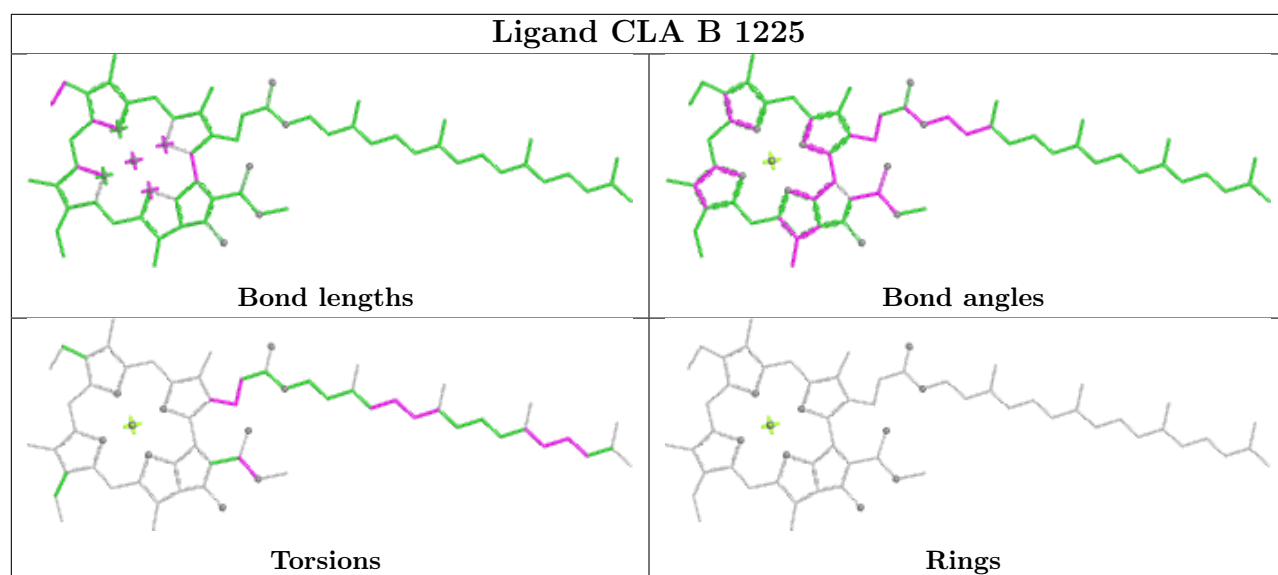
Bond angles

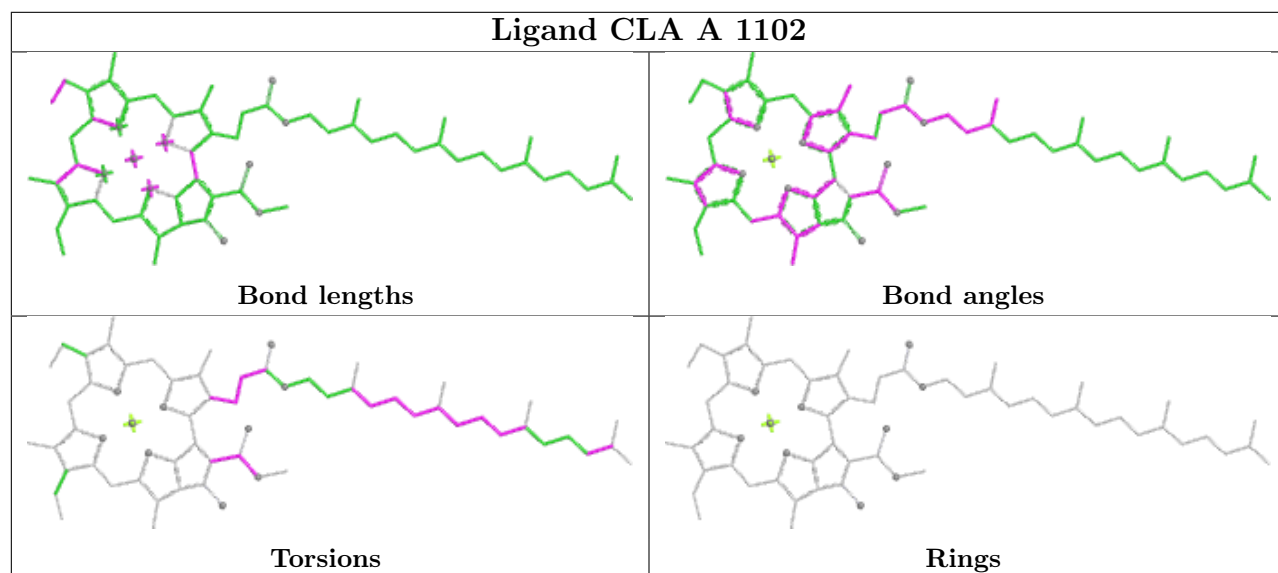
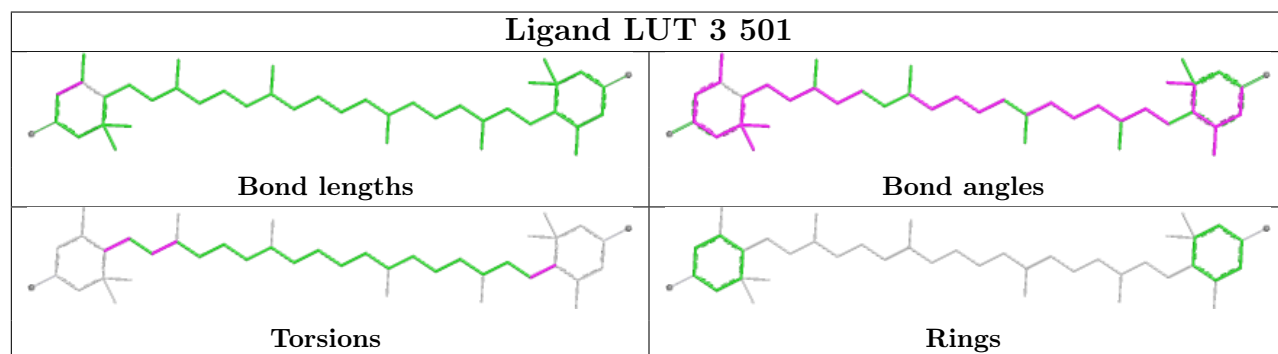
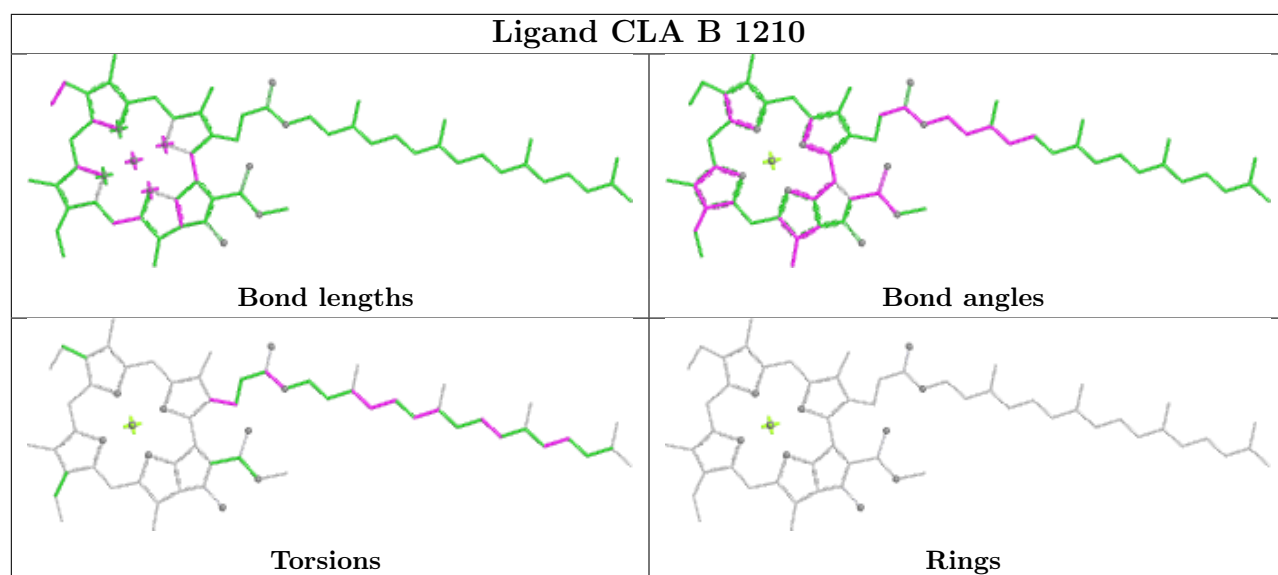


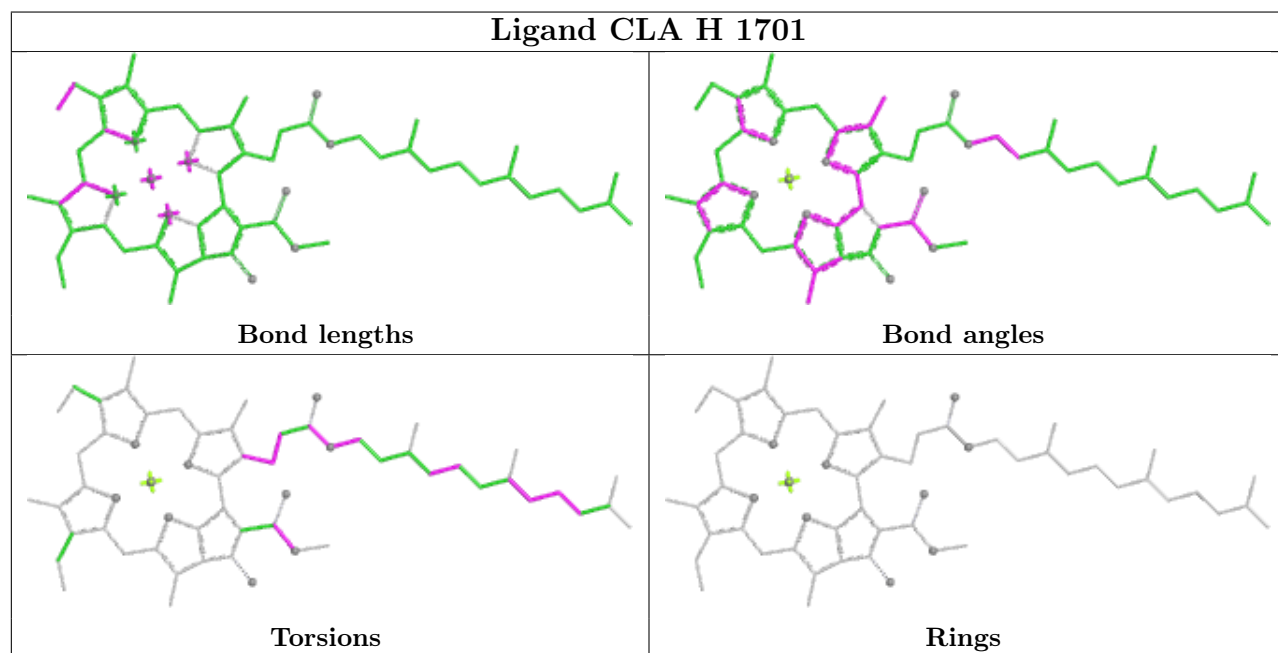
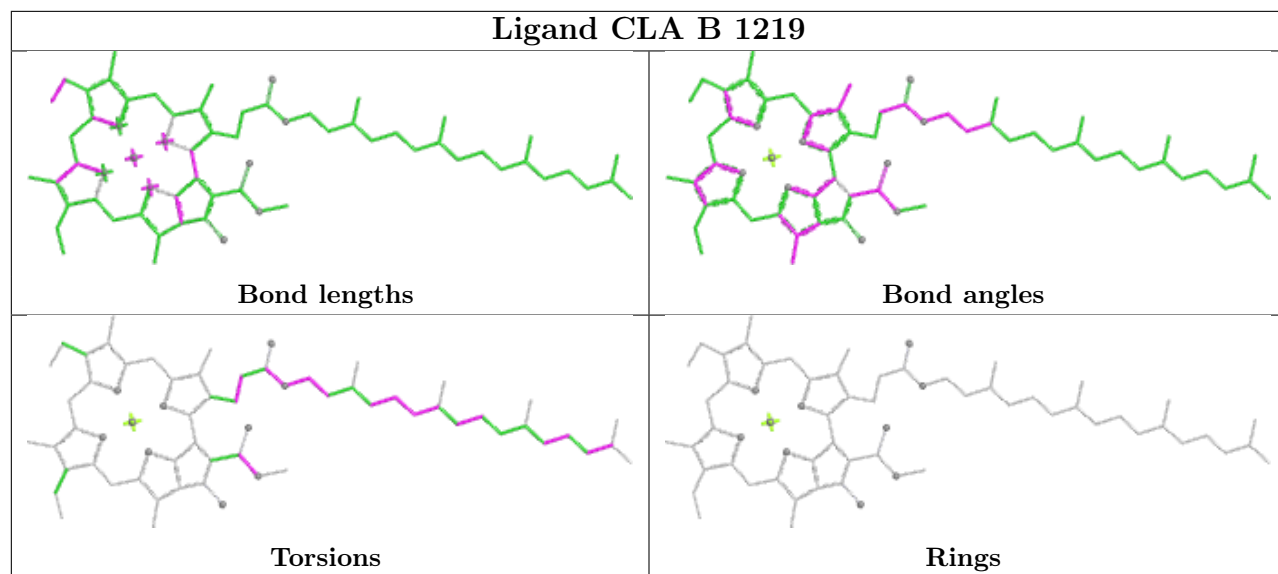
Torsions



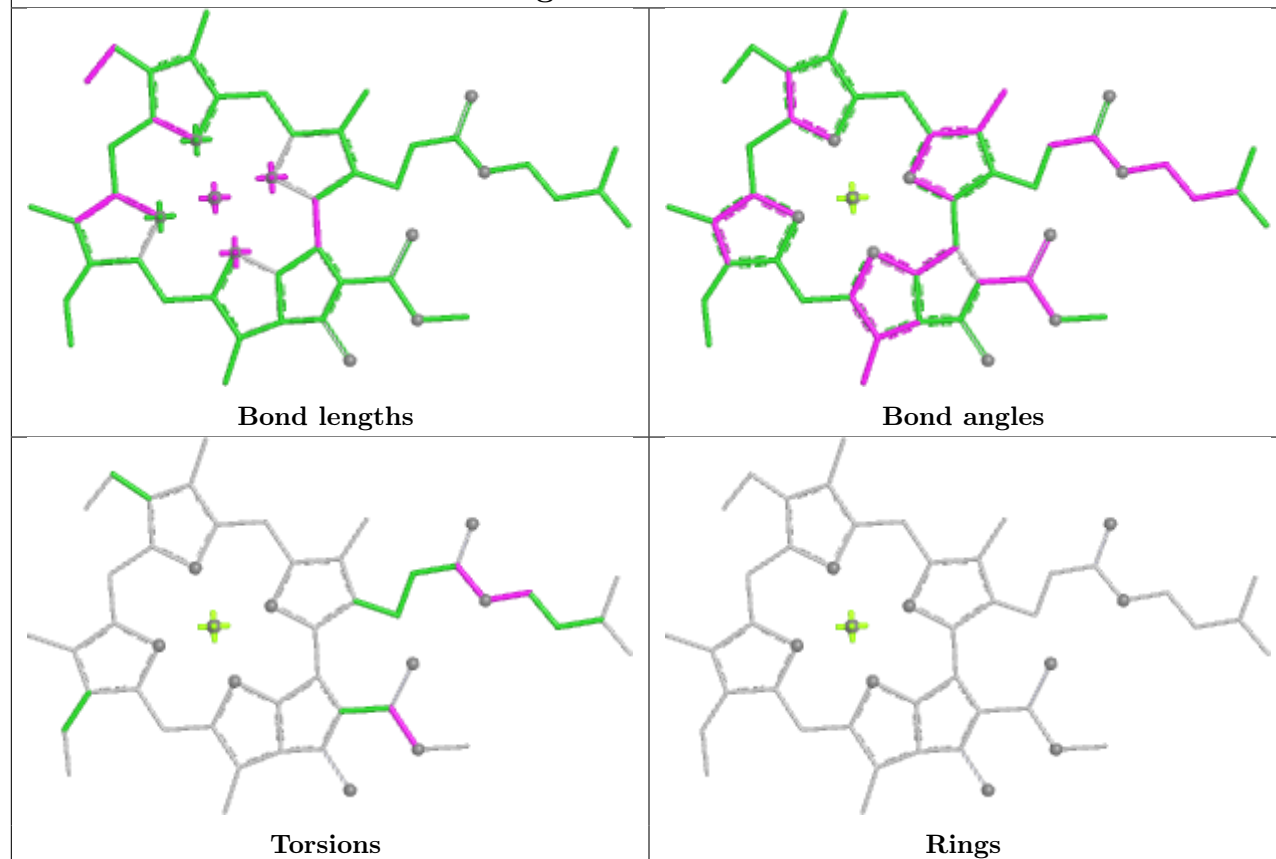
Rings



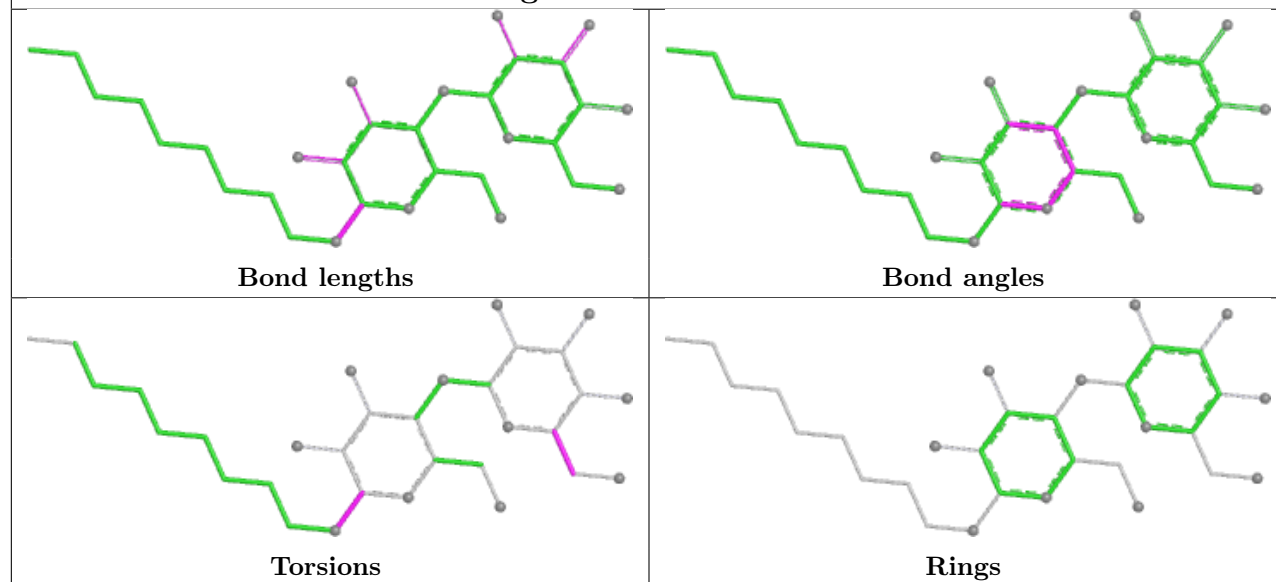


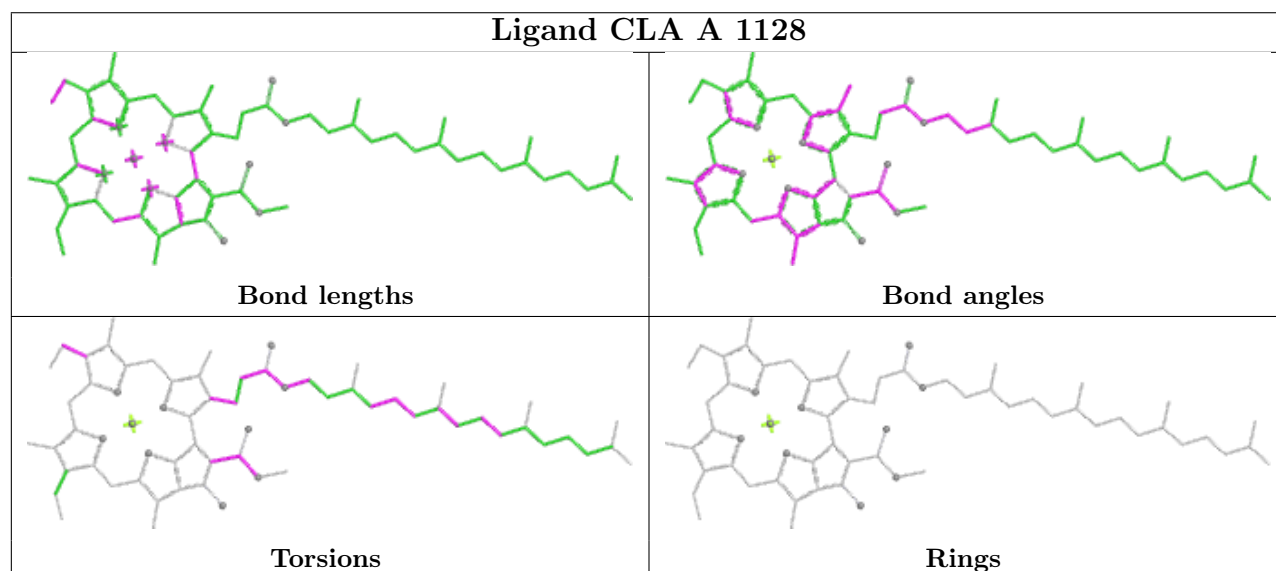
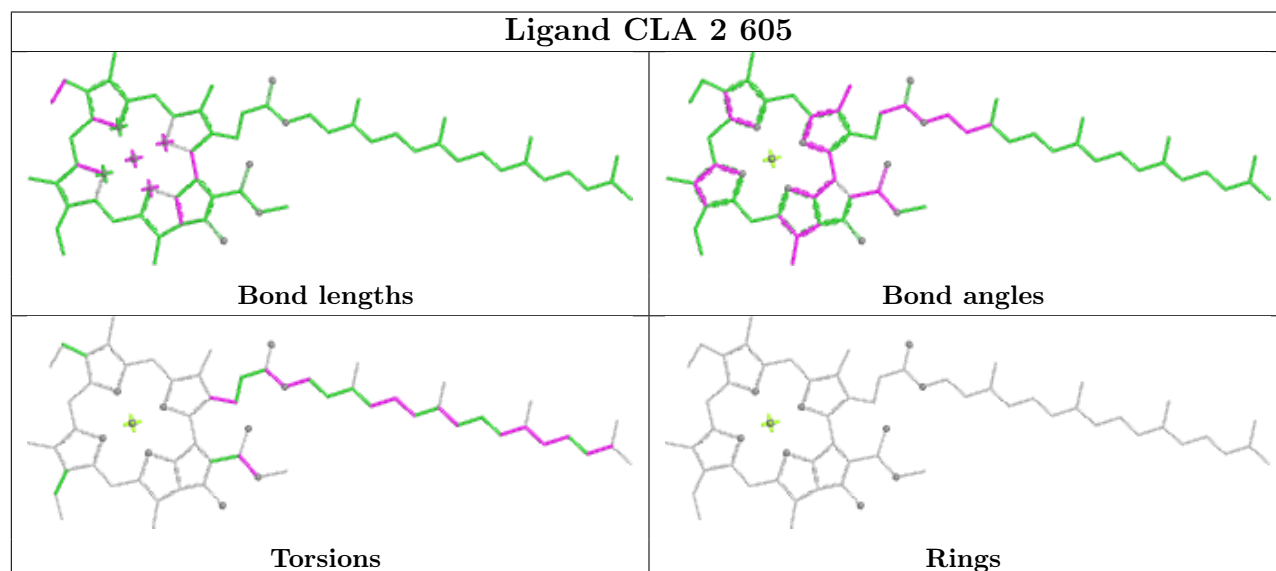
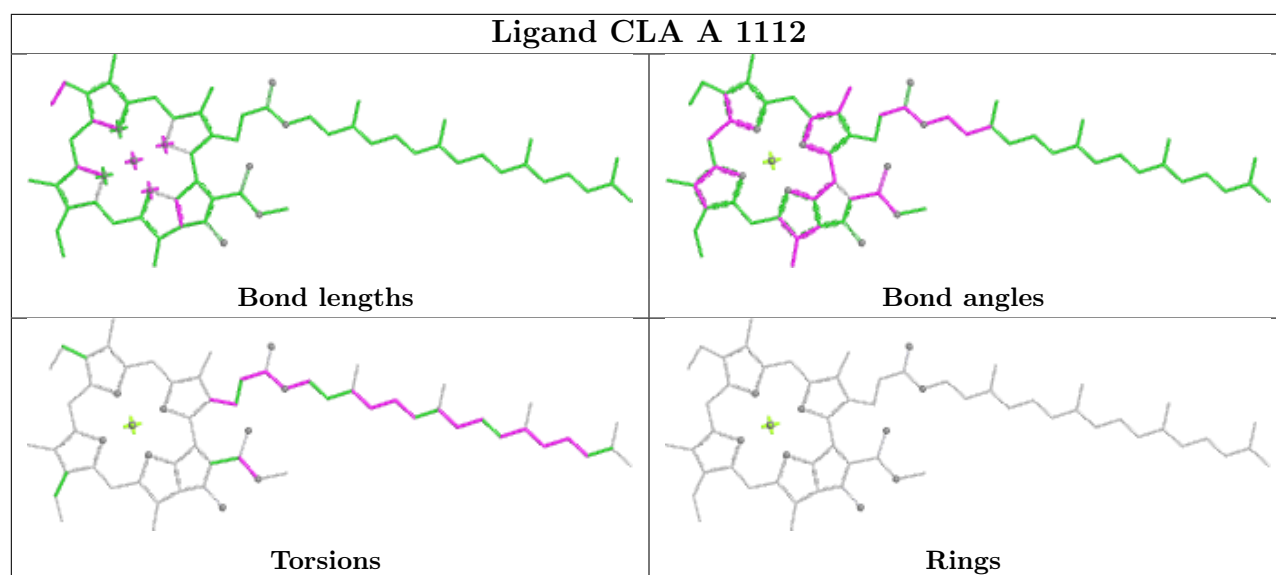


Ligand CLA 4 602

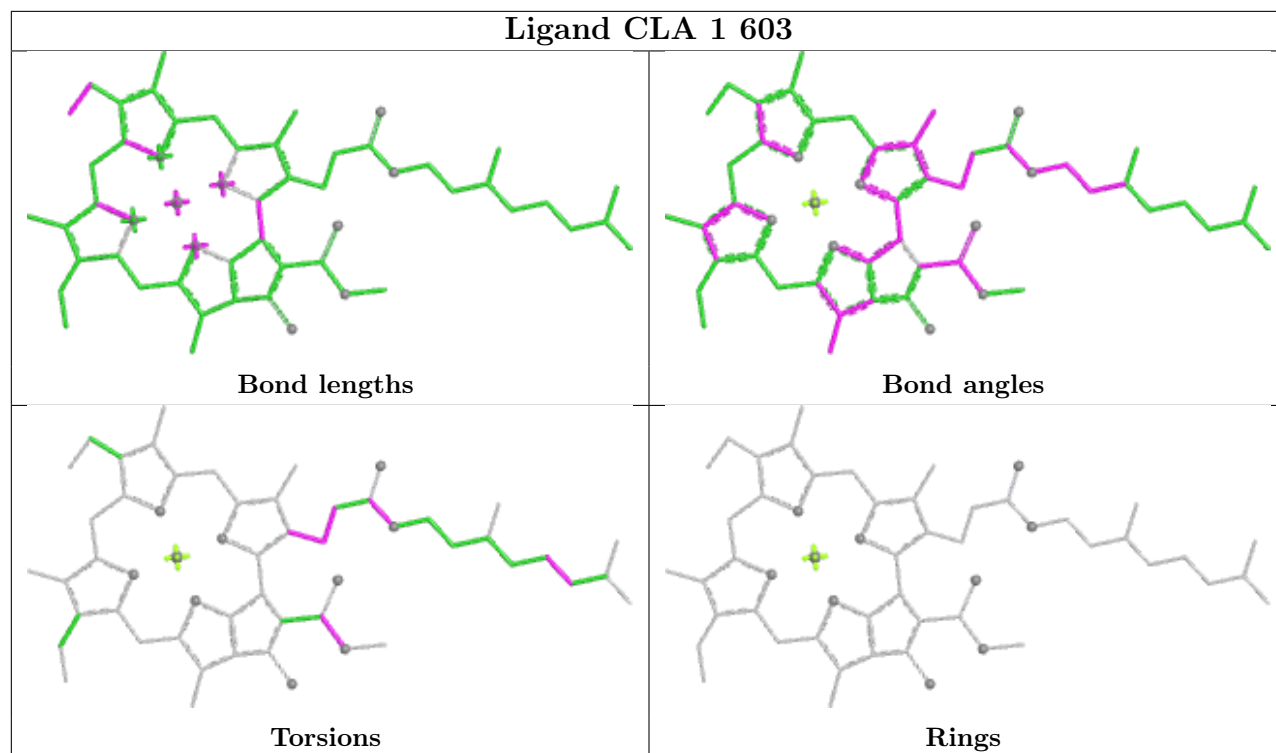


Ligand LMT B 5006

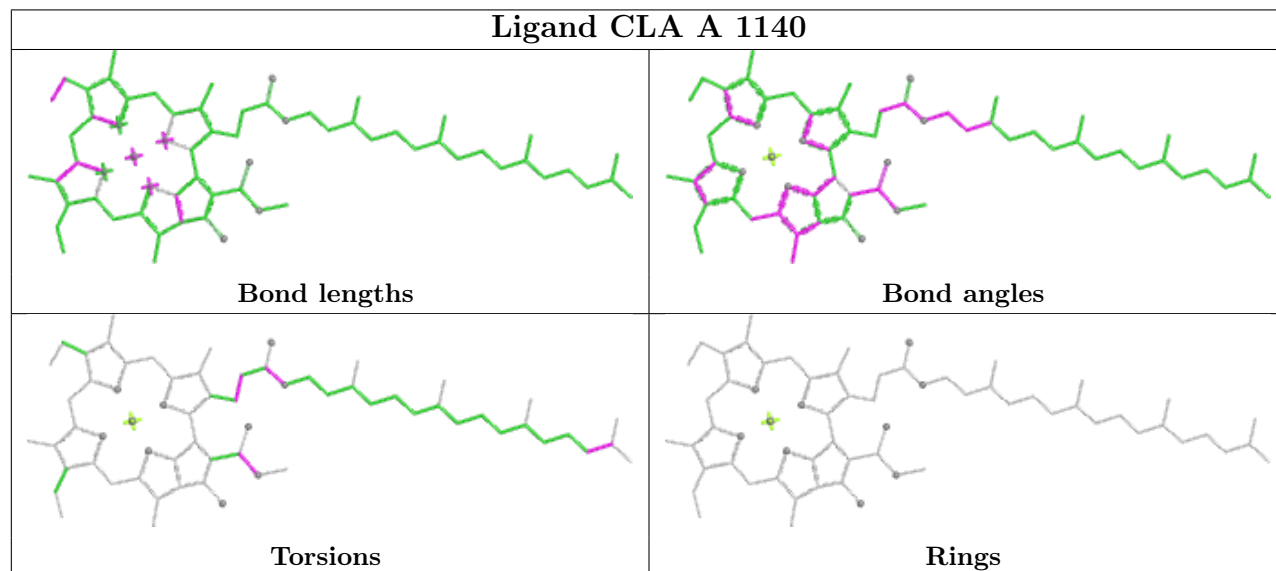




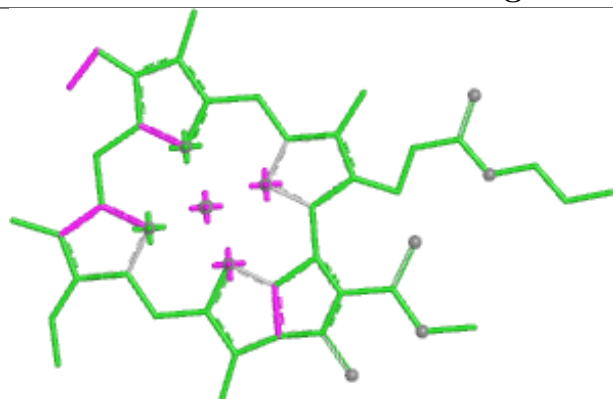
Ligand CLA 1 603



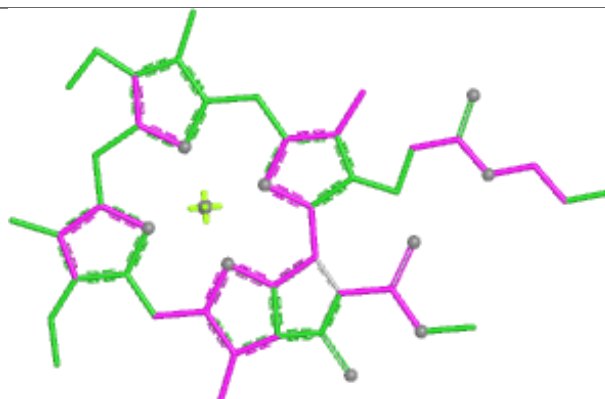
Ligand CLA A 1140



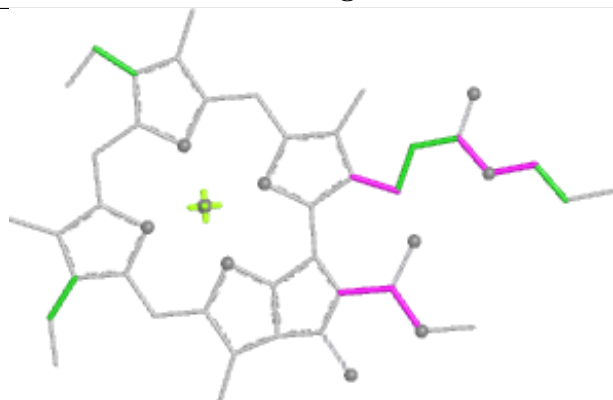
Ligand CLA K 1403



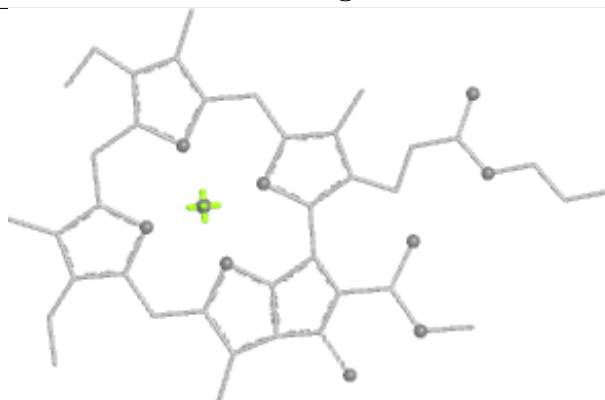
Bond lengths



Bond angles

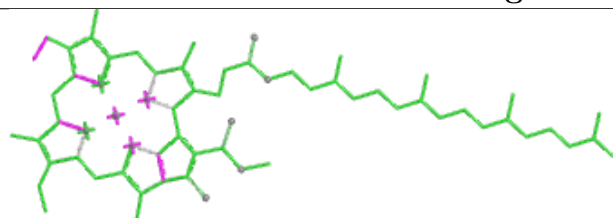


Torsions

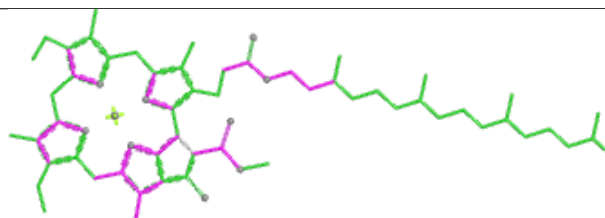


Rings

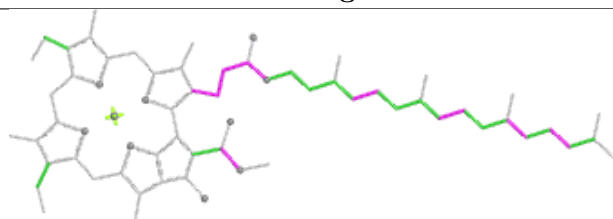
Ligand CLA B 1215



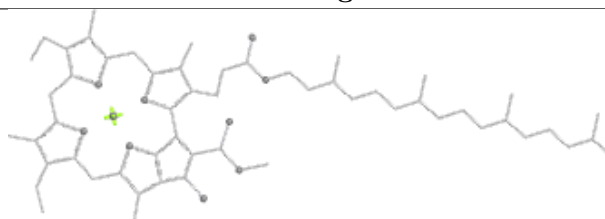
Bond lengths



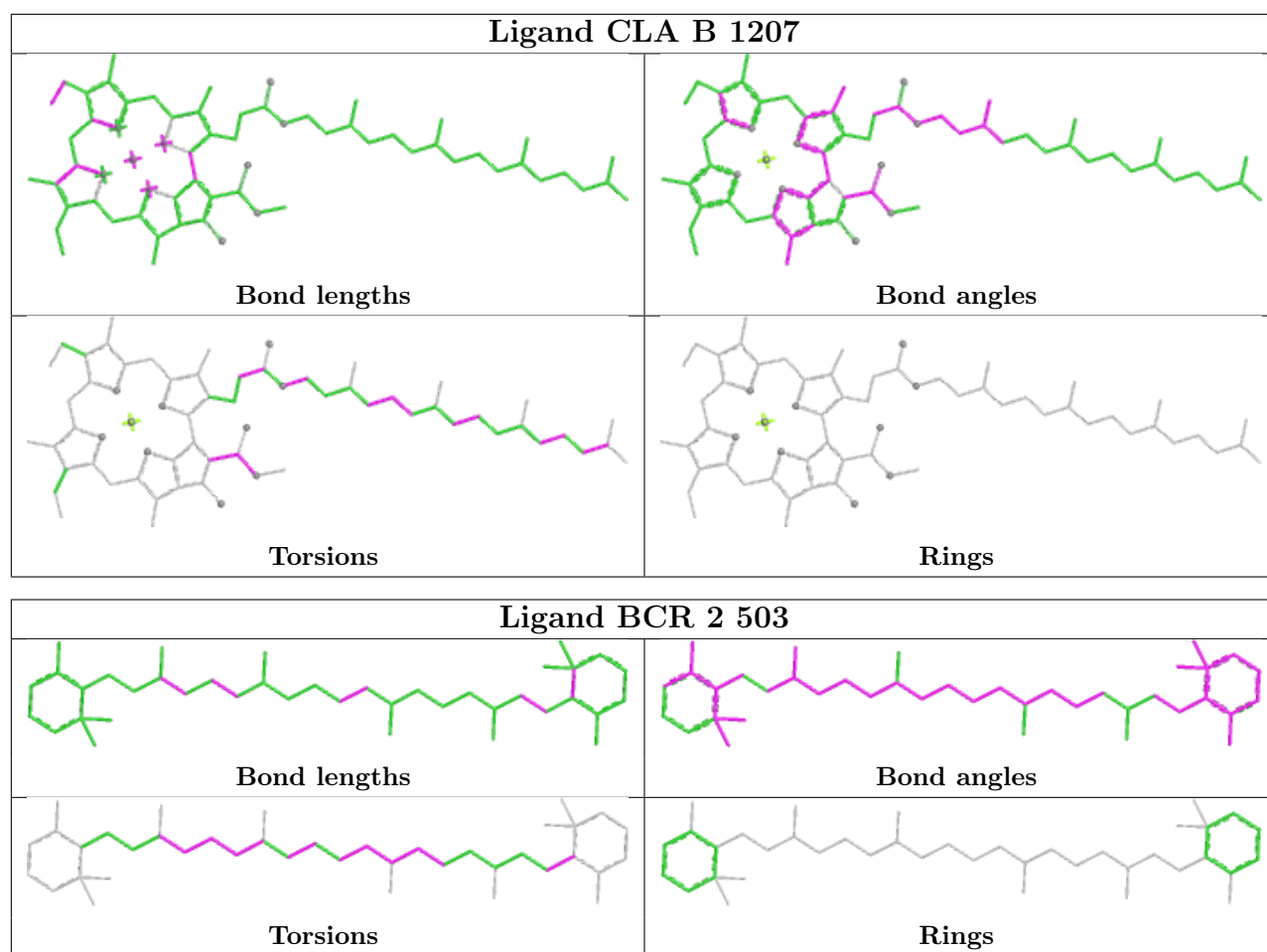
Bond angles



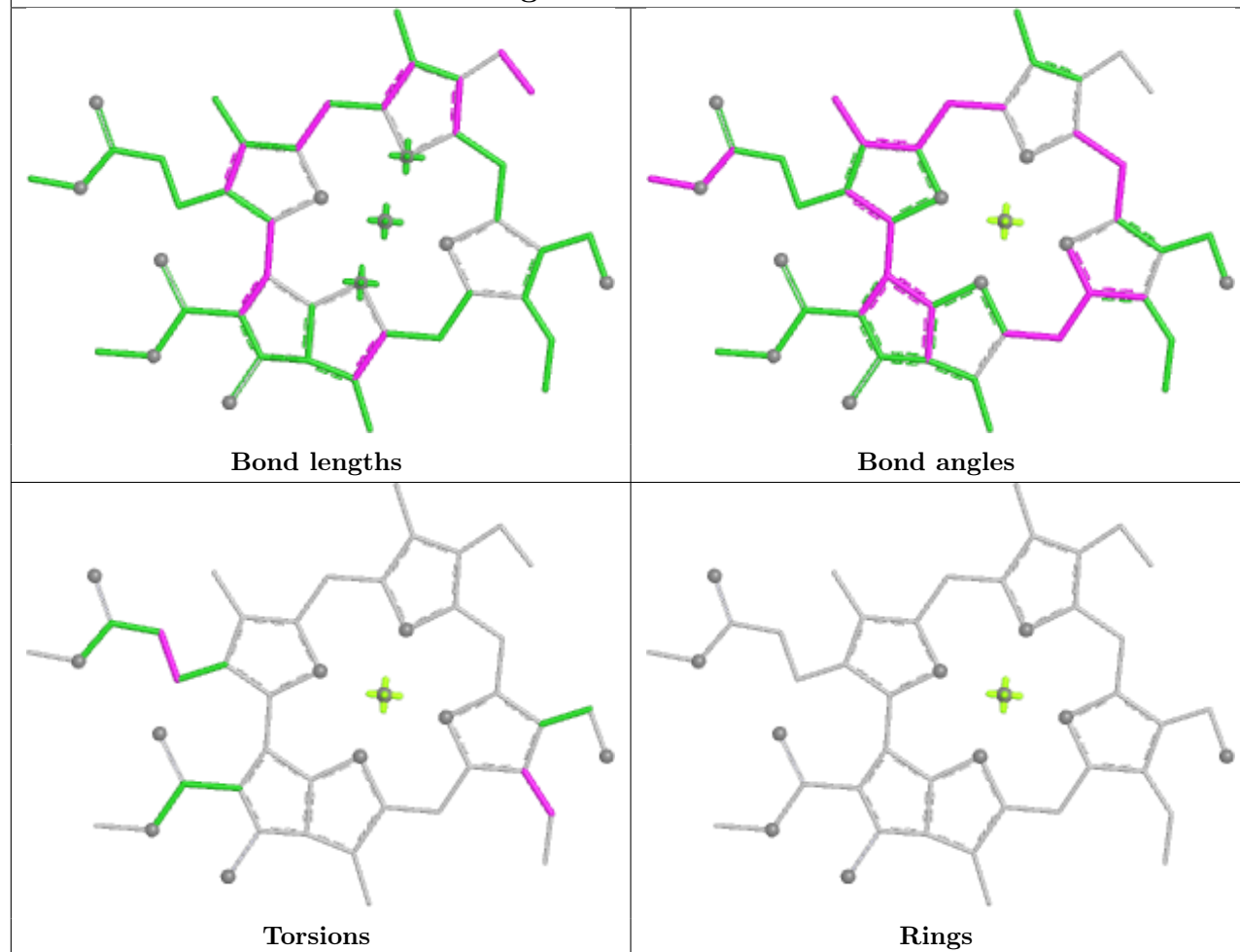
Torsions



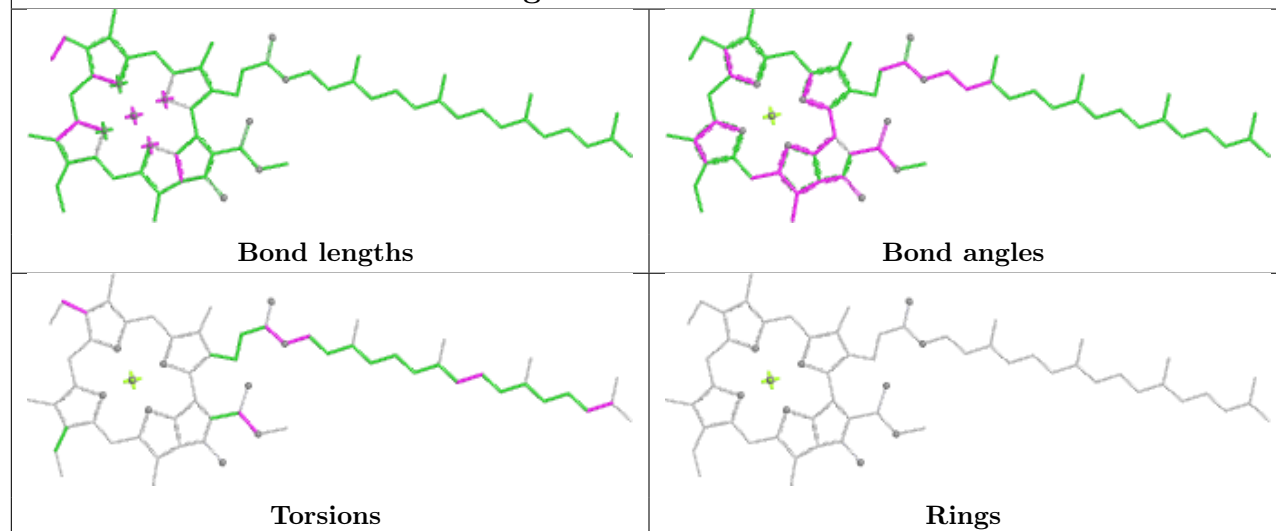
Rings

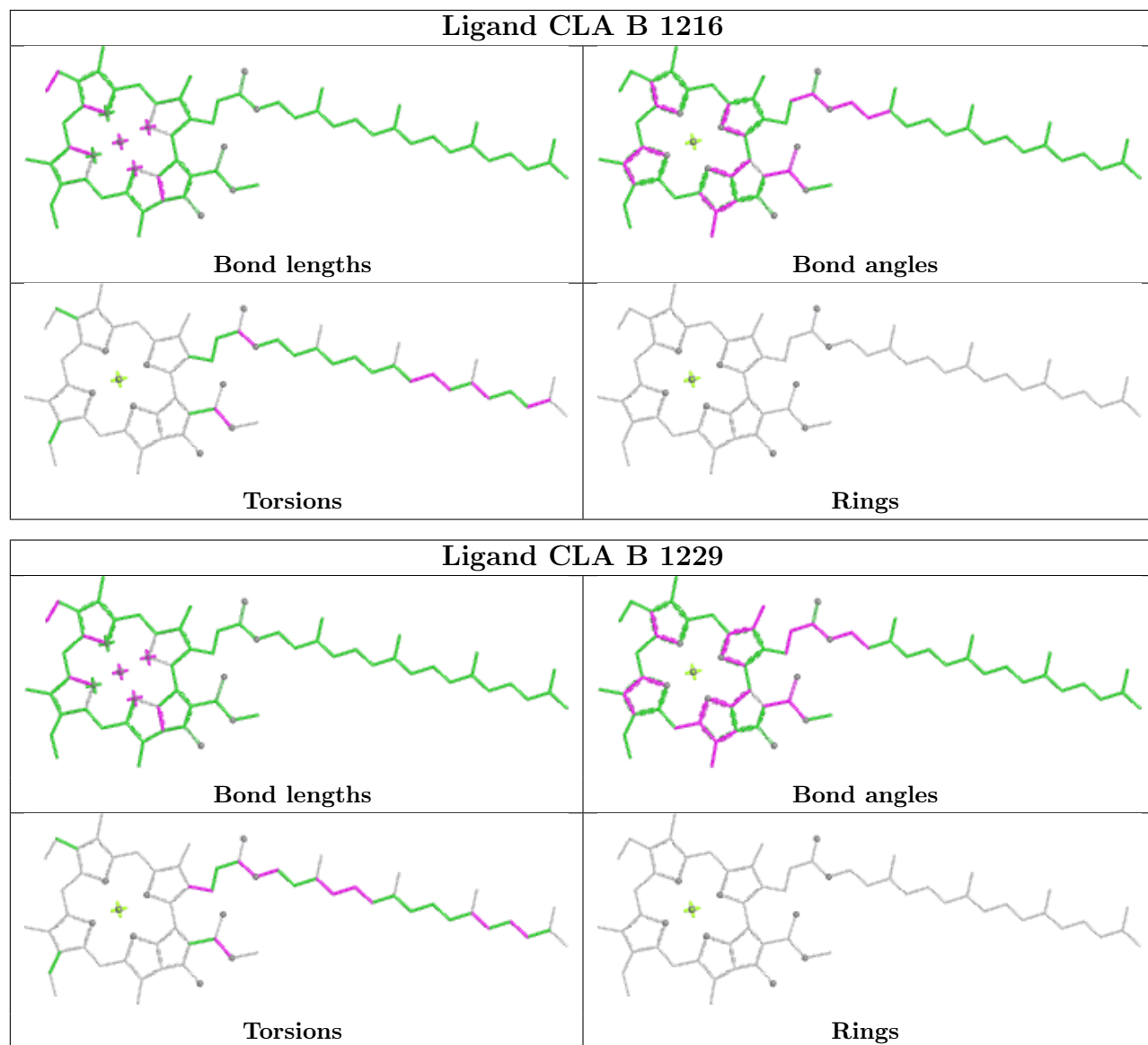


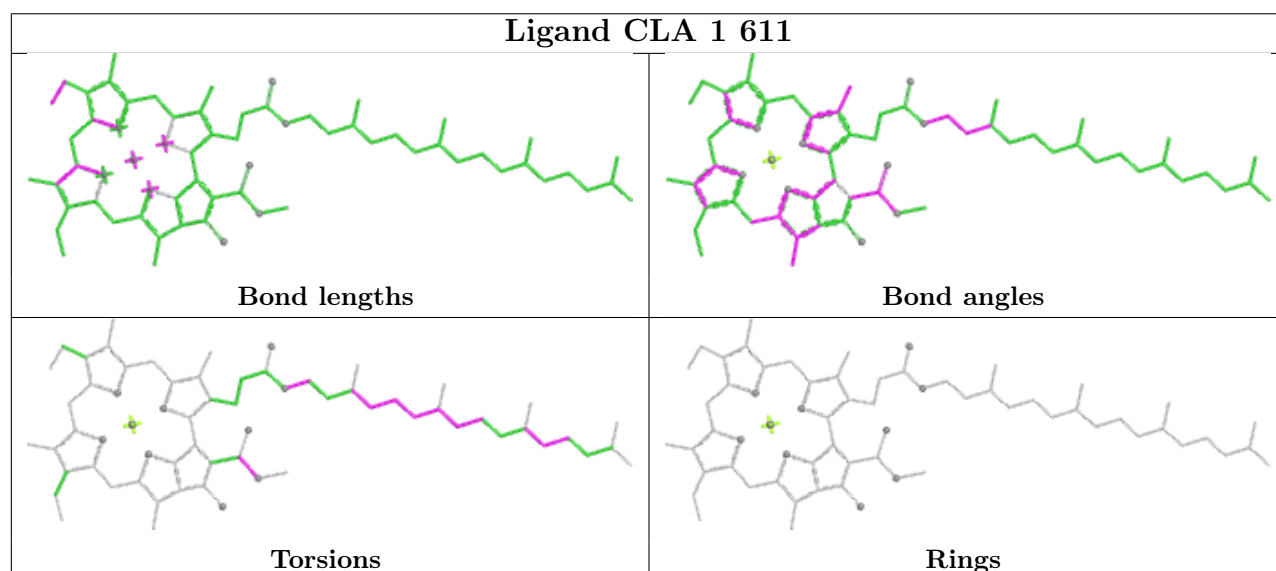
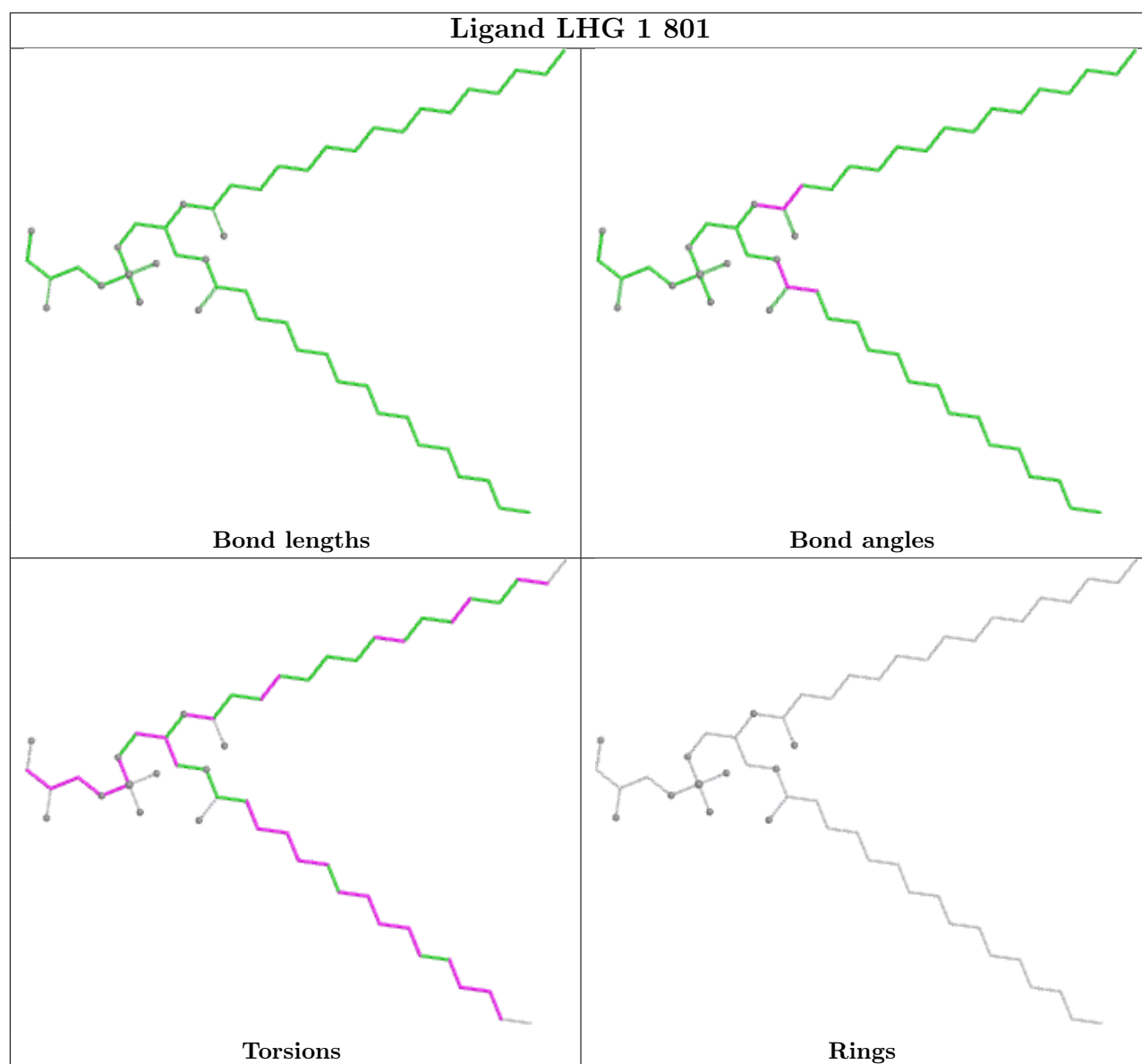
Ligand CHL 1 610



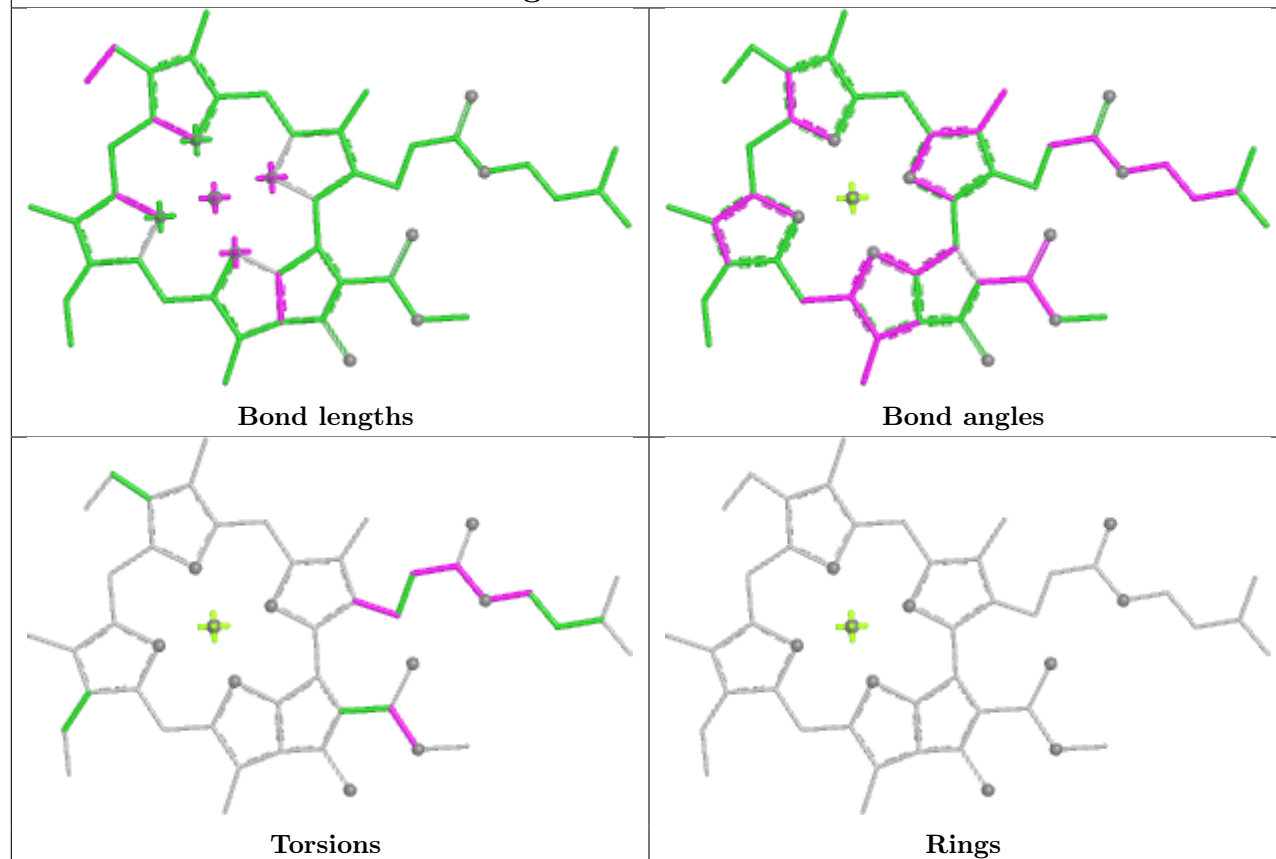
Ligand CLA B 1022



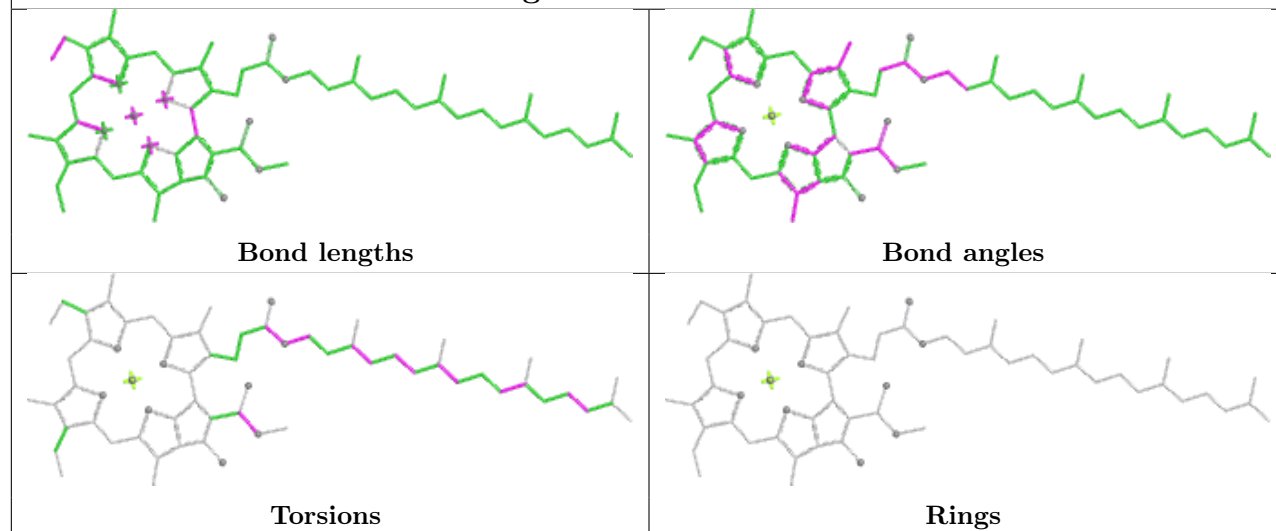


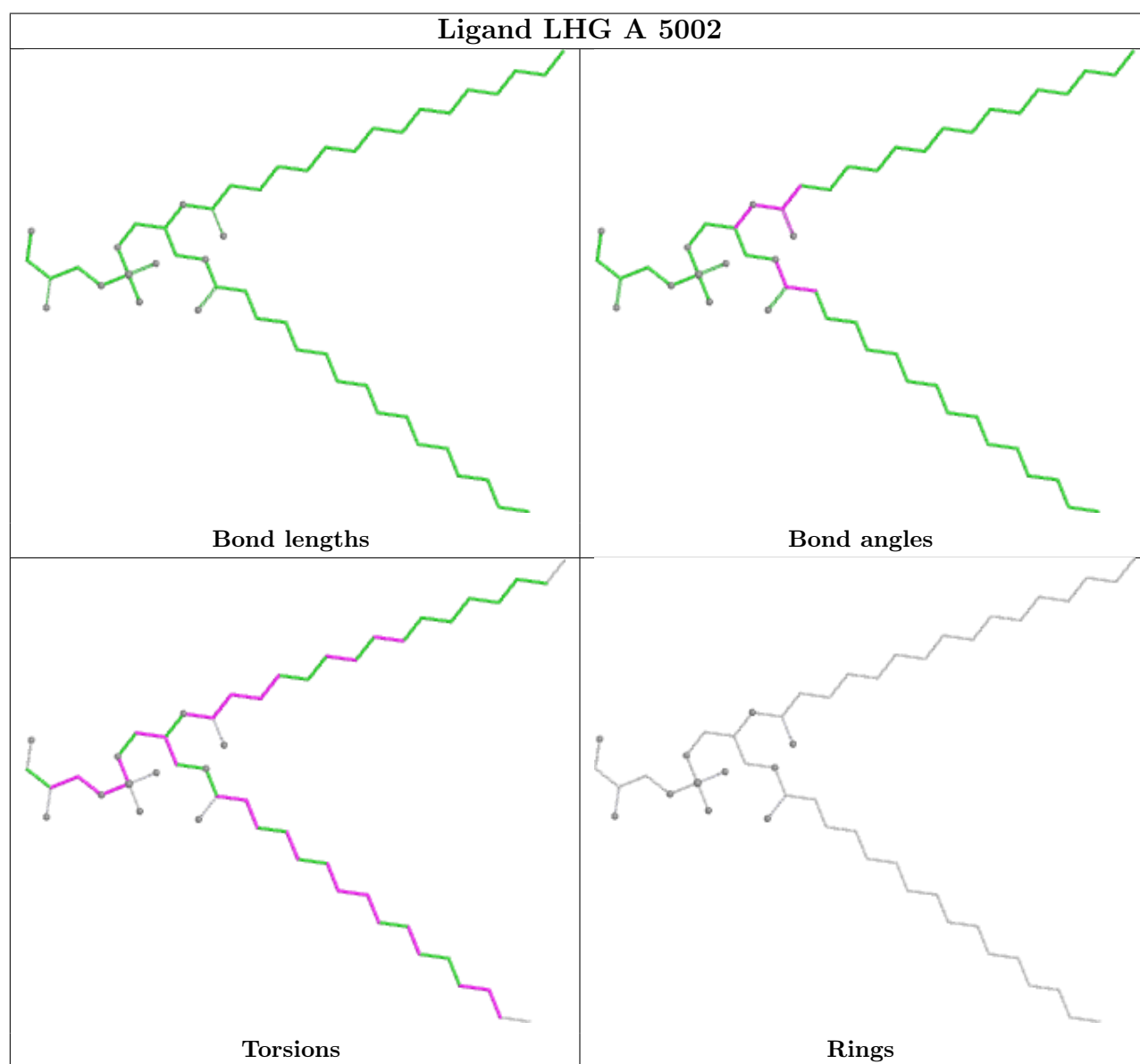
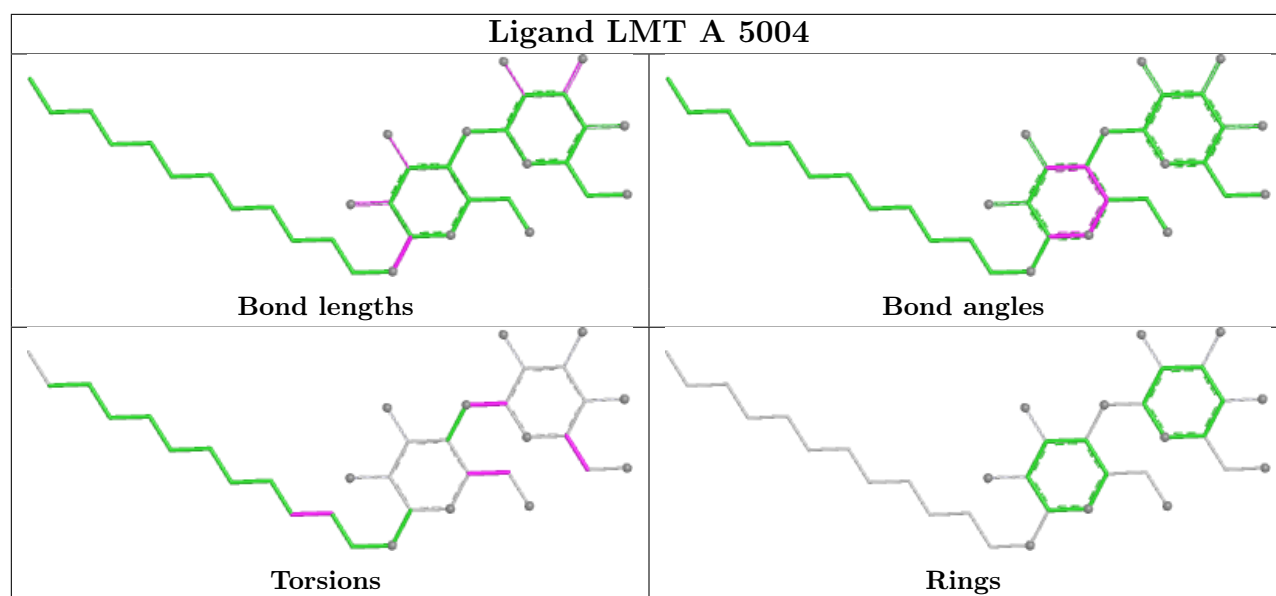


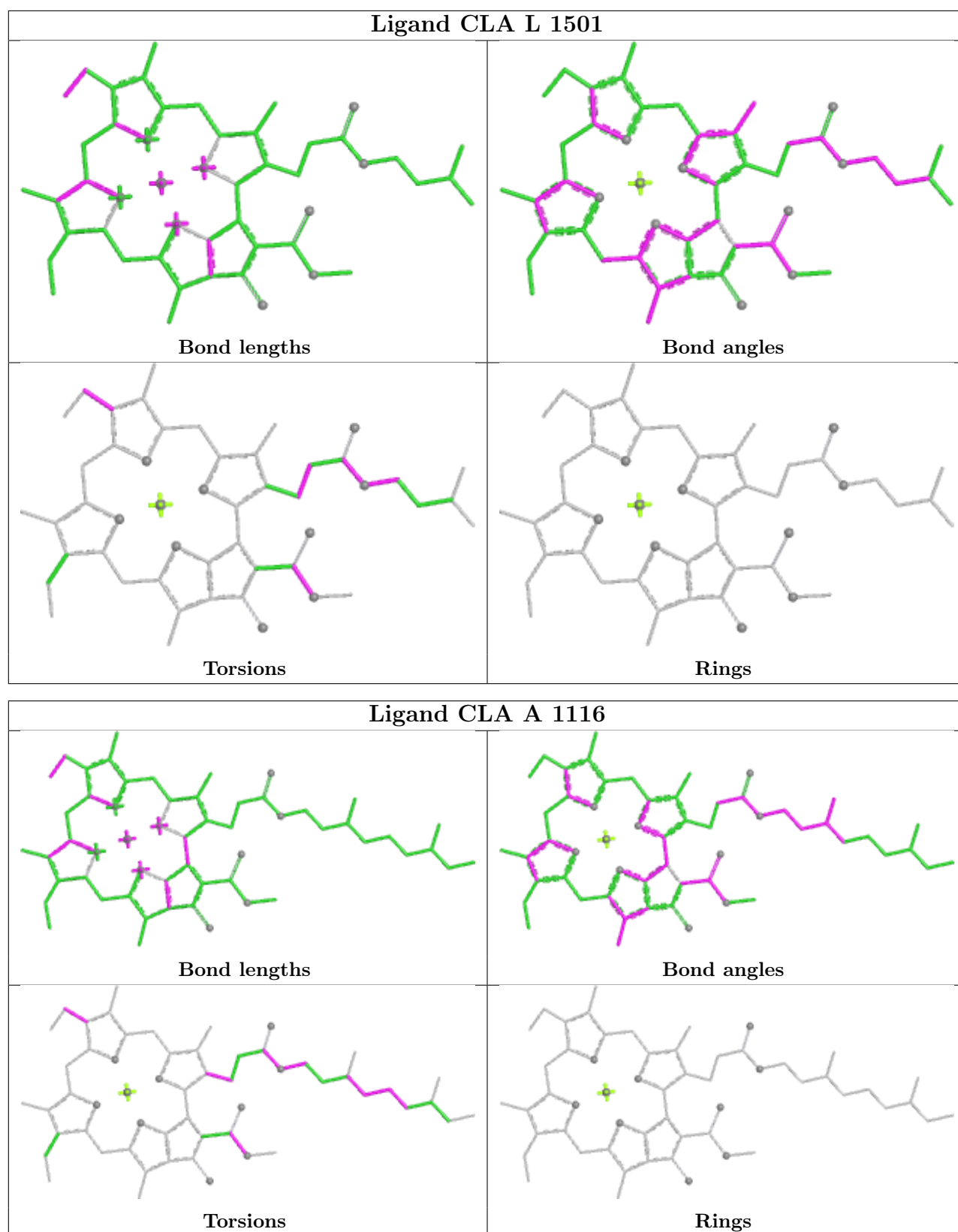
Ligand CLA B 1236

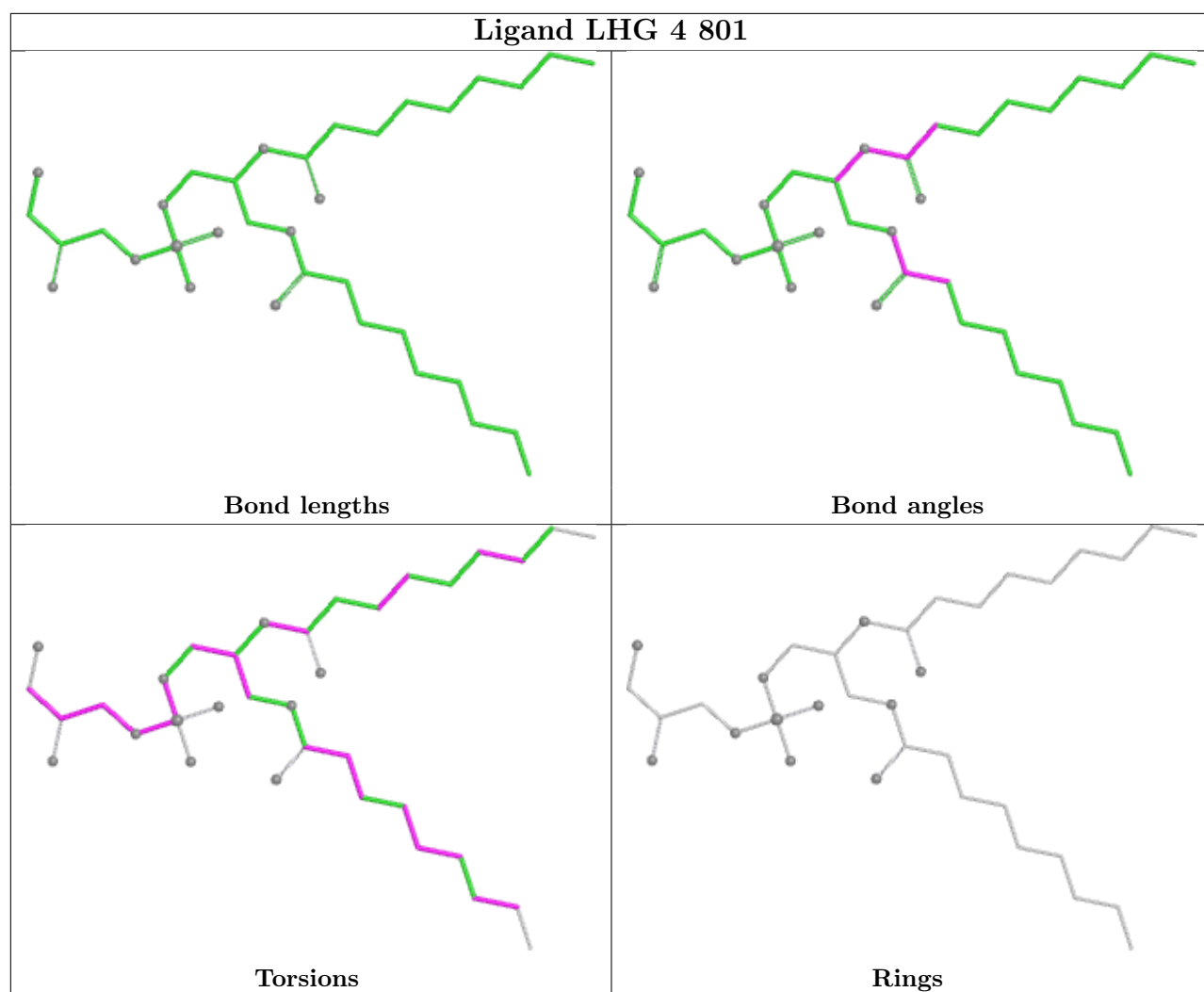


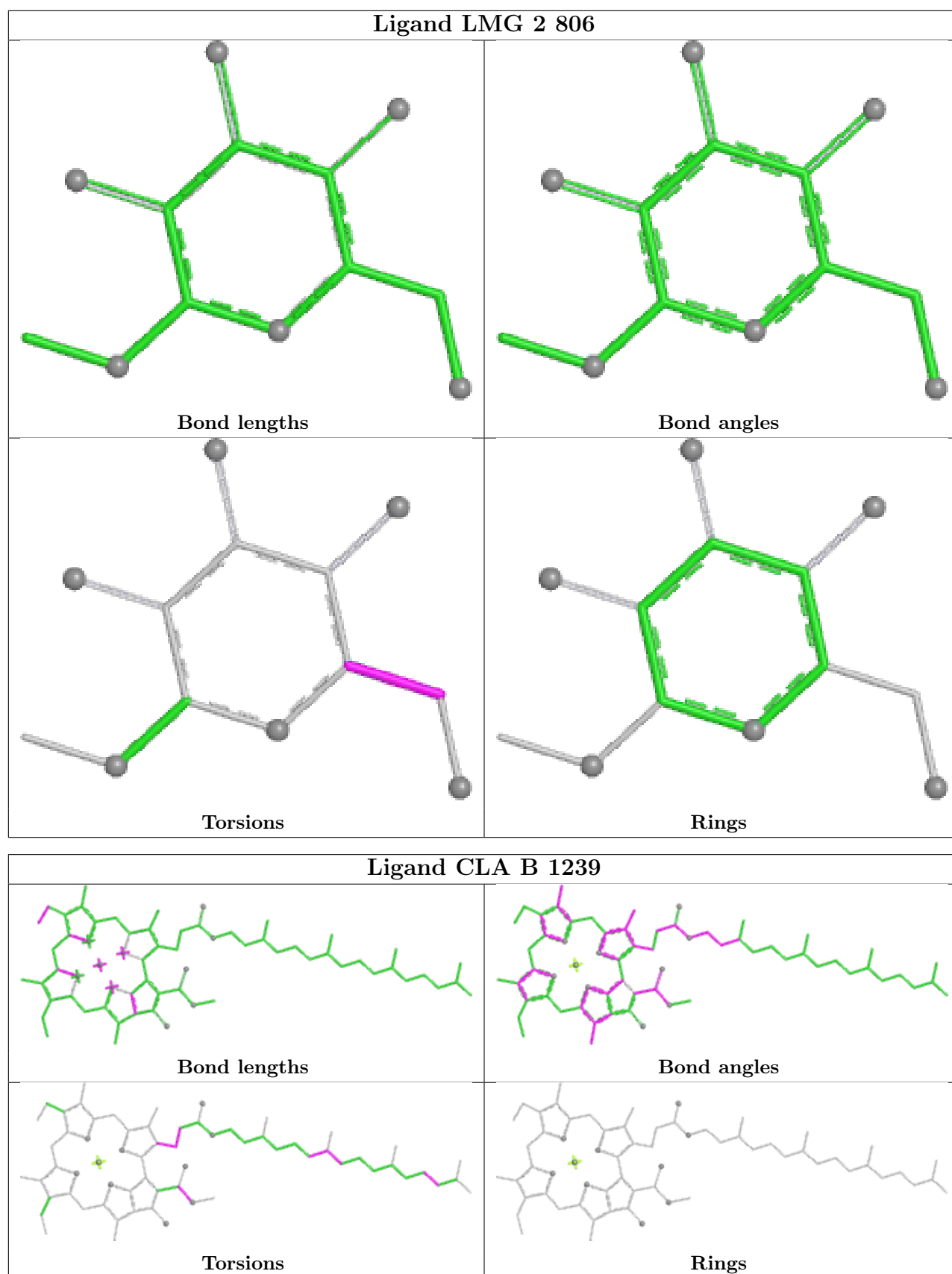
Ligand CLA A 1123

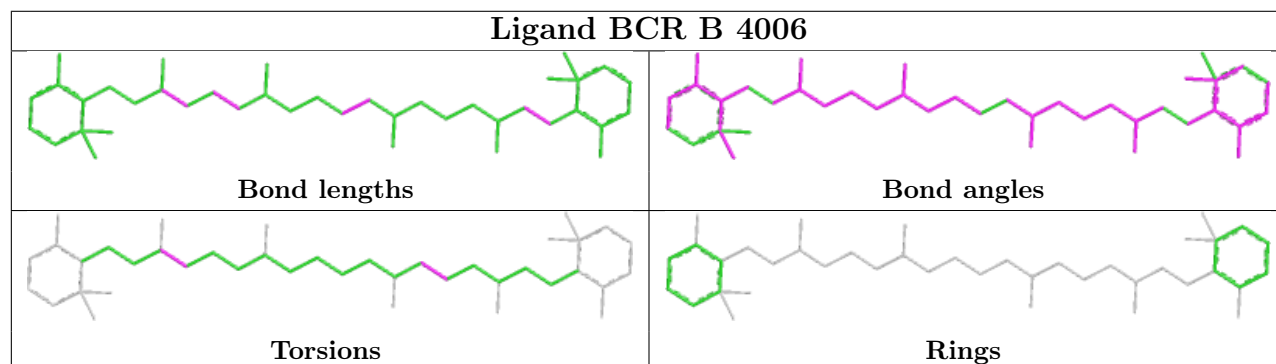
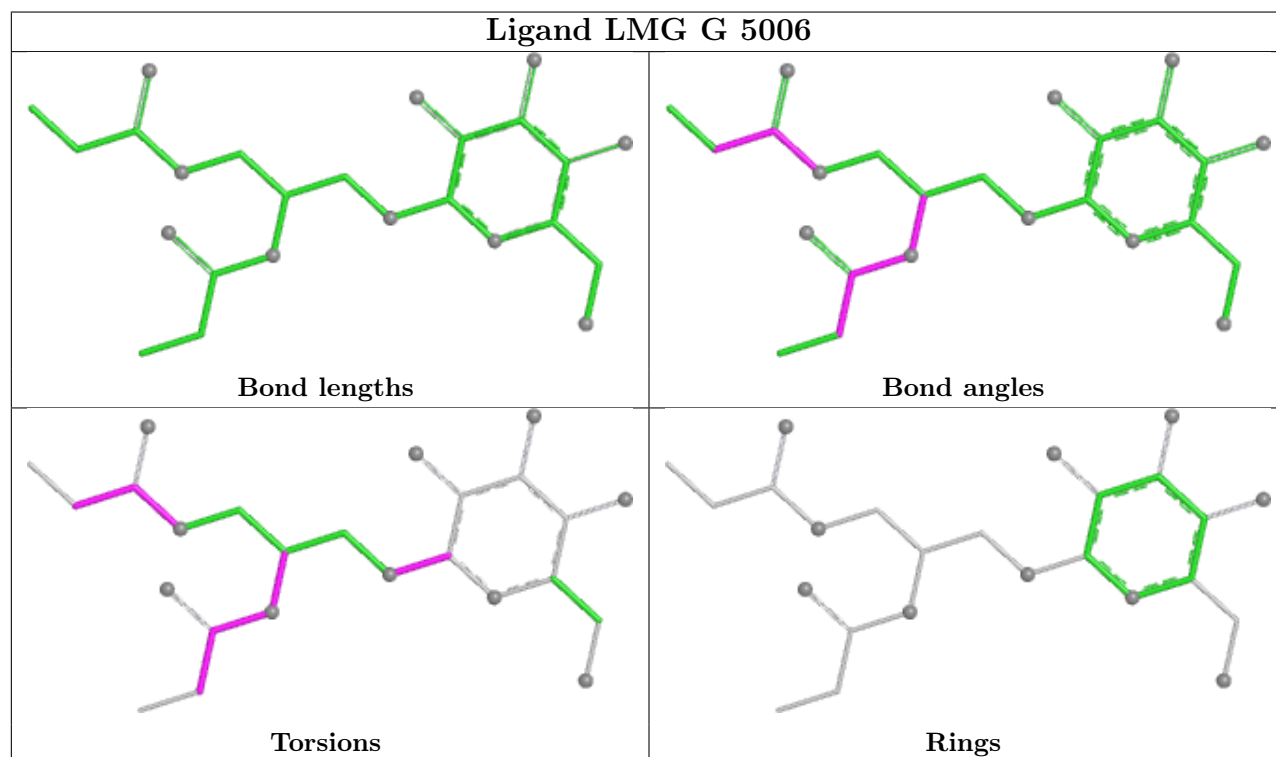
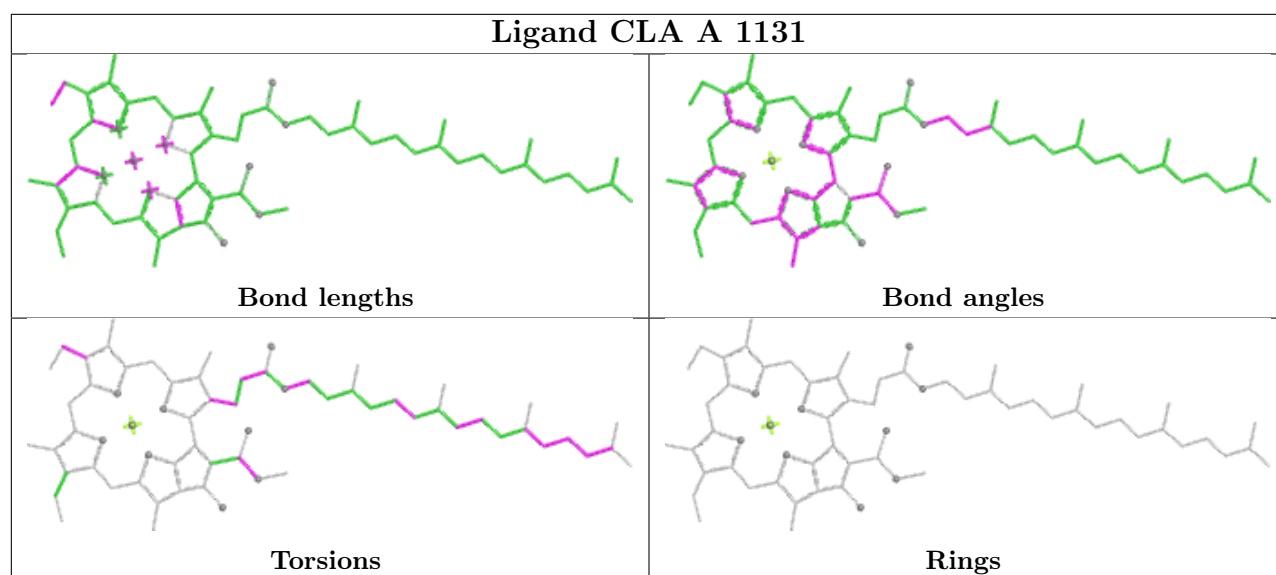


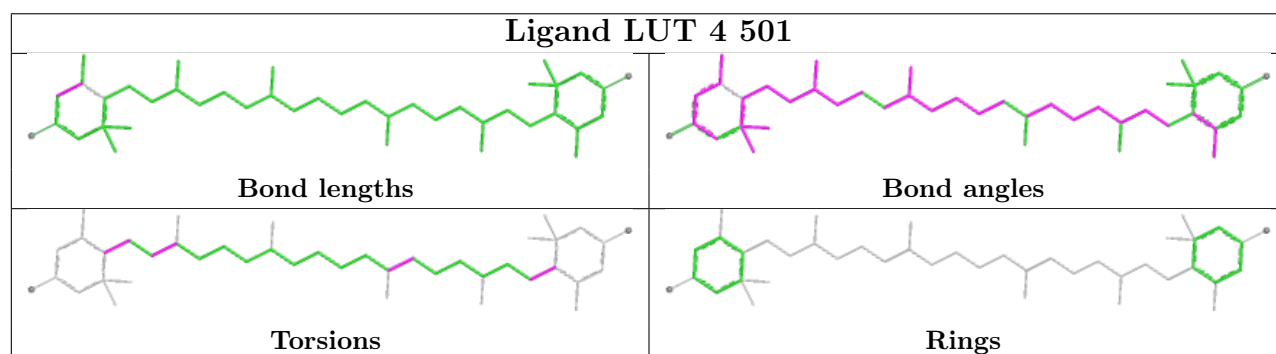
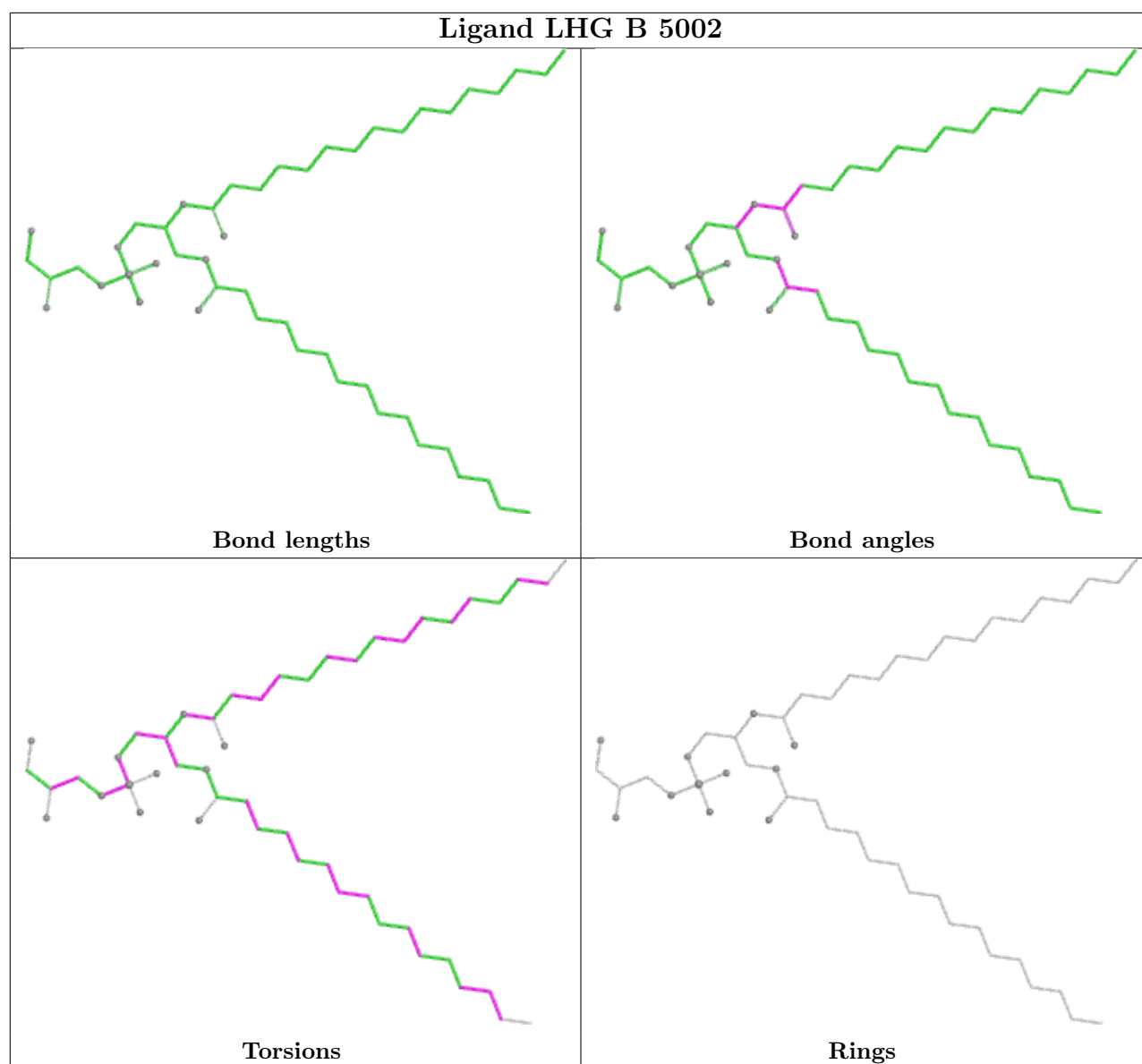




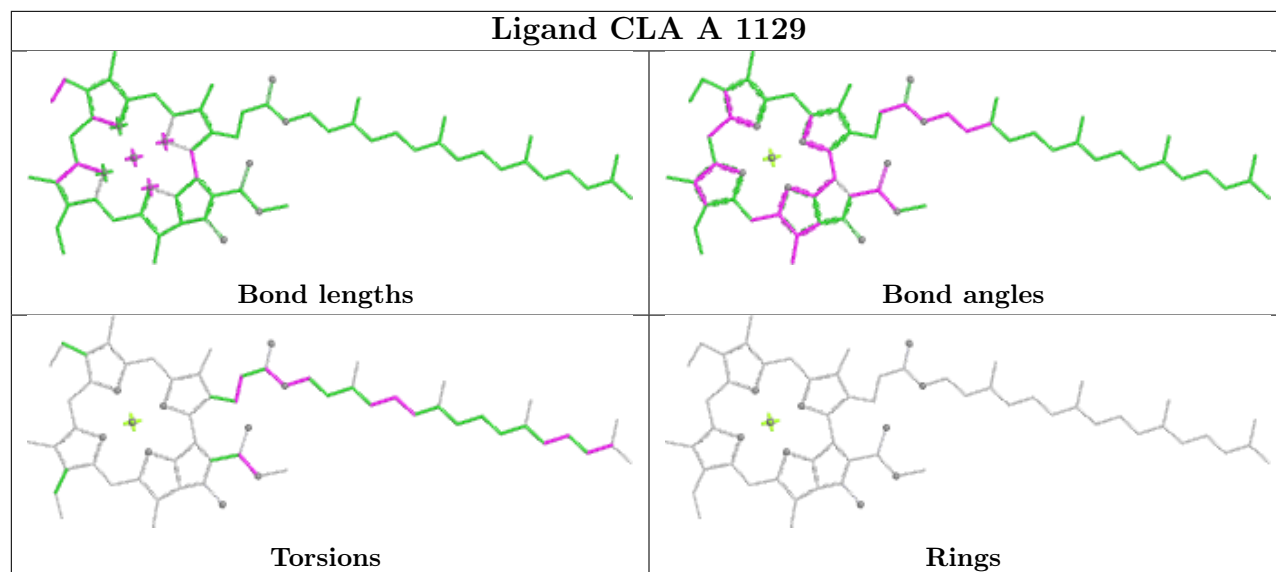




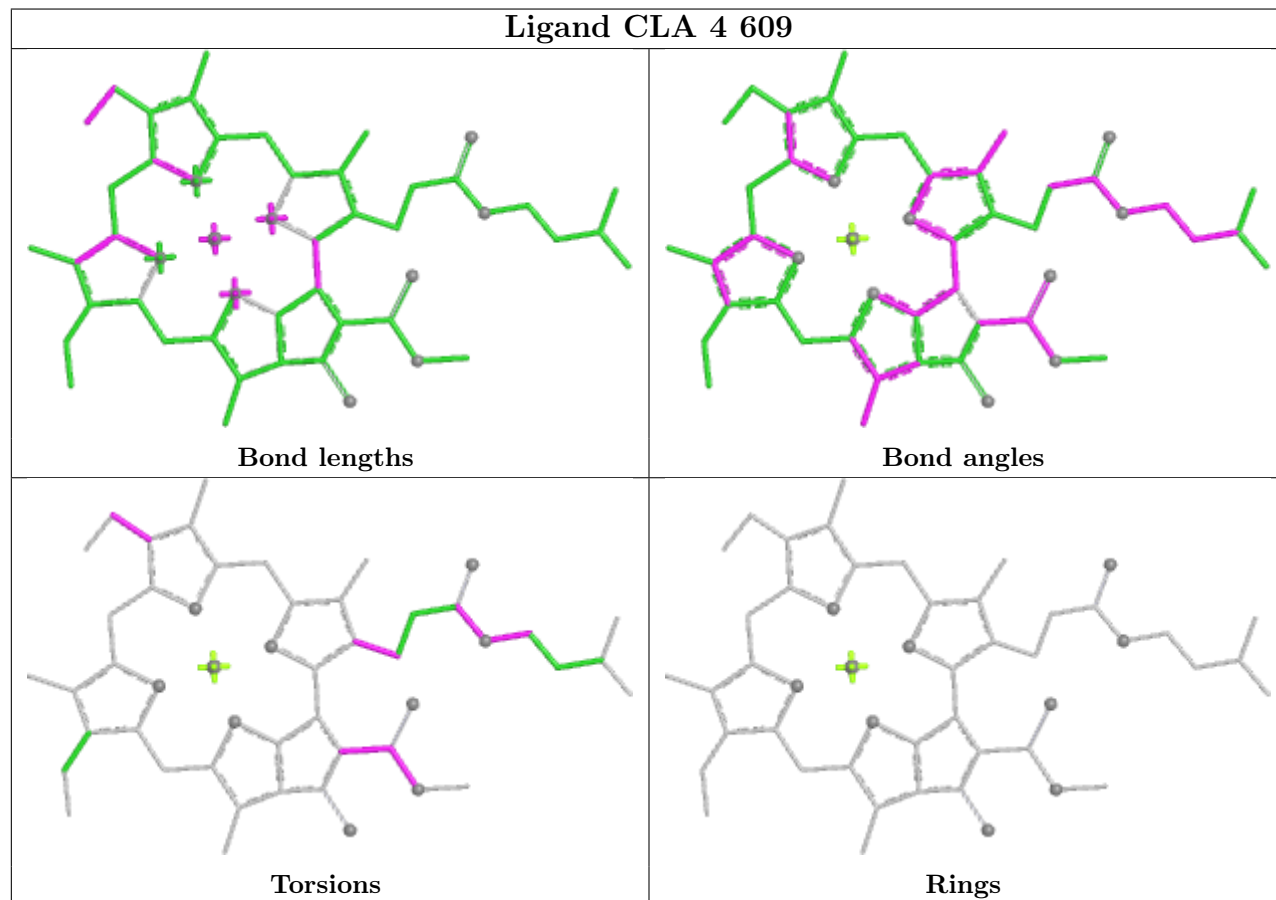


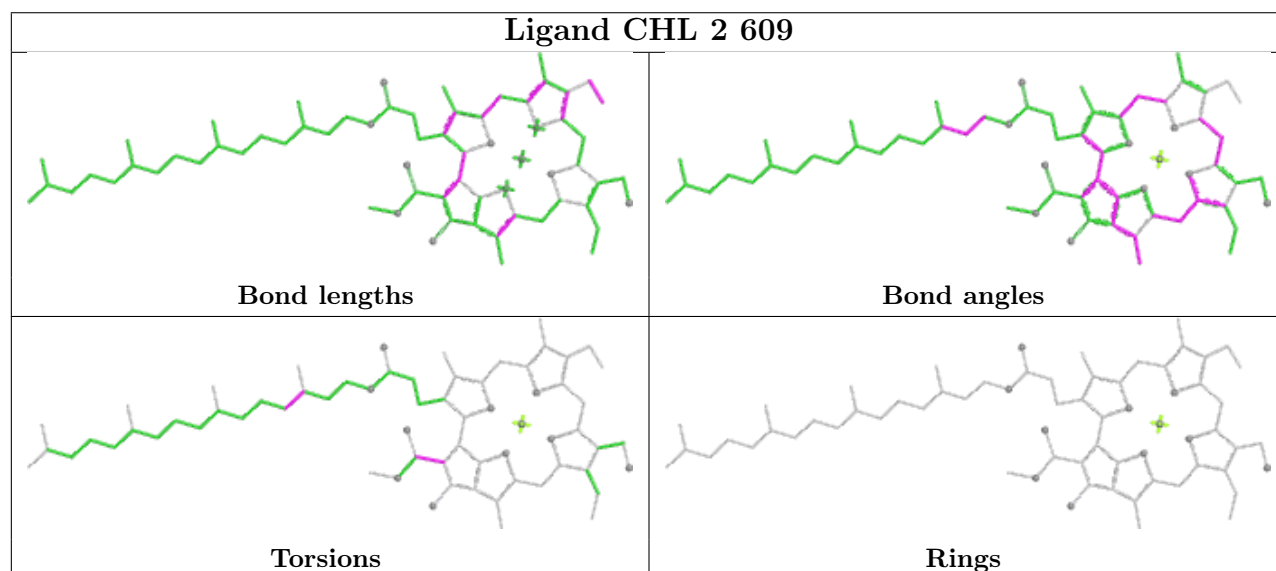
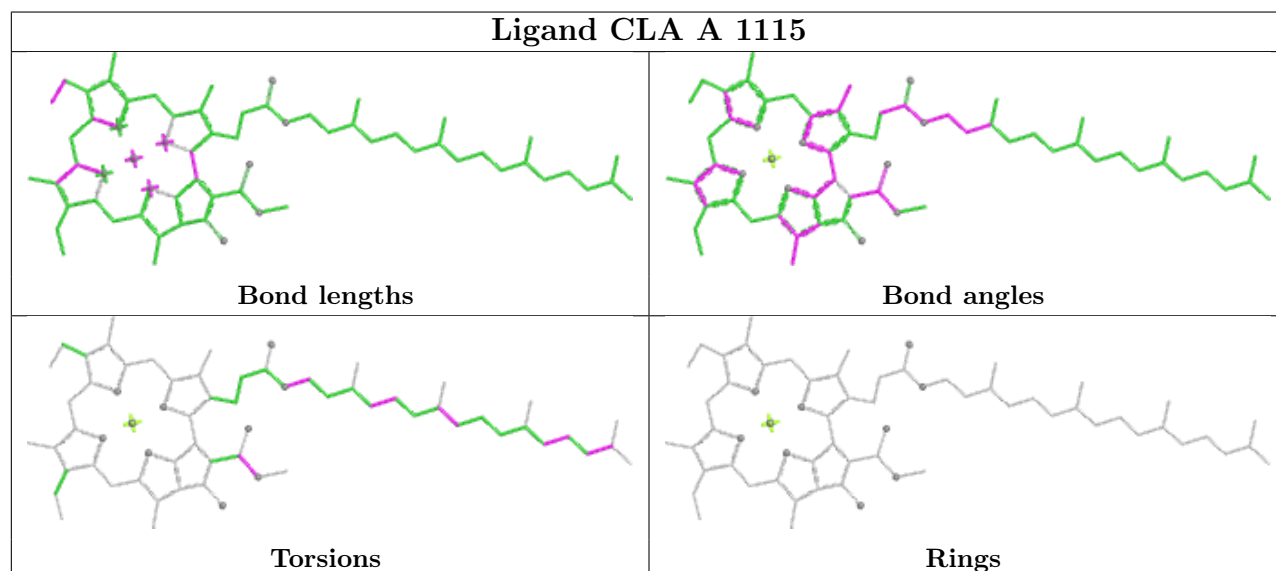
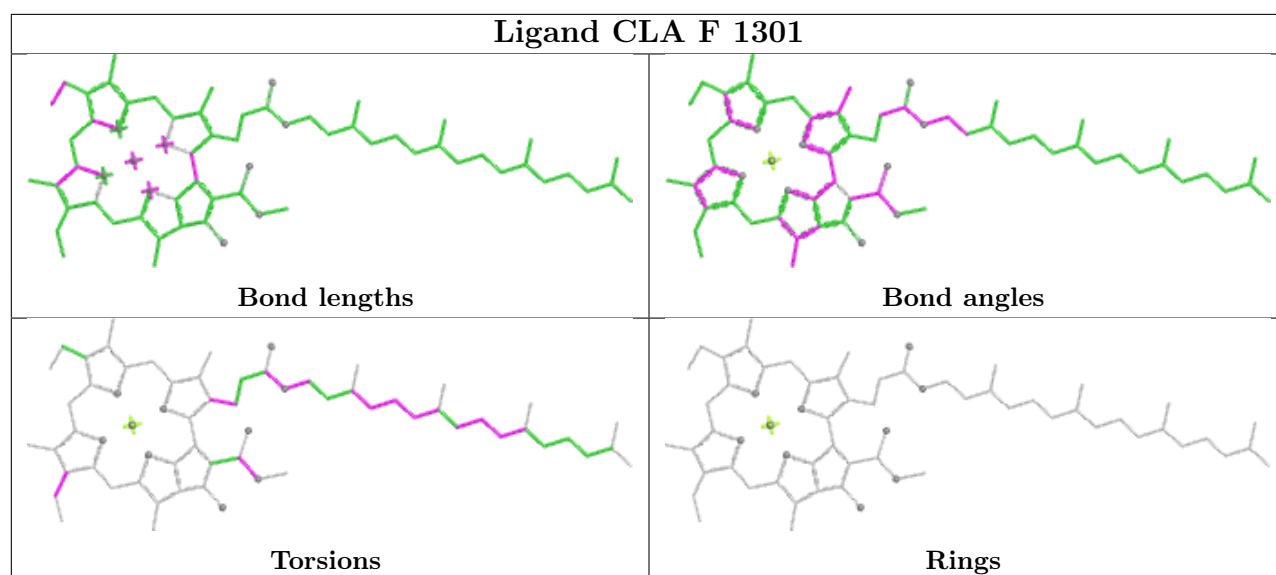


Ligand CLA A 1129

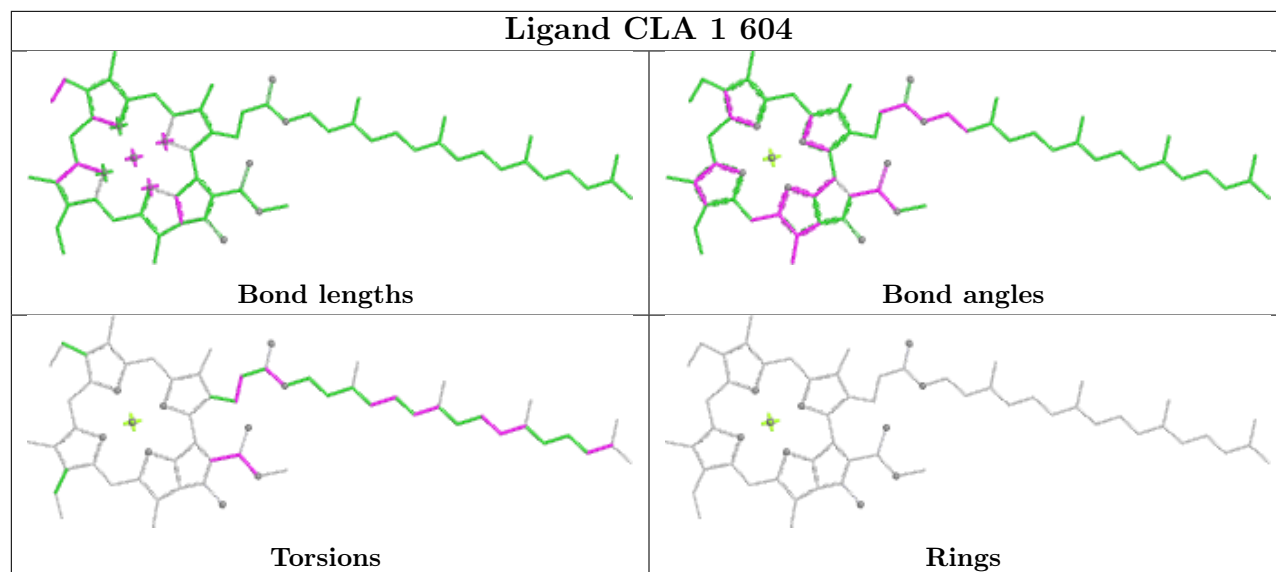


Ligand CLA 4 609

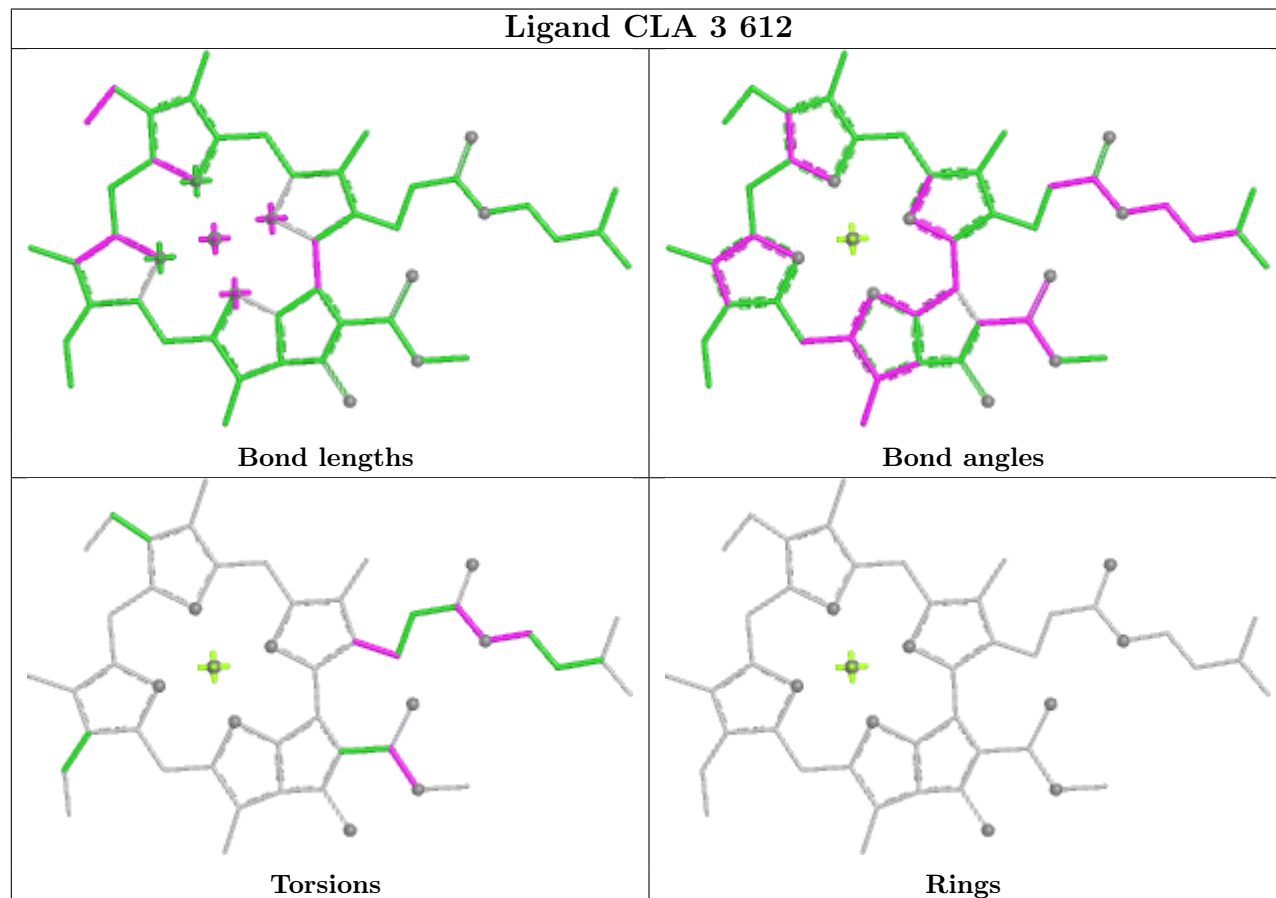




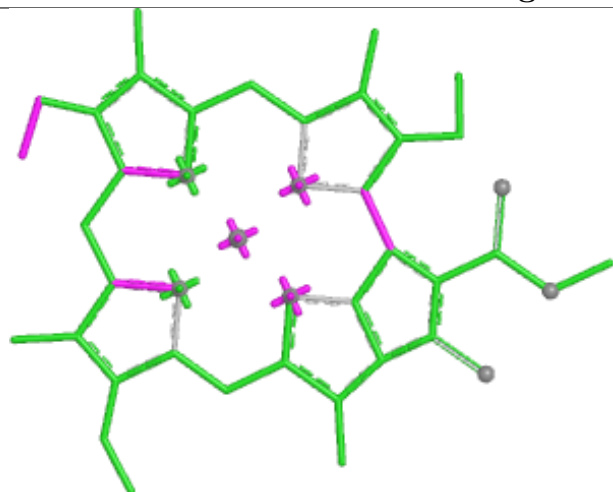
Ligand CLA 1 604



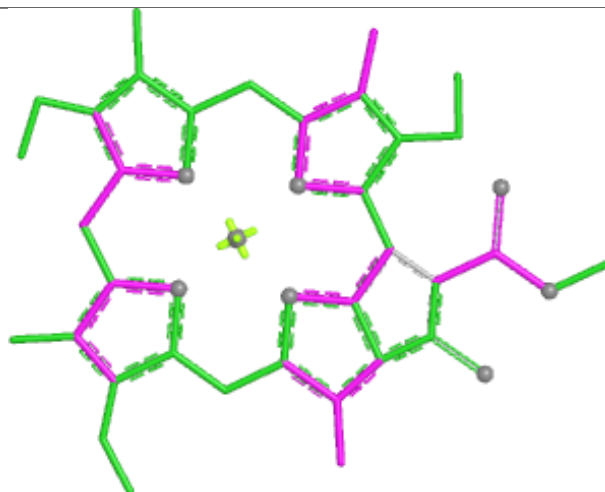
Ligand CLA 3 612



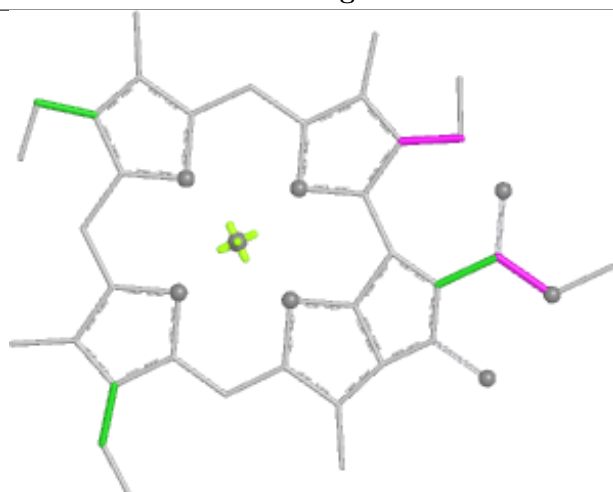
Ligand CLA 3 614



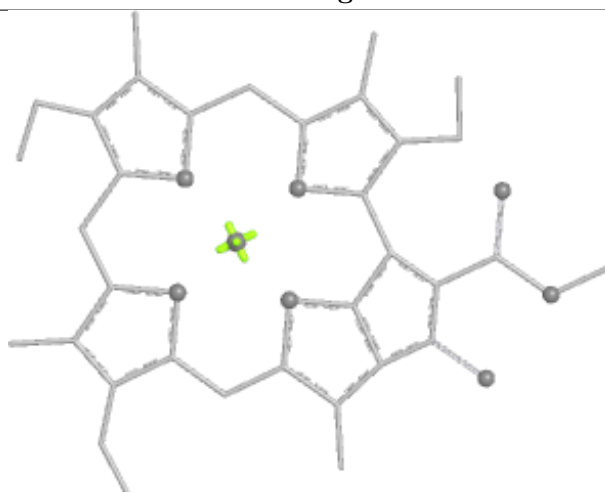
Bond lengths



Bond angles

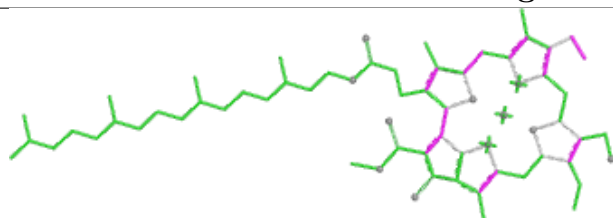


Torsions

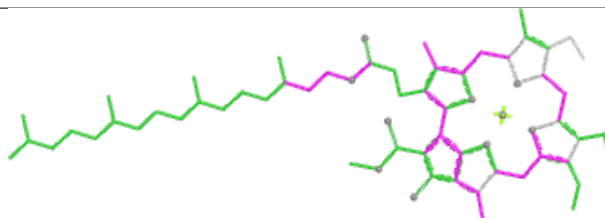


Rings

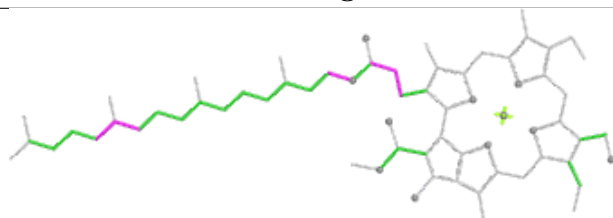
Ligand CHL 3 604



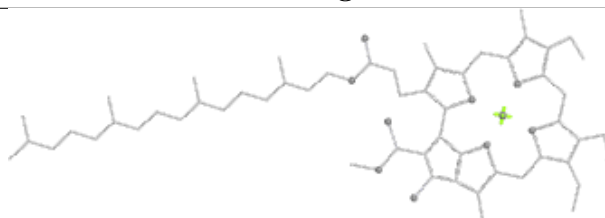
Bond lengths



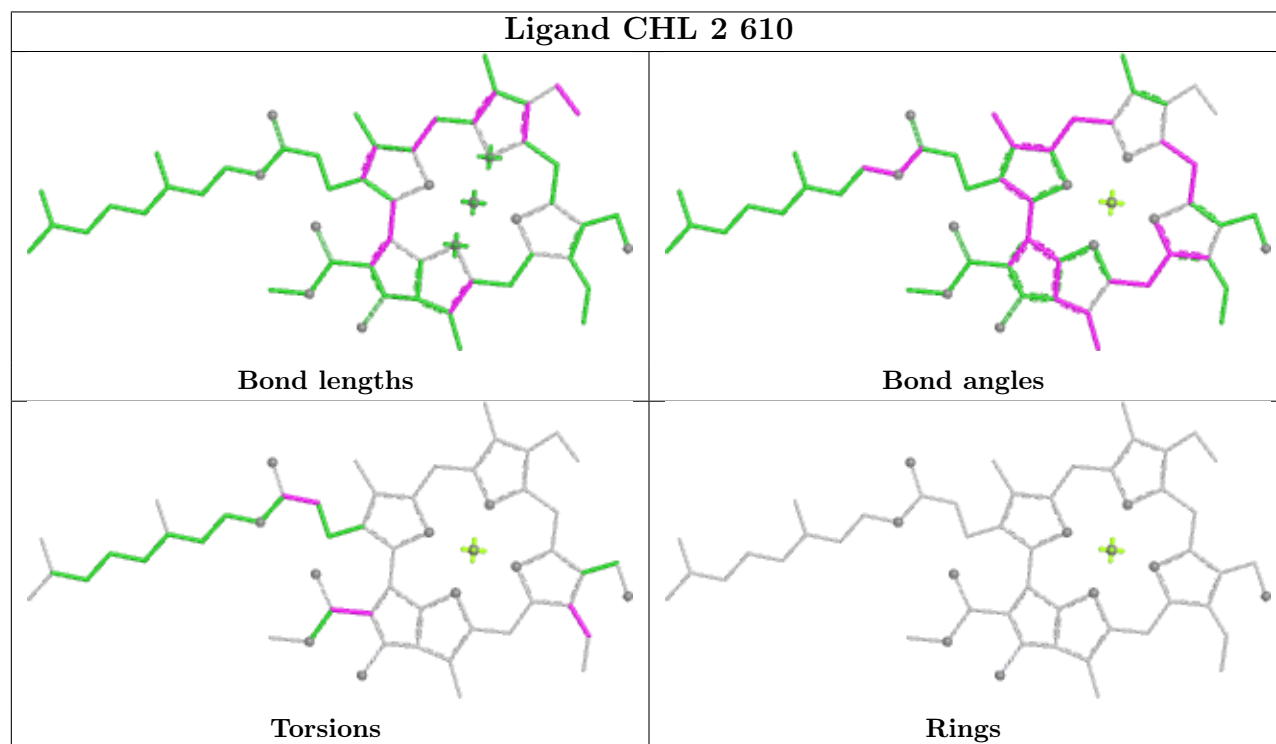
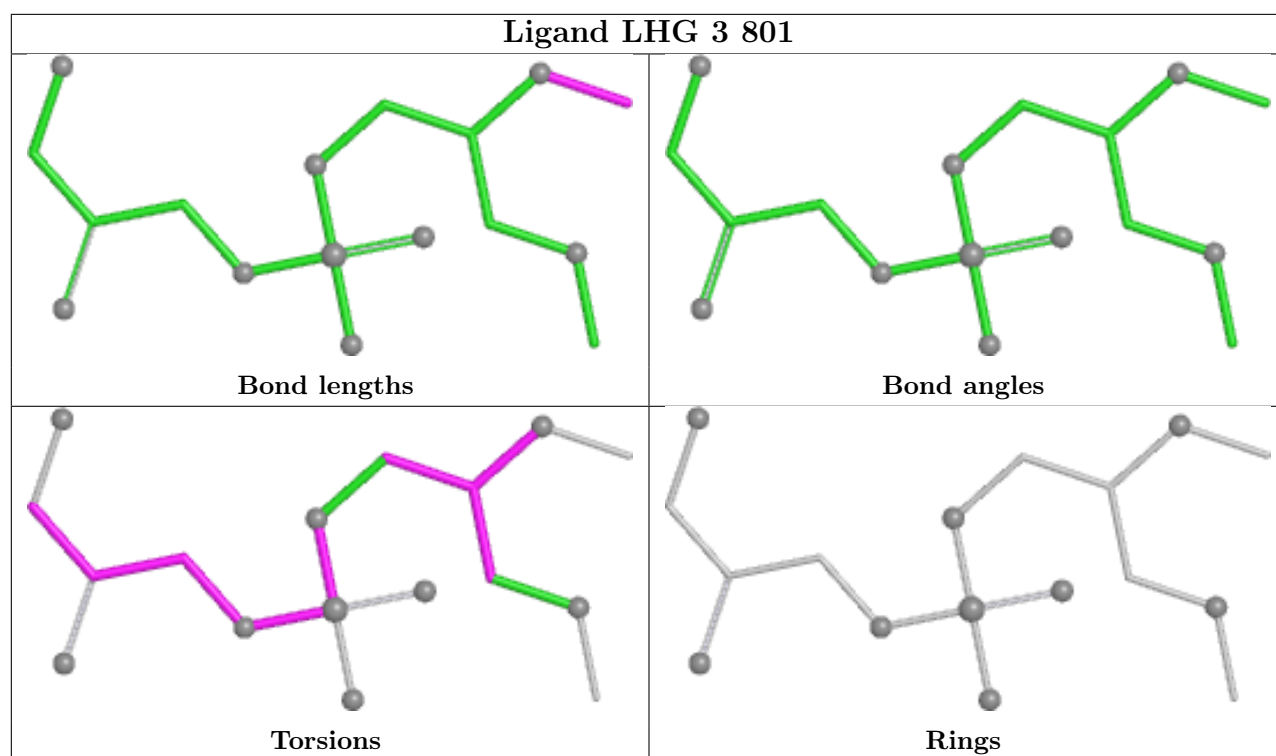
Bond angles



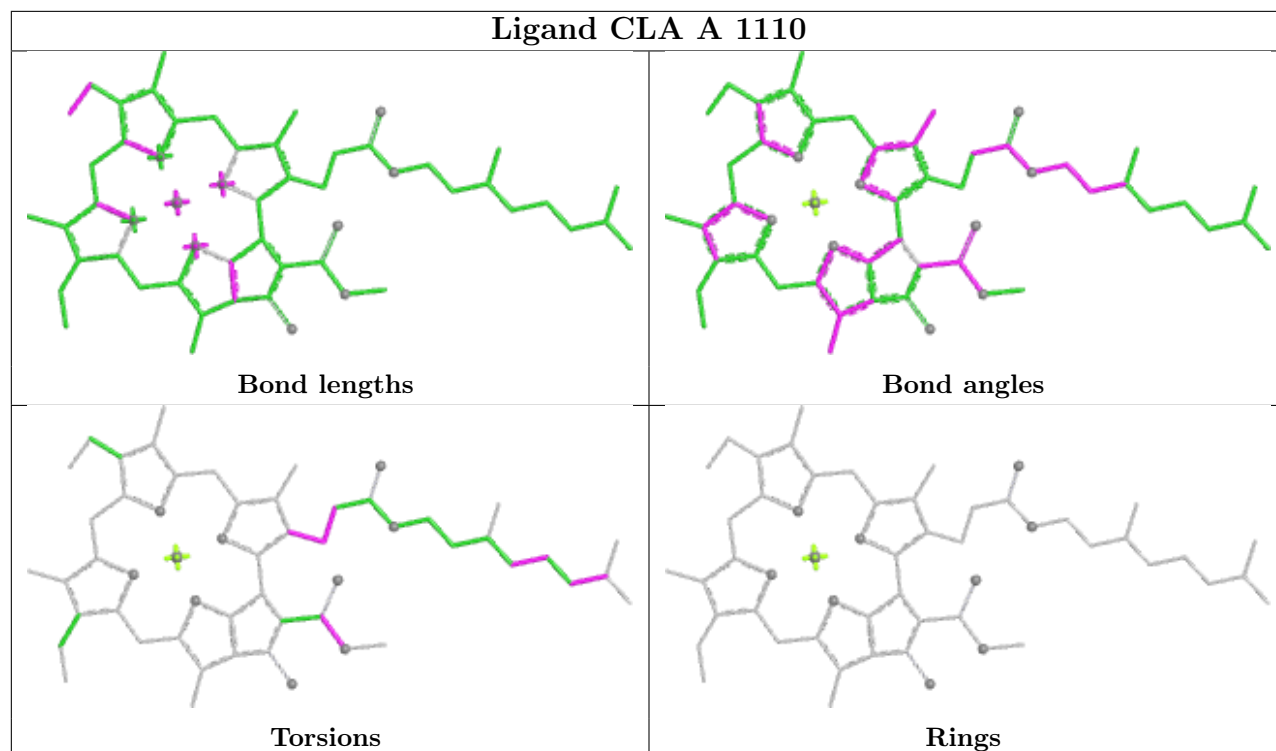
Torsions



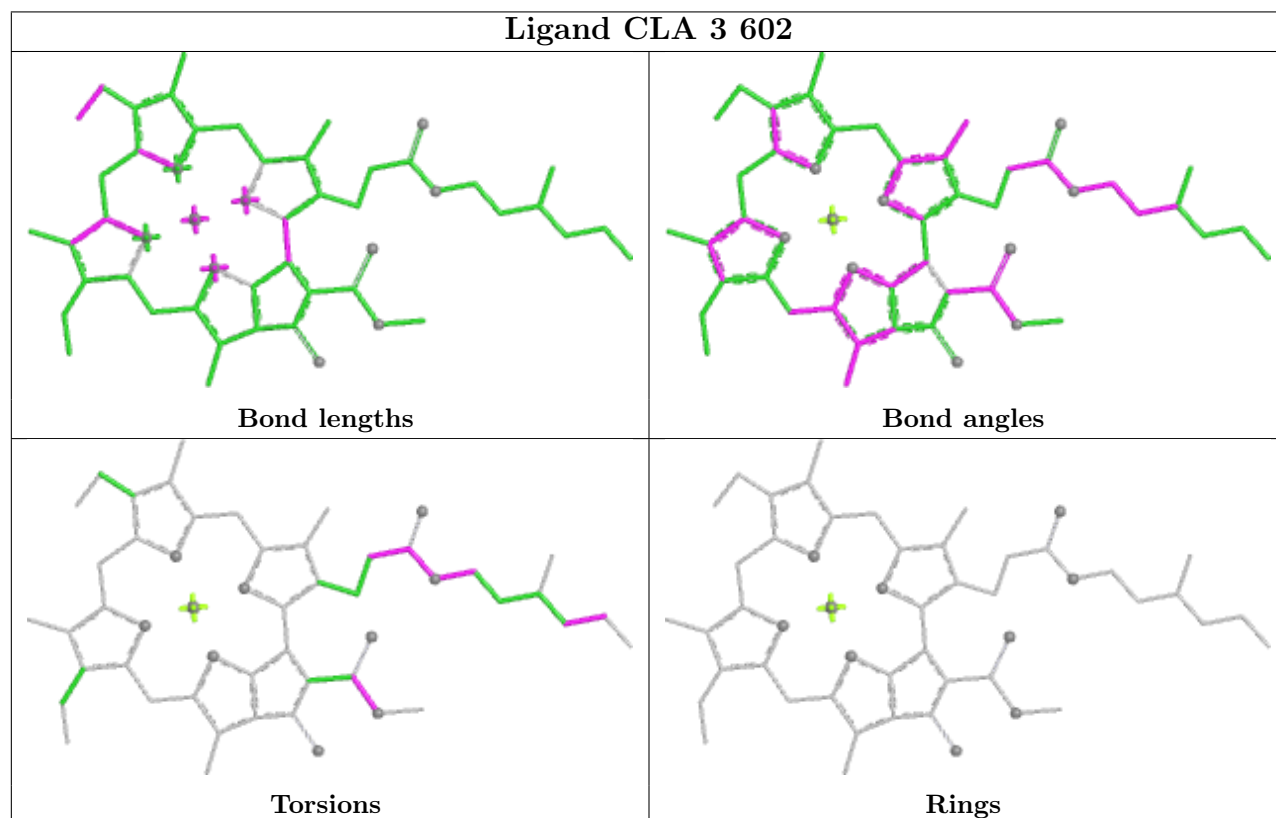
Rings

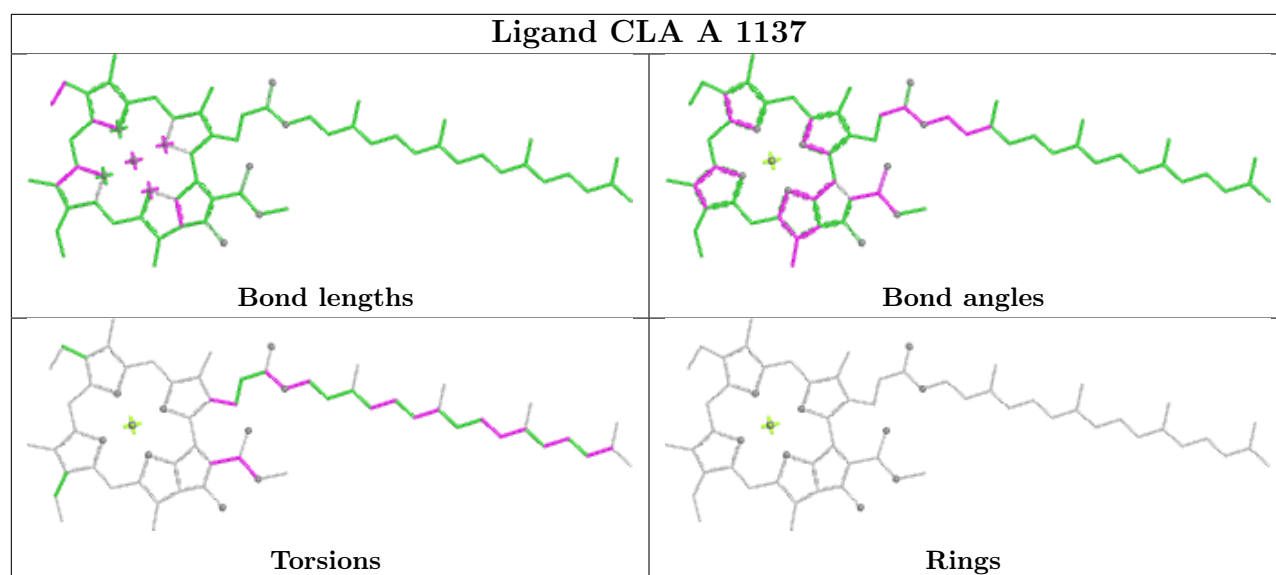


Ligand CLA A 1110



Ligand CLA 3 602





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

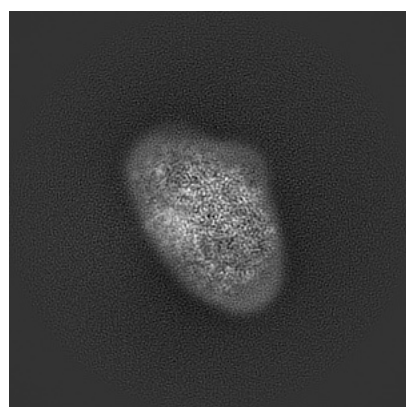
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-11326. These allow visual inspection of the internal detail of the map and identification of artifacts.

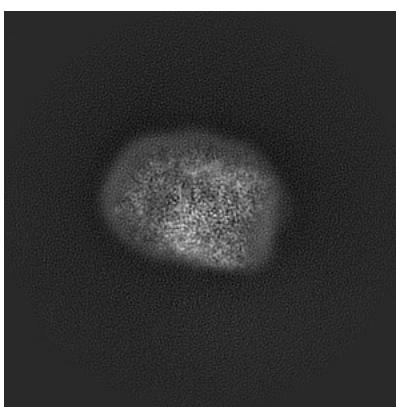
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

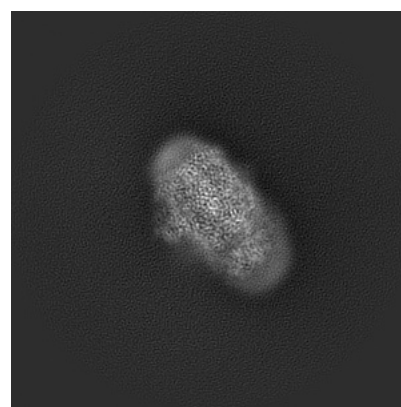
6.1.1 Primary map



X



Y

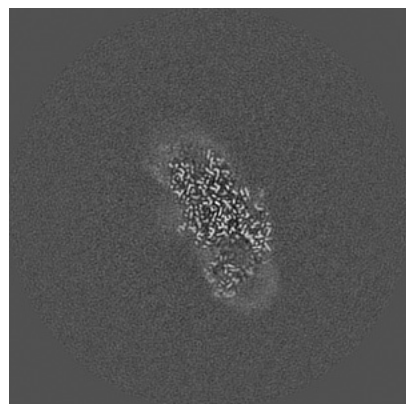


Z

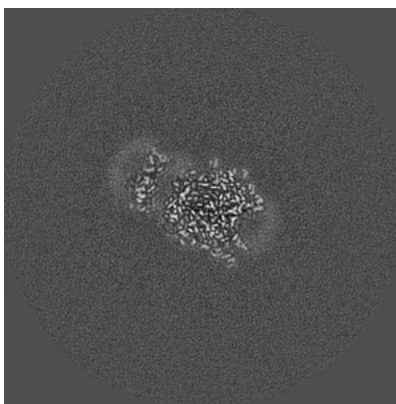
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

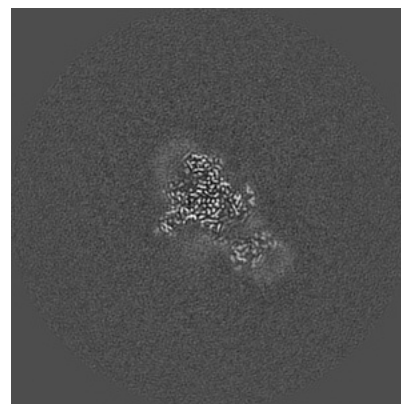
6.2.1 Primary map



X Index: 150



Y Index: 150

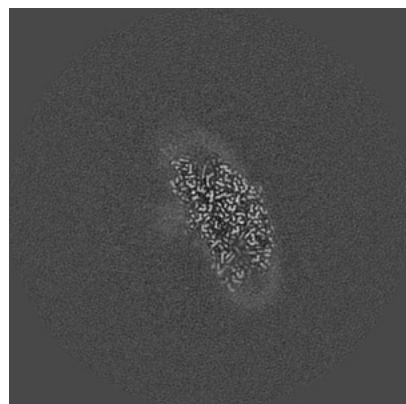


Z Index: 150

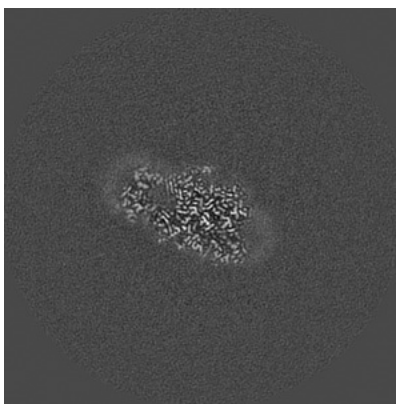
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

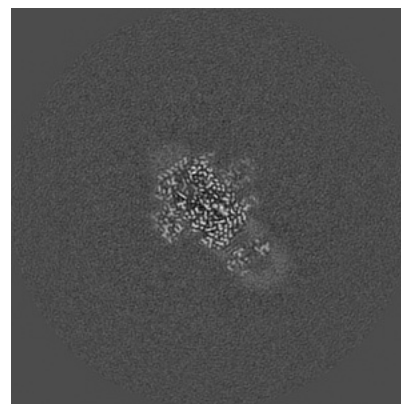
6.3.1 Primary map



X Index: 145



Y Index: 162

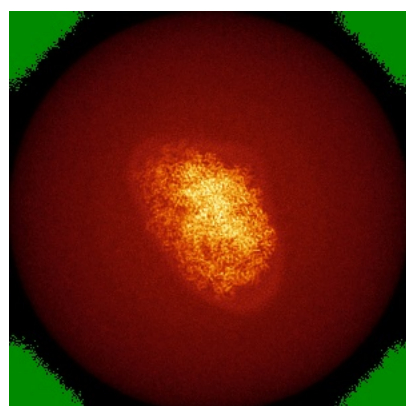


Z Index: 162

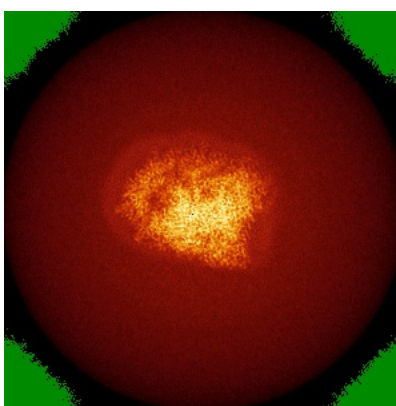
The images above show the largest variance slices of the map in three orthogonal directions.

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

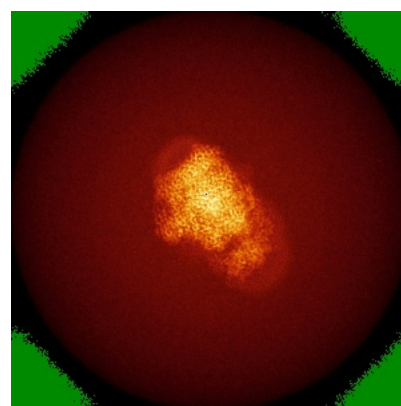
6.4.1 Primary map



X



Y

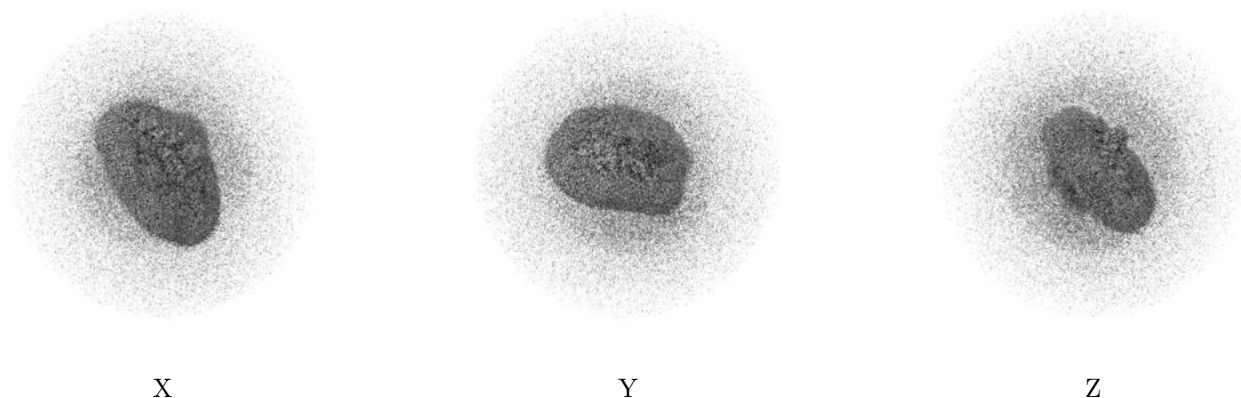


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0125. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

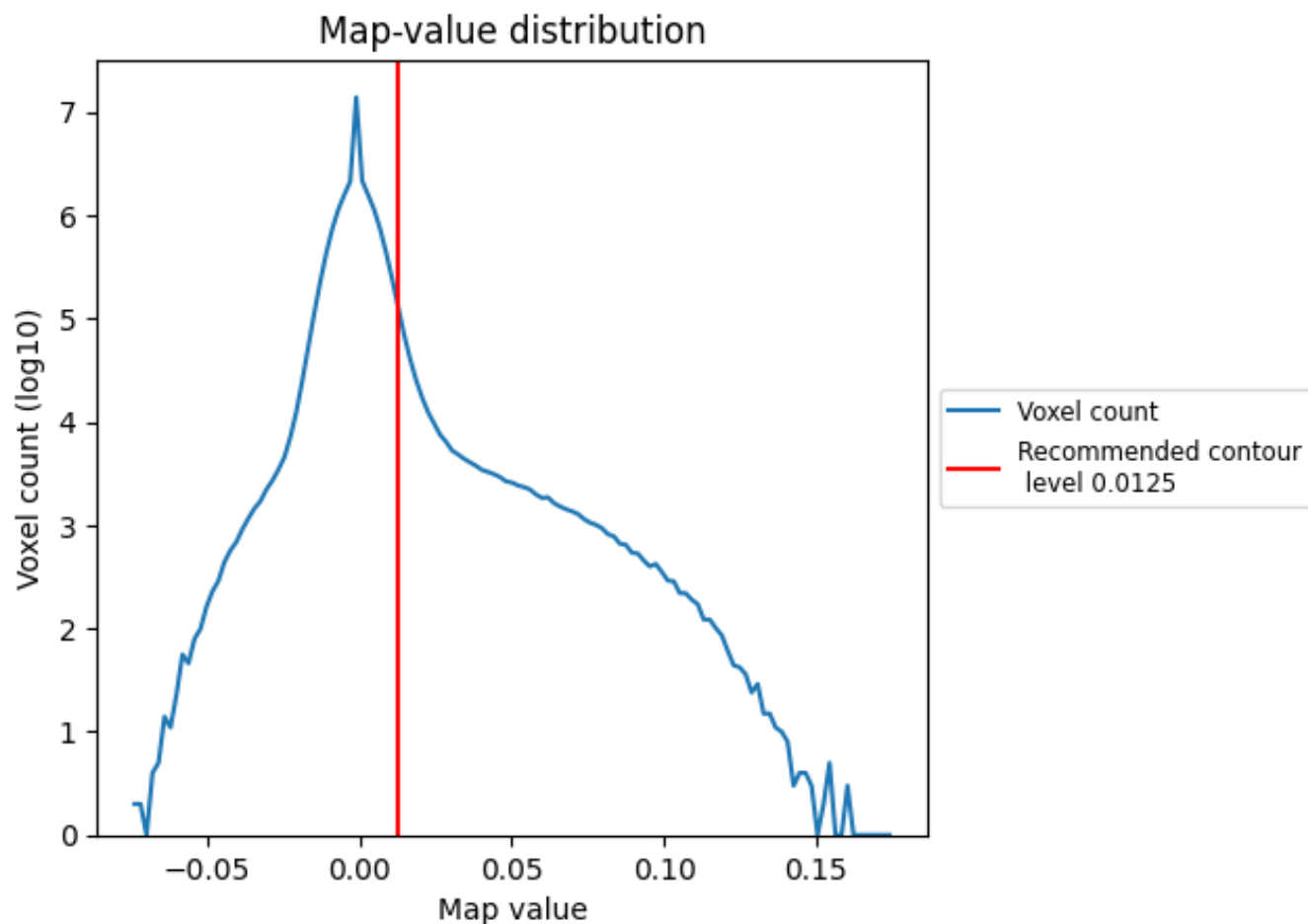
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

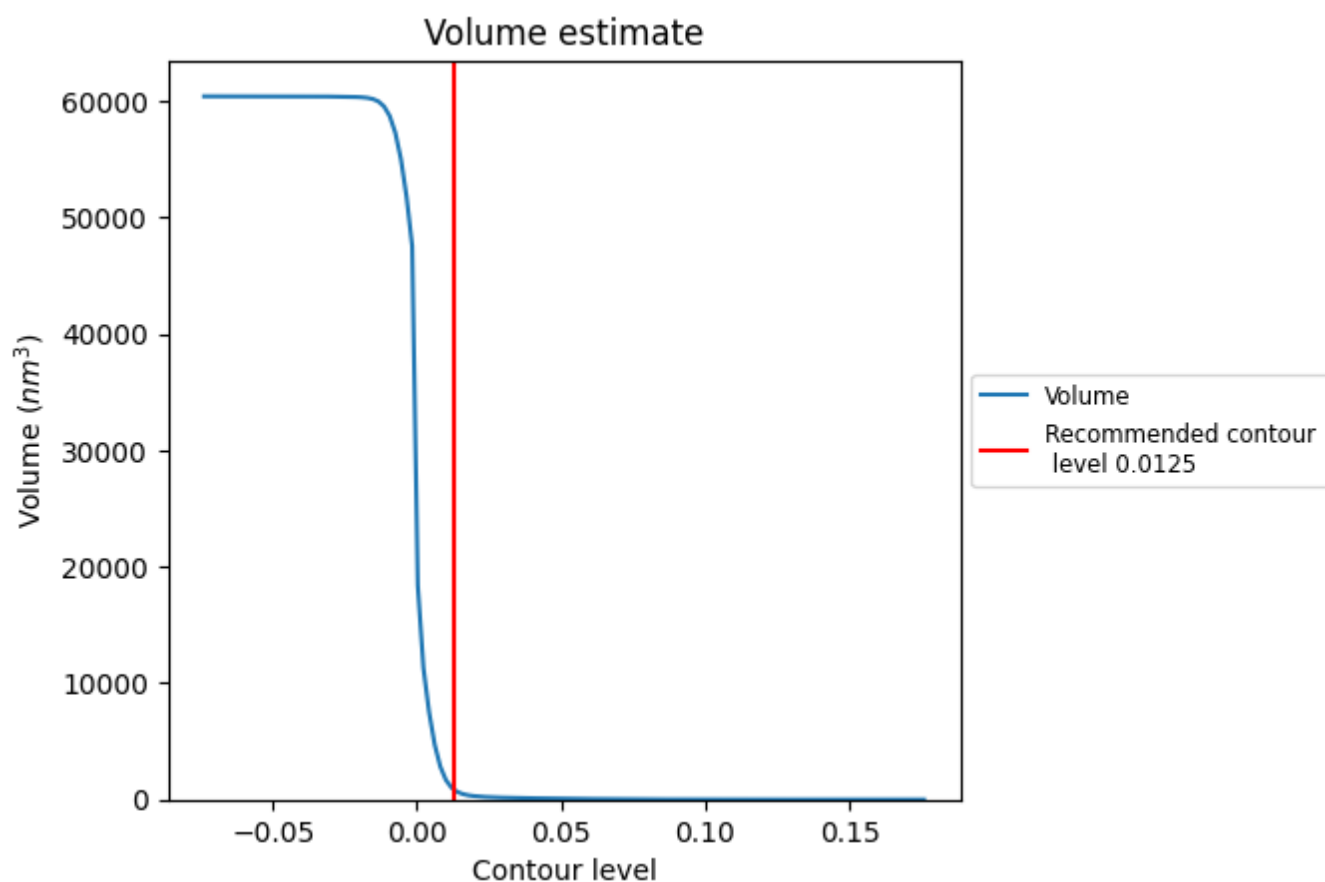
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

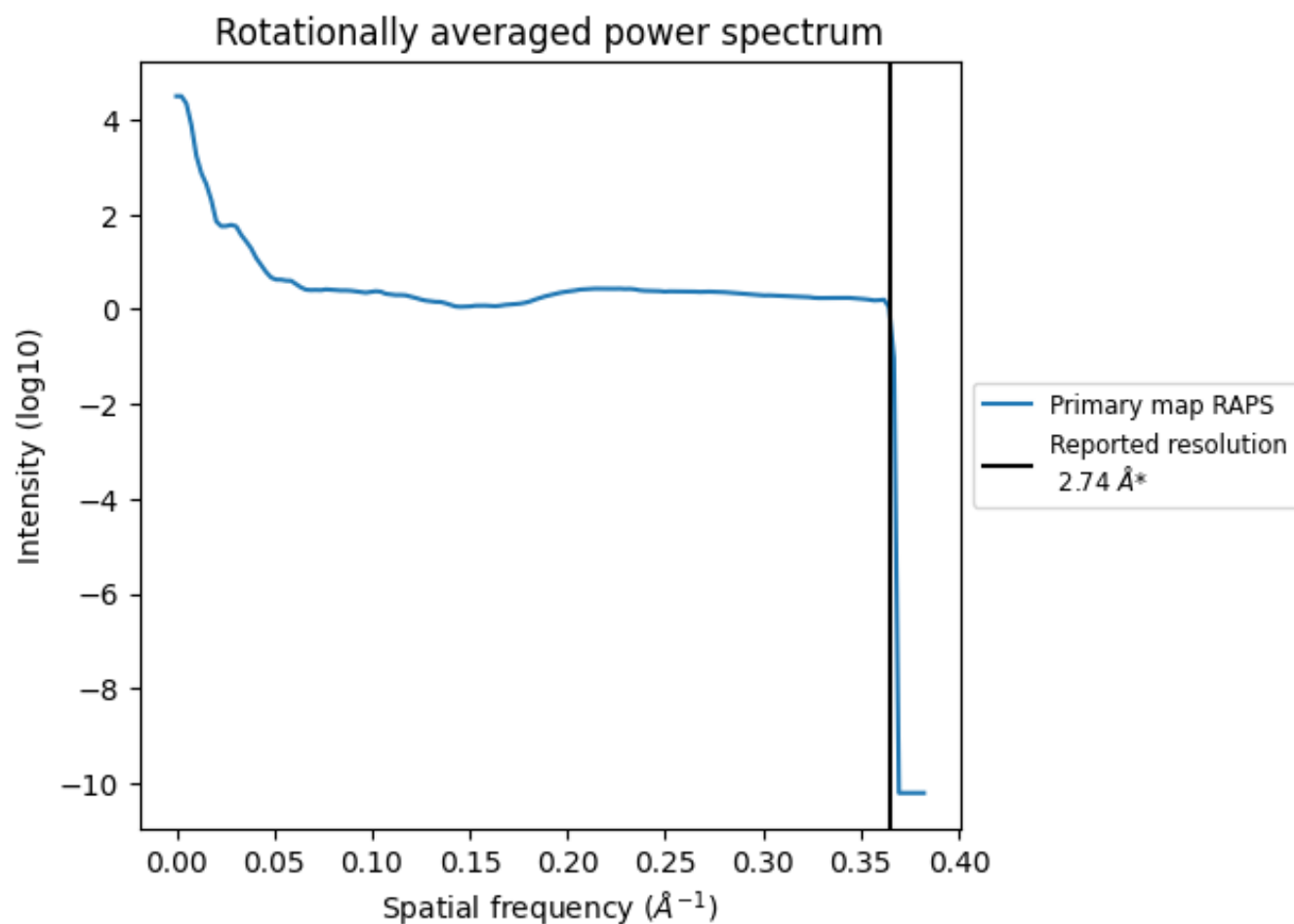
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 925 nm³; this corresponds to an approximate mass of 835 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

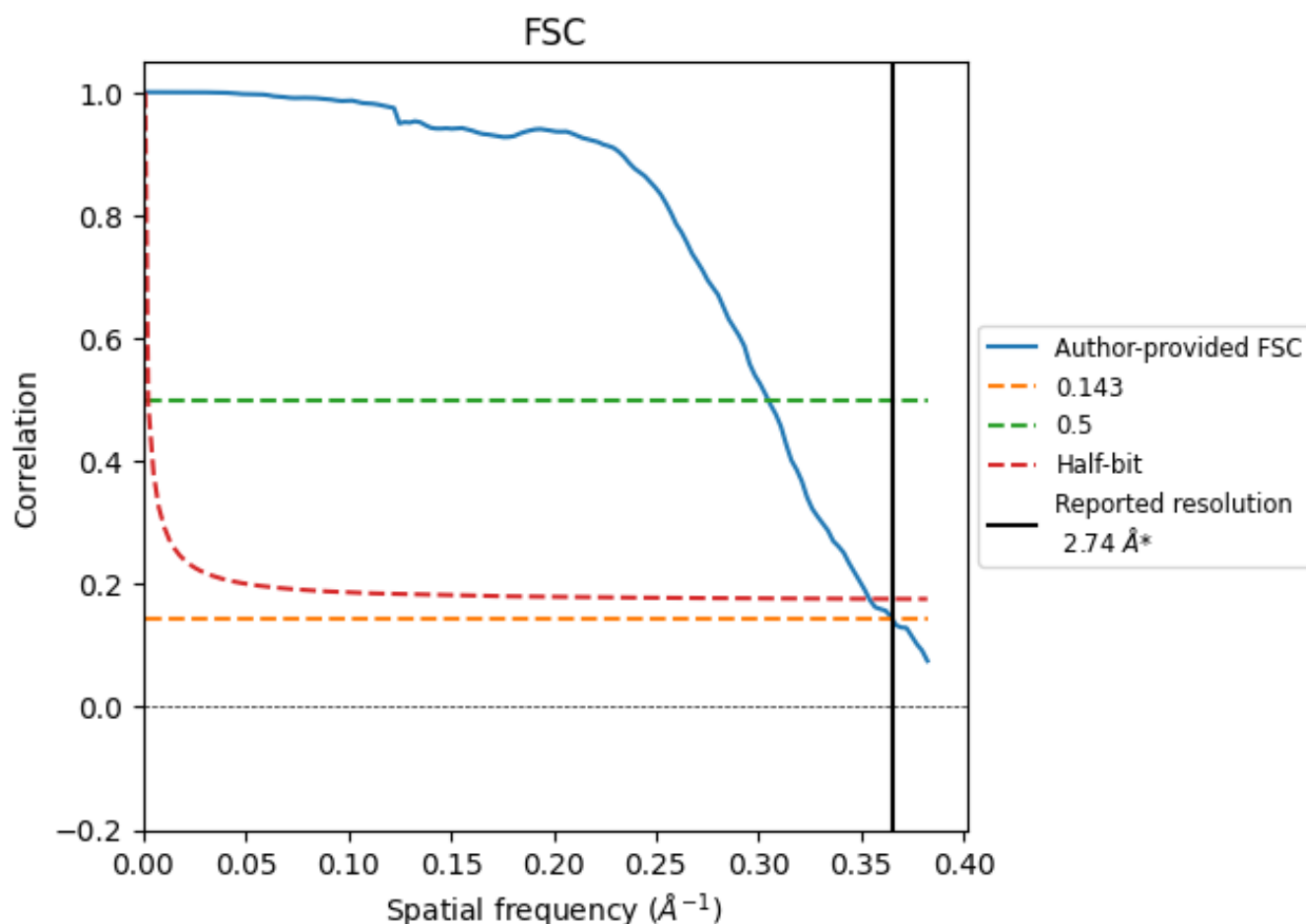


*Reported resolution corresponds to spatial frequency of 0.365 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.365 Å⁻¹

8.2 Resolution estimates [i](#)

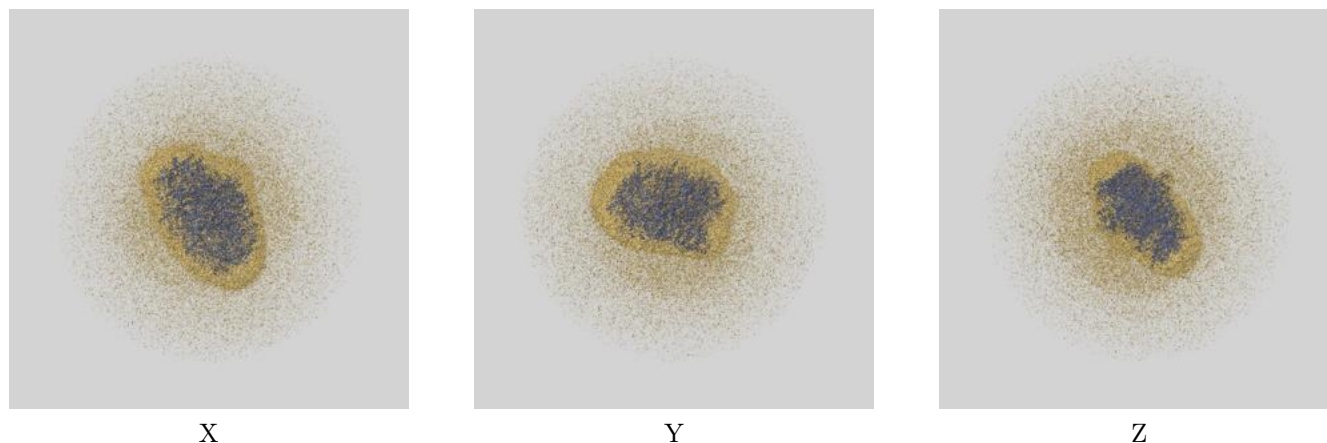
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.74	-	-
Author-provided FSC curve	2.74	3.28	2.82
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

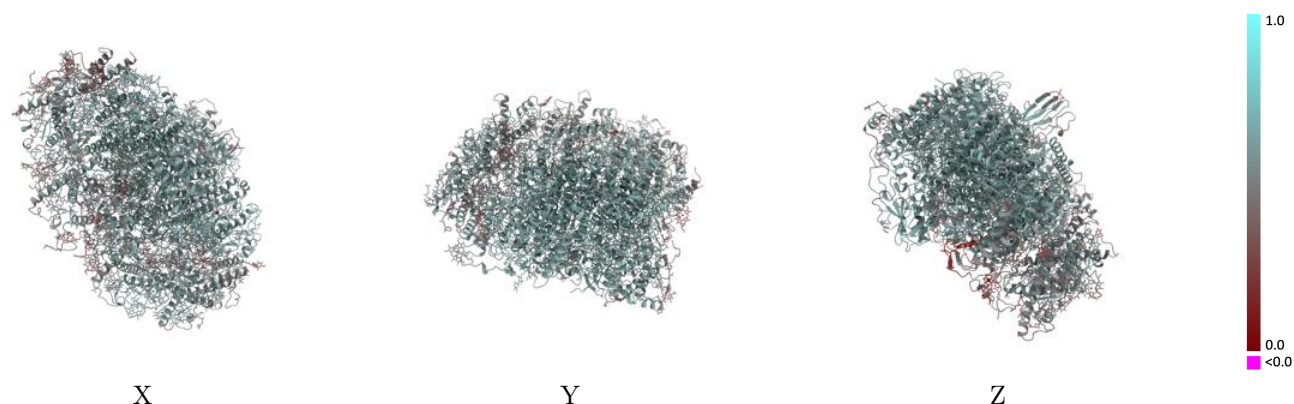
This section contains information regarding the fit between EMDB map EMD-11326 and PDB model 6ZOO. Per-residue inclusion information can be found in section 3 on page 32.

9.1 Map-model overlay [i](#)



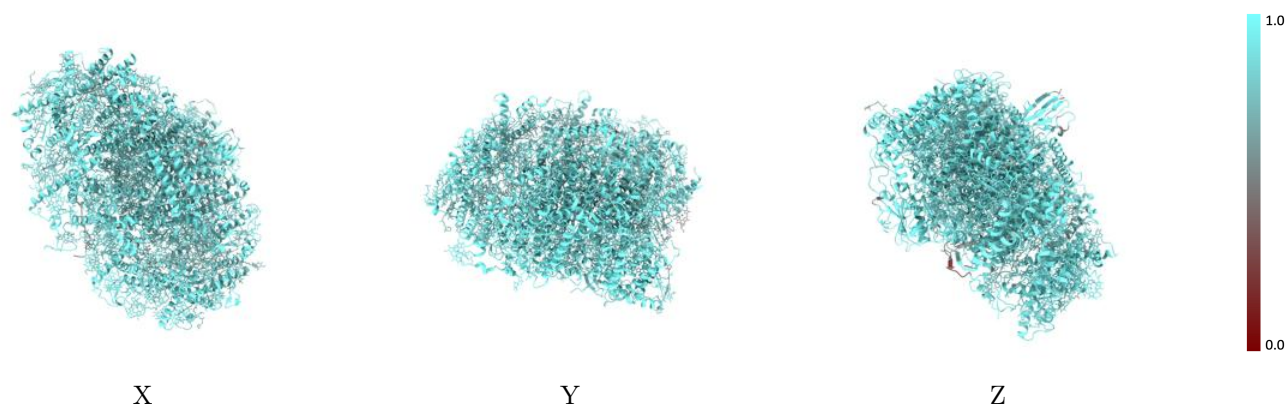
The images above show the 3D surface view of the map at the recommended contour level 0.0125 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



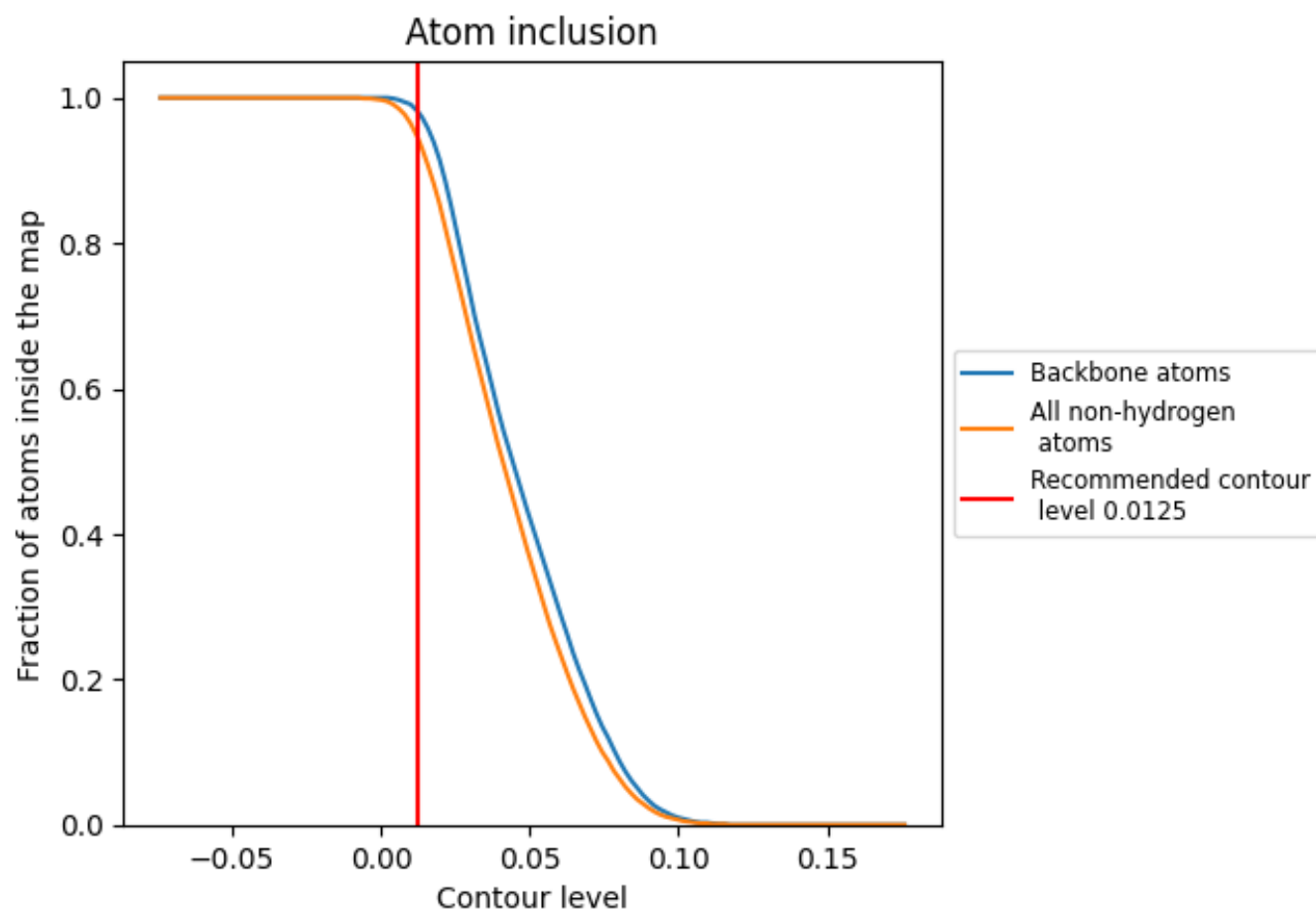
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0125).

9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 94% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.0125) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9450	0.5600
1	0.9360	0.5350
2	0.9140	0.5030
3	0.9260	0.4950
4	0.9290	0.5310
A	0.9590	0.5920
B	0.9720	0.6050
C	0.9870	0.5950
D	0.9830	0.5900
E	0.9690	0.5560
F	0.9370	0.5620
G	0.9130	0.5220
H	0.9110	0.5050
I	0.9750	0.5800
J	0.9170	0.5090
K	0.8040	0.3930
L	0.9690	0.5600
P	0.8760	0.5280

1.0

0.0

<0.0