



Full wwPDB EM Validation Report ⓘ

Mar 10, 2026 – 02:31 AM UTC

PDB ID : 6YEZ / pdb_00006yez
EMDB ID : EMD-10798
Title : Plant PSI-ferredoxin-plastocyanin supercomplex
Authors : Caspy, I.; Nelson, N.; Shkolnisky, Y.; Klaiman, D.; Sheinker, A.
Deposited on : 2020-03-25
Resolution : 2.70 Å(reported)
Based on initial model : 5L8R

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

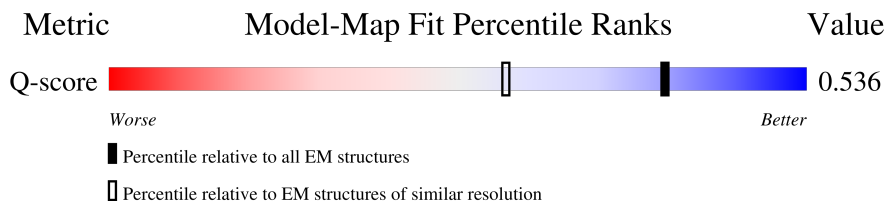
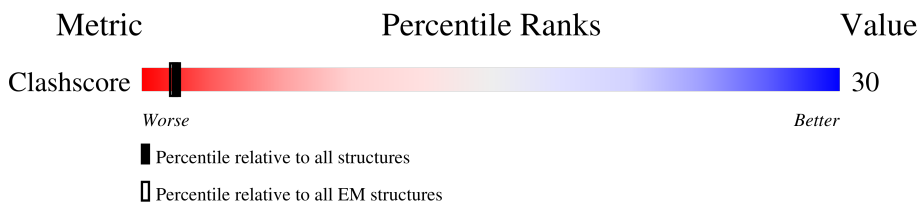
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

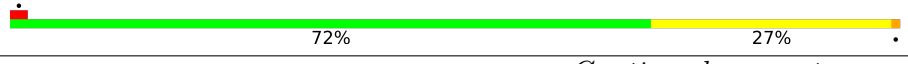
The reported resolution of this entry is 2.70 Å.

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	-
Q-score	-	25397	10327 (2.20 - 3.20)

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	 67% 32% .
2	B	733	 72% 28% .
3	C	80	 66% 32% .
4	D	143	 73% 27% .
5	E	66	 5% 88% 12% .
6	F	154	 72% 27% .

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Mol	Chain	Length	Quality of chain
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	N	97	
18	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
19	CL0	A	1011	X	-	-	-
20	CLA	1	601	X	-	-	-
20	CLA	1	602	X	-	-	-
20	CLA	1	603	X	-	X	-
20	CLA	1	604	X	-	-	-
20	CLA	1	605	X	-	-	-
20	CLA	1	606	X	-	-	-
20	CLA	1	607	X	-	-	-
20	CLA	1	608	X	-	-	-
20	CLA	1	611	X	-	-	-
20	CLA	1	613	X	-	-	-
20	CLA	1	614	X	-	-	-
20	CLA	2	601	X	-	-	-
20	CLA	2	602	X	-	-	-
20	CLA	2	603	X	-	-	-
20	CLA	2	604	X	-	X	-
20	CLA	2	605	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
20	CLA	2	606	X	-	-	-
20	CLA	2	607	X	-	-	-
20	CLA	2	608	X	-	-	-
20	CLA	2	612	X	-	-	-
20	CLA	3	601	X	-	-	-
20	CLA	3	602	X	-	-	-
20	CLA	3	603	X	-	-	-
20	CLA	3	605	X	-	-	-
20	CLA	3	606	X	-	-	-
20	CLA	3	608	X	-	-	-
20	CLA	3	610	X	-	-	-
20	CLA	3	612	X	-	-	-
20	CLA	3	613	X	-	-	-
20	CLA	3	614	X	-	-	-
20	CLA	3	617	X	-	-	-
20	CLA	4	601	X	-	X	-
20	CLA	4	602	X	-	-	-
20	CLA	4	603	X	-	-	-
20	CLA	4	604	X	-	X	-
20	CLA	4	606	X	-	-	-
20	CLA	4	607	X	-	-	-
20	CLA	4	608	X	-	-	-
20	CLA	4	609	X	-	-	-
20	CLA	4	612	X	-	-	-
20	CLA	4	617	X	-	-	-
20	CLA	A	1012	X	-	-	-
20	CLA	A	1013	X	-	-	-
20	CLA	A	1101	X	-	-	-
20	CLA	A	1102	X	-	-	-
20	CLA	A	1103	X	-	-	-
20	CLA	A	1104	X	-	-	-
20	CLA	A	1105	X	-	-	-
20	CLA	A	1106	X	-	-	-
20	CLA	A	1107	X	-	-	-
20	CLA	A	1108	X	-	-	-
20	CLA	A	1109	X	-	-	-
20	CLA	A	1110	X	-	-	-
20	CLA	A	1111	X	-	-	-
20	CLA	A	1112	X	-	-	-
20	CLA	A	1113	X	-	-	-
20	CLA	A	1114	X	-	-	-
20	CLA	A	1115	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
20	CLA	A	1116	X	-	-	-
20	CLA	A	1117	X	-	-	-
20	CLA	A	1118	X	-	-	-
20	CLA	A	1119	X	-	-	-
20	CLA	A	1120	X	-	-	-
20	CLA	A	1121	X	-	-	-
20	CLA	A	1122	X	-	-	-
20	CLA	A	1123	X	-	-	-
20	CLA	A	1124	X	-	-	-
20	CLA	A	1125	X	-	-	-
20	CLA	A	1126	X	-	-	-
20	CLA	A	1127	X	-	-	-
20	CLA	A	1128	X	-	-	-
20	CLA	A	1129	X	-	-	-
20	CLA	A	1130	X	-	-	-
20	CLA	A	1131	X	-	-	-
20	CLA	A	1132	X	-	X	-
20	CLA	A	1133	X	-	-	-
20	CLA	A	1134	X	-	-	-
20	CLA	A	1135	X	-	-	-
20	CLA	A	1136	X	-	-	-
20	CLA	A	1137	X	-	-	-
20	CLA	A	1138	X	-	-	-
20	CLA	A	1139	X	-	-	-
20	CLA	A	1140	X	-	-	-
20	CLA	A	1141	X	-	-	-
20	CLA	B	1021	X	-	-	-
20	CLA	B	1022	X	-	-	-
20	CLA	B	1023	X	-	-	-
20	CLA	B	1201	X	-	-	-
20	CLA	B	1202	X	-	-	-
20	CLA	B	1203	X	-	-	-
20	CLA	B	1204	X	-	-	-
20	CLA	B	1205	X	-	-	-
20	CLA	B	1206	X	-	-	-
20	CLA	B	1207	X	-	-	-
20	CLA	B	1208	X	-	-	-
20	CLA	B	1209	X	-	-	-
20	CLA	B	1210	X	-	-	-
20	CLA	B	1211	X	-	-	-
20	CLA	B	1212	X	-	-	-
20	CLA	B	1213	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
20	CLA	B	1214	X	-	-	-
20	CLA	B	1215	X	-	-	-
20	CLA	B	1216	X	-	-	-
20	CLA	B	1217	X	-	-	-
20	CLA	B	1218	X	-	-	-
20	CLA	B	1219	X	-	-	-
20	CLA	B	1220	X	-	-	-
20	CLA	B	1221	X	-	-	-
20	CLA	B	1222	X	-	-	-
20	CLA	B	1223	X	-	-	-
20	CLA	B	1224	X	-	-	-
20	CLA	B	1225	X	-	-	-
20	CLA	B	1226	X	-	-	-
20	CLA	B	1227	X	-	-	-
20	CLA	B	1228	X	-	-	-
20	CLA	B	1229	X	-	-	-
20	CLA	B	1230	X	-	-	-
20	CLA	B	1231	X	-	-	-
20	CLA	B	1232	X	-	-	-
20	CLA	B	1234	X	-	-	-
20	CLA	B	1235	X	-	-	-
20	CLA	B	1236	X	-	-	-
20	CLA	B	1237	X	-	-	-
20	CLA	B	1238	X	-	-	-
20	CLA	B	1239	X	-	-	-
20	CLA	B	1240	X	-	-	-
20	CLA	F	1301	X	-	-	-
20	CLA	F	1302	X	-	-	-
20	CLA	G	1601	X	-	-	-
20	CLA	G	1602	X	-	-	-
20	CLA	G	1603	X	-	-	-
20	CLA	H	1701	X	-	-	-
20	CLA	J	1901	X	-	-	-
20	CLA	K	1401	X	-	-	-
20	CLA	K	1402	X	-	-	-
20	CLA	K	1403	X	-	-	-
20	CLA	K	1404	X	-	-	-
20	CLA	L	1501	X	-	-	-
20	CLA	L	1502	X	-	-	-
20	CLA	L	1503	X	-	-	-
22	BCR	2	503	-	-	X	-
22	BCR	L	4019	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	SF4	C	3003	-	-	X	-
29	LUT	1	502	-	-	X	-
29	LUT	2	501	X	-	-	-
29	LUT	3	502	X	-	-	-
30	CHL	1	609	X	-	-	-
30	CHL	1	610	X	-	-	-
30	CHL	1	612	X	-	-	-
30	CHL	2	609	X	-	X	-
30	CHL	2	610	X	-	-	-
30	CHL	2	611	X	-	-	-
30	CHL	2	613	X	-	-	-
30	CHL	2	615	X	-	-	-
30	CHL	3	604	X	-	-	-
30	CHL	3	607	X	-	-	-
30	CHL	3	611	X	-	-	-
30	CHL	4	610	X	-	-	-
30	CHL	4	611	X	-	-	-
30	CHL	4	613	X	-	-	-
30	CHL	4	615	X	-	-	-
31	XAT	2	502	X	-	-	-
31	XAT	4	502	X	-	-	-

2 Entry composition

There are 36 unique types of molecules in this entry. The entry contains 39217 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	743	Total	C	N	O	S	0	0
			5858	3839	998	1003	18		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	80	Total	C	N	O	S	0	0
			612	379	107	115	11		

- Molecule 4 is a protein called PsaD.

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

- Molecule 5 is a protein called PsaE.

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

- Molecule 6 is a protein called PsaF.

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

- Molecule 7 is a protein called PsaG.

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

- Molecule 8 is a protein called PsaH.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	H	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 PsaJ.

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 12 is a protein called PsaL.

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

- Molecule 13 is a protein called Lhca1.

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

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

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

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

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

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

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

There are 3 discrepancies between the modelled and reference sequences:

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

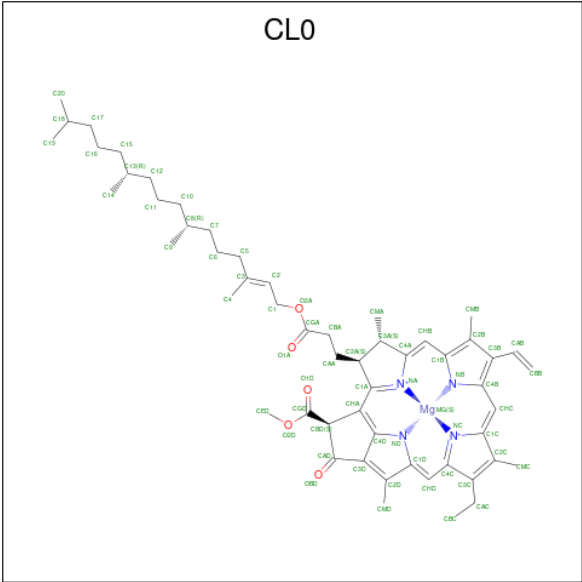
- Molecule 17 is a protein called Ferredoxin-1, chloroplastic.

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

- Molecule 18 is a protein called Plastocyanin, chloroplastic.

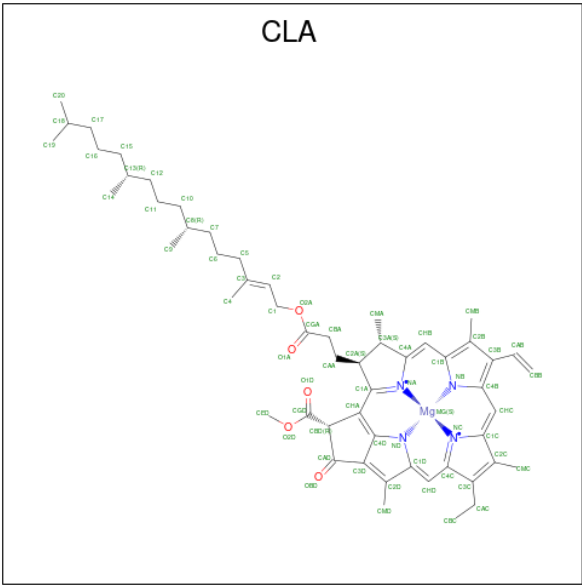
Mol	Chain	Residues	Atoms					AltConf	Trace
18	P	99	Total	C	N	O	S	0	0
			728	460	115	150	3		

- Molecule 19 is CHLOROPHYLL A ISOMER (CCD ID: CL0) (formula: C₅₅H₇₂MgN₄O₅).



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

- Molecule 20 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅).



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

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

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

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

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

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Mol	Chain	Residues	Atoms					AltConf
20	G	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
20	G	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
20	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	H	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
20	J	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
20	K	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
20	K	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
20	K	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
20	K	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
20	L	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
20	L	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
20	L	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
20	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	1	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
20	1	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
20	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	1	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
20	1	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
20	1	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
20	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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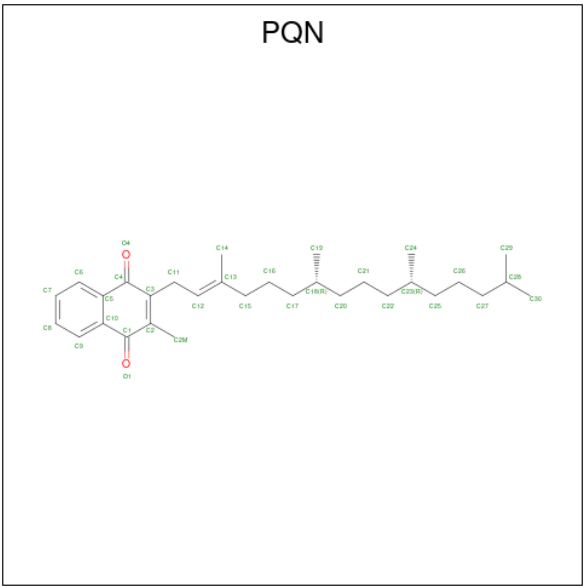
Mol	Chain	Residues	Atoms					AltConf
20	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
20	1	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
20	2	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
20	2	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
20	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	2	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
20	2	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
20	2	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
20	2	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
20	3	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
20	3	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
20	3	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
20	3	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
20	3	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
20	3	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
20	3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	3	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
20	3	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
20	3	1	Total	C	Mg	N	O	0
			42	34	1	4	3	

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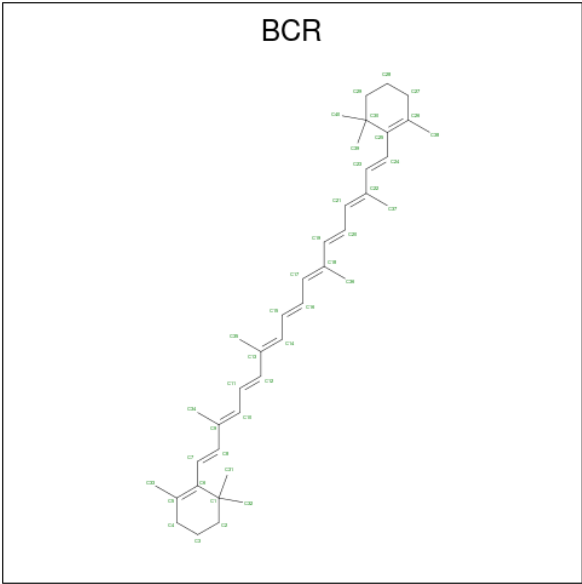
Mol	Chain	Residues	Atoms					AltConf
20	3	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
20	4	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
20	4	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
20	4	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
20	4	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	4	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
20	4	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
20	4	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
20	4	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
20	4	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
20	4	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	4	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

- Molecule 21 is PHYLLOQUINONE (CCD ID: PQN) (formula: C₃₁H₄₆O₂).



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

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



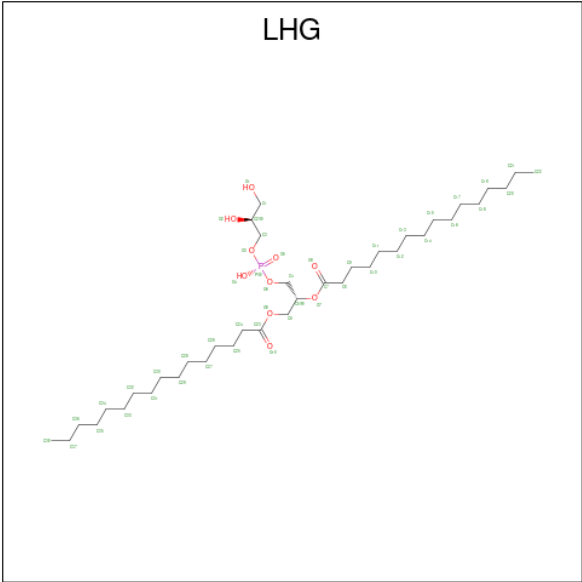
Mol	Chain	Residues	Atoms		AltConf
22	A	1	Total	C	0
			40	40	
22	A	1	Total	C	0
			40	40	
22	A	1	Total	C	0
			40	40	
22	A	1	Total	C	0
			40	40	
22	A	1	Total	C	0
			40	40	
22	A	1	Total	C	0
			40	40	
22	B	1	Total	C	0
			40	40	
22	B	1	Total	C	0
			40	40	
22	B	1	Total	C	0
			40	40	
22	B	1	Total	C	0
			40	40	

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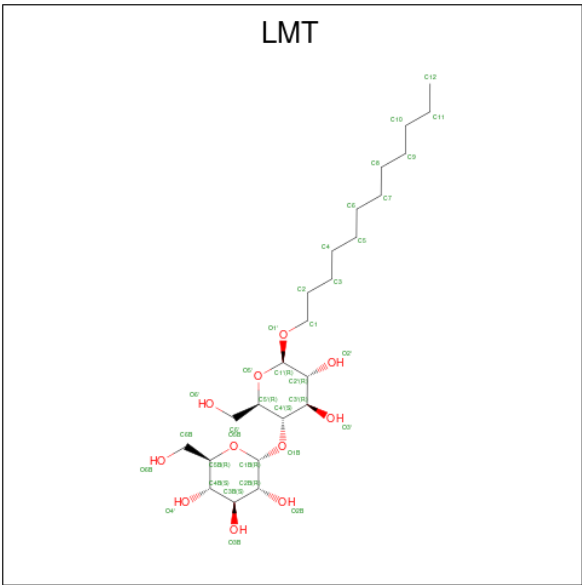
Mol	Chain	Residues	Atoms	AltConf
22	B	1	Total C 40 40	0
22	F	1	Total C 40 40	0
22	F	1	Total C 40 40	0
22	G	1	Total C 40 40	0
22	H	1	Total C 40 40	0
22	I	1	Total C 40 40	0
22	I	1	Total C 40 40	0
22	J	1	Total C 40 40	0
22	K	1	Total C 40 40	0
22	K	1	Total C 40 40	0
22	L	1	Total C 40 40	0
22	L	1	Total C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



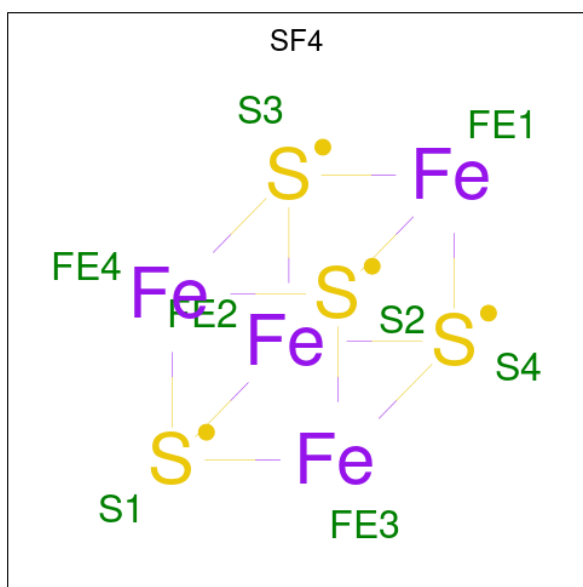
Mol	Chain	Residues	Atoms				AltConf
23	A	1	Total	C	O	P	0
			40	29	10	1	
23	A	1	Total	C	O	P	0
			49	38	10	1	
23	B	1	Total	C	O	P	0
			21	10	10	1	
23	B	1	Total	C	O	P	0
			49	38	10	1	
23	1	1	Total	C	O	P	0
			49	38	10	1	
23	2	1	Total	C	O	P	0
			35	24	10	1	
23	3	1	Total	C	O	P	0
			17	8	8	1	
23	4	1	Total	C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

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



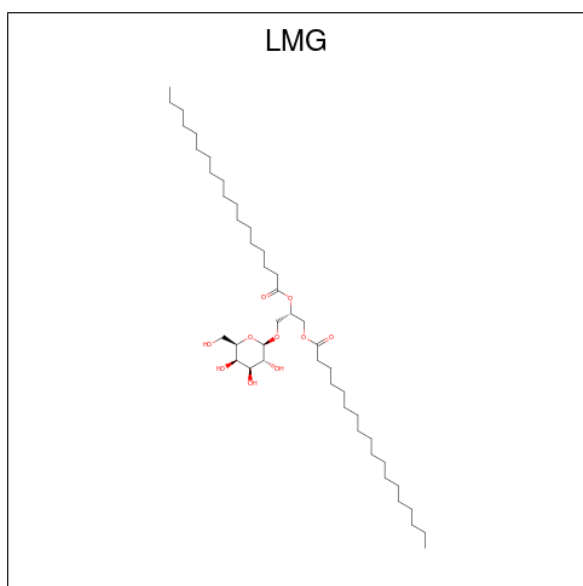
Mol	Chain	Residues	Atoms			AltConf
24	A	1	Total	C	O	0
			35	24	11	
24	B	1	Total	C	O	0
			32	21	11	
24	B	1	Total	C	O	0
			31	20	11	
24	G	1	Total	C	O	0
			31	20	11	
24	G	1	Total	C	O	0
			35	24	11	
24	2	1	Total	C	O	0
			35	24	11	

- Molecule 25 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



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

- Molecule 26 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: C₄₅H₈₆O₁₀).



Mol	Chain	Residues	Atoms			AltConf
26	A	1	Total	C	O	0
			50	40	10	
26	B	1	Total	C	O	0
			35	25	10	
26	B	1	Total	C	O	0
			33	23	10	
26	B	1	Total	C	O	0
			34	24	10	
26	F	1	Total	C	O	0
			47	37	10	
26	F	1	Total	C	O	0
			36	26	10	
26	F	1	Total	C	O	0
			34	24	10	
26	F	1	Total	C	O	0
			13	7	6	
26	F	1	Total	C	O	0
			30	20	10	
26	G	1	Total	C	O	0
			25	15	10	
26	G	1	Total	C	O	0
			49	39	10	
26	G	1	Total	C	O	0
			50	40	10	
26	1	1	Total	C	O	0
			46	36	10	
26	2	1	Total	C	O	0
			25	15	10	
26	2	1	Total	C	O	0
			36	26	10	
26	2	1	Total	C	O	0
			30	20	10	
26	2	1	Total	C	O	0
			30	20	10	
26	2	1	Total	C	O	0
			13	7	6	
26	3	1	Total	C	O	0
			30	20	10	

- Molecule 27 is CALCIUM ION (CCD ID: CA) (formula: Ca).

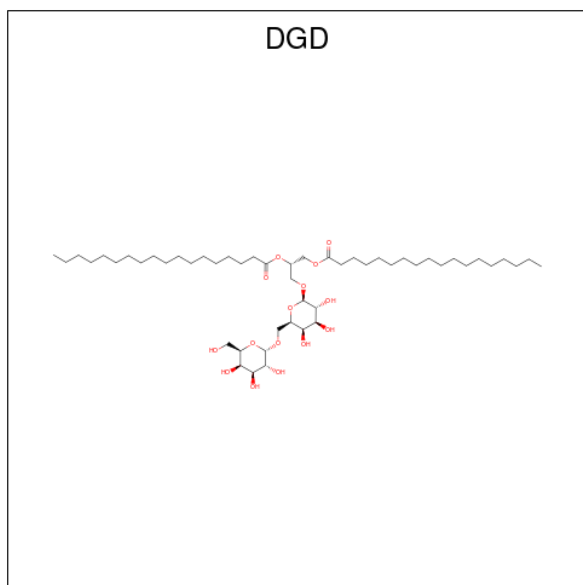
Mol	Chain	Residues	Atoms		AltConf
27	A	1	Total	Ca	0
			1	1	

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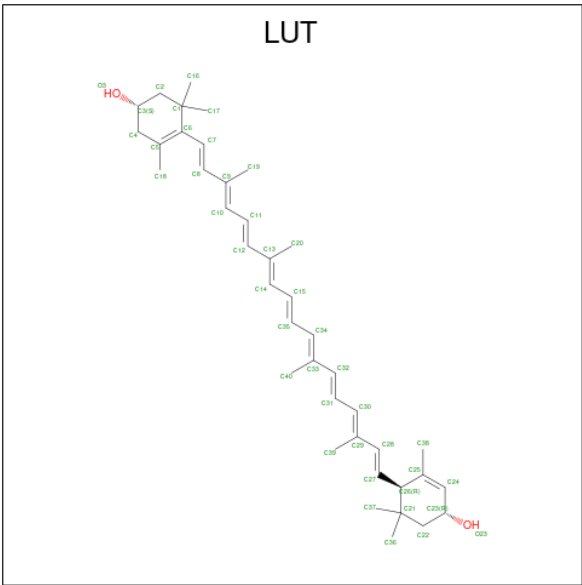
Mol	Chain	Residues	Atoms		AltConf
27	B	1	Total	Ca	0
			1	1	

- Molecule 28 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



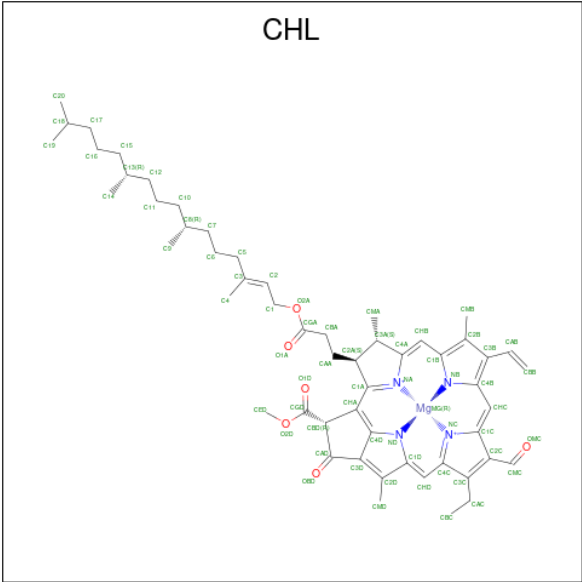
Mol	Chain	Residues	Atoms			AltConf
28	B	1	Total	C	O	0
			61	46	15	
28	F	1	Total	C	O	0
			57	42	15	
28	G	1	Total	C	O	0
			47	32	15	
28	J	1	Total	C	O	0
			58	43	15	
28	1	1	Total	C	O	0
			41	26	15	
28	3	1	Total	C	O	0
			51	36	15	
28	4	1	Total	C	O	0
			51	36	15	

- Molecule 29 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (CCD ID: LUT) (formula: $C_{40}H_{56}O_2$).



Mol	Chain	Residues	Atoms			AltConf
29	J	1	Total	C	O	0
			42	40	2	
29	1	1	Total	C	O	0
			42	40	2	
29	1	1	Total	C	O	0
			42	40	2	
29	2	1	Total	C	O	0
			42	40	2	
29	3	1	Total	C	O	0
			42	40	2	
29	3	1	Total	C	O	0
			42	40	2	
29	4	1	Total	C	O	0
			42	40	2	

- Molecule 30 is CHLOROPHYLL B (CCD ID: CHL) (formula: C₅₅H₇₀MgN₄O₆).



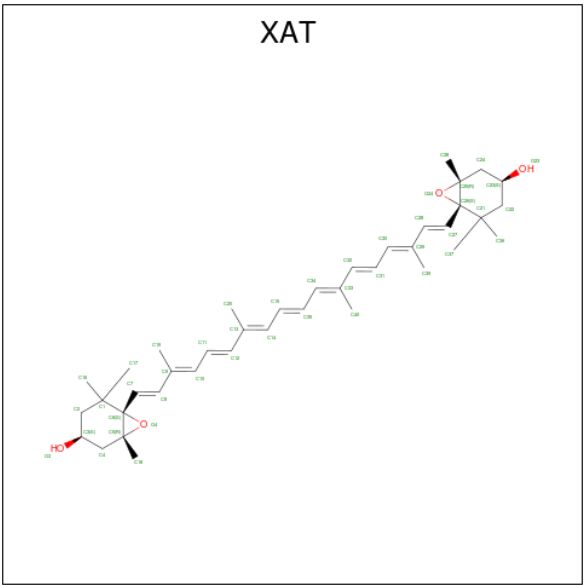
Mol	Chain	Residues	Atoms					AltConf
30	1	1	Total 47	C 36	Mg 1	N 4	O 6	0
30	1	1	Total 61	C 50	Mg 1	N 4	O 6	0
30	1	1	Total 56	C 45	Mg 1	N 4	O 6	0
30	2	1	Total 56	C 45	Mg 1	N 4	O 6	0
30	2	1	Total 48	C 37	Mg 1	N 4	O 6	0
30	2	1	Total 46	C 35	Mg 1	N 4	O 6	0
30	2	1	Total 56	C 45	Mg 1	N 4	O 6	0
30	2	1	Total 66	C 55	Mg 1	N 4	O 6	0
30	3	1	Total 66	C 55	Mg 1	N 4	O 6	0
30	3	1	Total 51	C 40	Mg 1	N 4	O 6	0
30	3	1	Total 47	C 36	Mg 1	N 4	O 6	0
30	4	1	Total 47	C 36	Mg 1	N 4	O 6	0
30	4	1	Total 51	C 40	Mg 1	N 4	O 6	0
30	4	1	Total 61	C 50	Mg 1	N 4	O 6	0

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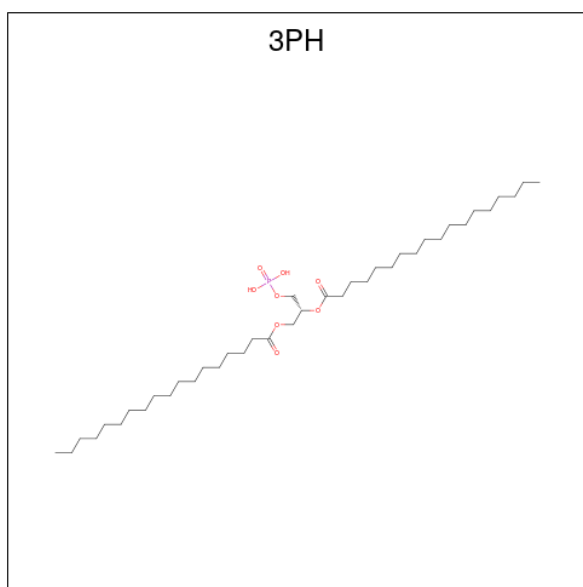
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
30	4	1	43	34	1	4	4	0

- Molecule 31 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).



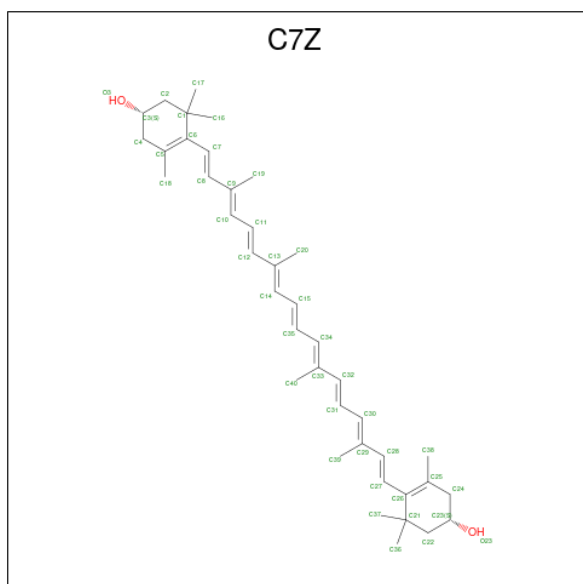
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
31	2	1	44	40	4	0
31	4	1	44	40	4	0

- Molecule 32 is 1,2-DIACYL-GLYCEROL-3-SN-PHOSPHATE (CCD ID: 3PH) (formula: C₃₉H₇₇O₈P).



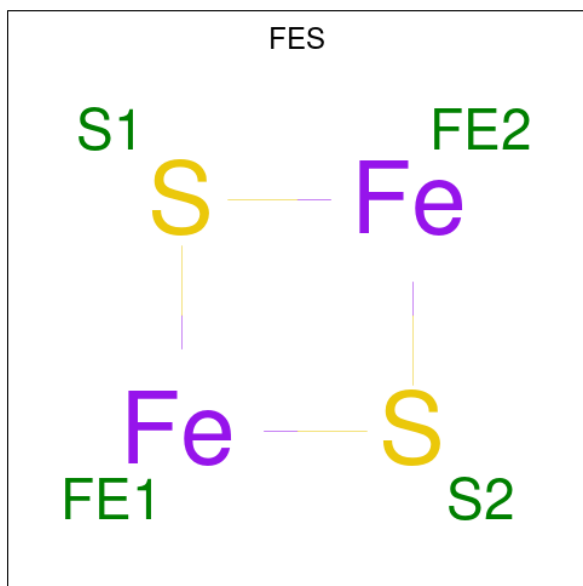
Mol	Chain	Residues	Atoms				AltConf
32	2	1	Total	C	O	P	0
			33	24	8	1	

- Molecule 33 is (1 {S})-3,5,5-trimethyl-4-[(1 {E},3 {E},5 {E},7 {E},9 {E},11 {E},13 {E},15 {E},17 {E})-3,7,12,16-tetramethyl-18-[(4 {S})-2,6,6-trimethyl-4-oxidanyl-cyclohexen-1-yl]octadeca-1,3,5,7,9,11,13,15,17-nonaenyl]cyclohex-3-en-1-ol (CCD ID: C7Z) (formula: $C_{40}H_{56}O_2$).



Mol	Chain	Residues	Atoms				AltConf
33	4	1	Total	C	O		0
			42	40	2		

- Molecule 34 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



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

- Molecule 35 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

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

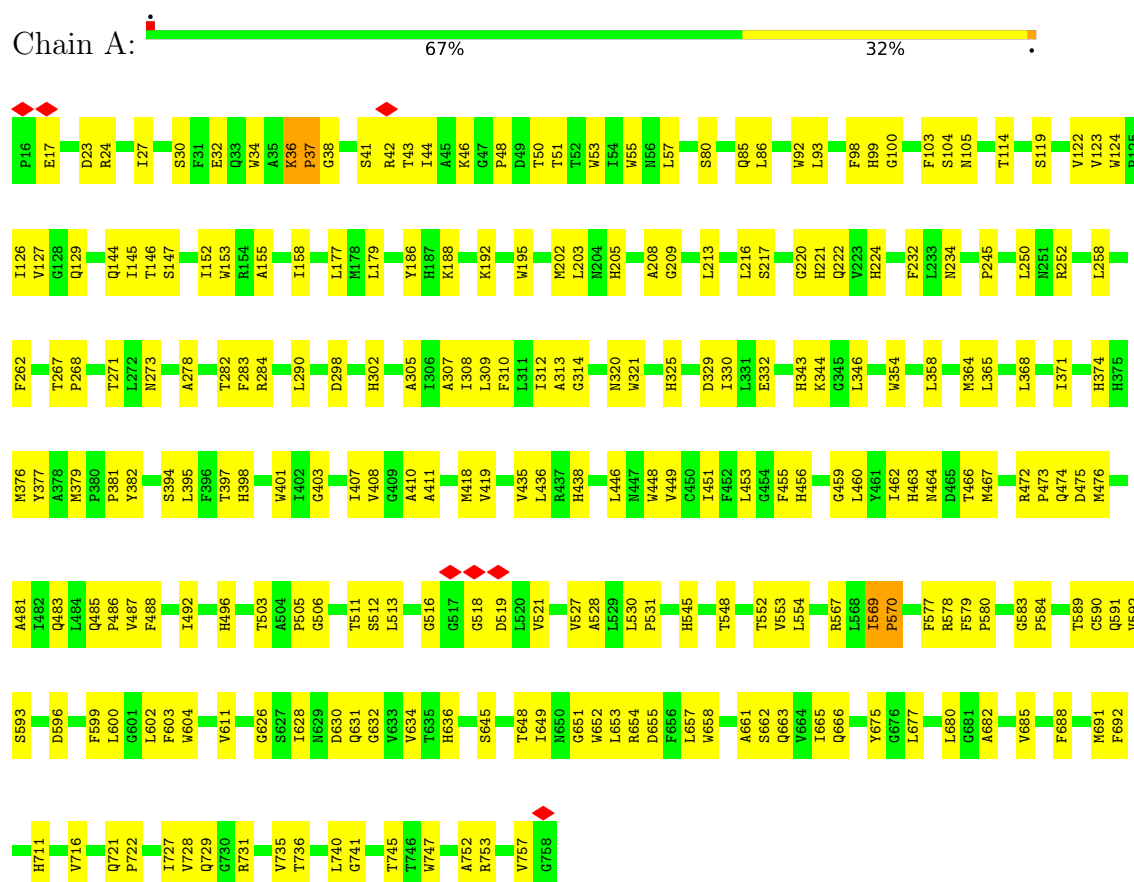
- Molecule 36 is water.

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

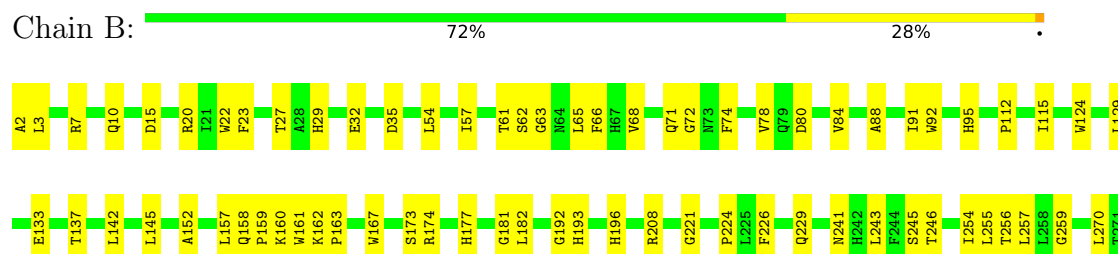
3 Residue-property plots

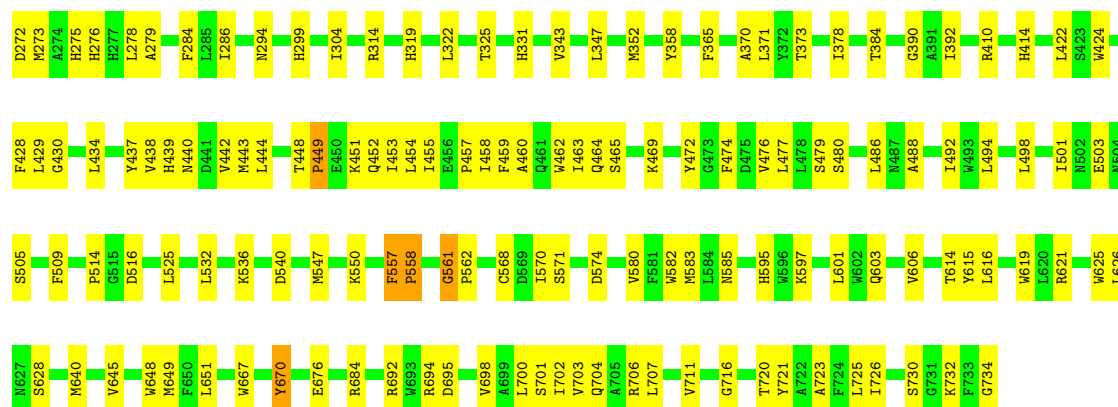
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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





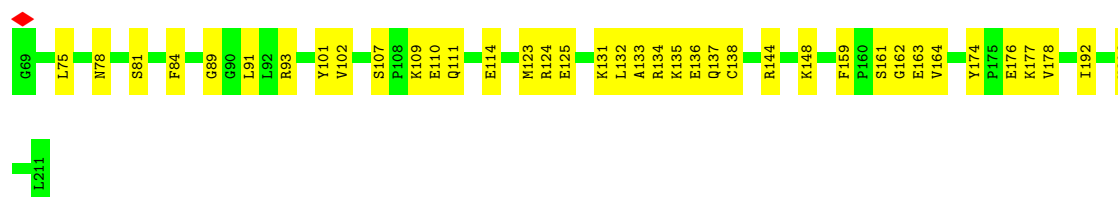
• Molecule 3: Photosystem I iron-sulfur center

Chain C: 66% 32% .



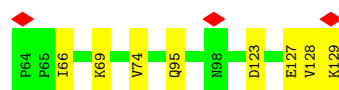
• Molecule 4: PsaD

Chain D: 73% 27%



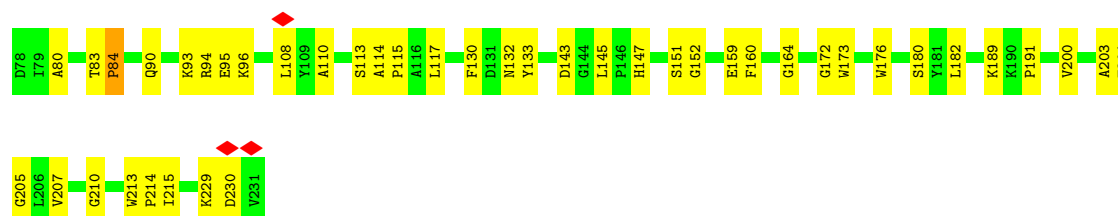
• Molecule 5: PsaE

Chain E: 5% 88% 12%



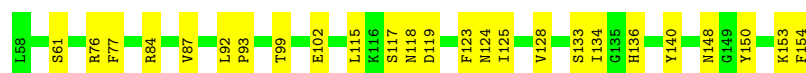
• Molecule 6: PsaF

Chain F: 72% 27%



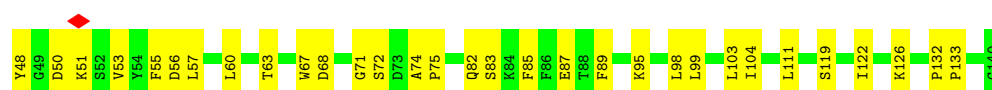
• Molecule 7: PsaG

Chain G:  74% 26%



• Molecule 8: PsaH

Chain H:  67% 33%



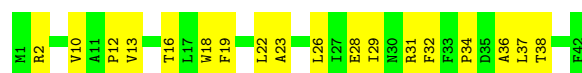
• Molecule 9: Photosystem I reaction center subunit VIII

Chain I:  61% 39%



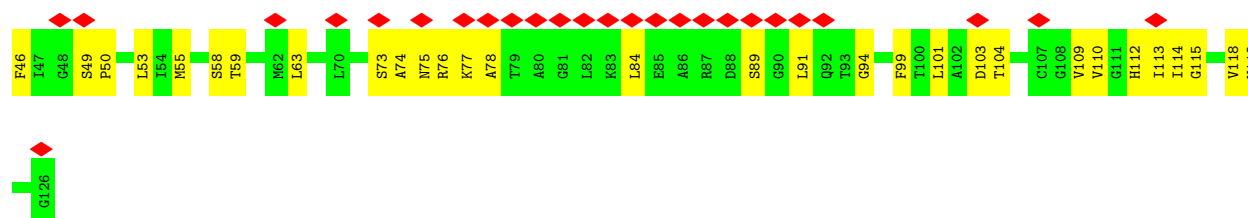
• Molecule 10: PsaJ

Chain J:  57% 43%



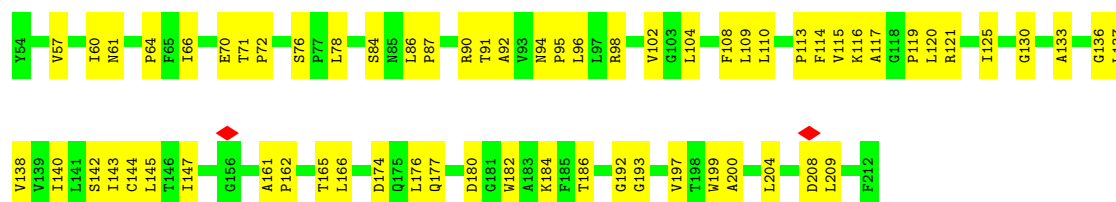
• Molecule 11: Photosystem I reaction center subunit X psaK

Chain K:  32% 63% 37%



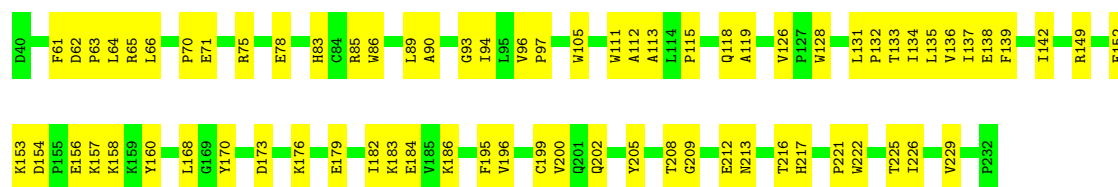
• Molecule 12: PsaL

Chain L:  60% 40%



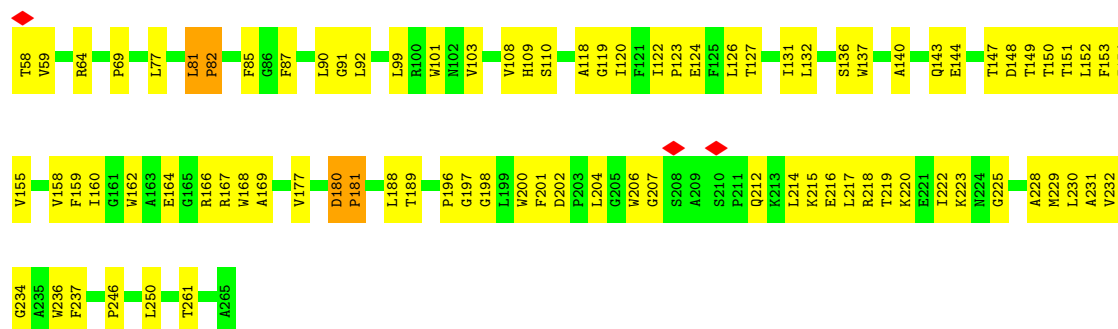
• Molecule 13: Lhca1

Chain 1:  63% 37%



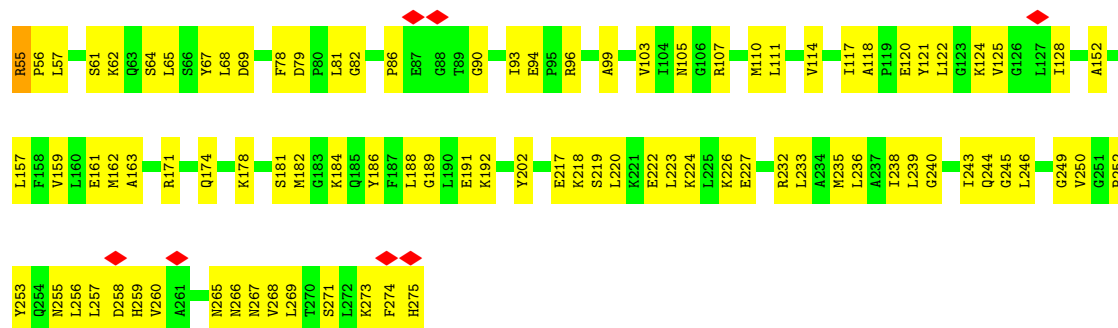
• Molecule 14: Chlorophyll a-b binding protein, chloroplastic

Chain 2:  58% 40%



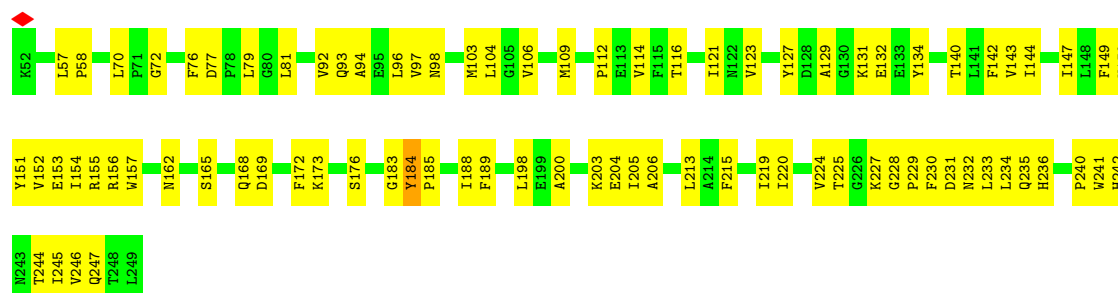
• Molecule 15: Chlorophyll a-b binding protein 3, chloroplastic

Chain 3:  58% 41%



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

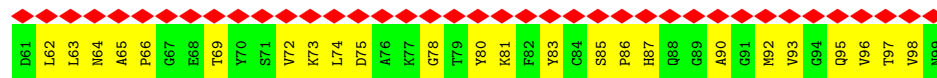
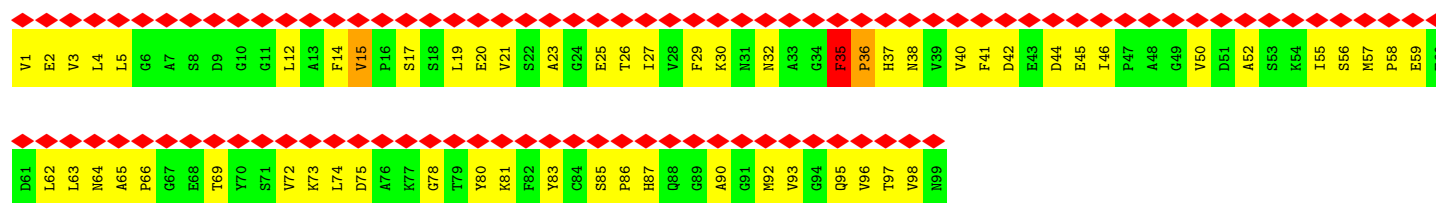
Chain 4:  58% 41%



● Molecule 17: Ferredoxin-1, chloroplastic



● Molecule 18: Plastocyanin, chloroplastic



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	102216	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 ($e^-/\text{\AA}^2$)	47.05	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.184	Depositor
Minimum map value	-0.047	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.022	Depositor
Map size ($\text{\AA}$)	246.6, 246.6, 246.6	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.822, 0.822, 0.822	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: SF4, CLA, FES, LMT, BCR, LMG, C7Z, XAT, DGD, CL0, 3PH, LUT, CHL, LHG, CU, PQN, CA

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	0.61	4/6057 (0.1%)	0.71	7/8264 (0.1%)
2	B	0.60	5/6069 (0.1%)	0.63	10/8286 (0.1%)
3	C	1.00	2/625 (0.3%)	1.21	4/846 (0.5%)
4	D	0.39	0/1163	0.55	0/1572
5	E	0.30	0/540	0.43	0/734
6	F	0.83	2/1234 (0.2%)	0.99	4/1670 (0.2%)
7	G	0.30	0/776	0.42	0/1054
8	H	0.61	0/733	0.78	0/995
9	I	0.32	0/246	0.57	0/335
10	J	0.42	0/349	0.52	0/476
11	K	0.65	0/576	0.87	0/779
12	L	0.80	2/1232 (0.2%)	1.18	7/1684 (0.4%)
13	1	0.36	0/1558	0.52	0/2125
14	2	0.86	4/1679 (0.2%)	1.11	6/2302 (0.3%)
15	3	0.60	1/1760 (0.1%)	0.85	5/2390 (0.2%)
16	4	0.55	1/1608 (0.1%)	0.76	4/2191 (0.2%)
17	N	1.19	2/736 (0.3%)	1.71	14/1000 (1.4%)
18	P	1.19	3/743 (0.4%)	1.20	3/1009 (0.3%)
All	All	0.67	26/27684 (0.1%)	0.83	64/37712 (0.2%)

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
18	P	0	2

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	561	GLY	C-N	20.63	1.50	1.33
1	A	37	PRO	N-CA	18.42	1.70	1.47
14	2	82	PRO	N-CA	18.38	1.70	1.47
1	A	570	PRO	N-CA	18.14	1.70	1.47
6	F	84	PRO	N-CA	18.13	1.70	1.47
2	B	558	PRO	N-CA	17.56	1.69	1.47
14	2	181	PRO	N-CA	17.22	1.70	1.47
2	B	449	PRO	N-CA	17.01	1.70	1.47
3	C	22	PRO	N-CA	16.59	1.69	1.47
15	3	55	ARG	C-N	13.81	1.50	1.33
17	N	18	CYS	C-N	13.30	1.50	1.33
18	P	36	PRO	N-CA	12.64	1.70	1.48
18	P	36	PRO	N-CD	-11.63	1.31	1.47
17	N	35	LEU	C-N	-11.37	1.19	1.33
14	2	180	ASP	C-N	9.73	1.45	1.33
3	C	21	CYS	C-N	9.63	1.44	1.34
2	B	448	THR	C-N	8.16	1.46	1.33
16	4	184	TYR	C-N	7.54	1.51	1.33
12	L	209	LEU	C-N	7.31	1.50	1.33
12	L	76	SER	C-N	7.16	1.50	1.33
18	P	35	PHE	C-N	5.30	1.46	1.33
2	B	557	PHE	C-N	5.08	1.45	1.33
1	A	36	LYS	C-N	5.07	1.45	1.33
6	F	83	THR	C-N	5.06	1.45	1.33
1	A	569	ILE	C-N	5.05	1.45	1.33
14	2	81	LEU	C-N	5.04	1.45	1.33

All (64) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	2	180	ASP	CA-C-N	19.71	139.66	119.56
14	2	180	ASP	C-N-CA	19.71	139.66	119.56
2	B	448	THR	CA-C-N	16.77	138.44	119.32
2	B	448	THR	C-N-CA	16.77	138.44	119.32
3	C	21	CYS	CA-C-N	16.74	137.28	119.87
3	C	21	CYS	C-N-CA	16.74	137.28	119.87
1	A	569	ILE	CA-C-N	15.93	139.75	119.84
1	A	569	ILE	C-N-CA	15.93	139.75	119.84
2	B	557	PHE	CA-C-N	15.83	139.63	119.84
2	B	557	PHE	C-N-CA	15.83	139.63	119.84
17	N	18	CYS	CA-C-N	15.68	135.91	119.76
17	N	18	CYS	C-N-CA	15.68	135.91	119.76
1	A	36	LYS	CA-C-N	14.97	138.55	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	36	LYS	C-N-CA	14.97	138.55	119.84
17	N	49	GLY	O-C-N	-14.94	103.28	122.70
14	2	81	LEU	CA-C-N	14.81	138.36	119.84
14	2	81	LEU	C-N-CA	14.81	138.36	119.84
15	3	55	ARG	CA-C-N	14.06	138.23	120.51
15	3	55	ARG	C-N-CA	14.06	138.23	120.51
6	F	83	THR	CA-C-N	14.05	137.40	119.84
6	F	83	THR	C-N-CA	14.05	137.40	119.84
17	N	49	GLY	CA-C-N	13.53	144.01	122.36
17	N	49	GLY	C-N-CA	13.53	144.01	122.36
12	L	76	SER	CA-C-N	12.95	136.03	119.84
12	L	76	SER	C-N-CA	12.95	136.03	119.84
12	L	209	LEU	CA-C-N	10.32	132.74	119.84
12	L	209	LEU	C-N-CA	10.32	132.74	119.84
17	N	35	LEU	O-C-N	-10.06	113.70	121.55
2	B	561	GLY	CA-C-N	9.69	132.76	121.04
2	B	561	GLY	C-N-CA	9.69	132.76	121.04
2	B	558	PRO	CA-N-CD	-9.41	98.83	112.00
16	4	184	TYR	CA-C-N	9.06	131.17	119.84
16	4	184	TYR	C-N-CA	9.06	131.17	119.84
1	A	570	PRO	CA-N-CD	-8.54	100.04	112.00
2	B	449	PRO	CA-N-CD	-8.35	100.31	112.00
1	A	37	PRO	CA-N-CD	-8.32	100.36	112.00
14	2	181	PRO	CA-N-CD	-7.97	100.84	112.00
14	2	82	PRO	CA-N-CD	-7.90	100.95	112.00
1	A	569	ILE	CA-C-O	-7.67	115.66	120.88
6	F	84	PRO	CA-N-CD	-7.63	101.32	112.00
3	C	22	PRO	CA-N-CD	-7.41	101.62	112.00
18	P	35	PHE	CA-C-N	7.38	137.01	120.56
18	P	35	PHE	C-N-CA	7.38	137.01	120.56
17	N	95	LEU	N-CA-C	-7.37	104.27	113.55
16	4	183	GLY	CA-C-N	-6.36	114.88	123.46
16	4	183	GLY	C-N-CA	-6.36	114.88	123.46
6	F	84	PRO	N-CA-C	-6.34	99.41	112.47
12	L	208	ASP	CA-C-N	6.29	137.15	121.80
12	L	208	ASP	C-N-CA	6.29	137.15	121.80
17	N	42	GLY	CA-C-N	-6.27	112.71	122.37
17	N	42	GLY	C-N-CA	-6.27	112.71	122.37
2	B	670	TYR	CB-CA-C	-6.23	100.84	110.81
12	L	208	ASP	O-C-N	6.20	128.48	122.03
15	3	191	GLU	N-CA-C	-6.13	105.93	113.41
17	N	35	LEU	CA-C-N	6.04	126.55	120.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	N	35	LEU	C-N-CA	6.04	126.55	120.14
17	N	87	ILE	CA-C-N	5.91	132.68	122.64
17	N	87	ILE	C-N-CA	5.91	132.68	122.64
15	3	258	ASP	CB-CA-C	5.87	120.53	110.79
17	N	46	SER	N-CA-C	5.75	118.02	111.11
15	3	189	GLY	CA-C-O	-5.65	115.29	122.01
18	P	78	GLY	CA-C-O	-5.16	117.93	122.16
3	C	53	ARG	N-CA-C	-5.07	105.83	111.36
2	B	561	GLY	O-C-N	-5.00	116.77	121.77

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
18	P	15	VAL	Peptide
18	P	35	PHE	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	5858	0	5719	336	0
2	B	5857	0	5653	231	0
3	C	612	0	591	31	0
4	D	1132	0	1141	47	0
5	E	528	0	528	5	0
6	F	1206	0	1231	48	0
7	G	757	0	743	24	0
8	H	712	0	701	38	0
9	I	240	0	264	30	0
10	J	338	0	345	35	0
11	K	569	0	596	38	0
12	L	1197	0	1197	87	0
13	1	1508	0	1489	117	0
14	2	1620	0	1557	135	0
15	3	1706	0	1661	125	0
16	4	1559	0	1527	144	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	N	724	0	672	69	0
18	P	728	0	699	92	0
19	A	65	0	72	11	0
20	1	608	0	563	96	0
20	2	522	0	499	95	0
20	3	578	0	495	60	0
20	4	631	0	595	169	0
20	A	2643	0	2749	345	0
20	B	2610	0	2747	241	0
20	F	130	0	144	21	0
20	G	166	0	153	21	0
20	H	60	0	58	18	0
20	J	50	0	38	7	0
20	K	199	0	158	16	0
20	L	160	0	134	49	0
21	A	33	0	46	8	0
21	B	33	0	46	3	0
22	1	80	0	105	5	0
22	2	40	0	53	23	0
22	3	80	0	105	10	0
22	A	240	0	316	25	0
22	B	200	0	265	19	0
22	F	80	0	105	12	0
22	G	40	0	53	4	0
22	H	40	0	53	18	0
22	I	80	0	105	17	0
22	J	40	0	53	5	0
22	K	80	0	106	15	0
22	L	80	0	106	46	0
23	1	49	0	74	11	0
23	2	35	0	40	7	0
23	3	17	0	12	0	0
23	4	35	0	40	11	0
23	A	89	0	127	3	0
23	B	70	0	86	6	0
24	2	35	0	46	7	0
24	A	35	0	45	1	0
24	B	63	0	68	1	0
24	G	66	0	79	0	0
25	A	8	0	0	0	0
25	C	16	0	0	3	0
26	1	46	0	65	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	2	134	0	133	17	0
26	3	30	0	30	0	0
26	A	50	0	73	3	0
26	B	102	0	114	16	0
26	F	160	0	188	8	0
26	G	124	0	161	15	0
27	A	1	0	0	0	0
27	B	1	0	0	0	0
28	1	41	0	40	1	0
28	3	51	0	60	3	0
28	4	51	0	60	4	0
28	B	61	0	83	7	0
28	F	57	0	75	18	0
28	G	47	0	52	3	0
28	J	58	0	77	11	0
29	1	84	0	110	39	0
29	2	42	0	55	12	0
29	3	84	0	110	7	0
29	4	42	0	55	19	0
29	J	42	0	55	9	0
30	1	164	0	134	28	0
30	2	272	0	223	52	0
30	3	164	0	136	8	0
30	4	202	0	152	11	0
31	2	44	0	56	13	0
31	4	44	0	56	14	0
32	2	33	0	39	5	0
33	4	42	0	0	4	0
34	N	4	0	0	0	0
35	P	1	0	0	0	0
36	B	2	0	0	0	0
All	All	39217	0	39245	2323	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 30.

All (2323) 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)
2:B:558:PRO:N	2:B:558:PRO:CA	1.69	1.44
14:2:181:PRO:CA	14:2:181:PRO:N	1.70	1.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:84:PRO:N	6:F:84:PRO:CA	1.70	1.41
1:A:570:PRO:N	1:A:570:PRO:CA	1.70	1.41
3:C:22:PRO:CA	3:C:22:PRO:N	1.69	1.38
1:A:37:PRO:CA	1:A:37:PRO:N	1.70	1.34
2:B:449:PRO:CA	2:B:449:PRO:N	1.70	1.32
18:P:36:PRO:N	18:P:36:PRO:CA	1.70	1.31
14:2:82:PRO:N	14:2:82:PRO:CA	1.70	1.31
1:A:666:GLN:NE2	18:P:86:PRO:HB3	1.55	1.21
17:N:73:PHE:CG	17:N:95:LEU:HD23	1.75	1.19
20:4:602:CLA:HBB1	20:4:602:CLA:HHC	1.23	1.16
28:F:5005:DGD:HAT2	28:F:5005:DGD:HB82	1.22	1.15
20:4:608:CLA:HHC	20:4:608:CLA:HBB1	1.28	1.15
23:1:801:LHG:H171	20:4:617:CLA:HED1	1.28	1.14
20:4:602:CLA:HED2	20:4:602:CLA:H2A	1.24	1.14
14:2:92:LEU:HD13	20:2:604:CLA:H42	1.17	1.14
20:K:1401:CLA:HBC3	22:K:4002:BCR:H313	1.28	1.13
18:P:81:LYS:HG2	18:P:95:GLN:HG2	1.27	1.12
29:4:501:LUT:H30	20:4:601:CLA:H51	1.28	1.10
18:P:65:ALA:HB1	18:P:66:PRO:HD2	1.33	1.10
20:3:617:CLA:H2	20:3:617:CLA:HMA2	1.21	1.10
1:A:453:LEU:HD21	20:A:1136:CLA:HAB	1.27	1.09
1:A:467:MET:HE2	1:A:467:MET:HA	1.34	1.09
12:L:110:LEU:HD13	12:L:137:LEU:HD23	1.17	1.08
6:F:159:GLU:HA	10:J:38:THR:HG22	1.35	1.08
14:2:122:ILE:HG12	20:2:606:CLA:HBC3	1.30	1.07
20:4:609:CLA:HHC	20:4:609:CLA:HBB1	1.28	1.06
20:B:1237:CLA:C14	22:I:4020:BCR:H14C	1.86	1.06
30:2:610:CHL:HBC2	30:2:610:CHL:HMC	1.38	1.05
1:A:50:THR:HG22	1:A:721:GLN:HB2	1.34	1.05
1:A:466:THR:HG21	20:A:1132:CLA:HBC3	1.38	1.05
20:B:1207:CLA:HBB1	20:B:1207:CLA:HHC	1.39	1.04
6:F:205:GLY:HA3	28:F:5005:DGD:C5E	1.87	1.04
6:F:205:GLY:CA	28:F:5005:DGD:HE5	1.88	1.03
20:K:1401:CLA:HBC3	22:K:4002:BCR:C31	1.88	1.03
20:3:617:CLA:HED2	20:3:617:CLA:H2A	1.05	1.03
20:3:612:CLA:HBB1	20:3:612:CLA:HMB3	1.41	1.02
15:3:268:VAL:O	15:3:271:SER:CB	2.07	1.02
1:A:310:PHE:HE1	20:A:1119:CLA:HAB	1.22	1.02
15:3:268:VAL:O	15:3:271:SER:HB2	1.60	1.02
20:4:617:CLA:HBB1	20:4:617:CLA:HMB1	1.41	1.02
12:L:71:THR:HB	12:L:72:PRO:HD2	1.39	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:L:4019:BCR:H382	20:L:1502:CLA:HAC2	1.42	1.01
16:4:81:LEU:HD13	20:4:604:CLA:H42	1.36	1.01
14:2:120:ILE:HG13	31:2:502:XAT:H163	1.43	1.00
14:2:120:ILE:HG13	31:2:502:XAT:C16	1.92	1.00
15:3:266:ASN:HD21	20:3:608:CLA:HED3	1.25	1.00
13:1:90:ALA:HB2	29:1:502:LUT:H392	1.44	0.99
20:3:617:CLA:HHC	20:3:617:CLA:HBB1	1.40	0.99
17:N:73:PHE:CD1	17:N:95:LEU:HD23	1.97	0.99
1:A:462:ILE:HG22	20:A:1132:CLA:HBC2	1.43	0.99
15:3:265:ASN:HA	15:3:269:LEU:HD23	1.39	0.99
16:4:150:HIS:CE1	16:4:154:ILE:HD11	1.96	0.99
13:1:195:PHE:CZ	29:1:502:LUT:H32	1.96	0.99
1:A:466:THR:HG21	20:A:1132:CLA:CBC	1.93	0.99
28:F:5005:DGD:HB82	28:F:5005:DGD:CAA	1.91	0.98
26:G:5002:LMG:O4	13:1:115:PRO:O	1.80	0.98
15:3:162:MET:HE1	20:3:617:CLA:H71	1.43	0.98
9:I:21:MET:HG2	22:L:4019:BCR:H10C	1.45	0.98
29:4:501:LUT:H28	20:4:601:CLA:H11	1.40	0.98
13:1:96:VAL:HG21	20:1:606:CLA:HAC2	1.46	0.98
20:K:1401:CLA:HED2	20:K:1401:CLA:H2A	1.45	0.97
20:2:608:CLA:O1A	30:2:609:CHL:H122	1.64	0.97
13:1:200:VAL:HG11	20:1:603:CLA:HAC2	1.48	0.96
22:L:4019:BCR:H331	22:L:4019:BCR:HC8	1.45	0.96
6:F:205:GLY:HA3	28:F:5005:DGD:HE5	0.97	0.95
23:1:801:LHG:H342	16:4:147:ILE:CD1	1.96	0.95
20:4:605:CLA:OBD	20:4:612:CLA:HBA2	1.65	0.95
16:4:215:PHE:CD1	31:4:502:XAT:H14	2.02	0.95
16:4:236:HIS:CG	20:4:603:CLA:HAA2	2.02	0.95
1:A:24:ARG:HE	15:3:90:GLY:HA2	1.32	0.95
20:4:601:CLA:H51	20:4:601:CLA:H93	1.47	0.95
1:A:41:SER:HB3	1:A:44:ILE:HG13	1.49	0.95
1:A:506:GLY:HA3	20:A:1134:CLA:HED3	1.45	0.95
20:1:604:CLA:HHH	30:1:609:CHL:HBB2	1.49	0.95
2:B:257:LEU:HD22	20:B:1214:CLA:HBB1	1.49	0.94
16:4:103:MET:SD	20:4:601:CLA:HAB	2.06	0.94
20:2:604:CLA:HMB3	20:2:604:CLA:HBB1	1.50	0.94
20:3:617:CLA:H2A	20:3:617:CLA:CED	1.95	0.94
17:N:58:GLN:HA	17:N:58:GLN:HE21	1.32	0.94
14:2:92:LEU:CD1	20:2:604:CLA:H42	1.97	0.94
11:K:73:SER:HB2	11:K:76:ARG:H	1.33	0.93
9:I:25:PHE:HB2	22:L:4019:BCR:H14C	1.51	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:L:1503:CLA:HMB1	20:L:1503:CLA:HBB1	1.48	0.92
14:2:149:THR:HG21	30:2:610:CHL:CMD	1.99	0.92
10:J:36:ALA:HB1	28:J:5001:DGD:HG2	1.50	0.92
20:4:604:CLA:HBB1	20:4:604:CLA:HMB3	1.48	0.92
29:1:502:LUT:H28	29:1:502:LUT:H361	1.50	0.92
18:P:20:GLU:HG2	18:P:97:THR:HG22	1.48	0.92
20:B:1237:CLA:H141	22:I:4020:BCR:H14C	1.50	0.91
23:B:5001:LHG:HC42	20:B:1240:CLA:HBA1	1.53	0.91
20:L:1501:CLA:HMB1	20:L:1501:CLA:HBB1	1.53	0.91
1:A:283:PHE:CD2	20:A:1116:CLA:HBB1	2.05	0.91
18:P:83:TYR:HB3	18:P:93:VAL:HG13	1.51	0.91
1:A:310:PHE:CE1	20:A:1119:CLA:HAB	2.06	0.91
13:1:90:ALA:CB	29:1:502:LUT:H392	2.00	0.91
20:B:1211:CLA:H3A	22:B:4006:BCR:H393	1.52	0.91
10:J:36:ALA:CB	28:J:5001:DGD:HG2	2.01	0.91
20:4:603:CLA:HBB1	20:4:603:CLA:HHC	1.52	0.91
29:4:501:LUT:H30	20:4:601:CLA:H93	1.51	0.91
20:K:1401:CLA:HBB1	20:K:1401:CLA:HMB3	1.53	0.90
15:3:250:VAL:CG2	15:3:255:ASN:HB2	2.01	0.90
28:F:5005:DGD:HB21	28:F:5005:DGD:HA21	1.54	0.90
14:2:149:THR:HG21	30:2:610:CHL:HMD2	1.54	0.89
20:H:1701:CLA:NB	22:H:4021:BCR:H362	1.86	0.89
20:2:606:CLA:HBA1	20:2:606:CLA:CHA	1.99	0.89
16:4:81:LEU:HD13	20:4:604:CLA:H11	1.55	0.89
15:3:250:VAL:HG23	15:3:255:ASN:HB2	1.54	0.89
29:1:502:LUT:H193	20:1:604:CLA:H13	1.55	0.88
31:2:502:XAT:H382	20:2:604:CLA:O1A	1.72	0.88
15:3:266:ASN:ND2	20:3:608:CLA:O1D	2.07	0.88
14:2:204:LEU:HD22	29:2:501:LUT:H22	1.55	0.88
2:B:694:ARG:HH12	9:I:30:LYS:HA	1.39	0.88
20:3:617:CLA:HED2	20:3:617:CLA:C2A	1.99	0.88
1:A:474:GLN:O	1:A:481:ALA:HB1	1.74	0.88
15:3:121:TYR:CD1	15:3:253:TYR:CE1	2.61	0.87
20:A:1101:CLA:HED2	21:A:2001:PQN:H241	1.56	0.87
16:4:245:ILE:HD11	20:4:603:CLA:C3D	2.05	0.87
13:1:195:PHE:CE2	29:1:502:LUT:H34	2.09	0.87
14:2:122:ILE:CG1	20:2:606:CLA:HBC3	2.04	0.87
1:A:126:ILE:HB	29:J:4013:LUT:H182	1.54	0.87
23:2:801:LHG:O4	23:2:801:LHG:HC12	1.75	0.87
1:A:98:PHE:CG	20:A:1105:CLA:HBC3	2.09	0.87
24:2:808:LMT:H6'2	15:3:186:TYR:HB2	1.57	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:25:PHE:CB	22:L:4019:BCR:H14C	2.06	0.86
20:4:602:CLA:HED2	20:4:602:CLA:C2A	2.06	0.86
16:4:76:PHE:HB3	20:4:604:CLA:CAD	2.05	0.86
20:A:1101:CLA:H93	20:A:1106:CLA:H171	1.56	0.85
1:A:41:SER:HB3	1:A:44:ILE:CG1	2.07	0.85
14:2:167:ARG:NH1	20:2:612:CLA:O1D	2.09	0.85
1:A:466:THR:CG2	20:A:1132:CLA:HBC3	2.05	0.85
20:K:1401:CLA:CBC	22:K:4002:BCR:H313	2.06	0.85
20:B:1237:CLA:H2	20:B:1237:CLA:HBA2	1.59	0.85
1:A:488:PHE:CE2	20:A:1136:CLA:H42	2.11	0.84
23:1:801:LHG:H342	16:4:147:ILE:HD12	1.58	0.84
29:4:501:LUT:C30	20:4:601:CLA:H93	2.06	0.84
1:A:98:PHE:CD2	20:A:1105:CLA:HBC3	2.13	0.84
16:4:58:PRO:HD2	20:4:609:CLA:HED2	1.58	0.84
1:A:453:LEU:CD2	20:A:1136:CLA:HAB	2.08	0.84
13:1:222:TRP:CD2	20:1:608:CLA:HMA3	2.14	0.83
16:4:241:TRP:CE3	20:4:608:CLA:HMA2	2.14	0.83
20:4:602:CLA:HBC1	20:4:603:CLA:H203	1.60	0.83
2:B:721:TYR:HB2	20:B:1021:CLA:HED3	1.60	0.83
29:1:502:LUT:H383	20:1:606:CLA:C2B	2.08	0.83
17:N:23:TYR:HD1	17:N:79:ALA:H	1.27	0.82
22:L:4019:BCR:H331	22:L:4019:BCR:C8	2.05	0.82
18:P:14:PHE:CZ	18:P:92:MET:HE2	2.13	0.82
1:A:220:GLY:HA3	20:A:1113:CLA:HAB	1.60	0.82
11:K:114:ILE:O	11:K:118:VAL:HG22	1.78	0.82
1:A:158:ILE:HA	20:A:1112:CLA:HED1	1.62	0.82
12:L:110:LEU:CD1	12:L:137:LEU:HD23	2.05	0.82
28:F:5005:DGD:HB82	28:F:5005:DGD:CBA	2.09	0.82
11:K:112:HIS:CE1	22:K:4002:BCR:H14C	2.15	0.82
16:4:76:PHE:HB3	20:4:604:CLA:OBD	1.80	0.81
16:4:244:THR:HB	20:4:608:CLA:HED3	1.62	0.81
20:4:607:CLA:HHC	20:4:607:CLA:HBB1	1.60	0.81
1:A:252:ARG:HD3	20:A:1113:CLA:HED2	1.62	0.81
14:2:90:LEU:O	26:2:804:LMG:H292	1.79	0.81
30:2:611:CHL:HHC	30:2:611:CHL:HBB1	1.63	0.81
18:P:1:VAL:HG21	18:P:21:VAL:HG12	1.62	0.81
1:A:205:HIS:CG	20:A:1111:CLA:HMC1	2.16	0.81
30:2:610:CHL:HBB1	30:2:610:CHL:HMB3	1.62	0.81
1:A:688:PHE:HZ	20:A:1140:CLA:HBC2	1.46	0.81
9:I:14:LEU:CD2	22:I:4018:BCR:H351	2.11	0.81
20:2:604:CLA:HMD3	30:2:609:CHL:CBB	2.10	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:2:613:CHL:HHC	30:2:613:CHL:HBB1	1.63	0.81
16:4:94:ALA:HA	20:4:612:CLA:HED2	1.61	0.80
20:B:1237:CLA:HMB1	20:B:1237:CLA:HBB1	1.64	0.80
6:F:114:ALA:HB3	6:F:115:PRO:HD3	1.62	0.80
20:2:604:CLA:CMD	30:2:609:CHL:CBB	2.60	0.80
12:L:87:PRO:CD	20:L:1502:CLA:HED2	2.11	0.80
14:2:92:LEU:HD13	20:2:604:CLA:C4	2.05	0.79
17:N:54:GLY:HA3	17:N:85:VAL:HG12	1.64	0.79
16:4:131:LYS:HE3	30:4:610:CHL:HED2	1.63	0.79
8:H:82:GLN:NE2	20:L:1501:CLA:HED2	1.97	0.79
18:P:57:MET:CE	18:P:62:LEU:HA	2.12	0.79
1:A:467:MET:HE2	1:A:467:MET:CA	2.12	0.79
18:P:57:MET:HE1	18:P:62:LEU:C	2.07	0.79
20:A:1101:CLA:HBB1	20:A:1101:CLA:HMB3	1.64	0.79
22:B:4004:BCR:H392	7:G:134:ILE:HD11	1.65	0.79
1:A:126:ILE:HG13	1:A:127:VAL:HG13	1.65	0.79
22:B:4004:BCR:H23C	7:G:134:ILE:HD11	1.64	0.79
14:2:127:THR:OG1	14:2:132:LEU:O	2.01	0.79
12:L:204:LEU:H	12:L:204:LEU:HD12	1.48	0.79
22:L:4020:BCR:H331	22:L:4020:BCR:C8	2.11	0.78
15:3:238:ILE:HG21	29:3:502:LUT:H12	1.65	0.78
1:A:51:THR:CG2	1:A:722:PRO:HA	2.13	0.78
1:A:221:HIS:HB2	20:A:1112:CLA:CHC	2.14	0.78
20:A:1139:CLA:H8	10:J:18:TRP:CE3	2.18	0.78
20:4:609:CLA:HBC3	23:4:801:LHG:HC42	1.65	0.78
4:D:91:LEU:HD23	4:D:133:ALA:HB2	1.66	0.78
17:N:9:THR:HG22	17:N:11:ASP:H	1.48	0.78
26:F:5003:LMG:HC92	26:F:5003:LMG:C14	2.14	0.78
1:A:245:PRO:HG2	20:A:1112:CLA:OBD	1.83	0.78
15:3:243:ILE:HD12	15:3:244:GLN:N	1.99	0.78
14:2:119:GLY:HA3	31:2:502:XAT:H172	1.66	0.78
20:4:604:CLA:HED2	20:4:604:CLA:H2A	1.64	0.78
13:1:85:ARG:HB3	20:1:601:CLA:HBC3	1.64	0.77
30:1:609:CHL:HED1	16:4:155:ARG:HA	1.65	0.77
1:A:41:SER:CB	1:A:44:ILE:HG13	2.13	0.77
3:C:15:THR:HG22	3:C:28:MET:SD	2.23	0.77
30:1:609:CHL:H43	16:4:147:ILE:HG22	1.64	0.77
15:3:188:LEU:HD12	22:3:503:BCR:H342	1.66	0.77
1:A:332:GLU:HG2	1:A:344:LYS:HA	1.67	0.77
20:4:608:CLA:HHC	20:4:608:CLA:CBB	2.12	0.77
1:A:666:GLN:NE2	18:P:86:PRO:CB	2.42	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:N:6:LYS:HZ2	17:N:6:LYS:HB2	1.49	0.77
20:A:1132:CLA:O1D	12:L:119:PRO:HB3	1.83	0.77
2:B:71:GLN:NE2	20:B:1204:CLA:O1D	2.16	0.77
3:C:38:GLN:OE1	4:D:178:VAL:CG1	2.33	0.77
30:2:609:CHL:HBD	30:2:609:CHL:HAA1	1.67	0.77
16:4:245:ILE:CD1	20:4:603:CLA:C3D	2.63	0.77
18:P:27:ILE:CG2	18:P:74:LEU:HD21	2.15	0.77
20:A:1101:CLA:CED	21:A:2001:PQN:H241	2.15	0.76
16:4:76:PHE:CE2	31:4:502:XAT:H383	2.20	0.76
1:A:408:VAL:HG11	1:A:602:LEU:CD2	2.16	0.76
13:1:195:PHE:CE2	29:1:502:LUT:H32	2.19	0.76
14:2:155:VAL:O	14:2:158:VAL:HG12	1.85	0.76
16:4:241:TRP:CZ3	20:4:608:CLA:HMA2	2.19	0.76
20:G:1603:CLA:HAC2	13:1:113:ALA:HA	1.68	0.76
14:2:122:ILE:HG12	20:2:606:CLA:CBC	2.12	0.76
16:4:81:LEU:CD1	20:4:604:CLA:H42	2.15	0.76
18:P:5:LEU:HG	18:P:14:PHE:CE1	2.21	0.76
16:4:241:TRP:CE3	20:4:608:CLA:CMA	2.69	0.76
20:B:1237:CLA:H72	20:B:1238:CLA:H43	1.68	0.75
3:C:16:GLN:HE21	17:N:44:CYS:HB2	1.52	0.75
20:4:602:CLA:HHC	20:4:602:CLA:CBB	2.09	0.75
10:J:28:GLU:HG3	20:J:1901:CLA:C1B	2.16	0.75
14:2:261:THR:HG21	15:3:156:THR:HG21	1.68	0.75
15:3:67:TYR:OH	15:3:82:GLY:HA2	1.87	0.75
1:A:37:PRO:HA	20:A:1101:CLA:HBC1	1.69	0.75
20:A:1107:CLA:H11	22:J:4012:BCR:H19C	1.69	0.75
12:L:204:LEU:HD12	12:L:204:LEU:N	2.01	0.75
20:1:608:CLA:HED1	16:4:140:THR:HG23	1.69	0.75
1:A:662:SER:OG	18:P:36:PRO:HG3	1.87	0.75
20:K:1401:CLA:HMC3	22:K:4002:BCR:H321	1.69	0.75
1:A:283:PHE:CE2	20:A:1116:CLA:HBB1	2.22	0.75
1:A:467:MET:HA	1:A:467:MET:CE	2.13	0.75
29:1:502:LUT:C28	29:1:502:LUT:H371	2.15	0.75
15:3:174:GLN:OE1	15:3:174:GLN:HA	1.86	0.75
20:4:609:CLA:HHC	20:4:609:CLA:CBB	2.12	0.75
6:F:108:LEU:O	6:F:108:LEU:HD12	1.86	0.74
30:2:609:CHL:HBB1	30:2:609:CHL:HHC	1.69	0.74
1:A:506:GLY:N	20:A:1134:CLA:O1D	2.19	0.74
20:L:1503:CLA:C2	20:L:1503:CLA:HBA1	2.17	0.74
16:4:104:LEU:HD13	20:4:601:CLA:HAC1	1.68	0.74
1:A:503:THR:HG23	20:A:1133:CLA:OBD	1.87	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:N:6:LYS:HB2	17:N:6:LYS:NZ	2.03	0.74
1:A:368:LEU:HD13	20:A:1125:CLA:H43	1.67	0.74
1:A:462:ILE:CG2	20:A:1132:CLA:HBC2	2.18	0.74
20:F:1301:CLA:HBC2	10:J:19:PHE:CZ	2.23	0.74
18:P:38:ASN:HB2	18:P:62:LEU:HB2	1.70	0.74
28:F:5005:DGD:HA22	28:F:5005:DGD:HA62	1.70	0.74
29:1:502:LUT:H28	29:1:502:LUT:H371	1.69	0.74
18:P:2:GLU:OE1	18:P:30:LYS:HD3	1.87	0.74
20:A:1114:CLA:HBB1	20:A:1114:CLA:HHC	1.70	0.74
2:B:514:PRO:HG2	6:F:147:HIS:CE1	2.22	0.74
11:K:73:SER:HB2	11:K:76:ARG:N	2.03	0.74
1:A:455:PHE:O	20:A:1132:CLA:HBB2	1.88	0.73
2:B:442:VAL:HG21	20:B:1230:CLA:HAC2	1.69	0.73
22:H:4021:BCR:H321	22:H:4021:BCR:C8	2.16	0.73
15:3:121:TYR:CD1	15:3:253:TYR:HE1	2.06	0.73
1:A:271:THR:HG23	1:A:273:ASN:H	1.54	0.73
1:A:93:LEU:HD12	20:A:1103:CLA:H91	1.70	0.73
20:3:617:CLA:HHC	20:3:617:CLA:CBB	2.18	0.73
16:4:76:PHE:HE2	31:4:502:XAT:H383	1.51	0.73
20:4:617:CLA:HBB1	20:4:617:CLA:CMB	2.19	0.73
22:2:503:BCR:H393	20:2:606:CLA:C2B	2.18	0.73
15:3:256:LEU:HD22	29:3:501:LUT:H172	1.71	0.73
20:A:1137:CLA:HBB1	20:A:1137:CLA:HHC	1.71	0.73
2:B:716:GLY:O	2:B:720:THR:HG22	1.89	0.73
23:1:801:LHG:C17	20:4:617:CLA:HED1	2.13	0.73
20:B:1207:CLA:HHC	20:B:1207:CLA:CBB	2.16	0.72
12:L:98:ARG:HH22	12:L:176:LEU:HB2	1.54	0.72
16:4:109:MET:HG3	31:4:502:XAT:O4	1.89	0.72
17:N:16:PHE:HZ	17:N:24:ILE:HG23	1.52	0.72
20:A:1109:CLA:H191	29:J:4013:LUT:H393	1.70	0.72
20:B:1239:CLA:HHC	20:B:1239:CLA:HBB1	1.70	0.72
29:1:502:LUT:H383	20:1:606:CLA:C3B	2.18	0.72
15:3:65:LEU:O	15:3:65:LEU:HD23	1.90	0.72
1:A:570:PRO:HB3	4:D:137:GLN:HG2	1.71	0.72
18:P:3:VAL:HG23	18:P:27:ILE:HD11	1.70	0.72
18:P:4:LEU:HD22	18:P:30:LYS:HE2	1.72	0.72
6:F:84:PRO:N	6:F:84:PRO:C	2.47	0.72
20:1:603:CLA:HBD	20:1:603:CLA:HBA1	1.71	0.72
20:A:1119:CLA:H122	22:A:4007:BCR:H10C	1.72	0.72
9:I:21:MET:CG	22:L:4019:BCR:H10C	2.19	0.72
11:K:73:SER:OG	11:K:76:ARG:HB2	1.90	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:2:228:ALA:O	14:2:232:VAL:HG22	1.90	0.72
15:3:257:LEU:HD23	15:3:257:LEU:C	2.14	0.72
30:2:615:CHL:HHC	30:2:615:CHL:HBB1	1.70	0.72
15:3:107:ARG:HB3	20:3:601:CLA:HBC3	1.72	0.72
2:B:159:PRO:O	2:B:160:LYS:HB3	1.90	0.72
16:4:198:LEU:C	16:4:198:LEU:HD23	2.15	0.72
22:L:4019:BCR:C38	20:L:1502:CLA:HAC2	2.20	0.72
20:2:608:CLA:O1A	30:2:609:CHL:C12	2.36	0.72
30:1:609:CHL:HHC	30:1:609:CHL:HBB1	1.70	0.71
9:I:21:MET:HG2	22:L:4019:BCR:C10	2.19	0.71
1:A:506:GLY:CA	20:A:1134:CLA:HED3	2.21	0.71
30:4:613:CHL:HHC	30:4:613:CHL:HBB1	1.73	0.71
13:1:142:ILE:HD13	22:1:504:BCR:H363	1.72	0.71
20:2:604:CLA:HBC1	23:2:801:LHG:H291	1.72	0.71
17:N:16:PHE:HB2	17:N:31:VAL:HG21	1.72	0.71
1:A:298:ASP:HB3	20:A:1116:CLA:HMA1	1.71	0.71
20:A:1109:CLA:HHC	20:A:1109:CLA:HBB1	1.72	0.71
20:A:1119:CLA:H52	20:A:1122:CLA:H42	1.73	0.71
10:J:29:ILE:HD11	28:J:5001:DGD:HB81	1.71	0.71
9:I:24:LEU:HD13	22:L:4019:BCR:H312	1.73	0.71
16:4:94:ALA:CA	20:4:612:CLA:HED2	2.21	0.71
11:K:53:LEU:HD13	11:K:53:LEU:C	2.16	0.71
20:B:1237:CLA:H162	22:I:4020:BCR:H363	1.73	0.70
1:A:590:CYS:HB2	2:B:667:TRP:HB3	1.73	0.70
18:P:62:LEU:C	18:P:62:LEU:HD23	2.16	0.70
1:A:250:LEU:HD23	28:3:803:DGD:HA21	1.73	0.70
2:B:440:ASN:O	2:B:444:LEU:HD12	1.92	0.70
3:C:58:CYS:HA	25:C:3003:SF4:S2	2.32	0.70
13:1:96:VAL:CG2	20:1:606:CLA:HAC2	2.20	0.70
18:P:14:PHE:HB2	18:P:17:SER:HA	1.74	0.70
14:2:108:VAL:HG11	20:2:612:CLA:O1D	1.92	0.70
22:H:4021:BCR:H372	22:L:4020:BCR:H10C	1.72	0.70
30:2:609:CHL:H71	30:2:609:CHL:H41	1.73	0.70
15:3:55:ARG:NH1	15:3:69:ASP:O	2.24	0.70
1:A:680:LEU:HD13	20:A:1012:CLA:H2	1.73	0.70
20:G:1603:CLA:CAC	13:1:113:ALA:HA	2.22	0.70
17:N:73:PHE:CD2	17:N:95:LEU:HD23	2.27	0.70
26:B:5003:LMG:H131	26:B:5003:LMG:HC91	1.73	0.69
29:1:502:LUT:H361	29:1:502:LUT:C28	2.22	0.69
10:J:38:THR:O	28:J:5001:DGD:O1G	2.11	0.69
20:L:1501:CLA:HBB1	20:L:1501:CLA:CMB	2.21	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:645:VAL:HG21	20:B:1205:CLA:HAC1	1.75	0.69
4:D:78:ASN:HA	8:H:53:VAL:HG21	1.74	0.69
4:D:174:TYR:HB3	4:D:176:GLU:OE2	1.93	0.69
23:1:801:LHG:C34	16:4:147:ILE:HD12	2.22	0.69
1:A:666:GLN:HE21	18:P:86:PRO:HB3	1.54	0.69
14:2:120:ILE:HG13	31:2:502:XAT:H162	1.74	0.69
22:2:503:BCR:H323	23:4:801:LHG:HC92	1.74	0.69
20:K:1401:CLA:HBB1	20:K:1401:CLA:CMB	2.22	0.69
13:1:225:THR:HG22	20:1:603:CLA:HBA2	1.73	0.69
2:B:694:ARG:NH1	9:I:30:LYS:HA	2.07	0.69
12:L:136:GLY:O	12:L:140:ILE:HG13	1.91	0.69
16:4:188:ILE:HG21	30:4:615:CHL:HBC3	1.73	0.69
29:4:501:LUT:H193	20:4:602:CLA:HMC3	1.74	0.69
9:I:14:LEU:HD22	22:I:4018:BCR:H351	1.74	0.69
29:4:501:LUT:C19	20:4:602:CLA:HMC3	2.23	0.69
20:L:1503:CLA:HBB1	20:L:1503:CLA:CMB	2.21	0.69
13:1:160:TYR:HB3	20:1:601:CLA:HED3	1.75	0.69
16:4:70:LEU:HD13	16:4:92:VAL:HG11	1.73	0.69
18:P:38:ASN:HB2	18:P:62:LEU:CB	2.22	0.69
18:P:57:MET:HE1	18:P:62:LEU:CA	2.22	0.69
18:P:65:ALA:HB1	18:P:66:PRO:CD	2.17	0.69
1:A:267:THR:O	1:A:271:THR:HG22	1.93	0.69
22:2:503:BCR:H321	22:2:503:BCR:HC8	1.75	0.69
1:A:57:LEU:HD21	20:A:1101:CLA:HBC2	1.75	0.69
1:A:569:ILE:HD12	1:A:592:VAL:HG21	1.74	0.69
20:2:604:CLA:HBB1	20:2:604:CLA:CMB	2.22	0.69
12:L:71:THR:HB	12:L:72:PRO:CD	2.20	0.68
18:P:57:MET:HE1	18:P:62:LEU:HA	1.74	0.68
1:A:124:TRP:HB3	29:J:4013:LUT:H183	1.76	0.68
20:G:1603:CLA:H42	26:G:5002:LMG:H222	1.76	0.68
17:N:65:ASP:C	17:N:67:GLU:H	2.02	0.68
14:2:220:LYS:HG2	20:2:607:CLA:O1D	1.94	0.68
22:A:4011:BCR:H23C	20:A:1013:CLA:H111	1.75	0.68
26:G:5002:LMG:H161	13:1:135:LEU:HG	1.76	0.68
13:1:226:ILE:CG2	20:1:603:CLA:H11	2.23	0.68
30:2:613:CHL:OMC	30:2:613:CHL:HBC2	1.93	0.68
1:A:152:ILE:HD11	20:A:1127:CLA:HAA1	1.75	0.68
2:B:63:GLY:HA3	20:B:1204:CLA:HAB	1.74	0.68
11:K:77:LYS:HA	11:K:77:LYS:HE2	1.74	0.68
31:2:502:XAT:H173	20:2:606:CLA:C2B	2.23	0.68
20:A:1012:CLA:HBC2	2:B:585:ASN:HB2	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:226:PHE:CE1	20:G:1601:CLA:HBC1	2.28	0.68
6:F:117:LEU:O	6:F:117:LEU:HD23	1.93	0.68
30:2:609:CHL:H71	30:2:609:CHL:C4	2.24	0.68
28:F:5005:DGD:HAT2	28:F:5005:DGD:C8B	2.14	0.68
7:G:148:ASN:HD22	20:G:1603:CLA:HED2	1.57	0.68
16:4:81:LEU:HD13	20:4:604:CLA:C4	2.21	0.68
1:A:224:HIS:HE1	20:A:1113:CLA:NB	1.92	0.67
20:L:1501:CLA:HBA1	22:L:4020:BCR:H352	1.74	0.67
20:4:604:CLA:HBB1	20:4:604:CLA:CMB	2.22	0.67
15:3:246:LEU:HD12	28:3:803:DGD:HB52	1.74	0.67
19:A:1011:CL0:H21	2:B:625:TRP:HD1	1.58	0.67
15:3:266:ASN:HD21	20:3:608:CLA:CED	2.03	0.67
20:A:1132:CLA:HMB1	20:A:1132:CLA:HBB1	1.75	0.67
29:J:4013:LUT:H371	29:J:4013:LUT:H28	1.76	0.67
2:B:547:MET:HE3	2:B:550:LYS:HG3	1.75	0.67
22:H:4021:BCR:H371	22:L:4020:BCR:C35	2.25	0.67
17:N:73:PHE:CG	17:N:95:LEU:CD2	2.68	0.67
18:P:62:LEU:HD23	18:P:62:LEU:O	1.95	0.67
20:H:1701:CLA:C4B	22:H:4021:BCR:H362	2.25	0.67
17:N:6:LYS:HZ2	17:N:6:LYS:CB	2.08	0.67
1:A:408:VAL:HG11	1:A:602:LEU:HD23	1.77	0.67
20:B:1206:CLA:H91	20:B:1239:CLA:H12	1.76	0.67
18:P:27:ILE:HG22	18:P:74:LEU:CD2	2.24	0.67
1:A:252:ARG:HB2	20:A:1113:CLA:HED2	1.77	0.66
20:A:1139:CLA:H8	10:J:18:TRP:CZ3	2.31	0.66
2:B:61:THR:HG23	2:B:142:LEU:HD13	1.78	0.66
14:2:153:PHE:HB2	30:2:610:CHL:HAC2	1.77	0.66
15:3:250:VAL:HG21	15:3:255:ASN:HB2	1.77	0.66
20:B:1023:CLA:H143	22:I:4018:BCR:H323	1.77	0.66
14:2:101:TRP:CD2	26:2:802:LMG:HC5	2.30	0.66
17:N:23:TYR:HA	17:N:79:ALA:O	1.95	0.66
20:2:606:CLA:HMC1	20:2:606:CLA:HBC2	1.77	0.66
20:A:1110:CLA:HBD	20:A:1110:CLA:HBA1	1.78	0.66
20:A:1122:CLA:H43	22:A:4008:BCR:H351	1.76	0.66
2:B:23:PHE:O	2:B:27:THR:HG22	1.95	0.66
23:1:801:LHG:H342	16:4:147:ILE:HD11	1.76	0.66
16:4:81:LEU:CD1	20:4:604:CLA:H11	2.24	0.66
16:4:213:LEU:CD1	20:4:604:CLA:HAC1	2.25	0.66
20:A:1132:CLA:HHD	20:B:1206:CLA:HBB2	1.77	0.66
15:3:152:ALA:HB3	15:3:157:LEU:HG	1.76	0.66
20:A:1116:CLA:HAC1	20:A:1133:CLA:H42	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:99:PHE:CD2	20:K:1404:CLA:HAB	2.30	0.66
22:I:4020:BCR:HC41	12:L:140:ILE:HD11	1.77	0.66
22:2:503:BCR:C8	22:2:503:BCR:H311	2.25	0.66
18:P:29:PHE:HE2	18:P:72:VAL:HG11	1.61	0.66
20:B:1208:CLA:HBB1	20:B:1208:CLA:HHC	1.77	0.66
10:J:32:PHE:CE2	20:J:1901:CLA:HMA2	2.31	0.66
2:B:439:HIS:NE2	2:B:453:ILE:HG13	2.10	0.65
3:C:73:THR:H	3:C:76:SER:HB3	1.60	0.65
17:N:49:GLY:HA2	17:N:91:LYS:HB2	1.77	0.65
1:A:579:PHE:CE1	1:A:593:SER:HB3	2.31	0.65
20:A:1119:CLA:H112	22:A:4008:BCR:H21C	1.78	0.65
18:P:19:LEU:HG	18:P:20:GLU:N	2.11	0.65
3:C:15:THR:HG22	3:C:28:MET:CE	2.27	0.65
20:1:604:CLA:CHD	30:1:609:CHL:HBB2	2.26	0.65
20:B:1237:CLA:HBB1	20:B:1237:CLA:CMB	2.26	0.65
15:3:239:LEU:HD13	20:3:605:CLA:HBB2	1.77	0.65
13:1:184:GLU:HB2	20:1:601:CLA:CHB	2.26	0.65
18:P:27:ILE:HG21	18:P:74:LEU:HD21	1.78	0.65
26:G:5001:LMG:H291	30:1:612:CHL:H11	1.77	0.65
15:3:121:TYR:HD1	15:3:253:TYR:CE1	2.09	0.65
1:A:371:ILE:HD13	20:A:1125:CLA:H12	1.77	0.65
22:H:4021:BCR:H24C	22:L:4020:BCR:H353	1.78	0.65
16:4:215:PHE:CG	31:4:502:XAT:H14	2.31	0.65
18:P:62:LEU:HD22	18:P:62:LEU:H	1.60	0.65
20:A:1123:CLA:HBA1	20:A:1127:CLA:H191	1.77	0.65
20:H:1701:CLA:HBB1	20:H:1701:CLA:HMB1	1.78	0.65
18:P:42:ASP:C	18:P:44:ASP:H	2.05	0.65
22:H:4021:BCR:H371	22:L:4020:BCR:H353	1.78	0.65
30:2:610:CHL:HMC	30:2:610:CHL:CBC	2.21	0.65
16:4:228:GLY:O	16:4:232:ASN:ND2	2.29	0.65
11:K:91:LEU:HD23	11:K:91:LEU:H	1.62	0.65
13:1:222:TRP:CE2	20:1:608:CLA:HMA3	2.32	0.65
18:P:20:GLU:HG2	18:P:97:THR:CG2	2.24	0.65
1:A:119:SER:HB2	1:A:144:GLN:HA	1.78	0.64
26:B:5003:LMG:H181	22:F:4016:BCR:H362	1.79	0.64
13:1:152:GLU:OE2	13:1:153:LYS:N	2.30	0.64
13:1:225:THR:HA	20:1:603:CLA:CBA	2.27	0.64
30:4:615:CHL:HHC	30:4:615:CHL:HBB1	1.77	0.64
20:A:1101:CLA:HBB1	20:A:1101:CLA:CMB	2.26	0.64
8:H:103:LEU:HD21	12:L:142:SER:HB2	1.79	0.64
12:L:71:THR:CB	12:L:72:PRO:HD2	2.21	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:503:THR:HG21	20:A:1133:CLA:CMD	2.27	0.64
20:A:1101:CLA:H43	21:A:2001:PQN:H303	1.79	0.64
11:K:49:SER:HB2	11:K:50:PRO:HD3	1.79	0.64
11:K:101:LEU:HA	11:K:104:THR:HG22	1.77	0.64
1:A:224:HIS:CE1	20:A:1113:CLA:NB	2.66	0.64
20:A:1131:CLA:HAA1	22:I:4020:BCR:C16	2.28	0.64
20:B:1207:CLA:HMD3	22:I:4018:BCR:H332	1.80	0.64
13:1:226:ILE:HD13	20:1:603:CLA:H42	1.78	0.64
16:4:184:TYR:HB3	20:4:601:CLA:O1D	1.98	0.64
18:P:46:ILE:HG22	18:P:80:TYR:HA	1.79	0.64
26:F:5002:LMG:C19	33:4:505:C7Z:C15	2.76	0.64
15:3:65:LEU:HD23	15:3:65:LEU:C	2.23	0.64
20:4:607:CLA:HHC	20:4:607:CLA:CBB	2.27	0.64
1:A:283:PHE:HD2	20:A:1116:CLA:HBB1	1.59	0.64
16:4:76:PHE:HB3	20:4:604:CLA:C3D	2.28	0.64
6:F:159:GLU:CA	10:J:38:THR:HG22	2.20	0.64
23:2:801:LHG:HC12	23:2:801:LHG:P	2.36	0.64
12:L:109:LEU:HD23	12:L:109:LEU:C	2.22	0.64
14:2:216:GLU:O	14:2:220:LYS:HG3	1.98	0.64
16:4:215:PHE:CD2	31:4:502:XAT:H12	2.33	0.64
20:B:1227:CLA:O2A	26:B:5003:LMG:H292	1.98	0.64
10:J:32:PHE:HE2	20:J:1901:CLA:HMA2	1.63	0.64
30:1:610:CHL:HHC	30:1:610:CHL:HBB1	1.79	0.63
1:A:177:LEU:HD22	20:A:1108:CLA:HBC1	1.80	0.63
22:A:4017:BCR:H343	20:B:1022:CLA:H202	1.81	0.63
20:B:1220:CLA:HBB1	20:B:1227:CLA:H13	1.80	0.63
12:L:199:TRP:CZ3	22:L:4020:BCR:H343	2.34	0.63
15:3:268:VAL:O	15:3:271:SER:HB3	1.95	0.63
26:B:5004:LMG:H112	20:1:614:CLA:H11	1.80	0.63
13:1:133:THR:HG23	13:1:134:ILE:N	2.12	0.63
29:4:501:LUT:C31	20:4:601:CLA:C9	2.76	0.63
20:B:1227:CLA:HBC1	22:B:4009:BCR:H21C	1.80	0.63
20:2:604:CLA:HMD3	30:2:609:CHL:HBB2	1.79	0.63
16:4:121:ILE:HD12	16:4:123:VAL:HG13	1.80	0.63
20:4:617:CLA:HMB1	20:4:617:CLA:CBB	2.25	0.63
17:N:56:VAL:CG1	17:N:80:TYR:O	2.47	0.63
20:A:1132:CLA:HBB1	20:A:1132:CLA:CMB	2.29	0.63
2:B:469:LYS:NZ	2:B:509:PHE:O	2.32	0.63
14:2:212:GLN:OE1	14:2:212:GLN:HA	1.99	0.63
18:P:27:ILE:HG22	18:P:74:LEU:HD21	1.77	0.63
2:B:458:ILE:HG21	6:F:151:SER:HB3	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:15:THR:HG22	3:C:28:MET:HE2	1.81	0.63
28:F:5005:DGD:HB82	28:F:5005:DGD:HAE1	1.81	0.63
1:A:662:SER:HA	1:A:665:ILE:HG12	1.81	0.63
1:A:747:TRP:HA	20:A:1126:CLA:HBB1	1.81	0.63
4:D:114:GLU:O	4:D:144:ARG:NH2	2.29	0.63
30:2:609:CHL:O1D	30:2:609:CHL:H2A	1.99	0.63
20:B:1238:CLA:HAA1	22:L:4019:BCR:H362	1.81	0.62
14:2:149:THR:HG21	30:2:610:CHL:HMD1	1.80	0.62
30:2:609:CHL:HAA1	30:2:609:CHL:CBD	2.29	0.62
17:N:92:GLU:O	17:N:95:LEU:HB3	1.99	0.62
1:A:711:HIS:NE2	20:A:1139:CLA:HAC1	2.14	0.62
20:B:1206:CLA:HBB1	20:B:1206:CLA:HMB1	1.81	0.62
6:F:117:LEU:HD23	6:F:117:LEU:C	2.24	0.62
30:1:612:CHL:HHC	30:1:612:CHL:HBB1	1.81	0.62
26:1:802:LMG:H152	26:1:802:LMG:H302	1.80	0.62
29:3:502:LUT:H32	30:3:604:CHL:HAB	1.80	0.62
20:4:605:CLA:HED2	20:4:605:CLA:H2A	1.81	0.62
28:F:5005:DGD:HA52	32:2:807:3PH:H2B2	1.81	0.62
9:I:25:PHE:CG	22:L:4019:BCR:H14C	2.34	0.62
14:2:189:THR:HG23	14:2:198:GLY:HA2	1.80	0.62
17:N:51:VAL:HG13	17:N:87:ILE:HD13	1.80	0.62
18:P:46:ILE:HG13	18:P:46:ILE:O	2.00	0.62
1:A:466:THR:HG21	20:A:1132:CLA:HBC1	1.79	0.62
2:B:15:ASP:HB3	2:B:20:ARG:HB2	1.81	0.62
12:L:144:CYS:HB3	22:L:4019:BCR:H19C	1.81	0.62
14:2:189:THR:OG1	14:2:198:GLY:N	2.28	0.62
20:A:1110:CLA:HED2	20:A:1111:CLA:HBC1	1.81	0.62
20:B:1237:CLA:H41	20:B:1238:CLA:H41	1.80	0.62
20:B:1229:CLA:H121	22:F:4016:BCR:H271	1.82	0.62
28:F:5005:DGD:HB21	28:F:5005:DGD:C2A	2.27	0.62
15:3:120:GLU:CD	15:3:253:TYR:HB3	2.25	0.62
16:4:231:ASP:OD1	16:4:232:ASN:N	2.33	0.62
20:4:601:CLA:O1A	20:4:601:CLA:H3A	1.99	0.62
1:A:448:TRP:HB2	20:B:1237:CLA:HED2	1.81	0.62
22:A:4007:BCR:H24C	26:A:5006:LMG:H382	1.79	0.62
13:1:195:PHE:CD2	29:1:502:LUT:H34	2.33	0.62
14:2:164:GLU:HG3	20:2:612:CLA:C4B	2.30	0.62
16:4:72:GLY:HA2	23:4:801:LHG:O2	1.99	0.62
16:4:103:MET:CB	20:4:601:CLA:HMC3	2.29	0.62
1:A:252:ARG:HD3	20:A:1113:CLA:CGD	2.29	0.62
1:A:51:THR:HG23	1:A:722:PRO:HA	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:A:1113:CLA:CGA	15:3:273:LYS:HZ2	2.13	0.62
5:E:128:VAL:HG22	5:E:129:LYS:H	1.65	0.62
13:1:128:TRP:NE1	20:1:613:CLA:HED2	2.15	0.62
20:2:604:CLA:HMD2	30:2:609:CHL:CBB	2.28	0.62
1:A:381:PRO:CB	20:A:1117:CLA:HAA2	2.29	0.61
1:A:394:SER:HB3	20:A:1126:CLA:HMA3	1.81	0.61
1:A:505:PRO:HD2	20:A:1134:CLA:C3D	2.30	0.61
2:B:95:HIS:CE1	20:B:1206:CLA:HMB3	2.35	0.61
20:B:1237:CLA:HBA2	20:B:1237:CLA:C2	2.29	0.61
23:B:5001:LHG:O10	23:B:5001:LHG:HC5	1.98	0.61
15:3:274:PHE:O	15:3:275:HIS:ND1	2.34	0.61
18:P:19:LEU:HG	18:P:20:GLU:H	1.65	0.61
3:C:2:SER:N	3:C:71:HIS:O	2.33	0.61
11:K:94:GLY:O	20:K:1404:CLA:HAA1	1.99	0.61
29:4:501:LUT:C31	20:4:601:CLA:H93	2.30	0.61
20:H:1701:CLA:HMA2	20:L:1501:CLA:H12	1.82	0.61
12:L:204:LEU:HD11	20:L:1503:CLA:CED	2.31	0.61
14:2:166:ARG:NH2	14:2:177:VAL:O	2.33	0.61
20:A:1138:CLA:HED2	2:B:424:TRP:HB2	1.82	0.61
2:B:160:LYS:HD2	2:B:160:LYS:O	1.99	0.61
7:G:99:THR:OG1	7:G:102:GLU:OE1	2.18	0.61
11:K:73:SER:CB	11:K:76:ARG:HB2	2.29	0.61
20:2:605:CLA:HBC1	30:2:610:CHL:HBB2	1.81	0.61
1:A:220:GLY:HA3	20:A:1113:CLA:CAB	2.29	0.61
12:L:114:PHE:HE1	12:L:137:LEU:HD22	1.64	0.61
20:1:604:CLA:H192	20:4:617:CLA:C9	2.30	0.61
15:3:174:GLN:HB3	15:3:182:MET:HE3	1.83	0.61
17:N:58:GLN:HE21	17:N:58:GLN:CA	2.05	0.61
22:2:503:BCR:H393	20:2:606:CLA:HMB2	1.82	0.61
30:3:607:CHL:HHC	30:3:607:CHL:HBB1	1.82	0.61
2:B:160:LYS:HG3	2:B:161:TRP:CE3	2.36	0.61
13:1:152:GLU:OE2	13:1:154:ASP:N	2.34	0.61
15:3:266:ASN:OD1	15:3:268:VAL:N	2.30	0.61
20:4:601:CLA:H42	20:4:602:CLA:HBA1	1.83	0.61
13:1:61:PHE:HB3	20:1:604:CLA:CAD	2.31	0.61
15:3:122:LEU:HD23	15:3:122:LEU:H	1.65	0.61
20:A:1129:CLA:HBA2	23:A:5001:LHG:HC81	1.83	0.60
2:B:429:LEU:HD11	20:B:1235:CLA:HMB1	1.83	0.60
8:H:50:ASP:O	8:H:51:LYS:HB3	2.00	0.60
11:K:78:ALA:HA	11:K:84:LEU:HD23	1.83	0.60
13:1:65:ARG:HH21	26:1:802:LMG:HC3	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:1:168:LEU:HD22	13:1:170:TYR:HE2	1.66	0.60
1:A:599:PHE:CE2	1:A:735:VAL:HB	2.36	0.60
20:H:1701:CLA:HBB1	20:H:1701:CLA:CMB	2.31	0.60
22:I:4020:BCR:HC41	12:L:140:ILE:CD1	2.31	0.60
30:2:610:CHL:HBC2	30:2:610:CHL:CMC	2.20	0.60
18:P:42:ASP:HA	18:P:83:TYR:HE1	1.67	0.60
17:N:23:TYR:HD1	17:N:79:ALA:N	1.97	0.60
9:I:24:LEU:HD13	22:L:4019:BCR:C31	2.31	0.60
18:P:26:THR:HG22	18:P:73:LYS:HG2	1.83	0.60
7:G:148:ASN:ND2	20:G:1603:CLA:HED2	2.14	0.60
8:H:89:PHE:HE1	22:H:4021:BCR:H331	1.67	0.60
13:1:226:ILE:HB	20:1:603:CLA:C1	2.32	0.60
1:A:298:ASP:HB3	20:A:1116:CLA:CMA	2.31	0.60
1:A:401:TRP:CD1	20:A:1126:CLA:HAB	2.36	0.60
20:A:1131:CLA:HBB1	20:A:1132:CLA:H2	1.83	0.60
13:1:225:THR:HA	20:1:603:CLA:HBA2	1.83	0.60
15:3:171:ARG:HD3	30:3:611:CHL:CBB	2.31	0.60
1:A:662:SER:CB	18:P:36:PRO:HG3	2.32	0.60
1:A:394:SER:CB	20:A:1126:CLA:HMA3	2.32	0.60
2:B:275:HIS:HB3	20:B:1214:CLA:HMB2	1.84	0.60
18:P:50:VAL:O	18:P:50:VAL:HG12	2.02	0.60
20:K:1401:CLA:HMC3	22:K:4002:BCR:C32	2.31	0.60
15:3:67:TYR:HH	15:3:82:GLY:HA2	1.65	0.60
15:3:266:ASN:ND2	20:3:608:CLA:HED3	2.08	0.60
30:1:609:CHL:H2	23:1:801:LHG:H291	1.84	0.59
1:A:371:ILE:HG21	20:A:1117:CLA:H191	1.83	0.59
20:B:1234:CLA:H71	26:F:5002:LMG:H401	1.84	0.59
6:F:189:LYS:O	6:F:191:PRO:HD3	2.03	0.59
20:3:612:CLA:HMB3	20:3:612:CLA:CBB	2.24	0.59
17:N:23:TYR:CE1	17:N:78:VAL:HA	2.37	0.59
12:L:86:LEU:O	12:L:90:ARG:HG3	2.01	0.59
14:2:250:LEU:HB2	29:2:501:LUT:O23	2.01	0.59
1:A:129:GLN:OE1	20:A:1107:CLA:ND	2.35	0.59
1:A:628:ILE:HD13	1:A:634:VAL:HG22	1.83	0.59
1:A:665:ILE:HD12	2:B:621:ARG:HG3	1.84	0.59
20:A:1013:CLA:H43	2:B:434:LEU:HD22	1.83	0.59
22:B:4004:BCR:H392	7:G:134:ILE:CD1	2.30	0.59
12:L:161:ALA:HB2	12:L:177:GLN:HG3	1.85	0.59
3:C:65:VAL:HB	25:C:3003:SF4:S1	2.43	0.59
16:4:213:LEU:HD11	20:4:604:CLA:HAC1	1.84	0.59
1:A:473:PRO:HA	1:A:476:MET:HE2	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:2:59:VAL:HG23	14:2:59:VAL:O	2.02	0.59
17:N:58:GLN:HA	17:N:58:GLN:NE2	2.09	0.59
20:A:1113:CLA:HAA1	15:3:273:LYS:HE3	1.84	0.59
2:B:476:VAL:HG12	2:B:477:LEU:HD12	1.85	0.59
12:L:115:VAL:HG22	12:L:130:GLY:HA3	1.83	0.59
13:1:149:ARG:HG3	20:1:611:CLA:CHD	2.33	0.59
15:3:99:ALA:O	15:3:103:VAL:HG23	2.02	0.59
20:4:601:CLA:H43	20:4:601:CLA:HMB2	1.84	0.59
1:A:680:LEU:CD1	20:A:1012:CLA:H2	2.33	0.59
2:B:133:GLU:O	2:B:137:THR:HG23	2.03	0.59
2:B:453:ILE:O	2:B:453:ILE:HG22	2.02	0.59
16:4:76:PHE:CB	20:4:604:CLA:OBD	2.50	0.59
16:4:134:TYR:CE1	30:4:613:CHL:HAC1	2.38	0.59
16:4:240:PRO:HG2	20:4:608:CLA:CMB	2.33	0.59
1:A:205:HIS:CD2	20:A:1111:CLA:HMC1	2.37	0.59
15:3:124:LYS:HZ3	15:3:253:TYR:HD2	1.51	0.59
17:N:56:VAL:HG13	17:N:80:TYR:O	2.01	0.59
18:P:40:VAL:HG11	18:P:85:SER:OG	2.02	0.59
3:C:12:ILE:HD12	17:N:39:CYS:HA	1.84	0.58
2:B:430:GLY:HA2	2:B:525:LEU:HD22	1.84	0.58
12:L:61:ASN:HD21	12:L:166:LEU:HD12	1.68	0.58
30:1:609:CHL:H11	16:4:151:TYR:HB2	1.83	0.58
16:4:162:ASN:O	16:4:165:SER:OG	2.19	0.58
1:A:245:PRO:HG2	20:A:1112:CLA:CAD	2.33	0.58
1:A:354:TRP:CZ2	20:A:1123:CLA:H203	2.38	0.58
20:B:1202:CLA:HHC	20:B:1202:CLA:HBB1	1.85	0.58
30:4:611:CHL:HHC	30:4:611:CHL:HBB1	1.85	0.58
1:A:92:TRP:CD2	20:A:1104:CLA:HAC2	2.39	0.58
1:A:278:ALA:N	20:A:1115:CLA:HMA2	2.18	0.58
1:A:584:PRO:HD3	2:B:561:GLY:HA2	1.84	0.58
11:K:59:THR:O	11:K:63:LEU:HD23	2.02	0.58
1:A:589:THR:HB	1:A:592:VAL:HG11	1.85	0.58
2:B:439:HIS:CD2	2:B:453:ILE:HG13	2.39	0.58
12:L:113:PRO:HA	20:L:1503:CLA:CMB	2.33	0.58
13:1:86:TRP:CD1	20:1:611:CLA:HED3	2.38	0.58
20:4:605:CLA:H43	20:4:605:CLA:HED3	1.85	0.58
17:N:18:CYS:O	17:N:18:CYS:SG	2.61	0.58
20:B:1201:CLA:H3A	23:B:5002:LHG:H291	1.86	0.58
15:3:90:GLY:H	15:3:93:ILE:HG22	1.68	0.58
16:4:76:PHE:N	20:4:604:CLA:OBD	2.36	0.58
16:4:96:LEU:HD11	16:4:205:ILE:HD11	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:364:MET:HG3	20:A:1123:CLA:HBB	1.86	0.58
20:B:1021:CLA:HMB1	20:B:1021:CLA:HBB1	1.85	0.58
20:B:1223:CLA:HBB1	20:B:1223:CLA:HMB3	1.86	0.58
14:2:231:ALA:HA	20:2:603:CLA:HBB1	1.85	0.58
17:N:93:GLU:HA	17:N:96:THR:HB	1.84	0.58
1:A:503:THR:HG21	20:A:1133:CLA:HMD2	1.85	0.58
20:B:1219:CLA:HBB2	22:B:4009:BCR:H343	1.84	0.58
20:H:1701:CLA:HMB2	20:L:1501:CLA:HAA2	1.86	0.58
16:4:94:ALA:HA	20:4:612:CLA:CED	2.34	0.58
16:4:97:VAL:HG11	20:4:612:CLA:O1D	2.03	0.58
16:4:233:LEU:HD22	29:4:501:LUT:H163	1.85	0.58
18:P:30:LYS:HG3	18:P:69:THR:CG2	2.34	0.58
1:A:93:LEU:CD1	20:A:1103:CLA:H91	2.32	0.58
1:A:145:ILE:HA	20:A:1106:CLA:HMD1	1.86	0.58
20:B:1238:CLA:H62	20:B:1239:CLA:H121	1.86	0.58
13:1:229:VAL:HG21	20:1:603:CLA:CMD	2.34	0.58
31:2:502:XAT:H28	20:2:604:CLA:H72	1.86	0.58
1:A:220:GLY:CA	20:A:1113:CLA:HAB	2.32	0.57
4:D:78:ASN:CA	8:H:53:VAL:HG21	2.34	0.57
8:H:74:ALA:O	12:L:92:ALA:HB3	2.04	0.57
13:1:61:PHE:HB3	20:1:604:CLA:C3D	2.33	0.57
13:1:112:ALA:HB1	13:1:131:LEU:HD12	1.86	0.57
20:4:601:CLA:H51	20:4:601:CLA:C9	2.27	0.57
1:A:505:PRO:HD2	20:A:1134:CLA:C4D	2.34	0.57
8:H:74:ALA:HB1	8:H:75:PRO:HD2	1.86	0.57
12:L:98:ARG:O	12:L:102:VAL:HG23	2.04	0.57
15:3:236:LEU:HD13	20:3:603:CLA:HBB2	1.85	0.57
20:4:603:CLA:H141	20:4:607:CLA:HAC2	1.86	0.57
17:N:95:LEU:C	17:N:95:LEU:HD13	2.29	0.57
1:A:51:THR:HG21	1:A:722:PRO:HA	1.85	0.57
3:C:38:GLN:OE1	4:D:178:VAL:HG11	2.04	0.57
9:I:31:ARG:NH1	9:I:31:ARG:HB2	2.19	0.57
12:L:87:PRO:CG	20:L:1502:CLA:HED2	2.33	0.57
15:3:267:ASN:HB2	20:3:603:CLA:O2A	2.05	0.57
16:4:244:THR:HG23	16:4:247:GLN:HE22	1.68	0.57
18:P:62:LEU:HD22	18:P:62:LEU:N	2.18	0.57
1:A:305:ALA:HB1	20:A:1115:CLA:HBC2	1.86	0.57
13:1:105:TRP:HE3	29:1:502:LUT:H373	1.68	0.57
15:3:61:SER:HB3	15:3:64:SER:HB3	1.87	0.57
15:3:156:THR:HA	15:3:159:VAL:HG12	1.86	0.57
1:A:278:ALA:HA	20:A:1115:CLA:HMA3	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:B:1240:CLA:HBB1	20:1:604:CLA:H92	1.86	0.57
4:D:134:ARG:HB2	4:D:137:GLN:HG3	1.85	0.57
13:1:64:LEU:HD12	29:1:502:LUT:C2	2.34	0.57
13:1:111:TRP:CH2	20:1:613:CLA:HAC1	2.39	0.57
14:2:169:ALA:CB	14:2:177:VAL:HG11	2.35	0.57
1:A:42:ARG:HB3	1:A:42:ARG:CZ	2.33	0.57
1:A:654:ARG:NE	1:A:655:ASP:OD1	2.36	0.57
1:A:252:ARG:HD3	20:A:1113:CLA:CED	2.31	0.57
1:A:591:GLN:HB3	1:A:596:ASP:HB3	1.87	0.57
20:A:1103:CLA:HED2	20:A:1128:CLA:HBB2	1.87	0.57
2:B:707:LEU:HD11	28:B:5005:DGD:HB71	1.85	0.57
20:B:1201:CLA:HAA2	23:B:5002:LHG:H242	1.86	0.57
20:G:1603:CLA:H141	30:1:610:CHL:CMC	2.35	0.57
20:H:1701:CLA:CMB	20:L:1501:CLA:HAA2	2.34	0.57
23:2:801:LHG:H142	23:2:801:LHG:HC92	1.85	0.57
20:4:609:CLA:H2A	20:4:609:CLA:O1D	2.05	0.57
20:4:604:CLA:HMB3	20:4:604:CLA:CBB	2.30	0.57
1:A:43:THR:HA	1:A:46:LYS:HD2	1.87	0.57
1:A:741:GLY:O	1:A:745:THR:HG22	2.05	0.57
28:F:5005:DGD:HA62	28:F:5005:DGD:C2A	2.33	0.57
12:L:110:LEU:HD13	12:L:137:LEU:CD2	2.12	0.57
15:3:218:LYS:HD2	15:3:219:SER:N	2.20	0.57
12:L:108:PHE:HB3	22:L:4020:BCR:H16C	1.85	0.57
30:1:610:CHL:HBB2	20:1:613:CLA:HBB2	1.85	0.57
16:4:245:ILE:CD1	20:4:603:CLA:CAD	2.82	0.57
29:4:501:LUT:C31	20:4:601:CLA:H101	2.35	0.57
1:A:86:LEU:HG	20:A:1111:CLA:HED1	1.86	0.57
22:2:503:BCR:H393	20:2:606:CLA:CMB	2.34	0.57
22:3:503:BCR:H402	20:3:606:CLA:C1B	2.35	0.57
17:N:93:GLU:O	17:N:97:ALA:N	2.37	0.57
18:P:35:PHE:HA	18:P:37:HIS:CD2	2.40	0.57
18:P:37:HIS:O	18:P:63:LEU:HB2	2.05	0.57
20:A:1140:CLA:H2	20:A:1013:CLA:H203	1.88	0.56
20:A:1012:CLA:HMA3	2:B:616:LEU:HD13	1.87	0.56
15:3:124:LYS:HG3	15:3:253:TYR:HE2	1.70	0.56
20:3:617:CLA:HBB1	20:3:617:CLA:CHC	2.25	0.56
16:4:103:MET:HB2	20:4:601:CLA:HMC3	1.85	0.56
20:4:601:CLA:H93	20:4:601:CLA:C5	2.26	0.56
18:P:81:LYS:HE3	18:P:95:GLN:HE21	1.69	0.56
12:L:204:LEU:H	12:L:204:LEU:CD1	2.17	0.56
30:2:610:CHL:HAA2	30:2:610:CHL:HBD	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:503:THR:OG1	20:A:1134:CLA:CHC	2.52	0.56
20:A:1013:CLA:C1D	2:B:582:TRP:HE1	2.17	0.56
20:B:1231:CLA:HBB1	20:B:1231:CLA:HMB1	1.87	0.56
20:L:1501:CLA:CBB	20:L:1502:CLA:HAA2	2.35	0.56
13:1:179:GLU:HA	13:1:182:ILE:HD12	1.86	0.56
14:2:101:TRP:HB2	26:2:802:LMG:HC3	1.86	0.56
14:2:122:ILE:HD12	14:2:123:PRO:N	2.20	0.56
20:2:603:CLA:H143	23:2:801:LHG:H141	1.87	0.56
15:3:118:ALA:HB2	20:3:606:CLA:HBC3	1.87	0.56
16:4:121:ILE:HD12	16:4:123:VAL:CG1	2.35	0.56
2:B:124:TRP:HB3	2:B:129:LEU:HD12	1.87	0.56
2:B:486:LEU:HD12	2:B:494:LEU:HD13	1.88	0.56
2:B:703:VAL:HG22	2:B:706:ARG:HH12	1.70	0.56
12:L:87:PRO:HD2	20:L:1502:CLA:HED2	1.86	0.56
20:L:1502:CLA:CMB	20:L:1502:CLA:HBB1	2.35	0.56
29:1:502:LUT:H12	20:1:604:CLA:CBB	2.35	0.56
32:2:807:3PH:H351	16:4:57:LEU:HD21	1.87	0.56
3:C:22:PRO:N	3:C:22:PRO:C	2.61	0.56
22:H:4021:BCR:H321	22:H:4021:BCR:HC8	1.85	0.56
14:2:122:ILE:CD1	20:2:606:CLA:HBC3	2.36	0.56
28:4:802:DGD:O5E	28:4:802:DGD:O4E	2.22	0.56
20:A:1115:CLA:C4D	20:A:1115:CLA:H12	2.36	0.56
22:A:4011:BCR:H362	20:A:1012:CLA:H43	1.87	0.56
2:B:226:PHE:HE1	20:G:1601:CLA:HBC1	1.70	0.56
30:2:609:CHL:HMA2	20:3:617:CLA:CGD	2.35	0.56
1:A:222:GLN:NE2	20:A:1117:CLA:O1D	2.39	0.56
1:A:492:ILE:HD11	20:A:1135:CLA:H2	1.86	0.56
2:B:370:ALA:HB1	20:B:1224:CLA:HMA1	1.87	0.56
11:K:110:VAL:HG21	22:K:4001:BCR:H383	1.86	0.56
14:2:217:LEU:HB3	20:2:601:CLA:HMA1	1.87	0.56
20:2:606:CLA:HBA1	20:2:606:CLA:CBD	2.34	0.56
20:A:1122:CLA:H12	22:A:4007:BCR:H15C	1.86	0.56
20:A:1131:CLA:HBB2	12:L:117:ALA:CB	2.35	0.56
13:1:105:TRP:CE3	29:1:502:LUT:H373	2.41	0.56
29:3:501:LUT:H373	20:3:601:CLA:H12	1.87	0.56
30:3:611:CHL:HHC	30:3:611:CHL:HBB1	1.86	0.56
1:A:371:ILE:CD1	20:A:1125:CLA:H12	2.36	0.56
14:2:202:ASP:OD1	20:2:601:CLA:HBD	2.06	0.56
20:2:604:CLA:CMD	30:2:609:CHL:HBB2	2.35	0.56
1:A:34:TRP:CD1	20:A:1109:CLA:HBA2	2.41	0.56
1:A:590:CYS:HB3	2:B:667:TRP:HE3	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:A:1013:CLA:C4	2:B:434:LEU:HD22	2.35	0.56
2:B:474:PHE:CE1	20:F:1302:CLA:HBC1	2.41	0.56
14:2:204:LEU:HD13	29:2:501:LUT:H22	1.88	0.56
16:4:245:ILE:HD12	20:4:603:CLA:HMD3	1.87	0.56
1:A:312:ILE:HD12	1:A:313:ALA:N	2.20	0.55
20:A:1123:CLA:HMB1	20:A:1123:CLA:HBB1	1.89	0.55
2:B:270:LEU:HD23	2:B:273:MET:HE3	1.87	0.55
20:B:1222:CLA:HAA2	20:B:1223:CLA:OBD	2.07	0.55
22:B:4004:BCR:H402	20:B:1218:CLA:C1D	2.36	0.55
20:2:604:CLA:HHD	30:2:609:CHL:HBB2	1.88	0.55
1:A:124:TRP:CH2	20:A:1105:CLA:O2A	2.60	0.55
14:2:137:TRP:HH2	14:2:236:TRP:HA	1.72	0.55
20:2:604:CLA:HED2	20:2:604:CLA:H2A	1.86	0.55
1:A:123:VAL:HA	20:A:1107:CLA:CED	2.36	0.55
1:A:475:ASP:HA	12:L:121:ARG:HH22	1.72	0.55
1:A:579:PHE:CZ	1:A:593:SER:HB3	2.41	0.55
20:B:1207:CLA:H143	12:L:136:GLY:HA2	1.88	0.55
28:F:5005:DGD:C8B	28:F:5005:DGD:HAE1	2.37	0.55
7:G:92:LEU:HD23	7:G:93:PRO:HD2	1.89	0.55
20:L:1502:CLA:CMA	22:L:4020:BCR:H373	2.36	0.55
13:1:168:LEU:HD13	29:1:501:LUT:H222	1.87	0.55
22:1:503:BCR:H271	20:4:606:CLA:NB	2.21	0.55
16:4:96:LEU:HD21	16:4:184:TYR:CZ	2.41	0.55
16:4:213:LEU:HD11	20:4:604:CLA:CBC	2.36	0.55
2:B:428:PHE:CE1	20:B:1235:CLA:HAB	2.41	0.55
13:1:226:ILE:HB	20:1:603:CLA:H11	1.88	0.55
1:A:221:HIS:HB2	20:A:1112:CLA:C4B	2.36	0.55
1:A:649:ILE:HD12	20:B:1022:CLA:HMA2	1.87	0.55
2:B:65:LEU:HD11	22:B:4006:BCR:H292	1.88	0.55
2:B:443:MET:SD	2:B:451:LYS:HE3	2.45	0.55
20:B:1231:CLA:H62	20:B:1232:CLA:H12	1.88	0.55
6:F:133:TYR:CE1	10:J:37:LEU:HD12	2.41	0.55
30:1:610:CHL:OMC	20:1:613:CLA:HAB	2.06	0.55
30:1:609:CHL:HED3	16:4:154:ILE:HG22	1.89	0.55
15:3:268:VAL:O	15:3:271:SER:N	2.38	0.55
16:4:150:HIS:ND1	16:4:154:ILE:HD11	2.21	0.55
20:4:609:CLA:HBC3	23:4:801:LHG:C4	2.36	0.55
1:A:692:PHE:HA	21:A:2001:PQN:H9	1.87	0.55
2:B:32:GLU:OE2	2:B:331:HIS:NE2	2.37	0.55
2:B:221:GLY:O	24:B:5008:LMT:O2B	2.16	0.55
2:B:626:LEU:CG	18:P:90:ALA:HB2	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:B:1228:CLA:HMB3	20:B:1228:CLA:HBB1	1.88	0.55
8:H:122:ILE:HD12	12:L:125:ILE:CD1	2.37	0.55
15:3:122:LEU:HB2	15:3:128:ILE:HD13	1.89	0.55
17:N:23:TYR:CD1	17:N:78:VAL:HA	2.42	0.55
1:A:44:ILE:HA	1:A:53:TRP:HE1	1.70	0.55
26:B:5003:LMG:H131	26:B:5003:LMG:O9	2.05	0.55
10:J:32:PHE:HE2	20:J:1901:CLA:CMA	2.19	0.55
12:L:109:LEU:HD11	20:L:1502:CLA:HMB2	1.88	0.55
13:1:78:GLU:OE1	13:1:158:LYS:HB3	2.07	0.55
13:1:212:GLU:O	13:1:216:THR:HG23	2.06	0.55
15:3:223:LEU:HB3	20:3:601:CLA:HMA2	1.89	0.55
16:4:112:PRO:O	16:4:116:THR:HG22	2.07	0.55
16:4:229:PRO:O	29:4:501:LUT:O3	2.25	0.55
2:B:707:LEU:HD22	28:B:5005:DGD:HB21	1.89	0.55
4:D:162:GLY:HA2	8:H:60:LEU:HD11	1.88	0.55
12:L:180:ASP:O	12:L:184:LYS:HG3	2.06	0.55
14:2:124:GLU:HA	14:2:127:THR:HG22	1.89	0.55
14:2:229:MET:HE1	20:2:604:CLA:CHC	2.37	0.55
20:A:1121:CLA:CAD	22:K:4001:BCR:H393	2.37	0.55
20:K:1401:CLA:HMB3	20:K:1401:CLA:CBB	2.32	0.55
12:L:104:LEU:HD23	12:L:192:GLY:O	2.07	0.55
13:1:64:LEU:HD12	29:1:502:LUT:H22	1.87	0.55
1:A:628:ILE:HD11	1:A:632:GLY:HA2	1.88	0.55
20:B:1207:CLA:HBB1	20:B:1207:CLA:CHC	2.24	0.55
20:B:1240:CLA:C4B	20:1:605:CLA:H52	2.37	0.55
9:I:5:PRO:O	9:I:9:VAL:HG12	2.06	0.55
17:N:60:ASP:OD2	17:N:80:TYR:CE2	2.60	0.55
18:P:57:MET:CE	18:P:62:LEU:CA	2.81	0.55
20:A:1131:CLA:HAA1	22:I:4020:BCR:H16C	1.89	0.54
28:G:5003:DGD:HB21	13:1:136:VAL:HG11	1.90	0.54
13:1:209:GLY:O	13:1:213:ASN:ND2	2.36	0.54
14:2:200:TRP:CZ2	30:2:615:CHL:NC	2.75	0.54
15:3:243:ILE:HD12	15:3:243:ILE:C	2.32	0.54
1:A:23:ASP:OD2	1:A:192:LYS:HD2	2.07	0.54
1:A:124:TRP:CB	29:J:4013:LUT:H183	2.37	0.54
20:A:1103:CLA:H151	20:A:1111:CLA:H51	1.88	0.54
20:A:1134:CLA:H8	20:K:1402:CLA:H51	1.89	0.54
20:B:1215:CLA:CGA	20:B:1215:CLA:H3A	2.35	0.54
1:A:354:TRP:CE2	20:A:1123:CLA:H203	2.43	0.54
1:A:462:ILE:CG2	20:A:1132:CLA:HMC2	2.37	0.54
2:B:476:VAL:O	2:B:480:SER:N	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:628:SER:O	2:B:628:SER:OG	2.25	0.54
20:B:1202:CLA:HBD	20:B:1202:CLA:H122	1.87	0.54
4:D:174:TYR:HB3	4:D:176:GLU:CD	2.32	0.54
11:K:115:GLY:O	11:K:119:VAL:HG23	2.07	0.54
14:2:164:GLU:HG3	20:2:612:CLA:NB	2.23	0.54
20:2:607:CLA:HMB1	24:2:808:LMT:H12	1.88	0.54
15:3:178:LYS:O	15:3:181:SER:OG	2.19	0.54
2:B:193:HIS:HB2	20:B:1211:CLA:CHC	2.37	0.54
2:B:455:ILE:HD11	28:J:5001:DGD:HAE2	1.89	0.54
2:B:492:ILE:HD11	7:G:150:TYR:CE1	2.43	0.54
2:B:558:PRO:HB3	2:B:702:ILE:HD12	1.90	0.54
11:K:74:ALA:N	11:K:103:ASP:OD1	2.40	0.54
33:4:505:C7Z:C37	33:4:505:C7Z:C38	2.86	0.54
1:A:282:THR:HB	1:A:284:ARG:HG3	1.88	0.54
1:A:377:TYR:C	1:A:377:TYR:CD2	2.86	0.54
1:A:736:THR:HG23	23:A:5002:LHG:H341	1.89	0.54
20:A:1138:CLA:H52	22:F:4014:BCR:H14C	1.89	0.54
1:A:578:ARG:HD2	1:A:728:VAL:HG11	1.88	0.54
2:B:459:PHE:HB3	20:B:1234:CLA:H42	1.90	0.54
15:3:124:LYS:HG3	15:3:253:TYR:CE2	2.43	0.54
2:B:558:PRO:N	2:B:558:PRO:C	2.60	0.54
10:J:13:VAL:HA	10:J:16:THR:HG22	1.90	0.54
1:A:464:ASN:HB3	1:A:648:THR:HG22	1.90	0.54
1:A:604:TRP:HE1	20:B:1023:CLA:C1D	2.20	0.54
20:A:1135:CLA:H12	20:A:1136:CLA:O1A	2.08	0.54
22:A:4017:BCR:HC41	2:B:648:TRP:CE3	2.43	0.54
6:F:189:LYS:C	6:F:191:PRO:HD3	2.32	0.54
7:G:124:ASN:O	7:G:128:VAL:HG13	2.07	0.54
26:G:5002:LMG:HC62	13:1:115:PRO:HA	1.90	0.54
14:2:91:GLY:HA3	26:2:804:LMG:HC92	1.90	0.54
20:4:602:CLA:HBB1	20:4:602:CLA:CHC	2.14	0.54
17:N:78:VAL:HG23	17:N:78:VAL:O	2.08	0.54
1:A:122:VAL:O	20:A:1107:CLA:HED2	2.08	0.54
2:B:174:ARG:HB2	20:B:1210:CLA:CBC	2.38	0.54
2:B:272:ASP:HB3	20:B:1214:CLA:HMA1	1.90	0.54
2:B:437:TYR:CE2	20:B:1021:CLA:H171	2.43	0.54
2:B:477:LEU:HD21	20:B:1232:CLA:HMC1	1.90	0.54
20:B:1237:CLA:HMB1	20:B:1237:CLA:CBB	2.37	0.54
29:1:502:LUT:H28	29:1:502:LUT:C36	2.24	0.54
14:2:101:TRP:CE3	26:2:802:LMG:HC5	2.43	0.54
26:2:802:LMG:O4	26:2:802:LMG:O5	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:740:LEU:HD22	20:A:1140:CLA:CMA	2.38	0.54
20:A:1110:CLA:HHC	20:A:1110:CLA:HBB1	1.89	0.54
2:B:157:LEU:HD11	23:B:5002:LHG:H281	1.90	0.54
14:2:167:ARG:NH2	20:2:612:CLA:O1D	2.40	0.54
24:2:808:LMT:C6B	15:3:186:TYR:HB2	2.35	0.54
15:3:107:ARG:HA	15:3:110:MET:HE3	1.90	0.54
15:3:128:ILE:H	15:3:128:ILE:HD12	1.73	0.54
20:4:601:CLA:CMB	20:4:601:CLA:HBB1	2.38	0.54
1:A:36:LYS:HA	1:A:36:LYS:HE3	1.90	0.53
1:A:203:LEU:HG	20:A:1123:CLA:HMD2	1.91	0.53
1:A:278:ALA:HA	20:A:1115:CLA:CMA	2.37	0.53
8:H:68:ASP:HB2	12:L:162:PRO:HG2	1.89	0.53
29:1:502:LUT:H12	20:1:604:CLA:CAB	2.38	0.53
14:2:124:GLU:OE2	14:2:136:SER:HA	2.08	0.53
15:3:110:MET:SD	20:3:601:CLA:HAB	2.48	0.53
30:4:610:CHL:HHC	30:4:610:CHL:HBB1	1.89	0.53
1:A:325:HIS:HB3	1:A:330:ILE:HD11	1.89	0.53
2:B:449:PRO:N	2:B:449:PRO:C	2.60	0.53
8:H:83:SER:O	8:H:87:GLU:HG3	2.08	0.53
1:A:343:HIS:HA	1:A:346:LEU:HD12	1.90	0.53
20:A:1132:CLA:HED3	12:L:121:ARG:HH12	1.73	0.53
2:B:626:LEU:HG	18:P:90:ALA:HB2	1.91	0.53
20:B:1218:CLA:H203	13:1:138:GLU:OE2	2.09	0.53
26:F:5003:LMG:C14	26:F:5003:LMG:C9	2.85	0.53
28:F:5005:DGD:HB71	16:4:79:LEU:HD21	1.90	0.53
13:1:200:VAL:CG1	20:1:603:CLA:HAC2	2.32	0.53
16:4:245:ILE:CD1	20:4:603:CLA:C2D	2.86	0.53
1:A:394:SER:HB3	20:A:1126:CLA:HBB	1.90	0.53
20:A:1101:CLA:H43	21:A:2001:PQN:C30	2.38	0.53
2:B:208:ARG:HA	20:B:1211:CLA:OBD	2.08	0.53
2:B:698:VAL:HG11	3:C:77:MET:HE3	1.89	0.53
3:C:8:TYR:CZ	4:D:192:ILE:HG13	2.43	0.53
12:L:147:ILE:HD11	22:L:4019:BCR:C17	2.38	0.53
20:1:614:CLA:H2	33:4:505:C7Z:O3	2.07	0.53
20:2:604:CLA:HMB3	20:2:604:CLA:CBB	2.30	0.53
15:3:217:GLU:H	15:3:217:GLU:CD	2.17	0.53
7:G:153:LYS:O	26:G:5006:LMG:C28	2.57	0.53
14:2:162:TRP:CH2	22:2:503:BCR:C32	2.92	0.53
1:A:486:PRO:HB3	20:A:1136:CLA:O1D	2.08	0.53
1:A:512:SER:OG	1:A:513:LEU:N	2.42	0.53
2:B:459:PHE:HB3	20:B:1234:CLA:H11	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:F:1301:CLA:HMB1	10:J:26:LEU:HD11	1.91	0.53
20:H:1701:CLA:CMA	20:L:1501:CLA:H12	2.38	0.53
10:J:31:ARG:NH2	20:J:1901:CLA:O1D	2.36	0.53
8:H:82:GLN:HE22	20:L:1501:CLA:HED2	1.71	0.53
20:H:1701:CLA:C10	20:H:1701:CLA:C14	2.86	0.53
22:L:4019:BCR:H393	20:L:1502:CLA:C3C	2.38	0.53
17:N:25:LEU:HB2	17:N:76:THR:HB	1.90	0.53
1:A:368:LEU:HD13	20:A:1125:CLA:C4	2.38	0.53
20:A:1101:CLA:HMB3	20:A:1101:CLA:CBB	2.37	0.53
4:D:109:LYS:HG3	4:D:111:GLN:HG2	1.91	0.53
26:1:802:LMG:H292	16:4:157:TRP:HH2	1.74	0.53
14:2:154:ILE:HD11	20:4:608:CLA:HED1	1.91	0.53
14:2:162:TRP:HH2	22:2:503:BCR:H313	1.74	0.53
1:A:381:PRO:HB2	20:A:1117:CLA:HAA2	1.91	0.53
20:L:1501:CLA:HMB1	20:L:1501:CLA:CBB	2.30	0.53
14:2:162:TRP:CH2	22:2:503:BCR:H322	2.44	0.53
15:3:105:ASN:ND2	20:3:612:CLA:OBD	2.42	0.53
16:4:103:MET:SD	20:4:601:CLA:HHC	2.49	0.53
16:4:236:HIS:CD2	20:4:603:CLA:HAA2	2.43	0.53
16:4:245:ILE:HD11	20:4:603:CLA:C2D	2.38	0.53
1:A:462:ILE:HB	20:A:1132:CLA:HMC2	1.90	0.53
2:B:488:ALA:HB1	20:B:1232:CLA:OBD	2.08	0.53
20:L:1503:CLA:C2	20:L:1503:CLA:CBA	2.87	0.53
14:2:140:ALA:HA	14:2:143:GLN:OE1	2.08	0.53
26:2:803:LMG:HC71	26:2:803:LMG:H122	1.91	0.53
16:4:213:LEU:HD11	20:4:604:CLA:CAC	2.39	0.53
2:B:378:ILE:HD13	20:B:1225:CLA:CAB	2.39	0.52
9:I:14:LEU:HD21	22:I:4018:BCR:H351	1.89	0.52
22:L:4019:BCR:H392	22:L:4019:BCR:H23C	1.91	0.52
20:L:1503:CLA:HMB1	20:L:1503:CLA:CBB	2.29	0.52
13:1:90:ALA:HB1	29:1:502:LUT:H392	1.88	0.52
13:1:119:ALA:HB3	13:1:126:VAL:HG22	1.91	0.52
15:3:267:ASN:HB2	20:3:603:CLA:C1	2.39	0.52
16:4:143:VAL:O	16:4:147:ILE:HG12	2.09	0.52
13:1:66:LEU:HD13	20:1:604:CLA:H42	1.91	0.52
14:2:92:LEU:CB	20:2:604:CLA:H11	2.40	0.52
15:3:266:ASN:OD1	15:3:267:ASN:N	2.42	0.52
16:4:93:GLN:O	16:4:97:VAL:HG12	2.09	0.52
20:4:601:CLA:C9	20:4:601:CLA:C5	2.86	0.52
1:A:213:LEU:HG	20:A:1118:CLA:HAC1	1.90	0.52
1:A:661:ALA:HB2	19:A:1011:CL0:H25	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:476:VAL:HG12	2:B:477:LEU:H	1.73	0.52
20:B:1227:CLA:H122	20:B:1227:CLA:H202	1.91	0.52
6:F:110:ALA:HB3	6:F:113:SER:HB3	1.90	0.52
12:L:182:TRP:O	12:L:186:THR:HG22	2.09	0.52
13:1:86:TRP:CE2	20:1:611:CLA:HED3	2.45	0.52
16:4:200:ALA:HB1	20:4:601:CLA:HMA3	1.91	0.52
13:1:217:HIS:ND1	20:1:603:CLA:HAA1	2.24	0.52
14:2:110:SER:HB2	14:2:225:GLY:HA3	1.91	0.52
16:4:104:LEU:HD11	20:4:601:CLA:HBC3	1.91	0.52
20:4:604:CLA:HBC1	23:4:801:LHG:H262	1.91	0.52
18:P:57:MET:HE2	18:P:62:LEU:HA	1.91	0.52
1:A:309:LEU:O	1:A:312:ILE:HG13	2.09	0.52
20:B:1218:CLA:H172	20:G:1603:CLA:H162	1.91	0.52
20:L:1501:CLA:HBA1	22:L:4020:BCR:C35	2.40	0.52
2:B:352:MET:HG2	20:B:1215:CLA:O1A	2.09	0.52
20:L:1502:CLA:HBB1	20:L:1502:CLA:HMB3	1.90	0.52
13:1:225:THR:HA	20:1:603:CLA:HBA1	1.91	0.52
20:1:601:CLA:H62	20:1:602:CLA:HMA2	1.91	0.52
14:2:101:TRP:CB	26:2:802:LMG:HC3	2.40	0.52
20:A:1101:CLA:CED	21:A:2001:PQN:C24	2.86	0.52
20:H:1701:CLA:H102	20:H:1701:CLA:H143	1.90	0.52
9:I:25:PHE:CE2	22:L:4019:BCR:H16C	2.45	0.52
11:K:77:LYS:HE2	11:K:77:LYS:CA	2.40	0.52
2:B:438:VAL:HB	20:B:1230:CLA:HMC2	1.91	0.52
28:G:5003:DGD:O1A	28:G:5003:DGD:O2D	2.27	0.52
20:K:1401:CLA:CMC	22:K:4002:BCR:H321	2.39	0.52
13:1:217:HIS:CG	20:1:603:CLA:HAA1	2.45	0.52
30:3:604:CHL:HBB1	30:3:604:CHL:HMB3	1.91	0.52
2:B:443:MET:HE1	20:B:1230:CLA:C2D	2.40	0.52
13:1:85:ARG:HH21	20:1:601:CLA:C4D	2.23	0.52
16:4:213:LEU:HD11	20:4:604:CLA:HBC1	1.92	0.52
1:A:496:HIS:NE2	20:A:1133:CLA:NB	2.58	0.52
1:A:591:GLN:CD	2:B:667:TRP:HB2	2.34	0.52
2:B:536:LYS:O	2:B:540:ASP:HB2	2.10	0.52
10:J:32:PHE:CE2	20:J:1901:CLA:CMA	2.92	0.52
13:1:226:ILE:HG21	20:1:603:CLA:H11	1.92	0.52
29:1:501:LUT:H32	20:1:601:CLA:HAB	1.91	0.52
20:3:617:CLA:HED2	20:3:617:CLA:O1A	2.10	0.52
13:1:202:GLN:NE2	13:1:208:THR:O	2.42	0.51
16:4:219:ILE:HG13	16:4:220:ILE:N	2.23	0.51
18:P:14:PHE:CE2	18:P:92:MET:HE2	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:P:81:LYS:CE	18:P:95:GLN:HE21	2.23	0.51
1:A:37:PRO:HB2	1:A:53:TRP:HH2	1.75	0.51
2:B:472:TYR:HB3	6:F:80:ALA:HA	1.92	0.51
20:B:1222:CLA:H92	20:B:1234:CLA:H62	1.91	0.51
20:B:1225:CLA:H8	22:B:4005:BCR:H21C	1.92	0.51
26:B:5007:LMG:H141	26:B:5007:LMG:O9	2.09	0.51
12:L:143:ILE:O	12:L:147:ILE:HG12	2.10	0.51
15:3:55:ARG:HH12	15:3:69:ASP:C	2.18	0.51
29:4:501:LUT:H31	20:4:601:CLA:H101	1.91	0.51
1:A:600:LEU:O	1:A:603:PHE:N	2.44	0.51
8:H:48:TYR:HB2	8:H:56:ASP:OD1	2.10	0.51
12:L:109:LEU:HD23	12:L:109:LEU:O	2.10	0.51
13:1:75:ARG:NH1	20:1:605:CLA:O1A	2.43	0.51
30:2:613:CHL:HAA2	30:2:613:CHL:HBD	1.91	0.51
16:4:241:TRP:CE3	20:4:608:CLA:HMA1	2.45	0.51
20:4:609:CLA:CBB	20:4:604:CLA:HMD3	2.40	0.51
1:A:548:THR:O	1:A:552:THR:HG22	2.10	0.51
1:A:740:LEU:HD22	20:A:1140:CLA:HMA2	1.90	0.51
2:B:92:TRP:CE3	9:I:9:VAL:HG11	2.45	0.51
3:C:23:THR:O	4:D:135:LYS:HE2	2.11	0.51
12:L:165:THR:OG1	12:L:166:LEU:N	2.42	0.51
13:1:222:TRP:CD2	20:1:608:CLA:CMA	2.91	0.51
14:2:167:ARG:CZ	20:2:612:CLA:O1D	2.59	0.51
15:3:233:LEU:O	15:3:236:LEU:HD12	2.11	0.51
20:4:605:CLA:HBC2	20:4:612:CLA:HAC1	1.92	0.51
17:N:29:GLU:HA	17:N:29:GLU:OE1	2.09	0.51
17:N:60:ASP:OD2	17:N:80:TYR:CZ	2.64	0.51
1:A:553:VAL:HG11	20:A:1137:CLA:HMB3	1.93	0.51
20:A:1120:CLA:H121	22:K:4001:BCR:H381	1.91	0.51
20:B:1227:CLA:H92	20:B:1240:CLA:HMA2	1.92	0.51
12:L:145:LEU:HD21	22:L:4019:BCR:H24C	1.92	0.51
20:1:608:CLA:HED2	16:4:144:ILE:HG13	1.92	0.51
18:P:62:LEU:N	18:P:62:LEU:CD2	2.73	0.51
20:A:1135:CLA:HBB1	20:A:1135:CLA:HMB1	1.91	0.51
20:B:1205:CLA:O1A	20:B:1224:CLA:HBD	2.10	0.51
28:F:5005:DGD:CBA	28:F:5005:DGD:C8B	2.86	0.51
11:K:49:SER:H	11:K:50:PRO:HD2	1.76	0.51
20:4:609:CLA:C1C	23:4:801:LHG:HC82	2.40	0.51
18:P:29:PHE:HE2	18:P:72:VAL:CG1	2.22	0.51
18:P:96:VAL:O	18:P:96:VAL:HG13	2.11	0.51
1:A:657:LEU:O	1:A:661:ALA:CB	2.59	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:A:1116:CLA:O1A	20:A:1125:CLA:HBB2	2.10	0.51
20:B:1220:CLA:HMD3	20:B:1221:CLA:HAB	1.93	0.51
20:2:603:CLA:HMA1	20:2:608:CLA:HBC3	1.93	0.51
30:2:610:CHL:HMB3	30:2:610:CHL:CBB	2.37	0.51
30:2:610:CHL:CBC	30:2:610:CHL:CMC	2.87	0.51
15:3:64:SER:HA	15:3:67:TYR:CZ	2.46	0.51
17:N:7:LEU:CD2	17:N:87:ILE:HB	2.40	0.51
17:N:23:TYR:CD1	17:N:77:CYS:O	2.64	0.51
1:A:381:PRO:CG	20:A:1117:CLA:HAA2	2.41	0.51
20:L:1503:CLA:HBA2	20:L:1503:CLA:CHA	2.40	0.51
13:1:154:ASP:OD1	13:1:156:GLU:N	2.29	0.51
22:A:4017:BCR:H362	20:B:1023:CLA:H122	1.92	0.51
2:B:428:PHE:HE1	20:B:1235:CLA:HAB	1.75	0.51
5:E:66:ILE:HD13	5:E:95:GLN:HA	1.93	0.51
12:L:90:ARG:HH22	20:L:1501:CLA:HAC2	1.76	0.51
16:4:220:ILE:O	16:4:224:VAL:HG12	2.10	0.51
1:A:48:PRO:HB3	1:A:53:TRP:CD2	2.46	0.51
1:A:666:GLN:HE22	18:P:86:PRO:HB3	1.60	0.51
2:B:254:ILE:HD12	20:B:1212:CLA:HAC2	1.93	0.51
2:B:284:PHE:HE1	20:B:1216:CLA:HAB	1.76	0.51
2:B:700:LEU:HB3	2:B:704:GLN:HG2	1.93	0.51
20:B:1230:CLA:H42	28:J:5001:DGD:HB21	1.92	0.51
13:1:133:THR:CG2	13:1:134:ILE:N	2.72	0.51
30:1:609:CHL:CED	16:4:154:ILE:HG22	2.41	0.51
14:2:92:LEU:HB2	20:2:604:CLA:H11	1.93	0.51
14:2:120:ILE:O	14:2:123:PRO:HD2	2.10	0.51
18:P:75:ASP:O	18:P:75:ASP:OD1	2.29	0.51
1:A:401:TRP:HD1	20:A:1126:CLA:HAB	1.76	0.50
1:A:503:THR:HG21	20:A:1133:CLA:HMD3	1.93	0.50
1:A:570:PRO:HG3	4:D:136:GLU:HG2	1.93	0.50
20:A:1139:CLA:H13	26:F:5001:LMG:H152	1.92	0.50
2:B:174:ARG:HB2	20:B:1210:CLA:HBC2	1.93	0.50
20:B:1216:CLA:HBB1	20:B:1221:CLA:H62	1.93	0.50
26:B:5003:LMG:C20	22:F:4016:BCR:H17C	2.41	0.50
8:H:95:LYS:HB2	8:H:98:LEU:HB3	1.93	0.50
15:3:202:TYR:HB3	20:3:601:CLA:HED3	1.93	0.50
4:D:107:SER:O	4:D:107:SER:OG	2.27	0.50
7:G:140:TYR:CD2	22:G:4011:BCR:H402	2.46	0.50
8:H:111:LEU:HD21	9:I:14:LEU:HD12	1.92	0.50
16:4:94:ALA:CB	20:4:612:CLA:HED2	2.40	0.50
20:4:601:CLA:HBB1	20:4:601:CLA:HMB1	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:SER:HB3	1:A:44:ILE:CD1	2.40	0.50
1:A:152:ILE:HD13	20:A:1127:CLA:O2A	2.10	0.50
1:A:376:MET:HE1	20:A:1127:CLA:O1D	2.11	0.50
20:A:1102:CLA:HBB1	20:A:1109:CLA:H151	1.92	0.50
2:B:2:ALA:O	2:B:3:LEU:HG	2.11	0.50
2:B:158:GLN:C	2:B:159:PRO:O	2.54	0.50
2:B:444:LEU:HD13	2:B:615:TYR:CG	2.46	0.50
13:1:205:TYR:O	13:1:208:THR:OG1	2.27	0.50
14:2:69:PRO:O	15:3:174:GLN:NE2	2.45	0.50
14:2:85:PHE:HZ	14:2:223:LYS:HE2	1.75	0.50
14:2:137:TRP:HE1	14:2:246:PRO:HD3	1.75	0.50
15:3:64:SER:HA	15:3:67:TYR:CE1	2.46	0.50
29:4:501:LUT:C31	20:4:601:CLA:H91	2.41	0.50
20:A:1104:CLA:O2D	20:A:1104:CLA:HBA2	2.11	0.50
20:A:1113:CLA:O2A	15:3:273:LYS:NZ	2.25	0.50
8:H:85:PHE:C	8:H:85:PHE:CD2	2.89	0.50
20:2:605:CLA:O2D	20:2:605:CLA:HBA2	2.11	0.50
15:3:181:SER:HA	15:3:184:LYS:NZ	2.26	0.50
20:3:617:CLA:H2A	20:3:617:CLA:O1A	2.10	0.50
16:4:245:ILE:HD12	20:4:603:CLA:CMD	2.42	0.50
20:A:1125:CLA:CAB	20:A:1133:CLA:HMA2	2.42	0.50
2:B:322:LEU:HA	2:B:325:THR:HG22	1.94	0.50
20:B:1215:CLA:HMB1	20:B:1215:CLA:HBB1	1.92	0.50
14:2:162:TRP:CZ3	22:2:503:BCR:H321	2.47	0.50
18:P:35:PHE:CE2	18:P:66:PRO:HA	2.46	0.50
1:A:466:THR:HG22	2:B:648:TRP:HE1	1.76	0.50
20:A:1138:CLA:HAA2	20:B:1228:CLA:HMB2	1.93	0.50
4:D:101:TYR:CE1	4:D:135:LYS:HB2	2.47	0.50
11:K:53:LEU:HD13	11:K:53:LEU:O	2.11	0.50
13:1:96:VAL:HG21	20:1:606:CLA:CAC	2.32	0.50
17:N:51:VAL:HG22	17:N:87:ILE:HD13	1.92	0.50
17:N:65:ASP:C	17:N:67:GLU:N	2.69	0.50
1:A:92:TRP:CG	20:A:1104:CLA:HAC2	2.47	0.50
20:B:1238:CLA:H111	20:B:1239:CLA:H13	1.94	0.50
4:D:176:GLU:CD	4:D:176:GLU:H	2.20	0.50
16:4:215:PHE:CE2	31:4:502:XAT:H12	2.47	0.50
16:4:236:HIS:CE1	20:4:603:CLA:HBA1	2.46	0.50
1:A:466:THR:CG2	20:A:1132:CLA:CBC	2.74	0.50
20:A:1130:CLA:HMB1	20:A:1130:CLA:HBB1	1.94	0.50
2:B:57:ILE:O	2:B:61:THR:HG22	2.11	0.50
2:B:465:SER:O	2:B:479:SER:OG	2.23	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:78:ASN:H	8:H:53:VAL:HG21	1.77	0.50
4:D:176:GLU:OE1	4:D:176:GLU:N	2.42	0.50
12:L:109:LEU:C	12:L:109:LEU:CD2	2.85	0.50
30:1:609:CHL:HBD	30:1:609:CHL:HAA1	1.94	0.50
14:2:147:THR:CG2	14:2:152:LEU:HG	2.41	0.50
14:2:215:LYS:O	14:2:219:THR:HG23	2.11	0.50
33:4:505:C7Z:C38	33:4:505:C7Z:C28	2.86	0.50
20:A:1103:CLA:H121	22:A:4002:BCR:HC41	1.93	0.50
20:A:1106:CLA:HAB	20:A:1126:CLA:H13	1.94	0.50
3:C:17:CYS:SG	3:C:18:VAL:N	2.85	0.50
17:N:56:VAL:HG12	17:N:80:TYR:O	2.12	0.50
1:A:645:SER:O	1:A:651:GLY:HA3	2.12	0.49
20:A:1105:CLA:HBB1	20:A:1105:CLA:HMB1	1.92	0.49
2:B:626:LEU:HD21	18:P:90:ALA:N	2.26	0.49
20:B:1022:CLA:H18	20:B:1206:CLA:H43	1.93	0.49
20:B:1205:CLA:HAB	20:B:1206:CLA:O1A	2.11	0.49
20:H:1701:CLA:HMB1	20:H:1701:CLA:CBB	2.42	0.49
20:H:1701:CLA:CHC	22:H:4021:BCR:H16C	2.41	0.49
20:L:1503:CLA:CMC	20:L:1503:CLA:HBC2	2.42	0.49
13:1:183:LYS:HD3	20:1:602:CLA:HBA1	1.93	0.49
17:N:93:GLU:HA	17:N:96:THR:CB	2.42	0.49
20:A:1132:CLA:CED	20:A:1132:CLA:H2A	2.42	0.49
3:C:52:LYS:HG2	3:C:67:VAL:HB	1.93	0.49
13:1:65:ARG:NH2	26:1:802:LMG:HC3	2.26	0.49
13:1:154:ASP:CG	13:1:157:LYS:H	2.20	0.49
20:2:608:CLA:C4D	30:2:609:CHL:H13	2.43	0.49
15:3:110:MET:O	15:3:114:VAL:HG12	2.11	0.49
16:4:225:THR:HG21	16:4:232:ASN:OD1	2.12	0.49
31:4:502:XAT:H183	20:4:606:CLA:C3B	2.42	0.49
1:A:252:ARG:NH1	1:A:262:PHE:O	2.44	0.49
20:A:1101:CLA:H102	20:A:1101:CLA:C5	2.42	0.49
2:B:74:PHE:O	2:B:78:VAL:HG13	2.12	0.49
2:B:365:PHE:HD2	2:B:734:GLY:HA2	1.76	0.49
20:3:601:CLA:H41	20:3:602:CLA:HMA2	1.94	0.49
20:B:1213:CLA:C1D	20:B:1214:CLA:HBB2	2.42	0.49
22:L:4019:BCR:H393	20:L:1502:CLA:C2C	2.42	0.49
20:4:609:CLA:CBB	20:4:604:CLA:CMD	2.90	0.49
17:N:25:LEU:HD23	17:N:77:CYS:HA	1.94	0.49
1:A:268:PRO:HA	1:A:271:THR:CG2	2.43	0.49
20:A:1113:CLA:O1A	15:3:273:LYS:HG2	2.12	0.49
20:A:1013:CLA:O1A	2:B:430:GLY:HA3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:123:ASP:OD2	5:E:123:ASP:N	2.43	0.49
20:1:614:CLA:CBB	16:4:142:PHE:CE2	2.96	0.49
14:2:147:THR:OG1	14:2:148:ASP:N	2.44	0.49
20:H:1701:CLA:C1C	22:H:4021:BCR:H16C	2.43	0.49
22:H:4021:BCR:H372	22:L:4020:BCR:C10	2.39	0.49
26:1:802:LMG:O8	26:1:802:LMG:H132	2.12	0.49
29:2:501:LUT:H21	20:2:601:CLA:H12	1.94	0.49
15:3:162:MET:CE	20:3:617:CLA:H71	2.29	0.49
2:B:278:LEU:HG	20:B:1213:CLA:HAB	1.95	0.49
2:B:365:PHE:CD2	2:B:734:GLY:HA2	2.48	0.49
2:B:443:MET:HG3	2:B:451:LYS:O	2.13	0.49
2:B:694:ARG:HB3	9:I:29:GLU:OE2	2.12	0.49
4:D:110:GLU:HA	4:D:123:MET:O	2.13	0.49
8:H:104:ILE:HD13	9:I:19:VAL:HG22	1.94	0.49
13:1:226:ILE:HB	20:1:603:CLA:O2A	2.12	0.49
15:3:65:LEU:C	15:3:65:LEU:CD2	2.86	0.49
22:3:503:BCR:H383	20:3:606:CLA:HHC	1.93	0.49
16:4:198:LEU:C	16:4:198:LEU:CD2	2.85	0.49
18:P:62:LEU:H	18:P:62:LEU:CD2	2.24	0.49
1:A:147:SER:OG	20:A:1106:CLA:O1D	2.19	0.49
1:A:411:ALA:HB2	22:A:4008:BCR:H292	1.95	0.49
6:F:173:TRP:CD1	6:F:210:GLY:HA3	2.48	0.49
15:3:117:ILE:HD12	15:3:252:PRO:HG2	1.95	0.49
1:A:30:SER:O	20:A:1109:CLA:HMA1	2.12	0.49
1:A:463:HIS:O	1:A:467:MET:HG2	2.12	0.49
1:A:486:PRO:C	20:A:1136:CLA:OBD	2.56	0.49
1:A:729:GLN:HB2	23:A:5002:LHG:HC41	1.93	0.49
20:A:1126:CLA:H8	22:A:4011:BCR:H343	1.95	0.49
7:G:61:SER:HA	20:G:1601:CLA:OBD	2.12	0.49
20:H:1701:CLA:C10	20:H:1701:CLA:H143	2.42	0.49
22:L:4020:BCR:H331	22:L:4020:BCR:HC8	1.93	0.49
13:1:133:THR:O	13:1:137:ILE:HG22	2.11	0.49
13:1:168:LEU:CD2	13:1:170:TYR:CE2	2.95	0.49
31:2:502:XAT:H173	20:2:606:CLA:C3B	2.41	0.49
30:2:610:CHL:HBB1	30:2:610:CHL:CMB	2.36	0.49
20:A:1012:CLA:H42	2:B:438:VAL:HG22	1.95	0.49
2:B:477:LEU:HD21	20:B:1232:CLA:CMC	2.43	0.49
2:B:477:LEU:CD2	20:B:1232:CLA:HBC2	2.43	0.49
4:D:164:VAL:HG11	8:H:57:LEU:HD21	1.94	0.49
6:F:90:GLN:OE1	6:F:90:GLN:N	2.41	0.49
7:G:77:PHE:CE1	20:G:1602:CLA:HAB	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:G:1603:CLA:HAC1	30:1:610:CHL:HMD3	1.95	0.49
26:G:5002:LMG:H392	30:1:610:CHL:NB	2.28	0.49
12:L:174:ASP:OD1	12:L:176:LEU:HB3	2.13	0.49
13:1:229:VAL:HG21	20:1:603:CLA:HMD2	1.93	0.49
22:2:503:BCR:HC22	20:4:609:CLA:HMD1	1.94	0.49
30:2:611:CHL:HHC	30:2:611:CHL:CBB	2.39	0.49
22:3:503:BCR:H383	20:3:606:CLA:CHC	2.42	0.49
16:4:106:VAL:HA	16:4:109:MET:HB2	1.95	0.49
20:4:602:CLA:C1D	20:4:607:CLA:H71	2.43	0.49
1:A:213:LEU:HD21	20:A:1118:CLA:HMC1	1.95	0.48
1:A:569:ILE:HD11	1:A:589:THR:HG21	1.94	0.48
4:D:81:SER:O	4:D:124:ARG:NH2	2.46	0.48
8:H:63:THR:O	12:L:66:ILE:HD11	2.13	0.48
10:J:10:VAL:HG13	10:J:12:PRO:HD2	1.95	0.48
22:1:504:BCR:H271	20:1:606:CLA:C4B	2.43	0.48
20:2:604:CLA:H61	20:2:604:CLA:H41	1.42	0.48
26:2:803:LMG:O7	26:2:803:LMG:H131	2.12	0.48
18:P:19:LEU:CG	18:P:20:GLU:H	2.26	0.48
1:A:34:TRP:HE1	20:A:1109:CLA:CHB	2.25	0.48
1:A:365:LEU:HD22	20:A:1103:CLA:HED3	1.95	0.48
19:A:1011:CL0:H15	19:A:1011:CL0:H11	1.95	0.48
20:A:1117:CLA:H172	20:A:1125:CLA:H42	1.95	0.48
20:A:1132:CLA:HMB1	20:A:1132:CLA:CBB	2.40	0.48
2:B:167:TRP:CZ2	20:B:1210:CLA:HAC2	2.48	0.48
6:F:203:ALA:O	6:F:207:VAL:HG13	2.12	0.48
7:G:136:HIS:CE1	22:G:4011:BCR:H16C	2.48	0.48
8:H:103:LEU:HD21	12:L:142:SER:CB	2.43	0.48
13:1:90:ALA:HB2	29:1:502:LUT:C39	2.30	0.48
20:1:605:CLA:H2A	20:1:605:CLA:HED2	1.96	0.48
14:2:200:TRP:CZ2	30:2:615:CHL:C4C	2.96	0.48
14:2:207:GLY:N	20:2:601:CLA:HBA1	2.28	0.48
2:B:88:ALA:HB1	20:B:1205:CLA:O2D	2.13	0.48
6:F:117:LEU:C	6:F:117:LEU:CD2	2.86	0.48
14:2:169:ALA:HB1	14:2:177:VAL:HG11	1.95	0.48
20:2:601:CLA:H41	20:2:602:CLA:HBA2	1.95	0.48
15:3:171:ARG:HD3	30:3:611:CHL:HBB1	1.95	0.48
20:3:612:CLA:O1A	20:3:612:CLA:H2	2.13	0.48
17:N:58:GLN:HG3	17:N:69:ILE:HG23	1.95	0.48
17:N:77:CYS:SG	17:N:78:VAL:N	2.85	0.48
18:P:4:LEU:HB3	18:P:32:ASN:HB2	1.94	0.48
18:P:21:VAL:HG23	18:P:98:VAL:HG22	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:P:30:LYS:HG3	18:P:69:THR:HG22	1.96	0.48
1:A:224:HIS:HE1	20:A:1113:CLA:C4B	2.25	0.48
22:B:4009:BCR:H332	26:G:5001:LMG:H392	1.95	0.48
13:1:226:ILE:CB	20:1:603:CLA:H11	2.42	0.48
14:2:167:ARG:HH22	20:2:612:CLA:CHA	2.26	0.48
15:3:122:LEU:HA	15:3:125:VAL:HG22	1.96	0.48
8:H:87:GLU:HB3	12:L:96:LEU:HD22	1.93	0.48
12:L:87:PRO:HG2	20:L:1502:CLA:HED2	1.95	0.48
12:L:114:PHE:CE1	12:L:137:LEU:HD22	2.47	0.48
13:1:128:TRP:HE1	20:1:613:CLA:HED2	1.78	0.48
30:1:609:CHL:HED1	16:4:155:ARG:CA	2.39	0.48
20:2:608:CLA:ND	30:2:609:CHL:H13	2.27	0.48
20:4:601:CLA:H62	20:4:601:CLA:H41	1.69	0.48
2:B:463:ILE:HD13	20:B:1231:CLA:HHC	1.95	0.48
4:D:164:VAL:CG1	8:H:57:LEU:HD21	2.44	0.48
13:1:83:HIS:CE1	30:1:612:CHL:OBD	2.66	0.48
13:1:168:LEU:CD2	13:1:170:TYR:HE2	2.25	0.48
15:3:56:PRO:C	15:3:57:LEU:HD22	2.39	0.48
20:3:610:CLA:HBB1	20:3:610:CLA:HMB1	1.96	0.48
20:4:601:CLA:HBA1	20:4:601:CLA:CHA	2.43	0.48
1:A:38:GLY:HA3	1:A:44:ILE:CG2	2.44	0.48
20:A:1122:CLA:H41	20:A:1122:CLA:H61	1.56	0.48
20:A:1140:CLA:HBB1	20:A:1013:CLA:H162	1.95	0.48
22:A:4017:BCR:H352	20:B:1022:CLA:H122	1.96	0.48
2:B:434:LEU:O	2:B:438:VAL:HG23	2.13	0.48
2:B:684:ARG:HD3	2:B:684:ARG:HA	1.61	0.48
20:B:1224:CLA:CGA	20:B:1224:CLA:H3A	2.40	0.48
20:B:1207:CLA:CMD	22:I:4018:BCR:H332	2.43	0.48
4:D:84:PHE:HB3	12:L:64:PRO:HB2	1.95	0.48
11:K:53:LEU:C	11:K:53:LEU:CD1	2.86	0.48
20:3:606:CLA:HMA3	20:3:613:CLA:C2C	2.43	0.48
1:A:17:GLU:OE2	1:A:17:GLU:HA	2.12	0.48
20:A:1110:CLA:O1A	15:3:81:LEU:HD23	2.14	0.48
22:A:4007:BCR:H15C	22:A:4007:BCR:H351	1.63	0.48
20:A:1139:CLA:H61	10:J:18:TRP:CD2	2.48	0.48
2:B:358:TYR:CE2	20:B:1225:CLA:HED2	2.49	0.48
7:G:125:ILE:O	7:G:128:VAL:HG22	2.13	0.48
20:L:1502:CLA:HMA3	22:L:4020:BCR:H373	1.95	0.48
13:1:94:ILE:HG23	13:1:105:TRP:HB3	1.95	0.48
14:2:162:TRP:HH2	22:2:503:BCR:H322	1.78	0.48
16:4:245:ILE:HD13	20:4:603:CLA:CAD	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:P:21:VAL:HG23	18:P:98:VAL:CG2	2.44	0.48
18:P:62:LEU:C	18:P:62:LEU:CD2	2.86	0.48
1:A:382:TYR:CE1	20:A:1127:CLA:HED2	2.49	0.48
20:A:1108:CLA:H12	20:A:1111:CLA:H193	1.95	0.48
20:A:1128:CLA:H62	20:A:1128:CLA:H41	1.57	0.48
20:G:1602:CLA:HBA2	20:G:1602:CLA:O2D	2.14	0.48
26:G:5001:LMG:H182	30:1:612:CHL:C1B	2.43	0.48
12:L:90:ARG:O	12:L:98:ARG:NE	2.47	0.48
20:1:601:CLA:HBB1	20:1:601:CLA:HMB1	1.95	0.48
14:2:162:TRP:CH2	22:2:503:BCR:H313	2.47	0.48
20:2:605:CLA:H61	20:2:605:CLA:H101	1.43	0.48
16:4:103:MET:HB2	20:4:601:CLA:CMC	2.44	0.48
1:A:472:ARG:NH2	20:A:1132:CLA:O1D	2.47	0.48
2:B:255:LEU:HD11	20:B:1212:CLA:HBC1	1.96	0.48
2:B:279:ALA:HA	20:B:1213:CLA:HMC3	1.95	0.48
26:B:5003:LMG:C18	22:F:4016:BCR:H362	2.42	0.48
6:F:159:GLU:HA	10:J:38:THR:CG2	2.26	0.48
6:F:213:TRP:CD1	6:F:214:PRO:HD3	2.48	0.48
20:2:606:CLA:HBD	20:2:606:CLA:CBA	2.44	0.48
1:A:583:GLY:HA3	3:C:51:CYS:O	2.14	0.47
2:B:694:ARG:NH1	9:I:29:GLU:O	2.46	0.47
20:B:1022:CLA:H193	20:B:1207:CLA:HMC2	1.95	0.47
20:B:1211:CLA:H3A	22:B:4006:BCR:C39	2.35	0.47
13:1:149:ARG:HA	20:1:611:CLA:HBC2	1.96	0.47
29:1:502:LUT:H15	29:1:502:LUT:H201	1.74	0.47
23:1:801:LHG:H322	16:4:147:ILE:HG23	1.95	0.47
20:2:601:CLA:HBA2	20:2:601:CLA:H3A	1.41	0.47
20:2:607:CLA:CHB	24:2:808:LMT:H32	2.44	0.47
16:4:96:LEU:HD21	16:4:184:TYR:CE1	2.49	0.47
2:B:314:ARG:HG2	26:B:5003:LMG:HC3	1.96	0.47
20:B:1237:CLA:H41	20:B:1237:CLA:H61	1.73	0.47
13:1:93:GLY:HA3	20:1:606:CLA:CHC	2.44	0.47
30:2:609:CHL:H41	30:2:609:CHL:C7	2.29	0.47
29:3:502:LUT:H35	29:3:502:LUT:H401	1.67	0.47
18:P:52:ALA:O	18:P:56:SER:HB3	2.13	0.47
2:B:152:ALA:HB2	20:B:1208:CLA:HBC2	1.95	0.47
2:B:464:GLN:HE21	20:B:1234:CLA:CAD	2.24	0.47
20:B:1205:CLA:CGA	20:B:1205:CLA:C1A	2.93	0.47
22:L:4019:BCR:H15C	22:L:4019:BCR:H351	1.63	0.47
17:N:93:GLU:C	17:N:95:LEU:H	2.20	0.47
1:A:716:VAL:O	1:A:716:VAL:HG22	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:B:1214:CLA:H141	20:B:1214:CLA:H161	1.62	0.47
28:F:5005:DGD:C5A	32:2:807:3PH:H2B2	2.44	0.47
7:G:154:PHE:CZ	30:1:610:CHL:HED2	2.49	0.47
20:1:601:CLA:O1A	20:1:601:CLA:H3A	2.14	0.47
14:2:188:LEU:HD22	14:2:198:GLY:HA3	1.95	0.47
15:3:218:LYS:O	15:3:222:GLU:HG3	2.15	0.47
30:4:610:CHL:CBB	30:4:613:CHL:HBB2	2.44	0.47
17:N:73:PHE:CE1	17:N:95:LEU:HB2	2.49	0.47
17:N:91:LYS:HE3	17:N:91:LYS:HB3	1.81	0.47
1:A:308:ILE:HD12	22:K:4001:BCR:H353	1.95	0.47
15:3:61:SER:HB3	15:3:64:SER:CB	2.44	0.47
22:3:506:BCR:H10C	30:3:611:CHL:HBA1	1.95	0.47
20:4:609:CLA:HBB2	20:4:604:CLA:HHD	1.97	0.47
20:4:602:CLA:H2A	20:4:602:CLA:CED	2.17	0.47
18:P:23:ALA:C	18:P:25:GLU:H	2.22	0.47
3:C:52:LYS:HE2	3:C:67:VAL:O	2.14	0.47
20:F:1302:CLA:H162	20:F:1302:CLA:H121	1.70	0.47
26:G:5001:LMG:H202	30:1:612:CHL:C4B	2.44	0.47
13:1:173:ASP:HB3	13:1:176:LYS:HB2	1.96	0.47
14:2:150:THR:HB	16:4:246:VAL:HG11	1.96	0.47
14:2:169:ALA:HB3	14:2:177:VAL:HG11	1.96	0.47
22:2:503:BCR:C39	20:2:606:CLA:C1B	2.93	0.47
15:3:64:SER:OG	15:3:79:ASP:HB3	2.14	0.47
16:4:98:ASN:OD1	20:4:612:CLA:HMD1	2.15	0.47
20:4:603:CLA:H111	20:4:603:CLA:H71	1.54	0.47
1:A:604:TRP:CH2	20:B:1022:CLA:HAB	2.50	0.47
1:A:688:PHE:CZ	20:A:1140:CLA:HBC2	2.37	0.47
20:A:1101:CLA:HED1	21:A:2001:PQN:C24	2.45	0.47
20:A:1013:CLA:H162	20:A:1013:CLA:H122	1.48	0.47
20:A:1139:CLA:H62	20:A:1139:CLA:H41	1.35	0.47
2:B:27:THR:O	2:B:27:THR:OG1	2.33	0.47
2:B:453:ILE:HD11	20:B:1230:CLA:CHB	2.43	0.47
20:B:1224:CLA:H112	20:B:1224:CLA:H72	1.71	0.47
7:G:133:SER:HB2	22:G:4011:BCR:H372	1.97	0.47
23:1:801:LHG:H151	23:1:801:LHG:H262	1.96	0.47
14:2:219:THR:O	14:2:222:ILE:HG22	2.14	0.47
30:2:613:CHL:HHC	30:2:613:CHL:CBB	2.39	0.47
15:3:249:GLY:HA3	15:3:274:PHE:CZ	2.49	0.47
15:3:257:LEU:HA	15:3:260:VAL:HG22	1.97	0.47
15:3:267:ASN:HB2	20:3:603:CLA:H11	1.97	0.47
1:A:527:VAL:HG11	1:A:530:LEU:HD23	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:147:ILE:HD11	22:L:4019:BCR:C16	2.44	0.47
22:L:4019:BCR:H403	22:L:4019:BCR:C23	2.45	0.47
29:1:501:LUT:H173	20:1:603:CLA:C3B	2.44	0.47
14:2:101:TRP:CE2	26:2:802:LMG:HC5	2.50	0.47
14:2:159:PHE:CD2	22:2:503:BCR:C15	2.98	0.47
20:4:612:CLA:C9	28:4:802:DGD:CCB	2.92	0.47
1:A:145:ILE:HB	20:A:1106:CLA:OBD	2.14	0.47
1:A:567:ARG:HB2	2:B:676:GLU:CD	2.40	0.47
20:A:1111:CLA:H191	20:3:605:CLA:H71	1.97	0.47
20:A:1115:CLA:H11	20:A:1115:CLA:H51	1.74	0.47
20:A:1132:CLA:HAA2	12:L:117:ALA:O	2.15	0.47
20:B:1204:CLA:H51	20:B:1204:CLA:H11	1.73	0.47
20:B:1223:CLA:C4B	20:B:1231:CLA:HMA3	2.45	0.47
20:B:1229:CLA:HBC3	6:F:164:GLY:HA2	1.97	0.47
3:C:38:GLN:OE1	4:D:178:VAL:HG12	2.12	0.47
20:F:1301:CLA:C2B	10:J:22:LEU:HD11	2.45	0.47
26:G:5002:LMG:H201	26:G:5002:LMG:H171	1.67	0.47
10:J:36:ALA:HB1	28:J:5001:DGD:C2G	2.34	0.47
29:J:4013:LUT:H27	29:J:4013:LUT:H381	1.72	0.47
20:2:608:CLA:C1D	30:2:609:CHL:H13	2.44	0.47
1:A:456:HIS:HA	20:A:1132:CLA:HBB2	1.97	0.47
1:A:583:GLY:HA2	2:B:562:PRO:HD3	1.97	0.47
2:B:181:GLY:HA3	20:B:1210:CLA:HBB1	1.97	0.47
2:B:299:HIS:HB3	2:B:304:ILE:HD11	1.97	0.47
2:B:422:LEU:HG	20:B:1236:CLA:CAB	2.45	0.47
2:B:726:ILE:O	2:B:730:SER:HB3	2.14	0.47
20:B:1235:CLA:H193	20:B:1235:CLA:H162	1.67	0.47
22:L:4020:BCR:H351	22:L:4020:BCR:H15C	1.56	0.47
13:1:196:VAL:HA	13:1:199:CYS:SG	2.55	0.47
20:1:605:CLA:H43	20:1:605:CLA:HED3	1.96	0.47
16:4:150:HIS:CE1	16:4:154:ILE:CD1	2.85	0.47
16:4:188:ILE:CG2	30:4:615:CHL:HBC3	2.42	0.47
20:4:601:CLA:C4	20:4:602:CLA:HBA1	2.44	0.47
1:A:224:HIS:HB2	20:A:1112:CLA:HBC3	1.97	0.46
1:A:579:PHE:CE1	1:A:593:SER:CB	2.98	0.46
20:A:1105:CLA:H111	20:A:1105:CLA:H72	1.60	0.46
20:A:1131:CLA:H152	20:A:1131:CLA:H112	1.66	0.46
2:B:221:GLY:HA3	20:B:1212:CLA:OBD	2.14	0.46
2:B:503:GLU:OE1	2:B:505:SER:N	2.42	0.46
2:B:711:VAL:HG11	20:B:1239:CLA:HED3	1.97	0.46
20:B:1216:CLA:HBC2	20:B:1220:CLA:H92	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:B:1207:CLA:H62	20:B:1207:CLA:H41	1.55	0.46
26:G:5002:LMG:O9	13:1:132:PRO:HG3	2.15	0.46
30:1:610:CHL:CBB	20:1:613:CLA:HBB2	2.45	0.46
30:2:609:CHL:C1	15:3:163:ALA:HA	2.45	0.46
15:3:257:LEU:C	15:3:257:LEU:CD2	2.86	0.46
16:4:132:GLU:N	16:4:132:GLU:OE2	2.48	0.46
1:A:122:VAL:CG2	20:A:1105:CLA:HED3	2.45	0.46
1:A:410:ALA:HB1	22:A:4008:BCR:H383	1.97	0.46
20:A:1136:CLA:CGA	20:A:1136:CLA:C1A	2.94	0.46
2:B:22:TRP:CG	2:B:704:GLN:HE22	2.33	0.46
6:F:159:GLU:HG2	10:J:38:THR:HG21	1.96	0.46
29:1:502:LUT:H31	20:1:605:CLA:HBC3	1.98	0.46
14:2:162:TRP:CH2	22:2:503:BCR:C31	2.98	0.46
16:4:198:LEU:HD23	16:4:198:LEU:O	2.15	0.46
29:4:501:LUT:H30	20:4:601:CLA:C5	2.21	0.46
1:A:467:MET:CA	1:A:467:MET:CE	2.86	0.46
20:B:1237:CLA:H143	22:I:4020:BCR:H14C	1.84	0.46
20:B:1205:CLA:H91	20:B:1206:CLA:H51	1.97	0.46
20:B:1219:CLA:H11	26:G:5001:LMG:H132	1.97	0.46
14:2:250:LEU:HD13	20:2:608:CLA:CBC	2.46	0.46
31:2:502:XAT:H15	31:2:502:XAT:H201	1.76	0.46
20:2:607:CLA:C1C	24:2:808:LMT:H72	2.45	0.46
15:3:233:LEU:HD12	15:3:236:LEU:HD11	1.97	0.46
20:4:603:CLA:HHC	20:4:603:CLA:CBB	2.34	0.46
1:A:252:ARG:HD2	20:A:1113:CLA:OBD	2.15	0.46
20:A:1102:CLA:HBA1	20:A:1109:CLA:C1D	2.46	0.46
2:B:516:ASP:OD1	2:B:597:LYS:NZ	2.47	0.46
20:B:1210:CLA:H172	22:B:4005:BCR:H271	1.98	0.46
20:B:1214:CLA:HBA2	20:B:1223:CLA:HBB2	1.97	0.46
20:B:1225:CLA:H142	22:B:4006:BCR:H372	1.96	0.46
3:C:15:THR:CG2	3:C:28:MET:HE2	2.45	0.46
6:F:93:LYS:O	6:F:96:LYS:HG3	2.15	0.46
12:L:61:ASN:HD21	12:L:166:LEU:CD1	2.27	0.46
12:L:94:ASN:HD21	12:L:184:LYS:HE3	1.79	0.46
20:1:614:CLA:HBB1	16:4:142:PHE:HE2	1.79	0.46
14:2:162:TRP:CH2	20:4:609:CLA:CAD	2.98	0.46
16:4:104:LEU:HD13	20:4:601:CLA:CAC	2.41	0.46
1:A:397:THR:HG22	20:A:1126:CLA:HAB	1.97	0.46
20:A:1126:CLA:H3A	20:A:1126:CLA:HBA2	1.45	0.46
20:A:1013:CLA:H41	20:A:1013:CLA:H61	1.50	0.46
20:B:1221:CLA:H61	20:B:1221:CLA:H41	1.64	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:102:VAL:HG21	8:H:55:PHE:CE1	2.50	0.46
11:K:99:PHE:CE2	20:K:1404:CLA:HAB	2.50	0.46
13:1:222:TRP:CE3	20:1:608:CLA:CMA	2.99	0.46
13:1:229:VAL:HG21	20:1:603:CLA:HMD1	1.97	0.46
20:2:606:CLA:HBA1	20:2:606:CLA:HBD	1.98	0.46
15:3:266:ASN:OD1	15:3:268:VAL:HG22	2.15	0.46
17:N:93:GLU:C	17:N:95:LEU:N	2.74	0.46
1:A:652:TRP:CE2	19:A:1011:CL0:H56	2.50	0.46
1:A:691:MET:SD	21:A:2001:PQN:H2M1	2.56	0.46
20:A:1102:CLA:H3A	20:A:1102:CLA:HBA2	1.30	0.46
20:A:1120:CLA:H93	20:A:1120:CLA:H111	1.68	0.46
20:B:1204:CLA:H61	20:B:1204:CLA:H41	1.47	0.46
20:B:1220:CLA:HBA2	20:B:1220:CLA:H3A	1.61	0.46
20:B:1228:CLA:C1	26:B:5003:LMG:H161	2.46	0.46
20:B:1229:CLA:HMB2	22:F:4014:BCR:H21C	1.98	0.46
12:L:113:PRO:HB3	20:L:1503:CLA:CAB	2.46	0.46
30:1:609:CHL:C4	16:4:147:ILE:HG22	2.40	0.46
14:2:206:TRP:HB2	20:2:601:CLA:O1A	2.16	0.46
26:2:802:LMG:HC8	26:2:802:LMG:H112	1.53	0.46
26:2:805:LMG:HC2	26:2:805:LMG:HC71	1.75	0.46
22:3:503:BCR:H402	20:3:606:CLA:NB	2.30	0.46
1:A:114:THR:O	1:A:114:THR:OG1	2.33	0.46
22:A:4017:BCR:C38	20:B:1237:CLA:HBC2	2.46	0.46
2:B:514:PRO:HG2	6:F:147:HIS:HE1	1.75	0.46
20:B:1238:CLA:HBB2	21:B:2002:PQN:H141	1.98	0.46
21:B:2002:PQN:H212	21:B:2002:PQN:H172	1.62	0.46
11:K:77:LYS:O	11:K:84:LEU:HD22	2.16	0.46
13:1:70:PRO:HB2	13:1:71:GLU:OE2	2.15	0.46
13:1:86:TRP:NE1	20:1:611:CLA:HED3	2.31	0.46
14:2:164:GLU:HB3	20:2:612:CLA:CHB	2.46	0.46
15:3:217:GLU:N	15:3:217:GLU:OE2	2.49	0.46
17:N:56:VAL:HG11	17:N:79:ALA:HB1	1.96	0.46
17:N:63:PHE:CD2	17:N:63:PHE:O	2.68	0.46
18:P:23:ALA:HA	18:P:98:VAL:HG11	1.97	0.46
1:A:283:PHE:CE2	20:A:1116:CLA:CBB	2.96	0.46
20:A:1110:CLA:H12	15:3:81:LEU:HD23	1.98	0.46
2:B:294:ASN:N	2:B:294:ASN:OD1	2.49	0.46
4:D:91:LEU:CD2	4:D:133:ALA:HB2	2.42	0.46
4:D:177:LYS:HE3	4:D:177:LYS:HB3	1.76	0.46
8:H:85:PHE:CD2	20:H:1701:CLA:HMC2	2.51	0.46
12:L:95:PRO:HD2	12:L:184:LYS:NZ	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:2:230:LEU:O	20:2:603:CLA:HMC3	2.15	0.46
31:2:502:XAT:H391	31:2:502:XAT:H31	1.73	0.46
16:4:215:PHE:CD1	31:4:502:XAT:C14	2.89	0.46
1:A:677:LEU:HD22	20:A:1012:CLA:H71	1.98	0.46
19:A:1011:CL0:H10	19:A:1011:CL0:H72	1.55	0.46
20:A:1131:CLA:HBB2	12:L:117:ALA:HB1	1.96	0.46
2:B:2:ALA:HB1	2:B:7:ARG:NE	2.31	0.46
2:B:66:PHE:CE2	20:B:1204:CLA:HBC3	2.51	0.46
2:B:243:LEU:HB2	2:B:246:THR:OG1	2.16	0.46
2:B:649:MET:HG2	2:B:723:ALA:HB2	1.98	0.46
20:B:1222:CLA:HED2	20:B:1223:CLA:HBD	1.98	0.46
20:B:1239:CLA:H3A	20:B:1239:CLA:HBA2	1.44	0.46
7:G:117:SER:OG	7:G:118:ASN:N	2.49	0.46
22:H:4021:BCR:C8	22:H:4021:BCR:C32	2.86	0.46
10:J:28:GLU:HG3	20:J:1901:CLA:NB	2.30	0.46
13:1:133:THR:CG2	13:1:134:ILE:H	2.28	0.46
14:2:124:GLU:OE1	14:2:246:PRO:HD2	2.15	0.46
14:2:159:PHE:HD2	22:2:503:BCR:C17	2.29	0.46
20:2:602:CLA:H61	20:2:602:CLA:H41	1.49	0.46
16:4:150:HIS:O	16:4:154:ILE:HG13	2.16	0.46
20:4:617:CLA:H111	20:4:617:CLA:H72	1.43	0.46
20:A:1119:CLA:H121	20:A:1122:CLA:H92	1.98	0.46
2:B:319:HIS:HB3	2:B:322:LEU:HD12	1.98	0.46
20:B:1238:CLA:H111	20:B:1238:CLA:H152	1.73	0.46
4:D:161:SER:OG	4:D:163:GLU:N	2.49	0.46
14:2:101:TRP:CG	26:2:802:LMG:HC3	2.51	0.46
20:3:608:CLA:HHC	20:3:608:CLA:HBB1	1.98	0.46
31:4:502:XAT:H31	31:4:502:XAT:H391	1.78	0.46
1:A:146:THR:O	20:A:1126:CLA:HMA1	2.16	0.45
1:A:245:PRO:CG	20:A:1112:CLA:CAD	2.94	0.45
1:A:250:LEU:HD21	20:A:1114:CLA:HAC2	1.97	0.45
1:A:459:GLY:HA3	20:A:1132:CLA:HAB	1.98	0.45
1:A:505:PRO:HG2	20:A:1134:CLA:C2D	2.47	0.45
1:A:649:ILE:HD12	20:B:1022:CLA:CMA	2.45	0.45
1:A:747:TRP:CA	20:A:1126:CLA:HBB1	2.45	0.45
1:A:757:VAL:HG13	18:P:64:ASN:ND2	2.31	0.45
20:A:1107:CLA:H93	20:A:1107:CLA:H61	1.70	0.45
20:A:1126:CLA:H71	20:A:1126:CLA:H112	1.37	0.45
20:A:1126:CLA:H92	20:A:1126:CLA:H61	1.68	0.45
20:A:1130:CLA:H62	20:A:1130:CLA:H41	1.58	0.45
20:A:1139:CLA:H143	20:A:1139:CLA:H112	1.72	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:H:1701:CLA:C1B	22:H:4021:BCR:H362	2.46	0.45
12:L:116:LYS:HG2	20:L:1503:CLA:HMA1	1.99	0.45
12:L:184:LYS:HB3	12:L:184:LYS:HE2	1.71	0.45
14:2:58:THR:HG23	14:2:58:THR:O	2.15	0.45
14:2:201:PHE:HB3	20:2:601:CLA:HMD2	1.98	0.45
20:2:603:CLA:NC	20:2:603:CLA:H51	2.31	0.45
20:2:604:CLA:CGA	20:2:604:CLA:C3A	2.92	0.45
23:2:801:LHG:HC92	23:2:801:LHG:C14	2.45	0.45
18:P:23:ALA:C	18:P:25:GLU:N	2.74	0.45
1:A:32:GLU:OE1	1:A:32:GLU:N	2.50	0.45
1:A:661:ALA:CB	19:A:1011:CL0:H3	2.46	0.45
2:B:343:VAL:CG2	22:B:4010:BCR:H362	2.47	0.45
26:B:5003:LMG:HC91	26:B:5003:LMG:O9	2.15	0.45
28:B:5005:DGD:HB21	28:B:5005:DGD:HB51	1.78	0.45
4:D:75:LEU:HA	4:D:75:LEU:HD23	1.69	0.45
4:D:109:LYS:HA	4:D:125:GLU:HG3	1.97	0.45
8:H:67:TRP:CZ3	12:L:60:ILE:HG23	2.52	0.45
8:H:89:PHE:CE1	22:H:4021:BCR:H331	2.51	0.45
14:2:180:ASP:OD1	14:2:181:PRO:HD2	2.15	0.45
14:2:189:THR:OG1	14:2:197:GLY:HA3	2.17	0.45
1:A:98:PHE:CE1	20:A:1105:CLA:CHD	3.00	0.45
1:A:757:VAL:HG13	18:P:64:ASN:HD21	1.81	0.45
20:A:1106:CLA:H12	22:J:4012:BCR:H371	1.97	0.45
2:B:145:LEU:HD23	2:B:145:LEU:HA	1.77	0.45
2:B:463:ILE:HG12	20:B:1231:CLA:HMC2	1.99	0.45
3:C:12:ILE:CD1	17:N:39:CYS:HA	2.45	0.45
12:L:108:PHE:CD2	12:L:200:ALA:HB2	2.51	0.45
16:4:206:ALA:HB2	23:4:801:LHG:HC32	1.98	0.45
1:A:123:VAL:HA	20:A:1107:CLA:HED2	1.98	0.45
1:A:208:ALA:HB2	1:A:314:GLY:HA3	1.98	0.45
1:A:657:LEU:O	1:A:661:ALA:HB2	2.16	0.45
2:B:62:SER:HB2	2:B:142:LEU:CB	2.47	0.45
2:B:259:GLY:HA2	20:B:1214:CLA:O2A	2.15	0.45
2:B:343:VAL:HG21	22:B:4010:BCR:H362	1.98	0.45
2:B:695:ASP:OD1	9:I:29:GLU:OE1	2.34	0.45
14:2:233:MET:HE2	20:2:605:CLA:HBB2	1.97	0.45
29:2:501:LUT:H191	29:2:501:LUT:H11	1.68	0.45
20:2:605:CLA:H41	20:2:605:CLA:H93	1.98	0.45
20:2:607:CLA:HMB1	24:2:808:LMT:C1	2.46	0.45
30:2:611:CHL:HBD	30:2:611:CHL:HAA1	1.98	0.45
20:2:612:CLA:H62	20:2:612:CLA:H41	1.54	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:P:42:ASP:C	18:P:44:ASP:N	2.73	0.45
1:A:398:HIS:CE1	20:A:1127:CLA:C1B	2.99	0.45
1:A:487:VAL:H	20:A:1136:CLA:HMD3	1.82	0.45
1:A:511:THR:HG22	20:A:1116:CLA:H2	1.99	0.45
1:A:591:GLN:HB3	1:A:596:ASP:CB	2.47	0.45
20:A:1105:CLA:H13	20:A:1107:CLA:H121	1.98	0.45
2:B:115:ILE:O	20:B:1205:CLA:HMD1	2.16	0.45
2:B:454:LEU:HD22	2:B:614:THR:HG21	1.97	0.45
20:G:1603:CLA:H101	13:1:135:LEU:HD11	1.98	0.45
29:J:4013:LUT:H15	29:J:4013:LUT:H201	1.76	0.45
22:2:503:BCR:HC8	22:2:503:BCR:H311	1.96	0.45
15:3:266:ASN:CG	15:3:267:ASN:N	2.74	0.45
16:4:233:LEU:HA	20:4:603:CLA:HMA3	1.99	0.45
18:P:19:LEU:CG	18:P:20:GLU:N	2.77	0.45
18:P:35:PHE:HA	18:P:37:HIS:HD2	1.80	0.45
20:A:1106:CLA:H11	22:J:4012:BCR:H392	1.99	0.45
20:A:1109:CLA:H62	20:A:1109:CLA:H41	1.35	0.45
20:A:1122:CLA:H162	20:A:1122:CLA:H121	1.73	0.45
20:A:1141:CLA:O1A	26:A:5006:LMG:H372	2.16	0.45
2:B:514:PRO:CG	6:F:147:HIS:CE1	2.98	0.45
20:B:1204:CLA:HED2	9:I:5:PRO:HB3	1.99	0.45
6:F:229:LYS:O	6:F:230:ASP:HB3	2.17	0.45
20:F:1301:CLA:HBA1	20:F:1301:CLA:H3A	1.55	0.45
20:G:1603:CLA:H11	20:G:1603:CLA:H52	1.69	0.45
29:1:502:LUT:C8	29:1:502:LUT:H181	2.44	0.45
14:2:162:TRP:CZ3	22:2:503:BCR:C32	2.99	0.45
15:3:240:GLY:O	15:3:244:GLN:HB2	2.17	0.45
17:N:65:ASP:HB3	17:N:68:GLN:HG2	1.98	0.45
1:A:374:HIS:CD2	20:A:1124:CLA:HED2	2.52	0.45
1:A:435:VAL:HA	1:A:438:HIS:CE1	2.52	0.45
20:A:1122:CLA:HMA1	20:A:1141:CLA:HAB	1.99	0.45
2:B:373:THR:HG21	2:B:721:TYR:HE2	1.81	0.45
20:B:1228:CLA:O2A	26:B:5003:LMG:H161	2.17	0.45
26:B:5004:LMG:H131	26:B:5004:LMG:HC8	1.98	0.45
11:K:73:SER:HB2	11:K:76:ARG:HB2	1.99	0.45
14:2:119:GLY:CA	31:2:502:XAT:H172	2.42	0.45
14:2:236:TRP:CD1	14:2:236:TRP:C	2.95	0.45
29:2:501:LUT:H201	29:2:501:LUT:H15	1.63	0.45
15:3:162:MET:HE3	20:3:612:CLA:CBB	2.46	0.45
15:3:220:LEU:HG	15:3:224:LYS:HE3	1.99	0.45
16:4:206:ALA:HB2	23:4:801:LHG:C3	2.45	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:N:45:SER:HB3	17:N:92:GLU:HG3	1.98	0.45
18:P:5:LEU:HD11	18:P:29:PHE:HB3	1.99	0.45
1:A:27:ILE:HD13	1:A:186:TYR:CZ	2.52	0.45
1:A:590:CYS:HB3	2:B:667:TRP:CE3	2.50	0.45
1:A:652:TRP:CZ2	19:A:1011:CL0:H56	2.51	0.45
20:A:1136:CLA:H92	20:A:1136:CLA:H61	1.81	0.45
20:B:1229:CLA:HAC1	6:F:160:PHE:CE1	2.52	0.45
20:B:1239:CLA:H61	20:B:1239:CLA:H41	1.71	0.45
6:F:95:GLU:HB2	6:F:130:PHE:CD1	2.51	0.45
6:F:132:ASN:HD22	6:F:132:ASN:HA	1.69	0.45
20:F:1302:CLA:H11	20:F:1302:CLA:H52	1.77	0.45
29:1:501:LUT:H35	29:1:501:LUT:H401	1.82	0.45
14:2:160:ILE:HD12	14:2:160:ILE:HA	1.85	0.45
16:4:94:ALA:CA	20:4:612:CLA:CED	2.93	0.45
20:4:607:CLA:H102	20:4:607:CLA:H13	1.52	0.45
1:A:626:GLY:HA3	1:A:636:HIS:HA	1.99	0.45
20:A:1124:CLA:H3A	20:A:1124:CLA:HBA2	1.44	0.45
20:A:1131:CLA:CAD	22:I:4020:BCR:H21C	2.47	0.45
22:A:4011:BCR:H362	20:A:1012:CLA:C4	2.47	0.45
2:B:91:ILE:CD1	20:B:1206:CLA:HMD1	2.47	0.45
2:B:503:GLU:OE1	2:B:505:SER:OG	2.32	0.45
20:F:1301:CLA:H92	20:F:1301:CLA:H61	1.67	0.45
11:K:46:PHE:O	11:K:46:PHE:CG	2.70	0.45
16:4:103:MET:HB3	20:4:601:CLA:HMC3	1.99	0.45
16:4:241:TRP:CZ3	20:4:608:CLA:CMA	2.92	0.45
20:4:609:CLA:HBB2	20:4:604:CLA:HMD3	1.98	0.45
1:A:221:HIS:ND1	20:A:1112:CLA:NB	2.65	0.45
1:A:487:VAL:N	20:A:1136:CLA:HMD3	2.31	0.45
2:B:159:PRO:C	2:B:161:TRP:H	2.25	0.45
2:B:462:TRP:CD1	20:F:1302:CLA:HAC1	2.52	0.45
6:F:176:TRP:O	6:F:180:SER:OG	2.33	0.45
8:H:119:SER:C	8:H:126:LYS:HD3	2.42	0.45
20:1:611:CLA:H62	20:1:611:CLA:H2	1.69	0.45
15:3:188:LEU:CD1	22:3:503:BCR:H342	2.43	0.45
20:4:609:CLA:HBB1	20:4:609:CLA:CHC	2.18	0.45
20:4:601:CLA:C3A	20:4:601:CLA:CGA	2.94	0.45
1:A:682:ALA:HA	1:A:685:VAL:HG12	1.98	0.44
20:A:1132:CLA:H2A	20:A:1132:CLA:HED2	1.97	0.44
20:A:1133:CLA:H41	20:A:1133:CLA:H61	1.63	0.44
2:B:410:ARG:O	2:B:414:HIS:ND1	2.44	0.44
2:B:726:ILE:O	2:B:730:SER:CB	2.65	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:B:1201:CLA:H162	20:B:1201:CLA:H122	1.33	0.44
20:B:1204:CLA:H11	22:I:4018:BCR:H281	1.98	0.44
20:B:1235:CLA:H142	20:B:1235:CLA:H112	1.79	0.44
22:B:4009:BCR:H353	20:B:1240:CLA:HED1	1.98	0.44
12:L:199:TRP:CE3	22:L:4020:BCR:H343	2.52	0.44
14:2:81:LEU:HD22	14:2:103:VAL:HG21	1.98	0.44
15:3:259:HIS:ND1	20:3:603:CLA:HAA2	2.32	0.44
20:4:608:CLA:HHD	20:4:608:CLA:HBC2	1.99	0.44
2:B:173:SER:O	2:B:177:HIS:ND1	2.34	0.44
2:B:257:LEU:HD13	20:B:1214:CLA:CMB	2.47	0.44
2:B:373:THR:HB	20:B:1224:CLA:HMB1	1.98	0.44
20:L:1503:CLA:HBA2	20:L:1503:CLA:HBD	1.98	0.44
13:1:118:GLN:NE2	13:1:126:VAL:O	2.48	0.44
20:1:604:CLA:H192	20:4:617:CLA:H93	1.98	0.44
15:3:245:GLY:O	15:3:249:GLY:HA2	2.17	0.44
31:4:502:XAT:H15	31:4:502:XAT:H201	1.78	0.44
20:4:612:CLA:H91	28:4:802:DGD:CCB	2.48	0.44
18:P:35:PHE:CD2	18:P:35:PHE:N	2.84	0.44
1:A:152:ILE:CD1	20:A:1127:CLA:HAA1	2.43	0.44
20:A:1104:CLA:H61	20:A:1104:CLA:H41	1.38	0.44
24:A:5004:LMT:O6B	24:A:5004:LMT:O4'	2.23	0.44
2:B:193:HIS:HB2	20:B:1211:CLA:C4B	2.46	0.44
2:B:670:TYR:CD2	2:B:670:TYR:C	2.94	0.44
6:F:172:GLY:HA3	6:F:213:TRP:CZ2	2.53	0.44
20:F:1302:CLA:HMB1	22:F:4016:BCR:HC7	1.99	0.44
20:F:1301:CLA:HBC2	10:J:19:PHE:HZ	1.77	0.44
22:H:4021:BCR:H371	22:L:4020:BCR:H352	1.99	0.44
20:L:1501:CLA:CMB	20:L:1501:CLA:CBB	2.93	0.44
13:1:62:ASP:N	13:1:63:PRO:HD3	2.32	0.44
13:1:90:ALA:HB1	29:1:502:LUT:H27	1.99	0.44
23:1:801:LHG:H223	20:4:617:CLA:O1A	2.17	0.44
30:2:610:CHL:HMD3	26:2:803:LMG:HC72	2.00	0.44
15:3:250:VAL:HG21	15:3:255:ASN:CB	2.46	0.44
20:3:602:CLA:H62	20:3:602:CLA:H41	1.73	0.44
16:4:234:LEU:HD12	16:4:235:GLN:N	2.32	0.44
29:4:501:LUT:H191	20:4:602:CLA:HMC3	1.99	0.44
20:4:604:CLA:H92	20:4:604:CLA:H61	1.64	0.44
1:A:448:TRP:HB2	20:B:1237:CLA:CED	2.47	0.44
1:A:462:ILE:HG22	20:A:1132:CLA:CBC	2.30	0.44
20:B:1237:CLA:H112	20:B:1237:CLA:H151	1.46	0.44
12:L:119:PRO:HG2	12:L:120:LEU:CD2	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:1:61:PHE:O	20:1:604:CLA:HBD	2.16	0.44
13:1:221:PRO:HG2	20:1:608:CLA:CMB	2.47	0.44
20:2:604:CLA:H162	20:2:604:CLA:H193	1.67	0.44
20:3:612:CLA:HBB1	20:3:612:CLA:CMB	2.28	0.44
16:4:127:TYR:OH	16:4:227:LYS:HA	2.17	0.44
16:4:215:PHE:CZ	20:4:605:CLA:HMC1	2.53	0.44
1:A:42:ARG:CZ	1:A:42:ARG:CB	2.96	0.44
1:A:209:GLY:O	1:A:213:LEU:HB2	2.17	0.44
1:A:408:VAL:HG11	1:A:602:LEU:HD21	1.96	0.44
20:A:1112:CLA:H143	20:A:1112:CLA:H162	1.80	0.44
20:A:1119:CLA:HMB2	20:A:1123:CLA:HMA3	2.00	0.44
20:A:1139:CLA:H42	20:F:1301:CLA:HBC3	1.99	0.44
20:B:1237:CLA:H151	20:B:1237:CLA:H8	1.98	0.44
20:B:1223:CLA:H152	20:B:1223:CLA:H111	1.72	0.44
20:L:1503:CLA:CMB	20:L:1503:CLA:CBB	2.93	0.44
20:2:605:CLA:C3	26:2:802:LMG:H291	2.47	0.44
26:2:803:LMG:HC8	26:2:803:LMG:O6	2.17	0.44
17:N:30:GLU:HA	17:N:30:GLU:OE2	2.16	0.44
18:P:45:GLU:OE1	18:P:45:GLU:N	2.51	0.44
1:A:42:ARG:CB	1:A:42:ARG:NH2	2.81	0.44
1:A:179:LEU:HG	20:A:1109:CLA:CMC	2.47	0.44
1:A:217:SER:OG	22:A:4002:BCR:C14	2.66	0.44
20:A:1131:CLA:CHC	20:A:1132:CLA:C9	2.96	0.44
20:A:1013:CLA:H91	20:A:1013:CLA:H112	1.55	0.44
20:B:1222:CLA:H142	22:F:4016:BCR:H341	2.00	0.44
20:B:1231:CLA:H42	20:B:1232:CLA:HBA1	2.00	0.44
12:L:166:LEU:HD12	12:L:166:LEU:HA	1.64	0.44
20:L:1502:CLA:HMB3	20:L:1502:CLA:CBB	2.47	0.44
13:1:85:ARG:O	20:1:601:CLA:HBC2	2.17	0.44
29:1:502:LUT:H11	29:1:502:LUT:H191	1.76	0.44
26:1:802:LMG:H291	26:1:802:LMG:C15	2.48	0.44
20:3:605:CLA:OBD	20:3:612:CLA:O1A	2.35	0.44
20:3:617:CLA:H2	20:3:617:CLA:CMA	2.16	0.44
16:4:203:LYS:HD3	20:4:602:CLA:HAA2	2.00	0.44
17:N:24:ILE:HD11	17:N:81:PRO:HB3	2.00	0.44
17:N:92:GLU:O	17:N:96:THR:N	2.44	0.44
20:A:1103:CLA:H2	20:A:1103:CLA:H62	1.74	0.44
20:B:1202:CLA:HBA1	20:B:1202:CLA:H3A	1.62	0.44
20:B:1203:CLA:H171	20:B:1225:CLA:HBB2	2.00	0.44
3:C:38:GLN:OE1	4:D:178:VAL:HB	2.17	0.44
6:F:94:ARG:NE	6:F:143:ASP:O	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:F:1301:CLA:HMB3	10:J:26:LEU:HD21	1.99	0.44
11:K:46:PHE:O	11:K:46:PHE:CD2	2.70	0.44
13:1:64:LEU:HD12	29:1:502:LUT:H21	2.00	0.44
15:3:78:PHE:HE2	29:3:502:LUT:H383	1.83	0.44
29:4:501:LUT:C19	20:4:602:CLA:CMC	2.95	0.44
17:N:47:CYS:HB2	17:N:76:THR:OG1	2.18	0.44
1:A:252:ARG:CD	20:A:1113:CLA:HED2	2.41	0.44
1:A:600:LEU:O	1:A:603:PHE:HB2	2.18	0.44
19:A:1011:CL0:CAC	2:B:625:TRP:HD1	2.26	0.44
20:A:1110:CLA:HED2	20:A:1111:CLA:CBC	2.48	0.44
2:B:460:ALA:HA	20:B:1234:CLA:O1A	2.18	0.44
2:B:597:LYS:HD3	20:B:1234:CLA:HBC2	1.98	0.44
20:B:1226:CLA:H92	28:B:5005:DGD:HB72	2.00	0.44
20:B:1207:CLA:H93	20:B:1207:CLA:H61	1.60	0.44
13:1:226:ILE:HG21	20:1:603:CLA:H42	2.00	0.44
20:1:614:CLA:CBB	16:4:142:PHE:HE2	2.30	0.44
14:2:162:TRP:HH2	22:2:503:BCR:C31	2.31	0.44
14:2:164:GLU:HB3	20:2:612:CLA:C1B	2.47	0.44
14:2:196:PRO:HB3	30:2:611:CHL:HBC2	2.00	0.44
29:2:501:LUT:H383	20:2:603:CLA:C2B	2.48	0.44
20:2:604:CLA:H61	20:2:604:CLA:H92	1.69	0.44
30:2:610:CHL:HAA2	30:2:610:CHL:CBD	2.48	0.44
1:A:403:GLY:O	1:A:407:ILE:HG13	2.18	0.44
20:A:1108:CLA:H11	20:A:1110:CLA:H43	2.00	0.44
20:A:1119:CLA:H122	22:A:4007:BCR:C10	2.45	0.44
26:B:5003:LMG:H201	22:F:4016:BCR:H17C	2.00	0.44
20:B:1218:CLA:H61	20:B:1218:CLA:H41	1.77	0.44
14:2:234:GLY:HA2	20:2:603:CLA:C3C	2.47	0.44
23:2:801:LHG:HC42	22:3:503:BCR:HC31	2.00	0.44
1:A:99:HIS:NE2	20:A:1105:CLA:NB	2.66	0.43
1:A:271:THR:HA	11:K:46:PHE:CZ	2.52	0.43
20:A:1119:CLA:H91	20:A:1119:CLA:H111	1.58	0.43
20:B:1230:CLA:H41	20:B:1230:CLA:H61	1.67	0.43
6:F:213:TRP:HZ3	22:F:4016:BCR:H381	1.83	0.43
12:L:110:LEU:HD12	12:L:138:VAL:CG2	2.48	0.43
20:L:1502:CLA:H62	20:L:1502:CLA:H41	1.58	0.43
14:2:118:ALA:O	14:2:122:ILE:HG13	2.17	0.43
15:3:249:GLY:HA3	15:3:274:PHE:HZ	1.83	0.43
16:4:244:THR:CB	20:4:608:CLA:HED3	2.41	0.43
1:A:57:LEU:HD11	20:A:1101:CLA:HBC2	2.00	0.43
1:A:511:THR:HG22	20:A:1116:CLA:O1A	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:591:GLN:HG2	1:A:731:ARG:CZ	2.48	0.43
19:A:1011:CL0:H22	2:B:625:TRP:CD1	2.53	0.43
20:A:1117:CLA:H192	20:A:1125:CLA:H11	2.00	0.43
20:A:1119:CLA:H2	20:A:1123:CLA:HBB1	1.99	0.43
2:B:224:PRO:HB3	2:B:229:GLN:O	2.17	0.43
20:B:1211:CLA:HMA3	22:B:4006:BCR:H271	1.99	0.43
20:B:1227:CLA:H41	20:B:1227:CLA:H61	1.80	0.43
6:F:215:ILE:HG12	20:4:605:CLA:H51	2.01	0.43
28:G:5003:DGD:HA61	28:G:5003:DGD:HA32	1.75	0.43
12:L:78:LEU:C	12:L:78:LEU:HD23	2.44	0.43
12:L:204:LEU:HD11	20:L:1503:CLA:HED1	1.99	0.43
13:1:97:PRO:HB3	20:1:606:CLA:C2D	2.48	0.43
14:2:81:LEU:HD13	14:2:103:VAL:HG22	2.00	0.43
22:2:503:BCR:H333	20:4:607:CLA:CHC	2.48	0.43
29:3:501:LUT:H15	29:3:501:LUT:H201	1.83	0.43
16:4:129:ALA:O	16:4:134:TYR:OH	2.32	0.43
1:A:86:LEU:HD23	1:A:86:LEU:HA	1.84	0.43
20:A:1102:CLA:HBB1	20:A:1109:CLA:C12	2.48	0.43
20:A:1113:CLA:H3A	20:A:1113:CLA:HBA2	1.50	0.43
20:A:1128:CLA:H92	20:A:1128:CLA:H61	1.66	0.43
2:B:390:GLY:HA2	22:B:4010:BCR:H393	2.00	0.43
20:B:1201:CLA:H3A	20:B:1201:CLA:HBA2	1.57	0.43
20:B:1232:CLA:HBA1	20:B:1232:CLA:H3A	1.95	0.43
3:C:65:VAL:O	3:C:65:VAL:HG13	2.18	0.43
4:D:131:LYS:NZ	8:H:63:THR:O	2.49	0.43
4:D:206:LYS:HE2	4:D:206:LYS:HB3	1.85	0.43
7:G:76:ARG:HH21	7:G:119:ASP:CG	2.26	0.43
20:G:1603:CLA:H112	20:G:1603:CLA:H142	1.63	0.43
8:H:122:ILE:HD12	12:L:125:ILE:HD12	2.00	0.43
12:L:57:VAL:HG22	12:L:71:THR:HG22	1.99	0.43
13:1:222:TRP:CE3	20:1:608:CLA:HMA3	2.51	0.43
29:1:502:LUT:H383	20:1:606:CLA:C1B	2.48	0.43
30:1:610:CHL:C2C	20:1:613:CLA:HMC3	2.48	0.43
20:1:611:CLA:H152	20:1:611:CLA:H111	1.68	0.43
15:3:67:TYR:HB2	15:3:86:PRO:HD3	2.00	0.43
17:N:91:LYS:HD2	17:N:94:ASP:OD2	2.18	0.43
1:A:460:LEU:HD21	20:A:1132:CLA:HMB1	2.00	0.43
20:A:1124:CLA:HBA1	20:A:1125:CLA:HED2	2.00	0.43
6:F:114:ALA:HB3	6:F:115:PRO:CD	2.43	0.43
20:2:603:CLA:H111	20:2:603:CLA:H142	1.72	0.43
20:3:605:CLA:H61	20:3:605:CLA:H93	1.81	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:P:81:LYS:HA	18:P:95:GLN:HA	2.00	0.43
1:A:418:MET:HE1	1:A:436:LEU:HD11	1.99	0.43
1:A:630:ASP:OD2	1:A:631:GLN:N	2.51	0.43
20:A:1109:CLA:HBA2	20:A:1109:CLA:H3A	1.51	0.43
2:B:245:SER:O	2:B:245:SER:OG	2.31	0.43
12:L:95:PRO:HA	12:L:98:ARG:HD3	2.00	0.43
13:1:142:ILE:CD1	22:1:504:BCR:H363	2.46	0.43
29:1:502:LUT:C8	29:1:502:LUT:C18	2.97	0.43
16:4:58:PRO:HD2	20:4:609:CLA:CED	2.39	0.43
17:N:7:LEU:HD23	17:N:87:ILE:HB	2.01	0.43
1:A:570:PRO:CG	4:D:136:GLU:HG2	2.49	0.43
1:A:747:TRP:CG	22:A:4011:BCR:HC41	2.54	0.43
20:B:1214:CLA:H111	20:B:1214:CLA:H143	1.75	0.43
9:I:7:LEU:O	9:I:10:PRO:HD2	2.19	0.43
11:K:73:SER:OG	11:K:76:ARG:HD3	2.19	0.43
14:2:87:PHE:HB3	20:2:604:CLA:CAD	2.49	0.43
14:2:90:LEU:HD23	14:2:90:LEU:HA	1.84	0.43
14:2:168:TRP:HB3	32:2:807:3PH:H341	2.01	0.43
20:4:604:CLA:C3A	20:4:604:CLA:CGA	2.96	0.43
20:4:605:CLA:H12	20:4:605:CLA:O1D	2.18	0.43
18:P:65:ALA:CB	18:P:66:PRO:HD2	2.21	0.43
18:P:98:VAL:O	18:P:98:VAL:HG12	2.18	0.43
1:A:41:SER:CB	1:A:44:ILE:CG1	2.85	0.43
1:A:85:GLN:HG2	20:A:1103:CLA:H3A	2.00	0.43
1:A:312:ILE:HD12	1:A:312:ILE:C	2.43	0.43
1:A:666:GLN:HE22	18:P:86:PRO:CB	2.23	0.43
2:B:257:LEU:HD13	20:B:1214:CLA:HMB1	2.01	0.43
20:B:1222:CLA:H91	20:B:1222:CLA:H112	1.80	0.43
20:B:1240:CLA:H41	20:B:1240:CLA:H62	1.57	0.43
20:F:1302:CLA:H3A	20:F:1302:CLA:HBA1	1.75	0.43
26:G:5002:LMG:O9	13:1:131:LEU:HD23	2.18	0.43
13:1:85:ARG:HD3	20:1:611:CLA:OBD	2.17	0.43
14:2:204:LEU:CD2	29:2:501:LUT:H22	2.36	0.43
20:2:604:CLA:CMB	20:2:604:CLA:CBB	2.94	0.43
15:3:232:ARG:HA	15:3:235:MET:HE3	2.01	0.43
20:3:603:CLA:H41	20:3:603:CLA:H62	1.69	0.43
20:3:610:CLA:H2	20:3:610:CLA:H61	1.73	0.43
29:4:501:LUT:C30	20:4:601:CLA:H101	2.48	0.43
20:4:612:CLA:H61	20:4:612:CLA:H101	1.36	0.43
17:N:63:PHE:O	17:N:63:PHE:CG	2.71	0.43
1:A:104:SER:OG	1:A:105:ASN:N	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:309:LEU:CD2	20:A:1119:CLA:HMC3	2.49	0.43
20:A:1120:CLA:HAB	20:A:1141:CLA:CBB	2.48	0.43
2:B:196:HIS:CG	20:B:1211:CLA:CBC	3.02	0.43
2:B:378:ILE:HD13	20:B:1225:CLA:HAB	2.01	0.43
20:B:1203:CLA:H111	20:B:1203:CLA:H71	1.65	0.43
20:B:1229:CLA:HBC3	6:F:164:GLY:CA	2.48	0.43
8:H:122:ILE:HD13	8:H:122:ILE:N	2.33	0.43
9:I:9:VAL:CG1	9:I:10:PRO:HD3	2.48	0.43
26:1:802:LMG:H291	26:1:802:LMG:C13	2.49	0.43
14:2:147:THR:HG23	14:2:152:LEU:HG	2.00	0.43
30:2:610:CHL:OMC	30:2:613:CHL:CBB	2.66	0.43
15:3:94:GLU:OE2	15:3:96:ARG:HB2	2.19	0.43
20:4:601:CLA:CGA	20:4:601:CLA:C4A	2.96	0.43
1:A:55:TRP:CG	1:A:729:GLN:HE22	2.36	0.43
1:A:483:GLN:HB3	1:A:485:GLN:HE21	1.83	0.43
19:A:1011:CL0:H61	19:A:1011:CL0:H53	1.72	0.43
20:A:1113:CLA:C4B	22:K:4001:BCR:HC21	2.48	0.43
20:A:1125:CLA:C3B	20:A:1133:CLA:HMA2	2.49	0.43
20:L:1502:CLA:HMA1	22:L:4020:BCR:H373	1.99	0.43
14:2:162:TRP:CD1	14:2:162:TRP:C	2.97	0.43
14:2:204:LEU:HD23	14:2:206:TRP:CD1	2.54	0.43
15:3:192:LYS:H	15:3:192:LYS:HG3	1.69	0.43
16:4:104:LEU:HD12	20:4:601:CLA:HMC2	2.01	0.43
17:N:58:GLN:HB3	17:N:69:ILE:HD12	2.01	0.43
1:A:395:LEU:HD11	20:A:1127:CLA:HED3	2.01	0.43
1:A:658:TRP:HD1	20:B:1021:CLA:HAC2	1.84	0.43
20:A:1115:CLA:H161	20:A:1115:CLA:H143	1.75	0.43
20:B:1203:CLA:H43	28:B:5005:DGD:HB61	2.00	0.43
20:B:1225:CLA:HBA2	20:B:1225:CLA:H3A	1.30	0.43
29:1:502:LUT:H27	29:1:502:LUT:H381	1.81	0.43
14:2:167:ARG:HH22	20:2:612:CLA:CGD	2.32	0.43
31:2:502:XAT:H35	31:2:502:XAT:H401	1.91	0.43
20:2:606:CLA:CMB	20:2:606:CLA:HBB1	2.49	0.43
15:3:67:TYR:CD2	15:3:68:LEU:HG	2.53	0.43
15:3:222:GLU:O	15:3:226:LYS:HG3	2.19	0.43
16:4:168:GLN:HA	16:4:176:SER:HA	2.01	0.43
20:4:601:CLA:HMB1	20:4:601:CLA:CBB	2.49	0.43
1:A:41:SER:OG	1:A:44:ILE:HG13	2.17	0.42
1:A:419:VAL:HG11	1:A:577:PHE:N	2.33	0.42
20:A:1112:CLA:H112	20:A:1112:CLA:H71	1.64	0.42
20:A:1119:CLA:H2	20:A:1119:CLA:H62	1.74	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:A:1138:CLA:CED	2:B:424:TRP:HB2	2.46	0.42
2:B:256:THR:OG1	2:B:257:LEU:N	2.52	0.42
2:B:640:MET:HE2	2:B:640:MET:HB2	1.94	0.42
20:B:1214:CLA:H62	20:B:1214:CLA:H101	1.66	0.42
3:C:22:PRO:HB2	4:D:136:GLU:HG3	2.01	0.42
20:K:1401:CLA:CMB	20:K:1401:CLA:CBB	2.94	0.42
14:2:82:PRO:O	14:2:222:ILE:HG21	2.18	0.42
22:2:503:BCR:HC42	20:4:607:CLA:C3B	2.49	0.42
20:4:607:CLA:CHD	23:4:801:LHG:HC62	2.49	0.42
18:P:30:LYS:HA	18:P:69:THR:HG22	2.01	0.42
1:A:86:LEU:CD1	20:A:1111:CLA:HED1	2.49	0.42
1:A:271:THR:HG23	1:A:273:ASN:HB2	2.01	0.42
1:A:521:VAL:HG13	1:A:528:ALA:HB3	2.01	0.42
1:A:580:PRO:HB3	1:A:727:ILE:HB	2.00	0.42
20:A:1111:CLA:H41	20:A:1111:CLA:H61	1.59	0.42
2:B:352:MET:HE3	20:B:1215:CLA:HBA1	2.01	0.42
2:B:392:ILE:HG21	20:B:1226:CLA:HED1	2.02	0.42
20:B:1211:CLA:H161	22:B:4005:BCR:H363	2.01	0.42
20:B:1238:CLA:H193	20:B:1238:CLA:H161	1.76	0.42
28:J:5001:DGD:HAS1	28:J:5001:DGD:HAH2	1.57	0.42
12:L:109:LEU:CD1	20:L:1503:CLA:HBC3	2.49	0.42
13:1:225:THR:HG21	20:1:608:CLA:O2D	2.19	0.42
14:2:122:ILE:HG13	14:2:123:PRO:HD3	2.01	0.42
14:2:144:GLU:H	14:2:144:GLU:CD	2.27	0.42
14:2:158:VAL:HG13	14:2:159:PHE:N	2.34	0.42
30:2:615:CHL:HHC	30:2:615:CHL:CBB	2.44	0.42
15:3:243:ILE:HD11	20:3:603:CLA:C4C	2.49	0.42
16:4:236:HIS:ND1	20:4:603:CLA:HAA2	2.32	0.42
30:4:613:CHL:HHC	30:4:613:CHL:CBB	2.46	0.42
1:A:55:TRP:HZ2	20:A:1139:CLA:HBB1	1.85	0.42
20:A:1106:CLA:H61	22:J:4012:BCR:H372	2.01	0.42
20:A:1013:CLA:H3A	20:A:1013:CLA:CGA	2.49	0.42
20:B:1202:CLA:H61	20:B:1202:CLA:H2	1.63	0.42
20:B:1229:CLA:H191	20:B:1235:CLA:H111	2.01	0.42
20:B:1218:CLA:H91	20:B:1218:CLA:H111	1.76	0.42
4:D:78:ASN:N	8:H:53:VAL:HG21	2.34	0.42
20:F:1301:CLA:C3B	10:J:22:LEU:HD21	2.49	0.42
9:I:31:ARG:HB2	9:I:31:ARG:HH11	1.84	0.42
20:L:1502:CLA:H62	20:L:1502:CLA:H93	1.72	0.42
16:4:173:LYS:HD2	16:4:173:LYS:HA	1.83	0.42
16:4:185:PRO:O	16:4:189:PHE:HB2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:P:23:ALA:O	18:P:25:GLU:N	2.52	0.42
20:A:1110:CLA:C4C	20:A:1110:CLA:H42	2.50	0.42
20:A:1130:CLA:HBA2	20:A:1130:CLA:H3A	1.52	0.42
2:B:29:HIS:HB2	20:B:1226:CLA:O1A	2.19	0.42
2:B:92:TRP:N	20:B:1206:CLA:O1D	2.50	0.42
2:B:286:ILE:O	20:B:1218:CLA:HBC1	2.19	0.42
31:2:502:XAT:H173	20:2:606:CLA:C1B	2.47	0.42
26:2:802:LMG:HO4	26:2:802:LMG:HO5	1.65	0.42
24:2:808:LMT:H111	24:2:808:LMT:H82	1.92	0.42
20:3:612:CLA:HBC2	20:3:613:CLA:HMB1	2.02	0.42
16:4:77:ASP:OD1	20:4:604:CLA:HBA2	2.19	0.42
16:4:94:ALA:HB2	20:4:612:CLA:HED2	2.01	0.42
16:4:242:HIS:C	16:4:247:GLN:HE21	2.26	0.42
20:4:602:CLA:HBC3	20:4:607:CLA:C9	2.49	0.42
1:A:123:VAL:HA	20:A:1107:CLA:HED3	2.02	0.42
1:A:195:TRP:CZ2	20:A:1111:CLA:HBC3	2.54	0.42
1:A:449:VAL:HG21	20:A:1137:CLA:HMC3	2.01	0.42
20:A:1126:CLA:H171	22:J:4012:BCR:H14C	2.01	0.42
2:B:557:PHE:O	2:B:571:SER:OG	2.36	0.42
20:B:1222:CLA:H92	20:B:1222:CLA:H61	1.83	0.42
20:B:1222:CLA:HBA2	20:B:1222:CLA:H3A	1.52	0.42
23:B:5002:LHG:H141	23:B:5002:LHG:H172	1.67	0.42
20:B:1207:CLA:H18	20:B:1207:CLA:H151	1.55	0.42
9:I:9:VAL:HG12	9:I:10:PRO:HD3	2.01	0.42
11:K:74:ALA:O	11:K:89:SER:OG	2.38	0.42
14:2:64:ARG:NH2	14:2:77:LEU:O	2.52	0.42
14:2:162:TRP:CE3	20:4:609:CLA:HBD	2.55	0.42
20:3:606:CLA:HMA3	20:3:613:CLA:C3C	2.50	0.42
16:4:134:TYR:CZ	30:4:613:CHL:HAC1	2.54	0.42
16:4:153:GLU:OE2	16:4:156:ARG:NH2	2.44	0.42
16:4:228:GLY:N	16:4:231:ASP:OD2	2.52	0.42
1:A:329:ASP:OD2	1:A:329:ASP:N	2.51	0.42
1:A:511:THR:CG2	20:A:1116:CLA:H2	2.49	0.42
20:A:1125:CLA:H91	20:A:1125:CLA:H111	1.81	0.42
22:A:4011:BCR:H24C	20:B:1230:CLA:HMC1	2.01	0.42
26:A:5006:LMG:H211	26:A:5006:LMG:H171	2.02	0.42
2:B:142:LEU:HA	2:B:142:LEU:HD23	1.80	0.42
2:B:177:HIS:CG	20:B:1210:CLA:HMC2	2.54	0.42
2:B:692:ARG:HE	4:D:93:ARG:NE	2.17	0.42
3:C:31:TRP:HE3	3:C:34:CYS:HG	1.67	0.42
3:C:61:ASP:HA	3:C:62:PHE:HA	1.81	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:132:LEU:HD12	4:D:138:CYS:SG	2.59	0.42
6:F:182:LEU:HD23	6:F:182:LEU:HA	1.88	0.42
6:F:200:VAL:O	6:F:204:THR:HG22	2.19	0.42
20:F:1301:CLA:H171	20:F:1301:CLA:H13	1.83	0.42
7:G:153:LYS:C	26:G:5006:LMG:O10	2.63	0.42
20:G:1603:CLA:H141	30:1:610:CHL:HMC	2.01	0.42
8:H:72:SER:OG	12:L:84:SER:O	2.33	0.42
8:H:99:LEU:O	8:H:103:LEU:HB2	2.20	0.42
13:1:89:LEU:HD12	13:1:89:LEU:HA	1.85	0.42
14:2:189:THR:HG1	14:2:198:GLY:H	1.59	0.42
30:2:609:CHL:CBB	30:2:609:CHL:HHC	2.44	0.42
22:3:503:BCR:H311	22:3:503:BCR:HC8	2.00	0.42
20:3:610:CLA:H3A	20:3:610:CLA:HBA2	1.38	0.42
16:4:240:PRO:HG2	20:4:608:CLA:HMB3	2.00	0.42
31:4:502:XAT:H183	20:4:606:CLA:C2B	2.50	0.42
20:4:605:CLA:H91	20:4:605:CLA:H111	1.85	0.42
20:4:605:CLA:HMD1	20:4:612:CLA:C4C	2.50	0.42
1:A:100:GLY:HA3	1:A:153:TRP:CH2	2.55	0.42
1:A:188:LYS:HD2	1:A:188:LYS:HA	1.85	0.42
1:A:232:PHE:CD1	1:A:258:LEU:HD11	2.54	0.42
1:A:473:PRO:CA	1:A:476:MET:HE2	2.50	0.42
2:B:160:LYS:HG3	2:B:161:TRP:CZ3	2.55	0.42
3:C:52:LYS:N	25:C:3002:SF4:S1	2.77	0.42
28:1:803:DGD:HA52	28:1:803:DGD:HA21	1.77	0.42
29:2:501:LUT:H401	29:2:501:LUT:H35	1.82	0.42
22:3:506:BCR:H351	22:3:506:BCR:H15C	1.63	0.42
28:3:803:DGD:O5E	28:3:803:DGD:O4E	2.33	0.42
20:4:612:CLA:H92	28:4:802:DGD:CCB	2.50	0.42
1:A:727:ILE:HD13	2:B:568:CYS:SG	2.59	0.42
20:A:1117:CLA:CAD	20:A:1127:CLA:H41	2.50	0.42
20:A:1132:CLA:H141	20:A:1132:CLA:H161	1.56	0.42
20:A:1133:CLA:H51	20:A:1133:CLA:H11	1.92	0.42
20:A:1136:CLA:H71	20:A:1136:CLA:H112	1.63	0.42
20:B:1230:CLA:H91	20:F:1301:CLA:HMA2	2.01	0.42
4:D:174:TYR:CB	4:D:176:GLU:OE2	2.64	0.42
13:1:134:ILE:HD12	20:1:613:CLA:C3D	2.50	0.42
14:2:151:THR:O	14:2:155:VAL:HG23	2.19	0.42
14:2:162:TRP:HH2	22:2:503:BCR:C32	2.31	0.42
20:3:605:CLA:H11	20:3:605:CLA:HED3	2.02	0.42
16:4:150:HIS:ND1	16:4:154:ILE:CD1	2.83	0.42
17:N:5:VAL:HG21	17:N:24:ILE:HG12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:N:58:GLN:CA	17:N:58:GLN:NE2	2.73	0.42
18:P:12:LEU:HD13	18:P:87:HIS:CD2	2.55	0.42
18:P:41:PHE:CD2	18:P:55:ILE:HD12	2.55	0.42
1:A:155:ALA:HB1	20:A:1117:CLA:HED2	2.02	0.42
20:A:1103:CLA:H161	20:A:1103:CLA:H143	1.72	0.42
20:A:1131:CLA:H93	20:A:1131:CLA:H61	1.72	0.42
2:B:444:LEU:HD11	2:B:452:GLN:OE1	2.20	0.42
2:B:514:PRO:HG2	6:F:147:HIS:ND1	2.34	0.42
20:B:1210:CLA:H141	20:B:1210:CLA:H162	1.59	0.42
20:B:1220:CLA:HMA2	20:B:1240:CLA:HED2	2.02	0.42
11:K:115:GLY:O	11:K:118:VAL:HG23	2.20	0.42
13:1:61:PHE:HE2	29:1:502:LUT:H183	1.84	0.42
14:2:81:LEU:HD11	14:2:99:LEU:HD11	2.00	0.42
15:3:161:GLU:HG3	20:3:613:CLA:CHB	2.50	0.42
17:N:16:PHE:CZ	17:N:24:ILE:HG23	2.43	0.42
1:A:92:TRP:CD1	20:A:1104:CLA:HBC1	2.55	0.42
1:A:371:ILE:HG21	20:A:1117:CLA:C19	2.50	0.42
20:A:1134:CLA:H92	20:A:1134:CLA:H61	1.71	0.42
2:B:410:ARG:HH22	26:B:5003:LMG:HC61	1.85	0.42
2:B:422:LEU:HD13	2:B:532:LEU:HA	2.02	0.42
20:B:1225:CLA:H61	20:B:1225:CLA:H41	1.80	0.42
20:B:1218:CLA:H121	13:1:139:PHE:HE1	1.85	0.42
20:G:1601:CLA:H41	20:G:1601:CLA:H61	1.36	0.42
12:L:113:PRO:HB3	20:L:1503:CLA:CBB	2.50	0.42
20:1:604:CLA:H2A	20:1:604:CLA:HED2	2.02	0.42
15:3:217:GLU:CD	15:3:217:GLU:N	2.77	0.42
1:A:34:TRP:NE1	20:A:1109:CLA:HBA2	2.35	0.41
1:A:158:ILE:HA	20:A:1112:CLA:CED	2.43	0.41
1:A:518:GLY:C	1:A:519:ASP:OD2	2.63	0.41
1:A:663:GLN:HG3	1:A:753:ARG:HD2	2.02	0.41
20:A:1103:CLA:H91	20:A:1103:CLA:H112	1.80	0.41
2:B:547:MET:HE2	2:B:570:ILE:HD13	2.02	0.41
3:C:58:CYS:HB3	3:C:63:LEU:CD2	2.50	0.41
4:D:134:ARG:HB2	4:D:137:GLN:CG	2.50	0.41
5:E:69:LYS:H	5:E:69:LYS:HG3	1.58	0.41
6:F:152:GLY:O	20:F:1302:CLA:HBD	2.20	0.41
6:F:159:GLU:HG2	10:J:38:THR:CG2	2.50	0.41
22:F:4014:BCR:H15C	22:F:4014:BCR:H351	1.92	0.41
8:H:68:ASP:OD2	8:H:71:GLY:N	2.51	0.41
11:K:77:LYS:O	11:K:84:LEU:CD2	2.68	0.41
12:L:110:LEU:HD12	12:L:138:VAL:HG23	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:2:250:LEU:HD13	20:2:608:CLA:HBC3	2.02	0.41
31:4:502:XAT:H35	31:4:502:XAT:H401	1.85	0.41
20:4:607:CLA:C4C	23:4:801:LHG:HC62	2.50	0.41
1:A:446:LEU:HD21	1:A:553:VAL:HG12	2.00	0.41
1:A:675:TYR:HB3	1:A:752:ALA:HB2	2.01	0.41
20:A:1127:CLA:H111	20:A:1127:CLA:H91	1.68	0.41
2:B:347:LEU:HD13	20:B:1223:CLA:HAA2	2.01	0.41
2:B:494:LEU:HD23	2:B:494:LEU:HA	1.77	0.41
20:B:1237:CLA:H141	20:B:1237:CLA:H161	1.77	0.41
5:E:74:VAL:HG12	5:E:127:GLU:HA	2.02	0.41
20:F:1301:CLA:H51	20:F:1301:CLA:H11	1.89	0.41
8:H:132:PRO:HA	8:H:133:PRO:HD3	1.93	0.41
11:K:113:ILE:HD11	22:K:4002:BCR:H333	2.01	0.41
12:L:144:CYS:HB3	22:L:4019:BCR:C20	2.50	0.41
13:1:168:LEU:HD23	13:1:170:TYR:CE2	2.54	0.41
29:1:501:LUT:H32	20:1:601:CLA:CAB	2.49	0.41
14:2:229:MET:O	14:2:232:VAL:HG23	2.20	0.41
15:3:267:ASN:OD1	20:3:603:CLA:HMD2	2.20	0.41
20:3:612:CLA:CBB	20:3:612:CLA:CMB	2.95	0.41
16:4:57:LEU:HD12	16:4:57:LEU:HA	1.85	0.41
18:P:14:PHE:CZ	18:P:92:MET:CE	2.96	0.41
1:A:86:LEU:CG	20:A:1111:CLA:HED1	2.49	0.41
20:A:1106:CLA:H61	20:A:1106:CLA:H101	1.82	0.41
20:A:1133:CLA:HMD1	20:A:1134:CLA:HAB	2.02	0.41
2:B:284:PHE:CE1	20:B:1216:CLA:HAB	2.55	0.41
20:B:1021:CLA:H3A	20:B:1021:CLA:HBA2	1.61	0.41
20:B:1021:CLA:O2D	20:B:1021:CLA:HAA2	2.20	0.41
20:B:1211:CLA:H141	20:B:1211:CLA:H162	1.72	0.41
29:J:4013:LUT:H35	29:J:4013:LUT:H401	1.84	0.41
12:L:199:TRP:HB2	22:L:4020:BCR:C33	2.50	0.41
14:2:204:LEU:HD13	29:2:501:LUT:C2	2.49	0.41
1:A:234:ASN:HB3	1:A:290:LEU:HD23	2.02	0.41
1:A:545:HIS:CE1	1:A:611:VAL:HG12	2.55	0.41
1:A:567:ARG:NH2	4:D:89:GLY:HA2	2.36	0.41
20:A:1111:CLA:HMA3	20:A:1111:CLA:H42	2.03	0.41
20:A:1125:CLA:H61	20:A:1125:CLA:H92	1.59	0.41
2:B:80:ASP:O	2:B:84:VAL:HG12	2.20	0.41
20:B:1237:CLA:CMB	20:B:1237:CLA:CBB	2.96	0.41
20:B:1202:CLA:H202	20:B:1202:CLA:H161	1.85	0.41
8:H:119:SER:O	8:H:122:ILE:HG12	2.20	0.41
22:I:4018:BCR:H341	22:I:4020:BCR:H323	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:3:243:ILE:HG12	20:3:603:CLA:HAC2	2.03	0.41
15:3:268:VAL:O	15:3:271:SER:CA	2.66	0.41
20:4:609:CLA:NC	23:4:801:LHG:HC82	2.35	0.41
20:4:605:CLA:H41	20:4:605:CLA:H62	1.79	0.41
17:N:25:LEU:HD23	17:N:77:CYS:CA	2.50	0.41
1:A:216:LEU:HB2	1:A:307:ALA:HB1	2.01	0.41
1:A:398:HIS:CE1	20:A:1127:CLA:C2B	3.03	0.41
1:A:462:ILE:CB	20:A:1132:CLA:HMC2	2.50	0.41
1:A:516:GLY:HA2	1:A:531:PRO:HB3	2.01	0.41
20:A:1012:CLA:CMA	2:B:616:LEU:HD13	2.50	0.41
2:B:241:ASN:OD1	2:B:241:ASN:N	2.53	0.41
2:B:453:ILE:HG21	28:J:5001:DGD:HA82	2.03	0.41
2:B:477:LEU:HD21	20:B:1232:CLA:HBC2	2.03	0.41
26:B:5003:LMG:H202	22:F:4016:BCR:H17C	2.02	0.41
4:D:101:TYR:CZ	4:D:135:LYS:HB2	2.55	0.41
11:K:75:ASN:HB2	11:K:76:ARG:HH11	1.85	0.41
14:2:109:HIS:HE1	20:2:605:CLA:HAA2	1.85	0.41
20:2:612:CLA:HBA1	20:2:612:CLA:H3A	1.84	0.41
15:3:111:LEU:HD23	15:3:111:LEU:HA	1.77	0.41
15:3:227:GLU:HB2	20:3:601:CLA:CHB	2.50	0.41
1:A:320:ASN:HB2	1:A:321:TRP:CZ3	2.56	0.41
20:A:1102:CLA:H52	20:A:1102:CLA:H11	1.88	0.41
20:A:1106:CLA:CHC	20:A:1107:CLA:HMD2	2.50	0.41
2:B:196:HIS:CG	20:B:1211:CLA:HBC3	2.56	0.41
20:B:1207:CLA:C4	12:L:133:ALA:HB2	2.51	0.41
10:J:34:PRO:O	28:J:5001:DGD:O2D	2.34	0.41
11:K:55:MET:HG2	20:K:1401:CLA:C3D	2.50	0.41
29:1:501:LUT:H23	20:1:611:CLA:H41	2.02	0.41
30:2:611:CHL:OMC	30:2:611:CHL:HAC1	2.21	0.41
16:4:114:VAL:HG12	16:4:230:PHE:CG	2.56	0.41
29:4:501:LUT:H191	29:4:501:LUT:H11	1.91	0.41
20:4:617:CLA:H161	20:4:617:CLA:H141	1.54	0.41
1:A:93:LEU:CD1	20:A:1103:CLA:H112	2.51	0.41
20:A:1101:CLA:H102	20:A:1101:CLA:H51	2.03	0.41
2:B:384:THR:HG21	2:B:580:VAL:HG22	2.03	0.41
2:B:477:LEU:CD2	20:B:1232:CLA:C2C	2.98	0.41
2:B:595:HIS:CD2	2:B:725:LEU:CD1	3.04	0.41
20:1:601:CLA:H3A	20:1:601:CLA:CGA	2.50	0.41
20:1:605:CLA:H111	20:1:605:CLA:H93	1.69	0.41
15:3:67:TYR:CB	15:3:86:PRO:HD3	2.50	0.41
16:4:149:PHE:HA	16:4:152:VAL:HG22	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:4:230:PHE:O	16:4:234:LEU:HG	2.19	0.41
1:A:302:HIS:CE1	20:A:1117:CLA:C1B	3.04	0.41
1:A:449:VAL:HG21	20:A:1137:CLA:CMC	2.51	0.41
2:B:439:HIS:HB2	20:B:1230:CLA:CHC	2.51	0.41
2:B:597:LYS:HD3	20:B:1234:CLA:CBC	2.51	0.41
4:D:159:PHE:HD2	4:D:163:GLU:OE2	2.03	0.41
26:F:5001:LMG:O5	10:J:2:ARG:O	2.37	0.41
7:G:61:SER:CB	20:G:1601:CLA:OBD	2.69	0.41
20:H:1701:CLA:HBC2	20:H:1701:CLA:HMC1	2.03	0.41
11:K:109:VAL:HG11	22:K:4001:BCR:C18	2.50	0.41
20:L:1502:CLA:CMB	20:L:1502:CLA:CBB	2.99	0.41
29:1:502:LUT:H35	29:1:502:LUT:H401	1.81	0.41
20:2:605:CLA:HBC1	30:2:610:CHL:CBB	2.49	0.41
16:4:103:MET:SD	20:4:601:CLA:CAB	2.94	0.41
18:P:58:PRO:C	18:P:59:GLU:O	2.64	0.41
1:A:41:SER:CB	1:A:44:ILE:CD1	2.98	0.41
1:A:202:MET:HE1	20:A:1123:CLA:H121	2.03	0.41
1:A:397:THR:HG22	20:A:1126:CLA:CAB	2.51	0.41
1:A:446:LEU:HG	1:A:554:LEU:HB2	2.02	0.41
20:A:1116:CLA:H62	20:A:1116:CLA:H41	1.40	0.41
20:A:1133:CLA:CMD	20:A:1134:CLA:HAB	2.50	0.41
20:A:1012:CLA:HMB3	20:B:1021:CLA:H201	2.02	0.41
20:A:1013:CLA:H202	20:A:1013:CLA:H161	1.60	0.41
2:B:182:LEU:HD13	20:B:1210:CLA:HHB	2.02	0.41
2:B:371:LEU:HD23	2:B:371:LEU:HA	1.84	0.41
2:B:459:PHE:CE2	20:F:1302:CLA:HBB1	2.56	0.41
20:B:1203:CLA:HED3	20:B:1226:CLA:H51	2.02	0.41
20:B:1206:CLA:H112	20:B:1206:CLA:H151	1.64	0.41
20:B:1226:CLA:H143	20:B:1226:CLA:H111	1.84	0.41
20:B:1232:CLA:H41	20:B:1232:CLA:H62	1.33	0.41
20:B:1234:CLA:H92	26:F:5002:LMG:H401	2.02	0.41
28:B:5005:DGD:HAE2	28:B:5005:DGD:HA82	1.84	0.41
6:F:133:TYR:CZ	10:J:37:LEU:HD12	2.56	0.41
6:F:213:TRP:CG	6:F:214:PRO:HD3	2.56	0.41
26:F:5003:LMG:O9	26:F:5003:LMG:HC91	2.14	0.41
20:G:1603:CLA:H71	20:G:1603:CLA:H111	1.83	0.41
20:G:1603:CLA:HBC1	13:1:112:ALA:O	2.21	0.41
9:I:24:LEU:HB3	22:L:4019:BCR:H333	2.02	0.41
29:J:4013:LUT:H191	29:J:4013:LUT:H11	1.71	0.41
13:1:133:THR:HG23	13:1:134:ILE:H	1.81	0.41
13:1:154:ASP:OD2	13:1:157:LYS:HG3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:1:154:ASP:OD2	13:1:157:LYS:NZ	2.53	0.41
26:1:802:LMG:H152	26:1:802:LMG:C30	2.48	0.41
14:2:120:ILE:C	14:2:123:PRO:HD2	2.46	0.41
20:2:608:CLA:HED1	15:3:156:THR:HG22	2.03	0.41
15:3:120:GLU:HG3	15:3:253:TYR:HB3	2.03	0.41
16:4:169:ASP:HB3	16:4:172:PHE:O	2.20	0.41
16:4:215:PHE:CG	31:4:502:XAT:H12	2.56	0.41
29:4:501:LUT:H15	29:4:501:LUT:H201	1.82	0.41
17:N:73:PHE:CD1	17:N:95:LEU:CD2	2.88	0.41
17:N:77:CYS:SG	17:N:78:VAL:HG13	2.60	0.41
1:A:381:PRO:HB3	20:A:1117:CLA:HMA2	2.02	0.41
1:A:451:ILE:HD11	22:A:4017:BCR:H402	2.02	0.41
20:A:1101:CLA:O2D	20:A:1101:CLA:HBA2	2.21	0.41
20:A:1131:CLA:H122	20:B:1238:CLA:H51	2.03	0.41
2:B:276:HIS:CE1	20:B:1215:CLA:C1B	3.04	0.41
2:B:449:PRO:HB2	6:F:145:LEU:HD21	2.03	0.41
20:B:1216:CLA:H3A	20:B:1216:CLA:HBA1	1.76	0.41
7:G:115:LEU:HD23	7:G:115:LEU:HA	1.87	0.41
20:H:1701:CLA:HBC2	22:H:4021:BCR:H14C	2.02	0.41
11:K:110:VAL:O	11:K:114:ILE:HG22	2.21	0.41
12:L:125:ILE:H	12:L:125:ILE:HG12	1.73	0.41
20:L:1503:CLA:HBC2	20:L:1503:CLA:HMC3	2.03	0.41
13:1:186:LYS:HB3	20:1:607:CLA:HMD1	2.02	0.41
22:1:504:BCR:H23C	22:1:504:BCR:H392	2.03	0.41
14:2:126:LEU:O	14:2:131:ILE:HB	2.21	0.41
14:2:214:LEU:O	14:2:218:ARG:HG3	2.21	0.41
14:2:229:MET:CE	20:2:604:CLA:CHC	2.98	0.41
29:2:501:LUT:H41	20:2:601:CLA:O2A	2.20	0.41
15:3:62:LYS:HA	15:3:62:LYS:HD3	1.91	0.41
15:3:269:LEU:HD12	15:3:269:LEU:O	2.21	0.41
17:N:73:PHE:CD1	17:N:95:LEU:HB2	2.56	0.41
18:P:4:LEU:HB2	18:P:15:VAL:HB	2.03	0.41
1:A:103:PHE:CZ	20:A:1105:CLA:CAD	3.03	0.40
1:A:492:ILE:CD1	20:A:1135:CLA:H2	2.50	0.40
20:A:1103:CLA:H202	20:A:1103:CLA:H162	1.90	0.40
2:B:10:GLN:N	2:B:35:ASP:OD2	2.52	0.40
2:B:66:PHE:CZ	20:B:1204:CLA:HBC3	2.56	0.40
2:B:162:LYS:HA	2:B:163:PRO:HD3	1.92	0.40
2:B:477:LEU:HD23	20:B:1232:CLA:HBC2	2.04	0.40
2:B:498:LEU:HA	2:B:501:ILE:HG22	2.03	0.40
2:B:601:LEU:HA	2:B:606:VAL:HG12	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:701:SER:OG	2:B:702:ILE:N	2.54	0.40
20:1:605:CLA:H62	20:1:605:CLA:H41	1.36	0.40
20:2:605:CLA:H162	20:2:605:CLA:H193	1.66	0.40
30:2:609:CHL:HED1	15:3:171:ARG:HG2	2.01	0.40
15:3:107:ARG:NH1	30:3:611:CHL:OBD	2.50	0.40
20:4:601:CLA:H41	20:4:602:CLA:HMA2	2.03	0.40
1:A:358:LEU:HD22	20:A:1103:CLA:HBC3	2.02	0.40
1:A:511:THR:HG22	20:A:1116:CLA:C2	2.51	0.40
20:A:1140:CLA:H193	10:J:23:ALA:HB2	2.03	0.40
20:A:1139:CLA:H112	20:A:1139:CLA:H72	1.80	0.40
2:B:54:LEU:HD23	2:B:54:LEU:HA	1.87	0.40
2:B:583:MET:HE3	2:B:583:MET:HB3	1.86	0.40
20:B:1216:CLA:H111	20:B:1216:CLA:H91	1.68	0.40
3:C:38:GLN:OE1	4:D:178:VAL:CB	2.69	0.40
9:I:25:PHE:CD2	22:L:4019:BCR:H16C	2.56	0.40
22:K:4001:BCR:H351	22:K:4001:BCR:H15C	1.83	0.40
12:L:193:GLY:O	12:L:197:VAL:HG23	2.21	0.40
14:2:233:MET:HE3	14:2:237:PHE:HE1	1.87	0.40
16:4:204:GLU:HB2	20:4:601:CLA:CHB	2.51	0.40
18:P:97:THR:OG1	18:P:98:VAL:N	2.54	0.40
1:A:278:ALA:CA	20:A:1115:CLA:HMA2	2.52	0.40
20:A:1115:CLA:H112	20:A:1115:CLA:H142	1.74	0.40
2:B:68:VAL:O	2:B:72:GLY:HA3	2.21	0.40
2:B:192:GLY:HA3	20:B:1212:CLA:HAB	2.02	0.40
2:B:571:SER:HB2	2:B:574:ASP:CG	2.45	0.40
2:B:603:GLN:HE21	2:B:732:LYS:HD3	1.87	0.40
20:B:1237:CLA:HBC1	21:B:2002:PQN:H191	2.04	0.40
4:D:148:LYS:HB3	4:D:148:LYS:HE2	1.73	0.40
28:F:5005:DGD:HA52	32:2:807:3PH:C2B	2.50	0.40
22:G:4011:BCR:H351	22:G:4011:BCR:H15C	1.55	0.40
22:H:4021:BCR:H271	22:H:4021:BCR:H393	2.03	0.40
9:I:21:MET:SD	22:L:4019:BCR:H10C	2.60	0.40
10:J:38:THR:N	28:J:5001:DGD:HA21	2.37	0.40
11:K:58:SER:OG	11:K:114:ILE:HG23	2.21	0.40
22:L:4019:BCR:C8	22:L:4019:BCR:C33	2.85	0.40
30:1:609:CHL:C1C	23:1:801:LHG:H242	2.51	0.40
14:2:198:GLY:O	14:2:202:ASP:N	2.55	0.40
14:2:204:LEU:HB2	29:2:501:LUT:O3	2.21	0.40
20:3:601:CLA:HBA2	20:3:601:CLA:H3A	1.36	0.40
20:4:604:CLA:CMB	20:4:604:CLA:CBB	2.94	0.40
1:A:37:PRO:N	1:A:37:PRO:C	2.67	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:80:SER:OG	1:A:186:TYR:HB2	2.21	0.40
1:A:376:MET:HE2	1:A:376:MET:HB3	1.99	0.40
1:A:530:LEU:HD21	1:A:636:HIS:HE1	1.85	0.40
1:A:653:LEU:HD22	2:B:651:LEU:HD21	2.03	0.40
1:A:747:TRP:CZ3	22:A:4011:BCR:H332	2.56	0.40
19:A:1011:CL0:H8	19:A:1011:CL0:CGD	2.51	0.40
22:A:4017:BCR:HC41	2:B:648:TRP:HE3	1.85	0.40
2:B:457:PRO:C	20:B:1235:CLA:OBD	2.65	0.40
20:B:1021:CLA:H62	20:B:1021:CLA:H102	1.82	0.40
28:B:5005:DGD:HA81	28:B:5005:DGD:HA52	1.88	0.40
20:F:1301:CLA:CMB	10:J:26:LEU:HD21	2.52	0.40
7:G:84:ARG:O	7:G:87:VAL:HG12	2.22	0.40
7:G:123:PHE:CE1	7:G:128:VAL:HG12	2.57	0.40
12:L:61:ASN:N	12:L:70:GLU:OE1	2.48	0.40
13:1:111:TRP:CD1	13:1:111:TRP:C	2.99	0.40
20:4:605:CLA:OBD	20:4:612:CLA:H2	2.22	0.40
1:A:374:HIS:CD2	20:A:1124:CLA:CED	3.05	0.40
1:A:379:MET:HE3	1:A:379:MET:HB2	1.99	0.40
1:A:397:THR:HB	20:A:1126:CLA:HMB2	2.04	0.40
2:B:91:ILE:HB	2:B:112:PRO:HB2	2.03	0.40
2:B:619:TRP:CG	20:B:1021:CLA:H112	2.57	0.40
12:L:91:THR:HG22	12:L:174:ASP:HB2	2.04	0.40
20:1:601:CLA:H61	20:1:601:CLA:H41	1.39	0.40
20:1:605:CLA:HBA1	20:1:605:CLA:H3A	1.61	0.40
18:P:75:ASP:O	18:P:75:ASP:CG	2.65	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 244 ligands modelled in this entry, 3 are monoatomic - leaving 241 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
20	CLA	A	1111	-	69,73,73	1.41	6 (8%)	82,113,113	1.96	19 (23%)
20	CLA	A	1128	-	69,73,73	1.41	6 (8%)	82,113,113	1.93	19 (23%)
20	CLA	A	1132	-	69,73,73	1.35	6 (8%)	82,113,113	1.93	18 (21%)
22	BCR	G	4011	-	41,41,41	1.63	4 (9%)	56,56,56	4.71	17 (30%)
20	CLA	3	614	-	46,50,73	1.67	7 (15%)	53,85,113	2.16	13 (24%)
31	XAT	4	502	-	41,47,47	0.76	1 (2%)	54,74,74	2.09	14 (25%)
20	CLA	A	1103	-	69,73,73	1.39	6 (8%)	82,113,113	1.99	20 (24%)
20	CLA	A	1106	1	69,73,73	1.40	6 (8%)	82,113,113	1.91	20 (24%)
26	LMG	B	5003	-	35,35,55	0.79	1 (2%)	43,43,63	1.15	4 (9%)
30	CHL	1	610	13	41,55,74	1.80	9 (21%)	35,91,114	2.10	9 (25%)
22	BCR	F	4016	-	41,41,41	1.68	5 (12%)	56,56,56	4.46	16 (28%)
26	LMG	F	5006	-	13,13,55	0.55	0	18,18,63	0.77	0
20	CLA	4	617	-	69,73,73	1.34	6 (8%)	82,113,113	1.98	18 (21%)
28	DGD	3	803	-	52,52,67	0.93	3 (5%)	66,66,81	1.15	4 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	CLA	B	1220	-	59,63,73	1.51	6 (10%)	70,101,113	1.95	16 (22%)
20	CLA	1	602	13	50,54,73	1.61	6 (12%)	59,90,113	2.02	16 (27%)
30	CHL	4	610	-	41,55,74	1.90	9 (21%)	35,91,114	1.98	9 (25%)
20	CLA	K	1403	-	52,56,73	1.57	6 (11%)	61,92,113	2.13	17 (27%)
20	CLA	4	604	-	64,68,73	1.40	6 (9%)	76,107,113	1.98	19 (25%)
33	C7Z	4	505	-	43,43,43	3.91	17 (39%)	56,60,60	5.58	32 (57%)
22	BCR	3	506	-	41,41,41	1.69	4 (9%)	56,56,56	4.57	17 (30%)
20	CLA	1	604	-	69,73,73	1.38	6 (8%)	82,113,113	1.89	18 (21%)
26	LMG	B	5007	-	34,34,55	0.51	0	42,42,63	1.08	3 (7%)
29	LUT	4	501	-	42,43,43	2.48	4 (9%)	51,60,60	2.13	15 (29%)
20	CLA	A	1136	-	69,73,73	1.38	6 (8%)	82,113,113	1.84	17 (20%)
22	BCR	A	4002	-	41,41,41	1.66	5 (12%)	56,56,56	4.41	17 (30%)
20	CLA	A	1112	-	69,73,73	1.40	6 (8%)	82,113,113	1.87	17 (20%)
30	CHL	2	609	-	60,74,74	1.27	9 (15%)	58,114,114	1.63	11 (18%)
22	BCR	1	503	-	41,41,41	1.65	4 (9%)	56,56,56	4.36	14 (25%)
20	CLA	A	1129	-	69,73,73	1.39	6 (8%)	82,113,113	1.89	17 (20%)
26	LMG	F	5003	-	36,36,55	0.78	1 (2%)	44,44,63	1.10	4 (9%)
26	LMG	2	803	-	36,36,55	0.69	1 (2%)	44,44,63	1.07	3 (6%)
20	CLA	B	1207	-	69,73,73	1.35	6 (8%)	82,113,113	1.93	19 (23%)
20	CLA	3	612	-	54,58,73	1.52	6 (11%)	64,95,113	2.12	17 (26%)
30	CHL	4	613	-	55,69,74	1.37	9 (16%)	52,108,114	1.79	12 (23%)
20	CLA	1	606	-	54,58,73	1.57	6 (11%)	64,95,113	2.09	19 (29%)
30	CHL	4	615	-	37,51,74	1.45	8 (21%)	30,86,114	2.37	11 (36%)
20	CLA	A	1113	-	49,53,73	1.61	6 (12%)	58,89,113	2.04	14 (24%)
20	CLA	B	1229	-	69,73,73	1.39	6 (8%)	82,113,113	1.97	21 (25%)
26	LMG	2	802	-	25,25,55	0.54	0	33,33,63	1.16	3 (9%)
20	CLA	B	1228	-	64,68,73	1.43	6 (9%)	76,107,113	1.91	13 (17%)
20	CLA	B	1022	-	69,73,73	1.45	6 (8%)	82,113,113	1.88	20 (24%)
20	CLA	1	608	-	50,54,73	1.61	6 (12%)	59,90,113	2.14	16 (27%)
20	CLA	3	601	-	59,63,73	1.49	6 (10%)	70,101,113	2.09	20 (28%)
26	LMG	2	805	-	30,30,55	0.53	0	38,38,63	1.10	2 (5%)
20	CLA	4	601	16	64,68,73	1.40	6 (9%)	76,107,113	1.94	18 (23%)
20	CLA	1	601	13	69,73,73	1.39	6 (8%)	82,113,113	1.95	21 (25%)
20	CLA	2	607	23	64,68,73	1.41	6 (9%)	76,107,113	2.04	20 (26%)
19	CL0	A	1011	-	58,73,73	2.94	16 (27%)	60,113,113	2.89	21 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	CLA	B	1218	-	69,73,73	1.37	6 (8%)	82,113,113	1.95	17 (20%)
20	CLA	B	1231	-	64,68,73	1.47	6 (9%)	76,107,113	1.97	15 (19%)
29	LUT	1	502	-	42,43,43	2.50	2 (4%)	51,60,60	2.06	11 (21%)
20	CLA	B	1023	-	69,73,73	1.42	7 (10%)	82,113,113	1.84	15 (18%)
20	CLA	B	1226	-	69,73,73	1.41	6 (8%)	82,113,113	1.99	17 (20%)
20	CLA	B	1235	-	69,73,73	1.38	6 (8%)	82,113,113	1.90	19 (23%)
20	CLA	B	1237	-	69,73,73	1.36	6 (8%)	82,113,113	2.00	21 (25%)
20	CLA	A	1013	-	69,73,73	1.43	6 (8%)	82,113,113	1.83	20 (24%)
20	CLA	G	1602	-	50,54,73	1.65	6 (12%)	59,90,113	2.04	17 (28%)
20	CLA	4	608	-	50,54,73	1.58	7 (14%)	59,90,113	2.11	17 (28%)
24	LMT	G	5005	-	32,32,36	1.20	4 (12%)	43,43,47	1.03	2 (4%)
20	CLA	K	1401	-	49,53,73	1.60	6 (12%)	58,89,113	2.09	15 (25%)
22	BCR	B	4005	-	41,41,41	1.64	4 (9%)	56,56,56	4.48	17 (30%)
20	CLA	G	1603	-	69,73,73	1.37	6 (8%)	82,113,113	2.06	20 (24%)
30	CHL	3	604	-	60,74,74	1.48	7 (11%)	58,114,114	1.67	10 (17%)
20	CLA	3	602	-	56,60,73	1.52	7 (12%)	65,97,113	2.11	19 (29%)
24	LMT	A	5004	-	36,36,36	1.19	7 (19%)	47,47,47	1.09	3 (6%)
26	LMG	A	5006	-	50,50,55	1.17	5 (10%)	58,58,63	1.20	3 (5%)
20	CLA	B	1210	-	69,73,73	1.43	6 (8%)	82,113,113	1.99	21 (25%)
22	BCR	A	4007	-	41,41,41	1.67	6 (14%)	56,56,56	4.54	16 (28%)
24	LMT	B	5008	-	32,32,36	1.28	6 (18%)	43,43,47	1.04	3 (6%)
22	BCR	3	503	-	41,41,41	1.61	4 (9%)	56,56,56	4.57	18 (32%)
22	BCR	L	4020	-	41,41,41	1.62	4 (9%)	56,56,56	4.61	15 (26%)
20	CLA	B	1202	-	69,73,73	1.36	6 (8%)	82,113,113	1.92	21 (25%)
20	CLA	4	606	-	54,58,73	1.54	6 (11%)	64,95,113	2.04	19 (29%)
20	CLA	L	1503	-	54,58,73	1.53	7 (12%)	64,95,113	2.08	20 (31%)
20	CLA	K	1404	11	50,54,73	1.59	7 (14%)	59,90,113	2.02	14 (23%)
26	LMG	G	5001	-	49,49,55	1.12	4 (8%)	57,57,63	1.18	6 (10%)
20	CLA	1	603	-	59,63,73	1.49	6 (10%)	70,101,113	2.10	20 (28%)
20	CLA	3	610	15	69,73,73	1.37	6 (8%)	82,113,113	1.88	21 (25%)
26	LMG	F	5004	-	34,34,55	0.46	0	42,42,63	1.13	3 (7%)
28	DGD	1	803	-	42,42,67	0.87	1 (2%)	56,56,81	1.06	3 (5%)
26	LMG	F	5001	-	30,30,55	0.53	0	38,38,63	1.18	2 (5%)
28	DGD	B	5005	-	62,62,67	1.21	6 (9%)	76,76,81	1.05	5 (6%)
20	CLA	1	614	13	64,68,73	1.43	6 (9%)	76,107,113	1.99	18 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	CLA	B	1222	36	69,73,73	1.41	6 (8%)	82,113,113	1.94	21 (25%)
20	CLA	A	1104	-	69,73,73	1.42	6 (8%)	82,113,113	1.93	19 (23%)
20	CLA	B	1205	-	69,73,73	1.39	6 (8%)	82,113,113	1.98	19 (23%)
20	CLA	A	1123	-	69,73,73	1.38	6 (8%)	82,113,113	1.89	19 (23%)
26	LMG	1	802	-	46,46,55	1.05	3 (6%)	54,54,63	1.08	2 (3%)
22	BCR	B	4010	-	41,41,41	1.66	5 (12%)	56,56,56	4.43	16 (28%)
20	CLA	B	1227	-	69,73,73	1.39	6 (8%)	82,113,113	1.91	20 (24%)
20	CLA	3	605	-	59,63,73	1.51	6 (10%)	70,101,113	2.09	21 (30%)
20	CLA	B	1232	-	59,63,73	1.52	6 (10%)	70,101,113	2.04	22 (31%)
30	CHL	1	612	-	55,69,74	1.77	9 (16%)	52,108,114	1.80	12 (23%)
20	CLA	2	612	-	59,63,73	1.48	6 (10%)	70,101,113	2.00	15 (21%)
20	CLA	4	605	-	64,68,73	1.48	6 (9%)	76,107,113	1.89	20 (26%)
22	BCR	B	4009	-	41,41,41	1.62	4 (9%)	56,56,56	4.36	12 (21%)
28	DGD	J	5001	-	59,59,67	1.16	6 (10%)	73,73,81	1.03	2 (2%)
20	CLA	A	1116	-	60,64,73	1.51	6 (10%)	71,102,113	2.00	17 (23%)
20	CLA	A	1139	-	69,73,73	1.41	6 (8%)	82,113,113	1.91	16 (19%)
20	CLA	3	613	-	50,54,73	1.59	6 (12%)	59,90,113	2.07	15 (25%)
22	BCR	F	4014	-	41,41,41	1.64	5 (12%)	56,56,56	4.43	16 (28%)
20	CLA	B	1236	-	54,58,73	1.59	6 (11%)	64,95,113	2.10	19 (29%)
20	CLA	B	1224	-	69,73,73	1.39	6 (8%)	82,113,113	1.93	17 (20%)
26	LMG	2	806	-	13,13,55	0.57	0	18,18,63	0.55	0
28	DGD	G	5003	-	48,48,67	0.86	2 (4%)	62,62,81	1.02	2 (3%)
20	CLA	B	1215	-	69,73,73	1.40	6 (8%)	82,113,113	1.98	20 (24%)
29	LUT	1	501	-	42,43,43	2.47	2 (4%)	51,60,60	1.91	16 (31%)
21	PQN	A	2001	-	34,34,34	0.39	0	43,45,45	1.27	4 (9%)
20	CLA	A	1117	-	69,73,73	1.41	6 (8%)	82,113,113	1.82	15 (18%)
23	LHG	4	801	-	34,34,48	0.42	0	37,40,54	1.16	3 (8%)
20	CLA	2	602	-	56,60,73	1.50	7 (12%)	65,97,113	2.04	18 (27%)
20	CLA	B	1213	-	64,68,73	1.45	6 (9%)	76,107,113	1.91	17 (22%)
23	LHG	B	5002	-	48,48,48	0.40	0	51,54,54	1.12	3 (5%)
23	LHG	1	801	-	48,48,48	0.45	1 (2%)	51,54,54	1.21	4 (7%)
20	CLA	B	1221	-	69,73,73	1.42	6 (8%)	82,113,113	1.94	20 (24%)
20	CLA	B	1214	-	69,73,73	1.42	6 (8%)	82,113,113	1.94	18 (21%)
26	LMG	F	5002	-	47,47,55	1.09	4 (8%)	55,55,63	1.22	4 (7%)
29	LUT	3	501	-	42,43,43	2.44	2 (4%)	51,60,60	2.08	19 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	CLA	J	1901	10	54,58,73	1.54	7 (12%)	64,95,113	2.12	19 (29%)
20	CLA	B	1239	-	69,73,73	1.42	6 (8%)	82,113,113	1.89	21 (25%)
20	CLA	4	607	-	64,68,73	1.41	8 (12%)	76,107,113	1.97	19 (25%)
22	BCR	I	4018	-	41,41,41	1.70	5 (12%)	56,56,56	4.02	19 (33%)
20	CLA	L	1501	12	54,58,73	1.52	7 (12%)	64,95,113	2.11	18 (28%)
20	CLA	A	1107	1	69,73,73	1.39	6 (8%)	82,113,113	1.96	19 (23%)
20	CLA	B	1217	-	50,54,73	1.63	6 (12%)	59,90,113	2.07	15 (25%)
26	LMG	2	804	-	30,30,55	0.55	0	38,38,63	1.15	4 (10%)
20	CLA	G	1601	-	59,63,73	1.55	6 (10%)	70,101,113	1.96	17 (24%)
20	CLA	B	1230	-	62,66,73	1.46	6 (9%)	73,104,113	2.04	20 (27%)
20	CLA	A	1133	-	69,73,73	1.40	7 (10%)	82,113,113	1.81	16 (19%)
23	LHG	A	5002	-	48,48,48	0.38	0	51,54,54	1.14	5 (9%)
26	LMG	B	5004	-	33,33,55	0.55	0	41,41,63	1.33	6 (14%)
30	CHL	3	611	-	41,55,74	1.80	9 (21%)	35,91,114	2.08	11 (31%)
20	CLA	B	1216	-	69,73,73	1.37	6 (8%)	82,113,113	1.83	17 (20%)
25	SF4	C	3003	3	0,12,12	-	-	-	-	-
30	CHL	4	611	-	45,59,74	1.58	9 (20%)	40,96,114	2.06	11 (27%)
22	BCR	A	4008	-	41,41,41	1.69	6 (14%)	56,56,56	4.21	19 (33%)
20	CLA	B	1208	-	64,68,73	1.42	6 (9%)	76,107,113	1.88	15 (19%)
20	CLA	F	1302	6	69,73,73	1.38	6 (8%)	82,113,113	1.85	15 (18%)
22	BCR	L	4019	-	41,41,41	1.62	4 (9%)	56,56,56	4.53	15 (26%)
22	BCR	I	4020	-	41,41,41	1.62	4 (9%)	56,56,56	4.51	14 (25%)
20	CLA	2	604	14	69,73,73	1.35	7 (10%)	82,113,113	1.90	19 (23%)
28	DGD	F	5005	-	58,58,67	1.13	4 (6%)	72,72,81	1.13	6 (8%)
22	BCR	A	4011	-	41,41,41	1.68	5 (12%)	56,56,56	4.46	19 (33%)
21	PQN	B	2002	-	34,34,34	0.43	0	43,45,45	1.30	5 (11%)
20	CLA	4	612	-	69,73,73	1.35	7 (10%)	82,113,113	1.91	18 (21%)
20	CLA	A	1115	-	69,73,73	1.37	6 (8%)	82,113,113	1.93	16 (19%)
20	CLA	A	1110	-	59,63,73	1.52	6 (10%)	70,101,113	2.04	21 (30%)
22	BCR	1	504	-	41,41,41	1.66	4 (9%)	56,56,56	4.81	15 (26%)
22	BCR	B	4004	-	41,41,41	1.64	4 (9%)	56,56,56	4.97	23 (41%)
22	BCR	K	4001	-	41,41,41	1.63	4 (9%)	56,56,56	4.53	15 (26%)
34	FES	N	101	17	0,4,4	-	-	-	-	-
20	CLA	A	1012	-	69,73,73	1.43	6 (8%)	82,113,113	1.95	17 (20%)
20	CLA	B	1225	-	69,73,73	1.41	6 (8%)	82,113,113	1.88	18 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	CLA	1	613	-	49,53,73	1.67	6 (12%)	58,89,113	1.97	13 (22%)
20	CLA	2	606	-	54,58,73	1.53	6 (11%)	64,95,113	2.12	20 (31%)
24	LMT	G	5004	-	36,36,36	1.18	6 (16%)	47,47,47	1.06	3 (6%)
20	CLA	A	1105	-	64,68,73	1.44	6 (9%)	76,107,113	2.00	16 (21%)
20	CLA	A	1121	-	64,68,73	1.45	6 (9%)	76,107,113	1.99	18 (23%)
30	CHL	2	611	-	42,56,74	1.60	9 (21%)	36,92,114	2.01	9 (25%)
29	LUT	2	501	-	42,43,43	2.41	2 (4%)	51,60,60	2.34	17 (33%)
20	CLA	3	617	-	64,68,73	1.39	6 (9%)	76,107,113	1.95	19 (25%)
20	CLA	A	1125	-	69,73,73	1.40	6 (8%)	82,113,113	1.97	20 (24%)
20	CLA	L	1502	-	64,68,73	1.39	6 (9%)	76,107,113	1.98	20 (26%)
22	BCR	B	4006	-	41,41,41	1.65	4 (9%)	56,56,56	4.38	21 (37%)
23	LHG	2	801	20	34,34,48	0.45	0	37,40,54	1.15	4 (10%)
20	CLA	A	1108	-	54,58,73	1.60	6 (11%)	64,95,113	2.05	18 (28%)
22	BCR	A	4003	-	41,41,41	1.65	4 (9%)	56,56,56	4.39	18 (32%)
20	CLA	B	1238	36	69,73,73	1.34	7 (10%)	82,113,113	1.92	18 (21%)
32	3PH	2	807	-	32,32,47	1.03	4 (12%)	35,37,52	1.23	2 (5%)
20	CLA	2	603	14	69,73,73	1.37	8 (11%)	82,113,113	1.91	19 (23%)
22	BCR	J	4012	-	41,41,41	1.65	4 (9%)	56,56,56	4.38	18 (32%)
22	BCR	K	4002	-	41,41,41	1.61	4 (9%)	56,56,56	4.63	18 (32%)
20	CLA	A	1127	-	69,73,73	1.42	7 (10%)	82,113,113	1.86	16 (19%)
25	SF4	C	3002	3	0,12,12	-	-	-	-	-
22	BCR	H	4021	-	41,41,41	1.62	4 (9%)	56,56,56	4.57	15 (26%)
31	XAT	2	502	-	41,47,47	0.79	1 (2%)	54,74,74	2.14	13 (24%)
20	CLA	3	606	-	54,58,73	1.58	7 (12%)	64,95,113	2.01	13 (20%)
20	CLA	A	1141	23	64,68,73	1.41	6 (9%)	76,107,113	1.93	19 (25%)
20	CLA	B	1240	23	69,73,73	1.42	6 (8%)	82,113,113	1.99	21 (25%)
20	CLA	B	1021	-	69,73,73	1.43	7 (10%)	82,113,113	1.92	18 (21%)
20	CLA	F	1301	-	69,73,73	1.38	6 (8%)	82,113,113	1.88	17 (20%)
20	CLA	4	609	16	54,58,73	1.52	6 (11%)	64,95,113	2.10	19 (29%)
20	CLA	K	1402	-	64,68,73	1.40	7 (10%)	76,107,113	2.00	21 (27%)
20	CLA	1	611	-	69,73,73	1.38	6 (8%)	82,113,113	1.90	17 (20%)
20	CLA	A	1122	-	69,73,73	1.38	6 (8%)	82,113,113	1.88	17 (20%)
20	CLA	B	1234	-	59,63,73	1.54	6 (10%)	70,101,113	1.97	14 (20%)
30	CHL	2	610	-	50,64,74	1.36	9 (18%)	46,102,114	1.86	11 (23%)
20	CLA	B	1211	-	69,73,73	1.39	6 (8%)	82,113,113	1.95	19 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	CLA	2	601	-	64,68,73	1.45	6 (9%)	76,107,113	1.89	17 (22%)
20	CLA	A	1109	-	69,73,73	1.39	6 (8%)	82,113,113	1.91	20 (24%)
23	LHG	B	5001	20	20,20,48	0.60	0	23,26,54	1.53	2 (8%)
20	CLA	B	1223	-	69,73,73	1.40	6 (8%)	82,113,113	1.94	17 (20%)
20	CLA	A	1124	-	59,63,73	1.51	6 (10%)	70,101,113	2.01	18 (25%)
28	DGD	4	802	-	52,52,67	0.93	2 (3%)	66,66,81	1.04	3 (4%)
20	CLA	B	1209	-	50,54,73	1.59	6 (12%)	59,90,113	2.02	12 (20%)
24	LMT	2	808	-	36,36,36	0.42	0	47,47,47	0.74	1 (2%)
20	CLA	A	1130	-	59,63,73	1.49	6 (10%)	70,101,113	1.95	17 (24%)
20	CLA	3	608	-	52,56,73	1.55	7 (13%)	61,92,113	2.09	19 (31%)
20	CLA	A	1119	-	69,73,73	1.42	6 (8%)	82,113,113	1.89	19 (23%)
30	CHL	1	609	13	50,64,74	1.47	9 (18%)	46,102,114	1.84	11 (23%)
30	CHL	2	613	-	40,54,74	1.43	9 (22%)	34,90,114	2.09	8 (23%)
20	CLA	1	605	-	69,73,73	1.38	6 (8%)	82,113,113	2.04	18 (21%)
30	CHL	2	615	-	50,64,74	1.25	9 (18%)	46,102,114	1.93	13 (28%)
20	CLA	A	1118	-	54,58,73	1.57	6 (11%)	64,95,113	2.20	20 (31%)
20	CLA	A	1137	-	69,73,73	1.38	6 (8%)	82,113,113	1.91	17 (20%)
20	CLA	B	1212	-	59,63,73	1.50	6 (10%)	70,101,113	2.04	17 (24%)
22	BCR	2	503	-	41,41,41	1.73	5 (12%)	56,56,56	5.47	26 (46%)
20	CLA	A	1126	-	69,73,73	1.41	6 (8%)	82,113,113	1.90	17 (20%)
30	CHL	3	607	23	45,59,74	1.68	10 (22%)	40,96,114	1.96	12 (30%)
25	SF4	A	3001	2,1	0,12,12	-	-	-	-	-
23	LHG	A	5001	20	39,39,48	0.46	0	42,45,54	1.27	4 (9%)
20	CLA	B	1206	2	69,73,73	1.42	6 (8%)	82,113,113	1.88	17 (20%)
20	CLA	A	1140	-	69,73,73	1.39	6 (8%)	82,113,113	1.87	21 (25%)
26	LMG	3	802	-	30,30,55	0.57	0	38,38,63	1.15	3 (7%)
20	CLA	4	603	-	69,73,73	1.34	7 (10%)	82,113,113	1.81	18 (21%)
29	LUT	3	502	-	42,43,43	2.41	1 (2%)	51,60,60	2.07	10 (19%)
24	LMT	B	5006	-	33,33,36	1.21	6 (18%)	44,44,47	1.01	3 (6%)
22	BCR	A	4017	-	41,41,41	1.64	5 (12%)	56,56,56	4.92	19 (33%)
20	CLA	B	1201	-	69,73,73	1.38	6 (8%)	82,113,113	1.87	16 (19%)
20	CLA	A	1101	-	69,73,73	1.35	6 (8%)	82,113,113	1.94	19 (23%)
20	CLA	A	1120	-	64,68,73	1.43	6 (9%)	76,107,113	1.93	16 (21%)
20	CLA	A	1131	-	69,73,73	1.41	6 (8%)	82,113,113	1.88	17 (20%)
23	LHG	3	801	30	16,16,48	0.85	1 (6%)	17,20,54	0.70	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	LUT	J	4013	-	42,43,43	2.33	2 (4%)	51,60,60	2.39	15 (29%)
20	CLA	A	1102	-	69,73,73	1.37	6 (8%)	82,113,113	1.93	20 (24%)
20	CLA	A	1134	1	59,63,73	1.47	6 (10%)	70,101,113	1.99	17 (24%)
20	CLA	A	1135	-	55,59,73	1.57	6 (10%)	64,96,113	2.08	16 (25%)
20	CLA	B	1204	-	69,73,73	1.39	6 (8%)	82,113,113	1.92	19 (23%)
20	CLA	B	1219	-	69,73,73	1.39	6 (8%)	82,113,113	1.90	16 (19%)
20	CLA	H	1701	8	64,68,73	1.39	6 (9%)	76,107,113	1.94	18 (23%)
20	CLA	1	607	-	50,54,73	1.63	6 (12%)	59,90,113	2.03	15 (25%)
20	CLA	2	608	-	54,58,73	1.59	6 (11%)	64,95,113	2.19	18 (28%)
26	LMG	G	5002	-	50,50,55	1.19	5 (10%)	58,58,63	1.23	5 (8%)
20	CLA	2	605	-	69,73,73	1.38	6 (8%)	82,113,113	1.95	18 (21%)
26	LMG	G	5006	-	25,25,55	0.57	0	33,33,63	1.25	4 (12%)
20	CLA	A	1138	-	69,73,73	1.40	6 (8%)	82,113,113	1.85	15 (18%)
20	CLA	3	603	15	59,63,73	1.47	6 (10%)	70,101,113	2.08	21 (30%)
20	CLA	B	1203	-	69,73,73	1.39	6 (8%)	82,113,113	1.87	20 (24%)
20	CLA	4	602	-	54,58,73	1.53	7 (12%)	64,95,113	2.02	17 (26%)
20	CLA	A	1114	-	50,54,73	1.61	6 (12%)	59,90,113	2.09	16 (27%)

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
20	CLA	A	1111	-	1/1/15/20	18/39/115/115	-
20	CLA	A	1128	-	1/1/15/20	16/39/115/115	-
20	CLA	A	1132	-	1/1/15/20	13/39/115/115	-
22	BCR	G	4011	-	-	8/29/63/63	0/2/2/2
20	CLA	3	614	-	1/1/10/20	3/12/88/115	-
31	XAT	4	502	-	2/2/12/26	2/31/93/93	0/4/4/4
20	CLA	A	1103	-	1/1/15/20	18/39/115/115	-
20	CLA	A	1106	1	1/1/15/20	17/39/115/115	-
30	CHL	1	610	13	3/3/16/26	5/17/115/137	-
26	LMG	B	5003	-	-	8/30/50/70	0/1/1/1
22	BCR	F	4016	-	-	14/29/63/63	0/2/2/2
26	LMG	F	5006	-	-	1/4/24/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	4	617	-	1/1/15/20	19/39/115/115	-
28	DGD	3	803	-	-	10/40/80/95	0/2/2/2
20	CLA	B	1220	-	1/1/13/20	10/27/103/115	-
20	CLA	1	602	13	1/1/11/20	8/17/93/115	-
30	CHL	4	610	-	3/3/16/26	3/17/115/137	-
20	CLA	K	1403	-	1/1/11/20	8/19/95/115	-
20	CLA	4	604	-	1/1/14/20	15/33/109/115	-
33	C7Z	4	505	-	-	16/29/67/67	0/2/2/2
22	BCR	3	506	-	-	14/29/63/63	0/2/2/2
20	CLA	1	604	-	1/1/15/20	14/39/115/115	-
26	LMG	B	5007	-	-	11/29/49/70	0/1/1/1
29	LUT	4	501	-	-	4/29/67/67	0/2/2/2
20	CLA	A	1136	-	1/1/15/20	14/39/115/115	-
30	CHL	2	609	-	4/4/20/26	9/39/137/137	-
20	CLA	A	1112	-	1/1/15/20	18/39/115/115	-
22	BCR	A	4002	-	-	11/29/63/63	0/2/2/2
22	BCR	1	503	-	-	16/29/63/63	0/2/2/2
20	CLA	A	1129	-	1/1/15/20	15/39/115/115	-
26	LMG	F	5003	-	-	6/31/51/70	0/1/1/1
26	LMG	2	803	-	-	12/31/51/70	0/1/1/1
20	CLA	B	1207	-	1/1/15/20	22/39/115/115	-
20	CLA	3	612	-	1/1/12/20	9/21/97/115	-
30	CHL	4	613	-	4/4/19/26	8/33/131/137	-
20	CLA	1	606	-	1/1/12/20	5/21/97/115	-
30	CHL	4	615	-	3/3/15/26	2/12/110/137	-
20	CLA	A	1113	-	1/1/11/20	7/15/91/115	-
20	CLA	B	1229	-	1/1/15/20	12/39/115/115	-
26	LMG	2	802	-	-	8/20/40/70	0/1/1/1
20	CLA	B	1228	-	1/1/14/20	11/33/109/115	-
20	CLA	B	1022	-	1/1/15/20	6/39/115/115	-
20	CLA	1	608	-	1/1/11/20	9/17/93/115	-
20	CLA	3	601	-	1/1/13/20	12/27/103/115	-
26	LMG	2	805	-	-	7/25/45/70	0/1/1/1
20	CLA	4	601	16	1/1/14/20	14/33/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	1	601	13	1/1/15/20	18/39/115/115	-
20	CLA	2	607	23	1/1/14/20	15/33/109/115	-
19	CL0	A	1011	-	3/3/20/25	8/37/135/135	-
20	CLA	B	1218	-	1/1/15/20	8/39/115/115	-
20	CLA	B	1231	-	1/1/14/20	10/33/109/115	-
29	LUT	1	502	-	-	5/29/67/67	0/2/2/2
20	CLA	B	1023	-	1/1/15/20	10/39/115/115	-
20	CLA	B	1226	-	1/1/15/20	21/39/115/115	-
20	CLA	B	1235	-	1/1/15/20	15/39/115/115	-
20	CLA	B	1237	-	1/1/15/20	18/39/115/115	-
20	CLA	A	1013	-	1/1/15/20	16/39/115/115	-
20	CLA	G	1602	-	1/1/11/20	6/17/93/115	-
20	CLA	4	608	-	1/1/11/20	5/17/93/115	-
24	LMT	G	5005	-	-	6/17/57/61	0/2/2/2
20	CLA	K	1401	-	1/1/11/20	7/15/91/115	-
22	BCR	B	4005	-	-	10/29/63/63	0/2/2/2
20	CLA	G	1603	-	1/1/15/20	17/39/115/115	-
30	CHL	3	604	-	4/4/20/26	9/39/137/137	-
20	CLA	3	602	-	1/1/12/20	11/24/100/115	-
24	LMT	A	5004	-	-	9/21/61/61	0/2/2/2
26	LMG	A	5006	-	-	11/45/65/70	0/1/1/1
20	CLA	B	1210	-	1/1/15/20	14/39/115/115	-
22	BCR	A	4007	-	-	9/29/63/63	0/2/2/2
24	LMT	B	5008	-	-	8/17/57/61	0/2/2/2
22	BCR	3	503	-	-	15/29/63/63	0/2/2/2
22	BCR	L	4020	-	-	9/29/63/63	0/2/2/2
20	CLA	B	1202	-	1/1/15/20	14/39/115/115	-
20	CLA	4	606	-	1/1/12/20	6/21/97/115	-
20	CLA	L	1503	-	1/1/12/20	10/21/97/115	-
20	CLA	K	1404	11	1/1/11/20	7/17/93/115	-
26	LMG	G	5001	-	-	21/44/64/70	0/1/1/1
20	CLA	1	603	-	1/1/13/20	7/27/103/115	-
20	CLA	3	610	15	1/1/15/20	21/39/115/115	-
26	LMG	F	5004	-	-	8/29/49/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	DGD	1	803	-	-	15/30/70/95	0/2/2/2
26	LMG	F	5001	-	-	6/25/45/70	0/1/1/1
28	DGD	B	5005	-	-	20/50/90/95	0/2/2/2
20	CLA	1	614	13	1/1/14/20	17/33/109/115	-
20	CLA	B	1222	36	1/1/15/20	21/39/115/115	-
20	CLA	A	1104	-	1/1/15/20	15/39/115/115	-
20	CLA	B	1205	-	1/1/15/20	17/39/115/115	-
20	CLA	A	1123	-	1/1/15/20	14/39/115/115	-
26	LMG	1	802	-	-	8/41/61/70	0/1/1/1
30	CHL	1	612	-	4/4/19/26	7/33/131/137	-
20	CLA	B	1227	-	1/1/15/20	14/39/115/115	-
20	CLA	3	605	-	1/1/13/20	10/27/103/115	-
20	CLA	B	1232	-	1/1/13/20	15/27/103/115	-
22	BCR	B	4010	-	-	14/29/63/63	0/2/2/2
20	CLA	2	612	-	1/1/13/20	10/27/103/115	-
20	CLA	4	605	-	-	14/33/109/115	-
22	BCR	B	4009	-	-	9/29/63/63	0/2/2/2
28	DGD	J	5001	-	-	14/47/87/95	0/2/2/2
20	CLA	A	1116	-	1/1/13/20	11/29/105/115	-
20	CLA	A	1139	-	1/1/15/20	12/39/115/115	-
20	CLA	3	613	-	1/1/11/20	7/17/93/115	-
22	BCR	F	4014	-	-	9/29/63/63	0/2/2/2
20	CLA	B	1236	-	1/1/12/20	8/21/97/115	-
20	CLA	B	1224	-	1/1/15/20	17/39/115/115	-
26	LMG	2	806	-	-	1/4/24/70	0/1/1/1
28	DGD	G	5003	-	-	12/36/76/95	0/2/2/2
20	CLA	B	1215	-	1/1/15/20	16/39/115/115	-
29	LUT	1	501	-	-	3/29/67/67	0/2/2/2
21	PQN	A	2001	-	-	3/23/43/43	0/2/2/2
20	CLA	A	1117	-	1/1/15/20	17/39/115/115	-
23	LHG	4	801	-	-	19/39/39/53	-
20	CLA	2	602	-	1/1/12/20	10/24/100/115	-
20	CLA	B	1213	-	1/1/14/20	7/33/109/115	-
23	LHG	B	5002	-	-	29/53/53/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	LHG	1	801	-	-	28/53/53/53	-
20	CLA	B	1221	-	1/1/15/20	21/39/115/115	-
20	CLA	B	1214	-	1/1/15/20	16/39/115/115	-
26	LMG	F	5002	-	-	10/42/62/70	0/1/1/1
29	LUT	3	501	-	-	5/29/67/67	0/2/2/2
20	CLA	J	1901	10	1/1/12/20	7/21/97/115	-
20	CLA	B	1239	-	1/1/15/20	18/39/115/115	-
20	CLA	4	607	-	1/1/14/20	13/33/109/115	-
22	BCR	I	4018	-	-	13/29/63/63	0/2/2/2
20	CLA	L	1501	12	1/1/12/20	10/21/97/115	-
20	CLA	A	1107	1	1/1/15/20	16/39/115/115	-
20	CLA	B	1217	-	1/1/11/20	9/17/93/115	-
26	LMG	2	804	-	-	7/25/45/70	0/1/1/1
20	CLA	G	1601	-	1/1/13/20	9/27/103/115	-
20	CLA	B	1230	-	1/1/13/20	14/31/107/115	-
20	CLA	A	1133	-	1/1/15/20	16/39/115/115	-
23	LHG	A	5002	-	-	35/53/53/53	-
26	LMG	B	5004	-	-	13/28/48/70	0/1/1/1
30	CHL	3	611	-	3/3/16/26	0/17/115/137	-
20	CLA	B	1216	-	1/1/15/20	11/39/115/115	-
25	SF4	C	3003	3	-	-	0/6/5/5
30	CHL	4	611	-	3/3/17/26	2/21/119/137	-
22	BCR	A	4008	-	-	12/29/63/63	0/2/2/2
20	CLA	B	1208	-	1/1/14/20	13/33/109/115	-
20	CLA	F	1302	6	1/1/15/20	17/39/115/115	-
22	BCR	L	4019	-	-	14/29/63/63	0/2/2/2
22	BCR	I	4020	-	-	15/29/63/63	0/2/2/2
20	CLA	2	604	14	1/1/15/20	17/39/115/115	-
28	DGD	F	5005	-	-	19/46/86/95	0/2/2/2
22	BCR	A	4011	-	-	15/29/63/63	0/2/2/2
21	PQN	B	2002	-	-	6/23/43/43	0/2/2/2
20	CLA	4	612	-	1/1/15/20	17/39/115/115	-
20	CLA	A	1115	-	1/1/15/20	19/39/115/115	-
20	CLA	A	1110	-	1/1/13/20	6/27/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	BCR	1	504	-	-	14/29/63/63	0/2/2/2
22	BCR	B	4004	-	-	12/29/63/63	0/2/2/2
22	BCR	K	4001	-	-	12/29/63/63	0/2/2/2
34	FES	N	101	17	-	-	0/1/1/1
20	CLA	A	1012	-	1/1/15/20	21/39/115/115	-
20	CLA	B	1225	-	1/1/15/20	14/39/115/115	-
20	CLA	1	613	-	1/1/11/20	6/15/91/115	-
20	CLA	2	606	-	1/1/12/20	9/21/97/115	-
24	LMT	G	5004	-	-	10/21/61/61	0/2/2/2
20	CLA	A	1105	-	1/1/14/20	18/33/109/115	-
20	CLA	A	1121	-	1/1/14/20	16/33/109/115	-
30	CHL	2	611	-	3/3/16/26	4/18/116/137	-
29	LUT	2	501	-	1/1/12/27	3/29/67/67	0/2/2/2
20	CLA	3	617	-	1/1/14/20	12/33/109/115	-
20	CLA	A	1125	-	1/1/15/20	16/39/115/115	-
20	CLA	L	1502	-	1/1/14/20	21/33/109/115	-
22	BCR	B	4006	-	-	11/29/63/63	0/2/2/2
23	LHG	2	801	20	-	19/39/39/53	-
20	CLA	A	1108	-	1/1/12/20	5/21/97/115	-
22	BCR	A	4003	-	-	13/29/63/63	0/2/2/2
20	CLA	B	1238	36	1/1/15/20	16/39/115/115	-
32	3PH	2	807	-	-	16/34/34/49	-
20	CLA	2	603	14	1/1/15/20	13/39/115/115	-
22	BCR	J	4012	-	-	12/29/63/63	0/2/2/2
22	BCR	K	4002	-	-	11/29/63/63	0/2/2/2
20	CLA	A	1127	-	1/1/15/20	16/39/115/115	-
25	SF4	C	3002	3	-	-	0/6/5/5
22	BCR	H	4021	-	-	12/29/63/63	0/2/2/2
31	XAT	2	502	-	2/2/12/26	4/31/93/93	0/4/4/4
20	CLA	3	606	-	1/1/12/20	10/21/97/115	-
20	CLA	A	1141	23	1/1/14/20	14/33/109/115	-
20	CLA	B	1240	23	1/1/15/20	18/39/115/115	-
20	CLA	B	1021	-	1/1/15/20	12/39/115/115	-
20	CLA	F	1301	-	1/1/15/20	17/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	4	609	16	1/1/12/20	9/21/97/115	-
20	CLA	K	1402	-	1/1/14/20	20/33/109/115	-
20	CLA	1	611	-	1/1/15/20	14/39/115/115	-
20	CLA	A	1122	-	1/1/15/20	15/39/115/115	-
20	CLA	B	1234	-	1/1/13/20	6/27/103/115	-
30	CHL	2	610	-	4/4/18/26	6/27/125/137	-
20	CLA	B	1211	-	1/1/15/20	21/39/115/115	-
20	CLA	2	601	-	1/1/14/20	14/33/109/115	-
20	CLA	A	1109	-	1/1/15/20	13/39/115/115	-
23	LHG	B	5001	20	-	14/23/23/53	-
20	CLA	B	1223	-	1/1/15/20	13/39/115/115	-
20	CLA	A	1124	-	1/1/13/20	8/27/103/115	-
28	DGD	4	802	-	-	16/40/80/95	0/2/2/2
20	CLA	B	1209	-	1/1/11/20	6/17/93/115	-
24	LMT	2	808	-	-	2/21/61/61	0/2/2/2
20	CLA	A	1130	-	1/1/13/20	12/27/103/115	-
20	CLA	3	608	-	1/1/11/20	4/19/95/115	-
20	CLA	A	1119	-	1/1/15/20	14/39/115/115	-
30	CHL	1	609	13	4/4/18/26	0/27/125/137	-
30	CHL	2	613	-	3/3/16/26	8/15/113/137	-
20	CLA	1	605	-	1/1/15/20	17/39/115/115	-
30	CHL	2	615	-	4/4/18/26	5/27/125/137	-
20	CLA	A	1118	-	1/1/12/20	8/21/97/115	-
20	CLA	A	1137	-	1/1/15/20	18/39/115/115	-
20	CLA	B	1212	-	1/1/13/20	9/27/103/115	-
22	BCR	2	503	-	-	14/29/63/63	0/2/2/2
20	CLA	A	1126	-	1/1/15/20	20/39/115/115	-
30	CHL	3	607	23	3/3/17/26	5/21/119/137	-
25	SF4	A	3001	2,1	-	-	0/6/5/5
23	LHG	A	5001	20	-	22/44/44/53	-
20	CLA	B	1206	2	1/1/15/20	17/39/115/115	-
20	CLA	A	1140	-	1/1/15/20	13/39/115/115	-
29	LUT	3	502	-	1/1/12/27	9/29/67/67	0/2/2/2
20	CLA	4	603	-	1/1/15/20	16/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	LMG	3	802	-	-	11/25/45/70	0/1/1/1
24	LMT	B	5006	-	-	7/18/58/61	0/2/2/2
22	BCR	A	4017	-	-	6/29/63/63	0/2/2/2
20	CLA	B	1201	-	1/1/15/20	17/39/115/115	-
20	CLA	A	1101	-	1/1/15/20	16/39/115/115	-
20	CLA	A	1120	-	1/1/14/20	15/33/109/115	-
20	CLA	A	1131	-	1/1/15/20	13/39/115/115	-
23	LHG	3	801	30	-	12/19/19/53	-
29	LUT	J	4013	-	-	7/29/67/67	0/2/2/2
20	CLA	A	1102	-	1/1/15/20	24/39/115/115	-
20	CLA	A	1134	1	1/1/13/20	13/27/103/115	-
20	CLA	A	1135	-	1/1/12/20	9/23/99/115	-
20	CLA	B	1204	-	1/1/15/20	20/39/115/115	-
20	CLA	B	1219	-	1/1/15/20	18/39/115/115	-
20	CLA	H	1701	8	1/1/14/20	15/33/109/115	-
20	CLA	1	607	-	1/1/11/20	5/17/93/115	-
20	CLA	2	608	-	1/1/12/20	8/21/97/115	-
26	LMG	G	5002	-	-	18/45/65/70	0/1/1/1
20	CLA	2	605	-	1/1/15/20	20/39/115/115	-
26	LMG	G	5006	-	-	11/20/40/70	0/1/1/1
20	CLA	A	1138	-	1/1/15/20	14/39/115/115	-
20	CLA	3	603	15	1/1/13/20	13/27/103/115	-
20	CLA	B	1203	-	1/1/15/20	13/39/115/115	-
20	CLA	4	602	-	1/1/12/20	7/21/97/115	-
20	CLA	A	1114	-	1/1/11/20	7/17/93/115	-

All (1256) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	1	502	LUT	C24-C25	15.26	1.51	1.33
29	4	501	LUT	C24-C25	14.96	1.50	1.33
29	1	501	LUT	C24-C25	14.95	1.50	1.33
29	3	501	LUT	C24-C25	14.84	1.50	1.33
29	3	502	LUT	C24-C25	14.70	1.50	1.33
29	2	501	LUT	C24-C25	14.62	1.50	1.33
29	J	4013	LUT	C24-C25	14.26	1.50	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	4	505	C7Z	C25-C26	11.39	1.53	1.34
33	4	505	C7Z	C5-C6	11.33	1.53	1.34
30	1	612	CHL	C3A-C2A	-9.02	1.46	1.54
19	A	1011	CL0	C1A-CHA	8.58	1.49	1.40
19	A	1011	CL0	C1D-C2D	8.53	1.49	1.39
33	4	505	C7Z	C34-C33	8.29	1.55	1.35
33	4	505	C7Z	C30-C29	8.21	1.54	1.35
33	4	505	C7Z	C14-C13	8.10	1.54	1.35
33	4	505	C7Z	C10-C9	8.06	1.54	1.35
19	A	1011	CL0	C1B-C2B	7.82	1.48	1.39
30	4	610	CHL	C3A-C2A	-7.16	1.48	1.54
30	1	610	CHL	C3A-C2A	-6.58	1.49	1.54
30	3	604	CHL	C3A-C2A	-6.41	1.49	1.54
19	A	1011	CL0	C3B-C4B	6.40	1.47	1.41
20	B	1207	CLA	MG-NA	6.39	2.21	2.06
20	K	1404	CLA	MG-NA	6.39	2.21	2.06
20	B	1237	CLA	MG-NA	6.38	2.21	2.06
20	K	1401	CLA	MG-NA	6.38	2.21	2.06
20	2	607	CLA	MG-NA	6.35	2.21	2.06
20	L	1503	CLA	MG-NA	6.32	2.21	2.06
20	3	612	CLA	MG-NA	6.31	2.21	2.06
20	4	608	CLA	MG-NA	6.30	2.21	2.06
20	4	609	CLA	MG-NA	6.30	2.21	2.06
20	2	606	CLA	MG-NA	6.29	2.21	2.06
20	K	1403	CLA	MG-NA	6.28	2.21	2.06
20	2	604	CLA	MG-NA	6.28	2.21	2.06
20	4	603	CLA	MG-NA	6.27	2.21	2.06
20	3	602	CLA	MG-NA	6.26	2.21	2.06
20	H	1701	CLA	MG-NA	6.25	2.21	2.06
20	B	1238	CLA	MG-NA	6.25	2.21	2.06
20	A	1101	CLA	MG-NA	6.25	2.21	2.06
20	2	608	CLA	MG-NA	6.25	2.21	2.06
20	L	1502	CLA	MG-NA	6.24	2.21	2.06
20	4	604	CLA	MG-NA	6.24	2.21	2.06
20	4	612	CLA	MG-NA	6.23	2.21	2.06
20	4	601	CLA	MG-NA	6.23	2.21	2.06
20	3	608	CLA	MG-NA	6.23	2.21	2.06
20	K	1402	CLA	MG-NA	6.22	2.21	2.06
20	4	602	CLA	MG-NA	6.21	2.21	2.06
20	4	606	CLA	MG-NA	6.20	2.21	2.06
20	L	1501	CLA	MG-NA	6.19	2.21	2.06
20	A	1132	CLA	MG-NA	6.19	2.21	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	J	1901	CLA	MG-NA	6.19	2.21	2.06
20	3	614	CLA	MG-NA	6.19	2.21	2.06
20	2	602	CLA	MG-NA	6.17	2.20	2.06
20	G	1602	CLA	MG-NA	6.17	2.20	2.06
20	G	1601	CLA	MG-NA	6.17	2.20	2.06
20	3	605	CLA	MG-NA	6.16	2.20	2.06
20	4	607	CLA	MG-NA	6.13	2.20	2.06
20	3	617	CLA	MG-NA	6.13	2.20	2.06
20	4	605	CLA	MG-NA	6.10	2.20	2.06
20	1	613	CLA	MG-NA	6.09	2.20	2.06
20	1	614	CLA	MG-NA	6.09	2.20	2.06
20	1	606	CLA	MG-NA	6.09	2.20	2.06
20	A	1141	CLA	MG-NA	6.09	2.20	2.06
22	L	4019	BCR	C24-C23	6.08	1.51	1.33
20	A	1110	CLA	MG-NA	6.08	2.20	2.06
20	4	617	CLA	MG-NA	6.08	2.20	2.06
20	A	1120	CLA	MG-NA	6.07	2.20	2.06
20	A	1139	CLA	MG-NA	6.06	2.20	2.06
20	1	607	CLA	MG-NA	6.05	2.20	2.06
20	B	1240	CLA	MG-NA	6.04	2.20	2.06
20	A	1108	CLA	MG-NA	6.04	2.20	2.06
20	3	613	CLA	MG-NA	6.03	2.20	2.06
30	3	607	CHL	C3A-C2A	-6.02	1.49	1.54
20	B	1213	CLA	MG-NA	6.02	2.20	2.06
20	B	1234	CLA	MG-NA	6.01	2.20	2.06
20	2	601	CLA	MG-NA	6.01	2.20	2.06
20	A	1114	CLA	MG-NA	6.01	2.20	2.06
20	3	610	CLA	MG-NA	6.01	2.20	2.06
20	A	1137	CLA	MG-NA	6.00	2.20	2.06
20	1	602	CLA	MG-NA	5.99	2.20	2.06
20	A	1109	CLA	MG-NA	5.99	2.20	2.06
20	A	1123	CLA	MG-NA	5.99	2.20	2.06
20	B	1210	CLA	MG-NA	5.98	2.20	2.06
20	B	1214	CLA	MG-NA	5.97	2.20	2.06
20	B	1239	CLA	MG-NA	5.97	2.20	2.06
20	2	603	CLA	MG-NA	5.97	2.20	2.06
20	A	1130	CLA	MG-NA	5.97	2.20	2.06
20	G	1603	CLA	MG-NA	5.97	2.20	2.06
20	1	611	CLA	MG-NA	5.97	2.20	2.06
20	F	1302	CLA	MG-NA	5.97	2.20	2.06
20	3	603	CLA	MG-NA	5.96	2.20	2.06
20	A	1116	CLA	MG-NA	5.96	2.20	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B	1231	CLA	MG-NA	5.96	2.20	2.06
20	B	1206	CLA	MG-NA	5.96	2.20	2.06
20	A	1112	CLA	MG-NA	5.95	2.20	2.06
20	A	1135	CLA	MG-NA	5.95	2.20	2.06
20	B	1232	CLA	MG-NA	5.94	2.20	2.06
20	A	1134	CLA	MG-NA	5.94	2.20	2.06
20	1	603	CLA	MG-NA	5.93	2.20	2.06
20	A	1122	CLA	MG-NA	5.93	2.20	2.06
20	B	1218	CLA	MG-NA	5.93	2.20	2.06
20	A	1128	CLA	MG-NA	5.92	2.20	2.06
20	B	1204	CLA	MG-NA	5.91	2.20	2.06
20	B	1223	CLA	MG-NA	5.90	2.20	2.06
20	B	1236	CLA	MG-NA	5.90	2.20	2.06
20	B	1022	CLA	MG-NA	5.89	2.20	2.06
20	A	1121	CLA	MG-NA	5.89	2.20	2.06
20	A	1129	CLA	MG-NA	5.88	2.20	2.06
20	A	1118	CLA	MG-NA	5.88	2.20	2.06
20	1	601	CLA	MG-NA	5.88	2.20	2.06
20	A	1136	CLA	MG-NA	5.88	2.20	2.06
30	3	611	CHL	C3A-C2A	-5.88	1.49	1.54
20	2	605	CLA	MG-NA	5.87	2.20	2.06
20	B	1221	CLA	MG-NA	5.87	2.20	2.06
20	B	1224	CLA	MG-NA	5.87	2.20	2.06
20	B	1230	CLA	MG-NA	5.87	2.20	2.06
20	A	1104	CLA	MG-NA	5.86	2.20	2.06
20	B	1203	CLA	MG-NA	5.86	2.20	2.06
20	F	1301	CLA	MG-NA	5.86	2.20	2.06
22	2	503	BCR	C24-C23	5.86	1.50	1.33
20	A	1140	CLA	MG-NA	5.86	2.20	2.06
20	1	604	CLA	MG-NA	5.85	2.20	2.06
22	I	4020	BCR	C24-C23	5.85	1.50	1.33
22	H	4021	BCR	C24-C23	5.84	1.50	1.33
20	B	1219	CLA	MG-NA	5.84	2.20	2.06
20	A	1117	CLA	MG-NA	5.84	2.20	2.06
20	B	1208	CLA	MG-NA	5.83	2.20	2.06
20	B	1212	CLA	MG-NA	5.83	2.20	2.06
20	B	1202	CLA	MG-NA	5.82	2.20	2.06
20	B	1227	CLA	MG-NA	5.82	2.20	2.06
20	B	1228	CLA	MG-NA	5.81	2.20	2.06
22	L	4020	BCR	C24-C23	5.81	1.50	1.33
20	A	1131	CLA	MG-NA	5.81	2.20	2.06
20	A	1105	CLA	MG-NA	5.80	2.20	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	A	1111	CLA	MG-NA	5.80	2.20	2.06
20	A	1107	CLA	MG-NA	5.80	2.20	2.06
20	A	1119	CLA	MG-NA	5.80	2.20	2.06
20	A	1115	CLA	MG-NA	5.80	2.20	2.06
22	1	504	BCR	C24-C23	5.80	1.50	1.33
20	B	1209	CLA	MG-NA	5.79	2.20	2.06
20	A	1124	CLA	MG-NA	5.79	2.20	2.06
20	B	1225	CLA	MG-NA	5.79	2.20	2.06
22	K	4002	BCR	C24-C23	5.79	1.50	1.33
20	A	1113	CLA	MG-NA	5.79	2.20	2.06
20	B	1229	CLA	MG-NA	5.78	2.20	2.06
20	A	1012	CLA	MG-NA	5.78	2.20	2.06
20	3	601	CLA	MG-NA	5.78	2.20	2.06
20	B	1216	CLA	MG-NA	5.78	2.20	2.06
20	B	1235	CLA	MG-NA	5.77	2.20	2.06
20	A	1138	CLA	MG-NA	5.77	2.20	2.06
22	I	4018	BCR	C24-C23	5.76	1.50	1.33
20	B	1217	CLA	MG-NA	5.75	2.19	2.06
20	A	1133	CLA	MG-NA	5.74	2.19	2.06
20	1	608	CLA	MG-NA	5.73	2.19	2.06
20	A	1125	CLA	MG-NA	5.73	2.19	2.06
20	B	1215	CLA	MG-NA	5.72	2.19	2.06
20	1	605	CLA	MG-NA	5.72	2.19	2.06
20	B	1220	CLA	MG-NA	5.71	2.19	2.06
20	B	1222	CLA	MG-NA	5.71	2.19	2.06
22	3	506	BCR	C24-C23	5.71	1.50	1.33
20	A	1102	CLA	MG-NA	5.71	2.19	2.06
22	1	503	BCR	C24-C23	5.70	1.50	1.33
20	A	1126	CLA	MG-NA	5.69	2.19	2.06
20	B	1201	CLA	MG-NA	5.69	2.19	2.06
20	A	1013	CLA	MG-NA	5.68	2.19	2.06
20	B	1226	CLA	MG-NA	5.68	2.19	2.06
20	A	1103	CLA	MG-NA	5.68	2.19	2.06
20	3	606	CLA	MG-NA	5.67	2.19	2.06
22	A	4008	BCR	C11-C12	-5.66	1.19	1.34
20	A	1127	CLA	MG-NA	5.66	2.19	2.06
22	3	503	BCR	C24-C23	5.66	1.49	1.33
20	B	1023	CLA	MG-NA	5.64	2.19	2.06
20	B	1205	CLA	MG-NA	5.63	2.19	2.06
20	B	1021	CLA	MG-NA	5.63	2.19	2.06
22	3	506	BCR	C11-C12	-5.62	1.20	1.34
20	A	1106	CLA	MG-NA	5.62	2.19	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	4007	BCR	C24-C23	5.62	1.49	1.33
22	B	4004	BCR	C24-C23	5.61	1.49	1.33
22	A	4002	BCR	C24-C23	5.61	1.49	1.33
22	B	4005	BCR	C24-C23	5.58	1.49	1.33
22	G	4011	BCR	C24-C23	5.58	1.49	1.33
22	F	4016	BCR	C11-C12	-5.54	1.20	1.34
22	A	4002	BCR	C11-C12	-5.54	1.20	1.34
22	K	4001	BCR	C24-C23	5.53	1.49	1.33
22	B	4010	BCR	C11-C12	-5.53	1.20	1.34
22	A	4003	BCR	C24-C23	5.52	1.49	1.33
20	B	1211	CLA	MG-NA	5.52	2.19	2.06
22	A	4011	BCR	C24-C23	5.49	1.49	1.33
22	F	4016	BCR	C24-C23	5.49	1.49	1.33
22	B	4010	BCR	C24-C23	5.49	1.49	1.33
22	A	4008	BCR	C24-C23	5.47	1.49	1.33
22	B	4009	BCR	C24-C23	5.47	1.49	1.33
22	F	4014	BCR	C24-C23	5.46	1.49	1.33
22	A	4017	BCR	C24-C23	5.45	1.49	1.33
22	I	4018	BCR	C11-C12	-5.41	1.20	1.34
22	J	4012	BCR	C24-C23	5.40	1.49	1.33
22	A	4011	BCR	C11-C12	-5.40	1.20	1.34
20	2	612	CLA	MG-NA	5.39	2.19	2.06
22	J	4012	BCR	C11-C12	-5.34	1.20	1.34
22	A	4017	BCR	C11-C12	-5.33	1.20	1.34
22	A	4003	BCR	C11-C12	-5.33	1.20	1.34
22	A	4007	BCR	C11-C12	-5.32	1.20	1.34
22	B	4009	BCR	C11-C12	-5.32	1.20	1.34
22	1	503	BCR	C11-C12	-5.29	1.20	1.34
22	F	4014	BCR	C11-C12	-5.29	1.20	1.34
19	A	1011	CL0	CHC-C4B	5.28	1.48	1.39
22	B	4006	BCR	C24-C23	5.28	1.48	1.33
19	A	1011	CL0	O2A-C1	5.25	1.60	1.46
22	B	4005	BCR	C11-C12	-5.23	1.21	1.34
22	B	4006	BCR	C11-C12	-5.21	1.21	1.34
22	K	4001	BCR	C11-C12	-5.18	1.21	1.34
22	3	503	BCR	C11-C12	-5.14	1.21	1.34
22	L	4020	BCR	C11-C12	-5.14	1.21	1.34
22	1	504	BCR	C11-C12	-5.13	1.21	1.34
22	H	4021	BCR	C11-C12	-5.11	1.21	1.34
22	I	4020	BCR	C11-C12	-5.04	1.21	1.34
30	4	611	CHL	C3A-C2A	-5.01	1.50	1.54
22	G	4011	BCR	C11-C12	-4.98	1.21	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	2	503	BCR	C11-C12	-4.97	1.21	1.34
19	A	1011	CL0	CHB-C1B	4.94	1.47	1.39
22	B	4004	BCR	C11-C12	-4.92	1.21	1.34
22	K	4002	BCR	C11-C12	-4.81	1.22	1.34
20	A	1012	CLA	MG-ND	-4.76	1.96	2.05
30	1	609	CHL	C3A-C2A	-4.72	1.50	1.54
30	3	607	CHL	C3B-C4B	4.69	1.46	1.41
19	A	1011	CL0	O2D-CGD	4.69	1.44	1.33
20	A	1127	CLA	MG-ND	-4.67	1.96	2.05
22	L	4019	BCR	C11-C12	-4.66	1.22	1.34
20	B	1022	CLA	MG-ND	-4.66	1.96	2.05
22	L	4019	BCR	C10-C9	4.62	1.46	1.35
30	4	613	CHL	C3B-C2B	-4.61	1.34	1.40
19	A	1011	CL0	CHD-C4C	4.60	1.48	1.39
20	B	1023	CLA	MG-ND	-4.59	1.96	2.05
19	A	1011	CL0	C3B-C2B	4.59	1.46	1.40
20	A	1133	CLA	MG-ND	-4.58	1.96	2.05
20	A	1013	CLA	MG-ND	-4.56	1.96	2.05
22	B	4010	BCR	C16-C17	-4.54	1.29	1.43
20	B	1021	CLA	MG-ND	-4.53	1.96	2.05
20	B	1214	CLA	MG-ND	-4.53	1.96	2.05
30	2	611	CHL	C1A-CHA	-4.53	1.34	1.40
20	B	1226	CLA	MG-ND	-4.52	1.96	2.05
22	B	4004	BCR	C10-C9	4.52	1.46	1.35
19	A	1011	CL0	CHD-C1D	4.51	1.46	1.39
20	A	1139	CLA	MG-ND	-4.51	1.96	2.05
30	2	610	CHL	C3B-C4B	4.50	1.45	1.41
22	J	4012	BCR	C16-C17	-4.49	1.29	1.43
20	1	613	CLA	MG-ND	-4.49	1.96	2.05
20	G	1601	CLA	MG-ND	-4.49	1.96	2.05
19	A	1011	CL0	OBD-CAD	4.49	1.28	1.22
20	A	1117	CLA	MG-ND	-4.48	1.96	2.05
20	2	608	CLA	CBB-CAB	4.48	1.51	1.30
22	1	504	BCR	C16-C17	-4.47	1.29	1.43
22	A	4003	BCR	C16-C17	-4.47	1.29	1.43
22	A	4011	BCR	C16-C17	-4.47	1.29	1.43
20	B	1228	CLA	MG-ND	-4.46	1.96	2.05
20	A	1113	CLA	MG-ND	-4.46	1.96	2.05
20	B	1234	CLA	MG-ND	-4.46	1.96	2.05
20	A	1116	CLA	MG-ND	-4.46	1.96	2.05
22	F	4016	BCR	C16-C17	-4.45	1.29	1.43
22	B	4009	BCR	C16-C17	-4.44	1.29	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	4008	BCR	C16-C17	-4.44	1.29	1.43
20	B	1201	CLA	MG-ND	-4.44	1.97	2.05
20	2	606	CLA	CBB-CAB	4.44	1.51	1.30
22	1	503	BCR	C16-C17	-4.44	1.29	1.43
20	A	1108	CLA	MG-ND	-4.43	1.97	2.05
20	4	605	CLA	MG-ND	-4.43	1.97	2.05
20	B	1239	CLA	MG-ND	-4.43	1.97	2.05
20	A	1130	CLA	MG-ND	-4.42	1.97	2.05
20	A	1131	CLA	MG-ND	-4.42	1.97	2.05
20	B	1231	CLA	MG-ND	-4.42	1.97	2.05
20	4	606	CLA	CBB-CAB	4.42	1.51	1.30
20	B	1220	CLA	MG-ND	-4.41	1.97	2.05
20	3	601	CLA	CBB-CAB	4.41	1.51	1.30
20	3	608	CLA	CBB-CAB	4.41	1.51	1.30
20	A	1119	CLA	MG-ND	-4.41	1.97	2.05
20	A	1137	CLA	MG-ND	-4.41	1.97	2.05
20	A	1126	CLA	MG-ND	-4.41	1.97	2.05
20	A	1112	CLA	MG-ND	-4.41	1.97	2.05
30	2	609	CHL	C3B-C4B	4.41	1.45	1.41
20	A	1129	CLA	CBB-CAB	4.41	1.51	1.30
20	4	607	CLA	CBB-CAB	4.40	1.51	1.30
20	K	1402	CLA	CBB-CAB	4.40	1.51	1.30
20	B	1223	CLA	MG-ND	-4.40	1.97	2.05
20	A	1106	CLA	MG-ND	-4.40	1.97	2.05
20	3	602	CLA	CBB-CAB	4.40	1.51	1.30
20	2	607	CLA	CBB-CAB	4.40	1.51	1.30
20	J	1901	CLA	CBB-CAB	4.39	1.51	1.30
20	4	608	CLA	CBB-CAB	4.39	1.51	1.30
20	B	1240	CLA	CBB-CAB	4.39	1.51	1.30
20	L	1503	CLA	CBB-CAB	4.39	1.51	1.30
20	3	610	CLA	CBB-CAB	4.39	1.51	1.30
22	G	4011	BCR	C16-C17	-4.39	1.29	1.43
20	1	611	CLA	CBB-CAB	4.39	1.51	1.30
20	A	1104	CLA	MG-ND	-4.39	1.97	2.05
20	K	1401	CLA	CBB-CAB	4.39	1.51	1.30
20	A	1128	CLA	MG-ND	-4.39	1.97	2.05
20	A	1110	CLA	CBB-CAB	4.39	1.51	1.30
20	A	1119	CLA	CBB-CAB	4.38	1.51	1.30
20	L	1502	CLA	CBB-CAB	4.38	1.51	1.30
20	K	1403	CLA	CBB-CAB	4.38	1.51	1.30
20	B	1206	CLA	CBB-CAB	4.38	1.51	1.30
20	B	1213	CLA	MG-ND	-4.38	1.97	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B	1221	CLA	CBB-CAB	4.38	1.51	1.30
22	F	4014	BCR	C16-C17	-4.38	1.29	1.43
20	A	1118	CLA	CBB-CAB	4.38	1.51	1.30
20	A	1121	CLA	CBB-CAB	4.38	1.51	1.30
20	A	1141	CLA	CBB-CAB	4.38	1.51	1.30
20	B	1227	CLA	MG-ND	-4.38	1.97	2.05
20	A	1125	CLA	CBB-CAB	4.38	1.51	1.30
20	1	606	CLA	CBB-CAB	4.38	1.51	1.30
20	4	601	CLA	CBB-CAB	4.38	1.51	1.30
20	4	602	CLA	CBB-CAB	4.37	1.51	1.30
20	B	1224	CLA	MG-ND	-4.37	1.97	2.05
20	B	1217	CLA	MG-ND	-4.37	1.97	2.05
20	A	1118	CLA	MG-ND	-4.37	1.97	2.05
20	A	1132	CLA	CBB-CAB	4.37	1.51	1.30
20	1	608	CLA	CBB-CAB	4.37	1.51	1.30
20	4	609	CLA	CBB-CAB	4.37	1.51	1.30
20	G	1603	CLA	CBB-CAB	4.37	1.51	1.30
20	3	612	CLA	CBB-CAB	4.37	1.51	1.30
20	A	1135	CLA	MG-ND	-4.37	1.97	2.05
20	2	604	CLA	CBB-CAB	4.37	1.51	1.30
20	4	617	CLA	CBB-CAB	4.37	1.51	1.30
20	B	1207	CLA	CBB-CAB	4.37	1.51	1.30
20	A	1101	CLA	CBB-CAB	4.36	1.51	1.30
20	B	1228	CLA	CBB-CAB	4.36	1.51	1.30
20	K	1404	CLA	CBB-CAB	4.36	1.51	1.30
20	B	1225	CLA	MG-ND	-4.36	1.97	2.05
22	A	4002	BCR	C16-C17	-4.36	1.29	1.43
20	A	1140	CLA	MG-ND	-4.36	1.97	2.05
20	2	612	CLA	CBB-CAB	4.36	1.51	1.30
20	B	1210	CLA	CBB-CAB	4.36	1.51	1.30
20	A	1105	CLA	MG-ND	-4.36	1.97	2.05
20	4	604	CLA	CBB-CAB	4.35	1.51	1.30
20	B	1240	CLA	MG-ND	-4.35	1.97	2.05
20	B	1213	CLA	CBB-CAB	4.35	1.51	1.30
20	2	605	CLA	CBB-CAB	4.35	1.51	1.30
20	B	1206	CLA	MG-ND	-4.35	1.97	2.05
20	B	1203	CLA	MG-ND	-4.35	1.97	2.05
20	B	1237	CLA	CBB-CAB	4.35	1.51	1.30
20	A	1121	CLA	MG-ND	-4.35	1.97	2.05
20	G	1602	CLA	CBB-CAB	4.35	1.51	1.30
20	4	605	CLA	CBB-CAB	4.35	1.51	1.30
20	H	1701	CLA	CBB-CAB	4.35	1.51	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	A	1135	CLA	CBB-CAB	4.35	1.51	1.30
20	2	601	CLA	MG-ND	-4.35	1.97	2.05
20	1	605	CLA	CBB-CAB	4.35	1.51	1.30
20	1	601	CLA	CBB-CAB	4.35	1.51	1.30
20	L	1501	CLA	CBB-CAB	4.34	1.51	1.30
20	A	1123	CLA	CBB-CAB	4.34	1.51	1.30
20	B	1210	CLA	MG-ND	-4.34	1.97	2.05
20	A	1130	CLA	CBB-CAB	4.34	1.51	1.30
20	B	1212	CLA	CBB-CAB	4.34	1.51	1.30
22	B	4006	BCR	C16-C17	-4.34	1.29	1.43
20	A	1111	CLA	CBB-CAB	4.34	1.51	1.30
20	A	1109	CLA	CBB-CAB	4.34	1.51	1.30
20	3	606	CLA	CBB-CAB	4.34	1.51	1.30
20	B	1235	CLA	CBB-CAB	4.34	1.51	1.30
20	3	605	CLA	CBB-CAB	4.34	1.51	1.30
20	B	1201	CLA	CBB-CAB	4.34	1.51	1.30
20	B	1238	CLA	CBB-CAB	4.34	1.51	1.30
20	A	1124	CLA	CBB-CAB	4.33	1.51	1.30
20	A	1106	CLA	CBB-CAB	4.33	1.51	1.30
20	B	1215	CLA	CBB-CAB	4.33	1.51	1.30
22	K	4001	BCR	C16-C17	-4.33	1.29	1.43
20	A	1136	CLA	MG-ND	-4.33	1.97	2.05
20	B	1236	CLA	MG-ND	-4.33	1.97	2.05
20	A	1133	CLA	CBB-CAB	4.33	1.51	1.30
20	1	613	CLA	CBB-CAB	4.32	1.51	1.30
20	B	1209	CLA	CBB-CAB	4.32	1.51	1.30
20	B	1227	CLA	CBB-CAB	4.32	1.51	1.30
20	A	1112	CLA	CBB-CAB	4.32	1.51	1.30
20	B	1222	CLA	CBB-CAB	4.32	1.51	1.30
20	B	1022	CLA	CBB-CAB	4.32	1.51	1.30
20	B	1230	CLA	CBB-CAB	4.32	1.51	1.30
20	G	1601	CLA	CBB-CAB	4.32	1.51	1.30
20	3	613	CLA	CBB-CAB	4.32	1.51	1.30
20	A	1134	CLA	CBB-CAB	4.31	1.51	1.30
20	B	1229	CLA	MG-ND	-4.31	1.97	2.05
20	3	603	CLA	CBB-CAB	4.31	1.51	1.30
20	1	604	CLA	CBB-CAB	4.31	1.51	1.30
20	A	1102	CLA	MG-ND	-4.31	1.97	2.05
20	B	1221	CLA	MG-ND	-4.31	1.97	2.05
20	A	1131	CLA	CBB-CAB	4.31	1.51	1.30
20	B	1211	CLA	CBB-CAB	4.31	1.51	1.30
20	B	1236	CLA	CBB-CAB	4.31	1.51	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B	1239	CLA	CBB-CAB	4.31	1.51	1.30
20	4	603	CLA	CBB-CAB	4.31	1.51	1.30
22	3	503	BCR	C16-C17	-4.31	1.29	1.43
20	A	1103	CLA	MG-ND	-4.31	1.97	2.05
20	A	1013	CLA	CBB-CAB	4.31	1.51	1.30
20	A	1107	CLA	CBB-CAB	4.31	1.51	1.30
20	B	1204	CLA	MG-ND	-4.31	1.97	2.05
30	3	604	CHL	C3B-C4B	4.31	1.45	1.41
28	1	803	DGD	O1G-C1A	4.31	1.45	1.33
20	A	1117	CLA	CBB-CAB	4.30	1.51	1.30
20	3	617	CLA	CBB-CAB	4.30	1.51	1.30
22	K	4002	BCR	C10-C9	4.30	1.45	1.35
20	B	1229	CLA	CBB-CAB	4.30	1.51	1.30
20	1	607	CLA	CBB-CAB	4.30	1.51	1.30
20	A	1126	CLA	CBB-CAB	4.30	1.51	1.30
20	1	603	CLA	CBB-CAB	4.30	1.51	1.30
20	B	1205	CLA	CBB-CAB	4.30	1.51	1.30
20	B	1232	CLA	CBB-CAB	4.30	1.51	1.30
20	B	1218	CLA	CBB-CAB	4.30	1.51	1.30
20	B	1205	CLA	MG-ND	-4.30	1.97	2.05
20	B	1224	CLA	CBB-CAB	4.30	1.51	1.30
30	2	611	CHL	C3A-C2A	-4.30	1.51	1.54
20	A	1114	CLA	CBB-CAB	4.30	1.51	1.30
20	A	1108	CLA	CBB-CAB	4.30	1.51	1.30
20	B	1231	CLA	CBB-CAB	4.30	1.51	1.30
20	2	605	CLA	MG-ND	-4.30	1.97	2.05
20	F	1301	CLA	CBB-CAB	4.29	1.51	1.30
20	1	602	CLA	CBB-CAB	4.29	1.51	1.30
30	1	609	CHL	C3B-C4B	4.29	1.45	1.41
20	A	1113	CLA	CBB-CAB	4.29	1.51	1.30
20	B	1220	CLA	CBB-CAB	4.29	1.51	1.30
20	A	1104	CLA	CBB-CAB	4.29	1.51	1.30
20	2	601	CLA	CBB-CAB	4.29	1.51	1.30
22	B	4005	BCR	C16-C17	-4.29	1.29	1.43
20	B	1204	CLA	CBB-CAB	4.29	1.51	1.30
20	3	605	CLA	MG-ND	-4.29	1.97	2.05
22	3	506	BCR	C16-C17	-4.29	1.29	1.43
20	A	1120	CLA	CBB-CAB	4.29	1.51	1.30
20	1	603	CLA	MG-ND	-4.29	1.97	2.05
22	A	4007	BCR	C16-C17	-4.29	1.29	1.43
20	B	1225	CLA	CBB-CAB	4.29	1.51	1.30
20	A	1138	CLA	CBB-CAB	4.29	1.51	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B	1222	CLA	MG-ND	-4.29	1.97	2.05
20	A	1127	CLA	CBB-CAB	4.28	1.51	1.30
20	1	607	CLA	MG-ND	-4.28	1.97	2.05
20	1	614	CLA	CBB-CAB	4.28	1.51	1.30
20	1	608	CLA	MG-ND	-4.28	1.97	2.05
20	B	1021	CLA	CBB-CAB	4.28	1.51	1.30
20	A	1140	CLA	CBB-CAB	4.28	1.51	1.30
20	A	1137	CLA	CBB-CAB	4.28	1.50	1.30
20	A	1139	CLA	CBB-CAB	4.28	1.50	1.30
20	B	1023	CLA	CBB-CAB	4.28	1.50	1.30
20	B	1216	CLA	CBB-CAB	4.28	1.50	1.30
20	A	1012	CLA	CBB-CAB	4.28	1.50	1.30
20	B	1217	CLA	CBB-CAB	4.28	1.50	1.30
20	B	1223	CLA	CBB-CAB	4.28	1.50	1.30
20	B	1219	CLA	CBB-CAB	4.28	1.50	1.30
30	4	610	CHL	C3B-C4B	4.28	1.45	1.41
20	2	602	CLA	CBB-CAB	4.28	1.50	1.30
20	B	1226	CLA	CBB-CAB	4.27	1.50	1.30
20	A	1120	CLA	MG-ND	-4.27	1.97	2.05
20	F	1301	CLA	MG-ND	-4.27	1.97	2.05
20	A	1122	CLA	CBB-CAB	4.27	1.50	1.30
20	B	1203	CLA	CBB-CAB	4.27	1.50	1.30
20	A	1136	CLA	CBB-CAB	4.27	1.50	1.30
20	B	1208	CLA	CBB-CAB	4.27	1.50	1.30
20	4	612	CLA	CBB-CAB	4.27	1.50	1.30
20	A	1123	CLA	MG-ND	-4.27	1.97	2.05
20	A	1129	CLA	MG-ND	-4.26	1.97	2.05
20	A	1116	CLA	CBB-CAB	4.26	1.50	1.30
20	B	1202	CLA	CBB-CAB	4.26	1.50	1.30
22	A	4017	BCR	C16-C17	-4.26	1.30	1.43
20	A	1128	CLA	CBB-CAB	4.26	1.50	1.30
20	2	603	CLA	CBB-CAB	4.25	1.50	1.30
20	A	1103	CLA	CBB-CAB	4.25	1.50	1.30
20	A	1105	CLA	CBB-CAB	4.25	1.50	1.30
20	A	1110	CLA	MG-ND	-4.25	1.97	2.05
20	B	1211	CLA	MG-ND	-4.24	1.97	2.05
20	3	614	CLA	CBB-CAB	4.24	1.50	1.30
20	3	603	CLA	MG-ND	-4.24	1.97	2.05
28	F	5005	DGD	O1G-C1A	4.23	1.45	1.33
20	B	1232	CLA	MG-ND	-4.23	1.97	2.05
20	A	1138	CLA	MG-ND	-4.23	1.97	2.05
20	B	1214	CLA	CBB-CAB	4.23	1.50	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	A	1102	CLA	CBB-CAB	4.23	1.50	1.30
20	3	610	CLA	MG-ND	-4.22	1.97	2.05
20	B	1234	CLA	CBB-CAB	4.22	1.50	1.30
20	A	1122	CLA	MG-ND	-4.22	1.97	2.05
22	2	503	BCR	C10-C9	4.22	1.45	1.35
20	A	1124	CLA	MG-ND	-4.22	1.97	2.05
20	1	611	CLA	MG-ND	-4.21	1.97	2.05
22	1	504	BCR	C10-C9	4.21	1.45	1.35
20	A	1115	CLA	CBB-CAB	4.20	1.50	1.30
20	A	1115	CLA	MG-ND	-4.20	1.97	2.05
20	1	606	CLA	MG-ND	-4.20	1.97	2.05
22	G	4011	BCR	C10-C9	4.20	1.45	1.35
28	4	802	DGD	O1G-C1A	4.19	1.45	1.33
20	B	1212	CLA	MG-ND	-4.19	1.97	2.05
20	F	1302	CLA	MG-ND	-4.19	1.97	2.05
20	3	606	CLA	MG-ND	-4.19	1.97	2.05
22	I	4018	BCR	C10-C9	4.19	1.45	1.35
20	F	1302	CLA	CBB-CAB	4.18	1.50	1.30
20	A	1134	CLA	MG-ND	-4.18	1.97	2.05
20	1	602	CLA	MG-ND	-4.18	1.97	2.05
22	H	4021	BCR	C10-C9	4.18	1.45	1.35
20	A	1114	CLA	MG-ND	-4.18	1.97	2.05
20	B	1209	CLA	MG-ND	-4.17	1.97	2.05
22	K	4002	BCR	C16-C17	-4.17	1.30	1.43
22	L	4020	BCR	C10-C9	4.17	1.45	1.35
20	B	1216	CLA	MG-ND	-4.16	1.97	2.05
20	B	1215	CLA	MG-ND	-4.16	1.97	2.05
20	B	1208	CLA	MG-ND	-4.16	1.97	2.05
22	I	4018	BCR	C16-C17	-4.16	1.30	1.43
28	G	5003	DGD	O1G-C1A	4.16	1.45	1.33
20	1	605	CLA	MG-ND	-4.16	1.97	2.05
20	A	1107	CLA	MG-ND	-4.16	1.97	2.05
20	A	1141	CLA	MG-ND	-4.16	1.97	2.05
22	B	4004	BCR	C16-C17	-4.15	1.30	1.43
20	3	614	CLA	MG-ND	-4.15	1.97	2.05
20	1	604	CLA	MG-ND	-4.15	1.97	2.05
20	2	612	CLA	MG-ND	-4.15	1.97	2.05
20	B	1202	CLA	MG-ND	-4.14	1.97	2.05
20	4	606	CLA	MG-ND	-4.14	1.97	2.05
20	A	1111	CLA	MG-ND	-4.14	1.97	2.05
22	I	4020	BCR	C10-C9	4.14	1.45	1.35
20	B	1219	CLA	MG-ND	-4.14	1.97	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	J	5001	DGD	O1G-C1A	4.13	1.45	1.33
20	A	1125	CLA	MG-ND	-4.13	1.97	2.05
20	B	1235	CLA	MG-ND	-4.12	1.97	2.05
20	B	1218	CLA	MG-ND	-4.12	1.97	2.05
28	3	803	DGD	O1G-C1A	4.12	1.45	1.33
20	G	1602	CLA	MG-ND	-4.12	1.97	2.05
22	3	506	BCR	C10-C9	4.11	1.45	1.35
22	I	4020	BCR	C16-C17	-4.11	1.30	1.43
20	3	613	CLA	MG-ND	-4.11	1.97	2.05
20	B	1230	CLA	MG-ND	-4.10	1.97	2.05
20	1	601	CLA	MG-ND	-4.10	1.97	2.05
22	L	4020	BCR	C16-C17	-4.10	1.30	1.43
30	2	611	CHL	C3B-C4B	4.09	1.45	1.41
20	J	1901	CLA	MG-ND	-4.09	1.97	2.05
22	H	4021	BCR	C16-C17	-4.08	1.30	1.43
20	B	1239	CLA	C1C-NC	-4.07	1.31	1.37
20	1	614	CLA	MG-ND	-4.06	1.97	2.05
22	K	4001	BCR	C10-C9	4.04	1.45	1.35
20	G	1603	CLA	MG-ND	-4.04	1.97	2.05
20	2	608	CLA	MG-ND	-4.04	1.97	2.05
22	2	503	BCR	C16-C17	-4.03	1.30	1.43
20	2	603	CLA	MG-ND	-4.03	1.97	2.05
20	2	602	CLA	MG-ND	-4.00	1.97	2.05
20	3	601	CLA	MG-ND	-3.99	1.97	2.05
20	A	1109	CLA	MG-ND	-3.96	1.97	2.05
28	B	5005	DGD	O1G-C1A	3.96	1.44	1.33
20	3	608	CLA	MG-ND	-3.96	1.97	2.05
20	K	1402	CLA	MG-ND	-3.96	1.97	2.05
20	K	1404	CLA	MG-ND	-3.95	1.98	2.05
30	3	611	CHL	C3B-C2B	-3.95	1.35	1.40
22	B	4006	BCR	C10-C9	3.95	1.44	1.35
22	3	503	BCR	C10-C9	3.94	1.44	1.35
30	1	609	CHL	C1A-CHA	-3.93	1.35	1.40
20	B	1210	CLA	C1C-NC	-3.92	1.31	1.37
22	B	4005	BCR	C10-C9	3.91	1.44	1.35
20	A	1125	CLA	C1C-NC	-3.86	1.31	1.37
22	A	4007	BCR	C10-C9	3.86	1.44	1.35
22	1	503	BCR	C10-C9	3.86	1.44	1.35
28	J	5001	DGD	CAA-C9A	-3.85	1.32	1.51
28	J	5001	DGD	CDA-CCA	-3.85	1.32	1.51
20	B	1225	CLA	C1C-NC	-3.85	1.31	1.37
20	K	1403	CLA	MG-ND	-3.84	1.98	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	L	4019	BCR	C16-C17	-3.84	1.31	1.43
20	A	1111	CLA	C1C-NC	-3.84	1.31	1.37
20	B	1215	CLA	C1C-NC	-3.84	1.31	1.37
20	B	1206	CLA	C1C-NC	-3.84	1.31	1.37
20	B	1205	CLA	C1C-NC	-3.83	1.31	1.37
20	B	1231	CLA	C1C-NC	-3.83	1.31	1.37
20	3	602	CLA	MG-ND	-3.83	1.98	2.05
20	A	1104	CLA	C1C-NC	-3.83	1.31	1.37
28	B	5005	DGD	CDB-CCB	-3.83	1.32	1.51
20	B	1023	CLA	C1C-NC	-3.82	1.31	1.37
20	B	1021	CLA	C1C-NC	-3.82	1.31	1.37
20	B	1240	CLA	C1C-NC	-3.82	1.31	1.37
20	A	1133	CLA	C1C-NC	-3.82	1.31	1.37
20	B	1226	CLA	C1C-NC	-3.81	1.31	1.37
20	B	1211	CLA	C1C-NC	-3.81	1.31	1.37
28	B	5005	DGD	CAB-C9B	-3.80	1.32	1.51
22	A	4003	BCR	C10-C9	3.80	1.44	1.35
28	J	5001	DGD	CGA-CFA	-3.80	1.32	1.51
22	2	503	BCR	C1-C6	-3.80	1.48	1.53
30	2	613	CHL	C1A-CHA	-3.80	1.35	1.40
20	B	1220	CLA	C1C-NC	-3.79	1.31	1.37
28	4	802	DGD	CAB-C9B	-3.79	1.32	1.51
20	A	1119	CLA	C1C-NC	-3.78	1.31	1.37
20	3	617	CLA	MG-ND	-3.77	1.98	2.05
26	G	5002	LMG	C37-C36	-3.77	1.33	1.51
33	4	505	C7Z	C35-C34	3.77	1.54	1.43
26	F	5002	LMG	C43-C42	-3.77	1.33	1.51
26	F	5002	LMG	C40-C39	-3.76	1.33	1.51
20	A	1138	CLA	C1C-NC	-3.76	1.32	1.37
26	1	802	LMG	C19-C18	-3.76	1.33	1.51
20	A	1106	CLA	C1C-NC	-3.76	1.32	1.37
20	A	1124	CLA	C1C-NC	-3.76	1.32	1.37
28	B	5005	DGD	CGB-CFB	-3.75	1.33	1.51
26	B	5003	LMG	C19-C18	-3.75	1.33	1.51
20	A	1105	CLA	C1C-NC	-3.75	1.32	1.37
20	B	1236	CLA	C1C-NC	-3.74	1.32	1.37
22	A	4017	BCR	C10-C9	3.74	1.44	1.35
20	A	1117	CLA	C1C-NC	-3.74	1.32	1.37
20	A	1013	CLA	C1C-NC	-3.74	1.32	1.37
26	G	5002	LMG	C19-C18	-3.74	1.33	1.51
20	A	1128	CLA	C1C-NC	-3.73	1.32	1.37
20	3	606	CLA	C1C-NC	-3.73	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	A	1138	CLA	C4B-NB	-3.73	1.33	1.37
26	G	5002	LMG	C40-C39	-3.72	1.33	1.51
20	A	1108	CLA	C1C-NC	-3.72	1.32	1.37
20	B	1212	CLA	C1C-NC	-3.71	1.32	1.37
26	A	5006	LMG	C25-C24	-3.71	1.33	1.51
20	A	1114	CLA	C1C-NC	-3.71	1.32	1.37
26	F	5002	LMG	C37-C36	-3.71	1.33	1.51
26	G	5001	LMG	C43-C42	-3.71	1.33	1.51
20	B	1222	CLA	C1C-NC	-3.71	1.32	1.37
28	B	5005	DGD	CAA-C9A	-3.71	1.33	1.51
20	A	1109	CLA	C1C-NC	-3.71	1.32	1.37
26	1	802	LMG	C22-C21	-3.71	1.33	1.51
28	F	5005	DGD	CGA-CFA	-3.71	1.33	1.51
30	4	611	CHL	C1A-CHA	-3.71	1.35	1.40
28	F	5005	DGD	CAA-C9A	-3.70	1.33	1.51
20	B	1214	CLA	C1C-NC	-3.69	1.32	1.37
20	A	1139	CLA	C1C-NC	-3.69	1.32	1.37
20	B	1217	CLA	C1C-NC	-3.69	1.32	1.37
26	G	5002	LMG	C22-C21	-3.69	1.33	1.51
26	G	5001	LMG	C19-C18	-3.69	1.33	1.51
22	F	4014	BCR	C10-C9	3.69	1.44	1.35
22	J	4012	BCR	C10-C9	3.69	1.44	1.35
28	F	5005	DGD	CDA-CCA	-3.68	1.33	1.51
20	B	1234	CLA	C1C-NC	-3.68	1.32	1.37
33	4	505	C7Z	C15-C14	3.68	1.54	1.43
20	A	1116	CLA	C1C-NC	-3.68	1.32	1.37
26	A	5006	LMG	C22-C21	-3.68	1.33	1.51
26	F	5003	LMG	C37-C36	-3.67	1.33	1.51
20	A	1121	CLA	C1C-NC	-3.67	1.32	1.37
26	A	5006	LMG	C37-C36	-3.67	1.33	1.51
20	4	602	CLA	MG-ND	-3.67	1.98	2.05
20	A	1140	CLA	C1C-NC	-3.67	1.32	1.37
20	B	1224	CLA	C1C-NC	-3.67	1.32	1.37
20	A	1110	CLA	C1C-NC	-3.67	1.32	1.37
26	1	802	LMG	C25-C24	-3.67	1.33	1.51
20	A	1107	CLA	C1C-NC	-3.67	1.32	1.37
20	1	603	CLA	C1C-NC	-3.67	1.32	1.37
30	4	611	CHL	CBB-CAB	3.66	1.52	1.29
20	A	1126	CLA	C1C-NC	-3.66	1.32	1.37
20	3	601	CLA	C1C-NC	-3.66	1.32	1.37
20	B	1022	CLA	C1C-NC	-3.65	1.32	1.37
26	G	5001	LMG	C37-C36	-3.65	1.33	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B	1235	CLA	C1C-NC	-3.65	1.32	1.37
20	B	1201	CLA	C1C-NC	-3.64	1.32	1.37
22	B	4009	BCR	C10-C9	3.64	1.44	1.35
20	4	605	CLA	C1C-NC	-3.64	1.32	1.37
20	A	1118	CLA	C1C-NC	-3.64	1.32	1.37
26	G	5001	LMG	C40-C39	-3.64	1.33	1.51
20	4	607	CLA	MG-ND	-3.64	1.98	2.05
20	3	603	CLA	C1C-NC	-3.64	1.32	1.37
20	B	1202	CLA	C1C-NC	-3.64	1.32	1.37
20	1	601	CLA	C1C-NC	-3.63	1.32	1.37
22	F	4016	BCR	C10-C9	3.63	1.44	1.35
20	F	1302	CLA	C1C-NC	-3.63	1.32	1.37
20	A	1103	CLA	C1C-NC	-3.62	1.32	1.37
22	A	4002	BCR	C10-C9	3.62	1.44	1.35
20	F	1301	CLA	C1C-NC	-3.62	1.32	1.37
20	G	1602	CLA	C1C-NC	-3.62	1.32	1.37
20	A	1122	CLA	C1C-NC	-3.62	1.32	1.37
20	3	606	CLA	C4B-NB	-3.61	1.33	1.37
30	3	604	CHL	CBB-CAB	3.61	1.52	1.29
20	2	607	CLA	MG-ND	-3.61	1.98	2.05
30	4	613	CHL	C3A-C2A	-3.61	1.51	1.54
20	A	1137	CLA	C1C-NC	-3.61	1.32	1.37
20	4	617	CLA	MG-ND	-3.61	1.98	2.05
22	A	4011	BCR	C10-C9	3.60	1.44	1.35
20	B	1229	CLA	C1C-NC	-3.60	1.32	1.37
20	A	1119	CLA	C4B-NB	-3.60	1.33	1.37
30	3	611	CHL	C3B-C4B	3.60	1.44	1.41
26	A	5006	LMG	C19-C18	-3.60	1.33	1.51
20	4	601	CLA	MG-ND	-3.60	1.98	2.05
30	2	609	CHL	C1A-CHA	-3.60	1.35	1.40
20	A	1111	CLA	C4B-NB	-3.60	1.33	1.37
20	1	613	CLA	C1C-NC	-3.60	1.32	1.37
20	A	1127	CLA	C1C-NC	-3.59	1.32	1.37
20	A	1136	CLA	C1C-NC	-3.59	1.32	1.37
20	B	1219	CLA	C4B-NB	-3.59	1.33	1.37
20	B	1214	CLA	C4B-NB	-3.59	1.33	1.37
20	B	1230	CLA	C1C-NC	-3.59	1.32	1.37
20	1	614	CLA	C1C-NC	-3.59	1.32	1.37
20	B	1234	CLA	C4B-NB	-3.58	1.33	1.37
20	B	1232	CLA	C1C-NC	-3.58	1.32	1.37
20	B	1023	CLA	C4B-NB	-3.58	1.33	1.37
20	B	1221	CLA	C1C-NC	-3.58	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B	1223	CLA	C1C-NC	-3.58	1.32	1.37
20	B	1211	CLA	C4B-NB	-3.58	1.33	1.37
20	4	612	CLA	MG-ND	-3.58	1.98	2.05
20	3	605	CLA	C1C-NC	-3.57	1.32	1.37
20	A	1127	CLA	C4B-NB	-3.57	1.33	1.37
20	A	1135	CLA	C1C-NC	-3.57	1.32	1.37
20	A	1131	CLA	C1C-NC	-3.57	1.32	1.37
20	A	1103	CLA	C4B-NB	-3.57	1.33	1.37
20	B	1208	CLA	C1C-NC	-3.56	1.32	1.37
30	1	610	CHL	C1A-CHA	-3.56	1.36	1.40
20	B	1225	CLA	C4B-NB	-3.56	1.33	1.37
20	A	1125	CLA	C4B-NB	-3.56	1.33	1.37
30	4	615	CHL	CBB-CAB	3.56	1.51	1.29
22	A	4008	BCR	C10-C9	3.55	1.44	1.35
20	B	1219	CLA	C1C-NC	-3.55	1.32	1.37
30	3	611	CHL	C1A-CHA	-3.55	1.36	1.40
20	B	1204	CLA	C4B-NB	-3.55	1.33	1.37
33	4	505	C7Z	C31-C30	3.55	1.54	1.43
20	B	1237	CLA	MG-ND	-3.55	1.98	2.05
20	A	1129	CLA	C1C-NC	-3.54	1.32	1.37
20	A	1117	CLA	C4B-NB	-3.54	1.33	1.37
33	4	505	C7Z	C11-C10	3.54	1.54	1.43
20	2	601	CLA	C1C-NC	-3.54	1.32	1.37
20	2	605	CLA	C1C-NC	-3.54	1.32	1.37
30	2	611	CHL	CBB-CAB	3.54	1.51	1.29
20	1	611	CLA	C1C-NC	-3.53	1.32	1.37
30	3	607	CHL	CBB-CAB	3.53	1.51	1.29
20	B	1227	CLA	C1C-NC	-3.53	1.32	1.37
20	B	1215	CLA	C4B-NB	-3.53	1.33	1.37
20	G	1603	CLA	C1C-NC	-3.53	1.32	1.37
20	A	1126	CLA	C4B-NB	-3.53	1.33	1.37
20	B	1222	CLA	C4B-NB	-3.52	1.33	1.37
20	4	604	CLA	MG-ND	-3.52	1.98	2.05
33	4	505	C7Z	C12-C13	3.52	1.53	1.46
20	4	609	CLA	MG-ND	-3.52	1.98	2.05
20	3	612	CLA	MG-ND	-3.51	1.98	2.05
20	B	1022	CLA	C4B-NB	-3.51	1.33	1.37
20	A	1101	CLA	MG-ND	-3.51	1.98	2.05
20	B	1204	CLA	C1C-NC	-3.51	1.32	1.37
20	1	605	CLA	C1C-NC	-3.51	1.32	1.37
30	2	610	CHL	C1A-CHA	-3.51	1.36	1.40
30	2	609	CHL	CBB-CAB	3.51	1.51	1.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	2	610	CHL	CBB-CAB	3.51	1.51	1.29
19	A	1011	CL0	CHB-C4A	-3.50	1.34	1.38
20	L	1501	CLA	MG-ND	-3.50	1.98	2.05
20	B	1231	CLA	C4B-NB	-3.50	1.33	1.37
30	2	615	CHL	CBB-CAB	3.50	1.51	1.29
20	A	1115	CLA	C1C-NC	-3.50	1.32	1.37
20	B	1210	CLA	C4B-NB	-3.50	1.33	1.37
20	G	1601	CLA	C1C-NC	-3.50	1.32	1.37
19	A	1011	CL0	C3A-C2A	-3.50	1.51	1.54
20	2	603	CLA	C1C-NC	-3.49	1.32	1.37
20	4	608	CLA	MG-ND	-3.49	1.98	2.05
20	2	604	CLA	MG-ND	-3.49	1.98	2.05
20	B	1228	CLA	C1C-NC	-3.49	1.32	1.37
20	A	1012	CLA	C1C-NC	-3.49	1.32	1.37
20	1	604	CLA	C1C-NC	-3.49	1.32	1.37
20	2	608	CLA	C1C-NC	-3.48	1.32	1.37
20	A	1102	CLA	C1C-NC	-3.48	1.32	1.37
20	B	1220	CLA	C4B-NB	-3.48	1.33	1.37
19	A	1011	CL0	CBB-CAB	3.48	1.51	1.29
20	B	1203	CLA	C1C-NC	-3.48	1.32	1.37
20	A	1106	CLA	C4B-NB	-3.48	1.33	1.37
30	2	613	CHL	CBB-CAB	3.47	1.51	1.29
20	B	1213	CLA	C1C-NC	-3.47	1.32	1.37
20	1	607	CLA	C1C-NC	-3.47	1.32	1.37
20	B	1229	CLA	C4B-NB	-3.47	1.33	1.37
20	2	606	CLA	MG-ND	-3.47	1.98	2.05
20	B	1021	CLA	C4B-NB	-3.47	1.33	1.37
20	L	1503	CLA	MG-ND	-3.47	1.98	2.05
22	B	4010	BCR	C10-C9	3.47	1.43	1.35
20	A	1112	CLA	C1C-NC	-3.46	1.32	1.37
20	A	1132	CLA	MG-ND	-3.46	1.98	2.05
20	3	613	CLA	C1C-NC	-3.46	1.32	1.37
30	1	609	CHL	CBB-CAB	3.46	1.51	1.29
20	A	1124	CLA	C4B-NB	-3.46	1.33	1.37
20	1	608	CLA	C1C-NC	-3.46	1.32	1.37
30	1	612	CHL	C3B-C4B	3.45	1.44	1.41
20	1	606	CLA	C1C-NC	-3.45	1.32	1.37
20	A	1108	CLA	C4B-NB	-3.45	1.33	1.37
30	2	613	CHL	C3B-C4B	3.45	1.44	1.41
20	4	603	CLA	MG-ND	-3.45	1.99	2.05
20	A	1130	CLA	C1C-NC	-3.45	1.32	1.37
20	K	1401	CLA	MG-ND	-3.44	1.99	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B	1223	CLA	C4B-NB	-3.44	1.33	1.37
20	F	1301	CLA	C4B-NB	-3.44	1.33	1.37
30	1	612	CHL	CBB-CAB	3.44	1.50	1.29
20	B	1216	CLA	C1C-NC	-3.44	1.32	1.37
30	1	610	CHL	C3B-C4B	3.44	1.44	1.41
20	A	1113	CLA	C1C-NC	-3.44	1.32	1.37
20	B	1212	CLA	C4B-NB	-3.43	1.33	1.37
20	A	1105	CLA	C4B-NB	-3.42	1.33	1.37
30	3	604	CHL	C1A-CHA	-3.42	1.36	1.40
20	1	602	CLA	C1C-NC	-3.41	1.32	1.37
20	A	1116	CLA	C4B-NB	-3.41	1.33	1.37
20	A	1139	CLA	C4B-NB	-3.41	1.33	1.37
20	2	612	CLA	C1C-NC	-3.41	1.32	1.37
20	H	1701	CLA	MG-ND	-3.40	1.99	2.05
20	A	1104	CLA	C4B-NB	-3.40	1.33	1.37
20	K	1403	CLA	C1C-NC	-3.40	1.32	1.37
20	3	602	CLA	C1C-NC	-3.40	1.32	1.37
30	4	611	CHL	C3B-C4B	3.40	1.44	1.41
20	B	1207	CLA	MG-ND	-3.40	1.99	2.05
20	L	1502	CLA	MG-ND	-3.40	1.99	2.05
30	4	610	CHL	CBB-CAB	3.40	1.50	1.29
30	4	613	CHL	CBB-CAB	3.39	1.50	1.29
20	B	1240	CLA	C4B-NB	-3.39	1.33	1.37
20	B	1238	CLA	MG-ND	-3.38	1.99	2.05
20	A	1131	CLA	C4B-NB	-3.38	1.33	1.37
20	A	1135	CLA	C4B-NB	-3.38	1.33	1.37
20	B	1218	CLA	C1C-NC	-3.37	1.32	1.37
20	B	1209	CLA	C1C-NC	-3.37	1.32	1.37
20	A	1013	CLA	C4B-NB	-3.37	1.33	1.37
20	A	1123	CLA	C1C-NC	-3.36	1.32	1.37
20	4	605	CLA	C4B-NB	-3.35	1.33	1.37
20	B	1221	CLA	C4B-NB	-3.35	1.33	1.37
20	B	1230	CLA	C4B-NB	-3.35	1.33	1.37
20	B	1203	CLA	C4B-NB	-3.35	1.33	1.37
20	B	1213	CLA	C4B-NB	-3.34	1.33	1.37
20	F	1302	CLA	C4B-NB	-3.34	1.33	1.37
20	A	1012	CLA	C4B-NB	-3.34	1.33	1.37
20	2	612	CLA	C4B-NB	-3.34	1.33	1.37
20	1	605	CLA	C4B-NB	-3.34	1.33	1.37
20	A	1134	CLA	C1C-NC	-3.34	1.32	1.37
20	2	605	CLA	C4B-NB	-3.34	1.33	1.37
20	1	607	CLA	C4B-NB	-3.34	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	1	610	CHL	CBB-CAB	3.34	1.50	1.29
20	B	1227	CLA	C4B-NB	-3.33	1.33	1.37
20	A	1120	CLA	C1C-NC	-3.33	1.32	1.37
20	B	1236	CLA	C4B-NB	-3.33	1.33	1.37
20	B	1201	CLA	C4B-NB	-3.32	1.33	1.37
20	B	1216	CLA	C4B-NB	-3.31	1.33	1.37
20	A	1118	CLA	C4B-NB	-3.31	1.33	1.37
20	J	1901	CLA	C1C-NC	-3.31	1.32	1.37
20	A	1123	CLA	C4B-NB	-3.30	1.33	1.37
20	A	1141	CLA	C1C-NC	-3.30	1.32	1.37
30	3	611	CHL	CBB-CAB	3.29	1.49	1.29
30	1	612	CHL	C3B-C2B	-3.29	1.35	1.40
20	A	1115	CLA	C4B-NB	-3.28	1.33	1.37
30	4	610	CHL	C3B-C2B	-3.28	1.35	1.40
20	3	614	CLA	C1C-NC	-3.28	1.32	1.37
20	A	1122	CLA	C4B-NB	-3.28	1.33	1.37
20	G	1601	CLA	C4B-NB	-3.28	1.33	1.37
20	3	610	CLA	C1C-NC	-3.28	1.32	1.37
20	4	606	CLA	C1C-NC	-3.28	1.32	1.37
20	3	601	CLA	C4B-NB	-3.27	1.33	1.37
30	4	610	CHL	C1A-CHA	-3.27	1.36	1.40
20	1	604	CLA	C4B-NB	-3.27	1.33	1.37
20	B	1206	CLA	C4B-NB	-3.26	1.33	1.37
20	G	1602	CLA	C4B-NB	-3.26	1.33	1.37
20	A	1107	CLA	C4B-NB	-3.26	1.33	1.37
20	B	1209	CLA	C4B-NB	-3.26	1.33	1.37
30	1	612	CHL	C1A-CHA	-3.25	1.36	1.40
20	A	1129	CLA	C4B-NB	-3.25	1.33	1.37
20	1	606	CLA	C4B-NB	-3.24	1.33	1.37
30	1	610	CHL	C3B-C2B	-3.22	1.36	1.40
20	A	1121	CLA	C4B-NB	-3.20	1.33	1.37
20	B	1224	CLA	C4B-NB	-3.19	1.33	1.37
20	A	1113	CLA	C4B-NB	-3.19	1.33	1.37
20	1	601	CLA	C4B-NB	-3.17	1.33	1.37
20	2	601	CLA	C4B-NB	-3.16	1.33	1.37
20	B	1232	CLA	C4B-NB	-3.16	1.33	1.37
20	3	605	CLA	C4B-NB	-3.16	1.33	1.37
20	A	1133	CLA	C4B-NB	-3.15	1.33	1.37
20	B	1205	CLA	C4B-NB	-3.15	1.33	1.37
20	4	602	CLA	C1C-NC	-3.14	1.32	1.37
20	K	1402	CLA	C1C-NC	-3.14	1.32	1.37
30	2	609	CHL	C3A-C2A	-3.14	1.52	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	1011	CL0	CBD-CGD	-3.14	1.48	1.52
20	3	608	CLA	C1C-NC	-3.13	1.32	1.37
33	4	505	C7Z	C28-C29	3.13	1.52	1.46
20	A	1112	CLA	C4B-NB	-3.13	1.33	1.37
20	A	1120	CLA	C4B-NB	-3.13	1.33	1.37
20	A	1130	CLA	C4B-NB	-3.12	1.33	1.37
20	A	1110	CLA	C4B-NB	-3.11	1.33	1.37
20	B	1217	CLA	C4B-NB	-3.11	1.33	1.37
20	3	610	CLA	C4B-NB	-3.11	1.33	1.37
20	A	1140	CLA	C4B-NB	-3.10	1.33	1.37
20	B	1226	CLA	C4B-NB	-3.10	1.33	1.37
20	4	617	CLA	C1C-NC	-3.09	1.33	1.37
20	B	1239	CLA	C4B-NB	-3.09	1.33	1.37
30	1	612	CHL	CHB-C4A	-3.09	1.34	1.38
20	4	604	CLA	C1C-NC	-3.09	1.33	1.37
20	4	612	CLA	C4B-NB	-3.08	1.33	1.37
20	B	1235	CLA	C4B-NB	-3.08	1.33	1.37
30	3	611	CHL	CHB-C4A	-3.08	1.34	1.38
20	B	1237	CLA	C1C-NC	-3.08	1.33	1.37
20	2	607	CLA	C1C-NC	-3.06	1.33	1.37
20	A	1128	CLA	C4B-NB	-3.06	1.33	1.37
20	2	604	CLA	C1C-NC	-3.06	1.33	1.37
20	3	612	CLA	C1C-NC	-3.06	1.33	1.37
20	1	611	CLA	C4B-NB	-3.05	1.33	1.37
20	3	614	CLA	C4B-NB	-3.05	1.33	1.37
20	B	1228	CLA	C4B-NB	-3.05	1.33	1.37
20	4	607	CLA	C4B-NB	-3.05	1.33	1.37
20	A	1132	CLA	C1C-NC	-3.04	1.33	1.37
20	4	601	CLA	C1C-NC	-3.04	1.33	1.37
20	A	1136	CLA	C4B-NB	-3.04	1.33	1.37
20	2	606	CLA	C1C-NC	-3.03	1.33	1.37
20	A	1102	CLA	C4B-NB	-3.03	1.33	1.37
20	1	614	CLA	C4B-NB	-3.02	1.33	1.37
20	4	617	CLA	C4B-NB	-3.02	1.33	1.37
20	A	1101	CLA	C1C-NC	-3.02	1.33	1.37
20	3	617	CLA	C4B-NB	-3.02	1.33	1.37
20	2	602	CLA	C1C-NC	-3.02	1.33	1.37
20	3	617	CLA	C1C-NC	-3.02	1.33	1.37
20	H	1701	CLA	C1C-NC	-3.02	1.33	1.37
20	1	608	CLA	C4B-NB	-3.00	1.33	1.37
20	L	1503	CLA	C1C-NC	-3.00	1.33	1.37
20	A	1109	CLA	C4B-NB	-2.99	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B	1207	CLA	C1C-NC	-2.98	1.33	1.37
30	4	615	CHL	C1B-C2B	2.98	1.42	1.39
20	3	613	CLA	C4B-NB	-2.98	1.33	1.37
20	1	613	CLA	C4B-NB	-2.98	1.33	1.37
20	4	612	CLA	C1C-NC	-2.97	1.33	1.37
20	L	1501	CLA	C1C-NC	-2.97	1.33	1.37
20	4	603	CLA	C1C-NC	-2.96	1.33	1.37
20	4	606	CLA	C4B-NB	-2.96	1.34	1.37
20	4	607	CLA	C1C-NC	-2.95	1.33	1.37
31	4	502	XAT	O24-C25	-2.94	1.42	1.46
30	4	613	CHL	C1A-CHA	-2.94	1.36	1.40
33	4	505	C7Z	C7-C6	2.93	1.55	1.45
20	4	609	CLA	C1C-NC	-2.93	1.33	1.37
20	K	1404	CLA	C1C-NC	-2.93	1.33	1.37
20	1	602	CLA	C4B-NB	-2.92	1.34	1.37
28	3	803	DGD	CAB-C9B	-2.92	1.33	1.51
30	3	604	CHL	CHB-C4A	-2.92	1.35	1.38
33	4	505	C7Z	C27-C26	2.92	1.55	1.45
26	2	803	LMG	C19-C18	-2.92	1.33	1.51
20	K	1401	CLA	C1C-NC	-2.91	1.33	1.37
33	4	505	C7Z	C32-C33	2.91	1.52	1.46
20	4	608	CLA	C1C-NC	-2.90	1.33	1.37
20	1	603	CLA	C4B-NB	-2.90	1.34	1.37
20	4	604	CLA	C4B-NB	-2.90	1.34	1.37
20	B	1207	CLA	C4B-NB	-2.90	1.34	1.37
20	B	1238	CLA	C1C-NC	-2.90	1.33	1.37
20	L	1503	CLA	C4B-NB	-2.89	1.34	1.37
20	B	1218	CLA	C4B-NB	-2.89	1.34	1.37
20	L	1502	CLA	C1C-NC	-2.89	1.33	1.37
20	2	608	CLA	C4B-NB	-2.89	1.34	1.37
20	A	1101	CLA	C4B-NB	-2.88	1.34	1.37
20	G	1603	CLA	C4B-NB	-2.88	1.34	1.37
30	2	615	CHL	C3B-C4B	2.87	1.44	1.41
20	L	1501	CLA	C4B-NB	-2.86	1.34	1.37
33	4	505	C7Z	C8-C9	2.85	1.52	1.46
20	K	1404	CLA	C4B-NB	-2.85	1.34	1.37
30	1	610	CHL	CHB-C4A	-2.84	1.35	1.38
20	K	1403	CLA	C4B-NB	-2.84	1.34	1.37
20	L	1502	CLA	C4B-NB	-2.84	1.34	1.37
20	H	1701	CLA	C4B-NB	-2.83	1.34	1.37
20	B	1237	CLA	C4B-NB	-2.83	1.34	1.37
30	2	610	CHL	C1B-C2B	2.82	1.42	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	2	603	CLA	C4B-NB	-2.81	1.34	1.37
20	A	1134	CLA	C4B-NB	-2.81	1.34	1.37
20	2	606	CLA	C4B-NB	-2.81	1.34	1.37
20	4	601	CLA	C4B-NB	-2.81	1.34	1.37
20	A	1114	CLA	C4B-NB	-2.80	1.34	1.37
30	3	607	CHL	C1A-CHA	-2.80	1.36	1.40
30	4	610	CHL	CHB-C4A	-2.80	1.35	1.38
31	2	502	XAT	O24-C25	-2.79	1.42	1.46
30	2	610	CHL	C3A-C2A	-2.79	1.52	1.54
20	K	1401	CLA	C4B-NB	-2.78	1.34	1.37
20	2	604	CLA	C4B-NB	-2.78	1.34	1.37
30	2	611	CHL	C1D-C2D	2.78	1.42	1.39
20	A	1132	CLA	C4B-NB	-2.78	1.34	1.37
20	4	608	CLA	C4B-NB	-2.78	1.34	1.37
30	4	613	CHL	CHB-C4A	-2.77	1.35	1.38
20	A	1141	CLA	C4B-NB	-2.77	1.34	1.37
30	1	609	CHL	C1B-C2B	2.77	1.42	1.39
20	2	607	CLA	C4B-NB	-2.77	1.34	1.37
20	4	602	CLA	C4B-NB	-2.77	1.34	1.37
30	3	604	CHL	C1D-C2D	2.76	1.42	1.39
30	1	609	CHL	C1D-C2D	2.76	1.42	1.39
30	2	613	CHL	C1B-C2B	2.76	1.42	1.39
20	4	609	CLA	C4B-NB	-2.74	1.34	1.37
30	4	615	CHL	C3B-C4B	2.74	1.44	1.41
30	2	609	CHL	C1D-C2D	2.74	1.42	1.39
24	G	5004	LMT	O3'-C3'	-2.74	1.36	1.43
20	B	1238	CLA	C4B-NB	-2.73	1.34	1.37
30	2	610	CHL	C1D-C2D	2.72	1.42	1.39
20	3	602	CLA	C4B-NB	-2.72	1.34	1.37
30	2	609	CHL	CHB-C4A	-2.72	1.35	1.38
20	B	1202	CLA	C4B-NB	-2.71	1.34	1.37
30	4	615	CHL	C1D-C2D	2.71	1.42	1.39
29	1	501	LUT	C1-C6	-2.71	1.50	1.53
30	3	607	CHL	CHB-C4A	-2.70	1.35	1.38
30	4	610	CHL	C1D-C2D	2.69	1.42	1.39
29	2	501	LUT	C1-C6	-2.69	1.50	1.53
20	J	1901	CLA	C4B-NB	-2.68	1.34	1.37
20	G	1601	CLA	C3D-C4D	-2.68	1.38	1.44
20	3	612	CLA	C4B-NB	-2.67	1.34	1.37
30	1	612	CHL	C1B-C2B	2.67	1.42	1.39
30	4	613	CHL	C1B-C2B	2.67	1.42	1.39
20	2	602	CLA	C4B-NB	-2.66	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	3	501	LUT	C1-C6	-2.66	1.50	1.53
30	2	611	CHL	CHB-C4A	-2.66	1.35	1.38
30	2	610	CHL	CHB-C4A	-2.66	1.35	1.38
30	2	609	CHL	C1B-C2B	2.66	1.42	1.39
32	2	807	3PH	O21-C2	-2.65	1.40	1.46
30	3	607	CHL	C1B-C2B	2.64	1.42	1.39
30	2	613	CHL	C1D-C2D	2.64	1.42	1.39
30	2	613	CHL	CHB-C4A	-2.63	1.35	1.38
20	A	1112	CLA	C3D-C4D	-2.63	1.38	1.44
30	3	607	CHL	C1D-C2D	2.63	1.42	1.39
30	2	615	CHL	C1B-C2B	2.62	1.42	1.39
20	B	1022	CLA	C3D-C4D	-2.61	1.38	1.44
20	A	1137	CLA	C4B-NB	-2.61	1.34	1.37
30	2	611	CHL	C1B-C2B	2.61	1.42	1.39
30	3	604	CHL	C1B-C2B	2.61	1.42	1.39
20	3	603	CLA	C4B-NB	-2.60	1.34	1.37
24	G	5005	LMT	O3'-C3'	-2.60	1.36	1.43
24	B	5008	LMT	O3'-C3'	-2.59	1.36	1.43
20	K	1402	CLA	C4B-NB	-2.58	1.34	1.37
30	3	607	CHL	C2C-C3C	2.58	1.38	1.36
30	4	610	CHL	C1B-C2B	2.57	1.42	1.39
30	1	609	CHL	CHB-C4A	-2.57	1.35	1.38
30	4	611	CHL	C1B-C2B	2.57	1.42	1.39
30	4	611	CHL	C1D-C2D	2.57	1.42	1.39
20	A	1013	CLA	C3D-C4D	-2.56	1.38	1.44
30	4	611	CHL	CHB-C4A	-2.56	1.35	1.38
30	4	615	CHL	CHB-C4A	-2.56	1.35	1.38
30	3	611	CHL	C1D-C2D	2.55	1.42	1.39
20	4	603	CLA	C4B-NB	-2.54	1.34	1.37
20	A	1103	CLA	C3D-C4D	-2.54	1.38	1.44
24	B	5008	LMT	O3B-C3B	-2.54	1.36	1.43
30	1	610	CHL	C1B-C2B	2.54	1.42	1.39
30	2	615	CHL	C1D-C2D	2.53	1.42	1.39
30	4	613	CHL	C1D-C2D	2.53	1.42	1.39
24	B	5006	LMT	O3'-C3'	-2.53	1.36	1.43
30	1	612	CHL	C1D-C2D	2.53	1.42	1.39
24	A	5004	LMT	O3B-C3B	-2.52	1.36	1.43
20	B	1211	CLA	C3D-C4D	-2.51	1.38	1.44
30	2	615	CHL	CHB-C4A	-2.51	1.35	1.38
20	B	1235	CLA	C3D-C4D	-2.50	1.38	1.44
20	A	1122	CLA	C3D-C4D	-2.50	1.38	1.44
20	A	1127	CLA	C3D-C4D	-2.50	1.38	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	A	1128	CLA	C3D-C4D	-2.49	1.38	1.44
30	2	615	CHL	C1A-CHA	-2.49	1.37	1.40
30	1	610	CHL	C1D-C2D	2.49	1.42	1.39
29	J	4013	LUT	C1-C6	-2.49	1.50	1.53
20	4	605	CLA	C3D-C4D	-2.49	1.38	1.44
30	4	615	CHL	C3A-C2A	-2.49	1.52	1.54
20	A	1121	CLA	C3D-C4D	-2.48	1.38	1.44
20	B	1204	CLA	C3D-C4D	-2.48	1.38	1.44
20	A	1119	CLA	C3D-C4D	-2.48	1.38	1.44
20	B	1228	CLA	C3D-C4D	-2.47	1.38	1.44
20	B	1234	CLA	C3D-C4D	-2.47	1.38	1.44
20	B	1221	CLA	C3D-C4D	-2.47	1.38	1.44
20	A	1106	CLA	C3D-C4D	-2.47	1.38	1.44
24	A	5004	LMT	O3'-C3'	-2.47	1.36	1.43
20	B	1021	CLA	C3D-C4D	-2.46	1.38	1.44
20	A	1104	CLA	C3D-C4D	-2.46	1.38	1.44
20	B	1208	CLA	C4B-NB	-2.46	1.34	1.37
24	G	5004	LMT	O2'-C2'	-2.45	1.36	1.43
20	3	608	CLA	C4B-NB	-2.45	1.34	1.37
20	B	1236	CLA	C3D-C4D	-2.45	1.38	1.44
20	A	1136	CLA	C3D-C4D	-2.45	1.38	1.44
20	A	1120	CLA	C3D-C4D	-2.45	1.38	1.44
20	A	1116	CLA	C3D-C4D	-2.44	1.38	1.44
30	3	611	CHL	C1B-C2B	2.44	1.42	1.39
20	A	1126	CLA	C3D-C4D	-2.44	1.38	1.44
20	2	601	CLA	C3D-C4D	-2.44	1.38	1.44
20	B	1203	CLA	C3D-C4D	-2.44	1.38	1.44
20	B	1023	CLA	C3D-C4D	-2.43	1.38	1.44
20	A	1129	CLA	C3D-C4D	-2.43	1.38	1.44
20	B	1206	CLA	C3D-C4D	-2.43	1.38	1.44
20	B	1205	CLA	C3D-C4D	-2.43	1.38	1.44
20	A	1117	CLA	C3D-C4D	-2.43	1.38	1.44
20	B	1240	CLA	C3D-C4D	-2.42	1.38	1.44
20	A	1135	CLA	C3D-C4D	-2.42	1.38	1.44
24	G	5005	LMT	O2B-C2B	-2.42	1.37	1.43
28	B	5005	DGD	CDA-CCA	-2.41	1.33	1.50
24	B	5008	LMT	O2B-C2B	-2.41	1.37	1.43
20	A	1125	CLA	C3D-C4D	-2.41	1.38	1.44
32	2	807	3PH	O31-C31	2.41	1.40	1.33
20	B	1226	CLA	C3D-C4D	-2.41	1.38	1.44
20	B	1231	CLA	C3D-C4D	-2.41	1.38	1.44
20	1	613	CLA	C3D-C4D	-2.41	1.38	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	A	5006	LMG	C40-C39	-2.40	1.33	1.50
20	A	1131	CLA	C3D-C4D	-2.40	1.38	1.44
20	A	1137	CLA	C3D-C4D	-2.40	1.38	1.44
20	B	1210	CLA	C3D-C4D	-2.40	1.38	1.44
20	A	1140	CLA	C3D-C4D	-2.40	1.38	1.44
20	2	612	CLA	C3D-C4D	-2.40	1.38	1.44
30	3	607	CHL	CHA-CBD	2.39	1.54	1.51
20	B	1225	CLA	C3D-C4D	-2.39	1.38	1.44
20	A	1108	CLA	C3D-C4D	-2.39	1.38	1.44
24	B	5008	LMT	O1'-C1'	-2.39	1.36	1.40
20	B	1201	CLA	C3D-C4D	-2.38	1.38	1.44
20	1	604	CLA	C3D-C4D	-2.38	1.38	1.44
20	A	1123	CLA	C3D-C4D	-2.38	1.38	1.44
20	A	1012	CLA	C3D-C4D	-2.38	1.38	1.44
20	A	1111	CLA	C3D-C4D	-2.38	1.38	1.44
20	3	605	CLA	C3D-C4D	-2.38	1.38	1.44
20	B	1227	CLA	C3D-C4D	-2.37	1.38	1.44
30	4	611	CHL	C3B-C2B	-2.37	1.37	1.40
20	B	1222	CLA	C3D-C4D	-2.37	1.38	1.44
30	2	609	CHL	C3B-C2B	-2.37	1.37	1.40
20	A	1115	CLA	C3D-C4D	-2.37	1.38	1.44
20	A	1114	CLA	C3D-C4D	-2.37	1.38	1.44
20	B	1216	CLA	C3D-C4D	-2.37	1.38	1.44
28	J	5001	DGD	CAB-C9B	-2.37	1.33	1.50
26	F	5002	LMG	C19-C18	-2.37	1.33	1.50
20	B	1208	CLA	C3D-C4D	-2.37	1.38	1.44
20	B	1202	CLA	C3D-C4D	-2.36	1.38	1.44
20	A	1139	CLA	C3D-C4D	-2.36	1.38	1.44
26	G	5002	LMG	C43-C42	-2.36	1.33	1.50
20	1	605	CLA	C3D-C4D	-2.36	1.38	1.44
20	1	606	CLA	C3D-C4D	-2.36	1.38	1.44
28	G	5003	DGD	CAB-C9B	-2.36	1.33	1.50
20	B	1217	CLA	C3D-C4D	-2.36	1.38	1.44
20	B	1220	CLA	C3D-C4D	-2.36	1.38	1.44
24	A	5004	LMT	O1'-C1'	-2.35	1.36	1.40
20	1	608	CLA	C3D-C4D	-2.35	1.38	1.44
28	3	803	DGD	CAA-C9A	-2.35	1.33	1.50
20	B	1214	CLA	C3D-C4D	-2.35	1.38	1.44
30	1	609	CHL	C3B-C2B	-2.35	1.37	1.40
20	B	1239	CLA	C3D-C4D	-2.35	1.38	1.44
20	B	1213	CLA	C3D-C4D	-2.35	1.38	1.44
22	A	4007	BCR	C1-C6	-2.35	1.50	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B	1223	CLA	C3D-C4D	-2.34	1.38	1.44
20	F	1301	CLA	C3D-C4D	-2.34	1.38	1.44
20	2	605	CLA	C3D-C4D	-2.33	1.38	1.44
24	B	5006	LMT	O2'-C2'	-2.33	1.37	1.43
20	B	1229	CLA	C3D-C4D	-2.33	1.38	1.44
20	B	1218	CLA	C3D-C4D	-2.33	1.38	1.44
20	2	608	CLA	C3D-C4D	-2.33	1.38	1.44
20	B	1224	CLA	C3D-C4D	-2.32	1.39	1.44
22	F	4016	BCR	C12-C13	-2.32	1.41	1.46
20	A	1133	CLA	C3D-C4D	-2.32	1.39	1.44
20	B	1209	CLA	C3D-C4D	-2.32	1.39	1.44
33	4	505	C7Z	C18-C5	2.32	1.54	1.50
20	A	1124	CLA	C3D-C4D	-2.32	1.39	1.44
20	A	1113	CLA	C3D-C4D	-2.32	1.39	1.44
20	A	1118	CLA	C3D-C4D	-2.31	1.39	1.44
30	2	613	CHL	C3B-C2B	-2.31	1.37	1.40
20	3	606	CLA	C3D-C4D	-2.31	1.39	1.44
20	4	607	CLA	C1C-C2C	2.31	1.49	1.44
20	A	1105	CLA	C3D-C4D	-2.30	1.39	1.44
20	1	607	CLA	C3D-C4D	-2.30	1.39	1.44
20	B	1232	CLA	C3D-C4D	-2.30	1.39	1.44
20	A	1110	CLA	C3D-C4D	-2.30	1.39	1.44
20	1	614	CLA	C3D-C4D	-2.30	1.39	1.44
23	3	801	LHG	O7-C7	-2.30	1.34	1.42
20	B	1212	CLA	C3D-C4D	-2.29	1.39	1.44
20	B	1219	CLA	C3D-C4D	-2.29	1.39	1.44
20	4	607	CLA	CHC-C1C	2.29	1.43	1.38
29	4	501	LUT	C1-C6	-2.29	1.50	1.53
20	A	1134	CLA	C3D-C4D	-2.29	1.39	1.44
20	B	1230	CLA	C3D-C4D	-2.28	1.39	1.44
24	G	5005	LMT	O2'-C2'	-2.28	1.37	1.43
20	A	1102	CLA	C3D-C4D	-2.28	1.39	1.44
22	A	4008	BCR	C12-C13	-2.28	1.41	1.46
24	B	5008	LMT	O2'-C2'	-2.28	1.37	1.43
20	3	613	CLA	C3D-C4D	-2.28	1.39	1.44
20	A	1107	CLA	C3D-C4D	-2.28	1.39	1.44
20	3	614	CLA	C3D-C4D	-2.27	1.39	1.44
20	A	1130	CLA	C3D-C4D	-2.27	1.39	1.44
20	A	1138	CLA	C3D-C4D	-2.27	1.39	1.44
20	A	1109	CLA	C3D-C4D	-2.26	1.39	1.44
20	B	1215	CLA	C3D-C4D	-2.25	1.39	1.44
24	B	5008	LMT	O4'-C4B	-2.25	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	1	611	CLA	C3D-C4D	-2.25	1.39	1.44
20	F	1302	CLA	C3D-C4D	-2.25	1.39	1.44
20	G	1602	CLA	C3D-C4D	-2.25	1.39	1.44
24	A	5004	LMT	O2'-C2'	-2.24	1.37	1.43
20	1	601	CLA	C3D-C4D	-2.24	1.39	1.44
30	4	610	CHL	C3D-C2D	-2.24	1.35	1.39
30	3	607	CHL	C3B-C2B	-2.24	1.37	1.40
30	4	613	CHL	CHC-C4B	-2.23	1.36	1.39
30	2	609	CHL	CHA-CBD	2.23	1.54	1.51
20	1	603	CLA	C3D-C4D	-2.23	1.39	1.44
24	A	5004	LMT	O2B-C2B	-2.22	1.37	1.43
20	1	602	CLA	C3D-C4D	-2.22	1.39	1.44
24	B	5006	LMT	O3B-C3B	-2.21	1.37	1.43
22	A	4008	BCR	C1-C6	-2.21	1.51	1.53
29	4	501	LUT	C26-C27	-2.21	1.47	1.50
20	2	603	CLA	C1C-C2C	2.21	1.49	1.44
30	1	610	CHL	CHA-CBD	2.20	1.54	1.51
20	2	602	CLA	C3D-C4D	-2.20	1.39	1.44
20	3	610	CLA	C3D-C4D	-2.20	1.39	1.44
30	2	615	CHL	C3B-C2B	-2.20	1.37	1.40
30	4	615	CHL	CHA-CBD	2.19	1.54	1.51
24	G	5004	LMT	O3B-C3B	-2.19	1.37	1.43
24	B	5006	LMT	O2B-C2B	-2.18	1.37	1.43
20	G	1603	CLA	C3D-C4D	-2.17	1.39	1.44
24	B	5006	LMT	O1'-C1'	-2.17	1.36	1.40
29	1	502	LUT	C1-C6	-2.17	1.51	1.53
30	1	612	CHL	CHA-CBD	2.16	1.54	1.51
22	B	4010	BCR	C12-C13	-2.15	1.41	1.46
20	2	603	CLA	C3D-C4D	-2.15	1.39	1.44
24	G	5004	LMT	O4'-C4B	-2.15	1.37	1.43
20	K	1404	CLA	C1A-CHA	2.14	1.51	1.43
22	A	4002	BCR	C12-C13	-2.14	1.41	1.46
30	2	610	CHL	C3B-C2B	-2.14	1.37	1.40
30	4	611	CHL	CHA-CBD	2.14	1.54	1.51
20	A	1141	CLA	C3D-C4D	-2.14	1.39	1.44
20	4	603	CLA	C1C-C2C	2.14	1.48	1.44
24	G	5005	LMT	O3B-C3B	-2.13	1.37	1.43
30	2	610	CHL	CHA-CBD	2.13	1.54	1.51
30	2	615	CHL	CHA-CBD	2.13	1.54	1.51
20	B	1238	CLA	C1C-C2C	2.13	1.48	1.44
24	G	5004	LMT	O1'-C1'	-2.13	1.36	1.40
22	F	4014	BCR	C1-C6	-2.13	1.51	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B	1207	CLA	C1C-C2C	2.12	1.48	1.44
32	2	807	3PH	O31-C3	-2.12	1.40	1.45
20	K	1402	CLA	C3D-C4D	-2.12	1.39	1.44
20	4	617	CLA	C3D-C4D	-2.12	1.39	1.44
22	A	4011	BCR	C12-C13	-2.12	1.41	1.46
20	K	1402	CLA	C1C-C2C	2.12	1.48	1.44
30	2	611	CHL	CHA-CBD	2.11	1.54	1.51
20	J	1901	CLA	C1A-CHA	2.11	1.51	1.43
30	2	613	CHL	C3A-C2A	-2.11	1.52	1.54
22	A	4017	BCR	C12-C13	-2.11	1.41	1.46
20	A	1133	CLA	C1D-ND	-2.11	1.35	1.37
29	4	501	LUT	C22-C21	-2.11	1.52	1.54
20	3	601	CLA	C3D-C4D	-2.11	1.39	1.44
32	2	807	3PH	O21-C21	2.10	1.40	1.34
20	B	1021	CLA	C1D-ND	-2.10	1.35	1.37
20	A	1127	CLA	C1D-ND	-2.10	1.35	1.37
20	3	602	CLA	C3D-C4D	-2.09	1.39	1.44
30	1	609	CHL	CHA-CBD	2.09	1.54	1.51
20	4	607	CLA	C3D-C4D	-2.09	1.39	1.44
20	4	603	CLA	CHC-C1C	2.08	1.42	1.38
20	3	603	CLA	C3D-C4D	-2.08	1.39	1.44
20	3	608	CLA	C1C-C2C	2.08	1.48	1.44
20	4	608	CLA	C1C-C2C	2.08	1.48	1.44
20	2	606	CLA	C1C-C2C	2.08	1.48	1.44
20	4	612	CLA	C3D-C4D	-2.08	1.39	1.44
30	2	611	CHL	C3B-C2B	-2.08	1.37	1.40
24	A	5004	LMT	O5'-C5'	-2.08	1.39	1.44
20	4	604	CLA	C1C-C2C	2.08	1.48	1.44
20	L	1503	CLA	C1C-C2C	2.07	1.48	1.44
20	K	1401	CLA	C1C-C2C	2.07	1.48	1.44
20	2	604	CLA	C1C-C2C	2.07	1.48	1.44
20	A	1132	CLA	C1C-C2C	2.07	1.48	1.44
20	K	1403	CLA	C3D-C4D	-2.07	1.39	1.44
24	G	5004	LMT	O2B-C2B	-2.07	1.37	1.43
20	2	604	CLA	C3D-C4D	-2.07	1.39	1.44
20	L	1501	CLA	C3D-C4D	-2.06	1.39	1.44
20	4	602	CLA	C1C-C2C	2.06	1.48	1.44
28	J	5001	DGD	O5D-C1E	2.06	1.43	1.40
30	4	613	CHL	CHA-CBD	2.06	1.54	1.51
20	3	608	CLA	C1A-CHA	2.06	1.51	1.43
30	2	615	CHL	C3A-C2A	-2.06	1.52	1.54
20	4	608	CLA	C3D-C4D	-2.06	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	2	613	CHL	CHA-CBD	2.05	1.54	1.51
20	B	1237	CLA	C1C-C2C	2.05	1.48	1.44
24	A	5004	LMT	O4'-C4B	-2.05	1.37	1.43
20	4	606	CLA	C1A-CHA	2.04	1.51	1.43
20	4	609	CLA	C1C-C2C	2.04	1.48	1.44
22	I	4018	BCR	C1-C6	-2.04	1.51	1.53
22	A	4007	BCR	C12-C13	-2.04	1.41	1.46
20	K	1404	CLA	C1C-C2C	2.04	1.48	1.44
20	L	1502	CLA	C1C-C2C	2.04	1.48	1.44
20	2	602	CLA	C1C-C2C	2.04	1.48	1.44
20	3	602	CLA	C1A-CHA	2.04	1.51	1.43
20	B	1023	CLA	C1D-ND	-2.04	1.35	1.37
24	B	5006	LMT	O4'-C4B	-2.03	1.37	1.43
20	B	1238	CLA	C3D-C4D	-2.03	1.39	1.44
20	A	1101	CLA	C3D-C4D	-2.03	1.39	1.44
20	3	612	CLA	C3D-C4D	-2.02	1.39	1.44
20	4	602	CLA	C3D-C4D	-2.02	1.39	1.44
23	1	801	LHG	O7-C5	-2.02	1.41	1.46
20	4	601	CLA	C1C-C2C	2.02	1.48	1.44
20	J	1901	CLA	C3D-C4D	-2.02	1.39	1.44
20	2	603	CLA	C1A-CHA	2.02	1.51	1.43
30	4	615	CHL	CHC-C4B	-2.02	1.36	1.39
20	3	606	CLA	C1A-CHA	2.02	1.51	1.43
20	4	612	CLA	C1C-C2C	2.02	1.48	1.44
20	H	1701	CLA	C3D-C4D	-2.02	1.39	1.44
20	L	1501	CLA	C1C-C2C	2.02	1.48	1.44
20	3	617	CLA	C1C-C2C	2.01	1.48	1.44
20	3	614	CLA	C1A-CHA	2.00	1.51	1.43
20	2	607	CLA	C1A-CHA	2.00	1.51	1.43
30	3	611	CHL	CHA-CBD	2.00	1.54	1.51
20	L	1503	CLA	C3D-C4D	-2.00	1.39	1.44

All (3472) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	H	4021	BCR	C10-C11-C12	19.50	179.72	123.20
22	3	506	BCR	C10-C11-C12	19.08	178.49	123.20
22	1	504	BCR	C10-C11-C12	18.96	178.15	123.20
22	L	4019	BCR	C10-C11-C12	18.96	178.13	123.20
22	3	503	BCR	C10-C11-C12	18.95	178.09	123.20
22	G	4011	BCR	C10-C11-C12	18.81	177.70	123.20
22	B	4004	BCR	C10-C11-C12	18.77	177.59	123.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	2	503	BCR	C10-C11-C12	18.74	177.50	123.20
22	L	4020	BCR	C10-C11-C12	18.71	177.43	123.20
22	1	503	BCR	C10-C11-C12	18.63	177.17	123.20
22	K	4001	BCR	C10-C11-C12	18.57	177.01	123.20
22	A	4007	BCR	C10-C11-C12	18.57	176.99	123.20
22	I	4020	BCR	C10-C11-C12	18.55	176.96	123.20
22	F	4014	BCR	C10-C11-C12	18.37	176.42	123.20
22	F	4016	BCR	C10-C11-C12	18.34	176.35	123.20
22	B	4010	BCR	C10-C11-C12	18.33	176.30	123.20
22	A	4008	BCR	C10-C11-C12	18.21	175.96	123.20
22	B	4009	BCR	C10-C11-C12	18.19	175.91	123.20
22	B	4004	BCR	C11-C10-C9	18.18	152.77	127.28
22	A	4017	BCR	C10-C11-C12	18.16	175.82	123.20
22	A	4017	BCR	C16-C15-C14	18.16	160.67	123.52
22	A	4003	BCR	C10-C11-C12	18.14	175.75	123.20
22	B	4006	BCR	C10-C11-C12	17.66	174.36	123.20
22	J	4012	BCR	C10-C11-C12	17.57	174.12	123.20
22	A	4002	BCR	C10-C11-C12	17.52	173.98	123.20
22	B	4005	BCR	C10-C11-C12	17.52	173.97	123.20
22	K	4002	BCR	C10-C11-C12	17.39	173.60	123.20
22	1	504	BCR	C16-C15-C14	17.20	158.71	123.52
22	A	4011	BCR	C10-C11-C12	17.09	172.72	123.20
22	I	4018	BCR	C10-C11-C12	16.66	171.47	123.20
22	B	4004	BCR	C21-C20-C19	15.17	167.16	123.20
22	B	4005	BCR	C11-C10-C9	15.01	148.33	127.28
22	2	503	BCR	C16-C15-C14	14.95	154.12	123.52
22	3	503	BCR	C16-C15-C14	14.93	154.07	123.52
22	2	503	BCR	C29-C30-C25	-14.92	88.77	110.44
22	2	503	BCR	C21-C20-C19	14.72	165.86	123.20
22	K	4001	BCR	C21-C20-C19	14.49	165.19	123.20
22	B	4006	BCR	C11-C10-C9	14.39	147.46	127.28
33	4	505	C7Z	C18-C5-C6	-14.36	108.82	124.48
22	L	4020	BCR	C16-C15-C14	14.17	152.51	123.52
22	K	4002	BCR	C11-C10-C9	14.16	147.14	127.28
22	3	506	BCR	C21-C20-C19	14.16	164.23	123.20
22	I	4020	BCR	C16-C15-C14	14.10	152.36	123.52
33	4	505	C7Z	C38-C25-C26	-13.97	109.24	124.48
22	A	4011	BCR	C11-C10-C9	13.96	146.85	127.28
22	H	4021	BCR	C16-C15-C14	13.86	151.88	123.52
22	G	4011	BCR	C21-C20-C19	13.70	162.88	123.20
22	G	4011	BCR	C16-C15-C14	13.67	151.50	123.52
22	A	4007	BCR	C16-C15-C14	13.64	151.42	123.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	4003	BCR	C21-C20-C19	13.63	162.71	123.20
22	A	4002	BCR	C11-C10-C9	13.56	146.29	127.28
22	K	4002	BCR	C21-C20-C19	13.47	162.23	123.20
22	1	504	BCR	C21-C20-C19	13.47	162.22	123.20
22	L	4019	BCR	C11-C10-C9	13.46	146.15	127.28
22	I	4018	BCR	C16-C15-C14	13.45	151.03	123.52
22	A	4017	BCR	C21-C20-C19	13.41	162.05	123.20
22	L	4020	BCR	C11-C10-C9	13.17	145.75	127.28
22	3	506	BCR	C16-C15-C14	13.16	150.46	123.52
22	J	4012	BCR	C21-C20-C19	13.11	161.19	123.20
22	A	4007	BCR	C21-C20-C19	13.11	161.19	123.20
22	J	4012	BCR	C11-C10-C9	13.07	145.61	127.28
22	A	4017	BCR	C11-C10-C9	13.00	145.51	127.28
22	B	4010	BCR	C11-C10-C9	12.98	145.48	127.28
22	H	4021	BCR	C21-C20-C19	12.97	160.78	123.20
22	K	4002	BCR	C11-C12-C13	12.88	161.67	126.36
22	I	4020	BCR	C21-C20-C19	12.86	160.47	123.20
22	F	4016	BCR	C11-C10-C9	12.83	145.28	127.28
19	A	1011	CL0	C1B-CHB-C4A	12.80	129.56	121.32
22	I	4020	BCR	C11-C10-C9	12.79	145.21	127.28
22	L	4020	BCR	C21-C20-C19	12.73	160.09	123.20
22	K	4001	BCR	C11-C10-C9	12.72	145.12	127.28
22	F	4016	BCR	C21-C20-C19	12.64	159.81	123.20
22	1	503	BCR	C11-C10-C9	12.60	144.95	127.28
22	A	4011	BCR	C11-C12-C13	12.53	160.71	126.36
22	F	4014	BCR	C11-C10-C9	12.52	144.84	127.28
22	2	503	BCR	C11-C10-C9	12.47	144.76	127.28
22	G	4011	BCR	C11-C10-C9	12.45	144.73	127.28
22	B	4005	BCR	C11-C12-C13	12.45	160.49	126.36
22	A	4007	BCR	C11-C10-C9	12.44	144.73	127.28
22	A	4003	BCR	C11-C10-C9	12.42	144.70	127.28
22	L	4019	BCR	C16-C15-C14	12.39	148.88	123.52
22	F	4016	BCR	C16-C15-C14	12.34	148.77	123.52
22	B	4009	BCR	C11-C12-C13	12.25	159.96	126.36
22	B	4009	BCR	C11-C10-C9	12.24	144.45	127.28
22	3	506	BCR	C11-C10-C9	12.22	144.42	127.28
22	L	4019	BCR	C21-C20-C19	12.21	158.58	123.20
22	A	4002	BCR	C21-C20-C19	12.09	158.23	123.20
22	J	4012	BCR	C11-C12-C13	12.08	159.48	126.36
22	B	4010	BCR	C21-C20-C19	12.05	158.11	123.20
22	B	4006	BCR	C11-C12-C13	12.04	159.38	126.36
22	1	503	BCR	C21-C20-C19	12.01	158.00	123.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	1	504	BCR	C11-C10-C9	12.00	144.10	127.28
22	K	4001	BCR	C16-C15-C14	11.96	148.00	123.52
22	A	4002	BCR	C11-C12-C13	11.90	159.00	126.36
22	A	4003	BCR	C11-C12-C13	11.87	158.92	126.36
22	K	4002	BCR	C16-C15-C14	11.80	147.67	123.52
22	B	4010	BCR	C16-C15-C14	11.66	147.37	123.52
22	F	4014	BCR	C16-C15-C14	11.64	147.33	123.52
22	F	4014	BCR	C11-C12-C13	11.58	158.11	126.36
22	A	4011	BCR	C21-C20-C19	11.54	156.62	123.20
33	4	505	C7Z	C31-C30-C29	-11.37	111.33	127.28
22	I	4018	BCR	C21-C20-C19	11.37	156.14	123.20
22	H	4021	BCR	C11-C10-C9	11.35	143.19	127.28
22	A	4008	BCR	C21-C20-C19	11.33	156.04	123.20
22	A	4008	BCR	C11-C10-C9	11.28	143.10	127.28
22	K	4001	BCR	C11-C12-C13	11.26	157.25	126.36
22	B	4009	BCR	C21-C20-C19	11.23	155.75	123.20
22	3	503	BCR	C21-C20-C19	11.12	155.44	123.20
22	1	503	BCR	C11-C12-C13	11.09	156.78	126.36
22	B	4010	BCR	C11-C12-C13	11.08	156.75	126.36
22	F	4014	BCR	C21-C20-C19	11.04	155.19	123.20
33	4	505	C7Z	C35-C34-C33	-11.01	111.84	127.28
33	4	505	C7Z	C15-C14-C13	-10.93	111.95	127.28
22	B	4009	BCR	C16-C15-C14	10.93	145.88	123.52
22	G	4011	BCR	C11-C12-C13	10.90	156.26	126.36
22	B	4005	BCR	C16-C15-C14	10.84	145.70	123.52
22	F	4016	BCR	C11-C12-C13	10.79	155.94	126.36
22	B	4005	BCR	C21-C20-C19	10.79	154.45	123.20
22	A	4007	BCR	C11-C12-C13	10.76	155.86	126.36
33	4	505	C7Z	C11-C10-C9	-10.68	112.30	127.28
22	A	4008	BCR	C11-C12-C13	10.64	155.54	126.36
22	B	4006	BCR	C16-C15-C14	10.57	145.15	123.52
22	A	4011	BCR	C16-C15-C14	10.56	145.12	123.52
22	1	504	BCR	C11-C12-C13	10.46	155.05	126.36
22	3	503	BCR	C11-C10-C9	10.44	141.93	127.28
22	1	503	BCR	C16-C15-C14	10.43	144.85	123.52
22	H	4021	BCR	C11-C12-C13	10.35	154.74	126.36
22	A	4002	BCR	C16-C15-C14	10.34	144.68	123.52
22	3	506	BCR	C11-C12-C13	10.33	154.69	126.36
22	L	4019	BCR	C11-C12-C13	10.19	154.30	126.36
20	A	1115	CLA	C4A-NA-C1A	10.05	111.26	106.68
22	3	503	BCR	C11-C12-C13	10.04	153.89	126.36
19	A	1011	CL0	O2D-CGD-CBD	9.98	121.91	110.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	3	503	BCR	C20-C19-C18	9.89	153.48	126.36
22	2	503	BCR	C11-C12-C13	9.77	153.16	126.36
20	G	1603	CLA	C4A-NA-C1A	9.74	111.12	106.68
20	B	1219	CLA	C4A-NA-C1A	9.72	111.11	106.68
20	A	1103	CLA	C4A-NA-C1A	9.71	111.11	106.68
20	A	1107	CLA	C4A-NA-C1A	9.69	111.10	106.68
22	I	4018	BCR	C20-C19-C18	9.68	152.90	126.36
22	A	4008	BCR	C16-C15-C14	9.67	143.29	123.52
20	A	1118	CLA	C4A-NA-C1A	9.60	111.06	106.68
22	J	4012	BCR	C16-C15-C14	9.55	143.07	123.52
20	3	601	CLA	C4A-NA-C1A	9.54	111.03	106.68
22	A	4017	BCR	C11-C12-C13	9.53	152.50	126.36
20	B	1205	CLA	C4A-NA-C1A	9.50	111.01	106.68
22	L	4020	BCR	C11-C12-C13	9.48	152.35	126.36
20	J	1901	CLA	C4A-NA-C1A	9.48	111.00	106.68
20	B	1206	CLA	C4A-NA-C1A	9.46	111.00	106.68
22	I	4020	BCR	C11-C12-C13	9.43	152.23	126.36
22	A	4017	BCR	C15-C14-C13	-9.36	114.14	127.28
20	A	1111	CLA	C4A-NA-C1A	9.34	110.94	106.68
20	B	1225	CLA	C4A-NA-C1A	9.32	110.93	106.68
20	3	602	CLA	C4A-NA-C1A	9.32	110.93	106.68
20	B	1201	CLA	C4A-NA-C1A	9.28	110.91	106.68
22	L	4019	BCR	C20-C19-C18	9.27	151.79	126.36
20	F	1301	CLA	C4A-NA-C1A	9.27	110.91	106.68
20	3	605	CLA	C4A-NA-C1A	9.23	110.89	106.68
20	A	1138	CLA	C4A-NA-C1A	9.23	110.89	106.68
22	A	4011	BCR	C20-C19-C18	9.23	151.66	126.36
22	K	4002	BCR	C20-C19-C18	9.21	151.62	126.36
20	1	608	CLA	C4A-NA-C1A	9.17	110.86	106.68
20	A	1125	CLA	C4A-NA-C1A	9.17	110.86	106.68
20	A	1139	CLA	C4A-NA-C1A	9.15	110.85	106.68
20	1	603	CLA	C4A-NA-C1A	9.15	110.85	106.68
20	B	1220	CLA	C4A-NA-C1A	9.13	110.84	106.68
20	A	1116	CLA	C4A-NA-C1A	9.12	110.84	106.68
20	A	1121	CLA	C4A-NA-C1A	9.11	110.84	106.68
20	A	1102	CLA	C4A-NA-C1A	9.11	110.83	106.68
20	1	605	CLA	C4A-NA-C1A	9.10	110.83	106.68
22	B	4009	BCR	C20-C19-C18	9.10	151.32	126.36
20	A	1105	CLA	C4A-NA-C1A	9.09	110.83	106.68
20	1	601	CLA	C4A-NA-C1A	9.08	110.82	106.68
20	A	1113	CLA	C4A-NA-C1A	9.07	110.82	106.68
20	2	612	CLA	C4A-NA-C1A	9.07	110.82	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	4005	BCR	C20-C19-C18	9.06	151.19	126.36
20	A	1126	CLA	C4A-NA-C1A	9.04	110.80	106.68
20	B	1223	CLA	C4A-NA-C1A	9.03	110.80	106.68
20	4	601	CLA	C4A-NA-C1A	9.00	110.78	106.68
20	3	612	CLA	C4A-NA-C1A	8.98	110.78	106.68
22	A	4003	BCR	C16-C15-C14	8.97	141.88	123.52
20	K	1402	CLA	C4A-NA-C1A	8.97	110.77	106.68
22	F	4014	BCR	C20-C19-C18	8.97	150.95	126.36
20	B	1230	CLA	C4A-NA-C1A	8.96	110.77	106.68
29	J	4013	LUT	C21-C26-C27	8.95	123.12	112.83
20	A	1122	CLA	C4A-NA-C1A	8.94	110.76	106.68
20	A	1109	CLA	C4A-NA-C1A	8.93	110.75	106.68
20	B	1231	CLA	C4A-NA-C1A	8.91	110.74	106.68
20	4	617	CLA	C4A-NA-C1A	8.90	110.74	106.68
20	F	1302	CLA	C4A-NA-C1A	8.88	110.73	106.68
20	B	1228	CLA	C4A-NA-C1A	8.88	110.73	106.68
20	B	1215	CLA	C4A-NA-C1A	8.88	110.73	106.68
20	B	1226	CLA	C4A-NA-C1A	8.88	110.73	106.68
20	B	1023	CLA	C4A-NA-C1A	8.86	110.72	106.68
20	1	611	CLA	C4A-NA-C1A	8.86	110.72	106.68
20	K	1404	CLA	C4A-NA-C1A	8.86	110.72	106.68
20	A	1110	CLA	C4A-NA-C1A	8.86	110.72	106.68
20	B	1211	CLA	C4A-NA-C1A	8.83	110.71	106.68
20	B	1224	CLA	C4A-NA-C1A	8.79	110.69	106.68
20	3	603	CLA	C4A-NA-C1A	8.79	110.69	106.68
20	B	1222	CLA	C4A-NA-C1A	8.78	110.69	106.68
20	B	1202	CLA	C4A-NA-C1A	8.77	110.68	106.68
20	B	1214	CLA	C4A-NA-C1A	8.76	110.68	106.68
20	2	601	CLA	C4A-NA-C1A	8.76	110.68	106.68
20	A	1106	CLA	C4A-NA-C1A	8.75	110.67	106.68
20	B	1227	CLA	C4A-NA-C1A	8.75	110.67	106.68
20	K	1403	CLA	C4A-NA-C1A	8.75	110.67	106.68
20	2	607	CLA	C4A-NA-C1A	8.74	110.67	106.68
20	3	613	CLA	C4A-NA-C1A	8.74	110.67	106.68
20	B	1207	CLA	C4A-NA-C1A	8.74	110.67	106.68
20	A	1140	CLA	C4A-NA-C1A	8.73	110.66	106.68
20	3	617	CLA	C4A-NA-C1A	8.73	110.66	106.68
20	B	1213	CLA	C4A-NA-C1A	8.73	110.66	106.68
20	A	1101	CLA	C4A-NA-C1A	8.72	110.66	106.68
20	2	605	CLA	C4A-NA-C1A	8.72	110.66	106.68
20	B	1021	CLA	C4A-NA-C1A	8.72	110.66	106.68
20	B	1212	CLA	C4A-NA-C1A	8.71	110.66	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	K	1401	CLA	C4A-NA-C1A	8.70	110.65	106.68
20	A	1012	CLA	C4A-NA-C1A	8.69	110.64	106.68
20	B	1204	CLA	C4A-NA-C1A	8.69	110.64	106.68
20	B	1235	CLA	C4A-NA-C1A	8.68	110.64	106.68
20	1	607	CLA	C4A-NA-C1A	8.67	110.64	106.68
20	2	606	CLA	C4A-NA-C1A	8.66	110.63	106.68
20	3	614	CLA	C4A-NA-C1A	8.66	110.63	106.68
20	A	1123	CLA	C4A-NA-C1A	8.63	110.61	106.68
20	B	1240	CLA	C4A-NA-C1A	8.61	110.61	106.68
20	3	610	CLA	C4A-NA-C1A	8.60	110.60	106.68
20	B	1217	CLA	C4A-NA-C1A	8.59	110.60	106.68
20	A	1134	CLA	C4A-NA-C1A	8.58	110.59	106.68
20	A	1104	CLA	C4A-NA-C1A	8.58	110.59	106.68
20	B	1209	CLA	C4A-NA-C1A	8.58	110.59	106.68
20	A	1013	CLA	C4A-NA-C1A	8.57	110.59	106.68
20	L	1502	CLA	C4A-NA-C1A	8.57	110.59	106.68
20	2	603	CLA	C4A-NA-C1A	8.57	110.59	106.68
20	A	1120	CLA	C4A-NA-C1A	8.56	110.58	106.68
20	H	1701	CLA	C4A-NA-C1A	8.56	110.58	106.68
22	B	4006	BCR	C21-C20-C19	8.55	147.97	123.20
22	B	4004	BCR	C16-C15-C14	8.54	141.00	123.52
20	B	1234	CLA	C4A-NA-C1A	8.54	110.57	106.68
20	4	612	CLA	C4A-NA-C1A	8.54	110.57	106.68
22	A	4008	BCR	C20-C19-C18	8.53	149.76	126.36
20	B	1203	CLA	C4A-NA-C1A	8.53	110.57	106.68
20	A	1128	CLA	C4A-NA-C1A	8.53	110.57	106.68
20	B	1229	CLA	C4A-NA-C1A	8.52	110.57	106.68
20	3	608	CLA	C4A-NA-C1A	8.52	110.56	106.68
22	B	4010	BCR	C20-C19-C18	8.51	149.71	126.36
20	2	604	CLA	C4A-NA-C1A	8.51	110.56	106.68
20	A	1132	CLA	C4A-NA-C1A	8.48	110.55	106.68
20	4	606	CLA	C4A-NA-C1A	8.48	110.55	106.68
20	A	1117	CLA	C4A-NA-C1A	8.48	110.55	106.68
20	1	602	CLA	C4A-NA-C1A	8.47	110.54	106.68
22	F	4016	BCR	C20-C19-C18	8.46	149.57	126.36
20	2	602	CLA	C4A-NA-C1A	8.46	110.54	106.68
33	4	505	C7Z	C39-C29-C30	-8.45	109.13	122.82
20	4	608	CLA	C4A-NA-C1A	8.44	110.53	106.68
33	4	505	C7Z	C1-C6-C5	-8.42	111.13	122.64
20	B	1239	CLA	C4A-NA-C1A	8.41	110.52	106.68
20	L	1501	CLA	C4A-NA-C1A	8.40	110.51	106.68
20	B	1236	CLA	C4A-NA-C1A	8.40	110.51	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	3	606	CLA	C4A-NA-C1A	8.40	110.51	106.68
20	B	1221	CLA	C4A-NA-C1A	8.39	110.51	106.68
22	L	4020	BCR	C20-C19-C18	8.39	149.36	126.36
20	4	609	CLA	C4A-NA-C1A	8.39	110.50	106.68
33	4	505	C7Z	C19-C9-C10	-8.38	109.24	122.82
20	A	1124	CLA	C4A-NA-C1A	8.37	110.50	106.68
20	A	1135	CLA	C4A-NA-C1A	8.36	110.50	106.68
20	B	1237	CLA	C4A-NA-C1A	8.36	110.50	106.68
20	A	1133	CLA	C4A-NA-C1A	8.36	110.49	106.68
20	A	1114	CLA	C4A-NA-C1A	8.32	110.48	106.68
20	A	1127	CLA	C4A-NA-C1A	8.30	110.47	106.68
20	A	1119	CLA	C4A-NA-C1A	8.28	110.46	106.68
20	A	1141	CLA	C4A-NA-C1A	8.28	110.46	106.68
20	A	1136	CLA	C4A-NA-C1A	8.26	110.45	106.68
20	1	614	CLA	C4A-NA-C1A	8.26	110.45	106.68
20	L	1503	CLA	C4A-NA-C1A	8.23	110.43	106.68
20	B	1218	CLA	C4A-NA-C1A	8.22	110.43	106.68
20	4	604	CLA	C4A-NA-C1A	8.22	110.43	106.68
20	A	1129	CLA	C4A-NA-C1A	8.22	110.43	106.68
20	2	608	CLA	C4A-NA-C1A	8.22	110.43	106.68
20	B	1216	CLA	C4A-NA-C1A	8.20	110.42	106.68
20	A	1108	CLA	C4A-NA-C1A	8.18	110.41	106.68
20	A	1130	CLA	C4A-NA-C1A	8.18	110.41	106.68
33	4	505	C7Z	C20-C13-C14	-8.17	109.58	122.82
33	4	505	C7Z	C40-C33-C34	-8.16	109.59	122.82
20	B	1238	CLA	C4A-NA-C1A	8.16	110.40	106.68
22	H	4021	BCR	C20-C19-C18	8.15	148.70	126.36
22	1	503	BCR	C20-C19-C18	8.14	148.67	126.36
20	4	605	CLA	C4A-NA-C1A	8.12	110.38	106.68
20	B	1232	CLA	C4A-NA-C1A	8.12	110.38	106.68
20	A	1131	CLA	C4A-NA-C1A	8.11	110.38	106.68
20	A	1137	CLA	C4A-NA-C1A	8.05	110.35	106.68
20	4	602	CLA	C4A-NA-C1A	8.01	110.33	106.68
22	A	4002	BCR	C20-C19-C18	8.01	148.32	126.36
30	4	615	CHL	C1B-CHB-C4A	8.00	126.47	121.32
22	I	4020	BCR	C20-C19-C18	7.95	148.17	126.36
20	B	1208	CLA	C4A-NA-C1A	7.94	110.30	106.68
20	G	1602	CLA	C4A-NA-C1A	7.94	110.30	106.68
20	1	613	CLA	C4A-NA-C1A	7.91	110.29	106.68
20	4	603	CLA	C4A-NA-C1A	7.90	110.28	106.68
22	B	4004	BCR	C11-C12-C13	7.85	147.88	126.36
20	A	1112	CLA	C4A-NA-C1A	7.79	110.23	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	1	606	CLA	C4A-NA-C1A	7.79	110.23	106.68
20	1	604	CLA	C4A-NA-C1A	7.72	110.20	106.68
22	2	503	BCR	C40-C30-C29	-7.71	79.34	108.95
20	B	1210	CLA	C4A-NA-C1A	7.70	110.19	106.68
20	4	607	CLA	C4A-NA-C1A	7.59	110.14	106.68
20	G	1601	CLA	C4A-NA-C1A	7.56	110.13	106.68
20	B	1022	CLA	C4A-NA-C1A	7.52	110.11	106.68
22	J	4012	BCR	C20-C19-C18	7.47	146.85	126.36
22	A	4007	BCR	C20-C19-C18	7.27	146.28	126.36
22	2	503	BCR	C33-C5-C6	-7.24	116.59	124.48
30	1	610	CHL	C1B-CHB-C4A	7.14	125.92	121.32
33	4	505	C7Z	C21-C26-C25	-7.14	112.88	122.64
22	G	4011	BCR	C20-C19-C18	6.87	145.19	126.36
20	2	608	CLA	CMD-C2D-C1D	6.82	136.74	124.73
22	3	506	BCR	C20-C19-C18	6.75	144.86	126.36
22	B	4004	BCR	C19-C18-C17	6.70	129.55	119.01
22	2	503	BCR	C20-C19-C18	6.66	144.62	126.36
20	B	1210	CLA	O2D-CGD-CBD	6.65	122.86	111.23
22	I	4018	BCR	C11-C10-C9	6.64	136.60	127.28
22	K	4001	BCR	C20-C19-C18	6.55	144.31	126.36
22	1	504	BCR	C20-C19-C18	6.53	144.26	126.36
29	2	501	LUT	C15-C14-C13	-6.51	118.14	127.28
30	1	612	CHL	C1B-CHB-C4A	6.51	125.51	121.32
22	A	4003	BCR	C20-C19-C18	6.51	144.20	126.36
22	B	4004	BCR	C8-C9-C10	6.45	129.16	119.01
30	4	611	CHL	C1B-CHB-C4A	6.44	125.47	121.32
20	A	1111	CLA	O2D-CGD-CBD	6.41	122.44	111.23
20	A	1106	CLA	O2D-CGD-CBD	6.40	122.42	111.23
20	A	1137	CLA	O2D-CGD-CBD	6.37	122.36	111.23
29	2	501	LUT	C11-C10-C9	-6.35	118.37	127.28
31	2	502	XAT	O4-C5-C18	-6.30	108.00	115.05
20	A	1112	CLA	O2D-CGD-CBD	6.29	122.23	111.23
22	2	503	BCR	C40-C30-C25	6.29	120.10	110.24
22	I	4018	BCR	C11-C12-C13	6.27	143.55	126.36
29	J	4013	LUT	C11-C10-C9	-6.25	118.52	127.28
20	1	614	CLA	O2D-CGD-CBD	6.18	122.04	111.23
20	B	1240	CLA	O2D-CGD-CBD	6.18	122.04	111.23
20	B	1226	CLA	O2D-CGD-CBD	6.18	122.04	111.23
20	1	608	CLA	O2D-CGD-CBD	6.14	121.96	111.23
22	B	4004	BCR	C12-C13-C14	6.13	128.66	119.01
20	B	1202	CLA	O2D-CGD-CBD	6.13	121.94	111.23
22	G	4011	BCR	C19-C18-C17	6.12	128.64	119.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	1128	CLA	O2D-CGD-CBD	6.12	121.93	111.23
20	B	1223	CLA	O2D-CGD-CBD	6.06	121.83	111.23
22	A	4017	BCR	C20-C19-C18	6.05	142.95	126.36
29	3	502	LUT	C21-C26-C27	6.05	119.78	112.83
20	3	614	CLA	CMD-C2D-C1D	6.05	135.38	124.73
20	B	1217	CLA	O2D-CGD-CBD	6.05	121.80	111.23
30	3	611	CHL	C1B-CHB-C4A	6.02	125.19	121.32
20	B	1205	CLA	O2D-CGD-CBD	6.01	121.74	111.23
33	4	505	C7Z	C40-C33-C32	-6.00	108.92	118.09
29	3	501	LUT	C21-C26-C27	5.98	119.70	112.83
20	A	1118	CLA	O2D-CGD-CBD	5.96	121.66	111.23
20	B	1236	CLA	O2D-CGD-CBD	5.94	121.61	111.23
20	B	1211	CLA	O2D-CGD-CBD	5.92	121.59	111.23
20	B	1229	CLA	O2D-CGD-CBD	5.90	121.54	111.23
20	1	604	CLA	CMD-C2D-C1D	5.89	135.11	124.73
20	B	1222	CLA	O2D-CGD-CBD	5.89	121.52	111.23
33	4	505	C7Z	C12-C13-C14	-5.88	109.75	119.01
33	4	505	C7Z	C20-C13-C12	-5.87	109.12	118.09
20	B	1237	CLA	C1-C2-C3	-5.87	116.59	126.20
20	K	1402	CLA	O2D-CGD-CBD	5.86	121.48	111.23
33	4	505	C7Z	C19-C9-C8	-5.86	109.13	118.09
20	B	1218	CLA	O2D-CGD-CBD	5.86	121.47	111.23
20	A	1105	CLA	O2D-CGD-CBD	5.85	121.46	111.23
33	4	505	C7Z	C39-C29-C28	-5.85	109.15	118.09
20	4	605	CLA	CMD-C2D-C1D	5.84	135.01	124.73
20	3	601	CLA	CMD-C2D-C1D	5.84	135.00	124.73
20	A	1102	CLA	O2D-CGD-CBD	5.84	121.43	111.23
20	B	1235	CLA	O2D-CGD-CBD	5.82	121.41	111.23
20	3	613	CLA	CMD-C2D-C1D	5.82	134.98	124.73
20	1	608	CLA	CMD-C2D-C1D	5.78	134.90	124.73
20	B	1212	CLA	O2D-CGD-CBD	5.77	121.32	111.23
20	A	1121	CLA	CMD-C2D-C1D	5.77	134.90	124.73
20	B	1224	CLA	O2D-CGD-CBD	5.77	121.32	111.23
20	B	1240	CLA	CMD-C2D-C1D	5.75	134.85	124.73
30	3	607	CHL	C1B-CHB-C4A	5.74	125.02	121.32
20	2	608	CLA	O2D-CGD-CBD	5.74	121.26	111.23
20	B	1202	CLA	CMD-C2D-C1D	5.73	134.83	124.73
20	B	1239	CLA	O2D-CGD-CBD	5.73	121.25	111.23
20	B	1231	CLA	CMD-C2D-C1D	5.73	134.82	124.73
20	A	1129	CLA	O2D-CGD-CBD	5.73	121.25	111.23
30	4	613	CHL	C1B-CHB-C4A	5.73	125.01	121.32
20	A	1109	CLA	CMD-C2D-C1D	5.72	134.80	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	1230	CLA	O2D-CGD-CBD	5.71	121.22	111.23
33	4	505	C7Z	C7-C6-C5	-5.71	108.40	121.56
20	B	1221	CLA	O2D-CGD-CBD	5.71	121.21	111.23
31	4	502	XAT	C18-C5-C4	5.69	120.63	114.24
20	A	1118	CLA	CMD-C2D-C1D	5.69	134.74	124.73
29	3	502	LUT	C35-C34-C33	-5.68	119.32	127.28
20	B	1221	CLA	CMD-C2D-C1D	5.67	134.72	124.73
20	B	1214	CLA	CMD-C2D-C1D	5.67	134.71	124.73
20	3	606	CLA	CMD-C2D-C1D	5.67	134.71	124.73
20	1	605	CLA	CMD-C2D-C1D	5.67	134.71	124.73
20	A	1108	CLA	CMD-C2D-C1D	5.66	134.70	124.73
20	3	612	CLA	CMD-C2D-C1D	5.66	134.70	124.73
20	B	1211	CLA	CMD-C2D-C1D	5.65	134.68	124.73
30	2	615	CHL	C1B-CHB-C4A	5.64	124.95	121.32
20	K	1402	CLA	CMD-C2D-C1D	5.62	134.63	124.73
20	A	1114	CLA	CMD-C2D-C1D	5.61	134.61	124.73
20	1	605	CLA	O2D-CGD-CBD	5.61	121.04	111.23
20	A	1125	CLA	CMD-C2D-C1D	5.61	134.61	124.73
31	2	502	XAT	O4-C5-C4	-5.61	108.23	113.49
20	A	1141	CLA	O2D-CGD-CBD	5.61	121.03	111.23
20	3	605	CLA	CMD-C2D-C1D	5.60	134.60	124.73
20	2	607	CLA	O2D-CGD-CBD	5.60	121.03	111.23
20	A	1131	CLA	CMD-C2D-C1D	5.59	134.58	124.73
22	B	4004	BCR	C15-C14-C13	5.59	135.12	127.28
20	A	1120	CLA	CMD-C2D-C1D	5.59	134.57	124.73
20	A	1116	CLA	O2D-CGD-CBD	5.59	121.00	111.23
20	A	1110	CLA	CMD-C2D-C1D	5.58	134.56	124.73
20	4	608	CLA	CMD-C2D-C1D	5.57	134.54	124.73
20	3	608	CLA	CMD-C2D-C1D	5.57	134.53	124.73
20	B	1209	CLA	O2D-CGD-CBD	5.56	120.96	111.23
20	2	603	CLA	CMD-C2D-C1D	5.56	134.52	124.73
20	A	1119	CLA	CMD-C2D-C1D	5.56	134.52	124.73
20	B	1210	CLA	CMD-C2D-C1D	5.56	134.51	124.73
20	2	606	CLA	CMD-C2D-C1D	5.56	134.51	124.73
20	G	1602	CLA	CMD-C2D-C1D	5.55	134.50	124.73
29	3	502	LUT	C31-C30-C29	-5.55	119.49	127.28
20	A	1103	CLA	O2D-CGD-CBD	5.54	120.92	111.23
20	3	610	CLA	CMD-C2D-C1D	5.54	134.49	124.73
20	1	605	CLA	C1-C2-C3	-5.54	117.11	126.20
20	G	1601	CLA	CMD-C2D-C1D	5.54	134.49	124.73
20	B	1204	CLA	O2D-CGD-CBD	5.54	120.92	111.23
20	4	608	CLA	O2D-CGD-CBD	5.53	120.90	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	1	614	CLA	CMD-C2D-C1D	5.53	134.46	124.73
20	3	603	CLA	CMD-C2D-C1D	5.52	134.46	124.73
20	A	1133	CLA	O2D-CGD-CBD	5.52	120.89	111.23
20	B	1208	CLA	CMD-C2D-C1D	5.52	134.46	124.73
20	4	606	CLA	CMD-C2D-C1D	5.52	134.45	124.73
20	A	1104	CLA	CMD-C2D-C1D	5.51	134.44	124.73
20	J	1901	CLA	CMD-C2D-C1D	5.51	134.44	124.73
20	K	1401	CLA	CMD-C2D-C1D	5.51	134.44	124.73
20	A	1125	CLA	O2D-CGD-CBD	5.51	120.87	111.23
20	B	1207	CLA	CMD-C2D-C1D	5.51	134.44	124.73
20	3	602	CLA	CMD-C2D-C1D	5.51	134.44	124.73
31	4	502	XAT	O4-C5-C18	-5.51	108.89	115.05
20	A	1101	CLA	CMD-C2D-C1D	5.51	134.43	124.73
20	A	1140	CLA	CMD-C2D-C1D	5.51	134.42	124.73
20	4	607	CLA	O2D-CGD-CBD	5.50	120.85	111.23
20	4	609	CLA	CMD-C2D-C1D	5.50	134.42	124.73
20	A	1101	CLA	O2D-CGD-CBD	5.50	120.85	111.23
20	A	1137	CLA	CMD-C2D-C1D	5.50	134.41	124.73
20	4	607	CLA	CMD-C2D-C1D	5.50	134.41	124.73
20	A	1102	CLA	CMD-C2D-C1D	5.50	134.41	124.73
20	H	1701	CLA	CMD-C2D-C1D	5.50	134.41	124.73
20	1	606	CLA	CMD-C2D-C1D	5.49	134.40	124.73
20	B	1204	CLA	CMD-C2D-C1D	5.49	134.40	124.73
20	3	617	CLA	CMD-C2D-C1D	5.49	134.40	124.73
20	L	1502	CLA	CMD-C2D-C1D	5.49	134.40	124.73
20	A	1129	CLA	CMD-C2D-C1D	5.49	134.40	124.73
20	A	1124	CLA	O2D-CGD-CBD	5.49	120.83	111.23
20	A	1116	CLA	CMD-C2D-C1D	5.49	134.39	124.73
20	B	1232	CLA	CMD-C2D-C1D	5.48	134.39	124.73
20	B	1238	CLA	CMD-C2D-C1D	5.48	134.39	124.73
20	A	1132	CLA	CMD-C2D-C1D	5.48	134.38	124.73
20	2	602	CLA	CMD-C2D-C1D	5.48	134.38	124.73
20	A	1130	CLA	O2D-CGD-CBD	5.47	120.80	111.23
20	L	1503	CLA	CMD-C2D-C1D	5.47	134.35	124.73
20	4	604	CLA	CMD-C2D-C1D	5.46	134.35	124.73
20	L	1501	CLA	CMD-C2D-C1D	5.46	134.35	124.73
20	A	1136	CLA	O2D-CGD-CBD	5.46	120.78	111.23
20	A	1131	CLA	O2D-CGD-CBD	5.46	120.77	111.23
20	K	1403	CLA	CMD-C2D-C1D	5.45	134.33	124.73
20	4	603	CLA	CMD-C2D-C1D	5.45	134.33	124.73
20	2	604	CLA	CMD-C2D-C1D	5.45	134.32	124.73
22	1	504	BCR	C15-C14-C13	-5.44	119.64	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	4	617	CLA	O2D-CGD-CBD	5.44	120.75	111.23
20	A	1111	CLA	CMD-C2D-C1D	5.44	134.31	124.73
30	2	613	CHL	C1B-CHB-C4A	5.43	124.82	121.32
20	B	1225	CLA	CMD-C2D-C1D	5.43	134.29	124.73
33	4	505	C7Z	C8-C9-C10	-5.43	110.47	119.01
20	B	1226	CLA	CMD-C2D-C1D	5.43	134.28	124.73
20	B	1235	CLA	CMD-C2D-C1D	5.43	134.28	124.73
20	B	1224	CLA	CMD-C2D-C1D	5.42	134.27	124.73
20	G	1603	CLA	CMD-C2D-C1D	5.42	134.26	124.73
20	B	1239	CLA	CMD-C2D-C1D	5.41	134.26	124.73
20	1	601	CLA	C1-C2-C3	-5.41	117.33	126.20
20	A	1107	CLA	CMD-C2D-C1D	5.41	134.26	124.73
20	B	1238	CLA	O2D-CGD-CBD	5.41	120.69	111.23
20	3	602	CLA	O2D-CGD-CBD	5.41	120.68	111.23
20	2	605	CLA	O2D-CGD-CBD	5.40	120.68	111.23
20	A	1134	CLA	CMD-C2D-C1D	5.40	134.24	124.73
20	3	601	CLA	O2D-CGD-CBD	5.40	120.66	111.23
20	B	1215	CLA	O2D-CGD-CBD	5.39	120.64	111.23
20	A	1141	CLA	CMD-C2D-C1D	5.38	134.21	124.73
20	K	1404	CLA	CMD-C2D-C1D	5.38	134.21	124.73
20	B	1203	CLA	CMD-C2D-C1D	5.36	134.17	124.73
20	B	1231	CLA	O2D-CGD-CBD	5.35	120.59	111.23
20	1	601	CLA	CMD-C2D-C1D	5.35	134.15	124.73
20	A	1012	CLA	C1-C2-C3	-5.35	117.43	126.20
20	A	1132	CLA	O2D-CGD-CBD	5.34	120.57	111.23
20	4	612	CLA	CMD-C2D-C1D	5.34	134.14	124.73
20	A	1103	CLA	CMD-C2D-C1D	5.34	134.13	124.73
20	B	1236	CLA	CMD-C2D-C1D	5.34	134.13	124.73
20	B	1214	CLA	O2D-CGD-CBD	5.34	120.56	111.23
19	A	1011	CL0	O2A-CGA-O1A	-5.34	110.28	123.63
33	4	505	C7Z	C32-C33-C34	-5.33	110.62	119.01
20	B	1201	CLA	O2D-CGD-CBD	5.33	120.55	111.23
20	1	606	CLA	O2D-CGD-CBD	5.33	120.55	111.23
20	A	1127	CLA	O2D-CGD-CBD	5.33	120.54	111.23
20	A	1123	CLA	CMD-C2D-C1D	5.32	134.10	124.73
20	B	1218	CLA	CMD-C2D-C1D	5.32	134.09	124.73
20	A	1135	CLA	CMD-C2D-C1D	5.31	134.08	124.73
20	B	1229	CLA	CMD-C2D-C1D	5.31	134.08	124.73
22	1	504	BCR	C19-C18-C17	5.31	127.36	119.01
20	A	1134	CLA	O2D-CGD-CBD	5.31	120.51	111.23
20	1	613	CLA	CMD-C2D-C1D	5.31	134.08	124.73
20	B	1237	CLA	CMD-C2D-C1D	5.31	134.07	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	1119	CLA	O2D-CGD-CBD	5.30	120.50	111.23
20	3	605	CLA	O2D-CGD-CBD	5.30	120.50	111.23
20	2	604	CLA	O2D-CGD-CBD	5.30	120.49	111.23
20	4	609	CLA	O2D-CGD-CBD	5.30	120.49	111.23
20	B	1022	CLA	CMD-C2D-C1D	5.30	134.06	124.73
20	2	612	CLA	CMD-C2D-C1D	5.30	134.05	124.73
20	B	1215	CLA	CMD-C2D-C1D	5.30	134.05	124.73
20	A	1105	CLA	CMD-C2D-C1D	5.29	134.05	124.73
20	3	610	CLA	O2D-CGD-CBD	5.29	120.47	111.23
20	L	1502	CLA	O2D-CGD-CBD	5.29	120.47	111.23
20	A	1122	CLA	CMD-C2D-C1D	5.28	134.03	124.73
20	L	1503	CLA	O2D-CGD-CBD	5.28	120.46	111.23
20	A	1140	CLA	O2D-CGD-CBD	5.28	120.46	111.23
29	2	501	LUT	C7-C8-C9	-5.28	118.43	126.23
20	A	1106	CLA	CMD-C2D-C1D	5.28	134.02	124.73
20	A	1115	CLA	O2D-CGD-CBD	5.28	120.46	111.23
20	B	1213	CLA	CMD-C2D-C1D	5.28	134.02	124.73
20	2	607	CLA	CMD-C2D-C1D	5.27	134.02	124.73
20	B	1226	CLA	C1-C2-C3	-5.27	117.56	126.20
20	A	1128	CLA	CMD-C2D-C1D	5.27	134.00	124.73
20	G	1603	CLA	O2D-CGD-CBD	5.26	120.42	111.23
29	4	501	LUT	C35-C34-C33	-5.25	119.92	127.28
20	1	602	CLA	CMD-C2D-C1D	5.23	133.94	124.73
20	A	1114	CLA	O2D-CGD-CBD	5.23	120.38	111.23
20	4	604	CLA	O2D-CGD-CBD	5.23	120.38	111.23
20	2	605	CLA	CMD-C2D-C1D	5.23	133.94	124.73
20	A	1127	CLA	C1-C2-C3	-5.23	117.63	126.20
20	B	1230	CLA	CMD-C2D-C1D	5.23	133.94	124.73
20	B	1021	CLA	C1-C2-C3	-5.23	117.64	126.20
20	B	1213	CLA	O2D-CGD-CBD	5.22	120.36	111.23
20	4	601	CLA	CMD-C2D-C1D	5.22	133.92	124.73
20	4	617	CLA	CMD-C2D-C1D	5.22	133.91	124.73
20	B	1207	CLA	O2D-CGD-CBD	5.21	120.34	111.23
20	B	1205	CLA	CMD-C2D-C1D	5.21	133.90	124.73
20	A	1113	CLA	CMD-C2D-C1D	5.20	133.89	124.73
20	B	1222	CLA	CMD-C2D-C1D	5.20	133.89	124.73
20	F	1302	CLA	CMD-C2D-C1D	5.20	133.89	124.73
22	2	503	BCR	C39-C30-C25	5.20	118.39	110.24
20	B	1223	CLA	CMD-C2D-C1D	5.19	133.88	124.73
20	B	1208	CLA	O2D-CGD-CBD	5.19	120.30	111.23
20	B	1021	CLA	O2D-CGD-CBD	5.19	120.30	111.23
33	4	505	C7Z	C27-C26-C25	-5.19	109.61	121.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	1232	CLA	O2D-CGD-CBD	5.18	120.28	111.23
20	A	1130	CLA	CMD-C2D-C1D	5.18	133.84	124.73
20	B	1227	CLA	O2D-CGD-CBD	5.17	120.28	111.23
20	B	1217	CLA	CMD-C2D-C1D	5.17	133.83	124.73
20	1	602	CLA	O2D-CGD-CBD	5.16	120.25	111.23
20	1	603	CLA	CMD-C2D-C1D	5.15	133.81	124.73
20	A	1117	CLA	O2D-CGD-CBD	5.15	120.24	111.23
23	B	5001	LHG	O7-C7-C8	5.15	120.28	111.09
22	3	503	BCR	C33-C5-C6	-5.14	118.87	124.48
31	4	502	XAT	C38-C25-C24	5.14	120.02	114.24
30	1	609	CHL	C1B-CHB-C4A	5.14	124.63	121.32
20	A	1122	CLA	O2D-CGD-CBD	5.14	120.21	111.23
20	1	601	CLA	O2D-CGD-CBD	5.14	120.21	111.23
20	A	1108	CLA	O2D-CGD-CBD	5.14	120.21	111.23
20	B	1204	CLA	C1-C2-C3	-5.13	117.79	126.20
20	F	1301	CLA	CMD-C2D-C1D	5.13	133.76	124.73
20	B	1227	CLA	CMD-C2D-C1D	5.13	133.75	124.73
20	3	608	CLA	O2D-CGD-CBD	5.12	120.19	111.23
20	1	611	CLA	O2D-CGD-CBD	5.12	120.19	111.23
20	B	1209	CLA	CMD-C2D-C1D	5.12	133.75	124.73
20	L	1501	CLA	O2D-CGD-CBD	5.12	120.18	111.23
33	4	505	C7Z	C28-C29-C30	-5.12	110.96	119.01
20	B	1228	CLA	CMD-C2D-C1D	5.11	133.73	124.73
20	B	1237	CLA	O2D-CGD-CBD	5.11	120.16	111.23
20	1	607	CLA	O2D-CGD-CBD	5.11	120.16	111.23
20	H	1701	CLA	O2D-CGD-CBD	5.10	120.15	111.23
20	B	1216	CLA	O2D-CGD-CBD	5.10	120.15	111.23
20	B	1216	CLA	CMD-C2D-C1D	5.10	133.71	124.73
20	B	1228	CLA	O2D-CGD-CBD	5.10	120.14	111.23
20	A	1120	CLA	O2D-CGD-CBD	5.09	120.12	111.23
20	A	1107	CLA	O2D-CGD-CBD	5.08	120.12	111.23
20	A	1109	CLA	O2D-CGD-CBD	5.07	120.10	111.23
29	1	502	LUT	C15-C14-C13	-5.07	120.17	127.28
20	K	1401	CLA	O2D-CGD-CBD	5.06	120.07	111.23
20	B	1234	CLA	O2D-CGD-CBD	5.05	120.07	111.23
20	B	1218	CLA	C1-C2-C3	-5.05	117.92	126.20
20	A	1115	CLA	CMD-C2D-C1D	5.05	133.62	124.73
20	A	1104	CLA	O2D-CGD-CBD	5.05	120.06	111.23
20	B	1219	CLA	CMD-C2D-C1D	5.05	133.62	124.73
20	G	1602	CLA	O2D-CGD-CBD	5.04	120.05	111.23
20	1	611	CLA	CMD-C2D-C1D	5.04	133.60	124.73
20	B	1220	CLA	CMD-C2D-C1D	5.03	133.59	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	1	603	CLA	O2D-CGD-CBD	5.03	120.03	111.23
20	3	617	CLA	O2D-CGD-CBD	5.03	120.02	111.23
20	3	613	CLA	O2D-CGD-CBD	5.03	120.02	111.23
20	A	1124	CLA	CMD-C2D-C1D	5.02	133.57	124.73
20	B	1225	CLA	O2D-CGD-CBD	5.02	120.01	111.23
20	1	604	CLA	O2D-CGD-CBD	5.02	120.00	111.23
20	A	1112	CLA	CMD-C2D-C1D	5.01	133.54	124.73
29	J	4013	LUT	C15-C14-C13	-5.00	120.26	127.28
20	A	1135	CLA	O2D-CGD-CBD	5.00	119.97	111.23
20	A	1138	CLA	CMD-C2D-C1D	4.99	133.52	124.73
33	4	505	C7Z	C27-C28-C29	-4.99	118.85	126.23
20	B	1212	CLA	CMD-C2D-C1D	4.99	133.52	124.73
20	F	1301	CLA	O2D-CGD-CBD	4.99	119.95	111.23
20	A	1126	CLA	O2D-CGD-CBD	4.98	119.94	111.23
20	2	606	CLA	O2D-CGD-CBD	4.97	119.92	111.23
30	3	604	CHL	C1C-CHC-C4B	4.97	133.84	116.07
20	B	1023	CLA	O2D-CGD-CBD	4.97	119.91	111.23
22	G	4011	BCR	C36-C18-C17	-4.96	114.78	122.82
20	K	1403	CLA	O2D-CGD-CBD	4.96	119.91	111.23
22	L	4020	BCR	C33-C5-C6	-4.96	119.07	124.48
20	G	1601	CLA	O2D-CGD-CBD	4.95	119.89	111.23
20	F	1302	CLA	O2D-CGD-CBD	4.95	119.88	111.23
20	A	1126	CLA	CMD-C2D-C1D	4.94	133.42	124.73
20	4	602	CLA	O2D-CGD-CBD	4.93	119.84	111.23
20	B	1203	CLA	O2D-CGD-CBD	4.92	119.84	111.23
30	4	611	CHL	C1C-CHC-C4B	4.91	133.62	116.07
20	A	1138	CLA	O2D-CGD-CBD	4.90	119.80	111.23
20	1	607	CLA	CMD-C2D-C1D	4.90	133.36	124.73
31	2	502	XAT	C15-C14-C13	-4.89	120.42	127.28
20	4	612	CLA	O2D-CGD-CBD	4.89	119.78	111.23
20	3	612	CLA	O2D-CGD-CBD	4.89	119.78	111.23
20	A	1123	CLA	O2D-CGD-CBD	4.89	119.78	111.23
30	2	615	CHL	C1C-CHC-C4B	4.89	133.56	116.07
20	2	601	CLA	O2D-CGD-CBD	4.89	119.77	111.23
30	4	610	CHL	C1B-CHB-C4A	4.88	124.47	121.32
20	3	603	CLA	O2D-CGD-CBD	4.88	119.76	111.23
30	2	609	CHL	C1C-CHC-C4B	4.88	133.52	116.07
30	2	611	CHL	C1C-CHC-C4B	4.87	133.51	116.07
20	A	1013	CLA	O2D-CGD-CBD	4.87	119.75	111.23
20	3	606	CLA	O2D-CGD-CBD	4.87	119.75	111.23
20	3	614	CLA	O2D-CGD-CBD	4.87	119.75	111.23
22	B	4006	BCR	C33-C5-C6	-4.86	119.18	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	2	610	CHL	C1B-CHB-C4A	4.85	124.44	121.32
20	A	1136	CLA	CMD-C2D-C1D	4.85	133.27	124.73
20	B	1021	CLA	CMD-C2D-C1D	4.85	133.27	124.73
20	B	1206	CLA	O2D-CGD-CBD	4.85	119.70	111.23
20	B	1022	CLA	O2D-CGD-CBD	4.85	119.70	111.23
30	4	610	CHL	C1C-CHC-C4B	4.85	133.41	116.07
29	J	4013	LUT	C31-C30-C29	-4.84	120.48	127.28
20	B	1219	CLA	O2D-CGD-CBD	4.84	119.69	111.23
29	1	502	LUT	C18-C5-C6	-4.84	119.21	124.48
20	A	1012	CLA	O2D-CGD-CBD	4.83	119.68	111.23
20	A	1125	CLA	C1-C2-C3	-4.83	118.28	126.20
22	L	4020	BCR	C15-C14-C13	-4.83	120.50	127.28
20	B	1201	CLA	CMD-C2D-C1D	4.81	133.21	124.73
20	A	1139	CLA	CMD-C2D-C1D	4.81	133.20	124.73
20	2	601	CLA	CMD-C2D-C1D	4.80	133.18	124.73
30	3	607	CHL	C1C-CHC-C4B	4.78	133.19	116.07
20	B	1234	CLA	CMD-C2D-C1D	4.78	133.15	124.73
20	B	1206	CLA	CMD-C2D-C1D	4.77	133.13	124.73
20	B	1220	CLA	O2D-CGD-CBD	4.76	119.56	111.23
30	2	610	CHL	C1C-CHC-C4B	4.76	133.11	116.07
22	K	4002	BCR	C33-C5-C6	-4.76	119.29	124.48
20	2	603	CLA	O2D-CGD-CBD	4.76	119.55	111.23
29	J	4013	LUT	C35-C34-C33	-4.75	120.61	127.28
22	B	4004	BCR	C20-C19-C18	4.75	139.38	126.36
20	A	1126	CLA	C1-C2-C3	-4.74	118.43	126.20
31	2	502	XAT	C38-C25-C24	4.74	119.56	114.24
20	1	613	CLA	O2D-CGD-CBD	4.74	119.51	111.23
20	A	1113	CLA	O2D-CGD-CBD	4.73	119.50	111.23
30	1	609	CHL	C1C-CHC-C4B	4.73	132.99	116.07
20	2	602	CLA	O2D-CGD-CBD	4.72	119.48	111.23
22	B	4006	BCR	C23-C24-C25	-4.72	114.39	127.00
20	A	1117	CLA	CMD-C2D-C1D	4.71	133.02	124.73
20	A	1013	CLA	CMD-C2D-C1D	4.69	132.99	124.73
20	K	1404	CLA	O2D-CGD-CBD	4.69	119.43	111.23
26	G	5002	LMG	O7-C10-C11	4.69	121.62	111.48
30	4	613	CHL	C1C-CHC-C4B	4.67	132.79	116.07
20	A	1139	CLA	O2D-CGD-CBD	4.66	119.38	111.23
20	A	1110	CLA	O2D-CGD-CBD	4.66	119.38	111.23
30	2	613	CHL	C1C-CHC-C4B	4.65	132.73	116.07
23	A	5001	LHG	O7-C7-C8	4.65	121.55	111.48
20	2	612	CLA	C1-C2-C3	-4.65	118.58	126.20
30	1	610	CHL	C1C-CHC-C4B	4.64	132.66	116.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	1	612	CHL	C1C-CHC-C4B	4.63	132.65	116.07
22	2	503	BCR	C33-C5-C4	4.62	123.45	113.60
30	2	611	CHL	CHA-C1A-C2A	-4.61	122.49	133.31
33	4	505	C7Z	C7-C8-C9	-4.60	119.42	126.23
20	A	1012	CLA	CMD-C2D-C1D	4.60	132.83	124.73
29	2	501	LUT	C21-C26-C27	4.59	118.11	112.83
20	A	1128	CLA	C1-C2-C3	-4.58	118.69	126.20
29	1	502	LUT	C11-C10-C9	-4.57	120.87	127.28
30	3	611	CHL	C1C-CHC-C4B	4.57	132.41	116.07
28	3	803	DGD	O2G-C1B-C2B	4.57	121.36	111.48
22	B	4006	BCR	C20-C19-C18	4.56	138.87	126.36
22	B	4006	BCR	C23-C22-C21	-4.56	111.84	119.01
30	4	615	CHL	C1C-CHC-C4B	4.56	132.38	116.07
20	4	601	CLA	O2D-CGD-CBD	4.55	119.19	111.23
20	4	617	CLA	C1-C2-C3	-4.55	118.75	126.20
26	F	5002	LMG	O7-C10-C11	4.55	121.32	111.48
31	4	502	XAT	C7-C8-C9	-4.53	118.50	125.53
31	2	502	XAT	C31-C30-C29	-4.52	120.93	127.28
29	4	501	LUT	C18-C5-C6	-4.50	119.57	124.48
22	K	4001	BCR	C33-C5-C6	-4.49	119.59	124.48
22	2	503	BCR	C39-C30-C29	-4.48	91.75	108.95
20	A	1119	CLA	C1-C2-C3	-4.47	118.87	126.20
20	A	1121	CLA	O2D-CGD-CBD	4.45	119.01	111.23
30	2	609	CHL	CHA-C1A-C2A	-4.44	122.88	133.31
20	2	612	CLA	O2D-CGD-CBD	4.44	118.99	111.23
30	2	610	CHL	CHA-C1A-C2A	-4.43	122.90	133.31
20	4	603	CLA	O2D-CGD-CBD	4.43	118.97	111.23
20	4	602	CLA	CMD-C2D-C1D	4.42	132.51	124.73
20	B	1222	CLA	C1-C2-C3	-4.42	118.96	126.20
19	A	1011	CL0	CBC-CAC-C3C	-4.41	106.56	112.87
20	J	1901	CLA	O2D-CGD-CBD	4.41	118.94	111.23
29	3	501	LUT	C35-C34-C33	-4.40	121.10	127.28
20	B	1232	CLA	O2A-C1-C2	4.40	125.05	108.11
33	4	505	C7Z	C24-C25-C26	-4.40	111.72	120.76
29	4	501	LUT	C26-C27-C28	-4.38	117.77	124.58
22	I	4020	BCR	C33-C5-C6	-4.38	119.71	124.48
26	F	5004	LMG	O7-C10-C11	4.37	120.94	111.48
20	G	1603	CLA	C1-C2-C3	-4.37	119.04	126.20
30	2	609	CHL	C1B-CHB-C4A	4.36	124.13	121.32
22	1	504	BCR	C36-C18-C17	-4.36	115.75	122.82
22	B	4004	BCR	C36-C18-C17	-4.35	115.78	122.82
30	3	604	CHL	C1A-CHA-C4D	4.34	126.23	118.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	4	606	CLA	O2D-CGD-CBD	4.34	118.82	111.23
22	3	506	BCR	C15-C14-C13	-4.34	121.19	127.28
33	4	505	C7Z	C4-C5-C6	-4.33	111.86	120.76
22	B	4005	BCR	C33-C5-C6	-4.32	119.77	124.48
23	A	5002	LHG	O7-C7-C8	4.32	120.83	111.48
30	2	615	CHL	C1A-CHA-C4D	4.32	126.19	118.98
19	A	1011	CL0	O2A-CGA-CBA	4.32	125.00	111.83
31	4	502	XAT	C31-C30-C29	-4.32	121.23	127.28
30	2	613	CHL	CHA-C1A-C2A	-4.31	123.19	133.31
20	3	605	CLA	C1-C2-C3	-4.30	119.15	126.20
20	1	614	CLA	C1-C2-C3	-4.30	119.16	126.20
20	B	1221	CLA	O2A-C1-C2	4.30	124.65	108.11
22	A	4003	BCR	C33-C5-C6	-4.29	119.80	124.48
29	4	501	LUT	C7-C8-C9	-4.29	119.89	126.23
30	3	604	CHL	C1-O2A-CGA	4.27	127.00	116.65
20	A	1131	CLA	C1-C2-C3	-4.27	119.20	126.20
23	B	5002	LHG	O7-C7-C8	4.27	120.72	111.48
19	A	1011	CL0	C1-C2-C3	-4.26	119.21	126.20
22	B	4004	BCR	C35-C13-C14	-4.26	115.92	122.82
20	1	604	CLA	C1-C2-C3	-4.26	119.22	126.20
20	B	1203	CLA	C1-C2-C3	-4.26	119.22	126.20
22	A	4017	BCR	C19-C18-C17	4.25	125.70	119.01
29	3	502	LUT	C7-C8-C9	-4.25	119.95	126.23
20	A	1110	CLA	O2A-C1-C2	4.25	124.45	108.11
26	B	5004	LMG	O7-C10-C11	4.25	120.67	111.48
20	B	1023	CLA	CMD-C2D-C1D	4.24	132.19	124.73
29	1	502	LUT	C7-C8-C9	-4.24	119.97	126.23
20	A	1127	CLA	CMD-C2D-C1D	4.24	132.19	124.73
30	1	609	CHL	CHA-C1A-C2A	-4.23	123.38	133.31
22	1	503	BCR	C33-C5-C6	-4.23	119.87	124.48
20	B	1215	CLA	C1-C2-C3	-4.22	119.28	126.20
20	1	605	CLA	O2A-C1-C2	4.21	124.32	108.11
19	A	1011	CL0	C1C-CHC-C4B	4.21	131.14	116.07
20	A	1115	CLA	C1-C2-C3	-4.21	119.31	126.20
20	B	1234	CLA	C1-C2-C3	-4.20	119.32	126.20
28	J	5001	DGD	O2G-C1B-C2B	4.19	120.56	111.48
29	2	501	LUT	C35-C34-C33	-4.19	121.40	127.28
22	H	4021	BCR	C33-C5-C6	-4.19	119.92	124.48
30	4	615	CHL	C3D-C4D-CHA	4.18	114.90	108.54
20	4	605	CLA	O2D-CGD-CBD	4.18	118.54	111.23
22	G	4011	BCR	C15-C14-C13	-4.17	121.43	127.28
20	B	1212	CLA	C1-C2-C3	-4.17	119.37	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	4006	BCR	C19-C18-C17	4.16	125.56	119.01
20	1	606	CLA	C1-C2-C3	-4.15	120.05	126.76
20	1	611	CLA	C1-C2-C3	-4.15	119.40	126.20
22	B	4004	BCR	C34-C9-C10	-4.15	116.09	122.82
30	2	611	CHL	C1A-CHA-C4D	4.14	125.89	118.98
30	1	612	CHL	C3D-C4D-CHA	4.14	114.83	108.54
22	I	4020	BCR	C15-C14-C13	-4.14	121.48	127.28
20	B	1240	CLA	C1-C2-C3	-4.13	119.43	126.20
22	F	4014	BCR	C23-C24-C25	-4.12	115.98	127.00
22	2	503	BCR	C40-C30-C39	4.12	120.44	108.63
21	B	2002	PQN	C11-C12-C13	-4.12	119.73	126.83
28	F	5005	DGD	O2G-C1B-C2B	4.11	120.38	111.48
29	1	502	LUT	C35-C34-C33	-4.11	121.52	127.28
20	4	604	CLA	C1-C2-C3	-4.11	119.47	126.20
22	A	4003	BCR	C19-C18-C17	4.10	125.46	119.01
29	2	501	LUT	C26-C27-C28	-4.10	118.20	124.58
30	2	611	CHL	C1B-CHB-C4A	4.10	123.96	121.32
29	3	501	LUT	C18-C5-C6	-4.10	120.01	124.48
29	1	501	LUT	C21-C26-C27	4.10	117.53	112.83
20	4	603	CLA	C1-C2-C3	-4.10	119.49	126.20
26	F	5003	LMG	O7-C10-C11	4.10	120.34	111.48
28	4	802	DGD	O2G-C1B-C2B	4.10	120.34	111.48
23	1	801	LHG	O7-C7-C8	4.09	120.33	111.48
29	1	502	LUT	C21-C26-C27	4.08	117.52	112.83
20	B	1215	CLA	O2A-C1-C2	4.08	123.83	108.11
23	2	801	LHG	O7-C7-C8	4.08	120.31	111.48
28	1	803	DGD	O2G-C1B-C2B	4.08	120.31	111.48
29	4	501	LUT	C15-C14-C13	-4.08	121.56	127.28
20	B	1211	CLA	C1-C2-C3	-4.07	119.53	126.20
22	A	4002	BCR	C23-C24-C25	-4.07	116.12	127.00
26	G	5001	LMG	O7-C10-C11	4.06	120.26	111.48
32	2	807	3PH	O21-C21-C22	4.04	120.23	111.48
20	A	1135	CLA	O2A-C1-C2	4.04	123.67	108.11
28	G	5003	DGD	O2G-C1B-C2B	4.04	120.22	111.48
30	2	615	CHL	C3D-C4D-CHA	4.04	114.68	108.54
20	G	1601	CLA	O2A-C1-C2	4.03	123.63	108.11
20	A	1104	CLA	C1-C2-C3	-4.03	119.60	126.20
20	4	602	CLA	C1-C2-C3	-4.02	120.25	126.76
30	4	613	CHL	C3D-C4D-CHA	4.02	114.65	108.54
30	2	609	CHL	C1A-CHA-C4D	4.01	125.68	118.98
20	A	1124	CLA	C1-C2-C3	-4.00	119.65	126.20
20	L	1501	CLA	C1-C2-C3	-3.99	120.30	126.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	3	503	BCR	C23-C24-C25	-3.99	116.34	127.00
22	3	506	BCR	C33-C5-C6	-3.98	120.14	124.48
22	G	4011	BCR	C23-C22-C21	3.97	125.26	119.01
20	B	1231	CLA	C1-C2-C3	-3.97	119.69	126.20
20	B	1206	CLA	C1-C2-C3	-3.97	119.69	126.20
30	2	610	CHL	C3D-C4D-CHA	3.97	114.58	108.54
20	4	609	CLA	C1-C2-C3	-3.97	120.34	126.76
20	2	608	CLA	O2A-C1-C2	3.97	123.38	108.11
20	B	1234	CLA	O2A-C1-C2	3.96	123.37	108.11
20	A	1109	CLA	O2A-C1-C2	3.96	123.34	108.11
30	3	611	CHL	C3D-C4D-CHA	3.95	114.55	108.54
30	2	613	CHL	C3D-C4D-CHA	3.95	114.54	108.54
30	2	613	CHL	C1A-CHA-C4D	3.95	125.57	118.98
30	3	607	CHL	C3D-C4D-CHA	3.94	114.54	108.54
26	B	5003	LMG	O7-C10-C11	3.94	120.01	111.48
30	2	609	CHL	C3D-C4D-CHA	3.94	114.53	108.54
30	4	613	CHL	C1A-CHA-C4D	3.94	125.56	118.98
26	2	804	LMG	O7-C10-C11	3.93	119.99	111.48
20	B	1227	CLA	C1-C2-C3	-3.93	119.75	126.20
29	3	501	LUT	C15-C14-C13	-3.93	121.77	127.28
20	J	1901	CLA	C1-C2-C3	-3.93	120.40	126.76
29	1	501	LUT	C26-C27-C28	-3.93	118.47	124.58
30	1	610	CHL	C3D-C4D-CHA	3.93	114.51	108.54
20	B	1230	CLA	C1-C2-C3	-3.92	119.77	126.20
30	2	610	CHL	C1A-CHA-C4D	3.92	125.52	118.98
22	B	4010	BCR	C33-C5-C6	-3.91	120.21	124.48
22	F	4014	BCR	C28-C27-C26	-3.91	107.08	114.06
20	A	1134	CLA	C1-C2-C3	-3.91	119.80	126.20
26	B	5007	LMG	O7-C10-C11	3.90	119.93	111.48
20	B	1214	CLA	C1-C2-C3	-3.90	119.81	126.20
28	B	5005	DGD	O2G-C1B-C2B	3.89	119.90	111.48
20	A	1138	CLA	C1-C2-C3	-3.89	119.83	126.20
22	A	4017	BCR	C33-C5-C6	-3.89	120.24	124.48
22	L	4019	BCR	C33-C5-C6	-3.88	120.25	124.48
20	A	1012	CLA	O2A-C1-C2	3.88	123.03	108.11
30	3	604	CHL	C1B-CHB-C4A	3.87	123.81	121.32
20	A	1103	CLA	C1-C2-C3	-3.86	119.86	126.20
26	A	5006	LMG	O7-C10-C11	3.86	119.84	111.48
29	2	501	LUT	C18-C5-C6	-3.86	120.28	124.48
20	3	606	CLA	C1-C2-C3	-3.85	120.53	126.76
22	B	4010	BCR	C23-C24-C25	-3.85	116.72	127.00
20	F	1301	CLA	O2A-C1-C2	3.85	122.91	108.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	2	611	CHL	C3D-C4D-CHA	3.85	114.39	108.54
26	2	803	LMG	O7-C10-C11	3.85	119.80	111.48
20	A	1121	CLA	C1-C2-C3	-3.85	119.90	126.20
26	2	805	LMG	O7-C10-C11	3.84	119.79	111.48
20	B	1230	CLA	O2A-C1-C2	3.84	122.89	108.11
20	A	1133	CLA	CMD-C2D-C1D	3.84	131.49	124.73
20	1	603	CLA	CAA-C2A-C3A	-3.83	102.64	113.00
20	A	1124	CLA	O2A-C1-C2	3.83	122.86	108.11
20	B	1201	CLA	C1-C2-C3	-3.83	119.92	126.20
20	A	1104	CLA	O2A-C1-C2	3.83	122.85	108.11
30	3	604	CHL	C3D-C4D-CHA	3.83	114.36	108.54
26	3	802	LMG	O7-C10-C11	3.83	119.76	111.48
30	4	611	CHL	CHA-C1A-C2A	-3.82	124.33	133.31
20	1	603	CLA	O2A-C1-C2	3.82	122.79	108.11
20	G	1603	CLA	O2A-C1-C2	3.82	122.79	108.11
20	A	1102	CLA	O2A-C1-C2	3.81	122.78	108.11
20	A	1129	CLA	C1-C2-C3	-3.81	119.95	126.20
20	A	1132	CLA	C1-C2-C3	-3.80	119.97	126.20
20	A	1130	CLA	O2A-C1-C2	3.79	122.71	108.11
20	L	1503	CLA	C1-C2-C3	-3.79	120.63	126.76
30	4	613	CHL	C1-O2A-CGA	3.79	125.82	116.65
20	4	606	CLA	O2A-C1-C2	3.79	122.68	108.11
31	4	502	XAT	C15-C14-C13	-3.77	121.99	127.28
20	4	612	CLA	C1-C2-C3	-3.77	120.02	126.20
20	B	1222	CLA	O2A-C1-C2	3.77	122.61	108.11
30	1	609	CHL	C3D-C4D-CHA	3.77	114.27	108.54
29	3	502	LUT	C27-C28-C29	-3.77	118.22	126.32
22	H	4021	BCR	C15-C14-C13	-3.76	122.00	127.28
20	B	1239	CLA	O2A-C1-C2	3.76	122.58	108.11
29	4	501	LUT	C31-C30-C29	-3.76	122.01	127.28
20	K	1403	CLA	O2A-C1-C2	3.76	122.02	109.44
30	4	610	CHL	CHA-C1A-C2A	-3.75	124.49	133.31
30	3	607	CHL	CHA-C1A-C2A	-3.75	124.51	133.31
20	B	1212	CLA	O2A-C1-C2	3.74	122.52	108.11
20	2	605	CLA	CAA-C2A-C3A	-3.74	102.89	113.00
20	B	1228	CLA	C1-C2-C3	-3.74	120.07	126.20
20	A	1125	CLA	O2A-C1-C2	3.74	122.49	108.11
30	4	611	CHL	C3D-C4D-CHA	3.74	114.22	108.54
22	I	4018	BCR	C33-C5-C6	-3.74	120.41	124.48
20	B	1220	CLA	O2A-C1-C2	3.74	122.49	108.11
29	3	502	LUT	C18-C5-C6	-3.73	120.41	124.48
22	J	4012	BCR	C33-C5-C6	-3.72	120.42	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	1129	CLA	O2A-C1-C2	3.72	122.42	108.11
20	2	606	CLA	C1-C2-C3	-3.71	120.75	126.76
31	2	502	XAT	C18-C5-C4	3.71	118.41	114.24
22	A	4007	BCR	C33-C5-C6	-3.71	120.44	124.48
20	A	1121	CLA	O2A-C1-C2	3.71	122.37	108.11
20	2	603	CLA	O2A-C1-C2	3.71	122.37	108.11
20	A	1122	CLA	O2A-C1-C2	3.70	122.36	108.11
20	A	1107	CLA	O2A-C1-C2	3.70	122.35	108.11
20	A	1137	CLA	O2A-C1-C2	3.69	122.32	108.11
26	1	802	LMG	O7-C10-C11	3.69	119.47	111.48
22	3	503	BCR	C27-C26-C25	-3.69	117.71	122.70
20	B	1216	CLA	C1-C2-C3	-3.69	120.15	126.20
20	B	1208	CLA	C1-C2-C3	-3.69	120.15	126.20
20	3	605	CLA	O2A-C1-C2	3.69	122.31	108.11
20	B	1236	CLA	C1-C2-C3	-3.69	120.80	126.76
20	2	605	CLA	C1-C2-C3	-3.69	120.16	126.20
30	1	609	CHL	C1A-CHA-C4D	3.68	125.12	118.98
20	A	1133	CLA	C1-C2-C3	-3.68	120.17	126.20
20	A	1105	CLA	C1-C2-C3	-3.68	120.17	126.20
20	3	603	CLA	C1-C2-C3	-3.68	120.17	126.20
23	A	5001	LHG	C5-O7-C7	-3.67	109.01	117.80
20	B	1022	CLA	C3B-C4B-NB	-3.66	107.26	110.53
20	B	1210	CLA	O2A-C1-C2	3.66	122.20	108.11
20	A	1103	CLA	O2A-C1-C2	3.66	122.19	108.11
20	A	1118	CLA	C1-C2-C3	-3.66	120.84	126.76
22	F	4016	BCR	C23-C24-C25	-3.66	117.23	127.00
20	A	1139	CLA	C1-C2-C3	-3.65	120.21	126.20
22	A	4002	BCR	C33-C5-C6	-3.65	120.50	124.48
29	1	501	LUT	C35-C34-C33	-3.65	122.16	127.28
20	B	1201	CLA	O2A-C1-C2	3.65	122.15	108.11
20	1	611	CLA	O2A-C1-C2	3.65	122.14	108.11
20	A	1115	CLA	O2A-C1-C2	3.64	122.12	108.11
23	1	801	LHG	C5-O7-C7	-3.64	109.09	117.80
20	A	1128	CLA	O2A-C1-C2	3.64	122.10	108.11
20	B	1023	CLA	O2A-C1-C2	3.63	122.07	108.11
20	A	1123	CLA	O2A-C1-C2	3.63	122.07	108.11
20	A	1119	CLA	O2A-C1-C2	3.62	122.04	108.11
20	A	1135	CLA	C1-C2-C3	-3.62	120.27	126.20
20	3	608	CLA	O2A-C1-C2	3.61	121.54	109.44
20	B	1231	CLA	O2A-C1-C2	3.61	122.02	108.11
20	B	1211	CLA	O2A-C1-C2	3.61	122.01	108.11
23	4	801	LHG	O7-C7-C8	3.61	119.29	111.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	1	603	CLA	C1-C2-C3	-3.61	120.28	126.20
30	4	610	CHL	C3D-C4D-CHA	3.60	114.02	108.54
22	A	4007	BCR	C15-C14-C13	-3.60	122.23	127.28
30	3	611	CHL	C1A-CHA-C4D	3.60	124.98	118.98
22	I	4018	BCR	C3-C4-C5	-3.59	107.65	114.06
20	2	604	CLA	C1-C2-C3	-3.59	120.31	126.20
20	4	607	CLA	C3B-C4B-NB	-3.59	107.33	110.53
20	B	1238	CLA	O2A-C1-C2	3.59	121.91	108.11
20	4	602	CLA	O2A-C1-C2	3.58	121.89	108.11
20	4	604	CLA	O2A-C1-C2	3.58	121.89	108.11
20	B	1236	CLA	O2A-C1-C2	3.57	121.85	108.11
20	4	617	CLA	O2A-C1-C2	3.57	121.85	108.11
20	2	607	CLA	C1-C2-C3	-3.57	120.35	126.20
30	3	604	CHL	CHA-C1A-C2A	-3.57	124.93	133.31
20	B	1203	CLA	O2A-C1-C2	3.57	121.84	108.11
20	1	614	CLA	O2A-C1-C2	3.57	121.84	108.11
20	A	1132	CLA	O2A-C1-C2	3.57	121.83	108.11
20	B	1022	CLA	O2A-C1-C2	3.56	121.80	108.11
20	4	612	CLA	O2A-C1-C2	3.55	121.79	108.11
30	1	612	CHL	C3C-C4C-NC	-3.55	105.97	114.65
20	B	1232	CLA	C1-C2-C3	-3.55	120.38	126.20
22	A	4002	BCR	C12-C13-C14	-3.55	113.42	119.01
31	4	502	XAT	C38-C25-C26	-3.55	116.46	122.30
22	A	4011	BCR	C23-C24-C25	-3.55	117.52	127.00
30	1	610	CHL	CHA-C1A-C2A	-3.55	124.98	133.31
22	A	4011	BCR	C4-C5-C6	-3.54	117.92	122.70
20	A	1139	CLA	O2A-C1-C2	3.54	121.74	108.11
20	B	1022	CLA	C1-C2-C3	-3.54	120.39	126.20
22	J	4012	BCR	C12-C13-C14	-3.54	113.44	119.01
22	3	503	BCR	C15-C14-C13	-3.54	122.31	127.28
22	G	4011	BCR	C33-C5-C6	-3.54	120.62	124.48
20	B	1223	CLA	C1-C2-C3	-3.53	120.41	126.20
22	B	4009	BCR	C35-C13-C12	3.53	123.48	118.09
20	B	1220	CLA	C1-C2-C3	-3.53	120.41	126.20
20	B	1225	CLA	O2A-C1-C2	3.53	121.69	108.11
20	3	601	CLA	O2A-C1-C2	3.53	121.69	108.11
20	L	1502	CLA	C1-C2-C3	-3.53	120.42	126.20
29	3	501	LUT	C16-C1-C6	-3.53	104.71	110.24
20	A	1107	CLA	CAA-CBA-CGA	-3.53	103.20	113.21
20	2	607	CLA	O2A-C1-C2	3.52	121.67	108.11
20	1	606	CLA	O2A-C1-C2	3.52	121.67	108.11
20	B	1224	CLA	C1-C2-C3	-3.52	120.43	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	1215	CLA	O2A-CGA-CBA	3.52	122.56	111.83
22	A	4007	BCR	C27-C26-C25	-3.52	117.95	122.70
20	B	1228	CLA	O2A-C1-C2	3.51	121.63	108.11
20	2	606	CLA	O2A-C1-C2	3.51	121.61	108.11
20	L	1502	CLA	O2A-C1-C2	3.51	121.60	108.11
20	3	612	CLA	C1-C2-C3	-3.51	121.09	126.76
20	A	1101	CLA	C1-C2-C3	-3.50	120.46	126.20
22	A	4017	BCR	C23-C24-C25	-3.50	117.65	127.00
30	4	611	CHL	C1A-CHA-C4D	3.50	124.82	118.98
22	B	4006	BCR	C27-C26-C25	-3.49	117.98	122.70
20	B	1227	CLA	O2A-C1-C2	3.49	121.54	108.11
20	A	1102	CLA	C1-C2-C3	-3.49	120.49	126.20
26	F	5001	LMG	O7-C10-C11	3.48	119.02	111.48
20	B	1204	CLA	O2A-C1-C2	3.48	121.51	108.11
20	B	1207	CLA	C1-C2-C3	-3.48	120.50	126.20
20	2	602	CLA	O2A-C1-C2	3.48	121.50	108.11
22	L	4020	BCR	C27-C26-C25	-3.48	118.00	122.70
22	1	503	BCR	C38-C26-C25	-3.48	120.69	124.48
20	2	607	CLA	CMA-C3A-C4A	3.48	121.12	111.77
20	B	1208	CLA	O2A-C1-C2	3.47	121.45	108.11
20	L	1501	CLA	O2A-C1-C2	3.46	121.44	108.11
30	4	610	CHL	C3C-C4C-NC	-3.46	106.18	114.65
20	4	603	CLA	O2A-C1-C2	3.46	121.42	108.11
22	A	4008	BCR	C23-C24-C25	-3.46	117.76	127.00
20	B	1216	CLA	O2A-C1-C2	3.45	121.40	108.11
29	1	501	LUT	C18-C5-C6	-3.45	120.72	124.48
20	A	1106	CLA	O2A-C1-C2	3.45	121.37	108.11
20	A	1130	CLA	C1-C2-C3	-3.45	120.55	126.20
20	4	601	CLA	C1-C2-C3	-3.44	120.56	126.20
22	B	4005	BCR	C23-C24-C25	-3.44	117.82	127.00
20	B	1232	CLA	C3B-C4B-NB	-3.43	107.46	110.53
20	L	1503	CLA	O2A-C1-C2	3.43	121.32	108.11
29	4	501	LUT	C21-C26-C27	3.43	116.77	112.83
22	2	503	BCR	C32-C1-C6	-3.43	104.86	110.24
20	A	1117	CLA	C1-C2-C3	-3.43	120.57	126.20
20	B	1219	CLA	C1-C2-C3	-3.43	120.58	126.20
22	H	4021	BCR	C27-C26-C25	-3.43	118.07	122.70
20	B	1238	CLA	C1-C2-C3	-3.42	120.59	126.20
20	A	1133	CLA	O2A-C1-C2	3.42	121.27	108.11
20	A	1104	CLA	CAA-C2A-C3A	-3.42	103.76	113.00
20	A	1105	CLA	O2A-C1-C2	3.42	121.27	108.11
20	A	1108	CLA	O2A-C1-C2	3.42	121.25	108.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	1213	CLA	O2A-C1-C2	3.41	121.23	108.11
20	B	1205	CLA	C1-C2-C3	-3.41	120.61	126.20
20	B	1206	CLA	O2A-C1-C2	3.41	121.22	108.11
20	B	1238	CLA	C3B-C4B-NB	-3.41	107.49	110.53
22	2	503	BCR	C15-C14-C13	-3.41	122.50	127.28
20	A	1137	CLA	C3B-C4B-NB	-3.41	107.49	110.53
20	A	1134	CLA	O2A-C1-C2	3.40	121.21	108.11
22	B	4009	BCR	C23-C24-C25	-3.40	117.91	127.00
20	A	1139	CLA	C2C-C1C-NC	3.40	113.55	109.98
20	1	601	CLA	O2A-C1-C2	3.40	121.18	108.11
20	J	1901	CLA	O2A-C1-C2	3.39	121.17	108.11
22	1	504	BCR	C33-C5-C6	-3.39	120.78	124.48
20	4	606	CLA	C1-C2-C3	-3.39	121.27	126.76
30	3	607	CHL	C1A-CHA-C4D	3.39	124.64	118.98
22	A	4002	BCR	C27-C26-C25	-3.39	118.12	122.70
20	A	1131	CLA	O2A-C1-C2	3.39	121.15	108.11
20	B	1240	CLA	O2A-C1-C2	3.38	121.12	108.11
30	2	615	CHL	CHA-C1A-C2A	-3.38	125.37	133.31
20	4	603	CLA	C3B-C4B-NB	-3.38	107.52	110.53
20	2	608	CLA	CMD-C2D-C3D	-3.38	119.95	127.69
20	B	1226	CLA	O2A-C1-C2	3.38	121.10	108.11
20	B	1223	CLA	O2A-C1-C2	3.37	121.10	108.11
20	2	602	CLA	C1-C2-C3	-3.37	120.67	126.20
20	3	610	CLA	C1-C2-C3	-3.37	120.67	126.20
22	J	4012	BCR	C35-C13-C12	3.37	123.24	118.09
20	B	1237	CLA	C3B-C4B-NB	-3.37	107.52	110.53
20	K	1403	CLA	C2C-C1C-NC	3.36	113.52	109.98
30	1	609	CHL	C1-O2A-CGA	3.36	124.80	116.65
20	A	1137	CLA	C1-C2-C3	-3.36	120.69	126.20
20	A	1141	CLA	O2A-C1-C2	3.36	121.03	108.11
22	A	4011	BCR	C12-C13-C14	-3.36	113.73	119.01
20	A	1105	CLA	C2C-C1C-NC	3.36	113.51	109.98
20	3	603	CLA	O2A-C1-C2	3.35	121.02	108.11
22	B	4009	BCR	C33-C5-C6	-3.35	120.83	124.48
22	I	4020	BCR	C38-C26-C25	-3.35	120.83	124.48
20	3	610	CLA	O2A-C1-C2	3.35	121.00	108.11
20	B	1221	CLA	C1-O2A-CGA	3.34	124.75	116.65
30	3	611	CHL	CHA-C1A-C2A	-3.34	125.46	133.31
20	B	1214	CLA	O2A-C1-C2	3.34	120.97	108.11
20	2	604	CLA	O2A-C1-C2	3.34	120.95	108.11
30	3	611	CHL	C3C-C4C-NC	-3.33	106.50	114.65
20	1	613	CLA	C3B-C4B-NB	-3.33	107.56	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	4003	BCR	C36-C18-C17	-3.33	117.42	122.82
20	B	1215	CLA	CAA-C2A-C1A	-3.33	101.08	111.97
20	A	1123	CLA	C1-C2-C3	-3.32	120.75	126.20
19	A	1011	CL0	O1D-CGD-CBD	-3.32	119.68	124.72
20	B	1210	CLA	CAC-C3C-C4C	3.32	129.11	124.79
20	2	601	CLA	CMA-C3A-C4A	3.32	120.69	111.77
20	4	607	CLA	O2A-C1-C2	3.31	120.86	108.11
20	F	1302	CLA	C1-C2-C3	-3.31	120.77	126.20
21	A	2001	PQN	C11-C12-C13	-3.31	121.13	126.83
29	3	501	LUT	C7-C8-C9	-3.31	121.34	126.23
20	1	604	CLA	O2A-C1-C2	3.31	120.84	108.11
23	B	5001	LHG	C5-O7-C7	-3.30	112.01	117.85
20	4	609	CLA	O2A-C1-C2	3.30	120.82	108.11
20	A	1122	CLA	C1-C2-C3	-3.30	120.79	126.20
20	B	1210	CLA	C1-C2-C3	-3.30	120.79	126.20
20	B	1219	CLA	O2A-C1-C2	3.30	120.81	108.11
19	A	1011	CL0	CHA-C1A-C2A	-3.30	125.56	133.31
30	4	613	CHL	CHA-C1A-C2A	-3.29	125.59	133.31
20	2	608	CLA	C1-C2-C3	-3.29	121.45	126.76
20	4	602	CLA	C3B-C4B-NB	-3.29	107.60	110.53
20	A	1101	CLA	O2A-C1-C2	3.28	120.75	108.11
20	B	1207	CLA	O2A-C1-C2	3.28	120.74	108.11
29	1	501	LUT	C8-C7-C6	-3.28	118.23	127.00
20	3	617	CLA	O2A-C1-C2	3.28	120.74	108.11
20	B	1213	CLA	O2A-CGA-CBA	3.28	121.83	111.83
20	2	605	CLA	CBC-CAC-C3C	-3.28	103.54	112.42
22	A	4002	BCR	C35-C13-C12	3.28	123.09	118.09
30	4	615	CHL	CHA-C1A-C2A	-3.27	125.62	133.31
33	4	505	C7Z	C38-C25-C24	-3.27	108.40	114.42
22	A	4007	BCR	C23-C24-C25	-3.27	118.25	127.00
20	4	601	CLA	O2A-C1-C2	3.27	120.70	108.11
22	A	4011	BCR	C2-C1-C6	3.27	115.19	110.44
22	F	4014	BCR	C23-C22-C21	-3.27	113.87	119.01
20	K	1402	CLA	O2A-C1-C2	3.26	120.67	108.11
20	4	617	CLA	C3B-C4B-NB	-3.26	107.62	110.53
31	2	502	XAT	C38-C25-C26	-3.26	116.93	122.30
20	A	1136	CLA	C3B-C4B-NB	-3.26	107.62	110.53
29	1	502	LUT	C26-C27-C28	-3.26	119.51	124.58
20	3	617	CLA	C1-C2-C3	-3.26	120.86	126.20
26	G	5001	LMG	O8-C28-C29	3.26	121.76	111.83
26	B	5004	LMG	O8-C28-C29	3.26	121.76	111.83
31	2	502	XAT	C7-C8-C9	-3.25	120.49	125.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	L	1502	CLA	C3B-C4B-NB	-3.25	107.63	110.53
22	B	4006	BCR	C37-C22-C23	3.25	123.05	118.09
20	B	1202	CLA	C3B-C4B-NB	-3.25	107.63	110.53
22	I	4018	BCR	C33-C5-C4	3.25	120.52	113.60
20	B	1207	CLA	C3B-C4B-NB	-3.24	107.63	110.53
20	B	1218	CLA	C3B-C4B-NB	-3.24	107.64	110.53
20	B	1229	CLA	C1-C2-C3	-3.24	120.89	126.20
20	A	1120	CLA	O2A-C1-C2	3.24	120.58	108.11
20	G	1603	CLA	CMA-C3A-C4A	3.24	120.48	111.77
30	4	610	CHL	C1A-CHA-C4D	3.24	124.39	118.98
20	4	605	CLA	O2A-C1-C2	3.23	120.56	108.11
22	F	4016	BCR	C33-C5-C6	-3.23	120.96	124.48
22	B	4006	BCR	C35-C13-C12	3.23	123.02	118.09
20	A	1140	CLA	C1-C2-C3	-3.23	120.91	126.20
20	B	1238	CLA	C1D-ND-C4D	-3.23	104.05	106.31
30	1	609	CHL	C3C-C4C-NC	-3.22	106.78	114.65
20	B	1229	CLA	O2A-C1-C2	3.22	120.50	108.11
30	2	611	CHL	C3C-C4C-NC	-3.22	106.78	114.65
20	3	601	CLA	C1-O2A-CGA	3.22	124.45	116.65
20	4	602	CLA	C1D-ND-C4D	-3.22	104.05	106.31
20	B	1208	CLA	C3B-C4B-NB	-3.22	107.66	110.53
20	3	602	CLA	C1-C2-C3	-3.22	120.93	126.20
20	A	1112	CLA	C1-C2-C3	-3.21	120.93	126.20
20	B	1022	CLA	OBD-CAD-C3D	-3.21	120.92	128.42
22	2	503	BCR	C28-C27-C26	-3.21	108.33	114.06
20	A	1136	CLA	O2A-C1-C2	3.21	120.45	108.11
20	B	1239	CLA	C2C-C1C-NC	3.21	113.35	109.98
20	B	1239	CLA	C1-C2-C3	-3.20	120.95	126.20
20	B	1229	CLA	O2A-CGA-CBA	3.20	121.59	111.83
22	F	4014	BCR	C37-C22-C23	3.20	122.98	118.09
20	A	1103	CLA	CAA-C2A-C3A	-3.20	104.35	113.00
20	B	1237	CLA	O2A-C1-C2	3.20	120.41	108.11
20	H	1701	CLA	O2A-C1-C2	3.20	120.41	108.11
20	B	1207	CLA	C1D-ND-C4D	-3.19	104.07	106.31
29	4	501	LUT	C31-C32-C33	-3.19	117.62	126.36
20	2	603	CLA	O2A-CGA-CBA	3.19	121.55	111.83
30	4	611	CHL	C3C-C4C-NC	-3.19	106.86	114.65
22	A	4007	BCR	C19-C18-C17	3.18	124.01	119.01
20	4	608	CLA	C3B-C4B-NB	-3.18	107.69	110.53
20	1	608	CLA	O2D-CGD-O1D	-3.18	117.66	123.85
22	H	4021	BCR	C30-C25-C26	-3.18	118.30	122.64
20	B	1235	CLA	O2A-C1-C2	3.18	120.33	108.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	4	617	CLA	C1D-ND-C4D	-3.17	104.08	106.31
20	A	1121	CLA	C3B-C4B-NB	-3.17	107.70	110.53
20	G	1601	CLA	C1-C2-C3	-3.17	121.00	126.20
20	A	1134	CLA	C3B-C4B-NB	-3.17	107.70	110.53
20	2	605	CLA	O2A-C1-C2	3.17	120.30	108.11
20	A	1118	CLA	O2A-C1-C2	3.16	120.28	108.11
20	3	602	CLA	O2A-C1-C2	3.16	120.28	108.11
20	2	604	CLA	C1D-ND-C4D	-3.16	104.09	106.31
30	4	611	CHL	C1-O2A-CGA	3.16	124.30	116.65
30	2	609	CHL	C3C-C4C-NC	-3.16	106.93	114.65
22	A	4011	BCR	C33-C5-C4	3.16	120.32	113.60
20	A	1132	CLA	C3B-C4B-NB	-3.15	107.72	110.53
20	H	1701	CLA	C1-C2-C3	-3.15	121.04	126.20
20	4	608	CLA	C1D-ND-C4D	-3.15	104.10	106.31
20	4	607	CLA	C4B-CHC-C1C	3.14	133.64	126.25
20	4	607	CLA	C1D-ND-C4D	-3.14	104.11	106.31
22	A	4003	BCR	C35-C13-C12	3.14	122.89	118.09
20	L	1501	CLA	C1D-ND-C4D	-3.14	104.11	106.31
30	2	613	CHL	C3C-C4C-NC	-3.14	106.98	114.65
20	G	1603	CLA	C1C-C2C-C3C	-3.14	103.68	106.98
20	2	603	CLA	C1-C2-C3	-3.14	121.06	126.20
20	A	1139	CLA	C1C-C2C-C3C	-3.14	103.68	106.98
30	4	613	CHL	C3C-C4C-NC	-3.13	106.99	114.65
20	B	1021	CLA	O2A-C1-C2	3.13	120.15	108.11
22	F	4014	BCR	C33-C5-C6	-3.13	121.07	124.48
20	A	1118	CLA	C2C-C1C-NC	3.13	113.27	109.98
20	4	601	CLA	C1D-ND-C4D	-3.12	104.12	106.31
20	4	604	CLA	C1D-ND-C4D	-3.12	104.12	106.31
20	A	1113	CLA	C2C-C1C-NC	3.12	113.26	109.98
20	4	609	CLA	C1D-ND-C4D	-3.12	104.12	106.31
20	A	1110	CLA	C1-C2-C3	-3.12	121.09	126.20
20	A	1127	CLA	O2A-C1-C2	3.12	120.10	108.11
22	B	4004	BCR	C30-C25-C24	3.11	124.10	115.65
20	A	1106	CLA	O2D-CGD-O1D	-3.11	117.79	123.85
30	2	610	CHL	C3C-C4C-NC	-3.11	107.05	114.65
20	2	607	CLA	C2C-C1C-NC	3.11	113.25	109.98
30	1	612	CHL	C4D-CHA-CBD	-3.11	105.83	108.97
20	B	1202	CLA	O2D-CGD-O1D	-3.11	117.80	123.85
21	A	2001	PQN	C14-C13-C15	3.11	120.62	115.23
20	G	1602	CLA	C3B-C4B-NB	-3.11	107.76	110.53
20	L	1502	CLA	C1D-ND-C4D	-3.10	104.14	106.31
22	A	4003	BCR	C28-C27-C26	-3.10	108.53	114.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	J	5001	DGD	O1G-C1A-C2A	3.10	121.28	111.83
20	A	1013	CLA	C6-C5-C3	-3.10	105.92	113.47
20	A	1133	CLA	CAA-C2A-C3A	-3.10	104.63	113.00
29	4	501	LUT	C39-C29-C28	3.09	122.81	118.09
20	F	1302	CLA	O2A-C1-C2	3.09	120.01	108.11
30	4	613	CHL	C4D-CHA-CBD	-3.09	105.85	108.97
20	3	617	CLA	C3B-C4B-NB	-3.09	107.77	110.53
29	1	501	LUT	C16-C1-C6	-3.09	105.39	110.24
20	A	1112	CLA	C3B-C4B-NB	-3.09	107.77	110.53
20	A	1114	CLA	C2C-C1C-NC	3.09	113.23	109.98
20	2	606	CLA	C1D-ND-C4D	-3.09	104.14	106.31
20	3	612	CLA	O2A-C1-C2	3.09	120.00	108.11
20	2	606	CLA	CMA-C3A-C4A	3.08	120.06	111.77
20	3	614	CLA	C2C-C1C-NC	3.08	113.22	109.98
22	A	4008	BCR	C4-C5-C6	-3.08	118.54	122.70
20	3	603	CLA	C1D-ND-C4D	-3.08	104.15	106.31
20	L	1503	CLA	C3B-C4B-NB	-3.08	107.78	110.53
26	F	5001	LMG	O8-C28-C29	3.08	120.49	111.15
20	A	1141	CLA	C1-C2-C3	-3.08	121.16	126.20
20	B	1237	CLA	CMA-C3A-C4A	3.07	120.03	111.77
20	2	607	CLA	O2A-CGA-CBA	3.07	121.20	111.83
20	2	606	CLA	C3B-C4B-NB	-3.07	107.79	110.53
20	4	612	CLA	C3B-C4B-NB	-3.07	107.79	110.53
20	4	603	CLA	C1D-ND-C4D	-3.07	104.16	106.31
26	2	802	LMG	O8-C28-C29	3.07	120.45	111.15
20	B	1202	CLA	C1-C2-C3	-3.07	121.17	126.20
20	A	1132	CLA	C1D-ND-C4D	-3.06	104.16	106.31
30	1	612	CHL	C1-O2A-CGA	3.06	124.06	116.65
20	2	603	CLA	CMA-C3A-C4A	3.06	120.00	111.77
28	B	5005	DGD	O1G-C1A-C2A	3.06	121.16	111.83
26	G	5006	LMG	O8-C28-C29	3.06	120.43	111.15
30	2	615	CHL	C4D-CHA-CBD	-3.06	105.89	108.97
22	A	4017	BCR	C34-C9-C10	-3.06	117.86	122.82
20	B	1210	CLA	O2D-CGD-O1D	-3.06	117.90	123.85
30	3	604	CHL	C3C-C4C-NC	-3.06	107.18	114.65
26	G	5002	LMG	C8-O7-C10	-3.05	110.49	117.80
30	1	612	CHL	CHA-C1A-C2A	-3.05	126.14	133.31
20	K	1403	CLA	CMA-C3A-C4A	3.05	119.97	111.77
20	G	1603	CLA	C1D-ND-C4D	-3.05	104.17	106.31
20	4	604	CLA	CMA-C3A-C4A	3.05	119.96	111.77
20	B	1226	CLA	O2D-CGD-O1D	-3.04	117.92	123.85
20	4	609	CLA	C3B-C4B-NB	-3.04	107.81	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	4	615	CHL	C3C-C4C-NC	-3.04	107.21	114.65
20	A	1136	CLA	C6-C5-C3	-3.04	106.06	113.47
23	A	5002	LHG	O8-C23-C24	3.04	121.11	111.83
20	B	1223	CLA	O2D-CGD-O1D	-3.04	117.93	123.85
20	L	1501	CLA	C3B-C4B-NB	-3.04	107.82	110.53
20	B	1224	CLA	O2A-C1-C2	3.04	119.79	108.11
29	3	502	LUT	C10-C11-C12	-3.04	114.40	123.20
30	1	610	CHL	C3C-C4C-NC	-3.04	107.23	114.65
26	3	802	LMG	O8-C28-C29	3.04	121.09	111.83
20	K	1402	CLA	CMA-C3A-C4A	3.03	119.93	111.77
20	1	605	CLA	CAA-C2A-C1A	-3.03	102.03	111.97
33	4	505	C7Z	C18-C5-C4	-3.03	108.85	114.42
20	L	1503	CLA	C1D-ND-C4D	-3.03	104.19	106.31
22	G	4011	BCR	C23-C24-C25	-3.03	118.92	127.00
22	2	503	BCR	C23-C24-C25	-3.02	118.92	127.00
19	A	1011	CL0	O2A-C1-C2	3.02	119.75	108.11
20	2	603	CLA	C3B-C4B-NB	-3.02	107.83	110.53
20	3	612	CLA	C3B-C4B-NB	-3.02	107.83	110.53
20	A	1111	CLA	O2D-CGD-O1D	-3.01	117.98	123.85
20	K	1401	CLA	CMA-C3A-C4A	3.01	119.87	111.77
30	2	610	CHL	C1-C2-C3	-3.01	121.26	126.20
22	B	4010	BCR	C8-C7-C6	-3.01	118.95	127.00
24	A	5004	LMT	C1'-O5'-C5'	-3.01	107.84	113.72
22	3	503	BCR	C34-C9-C10	-3.01	117.94	122.82
20	3	603	CLA	CHD-C1D-ND	-3.01	120.56	124.80
20	K	1404	CLA	C2C-C1C-NC	3.01	113.14	109.98
20	G	1601	CLA	OBD-CAD-C3D	-3.01	121.38	128.42
20	2	605	CLA	C1C-C2C-C3C	-3.01	103.81	106.98
30	2	615	CHL	C3C-C4C-NC	-3.01	107.30	114.65
20	K	1401	CLA	C3B-C4B-NB	-3.01	107.85	110.53
20	4	608	CLA	CMA-C3A-C4A	3.00	119.84	111.77
22	L	4020	BCR	C30-C25-C26	-3.00	118.53	122.64
30	1	612	CHL	C1A-CHA-C4D	3.00	123.99	118.98
22	A	4011	BCR	C3-C4-C5	-3.00	108.70	114.06
20	3	602	CLA	C2C-C1C-NC	3.00	113.13	109.98
26	2	802	LMG	O7-C10-C11	3.00	121.94	110.93
20	A	1102	CLA	C3B-C4B-NB	-3.00	107.85	110.53
20	L	1501	CLA	CMA-C3A-C4A	3.00	119.83	111.77
20	A	1136	CLA	C1-C2-C3	-2.99	121.29	126.20
20	2	604	CLA	CMA-C3A-C4A	2.99	119.82	111.77
20	1	607	CLA	CMA-C3A-C4A	2.99	119.81	111.77
20	4	607	CLA	CMA-C3A-C4A	2.99	119.80	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	1217	CLA	O2D-CGD-O1D	-2.98	118.04	123.85
20	3	608	CLA	CMA-C3A-C4A	2.98	119.80	111.77
30	3	611	CHL	C4D-CHA-CBD	-2.98	105.96	108.97
20	A	1140	CLA	O2A-C1-C2	2.98	119.58	108.11
20	A	1120	CLA	C2C-C1C-NC	2.98	113.11	109.98
20	A	1107	CLA	O2A-CGA-CBA	2.98	120.92	111.83
20	A	1012	CLA	C3B-C4B-NB	-2.98	107.87	110.53
20	4	607	CLA	C1-C2-C3	-2.98	121.32	126.20
29	1	501	LUT	C10-C11-C12	-2.98	114.58	123.20
20	G	1603	CLA	C3B-C4B-NB	-2.98	107.87	110.53
22	1	504	BCR	C33-C5-C4	2.97	119.94	113.60
22	B	4005	BCR	C34-C9-C10	-2.97	118.00	122.82
20	A	1132	CLA	CMA-C3A-C4A	2.97	119.76	111.77
20	B	1021	CLA	C1C-C2C-C3C	-2.97	103.86	106.98
20	B	1235	CLA	O2A-CGA-CBA	2.97	120.89	111.83
20	A	1112	CLA	O2D-CGD-O1D	-2.97	118.07	123.85
20	A	1112	CLA	O2A-C1-C2	2.97	119.54	108.11
29	1	501	LUT	C15-C14-C13	-2.97	123.12	127.28
20	B	1214	CLA	C2C-C1C-NC	2.97	113.10	109.98
20	4	604	CLA	C3B-C4B-NB	-2.97	107.88	110.53
22	I	4018	BCR	C31-C1-C6	-2.96	105.59	110.24
20	A	1109	CLA	C3B-C4B-NB	-2.96	107.89	110.53
22	K	4001	BCR	C40-C30-C25	-2.96	105.60	110.24
20	L	1503	CLA	CMA-C3A-C4A	2.96	119.73	111.77
20	4	601	CLA	C3B-C4B-NB	-2.96	107.89	110.53
20	2	612	CLA	O2A-C1-C2	2.96	119.50	108.11
20	A	1114	CLA	C1C-C2C-C3C	-2.96	103.87	106.98
29	1	502	LUT	C31-C30-C29	-2.96	123.13	127.28
20	4	617	CLA	C1C-C2C-C3C	-2.96	103.87	106.98
19	A	1011	CL0	CMB-C2B-C3B	2.95	130.59	124.68
30	4	611	CHL	C4D-CHA-CBD	-2.95	105.99	108.97
20	B	1229	CLA	C2C-C1C-NC	2.95	113.08	109.98
20	A	1141	CLA	C3B-C4B-NB	-2.95	107.89	110.53
20	L	1502	CLA	CMA-C3A-C4A	2.95	119.71	111.77
22	I	4018	BCR	C12-C13-C14	2.95	123.65	119.01
22	I	4018	BCR	C23-C24-C25	-2.95	119.11	127.00
20	3	606	CLA	C2C-C1C-NC	2.95	113.08	109.98
20	B	1205	CLA	O2A-C1-C2	2.95	119.46	108.11
20	2	602	CLA	C1C-C2C-C3C	-2.95	103.88	106.98
20	2	604	CLA	C3B-C4B-NB	-2.95	107.90	110.53
20	B	1224	CLA	O2A-CGA-CBA	2.95	120.82	111.83
20	B	1207	CLA	CMA-C3A-C4A	2.95	119.69	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	4017	BCR	C8-C9-C10	2.95	123.64	119.01
20	2	612	CLA	C1C-C2C-C3C	-2.95	103.88	106.98
20	G	1601	CLA	CHA-C4D-ND	2.94	138.62	132.55
20	A	1114	CLA	C3B-C4B-NB	-2.94	107.90	110.53
20	A	1117	CLA	O2A-C1-C2	2.94	119.43	108.11
20	4	609	CLA	CMA-C3A-C4A	2.94	119.68	111.77
20	A	1140	CLA	C3B-C4B-NB	-2.94	107.91	110.53
20	2	608	CLA	C3B-C4B-NB	-2.94	107.91	110.53
29	3	501	LUT	C35-C15-C14	-2.94	117.51	123.52
30	3	607	CHL	C3C-C4C-NC	-2.94	107.47	114.65
20	1	611	CLA	CMA-C3A-C4A	2.94	119.67	111.77
20	1	604	CLA	O2A-CGA-CBA	2.94	120.79	111.83
20	A	1108	CLA	C2C-C1C-NC	2.94	113.07	109.98
20	B	1232	CLA	O2A-CGA-CBA	2.94	120.79	111.83
21	B	2002	PQN	C14-C13-C15	2.94	120.32	115.23
20	1	602	CLA	C3B-C4B-NB	-2.93	107.91	110.53
20	1	603	CLA	O2A-CGA-CBA	2.93	120.78	111.83
20	G	1602	CLA	CMA-C3A-C4A	2.93	119.66	111.77
20	4	605	CLA	C1C-C2C-C3C	-2.93	103.90	106.98
20	2	608	CLA	O1D-CGD-CBD	-2.92	118.75	124.52
20	B	1239	CLA	C1C-C2C-C3C	-2.92	103.91	106.98
22	K	4002	BCR	C23-C24-C25	-2.92	119.19	127.00
20	A	1120	CLA	CMA-C3A-C4A	2.92	119.63	111.77
20	3	614	CLA	CMA-C3A-C4A	2.92	119.62	111.77
22	L	4019	BCR	C28-C27-C26	-2.92	108.85	114.06
20	H	1701	CLA	CMA-C3A-C4A	2.92	119.62	111.77
20	A	1109	CLA	CMA-C3A-C4A	2.92	119.62	111.77
20	A	1101	CLA	CMA-C3A-C4A	2.92	119.61	111.77
20	3	603	CLA	C3B-C4B-NB	-2.92	107.93	110.53
29	J	4013	LUT	C30-C31-C32	-2.92	114.75	123.20
20	B	1209	CLA	O2D-CGD-O1D	-2.91	118.17	123.85
22	A	4003	BCR	C12-C13-C14	-2.91	114.42	119.01
20	A	1012	CLA	OBD-CAD-C3D	-2.91	121.61	128.42
20	J	1901	CLA	C2C-C1C-NC	2.91	113.04	109.98
20	A	1129	CLA	O2D-CGD-O1D	-2.91	118.18	123.85
20	2	603	CLA	C1D-ND-C4D	-2.91	104.27	106.31
22	B	4005	BCR	C35-C13-C12	2.91	122.53	118.09
20	K	1404	CLA	C1C-C2C-C3C	-2.91	103.92	106.98
20	H	1701	CLA	C3B-C4B-NB	-2.91	107.94	110.53
20	1	603	CLA	C3B-C4B-NB	-2.90	107.94	110.53
20	K	1401	CLA	C1D-ND-C4D	-2.90	104.28	106.31
22	A	4008	BCR	C36-C18-C17	-2.90	118.11	122.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	K	4001	BCR	C37-C22-C21	-2.90	118.12	122.82
20	3	612	CLA	C1D-ND-C4D	-2.90	104.28	106.31
22	A	4008	BCR	C33-C5-C4	2.90	119.78	113.60
24	G	5005	LMT	C3'-C4'-C5'	-2.90	104.51	110.93
20	B	1206	CLA	C2C-C1C-NC	2.90	113.02	109.98
20	B	1212	CLA	C2C-C1C-NC	2.90	113.02	109.98
20	A	1105	CLA	C1C-C2C-C3C	-2.90	103.94	106.98
20	B	1226	CLA	C1C-C2C-C3C	-2.90	103.94	106.98
22	1	504	BCR	C38-C26-C25	-2.90	121.33	124.48
20	F	1302	CLA	C2C-C1C-NC	2.89	113.02	109.98
22	K	4002	BCR	C35-C13-C12	2.89	122.51	118.09
30	2	609	CHL	C1-C2-C3	-2.89	121.46	126.20
20	A	1123	CLA	C2C-C1C-NC	2.89	113.02	109.98
20	1	611	CLA	C2C-C1C-NC	2.89	113.02	109.98
20	B	1206	CLA	C1C-C2C-C3C	-2.89	103.94	106.98
28	4	802	DGD	O1G-C1A-C2A	2.89	120.65	111.83
20	B	1234	CLA	O2A-CGA-CBA	2.89	120.64	111.83
20	1	614	CLA	C2C-C1C-NC	2.89	113.02	109.98
20	A	1101	CLA	C1D-ND-C4D	-2.89	104.29	106.31
20	B	1238	CLA	CMA-C3A-C4A	2.89	119.53	111.77
20	B	1235	CLA	C1-C2-C3	-2.88	121.47	126.20
20	H	1701	CLA	C1D-ND-C4D	-2.88	104.29	106.31
20	B	1228	CLA	C2C-C1C-NC	2.88	113.01	109.98
26	1	802	LMG	O8-C28-C29	2.88	120.61	111.83
20	B	1210	CLA	O2A-CGA-CBA	2.88	120.61	111.83
30	3	607	CHL	C4D-CHA-CBD	-2.88	106.06	108.97
20	A	1013	CLA	CAA-C2A-C3A	-2.88	105.22	113.00
20	A	1138	CLA	O2A-C1-C2	2.88	119.18	108.11
29	3	501	LUT	C31-C30-C29	-2.88	123.24	127.28
28	F	5005	DGD	O1G-C1A-C2A	2.88	120.60	111.83
20	G	1603	CLA	O2D-CGD-O1D	-2.87	118.25	123.85
20	A	1104	CLA	C1C-C2C-C3C	-2.87	103.96	106.98
20	2	601	CLA	O2A-C1-C2	2.87	119.16	108.11
20	B	1023	CLA	C1-C2-C3	-2.87	121.49	126.20
20	B	1219	CLA	CMA-C3A-C4A	2.87	119.49	111.77
20	3	617	CLA	CMA-C3A-C4A	2.87	119.48	111.77
20	A	1116	CLA	O2A-C1-C2	2.87	119.15	108.11
20	J	1901	CLA	CMA-C3A-C4A	2.87	119.47	111.77
20	3	601	CLA	C1-C2-C3	-2.86	121.50	126.20
20	3	603	CLA	C2D-C1D-ND	2.86	112.96	110.13
22	L	4019	BCR	C8-C9-C10	2.86	123.51	119.01
20	B	1237	CLA	C1D-ND-C4D	-2.86	104.30	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	1023	CLA	C3B-C4B-NB	-2.86	107.97	110.53
20	B	1224	CLA	C3B-C4B-NB	-2.86	107.97	110.53
20	J	1901	CLA	C3B-C4B-NB	-2.86	107.98	110.53
20	3	606	CLA	O2A-C1-C2	2.86	119.11	108.11
20	B	1229	CLA	CAA-CBA-CGA	-2.86	105.09	113.21
20	A	1110	CLA	C3B-C4B-NB	-2.86	107.98	110.53
30	3	604	CHL	C4D-CHA-CBD	-2.86	106.09	108.97
20	K	1402	CLA	C1-C2-C3	-2.86	121.52	126.20
20	1	606	CLA	CMA-C3A-C4A	2.85	119.44	111.77
30	1	612	CHL	C1-C2-C3	-2.85	121.52	126.20
20	2	605	CLA	C2C-C1C-NC	2.85	112.98	109.98
20	1	611	CLA	C1C-C2C-C3C	-2.85	103.98	106.98
20	G	1601	CLA	C2C-C1C-NC	2.85	112.98	109.98
20	A	1120	CLA	C1C-C2C-C3C	-2.85	103.98	106.98
20	A	1108	CLA	CMA-C3A-C4A	2.85	119.43	111.77
20	A	1105	CLA	O2D-CGD-O1D	-2.85	118.30	123.85
20	G	1603	CLA	C2D-C1D-ND	2.84	112.94	110.13
19	A	1011	CL0	C4D-ND-C1D	-2.84	103.06	105.22
20	3	613	CLA	C2C-C1C-NC	2.84	112.97	109.98
31	4	502	XAT	C26-C27-C28	-2.84	119.98	125.99
20	A	1108	CLA	C1C-C2C-C3C	-2.84	103.99	106.98
22	A	4011	BCR	C35-C13-C12	2.84	122.43	118.09
20	B	1231	CLA	C2C-C1C-NC	2.84	112.97	109.98
20	B	1221	CLA	CAA-C2A-C3A	-2.84	105.33	113.00
20	3	606	CLA	C1C-C2C-C3C	-2.84	104.00	106.98
20	1	603	CLA	CBA-CAA-C2A	2.84	122.23	113.79
20	A	1110	CLA	O2A-CGA-CBA	2.84	120.48	111.83
24	G	5004	LMT	C1'-O5'-C5'	-2.84	108.18	113.72
22	F	4014	BCR	C29-C30-C25	2.84	114.56	110.44
20	A	1106	CLA	C1C-C2C-C3C	-2.84	104.00	106.98
26	B	5007	LMG	O8-C28-C29	2.84	120.48	111.83
20	A	1101	CLA	C3B-C4B-NB	-2.84	108.00	110.53
20	B	1236	CLA	C1C-C2C-C3C	-2.84	104.00	106.98
20	B	1239	CLA	C3B-C4B-NB	-2.83	108.00	110.53
20	B	1219	CLA	C2C-C1C-NC	2.83	112.96	109.98
22	K	4002	BCR	C27-C26-C25	-2.83	118.88	122.70
20	A	1131	CLA	C1C-C2C-C3C	-2.83	104.00	106.98
26	A	5006	LMG	O8-C28-C29	2.83	120.46	111.83
22	B	4009	BCR	C12-C13-C14	-2.83	114.56	119.01
26	B	5003	LMG	O8-C28-C29	2.83	120.46	111.83
20	A	1103	CLA	CAA-C2A-C1A	-2.83	102.71	111.97
20	A	1131	CLA	C3B-C4B-NB	-2.83	108.01	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	1128	CLA	O2D-CGD-O1D	-2.83	118.34	123.85
20	A	1126	CLA	C3B-C4B-NB	-2.83	108.01	110.53
20	B	1224	CLA	C1C-C2C-C3C	-2.82	104.01	106.98
20	2	608	CLA	CHD-C1D-ND	-2.82	120.83	124.80
20	B	1236	CLA	O2D-CGD-O1D	-2.82	118.36	123.85
29	1	501	LUT	C22-C23-C24	-2.82	107.00	111.18
24	B	5006	LMT	C1'-O5'-C5'	-2.81	108.22	113.72
20	3	614	CLA	C1C-C2C-C3C	-2.81	104.02	106.98
20	1	614	CLA	O2D-CGD-O1D	-2.81	118.37	123.85
20	1	605	CLA	CAA-CBA-CGA	-2.81	105.23	113.21
20	B	1225	CLA	C1C-C2C-C3C	-2.81	104.02	106.98
20	G	1601	CLA	O2A-CGA-CBA	2.81	120.40	111.83
22	H	4021	BCR	C33-C5-C4	2.81	119.59	113.60
20	4	602	CLA	CMA-C3A-C4A	2.81	119.32	111.77
22	L	4019	BCR	C34-C9-C10	-2.81	118.27	122.82
20	4	612	CLA	C1D-ND-C4D	-2.80	104.34	106.31
20	B	1213	CLA	C3B-C4B-NB	-2.80	108.03	110.53
20	B	1237	CLA	C2C-C1C-NC	2.80	112.92	109.98
20	A	1012	CLA	C1C-C2C-C3C	-2.80	104.03	106.98
20	B	1216	CLA	C3B-C4B-NB	-2.80	108.03	110.53
20	B	1230	CLA	O2A-CGA-CBA	2.80	120.37	111.83
19	A	1011	CL0	O2D-CGD-O1D	-2.80	118.40	123.85
20	1	606	CLA	C2C-C1C-NC	2.80	112.92	109.98
20	B	1203	CLA	C1C-C2C-C3C	-2.80	104.04	106.98
20	B	1215	CLA	C1C-C2C-C3C	-2.80	104.04	106.98
20	A	1114	CLA	CMA-C3A-C4A	2.79	119.28	111.77
22	I	4020	BCR	C33-C5-C4	2.79	119.55	113.60
22	1	503	BCR	C33-C5-C4	2.79	119.55	113.60
29	2	501	LUT	C15-C35-C34	-2.79	117.81	123.52
20	3	601	CLA	C1D-ND-C4D	-2.79	104.35	106.31
20	4	605	CLA	C2C-C1C-NC	2.79	112.91	109.98
20	A	1129	CLA	C2C-C1C-NC	2.79	112.91	109.98
20	B	1205	CLA	C3B-C4B-NB	-2.79	108.04	110.53
20	B	1228	CLA	C1C-C2C-C3C	-2.79	104.05	106.98
20	B	1222	CLA	O2D-CGD-O1D	-2.79	118.42	123.85
20	A	1012	CLA	C2C-C1C-NC	2.79	112.91	109.98
22	B	4004	BCR	C29-C30-C25	-2.79	106.39	110.44
20	3	603	CLA	C2C-C1C-NC	2.79	112.91	109.98
22	2	503	BCR	C1-C6-C5	-2.79	118.83	122.64
20	B	1229	CLA	C1C-C2C-C3C	-2.79	104.05	106.98
20	B	1022	CLA	C1C-C2C-C3C	-2.78	104.05	106.98
29	4	501	LUT	C10-C11-C12	-2.78	115.14	123.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	L	4020	BCR	C33-C5-C4	2.78	119.53	113.60
20	4	605	CLA	CMA-C3A-C4A	2.78	119.25	111.77
20	B	1214	CLA	C1C-C2C-C3C	-2.78	104.06	106.98
20	3	612	CLA	C1C-C2C-C3C	-2.78	104.06	106.98
22	A	4003	BCR	C33-C5-C4	2.78	119.52	113.60
30	1	610	CHL	C1A-CHA-C4D	2.78	123.62	118.98
20	A	1118	CLA	O2D-CGD-O1D	-2.78	118.44	123.85
20	G	1601	CLA	CMA-C3A-C4A	2.78	119.24	111.77
20	4	617	CLA	CMA-C3A-C4A	2.78	119.24	111.77
20	B	1223	CLA	C2C-C1C-NC	2.78	112.90	109.98
20	B	1219	CLA	C1C-C2C-C3C	-2.78	104.06	106.98
20	A	1118	CLA	C1C-C2C-C3C	-2.77	104.06	106.98
20	1	607	CLA	C2C-C1C-NC	2.77	112.89	109.98
20	4	607	CLA	C2D-C1D-ND	2.77	112.87	110.13
29	2	501	LUT	C11-C12-C13	-2.77	118.78	126.36
20	4	607	CLA	CMC-C2C-C1C	2.77	129.36	125.03
20	B	1217	CLA	C3B-C4B-NB	-2.77	108.06	110.53
22	B	4004	BCR	C38-C26-C25	-2.77	121.47	124.48
20	4	612	CLA	CMA-C3A-C4A	2.77	119.21	111.77
20	B	1202	CLA	O2A-CGA-CBA	2.77	120.27	111.83
30	2	615	CHL	C1-O2A-CGA	2.76	123.34	116.65
20	A	1117	CLA	O2A-CGA-CBA	2.76	120.26	111.83
20	A	1135	CLA	C2C-C1C-NC	2.76	112.88	109.98
20	B	1226	CLA	C2C-C1C-NC	2.76	112.88	109.98
20	2	606	CLA	C1C-C2C-C3C	-2.76	104.08	106.98
26	2	805	LMG	O8-C28-C29	2.76	120.25	111.83
20	B	1205	CLA	O2A-CGA-CBA	2.76	120.25	111.83
20	A	1137	CLA	O2D-CGD-O1D	-2.76	118.48	123.85
22	A	4007	BCR	C36-C18-C17	-2.76	118.35	122.82
22	A	4008	BCR	C19-C18-C17	2.76	123.34	119.01
23	2	801	LHG	O8-C23-C24	2.76	120.24	111.83
20	3	612	CLA	C2C-C1C-NC	2.76	112.88	109.98
20	K	1403	CLA	C1C-C2C-C3C	-2.75	104.08	106.98
22	3	503	BCR	C33-C5-C4	2.75	119.47	113.60
20	H	1701	CLA	C2C-C1C-NC	2.75	112.87	109.98
30	4	615	CHL	C1A-CHA-C4D	2.75	123.57	118.98
20	A	1122	CLA	CMA-C3A-C4A	2.75	119.17	111.77
20	A	1105	CLA	C6-C5-C3	-2.75	106.77	113.47
20	B	1224	CLA	C2C-C1C-NC	2.75	112.87	109.98
20	A	1109	CLA	C4B-CHC-C1C	2.75	132.71	126.25
20	B	1240	CLA	CMA-C3A-C4A	2.75	119.16	111.77
20	A	1121	CLA	C1C-C2C-C3C	-2.75	104.09	106.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	F	1301	CLA	C2C-C1C-NC	2.75	112.87	109.98
30	3	607	CHL	C1-O2A-CGA	2.75	123.30	116.65
20	B	1229	CLA	CMA-C3A-C4A	2.74	119.15	111.77
20	2	603	CLA	C1-O2A-CGA	2.74	123.29	116.65
22	1	503	BCR	C36-C18-C17	-2.74	118.37	122.82
20	F	1301	CLA	C1-C2-C3	-2.74	121.71	126.20
20	B	1239	CLA	C4B-CHC-C1C	2.74	132.69	126.25
20	1	604	CLA	CMD-C2D-C3D	-2.74	121.41	127.69
20	B	1208	CLA	C1C-C2C-C3C	-2.74	104.10	106.98
20	G	1601	CLA	C1C-C2C-C3C	-2.74	104.10	106.98
20	B	1226	CLA	O2A-CGA-CBA	2.74	120.19	111.83
20	A	1119	CLA	C3B-C4B-NB	-2.74	108.08	110.53
20	3	614	CLA	CMD-C2D-C3D	-2.74	121.41	127.69
20	B	1210	CLA	C2C-C1C-NC	2.74	112.86	109.98
20	1	601	CLA	CMA-C3A-C4A	2.74	119.13	111.77
22	3	506	BCR	C33-C5-C4	2.74	119.43	113.60
20	B	1222	CLA	CAA-C2A-C3A	-2.74	105.61	113.00
20	A	1104	CLA	C3B-C4B-NB	-2.74	108.09	110.53
22	A	4002	BCR	C36-C18-C17	-2.73	118.39	122.82
20	A	1140	CLA	CMA-C3A-C4A	2.73	119.12	111.77
20	3	608	CLA	C1C-C2C-C3C	-2.73	104.11	106.98
20	A	1121	CLA	CMA-C3A-C4A	2.73	119.12	111.77
20	3	605	CLA	CMA-C3A-C4A	2.73	119.12	111.77
22	A	4017	BCR	C35-C13-C14	-2.73	118.39	122.82
20	A	1113	CLA	C1C-C2C-C3C	-2.73	104.11	106.98
20	B	1212	CLA	C1C-C2C-C3C	-2.73	104.11	106.98
20	A	1123	CLA	C1C-C2C-C3C	-2.73	104.11	106.98
22	B	4010	BCR	C37-C22-C23	2.73	122.26	118.09
26	G	5002	LMG	O8-C28-C29	2.73	120.16	111.83
28	G	5003	DGD	O1G-C1A-C2A	2.73	120.16	111.83
20	B	1235	CLA	C1C-C2C-C3C	-2.73	104.11	106.98
29	J	4013	LUT	C18-C5-C6	-2.73	121.51	124.48
22	K	4001	BCR	C27-C26-C25	-2.73	119.02	122.70
20	2	602	CLA	C2C-C1C-NC	2.73	112.85	109.98
20	A	1103	CLA	O2D-CGD-O1D	-2.73	118.54	123.85
20	A	1101	CLA	C2C-C1C-NC	2.73	112.84	109.98
20	3	608	CLA	C2C-C1C-NC	2.72	112.84	109.98
20	3	602	CLA	C1C-C2C-C3C	-2.72	104.11	106.98
20	B	1236	CLA	C2C-C1C-NC	2.72	112.84	109.98
22	B	4010	BCR	C35-C13-C12	2.72	122.25	118.09
20	A	1127	CLA	CAA-C2A-C3A	-2.72	105.64	113.00
22	I	4018	BCR	C4-C5-C6	-2.72	119.03	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	1117	CLA	C2C-C1C-NC	2.72	112.84	109.98
20	3	605	CLA	CHA-C4D-ND	2.72	138.16	132.55
20	K	1402	CLA	O2A-CGA-CBA	2.72	120.13	111.83
29	3	501	LUT	C10-C11-C12	-2.72	115.32	123.20
20	3	602	CLA	CMA-C3A-C4A	2.72	119.08	111.77
20	A	1137	CLA	O1D-CGD-CBD	-2.72	119.15	124.52
20	B	1229	CLA	C3B-C4B-NB	-2.72	108.10	110.53
20	A	1102	CLA	C1-O2A-CGA	2.72	123.23	116.65
20	4	617	CLA	C2C-C1C-NC	2.72	112.84	109.98
22	A	4002	BCR	C19-C18-C17	2.72	123.28	119.01
20	B	1214	CLA	O2A-CGA-CBA	2.72	120.12	111.83
20	1	614	CLA	C1C-C2C-C3C	-2.72	104.12	106.98
22	F	4016	BCR	C35-C13-C12	2.72	122.24	118.09
23	B	5002	LHG	C5-O7-C7	-2.72	111.29	117.80
20	B	1205	CLA	O2D-CGD-O1D	-2.72	118.56	123.85
20	B	1214	CLA	C3B-C4B-NB	-2.72	108.11	110.53
20	1	614	CLA	C3B-C4B-NB	-2.72	108.11	110.53
20	4	605	CLA	C3B-C4B-NB	-2.72	108.11	110.53
20	A	1129	CLA	C1C-C2C-C3C	-2.72	104.12	106.98
22	B	4006	BCR	C36-C18-C17	-2.72	118.42	122.82
20	2	602	CLA	C3B-C4B-NB	-2.72	108.11	110.53
22	A	4017	BCR	C12-C13-C14	2.71	123.28	119.01
20	3	610	CLA	C1C-C2C-C3C	-2.71	104.12	106.98
20	4	604	CLA	C1C-C2C-C3C	-2.71	104.12	106.98
30	1	610	CHL	C4D-CHA-CBD	-2.71	106.23	108.97
20	1	601	CLA	O2A-CGA-CBA	2.71	120.11	111.83
22	3	506	BCR	C37-C22-C21	-2.71	118.42	122.82
20	B	1201	CLA	C1C-C2C-C3C	-2.71	104.13	106.98
20	B	1205	CLA	C1C-C2C-C3C	-2.71	104.13	106.98
20	A	1104	CLA	C2C-C1C-NC	2.71	112.83	109.98
20	2	608	CLA	C2C-C1C-NC	2.71	112.83	109.98
20	B	1201	CLA	O2D-CGD-O1D	-2.71	118.57	123.85
30	4	615	CHL	CMA-C3A-C4A	2.71	120.45	114.61
20	B	1240	CLA	C3B-C4B-NB	-2.71	108.11	110.53
20	B	1237	CLA	C1C-C2C-C3C	-2.71	104.13	106.98
29	1	502	LUT	C8-C7-C6	-2.71	119.76	127.00
20	A	1117	CLA	C1C-C2C-C3C	-2.71	104.13	106.98
23	A	5001	LHG	O8-C23-C24	2.71	120.08	111.83
20	A	1101	CLA	C1C-C2C-C3C	-2.70	104.14	106.98
20	3	612	CLA	CMA-C3A-C4A	2.70	119.04	111.77
20	B	1021	CLA	C2C-C1C-NC	2.70	112.82	109.98
22	F	4014	BCR	C31-C1-C6	-2.70	106.00	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	1237	CLA	C11-C12-C13	-2.70	106.98	115.97
20	B	1218	CLA	O2A-C1-C2	2.70	118.51	108.11
24	A	5004	LMT	C3'-C4'-C5'	-2.70	104.94	110.93
20	F	1302	CLA	C1C-C2C-C3C	-2.70	104.14	106.98
20	A	1137	CLA	O2A-CGA-CBA	2.70	120.07	111.83
20	B	1204	CLA	C2C-C1C-NC	2.70	112.82	109.98
22	B	4010	BCR	C12-C13-C14	-2.70	114.77	119.01
20	3	605	CLA	C3B-C4B-NB	-2.70	108.12	110.53
20	B	1223	CLA	C1C-C2C-C3C	-2.70	104.14	106.98
24	G	5004	LMT	C3'-C4'-C5'	-2.70	104.95	110.93
26	2	804	LMG	O8-C28-C29	2.70	120.06	111.83
20	1	604	CLA	C1C-C2C-C3C	-2.70	104.14	106.98
20	K	1402	CLA	C1C-C2C-C3C	-2.69	104.15	106.98
20	B	1211	CLA	O2D-CGD-O1D	-2.69	118.60	123.85
20	4	601	CLA	CMA-C3A-C4A	2.69	119.01	111.77
20	B	1234	CLA	C2C-C1C-NC	2.69	112.81	109.98
20	1	608	CLA	C1C-C2C-C3C	-2.69	104.15	106.98
22	F	4016	BCR	C38-C26-C25	-2.69	121.55	124.48
20	B	1223	CLA	CHA-C4D-ND	2.69	138.10	132.55
20	A	1138	CLA	C3B-C4B-NB	-2.69	108.13	110.53
30	2	611	CHL	CMA-C3A-C4A	2.69	120.41	114.61
20	B	1223	CLA	CMA-C3A-C4A	2.69	119.01	111.77
20	K	1402	CLA	C3B-C4B-NB	-2.69	108.13	110.53
20	A	1108	CLA	CAA-C2A-C3A	-2.69	105.73	113.00
20	3	613	CLA	CMD-C2D-C3D	-2.69	121.52	127.69
20	4	605	CLA	CHA-C4D-ND	2.69	138.09	132.55
22	B	4005	BCR	C12-C13-C14	-2.69	114.78	119.01
20	A	1102	CLA	O2D-CGD-O1D	-2.69	118.62	123.85
20	3	614	CLA	CHA-C4D-ND	2.69	138.09	132.55
20	2	606	CLA	C2C-C1C-NC	2.69	112.80	109.98
20	B	1235	CLA	C3B-C4B-NB	-2.69	108.13	110.53
22	J	4012	BCR	C3-C4-C5	-2.69	109.27	114.06
20	B	1230	CLA	O2D-CGD-O1D	-2.69	118.62	123.85
20	B	1227	CLA	C2C-C1C-NC	2.68	112.80	109.98
20	1	604	CLA	CAA-CBA-CGA	-2.68	105.59	113.21
20	1	608	CLA	CHA-C4D-ND	2.68	138.08	132.55
20	4	612	CLA	C2C-C1C-NC	2.68	112.80	109.98
20	A	1122	CLA	C3B-C4B-NB	-2.68	108.14	110.53
24	B	5008	LMT	C1'-O5'-C5'	-2.68	108.48	113.72
26	2	803	LMG	O8-C28-C29	2.68	120.01	111.83
20	A	1130	CLA	C1C-C2C-C3C	-2.68	104.16	106.98
29	J	4013	LUT	C15-C35-C34	-2.68	118.03	123.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	2	612	CLA	C2C-C1C-NC	2.68	112.80	109.98
22	L	4020	BCR	C23-C24-C25	-2.68	119.84	127.00
20	K	1402	CLA	O2D-CGD-O1D	-2.68	118.63	123.85
20	B	1235	CLA	O2D-CGD-O1D	-2.68	118.63	123.85
22	F	4016	BCR	C19-C18-C17	-2.68	114.80	119.01
20	A	1131	CLA	C2C-C1C-NC	2.68	112.80	109.98
20	B	1240	CLA	O2D-CGD-O1D	-2.68	118.64	123.85
20	B	1210	CLA	O1D-CGD-CBD	-2.68	119.24	124.52
29	4	501	LUT	C27-C28-C29	-2.68	120.56	126.32
20	4	606	CLA	O2A-CGA-CBA	2.67	119.99	111.83
29	3	502	LUT	C31-C32-C33	-2.67	119.04	126.36
20	1	605	CLA	C1C-C2C-C3C	-2.67	104.17	106.98
20	4	602	CLA	C2D-C1D-ND	2.67	112.77	110.13
20	A	1124	CLA	C3B-C4B-NB	-2.67	108.15	110.53
20	A	1122	CLA	C2C-C1C-NC	2.67	112.78	109.98
20	A	1110	CLA	CAA-C2A-C3A	-2.67	105.79	113.00
20	A	1115	CLA	C1C-C2C-C3C	-2.67	104.17	106.98
29	1	501	LUT	C11-C10-C9	-2.67	123.54	127.28
22	3	503	BCR	C38-C26-C27	2.67	119.28	113.60
20	2	608	CLA	CMA-C3A-C4A	2.67	118.94	111.77
20	K	1403	CLA	C4B-CHC-C1C	2.67	132.51	126.25
20	A	1117	CLA	CMA-C3A-C4A	2.67	118.94	111.77
20	1	608	CLA	C3B-C4B-NB	-2.66	108.15	110.53
20	B	1022	CLA	CHA-C4D-ND	2.66	138.04	132.55
20	B	1210	CLA	C4B-CHC-C1C	2.66	132.51	126.25
22	I	4018	BCR	C15-C14-C13	-2.66	123.54	127.28
20	A	1136	CLA	C2C-C1C-NC	2.66	112.78	109.98
20	A	1127	CLA	C1C-C2C-C3C	-2.66	104.18	106.98
22	L	4019	BCR	C27-C26-C25	-2.66	119.11	122.70
26	G	5006	LMG	O7-C10-C11	2.66	120.70	110.93
20	3	608	CLA	C4B-CHC-C1C	2.66	132.50	126.25
22	2	503	BCR	C34-C9-C10	-2.66	118.51	122.82
20	1	604	CLA	C2C-C1C-NC	2.66	112.78	109.98
20	B	1240	CLA	CHA-C4D-ND	2.66	138.03	132.55
24	B	5008	LMT	C3'-C4'-C5'	-2.66	105.04	110.93
22	A	4003	BCR	C23-C24-C25	-2.66	119.90	127.00
30	2	615	CHL	CMA-C3A-C4A	2.66	120.33	114.61
20	4	612	CLA	C1C-C2C-C3C	-2.66	104.19	106.98
20	A	1127	CLA	C2C-C1C-NC	2.66	112.77	109.98
20	A	1122	CLA	C1C-C2C-C3C	-2.66	104.19	106.98
20	2	607	CLA	C1C-C2C-C3C	-2.66	104.19	106.98
20	K	1401	CLA	C2C-C1C-NC	2.65	112.77	109.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	1141	CLA	O2A-CGA-CBA	2.65	119.93	111.83
20	K	1401	CLA	C1C-C2C-C3C	-2.65	104.19	106.98
20	4	608	CLA	C1C-C2C-C3C	-2.65	104.19	106.98
20	B	1221	CLA	C3B-C4B-NB	-2.65	108.16	110.53
20	3	613	CLA	C3B-C4B-NB	-2.65	108.16	110.53
30	2	610	CHL	CMA-C3A-C4A	2.65	120.33	114.61
20	A	1109	CLA	C1D-ND-C4D	-2.65	104.45	106.31
20	1	605	CLA	C1D-ND-C4D	-2.65	104.45	106.31
22	B	4005	BCR	C38-C26-C25	-2.65	121.59	124.48
29	3	501	LUT	C22-C23-C24	-2.65	107.25	111.18
20	A	1141	CLA	CMA-C3A-C4A	2.65	118.90	111.77
28	F	5005	DGD	C2G-O2G-C1B	-2.65	111.45	117.80
20	A	1109	CLA	O2D-CGD-O1D	-2.65	118.69	123.85
22	G	4011	BCR	C38-C26-C25	-2.65	121.59	124.48
20	2	607	CLA	C1D-ND-C4D	-2.65	104.45	106.31
22	B	4006	BCR	C34-C9-C10	-2.65	118.53	122.82
20	K	1404	CLA	C3B-C4B-NB	-2.65	108.17	110.53
29	J	4013	LUT	C37-C21-C22	-2.65	104.47	109.41
30	3	604	CHL	CMA-C3A-C4A	2.64	120.31	114.61
33	4	505	C7Z	C21-C26-C27	-2.64	108.48	115.65
20	A	1125	CLA	C3B-C4B-NB	-2.64	108.17	110.53
20	A	1108	CLA	C1-C2-C3	-2.64	122.48	126.76
20	2	601	CLA	CHA-C4D-ND	2.64	138.00	132.55
20	2	608	CLA	C1-O2A-CGA	2.64	123.05	116.65
20	1	606	CLA	C1C-C2C-C3C	-2.64	104.20	106.98
20	B	1218	CLA	C4B-CHC-C1C	2.64	132.46	126.25
22	L	4019	BCR	C33-C5-C4	2.64	119.23	113.60
20	A	1108	CLA	CHA-C4D-ND	2.64	138.00	132.55
20	A	1114	CLA	O2D-CGD-O1D	-2.64	118.71	123.85
20	4	602	CLA	C1C-C2C-C3C	-2.64	104.20	106.98
20	A	1112	CLA	C1C-C2C-C3C	-2.64	104.20	106.98
20	2	608	CLA	CHA-C4D-ND	2.64	137.99	132.55
20	A	1116	CLA	CAA-CBA-CGA	-2.64	105.72	113.21
20	1	607	CLA	C1C-C2C-C3C	-2.64	104.21	106.98
20	A	1116	CLA	C2C-C1C-NC	2.64	112.75	109.98
33	4	505	C7Z	C31-C32-C33	-2.64	119.13	126.36
20	A	1116	CLA	CHA-C4D-ND	2.64	137.99	132.55
20	G	1603	CLA	CHD-C1D-ND	-2.64	121.09	124.80
20	2	604	CLA	C1C-C2C-C3C	-2.64	104.21	106.98
20	B	1201	CLA	C2C-C1C-NC	2.64	112.75	109.98
20	A	1012	CLA	CHA-C4D-ND	2.64	137.99	132.55
20	A	1013	CLA	O2A-C1-C2	2.64	118.25	108.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	4	617	CLA	O2A-CGA-CBA	2.63	119.87	111.83
20	B	1221	CLA	CHA-C4D-ND	2.63	137.99	132.55
20	J	1901	CLA	CHA-C4D-ND	2.63	137.99	132.55
20	A	1126	CLA	C6-C5-C3	-2.63	107.05	113.47
20	B	1240	CLA	O1D-CGD-CBD	-2.63	119.32	124.52
20	B	1204	CLA	C1C-C2C-C3C	-2.63	104.21	106.98
20	A	1116	CLA	O2A-CGA-CBA	2.63	119.86	111.83
26	F	5002	LMG	O8-C28-C29	2.63	119.86	111.83
20	A	1133	CLA	C2C-C1C-NC	2.63	112.75	109.98
20	L	1501	CLA	C2C-C1C-NC	2.63	112.75	109.98
20	A	1111	CLA	C1-C2-C3	-2.63	121.89	126.20
20	A	1013	CLA	C1C-C2C-C3C	-2.63	104.21	106.98
20	L	1503	CLA	C2C-C1C-NC	2.63	112.74	109.98
20	B	1231	CLA	O2D-CGD-O1D	-2.63	118.73	123.85
30	4	610	CHL	C4D-CHA-CBD	-2.63	106.32	108.97
20	B	1208	CLA	O2D-CGD-O1D	-2.63	118.73	123.85
20	3	606	CLA	CHA-C4D-ND	2.63	137.97	132.55
29	3	502	LUT	C15-C14-C13	-2.63	123.59	127.28
20	3	617	CLA	C1C-C2C-C3C	-2.63	104.22	106.98
22	B	4006	BCR	C30-C25-C26	-2.63	119.05	122.64
26	A	5006	LMG	C8-O7-C10	-2.63	111.51	117.80
20	1	603	CLA	CMA-C3A-C4A	2.63	118.83	111.77
20	A	1135	CLA	C1C-C2C-C3C	-2.63	104.22	106.98
20	B	1213	CLA	CMA-C3A-C4A	2.62	118.83	111.77
20	A	1134	CLA	O2D-CGD-O1D	-2.62	118.74	123.85
20	B	1224	CLA	C6-C5-C3	-2.62	107.08	113.47
20	3	608	CLA	C3B-C4B-NB	-2.62	108.19	110.53
20	A	1124	CLA	C2C-C1C-NC	2.62	112.74	109.98
20	2	601	CLA	C2C-C1C-NC	2.62	112.73	109.98
22	G	4011	BCR	C33-C5-C4	2.62	119.18	113.60
20	B	1221	CLA	O2D-CGD-O1D	-2.62	118.75	123.85
20	A	1133	CLA	C1C-C2C-C3C	-2.62	104.22	106.98
20	B	1231	CLA	C1C-C2C-C3C	-2.62	104.22	106.98
20	2	607	CLA	O2D-CGD-O1D	-2.62	118.75	123.85
29	4	501	LUT	C11-C10-C9	-2.62	123.61	127.28
20	2	604	CLA	C2C-C1C-NC	2.62	112.73	109.98
20	A	1131	CLA	O2A-CGA-CBA	2.62	119.82	111.83
22	B	4006	BCR	C33-C5-C4	2.62	119.18	113.60
20	B	1208	CLA	C4B-CHC-C1C	2.62	132.40	126.25
22	I	4020	BCR	C34-C9-C10	-2.62	118.58	122.82
20	B	1203	CLA	C2C-C1C-NC	2.62	112.73	109.98
32	2	807	3PH	O31-C31-C32	2.62	119.81	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	1128	CLA	C1C-C2C-C3C	-2.62	104.23	106.98
20	L	1502	CLA	C1C-C2C-C3C	-2.62	104.23	106.98
20	4	607	CLA	O2D-CGD-O1D	-2.61	118.76	123.85
20	J	1901	CLA	C1C-C2C-C3C	-2.61	104.23	106.98
20	L	1501	CLA	C1C-C2C-C3C	-2.61	104.23	106.98
20	2	608	CLA	C1C-C2C-C3C	-2.61	104.23	106.98
20	B	1224	CLA	O1D-CGD-CBD	-2.61	119.36	124.52
20	B	1228	CLA	O2D-CGD-O1D	-2.61	118.76	123.85
22	A	4007	BCR	C38-C26-C27	2.61	119.17	113.60
20	B	1239	CLA	CHA-C4D-ND	2.61	137.94	132.55
20	A	1121	CLA	CHA-C4D-ND	2.61	137.94	132.55
20	4	601	CLA	C2C-C1C-NC	2.61	112.73	109.98
20	2	612	CLA	CHD-C1D-ND	-2.61	121.13	124.80
20	A	1124	CLA	O2D-CGD-O1D	-2.61	118.76	123.85
20	2	602	CLA	CMA-C3A-C4A	2.61	118.79	111.77
20	A	1107	CLA	C1C-C2C-C3C	-2.61	104.23	106.98
20	A	1114	CLA	C4B-CHC-C1C	2.61	132.39	126.25
20	3	617	CLA	C1D-ND-C4D	-2.61	104.48	106.31
20	1	601	CLA	CHD-C1D-ND	-2.61	121.13	124.80
20	B	1218	CLA	O2D-CGD-O1D	-2.61	118.77	123.85
30	2	609	CHL	CMA-C3A-C4A	2.61	120.23	114.61
20	G	1602	CLA	C1C-C2C-C3C	-2.61	104.23	106.98
20	B	1023	CLA	O2A-CGA-CBA	2.61	119.79	111.83
29	J	4013	LUT	C7-C8-C9	-2.61	122.38	126.23
20	B	1223	CLA	OBD-CAD-C3D	-2.61	122.32	128.42
20	4	601	CLA	C4B-CHC-C1C	2.61	132.38	126.25
20	3	601	CLA	CHD-C1D-ND	-2.60	121.14	124.80
20	B	1235	CLA	CHD-C1D-ND	-2.60	121.14	124.80
20	4	608	CLA	C4B-CHC-C1C	2.60	132.37	126.25
20	2	607	CLA	C1-O2A-CGA	2.60	122.95	116.65
20	B	1240	CLA	C2C-C1C-NC	2.60	112.71	109.98
20	B	1203	CLA	C3B-C4B-NB	-2.60	108.21	110.53
20	B	1207	CLA	C4B-CHC-C1C	2.60	132.36	126.25
31	2	502	XAT	C40-C33-C34	-2.60	118.61	122.82
20	B	1240	CLA	C4B-CHC-C1C	2.60	132.36	126.25
20	G	1601	CLA	CHA-C1A-NA	-2.60	120.51	126.39
19	A	1011	CL0	C4-C3-C5	2.60	119.74	115.23
20	L	1503	CLA	C1C-C2C-C3C	-2.60	104.25	106.98
20	4	604	CLA	C2C-C1C-NC	2.60	112.71	109.98
22	3	503	BCR	C30-C25-C26	-2.60	119.09	122.64
20	1	606	CLA	O2D-CGD-O1D	-2.60	118.80	123.85
20	A	1137	CLA	C1C-C2C-C3C	-2.59	104.25	106.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	1	613	CLA	CHA-C4D-ND	2.59	137.90	132.55
20	B	1231	CLA	CHA-C4D-ND	2.59	137.90	132.55
19	A	1011	CL0	CAA-C2A-C3A	-2.59	105.99	113.00
22	A	4011	BCR	C32-C1-C6	-2.59	106.18	110.24
20	1	608	CLA	C2C-C1C-NC	2.59	112.70	109.98
20	A	1126	CLA	O2A-C1-C2	2.59	118.08	108.11
20	A	1131	CLA	CHA-C4D-ND	2.59	137.89	132.55
20	F	1301	CLA	C1C-C2C-C3C	-2.59	104.26	106.98
20	B	1218	CLA	CHD-C1D-ND	-2.59	121.16	124.80
31	2	502	XAT	O24-C25-C24	2.59	115.92	113.49
20	A	1140	CLA	O2A-CGA-CBA	2.59	119.73	111.83
20	2	603	CLA	C4B-CHC-C1C	2.59	132.33	126.25
20	A	1101	CLA	O2D-CGD-O1D	-2.59	118.81	123.85
20	B	1229	CLA	O2D-CGD-O1D	-2.59	118.81	123.85
22	K	4001	BCR	C19-C18-C17	2.59	123.08	119.01
20	B	1205	CLA	C2C-C1C-NC	2.59	112.70	109.98
20	A	1107	CLA	O2D-CGD-O1D	-2.59	118.81	123.85
20	B	1212	CLA	O2D-CGD-O1D	-2.59	118.82	123.85
20	A	1118	CLA	O2A-CGA-CBA	2.58	119.72	111.83
20	B	1237	CLA	C4B-CHC-C1C	2.58	132.32	126.25
20	A	1012	CLA	O2A-CGA-CBA	2.58	119.72	111.83
20	A	1118	CLA	CHA-C4D-ND	2.58	137.88	132.55
20	4	608	CLA	C2C-C1C-NC	2.58	112.70	109.98
20	B	1236	CLA	C3B-C4B-NB	-2.58	108.22	110.53
20	B	1204	CLA	O2D-CGD-O1D	-2.58	118.82	123.85
20	B	1211	CLA	C1C-C2C-C3C	-2.58	104.27	106.98
29	3	501	LUT	C8-C7-C6	-2.58	120.10	127.00
20	1	614	CLA	CHA-C4D-ND	2.58	137.87	132.55
20	B	1225	CLA	C2C-C1C-NC	2.58	112.69	109.98
20	4	617	CLA	O2D-CGD-O1D	-2.58	118.83	123.85
20	A	1135	CLA	CHA-C4D-ND	2.58	137.87	132.55
20	B	1227	CLA	C1C-C2C-C3C	-2.58	104.27	106.98
31	4	502	XAT	C6-C7-C8	-2.58	120.54	125.99
20	A	1136	CLA	C1C-C2C-C3C	-2.58	104.27	106.98
20	B	1231	CLA	CMD-C2D-C3D	-2.58	121.78	127.69
20	A	1132	CLA	C1C-C2C-C3C	-2.58	104.27	106.98
22	F	4014	BCR	C27-C26-C25	-2.58	119.22	122.70
20	A	1128	CLA	O2A-CGA-CBA	2.57	119.69	111.83
31	2	502	XAT	C26-C27-C28	-2.57	120.55	125.99
20	A	1116	CLA	CMA-C3A-C4A	2.57	118.69	111.77
20	3	603	CLA	O2A-CGA-CBA	2.57	119.68	111.83
20	A	1109	CLA	C1C-C2C-C3C	-2.57	104.27	106.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	4	609	CLA	C4B-CHC-C1C	2.57	132.30	126.25
20	G	1603	CLA	C2C-C1C-NC	2.57	112.68	109.98
20	B	1238	CLA	C4B-CHC-C1C	2.57	132.30	126.25
20	A	1110	CLA	C4B-CHC-C1C	2.57	132.29	126.25
22	B	4004	BCR	C39-C30-C25	2.57	114.28	110.24
20	2	608	CLA	O2A-CGA-CBA	2.57	119.67	111.83
20	B	1210	CLA	C6-C5-C3	-2.57	107.21	113.47
20	4	609	CLA	C1C-C2C-C3C	-2.57	104.28	106.98
20	4	604	CLA	C4B-CHC-C1C	2.57	132.29	126.25
20	4	606	CLA	CHD-C1D-ND	-2.57	121.19	124.80
20	2	604	CLA	C4B-CHC-C1C	2.57	132.28	126.25
20	B	1021	CLA	CHA-C4D-ND	2.57	137.84	132.55
20	L	1502	CLA	C4B-CHC-C1C	2.57	132.28	126.25
20	B	1234	CLA	CHA-C4D-ND	2.57	137.84	132.55
20	2	607	CLA	C3B-C4B-NB	-2.57	108.24	110.53
22	A	4008	BCR	C33-C5-C6	-2.57	121.69	124.48
29	1	502	LUT	C27-C28-C29	-2.56	120.81	126.32
22	A	4003	BCR	C27-C26-C25	-2.56	119.24	122.70
20	A	1125	CLA	O2D-CGD-O1D	-2.56	118.86	123.85
20	4	609	CLA	C2C-C1C-NC	2.56	112.67	109.98
20	2	607	CLA	CHA-C4D-ND	2.56	137.84	132.55
22	K	4001	BCR	C36-C18-C17	-2.56	118.67	122.82
20	A	1109	CLA	O2A-CGA-CBA	2.56	119.65	111.83
20	A	1128	CLA	C2C-C1C-NC	2.56	112.67	109.98
20	B	1224	CLA	CHD-C1D-ND	-2.56	121.20	124.80
20	A	1135	CLA	CMA-C3A-C4A	2.56	118.66	111.77
29	2	501	LUT	C22-C23-C24	-2.56	107.38	111.18
20	B	1203	CLA	O2D-CGD-O1D	-2.56	118.86	123.85
20	B	1022	CLA	C2C-C1C-NC	2.56	112.67	109.98
20	A	1107	CLA	CHA-C4D-ND	2.56	137.83	132.55
20	4	606	CLA	C2C-C1C-NC	2.56	112.67	109.98
30	2	615	CHL	C1-C2-C3	-2.56	122.00	126.20
20	B	1223	CLA	O2A-CGA-CBA	2.56	119.63	111.83
20	A	1111	CLA	C1C-C2C-C3C	-2.56	104.29	106.98
20	1	602	CLA	C1C-C2C-C3C	-2.56	104.29	106.98
22	B	4005	BCR	C8-C9-C10	2.56	123.03	119.01
20	B	1218	CLA	CMA-C3A-C4A	2.56	118.64	111.77
20	4	603	CLA	C2D-C1D-ND	2.56	112.66	110.13
20	A	1128	CLA	CHA-C4D-ND	2.56	137.82	132.55
20	1	604	CLA	CHD-C1D-ND	-2.55	121.21	124.80
20	A	1137	CLA	CHA-C4D-ND	2.55	137.82	132.55
22	A	4017	BCR	C36-C18-C17	-2.55	118.68	122.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	3	606	CLA	CAA-C2A-C3A	-2.55	106.10	113.00
20	A	1110	CLA	O2D-CGD-O1D	-2.55	118.88	123.85
20	A	1132	CLA	C4B-CHC-C1C	2.55	132.25	126.25
20	A	1102	CLA	C1C-C2C-C3C	-2.55	104.30	106.98
20	B	1226	CLA	CHA-C4D-ND	2.55	137.81	132.55
20	B	1202	CLA	O2A-C1-C2	2.55	117.92	108.11
20	L	1502	CLA	C2C-C1C-NC	2.55	112.66	109.98
26	F	5003	LMG	O8-C28-C29	2.55	119.61	111.83
20	2	601	CLA	C1C-C2C-C3C	-2.55	104.30	106.98
20	B	1204	CLA	CHA-C4D-ND	2.55	137.81	132.55
20	3	613	CLA	CHA-C4D-ND	2.55	137.81	132.55
20	2	602	CLA	O2A-CGA-CBA	2.55	119.60	111.83
20	A	1104	CLA	CHA-C4D-ND	2.55	137.81	132.55
20	3	603	CLA	C1C-C2C-C3C	-2.55	104.30	106.98
20	H	1701	CLA	C4B-CHC-C1C	2.55	132.23	126.25
20	B	1239	CLA	O2D-CGD-O1D	-2.54	118.89	123.85
20	A	1126	CLA	C2C-C1C-NC	2.54	112.65	109.98
20	B	1225	CLA	CHA-C4D-ND	2.54	137.80	132.55
20	A	1129	CLA	CHD-C1D-ND	-2.54	121.22	124.80
20	K	1401	CLA	C4B-CHC-C1C	2.54	132.23	126.25
29	1	502	LUT	C18-C5-C4	2.54	119.10	114.42
20	3	610	CLA	CMA-C3A-C4A	2.54	118.61	111.77
20	B	1238	CLA	O2D-CGD-O1D	-2.54	118.90	123.85
20	B	1222	CLA	C4B-CHC-C1C	2.54	132.22	126.25
20	3	601	CLA	O1D-CGD-CBD	-2.54	119.51	124.52
20	B	1236	CLA	O2A-CGA-CBA	2.54	119.58	111.83
20	K	1402	CLA	C1D-ND-C4D	-2.54	104.53	106.31
20	H	1701	CLA	C1C-C2C-C3C	-2.54	104.31	106.98
20	2	601	CLA	C3B-C4B-NB	-2.54	108.26	110.53
26	2	804	LMG	C8-O7-C10	-2.54	111.72	117.80
20	B	1203	CLA	CHA-C4D-ND	2.54	137.79	132.55
20	A	1136	CLA	O2A-CGA-CBA	2.54	119.57	111.83
20	3	617	CLA	C2C-C1C-NC	2.54	112.65	109.98
20	A	1108	CLA	O2D-CGD-O1D	-2.54	118.91	123.85
22	1	504	BCR	C4-C5-C6	-2.54	119.28	122.70
20	A	1113	CLA	CAA-CBA-CGA	-2.54	105.72	112.49
20	4	603	CLA	CHA-C4D-ND	2.54	137.78	132.55
20	3	612	CLA	O2A-CGA-CBA	2.54	119.57	111.83
20	2	602	CLA	CHA-C4D-ND	2.54	137.78	132.55
20	A	1130	CLA	O2D-CGD-O1D	-2.54	118.91	123.85
20	J	1901	CLA	C4B-CHC-C1C	2.53	132.21	126.25
20	B	1202	CLA	C4B-CHC-C1C	2.53	132.20	126.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	1	609	CHL	CMA-C3A-C4A	2.53	120.07	114.61
20	2	605	CLA	CHA-C4D-ND	2.53	137.77	132.55
20	B	1216	CLA	O2A-CGA-CBA	2.53	119.55	111.83
20	L	1501	CLA	C4B-CHC-C1C	2.53	132.20	126.25
20	B	1023	CLA	CAA-C2A-C3A	-2.53	106.16	113.00
20	4	601	CLA	C1C-C2C-C3C	-2.53	104.32	106.98
20	3	612	CLA	CHA-C4D-ND	2.53	137.76	132.55
20	3	602	CLA	O2A-CGA-CBA	2.53	119.54	111.83
20	3	606	CLA	O2D-CGD-O1D	-2.53	118.93	123.85
20	L	1503	CLA	C4B-CHC-C1C	2.53	132.19	126.25
20	A	1135	CLA	C3B-C4B-NB	-2.52	108.28	110.53
20	B	1022	CLA	O2D-CGD-O1D	-2.52	118.93	123.85
20	1	604	CLA	CHA-C4D-ND	2.52	137.76	132.55
20	A	1102	CLA	CHD-C1D-ND	-2.52	121.25	124.80
20	3	603	CLA	C4B-CHC-C1C	2.52	132.18	126.25
20	1	603	CLA	CHA-C4D-ND	2.52	137.75	132.55
20	B	1212	CLA	CMA-C3A-C4A	2.52	118.55	111.77
22	L	4020	BCR	C38-C26-C27	2.52	118.97	113.60
20	B	1218	CLA	C1C-C2C-C3C	-2.52	104.33	106.98
22	L	4019	BCR	C35-C13-C14	-2.52	118.73	122.82
20	G	1602	CLA	C4B-CHC-C1C	2.52	132.17	126.25
20	B	1230	CLA	CHA-C4D-ND	2.52	137.75	132.55
20	4	603	CLA	O2D-CGD-O1D	-2.52	118.95	123.85
20	A	1130	CLA	C2C-C1C-NC	2.52	112.63	109.98
20	A	1132	CLA	C2C-C1C-NC	2.52	112.63	109.98
20	3	613	CLA	C1C-C2C-C3C	-2.52	104.33	106.98
24	G	5004	LMT	O5B-C5B-C4B	2.52	114.23	109.70
20	A	1107	CLA	C2C-C1C-NC	2.52	112.62	109.98
20	A	1125	CLA	C4B-CHC-C1C	2.51	132.16	126.25
20	B	1213	CLA	O2D-CGD-O1D	-2.51	118.95	123.85
20	A	1109	CLA	CHA-C4D-ND	2.51	137.73	132.55
20	A	1119	CLA	C2C-C1C-NC	2.51	112.62	109.98
20	2	606	CLA	C4B-CHC-C1C	2.51	132.16	126.25
20	B	1237	CLA	CHA-C4D-ND	2.51	137.73	132.55
20	3	608	CLA	CHA-C4D-ND	2.51	137.73	132.55
20	4	603	CLA	C4B-CHC-C1C	2.51	132.15	126.25
20	B	1219	CLA	CHA-C4D-ND	2.51	137.73	132.55
22	3	503	BCR	C8-C9-C10	2.51	122.96	119.01
30	4	611	CHL	CMA-C3A-C4A	2.51	120.02	114.61
20	2	606	CLA	C2D-C1D-ND	2.51	112.61	110.13
20	3	602	CLA	O2D-CGD-O1D	-2.51	118.96	123.85
20	3	617	CLA	C2D-C1D-ND	2.51	112.61	110.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	1238	CLA	C1C-C2C-C3C	-2.51	104.34	106.98
20	1	601	CLA	C1C-C2C-C3C	-2.51	104.34	106.98
20	B	1209	CLA	CMA-C3A-C4A	2.51	118.51	111.77
20	B	1213	CLA	C2C-C1C-NC	2.51	112.62	109.98
29	1	501	LUT	C35-C15-C14	-2.51	118.39	123.52
20	K	1403	CLA	O2A-CGA-CBA	2.51	119.48	111.83
20	1	607	CLA	CHA-C4D-ND	2.51	137.72	132.55
20	B	1216	CLA	C1C-C2C-C3C	-2.51	104.34	106.98
20	L	1502	CLA	O2D-CGD-O1D	-2.51	118.97	123.85
20	1	603	CLA	O2D-CGD-O1D	-2.51	118.97	123.85
20	A	1141	CLA	C2C-C1C-NC	2.50	112.61	109.98
20	B	1222	CLA	CHA-C4D-ND	2.50	137.72	132.55
20	A	1111	CLA	O1D-CGD-CBD	-2.50	119.58	124.52
20	A	1110	CLA	CHA-C4D-ND	2.50	137.72	132.55
20	4	603	CLA	CMA-C3A-C4A	2.50	118.50	111.77
20	A	1101	CLA	C4B-CHC-C1C	2.50	132.13	126.25
20	1	614	CLA	O1D-CGD-CBD	-2.50	119.58	124.52
20	A	1120	CLA	C3B-C4B-NB	-2.50	108.30	110.53
20	A	1125	CLA	C2D-C1D-ND	2.50	112.60	110.13
20	A	1119	CLA	CHD-C1D-ND	-2.50	121.28	124.80
20	A	1123	CLA	CMA-C3A-C4A	2.50	118.50	111.77
20	B	1211	CLA	CHA-C4D-ND	2.50	137.71	132.55
20	4	606	CLA	C3B-C4B-NB	-2.50	108.30	110.53
20	B	1229	CLA	CHA-C4D-ND	2.50	137.71	132.55
20	4	606	CLA	C1-O2A-CGA	2.50	122.70	116.65
29	2	501	LUT	C30-C31-C32	-2.50	115.96	123.20
20	A	1141	CLA	CHA-C4D-ND	2.50	137.71	132.55
20	A	1120	CLA	CHA-C4D-ND	2.50	137.71	132.55
20	B	1220	CLA	CHA-C4D-ND	2.50	137.71	132.55
29	2	501	LUT	C8-C7-C6	-2.50	120.32	127.00
20	A	1134	CLA	CMA-C3A-C4A	2.50	118.48	111.77
20	A	1126	CLA	CHA-C4D-ND	2.50	137.70	132.55
22	H	4021	BCR	C38-C26-C27	2.50	118.92	113.60
20	A	1117	CLA	O2D-CGD-O1D	-2.50	118.99	123.85
20	1	605	CLA	CHA-C4D-ND	2.50	137.70	132.55
30	2	613	CHL	CMA-C3A-C4A	2.50	119.99	114.61
20	B	1232	CLA	CHD-C1D-ND	-2.50	121.29	124.80
22	A	4011	BCR	C33-C5-C6	-2.49	121.76	124.48
20	B	1216	CLA	C2C-C1C-NC	2.49	112.60	109.98
30	3	607	CHL	C1-C2-C3	-2.49	122.73	126.76
20	A	1141	CLA	C1C-C2C-C3C	-2.49	104.36	106.98
20	A	1129	CLA	CHA-C4D-ND	2.49	137.69	132.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	3	610	CLA	C2C-C1C-NC	2.49	112.60	109.98
22	3	506	BCR	C30-C25-C24	2.49	122.41	115.65
20	B	1213	CLA	C1C-C2C-C3C	-2.49	104.36	106.98
20	B	1236	CLA	CHD-C1D-ND	-2.49	121.30	124.80
20	B	1225	CLA	O2A-CGA-CBA	2.49	119.43	111.83
20	A	1013	CLA	C3B-C4B-NB	-2.49	108.31	110.53
20	3	613	CLA	CMA-C3A-C4A	2.49	118.46	111.77
20	3	606	CLA	C4B-CHC-C1C	2.49	132.10	126.25
20	A	1114	CLA	CHA-C4D-ND	2.49	137.68	132.55
20	G	1602	CLA	C2C-C1C-NC	2.49	112.60	109.98
20	B	1214	CLA	CHA-C4D-ND	2.49	137.68	132.55
20	B	1236	CLA	CHA-C4D-ND	2.49	137.68	132.55
20	A	1126	CLA	C1C-C2C-C3C	-2.49	104.36	106.98
20	A	1136	CLA	O2D-CGD-O1D	-2.49	119.00	123.85
20	A	1101	CLA	CHA-C4D-ND	2.49	137.68	132.55
20	L	1503	CLA	O2D-CGD-O1D	-2.49	119.01	123.85
20	4	617	CLA	C4B-CHC-C1C	2.49	132.09	126.25
20	B	1232	CLA	C2C-C1C-NC	2.49	112.59	109.98
20	A	1140	CLA	CHA-C4D-ND	2.49	137.68	132.55
20	B	1215	CLA	CHA-C4D-ND	2.49	137.68	132.55
20	F	1302	CLA	CHA-C4D-ND	2.49	137.68	132.55
20	K	1401	CLA	CHA-C4D-ND	2.49	137.68	132.55
20	B	1204	CLA	C3B-C4B-NB	-2.49	108.31	110.53
20	4	612	CLA	C4B-CHC-C1C	2.49	132.09	126.25
20	A	1130	CLA	C3B-C4B-NB	-2.48	108.31	110.53
20	3	610	CLA	CHA-C4D-ND	2.48	137.67	132.55
20	3	610	CLA	O2D-CGD-O1D	-2.48	119.01	123.85
20	B	1230	CLA	C3B-C4B-NB	-2.48	108.31	110.53
20	A	1120	CLA	O2A-CGA-CBA	2.48	119.41	111.83
20	A	1121	CLA	C4B-CHC-C1C	2.48	132.09	126.25
30	2	610	CHL	C1-O2A-CGA	2.48	122.66	116.65
20	A	1136	CLA	CMA-C3A-C4A	2.48	118.44	111.77
20	B	1215	CLA	C4B-CHC-C1C	2.48	132.08	126.25
20	B	1217	CLA	CHA-C4D-ND	2.48	137.67	132.55
20	H	1701	CLA	O2A-CGA-CBA	2.48	119.40	111.83
20	A	1140	CLA	C4B-CHC-C1C	2.48	132.08	126.25
20	3	617	CLA	C4B-CHC-C1C	2.48	132.08	126.25
20	A	1123	CLA	CHA-C4D-ND	2.48	137.67	132.55
20	A	1109	CLA	C1-O2A-CGA	2.48	122.65	116.65
20	A	1106	CLA	C4B-CHC-C1C	2.48	132.08	126.25
20	A	1105	CLA	CMA-C3A-C4A	2.48	118.44	111.77
20	B	1209	CLA	CHA-C4D-ND	2.48	137.66	132.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	3	601	CLA	C4B-CHC-C1C	2.48	132.07	126.25
20	L	1501	CLA	O2D-CGD-O1D	-2.48	119.03	123.85
20	K	1402	CLA	CHA-C4D-ND	2.48	137.66	132.55
22	H	4021	BCR	C8-C7-C6	-2.48	120.38	127.00
20	B	1209	CLA	C1C-C2C-C3C	-2.48	104.38	106.98
20	A	1104	CLA	O2D-CGD-O1D	-2.48	119.03	123.85
20	A	1119	CLA	O2A-CGA-CBA	2.47	119.38	111.83
20	B	1232	CLA	CHA-C4D-ND	2.47	137.65	132.55
20	A	1112	CLA	O2A-CGA-CBA	2.47	119.38	111.83
20	B	1224	CLA	CHA-C4D-ND	2.47	137.65	132.55
20	A	1140	CLA	O2D-CGD-O1D	-2.47	119.03	123.85
20	A	1012	CLA	O2D-CGD-O1D	-2.47	119.03	123.85
20	B	1023	CLA	CAC-C3C-C4C	2.47	128.01	124.79
29	4	501	LUT	C35-C15-C14	-2.47	118.46	123.52
20	A	1125	CLA	CHA-C4D-ND	2.47	137.65	132.55
20	2	608	CLA	C4B-CHC-C1C	2.47	132.06	126.25
20	1	605	CLA	CMD-C2D-C3D	-2.47	122.02	127.69
20	A	1124	CLA	CHA-C4D-ND	2.47	137.65	132.55
20	B	1229	CLA	O1D-CGD-CBD	-2.47	119.64	124.52
20	B	1207	CLA	O2D-CGD-O1D	-2.47	119.04	123.85
20	B	1210	CLA	CHA-C4D-ND	2.47	137.65	132.55
20	A	1131	CLA	CHD-C1D-ND	-2.47	121.33	124.80
20	A	1123	CLA	O2D-CGD-O1D	-2.47	119.04	123.85
20	A	1115	CLA	C2C-C1C-NC	2.47	112.58	109.98
20	B	1230	CLA	C1C-C2C-C3C	-2.47	104.38	106.98
20	B	1232	CLA	C1C-C2C-C3C	-2.47	104.38	106.98
20	B	1022	CLA	CHD-C1D-ND	-2.47	121.33	124.80
20	3	602	CLA	C4B-CHC-C1C	2.47	132.05	126.25
20	A	1127	CLA	O2A-CGA-CBA	2.47	119.36	111.83
20	B	1207	CLA	C2C-C1C-NC	2.47	112.57	109.98
20	4	602	CLA	C2C-C1C-NC	2.47	112.57	109.98
20	4	605	CLA	CHA-C1A-NA	-2.47	120.80	126.39
20	B	1234	CLA	C1C-C2C-C3C	-2.47	104.39	106.98
20	A	1137	CLA	C4B-CHC-C1C	2.47	132.05	126.25
20	A	1129	CLA	C3B-C4B-NB	-2.47	108.33	110.53
20	A	1134	CLA	CHA-C4D-ND	2.47	137.64	132.55
22	A	4002	BCR	C38-C26-C27	2.47	118.86	113.60
20	A	1111	CLA	C4B-CHC-C1C	2.47	132.04	126.25
20	A	1102	CLA	CHA-C4D-ND	2.46	137.63	132.55
20	B	1232	CLA	CMA-C3A-C4A	2.46	118.40	111.77
22	B	4004	BCR	C24-C25-C26	-2.46	115.88	121.56
20	B	1205	CLA	CHA-C4D-ND	2.46	137.63	132.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	3	612	CLA	C4B-CHC-C1C	2.46	132.04	126.25
22	2	503	BCR	C36-C18-C17	-2.46	118.83	122.82
20	1	606	CLA	C3B-C4B-NB	-2.46	108.33	110.53
20	A	1105	CLA	CHA-C4D-ND	2.46	137.63	132.55
20	A	1140	CLA	C1-O2A-CGA	2.46	122.61	116.65
20	F	1302	CLA	O2D-CGD-O1D	-2.46	119.05	123.85
20	3	602	CLA	C3B-C4B-NB	-2.46	108.33	110.53
29	4	501	LUT	C22-C23-C24	-2.46	107.53	111.18
20	B	1211	CLA	O2A-CGA-CBA	2.46	119.34	111.83
20	B	1205	CLA	C4B-CHC-C1C	2.46	132.03	126.25
20	B	1215	CLA	C2C-C1C-NC	2.46	112.57	109.98
20	B	1205	CLA	CMA-C3A-C4A	2.46	118.39	111.77
22	I	4018	BCR	C30-C25-C26	-2.46	119.27	122.64
29	1	501	LUT	C7-C8-C9	-2.46	122.60	126.23
20	A	1127	CLA	CHA-C4D-ND	2.46	137.62	132.55
20	A	1112	CLA	CHA-C4D-ND	2.46	137.62	132.55
20	B	1023	CLA	O2D-CGD-O1D	-2.46	119.06	123.85
20	A	1130	CLA	CHA-C4D-ND	2.46	137.62	132.55
20	4	612	CLA	CHA-C4D-ND	2.46	137.62	132.55
20	B	1202	CLA	C1C-C2C-C3C	-2.46	104.40	106.98
20	B	1211	CLA	CMD-C2D-C3D	-2.46	122.06	127.69
20	3	601	CLA	CHA-C4D-ND	2.46	137.62	132.55
20	3	602	CLA	CHA-C4D-ND	2.46	137.62	132.55
20	A	1132	CLA	O2D-CGD-O1D	-2.46	119.07	123.85
20	B	1220	CLA	C2C-C1C-NC	2.46	112.56	109.98
22	A	4008	BCR	C12-C13-C14	-2.46	115.15	119.01
22	F	4016	BCR	C12-C13-C14	-2.46	115.15	119.01
20	B	1021	CLA	O2A-CGA-CBA	2.45	119.32	111.83
20	4	604	CLA	O2D-CGD-O1D	-2.45	119.07	123.85
20	3	614	CLA	C3B-C4B-NB	-2.45	108.34	110.53
20	A	1135	CLA	O2D-CGD-O1D	-2.45	119.07	123.85
20	B	1214	CLA	O2D-CGD-O1D	-2.45	119.07	123.85
29	J	4013	LUT	C8-C7-C6	-2.45	120.44	127.00
20	3	605	CLA	C1D-ND-C4D	-2.45	104.59	106.31
20	4	607	CLA	C3D-C2D-C1D	-2.45	102.48	105.83
20	4	607	CLA	CHA-C4D-ND	2.45	137.61	132.55
20	A	1139	CLA	CHA-C4D-ND	2.45	137.61	132.55
20	A	1121	CLA	C2C-C1C-NC	2.45	112.56	109.98
20	B	1215	CLA	O2D-CGD-O1D	-2.45	119.08	123.85
22	J	4012	BCR	C36-C18-C17	-2.45	118.84	122.82
20	K	1404	CLA	CHA-C4D-ND	2.45	137.60	132.55
20	A	1112	CLA	CMA-C3A-C4A	2.45	118.36	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	1209	CLA	C2C-C1C-NC	2.45	112.56	109.98
20	B	1212	CLA	CHA-C4D-ND	2.45	137.60	132.55
20	3	617	CLA	CHD-C1D-ND	-2.45	121.36	124.80
22	2	503	BCR	C38-C26-C25	-2.45	121.81	124.48
22	G	4011	BCR	C29-C28-C27	2.45	116.66	111.28
20	A	1141	CLA	CHD-C1D-ND	-2.45	121.36	124.80
22	1	503	BCR	C35-C13-C12	2.45	121.83	118.09
20	B	1210	CLA	CMD-C2D-C3D	-2.45	122.08	127.69
28	3	803	DGD	C2G-O2G-C1B	-2.45	111.94	117.80
20	B	1205	CLA	O1D-CGD-CBD	-2.45	119.69	124.52
20	B	1227	CLA	CHA-C4D-ND	2.45	137.59	132.55
20	3	606	CLA	CMD-C2D-C3D	-2.45	122.08	127.69
20	B	1232	CLA	C1-O2A-CGA	2.45	122.57	116.65
20	B	1206	CLA	CHA-C4D-ND	2.45	137.59	132.55
20	B	1214	CLA	CMD-C2D-C3D	-2.44	122.08	127.69
20	B	1222	CLA	C1C-C2C-C3C	-2.44	104.41	106.98
20	A	1110	CLA	C1D-ND-C4D	-2.44	104.60	106.31
20	B	1211	CLA	CHD-C1D-ND	-2.44	121.36	124.80
20	3	601	CLA	C1C-C2C-C3C	-2.44	104.41	106.98
20	B	1232	CLA	C4B-CHC-C1C	2.44	131.99	126.25
20	B	1214	CLA	CMA-C3A-C4A	2.44	118.34	111.77
20	A	1112	CLA	O1D-CGD-CBD	-2.44	119.70	124.52
20	B	1221	CLA	C2C-C1C-NC	2.44	112.55	109.98
20	A	1137	CLA	CHA-C1A-NA	-2.44	120.86	126.39
20	1	602	CLA	C2C-C1C-NC	2.44	112.55	109.98
20	A	1101	CLA	O2A-CGA-CBA	2.44	119.28	111.83
23	4	801	LHG	O8-C23-C24	2.44	119.28	111.83
20	3	601	CLA	CMD-C2D-C3D	-2.44	122.09	127.69
20	B	1228	CLA	CHA-C4D-ND	2.44	137.58	132.55
20	A	1138	CLA	CHA-C4D-ND	2.44	137.58	132.55
20	B	1218	CLA	CHA-C4D-ND	2.44	137.58	132.55
20	B	1240	CLA	C1C-C2C-C3C	-2.44	104.42	106.98
20	G	1601	CLA	C3D-C2D-C1D	-2.44	102.50	105.83
20	K	1403	CLA	CHA-C4D-ND	2.44	137.58	132.55
22	F	4014	BCR	C35-C13-C12	2.44	121.81	118.09
20	1	614	CLA	O2A-CGA-CBA	2.44	119.27	111.83
20	G	1602	CLA	CHD-C1D-ND	-2.44	121.37	124.80
29	1	501	LUT	C39-C29-C28	2.44	121.81	118.09
20	B	1202	CLA	CHA-C4D-ND	2.44	137.57	132.55
20	B	1208	CLA	CHA-C4D-ND	2.44	137.57	132.55
20	L	1502	CLA	CHA-C4D-ND	2.44	137.57	132.55
20	B	1215	CLA	CHD-C1D-ND	-2.44	121.38	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	1	611	CLA	CHA-C4D-ND	2.44	137.57	132.55
20	A	1125	CLA	C3D-C2D-C1D	-2.44	102.51	105.83
20	4	602	CLA	C4B-CHC-C1C	2.43	131.97	126.25
20	A	1137	CLA	C2C-C1C-NC	2.43	112.54	109.98
20	K	1403	CLA	C3B-C4B-NB	-2.43	108.36	110.53
20	2	605	CLA	CMA-C3A-C4A	2.43	118.31	111.77
20	A	1112	CLA	C2C-C1C-NC	2.43	112.54	109.98
20	A	1116	CLA	O1D-CGD-CBD	-2.43	119.72	124.52
20	B	1207	CLA	C2D-C1D-ND	2.43	112.53	110.13
29	3	502	LUT	C35-C15-C14	-2.43	118.54	123.52
20	A	1128	CLA	O1D-CGD-CBD	-2.43	119.72	124.52
20	3	610	CLA	C1D-ND-C4D	-2.43	104.61	106.31
20	4	608	CLA	CHA-C4D-ND	2.43	137.56	132.55
29	3	501	LUT	C27-C28-C29	-2.43	121.09	126.32
26	F	5002	LMG	C8-O7-C10	-2.43	111.98	117.80
20	J	1901	CLA	O2D-CGD-O1D	-2.43	119.12	123.85
20	4	609	CLA	O2D-CGD-O1D	-2.43	119.12	123.85
20	1	601	CLA	CAA-C2A-C3A	-2.43	106.43	113.00
22	B	4010	BCR	C23-C22-C21	-2.43	115.19	119.01
20	F	1301	CLA	CHA-C4D-ND	2.43	137.56	132.55
20	B	1202	CLA	CMD-C2D-C3D	-2.43	122.12	127.69
20	A	1139	CLA	O2A-CGA-CBA	2.43	119.24	111.83
23	B	5002	LHG	O8-C23-C24	2.43	119.24	111.83
20	B	1211	CLA	C3B-C4B-NB	-2.43	108.36	110.53
20	2	612	CLA	CHA-C4D-ND	2.43	137.56	132.55
20	3	601	CLA	C2D-C1D-ND	2.43	112.53	110.13
23	1	801	LHG	O8-C23-C24	2.43	119.24	111.83
20	A	1106	CLA	C2C-C1C-NC	2.43	112.53	109.98
20	1	603	CLA	C2C-C1C-NC	2.43	112.53	109.98
20	B	1204	CLA	CHD-C1D-ND	-2.43	121.39	124.80
20	A	1013	CLA	CHA-C4D-ND	2.43	137.56	132.55
20	A	1125	CLA	C1D-ND-C4D	-2.43	104.61	106.31
26	F	5004	LMG	O8-C28-C29	2.43	119.23	111.83
20	B	1207	CLA	C1C-C2C-C3C	-2.43	104.43	106.98
20	4	603	CLA	C1C-C2C-C3C	-2.43	104.43	106.98
20	3	605	CLA	C4B-CHC-C1C	2.43	131.95	126.25
20	1	601	CLA	C2C-C1C-NC	2.43	112.53	109.98
20	1	607	CLA	O2D-CGD-O1D	-2.43	119.13	123.85
20	4	601	CLA	C2D-C1D-ND	2.42	112.53	110.13
20	A	1135	CLA	O2A-CGA-CBA	2.42	119.23	111.83
20	B	1221	CLA	C1C-C2C-C3C	-2.42	104.43	106.98
20	A	1102	CLA	C1D-ND-C4D	-2.42	104.61	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	2	606	CLA	CHA-C4D-ND	2.42	137.55	132.55
20	4	606	CLA	C1C-C2C-C3C	-2.42	104.43	106.98
20	1	602	CLA	CMA-C3A-C4A	2.42	118.29	111.77
22	B	4004	BCR	C2-C1-C6	2.42	113.96	110.44
28	3	803	DGD	O1G-C1A-C2A	2.42	119.22	111.83
20	B	1218	CLA	O1D-CGD-CBD	-2.42	119.74	124.52
20	3	608	CLA	CAA-C2A-C3A	-2.42	106.45	113.00
22	H	4021	BCR	C23-C24-C25	-2.42	120.53	127.00
20	1	602	CLA	CHA-C4D-ND	2.42	137.54	132.55
20	B	1217	CLA	C2C-C1C-NC	2.42	112.52	109.98
20	A	1131	CLA	O2D-CGD-O1D	-2.42	119.14	123.85
20	B	1216	CLA	CHA-C4D-ND	2.42	137.54	132.55
20	1	601	CLA	C4B-CHC-C1C	2.42	131.93	126.25
20	4	612	CLA	O2A-CGA-CBA	2.42	119.20	111.83
20	1	603	CLA	C4B-CHC-C1C	2.42	131.93	126.25
20	H	1701	CLA	CHA-C4D-ND	2.42	137.53	132.55
20	A	1013	CLA	C11-C10-C8	-2.42	107.93	115.97
20	4	604	CLA	O2A-CGA-CBA	2.42	119.20	111.83
20	B	1226	CLA	CMA-C3A-C4A	2.42	118.27	111.77
20	3	603	CLA	CAC-C3C-C4C	2.42	127.93	124.79
22	3	506	BCR	C38-C26-C25	-2.42	121.85	124.48
20	B	1230	CLA	C2C-C1C-NC	2.42	112.52	109.98
20	4	604	CLA	CHA-C4D-ND	2.41	137.53	132.55
22	B	4006	BCR	C12-C13-C14	-2.41	115.21	119.01
20	F	1301	CLA	O2A-CGA-CBA	2.41	119.20	111.83
20	B	1229	CLA	CHD-C1D-ND	-2.41	121.41	124.80
20	B	1221	CLA	C4B-CHC-C1C	2.41	131.92	126.25
20	A	1141	CLA	O2D-CGD-O1D	-2.41	119.15	123.85
20	K	1403	CLA	O2D-CGD-O1D	-2.41	119.15	123.85
20	3	610	CLA	CHD-C1D-ND	-2.41	121.41	124.80
20	B	1208	CLA	CHD-C1D-ND	-2.41	121.41	124.80
22	1	503	BCR	C19-C18-C17	2.41	122.80	119.01
20	K	1401	CLA	O2D-CGD-O1D	-2.41	119.15	123.85
20	F	1301	CLA	C4B-CHC-C1C	2.41	131.92	126.25
20	2	603	CLA	C2D-C1D-ND	2.41	112.51	110.13
22	A	4007	BCR	C30-C25-C26	-2.41	119.34	122.64
20	B	1234	CLA	CHA-C1A-NA	-2.41	120.93	126.39
20	G	1603	CLA	C3D-C2D-C1D	-2.41	102.54	105.83
20	A	1109	CLA	CMD-C2D-C3D	-2.41	122.16	127.69
20	B	1215	CLA	CMA-C3A-C4A	2.41	118.25	111.77
20	A	1106	CLA	C3B-C4B-NB	-2.41	108.38	110.53
33	4	505	C7Z	C8-C7-C6	-2.41	120.57	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	1239	CLA	O2A-CGA-CBA	2.41	119.17	111.83
20	A	1111	CLA	CHA-C4D-ND	2.41	137.51	132.55
20	A	1119	CLA	CHA-C4D-ND	2.41	137.51	132.55
20	A	1122	CLA	O2A-CGA-CBA	2.41	119.17	111.83
20	1	611	CLA	O2D-CGD-O1D	-2.41	119.17	123.85
20	3	612	CLA	CMD-C2D-C3D	-2.40	122.17	127.69
22	A	4011	BCR	C27-C26-C25	-2.40	119.45	122.70
20	K	1403	CLA	CHD-C1D-ND	-2.40	121.42	124.80
20	L	1502	CLA	C2D-C1D-ND	2.40	112.50	110.13
20	B	1201	CLA	CHA-C4D-ND	2.40	137.51	132.55
20	A	1103	CLA	C2C-C1C-NC	2.40	112.51	109.98
20	A	1120	CLA	CMD-C2D-C3D	-2.40	122.18	127.69
20	1	605	CLA	CHD-C1D-ND	-2.40	121.42	124.80
20	A	1103	CLA	CHA-C4D-ND	2.40	137.50	132.55
20	4	605	CLA	CAA-C2A-C3A	-2.40	106.51	113.00
20	4	604	CLA	C2D-C1D-ND	2.40	112.50	110.13
20	A	1106	CLA	C1D-ND-C4D	-2.40	104.63	106.31
20	A	1115	CLA	O2D-CGD-O1D	-2.40	119.18	123.85
20	1	605	CLA	O2D-CGD-O1D	-2.40	119.18	123.85
20	A	1106	CLA	O1D-CGD-CBD	-2.40	119.78	124.52
20	1	605	CLA	O1D-CGD-CBD	-2.40	119.78	124.52
20	B	1208	CLA	CMD-C2D-C3D	-2.40	122.19	127.69
20	B	1021	CLA	CAA-C2A-C3A	-2.40	106.52	113.00
20	1	606	CLA	CHD-C1D-ND	-2.40	121.43	124.80
30	4	610	CHL	C1-O2A-CGA	2.40	123.75	116.07
20	B	1226	CLA	CMD-C2D-C3D	-2.40	122.19	127.69
20	L	1503	CLA	CHA-C4D-ND	2.40	137.49	132.55
20	B	1235	CLA	C2C-C1C-NC	2.40	112.50	109.98
20	A	1139	CLA	CHA-C1A-NA	-2.40	120.97	126.39
22	A	4007	BCR	C33-C5-C4	2.40	118.70	113.60
20	A	1116	CLA	C1C-C2C-C3C	-2.40	104.46	106.98
20	B	1208	CLA	C2C-C1C-NC	2.39	112.50	109.98
20	B	1206	CLA	O2A-CGA-CBA	2.39	119.14	111.83
22	B	4004	BCR	C33-C5-C6	-2.39	121.87	124.48
20	A	1013	CLA	O2A-CGA-CBA	2.39	119.13	111.83
20	B	1213	CLA	CHA-C4D-ND	2.39	137.49	132.55
20	A	1013	CLA	C6-C7-C8	-2.39	108.01	115.97
20	B	1235	CLA	CHA-C4D-ND	2.39	137.48	132.55
26	B	5003	LMG	C8-O7-C10	-2.39	112.07	117.80
20	A	1117	CLA	CAA-C2A-C3A	-2.39	106.54	113.00
20	4	617	CLA	C2D-C1D-ND	2.39	112.49	110.13
20	A	1106	CLA	CHA-C4D-ND	2.39	137.48	132.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	2	503	BCR	C8-C7-C6	-2.39	120.61	127.00
20	L	1503	CLA	C2D-C1D-ND	2.39	112.49	110.13
20	A	1119	CLA	C1C-C2C-C3C	-2.39	104.47	106.98
20	A	1013	CLA	O2D-CGD-O1D	-2.39	119.20	123.85
20	1	613	CLA	CMA-C3A-C4A	2.39	118.19	111.77
20	B	1210	CLA	C3B-C4B-NB	-2.39	108.40	110.53
20	F	1301	CLA	C1-O2A-CGA	2.39	122.43	116.65
20	B	1211	CLA	O1D-CGD-CBD	-2.39	119.81	124.52
20	2	604	CLA	O2D-CGD-O1D	-2.39	119.20	123.85
20	A	1134	CLA	CHD-C1D-ND	-2.39	121.44	124.80
20	1	608	CLA	C4B-CHC-C1C	2.39	131.86	126.25
20	A	1133	CLA	O1D-CGD-CBD	-2.39	119.81	124.52
20	A	1134	CLA	C2C-C1C-NC	2.38	112.49	109.98
30	2	611	CHL	C1-O2A-CGA	2.38	123.44	116.67
20	1	606	CLA	O2A-CGA-CBA	2.38	119.10	111.83
20	B	1023	CLA	CHA-C4D-ND	2.38	137.47	132.55
20	1	608	CLA	CMD-C2D-C3D	-2.38	122.22	127.69
20	1	604	CLA	CMA-C3A-C4A	2.38	118.18	111.77
20	A	1141	CLA	O1D-CGD-CBD	-2.38	119.82	124.52
20	4	606	CLA	CHA-C4D-ND	2.38	137.46	132.55
20	A	1122	CLA	CHA-C4D-ND	2.38	137.46	132.55
20	B	1206	CLA	O2D-CGD-O1D	-2.38	119.21	123.85
20	A	1111	CLA	C2C-C1C-NC	2.38	112.48	109.98
20	A	1138	CLA	O2D-CGD-O1D	-2.38	119.22	123.85
22	I	4020	BCR	C36-C18-C17	-2.38	118.96	122.82
20	1	611	CLA	O2A-CGA-CBA	2.38	119.09	111.83
20	B	1207	CLA	CHA-C4D-ND	2.38	137.46	132.55
20	2	603	CLA	C1C-C2C-C3C	-2.38	104.48	106.98
20	F	1301	CLA	O2D-CGD-O1D	-2.38	119.22	123.85
20	A	1113	CLA	CHA-C4D-ND	2.38	137.45	132.55
20	B	1208	CLA	C1D-ND-C4D	-2.38	104.64	106.31
20	B	1231	CLA	O2A-CGA-CBA	2.38	119.08	111.83
20	4	608	CLA	O2D-CGD-O1D	-2.38	119.22	123.85
20	A	1132	CLA	CHA-C4D-ND	2.38	137.45	132.55
20	4	617	CLA	CHA-C4D-ND	2.37	137.45	132.55
20	G	1602	CLA	C1D-ND-C4D	-2.37	104.65	106.31
29	4	501	LUT	C15-C35-C34	-2.37	118.66	123.52
20	A	1130	CLA	C4B-CHC-C1C	2.37	131.83	126.25
20	1	601	CLA	CHA-C4D-ND	2.37	137.45	132.55
20	A	1124	CLA	C1C-C2C-C3C	-2.37	104.48	106.98
20	3	614	CLA	C4B-CHC-C1C	2.37	131.83	126.25
20	A	1127	CLA	C3B-C4B-NB	-2.37	108.41	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	1107	CLA	C1-C2-C3	-2.37	122.31	126.20
20	4	608	CLA	C2D-C1D-ND	2.37	112.47	110.13
20	G	1602	CLA	CHA-C4D-ND	2.37	137.44	132.55
20	4	602	CLA	O2D-CGD-O1D	-2.37	119.23	123.85
20	B	1238	CLA	C2C-C1C-NC	2.37	112.47	109.98
22	J	4012	BCR	C23-C24-C25	-2.37	120.66	127.00
20	1	604	CLA	O2D-CGD-O1D	-2.37	119.23	123.85
20	A	1119	CLA	CMD-C2D-C3D	-2.37	122.25	127.69
20	B	1226	CLA	CAA-C2A-C3A	-2.37	106.59	113.00
20	B	1202	CLA	CHD-C1D-ND	-2.37	121.47	124.80
20	A	1115	CLA	CHA-C4D-ND	2.37	137.44	132.55
22	J	4012	BCR	C33-C5-C4	2.37	118.65	113.60
22	A	4011	BCR	C34-C9-C10	-2.37	118.98	122.82
20	A	1110	CLA	CHA-C1A-NA	-2.37	121.03	126.39
20	B	1225	CLA	CHD-C1D-ND	-2.37	121.47	124.80
20	2	612	CLA	CMD-C2D-C3D	-2.37	122.26	127.69
20	B	1234	CLA	O2D-CGD-O1D	-2.37	119.24	123.85
20	A	1111	CLA	C1D-ND-C4D	-2.37	104.65	106.31
20	A	1112	CLA	CHA-C1A-NA	-2.37	121.03	126.39
20	A	1135	CLA	C4B-CHC-C1C	2.37	131.81	126.25
20	2	601	CLA	O2D-CGD-O1D	-2.37	119.24	123.85
20	B	1227	CLA	O2D-CGD-O1D	-2.37	119.24	123.85
20	B	1239	CLA	O1D-CGD-CBD	-2.37	119.85	124.52
20	B	1202	CLA	C2C-C1C-NC	2.36	112.47	109.98
20	2	603	CLA	CHA-C4D-ND	2.36	137.43	132.55
22	B	4009	BCR	C33-C5-C4	2.36	118.64	113.60
28	F	5005	DGD	C1D-O6D-C5D	-2.36	109.10	113.72
20	B	1227	CLA	C3B-C4B-NB	-2.36	108.42	110.53
30	4	615	CHL	C4D-CHA-CBD	-2.36	106.58	108.97
20	B	1021	CLA	C6-C5-C3	-2.36	107.71	113.47
20	3	603	CLA	C3D-C2D-C1D	-2.36	102.61	105.83
20	1	602	CLA	C1D-ND-C4D	-2.36	104.65	106.31
20	G	1601	CLA	C3B-C4B-NB	-2.36	108.42	110.53
20	A	1105	CLA	CHD-C1D-ND	-2.36	121.48	124.80
20	A	1125	CLA	O2A-CGA-CBA	2.36	119.04	111.83
20	B	1220	CLA	C1C-C2C-C3C	-2.36	104.50	106.98
20	B	1237	CLA	O2D-CGD-O1D	-2.36	119.25	123.85
20	A	1118	CLA	CMD-C2D-C3D	-2.36	122.27	127.69
20	A	1115	CLA	CHD-C1D-ND	-2.36	121.48	124.80
20	B	1212	CLA	O1D-CGD-CBD	-2.36	119.86	124.52
20	H	1701	CLA	O2D-CGD-O1D	-2.36	119.25	123.85
20	3	617	CLA	CHA-C4D-ND	2.36	137.42	132.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	1238	CLA	C2D-C1D-ND	2.36	112.46	110.13
20	A	1116	CLA	C3B-C4B-NB	-2.36	108.42	110.53
20	B	1214	CLA	CHD-C1D-ND	-2.36	121.48	124.80
20	B	1221	CLA	CHD-C1D-ND	-2.36	121.48	124.80
20	1	606	CLA	CHA-C4D-ND	2.36	137.42	132.55
20	A	1125	CLA	CHD-C1D-ND	-2.36	121.48	124.80
20	A	1135	CLA	CHA-C1A-NA	-2.36	121.05	126.39
22	K	4002	BCR	C36-C18-C17	-2.36	119.00	122.82
20	A	1117	CLA	CHA-C4D-ND	2.36	137.41	132.55
20	1	603	CLA	CAC-C3C-C4C	2.36	127.86	124.79
22	B	4005	BCR	C19-C18-C17	2.36	122.72	119.01
20	4	608	CLA	O1D-CGD-CBD	-2.36	119.87	124.52
20	A	1109	CLA	CHD-C1D-ND	-2.36	121.49	124.80
20	B	1231	CLA	CHD-C1D-ND	-2.36	121.49	124.80
20	3	610	CLA	O2A-CGA-CBA	2.36	119.02	111.83
20	K	1402	CLA	CHD-C1D-ND	-2.35	121.49	124.80
22	L	4020	BCR	C34-C9-C10	-2.35	119.00	122.82
20	4	605	CLA	CMD-C2D-C3D	-2.35	122.29	127.69
20	A	1130	CLA	CHD-C1D-ND	-2.35	121.49	124.80
20	B	1212	CLA	C4B-CHC-C1C	2.35	131.78	126.25
22	A	4002	BCR	C30-C25-C26	-2.35	119.42	122.64
20	1	614	CLA	C4B-CHC-C1C	2.35	131.78	126.25
20	B	1221	CLA	O2A-CGA-CBA	2.35	119.00	111.83
20	A	1129	CLA	CHA-C1A-NA	-2.35	121.07	126.39
20	A	1116	CLA	O2D-CGD-O1D	-2.35	119.27	123.85
20	1	605	CLA	CBC-CAC-C3C	-2.35	106.05	112.42
20	L	1501	CLA	CHA-C4D-ND	2.35	137.40	132.55
20	4	609	CLA	CHA-C4D-ND	2.35	137.40	132.55
20	3	610	CLA	C4B-CHC-C1C	2.35	131.77	126.25
20	A	1109	CLA	C1-C2-C3	-2.35	122.35	126.20
20	A	1134	CLA	C1C-C2C-C3C	-2.35	104.51	106.98
20	A	1138	CLA	C4B-CHC-C1C	2.35	131.77	126.25
20	A	1133	CLA	C3B-C4B-NB	-2.35	108.43	110.53
21	B	2002	PQN	C16-C15-C13	-2.35	107.75	113.47
20	A	1138	CLA	C1C-C2C-C3C	-2.35	104.51	106.98
22	2	503	BCR	C1-C6-C7	2.35	122.02	115.65
20	1	604	CLA	C4B-CHC-C1C	2.35	131.77	126.25
20	A	1128	CLA	CHD-C1D-ND	-2.35	121.50	124.80
20	B	1226	CLA	CHD-C1D-ND	-2.35	121.50	124.80
20	A	1118	CLA	O1D-CGD-CBD	-2.35	119.89	124.52
20	A	1108	CLA	O2A-CGA-CBA	2.35	118.99	111.83
20	K	1402	CLA	O1D-CGD-CBD	-2.35	119.89	124.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	1234	CLA	C3B-C4B-NB	-2.35	108.44	110.53
20	1	604	CLA	C3B-C4B-NB	-2.35	108.44	110.53
20	3	617	CLA	O2A-CGA-CBA	2.35	118.99	111.83
20	A	1103	CLA	C1-O2A-CGA	2.35	122.33	116.65
20	A	1012	CLA	CHA-C1A-NA	-2.35	121.08	126.39
20	3	601	CLA	C6-C5-C3	-2.34	107.76	113.47
20	A	1108	CLA	C3B-C4B-NB	-2.34	108.44	110.53
30	4	613	CHL	C4D-ND-C1D	2.34	107.00	105.22
20	1	605	CLA	C2C-C1C-NC	2.34	112.44	109.98
20	A	1129	CLA	CMD-C2D-C3D	-2.34	122.31	127.69
22	B	4010	BCR	C28-C27-C26	-2.34	109.88	114.06
20	B	1023	CLA	CHA-C1A-NA	-2.34	121.08	126.39
20	1	601	CLA	O1D-CGD-CBD	-2.34	119.90	124.52
20	A	1121	CLA	C3D-C2D-C1D	-2.34	102.64	105.83
20	A	1133	CLA	O2D-CGD-O1D	-2.34	119.29	123.85
20	K	1402	CLA	CMD-C2D-C3D	-2.34	122.32	127.69
22	K	4002	BCR	C38-C26-C27	2.34	118.59	113.60
20	B	1201	CLA	C4B-CHC-C1C	2.34	131.75	126.25
20	A	1121	CLA	O2A-CGA-CBA	2.34	118.97	111.83
20	2	605	CLA	O1D-CGD-CBD	-2.34	119.90	124.52
20	K	1402	CLA	C2C-C1C-NC	2.34	112.44	109.98
26	2	802	LMG	O7-C10-O9	-2.34	118.24	123.70
20	K	1404	CLA	CMA-C3A-C4A	2.34	118.06	111.77
20	A	1108	CLA	C4B-CHC-C1C	2.34	131.74	126.25
20	B	1204	CLA	C4B-CHC-C1C	2.34	131.74	126.25
22	B	4005	BCR	C36-C18-C17	-2.34	119.03	122.82
28	1	803	DGD	C2G-O2G-C1B	-2.34	112.21	117.80
20	B	1221	CLA	CHA-C1A-NA	-2.34	121.10	126.39
20	A	1104	CLA	CHD-C1D-ND	-2.34	121.52	124.80
22	J	4012	BCR	C38-C26-C25	-2.34	121.94	124.48
20	B	1235	CLA	C4B-CHC-C1C	2.33	131.74	126.25
20	B	1231	CLA	C3B-C4B-NB	-2.33	108.45	110.53
29	2	501	LUT	C39-C29-C28	2.33	121.65	118.09
20	F	1302	CLA	CMA-C3A-C4A	2.33	118.05	111.77
20	A	1141	CLA	CHA-C1A-NA	-2.33	121.11	126.39
20	A	1106	CLA	CHD-C1D-ND	-2.33	121.52	124.80
20	B	1202	CLA	CMA-C3A-C4A	2.33	118.05	111.77
20	B	1023	CLA	C2C-C1C-NC	2.33	112.43	109.98
20	A	1110	CLA	CHD-C1D-ND	-2.33	121.52	124.80
20	A	1122	CLA	C4B-CHC-C1C	2.33	131.73	126.25
26	B	5004	LMG	C1-O6-C5	2.33	118.27	113.72
20	1	606	CLA	CAC-C3C-C4C	2.33	127.82	124.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	1222	CLA	C3B-C4B-NB	-2.33	108.45	110.53
20	4	607	CLA	O2A-CGA-CBA	2.33	118.94	111.83
20	B	1224	CLA	O2D-CGD-O1D	-2.33	119.31	123.85
20	K	1402	CLA	C4B-CHC-C1C	2.33	131.73	126.25
20	A	1118	CLA	CMA-C3A-C4A	2.33	118.03	111.77
28	1	803	DGD	O1G-C1A-C2A	2.33	118.94	111.83
20	A	1108	CLA	CHD-C1D-ND	-2.33	121.53	124.80
20	1	606	CLA	CAA-C2A-C3A	-2.33	106.71	113.00
20	A	1120	CLA	O2D-CGD-O1D	-2.33	119.32	123.85
22	3	503	BCR	C37-C22-C23	2.33	121.64	118.09
30	1	610	CHL	CMA-C3A-C4A	2.33	119.62	114.61
20	F	1302	CLA	C3B-C4B-NB	-2.33	108.45	110.53
20	B	1216	CLA	CAA-C2A-C3A	-2.33	106.72	113.00
20	J	1901	CLA	CMA-C3A-C2A	2.32	122.97	113.98
20	B	1237	CLA	C2D-C1D-ND	2.32	112.43	110.13
20	4	609	CLA	C2D-C1D-ND	2.32	112.43	110.13
20	A	1113	CLA	O2D-CGD-O1D	-2.32	119.32	123.85
22	A	4017	BCR	C27-C26-C25	-2.32	119.56	122.70
20	B	1221	CLA	CMD-C2D-C3D	-2.32	122.36	127.69
20	B	1236	CLA	CHA-C1A-NA	-2.32	121.13	126.39
20	B	1231	CLA	C4B-CHC-C1C	2.32	131.71	126.25
22	3	506	BCR	C36-C18-C17	-2.32	119.06	122.82
20	K	1404	CLA	C4B-CHC-C1C	2.32	131.70	126.25
20	B	1022	CLA	C4B-CHC-C1C	2.32	131.70	126.25
20	B	1210	CLA	CMA-C3A-C4A	2.32	118.00	111.77
20	A	1140	CLA	CHD-C1D-ND	-2.32	121.54	124.80
20	B	1222	CLA	CHD-C1D-ND	-2.32	121.54	124.80
20	B	1240	CLA	CMD-C2D-C3D	-2.32	122.38	127.69
20	J	1901	CLA	O2A-CGA-CBA	2.32	118.90	111.83
20	2	605	CLA	CHA-C1A-NA	-2.32	121.14	126.39
20	L	1501	CLA	C2D-C1D-ND	2.32	112.42	110.13
20	A	1122	CLA	O2D-CGD-O1D	-2.32	119.34	123.85
20	B	1202	CLA	C1D-ND-C4D	-2.32	104.69	106.31
20	B	1219	CLA	O2A-CGA-CBA	2.32	118.90	111.83
20	A	1102	CLA	O1D-CGD-CBD	-2.32	119.95	124.52
20	B	1235	CLA	O1D-CGD-CBD	-2.32	119.95	124.52
20	A	1127	CLA	O2D-CGD-O1D	-2.32	119.34	123.85
20	2	604	CLA	CHA-C4D-ND	2.32	137.33	132.55
28	B	5005	DGD	C2G-O2G-C1B	-2.31	112.26	117.80
20	B	1209	CLA	C4B-CHC-C1C	2.31	131.69	126.25
20	B	1211	CLA	C4B-CHC-C1C	2.31	131.69	126.25
20	A	1114	CLA	CMD-C2D-C3D	-2.31	122.38	127.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	1110	CLA	C2C-C1C-NC	2.31	112.41	109.98
20	K	1403	CLA	C1D-ND-C4D	-2.31	104.69	106.31
23	A	5002	LHG	C5-O7-C7	-2.31	112.26	117.80
20	A	1111	CLA	O2A-C1-C2	2.31	117.00	108.11
20	A	1119	CLA	O2D-CGD-O1D	-2.31	119.35	123.85
20	A	1116	CLA	CMD-C2D-C3D	-2.31	122.39	127.69
20	A	1130	CLA	O2A-CGA-CBA	2.31	118.88	111.83
20	B	1239	CLA	CHD-C1D-ND	-2.31	121.55	124.80
20	B	1230	CLA	C4B-CHC-C1C	2.31	131.68	126.25
20	A	1108	CLA	CMD-C2D-C3D	-2.31	122.39	127.69
22	1	503	BCR	C37-C22-C23	2.31	121.62	118.09
19	A	1011	CL0	C4C-CHD-C1D	2.31	124.33	116.07
20	A	1102	CLA	C2D-C1D-ND	2.31	112.41	110.13
20	4	605	CLA	C3D-C2D-C1D	-2.31	102.68	105.83
20	3	602	CLA	CHD-C1D-ND	-2.31	121.55	124.80
20	4	604	CLA	CHD-C1D-ND	-2.31	121.55	124.80
20	4	609	CLA	O2A-CGA-CBA	2.31	118.87	111.83
20	A	1110	CLA	C1C-C2C-C3C	-2.31	104.55	106.98
20	G	1601	CLA	O2D-CGD-O1D	-2.31	119.36	123.85
20	A	1104	CLA	O2A-CGA-CBA	2.31	118.87	111.83
20	B	1218	CLA	C2C-C1C-NC	2.31	112.41	109.98
26	G	5001	LMG	C8-O7-C10	-2.31	112.27	117.80
20	A	1132	CLA	CMD-C2D-C3D	-2.31	122.40	127.69
20	A	1133	CLA	CHA-C4D-ND	2.31	137.31	132.55
20	A	1124	CLA	C4B-CHC-C1C	2.31	131.67	126.25
20	A	1109	CLA	C2D-C1D-ND	2.31	112.41	110.13
20	4	609	CLA	CMD-C2D-C3D	-2.31	122.40	127.69
20	A	1137	CLA	CHD-C1D-ND	-2.31	121.56	124.80
20	1	606	CLA	C4B-CHC-C1C	2.31	131.67	126.25
30	4	611	CHL	C1-C2-C3	-2.31	123.03	126.76
29	3	501	LUT	C11-C10-C9	-2.31	124.05	127.28
20	B	1210	CLA	CAA-C2A-C3A	-2.31	106.77	113.00
20	A	1104	CLA	CHA-C1A-NA	-2.30	121.17	126.39
20	A	1136	CLA	CHA-C4D-ND	2.30	137.30	132.55
20	A	1103	CLA	C1C-C2C-C3C	-2.30	104.56	106.98
20	G	1603	CLA	C4B-CHC-C1C	2.30	131.66	126.25
20	B	1216	CLA	CHD-C1D-ND	-2.30	121.56	124.80
20	A	1101	CLA	CMD-C2D-C3D	-2.30	122.41	127.69
20	F	1302	CLA	C4B-CHC-C1C	2.30	131.66	126.25
20	2	612	CLA	O2D-CGD-O1D	-2.30	119.37	123.85
31	2	502	XAT	C16-C1-C6	-2.30	103.83	110.05
20	B	1210	CLA	CHD-C1D-ND	-2.30	121.56	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	1238	CLA	CHD-C1D-ND	-2.30	121.56	124.80
20	1	608	CLA	CHD-C1D-ND	-2.30	121.56	124.80
20	1	603	CLA	C1C-C2C-C3C	-2.30	104.56	106.98
20	B	1238	CLA	CHA-C4D-ND	2.30	137.30	132.55
20	A	1111	CLA	C2D-C1D-ND	2.30	112.40	110.13
20	1	614	CLA	CMA-C3A-C4A	2.30	117.96	111.77
20	A	1111	CLA	C6-C7-C8	-2.30	108.31	115.97
20	B	1228	CLA	CHD-C1D-ND	-2.30	121.56	124.80
22	B	4006	BCR	C38-C26-C27	2.30	118.50	113.60
24	B	5006	LMT	O1'-C1'-C2'	2.30	111.77	108.27
20	A	1131	CLA	CMD-C2D-C3D	-2.30	122.41	127.69
20	3	613	CLA	C4B-CHC-C1C	2.30	131.66	126.25
20	A	1110	CLA	CMD-C2D-C3D	-2.30	122.41	127.69
20	B	1226	CLA	CAA-CBA-CGA	-2.30	106.68	113.21
20	3	601	CLA	CMA-C3A-C4A	2.30	117.95	111.77
20	A	1110	CLA	C2D-C1D-ND	2.30	112.40	110.13
20	A	1106	CLA	C1-C2-C3	-2.30	122.43	126.20
31	4	502	XAT	C24-C23-C22	-2.30	106.49	110.79
20	A	1132	CLA	O2A-CGA-CBA	2.30	118.84	111.83
26	B	5004	LMG	C8-O7-C10	-2.30	112.30	117.80
20	1	614	CLA	CMD-C2D-C3D	-2.30	122.42	127.69
20	3	602	CLA	C1D-ND-C4D	-2.30	104.70	106.31
20	A	1113	CLA	CHD-C1D-ND	-2.30	121.57	124.80
20	A	1013	CLA	C2C-C1C-NC	2.30	112.39	109.98
20	4	604	CLA	CMD-C2D-C3D	-2.30	122.42	127.69
20	A	1105	CLA	O2A-CGA-CBA	2.30	118.83	111.83
20	1	601	CLA	C1D-ND-C4D	-2.29	104.70	106.31
20	2	607	CLA	C4B-CHC-C1C	2.29	131.64	126.25
20	2	604	CLA	O2A-CGA-CBA	2.29	118.83	111.83
20	3	613	CLA	CHD-C1D-ND	-2.29	121.57	124.80
20	A	1118	CLA	CHD-C1D-ND	-2.29	121.58	124.80
20	2	603	CLA	CMD-C2D-C3D	-2.29	122.43	127.69
20	4	608	CLA	CMD-C2D-C3D	-2.29	122.43	127.69
20	B	1213	CLA	CHD-C1D-ND	-2.29	121.58	124.80
29	J	4013	LUT	C39-C29-C28	2.29	121.59	118.09
20	A	1136	CLA	CHD-C1D-ND	-2.29	121.58	124.80
23	A	5001	LHG	O7-C7-O9	-2.29	118.35	123.70
20	A	1123	CLA	CHD-C1D-ND	-2.29	121.58	124.80
20	A	1136	CLA	C4B-CHC-C1C	2.29	131.63	126.25
20	A	1138	CLA	C2C-C1C-NC	2.29	112.39	109.98
20	B	1232	CLA	O2D-CGD-O1D	-2.29	119.39	123.85
22	3	506	BCR	C34-C9-C10	-2.29	119.11	122.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	1220	CLA	C4B-CHC-C1C	2.29	131.63	126.25
20	A	1102	CLA	C4B-CHC-C1C	2.29	131.63	126.25
22	L	4019	BCR	C15-C14-C13	-2.29	124.07	127.28
22	K	4002	BCR	C33-C5-C4	2.29	118.48	113.60
20	2	601	CLA	C6-C5-C3	-2.29	107.89	113.47
20	1	602	CLA	C2D-C1D-ND	2.29	112.39	110.13
20	2	602	CLA	CMD-C2D-C3D	-2.29	122.44	127.69
20	3	605	CLA	CMD-C2D-C3D	-2.29	122.44	127.69
20	B	1022	CLA	CHA-C1A-NA	-2.29	121.21	126.39
22	3	506	BCR	C29-C28-C27	2.29	116.31	111.28
20	A	1139	CLA	CMA-C3A-C4A	2.29	117.92	111.77
20	3	617	CLA	O2D-CGD-O1D	-2.29	119.40	123.85
22	1	504	BCR	C34-C9-C10	-2.29	119.11	122.82
26	B	5004	LMG	O6-C5-C6	2.29	112.11	106.44
22	B	4006	BCR	C28-C27-C26	-2.29	109.98	114.06
20	K	1401	CLA	CMD-C2D-C3D	-2.28	122.45	127.69
20	A	1126	CLA	O2A-CGA-CBA	2.28	118.80	111.83
20	B	1225	CLA	C3B-C4B-NB	-2.28	108.49	110.53
20	H	1701	CLA	CMD-C2D-C3D	-2.28	122.45	127.69
20	B	1217	CLA	C1C-C2C-C3C	-2.28	104.58	106.98
22	A	4008	BCR	C37-C22-C23	2.28	121.58	118.09
20	3	608	CLA	O2D-CGD-O1D	-2.28	119.40	123.85
20	A	1125	CLA	CMA-C3A-C4A	2.28	117.91	111.77
20	A	1129	CLA	CAA-C2A-C3A	-2.28	106.83	113.00
20	A	1119	CLA	C7-C6-C5	-2.28	107.18	113.26
20	B	1217	CLA	CHD-C1D-ND	-2.28	121.59	124.80
20	2	604	CLA	CMD-C2D-C3D	-2.28	122.45	127.69
20	1	613	CLA	C2C-C1C-NC	2.28	112.38	109.98
20	B	1205	CLA	CAA-C2A-C3A	-2.28	106.83	113.00
20	B	1216	CLA	O2D-CGD-O1D	-2.28	119.41	123.85
20	B	1021	CLA	CHD-C1D-ND	-2.28	121.59	124.80
20	B	1238	CLA	CMD-C2D-C3D	-2.28	122.46	127.69
20	3	608	CLA	C2D-C1D-ND	2.28	112.38	110.13
20	A	1106	CLA	CAA-C2A-C1A	-2.28	104.50	111.97
20	1	613	CLA	CHA-C1A-NA	-2.28	121.23	126.39
20	K	1401	CLA	C2D-C1D-ND	2.28	112.38	110.13
19	A	1011	CL0	CMC-C2C-C1C	2.28	128.84	124.73
20	B	1021	CLA	C3B-C4B-NB	-2.28	108.50	110.53
20	3	608	CLA	CHA-C1A-NA	-2.28	121.23	126.39
20	2	612	CLA	C1D-ND-C4D	-2.28	104.71	106.31
22	F	4016	BCR	C36-C18-C19	2.28	121.57	118.09
30	2	609	CHL	C1-O2A-CGA	2.28	122.17	116.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	1121	CLA	CMD-C2D-C3D	-2.28	122.47	127.69
20	3	605	CLA	O2D-CGD-O1D	-2.28	119.41	123.85
20	A	1123	CLA	CHA-C1A-NA	-2.28	121.23	126.39
20	B	1236	CLA	O1D-CGD-CBD	-2.28	120.03	124.52
20	A	1124	CLA	C1-O2A-CGA	2.28	122.16	116.65
30	3	607	CHL	CMA-C3A-C4A	2.28	119.52	114.61
20	B	1236	CLA	C2D-C1D-ND	2.28	112.38	110.13
20	B	1212	CLA	O2A-CGA-CBA	2.28	118.78	111.83
20	3	617	CLA	C3D-C2D-C1D	-2.28	102.72	105.83
20	2	605	CLA	O2D-CGD-O1D	-2.28	119.42	123.85
20	4	605	CLA	CHD-C1D-ND	-2.28	121.60	124.80
20	B	1223	CLA	C3D-C2D-C1D	-2.28	102.73	105.83
20	B	1234	CLA	OBD-CAD-C3D	-2.28	123.10	128.42
20	B	1203	CLA	CHD-C1D-ND	-2.27	121.60	124.80
20	4	607	CLA	CHD-C1D-ND	-2.27	121.60	124.80
20	B	1222	CLA	C1D-ND-C4D	-2.27	104.72	106.31
20	A	1132	CLA	C2D-C1D-ND	2.27	112.38	110.13
20	A	1119	CLA	C4B-CHC-C1C	2.27	131.59	126.25
20	2	602	CLA	O2D-CGD-O1D	-2.27	119.42	123.85
20	3	601	CLA	O2A-CGA-CBA	2.27	118.77	111.83
24	G	5005	LMT	C1'-O5'-C5'	-2.27	109.28	113.72
20	A	1123	CLA	C4B-CHC-C1C	2.27	131.59	126.25
20	A	1111	CLA	CHD-C1D-ND	-2.27	121.60	124.80
20	A	1122	CLA	CHD-C1D-ND	-2.27	121.60	124.80
20	3	613	CLA	O2D-CGD-O1D	-2.27	119.43	123.85
20	3	605	CLA	C2C-C1C-NC	2.27	112.37	109.98
20	3	612	CLA	C2D-C1D-ND	2.27	112.37	110.13
20	B	1226	CLA	O1D-CGD-CBD	-2.27	120.04	124.52
20	4	617	CLA	CHD-C1D-ND	-2.27	121.61	124.80
30	4	615	CHL	C4D-ND-C1D	2.27	106.94	105.22
20	2	612	CLA	CBC-CAC-C3C	-2.27	106.27	112.42
20	A	1138	CLA	C2D-C1D-ND	2.27	112.37	110.13
20	3	610	CLA	CMD-C2D-C3D	-2.27	122.49	127.69
20	2	603	CLA	CMC-C2C-C1C	2.27	128.58	125.03
20	1	604	CLA	C6-C5-C3	-2.27	107.94	113.47
20	2	601	CLA	C3D-C2D-C1D	-2.27	102.74	105.83
20	B	1221	CLA	O1D-CGD-CBD	-2.27	120.05	124.52
20	1	613	CLA	C1C-C2C-C3C	-2.27	104.59	106.98
20	1	613	CLA	C4B-CHC-C1C	2.27	131.58	126.25
29	J	4013	LUT	C19-C9-C10	-2.27	119.14	122.82
20	K	1404	CLA	O2D-CGD-O1D	-2.27	119.44	123.85
20	B	1239	CLA	C1-O2A-CGA	2.27	122.14	116.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	4	610	CHL	CMA-C3A-C4A	2.27	119.49	114.61
20	B	1230	CLA	CAA-CBA-CGA	-2.27	106.78	113.21
20	3	601	CLA	C3B-C4B-NB	-2.27	108.51	110.53
20	L	1502	CLA	CHD-C1D-ND	-2.26	121.61	124.80
20	1	607	CLA	OBD-CAD-C3D	-2.26	123.12	128.42
20	A	1105	CLA	C4B-CHC-C1C	2.26	131.57	126.25
20	A	1115	CLA	C3B-C4B-NB	-2.26	108.51	110.53
20	B	1225	CLA	CBC-CAC-C3C	-2.26	106.28	112.42
20	B	1222	CLA	O1D-CGD-CBD	-2.26	120.05	124.52
20	B	1213	CLA	C4B-CHC-C1C	2.26	131.57	126.25
20	B	1220	CLA	O2D-CGD-O1D	-2.26	119.44	123.85
20	A	1103	CLA	CHD-C1D-ND	-2.26	121.62	124.80
20	3	603	CLA	O2D-CGD-O1D	-2.26	119.44	123.85
20	A	1121	CLA	C2D-C1D-ND	2.26	112.36	110.13
20	A	1120	CLA	CHA-C1A-NA	-2.26	121.27	126.39
20	A	1130	CLA	CMA-C3A-C4A	2.26	117.85	111.77
20	1	606	CLA	CMD-C2D-C3D	-2.26	122.50	127.69
20	A	1121	CLA	C1D-ND-C4D	-2.26	104.73	106.31
20	G	1603	CLA	CHA-C4D-ND	2.26	137.21	132.55
20	B	1021	CLA	CHA-C1A-NA	-2.26	121.27	126.39
20	B	1207	CLA	CMD-C2D-C3D	-2.26	122.51	127.69
20	4	612	CLA	O2D-CGD-O1D	-2.26	119.45	123.85
20	A	1117	CLA	C4B-CHC-C1C	2.26	131.56	126.25
20	A	1106	CLA	CMA-C3A-C4A	2.26	117.84	111.77
20	4	605	CLA	C1-C2-C3	-2.26	122.50	126.20
20	A	1120	CLA	C4B-CHC-C1C	2.26	131.56	126.25
22	A	4003	BCR	C39-C30-C25	-2.26	106.70	110.24
20	A	1102	CLA	CMD-C2D-C3D	-2.26	122.51	127.69
28	3	803	DGD	O6D-C5D-C6D	2.26	111.17	106.69
20	3	602	CLA	C2D-C1D-ND	2.26	112.36	110.13
20	4	605	CLA	C4B-CHC-C1C	2.26	131.55	126.25
20	4	608	CLA	CHD-C1D-ND	-2.26	121.63	124.80
20	B	1240	CLA	CMC-C2C-C1C	2.26	128.56	125.03
22	I	4018	BCR	C27-C26-C25	-2.25	119.66	122.70
20	B	1222	CLA	CMA-C3A-C4A	2.25	117.83	111.77
20	A	1123	CLA	O2A-CGA-CBA	2.25	118.71	111.83
20	L	1502	CLA	CMD-C2D-C3D	-2.25	122.52	127.69
22	K	4001	BCR	C23-C22-C21	2.25	122.56	119.01
20	2	606	CLA	CHD-C1D-ND	-2.25	121.63	124.80
20	2	602	CLA	C4B-CHC-C1C	2.25	131.55	126.25
20	A	1119	CLA	CMA-C3A-C4A	2.25	117.83	111.77
20	B	1225	CLA	O2D-CGD-O1D	-2.25	119.47	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	1218	CLA	CMD-C2D-C3D	-2.25	122.53	127.69
21	B	2002	PQN	C2M-C2-C3	-2.25	120.75	124.45
20	B	1234	CLA	C4B-CHC-C1C	2.25	131.54	126.25
20	L	1501	CLA	CMD-C2D-C3D	-2.25	122.53	127.69
20	K	1404	CLA	CHA-C1A-NA	-2.25	121.29	126.39
20	A	1104	CLA	C2D-C1D-ND	2.25	112.35	110.13
20	A	1129	CLA	O2A-CGA-CBA	2.25	118.69	111.83
22	K	4002	BCR	C12-C13-C14	-2.25	115.47	119.01
31	4	502	XAT	C40-C33-C34	-2.25	119.17	122.82
20	A	1131	CLA	O1D-CGD-CBD	-2.25	120.08	124.52
20	B	1237	CLA	C11-C10-C8	-2.25	108.49	115.97
20	3	605	CLA	O1D-CGD-CBD	-2.25	120.08	124.52
20	4	606	CLA	CMA-C3A-C4A	2.25	117.81	111.77
20	A	1101	CLA	C2D-C1D-ND	2.25	112.35	110.13
20	K	1403	CLA	CMD-C2D-C3D	-2.25	122.54	127.69
22	B	4004	BCR	C36-C18-C19	-2.25	114.66	118.09
20	A	1103	CLA	C4B-CHC-C1C	2.25	131.53	126.25
20	2	604	CLA	CHD-C1D-ND	-2.25	121.64	124.80
20	1	602	CLA	C4B-CHC-C1C	2.25	131.53	126.25
20	2	606	CLA	CMD-C2D-C3D	-2.25	122.54	127.69
20	A	1111	CLA	C3D-C2D-C1D	-2.25	102.77	105.83
20	4	602	CLA	CHA-C4D-ND	2.25	137.18	132.55
20	A	1112	CLA	CHD-C1D-ND	-2.25	121.64	124.80
22	G	4011	BCR	C37-C22-C21	-2.24	119.18	122.82
20	B	1225	CLA	C4B-CHC-C1C	2.24	131.53	126.25
20	2	604	CLA	C2D-C1D-ND	2.24	112.35	110.13
20	A	1134	CLA	CMD-C2D-C3D	-2.24	122.54	127.69
20	1	613	CLA	CMD-C2D-C3D	-2.24	122.54	127.69
20	1	611	CLA	CHD-C1D-ND	-2.24	121.64	124.80
20	2	612	CLA	CAA-CBA-CGA	-2.24	106.84	113.21
20	A	1135	CLA	C3D-C2D-C1D	-2.24	102.77	105.83
20	2	607	CLA	C2D-C1D-ND	2.24	112.34	110.13
20	B	1236	CLA	C4B-CHC-C1C	2.24	131.52	126.25
23	4	801	LHG	C5-O7-C7	-2.24	112.43	117.80
20	B	1022	CLA	O2A-CGA-CBA	2.24	118.67	111.83
20	G	1601	CLA	C4B-CHC-C1C	2.24	131.52	126.25
26	F	5003	LMG	C8-O7-C10	-2.24	112.43	117.80
20	B	1214	CLA	CHA-C1A-NA	-2.24	121.32	126.39
20	G	1603	CLA	C11-C10-C8	-2.24	108.52	115.97
20	1	606	CLA	CHA-C1A-NA	-2.24	121.32	126.39
20	A	1107	CLA	CMD-C2D-C3D	-2.24	122.55	127.69
20	B	1222	CLA	C2D-C1D-ND	2.24	112.34	110.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	3	608	CLA	CHD-C1D-ND	-2.24	121.65	124.80
20	4	603	CLA	CMD-C2D-C3D	-2.24	122.56	127.69
20	B	1240	CLA	C3D-C2D-C1D	-2.24	102.78	105.83
20	4	606	CLA	CHA-C1A-NA	-2.24	121.32	126.39
21	A	2001	PQN	C12-C11-C3	-2.24	106.57	112.08
20	B	1204	CLA	C1D-ND-C4D	-2.24	104.74	106.31
20	3	602	CLA	CMD-C2D-C3D	-2.24	122.56	127.69
20	3	610	CLA	C3B-C4B-NB	-2.24	108.53	110.53
20	4	606	CLA	C3D-C2D-C1D	-2.24	102.78	105.83
20	2	605	CLA	C4B-CHC-C1C	2.24	131.50	126.25
20	2	601	CLA	C4B-CHC-C1C	2.24	131.50	126.25
20	B	1214	CLA	C4B-CHC-C1C	2.23	131.50	126.25
20	F	1302	CLA	O2A-CGA-CBA	2.23	118.65	111.83
20	3	612	CLA	O2D-CGD-O1D	-2.23	119.50	123.85
20	A	1141	CLA	C4B-CHC-C1C	2.23	131.50	126.25
20	A	1012	CLA	C6-C5-C3	-2.23	108.03	113.47
20	B	1224	CLA	CMD-C2D-C3D	-2.23	122.57	127.69
20	B	1232	CLA	C2D-C1D-ND	2.23	112.34	110.13
20	B	1207	CLA	O2A-CGA-CBA	2.23	118.64	111.83
20	B	1239	CLA	CMA-C3A-C4A	2.23	117.77	111.77
20	A	1127	CLA	O1D-CGD-CBD	-2.23	120.11	124.52
20	1	602	CLA	O1D-CGD-CBD	-2.23	120.11	124.52
20	A	1108	CLA	CHA-C1A-NA	-2.23	121.34	126.39
20	A	1123	CLA	C1-O2A-CGA	2.23	122.05	116.65
20	B	1204	CLA	CMD-C2D-C3D	-2.23	122.57	127.69
20	A	1129	CLA	C4B-CHC-C1C	2.23	131.50	126.25
20	B	1215	CLA	C3B-C4B-NB	-2.23	108.54	110.53
20	B	1021	CLA	O1D-CGD-CBD	-2.23	120.12	124.52
20	A	1125	CLA	C1C-C2C-C3C	-2.23	104.63	106.98
20	4	601	CLA	CHA-C4D-ND	2.23	137.15	132.55
20	A	1104	CLA	C4B-CHC-C1C	2.23	131.49	126.25
20	B	1222	CLA	O2A-CGA-CBA	2.23	118.63	111.83
20	2	601	CLA	C1-C2-C3	-2.23	122.54	126.20
20	1	607	CLA	C3B-C4B-NB	-2.23	108.54	110.53
20	L	1501	CLA	O2A-CGA-CBA	2.23	118.63	111.83
20	B	1230	CLA	CAA-C2A-C1A	-2.23	104.67	111.97
20	A	1131	CLA	C4B-CHC-C1C	2.23	131.49	126.25
20	1	605	CLA	C4B-CHC-C1C	2.23	131.49	126.25
20	A	1140	CLA	C2D-C1D-ND	2.23	112.33	110.13
20	G	1602	CLA	C2D-C1D-ND	2.23	112.33	110.13
20	B	1215	CLA	CAA-C2A-C3A	-2.23	106.98	113.00
20	A	1107	CLA	C4B-CHC-C1C	2.23	131.48	126.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	J	1901	CLA	CMD-C2D-C3D	-2.23	122.58	127.69
20	B	1021	CLA	C2A-C3A-C4A	2.23	105.46	101.87
20	1	601	CLA	C3B-C4B-NB	-2.22	108.54	110.53
20	A	1120	CLA	CHD-C1D-ND	-2.22	121.67	124.80
20	A	1013	CLA	C11-C12-C13	-2.22	108.57	115.97
30	4	613	CHL	C3D-C4D-ND	-2.22	109.37	112.94
20	3	614	CLA	O2D-CGD-O1D	-2.22	119.52	123.85
20	B	1227	CLA	O2A-CGA-CBA	2.22	118.61	111.83
20	A	1105	CLA	CMD-C2D-C3D	-2.22	122.59	127.69
24	A	5004	LMT	O5B-C5B-C4B	2.22	113.70	109.70
20	H	1701	CLA	C2D-C1D-ND	2.22	112.33	110.13
20	L	1503	CLA	CMD-C2D-C3D	-2.22	122.59	127.69
26	G	5001	LMG	O8-C28-O10	-2.22	118.07	123.63
22	H	4021	BCR	C36-C18-C17	-2.22	119.22	122.82
22	B	4010	BCR	C33-C5-C4	2.22	118.33	113.60
20	A	1115	CLA	C1D-ND-C4D	-2.22	104.75	106.31
20	A	1140	CLA	C1D-ND-C4D	-2.22	104.75	106.31
22	3	503	BCR	C7-C6-C5	-2.22	116.45	121.56
20	2	601	CLA	C2D-C1D-ND	2.22	112.32	110.13
30	2	615	CHL	C3D-C4D-ND	-2.22	109.38	112.94
20	A	1107	CLA	CMA-C3A-C4A	2.22	117.73	111.77
20	A	1119	CLA	O1D-CGD-CBD	-2.22	120.14	124.52
22	B	4004	BCR	C37-C22-C21	-2.22	119.22	122.82
20	3	608	CLA	CMD-C2D-C3D	-2.22	122.61	127.69
20	A	1126	CLA	CHD-C1D-ND	-2.22	121.68	124.80
29	2	501	LUT	C1-C2-C3	-2.22	108.73	113.59
22	K	4002	BCR	C34-C9-C10	-2.22	119.23	122.82
20	B	1235	CLA	CAA-C2A-C3A	-2.22	107.01	113.00
20	B	1223	CLA	CHA-C1A-NA	-2.22	121.37	126.39
22	K	4001	BCR	C33-C5-C4	2.22	118.32	113.60
22	I	4020	BCR	C8-C9-C10	2.21	122.49	119.01
20	4	601	CLA	O2D-CGD-O1D	-2.21	119.54	123.85
20	B	1237	CLA	CHA-C1A-NA	-2.21	121.38	126.39
20	A	1111	CLA	O2A-CGA-CBA	2.21	118.59	111.83
20	A	1138	CLA	O2A-CGA-CBA	2.21	118.59	111.83
20	L	1503	CLA	CHD-C1D-ND	-2.21	121.69	124.80
20	4	603	CLA	CHA-C1A-NA	-2.21	121.39	126.39
20	A	1128	CLA	CMA-C3A-C4A	2.21	117.71	111.77
20	3	603	CLA	CHA-C1A-NA	-2.21	121.39	126.39
20	B	1217	CLA	O1D-CGD-CBD	-2.21	120.16	124.52
20	F	1301	CLA	CHD-C1D-ND	-2.21	121.69	124.80
20	L	1501	CLA	CHD-C1D-ND	-2.21	121.69	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	1230	CLA	CMA-C3A-C4A	2.21	117.71	111.77
20	B	1230	CLA	O1D-CGD-CBD	-2.21	120.16	124.52
20	1	607	CLA	CHA-C1A-NA	-2.21	121.39	126.39
20	B	1240	CLA	CHD-C1D-ND	-2.21	121.69	124.80
20	G	1602	CLA	C3D-C2D-C1D	-2.21	102.82	105.83
20	B	1237	CLA	C4-C3-C5	2.21	119.06	115.23
20	4	609	CLA	CHD-C1D-ND	-2.21	121.70	124.80
29	3	501	LUT	C20-C13-C12	2.20	121.46	118.09
20	B	1238	CLA	O2A-CGA-CBA	2.20	118.56	111.83
20	G	1603	CLA	CAA-C2A-C3A	-2.20	107.04	113.00
20	4	605	CLA	CBC-CAC-C3C	-2.20	106.45	112.42
20	A	1109	CLA	C2C-C1C-NC	2.20	112.30	109.98
20	B	1208	CLA	CAA-C2A-C3A	-2.20	107.05	113.00
20	1	614	CLA	CHD-C1D-ND	-2.20	121.70	124.80
20	B	1218	CLA	CHA-C1A-NA	-2.20	121.40	126.39
20	B	1229	CLA	CHA-C1A-NA	-2.20	121.41	126.39
20	B	1236	CLA	C3D-C2D-C1D	-2.20	102.83	105.83
20	G	1602	CLA	O1D-CGD-CBD	-2.20	120.18	124.52
31	4	502	XAT	O24-C26-C27	-2.20	110.57	116.88
20	B	1227	CLA	CAA-CBA-CGA	-2.20	106.96	113.21
20	4	612	CLA	CHA-C1A-NA	-2.20	121.41	126.39
20	B	1225	CLA	CMD-C2D-C3D	-2.20	122.64	127.69
20	A	1118	CLA	C2D-C1D-ND	2.20	112.30	110.13
20	B	1207	CLA	CHD-C1D-ND	-2.20	121.71	124.80
20	B	1224	CLA	C4B-CHC-C1C	2.20	131.41	126.25
20	A	1106	CLA	C2D-C1D-ND	2.20	112.30	110.13
22	A	4003	BCR	C31-C1-C6	-2.20	106.80	110.24
20	A	1132	CLA	CHD-C1D-ND	-2.20	121.71	124.80
20	B	1021	CLA	C4B-CHC-C1C	2.20	131.41	126.25
20	2	607	CLA	CHA-C1A-NA	-2.20	121.42	126.39
20	K	1404	CLA	CHD-C1D-ND	-2.20	121.71	124.80
20	A	1122	CLA	CMD-C2D-C3D	-2.20	122.65	127.69
20	A	1127	CLA	CMA-C3A-C4A	2.20	117.67	111.77
22	K	4002	BCR	C30-C25-C26	-2.20	119.64	122.64
20	B	1211	CLA	C2C-C1C-NC	2.20	112.29	109.98
20	A	1118	CLA	C3B-C4B-NB	-2.19	108.57	110.53
20	B	1220	CLA	C3B-C4B-NB	-2.19	108.57	110.53
20	B	1227	CLA	C4B-CHC-C1C	2.19	131.41	126.25
20	A	1116	CLA	CHD-C1D-ND	-2.19	121.72	124.80
20	B	1240	CLA	CHA-C1A-NA	-2.19	121.42	126.39
20	B	1221	CLA	C6-C5-C3	-2.19	108.12	113.47
20	B	1203	CLA	C4B-CHC-C1C	2.19	131.41	126.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	1102	CLA	CHA-C1A-NA	-2.19	121.42	126.39
20	A	1013	CLA	CHD-C1D-ND	-2.19	121.72	124.80
20	B	1021	CLA	O2D-CGD-O1D	-2.19	119.58	123.85
20	B	1201	CLA	C2D-C1D-ND	2.19	112.30	110.13
20	B	1229	CLA	C4B-CHC-C1C	2.19	131.40	126.25
20	A	1123	CLA	C3B-C4B-NB	-2.19	108.57	110.53
20	A	1133	CLA	C1-O2A-CGA	2.19	121.95	116.65
20	A	1104	CLA	C3D-C2D-C1D	-2.19	102.84	105.83
30	1	612	CHL	CMD-C2D-C3D	2.19	129.06	124.68
22	B	4004	BCR	C34-C9-C8	-2.19	114.74	118.09
31	4	502	XAT	C18-C5-C6	-2.19	118.70	122.30
20	B	1204	CLA	CMA-C3A-C4A	2.19	117.66	111.77
20	L	1502	CLA	O2A-CGA-CBA	2.19	118.51	111.83
20	A	1136	CLA	O1D-CGD-CBD	-2.19	120.20	124.52
20	4	602	CLA	O2A-CGA-CBA	2.19	118.51	111.83
26	G	5001	LMG	C9-C8-C7	-2.19	106.68	111.78
20	3	610	CLA	C2D-C1D-ND	2.19	112.29	110.13
26	2	803	LMG	C8-O7-C10	-2.19	112.56	117.80
20	1	607	CLA	C4B-CHC-C1C	2.19	131.39	126.25
20	1	608	CLA	C2D-C1D-ND	2.19	112.29	110.13
20	B	1215	CLA	CMD-C2D-C3D	-2.19	122.67	127.69
20	B	1232	CLA	CMD-C2D-C3D	-2.19	122.67	127.69
20	G	1602	CLA	CMD-C2D-C3D	-2.19	122.68	127.69
20	K	1404	CLA	CMD-C2D-C3D	-2.19	122.68	127.69
20	J	1901	CLA	CHD-C1D-ND	-2.19	121.73	124.80
20	A	1112	CLA	C4B-CHC-C1C	2.18	131.38	126.25
20	B	1211	CLA	C1D-ND-C4D	-2.18	104.78	106.31
20	A	1130	CLA	CHA-C1A-NA	-2.18	121.44	126.39
20	B	1240	CLA	C2D-C1D-ND	2.18	112.29	110.13
20	B	1220	CLA	O2A-CGA-CBA	2.18	118.49	111.83
20	A	1140	CLA	C3D-C2D-C1D	-2.18	102.85	105.83
20	B	1220	CLA	C1D-ND-C4D	-2.18	104.78	106.31
20	A	1101	CLA	CHD-C1D-ND	-2.18	121.73	124.80
20	3	605	CLA	C1C-C2C-C3C	-2.18	104.68	106.98
20	1	603	CLA	CHA-C1A-NA	-2.18	121.45	126.39
20	A	1126	CLA	OBD-CAD-C3D	-2.18	123.31	128.42
20	4	606	CLA	C4B-CHC-C1C	2.18	131.38	126.25
20	B	1235	CLA	CMD-C2D-C3D	-2.18	122.69	127.69
20	A	1118	CLA	C1D-ND-C4D	-2.18	104.78	106.31
22	K	4002	BCR	C2-C3-C4	-2.18	106.48	111.28
20	2	605	CLA	CMD-C2D-C3D	-2.18	122.69	127.69
20	3	617	CLA	CHA-C1A-NA	-2.18	121.45	126.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	4	601	CLA	CHD-C1D-ND	-2.18	121.74	124.80
30	4	615	CHL	C4C-CHD-C1D	2.18	123.86	116.07
22	K	4002	BCR	C30-C25-C24	2.18	121.56	115.65
20	2	607	CLA	O1D-CGD-CBD	-2.18	120.22	124.52
20	2	603	CLA	CHD-C1D-ND	-2.18	121.74	124.80
20	3	608	CLA	C3D-C2D-C1D	-2.18	102.86	105.83
20	B	1216	CLA	C4B-CHC-C1C	2.18	131.37	126.25
20	A	1128	CLA	C3B-C4B-NB	-2.18	108.59	110.53
20	K	1401	CLA	CHD-C1D-ND	-2.18	121.74	124.80
20	A	1137	CLA	CMD-C2D-C3D	-2.18	122.70	127.69
20	A	1111	CLA	C3B-C4B-NB	-2.18	108.59	110.53
20	4	612	CLA	CMD-C2D-C3D	-2.18	122.70	127.69
20	A	1139	CLA	C6-C7-C8	-2.17	108.74	115.97
20	B	1205	CLA	CMD-C2D-C3D	-2.17	122.70	127.69
20	A	1103	CLA	CMD-C2D-C3D	-2.17	122.70	127.69
20	1	602	CLA	CHA-C1A-NA	-2.17	121.47	126.39
20	B	1206	CLA	CHD-C1D-ND	-2.17	121.74	124.80
22	A	4002	BCR	C37-C22-C23	2.17	121.41	118.09
22	B	4009	BCR	C37-C22-C23	2.17	121.41	118.09
20	1	601	CLA	CMD-C2D-C3D	-2.17	122.71	127.69
20	A	1105	CLA	O1D-CGD-CBD	-2.17	120.24	124.52
20	B	1223	CLA	O1D-CGD-CBD	-2.17	120.24	124.52
20	3	605	CLA	C2D-C1D-ND	2.17	112.27	110.13
22	A	4017	BCR	C33-C5-C4	2.17	118.22	113.60
20	L	1503	CLA	O2A-CGA-CBA	2.17	118.45	111.83
30	3	611	CHL	CMD-C2D-C3D	2.17	129.02	124.68
31	4	502	XAT	O4-C6-C7	-2.17	110.67	116.88
20	1	602	CLA	O2D-CGD-O1D	-2.17	119.63	123.85
20	B	1218	CLA	C6-C5-C3	-2.17	108.19	113.47
20	3	613	CLA	CBA-CAA-C2A	-2.17	107.34	113.79
20	3	614	CLA	CHD-C1D-ND	-2.17	121.75	124.80
20	A	1104	CLA	CMD-C2D-C3D	-2.17	122.72	127.69
22	1	503	BCR	C29-C28-C27	2.17	116.04	111.28
20	1	608	CLA	C3D-C2D-C1D	-2.17	102.87	105.83
30	4	615	CHL	C3D-C4D-ND	-2.17	109.46	112.94
26	B	5004	LMG	O8-C28-O10	-2.17	118.21	123.63
20	F	1301	CLA	C3B-C4B-NB	-2.17	108.60	110.53
20	B	1231	CLA	CHA-C1A-NA	-2.17	121.49	126.39
20	2	606	CLA	O1D-CGD-CBD	-2.16	120.25	124.52
20	B	1227	CLA	CMA-C3A-C4A	2.16	117.59	111.77
20	4	612	CLA	C2D-C1D-ND	2.16	112.27	110.13
20	A	1140	CLA	CMD-C2D-C3D	-2.16	122.73	127.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	1116	CLA	C4B-CHC-C1C	2.16	131.34	126.25
20	B	1210	CLA	CHA-C1A-NA	-2.16	121.49	126.39
20	B	1202	CLA	O1D-CGD-CBD	-2.16	120.25	124.52
20	A	1140	CLA	C1C-C2C-C3C	-2.16	104.71	106.98
20	2	612	CLA	C4B-CHC-C1C	2.16	131.33	126.25
20	B	1235	CLA	CMA-C3A-C4A	2.16	117.58	111.77
20	2	606	CLA	O2A-CGA-CBA	2.16	118.42	111.83
20	A	1124	CLA	CAA-C2A-C1A	-2.16	104.89	111.97
20	A	1124	CLA	CAC-C3C-C4C	2.16	127.60	124.79
20	A	1114	CLA	CHD-C1D-ND	-2.16	121.76	124.80
20	B	1232	CLA	CHA-C1A-NA	-2.16	121.50	126.39
20	B	1228	CLA	CHA-C1A-NA	-2.16	121.50	126.39
20	4	603	CLA	CHD-C1D-ND	-2.16	121.76	124.80
20	B	1204	CLA	O1D-CGD-CBD	-2.16	120.26	124.52
20	B	1219	CLA	O2D-CGD-O1D	-2.16	119.64	123.85
20	B	1201	CLA	CHD-C1D-ND	-2.16	121.76	124.80
20	B	1206	CLA	CMA-C3A-C4A	2.16	117.58	111.77
20	B	1203	CLA	O2A-CGA-CBA	2.16	118.42	111.83
20	B	1212	CLA	C3B-C4B-NB	-2.16	108.60	110.53
30	1	612	CHL	C4C-CHD-C1D	2.16	123.79	116.07
20	J	1901	CLA	CHA-C1A-NA	-2.16	121.50	126.39
20	K	1402	CLA	CHA-C1A-NA	-2.16	121.50	126.39
20	4	606	CLA	C2D-C1D-ND	2.16	112.26	110.13
20	A	1137	CLA	C3D-C2D-C1D	-2.16	102.89	105.83
20	B	1240	CLA	C1D-ND-C4D	-2.16	104.80	106.31
24	2	808	LMT	C1B-O1B-C4'	-2.16	112.86	117.98
20	A	1128	CLA	CMD-C2D-C3D	-2.16	122.74	127.69
22	J	4012	BCR	C19-C18-C17	2.16	122.40	119.01
20	B	1227	CLA	C6-C5-C3	-2.16	108.22	113.47
24	B	5006	LMT	C3'-C4'-C5'	-2.15	106.16	110.93
20	B	1212	CLA	CHA-C1A-NA	-2.15	121.51	126.39
30	2	609	CHL	CMD-C2D-C3D	2.15	128.99	124.68
20	B	1203	CLA	C1-O2A-CGA	2.15	121.86	116.65
20	A	1125	CLA	O1D-CGD-CBD	-2.15	120.27	124.52
20	K	1403	CLA	C1-O2A-CGA	2.15	121.86	116.65
20	B	1211	CLA	CAA-C2A-C3A	-2.15	107.19	113.00
20	A	1126	CLA	O1D-CGD-CBD	-2.15	120.28	124.52
20	4	612	CLA	CHD-C1D-ND	-2.15	121.78	124.80
20	B	1023	CLA	C4B-CHC-C1C	2.15	131.30	126.25
20	B	1215	CLA	O1D-CGD-CBD	-2.15	120.28	124.52
20	A	1124	CLA	O2A-CGA-CBA	2.15	118.39	111.83
20	1	611	CLA	C4B-CHC-C1C	2.15	131.30	126.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	1136	CLA	CAA-C2A-C3A	-2.15	107.19	113.00
20	A	1114	CLA	CHA-C1A-NA	-2.15	121.52	126.39
26	F	5002	LMG	O7-C10-O9	-2.15	118.68	123.70
30	2	609	CHL	C4D-CHA-CBD	-2.15	106.80	108.97
20	4	603	CLA	C2C-C1C-NC	2.15	112.24	109.98
20	B	1022	CLA	C3D-C2D-C1D	-2.15	102.90	105.83
20	A	1107	CLA	CHD-C1D-ND	-2.15	121.78	124.80
20	A	1130	CLA	O1D-CGD-CBD	-2.15	120.28	124.52
22	F	4016	BCR	C38-C26-C27	2.15	118.18	113.60
22	I	4020	BCR	C37-C22-C21	-2.15	119.34	122.82
20	B	1223	CLA	C4B-CHC-C1C	2.15	131.30	126.25
20	3	614	CLA	CHA-C1A-NA	-2.15	121.53	126.39
20	L	1503	CLA	CHA-C1A-NA	-2.15	121.53	126.39
20	3	601	CLA	C3D-C2D-C1D	-2.15	102.90	105.83
20	3	605	CLA	O2A-CGA-CBA	2.15	118.38	111.83
19	A	1011	CL0	C4C-C3C-C2C	-2.14	104.90	113.37
20	4	606	CLA	CMD-C2D-C3D	-2.14	122.77	127.69
20	A	1117	CLA	C3B-C4B-NB	-2.14	108.62	110.53
20	A	1108	CLA	C3D-C2D-C1D	-2.14	102.91	105.83
20	A	1107	CLA	C3B-C4B-NB	-2.14	108.62	110.53
20	G	1603	CLA	C11-C12-C13	-2.14	108.85	115.97
20	B	1239	CLA	CMD-C2D-C3D	-2.14	122.78	127.69
20	B	1237	CLA	O2A-CGA-CBA	2.14	118.36	111.83
30	2	610	CHL	C4D-CHA-CBD	-2.14	106.81	108.97
20	B	1217	CLA	CAC-C3C-C4C	2.14	127.58	124.79
20	B	1222	CLA	C1-O2A-CGA	2.14	121.83	116.65
20	3	608	CLA	C1D-ND-C4D	-2.14	104.81	106.31
20	3	606	CLA	CHD-C1D-ND	-2.14	121.79	124.80
20	B	1221	CLA	C3D-C2D-C1D	-2.14	102.91	105.83
23	A	5002	LHG	O7-C7-O9	-2.14	118.71	123.70
20	G	1603	CLA	O2A-CGA-CBA	2.14	118.35	111.83
20	B	1022	CLA	C6-C5-C3	-2.14	108.26	113.47
20	A	1102	CLA	C2C-C1C-NC	2.14	112.23	109.98
28	F	5005	DGD	O5D-C1E-C2E	2.14	111.52	108.27
22	3	506	BCR	C23-C22-C21	2.14	122.37	119.01
20	2	603	CLA	O2D-CGD-O1D	-2.14	119.69	123.85
20	B	1230	CLA	CHD-C1D-ND	-2.13	121.80	124.80
20	A	1141	CLA	CMD-C2D-C3D	-2.13	122.80	127.69
20	A	1013	CLA	CHA-C1A-NA	-2.13	121.56	126.39
20	2	604	CLA	O1D-CGD-CBD	-2.13	120.31	124.52
20	A	1123	CLA	CMD-C2D-C3D	-2.13	122.80	127.69
20	F	1301	CLA	CHA-C1A-NA	-2.13	121.56	126.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	4007	BCR	C31-C1-C6	-2.13	106.90	110.24
20	B	1210	CLA	C6-C7-C8	-2.13	108.88	115.97
20	A	1012	CLA	C4B-CHC-C1C	2.13	131.26	126.25
20	B	1222	CLA	C2C-C1C-NC	2.13	112.22	109.98
22	A	4011	BCR	C38-C26-C27	2.13	118.14	113.60
20	B	1230	CLA	C1D-ND-C4D	-2.13	104.82	106.31
20	H	1701	CLA	CHD-C1D-ND	-2.13	121.81	124.80
20	4	601	CLA	O2A-CGA-CBA	2.13	118.32	111.83
20	3	610	CLA	CHA-C1A-NA	-2.13	121.57	126.39
20	B	1235	CLA	C1D-ND-C4D	-2.13	104.82	106.31
20	A	1123	CLA	OBD-CAD-C3D	-2.13	123.45	128.42
20	B	1209	CLA	CHD-C1D-ND	-2.13	121.81	124.80
20	B	1232	CLA	C1D-ND-C4D	-2.13	104.82	106.31
20	B	1232	CLA	O1D-CGD-CBD	-2.12	120.33	124.52
22	L	4019	BCR	C36-C18-C17	-2.12	119.38	122.82
20	A	1117	CLA	CHD-C1D-ND	-2.12	121.81	124.80
20	1	603	CLA	C1D-ND-C4D	-2.12	104.82	106.31
30	1	609	CHL	C4D-CHA-CBD	-2.12	106.83	108.97
20	B	1202	CLA	C2D-C1D-ND	2.12	112.23	110.13
20	B	1237	CLA	CMD-C2D-C3D	-2.12	122.82	127.69
26	G	5002	LMG	O8-C28-O10	-2.12	118.32	123.63
29	3	501	LUT	C19-C9-C8	2.12	121.33	118.09
19	A	1011	CL0	C11-C10-C8	-2.12	108.91	115.97
20	2	602	CLA	CHD-C1D-ND	-2.12	121.82	124.80
22	A	4003	BCR	C34-C9-C10	-2.12	119.38	122.82
20	B	1220	CLA	CHD-C1D-ND	-2.12	121.82	124.80
20	A	1104	CLA	C1D-ND-C4D	-2.12	104.82	106.31
20	B	1203	CLA	C6-C5-C3	-2.12	108.30	113.47
20	A	1118	CLA	C4B-CHC-C1C	2.12	131.23	126.25
20	B	1232	CLA	C3D-C2D-C1D	-2.12	102.94	105.83
20	B	1227	CLA	CHD-C1D-ND	-2.12	121.82	124.80
20	3	612	CLA	CHD-C1D-ND	-2.12	121.82	124.80
20	K	1402	CLA	C2D-C1D-ND	2.12	112.22	110.13
20	B	1206	CLA	C4B-CHC-C1C	2.12	131.23	126.25
20	3	613	CLA	CHA-C1A-NA	-2.12	121.59	126.39
20	A	1115	CLA	C2D-C1D-ND	2.12	112.22	110.13
20	B	1212	CLA	CHD-C1D-ND	-2.12	121.82	124.80
20	A	1125	CLA	C2C-C1C-NC	2.12	112.21	109.98
20	B	1213	CLA	CMD-C2D-C3D	-2.12	122.83	127.69
29	3	501	LUT	C18-C5-C4	2.12	118.32	114.42
20	A	1128	CLA	C6-C5-C3	-2.12	108.31	113.47
20	A	1101	CLA	O1D-CGD-CBD	-2.12	120.34	124.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	J	4013	LUT	C11-C12-C13	-2.12	120.56	126.36
20	B	1217	CLA	CMA-C3A-C4A	2.12	117.46	111.77
20	A	1124	CLA	CHD-C1D-ND	-2.12	121.82	124.80
20	A	1135	CLA	CHD-C1D-ND	-2.12	121.82	124.80
20	B	1203	CLA	C3D-C2D-C1D	-2.12	102.94	105.83
22	A	4008	BCR	C27-C26-C25	-2.12	119.84	122.70
20	A	1101	CLA	CHA-C1A-NA	-2.12	121.60	126.39
20	B	1209	CLA	C1D-ND-C4D	-2.12	104.83	106.31
20	2	608	CLA	C1D-ND-C4D	-2.12	104.83	106.31
20	B	1202	CLA	C1-O2A-CGA	2.11	121.77	116.65
20	A	1112	CLA	C3D-C2D-C1D	-2.11	102.94	105.83
20	A	1127	CLA	C4B-CHC-C1C	2.11	131.22	126.25
20	2	605	CLA	O2A-CGA-CBA	2.11	118.28	111.83
20	A	1013	CLA	C4B-CHC-C1C	2.11	131.22	126.25
20	1	608	CLA	O1D-CGD-CBD	-2.11	120.35	124.52
20	1	608	CLA	CHA-C1A-NA	-2.11	121.61	126.39
20	2	606	CLA	C3D-C2D-C1D	-2.11	102.95	105.83
30	2	611	CHL	C1A-CHA-CBD	-2.11	126.95	132.36
20	1	603	CLA	CHD-C1D-ND	-2.11	121.83	124.80
29	J	4013	LUT	C26-C27-C28	-2.11	121.29	124.58
20	4	609	CLA	CHA-C1A-NA	-2.11	121.61	126.39
20	3	602	CLA	O1D-CGD-CBD	-2.11	120.35	124.52
22	A	4011	BCR	C8-C7-C6	-2.11	121.36	127.00
20	B	1216	CLA	CHA-C1A-NA	-2.11	121.61	126.39
20	A	1128	CLA	CAA-C2A-C3A	-2.11	107.30	113.00
20	A	1115	CLA	O1D-CGD-CBD	-2.11	120.36	124.52
20	A	1132	CLA	O1D-CGD-CBD	-2.11	120.36	124.52
20	A	1127	CLA	CHA-C1A-NA	-2.11	121.61	126.39
20	B	1215	CLA	C1D-ND-C4D	-2.11	104.83	106.31
20	B	1205	CLA	C16-C15-C13	-2.11	108.95	115.97
20	A	1126	CLA	C4B-CHC-C1C	2.11	131.21	126.25
20	A	1119	CLA	C1D-ND-C4D	-2.11	104.83	106.31
20	1	607	CLA	CHD-C1D-ND	-2.11	121.84	124.80
20	2	606	CLA	CHA-C1A-NA	-2.11	121.62	126.39
20	K	1403	CLA	CHA-C1A-NA	-2.11	121.62	126.39
20	B	1225	CLA	CHA-C1A-NA	-2.11	121.62	126.39
20	3	605	CLA	C3D-C2D-C1D	-2.11	102.96	105.83
24	B	5008	LMT	C3B-C4B-C5B	-2.11	106.42	110.23
20	4	601	CLA	CHA-C1A-NA	-2.11	121.62	126.39
20	B	1214	CLA	O1D-CGD-CBD	-2.11	120.37	124.52
30	4	613	CHL	CMD-C2D-C3D	2.10	128.89	124.68
20	3	605	CLA	OBD-CAD-C3D	-2.10	123.50	128.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	1115	CLA	C4B-CHC-C1C	2.10	131.19	126.25
20	B	1239	CLA	CHA-C1A-NA	-2.10	121.63	126.39
20	A	1138	CLA	C1D-ND-C4D	-2.10	104.84	106.31
20	B	1227	CLA	CHA-C1A-NA	-2.10	121.63	126.39
20	F	1302	CLA	CMD-C2D-C3D	-2.10	122.87	127.69
20	B	1239	CLA	C3D-C2D-C1D	-2.10	102.96	105.83
20	2	605	CLA	CHD-C1D-ND	-2.10	121.84	124.80
20	B	1204	CLA	O2A-CGA-CBA	2.10	118.24	111.83
20	A	1139	CLA	C1-O2A-CGA	2.10	121.73	116.65
22	1	504	BCR	C30-C25-C24	2.10	121.35	115.65
20	3	617	CLA	CMD-C2D-C3D	-2.10	122.87	127.69
20	A	1113	CLA	CMA-C3A-C4A	2.10	117.42	111.77
20	B	1219	CLA	C4B-CHC-C1C	2.10	131.19	126.25
20	A	1116	CLA	CHA-C1A-NA	-2.10	121.64	126.39
20	G	1602	CLA	O2D-CGD-O1D	-2.10	119.76	123.85
20	B	1239	CLA	CAA-CBA-CGA	-2.10	107.25	113.21
30	1	610	CHL	C4C-CHD-C1D	2.10	123.58	116.07
20	2	602	CLA	C1D-ND-C4D	-2.10	104.84	106.31
20	B	1229	CLA	C3D-C2D-C1D	-2.10	102.97	105.83
20	4	607	CLA	O1D-CGD-CBD	-2.10	120.38	124.52
20	A	1133	CLA	C4B-CHC-C1C	2.10	131.18	126.25
30	3	611	CHL	C3D-C4D-ND	-2.10	109.58	112.94
22	2	503	BCR	C8-C9-C10	2.10	122.31	119.01
20	A	1126	CLA	C11-C12-C13	-2.09	109.00	115.97
20	A	1125	CLA	CMD-C2D-C3D	-2.09	122.89	127.69
20	A	1113	CLA	C4B-CHC-C1C	2.09	131.17	126.25
20	B	1230	CLA	CMD-C2D-C3D	-2.09	122.89	127.69
20	1	601	CLA	C2D-C1D-ND	2.09	112.20	110.13
20	B	1203	CLA	CMD-C2D-C3D	-2.09	122.89	127.69
30	2	615	CHL	CMD-C2D-C3D	2.09	128.87	124.68
30	3	604	CHL	CMD-C2D-C3D	2.09	128.87	124.68
20	4	606	CLA	O1D-CGD-CBD	-2.09	120.39	124.52
20	A	1134	CLA	CHA-C1A-NA	-2.09	121.65	126.39
20	B	1236	CLA	C1D-ND-C4D	-2.09	104.84	106.31
20	B	1217	CLA	C3D-C2D-C1D	-2.09	102.98	105.83
20	A	1103	CLA	C6-C5-C3	-2.09	108.37	113.47
20	A	1141	CLA	C2D-C1D-ND	2.09	112.20	110.13
20	4	609	CLA	O1D-CGD-CBD	-2.09	120.39	124.52
20	J	1901	CLA	C3D-C2D-C1D	-2.09	102.98	105.83
29	3	501	LUT	C26-C27-C28	-2.09	121.33	124.58
20	B	1227	CLA	CAC-C3C-C4C	2.09	127.51	124.79
20	J	1901	CLA	C2D-C1D-ND	2.09	112.19	110.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	4008	BCR	C8-C7-C6	-2.09	121.42	127.00
20	A	1126	CLA	O2D-CGD-O1D	-2.09	119.78	123.85
20	A	1133	CLA	CHA-C1A-NA	-2.09	121.66	126.39
20	2	608	CLA	CHA-C1A-NA	-2.09	121.66	126.39
20	A	1124	CLA	CMA-C3A-C4A	2.09	117.39	111.77
20	B	1205	CLA	C1D-ND-C4D	-2.09	104.85	106.31
20	B	1205	CLA	CHD-C1D-ND	-2.09	121.86	124.80
20	B	1203	CLA	CHA-C1A-NA	-2.09	121.66	126.39
30	1	609	CHL	C1-C2-C3	-2.09	122.78	126.20
20	B	1204	CLA	C2D-C1D-ND	2.09	112.19	110.13
20	B	1215	CLA	C2D-C1D-ND	2.09	112.19	110.13
20	A	1118	CLA	C3D-C2D-C1D	-2.09	102.98	105.83
20	4	605	CLA	C2D-C1D-ND	2.09	112.19	110.13
20	3	608	CLA	O1D-CGD-CBD	-2.09	120.40	124.52
20	2	601	CLA	O2A-CGA-CBA	2.09	118.20	111.83
20	3	603	CLA	CMB-C2B-C1B	2.09	128.59	125.42
30	2	613	CHL	C4D-CHA-CBD	-2.09	106.86	108.97
26	G	5006	LMG	C7-O1-C1	-2.09	109.33	113.80
20	3	605	CLA	CHA-C1A-NA	-2.08	121.67	126.39
20	B	1219	CLA	C3D-C2D-C1D	-2.08	102.99	105.83
20	B	1219	CLA	CAA-CBA-CGA	-2.08	107.29	113.21
20	B	1237	CLA	C4-C3-C2	-2.08	118.28	123.63
20	A	1124	CLA	O1D-CGD-CBD	-2.08	120.41	124.52
29	1	501	LUT	C38-C25-C24	-2.08	118.43	123.36
20	2	607	CLA	CMD-C2D-C3D	-2.08	122.91	127.69
19	A	1011	CL0	C16-C15-C13	-2.08	109.04	115.97
20	B	1239	CLA	C2D-C1D-ND	2.08	112.19	110.13
20	A	1103	CLA	CMA-C3A-C4A	2.08	117.37	111.77
20	1	611	CLA	C2D-C1D-ND	2.08	112.19	110.13
20	A	1119	CLA	CHA-C1A-NA	-2.08	121.68	126.39
20	A	1110	CLA	CMA-C3A-C4A	2.08	117.37	111.77
20	F	1302	CLA	CHD-C1D-ND	-2.08	121.87	124.80
20	B	1240	CLA	CGD-CBD-CAD	-2.08	104.11	110.85
30	2	610	CHL	CMD-C2D-C3D	2.08	128.84	124.68
20	B	1238	CLA	O1D-CGD-CBD	-2.08	120.41	124.52
29	2	501	LUT	C40-C33-C32	2.08	121.27	118.09
20	B	1213	CLA	C1D-ND-C4D	-2.08	104.85	106.31
26	B	5007	LMG	C8-O7-C10	-2.08	112.82	117.80
20	B	1216	CLA	CMD-C2D-C3D	-2.08	122.92	127.69
20	A	1110	CLA	CBA-CAA-C2A	2.08	119.98	113.79
20	3	603	CLA	CHA-C4D-ND	2.08	136.84	132.55
29	1	501	LUT	C31-C32-C33	-2.08	120.66	126.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	1221	CLA	CMA-C3A-C4A	2.08	117.36	111.77
20	4	601	CLA	CMD-C2D-C3D	-2.08	122.92	127.69
20	A	1121	CLA	CHD-C1D-ND	-2.08	121.88	124.80
20	A	1012	CLA	C2D-C1D-ND	2.08	112.18	110.13
33	4	505	C7Z	C11-C12-C13	-2.08	120.67	126.36
20	A	1113	CLA	CMD-C2D-C3D	-2.08	122.92	127.69
20	4	602	CLA	CHA-C1A-NA	-2.08	121.69	126.39
20	B	1022	CLA	C6-C7-C8	-2.08	109.06	115.97
20	A	1013	CLA	C1D-ND-C4D	-2.08	104.86	106.31
20	A	1111	CLA	CMD-C2D-C3D	-2.08	122.93	127.69
20	4	617	CLA	O1D-CGD-CBD	-2.08	120.42	124.52
20	1	601	CLA	CHA-C1A-NA	-2.08	121.69	126.39
20	A	1102	CLA	O2A-CGA-CBA	2.08	118.16	111.83
20	3	603	CLA	CMA-C3A-C4A	2.08	117.35	111.77
20	B	1202	CLA	CHA-C1A-NA	-2.07	121.69	126.39
20	K	1401	CLA	CHA-C1A-NA	-2.07	121.69	126.39
20	A	1141	CLA	C3D-C2D-C1D	-2.07	103.00	105.83
20	1	605	CLA	C2D-C1D-ND	2.07	112.18	110.13
20	B	1216	CLA	O1D-CGD-CBD	-2.07	120.43	124.52
20	1	603	CLA	CMD-C2D-C3D	-2.07	122.93	127.69
20	H	1701	CLA	CHA-C1A-NA	-2.07	121.70	126.39
28	B	5005	DGD	O1G-C1A-O1A	-2.07	118.44	123.63
20	B	1201	CLA	C3D-C2D-C1D	-2.07	103.00	105.83
30	2	615	CHL	C4D-ND-C1D	2.07	106.79	105.22
30	4	613	CHL	CMA-C3A-C4A	2.07	119.08	114.61
20	3	603	CLA	CMD-C2D-C3D	-2.07	122.94	127.69
20	A	1118	CLA	CHA-C1A-NA	-2.07	121.70	126.39
20	A	1114	CLA	C3D-C2D-C1D	-2.07	103.00	105.83
30	3	607	CHL	CMD-C2D-C3D	2.07	128.82	124.68
20	1	607	CLA	C2D-C1D-ND	2.07	112.17	110.13
20	A	1107	CLA	CHA-C1A-NA	-2.07	121.70	126.39
20	3	602	CLA	C3D-C2D-C1D	-2.07	103.01	105.83
22	B	4005	BCR	C33-C5-C4	2.07	118.01	113.60
20	1	602	CLA	CMD-C2D-C3D	-2.07	122.94	127.69
22	A	4017	BCR	C38-C26-C27	2.07	118.01	113.60
20	B	1203	CLA	C2D-C1D-ND	2.07	112.17	110.13
20	A	1138	CLA	C3D-C2D-C1D	-2.07	103.01	105.83
20	A	1130	CLA	CMD-C2D-C3D	-2.07	122.95	127.69
20	A	1134	CLA	O2A-CGA-CBA	2.07	118.14	111.83
20	B	1217	CLA	CAA-C2A-C3A	-2.07	107.41	113.00
20	1	613	CLA	O2D-CGD-O1D	-2.07	119.82	123.85
20	A	1131	CLA	C3D-C2D-C1D	-2.07	103.01	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	1	611	CLA	C3D-C2D-C1D	-2.07	103.01	105.83
20	B	1023	CLA	C1C-C2C-C3C	-2.07	104.81	106.98
23	1	801	LHG	O7-C7-O9	-2.07	118.87	123.70
20	2	602	CLA	CHA-C1A-NA	-2.07	121.71	126.39
20	B	1229	CLA	CMD-C2D-C3D	-2.07	122.95	127.69
20	1	614	CLA	CHA-C1A-NA	-2.07	121.71	126.39
20	3	601	CLA	O2D-CGD-O1D	-2.07	119.83	123.85
26	3	802	LMG	C8-O7-C10	-2.07	112.85	117.80
26	G	5006	LMG	C9-C8-C7	-2.06	106.97	111.78
26	2	804	LMG	O7-C10-O9	-2.06	118.88	123.70
20	A	1122	CLA	O1D-CGD-CBD	-2.06	120.45	124.52
22	B	4006	BCR	C40-C30-C39	-2.06	102.72	108.63
20	K	1402	CLA	CMC-C2C-C1C	2.06	128.26	125.03
20	F	1301	CLA	C3D-C2D-C1D	-2.06	103.02	105.83
20	A	1113	CLA	CHA-C1A-NA	-2.06	121.72	126.39
20	G	1602	CLA	CHA-C1A-NA	-2.06	121.72	126.39
20	2	606	CLA	O2D-CGD-O1D	-2.06	119.83	123.85
20	A	1106	CLA	CMD-C2D-C3D	-2.06	122.96	127.69
20	A	1122	CLA	CAA-C2A-C3A	-2.06	107.43	113.00
22	J	4012	BCR	C29-C28-C27	2.06	115.81	111.28
20	B	1206	CLA	CHA-C1A-NA	-2.06	121.72	126.39
21	B	2002	PQN	C11-C3-C2	-2.06	121.36	124.89
20	A	1106	CLA	C3D-C2D-C1D	-2.06	103.02	105.83
20	B	1223	CLA	C2D-C1D-ND	2.06	112.17	110.13
28	B	5005	DGD	O2G-C1B-O1B	-2.06	118.89	123.70
20	4	605	CLA	CGD-CBD-CAD	-2.06	104.18	110.85
20	B	1219	CLA	C2D-C1D-ND	2.06	112.16	110.13
20	B	1230	CLA	C2D-C1D-ND	2.06	112.16	110.13
20	A	1103	CLA	C3B-C4B-NB	-2.06	108.69	110.53
20	3	610	CLA	C3D-C2D-C1D	-2.06	103.02	105.83
20	B	1227	CLA	CMD-C2D-C3D	-2.06	122.97	127.69
20	B	1214	CLA	C6-C5-C3	-2.06	108.46	113.47
30	1	612	CHL	C3D-C4D-ND	-2.06	109.64	112.94
20	4	617	CLA	CMD-C2D-C3D	-2.06	122.97	127.69
22	A	4017	BCR	C31-C1-C6	-2.06	107.02	110.24
22	2	503	BCR	C4-C5-C6	-2.06	119.93	122.70
20	B	1204	CLA	C3D-C2D-C1D	-2.06	103.03	105.83
20	B	1235	CLA	C3D-C2D-C1D	-2.06	103.03	105.83
20	A	1106	CLA	O2A-CGA-CBA	2.05	118.10	111.83
20	1	613	CLA	CHD-C1D-ND	-2.05	121.91	124.80
20	B	1022	CLA	C2D-C1D-ND	2.05	112.16	110.13
20	A	1110	CLA	C3D-C2D-C1D	-2.05	103.03	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	1140	CLA	C2C-C1C-NC	2.05	112.14	109.98
23	A	5002	LHG	O8-C23-O10	-2.05	118.49	123.63
20	A	1134	CLA	C4B-CHC-C1C	2.05	131.07	126.25
20	B	1201	CLA	C3B-C4B-NB	-2.05	108.70	110.53
20	4	607	CLA	CHA-C1A-NA	-2.05	121.74	126.39
20	A	1109	CLA	C3D-C2D-C1D	-2.05	103.03	105.83
20	A	1113	CLA	CAC-C3C-C4C	2.05	127.46	124.79
22	B	4005	BCR	C37-C22-C23	2.05	121.22	118.09
20	4	608	CLA	C3D-C2D-C1D	-2.05	103.03	105.83
20	B	1227	CLA	O1D-CGD-CBD	-2.05	120.47	124.52
22	J	4012	BCR	C31-C1-C6	-2.05	107.03	110.24
22	A	4008	BCR	C35-C13-C12	2.05	121.22	118.09
22	A	4008	BCR	C30-C25-C26	-2.05	119.84	122.64
20	2	604	CLA	CHA-C1A-NA	-2.05	121.75	126.39
22	F	4016	BCR	C33-C5-C4	2.05	117.96	113.60
20	3	610	CLA	C6-C5-C3	-2.05	108.48	113.47
20	L	1501	CLA	CHA-C1A-NA	-2.05	121.76	126.39
30	3	607	CHL	C4C-CHD-C1D	2.05	123.39	116.07
31	2	502	XAT	C24-C23-C22	-2.05	106.96	110.79
20	B	1207	CLA	CHA-C1A-NA	-2.05	121.76	126.39
20	A	1139	CLA	C4B-CHC-C1C	2.05	131.06	126.25
20	B	1220	CLA	C2D-C1D-ND	2.04	112.15	110.13
22	A	4002	BCR	C33-C5-C4	2.04	117.95	113.60
20	A	1103	CLA	C1D-ND-C4D	-2.04	104.88	106.31
20	B	1220	CLA	CAA-CBA-CGA	-2.04	107.41	113.21
20	G	1601	CLA	CMD-C2D-C3D	-2.04	123.01	127.69
20	B	1232	CLA	CAA-C2A-C3A	-2.04	107.48	113.00
20	K	1402	CLA	C3D-C2D-C1D	-2.04	103.05	105.83
20	2	603	CLA	C3D-C2D-C1D	-2.04	103.05	105.83
22	A	4008	BCR	C34-C9-C10	-2.04	119.51	122.82
29	3	501	LUT	C38-C25-C24	-2.04	118.53	123.36
20	B	1203	CLA	C1D-ND-C4D	-2.04	104.88	106.31
20	A	1012	CLA	CAA-C2A-C3A	-2.04	107.48	113.00
22	K	4001	BCR	C29-C28-C27	2.04	115.76	111.28
20	1	611	CLA	CHA-C1A-NA	-2.04	121.77	126.39
20	A	1134	CLA	C6-C5-C3	-2.04	108.50	113.47
20	B	1210	CLA	C1C-C2C-C3C	-2.04	104.84	106.98
20	4	608	CLA	CHA-C1A-NA	-2.04	121.78	126.39
20	K	1404	CLA	C2D-C1D-ND	2.04	112.14	110.13
20	L	1502	CLA	CHA-C1A-NA	-2.04	121.78	126.39
20	B	1217	CLA	C4B-CHC-C1C	2.04	131.04	126.25
20	A	1121	CLA	OBD-CAD-C3D	-2.04	123.66	128.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	3	611	CHL	C1-O2A-CGA	2.04	122.59	116.07
20	A	1114	CLA	C1D-ND-C4D	-2.04	104.88	106.31
22	B	4010	BCR	C34-C9-C8	2.04	121.20	118.09
20	L	1503	CLA	C3D-C2D-C1D	-2.04	103.05	105.83
22	J	4012	BCR	C2-C1-C6	2.04	113.40	110.44
20	4	607	CLA	C1C-C2C-C3C	-2.03	104.84	106.98
20	A	1140	CLA	O1D-CGD-CBD	-2.03	120.50	124.52
20	A	1131	CLA	CHA-C1A-NA	-2.03	121.78	126.39
22	3	506	BCR	C24-C25-C26	-2.03	116.87	121.56
20	A	1013	CLA	C2D-C1D-ND	2.03	112.14	110.13
20	1	601	CLA	O2D-CGD-O1D	-2.03	119.89	123.85
20	B	1202	CLA	C3D-C2D-C1D	-2.03	103.06	105.83
30	4	611	CHL	CMD-C2D-C3D	2.03	128.75	124.68
20	B	1207	CLA	C3D-C2D-C1D	-2.03	103.06	105.83
20	3	610	CLA	O1D-CGD-CBD	-2.03	120.51	124.52
20	4	604	CLA	CHA-C1A-NA	-2.03	121.79	126.39
29	3	501	LUT	C30-C31-C32	-2.03	117.31	123.20
20	B	1213	CLA	CHA-C1A-NA	-2.03	121.79	126.39
20	B	1229	CLA	C2D-C1D-ND	2.03	112.14	110.13
20	1	601	CLA	C6-C5-C3	-2.03	108.52	113.47
20	2	601	CLA	CHA-C1A-NA	-2.03	121.80	126.39
20	1	614	CLA	C1D-ND-C4D	-2.03	104.89	106.31
19	A	1011	CL0	C1-O2A-CGA	2.03	121.56	116.65
26	B	5003	LMG	O7-C10-O9	-2.03	118.96	123.70
20	B	1225	CLA	C3D-C2D-C1D	-2.03	103.06	105.83
20	3	605	CLA	CAA-C2A-C3A	-2.03	107.52	113.00
20	4	603	CLA	O2A-CGA-CBA	2.03	118.02	111.83
20	A	1139	CLA	O2D-CGD-O1D	-2.03	119.90	123.85
20	1	608	CLA	C1D-ND-C4D	-2.03	104.89	106.31
20	B	1226	CLA	C4B-CHC-C1C	2.03	131.02	126.25
20	A	1109	CLA	C11-C10-C8	-2.03	109.22	115.97
23	3	801	LHG	C23-O8-C6	2.03	120.50	112.37
20	B	1236	CLA	CMD-C2D-C3D	-2.03	123.04	127.69
20	B	1219	CLA	CHD-C1D-ND	-2.03	121.95	124.80
20	A	1125	CLA	CHA-C1A-NA	-2.03	121.80	126.39
20	B	1222	CLA	C3D-C2D-C1D	-2.03	103.07	105.83
20	B	1222	CLA	CMD-C2D-C3D	-2.03	123.04	127.69
29	2	501	LUT	C38-C25-C24	-2.03	118.57	123.36
20	B	1022	CLA	CMD-C2D-C3D	-2.03	123.04	127.69
20	A	1107	CLA	C1D-ND-C4D	-2.03	104.89	106.31
20	4	605	CLA	O2A-CGA-CBA	2.03	118.01	111.83
21	A	2001	PQN	C21-C20-C18	-2.02	109.23	115.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	1201	CLA	CMA-C3A-C4A	2.02	117.22	111.77
20	B	1228	CLA	O2A-CGA-CBA	2.02	118.01	111.83
20	B	1228	CLA	CMD-C2D-C3D	-2.02	123.05	127.69
20	B	1212	CLA	C1-O2A-CGA	2.02	121.55	116.65
20	B	1225	CLA	O1D-CGD-CBD	-2.02	120.53	124.52
20	B	1229	CLA	C6-C7-C8	-2.02	109.24	115.97
20	A	1128	CLA	C4B-CHC-C1C	2.02	131.00	126.25
22	F	4016	BCR	C31-C1-C6	-2.02	107.07	110.24
23	2	801	LHG	O7-C7-O9	-2.02	118.98	123.70
23	2	801	LHG	C5-O7-C7	-2.02	112.96	117.80
22	F	4014	BCR	C33-C5-C4	2.02	117.91	113.60
20	L	1503	CLA	O1D-CGD-CBD	-2.02	120.53	124.52
20	2	607	CLA	C3D-C2D-C1D	-2.02	103.07	105.83
26	F	5004	LMG	O7-C10-O9	-2.02	118.98	123.70
22	L	4020	BCR	C8-C7-C6	-2.02	121.60	127.00
20	A	1140	CLA	CHA-C1A-NA	-2.02	121.82	126.39
20	A	1103	CLA	O1D-CGD-CBD	-2.02	120.53	124.52
29	1	501	LUT	C18-C5-C4	2.02	118.13	114.42
20	B	1201	CLA	O2A-CGA-CBA	2.02	117.99	111.83
20	B	1211	CLA	CMA-C3A-C4A	2.02	117.20	111.77
20	1	602	CLA	CHD-C1D-ND	-2.02	121.96	124.80
20	B	1225	CLA	CMA-C3A-C4A	2.02	117.19	111.77
20	A	1102	CLA	C3D-C2D-C1D	-2.02	103.08	105.83
20	A	1107	CLA	C2D-C1D-ND	2.01	112.12	110.13
22	I	4018	BCR	C35-C13-C14	-2.01	119.55	122.82
20	L	1502	CLA	C3D-C2D-C1D	-2.01	103.08	105.83
22	I	4018	BCR	C38-C26-C27	2.01	117.89	113.60
20	B	1213	CLA	C2D-C1D-ND	2.01	112.12	110.13
20	A	1139	CLA	C11-C10-C8	-2.01	109.27	115.97
20	B	1211	CLA	CHA-C1A-NA	-2.01	121.83	126.39
26	G	5002	LMG	O7-C10-O9	-2.01	119.00	123.70
20	A	1114	CLA	C2D-C1D-ND	2.01	112.12	110.13
26	G	5001	LMG	O7-C10-O9	-2.01	119.00	123.70
20	B	1206	CLA	C2D-C1D-ND	2.01	112.11	110.13
22	3	503	BCR	C35-C13-C12	2.01	121.16	118.09
20	4	604	CLA	O1D-CGD-CBD	-2.01	120.56	124.52
20	L	1502	CLA	O1D-CGD-CBD	-2.01	120.56	124.52
26	F	5003	LMG	O7-C10-O9	-2.01	119.01	123.70
20	A	1115	CLA	CMD-C2D-C3D	-2.01	123.08	127.69
20	A	1120	CLA	O1D-CGD-CBD	-2.01	120.56	124.52
20	3	613	CLA	O1D-CGD-CBD	-2.01	120.56	124.52
20	F	1301	CLA	C2D-C1D-ND	2.01	112.11	110.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	I	4018	BCR	C8-C7-C6	-2.01	121.64	127.00
20	1	606	CLA	C3D-C2D-C1D	-2.01	103.09	105.83
20	1	611	CLA	C3B-C4B-NB	-2.01	108.74	110.53
20	B	1209	CLA	CMD-C2D-C3D	-2.01	123.09	127.69
29	2	501	LUT	C31-C32-C33	-2.01	120.86	126.36
20	B	1206	CLA	C6-C7-C8	-2.00	109.30	115.97
30	3	611	CHL	C1C-C2C-CMC	2.00	130.41	126.80
20	B	1224	CLA	CAA-C2A-C3A	-2.00	107.58	113.00
20	2	602	CLA	C2D-C1D-ND	2.00	112.11	110.13
28	4	802	DGD	O3G-C1D-C2D	2.00	111.31	108.27
30	1	609	CHL	C4C-CHD-C1D	2.00	123.23	116.07
20	1	607	CLA	C1D-ND-C4D	-2.00	104.91	106.31
20	B	1206	CLA	C3B-C4B-NB	-2.00	108.74	110.53
20	A	1133	CLA	C2D-C1D-ND	2.00	112.11	110.13
20	A	1128	CLA	CHA-C1A-NA	-2.00	121.86	126.39
28	F	5005	DGD	O2G-C1B-O1B	-2.00	119.03	123.70
20	A	1123	CLA	C3D-C2D-C1D	-2.00	103.10	105.83
20	4	602	CLA	C3D-C2D-C1D	-2.00	103.10	105.83
20	A	1129	CLA	O1D-CGD-CBD	-2.00	120.57	124.52
22	G	4011	BCR	C35-C13-C14	-2.00	119.58	122.82
20	1	604	CLA	CHA-C1A-NA	-2.00	121.86	126.39

All (201) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
19	A	1011	CL0	NA
19	A	1011	CL0	ND
19	A	1011	CL0	NC
20	A	1101	CLA	ND
20	A	1102	CLA	ND
20	A	1103	CLA	ND
20	A	1104	CLA	ND
20	A	1105	CLA	ND
20	A	1106	CLA	ND
20	A	1107	CLA	ND
20	A	1108	CLA	ND
20	A	1109	CLA	ND
20	A	1110	CLA	ND
20	A	1111	CLA	ND
20	A	1112	CLA	ND
20	A	1113	CLA	ND
20	A	1114	CLA	ND

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Mol	Chain	Res	Type	Atom
20	A	1115	CLA	ND
20	A	1116	CLA	ND
20	A	1117	CLA	ND
20	A	1118	CLA	ND
20	A	1119	CLA	ND
20	A	1120	CLA	ND
20	A	1121	CLA	ND
20	A	1122	CLA	ND
20	A	1123	CLA	ND
20	A	1124	CLA	ND
20	A	1125	CLA	ND
20	A	1126	CLA	ND
20	A	1127	CLA	ND
20	A	1128	CLA	ND
20	A	1129	CLA	ND
20	A	1130	CLA	ND
20	A	1131	CLA	ND
20	A	1132	CLA	ND
20	A	1133	CLA	ND
20	A	1134	CLA	ND
20	A	1135	CLA	ND
20	A	1136	CLA	ND
20	A	1137	CLA	ND
20	A	1140	CLA	ND
20	A	1141	CLA	ND
20	A	1012	CLA	ND
20	A	1013	CLA	ND
20	A	1138	CLA	ND
20	A	1139	CLA	ND
20	B	1022	CLA	ND
20	B	1023	CLA	ND
20	B	1237	CLA	ND
20	B	1021	CLA	ND
20	B	1201	CLA	ND
20	B	1202	CLA	ND
20	B	1203	CLA	ND
20	B	1204	CLA	ND
20	B	1205	CLA	ND
20	B	1206	CLA	ND
20	B	1208	CLA	ND
20	B	1209	CLA	ND
20	B	1210	CLA	ND

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Mol	Chain	Res	Type	Atom
20	B	1211	CLA	ND
20	B	1212	CLA	ND
20	B	1213	CLA	ND
20	B	1214	CLA	ND
20	B	1215	CLA	ND
20	B	1216	CLA	ND
20	B	1217	CLA	ND
20	B	1219	CLA	ND
20	B	1220	CLA	ND
20	B	1221	CLA	ND
20	B	1222	CLA	ND
20	B	1223	CLA	ND
20	B	1224	CLA	ND
20	B	1225	CLA	ND
20	B	1226	CLA	ND
20	B	1227	CLA	ND
20	B	1228	CLA	ND
20	B	1229	CLA	ND
20	B	1230	CLA	ND
20	B	1231	CLA	ND
20	B	1232	CLA	ND
20	B	1234	CLA	ND
20	B	1235	CLA	ND
20	B	1236	CLA	ND
20	B	1238	CLA	ND
20	B	1239	CLA	ND
20	B	1207	CLA	ND
20	B	1218	CLA	ND
20	B	1240	CLA	ND
20	F	1302	CLA	ND
20	F	1301	CLA	ND
20	G	1601	CLA	ND
20	G	1602	CLA	ND
20	G	1603	CLA	ND
20	H	1701	CLA	ND
20	J	1901	CLA	ND
20	K	1401	CLA	ND
20	K	1402	CLA	ND
20	K	1403	CLA	ND
20	K	1404	CLA	ND
20	L	1501	CLA	ND
20	L	1502	CLA	ND

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Mol	Chain	Res	Type	Atom
20	L	1503	CLA	ND
20	1	601	CLA	ND
20	1	602	CLA	ND
20	1	603	CLA	ND
20	1	604	CLA	ND
20	1	605	CLA	ND
20	1	606	CLA	ND
20	1	607	CLA	ND
20	1	608	CLA	ND
20	1	611	CLA	ND
20	1	613	CLA	ND
20	1	614	CLA	ND
20	2	601	CLA	ND
20	2	602	CLA	ND
20	2	603	CLA	ND
20	2	604	CLA	ND
20	2	605	CLA	ND
20	2	606	CLA	ND
20	2	607	CLA	ND
20	2	608	CLA	ND
20	2	612	CLA	ND
20	3	601	CLA	ND
20	3	602	CLA	ND
20	3	603	CLA	ND
20	3	605	CLA	ND
20	3	606	CLA	ND
20	3	608	CLA	ND
20	3	610	CLA	ND
20	3	612	CLA	ND
20	3	613	CLA	ND
20	3	614	CLA	ND
20	3	617	CLA	ND
20	4	609	CLA	ND
20	4	601	CLA	ND
20	4	602	CLA	ND
20	4	603	CLA	ND
20	4	604	CLA	ND
20	4	606	CLA	ND
20	4	607	CLA	ND
20	4	608	CLA	ND
20	4	612	CLA	ND
20	4	617	CLA	ND

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Mol	Chain	Res	Type	Atom
29	2	501	LUT	C26
29	3	502	LUT	C26
30	1	610	CHL	NA
30	1	610	CHL	ND
30	1	610	CHL	NC
30	1	612	CHL	NA
30	1	612	CHL	ND
30	1	612	CHL	NC
30	1	612	CHL	C8
30	1	609	CHL	NA
30	1	609	CHL	ND
30	1	609	CHL	NC
30	1	609	CHL	C8
30	2	610	CHL	NA
30	2	610	CHL	ND
30	2	610	CHL	NC
30	2	610	CHL	C8
30	2	611	CHL	NA
30	2	611	CHL	ND
30	2	611	CHL	NC
30	2	613	CHL	NA
30	2	613	CHL	ND
30	2	613	CHL	NC
30	2	615	CHL	NA
30	2	615	CHL	ND
30	2	615	CHL	NC
30	2	615	CHL	C8
30	2	609	CHL	NA
30	2	609	CHL	ND
30	2	609	CHL	NC
30	2	609	CHL	C8
30	3	604	CHL	NA
30	3	604	CHL	ND
30	3	604	CHL	NC
30	3	604	CHL	C8
30	3	607	CHL	NA
30	3	607	CHL	ND
30	3	607	CHL	NC
30	3	611	CHL	NA
30	3	611	CHL	ND
30	3	611	CHL	NC
30	4	610	CHL	NA

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Mol	Chain	Res	Type	Atom
30	4	610	CHL	ND
30	4	610	CHL	NC
30	4	611	CHL	NA
30	4	611	CHL	ND
30	4	611	CHL	NC
30	4	613	CHL	NA
30	4	613	CHL	ND
30	4	613	CHL	NC
30	4	613	CHL	C8
30	4	615	CHL	NA
30	4	615	CHL	ND
30	4	615	CHL	NC
31	2	502	XAT	C5
31	2	502	XAT	C26
31	4	502	XAT	C6
31	4	502	XAT	C26

All (2850) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
20	A	1101	CLA	C2-C1-O2A-CGA
20	A	1102	CLA	C3A-C2A-CAA-CBA
20	A	1102	CLA	CHA-CBD-CGD-O1D
20	A	1102	CLA	CHA-CBD-CGD-O2D
20	A	1103	CLA	C1A-C2A-CAA-CBA
20	A	1103	CLA	C3A-C2A-CAA-CBA
20	A	1103	CLA	CAD-CBD-CGD-O1D
20	A	1103	CLA	CAD-CBD-CGD-O2D
20	A	1105	CLA	C1A-C2A-CAA-CBA
20	A	1105	CLA	C2-C1-O2A-CGA
20	A	1106	CLA	C3A-C2A-CAA-CBA
20	A	1106	CLA	CHA-CBD-CGD-O1D
20	A	1106	CLA	CHA-CBD-CGD-O2D
20	A	1107	CLA	C1A-C2A-CAA-CBA
20	A	1107	CLA	CBD-CGD-O2D-CED
20	A	1109	CLA	C1A-C2A-CAA-CBA
20	A	1109	CLA	C3A-C2A-CAA-CBA
20	A	1110	CLA	C1A-C2A-CAA-CBA
20	A	1112	CLA	C2-C1-O2A-CGA
20	A	1113	CLA	C1A-C2A-CAA-CBA
20	A	1113	CLA	C3A-C2A-CAA-CBA
20	A	1114	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
20	A	1114	CLA	CHA-CBD-CGD-O1D
20	A	1114	CLA	CHA-CBD-CGD-O2D
20	A	1115	CLA	CBD-CGD-O2D-CED
20	A	1116	CLA	C1A-C2A-CAA-CBA
20	A	1116	CLA	C3A-C2A-CAA-CBA
20	A	1116	CLA	CBD-CGD-O2D-CED
20	A	1119	CLA	C1A-C2A-CAA-CBA
20	A	1119	CLA	C3A-C2A-CAA-CBA
20	A	1121	CLA	C1A-C2A-CAA-CBA
20	A	1121	CLA	C3A-C2A-CAA-CBA
20	A	1121	CLA	CBD-CGD-O2D-CED
20	A	1122	CLA	CBD-CGD-O2D-CED
20	A	1122	CLA	C4-C3-C5-C6
20	A	1123	CLA	C2-C1-O2A-CGA
20	A	1124	CLA	C1A-C2A-CAA-CBA
20	A	1124	CLA	C3A-C2A-CAA-CBA
20	A	1126	CLA	C1A-C2A-CAA-CBA
20	A	1126	CLA	C3A-C2A-CAA-CBA
20	A	1126	CLA	C2-C1-O2A-CGA
20	A	1128	CLA	CHA-CBD-CGD-O1D
20	A	1128	CLA	CHA-CBD-CGD-O2D
20	A	1130	CLA	C1A-C2A-CAA-CBA
20	A	1130	CLA	C3A-C2A-CAA-CBA
20	A	1131	CLA	CBD-CGD-O2D-CED
20	A	1132	CLA	CHA-CBD-CGD-O1D
20	A	1132	CLA	CHA-CBD-CGD-O2D
20	A	1134	CLA	C2B-C3B-CAB-CBB
20	A	1134	CLA	C4B-C3B-CAB-CBB
20	A	1134	CLA	CBD-CGD-O2D-CED
20	A	1135	CLA	C1A-C2A-CAA-CBA
20	A	1135	CLA	C3A-C2A-CAA-CBA
20	A	1137	CLA	CBD-CGD-O2D-CED
20	A	1141	CLA	CBD-CGD-O2D-CED
20	A	1012	CLA	CBD-CGD-O2D-CED
20	A	1013	CLA	C2-C1-O2A-CGA
20	B	1022	CLA	CBD-CGD-O2D-CED
20	B	1237	CLA	CBD-CGD-O2D-CED
20	B	1201	CLA	C1A-C2A-CAA-CBA
20	B	1201	CLA	C3A-C2A-CAA-CBA
20	B	1202	CLA	C1A-C2A-CAA-CBA
20	B	1202	CLA	C3A-C2A-CAA-CBA
20	B	1203	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
20	B	1205	CLA	CHA-CBD-CGD-O1D
20	B	1205	CLA	CHA-CBD-CGD-O2D
20	B	1208	CLA	C11-C10-C8-C9
20	B	1210	CLA	C1A-C2A-CAA-CBA
20	B	1210	CLA	C3A-C2A-CAA-CBA
20	B	1212	CLA	CHA-CBD-CGD-O1D
20	B	1212	CLA	CHA-CBD-CGD-O2D
20	B	1213	CLA	C1A-C2A-CAA-CBA
20	B	1214	CLA	C4B-C3B-CAB-CBB
20	B	1214	CLA	C11-C10-C8-C9
20	B	1217	CLA	CBA-CGA-O2A-C1
20	B	1219	CLA	C2-C1-O2A-CGA
20	B	1221	CLA	C1A-C2A-CAA-CBA
20	B	1221	CLA	C2-C1-O2A-CGA
20	B	1221	CLA	CHA-CBD-CGD-O1D
20	B	1221	CLA	CHA-CBD-CGD-O2D
20	B	1222	CLA	C1A-C2A-CAA-CBA
20	B	1222	CLA	C3A-C2A-CAA-CBA
20	B	1222	CLA	CHA-CBD-CGD-O1D
20	B	1222	CLA	CHA-CBD-CGD-O2D
20	B	1222	CLA	C6-C7-C8-C9
20	B	1223	CLA	C1A-C2A-CAA-CBA
20	B	1223	CLA	C3A-C2A-CAA-CBA
20	B	1224	CLA	C1A-C2A-CAA-CBA
20	B	1224	CLA	C3A-C2A-CAA-CBA
20	B	1224	CLA	CBD-CGD-O2D-CED
20	B	1225	CLA	C1A-C2A-CAA-CBA
20	B	1225	CLA	C3A-C2A-CAA-CBA
20	B	1226	CLA	C11-C12-C13-C14
20	B	1229	CLA	C2-C1-O2A-CGA
20	B	1230	CLA	CHA-CBD-CGD-O1D
20	B	1230	CLA	CHA-CBD-CGD-O2D
20	B	1232	CLA	C1A-C2A-CAA-CBA
20	B	1232	CLA	C3A-C2A-CAA-CBA
20	B	1234	CLA	CBD-CGD-O2D-CED
20	B	1239	CLA	C3A-C2A-CAA-CBA
20	B	1207	CLA	C2-C1-O2A-CGA
20	B	1207	CLA	CAD-CBD-CGD-O1D
20	B	1207	CLA	CAD-CBD-CGD-O2D
20	B	1207	CLA	CBD-CGD-O2D-CED
20	B	1207	CLA	C12-C13-C15-C16
20	F	1302	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
20	F	1301	CLA	C2-C1-O2A-CGA
20	F	1301	CLA	CBD-CGD-O2D-CED
20	G	1601	CLA	C1A-C2A-CAA-CBA
20	G	1601	CLA	C3A-C2A-CAA-CBA
20	H	1701	CLA	C2-C1-O2A-CGA
20	H	1701	CLA	CBD-CGD-O2D-CED
20	J	1901	CLA	CBD-CGD-O2D-CED
20	K	1401	CLA	C1A-C2A-CAA-CBA
20	K	1401	CLA	C3A-C2A-CAA-CBA
20	K	1401	CLA	CHA-CBD-CGD-O1D
20	K	1401	CLA	CHA-CBD-CGD-O2D
20	K	1401	CLA	CBD-CGD-O2D-CED
20	K	1402	CLA	C1A-C2A-CAA-CBA
20	K	1403	CLA	CBA-CGA-O2A-C1
20	K	1403	CLA	O1A-CGA-O2A-C1
20	K	1403	CLA	CBD-CGD-O2D-CED
20	L	1501	CLA	C1A-C2A-CAA-CBA
20	L	1501	CLA	C3A-C2A-CAA-CBA
20	L	1501	CLA	CBD-CGD-O2D-CED
20	L	1502	CLA	C1A-C2A-CAA-CBA
20	L	1502	CLA	C3A-C2A-CAA-CBA
20	L	1502	CLA	CBD-CGD-O2D-CED
20	L	1502	CLA	C4-C3-C5-C6
20	L	1503	CLA	C1A-C2A-CAA-CBA
20	L	1503	CLA	CBA-CGA-O2A-C1
20	L	1503	CLA	O1A-CGA-O2A-C1
20	1	602	CLA	CBA-CGA-O2A-C1
20	1	602	CLA	CBD-CGD-O2D-CED
20	1	603	CLA	C1A-C2A-CAA-CBA
20	1	603	CLA	CBD-CGD-O2D-CED
20	1	606	CLA	CBD-CGD-O2D-CED
20	1	608	CLA	CBD-CGD-O2D-CED
20	1	611	CLA	CBD-CGD-O2D-CED
20	1	613	CLA	CBD-CGD-O2D-CED
20	1	614	CLA	C2B-C3B-CAB-CBB
20	1	614	CLA	C4B-C3B-CAB-CBB
20	1	614	CLA	CHA-CBD-CGD-O1D
20	1	614	CLA	CHA-CBD-CGD-O2D
20	1	614	CLA	C6-C7-C8-C9
20	2	601	CLA	C1A-C2A-CAA-CBA
20	2	601	CLA	C3A-C2A-CAA-CBA
20	2	602	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
20	2	602	CLA	C3-C5-C6-C7
20	2	603	CLA	CBD-CGD-O2D-CED
20	2	604	CLA	C3A-C2A-CAA-CBA
20	2	604	CLA	CBD-CGD-O2D-CED
20	2	605	CLA	C1A-C2A-CAA-CBA
20	2	606	CLA	C1A-C2A-CAA-CBA
20	2	606	CLA	C3A-C2A-CAA-CBA
20	2	607	CLA	CBA-CGA-O2A-C1
20	2	607	CLA	O1A-CGA-O2A-C1
20	2	608	CLA	CBD-CGD-O2D-CED
20	2	612	CLA	C1A-C2A-CAA-CBA
20	2	612	CLA	C3A-C2A-CAA-CBA
20	3	601	CLA	C1A-C2A-CAA-CBA
20	3	601	CLA	C3A-C2A-CAA-CBA
20	3	601	CLA	CBD-CGD-O2D-CED
20	3	606	CLA	CAD-CBD-CGD-O1D
20	3	606	CLA	CAD-CBD-CGD-O2D
20	3	606	CLA	CBD-CGD-O2D-CED
20	3	608	CLA	C1A-C2A-CAA-CBA
20	3	610	CLA	C3A-C2A-CAA-CBA
20	3	612	CLA	C1A-C2A-CAA-CBA
20	3	612	CLA	C3A-C2A-CAA-CBA
20	3	612	CLA	C2-C1-O2A-CGA
20	3	614	CLA	C1A-C2A-CAA-CBA
20	3	617	CLA	C1A-C2A-CAA-CBA
20	3	617	CLA	C3A-C2A-CAA-CBA
20	3	617	CLA	CHA-CBD-CGD-O1D
20	3	617	CLA	CHA-CBD-CGD-O2D
20	4	609	CLA	C1A-C2A-CAA-CBA
20	4	609	CLA	C3A-C2A-CAA-CBA
20	4	609	CLA	CAD-CBD-CGD-O1D
20	4	609	CLA	CAD-CBD-CGD-O2D
20	4	609	CLA	CBD-CGD-O2D-CED
20	4	602	CLA	CHA-CBD-CGD-O1D
20	4	602	CLA	CHA-CBD-CGD-O2D
20	4	604	CLA	CBD-CGD-O2D-CED
20	4	604	CLA	C2-C3-C5-C6
20	4	604	CLA	C4-C3-C5-C6
20	4	605	CLA	C1A-C2A-CAA-CBA
20	4	606	CLA	CBD-CGD-O2D-CED
20	4	607	CLA	C3A-C2A-CAA-CBA
20	4	612	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
20	4	612	CLA	O1A-CGA-O2A-C1
22	A	4002	BCR	C10-C11-C12-C13
22	A	4002	BCR	C11-C12-C13-C14
22	A	4003	BCR	C11-C10-C9-C8
22	A	4003	BCR	C11-C10-C9-C34
22	A	4007	BCR	C21-C22-C23-C24
22	A	4008	BCR	C11-C10-C9-C8
22	A	4008	BCR	C11-C10-C9-C34
22	A	4008	BCR	C10-C11-C12-C13
22	A	4011	BCR	C11-C10-C9-C8
22	A	4011	BCR	C11-C10-C9-C34
22	A	4011	BCR	C17-C18-C19-C20
22	A	4011	BCR	C36-C18-C19-C20
22	A	4017	BCR	C11-C10-C9-C8
22	A	4017	BCR	C11-C10-C9-C34
22	A	4017	BCR	C10-C11-C12-C13
22	B	4005	BCR	C11-C10-C9-C8
22	B	4005	BCR	C11-C10-C9-C34
22	B	4005	BCR	C21-C22-C23-C24
22	B	4005	BCR	C37-C22-C23-C24
22	B	4006	BCR	C1-C6-C7-C8
22	B	4006	BCR	C5-C6-C7-C8
22	B	4006	BCR	C7-C8-C9-C10
22	B	4009	BCR	C7-C8-C9-C10
22	B	4009	BCR	C11-C10-C9-C8
22	B	4009	BCR	C11-C10-C9-C34
22	B	4010	BCR	C11-C10-C9-C8
22	B	4010	BCR	C11-C10-C9-C34
22	B	4010	BCR	C17-C18-C19-C20
22	B	4010	BCR	C36-C18-C19-C20
22	B	4010	BCR	C21-C22-C23-C24
22	B	4004	BCR	C11-C10-C9-C8
22	B	4004	BCR	C11-C10-C9-C34
22	B	4004	BCR	C23-C24-C25-C26
22	B	4004	BCR	C23-C24-C25-C30
22	F	4014	BCR	C7-C8-C9-C10
22	F	4014	BCR	C7-C8-C9-C34
22	F	4014	BCR	C11-C10-C9-C8
22	F	4014	BCR	C11-C10-C9-C34
22	F	4016	BCR	C7-C8-C9-C10
22	F	4016	BCR	C7-C8-C9-C34
22	F	4016	BCR	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
22	F	4016	BCR	C11-C10-C9-C34
22	F	4016	BCR	C10-C11-C12-C13
22	H	4021	BCR	C17-C18-C19-C20
22	H	4021	BCR	C19-C20-C21-C22
22	I	4018	BCR	C7-C8-C9-C10
22	I	4018	BCR	C7-C8-C9-C34
22	I	4018	BCR	C17-C18-C19-C20
22	I	4020	BCR	C11-C10-C9-C8
22	I	4020	BCR	C11-C10-C9-C34
22	I	4020	BCR	C11-C12-C13-C14
22	J	4012	BCR	C7-C8-C9-C10
22	J	4012	BCR	C11-C12-C13-C14
22	J	4012	BCR	C11-C12-C13-C35
22	J	4012	BCR	C21-C22-C23-C24
22	J	4012	BCR	C37-C22-C23-C24
22	K	4001	BCR	C1-C6-C7-C8
22	K	4001	BCR	C5-C6-C7-C8
22	K	4001	BCR	C7-C8-C9-C10
22	K	4001	BCR	C7-C8-C9-C34
22	K	4001	BCR	C11-C10-C9-C8
22	K	4001	BCR	C11-C10-C9-C34
22	K	4002	BCR	C11-C10-C9-C8
22	K	4002	BCR	C11-C10-C9-C34
22	K	4002	BCR	C21-C22-C23-C24
22	L	4019	BCR	C11-C10-C9-C8
22	L	4019	BCR	C11-C10-C9-C34
22	L	4019	BCR	C15-C16-C17-C18
22	L	4019	BCR	C17-C18-C19-C20
22	L	4019	BCR	C21-C22-C23-C24
22	L	4020	BCR	C11-C10-C9-C8
22	L	4020	BCR	C11-C10-C9-C34
22	L	4020	BCR	C17-C18-C19-C20
22	L	4020	BCR	C19-C20-C21-C22
22	1	504	BCR	C7-C8-C9-C10
22	1	504	BCR	C7-C8-C9-C34
22	1	504	BCR	C11-C10-C9-C8
22	1	504	BCR	C11-C10-C9-C34
22	1	504	BCR	C11-C12-C13-C35
22	1	504	BCR	C21-C22-C23-C24
22	1	504	BCR	C37-C22-C23-C24
22	1	504	BCR	C23-C24-C25-C26
22	1	504	BCR	C23-C24-C25-C30

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Mol	Chain	Res	Type	Atoms
22	1	503	BCR	C5-C6-C7-C8
22	1	503	BCR	C11-C10-C9-C8
22	1	503	BCR	C11-C10-C9-C34
22	1	503	BCR	C23-C24-C25-C26
22	1	503	BCR	C23-C24-C25-C30
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	C23-C24-C25-C26
22	2	503	BCR	C23-C24-C25-C30
22	3	503	BCR	C1-C6-C7-C8
22	3	503	BCR	C5-C6-C7-C8
22	3	503	BCR	C7-C8-C9-C10
22	3	503	BCR	C7-C8-C9-C34
22	3	503	BCR	C11-C10-C9-C8
22	3	503	BCR	C11-C10-C9-C34
22	3	503	BCR	C10-C11-C12-C13
22	3	503	BCR	C17-C18-C19-C20
22	3	503	BCR	C36-C18-C19-C20
22	3	503	BCR	C19-C20-C21-C22
22	3	506	BCR	C5-C6-C7-C8
22	3	506	BCR	C7-C8-C9-C10
22	3	506	BCR	C7-C8-C9-C34
22	3	506	BCR	C11-C10-C9-C8
22	3	506	BCR	C11-C10-C9-C34
22	3	506	BCR	C23-C24-C25-C26
22	3	506	BCR	C23-C24-C25-C30
23	A	5001	LHG	O1-C1-C2-C3
23	A	5001	LHG	O2-C2-C3-O3
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	O1-C1-C2-C3
23	A	5002	LHG	C3-O3-P-O5
23	A	5002	LHG	C4-O6-P-O3
23	A	5002	LHG	C4-O6-P-O4
23	A	5002	LHG	C4-O6-P-O5
23	A	5002	LHG	O7-C5-C6-O8
23	B	5001	LHG	C3-O3-P-O6
23	B	5001	LHG	C4-O6-P-O3
23	B	5001	LHG	C4-O6-P-O4

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Mol	Chain	Res	Type	Atoms
23	B	5001	LHG	C4-O6-P-O5
23	B	5001	LHG	C8-C7-O7-C5
23	B	5002	LHG	C3-O3-P-O6
23	B	5002	LHG	C8-C7-O7-C5
23	1	801	LHG	O1-C1-C2-O2
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	O1-C1-C2-C3
23	2	801	LHG	C1-C2-C3-O3
23	2	801	LHG	C3-O3-P-O4
23	2	801	LHG	C4-O6-P-O3
23	2	801	LHG	C4-O6-P-O5
23	2	801	LHG	C8-C7-O7-C5
23	3	801	LHG	C3-O3-P-O5
23	3	801	LHG	C4-O6-P-O3
23	3	801	LHG	C4-O6-P-O5
23	4	801	LHG	O1-C1-C2-C3
23	4	801	LHG	C2-C3-O3-P
23	4	801	LHG	O7-C5-C6-O8
23	4	801	LHG	C8-C7-O7-C5
24	B	5008	LMT	C2'-C1'-O1'-C1
24	G	5005	LMT	C2'-C1'-O1'-C1
24	G	5005	LMT	O5'-C1'-O1'-C1
24	G	5005	LMT	C2-C1-O1'-C1'
26	A	5006	LMG	O6-C1-O1-C7
26	A	5006	LMG	O9-C10-O7-C8
26	B	5003	LMG	C11-C10-O7-C8
26	B	5004	LMG	O6-C1-O1-C7
26	B	5004	LMG	C11-C10-O7-C8
26	F	5002	LMG	O6-C1-O1-C7
26	F	5002	LMG	C11-C10-O7-C8
26	F	5004	LMG	C11-C10-O7-C8
26	G	5006	LMG	O9-C10-O7-C8
26	G	5001	LMG	O9-C10-O7-C8
26	G	5002	LMG	O6-C1-O1-C7
26	G	5002	LMG	O1-C7-C8-O7
26	G	5002	LMG	O9-C10-O7-C8
26	G	5002	LMG	C11-C10-O7-C8
26	2	802	LMG	O9-C10-O7-C8
26	2	802	LMG	C11-C10-O7-C8
26	3	802	LMG	O6-C1-O1-C7

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Mol	Chain	Res	Type	Atoms
26	3	802	LMG	C11-C10-O7-C8
28	B	5005	DGD	O1B-C1B-O2G-C2G
28	F	5005	DGD	C2B-C1B-O2G-C2G
28	F	5005	DGD	O1B-C1B-O2G-C2G
28	J	5001	DGD	O1B-C1B-O2G-C2G
28	J	5001	DGD	O6E-C1E-O5D-C6D
28	1	803	DGD	O6E-C1E-O5D-C6D
28	3	803	DGD	O6D-C1D-O3G-C3G
28	4	802	DGD	C2B-C1B-O2G-C2G
28	4	802	DGD	O6D-C1D-O3G-C3G
29	J	4013	LUT	C7-C8-C9-C10
29	J	4013	LUT	C7-C8-C9-C19
29	J	4013	LUT	C21-C26-C27-C28
29	J	4013	LUT	C25-C26-C27-C28
29	J	4013	LUT	C29-C30-C31-C32
29	1	502	LUT	C21-C26-C27-C28
29	1	502	LUT	C25-C26-C27-C28
29	1	502	LUT	C27-C28-C29-C30
29	1	502	LUT	C27-C28-C29-C39
29	1	502	LUT	C29-C30-C31-C32
29	2	501	LUT	C21-C26-C27-C28
29	3	502	LUT	C21-C26-C27-C28
29	4	501	LUT	C25-C26-C27-C28
30	1	610	CHL	C4C-C3C-CAC-CBC
30	2	610	CHL	C4C-C3C-CAC-CBC
30	2	613	CHL	C4C-C3C-CAC-CBC
30	2	613	CHL	CHA-CBD-CGD-O1D
30	2	613	CHL	CHA-CBD-CGD-O2D
30	3	607	CHL	C3A-C2A-CAA-CBA
30	4	613	CHL	C1A-C2A-CAA-CBA
30	4	613	CHL	C3A-C2A-CAA-CBA
30	4	615	CHL	C4C-C3C-CAC-CBC
31	2	502	XAT	C5-C6-C7-C8
31	2	502	XAT	C27-C28-C29-C30
33	4	505	C7Z	C5-C6-C7-C8
33	4	505	C7Z	C7-C8-C9-C19
33	4	505	C7Z	C11-C10-C9-C8
33	4	505	C7Z	C12-C13-C14-C15
33	4	505	C7Z	C32-C33-C34-C35
33	4	505	C7Z	C39-C29-C30-C31
33	4	505	C7Z	C27-C28-C29-C39
20	A	1104	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
20	A	1139	CLA	O1D-CGD-O2D-CED
20	B	1021	CLA	O1D-CGD-O2D-CED
20	B	1219	CLA	O1D-CGD-O2D-CED
20	K	1404	CLA	O1D-CGD-O2D-CED
20	2	606	CLA	O1D-CGD-O2D-CED
20	2	612	CLA	O1D-CGD-O2D-CED
20	3	613	CLA	O1D-CGD-O2D-CED
20	A	1121	CLA	O1D-CGD-O2D-CED
20	A	1126	CLA	O1D-CGD-O2D-CED
20	2	605	CLA	O1D-CGD-O2D-CED
20	3	612	CLA	O1D-CGD-O2D-CED
20	3	614	CLA	O1D-CGD-O2D-CED
20	4	601	CLA	O1D-CGD-O2D-CED
20	4	606	CLA	O1D-CGD-O2D-CED
23	B	5001	LHG	O9-C7-O7-C5
20	A	1101	CLA	CBD-CGD-O2D-CED
20	A	1103	CLA	CBD-CGD-O2D-CED
20	A	1104	CLA	CBD-CGD-O2D-CED
20	A	1108	CLA	CBD-CGD-O2D-CED
20	A	1109	CLA	CBD-CGD-O2D-CED
20	A	1117	CLA	CBD-CGD-O2D-CED
20	A	1119	CLA	CBD-CGD-O2D-CED
20	A	1126	CLA	CBD-CGD-O2D-CED
20	A	1127	CLA	CBD-CGD-O2D-CED
20	A	1132	CLA	CBD-CGD-O2D-CED
20	A	1140	CLA	CBD-CGD-O2D-CED
20	A	1013	CLA	CBD-CGD-O2D-CED
20	A	1139	CLA	CBD-CGD-O2D-CED
20	B	1023	CLA	CBD-CGD-O2D-CED
20	B	1021	CLA	CBD-CGD-O2D-CED
20	B	1201	CLA	CBD-CGD-O2D-CED
20	B	1206	CLA	CBD-CGD-O2D-CED
20	B	1208	CLA	CBD-CGD-O2D-CED
20	B	1209	CLA	CBD-CGD-O2D-CED
20	B	1213	CLA	CBD-CGD-O2D-CED
20	B	1216	CLA	CBD-CGD-O2D-CED
20	B	1219	CLA	CBD-CGD-O2D-CED
20	B	1227	CLA	CBD-CGD-O2D-CED
20	B	1228	CLA	CBD-CGD-O2D-CED
20	B	1229	CLA	CBD-CGD-O2D-CED
20	B	1232	CLA	CBD-CGD-O2D-CED
20	B	1238	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
20	G	1601	CLA	CBD-CGD-O2D-CED
20	G	1602	CLA	CBD-CGD-O2D-CED
20	K	1404	CLA	CBD-CGD-O2D-CED
20	L	1503	CLA	CBD-CGD-O2D-CED
20	1	601	CLA	CBD-CGD-O2D-CED
20	1	605	CLA	CBD-CGD-O2D-CED
20	2	605	CLA	CBD-CGD-O2D-CED
20	2	606	CLA	CBD-CGD-O2D-CED
20	2	607	CLA	CBD-CGD-O2D-CED
20	2	612	CLA	CBD-CGD-O2D-CED
20	3	603	CLA	CBD-CGD-O2D-CED
20	3	608	CLA	CBD-CGD-O2D-CED
20	3	610	CLA	CBD-CGD-O2D-CED
20	3	612	CLA	CBD-CGD-O2D-CED
20	3	613	CLA	CBD-CGD-O2D-CED
20	3	614	CLA	CBD-CGD-O2D-CED
20	3	617	CLA	CBD-CGD-O2D-CED
20	4	601	CLA	CBD-CGD-O2D-CED
20	4	602	CLA	CBD-CGD-O2D-CED
20	4	603	CLA	CBD-CGD-O2D-CED
20	4	605	CLA	CBD-CGD-O2D-CED
20	4	607	CLA	CBD-CGD-O2D-CED
20	4	612	CLA	CBD-CGD-O2D-CED
20	4	617	CLA	CBD-CGD-O2D-CED
20	B	1214	CLA	O1A-CGA-O2A-C1
20	F	1302	CLA	O1A-CGA-O2A-C1
26	F	5002	LMG	O10-C28-O8-C9
20	A	1114	CLA	O1A-CGA-O2A-C1
20	G	1602	CLA	O1A-CGA-O2A-C1
20	K	1404	CLA	O1A-CGA-O2A-C1
20	1	602	CLA	O1A-CGA-O2A-C1
24	G	5004	LMT	O5B-C1B-O1B-C4'
20	K	1404	CLA	CBA-CGA-O2A-C1
20	3	613	CLA	CBA-CGA-O2A-C1
30	2	610	CHL	C2C-C3C-CAC-CBC
20	B	1201	CLA	O1D-CGD-O2D-CED
20	B	1206	CLA	O1D-CGD-O2D-CED
20	B	1232	CLA	O1D-CGD-O2D-CED
20	G	1602	CLA	O1D-CGD-O2D-CED
20	3	617	CLA	O1D-CGD-O2D-CED
20	4	602	CLA	O1D-CGD-O2D-CED
20	4	612	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
20	B	1214	CLA	CBA-CGA-O2A-C1
20	B	1227	CLA	CBA-CGA-O2A-C1
20	4	609	CLA	CBA-CGA-O2A-C1
26	F	5002	LMG	C29-C28-O8-C9
20	A	1120	CLA	CBD-CGD-O2D-CED
20	A	1104	CLA	O1A-CGA-O2A-C1
20	A	1121	CLA	O1A-CGA-O2A-C1
20	A	1122	CLA	O1A-CGA-O2A-C1
20	B	1237	CLA	O1A-CGA-O2A-C1
20	B	1227	CLA	O1A-CGA-O2A-C1
20	J	1901	CLA	O1A-CGA-O2A-C1
20	1	606	CLA	O1A-CGA-O2A-C1
20	2	603	CLA	O1A-CGA-O2A-C1
20	2	612	CLA	O1A-CGA-O2A-C1
20	3	602	CLA	O1A-CGA-O2A-C1
20	3	610	CLA	O1A-CGA-O2A-C1
20	4	609	CLA	O1A-CGA-O2A-C1
20	4	605	CLA	O1A-CGA-O2A-C1
20	4	606	CLA	O1A-CGA-O2A-C1
26	B	5003	LMG	O10-C28-O8-C9
26	F	5003	LMG	O10-C28-O8-C9
26	G	5006	LMG	O10-C28-O8-C9
26	G	5002	LMG	O10-C28-O8-C9
26	2	803	LMG	O10-C28-O8-C9
20	4	607	CLA	C10-C11-C12-C13
20	B	1217	CLA	O1A-CGA-O2A-C1
20	3	613	CLA	O1A-CGA-O2A-C1
20	B	1203	CLA	O1D-CGD-O2D-CED
20	G	1601	CLA	O1D-CGD-O2D-CED
20	J	1901	CLA	O1D-CGD-O2D-CED
20	2	602	CLA	O1D-CGD-O2D-CED
20	3	601	CLA	O1D-CGD-O2D-CED
20	3	603	CLA	O1D-CGD-O2D-CED
20	3	608	CLA	O1D-CGD-O2D-CED
20	A	1115	CLA	O1D-CGD-O2D-CED
20	A	1137	CLA	O1D-CGD-O2D-CED
20	A	1141	CLA	O1D-CGD-O2D-CED
20	B	1237	CLA	O1D-CGD-O2D-CED
20	B	1207	CLA	O1D-CGD-O2D-CED
20	F	1302	CLA	O1D-CGD-O2D-CED
20	F	1301	CLA	O1D-CGD-O2D-CED
20	H	1701	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
20	K	1401	CLA	O1D-CGD-O2D-CED
20	K	1403	CLA	O1D-CGD-O2D-CED
20	L	1501	CLA	O1D-CGD-O2D-CED
20	L	1502	CLA	O1D-CGD-O2D-CED
20	1	602	CLA	O1D-CGD-O2D-CED
20	1	603	CLA	O1D-CGD-O2D-CED
20	1	613	CLA	O1D-CGD-O2D-CED
20	2	603	CLA	O1D-CGD-O2D-CED
20	2	604	CLA	O1D-CGD-O2D-CED
20	3	606	CLA	O1D-CGD-O2D-CED
20	4	604	CLA	O1D-CGD-O2D-CED
20	A	1105	CLA	CBD-CGD-O2D-CED
20	4	607	CLA	O1A-CGA-O2A-C1
26	B	5004	LMG	O10-C28-O8-C9
23	4	801	LHG	O9-C7-O7-C5
26	B	5004	LMG	O9-C10-O7-C8
26	F	5002	LMG	O9-C10-O7-C8
26	F	5004	LMG	O9-C10-O7-C8
26	2	803	LMG	O9-C10-O7-C8
26	3	802	LMG	O9-C10-O7-C8
28	4	802	DGD	O1B-C1B-O2G-C2G
20	A	1102	CLA	C3-C5-C6-C7
20	A	1105	CLA	C3-C5-C6-C7
20	A	1107	CLA	C3-C5-C6-C7
20	A	1109	CLA	C3-C5-C6-C7
20	A	1110	CLA	C3-C5-C6-C7
20	A	1112	CLA	C3-C5-C6-C7
20	A	1119	CLA	C3-C5-C6-C7
20	A	1125	CLA	C3-C5-C6-C7
20	A	1126	CLA	C3-C5-C6-C7
20	A	1134	CLA	C3-C5-C6-C7
20	B	1203	CLA	C3-C5-C6-C7
20	B	1206	CLA	C3-C5-C6-C7
20	B	1215	CLA	C3-C5-C6-C7
20	B	1219	CLA	C3-C5-C6-C7
20	B	1223	CLA	C3-C5-C6-C7
20	B	1228	CLA	C3-C5-C6-C7
20	B	1232	CLA	C3-C5-C6-C7
20	B	1238	CLA	C3-C5-C6-C7
20	F	1302	CLA	C3-C5-C6-C7
20	1	605	CLA	C3-C5-C6-C7
20	2	604	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
20	2	605	CLA	C3-C5-C6-C7
20	3	601	CLA	C3-C5-C6-C7
20	3	605	CLA	C3-C5-C6-C7
20	3	610	CLA	C3-C5-C6-C7
30	4	613	CHL	C3-C5-C6-C7
20	B	1022	CLA	O1D-CGD-O2D-CED
20	B	1234	CLA	O1D-CGD-O2D-CED
20	A	1108	CLA	CBA-CGA-O2A-C1
20	A	1122	CLA	CBA-CGA-O2A-C1
20	A	1126	CLA	CBA-CGA-O2A-C1
20	A	1127	CLA	CBA-CGA-O2A-C1
20	B	1237	CLA	CBA-CGA-O2A-C1
20	B	1219	CLA	CBA-CGA-O2A-C1
20	B	1232	CLA	CBA-CGA-O2A-C1
20	F	1302	CLA	CBA-CGA-O2A-C1
20	J	1901	CLA	CBA-CGA-O2A-C1
20	2	603	CLA	CBA-CGA-O2A-C1
20	2	605	CLA	CBA-CGA-O2A-C1
20	2	612	CLA	CBA-CGA-O2A-C1
20	3	602	CLA	CBA-CGA-O2A-C1
20	4	606	CLA	CBA-CGA-O2A-C1
26	B	5003	LMG	C29-C28-O8-C9
26	F	5003	LMG	C29-C28-O8-C9
26	G	5006	LMG	C29-C28-O8-C9
26	2	803	LMG	C29-C28-O8-C9
20	A	1113	CLA	CBD-CGD-O2D-CED
20	A	1125	CLA	CBD-CGD-O2D-CED
20	A	1129	CLA	CBD-CGD-O2D-CED
20	A	1130	CLA	CBD-CGD-O2D-CED
20	A	1135	CLA	CBD-CGD-O2D-CED
20	A	1138	CLA	CBD-CGD-O2D-CED
20	B	1214	CLA	CBD-CGD-O2D-CED
20	B	1215	CLA	CBD-CGD-O2D-CED
20	B	1226	CLA	CBD-CGD-O2D-CED
20	B	1230	CLA	CBD-CGD-O2D-CED
20	B	1236	CLA	CBD-CGD-O2D-CED
20	B	1239	CLA	CBD-CGD-O2D-CED
20	1	604	CLA	CBD-CGD-O2D-CED
20	1	614	CLA	CBD-CGD-O2D-CED
20	2	601	CLA	CBD-CGD-O2D-CED
20	3	602	CLA	CBD-CGD-O2D-CED
20	4	608	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
26	A	5006	LMG	C11-C10-O7-C8
26	G	5006	LMG	C11-C10-O7-C8
26	G	5001	LMG	C11-C10-O7-C8
26	2	803	LMG	C11-C10-O7-C8
28	B	5005	DGD	C2B-C1B-O2G-C2G
28	J	5001	DGD	C2B-C1B-O2G-C2G
20	A	1107	CLA	O1D-CGD-O2D-CED
20	A	1116	CLA	O1D-CGD-O2D-CED
20	A	1122	CLA	O1D-CGD-O2D-CED
20	A	1131	CLA	O1D-CGD-O2D-CED
20	A	1134	CLA	O1D-CGD-O2D-CED
20	A	1012	CLA	O1D-CGD-O2D-CED
20	B	1208	CLA	O1D-CGD-O2D-CED
20	B	1224	CLA	O1D-CGD-O2D-CED
20	1	606	CLA	O1D-CGD-O2D-CED
20	1	608	CLA	O1D-CGD-O2D-CED
20	1	611	CLA	O1D-CGD-O2D-CED
20	2	608	CLA	O1D-CGD-O2D-CED
20	4	609	CLA	O1D-CGD-O2D-CED
20	4	617	CLA	O1D-CGD-O2D-CED
26	2	804	LMG	O10-C28-O8-C9
20	L	1503	CLA	C2C-C3C-CAC-CBC
20	A	1104	CLA	C4-C3-C5-C6
20	A	1109	CLA	C4-C3-C5-C6
20	A	1133	CLA	C4-C3-C5-C6
20	A	1012	CLA	C4-C3-C5-C6
20	B	1204	CLA	C4-C3-C5-C6
20	B	1230	CLA	C4-C3-C5-C6
20	B	1239	CLA	C4-C3-C5-C6
20	B	1207	CLA	C4-C3-C5-C6
20	B	1240	CLA	C4-C3-C5-C6
20	G	1601	CLA	C4-C3-C5-C6
20	K	1402	CLA	C4-C3-C5-C6
20	1	601	CLA	C4-C3-C5-C6
20	2	602	CLA	C4-C3-C5-C6
20	2	604	CLA	C4-C3-C5-C6
20	2	612	CLA	C4-C3-C5-C6
20	3	602	CLA	C4-C3-C5-C6
20	3	603	CLA	C4-C3-C5-C6
20	A	1104	CLA	C2-C3-C5-C6
20	A	1122	CLA	C2-C3-C5-C6
20	A	1133	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
20	B	1204	CLA	C2-C3-C5-C6
20	B	1207	CLA	C2-C3-C5-C6
20	K	1402	CLA	C2-C3-C5-C6
20	L	1502	CLA	C2-C3-C5-C6
20	1	601	CLA	C2-C3-C5-C6
20	2	602	CLA	C2-C3-C5-C6
20	2	604	CLA	C2-C3-C5-C6
20	2	612	CLA	C2-C3-C5-C6
20	3	603	CLA	C2-C3-C5-C6
20	G	1602	CLA	CBA-CGA-O2A-C1
20	A	1124	CLA	CBD-CGD-O2D-CED
20	B	1023	CLA	O1D-CGD-O2D-CED
20	B	1228	CLA	O1D-CGD-O2D-CED
20	4	603	CLA	O1D-CGD-O2D-CED
20	A	1121	CLA	C2A-CAA-CBA-CGA
20	B	1214	CLA	C2A-CAA-CBA-CGA
20	4	608	CLA	C2A-CAA-CBA-CGA
20	A	1106	CLA	C3-C5-C6-C7
20	B	1211	CLA	C3-C5-C6-C7
20	B	1226	CLA	C3-C5-C6-C7
20	B	1207	CLA	C3-C5-C6-C7
20	1	611	CLA	C3-C5-C6-C7
20	2	603	CLA	C3-C5-C6-C7
20	3	603	CLA	C3-C5-C6-C7
20	4	617	CLA	C3-C5-C6-C7
20	A	1104	CLA	CBA-CGA-O2A-C1
20	A	1118	CLA	CBA-CGA-O2A-C1
20	A	1121	CLA	CBA-CGA-O2A-C1
20	B	1202	CLA	CBA-CGA-O2A-C1
20	B	1208	CLA	CBA-CGA-O2A-C1
20	B	1222	CLA	CBA-CGA-O2A-C1
20	B	1230	CLA	CBA-CGA-O2A-C1
20	G	1603	CLA	CBA-CGA-O2A-C1
20	1	606	CLA	CBA-CGA-O2A-C1
20	2	602	CLA	CBA-CGA-O2A-C1
20	3	610	CLA	CBA-CGA-O2A-C1
20	4	605	CLA	CBA-CGA-O2A-C1
20	4	607	CLA	CBA-CGA-O2A-C1
26	B	5004	LMG	C29-C28-O8-C9
26	G	5002	LMG	C29-C28-O8-C9
28	B	5005	DGD	C8A-C9A-CAA-CBA
20	B	1202	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
20	B	1212	CLA	CBD-CGD-O2D-CED
26	G	5002	LMG	C35-C36-C37-C38
30	2	611	CHL	C2-C1-O2A-CGA
22	H	4021	BCR	C9-C10-C11-C12
22	2	503	BCR	C9-C10-C11-C12
22	2	503	BCR	C19-C20-C21-C22
22	3	503	BCR	C15-C16-C17-C18
29	4	501	LUT	C29-C30-C31-C32
20	A	1126	CLA	O1A-CGA-O2A-C1
20	A	1127	CLA	O1A-CGA-O2A-C1
20	A	1129	CLA	O1A-CGA-O2A-C1
20	B	1208	CLA	O1A-CGA-O2A-C1
20	B	1219	CLA	O1A-CGA-O2A-C1
20	B	1222	CLA	O1A-CGA-O2A-C1
20	B	1232	CLA	O1A-CGA-O2A-C1
20	G	1603	CLA	O1A-CGA-O2A-C1
20	2	602	CLA	O1A-CGA-O2A-C1
20	2	605	CLA	O1A-CGA-O2A-C1
23	B	5002	LHG	O9-C7-O7-C5
23	2	801	LHG	O9-C7-O7-C5
26	B	5003	LMG	O9-C10-O7-C8
20	A	1127	CLA	O1D-CGD-O2D-CED
20	L	1503	CLA	O1D-CGD-O2D-CED
26	G	5002	LMG	C17-C18-C19-C20
26	A	5006	LMG	C17-C18-C19-C20
26	G	5001	LMG	C35-C36-C37-C38
26	G	5001	LMG	C38-C39-C40-C41
28	F	5005	DGD	C8A-C9A-CAA-CBA
24	G	5004	LMT	C4B-C5B-C6B-O6B
26	2	802	LMG	C4-C5-C6-O5
20	A	1101	CLA	O1D-CGD-O2D-CED
20	A	1119	CLA	O1D-CGD-O2D-CED
20	B	1216	CLA	O1D-CGD-O2D-CED
20	2	607	CLA	O1D-CGD-O2D-CED
20	4	607	CLA	O1D-CGD-O2D-CED
20	A	1012	CLA	C3-C5-C6-C7
20	K	1402	CLA	CBD-CGD-O2D-CED
20	1	607	CLA	CBD-CGD-O2D-CED
23	A	5002	LHG	O2-C2-C3-O3
20	A	1108	CLA	O1D-CGD-O2D-CED
20	A	1109	CLA	O1D-CGD-O2D-CED
20	B	1209	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
20	B	1213	CLA	O1D-CGD-O2D-CED
20	B	1227	CLA	O1D-CGD-O2D-CED
20	1	601	CLA	O1D-CGD-O2D-CED
20	B	1206	CLA	CBA-CGA-O2A-C1
20	B	1211	CLA	CBA-CGA-O2A-C1
20	B	1220	CLA	CBA-CGA-O2A-C1
20	3	603	CLA	CBA-CGA-O2A-C1
20	A	1108	CLA	O1A-CGA-O2A-C1
20	A	1118	CLA	O1A-CGA-O2A-C1
20	2	601	CLA	O1A-CGA-O2A-C1
20	A	1132	CLA	O1D-CGD-O2D-CED
20	B	1238	CLA	O1D-CGD-O2D-CED
20	3	610	CLA	O1D-CGD-O2D-CED
24	A	5004	LMT	O5B-C5B-C6B-O6B
24	G	5004	LMT	O5'-C5'-C6'-O6'
24	A	5004	LMT	C4B-C5B-C6B-O6B
24	B	5006	LMT	C4B-C5B-C6B-O6B
20	A	1106	CLA	CBD-CGD-O2D-CED
20	A	1114	CLA	CBD-CGD-O2D-CED
20	A	1128	CLA	CBD-CGD-O2D-CED
20	B	1225	CLA	CBD-CGD-O2D-CED
20	G	1603	CLA	CBD-CGD-O2D-CED
20	B	1209	CLA	CBA-CGA-O2A-C1
20	A	1103	CLA	O1D-CGD-O2D-CED
20	A	1140	CLA	O1D-CGD-O2D-CED
20	A	1013	CLA	O1D-CGD-O2D-CED
20	1	605	CLA	O1D-CGD-O2D-CED
20	B	1222	CLA	C3-C5-C6-C7
20	G	1601	CLA	C3-C5-C6-C7
24	B	5006	LMT	O5B-C5B-C6B-O6B
20	A	1117	CLA	O1D-CGD-O2D-CED
20	B	1229	CLA	O1D-CGD-O2D-CED
20	4	605	CLA	O1D-CGD-O2D-CED
20	A	1129	CLA	CBA-CGA-O2A-C1
20	A	1013	CLA	CBA-CGA-O2A-C1
20	2	601	CLA	CBA-CGA-O2A-C1
20	2	604	CLA	CBA-CGA-O2A-C1
26	2	804	LMG	C29-C28-O8-C9
20	A	1111	CLA	C4-C3-C5-C6
20	A	1139	CLA	C4-C3-C5-C6
20	B	1221	CLA	C4-C3-C5-C6
20	B	1222	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
20	B	1225	CLA	C4-C3-C5-C6
20	B	1232	CLA	C4-C3-C5-C6
20	1	605	CLA	C4-C3-C5-C6
30	3	604	CHL	C4-C3-C5-C6
20	A	1109	CLA	C2-C3-C5-C6
20	A	1012	CLA	C2-C3-C5-C6
20	A	1139	CLA	C2-C3-C5-C6
20	B	1225	CLA	C2-C3-C5-C6
20	B	1230	CLA	C2-C3-C5-C6
20	B	1232	CLA	C2-C3-C5-C6
20	B	1239	CLA	C2-C3-C5-C6
20	1	605	CLA	C2-C3-C5-C6
20	B	1207	CLA	C15-C16-C17-C18
20	B	1202	CLA	O1A-CGA-O2A-C1
20	B	1206	CLA	O1A-CGA-O2A-C1
20	B	1230	CLA	O1A-CGA-O2A-C1
24	B	5008	LMT	O5'-C5'-C6'-O6'
20	A	1136	CLA	CBD-CGD-O2D-CED
20	B	1222	CLA	CBD-CGD-O2D-CED
24	A	5004	LMT	O5'-C5'-C6'-O6'
24	G	5004	LMT	O5B-C5B-C6B-O6B
20	A	1105	CLA	C2A-CAA-CBA-CGA
20	A	1141	CLA	C2A-CAA-CBA-CGA
20	A	1120	CLA	O1D-CGD-O2D-CED
20	A	1105	CLA	O1A-CGA-O2A-C1
20	A	1013	CLA	O1A-CGA-O2A-C1
20	B	1220	CLA	O1A-CGA-O2A-C1
26	G	5006	LMG	O6-C1-O1-C7
28	B	5005	DGD	O6D-C1D-O3G-C3G
28	G	5003	DGD	O6D-C1D-O3G-C3G
28	1	803	DGD	O6D-C1D-O3G-C3G
26	2	802	LMG	O6-C5-C6-O5
20	A	1105	CLA	CBA-CGA-O2A-C1
20	A	1112	CLA	CBA-CGA-O2A-C1
20	A	1124	CLA	CBA-CGA-O2A-C1
20	K	1402	CLA	CBA-CGA-O2A-C1
20	3	606	CLA	CBA-CGA-O2A-C1
20	4	603	CLA	CBA-CGA-O2A-C1
20	A	1102	CLA	CBD-CGD-O2D-CED
20	B	1204	CLA	CBD-CGD-O2D-CED
20	B	1205	CLA	CBD-CGD-O2D-CED
20	B	1211	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
20	B	1231	CLA	CBD-CGD-O2D-CED
20	B	1235	CLA	CBD-CGD-O2D-CED
20	3	605	CLA	CBD-CGD-O2D-CED
20	L	1503	CLA	C4C-C3C-CAC-CBC
20	1	608	CLA	CBA-CGA-O2A-C1
20	B	1211	CLA	O1A-CGA-O2A-C1
20	2	604	CLA	O1A-CGA-O2A-C1
20	3	603	CLA	O1A-CGA-O2A-C1
22	F	4016	BCR	C19-C20-C21-C22
22	L	4019	BCR	C19-C20-C21-C22
22	3	503	BCR	C13-C14-C15-C16
20	K	1402	CLA	O1A-CGA-O2A-C1
23	B	5001	LHG	C1-C2-C3-O3
23	4	801	LHG	C1-C2-C3-O3
20	A	1101	CLA	CBA-CGA-O2A-C1
20	A	1123	CLA	CBA-CGA-O2A-C1
20	A	1130	CLA	CBA-CGA-O2A-C1
20	A	1134	CLA	CBA-CGA-O2A-C1
20	B	1204	CLA	CBA-CGA-O2A-C1
20	B	1231	CLA	CBA-CGA-O2A-C1
20	H	1701	CLA	CBA-CGA-O2A-C1
20	1	604	CLA	CBA-CGA-O2A-C1
20	2	608	CLA	CBA-CGA-O2A-C1
20	3	605	CLA	CBA-CGA-O2A-C1
20	3	612	CLA	CBA-CGA-O2A-C1
20	4	617	CLA	CBA-CGA-O2A-C1
28	G	5003	DGD	C2A-C1A-O1G-C1G
28	3	803	DGD	C2A-C1A-O1G-C1G
28	4	802	DGD	C2A-C1A-O1G-C1G
20	A	1105	CLA	O1D-CGD-O2D-CED
20	A	1125	CLA	O1D-CGD-O2D-CED
20	B	1214	CLA	O1D-CGD-O2D-CED
20	B	1239	CLA	O1D-CGD-O2D-CED
23	A	5001	LHG	C13-C14-C15-C16
20	A	1116	CLA	C4-C3-C5-C6
20	A	1130	CLA	C4-C3-C5-C6
30	2	609	CHL	C4-C3-C5-C6
20	A	1116	CLA	C2-C3-C5-C6
20	A	1130	CLA	C2-C3-C5-C6
20	B	1240	CLA	C2-C3-C5-C6
20	G	1601	CLA	C2-C3-C5-C6
20	3	602	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
30	2	609	CHL	C2-C3-C5-C6
20	A	1102	CLA	C11-C10-C8-C9
20	A	1115	CLA	C11-C10-C8-C9
20	A	1119	CLA	C11-C10-C8-C9
20	A	1120	CLA	C11-C10-C8-C9
20	A	1125	CLA	C11-C10-C8-C9
20	A	1126	CLA	C6-C7-C8-C9
20	A	1132	CLA	C14-C13-C15-C16
20	A	1137	CLA	C6-C7-C8-C9
20	A	1139	CLA	C11-C12-C13-C14
20	B	1203	CLA	C6-C7-C8-C9
20	B	1205	CLA	C11-C12-C13-C14
20	B	1206	CLA	C14-C13-C15-C16
20	B	1211	CLA	C14-C13-C15-C16
20	B	1214	CLA	C14-C13-C15-C16
20	B	1216	CLA	C14-C13-C15-C16
20	B	1221	CLA	C14-C13-C15-C16
20	B	1239	CLA	C11-C10-C8-C9
20	B	1207	CLA	C6-C7-C8-C9
20	B	1207	CLA	C11-C12-C13-C14
20	B	1218	CLA	C14-C13-C15-C16
20	B	1240	CLA	C14-C13-C15-C16
20	F	1302	CLA	C11-C12-C13-C14
20	F	1301	CLA	C6-C7-C8-C9
20	G	1603	CLA	C14-C13-C15-C16
20	H	1701	CLA	C11-C10-C8-C9
20	L	1502	CLA	C6-C7-C8-C9
20	2	604	CLA	C6-C7-C8-C9
20	2	607	CLA	C6-C7-C8-C9
20	4	601	CLA	C6-C7-C8-C9
20	4	604	CLA	C6-C7-C8-C9
20	4	612	CLA	C14-C13-C15-C16
20	4	617	CLA	C14-C13-C15-C16
20	A	1138	CLA	O1D-CGD-O2D-CED
20	B	1230	CLA	O1D-CGD-O2D-CED
20	1	604	CLA	O1D-CGD-O2D-CED
20	2	601	CLA	O1D-CGD-O2D-CED
26	A	5006	LMG	C2-C1-O1-C7
26	G	5006	LMG	C2-C1-O1-C7
26	3	802	LMG	C2-C1-O1-C7
28	B	5005	DGD	C2D-C1D-O3G-C3G
28	G	5003	DGD	C2D-C1D-O3G-C3G

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Mol	Chain	Res	Type	Atoms
28	1	803	DGD	C2D-C1D-O3G-C3G
23	B	5001	LHG	O2-C2-C3-O3
23	B	5002	LHG	O2-C2-C3-O3
20	A	1135	CLA	O1D-CGD-O2D-CED
20	A	1101	CLA	O1A-CGA-O2A-C1
20	1	604	CLA	O1A-CGA-O2A-C1
20	3	606	CLA	O1A-CGA-O2A-C1
20	B	1215	CLA	O1D-CGD-O2D-CED
20	B	1236	CLA	O1D-CGD-O2D-CED
20	3	602	CLA	O1D-CGD-O2D-CED
22	A	4002	BCR	C11-C12-C13-C35
22	A	4003	BCR	C36-C18-C19-C20
22	A	4007	BCR	C37-C22-C23-C24
22	A	4011	BCR	C37-C22-C23-C24
22	B	4005	BCR	C36-C18-C19-C20
22	B	4006	BCR	C7-C8-C9-C34
22	B	4006	BCR	C37-C22-C23-C24
22	B	4009	BCR	C7-C8-C9-C34
22	B	4010	BCR	C37-C22-C23-C24
22	F	4016	BCR	C36-C18-C19-C20
22	G	4011	BCR	C37-C22-C23-C24
22	H	4021	BCR	C36-C18-C19-C20
22	H	4021	BCR	C37-C22-C23-C24
22	I	4018	BCR	C36-C18-C19-C20
22	I	4020	BCR	C11-C12-C13-C35
22	I	4020	BCR	C36-C18-C19-C20
22	J	4012	BCR	C7-C8-C9-C34
22	K	4002	BCR	C37-C22-C23-C24
22	L	4019	BCR	C36-C18-C19-C20
22	L	4019	BCR	C37-C22-C23-C24
22	L	4020	BCR	C36-C18-C19-C20
22	1	503	BCR	C7-C8-C9-C34
22	2	503	BCR	C11-C12-C13-C35
22	2	503	BCR	C36-C18-C19-C20
29	3	502	LUT	C27-C28-C29-C39
31	2	502	XAT	C27-C28-C29-C39
31	4	502	XAT	C27-C28-C29-C39
22	A	4008	BCR	C7-C8-C9-C10
22	A	4011	BCR	C21-C22-C23-C24
22	G	4011	BCR	C21-C22-C23-C24
22	1	504	BCR	C11-C12-C13-C14
22	1	503	BCR	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
22	2	503	BCR	C17-C18-C19-C20
29	3	502	LUT	C27-C28-C29-C30
20	A	1113	CLA	C2A-CAA-CBA-CGA
20	B	1201	CLA	C2A-CAA-CBA-CGA
20	B	1225	CLA	C2A-CAA-CBA-CGA
20	2	603	CLA	C2A-CAA-CBA-CGA
24	A	5004	LMT	C2B-C1B-O1B-C4'
20	A	1123	CLA	O1A-CGA-O2A-C1
20	A	1134	CLA	O1A-CGA-O2A-C1
20	2	608	CLA	O1A-CGA-O2A-C1
20	4	617	CLA	O1A-CGA-O2A-C1
28	G	5003	DGD	O1A-C1A-O1G-C1G
28	3	803	DGD	O1A-C1A-O1G-C1G
28	4	802	DGD	O1A-C1A-O1G-C1G
20	K	1402	CLA	C8-C10-C11-C12
20	A	1103	CLA	C2-C1-O2A-CGA
20	A	1107	CLA	C2-C1-O2A-CGA
20	A	1120	CLA	C2-C1-O2A-CGA
20	B	1214	CLA	C2-C1-O2A-CGA
20	B	1238	CLA	C2-C1-O2A-CGA
20	F	1302	CLA	C2-C1-O2A-CGA
20	L	1501	CLA	C2-C1-O2A-CGA
20	2	601	CLA	C2-C1-O2A-CGA
20	2	604	CLA	C2-C1-O2A-CGA
20	2	612	CLA	C2-C1-O2A-CGA
20	3	602	CLA	C2-C1-O2A-CGA
20	3	617	CLA	C2-C1-O2A-CGA
20	4	609	CLA	C2-C1-O2A-CGA
20	4	606	CLA	C2-C1-O2A-CGA
20	4	607	CLA	C2-C1-O2A-CGA
30	3	604	CHL	C2-C1-O2A-CGA
20	A	1130	CLA	O1D-CGD-O2D-CED
20	4	608	CLA	O1D-CGD-O2D-CED
23	2	801	LHG	C9-C10-C11-C12
20	A	1111	CLA	C10-C11-C12-C13
20	A	1128	CLA	C5-C6-C7-C8
20	A	1013	CLA	C5-C6-C7-C8
20	B	1208	CLA	C5-C6-C7-C8
20	1	601	CLA	C8-C10-C11-C12
20	A	1113	CLA	O1D-CGD-O2D-CED
20	B	1205	CLA	C3-C5-C6-C7
20	F	1301	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
23	2	801	LHG	C7-C8-C9-C10
20	B	1240	CLA	CBD-CGD-O2D-CED
20	A	1105	CLA	C11-C10-C8-C7
20	A	1122	CLA	C6-C7-C8-C10
20	A	1129	CLA	C6-C7-C8-C10
20	A	1136	CLA	C11-C10-C8-C7
20	A	1013	CLA	C12-C13-C15-C16
20	B	1201	CLA	C12-C13-C15-C16
20	B	1203	CLA	C11-C10-C8-C7
20	3	610	CLA	C12-C13-C15-C16
21	B	2002	PQN	C17-C18-C20-C21
20	2	606	CLA	CBA-CGA-O2A-C1
20	A	1115	CLA	C4-C3-C5-C6
22	A	4017	BCR	C9-C10-C11-C12
22	I	4020	BCR	C9-C10-C11-C12
22	I	4020	BCR	C19-C20-C21-C22
22	1	504	BCR	C19-C20-C21-C22
22	3	503	BCR	C9-C10-C11-C12
22	3	506	BCR	C19-C20-C21-C22
20	B	1209	CLA	O1A-CGA-O2A-C1
20	A	1129	CLA	O1D-CGD-O2D-CED
20	B	1202	CLA	C15-C16-C17-C18
20	G	1603	CLA	C10-C11-C12-C13
20	1	611	CLA	C13-C15-C16-C17
20	2	603	CLA	C10-C11-C12-C13
20	2	605	CLA	C5-C6-C7-C8
28	B	5005	DGD	C2G-C1G-O1G-C1A
24	B	5008	LMT	O5B-C5B-C6B-O6B
23	B	5002	LHG	C23-C24-C25-C26
20	A	1130	CLA	O1A-CGA-O2A-C1
20	B	1204	CLA	O1A-CGA-O2A-C1
20	B	1231	CLA	O1A-CGA-O2A-C1
20	4	603	CLA	O1A-CGA-O2A-C1
20	A	1118	CLA	CBD-CGD-O2D-CED
20	A	1102	CLA	C8-C10-C11-C12
20	A	1112	CLA	C8-C10-C11-C12
20	A	1117	CLA	C5-C6-C7-C8
20	A	1127	CLA	C8-C10-C11-C12
20	A	1139	CLA	C8-C10-C11-C12
20	B	1021	CLA	C13-C15-C16-C17
20	4	617	CLA	C13-C15-C16-C17
20	4	617	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
20	A	1106	CLA	C2A-CAA-CBA-CGA
20	A	1114	CLA	C2A-CAA-CBA-CGA
20	B	1239	CLA	C2A-CAA-CBA-CGA
20	K	1403	CLA	C2A-CAA-CBA-CGA
20	1	607	CLA	C2A-CAA-CBA-CGA
20	2	601	CLA	C2A-CAA-CBA-CGA
20	4	606	CLA	C2A-CAA-CBA-CGA
30	4	613	CHL	C2A-CAA-CBA-CGA
22	A	4011	BCR	C10-C11-C12-C13
22	B	4010	BCR	C10-C11-C12-C13
22	B	4004	BCR	C10-C11-C12-C13
22	J	4012	BCR	C10-C11-C12-C13
22	K	4001	BCR	C10-C11-C12-C13
22	3	506	BCR	C10-C11-C12-C13
20	A	1106	CLA	C5-C6-C7-C8
20	A	1107	CLA	C13-C15-C16-C17
20	A	1119	CLA	C13-C15-C16-C17
20	A	1121	CLA	C10-C11-C12-C13
20	A	1125	CLA	C5-C6-C7-C8
20	A	1140	CLA	C10-C11-C12-C13
20	A	1013	CLA	C15-C16-C17-C18
20	B	1237	CLA	C15-C16-C17-C18
20	B	1216	CLA	C10-C11-C12-C13
20	B	1219	CLA	C5-C6-C7-C8
20	B	1225	CLA	C5-C6-C7-C8
20	B	1227	CLA	C8-C10-C11-C12
20	B	1227	CLA	C15-C16-C17-C18
20	B	1235	CLA	C13-C15-C16-C17
20	B	1207	CLA	C5-C6-C7-C8
20	B	1240	CLA	C10-C11-C12-C13
20	F	1302	CLA	C5-C6-C7-C8
20	1	603	CLA	C5-C6-C7-C8
20	4	603	CLA	C10-C11-C12-C13
23	A	5001	LHG	C23-C24-C25-C26
23	A	5002	LHG	C7-C8-C9-C10
26	3	802	LMG	C10-C11-C12-C13
20	3	605	CLA	O1A-CGA-O2A-C1
20	A	1101	CLA	C3-C5-C6-C7
24	B	5008	LMT	O5'-C1'-O1'-C1
28	1	803	DGD	C2G-C1G-O1G-C1A
20	B	1226	CLA	O1D-CGD-O2D-CED
20	1	614	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
20	A	1101	CLA	C8-C10-C11-C12
20	A	1101	CLA	C10-C11-C12-C13
20	A	1115	CLA	C10-C11-C12-C13
20	A	1117	CLA	C13-C15-C16-C17
20	A	1120	CLA	C8-C10-C11-C12
20	A	1122	CLA	C13-C15-C16-C17
20	A	1123	CLA	C15-C16-C17-C18
20	A	1129	CLA	C5-C6-C7-C8
20	A	1133	CLA	C10-C11-C12-C13
20	A	1133	CLA	C13-C15-C16-C17
20	A	1013	CLA	C10-C11-C12-C13
20	B	1214	CLA	C10-C11-C12-C13
20	B	1219	CLA	C8-C10-C11-C12
20	B	1226	CLA	C15-C16-C17-C18
20	B	1230	CLA	C5-C6-C7-C8
20	B	1207	CLA	C13-C15-C16-C17
20	B	1240	CLA	C15-C16-C17-C18
20	G	1603	CLA	C8-C10-C11-C12
20	L	1502	CLA	C8-C10-C11-C12
20	2	601	CLA	C10-C11-C12-C13
20	2	605	CLA	C15-C16-C17-C18
20	4	612	CLA	C5-C6-C7-C8
20	B	1235	CLA	CBA-CGA-O2A-C1
20	A	1112	CLA	O1A-CGA-O2A-C1
20	A	1124	CLA	O1A-CGA-O2A-C1
20	H	1701	CLA	O1A-CGA-O2A-C1
23	4	801	LHG	C23-C24-C25-C26
20	A	1012	CLA	C15-C16-C17-C18
20	B	1201	CLA	C5-C6-C7-C8
20	1	614	CLA	C10-C11-C12-C13
20	A	1132	CLA	C3-C5-C6-C7
20	H	1701	CLA	C3-C5-C6-C7
20	A	1124	CLA	O1D-CGD-O2D-CED
20	B	1202	CLA	O1D-CGD-O2D-CED
20	B	1212	CLA	O1D-CGD-O2D-CED
20	A	1103	CLA	C13-C15-C16-C17
20	A	1112	CLA	C15-C16-C17-C18
20	A	1133	CLA	C15-C16-C17-C18
20	B	1210	CLA	C13-C15-C16-C17
20	B	1214	CLA	C13-C15-C16-C17
20	1	601	CLA	C5-C6-C7-C8
20	1	605	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
20	2	601	CLA	C5-C6-C7-C8
20	2	603	CLA	C13-C15-C16-C17
20	3	610	CLA	C15-C16-C17-C18
20	3	612	CLA	O1A-CGA-O2A-C1
20	A	1111	CLA	C2-C3-C5-C6
20	B	1221	CLA	C2-C3-C5-C6
20	2	607	CLA	C2C-C3C-CAC-CBC
20	A	1102	CLA	C5-C6-C7-C8
20	B	1204	CLA	C15-C16-C17-C18
20	B	1214	CLA	C8-C10-C11-C12
20	B	1224	CLA	C13-C15-C16-C17
20	B	1235	CLA	C15-C16-C17-C18
20	B	1240	CLA	C8-C10-C11-C12
20	4	605	CLA	C8-C10-C11-C12
20	4	612	CLA	C13-C15-C16-C17
28	J	5001	DGD	C2A-C1A-O1G-C1G
26	2	805	LMG	C11-C10-O7-C8
24	A	5004	LMT	O5B-C1B-O1B-C4'
28	J	5001	DGD	CDA-CEA-CFA-CGA
20	B	1211	CLA	C15-C16-C17-C18
20	B	1224	CLA	C15-C16-C17-C18
20	A	1139	CLA	C3-C5-C6-C7
20	B	1230	CLA	C3-C5-C6-C7
33	4	505	C7Z	C9-C10-C11-C12
20	H	1701	CLA	C5-C6-C7-C8
20	4	605	CLA	C5-C6-C7-C8
26	2	805	LMG	O9-C10-O7-C8
23	A	5001	LHG	C1-C2-C3-O3
23	A	5002	LHG	C1-C2-C3-O3
23	B	5002	LHG	C1-C2-C3-O3
23	1	801	LHG	C1-C2-C3-O3
20	A	1119	CLA	C2A-CAA-CBA-CGA
20	3	603	CLA	C2A-CAA-CBA-CGA
20	1	607	CLA	O1D-CGD-O2D-CED
20	A	1141	CLA	CBA-CGA-O2A-C1
20	B	1228	CLA	CBA-CGA-O2A-C1
20	B	1240	CLA	CBA-CGA-O2A-C1
20	F	1301	CLA	CBA-CGA-O2A-C1
20	A	1136	CLA	C8-C10-C11-C12
20	A	1137	CLA	C10-C11-C12-C13
20	A	1137	CLA	C13-C15-C16-C17
20	A	1138	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
20	B	1201	CLA	C8-C10-C11-C12
20	B	1201	CLA	C13-C15-C16-C17
20	B	1212	CLA	C5-C6-C7-C8
20	B	1223	CLA	C13-C15-C16-C17
20	B	1228	CLA	C10-C11-C12-C13
20	B	1239	CLA	C10-C11-C12-C13
20	B	1207	CLA	C8-C10-C11-C12
20	F	1301	CLA	C5-C6-C7-C8
20	F	1301	CLA	C8-C10-C11-C12
20	K	1402	CLA	C10-C11-C12-C13
20	1	601	CLA	C15-C16-C17-C18
20	1	611	CLA	C5-C6-C7-C8
20	2	607	CLA	C8-C10-C11-C12
20	B	1225	CLA	O1D-CGD-O2D-CED
20	K	1402	CLA	O1D-CGD-O2D-CED
20	A	1127	CLA	C15-C16-C17-C18
20	B	1203	CLA	C5-C6-C7-C8
20	B	1214	CLA	C15-C16-C17-C18
20	B	1228	CLA	C8-C10-C11-C12
20	B	1218	CLA	C8-C10-C11-C12
20	B	1218	CLA	C15-C16-C17-C18
20	4	604	CLA	C8-C10-C11-C12
20	4	612	CLA	C10-C11-C12-C13
20	4	617	CLA	C10-C11-C12-C13
20	A	1111	CLA	C2C-C3C-CAC-CBC
20	A	1107	CLA	C10-C11-C12-C13
20	A	1111	CLA	C13-C15-C16-C17
20	A	1115	CLA	C13-C15-C16-C17
20	A	1119	CLA	C8-C10-C11-C12
20	A	1122	CLA	C10-C11-C12-C13
20	A	1132	CLA	C13-C15-C16-C17
20	A	1134	CLA	C5-C6-C7-C8
20	B	1202	CLA	C13-C15-C16-C17
20	B	1205	CLA	C15-C16-C17-C18
20	B	1216	CLA	C8-C10-C11-C12
20	B	1219	CLA	C13-C15-C16-C17
20	B	1238	CLA	C13-C15-C16-C17
20	B	1218	CLA	C5-C6-C7-C8
20	1	614	CLA	C5-C6-C7-C8
20	3	605	CLA	C5-C6-C7-C8
20	3	610	CLA	C13-C15-C16-C17
20	4	603	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
20	A	1120	CLA	CBA-CGA-O2A-C1
28	B	5005	DGD	C2A-C1A-O1G-C1G
20	B	1237	CLA	C4-C3-C5-C6
20	4	605	CLA	C4-C3-C5-C6
20	B	1222	CLA	C2-C3-C5-C6
30	3	604	CHL	C2-C3-C5-C6
20	A	1114	CLA	O1D-CGD-O2D-CED
20	A	1136	CLA	O1D-CGD-O2D-CED
20	G	1603	CLA	O1D-CGD-O2D-CED
20	1	608	CLA	O1A-CGA-O2A-C1
20	A	1136	CLA	C15-C16-C17-C18
20	B	1021	CLA	C8-C10-C11-C12
26	F	5001	LMG	C11-C10-O7-C8
20	B	1023	CLA	C14-C13-C15-C16
20	B	1222	CLA	C14-C13-C15-C16
26	G	5002	LMG	C39-C40-C41-C42
26	F	5001	LMG	O9-C10-O7-C8
26	G	5001	LMG	C2-C1-O1-C7
28	F	5005	DGD	C2E-C1E-O5D-C6D
20	A	1121	CLA	C8-C10-C11-C12
20	A	1141	CLA	C5-C6-C7-C8
20	B	1226	CLA	C10-C11-C12-C13
23	A	5001	LHG	C7-C8-C9-C10
20	A	1128	CLA	O1D-CGD-O2D-CED
20	1	607	CLA	CBA-CGA-O2A-C1
23	2	801	LHG	O2-C2-C3-O3
23	3	801	LHG	O2-C2-C3-O3
23	4	801	LHG	O2-C2-C3-O3
20	A	1111	CLA	C16-C17-C18-C20
20	A	1126	CLA	C16-C17-C18-C19
20	B	1232	CLA	C6-C7-C8-C9
20	4	604	CLA	C11-C12-C13-C14
20	2	606	CLA	O1A-CGA-O2A-C1
22	A	4002	BCR	C11-C10-C9-C34
22	A	4007	BCR	C11-C10-C9-C34
22	I	4018	BCR	C11-C10-C9-C34
22	J	4012	BCR	C11-C10-C9-C34
33	4	505	C7Z	C11-C10-C9-C19
20	A	1124	CLA	C3-C5-C6-C7
20	A	1129	CLA	C3-C5-C6-C7
20	1	614	CLA	C3-C5-C6-C7
20	A	1106	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
22	A	4008	BCR	C7-C8-C9-C34
22	A	4011	BCR	C7-C8-C9-C34
22	F	4014	BCR	C11-C12-C13-C35
22	F	4016	BCR	C11-C12-C13-C35
22	H	4021	BCR	C11-C12-C13-C35
22	K	4001	BCR	C37-C22-C23-C24
22	K	4002	BCR	C7-C8-C9-C34
22	L	4019	BCR	C11-C12-C13-C35
22	3	506	BCR	C37-C22-C23-C24
29	J	4013	LUT	C11-C12-C13-C20
29	2	501	LUT	C31-C32-C33-C40
29	3	502	LUT	C7-C8-C9-C19
29	3	502	LUT	C11-C12-C13-C20
29	4	501	LUT	C27-C28-C29-C39
33	4	505	C7Z	C11-C12-C13-C20
33	4	505	C7Z	C31-C32-C33-C40
22	A	4003	BCR	C17-C18-C19-C20
22	B	4005	BCR	C17-C18-C19-C20
22	F	4016	BCR	C17-C18-C19-C20
22	H	4021	BCR	C21-C22-C23-C24
22	K	4001	BCR	C21-C22-C23-C24
22	2	503	BCR	C11-C12-C13-C14
22	3	506	BCR	C21-C22-C23-C24
29	4	501	LUT	C27-C28-C29-C30
28	F	5005	DGD	O6D-C5D-C6D-O5D
20	A	1141	CLA	O1A-CGA-O2A-C1
20	A	1135	CLA	C2A-CAA-CBA-CGA
20	B	1217	CLA	C2A-CAA-CBA-CGA
20	L	1502	CLA	C2A-CAA-CBA-CGA
20	3	610	CLA	C2A-CAA-CBA-CGA
20	A	1109	CLA	C10-C11-C12-C13
20	L	1502	CLA	C5-C6-C7-C8
20	2	603	CLA	C5-C6-C7-C8
23	B	5001	LHG	O1-C1-C2-C3
23	1	801	LHG	O1-C1-C2-C3
23	3	801	LHG	O1-C1-C2-C3
20	2	606	CLA	C2C-C3C-CAC-CBC
20	A	1131	CLA	C16-C17-C18-C19
20	B	1204	CLA	C16-C17-C18-C20
20	B	1219	CLA	C16-C17-C18-C20
20	B	1221	CLA	C16-C17-C18-C19
20	G	1603	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
20	1	603	CLA	C6-C7-C8-C10
20	3	603	CLA	C6-C7-C8-C10
20	B	1222	CLA	O1D-CGD-O2D-CED
20	F	1301	CLA	O1A-CGA-O2A-C1
20	B	1225	CLA	C13-C15-C16-C17
24	G	5004	LMT	C4'-C5'-C6'-O6'
22	A	4002	BCR	C11-C10-C9-C8
22	A	4007	BCR	C11-C10-C9-C8
22	I	4018	BCR	C11-C10-C9-C8
22	J	4012	BCR	C11-C10-C9-C8
28	F	5005	DGD	O6E-C1E-O5D-C6D
26	B	5007	LMG	C11-C10-O7-C8
26	2	804	LMG	C11-C10-O7-C8
32	2	807	3PH	C22-C21-O21-C2
20	L	1502	CLA	C10-C11-C12-C13
28	F	5005	DGD	C4D-C5D-C6D-O5D
20	A	1102	CLA	O1D-CGD-O2D-CED
28	1	803	DGD	C2A-C1A-O1G-C1G
20	A	1112	CLA	C13-C15-C16-C17
20	A	1126	CLA	C15-C16-C17-C18
20	4	604	CLA	C3-C5-C6-C7
20	B	1231	CLA	O1D-CGD-O2D-CED
20	A	1118	CLA	C2-C1-O2A-CGA
20	B	1206	CLA	C2-C1-O2A-CGA
20	B	1213	CLA	C2-C1-O2A-CGA
20	B	1225	CLA	C2-C1-O2A-CGA
20	B	1227	CLA	C2-C1-O2A-CGA
20	B	1230	CLA	C2-C1-O2A-CGA
20	B	1232	CLA	C2-C1-O2A-CGA
20	B	1236	CLA	C2-C1-O2A-CGA
20	B	1239	CLA	C2-C1-O2A-CGA
20	L	1502	CLA	C2-C1-O2A-CGA
20	L	1503	CLA	C2-C1-O2A-CGA
20	1	605	CLA	C2-C1-O2A-CGA
20	1	611	CLA	C2-C1-O2A-CGA
20	2	608	CLA	C2-C1-O2A-CGA
20	4	612	CLA	C2-C1-O2A-CGA
19	A	1011	CL0	C16-C17-C18-C19
20	A	1104	CLA	C16-C17-C18-C20
20	A	1107	CLA	C16-C17-C18-C19
20	A	1112	CLA	C16-C17-C18-C20
20	A	1122	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
20	A	1133	CLA	C16-C17-C18-C19
20	B	1212	CLA	C6-C7-C8-C10
20	B	1221	CLA	C16-C17-C18-C20
20	B	1207	CLA	C16-C17-C18-C19
20	B	1240	CLA	C16-C17-C18-C19
20	G	1603	CLA	C16-C17-C18-C20
20	K	1402	CLA	C11-C12-C13-C14
20	1	604	CLA	C16-C17-C18-C19
20	2	607	CLA	C11-C12-C13-C14
20	4	603	CLA	C16-C17-C18-C19
20	4	604	CLA	C11-C12-C13-C15
20	4	617	CLA	C16-C17-C18-C19
30	1	612	CHL	C11-C12-C13-C15
20	B	1240	CLA	O1A-CGA-O2A-C1
23	A	5001	LHG	C11-C12-C13-C14
23	1	801	LHG	C30-C31-C32-C33
20	B	1235	CLA	O1A-CGA-O2A-C1
28	J	5001	DGD	O1A-C1A-O1G-C1G
23	A	5002	LHG	C12-C13-C14-C15
26	B	5007	LMG	O9-C10-O7-C8
26	2	804	LMG	O9-C10-O7-C8
23	2	801	LHG	O1-C1-C2-O2
23	4	801	LHG	O1-C1-C2-O2
20	B	1217	CLA	CBD-CGD-O2D-CED
26	G	5001	LMG	C13-C14-C15-C16
20	B	1217	CLA	C4B-C3B-CAB-CBB
20	F	1302	CLA	C4B-C3B-CAB-CBB
20	K	1404	CLA	C4B-C3B-CAB-CBB
20	1	602	CLA	C4B-C3B-CAB-CBB
20	2	608	CLA	C4B-C3B-CAB-CBB
20	3	605	CLA	C4B-C3B-CAB-CBB
23	A	5001	LHG	C15-C16-C17-C18
20	A	1106	CLA	C16-C17-C18-C20
20	A	1111	CLA	C16-C17-C18-C19
20	A	1112	CLA	C16-C17-C18-C19
20	A	1131	CLA	C16-C17-C18-C20
20	A	1133	CLA	C16-C17-C18-C20
20	B	1219	CLA	C16-C17-C18-C19
20	B	1223	CLA	C16-C17-C18-C19
20	B	1232	CLA	C6-C7-C8-C10
20	B	1207	CLA	C16-C17-C18-C20
20	B	1240	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
20	L	1502	CLA	C11-C12-C13-C14
20	3	603	CLA	C6-C7-C8-C9
20	4	603	CLA	C16-C17-C18-C20
20	B	1204	CLA	O1D-CGD-O2D-CED
20	H	1701	CLA	C2A-CAA-CBA-CGA
20	2	606	CLA	C2A-CAA-CBA-CGA
30	3	604	CHL	C2A-CAA-CBA-CGA
28	F	5005	DGD	C2A-C3A-C4A-C5A
20	A	1131	CLA	C5-C6-C7-C8
20	B	1221	CLA	C5-C6-C7-C8
20	B	1231	CLA	C8-C10-C11-C12
20	4	617	CLA	C5-C6-C7-C8
26	F	5003	LMG	C11-C10-O7-C8
20	A	1131	CLA	C11-C12-C13-C15
20	B	1208	CLA	C6-C7-C8-C10
20	B	1210	CLA	C11-C10-C8-C7
20	2	605	CLA	C6-C7-C8-C10
20	2	605	CLA	C11-C12-C13-C15
20	4	612	CLA	C6-C7-C8-C10
23	1	801	LHG	C13-C14-C15-C16
28	J	5001	DGD	C1A-C2A-C3A-C4A
20	B	1205	CLA	O1D-CGD-O2D-CED
20	A	1139	CLA	C13-C15-C16-C17
20	G	1603	CLA	C5-C6-C7-C8
23	A	5002	LHG	C31-C32-C33-C34
20	A	1104	CLA	C3-C5-C6-C7
20	A	1101	CLA	C3A-C2A-CAA-CBA
20	A	1104	CLA	C3A-C2A-CAA-CBA
20	A	1105	CLA	C3A-C2A-CAA-CBA
20	A	1110	CLA	C3A-C2A-CAA-CBA
20	B	1221	CLA	C3A-C2A-CAA-CBA
20	G	1602	CLA	C3A-C2A-CAA-CBA
20	J	1901	CLA	C3A-C2A-CAA-CBA
20	K	1403	CLA	C3A-C2A-CAA-CBA
20	L	1503	CLA	C3A-C2A-CAA-CBA
20	1	602	CLA	C3A-C2A-CAA-CBA
20	1	603	CLA	C3A-C2A-CAA-CBA
20	2	605	CLA	C3A-C2A-CAA-CBA
20	3	605	CLA	C3A-C2A-CAA-CBA
20	3	613	CLA	C3A-C2A-CAA-CBA
20	4	617	CLA	C3A-C2A-CAA-CBA
30	2	613	CHL	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
20	B	1211	CLA	O1D-CGD-O2D-CED
20	3	605	CLA	O1D-CGD-O2D-CED
28	B	5005	DGD	CCB-CDB-CEB-CFB
20	A	1101	CLA	C5-C6-C7-C8
20	A	1131	CLA	C13-C15-C16-C17
20	A	1133	CLA	C8-C10-C11-C12
20	B	1211	CLA	C13-C15-C16-C17
20	2	603	CLA	C15-C16-C17-C18
26	2	805	LMG	C8-C9-O8-C28
22	F	4016	BCR	C9-C10-C11-C12
20	A	1115	CLA	C16-C17-C18-C19
20	A	1115	CLA	C16-C17-C18-C20
20	B	1222	CLA	C16-C17-C18-C19
20	B	1222	CLA	C16-C17-C18-C20
20	B	1223	CLA	C16-C17-C18-C20
20	L	1502	CLA	C11-C12-C13-C15
20	3	601	CLA	C6-C7-C8-C10
20	A	1120	CLA	O1A-CGA-O2A-C1
20	B	1228	CLA	O1A-CGA-O2A-C1
23	B	5002	LHG	C31-C32-C33-C34
32	2	807	3PH	O22-C21-O21-C2
20	B	1235	CLA	O1D-CGD-O2D-CED
20	A	1128	CLA	CBA-CGA-O2A-C1
20	B	1234	CLA	CBA-CGA-O2A-C1
26	G	5001	LMG	C7-C8-C9-O8
28	4	802	DGD	O1G-C1G-C2G-C3G
20	A	1137	CLA	C3-C5-C6-C7
20	B	1229	CLA	C3-C5-C6-C7
26	F	5003	LMG	C10-C11-C12-C13
23	A	5002	LHG	C28-C29-C30-C31
23	1	801	LHG	C11-C12-C13-C14
28	B	5005	DGD	O1A-C1A-O1G-C1G
28	1	803	DGD	O1A-C1A-O1G-C1G
24	B	5008	LMT	C4'-C5'-C6'-O6'
19	A	1011	CL0	C16-C17-C18-C20
20	A	1110	CLA	C6-C7-C8-C9
20	A	1122	CLA	C16-C17-C18-C20
20	B	1205	CLA	C16-C17-C18-C20
20	B	1212	CLA	C6-C7-C8-C9
20	B	1226	CLA	C16-C17-C18-C19
20	K	1402	CLA	C11-C12-C13-C15
26	B	5004	LMG	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
20	B	1214	CLA	C2B-C3B-CAB-CBB
20	B	1217	CLA	C2B-C3B-CAB-CBB
20	1	602	CLA	C2B-C3B-CAB-CBB
20	2	608	CLA	C2B-C3B-CAB-CBB
22	A	4003	BCR	C23-C24-C25-C30
22	B	4009	BCR	C23-C24-C25-C26
22	B	4009	BCR	C23-C24-C25-C30
22	B	4010	BCR	C1-C6-C7-C8
22	B	4010	BCR	C5-C6-C7-C8
22	G	4011	BCR	C23-C24-C25-C26
22	G	4011	BCR	C23-C24-C25-C30
22	H	4021	BCR	C1-C6-C7-C8
22	H	4021	BCR	C5-C6-C7-C8
22	I	4020	BCR	C23-C24-C25-C26
22	I	4020	BCR	C23-C24-C25-C30
22	J	4012	BCR	C1-C6-C7-C8
22	L	4019	BCR	C23-C24-C25-C26
22	L	4019	BCR	C23-C24-C25-C30
22	1	503	BCR	C1-C6-C7-C8
22	2	503	BCR	C1-C6-C7-C8
22	2	503	BCR	C5-C6-C7-C8
22	3	506	BCR	C1-C6-C7-C8
29	1	501	LUT	C1-C6-C7-C8
29	1	501	LUT	C5-C6-C7-C8
33	4	505	C7Z	C25-C26-C27-C28
28	B	5005	DGD	C4A-C5A-C6A-C7A
20	A	1111	CLA	C15-C16-C17-C18
20	H	1701	CLA	C8-C10-C11-C12
20	4	601	CLA	C8-C10-C11-C12
20	A	1116	CLA	C3-C5-C6-C7
23	B	5001	LHG	C24-C23-O8-C6
20	A	1109	CLA	C2A-CAA-CBA-CGA
20	B	1224	CLA	C2A-CAA-CBA-CGA
20	1	604	CLA	C2A-CAA-CBA-CGA
26	F	5003	LMG	O9-C10-O7-C8
20	A	1102	CLA	C4-C3-C5-C6
26	G	5002	LMG	C12-C13-C14-C15
22	A	4007	BCR	C10-C11-C12-C13
22	B	4006	BCR	C10-C11-C12-C13
22	B	4009	BCR	C10-C11-C12-C13
22	I	4018	BCR	C10-C11-C12-C13
22	I	4020	BCR	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
22	K	4002	BCR	C18-C19-C20-C21
22	1	503	BCR	C10-C11-C12-C13
20	A	1109	CLA	C13-C15-C16-C17
20	A	1115	CLA	C2-C3-C5-C6
20	4	605	CLA	C2-C3-C5-C6
20	A	1126	CLA	C16-C17-C18-C20
20	1	605	CLA	C16-C17-C18-C19
30	1	612	CHL	C11-C12-C13-C14
23	A	5002	LHG	C26-C27-C28-C29
20	B	1215	CLA	CBA-CGA-O2A-C1
20	B	1226	CLA	CBA-CGA-O2A-C1
20	B	1238	CLA	CBA-CGA-O2A-C1
20	B	1207	CLA	CBA-CGA-O2A-C1
20	4	604	CLA	CBA-CGA-O2A-C1
20	A	1112	CLA	C14-C13-C15-C16
20	A	1103	CLA	C5-C6-C7-C8
20	B	1211	CLA	C5-C6-C7-C8
23	B	5002	LHG	C14-C15-C16-C17
24	B	5006	LMT	O5'-C1'-O1'-C1
20	A	1122	CLA	C15-C16-C17-C18
20	1	614	CLA	C8-C10-C11-C12
20	2	605	CLA	C8-C10-C11-C12
23	A	5002	LHG	C27-C28-C29-C30
23	A	5002	LHG	C32-C33-C34-C35
23	B	5002	LHG	C11-C12-C13-C14
23	4	801	LHG	C11-C12-C13-C14
30	2	613	CHL	C2C-C3C-CAC-CBC
20	B	1210	CLA	C3-C5-C6-C7
20	B	1212	CLA	CBA-CGA-O2A-C1
20	A	1130	CLA	C6-C7-C8-C9
20	B	1235	CLA	C16-C17-C18-C20
20	A	1112	CLA	CBD-CGD-O2D-CED
23	A	5001	LHG	C8-C7-O7-C5
23	A	5002	LHG	C8-C7-O7-C5
23	1	801	LHG	C8-C7-O7-C5
26	1	802	LMG	C11-C10-O7-C8
20	A	1104	CLA	C8-C10-C11-C12
20	3	617	CLA	C10-C11-C12-C13
20	4	604	CLA	C5-C6-C7-C8
23	1	801	LHG	O9-C7-O7-C5
23	1	801	LHG	C35-C36-C37-C38
20	B	1215	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
20	B	1227	CLA	C5-C6-C7-C8
22	1	503	BCR	C36-C18-C19-C20
22	I	4020	BCR	C17-C18-C19-C20
29	2	501	LUT	C31-C32-C33-C34
31	4	502	XAT	C27-C28-C29-C30
26	B	5007	LMG	C8-C7-O1-C1
20	L	1501	CLA	C2A-CAA-CBA-CGA
20	A	1107	CLA	C16-C17-C18-C20
20	A	1110	CLA	C6-C7-C8-C10
20	A	1117	CLA	C16-C17-C18-C19
20	A	1117	CLA	C16-C17-C18-C20
20	A	1130	CLA	C6-C7-C8-C10
20	A	1141	CLA	C11-C12-C13-C14
20	A	1141	CLA	C11-C12-C13-C15
20	B	1205	CLA	C16-C17-C18-C19
20	2	607	CLA	C11-C12-C13-C15
20	A	1103	CLA	C4-C3-C5-C6
20	A	1117	CLA	C4-C3-C5-C6
20	A	1117	CLA	C2-C3-C5-C6
20	B	1237	CLA	C2-C3-C5-C6
26	G	5002	LMG	C16-C17-C18-C19
20	A	1128	CLA	O1A-CGA-O2A-C1
20	4	604	CLA	O1A-CGA-O2A-C1
26	F	5006	LMG	O6-C5-C6-O5
20	A	1105	CLA	C10-C11-C12-C13
20	B	1229	CLA	C5-C6-C7-C8
20	1	604	CLA	C8-C10-C11-C12
26	G	5002	LMG	C31-C32-C33-C34
20	B	1225	CLA	C15-C16-C17-C18
20	B	1229	CLA	C15-C16-C17-C18
20	B	1204	CLA	C16-C17-C18-C19
20	1	605	CLA	C16-C17-C18-C20
20	B	1234	CLA	O1A-CGA-O2A-C1
24	G	5005	LMT	O5B-C5B-C6B-O6B
28	3	803	DGD	O6E-C5E-C6E-O5E
23	1	801	LHG	C28-C29-C30-C31
26	B	5004	LMG	C28-C29-C30-C31
20	A	1136	CLA	C10-C11-C12-C13
20	A	1141	CLA	C8-C10-C11-C12
20	B	1215	CLA	C15-C16-C17-C18
26	B	5007	LMG	O6-C5-C6-O5
28	B	5005	DGD	O6E-C5E-C6E-O5E

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Mol	Chain	Res	Type	Atoms
26	G	5001	LMG	O7-C8-C9-O8
28	4	802	DGD	O2G-C2G-C3G-O3G
20	A	1140	CLA	CBA-CGA-O2A-C1
20	B	1229	CLA	CBA-CGA-O2A-C1
20	A	1126	CLA	C5-C6-C7-C8
20	B	1216	CLA	C13-C15-C16-C17
20	A	1124	CLA	C2-C1-O2A-CGA
20	B	1022	CLA	C2-C1-O2A-CGA
20	B	1220	CLA	C2-C1-O2A-CGA
20	J	1901	CLA	C2-C1-O2A-CGA
20	1	606	CLA	C2-C1-O2A-CGA
20	4	602	CLA	C2-C1-O2A-CGA
20	A	1134	CLA	C6-C7-C8-C10
28	F	5005	DGD	O6E-C5E-C6E-O5E
23	B	5002	LHG	C17-C18-C19-C20
20	A	1128	CLA	C4-C3-C5-C6
20	A	1101	CLA	C2-C3-C5-C6
20	A	1102	CLA	C2-C3-C5-C6
20	A	1103	CLA	C2-C3-C5-C6
30	2	615	CHL	C2-C3-C5-C6
23	3	801	LHG	C1-C2-C3-O3
23	A	5002	LHG	C11-C12-C13-C14
23	A	5002	LHG	C13-C14-C15-C16
28	J	5001	DGD	C2B-C3B-C4B-C5B
20	A	1130	CLA	C2A-CAA-CBA-CGA
20	B	1022	CLA	C2A-CAA-CBA-CGA
20	2	602	CLA	C2A-CAA-CBA-CGA
30	1	610	CHL	C2A-CAA-CBA-CGA
20	A	1118	CLA	O1D-CGD-O2D-CED
20	B	1218	CLA	C16-C17-C18-C20
20	4	617	CLA	C16-C17-C18-C20
23	A	5001	LHG	O1-C1-C2-O2
20	B	1229	CLA	O1A-CGA-O2A-C1
20	B	1238	CLA	O1A-CGA-O2A-C1
20	1	604	CLA	C3-C5-C6-C7
20	A	1101	CLA	C1A-C2A-CAA-CBA
20	A	1102	CLA	C1A-C2A-CAA-CBA
20	A	1104	CLA	C1A-C2A-CAA-CBA
20	A	1106	CLA	C1A-C2A-CAA-CBA
20	A	1120	CLA	C1A-C2A-CAA-CBA
20	A	1127	CLA	C1A-C2A-CAA-CBA
20	A	1133	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
20	A	1137	CLA	C1A-C2A-CAA-CBA
20	B	1208	CLA	C1A-C2A-CAA-CBA
20	B	1209	CLA	C1A-C2A-CAA-CBA
20	B	1211	CLA	C1A-C2A-CAA-CBA
20	B	1226	CLA	C1A-C2A-CAA-CBA
20	B	1236	CLA	C1A-C2A-CAA-CBA
20	B	1239	CLA	C1A-C2A-CAA-CBA
20	B	1218	CLA	C1A-C2A-CAA-CBA
20	G	1602	CLA	C1A-C2A-CAA-CBA
20	G	1603	CLA	C1A-C2A-CAA-CBA
20	J	1901	CLA	C1A-C2A-CAA-CBA
20	K	1403	CLA	C1A-C2A-CAA-CBA
20	1	601	CLA	C1A-C2A-CAA-CBA
20	1	602	CLA	C1A-C2A-CAA-CBA
20	1	608	CLA	C1A-C2A-CAA-CBA
20	2	603	CLA	C1A-C2A-CAA-CBA
20	2	604	CLA	C1A-C2A-CAA-CBA
20	3	605	CLA	C1A-C2A-CAA-CBA
20	3	606	CLA	C1A-C2A-CAA-CBA
20	3	610	CLA	C1A-C2A-CAA-CBA
20	3	613	CLA	C1A-C2A-CAA-CBA
20	4	601	CLA	C1A-C2A-CAA-CBA
20	4	607	CLA	C1A-C2A-CAA-CBA
23	2	801	LHG	C25-C26-C27-C28
20	B	1226	CLA	O1A-CGA-O2A-C1
20	A	1111	CLA	C4C-C3C-CAC-CBC
30	3	604	CHL	C5-C6-C7-C8
32	2	807	3PH	O11-C1-C2-C3
26	G	5002	LMG	O6-C5-C6-O5
26	2	803	LMG	O6-C5-C6-O5
23	A	5002	LHG	O9-C7-O7-C5
20	A	1102	CLA	C11-C12-C13-C15
20	A	1117	CLA	C11-C10-C8-C7
20	A	1126	CLA	C11-C10-C8-C7
20	A	1139	CLA	C12-C13-C15-C16
20	B	1201	CLA	C11-C10-C8-C7
20	B	1201	CLA	C11-C12-C13-C15
20	B	1203	CLA	C11-C12-C13-C15
20	B	1204	CLA	C11-C12-C13-C15
20	B	1204	CLA	C12-C13-C15-C16
20	B	1216	CLA	C12-C13-C15-C16
20	B	1219	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
20	B	1226	CLA	C11-C12-C13-C15
20	B	1226	CLA	C12-C13-C15-C16
20	B	1227	CLA	C11-C12-C13-C15
20	B	1229	CLA	C12-C13-C15-C16
20	B	1231	CLA	C6-C7-C8-C10
20	B	1218	CLA	C12-C13-C15-C16
20	F	1302	CLA	C11-C10-C8-C7
20	G	1603	CLA	C12-C13-C15-C16
20	L	1502	CLA	C6-C7-C8-C10
20	1	604	CLA	C11-C12-C13-C15
20	2	607	CLA	C6-C7-C8-C10
20	4	601	CLA	C11-C10-C8-C7
20	4	603	CLA	C12-C13-C15-C16
20	4	617	CLA	C11-C10-C8-C7
21	B	2002	PQN	C16-C17-C18-C20
20	A	1012	CLA	C16-C17-C18-C19
20	A	1129	CLA	C13-C15-C16-C17
20	2	604	CLA	C15-C16-C17-C18
20	A	1140	CLA	O1A-CGA-O2A-C1
20	B	1207	CLA	O1A-CGA-O2A-C1
20	B	1210	CLA	CBA-CGA-O2A-C1
20	F	1302	CLA	C8-C10-C11-C12
20	4	603	CLA	C5-C6-C7-C8
26	B	5003	LMG	C10-C11-C12-C13
20	3	610	CLA	C2-C3-C5-C6
23	1	801	LHG	C24-C25-C26-C27
23	2	801	LHG	C11-C12-C13-C14
26	A	5006	LMG	O6-C5-C6-O5
20	A	1111	CLA	C8-C10-C11-C12
20	B	1224	CLA	C10-C11-C12-C13
20	A	1105	CLA	C2C-C3C-CAC-CBC
20	A	1140	CLA	C2A-CAA-CBA-CGA
20	2	605	CLA	C2A-CAA-CBA-CGA
20	A	1103	CLA	C11-C12-C13-C14
20	A	1104	CLA	C11-C12-C13-C14
20	A	1129	CLA	C6-C7-C8-C9
20	A	1132	CLA	C11-C12-C13-C14
20	A	1012	CLA	C6-C7-C8-C9
20	A	1139	CLA	C14-C13-C15-C16
20	B	1237	CLA	C11-C10-C8-C9
20	B	1201	CLA	C11-C10-C8-C9
20	B	1203	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
20	B	1219	CLA	C11-C12-C13-C14
20	B	1226	CLA	C6-C7-C8-C9
20	B	1229	CLA	C14-C13-C15-C16
20	1	611	CLA	C6-C7-C8-C9
20	3	610	CLA	C14-C13-C15-C16
20	4	605	CLA	C6-C7-C8-C9
21	B	2002	PQN	C16-C17-C18-C19
30	3	604	CHL	C11-C12-C13-C14
28	1	803	DGD	O6E-C5E-C6E-O5E
26	F	5001	LMG	C10-C11-C12-C13
22	K	4002	BCR	C19-C20-C21-C22
28	1	803	DGD	O6D-C5D-C6D-O5D
20	A	1106	CLA	CBA-CGA-O2A-C1
23	A	5002	LHG	C24-C23-O8-C6
20	A	1129	CLA	C15-C16-C17-C18
20	A	1139	CLA	C10-C11-C12-C13
26	G	5001	LMG	O6-C5-C6-O5
23	B	5001	LHG	C5-C6-O8-C23
28	J	5001	DGD	C2E-C1E-O5D-C6D
28	4	802	DGD	C2D-C1D-O3G-C3G
24	G	5004	LMT	C2B-C1B-O1B-C4'
20	B	1237	CLA	C10-C11-C12-C13
20	B	1205	CLA	C8-C10-C11-C12
20	B	1238	CLA	C5-C6-C7-C8
26	B	5004	LMG	O6-C5-C6-O5
26	F	5002	LMG	O1-C7-C8-C9
26	F	5004	LMG	C7-C8-C9-O8
32	2	807	3PH	C1-C2-C3-O31
20	B	1212	CLA	O1A-CGA-O2A-C1
20	A	1127	CLA	C3-C5-C6-C7
24	A	5004	LMT	C1-C2-C3-C4
24	B	5006	LMT	C4'-C5'-C6'-O6'
20	A	1111	CLA	CBA-CGA-O2A-C1
20	A	1116	CLA	CBA-CGA-O2A-C1
20	B	1236	CLA	CBA-CGA-O2A-C1
26	1	802	LMG	O6-C5-C6-O5
28	4	802	DGD	O6E-C5E-C6E-O5E
20	1	601	CLA	C16-C17-C18-C20
20	1	604	CLA	C16-C17-C18-C20
23	B	5002	LHG	C34-C35-C36-C37
30	3	607	CHL	CHA-CBD-CGD-O1D
30	3	607	CHL	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
20	A	1128	CLA	C10-C11-C12-C13
20	B	1023	CLA	C8-C10-C11-C12
20	B	1224	CLA	C8-C10-C11-C12
24	A	5004	LMT	C4'-C5'-C6'-O6'
20	A	1101	CLA	C4-C3-C5-C6
30	2	615	CHL	C4-C3-C5-C6
20	A	1102	CLA	C10-C11-C12-C13
20	A	1104	CLA	C5-C6-C7-C8
20	A	1120	CLA	C5-C6-C7-C8
20	A	1123	CLA	C8-C10-C11-C12
20	B	1023	CLA	C13-C15-C16-C17
22	A	4003	BCR	C37-C22-C23-C24
22	1	503	BCR	C37-C22-C23-C24
26	1	802	LMG	O9-C10-O7-C8
20	B	1218	CLA	C16-C17-C18-C19
23	B	5002	LHG	C13-C14-C15-C16
26	2	806	LMG	O6-C5-C6-O5
22	A	4003	BCR	C21-C22-C23-C24
22	B	4006	BCR	C21-C22-C23-C24
22	K	4002	BCR	C7-C8-C9-C10
22	1	503	BCR	C21-C22-C23-C24
20	4	603	CLA	C13-C15-C16-C17
23	1	801	LHG	C33-C34-C35-C36
20	A	1119	CLA	CBA-CGA-O2A-C1
20	4	602	CLA	CBA-CGA-O2A-C1
30	2	609	CHL	O2A-C1-C2-C3
24	G	5004	LMT	C6-C7-C8-C9
26	G	5001	LMG	C31-C32-C33-C34
22	J	4012	BCR	C19-C20-C21-C22
29	1	501	LUT	C29-C30-C31-C32
29	3	501	LUT	C29-C30-C31-C32
23	1	801	LHG	C23-C24-C25-C26
26	F	5002	LMG	C34-C35-C36-C37
26	G	5001	LMG	O6-C1-O1-C7
20	B	1221	CLA	CBD-CGD-O2D-CED
20	B	1210	CLA	O1A-CGA-O2A-C1
20	4	601	CLA	C4-C3-C5-C6
20	A	1138	CLA	C2-C3-C5-C6
20	A	1104	CLA	C16-C17-C18-C19
20	A	1012	CLA	C16-C17-C18-C20
20	B	1206	CLA	C16-C17-C18-C20
28	F	5005	DGD	O1G-C1G-C2G-O2G

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Mol	Chain	Res	Type	Atoms
20	A	1117	CLA	CBA-CGA-O2A-C1
30	4	615	CHL	C2C-C3C-CAC-CBC
26	G	5002	LMG	C29-C30-C31-C32
20	3	612	CLA	C2A-CAA-CBA-CGA
20	4	617	CLA	C2A-CAA-CBA-CGA
20	1	601	CLA	C3-C5-C6-C7
20	3	617	CLA	C3-C5-C6-C7
20	B	1240	CLA	O1D-CGD-O2D-CED
20	3	606	CLA	C2-C1-O2A-CGA
20	A	1121	CLA	C11-C12-C13-C15
26	3	802	LMG	C11-C12-C13-C14
20	B	1216	CLA	CBA-CGA-O2A-C1
26	G	5002	LMG	C32-C33-C34-C35
20	1	607	CLA	O1A-CGA-O2A-C1
20	A	1116	CLA	C5-C6-C7-C8
20	A	1132	CLA	C8-C10-C11-C12
20	A	1140	CLA	C15-C16-C17-C18
20	B	1221	CLA	C10-C11-C12-C13
20	B	1222	CLA	C5-C6-C7-C8
20	A	1117	CLA	C8-C10-C11-C12
20	1	611	CLA	C8-C10-C11-C12
20	A	1105	CLA	C11-C12-C13-C15
20	A	1121	CLA	C4-C3-C5-C6
20	A	1136	CLA	C4-C3-C5-C6
30	1	612	CHL	C4-C3-C5-C6
20	A	1115	CLA	CBA-CGA-O2A-C1
20	B	1201	CLA	CBA-CGA-O2A-C1
20	1	614	CLA	CBA-CGA-O2A-C1
20	A	1101	CLA	C13-C15-C16-C17
20	4	603	CLA	C15-C16-C17-C18
23	A	5001	LHG	O9-C7-O7-C5
23	A	5002	LHG	O1-C1-C2-O2
24	B	5008	LMT	C2-C1-O1'-C1'
20	A	1102	CLA	C11-C12-C13-C14
20	A	1102	CLA	C14-C13-C15-C16
20	A	1103	CLA	C14-C13-C15-C16
20	A	1106	CLA	C11-C12-C13-C14
20	A	1117	CLA	C11-C10-C8-C9
20	A	1123	CLA	C11-C10-C8-C9
20	A	1123	CLA	C11-C12-C13-C14
20	A	1128	CLA	C11-C10-C8-C9
20	A	1133	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
20	A	1133	CLA	C11-C12-C13-C14
20	A	1012	CLA	C11-C10-C8-C9
20	A	1013	CLA	C14-C13-C15-C16
20	A	1138	CLA	C11-C12-C13-C14
20	B	1023	CLA	C11-C12-C13-C14
20	B	1201	CLA	C11-C12-C13-C14
20	B	1206	CLA	C11-C10-C8-C9
20	B	1208	CLA	C6-C7-C8-C9
20	B	1211	CLA	C6-C7-C8-C9
20	B	1215	CLA	C14-C13-C15-C16
20	B	1221	CLA	C6-C7-C8-C9
20	B	1226	CLA	C14-C13-C15-C16
20	B	1227	CLA	C11-C12-C13-C14
20	F	1302	CLA	C11-C10-C8-C9
20	F	1301	CLA	C11-C12-C13-C14
20	1	601	CLA	C14-C13-C15-C16
20	1	604	CLA	C11-C12-C13-C14
20	1	605	CLA	C6-C7-C8-C9
20	2	605	CLA	C11-C12-C13-C14
20	3	610	CLA	C11-C12-C13-C14
20	4	601	CLA	C11-C10-C8-C9
20	B	1222	CLA	C8-C10-C11-C12
20	B	1232	CLA	C5-C6-C7-C8
20	B	1239	CLA	C15-C16-C17-C18
20	B	1215	CLA	O1A-CGA-O2A-C1
20	A	1102	CLA	C4B-C3B-CAB-CBB
20	A	1120	CLA	C4B-C3B-CAB-CBB
20	A	1126	CLA	C4B-C3B-CAB-CBB
20	A	1131	CLA	C4B-C3B-CAB-CBB
20	A	1012	CLA	C4B-C3B-CAB-CBB
20	B	1022	CLA	C4B-C3B-CAB-CBB
20	G	1603	CLA	C4B-C3B-CAB-CBB
20	1	613	CLA	C4B-C3B-CAB-CBB
20	2	607	CLA	C4C-C3C-CAC-CBC
26	1	802	LMG	O7-C10-C11-C12
28	1	803	DGD	C2A-C3A-C4A-C5A
21	A	2001	PQN	C18-C20-C21-C22
20	G	1603	CLA	C2A-CAA-CBA-CGA
20	B	1217	CLA	O1D-CGD-O2D-CED
24	B	5006	LMT	C2'-C1'-O1'-C1
26	B	5004	LMG	C2-C1-O1-C7
26	2	805	LMG	C2-C1-O1-C7

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Mol	Chain	Res	Type	Atoms
28	F	5005	DGD	C2D-C1D-O3G-C3G
28	1	803	DGD	C2E-C1E-O5D-C6D
23	1	801	LHG	C29-C30-C31-C32
23	A	5002	LHG	O6-C4-C5-C6
23	B	5002	LHG	O6-C4-C5-C6
23	3	801	LHG	O6-C4-C5-C6
28	1	803	DGD	O1G-C1A-C2A-C3A
20	A	1103	CLA	C11-C12-C13-C15
20	A	1104	CLA	C11-C12-C13-C15
20	A	1106	CLA	C11-C12-C13-C15
20	A	1115	CLA	C11-C10-C8-C7
20	A	1123	CLA	C11-C10-C8-C7
20	A	1128	CLA	C11-C10-C8-C7
20	A	1132	CLA	C11-C12-C13-C15
20	A	1133	CLA	C6-C7-C8-C10
20	A	1133	CLA	C11-C12-C13-C15
20	A	1137	CLA	C11-C12-C13-C15
20	A	1012	CLA	C6-C7-C8-C10
20	B	1023	CLA	C11-C12-C13-C15
20	B	1237	CLA	C11-C10-C8-C7
20	B	1206	CLA	C11-C10-C8-C7
20	B	1208	CLA	C11-C10-C8-C7
20	B	1211	CLA	C11-C10-C8-C7
20	B	1214	CLA	C11-C10-C8-C7
20	B	1215	CLA	C12-C13-C15-C16
20	B	1221	CLA	C6-C7-C8-C10
20	B	1221	CLA	C12-C13-C15-C16
20	B	1222	CLA	C6-C7-C8-C10
20	B	1226	CLA	C6-C7-C8-C10
20	B	1226	CLA	C11-C10-C8-C7
20	B	1235	CLA	C6-C7-C8-C10
20	F	1301	CLA	C11-C12-C13-C15
20	1	601	CLA	C12-C13-C15-C16
20	1	605	CLA	C6-C7-C8-C10
20	1	611	CLA	C6-C7-C8-C10
20	3	610	CLA	C11-C12-C13-C15
20	4	605	CLA	C6-C7-C8-C10
20	4	617	CLA	C6-C7-C8-C10
20	B	1222	CLA	C10-C11-C12-C13
20	1	605	CLA	C15-C16-C17-C18
28	4	802	DGD	C2B-C3B-C4B-C5B
20	A	1111	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
20	B	1236	CLA	O1A-CGA-O2A-C1
20	A	1134	CLA	C3A-C2A-CAA-CBA
20	B	1204	CLA	C3A-C2A-CAA-CBA
20	B	1213	CLA	C3A-C2A-CAA-CBA
20	B	1228	CLA	C3A-C2A-CAA-CBA
20	B	1207	CLA	C3A-C2A-CAA-CBA
20	H	1701	CLA	C3A-C2A-CAA-CBA
20	3	610	CLA	C4-C3-C5-C6
20	4	605	CLA	C3A-C2A-CAA-CBA
30	2	611	CHL	C3A-C2A-CAA-CBA
30	4	611	CHL	C3A-C2A-CAA-CBA
20	1	605	CLA	C13-C15-C16-C17
20	B	1240	CLA	CAA-CBA-CGA-O2A
20	A	1106	CLA	O1A-CGA-O2A-C1
20	A	1119	CLA	O1A-CGA-O2A-C1
23	A	5002	LHG	O10-C23-O8-C6
20	A	1125	CLA	C10-C11-C12-C13
20	B	1222	CLA	C13-C15-C16-C17
19	A	1011	CL0	CBA-CGA-O2A-C1
26	B	5007	LMG	C10-C11-C12-C13
22	A	4008	BCR	C13-C14-C15-C16
22	K	4002	BCR	C13-C14-C15-C16
22	1	504	BCR	C13-C14-C15-C16
22	1	503	BCR	C19-C20-C21-C22
22	2	503	BCR	C13-C14-C15-C16
20	A	1121	CLA	C11-C12-C13-C14
22	A	4003	BCR	C7-C8-C9-C34
30	1	610	CHL	CAA-CBA-CGA-O2A
23	4	801	LHG	C28-C29-C30-C31
20	A	1112	CLA	O1D-CGD-O2D-CED
20	4	607	CLA	C5-C6-C7-C8
22	A	4011	BCR	C7-C8-C9-C10
29	3	502	LUT	C7-C8-C9-C10
23	4	801	LHG	C26-C27-C28-C29
28	J	5001	DGD	CCA-CDA-CEA-CFA
20	A	1136	CLA	C5-C6-C7-C8
23	1	801	LHG	C4-C5-C6-O8
23	3	801	LHG	C4-C5-C6-O8
26	G	5001	LMG	O1-C7-C8-C9
26	G	5002	LMG	O1-C7-C8-C9
28	F	5005	DGD	O1G-C1G-C2G-C3G
20	A	1105	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
20	1	601	CLA	C16-C17-C18-C19
20	B	1213	CLA	C8-C10-C11-C12
30	2	613	CHL	C1A-C2A-CAA-CBA
30	3	607	CHL	C1A-C2A-CAA-CBA
23	A	5001	LHG	C26-C27-C28-C29
20	B	1206	CLA	C5-C6-C7-C8
23	A	5001	LHG	C16-C17-C18-C19
20	A	1138	CLA	C4-C3-C5-C6
26	A	5006	LMG	C22-C23-C24-C25
20	A	1123	CLA	C2-C3-C5-C6
20	A	1136	CLA	C2-C3-C5-C6
30	1	612	CHL	C2-C3-C5-C6
20	4	612	CLA	C3-C5-C6-C7
24	2	808	LMT	C4B-C5B-C6B-O6B
24	B	5006	LMT	C6-C7-C8-C9
20	2	606	CLA	C4C-C3C-CAC-CBC
20	A	1102	CLA	C16-C17-C18-C19
20	B	1226	CLA	C16-C17-C18-C20
23	3	801	LHG	O6-C4-C5-O7
20	A	1102	CLA	C2B-C3B-CAB-CBB
22	A	4008	BCR	C1-C6-C7-C8
22	B	4006	BCR	C23-C24-C25-C30
22	I	4018	BCR	C1-C6-C7-C8
22	K	4002	BCR	C1-C6-C7-C8
22	K	4002	BCR	C5-C6-C7-C8
22	L	4020	BCR	C23-C24-C25-C30
22	3	503	BCR	C23-C24-C25-C30
20	G	1603	CLA	C15-C16-C17-C18
23	B	5001	LHG	O10-C23-O8-C6
20	4	602	CLA	O1A-CGA-O2A-C1
26	G	5001	LMG	C33-C34-C35-C36
20	A	1127	CLA	C13-C15-C16-C17
26	G	5001	LMG	C11-C12-C13-C14
23	A	5002	LHG	C35-C36-C37-C38
23	1	801	LHG	O7-C5-C6-O8
23	3	801	LHG	O7-C5-C6-O8
26	G	5001	LMG	O1-C7-C8-O7
28	B	5005	DGD	O2G-C2G-C3G-O3G
32	2	807	3PH	O21-C2-C3-O31
23	B	5002	LHG	C32-C33-C34-C35
28	4	802	DGD	C1A-C2A-C3A-C4A
20	4	608	CLA	C2C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
20	A	1123	CLA	C4-C3-C5-C6
20	A	1130	CLA	C5-C6-C7-C8
20	K	1402	CLA	C5-C6-C7-C8
20	2	612	CLA	C5-C6-C7-C8
20	A	1121	CLA	C2-C3-C5-C6
20	A	1134	CLA	C6-C7-C8-C9
20	B	1235	CLA	C16-C17-C18-C19
28	B	5005	DGD	C7A-C8A-C9A-CAA
20	K	1402	CLA	C3-C5-C6-C7
20	A	1103	CLA	C6-C7-C8-C9
20	B	1204	CLA	C11-C12-C13-C14
20	B	1204	CLA	C14-C13-C15-C16
20	B	1239	CLA	C14-C13-C15-C16
20	B	1207	CLA	C14-C13-C15-C16
20	4	603	CLA	C14-C13-C15-C16
32	2	807	3PH	C22-C23-C24-C25
20	A	1138	CLA	C5-C6-C7-C8
20	B	1215	CLA	CAA-CBA-CGA-O2A
20	1	603	CLA	C6-C7-C8-C9
26	2	803	LMG	C2-C1-O1-C7
28	3	803	DGD	C2D-C1D-O3G-C3G
28	4	802	DGD	C9B-CAB-CBB-CCB
20	A	1103	CLA	C8-C10-C11-C12
20	A	1106	CLA	C8-C10-C11-C12
23	3	801	LHG	O1-C1-C2-O2
20	3	606	CLA	C2C-C3C-CAC-CBC
20	B	1202	CLA	C3-C5-C6-C7
20	B	1234	CLA	C3-C5-C6-C7
22	A	4008	BCR	C19-C20-C21-C22
22	B	4005	BCR	C13-C14-C15-C16
20	A	1106	CLA	C16-C17-C18-C19
20	B	1238	CLA	C16-C17-C18-C19
20	A	1116	CLA	O1A-CGA-O2A-C1
28	F	5005	DGD	C3A-C4A-C5A-C6A
23	A	5002	LHG	C33-C34-C35-C36
20	A	1107	CLA	C8-C10-C11-C12
22	G	4011	BCR	C11-C10-C9-C34
19	A	1011	CL0	O1A-CGA-O2A-C1
20	4	601	CLA	CBA-CGA-O2A-C1
20	B	1240	CLA	C5-C6-C7-C8
23	2	801	LHG	C26-C27-C28-C29
23	A	5001	LHG	O6-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
20	B	1206	CLA	C16-C17-C18-C19
20	3	601	CLA	C6-C7-C8-C9
20	B	1021	CLA	C15-C16-C17-C18
20	3	610	CLA	C8-C10-C11-C12
22	A	4011	BCR	C11-C12-C13-C35
22	B	4010	BCR	C11-C12-C13-C35
20	A	1103	CLA	C6-C7-C8-C10
20	A	1112	CLA	C11-C12-C13-C15
20	A	1126	CLA	C6-C7-C8-C10
20	A	1127	CLA	C11-C12-C13-C15
20	A	1131	CLA	C12-C13-C15-C16
20	A	1136	CLA	C11-C12-C13-C15
20	B	1203	CLA	C6-C7-C8-C10
20	B	1206	CLA	C12-C13-C15-C16
20	B	1211	CLA	C6-C7-C8-C10
20	B	1223	CLA	C12-C13-C15-C16
20	B	1239	CLA	C11-C10-C8-C7
20	H	1701	CLA	C11-C10-C8-C7
20	1	604	CLA	C6-C7-C8-C10
20	1	614	CLA	C6-C7-C8-C10
20	2	607	CLA	C11-C10-C8-C7
20	4	601	CLA	C6-C7-C8-C10
20	4	604	CLA	C6-C7-C8-C10
20	4	612	CLA	C12-C13-C15-C16
23	A	5002	LHG	C34-C35-C36-C37
20	A	1105	CLA	C8-C10-C11-C12
22	F	4016	BCR	C11-C12-C13-C14
22	H	4021	BCR	C11-C12-C13-C14
22	L	4019	BCR	C11-C12-C13-C14
29	J	4013	LUT	C11-C12-C13-C14
33	4	505	C7Z	C27-C28-C29-C30
20	A	1117	CLA	O1A-CGA-O2A-C1
20	B	1201	CLA	O1A-CGA-O2A-C1
20	1	614	CLA	O1A-CGA-O2A-C1
26	2	803	LMG	C8-C7-O1-C1
20	F	1301	CLA	C10-C11-C12-C13
20	A	1013	CLA	C2A-CAA-CBA-CGA
20	G	1601	CLA	C2A-CAA-CBA-CGA
20	A	1127	CLA	C16-C17-C18-C20
24	A	5004	LMT	O1'-C1-C2-C3
20	A	1013	CLA	C4-C3-C5-C6
20	B	1224	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
20	1	611	CLA	C4-C3-C5-C6
20	B	1220	CLA	CAA-CBA-CGA-O2A
20	A	1115	CLA	O1A-CGA-O2A-C1
20	B	1205	CLA	C5-C6-C7-C8
20	2	607	CLA	C10-C11-C12-C13
23	4	801	LHG	C12-C13-C14-C15
20	A	1127	CLA	C10-C11-C12-C13
26	B	5003	LMG	C9-C8-O7-C10
26	F	5004	LMG	C9-C8-O7-C10
28	J	5001	DGD	C1G-C2G-O2G-C1B
22	F	4016	BCR	C13-C14-C15-C16
20	A	1123	CLA	C16-C17-C18-C19
20	B	1208	CLA	C11-C12-C13-C14
20	B	1216	CLA	O1A-CGA-O2A-C1
26	2	803	LMG	O7-C10-C11-C12
23	A	5002	LHG	O6-C4-C5-O7
23	B	5002	LHG	O6-C4-C5-O7
23	4	801	LHG	O6-C4-C5-O7
20	A	1105	CLA	C4C-C3C-CAC-CBC
26	B	5003	LMG	O6-C1-O1-C7
23	A	5002	LHG	C4-C5-C6-O8
23	B	5002	LHG	C19-C20-C21-C22
20	B	1221	CLA	O1D-CGD-O2D-CED
28	1	803	DGD	C4D-C5D-C6D-O5D
20	B	1211	CLA	C4-C3-C5-C6
20	B	1219	CLA	C4-C3-C5-C6
20	B	1224	CLA	C2-C3-C5-C6
20	B	1021	CLA	C5-C6-C7-C8
20	A	1121	CLA	C3-C5-C6-C7
26	F	5004	LMG	O7-C8-C9-O8
26	3	802	LMG	O1-C7-C8-O7
28	G	5003	DGD	O1G-C1G-C2G-O2G
28	3	803	DGD	O1G-C1G-C2G-O2G
20	A	1127	CLA	C11-C12-C13-C14
20	A	1131	CLA	C14-C13-C15-C16
20	A	1140	CLA	C6-C7-C8-C9
20	B	1225	CLA	C11-C12-C13-C14
20	B	1240	CLA	C11-C10-C8-C9
20	1	604	CLA	C6-C7-C8-C9
20	2	607	CLA	C11-C10-C8-C9
20	A	1125	CLA	CBA-CGA-O2A-C1
23	1	801	LHG	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
28	J	5001	DGD	C6A-C7A-C8A-C9A
28	G	5003	DGD	C2B-C3B-C4B-C5B
26	F	5002	LMG	C14-C15-C16-C17
20	B	1224	CLA	C5-C6-C7-C8
20	A	1115	CLA	C2-C1-O2A-CGA
20	A	1133	CLA	C2-C1-O2A-CGA
20	3	610	CLA	C2-C1-O2A-CGA
22	A	4011	BCR	C19-C20-C21-C22
22	B	4009	BCR	C19-C20-C21-C22
22	I	4018	BCR	C19-C20-C21-C22
20	4	612	CLA	C16-C17-C18-C20
20	A	1125	CLA	C8-C10-C11-C12
23	B	5002	LHG	C30-C31-C32-C33
20	B	1203	CLA	C10-C11-C12-C13
20	2	604	CLA	C5-C6-C7-C8
20	A	1012	CLA	C2A-CAA-CBA-CGA
20	B	1215	CLA	C2A-CAA-CBA-CGA
26	G	5002	LMG	C18-C19-C20-C21
20	A	1123	CLA	C16-C17-C18-C20
20	B	1211	CLA	C16-C17-C18-C19
30	4	610	CHL	C2C-C3C-CAC-CBC
24	B	5006	LMT	O5'-C5'-C6'-O6'
24	G	5004	LMT	C2-C1-O1'-C1'
20	B	1237	CLA	C3-C5-C6-C7
22	A	4002	BCR	C36-C18-C19-C20
22	B	4004	BCR	C7-C8-C9-C34
22	K	4001	BCR	C36-C18-C19-C20
20	A	1121	CLA	C4B-C3B-CAB-CBB
20	A	1136	CLA	C4B-C3B-CAB-CBB
20	A	1140	CLA	C4B-C3B-CAB-CBB
20	A	1141	CLA	C1A-C2A-CAA-CBA
20	B	1205	CLA	C4B-C3B-CAB-CBB
20	B	1215	CLA	C1A-C2A-CAA-CBA
20	B	1232	CLA	C4B-C3B-CAB-CBB
20	B	1207	CLA	C1A-C2A-CAA-CBA
20	H	1701	CLA	C1A-C2A-CAA-CBA
20	K	1402	CLA	C4B-C3B-CAB-CBB
20	1	608	CLA	C4B-C3B-CAB-CBB
20	2	602	CLA	C4B-C3B-CAB-CBB
20	3	602	CLA	C4B-C3B-CAB-CBB
20	4	617	CLA	C1A-C2A-CAA-CBA
20	A	1119	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
20	B	1211	CLA	C2-C3-C5-C6
22	A	4003	BCR	C7-C8-C9-C10
22	B	4004	BCR	C7-C8-C9-C10
22	K	4001	BCR	C17-C18-C19-C20
22	1	503	BCR	C17-C18-C19-C20
29	3	502	LUT	C11-C12-C13-C14
28	G	5003	DGD	C2A-C3A-C4A-C5A
20	B	1239	CLA	C2C-C3C-CAC-CBC
20	B	1204	CLA	C2A-CAA-CBA-CGA
23	B	5002	LHG	C28-C29-C30-C31
24	G	5004	LMT	C11-C10-C9-C8
20	A	1101	CLA	C11-C10-C8-C7
20	A	1102	CLA	C6-C7-C8-C10
20	A	1117	CLA	C11-C12-C13-C15
20	A	1129	CLA	C11-C10-C8-C7
20	A	1013	CLA	C11-C12-C13-C15
20	A	1139	CLA	C11-C12-C13-C15
20	B	1021	CLA	C11-C12-C13-C15
20	B	1205	CLA	C11-C12-C13-C15
20	B	1211	CLA	C12-C13-C15-C16
20	B	1223	CLA	C6-C7-C8-C10
20	B	1231	CLA	C11-C10-C8-C7
20	4	607	CLA	C6-C7-C8-C10
20	4	617	CLA	C12-C13-C15-C16
20	A	1102	CLA	C16-C17-C18-C20
26	2	803	LMG	C13-C14-C15-C16
20	4	601	CLA	O1A-CGA-O2A-C1
23	1	801	LHG	C2-C3-O3-P
23	2	801	LHG	C2-C3-O3-P
20	3	608	CLA	C3A-C2A-CAA-CBA
20	A	1127	CLA	C16-C17-C18-C19
23	A	5001	LHG	O6-C4-C5-O7
23	1	801	LHG	O6-C4-C5-O7
32	2	807	3PH	O11-C1-C2-O21
20	A	1105	CLA	C11-C10-C8-C9
20	A	1112	CLA	C11-C12-C13-C14
20	A	1117	CLA	C11-C12-C13-C14
20	A	1137	CLA	C11-C12-C13-C14
20	B	1203	CLA	C11-C10-C8-C9
20	B	1211	CLA	C11-C10-C8-C9
20	B	1223	CLA	C14-C13-C15-C16
20	B	1226	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
20	B	1235	CLA	C6-C7-C8-C9
20	4	612	CLA	C11-C10-C8-C9
20	4	617	CLA	C6-C7-C8-C9
21	B	2002	PQN	C19-C18-C20-C21
22	A	4008	BCR	C15-C16-C17-C18
22	B	4004	BCR	C19-C20-C21-C22
22	L	4019	BCR	C9-C10-C11-C12
20	A	1138	CLA	C16-C17-C18-C20
20	A	1012	CLA	C8-C10-C11-C12
23	1	801	LHG	C19-C20-C21-C22
26	F	5002	LMG	O1-C7-C8-O7
28	3	803	DGD	O2G-C2G-C3G-O3G
28	4	802	DGD	O1G-C1G-C2G-O2G
23	4	801	LHG	C4-C5-C6-O8
26	3	802	LMG	O1-C7-C8-C9
28	B	5005	DGD	C1G-C2G-C3G-O3G
28	4	802	DGD	C1G-C2G-C3G-O3G
20	F	1302	CLA	C13-C15-C16-C17
20	B	1202	CLA	CAD-CBD-CGD-O2D
30	2	609	CHL	CAD-CBD-CGD-O2D
21	B	2002	PQN	C25-C26-C27-C28
20	A	1107	CLA	CBA-CGA-O2A-C1
20	B	1224	CLA	CBA-CGA-O2A-C1
20	A	1013	CLA	C16-C17-C18-C20
20	B	1237	CLA	C13-C15-C16-C17
20	A	1107	CLA	O1A-CGA-O2A-C1
20	A	1125	CLA	O1A-CGA-O2A-C1
19	A	1011	CL0	CHA-CBD-CGD-O2D
20	A	1135	CLA	CHA-CBD-CGD-O1D
20	A	1135	CLA	CHA-CBD-CGD-O2D
20	B	1202	CLA	CAD-CBD-CGD-O1D
20	B	1217	CLA	CHA-CBD-CGD-O1D
20	B	1217	CLA	CHA-CBD-CGD-O2D
20	1	608	CLA	CHA-CBD-CGD-O1D
20	1	608	CLA	CHA-CBD-CGD-O2D
20	4	604	CLA	CHA-CBD-CGD-O1D
20	4	604	CLA	CHA-CBD-CGD-O2D
20	4	605	CLA	CHA-CBD-CGD-O1D
20	4	605	CLA	CHA-CBD-CGD-O2D
22	B	4010	BCR	C19-C20-C21-C22
22	L	4020	BCR	C9-C10-C11-C12
23	A	5001	LHG	C3-O3-P-O5

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Mol	Chain	Res	Type	Atoms
23	B	5001	LHG	C3-O3-P-O5
23	B	5002	LHG	C3-O3-P-O5
23	1	801	LHG	C3-O3-P-O5
23	2	801	LHG	C3-O3-P-O6
23	4	801	LHG	C3-O3-P-O5
29	3	502	LUT	C25-C26-C27-C28
29	3	502	LUT	C29-C30-C31-C32
30	2	610	CHL	CHA-CBD-CGD-O1D
30	2	610	CHL	CHA-CBD-CGD-O2D
30	2	611	CHL	CHA-CBD-CGD-O2D
30	2	609	CHL	CAD-CBD-CGD-O1D
30	4	611	CHL	CHA-CBD-CGD-O2D
20	3	603	CLA	C5-C6-C7-C8
20	2	605	CLA	C4-C3-C5-C6
20	A	1140	CLA	C2B-C3B-CAB-CBB
20	B	1232	CLA	C2B-C3B-CAB-CBB
20	F	1302	CLA	C2B-C3B-CAB-CBB
20	K	1402	CLA	C2B-C3B-CAB-CBB
20	K	1404	CLA	C2B-C3B-CAB-CBB
20	2	602	CLA	C2B-C3B-CAB-CBB
20	3	605	CLA	C2B-C3B-CAB-CBB
22	J	4012	BCR	C5-C6-C7-C8
26	G	5006	LMG	O7-C10-C11-C12
26	2	802	LMG	O7-C10-C11-C12
20	4	608	CLA	CAA-CBA-CGA-O2A
20	A	1119	CLA	C2-C3-C5-C6
20	A	1128	CLA	C2-C3-C5-C6
20	1	611	CLA	C2-C3-C5-C6
23	A	5001	LHG	C11-C10-C9-C8
22	A	4007	BCR	C36-C18-C19-C20
22	1	503	BCR	C11-C12-C13-C35
32	2	807	3PH	C1-O11-P-O12
20	3	617	CLA	C2C-C3C-CAC-CBC
23	B	5001	LHG	O1-C1-C2-O2
26	3	802	LMG	O10-C28-O8-C9
26	F	5003	LMG	C9-C8-O7-C10
26	F	5001	LMG	C9-C8-O7-C10
26	G	5001	LMG	C7-C8-O7-C10
26	2	803	LMG	C7-C8-O7-C10
22	B	4006	BCR	C18-C19-C20-C21
22	L	4019	BCR	C10-C11-C12-C13
22	L	4020	BCR	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
33	4	505	C7Z	C10-C11-C12-C13
23	4	801	LHG	O8-C23-C24-C25
20	4	601	CLA	C2-C3-C5-C6
26	1	802	LMG	C10-C11-C12-C13
28	B	5005	DGD	C1B-C2B-C3B-C4B
20	B	1211	CLA	C16-C17-C18-C20
30	4	613	CHL	C11-C12-C13-C15
20	B	1211	CLA	C10-C11-C12-C13
26	G	5006	LMG	O9-C10-C11-C12
26	G	5006	LMG	O10-C28-C29-C30
23	1	801	LHG	O6-C4-C5-C6
26	3	802	LMG	C29-C28-O8-C9
20	B	1224	CLA	O1A-CGA-O2A-C1
28	B	5005	DGD	O6D-C5D-C6D-O5D
20	A	1101	CLA	C11-C10-C8-C9
20	A	1109	CLA	C14-C13-C15-C16
20	A	1136	CLA	C11-C10-C8-C9
20	A	1136	CLA	C11-C12-C13-C14
20	A	1141	CLA	C11-C10-C8-C9
20	B	1021	CLA	C11-C12-C13-C14
20	B	1201	CLA	C14-C13-C15-C16
23	1	801	LHG	C27-C28-C29-C30
20	B	1239	CLA	C6-C7-C8-C10
20	2	604	CLA	C6-C7-C8-C10
24	B	5008	LMT	O1'-C1-C2-C3
23	B	5002	LHG	C11-C10-C9-C8
23	1	801	LHG	C34-C35-C36-C37
26	F	5001	LMG	O6-C1-O1-C7
20	B	1235	CLA	C2A-CAA-CBA-CGA
26	2	805	LMG	O10-C28-O8-C9
20	B	1219	CLA	C2-C3-C5-C6
26	F	5002	LMG	C15-C16-C17-C18
20	1	601	CLA	C13-C15-C16-C17
22	A	4002	BCR	C9-C10-C11-C12
26	B	5003	LMG	C11-C12-C13-C14
20	F	1301	CLA	CAA-CBA-CGA-O2A
26	2	805	LMG	C29-C28-O8-C9
20	A	1137	CLA	C2-C1-O2A-CGA
20	B	1204	CLA	C2-C1-O2A-CGA
20	4	601	CLA	C2-C1-O2A-CGA
20	B	1206	CLA	C4-C3-C5-C6
20	4	607	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
32	2	807	3PH	C28-C29-C2A-C2B
24	2	808	LMT	O5B-C5B-C6B-O6B
20	3	606	CLA	C4C-C3C-CAC-CBC
20	B	1224	CLA	CAA-CBA-CGA-O2A
22	A	4008	BCR	C36-C18-C19-C20
20	2	605	CLA	C16-C17-C18-C19
30	2	615	CHL	C1C-C2C-CMC-OMC
22	B	4010	BCR	C11-C12-C13-C14
26	2	802	LMG	O9-C10-C11-C12
26	F	5004	LMG	C8-C7-O1-C1
28	1	803	DGD	C2G-C3G-O3G-C1D
20	B	1023	CLA	C2A-CAA-CBA-CGA
20	B	1219	CLA	C2A-CAA-CBA-CGA
30	2	615	CHL	C2A-CAA-CBA-CGA
22	A	4011	BCR	C9-C10-C11-C12
22	B	4009	BCR	C13-C14-C15-C16
22	K	4001	BCR	C19-C20-C21-C22
20	A	1127	CLA	C4-C3-C5-C6
19	A	1011	CL0	CBD-CGD-O2D-CED
26	1	802	LMG	O9-C10-C11-C12
26	G	5006	LMG	O8-C28-C29-C30
20	B	1220	CLA	O1D-CGD-O2D-CED
20	B	1021	CLA	C16-C17-C18-C19
20	B	1238	CLA	C16-C17-C18-C20
24	G	5005	LMT	C1-C2-C3-C4
20	A	1137	CLA	C11-C10-C8-C9
20	B	1223	CLA	C6-C7-C8-C9
20	4	612	CLA	C6-C7-C8-C9
23	A	5001	LHG	C2-C3-O3-P
20	2	601	CLA	C4B-C3B-CAB-CBB
20	H	1701	CLA	C10-C11-C12-C13
20	B	1203	CLA	C8-C10-C11-C12
20	3	617	CLA	CBA-CGA-O2A-C1
20	4	612	CLA	C8-C10-C11-C12
20	3	617	CLA	O1A-CGA-O2A-C1
20	B	1221	CLA	C2A-CAA-CBA-CGA
20	A	1126	CLA	CAA-CBA-CGA-O2A
22	A	4002	BCR	C19-C20-C21-C22
20	A	1132	CLA	C11-C10-C8-C7
20	A	1137	CLA	C6-C7-C8-C10
20	A	1137	CLA	C11-C10-C8-C7
20	B	1204	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
20	L	1502	CLA	C11-C10-C8-C7
20	1	611	CLA	C11-C10-C8-C7
20	2	603	CLA	C6-C7-C8-C10
20	B	1021	CLA	O1A-CGA-O2A-C1
26	G	5002	LMG	C19-C20-C21-C22
20	B	1239	CLA	C4C-C3C-CAC-CBC
23	B	5002	LHG	C29-C30-C31-C32
30	2	609	CHL	C3A-C2A-CAA-CBA
20	B	1208	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	4006	BCR	C11-C10-C9-C34
22	B	4004	BCR	C35-C13-C14-C15
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	H	4021	BCR	C11-C10-C9-C34
22	I	4018	BCR	C35-C13-C14-C15
22	I	4020	BCR	C16-C17-C18-C36
22	I	4020	BCR	C20-C21-C22-C37
22	1	504	BCR	C16-C17-C18-C36
22	3	506	BCR	C16-C17-C18-C36
23	A	5002	LHG	C14-C15-C16-C17
20	B	1204	CLA	C5-C6-C7-C8
20	A	1140	CLA	C2-C1-O2A-CGA
20	K	1403	CLA	C2-C1-O2A-CGA
22	B	4005	BCR	C15-C16-C17-C18
20	1	614	CLA	C11-C12-C13-C14
20	B	1223	CLA	C8-C10-C11-C12
22	1	503	BCR	C11-C12-C13-C14
30	2	615	CHL	CAA-CBA-CGA-O2A
20	B	1237	CLA	C16-C17-C18-C20
20	B	1237	CLA	C2A-CAA-CBA-CGA
20	L	1501	CLA	O1A-CGA-O2A-C1
20	A	1111	CLA	C14-C13-C15-C16
20	A	1115	CLA	C11-C12-C13-C14
20	A	1116	CLA	C6-C7-C8-C9
20	A	1125	CLA	C6-C7-C8-C9
20	A	1138	CLA	C6-C7-C8-C9
20	A	1138	CLA	C11-C10-C8-C9
20	B	1230	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
20	K	1402	CLA	C6-C7-C8-C9
20	L	1502	CLA	C11-C10-C8-C9
20	1	605	CLA	C11-C10-C8-C9
20	1	611	CLA	C11-C10-C8-C9
20	2	603	CLA	C11-C10-C8-C9
20	2	605	CLA	C11-C10-C8-C9
20	3	610	CLA	C6-C7-C8-C9
20	4	607	CLA	C6-C7-C8-C9
21	A	2001	PQN	C19-C18-C20-C21
30	1	612	CHL	C6-C7-C8-C9
30	3	604	CHL	C14-C13-C15-C16
26	G	5006	LMG	C9-C8-O7-C10
28	B	5005	DGD	C3G-C2G-O2G-C1B
30	2	611	CHL	C1A-C2A-CAA-CBA
30	3	604	CHL	C1A-C2A-CAA-CBA
20	A	1133	CLA	O1D-CGD-O2D-CED
20	B	1209	CLA	CAA-CBA-CGA-O2A
20	A	1127	CLA	C2-C3-C5-C6
30	1	610	CHL	C2C-C3C-CAC-CBC
30	2	613	CHL	CAA-CBA-CGA-O1A
30	2	613	CHL	CAA-CBA-CGA-O2A
32	2	807	3PH	C25-C26-C27-C28
20	A	1118	CLA	C2A-CAA-CBA-CGA
20	A	1117	CLA	C1A-C2A-CAA-CBA
20	A	1128	CLA	C1A-C2A-CAA-CBA
20	A	1134	CLA	C1A-C2A-CAA-CBA
20	B	1204	CLA	C1A-C2A-CAA-CBA
20	B	1220	CLA	C1A-C2A-CAA-CBA
20	B	1230	CLA	C1A-C2A-CAA-CBA
20	F	1301	CLA	C1A-C2A-CAA-CBA
20	1	605	CLA	C1A-C2A-CAA-CBA
20	1	611	CLA	C1A-C2A-CAA-CBA
22	A	4007	BCR	C16-C17-C18-C19
22	A	4011	BCR	C16-C17-C18-C19
22	A	4017	BCR	C16-C17-C18-C19
22	B	4006	BCR	C11-C10-C9-C8
22	B	4004	BCR	C12-C13-C14-C15
22	B	4004	BCR	C16-C17-C18-C19
22	F	4016	BCR	C16-C17-C18-C19
22	G	4011	BCR	C11-C10-C9-C8
22	G	4011	BCR	C16-C17-C18-C19
22	H	4021	BCR	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
22	I	4018	BCR	C12-C13-C14-C15
22	I	4020	BCR	C16-C17-C18-C19
22	I	4020	BCR	C20-C21-C22-C23
22	1	504	BCR	C16-C17-C18-C19
22	3	506	BCR	C16-C17-C18-C19
20	1	601	CLA	C2C-C3C-CAC-CBC
20	A	1120	CLA	C2B-C3B-CAB-CBB
20	A	1121	CLA	C2B-C3B-CAB-CBB
20	A	1126	CLA	C2B-C3B-CAB-CBB
20	A	1136	CLA	C2B-C3B-CAB-CBB
20	B	1022	CLA	C2B-C3B-CAB-CBB
20	B	1205	CLA	C2B-C3B-CAB-CBB
20	G	1603	CLA	C2B-C3B-CAB-CBB
20	1	608	CLA	C2B-C3B-CAB-CBB
20	1	613	CLA	C2B-C3B-CAB-CBB
20	2	601	CLA	C2B-C3B-CAB-CBB
20	3	602	CLA	C2B-C3B-CAB-CBB
22	A	4002	BCR	C1-C6-C7-C8
22	A	4003	BCR	C23-C24-C25-C26
22	A	4008	BCR	C5-C6-C7-C8
22	B	4005	BCR	C1-C6-C7-C8
22	I	4018	BCR	C5-C6-C7-C8
22	L	4020	BCR	C23-C24-C25-C26
22	3	503	BCR	C23-C24-C25-C26
20	B	1211	CLA	C8-C10-C11-C12
23	A	5002	LHG	C2-C3-O3-P
20	A	1131	CLA	C4-C3-C5-C6
20	A	1102	CLA	C11-C10-C8-C7
20	A	1111	CLA	C6-C7-C8-C10
20	A	1125	CLA	C11-C12-C13-C15
20	A	1132	CLA	C12-C13-C15-C16
20	A	1138	CLA	C11-C10-C8-C7
20	B	1202	CLA	C12-C13-C15-C16
20	B	1215	CLA	C11-C10-C8-C7
20	B	1227	CLA	C11-C10-C8-C7
20	B	1230	CLA	C11-C10-C8-C7
20	B	1240	CLA	C12-C13-C15-C16
20	K	1402	CLA	C6-C7-C8-C10
21	A	2001	PQN	C17-C18-C20-C21
30	3	604	CHL	C11-C12-C13-C15
20	4	607	CLA	C11-C12-C13-C14
20	A	1117	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
20	B	1223	CLA	O1D-CGD-O2D-CED
26	F	5004	LMG	C28-C29-C30-C31
20	B	1237	CLA	C8-C10-C11-C12
32	2	807	3PH	C27-C28-C29-C2A
20	B	1204	CLA	C3-C5-C6-C7
20	B	1235	CLA	C5-C6-C7-C8
23	1	801	LHG	C16-C17-C18-C19
26	B	5004	LMG	C11-C12-C13-C14
21	B	2002	PQN	C23-C25-C26-C27
22	F	4014	BCR	C36-C18-C19-C20
29	3	501	LUT	C11-C12-C13-C20
24	G	5004	LMT	C7-C8-C9-C10
20	B	1205	CLA	C4-C3-C5-C6
20	B	1220	CLA	C4-C3-C5-C6
20	B	1226	CLA	C4-C3-C5-C6
20	L	1501	CLA	CBA-CGA-O2A-C1
32	2	807	3PH	O21-C21-C22-C23
20	B	1202	CLA	C10-C11-C12-C13
20	A	1013	CLA	C2-C3-C5-C6
22	A	4011	BCR	C11-C12-C13-C14
26	G	5001	LMG	C14-C15-C16-C17
20	A	1134	CLA	C2A-CAA-CBA-CGA
20	B	1206	CLA	C6-C7-C8-C9
20	B	1210	CLA	C14-C13-C15-C16
20	B	1221	CLA	C11-C12-C13-C14
22	F	4014	BCR	C15-C16-C17-C18
20	B	1210	CLA	C4-C3-C5-C6
20	A	1107	CLA	C15-C16-C17-C18
28	3	803	DGD	O1G-C1G-C2G-C3G
28	3	803	DGD	C1G-C2G-C3G-O3G
20	K	1402	CLA	C2A-CAA-CBA-CGA
20	2	608	CLA	C2A-CAA-CBA-CGA
20	B	1208	CLA	C11-C12-C13-C15
20	1	601	CLA	C4C-C3C-CAC-CBC
23	A	5002	LHG	C17-C18-C19-C20
24	B	5008	LMT	C4B-C5B-C6B-O6B
20	A	1138	CLA	C13-C15-C16-C17
23	A	5002	LHG	C25-C26-C27-C28
20	B	1238	CLA	C4-C3-C5-C6
30	1	610	CHL	CAA-CBA-CGA-O1A
20	B	1021	CLA	C16-C17-C18-C20
20	A	1122	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
20	A	1141	CLA	C4B-C3B-CAB-CBB
20	B	1023	CLA	C4B-C3B-CAB-CBB
20	B	1227	CLA	C4B-C3B-CAB-CBB
20	A	1137	CLA	O1A-CGA-O2A-C1
20	L	1502	CLA	O1A-CGA-O2A-C1
26	2	802	LMG	O10-C28-O8-C9
19	A	1011	CL0	O1D-CGD-O2D-CED
26	F	5004	LMG	C11-C12-C13-C14
23	4	801	LHG	C9-C10-C11-C12
32	2	807	3PH	O32-C31-O31-C3
20	1	613	CLA	CAA-CBA-CGA-O2A
20	B	1210	CLA	C16-C17-C18-C19
20	2	604	CLA	C16-C17-C18-C19
30	4	610	CHL	CHA-CBD-CGD-O1D
30	4	610	CHL	CHA-CBD-CGD-O2D
33	4	505	C7Z	C20-C13-C14-C15
32	2	807	3PH	C29-C2A-C2B-C2C
20	B	1216	CLA	C16-C17-C18-C20
30	4	613	CHL	C11-C12-C13-C14
23	B	5002	LHG	O7-C5-C6-O8
26	B	5007	LMG	O1-C7-C8-O7
20	B	1240	CLA	CAA-CBA-CGA-O1A
20	B	1205	CLA	C2-C3-C5-C6
20	B	1210	CLA	C2-C3-C5-C6
28	J	5001	DGD	C5B-C6B-C7B-C8B
20	A	1012	CLA	C11-C12-C13-C15
20	B	1206	CLA	C6-C7-C8-C10
20	3	610	CLA	C6-C7-C8-C10
26	2	803	LMG	C11-C12-C13-C14
26	A	5006	LMG	C19-C20-C21-C22
28	1	803	DGD	O1A-C1A-C2A-C3A
22	F	4014	BCR	C11-C12-C13-C14
20	A	1122	CLA	C6-C7-C8-C9
20	A	1128	CLA	C6-C7-C8-C9
20	A	1129	CLA	C14-C13-C15-C16
20	A	1141	CLA	C6-C7-C8-C9
20	B	1225	CLA	C14-C13-C15-C16
20	B	1231	CLA	C11-C10-C8-C9
20	B	1238	CLA	C6-C7-C8-C9
20	4	603	CLA	C11-C12-C13-C14
26	2	804	LMG	C11-C12-C13-C14
26	B	5004	LMG	C8-C7-O1-C1

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Mol	Chain	Res	Type	Atoms
26	1	802	LMG	C8-C7-O1-C1
28	3	803	DGD	C5D-C6D-O5D-C1E
20	F	1301	CLA	C2A-CAA-CBA-CGA
20	3	613	CLA	C2A-CAA-CBA-CGA
20	A	1108	CLA	C2-C1-O2A-CGA
20	2	607	CLA	C2-C1-O2A-CGA
30	2	609	CHL	C2-C1-O2A-CGA
20	B	1021	CLA	CBA-CGA-O2A-C1
32	2	807	3PH	C32-C31-O31-C3
23	A	5002	LHG	C30-C31-C32-C33
20	A	1107	CLA	C3A-C2A-CAA-CBA
20	A	1111	CLA	C3A-C2A-CAA-CBA
20	A	1115	CLA	C3A-C2A-CAA-CBA
20	B	1215	CLA	C3A-C2A-CAA-CBA
20	B	1220	CLA	C3A-C2A-CAA-CBA
20	B	1231	CLA	C3A-C2A-CAA-CBA
20	B	1235	CLA	C3A-C2A-CAA-CBA
20	F	1301	CLA	C3A-C2A-CAA-CBA
30	1	612	CHL	C3A-C2A-CAA-CBA
28	F	5005	DGD	C9A-CAA-CBA-CCA
20	A	1125	CLA	C16-C17-C18-C19
30	3	607	CHL	CAA-CBA-CGA-O2A
28	B	5005	DGD	C1G-C2G-O2G-C1B
22	A	4003	BCR	C10-C11-C12-C13
20	A	1109	CLA	C15-C16-C17-C18
29	3	501	LUT	C33-C34-C35-C15
20	A	1137	CLA	C16-C17-C18-C19
20	B	1229	CLA	C4-C3-C5-C6
20	1	613	CLA	CAA-CBA-CGA-O1A
20	B	1206	CLA	C2-C3-C5-C6
31	2	502	XAT	O4-C6-C7-C8
20	A	1113	CLA	CAA-CBA-CGA-O1A
26	2	802	LMG	C29-C28-O8-C9
23	B	5002	LHG	C4-C5-C6-O8
30	4	613	CHL	C8-C10-C11-C12
20	A	1123	CLA	O1D-CGD-O2D-CED
28	F	5005	DGD	C1B-C2B-C3B-C4B
20	B	1238	CLA	C2A-CAA-CBA-CGA
20	2	601	CLA	CAA-CBA-CGA-O2A
20	A	1113	CLA	CAA-CBA-CGA-O2A
22	B	4010	BCR	C9-C10-C11-C12
26	1	802	LMG	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
26	G	5001	LMG	C12-C13-C14-C15
20	A	1126	CLA	C10-C11-C12-C13
20	A	1123	CLA	CBD-CGD-O2D-CED
20	1	614	CLA	CAA-CBA-CGA-O2A
20	3	603	CLA	CAA-CBA-CGA-O2A
23	2	801	LHG	O8-C23-C24-C25
26	B	5007	LMG	O7-C8-C9-O8
20	A	1102	CLA	C6-C7-C8-C9
20	A	1106	CLA	C11-C10-C8-C9
20	A	1112	CLA	C6-C7-C8-C9
20	A	1126	CLA	C14-C13-C15-C16
20	A	1013	CLA	C11-C12-C13-C14
24	A	5004	LMT	C9-C10-C11-C12
22	F	4014	BCR	C17-C18-C19-C20
20	B	1235	CLA	CAA-CBA-CGA-O2A
20	A	1137	CLA	CBA-CGA-O2A-C1
20	A	1111	CLA	C2A-CAA-CBA-CGA
20	B	1220	CLA	CBD-CGD-O2D-CED
20	A	1120	CLA	C11-C10-C8-C7
20	A	1141	CLA	C6-C7-C8-C10
20	B	1205	CLA	C6-C7-C8-C10
20	B	1214	CLA	C12-C13-C15-C16
20	B	1221	CLA	C11-C12-C13-C15
20	B	1225	CLA	C12-C13-C15-C16
20	B	1228	CLA	C6-C7-C8-C10
20	B	1238	CLA	C6-C7-C8-C10
20	B	1238	CLA	C11-C10-C8-C7
20	F	1301	CLA	C6-C7-C8-C10
20	4	603	CLA	C11-C10-C8-C7
20	4	603	CLA	C11-C12-C13-C15
30	2	609	CHL	C12-C13-C15-C16
20	A	1118	CLA	C2B-C3B-CAB-CBB
20	A	1122	CLA	C2B-C3B-CAB-CBB
20	A	1131	CLA	C2B-C3B-CAB-CBB
20	A	1012	CLA	C2B-C3B-CAB-CBB
20	B	1227	CLA	C2B-C3B-CAB-CBB
20	L	1503	CLA	C2B-C3B-CAB-CBB
20	2	604	CLA	C2B-C3B-CAB-CBB
22	A	4002	BCR	C5-C6-C7-C8
22	A	4003	BCR	C1-C6-C7-C8
22	A	4003	BCR	C5-C6-C7-C8
22	B	4005	BCR	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
22	I	4018	BCR	C23-C24-C25-C30
28	G	5003	DGD	O1B-C1B-O2G-C2G
23	A	5002	LHG	C24-C25-C26-C27
20	B	1237	CLA	C2-C1-O2A-CGA
20	B	1234	CLA	C2-C1-O2A-CGA
20	B	1240	CLA	C2-C1-O2A-CGA
20	B	1201	CLA	C10-C11-C12-C13
23	3	801	LHG	C2-C3-O3-P
20	B	1236	CLA	CAA-CBA-CGA-O2A
20	3	602	CLA	CAA-CBA-CGA-O2A
20	B	1223	CLA	CBD-CGD-O2D-CED
20	L	1502	CLA	CBA-CGA-O2A-C1
23	B	5002	LHG	C24-C23-O8-C6
20	B	1229	CLA	C2-C3-C5-C6
20	2	605	CLA	C2-C3-C5-C6
20	B	1210	CLA	C2A-CAA-CBA-CGA
20	K	1404	CLA	C2A-CAA-CBA-CGA
20	A	1140	CLA	CAA-CBA-CGA-O2A
20	L	1501	CLA	CAA-CBA-CGA-O2A
28	G	5003	DGD	O1G-C1A-C2A-C3A
20	B	1237	CLA	C16-C17-C18-C19
20	B	1219	CLA	CAA-CBA-CGA-O2A
20	1	605	CLA	CAA-CBA-CGA-O2A
20	3	601	CLA	CAA-CBA-CGA-O2A
26	G	5001	LMG	O8-C28-C29-C30
28	F	5005	DGD	O1G-C1A-C2A-C3A
30	2	610	CHL	CAA-CBA-CGA-O2A
20	A	1112	CLA	CAA-CBA-CGA-O2A
23	B	5002	LHG	O10-C23-O8-C6
20	A	1012	CLA	C13-C15-C16-C17
20	A	1107	CLA	C6-C7-C8-C9
20	A	1012	CLA	C11-C12-C13-C14
20	B	1202	CLA	C14-C13-C15-C16
20	B	1227	CLA	C11-C10-C8-C9
20	A	1125	CLA	CAA-CBA-CGA-O2A
20	B	1210	CLA	CAA-CBA-CGA-O2A
28	G	5003	DGD	O1G-C1G-C2G-C3G
20	A	1111	CLA	C1A-C2A-CAA-CBA
20	A	1118	CLA	C4B-C3B-CAB-CBB
20	B	1237	CLA	C1A-C2A-CAA-CBA
20	B	1224	CLA	C4B-C3B-CAB-CBB
20	F	1302	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
20	A	1120	CLA	C4-C3-C5-C6
20	A	1115	CLA	CAA-CBA-CGA-O2A
20	A	1120	CLA	CAA-CBA-CGA-O2A
23	A	5002	LHG	O8-C23-C24-C25
23	B	5002	LHG	C16-C17-C18-C19
22	A	4002	BCR	C17-C18-C19-C20
22	A	4007	BCR	C17-C18-C19-C20
22	A	4008	BCR	C17-C18-C19-C20
29	3	501	LUT	C11-C12-C13-C14
33	4	505	C7Z	C7-C8-C9-C10
20	4	612	CLA	C16-C17-C18-C19
20	B	1228	CLA	CAA-CBA-CGA-O2A
23	B	5002	LHG	O8-C23-C24-C25
26	B	5007	LMG	O7-C10-C11-C12
20	B	1203	CLA	O1A-CGA-O2A-C1
28	F	5005	DGD	O1A-C1A-O1G-C1G
20	A	1137	CLA	CAA-CBA-CGA-O2A
20	L	1502	CLA	CAA-CBA-CGA-O2A
26	A	5006	LMG	O7-C10-C11-C12
26	F	5001	LMG	O7-C10-C11-C12
20	F	1302	CLA	C10-C11-C12-C13
20	G	1603	CLA	C13-C15-C16-C17
20	A	1135	CLA	C2-C3-C5-C6
28	B	5005	DGD	C2A-C3A-C4A-C5A
20	B	1222	CLA	C2-C1-O2A-CGA
20	B	1224	CLA	C2-C1-O2A-CGA
20	G	1601	CLA	C2-C1-O2A-CGA
20	1	601	CLA	C2-C1-O2A-CGA
20	A	1119	CLA	C11-C10-C8-C7
20	A	1125	CLA	C11-C10-C8-C7
20	A	1129	CLA	C12-C13-C15-C16
20	A	1012	CLA	C12-C13-C15-C16
20	B	1023	CLA	C11-C10-C8-C7
20	F	1302	CLA	C11-C12-C13-C15
20	K	1402	CLA	C11-C10-C8-C7
20	2	604	CLA	C11-C10-C8-C7
20	B	1231	CLA	C11-C12-C13-C14
24	G	5005	LMT	O1'-C1-C2-C3
26	2	804	LMG	C9-C8-O7-C10
20	H	1701	CLA	C2C-C3C-CAC-CBC
30	4	613	CHL	C10-C11-C12-C13
26	2	803	LMG	O9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
20	A	1115	CLA	C2A-CAA-CBA-CGA
20	A	1138	CLA	C2A-CAA-CBA-CGA
20	1	601	CLA	C2A-CAA-CBA-CGA
20	3	601	CLA	C2A-CAA-CBA-CGA
20	A	1105	CLA	C5-C6-C7-C8
20	A	1128	CLA	C16-C17-C18-C19
20	A	1129	CLA	C8-C10-C11-C12
23	2	801	LHG	O10-C23-C24-C25
20	A	1012	CLA	C3A-C2A-CAA-CBA
20	K	1402	CLA	C3A-C2A-CAA-CBA
20	B	1220	CLA	CAA-CBA-CGA-O1A
30	2	610	CHL	CAA-CBA-CGA-O1A
20	A	1128	CLA	C13-C15-C16-C17
20	3	610	CLA	C10-C11-C12-C13
19	A	1011	CL0	CAA-CBA-CGA-O2A
20	B	1226	CLA	C2-C3-C5-C6
26	A	5006	LMG	C28-C29-C30-C31
26	B	5007	LMG	C30-C31-C32-C33
20	K	1401	CLA	CAA-CBA-CGA-O2A
20	3	601	CLA	C4C-C3C-CAC-CBC
20	2	605	CLA	C10-C11-C12-C13
20	B	1215	CLA	CAA-CBA-CGA-O1A
20	3	601	CLA	CAA-CBA-CGA-O1A
20	4	601	CLA	C5-C6-C7-C8
20	B	1239	CLA	CAA-CBA-CGA-O2A
20	3	612	CLA	C2C-C3C-CAC-CBC
20	B	1235	CLA	CAA-CBA-CGA-O1A
20	L	1501	CLA	CAA-CBA-CGA-O1A
20	A	1107	CLA	C11-C12-C13-C14
20	A	1111	CLA	C6-C7-C8-C9
20	A	1115	CLA	C6-C7-C8-C9
20	A	1125	CLA	C11-C12-C13-C14
20	A	1129	CLA	C11-C10-C8-C9
20	A	1131	CLA	C11-C12-C13-C14
20	A	1012	CLA	C14-C13-C15-C16
20	B	1215	CLA	C11-C10-C8-C9
20	B	1239	CLA	C6-C7-C8-C9
20	2	605	CLA	C6-C7-C8-C9
20	A	1137	CLA	CAA-CBA-CGA-O1A
20	L	1502	CLA	CAA-CBA-CGA-O1A
20	2	601	CLA	CAA-CBA-CGA-O1A
20	3	602	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
20	3	603	CLA	CAA-CBA-CGA-O1A
26	G	5001	LMG	C37-C38-C39-C40
23	B	5002	LHG	C35-C36-C37-C38
29	3	501	LUT	C21-C26-C27-C28
20	A	1140	CLA	CAA-CBA-CGA-O1A
20	B	1210	CLA	CAA-CBA-CGA-O1A
20	B	1219	CLA	CAA-CBA-CGA-O1A
20	1	614	CLA	CAA-CBA-CGA-O1A
28	4	802	DGD	O2G-C1B-C2B-C3B
20	1	605	CLA	CAA-CBA-CGA-O1A
23	2	801	LHG	C23-C24-C25-C26
28	B	5005	DGD	C5D-C6D-O5D-C1E
28	F	5005	DGD	C5D-C6D-O5D-C1E
28	J	5001	DGD	O1G-C1G-C2G-O2G
20	3	601	CLA	C2C-C3C-CAC-CBC
26	A	5006	LMG	O9-C10-C11-C12
26	G	5001	LMG	O10-C28-C29-C30
26	B	5004	LMG	O8-C28-C29-C30
20	A	1109	CLA	C8-C10-C11-C12
20	B	1221	CLA	C15-C16-C17-C18
26	B	5007	LMG	C11-C12-C13-C14
20	A	1120	CLA	CAA-CBA-CGA-O1A
23	B	5002	LHG	O10-C23-C24-C25
28	F	5005	DGD	O1A-C1A-C2A-C3A
20	A	1102	CLA	C13-C15-C16-C17
20	A	1112	CLA	C5-C6-C7-C8
22	B	4010	BCR	C13-C14-C15-C16
20	A	1125	CLA	CAA-CBA-CGA-O1A
20	B	1236	CLA	CAA-CBA-CGA-O1A
28	G	5003	DGD	O1A-C1A-C2A-C3A
20	A	1135	CLA	CAD-CBD-CGD-O2D
28	G	5003	DGD	C2B-C1B-O2G-C2G
26	2	805	LMG	O7-C10-C11-C12
20	A	1132	CLA	C2C-C3C-CAC-CBC
32	2	807	3PH	C36-C37-C38-C39
23	4	801	LHG	O6-C4-C5-C6
20	B	1226	CLA	C13-C15-C16-C17
20	A	1110	CLA	C2-C1-O2A-CGA
20	1	604	CLA	C2-C1-O2A-CGA
30	1	612	CHL	C2-C1-O2A-CGA
20	A	1103	CLA	CAA-CBA-CGA-O2A
20	A	1138	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
20	B	1238	CLA	CAA-CBA-CGA-O2A
20	B	1216	CLA	C16-C17-C18-C19
30	2	609	CHL	C2A-CAA-CBA-CGA
20	B	1228	CLA	CAA-CBA-CGA-O1A
20	A	1133	CLA	C12-C13-C15-C16
20	B	1213	CLA	CAA-CBA-CGA-O2A
26	2	804	LMG	O7-C10-C11-C12
26	3	802	LMG	O7-C10-C11-C12
28	1	803	DGD	O2G-C1B-C2B-C3B
26	B	5004	LMG	O10-C28-C29-C30
26	B	5007	LMG	O9-C10-C11-C12
20	A	1112	CLA	CAA-CBA-CGA-O1A
20	A	1115	CLA	CAA-CBA-CGA-O1A
28	4	802	DGD	O1B-C1B-C2B-C3B

There are no ring outliers.

226 monomers are involved in 1507 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	A	1111	CLA	13	0
20	A	1128	CLA	3	0
20	A	1132	CLA	28	0
22	G	4011	BCR	4	0
31	4	502	XAT	14	0
20	A	1103	CLA	13	0
20	A	1106	CLA	10	0
26	B	5003	LMG	13	0
30	1	610	CHL	10	0
22	F	4016	BCR	9	0
20	4	617	CLA	10	0
28	3	803	DGD	3	0
20	B	1220	CLA	5	0
20	1	602	CLA	2	0
30	4	610	CHL	3	0
20	4	604	CLA	28	0
33	4	505	C7Z	4	0
22	3	506	BCR	2	0
20	1	604	CLA	13	0
26	B	5007	LMG	1	0
29	4	501	LUT	19	0
20	A	1136	CLA	11	0
22	A	4002	BCR	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	A	1112	CLA	11	0
30	2	609	CHL	22	0
22	1	503	BCR	1	0
20	A	1129	CLA	1	0
26	F	5003	LMG	3	0
26	2	803	LMG	4	0
20	B	1207	CLA	11	0
20	3	612	CLA	9	0
30	4	613	CHL	5	0
20	1	606	CLA	9	0
30	4	615	CHL	3	0
20	A	1113	CLA	18	0
20	B	1229	CLA	6	0
26	2	802	LMG	10	0
20	B	1228	CLA	4	0
20	B	1022	CLA	7	0
20	1	608	CLA	9	0
20	3	601	CLA	8	0
26	2	805	LMG	1	0
20	4	601	CLA	41	0
20	1	601	CLA	12	0
20	2	607	CLA	5	0
19	A	1011	CL0	11	0
20	B	1218	CLA	7	0
20	B	1231	CLA	6	0
29	1	502	LUT	33	0
20	B	1023	CLA	3	0
20	B	1226	CLA	5	0
20	B	1235	CLA	7	0
20	B	1237	CLA	20	0
20	A	1013	CLA	12	0
20	G	1602	CLA	2	0
20	4	608	CLA	13	0
20	K	1401	CLA	12	0
22	B	4005	BCR	3	0
20	G	1603	CLA	14	0
30	3	604	CHL	2	0
20	3	602	CLA	2	0
24	A	5004	LMT	1	0
26	A	5006	LMG	3	0
20	B	1210	CLA	8	0
22	A	4007	BCR	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	B	5008	LMT	1	0
22	3	503	BCR	8	0
22	L	4020	BCR	18	0
20	B	1202	CLA	5	0
20	4	606	CLA	3	0
20	L	1503	CLA	17	0
20	K	1404	CLA	3	0
26	G	5001	LMG	5	0
20	1	603	CLA	21	0
20	3	610	CLA	3	0
28	1	803	DGD	1	0
26	F	5001	LMG	2	0
28	B	5005	DGD	7	0
20	1	614	CLA	5	0
20	B	1222	CLA	7	0
20	A	1104	CLA	5	0
20	B	1205	CLA	7	0
20	A	1123	CLA	9	0
26	1	802	LMG	8	0
22	B	4010	BCR	3	0
20	B	1227	CLA	6	0
20	3	605	CLA	5	0
20	B	1232	CLA	11	0
30	1	612	CHL	5	0
20	2	612	CLA	12	0
20	4	605	CLA	11	0
22	B	4009	BCR	4	0
28	J	5001	DGD	11	0
20	A	1116	CLA	13	0
20	A	1139	CLA	10	0
20	3	613	CLA	4	0
22	F	4014	BCR	3	0
20	B	1236	CLA	1	0
20	B	1224	CLA	5	0
28	G	5003	DGD	3	0
20	B	1215	CLA	5	0
29	1	501	LUT	6	0
21	A	2001	PQN	8	0
20	A	1117	CLA	12	0
23	4	801	LHG	11	0
20	2	602	CLA	2	0
20	B	1213	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	B	5002	LHG	4	0
23	1	801	LHG	11	0
20	B	1221	CLA	3	0
20	B	1214	CLA	11	0
26	F	5002	LMG	3	0
29	3	501	LUT	3	0
20	J	1901	CLA	7	0
20	B	1239	CLA	7	0
20	4	607	CLA	10	0
22	I	4018	BCR	8	0
20	L	1501	CLA	14	0
20	A	1107	CLA	9	0
26	2	804	LMG	2	0
20	G	1601	CLA	5	0
20	B	1230	CLA	9	0
20	A	1133	CLA	12	0
23	A	5002	LHG	2	0
26	B	5004	LMG	2	0
30	3	611	CHL	5	0
20	B	1216	CLA	6	0
25	C	3003	SF4	2	0
30	4	611	CHL	1	0
22	A	4008	BCR	4	0
20	B	1208	CLA	2	0
20	F	1302	CLA	8	0
22	L	4019	BCR	28	0
22	I	4020	BCR	10	0
20	2	604	CLA	26	0
28	F	5005	DGD	18	0
22	A	4011	BCR	7	0
21	B	2002	PQN	3	0
20	4	612	CLA	16	0
20	A	1115	CLA	9	0
20	A	1110	CLA	8	0
22	1	504	BCR	4	0
22	B	4004	BCR	4	0
22	K	4001	BCR	7	0
20	A	1012	CLA	10	0
20	B	1225	CLA	8	0
20	1	613	CLA	8	0
20	2	606	CLA	17	0
20	A	1105	CLA	10	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	A	1121	CLA	1	0
30	2	611	CHL	5	0
29	2	501	LUT	12	0
20	3	617	CLA	13	0
20	A	1125	CLA	12	0
20	L	1502	CLA	19	0
22	B	4006	BCR	5	0
23	2	801	LHG	7	0
20	A	1108	CLA	3	0
20	B	1238	CLA	9	0
32	2	807	3PH	5	0
20	2	603	CLA	8	0
22	J	4012	BCR	5	0
22	K	4002	BCR	8	0
20	A	1127	CLA	11	0
25	C	3002	SF4	1	0
22	H	4021	BCR	18	0
31	2	502	XAT	13	0
20	3	606	CLA	7	0
20	A	1141	CLA	3	0
20	B	1240	CLA	7	0
20	B	1021	CLA	9	0
20	F	1301	CLA	13	0
20	4	609	CLA	17	0
20	K	1402	CLA	1	0
20	1	611	CLA	9	0
20	A	1122	CLA	7	0
20	B	1234	CLA	9	0
30	2	610	CHL	17	0
20	B	1211	CLA	10	0
20	2	601	CLA	9	0
20	A	1109	CLA	12	0
23	B	5001	LHG	2	0
20	B	1223	CLA	7	0
20	A	1124	CLA	4	0
28	4	802	DGD	4	0
24	2	808	LMT	7	0
20	A	1130	CLA	3	0
20	3	608	CLA	5	0
20	A	1119	CLA	12	0
30	1	609	CHL	13	0
30	2	613	CHL	5	0

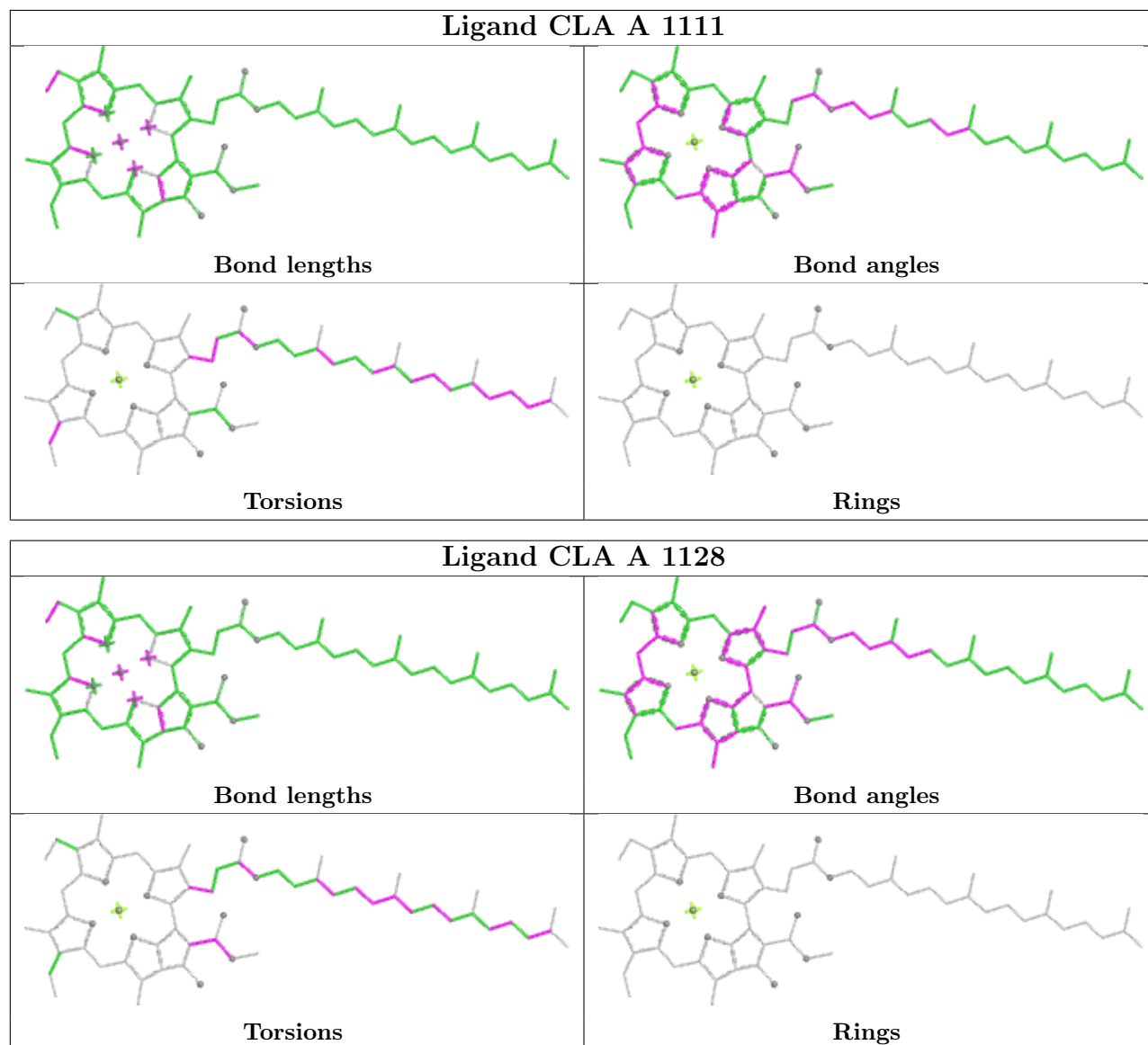
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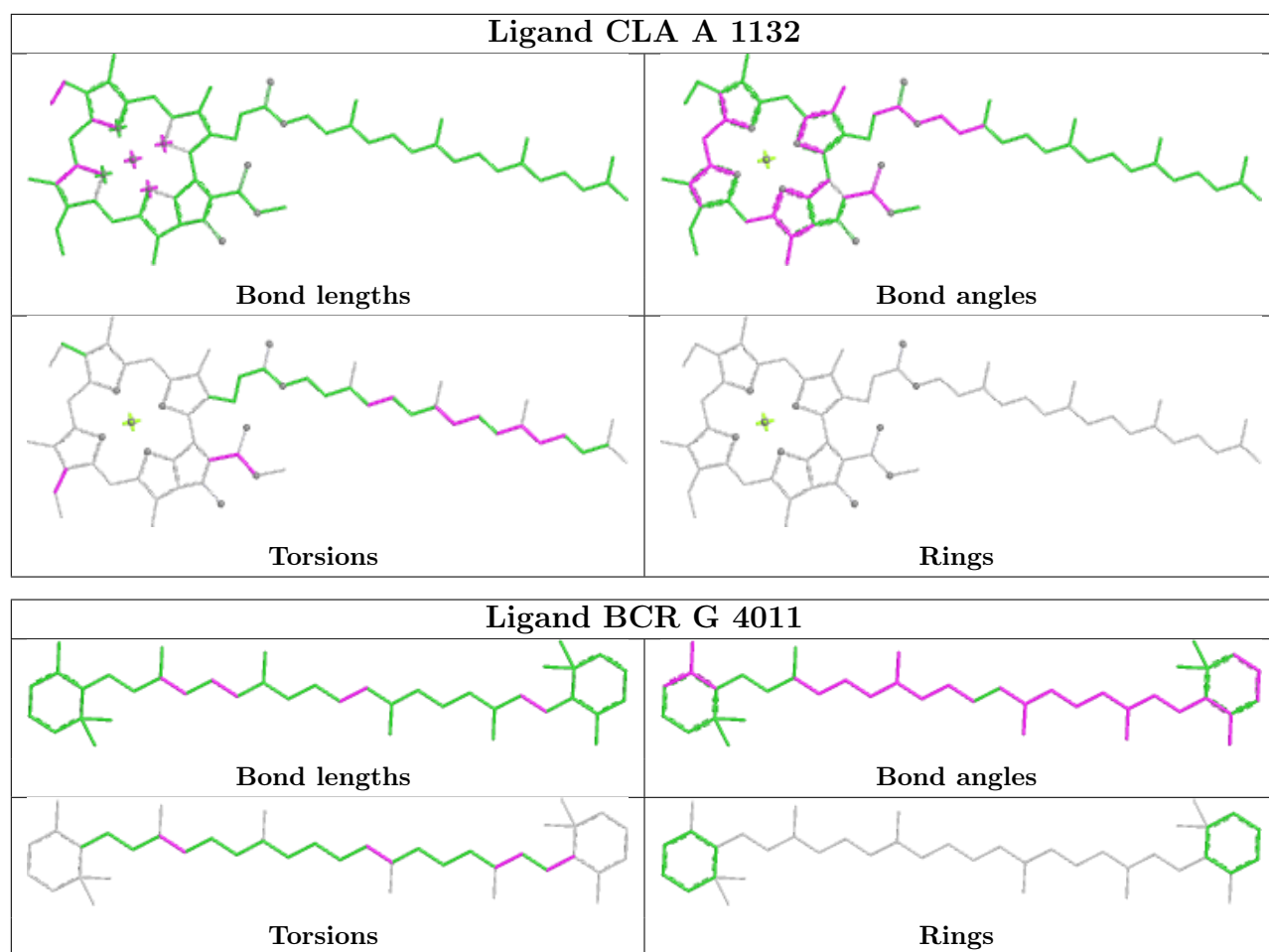
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	1	605	CLA	8	0
30	2	615	CHL	4	0
20	A	1118	CLA	2	0
20	A	1137	CLA	4	0
20	B	1212	CLA	4	0
22	2	503	BCR	23	0
20	A	1126	CLA	17	0
30	3	607	CHL	1	0
23	A	5001	LHG	1	0
20	B	1206	CLA	10	0
20	A	1140	CLA	7	0
20	4	603	CLA	18	0
29	3	502	LUT	4	0
22	A	4017	BCR	7	0
20	B	1201	CLA	4	0
20	A	1101	CLA	16	0
20	A	1120	CLA	3	0
20	A	1131	CLA	10	0
29	J	4013	LUT	9	0
20	A	1102	CLA	5	0
20	A	1134	CLA	11	0
20	A	1135	CLA	4	0
20	B	1204	CLA	8	0
20	B	1219	CLA	2	0
20	H	1701	CLA	18	0
20	1	607	CLA	1	0
20	2	608	CLA	9	0
26	G	5002	LMG	8	0
20	2	605	CLA	9	0
26	G	5006	LMG	2	0
20	A	1138	CLA	4	0
20	3	603	CLA	9	0
20	B	1203	CLA	4	0
20	4	602	CLA	17	0
20	A	1114	CLA	2	0

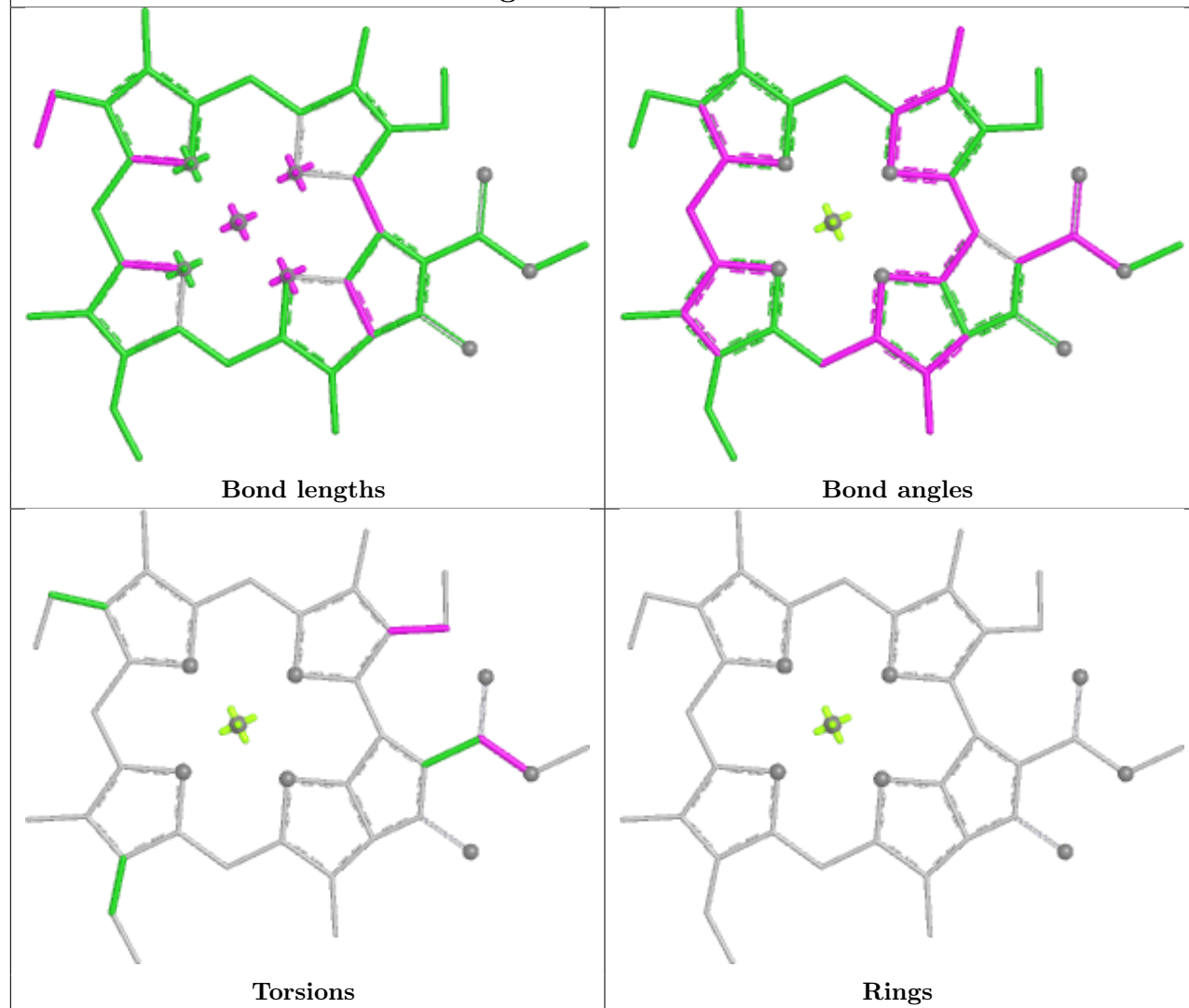
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

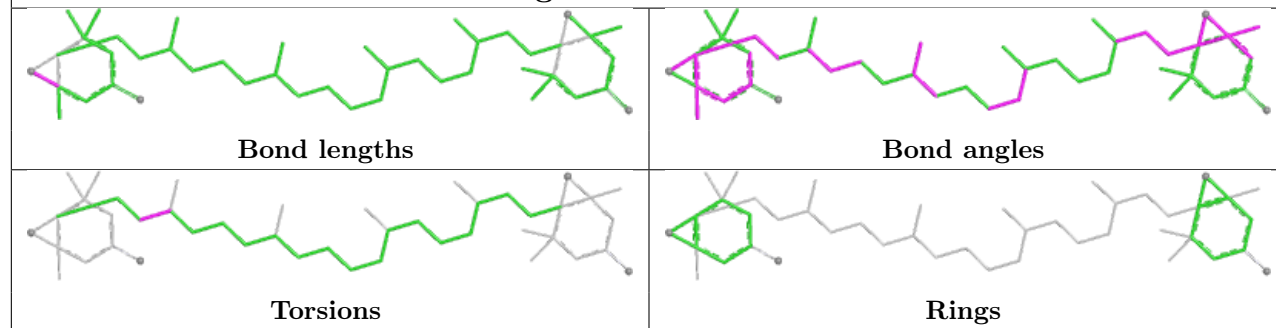


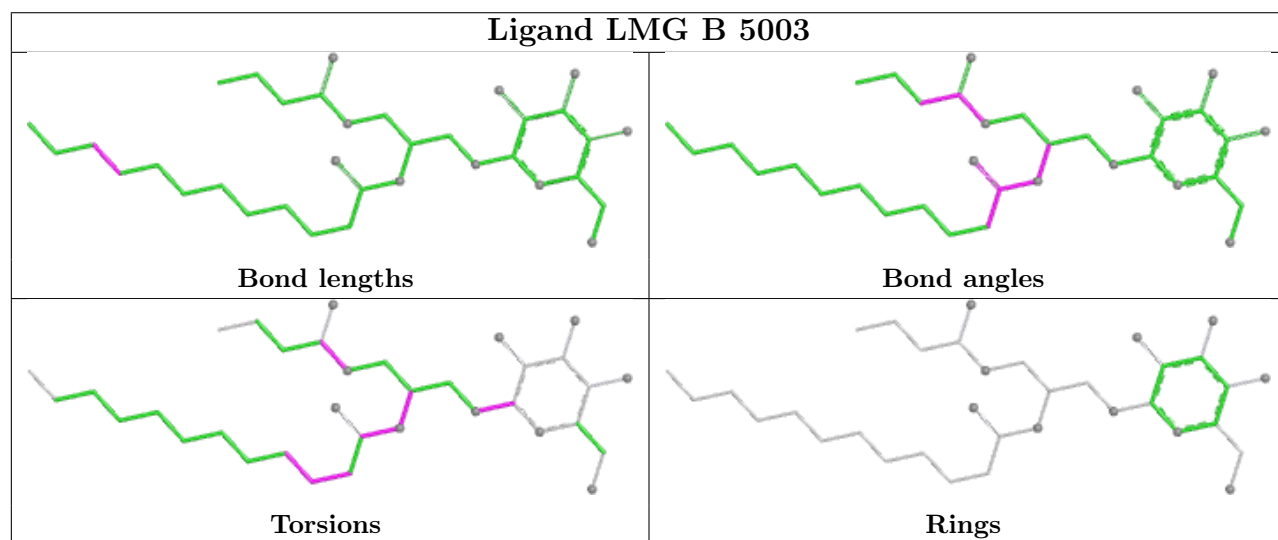
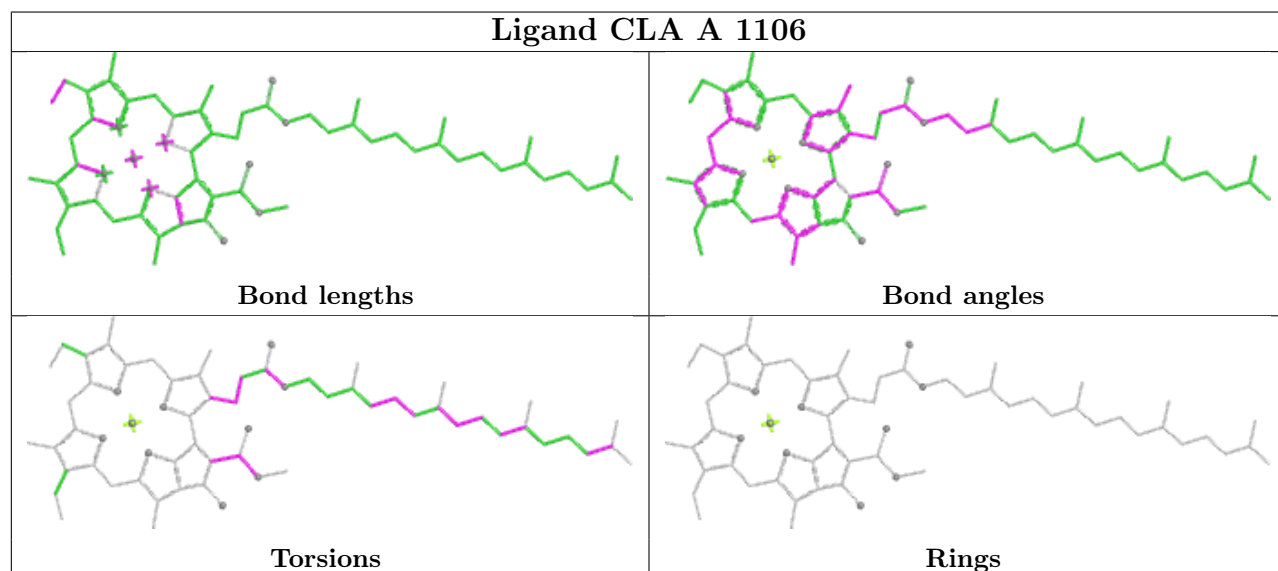
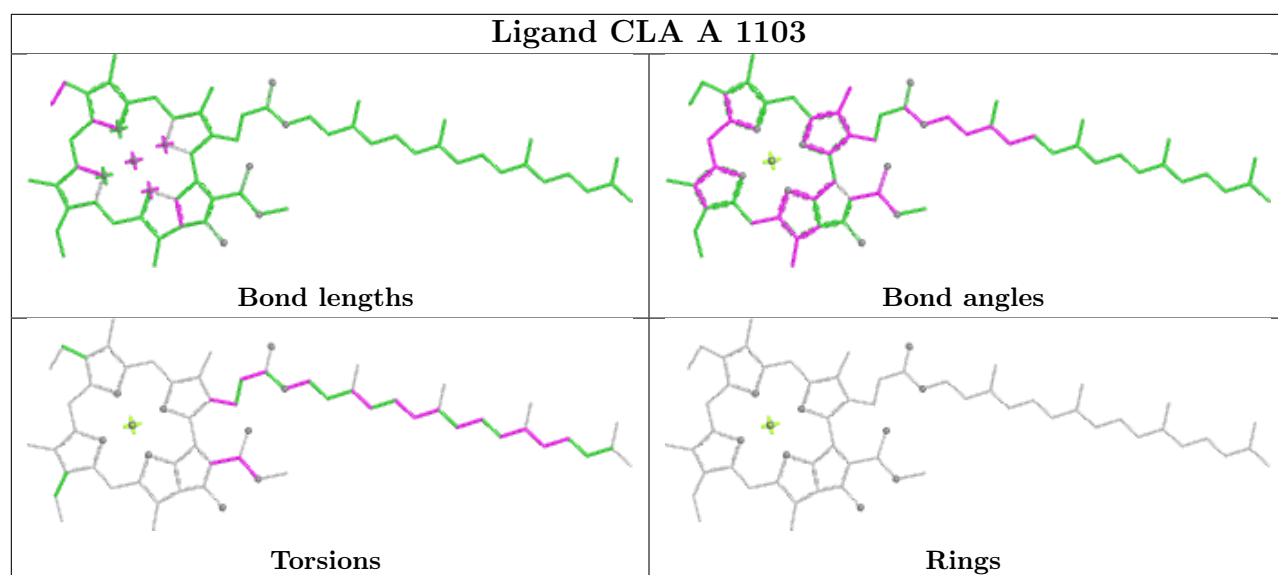


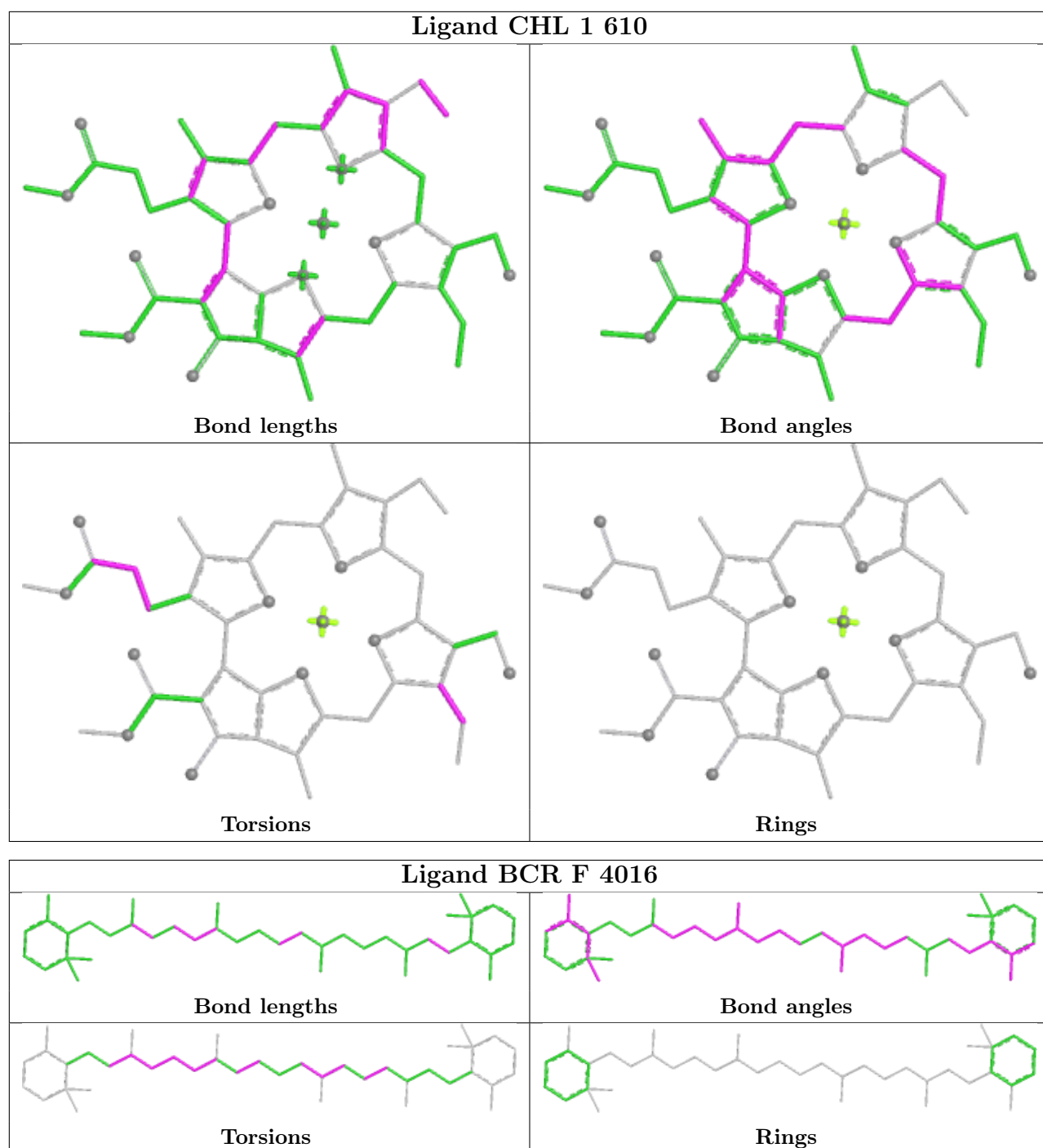
Ligand CLA 3 614

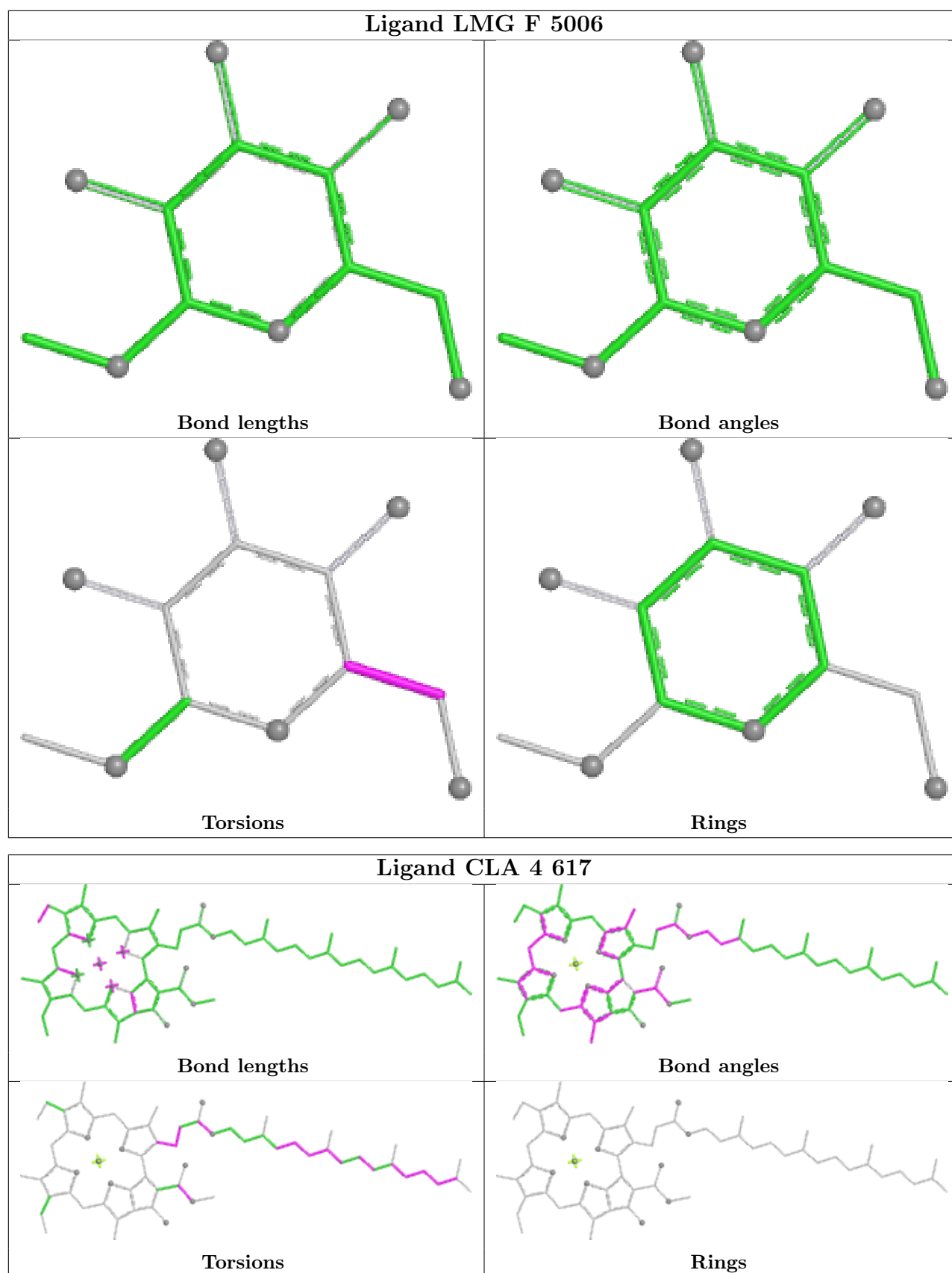


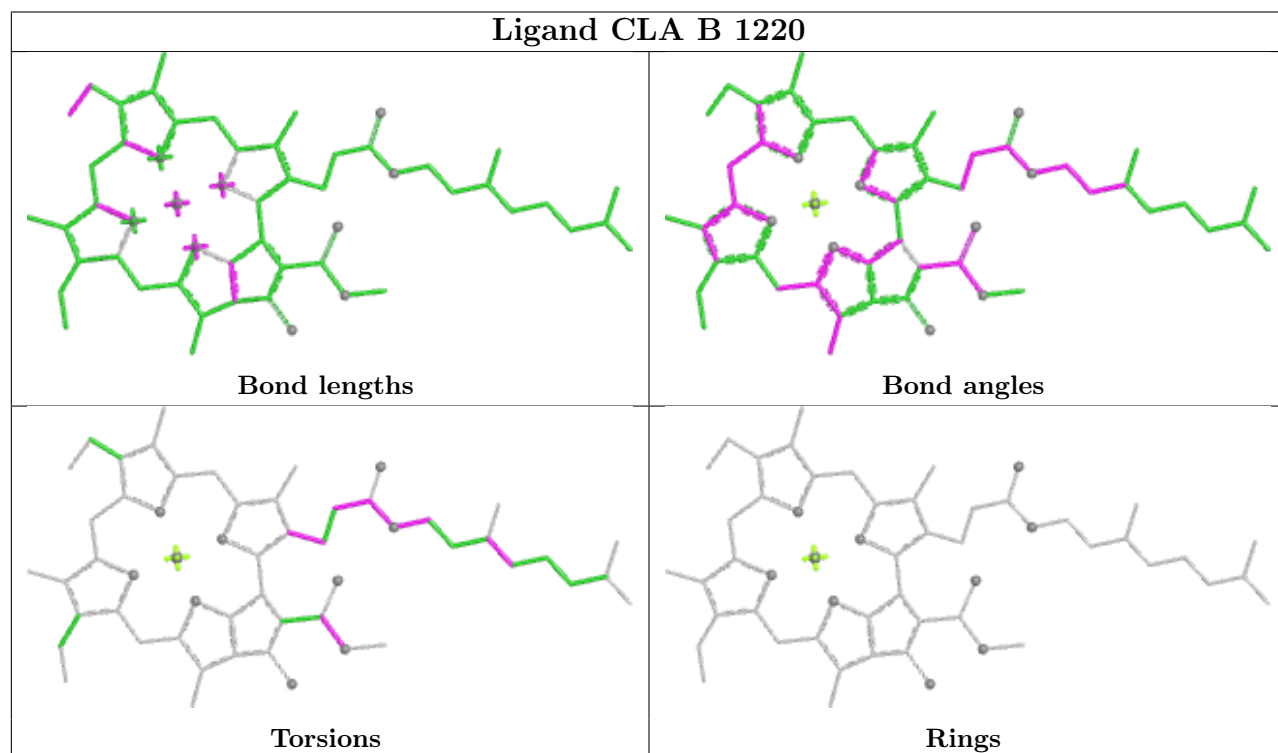
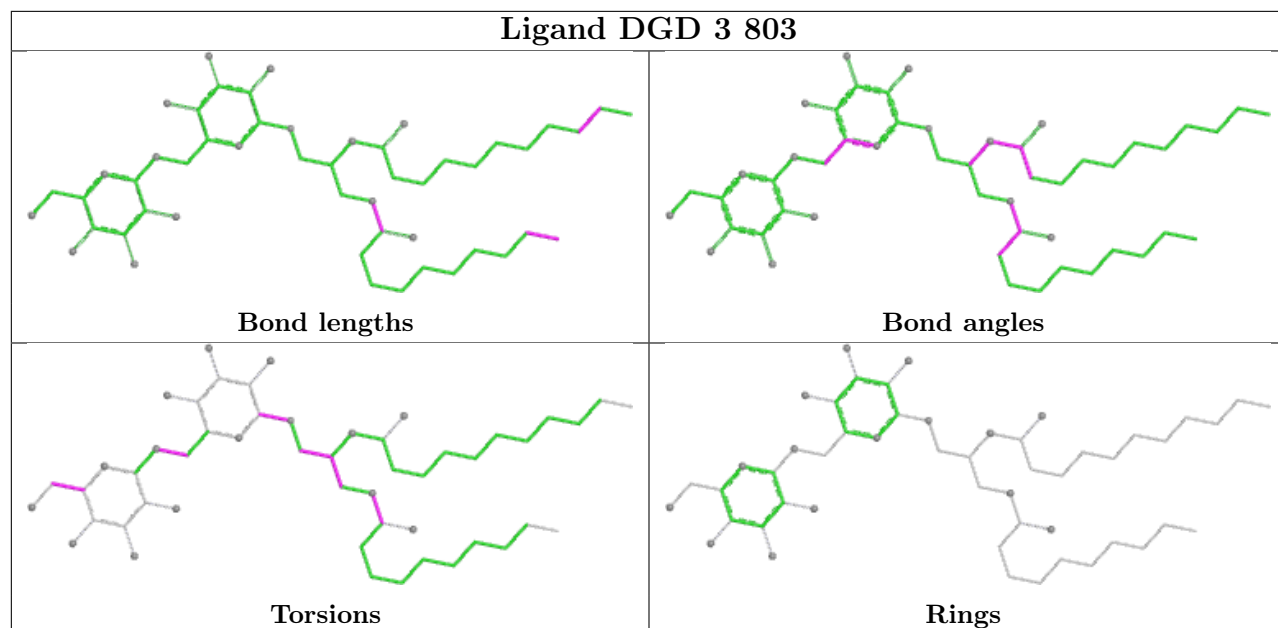
Ligand XAT 4 502



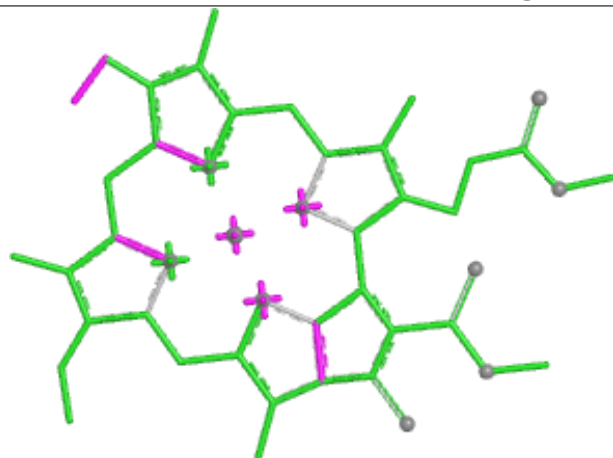




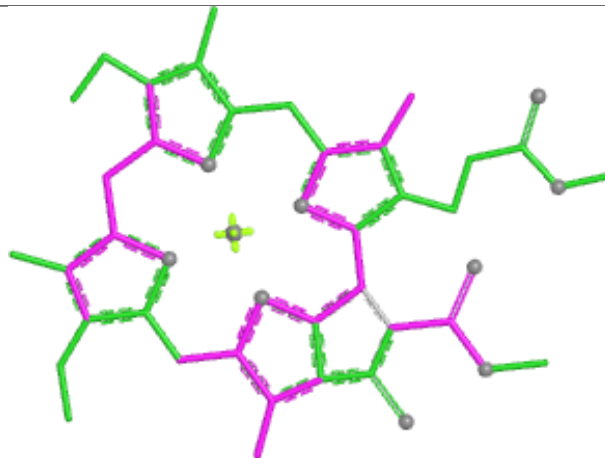




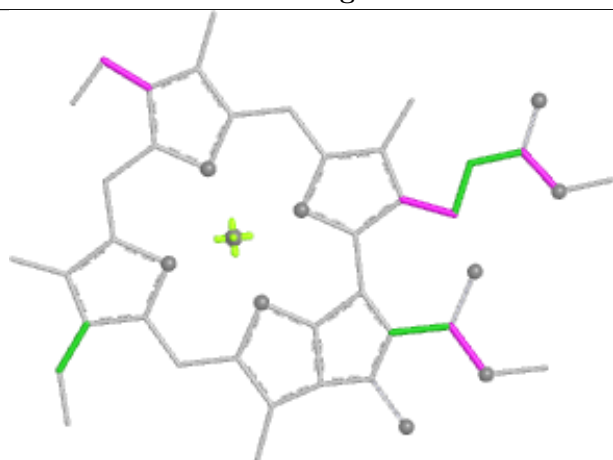
Ligand CLA 1 602



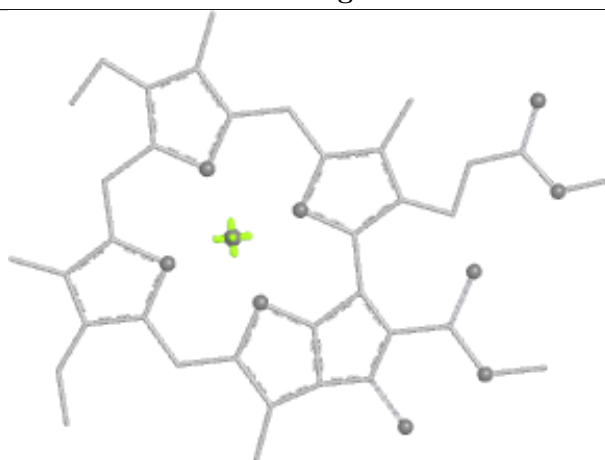
Bond lengths



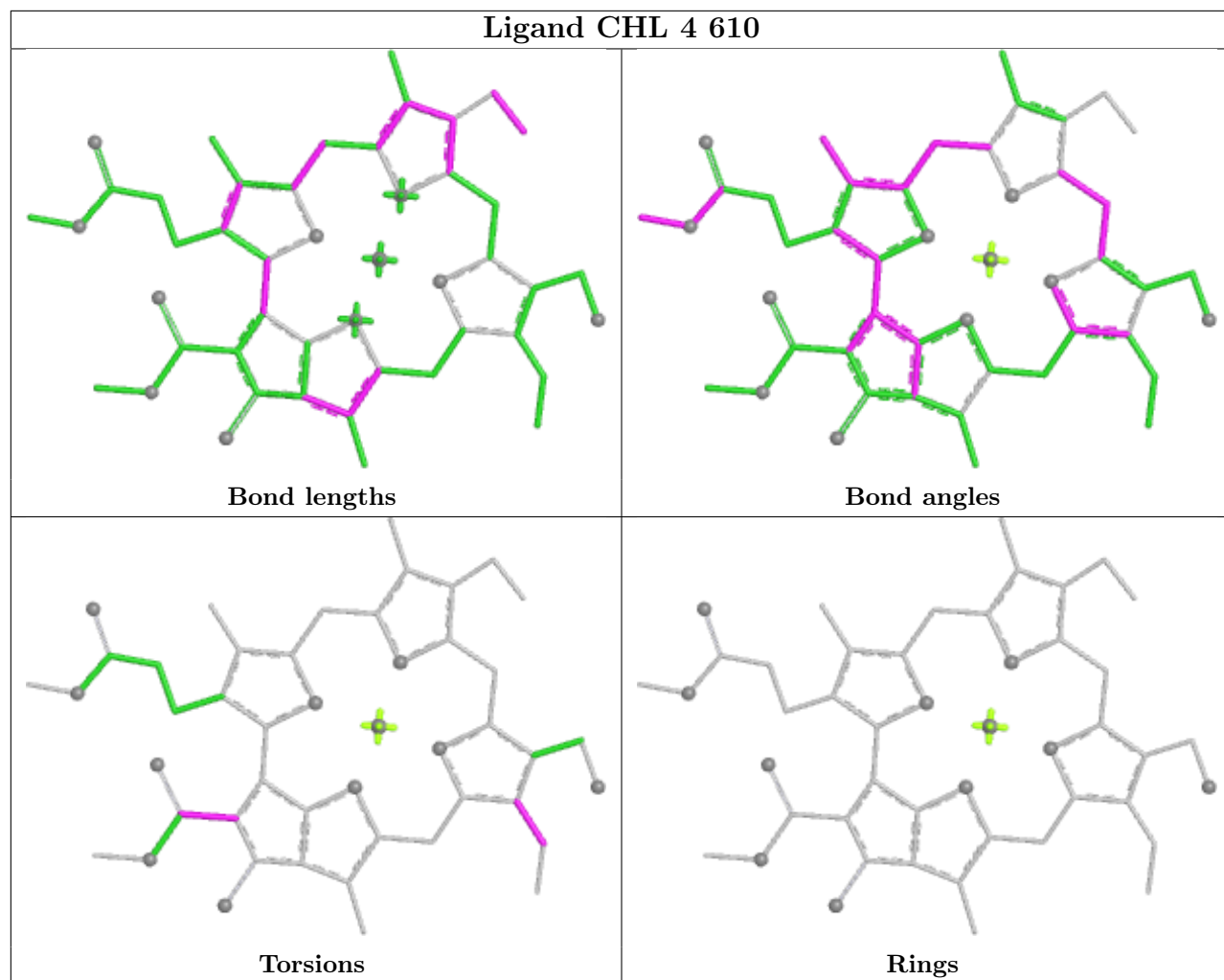
Bond angles



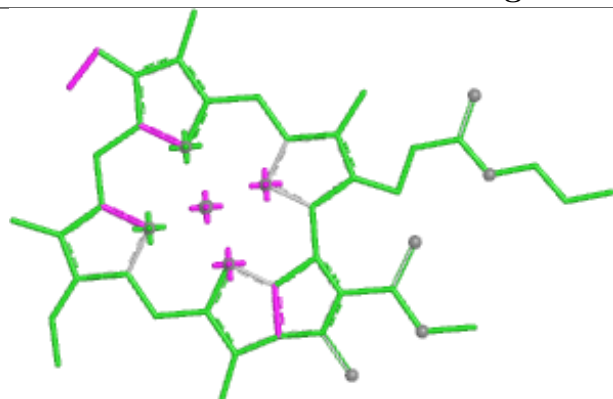
Torsions



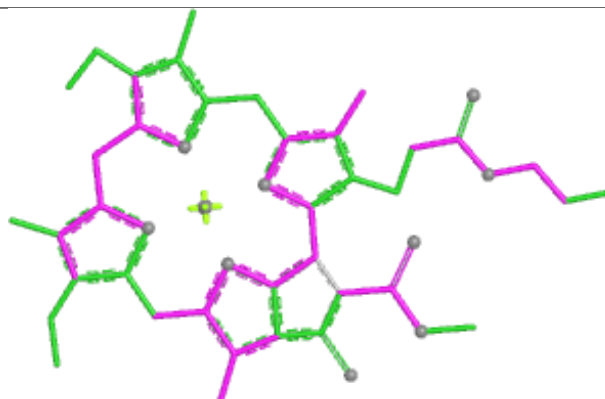
Rings



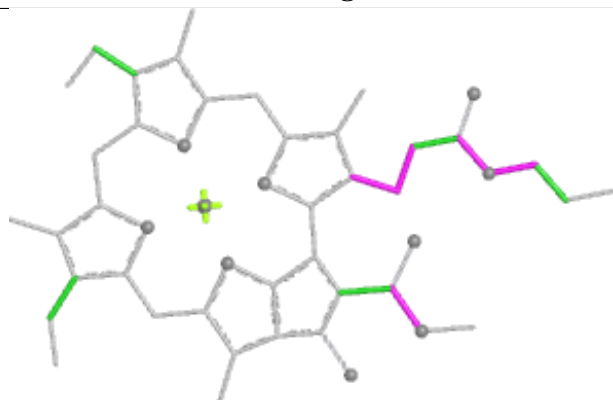
Ligand CLA K 1403



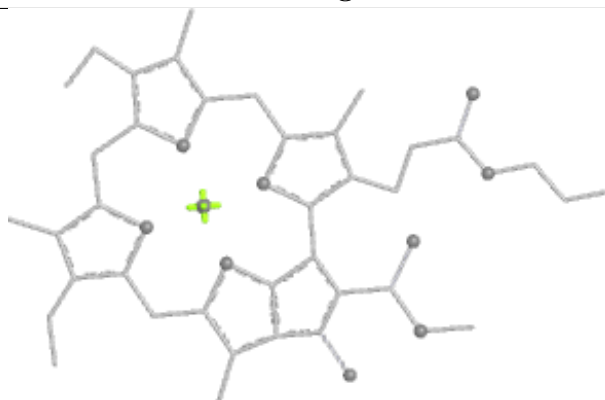
Bond lengths



Bond angles

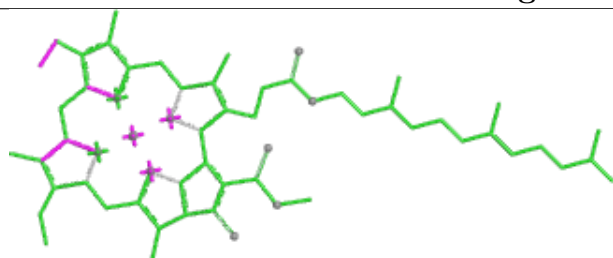


Torsions

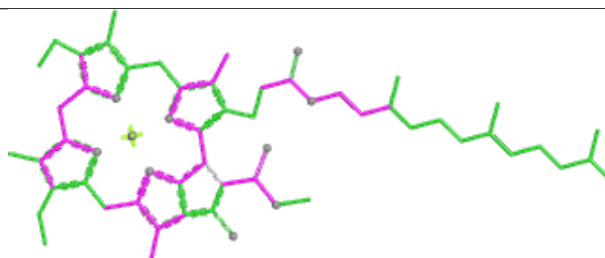


Rings

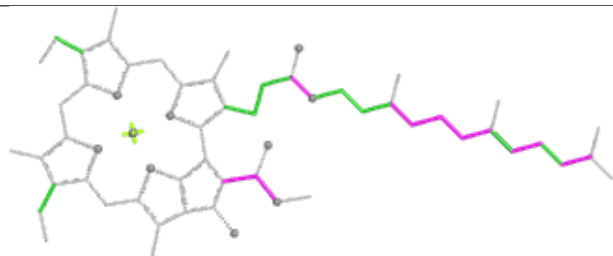
Ligand CLA 4 604



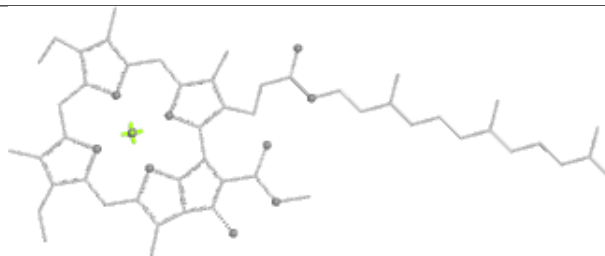
Bond lengths



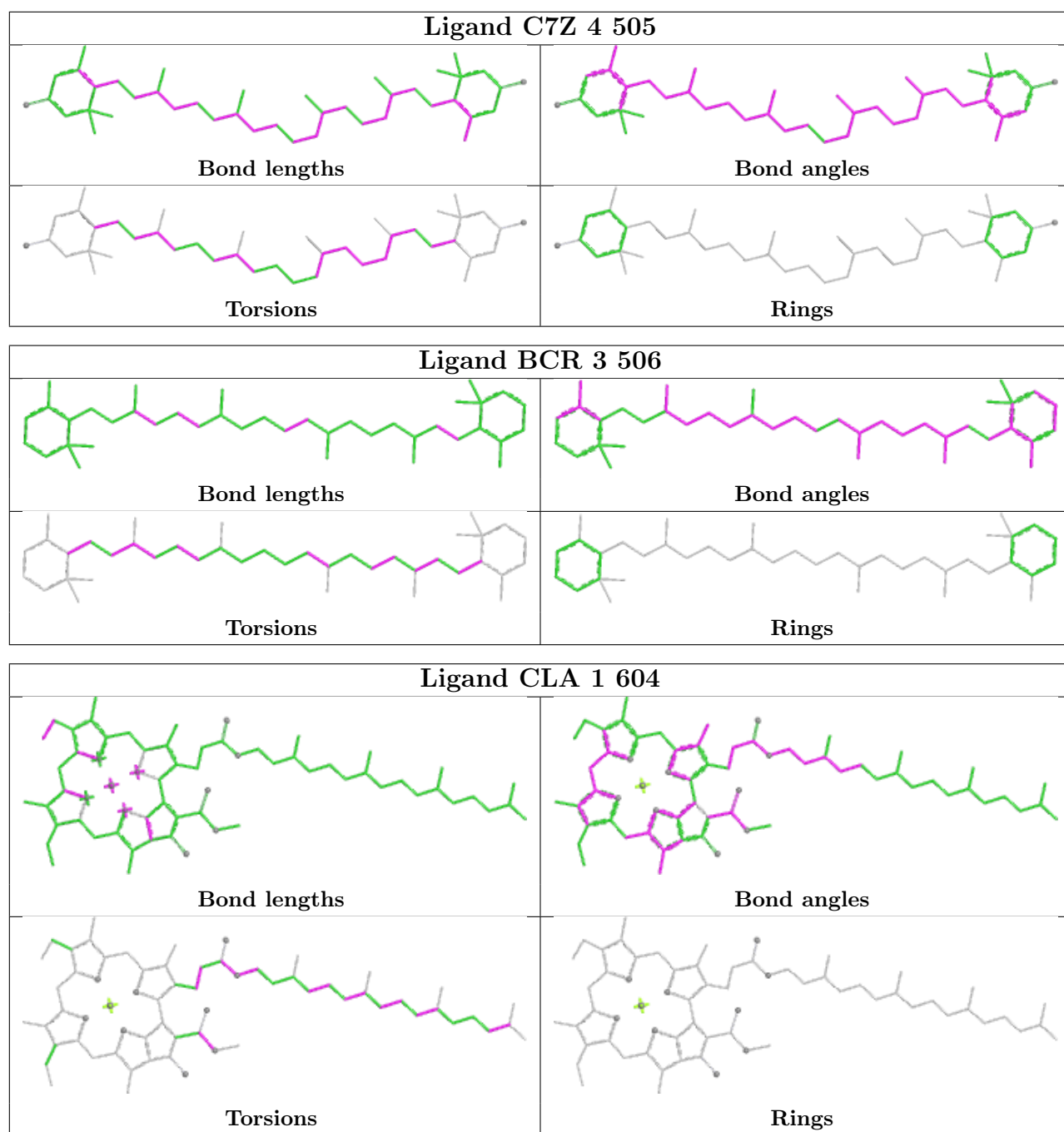
Bond angles

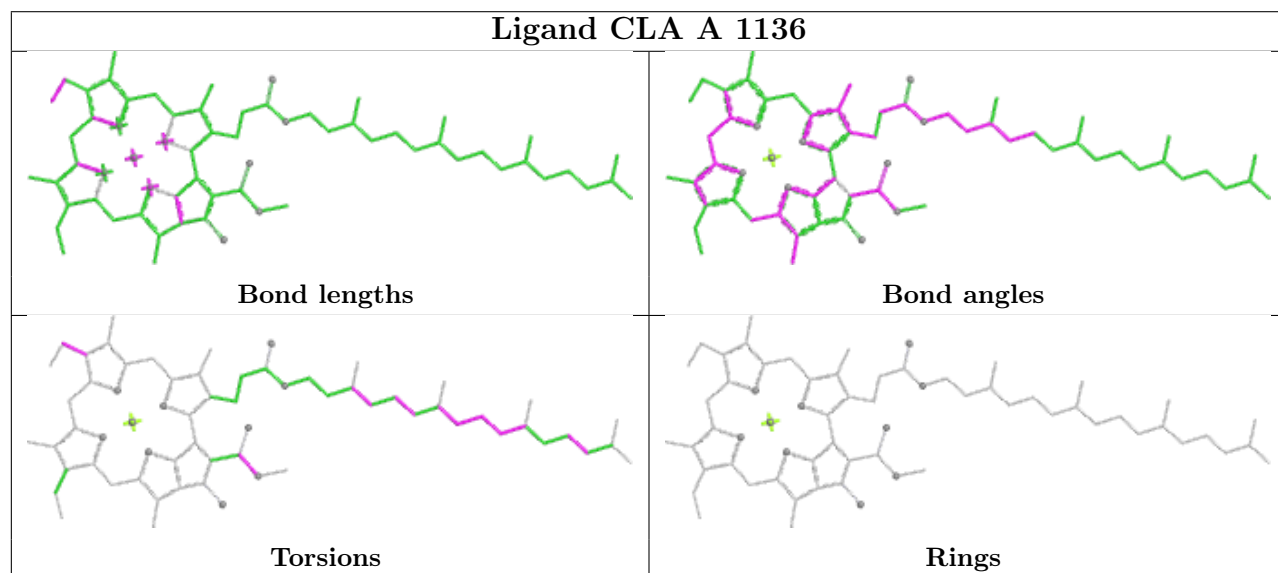
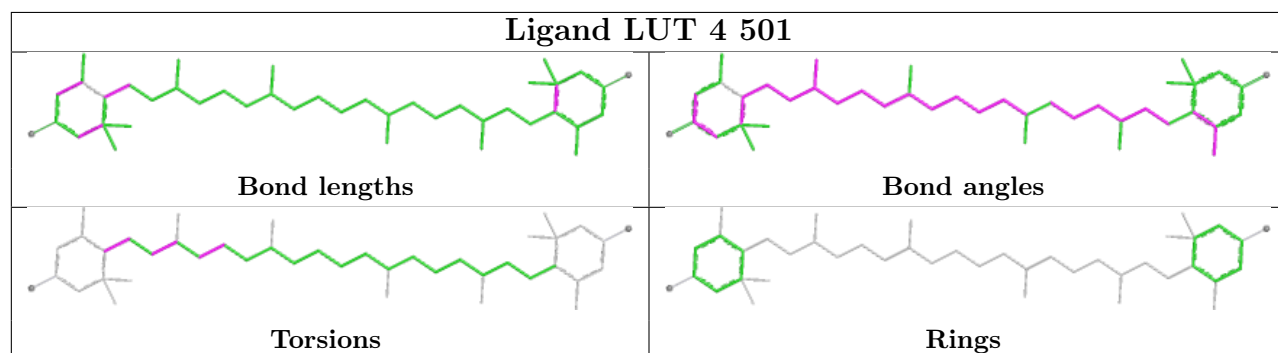
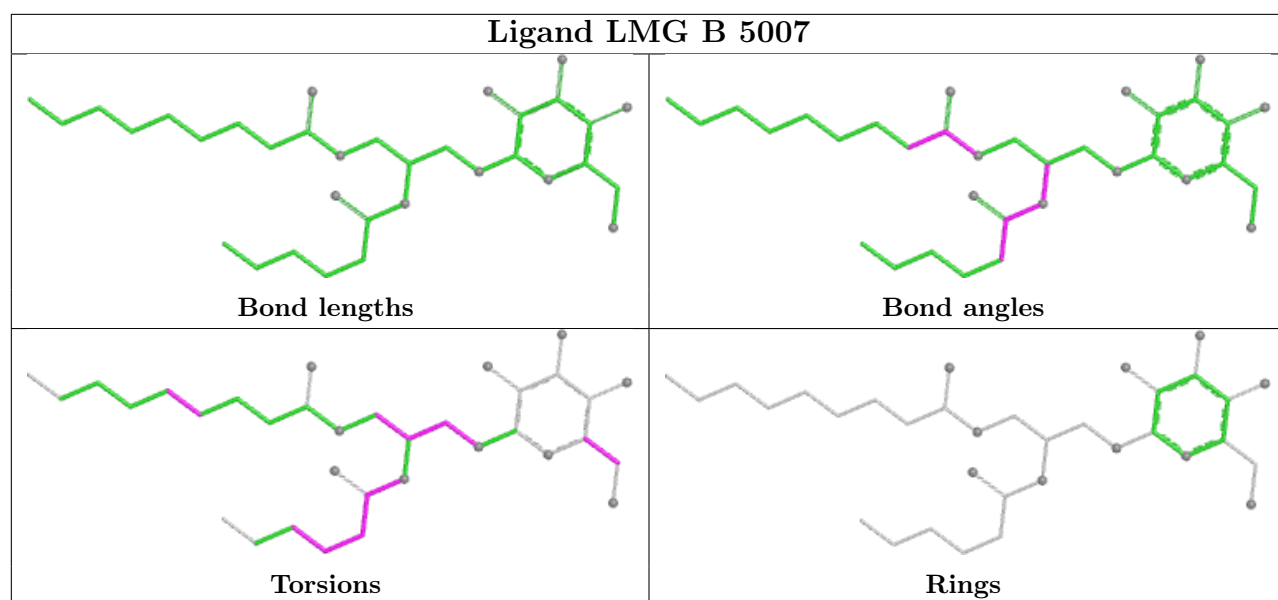


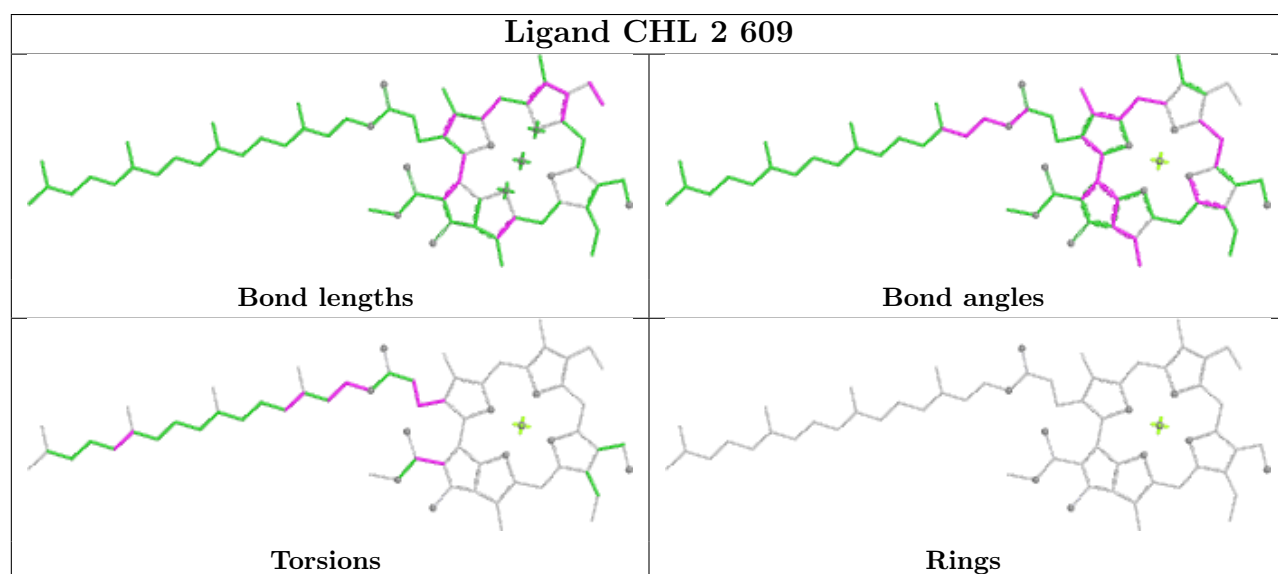
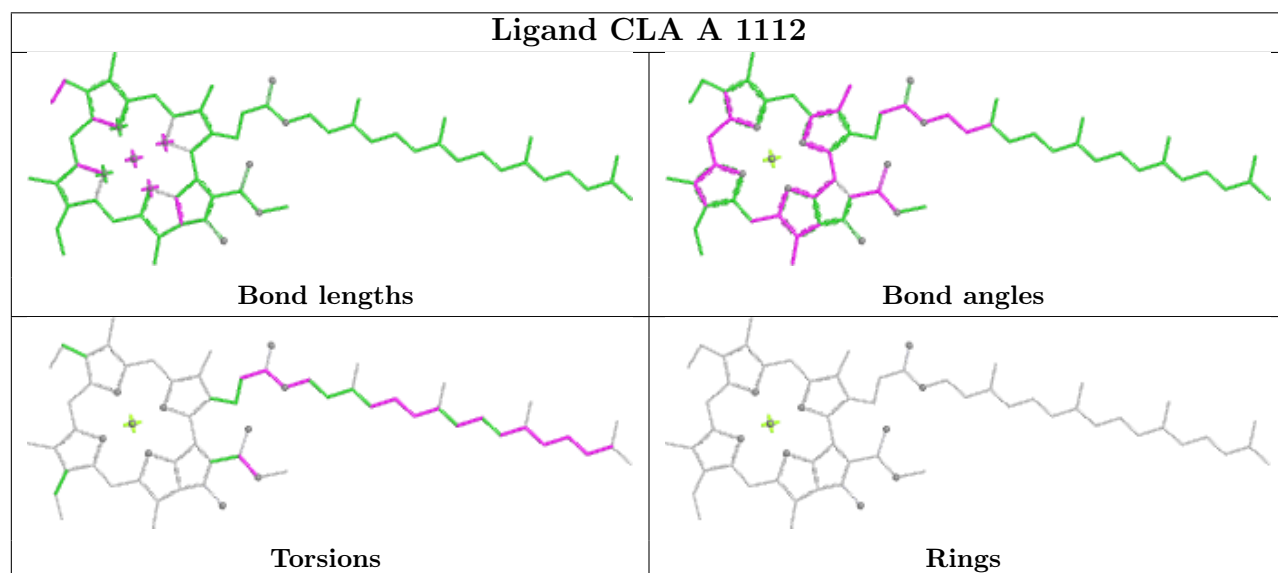
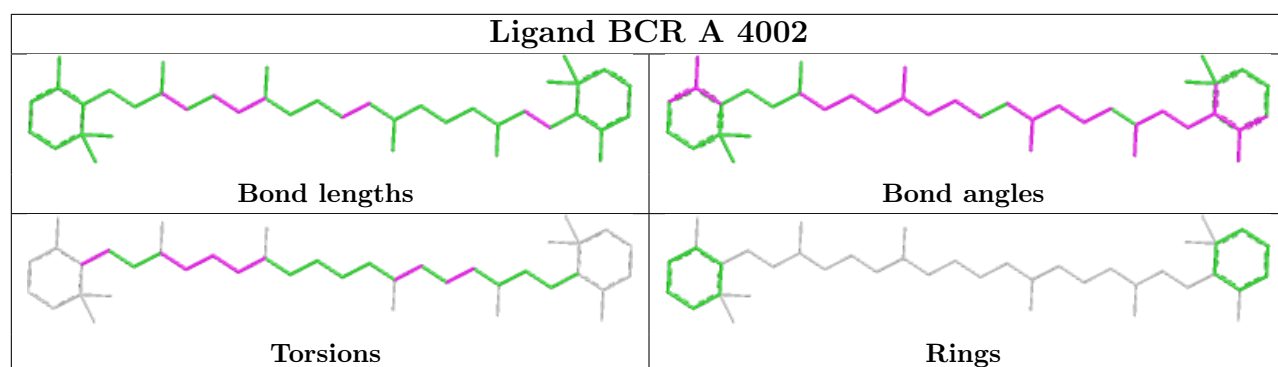
Torsions

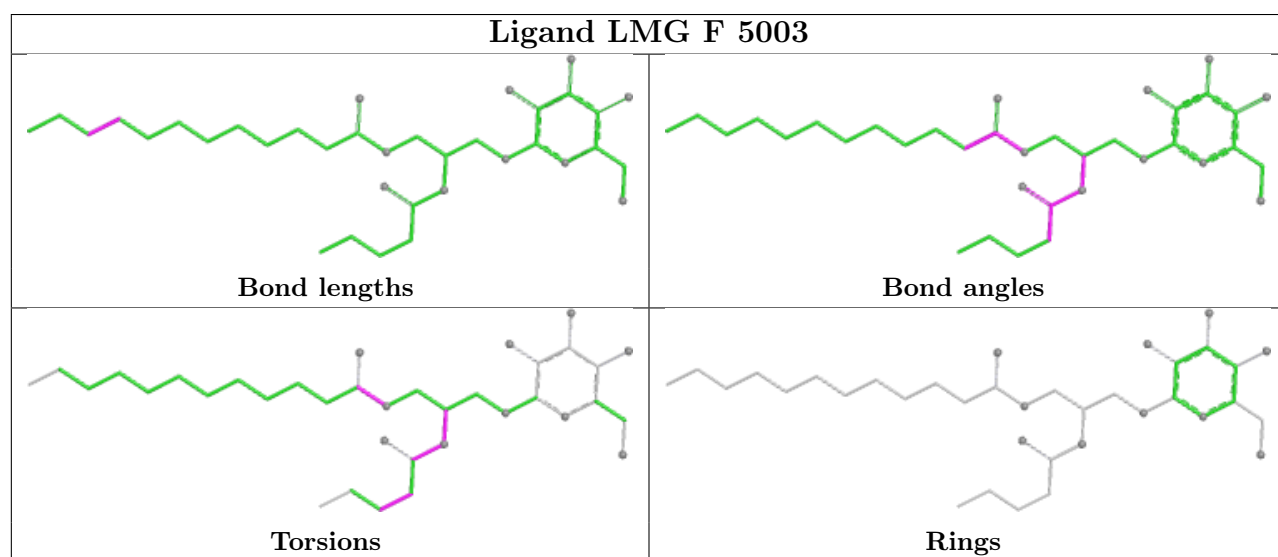
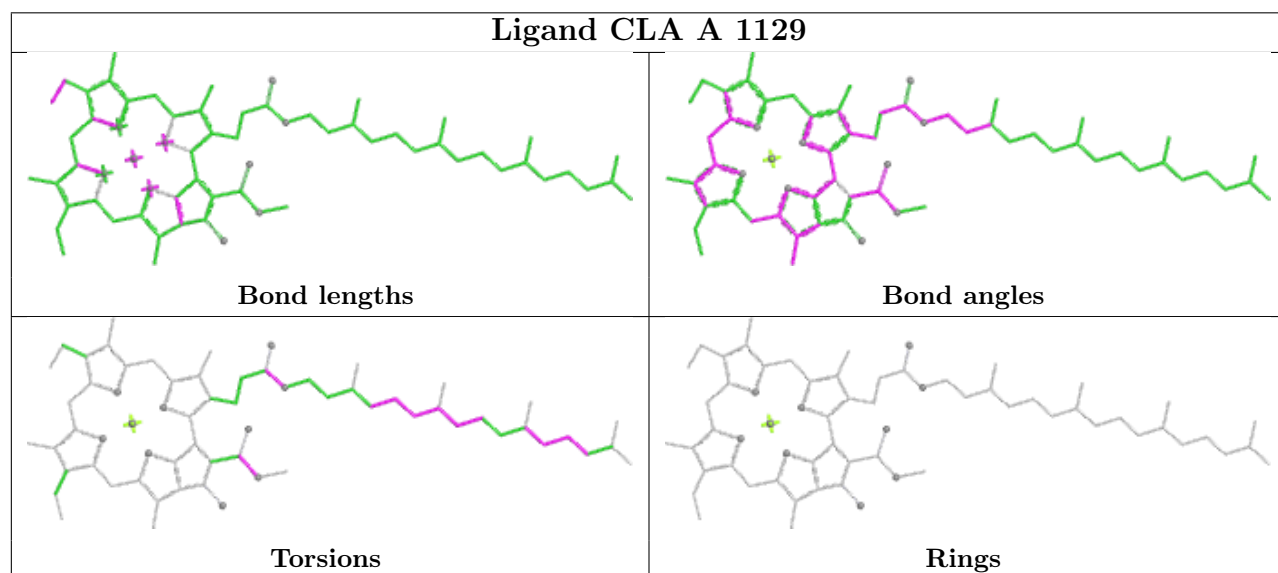
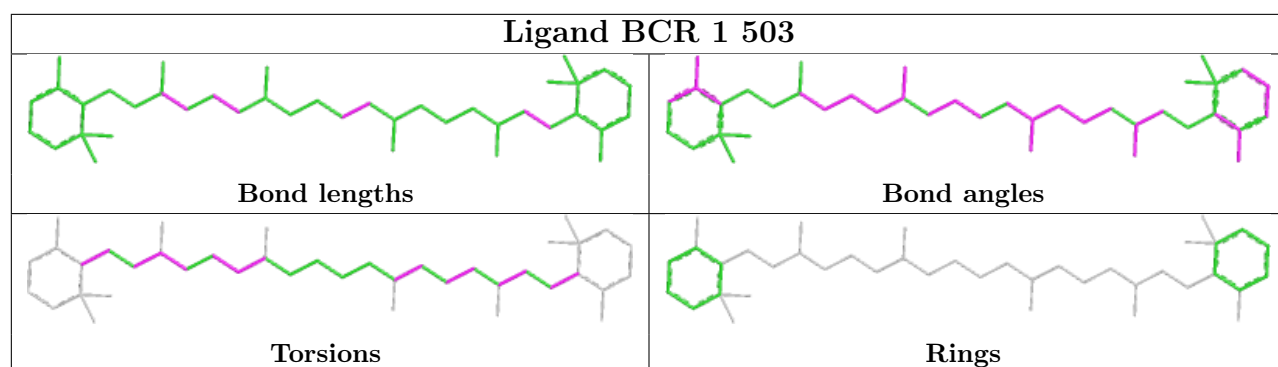


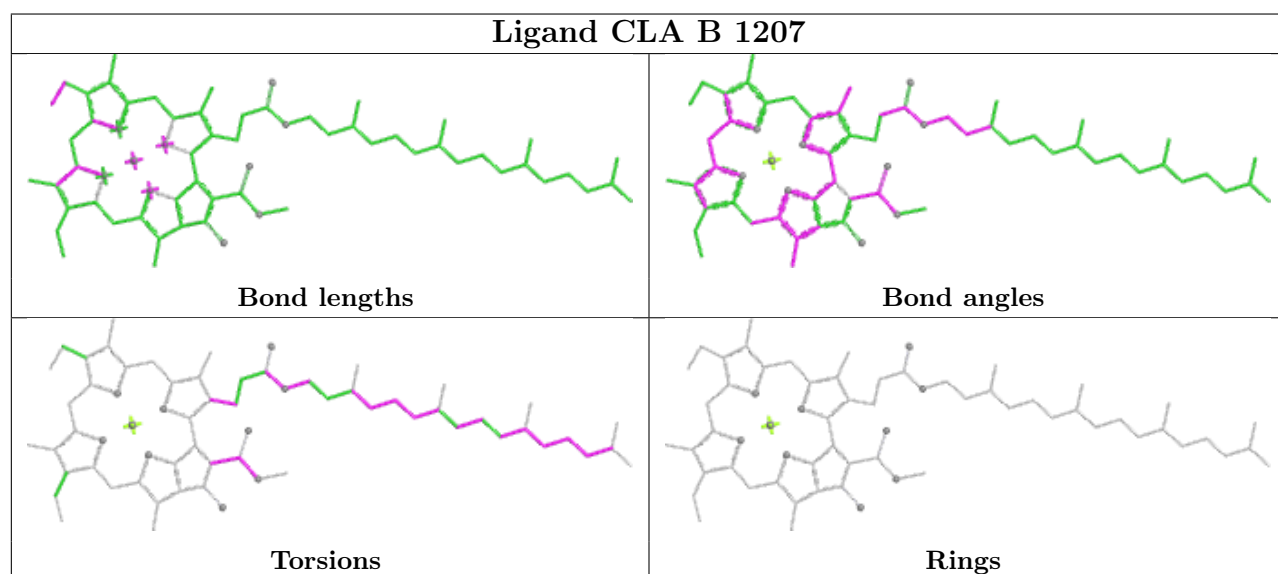
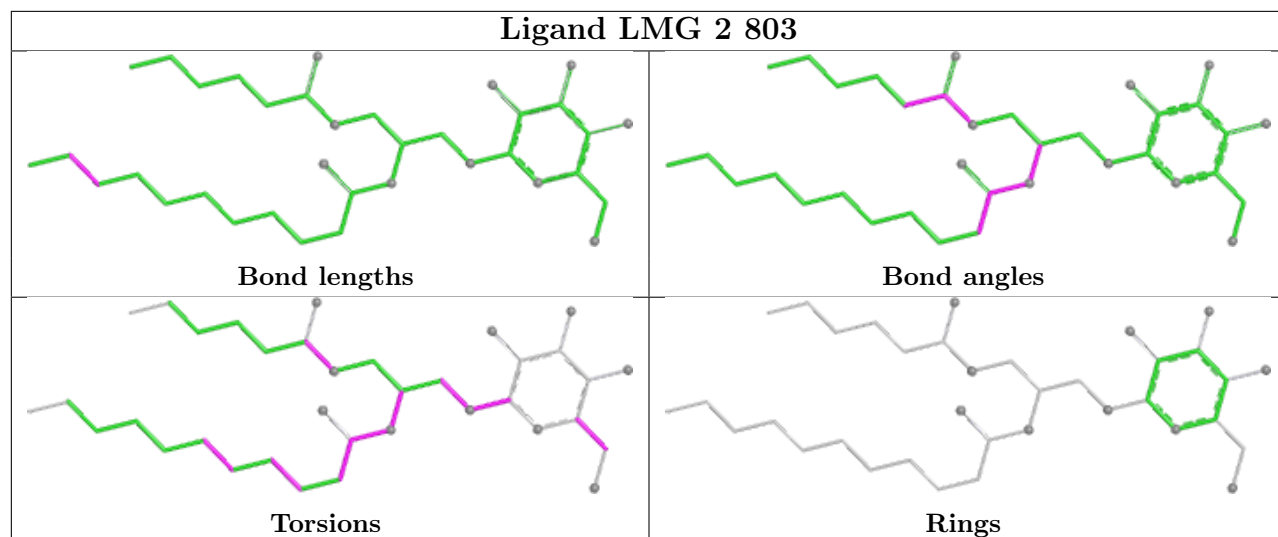
Rings



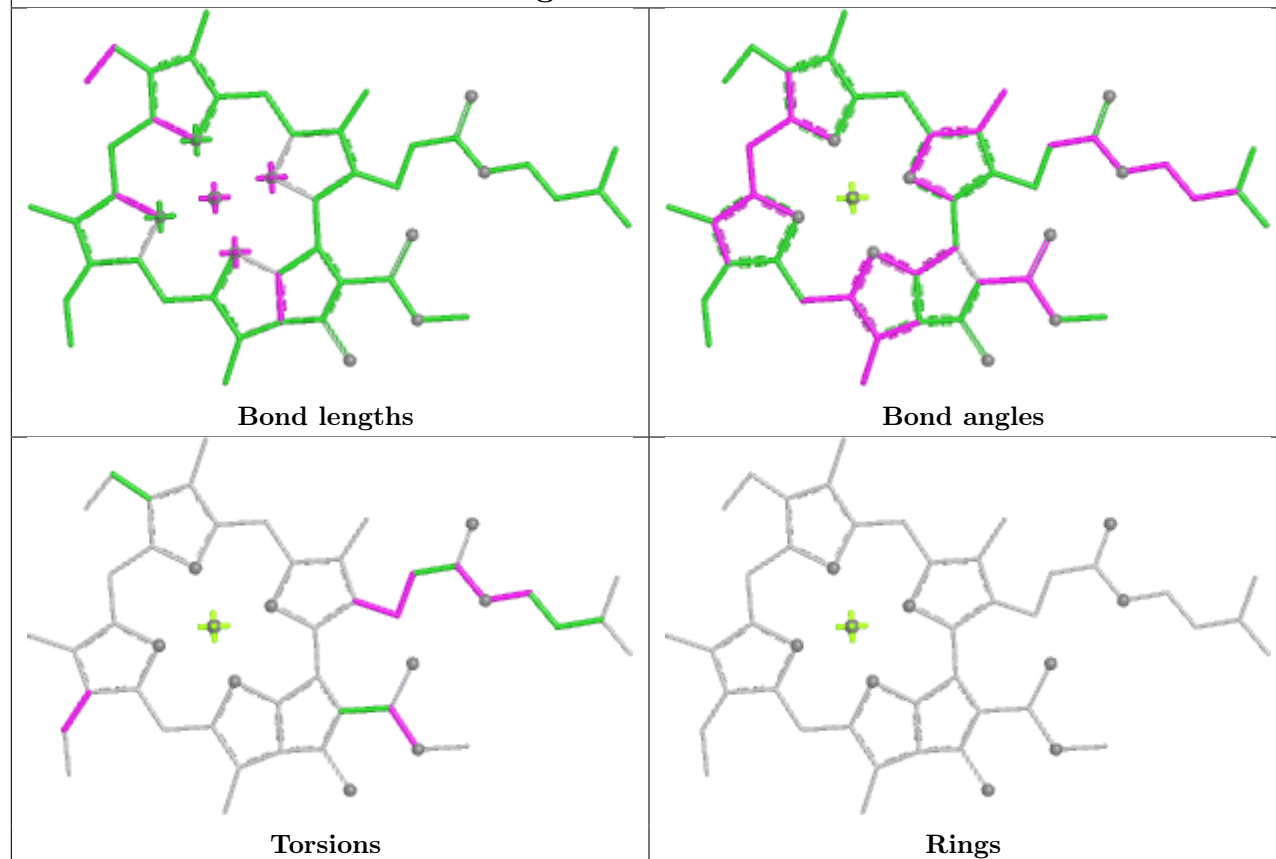




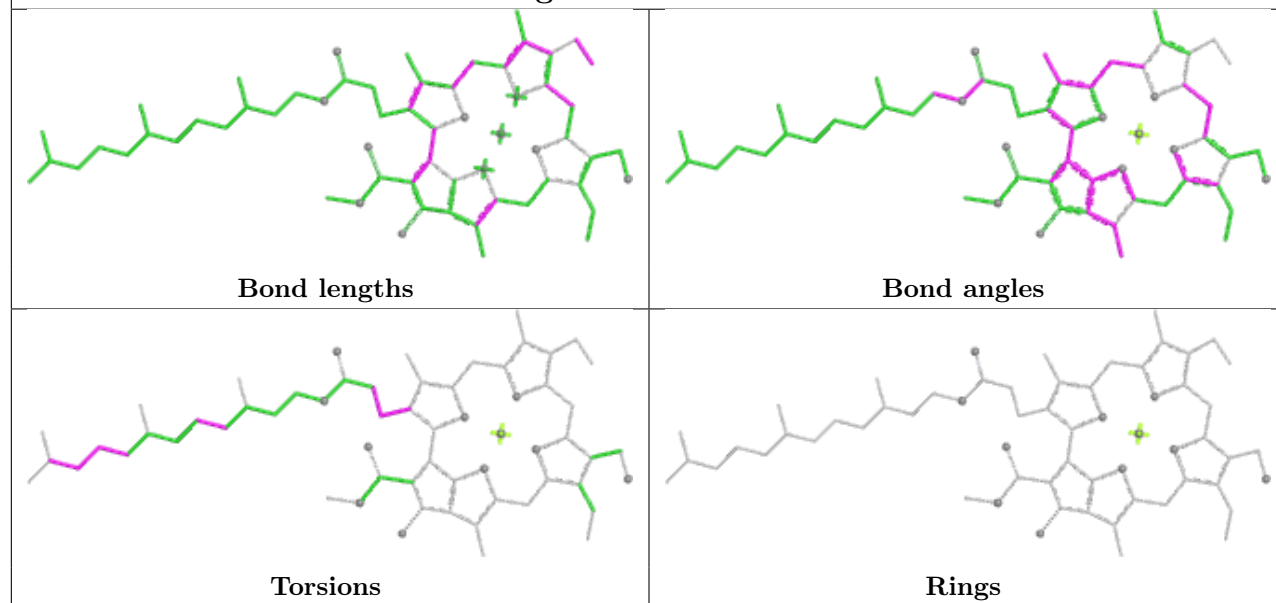


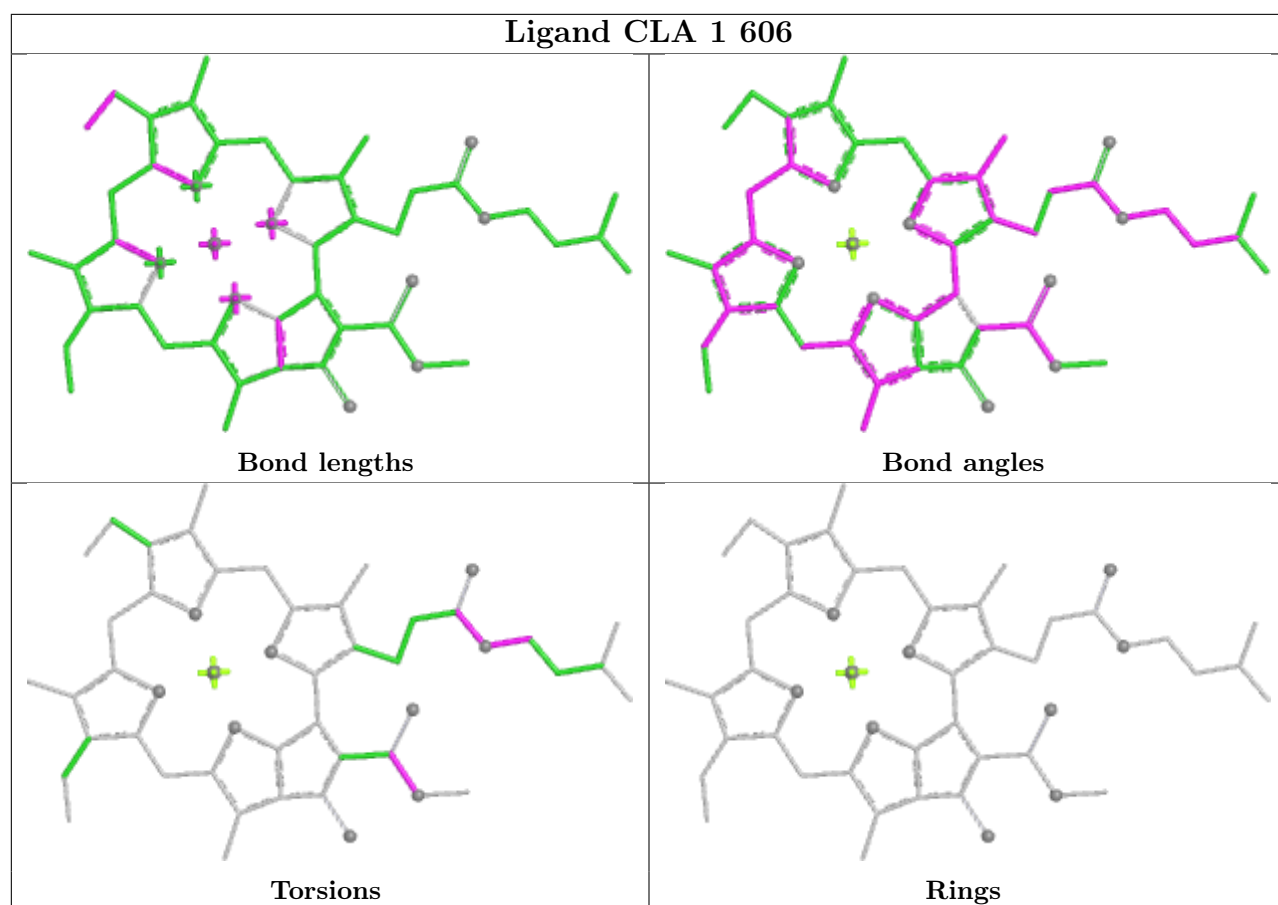


Ligand CLA 3 612

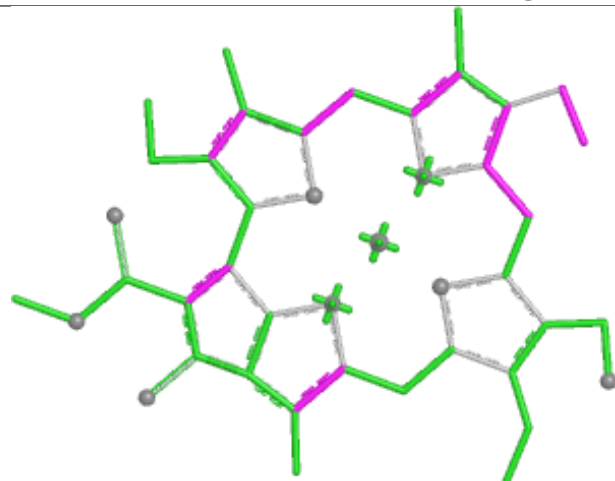


Ligand CHL 4 613

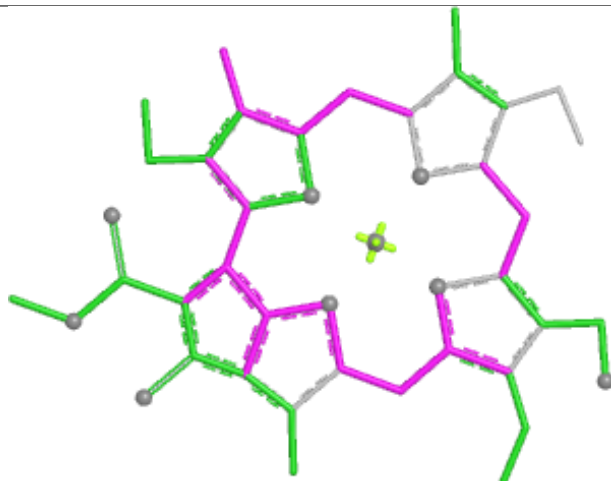




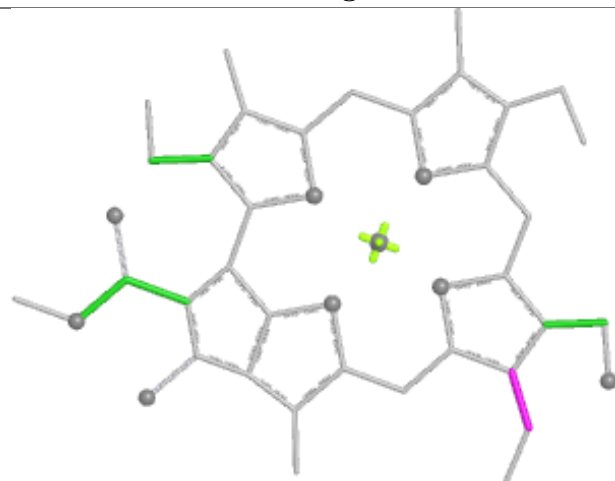
Ligand CHL 4 615



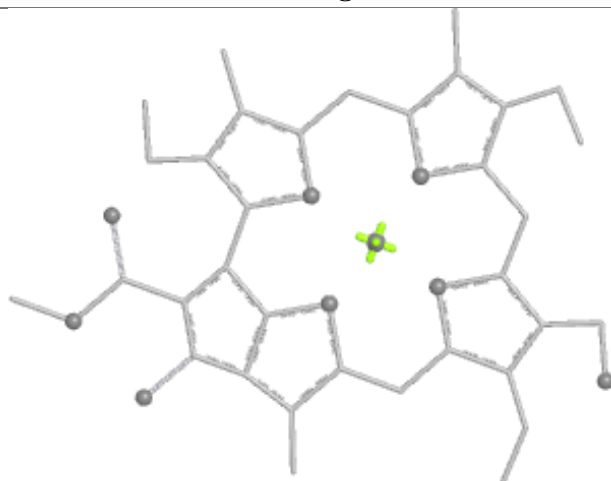
Bond lengths



Bond angles

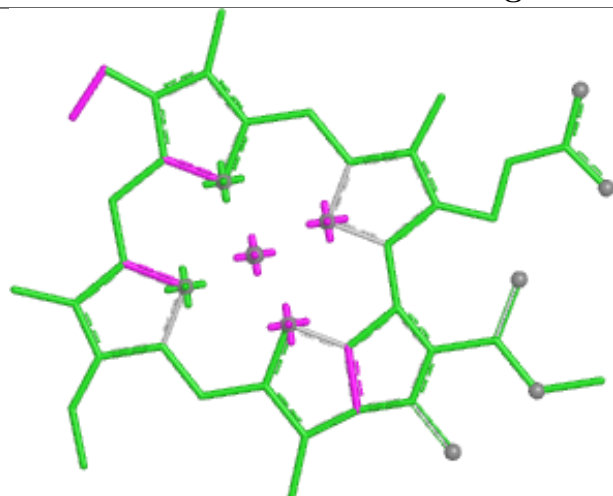


Torsions

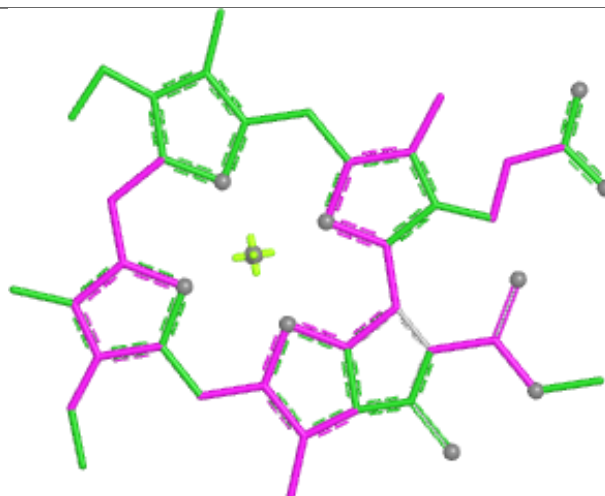


Rings

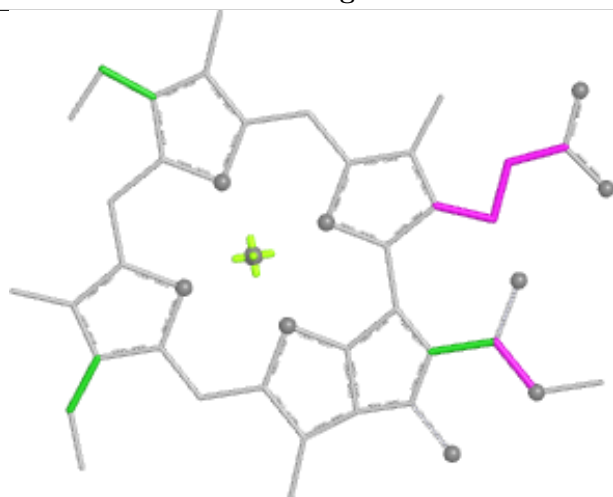
Ligand CLA A 1113



Bond lengths



Bond angles

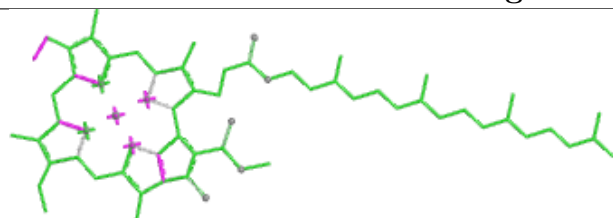


Torsions

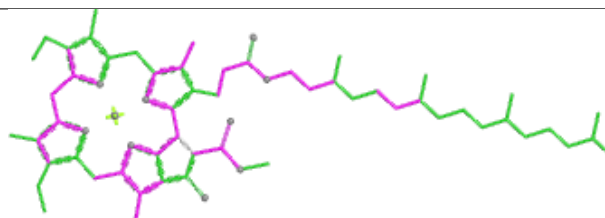


Rings

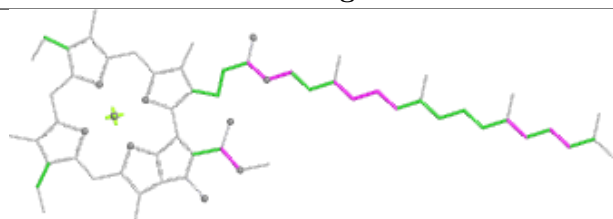
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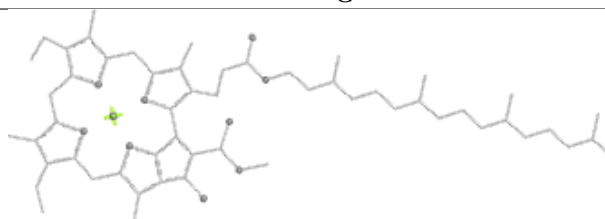
Bond lengths



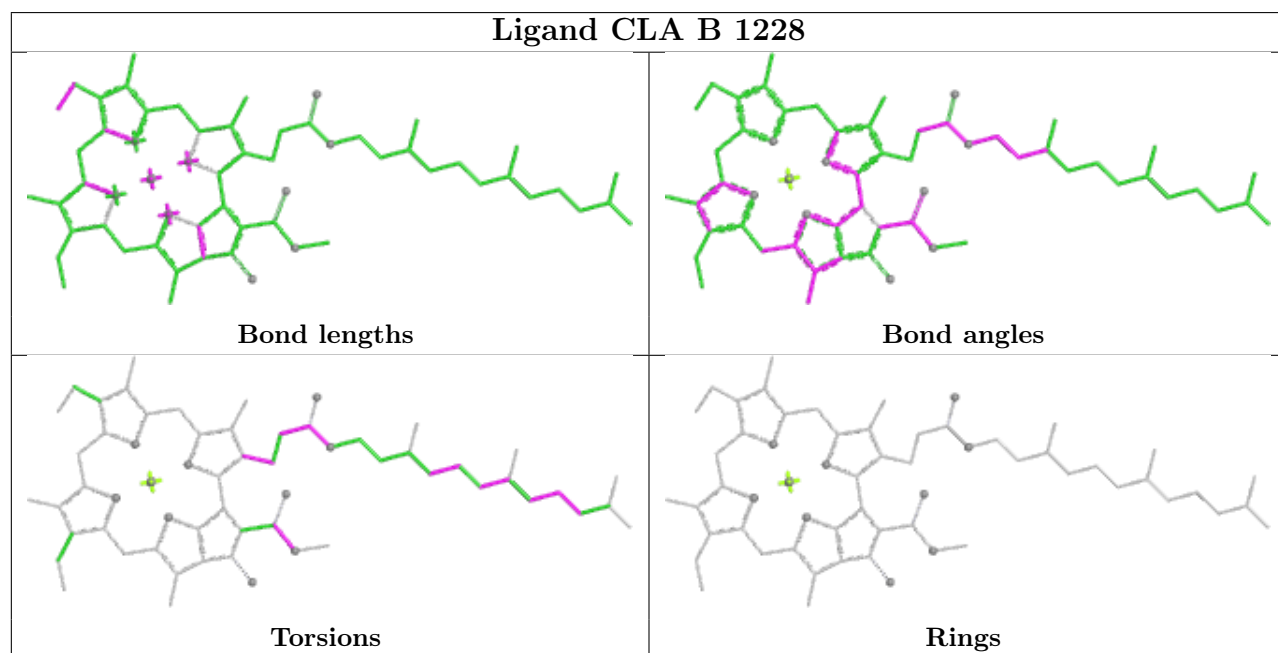
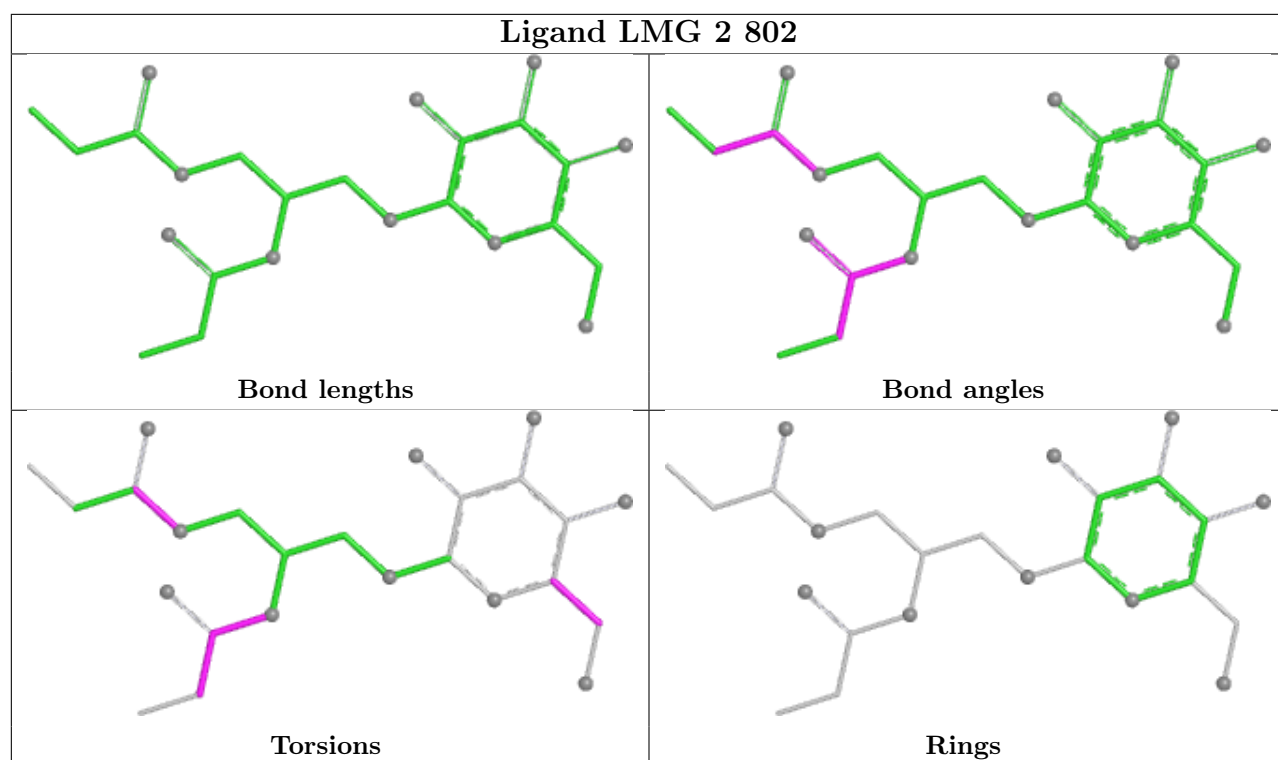
Bond angles

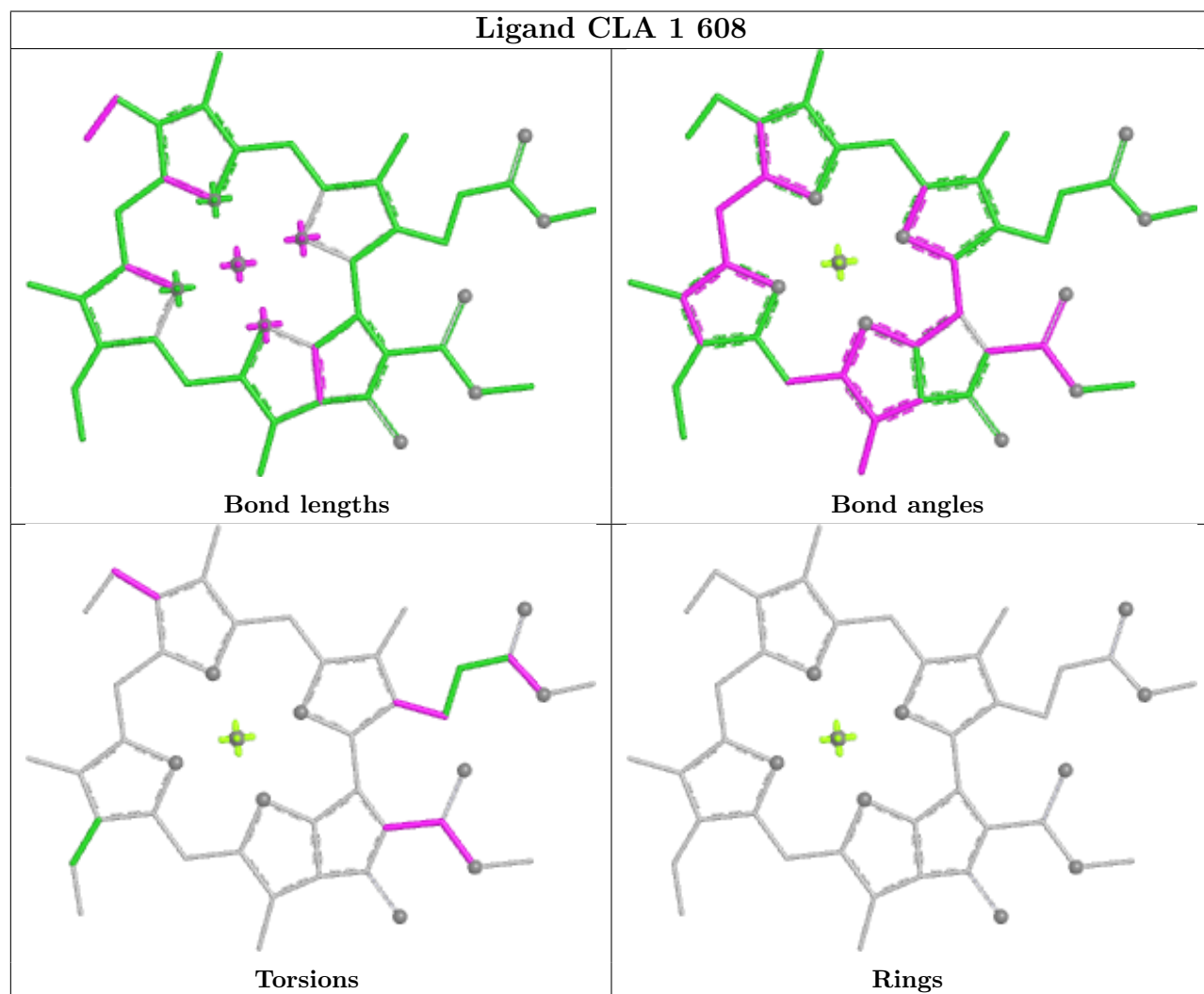
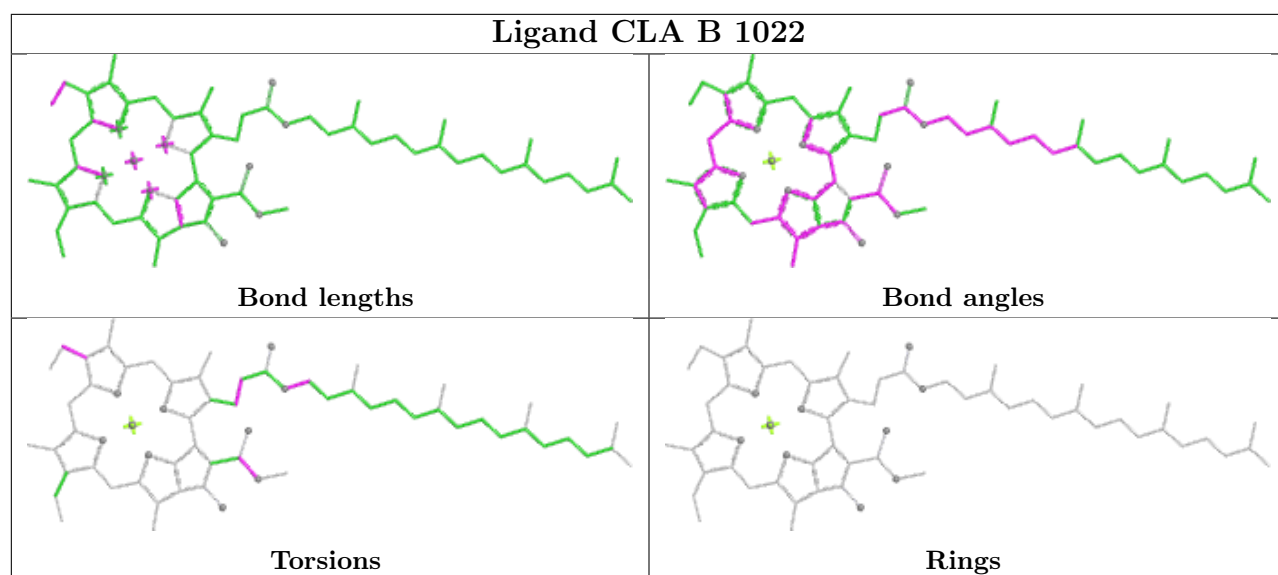


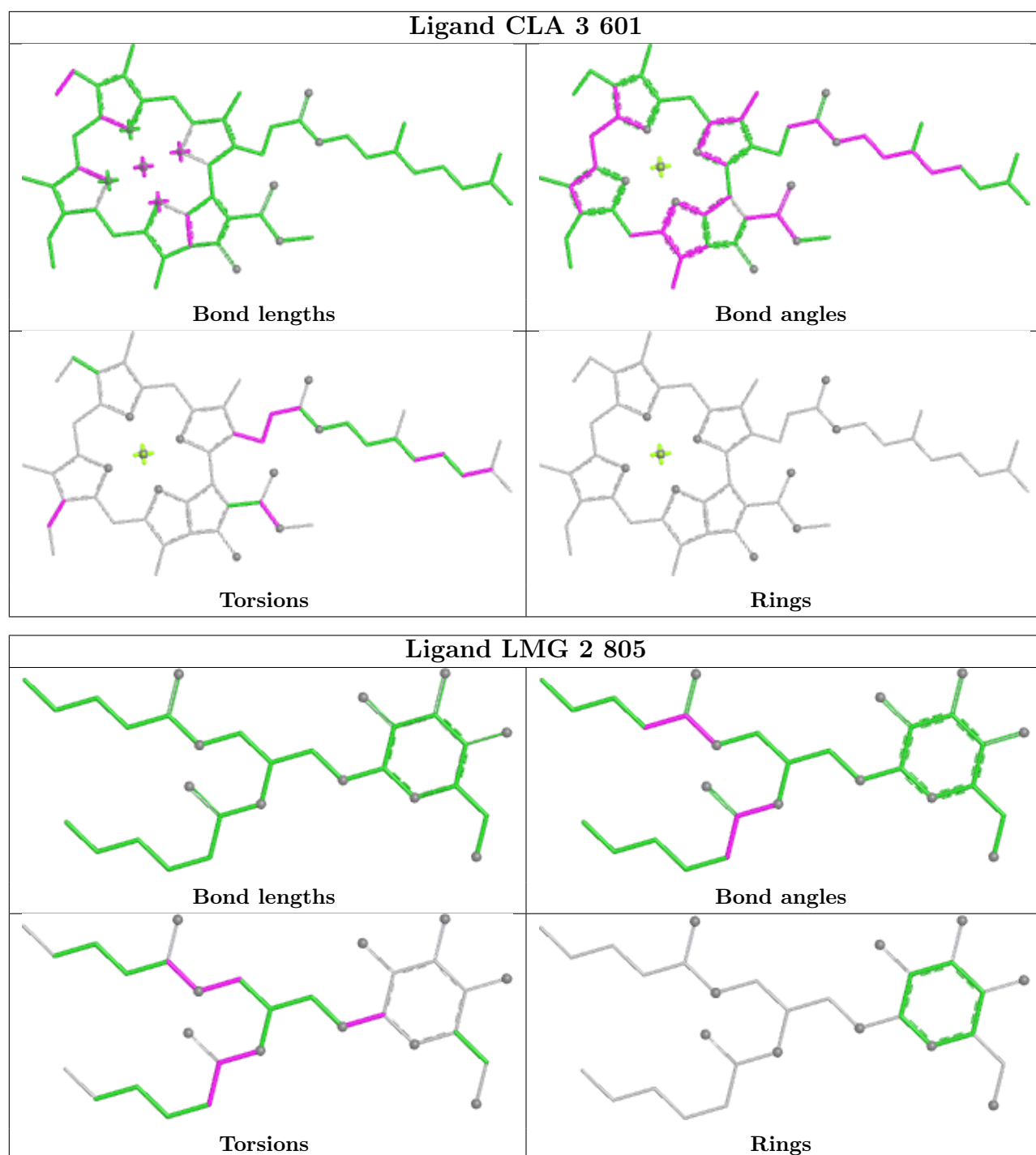
Torsions

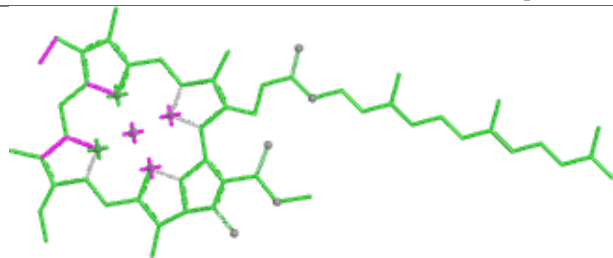
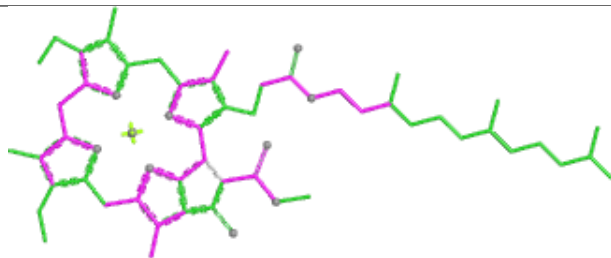
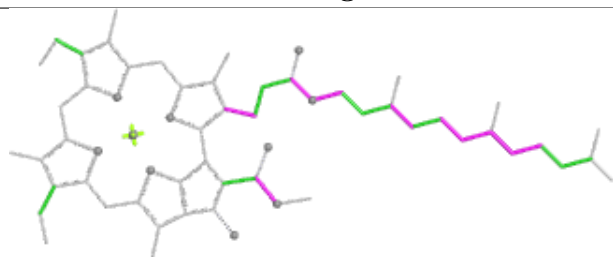
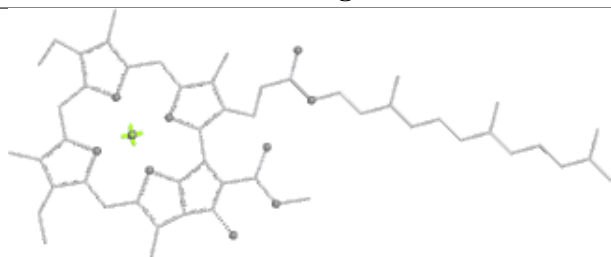
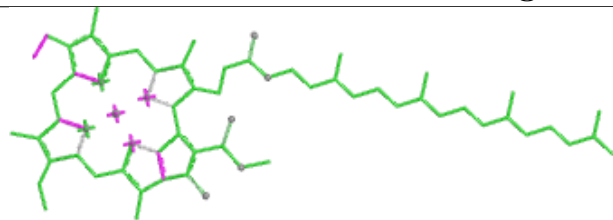
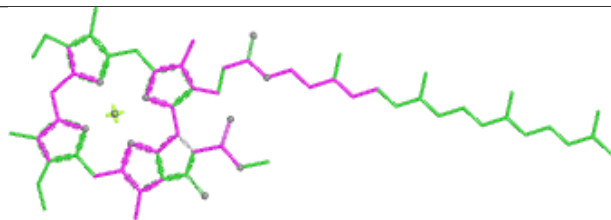
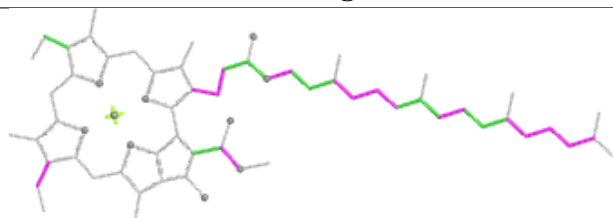
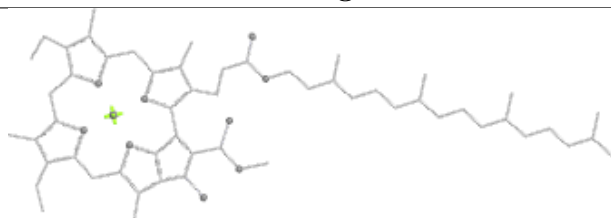


Rings

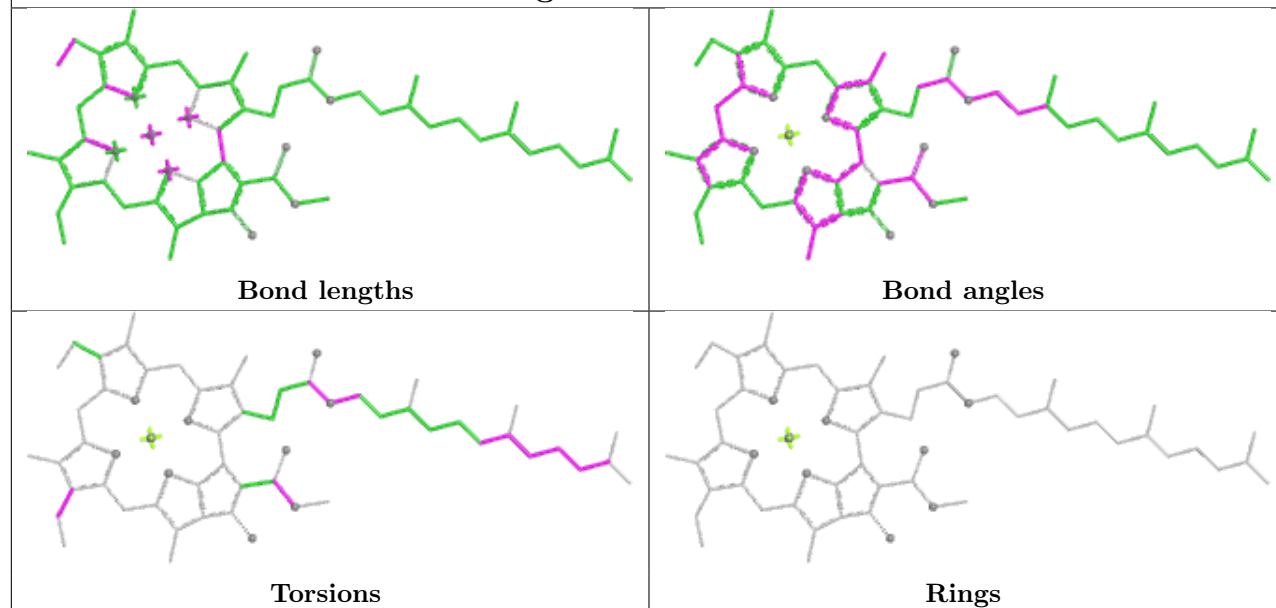




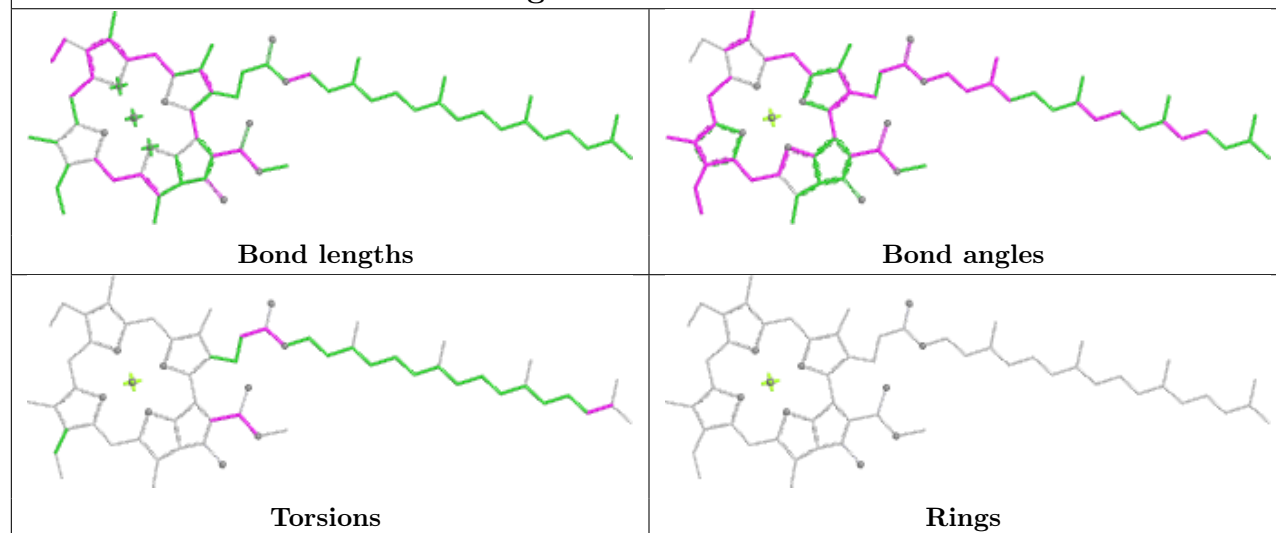


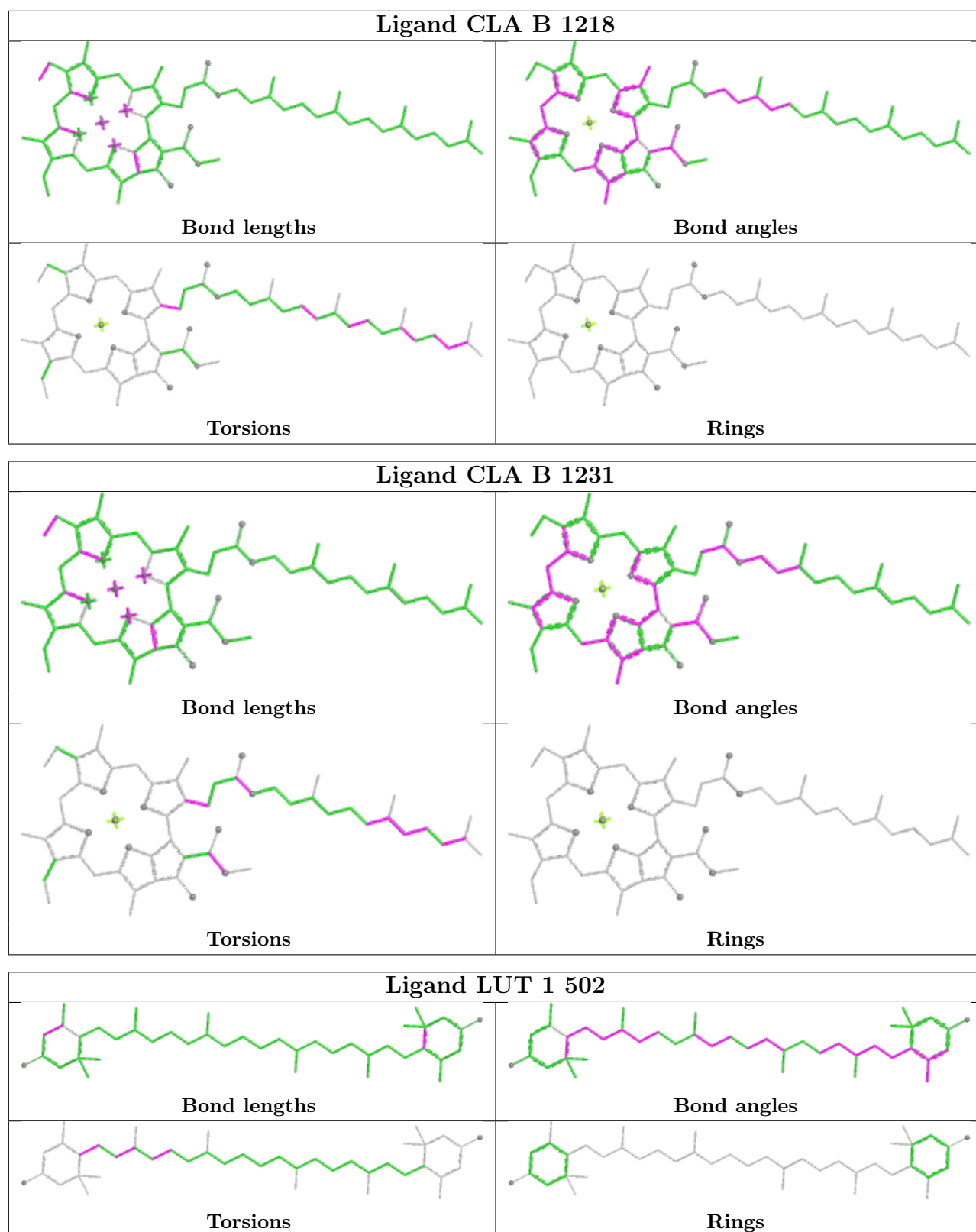
Ligand CLA 4 601**Bond lengths****Bond angles****Torsions****Rings****Ligand CLA 1 601****Bond lengths****Bond angles****Torsions****Rings**

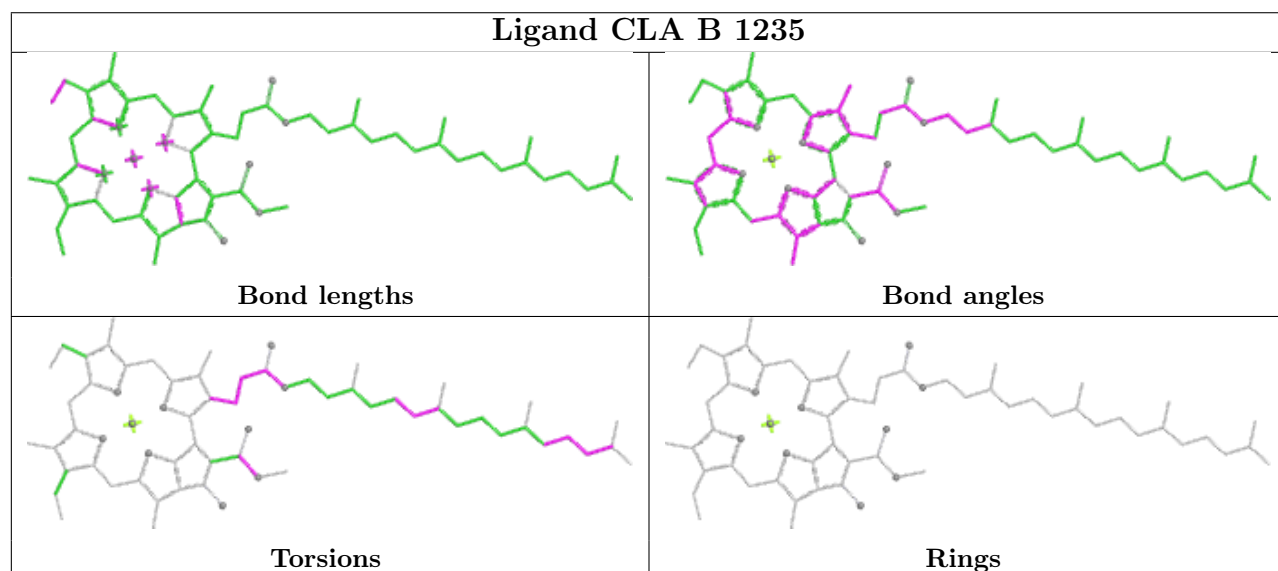
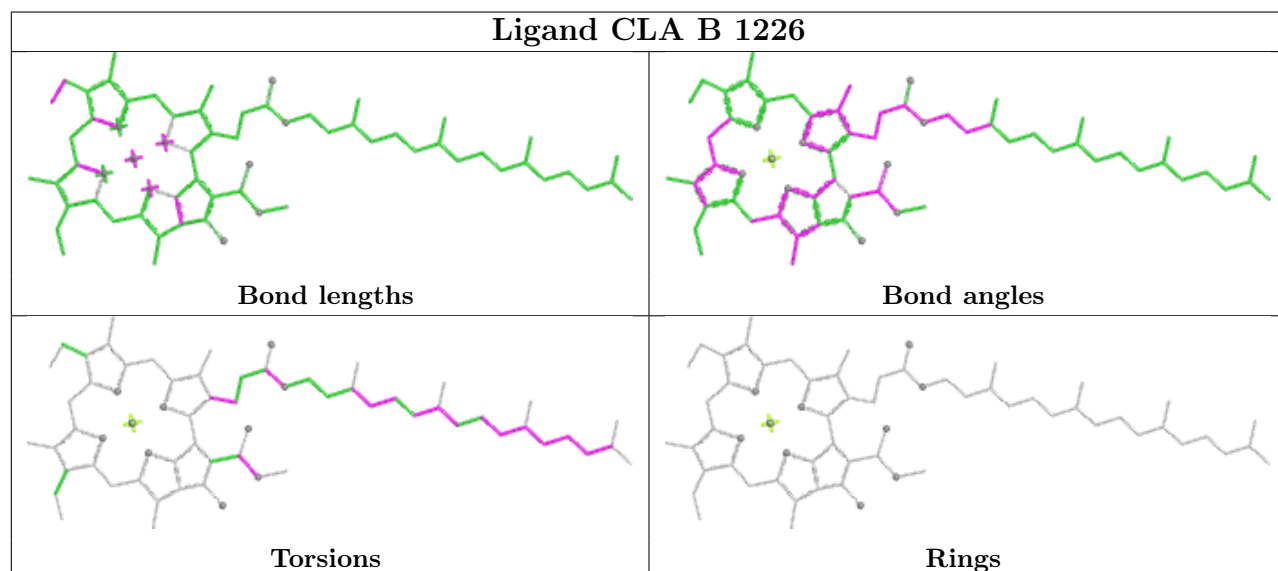
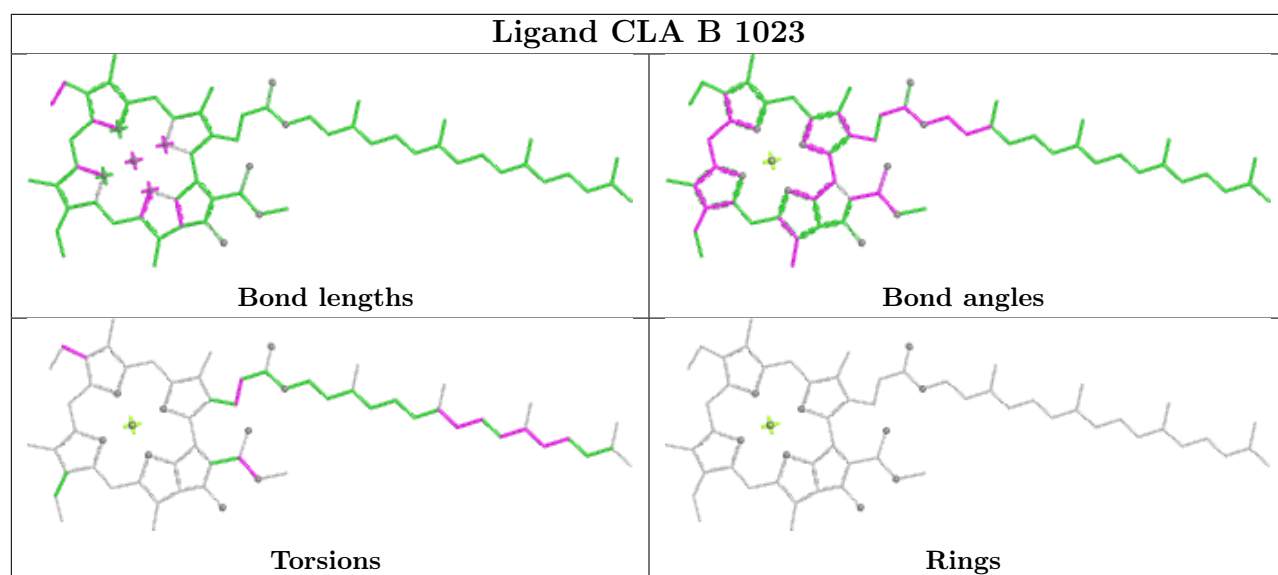
Ligand CLA 2 607

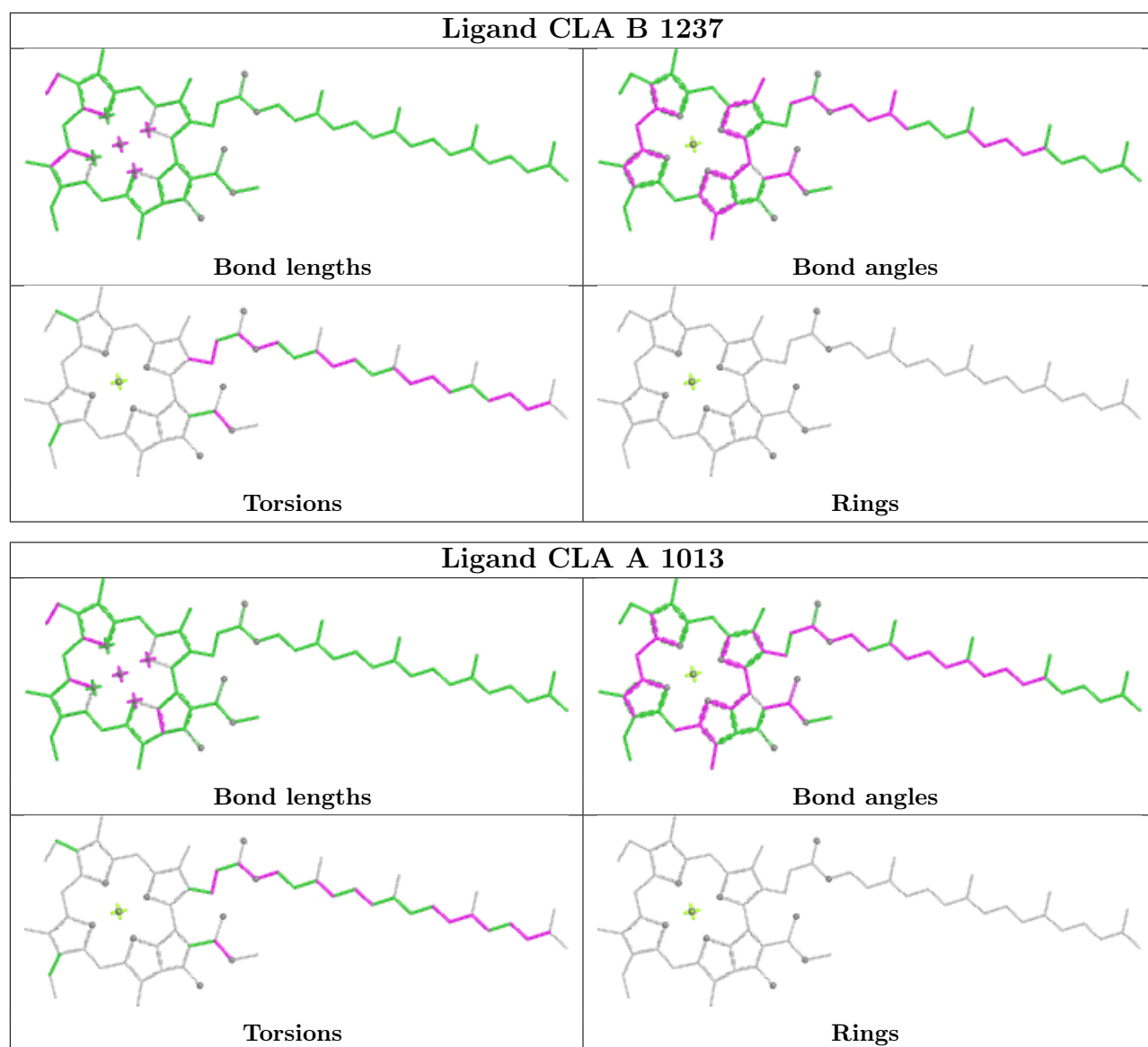


Ligand CL0 A 1011

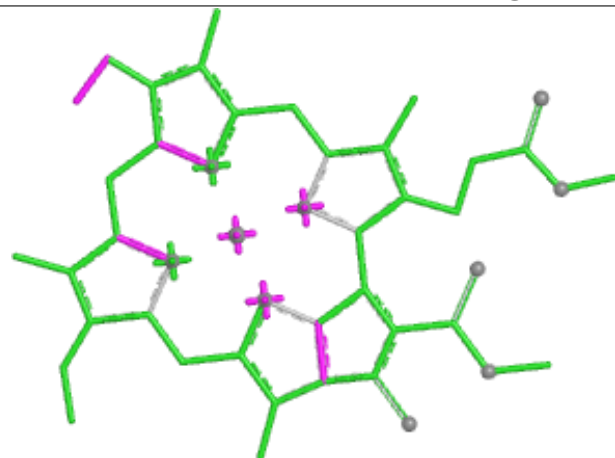




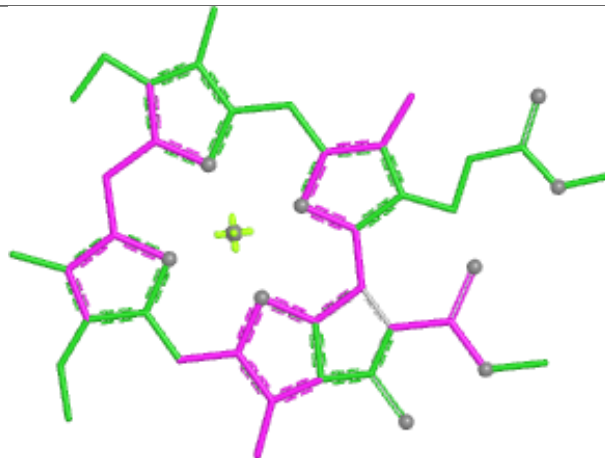




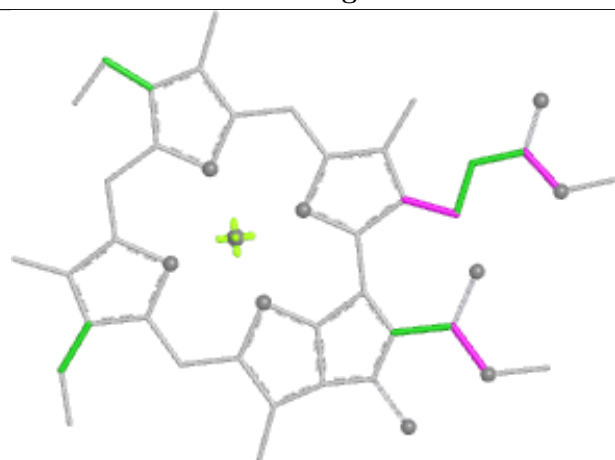
Ligand CLA G 1602



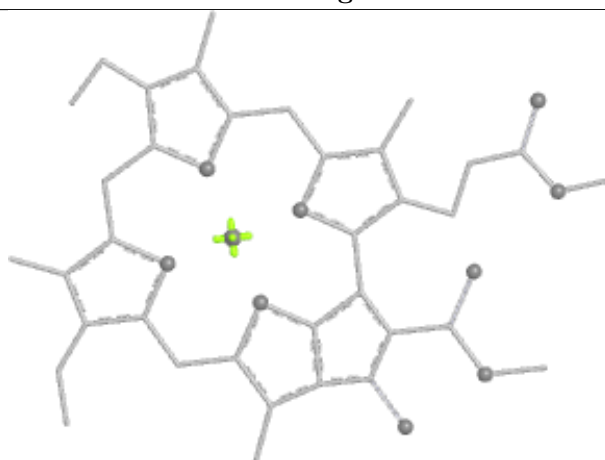
Bond lengths



Bond angles

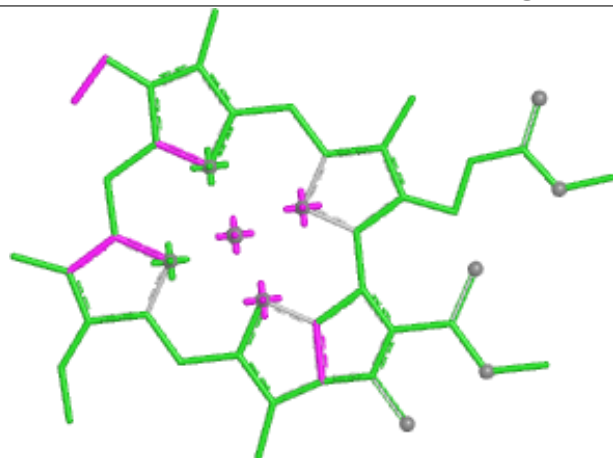


Torsions

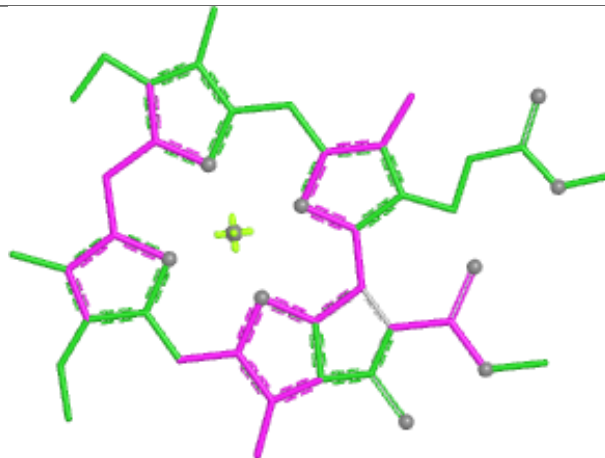


Rings

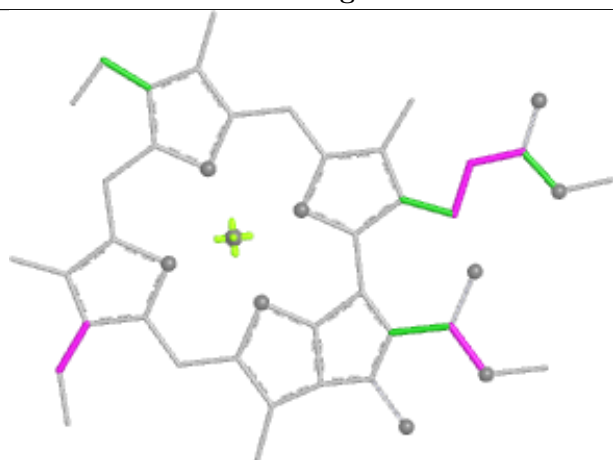
Ligand CLA 4 608



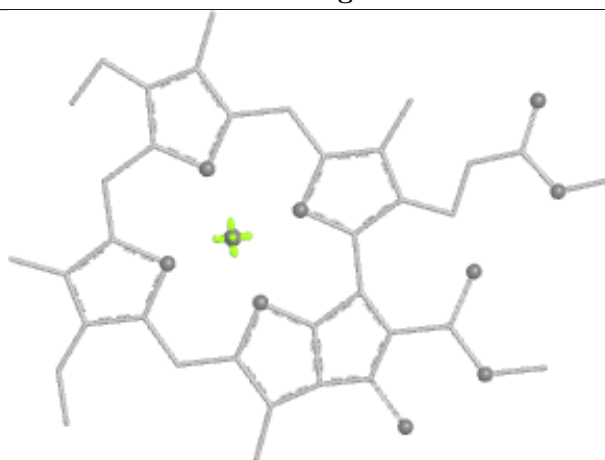
Bond lengths



Bond angles

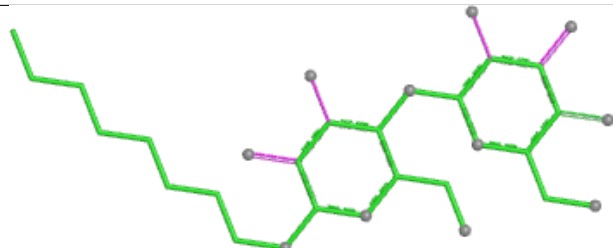


Torsions

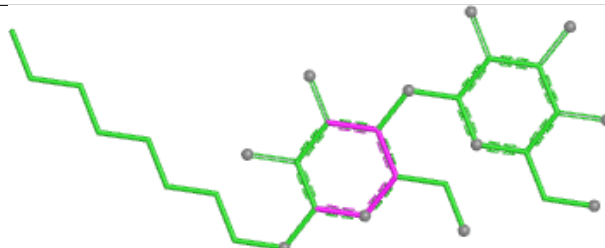


Rings

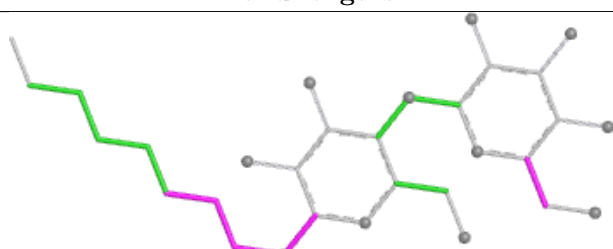
Ligand LMT G 5005



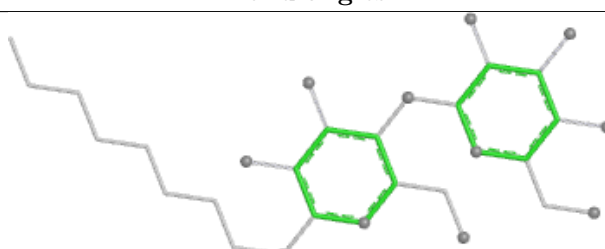
Bond lengths



Bond angles

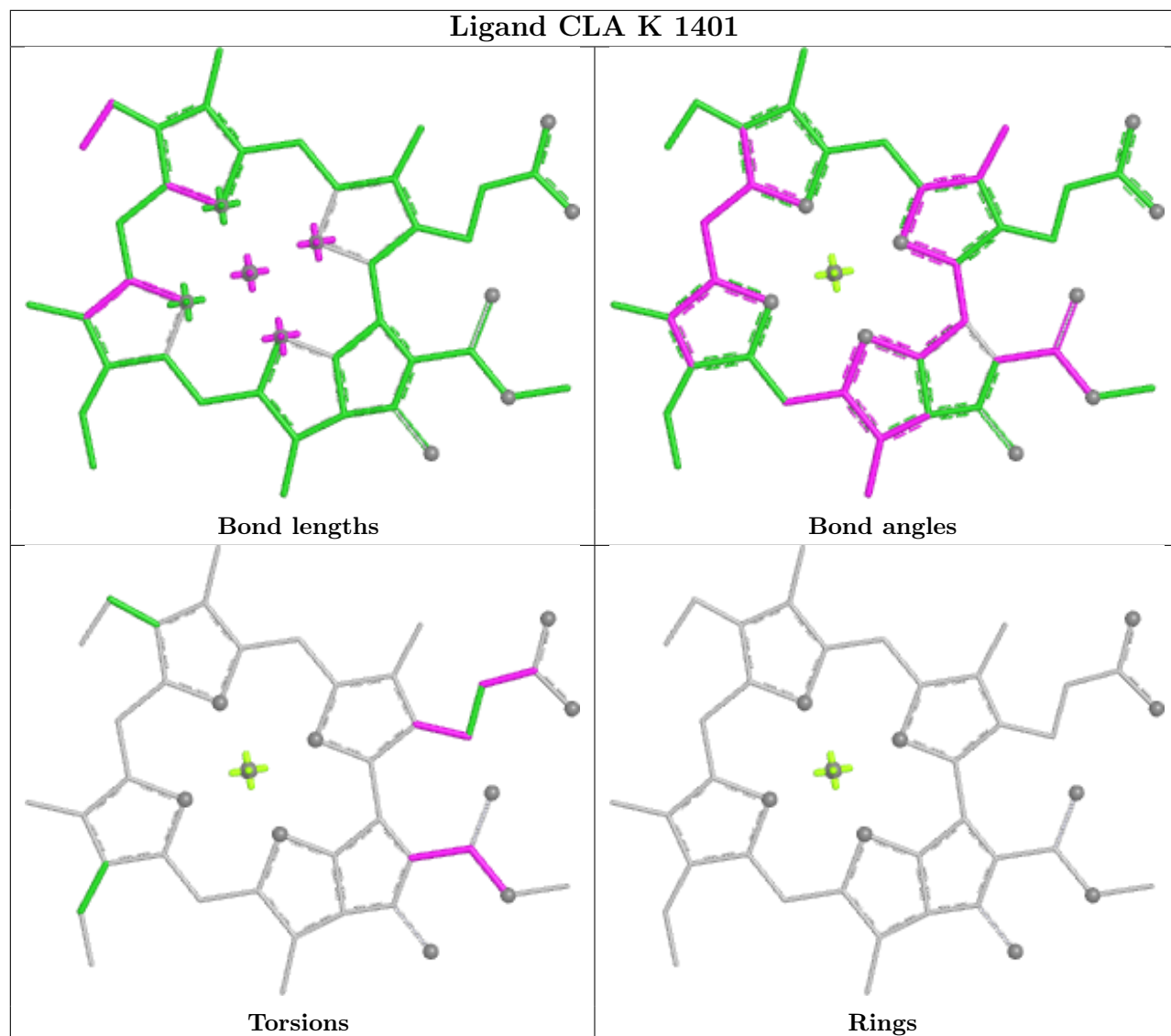


Torsions

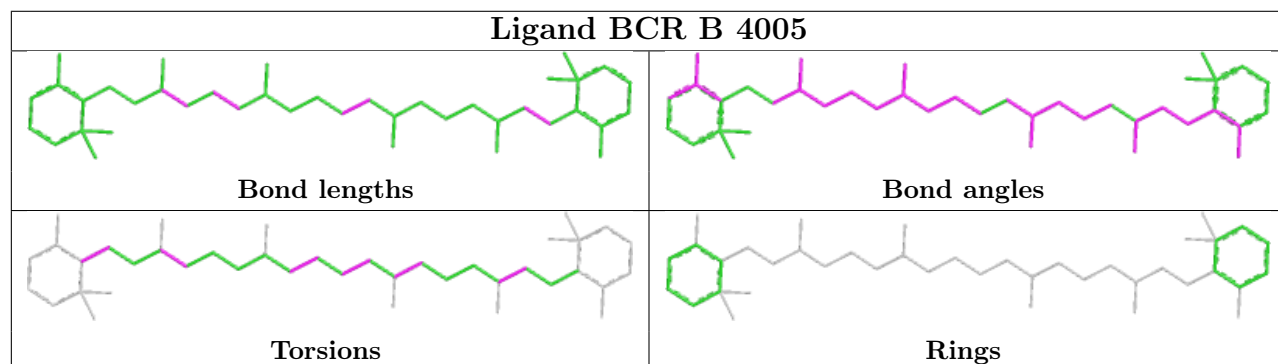


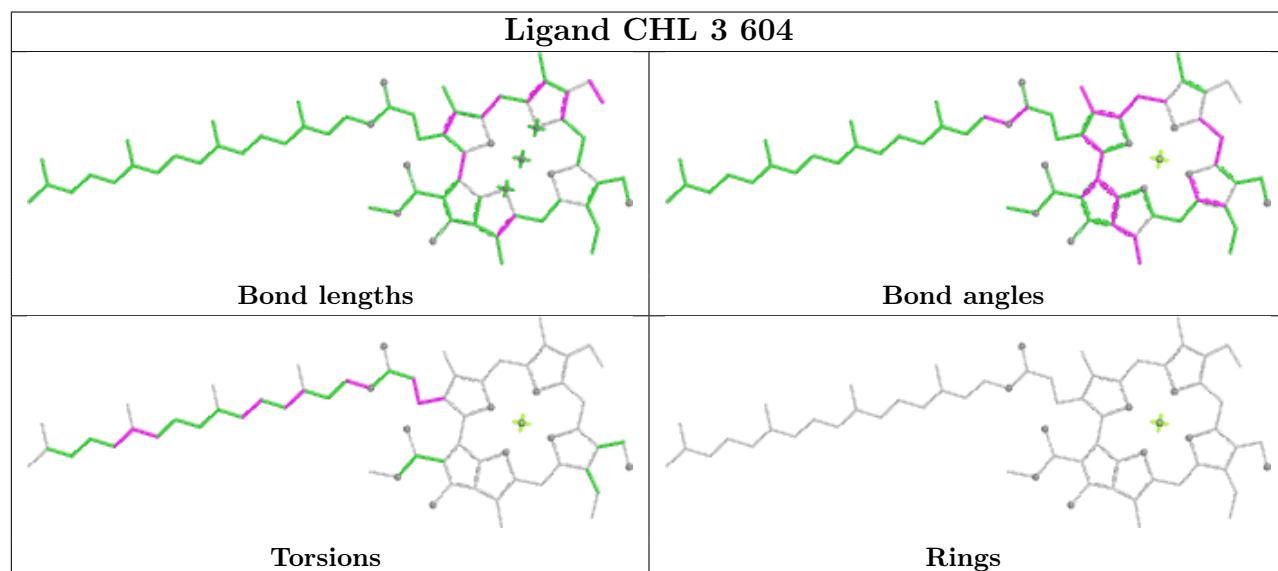
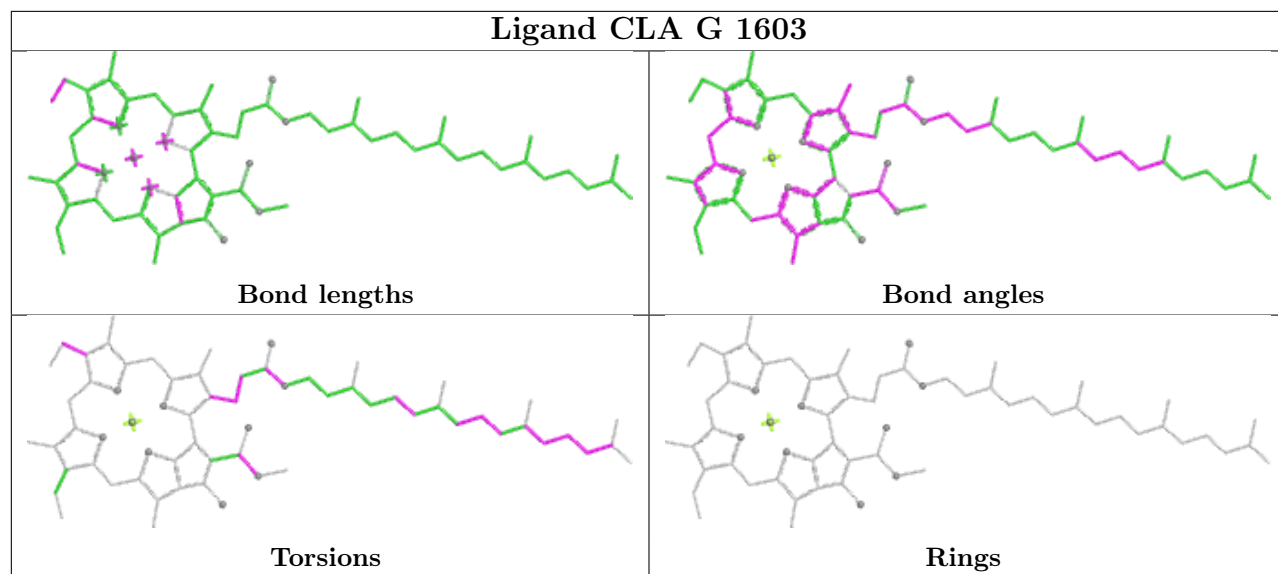
Rings

Ligand CLA K 1401

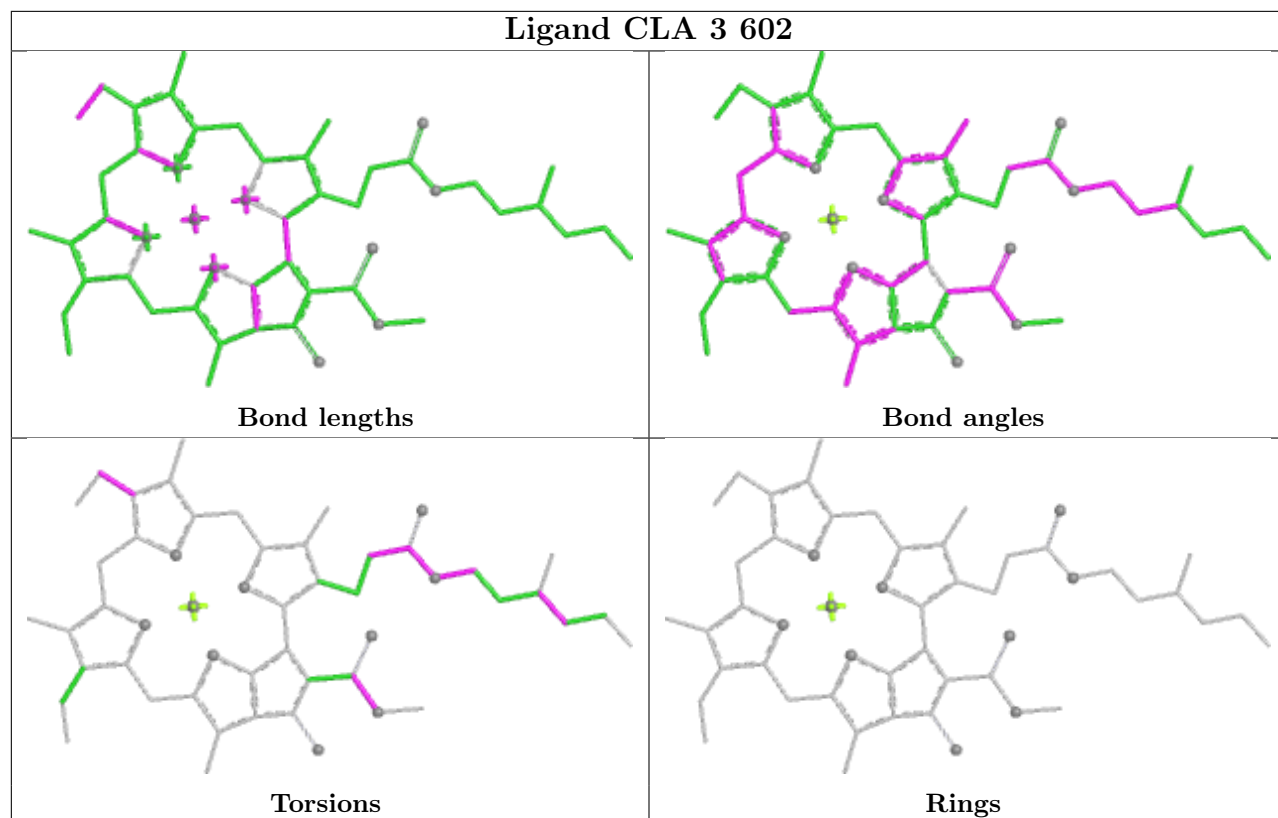


Ligand BCR B 4005

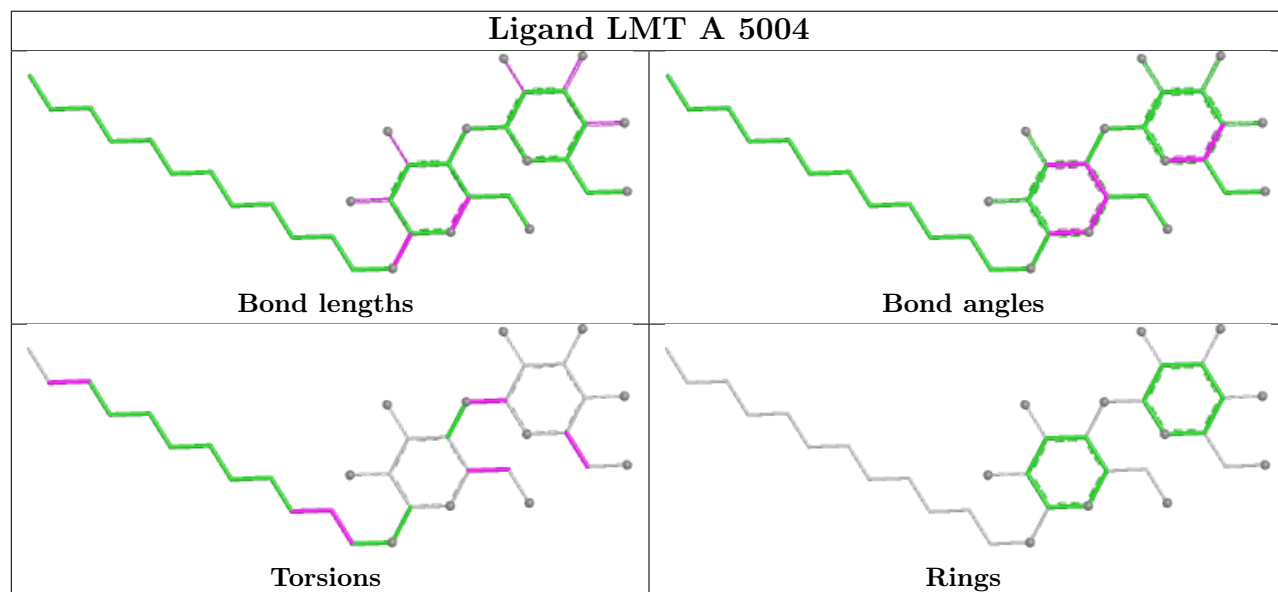


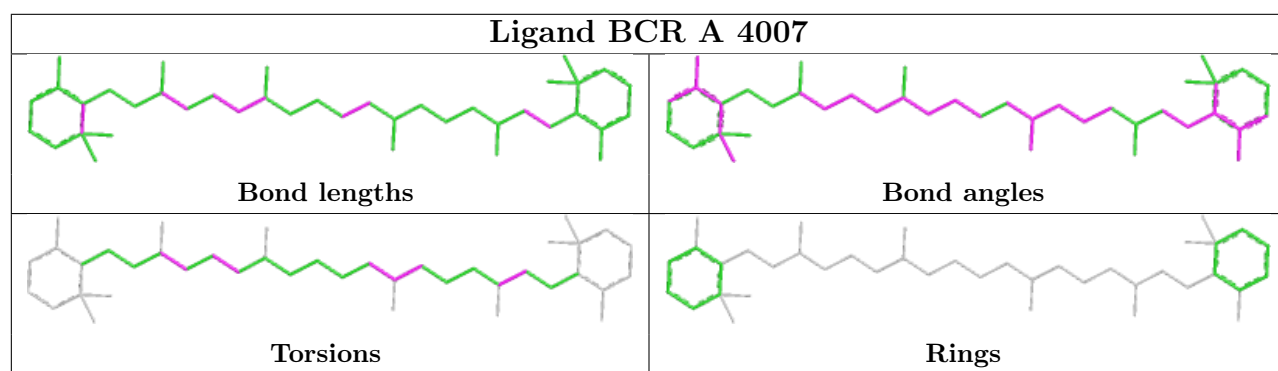
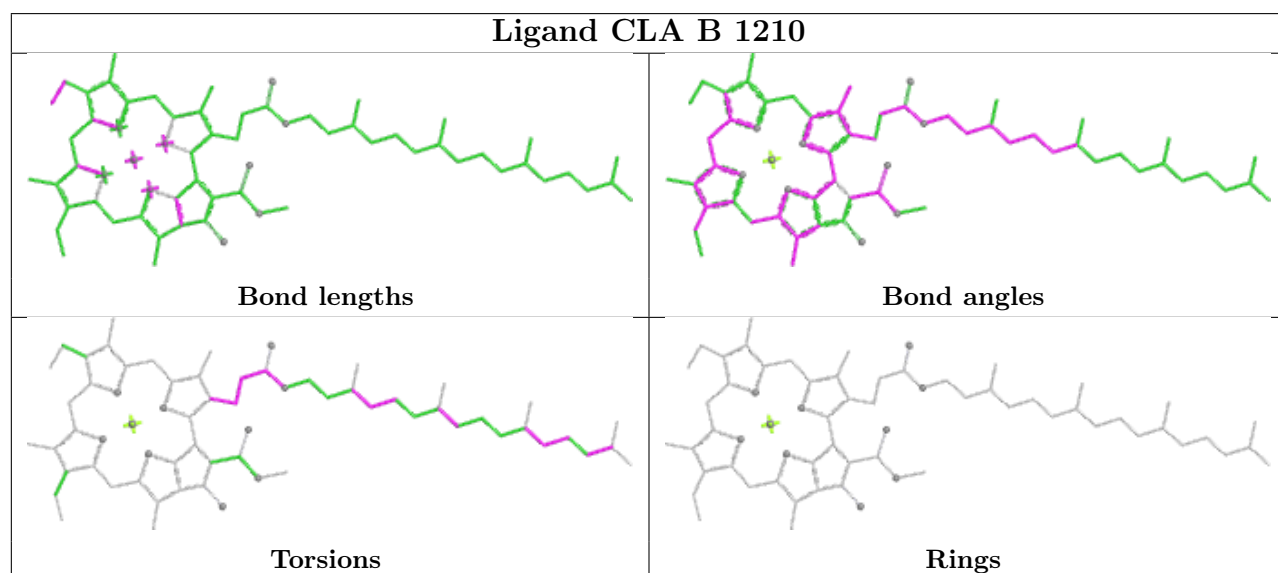
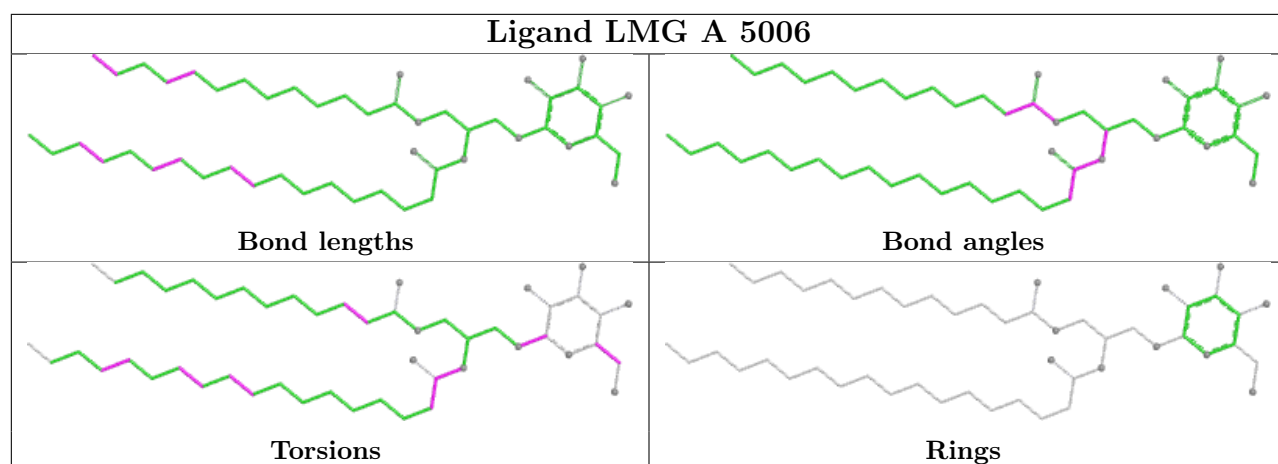


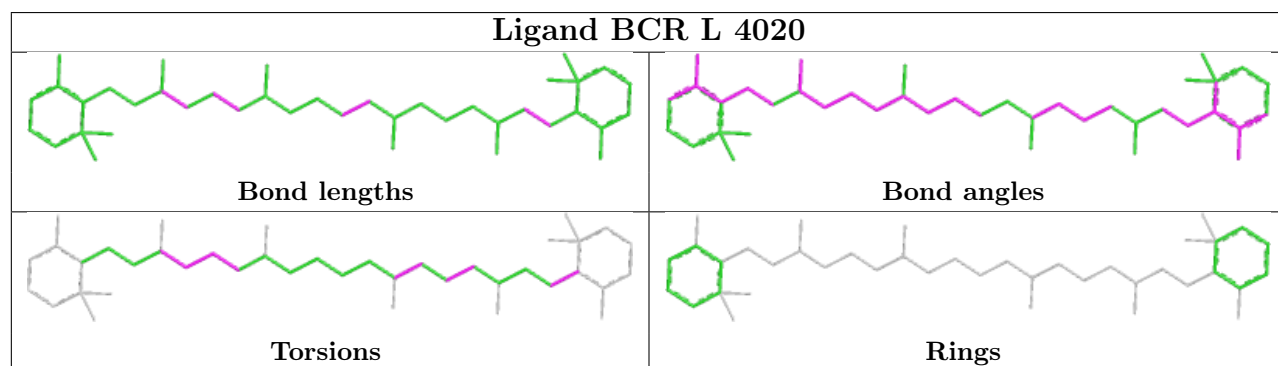
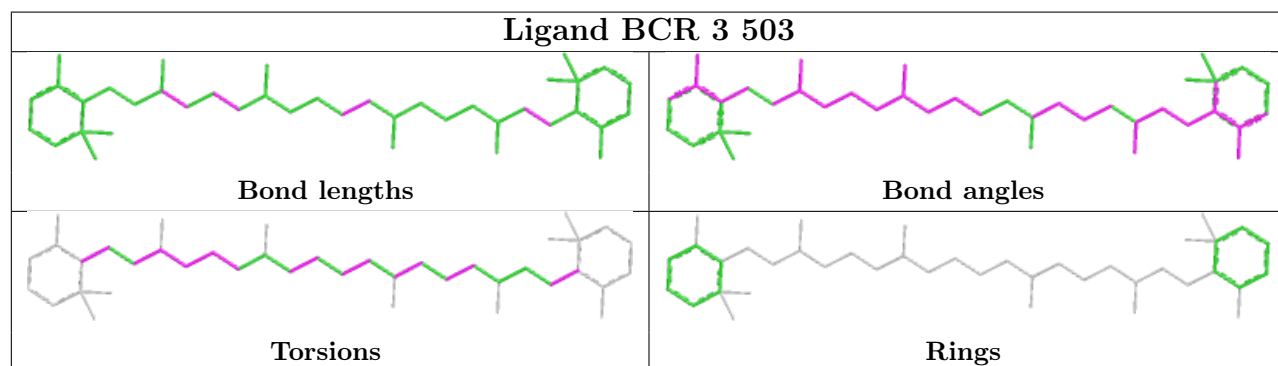
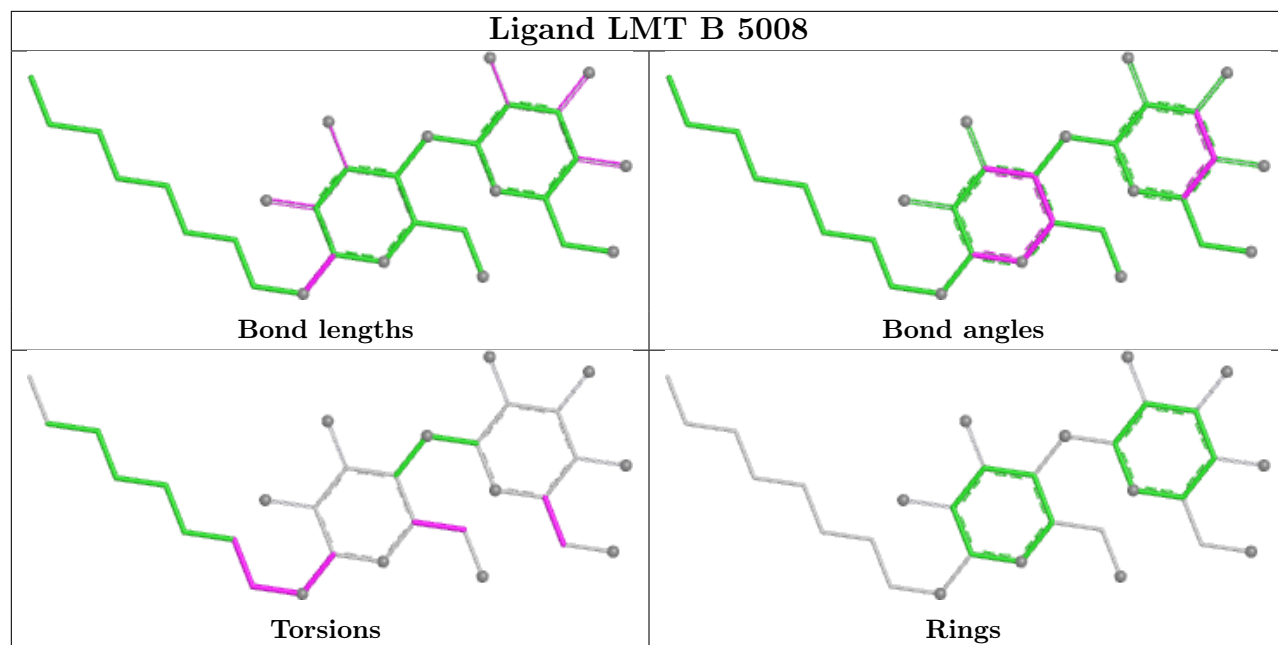
Ligand CLA 3 602

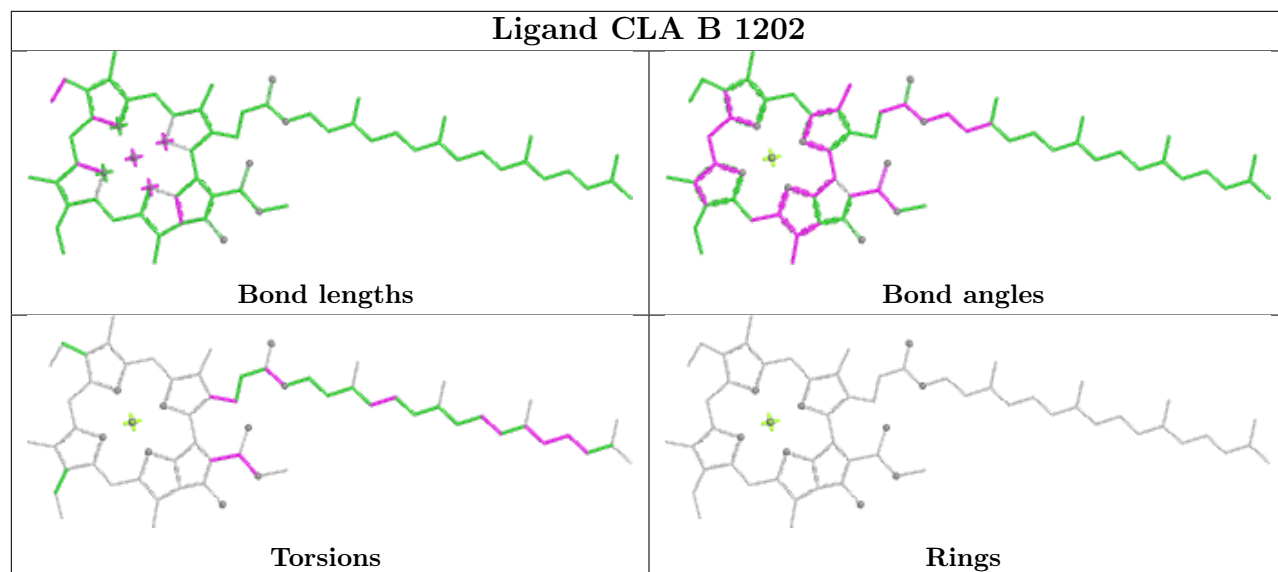
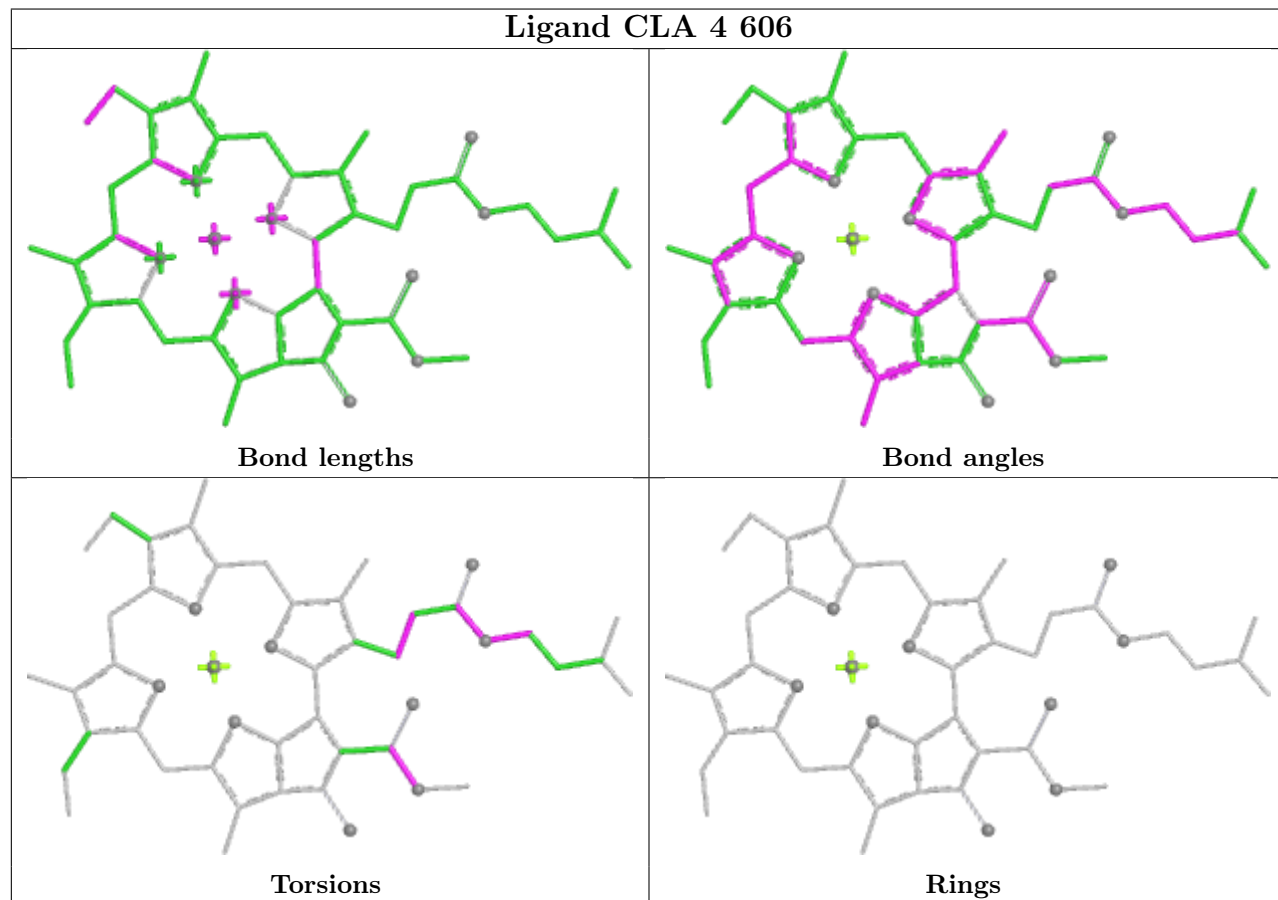


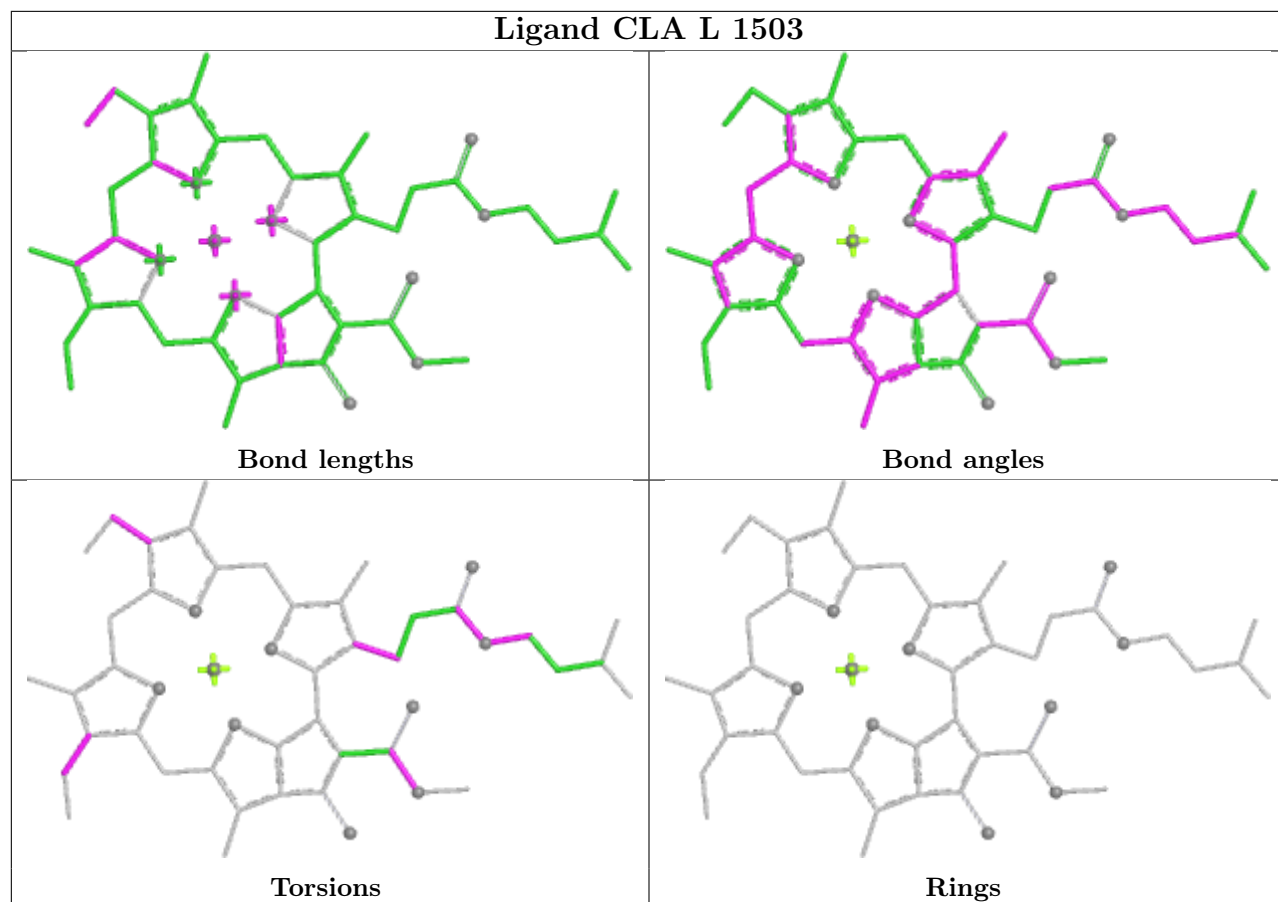
Ligand LMT A 5004



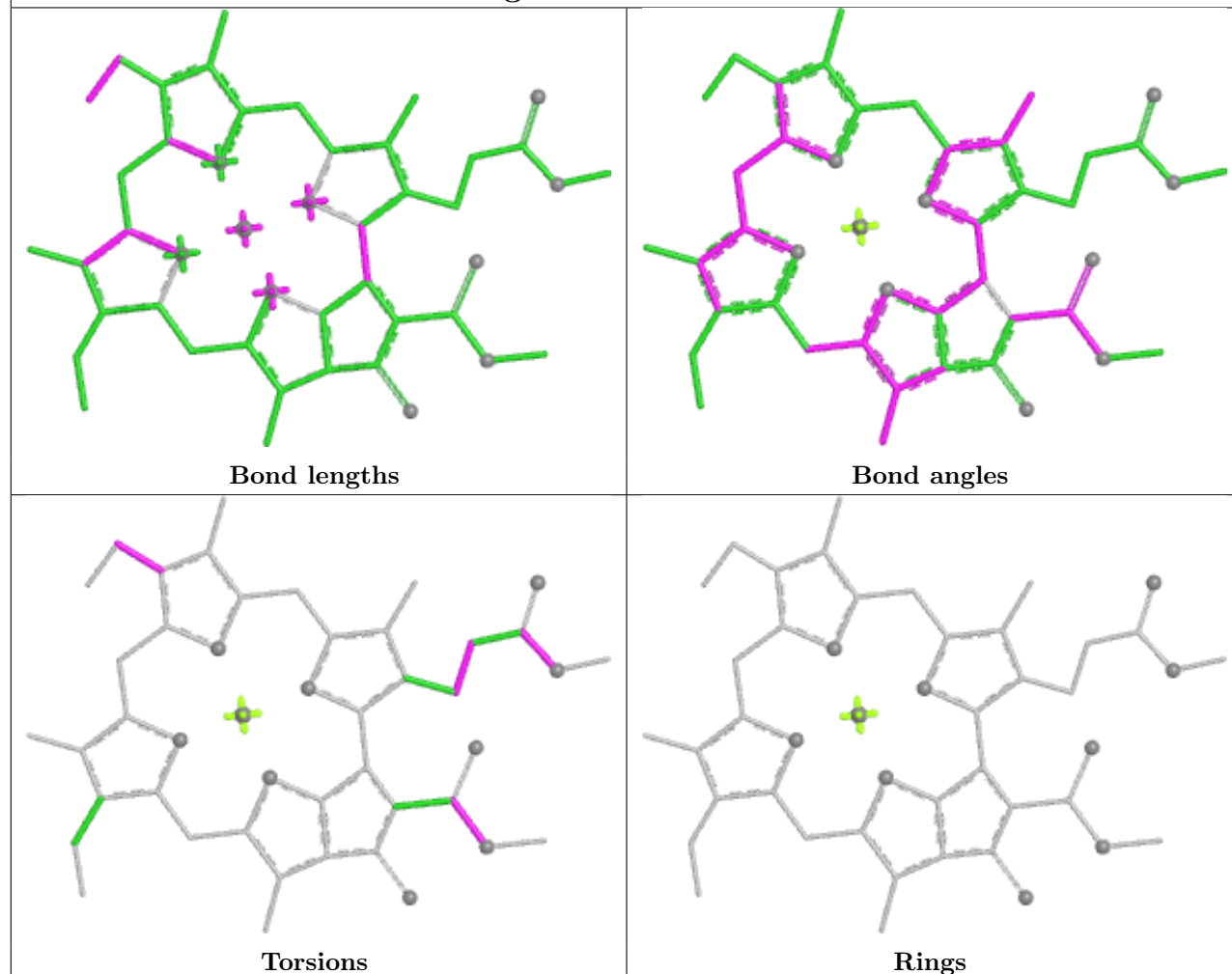




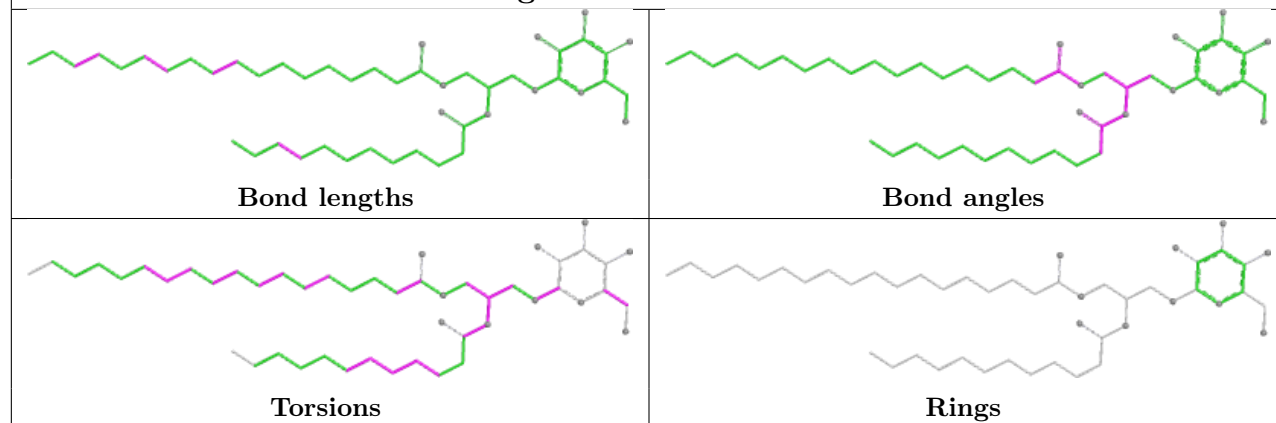
Ligand CLA B 1202**Ligand CLA 4 606**

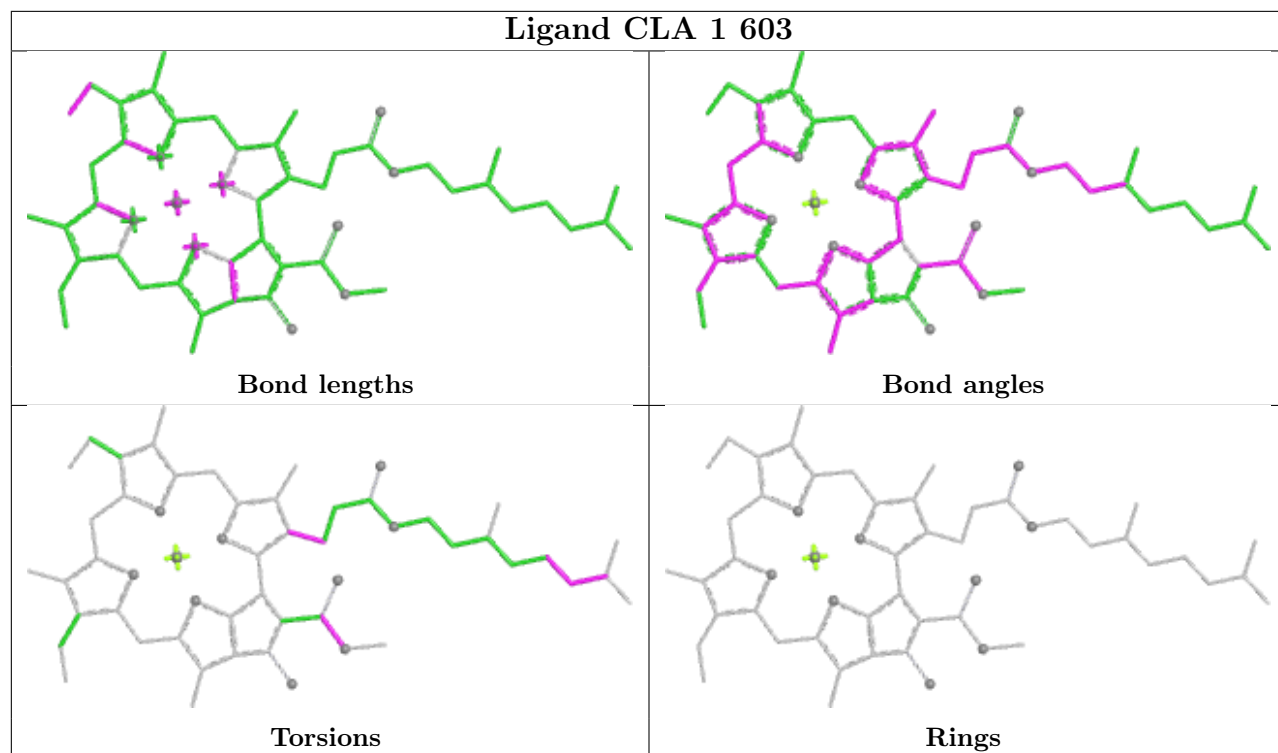
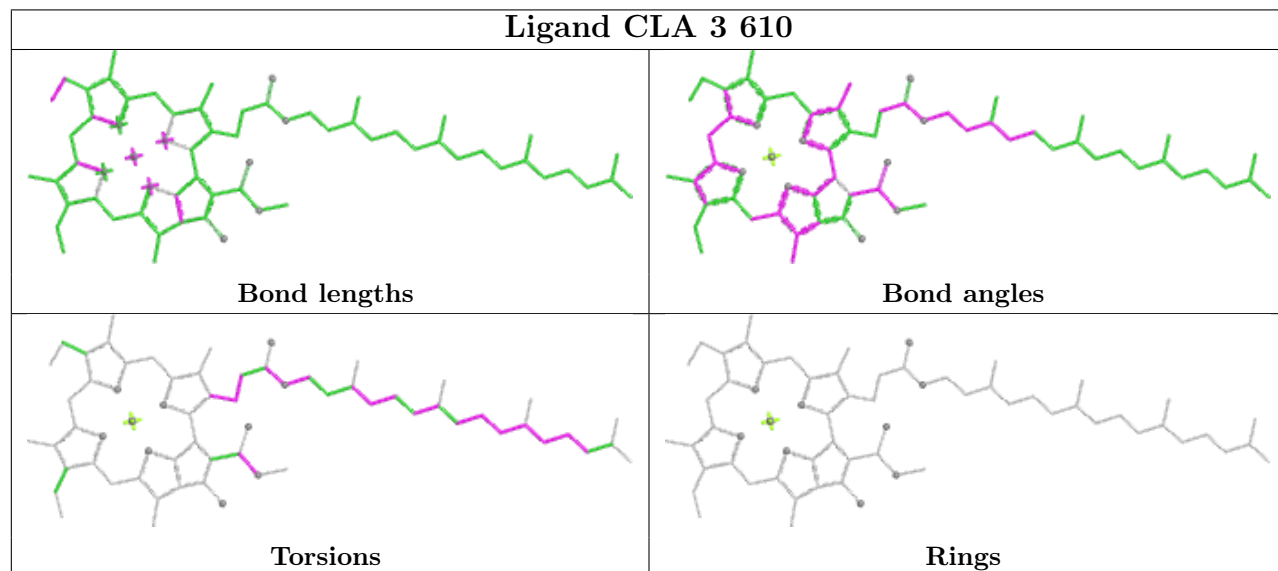


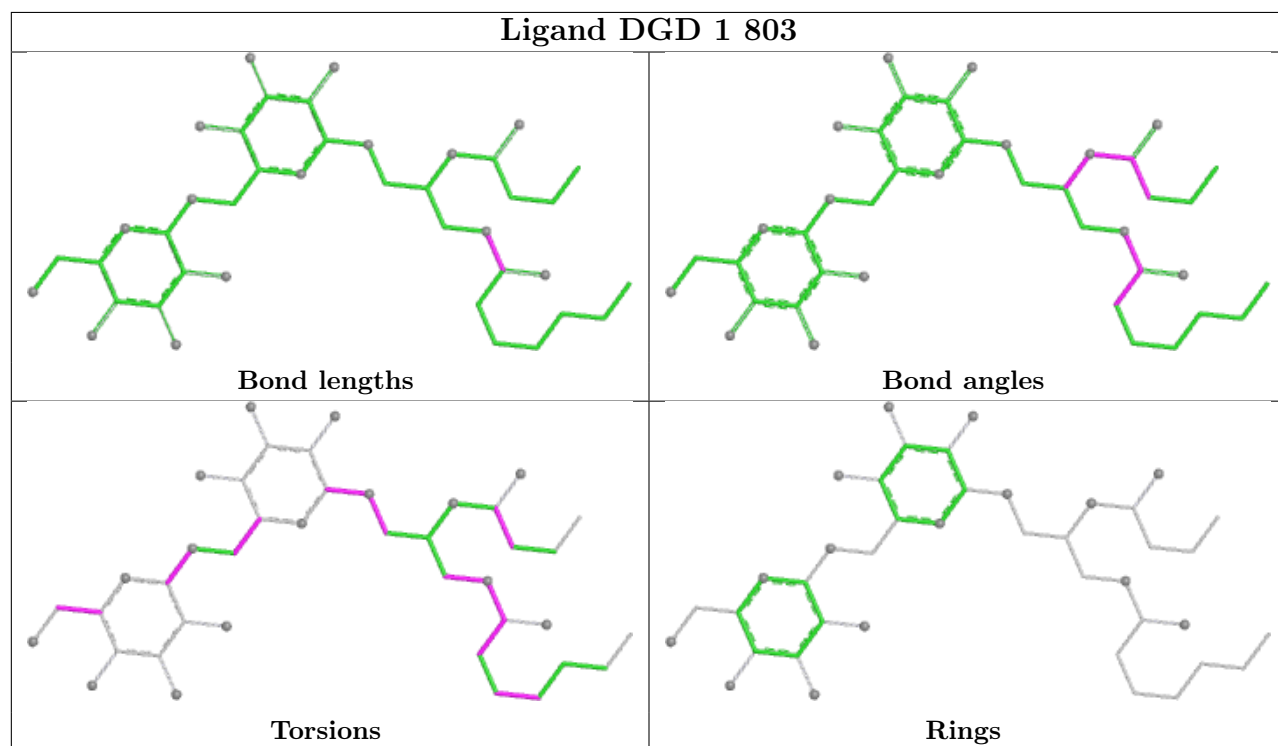
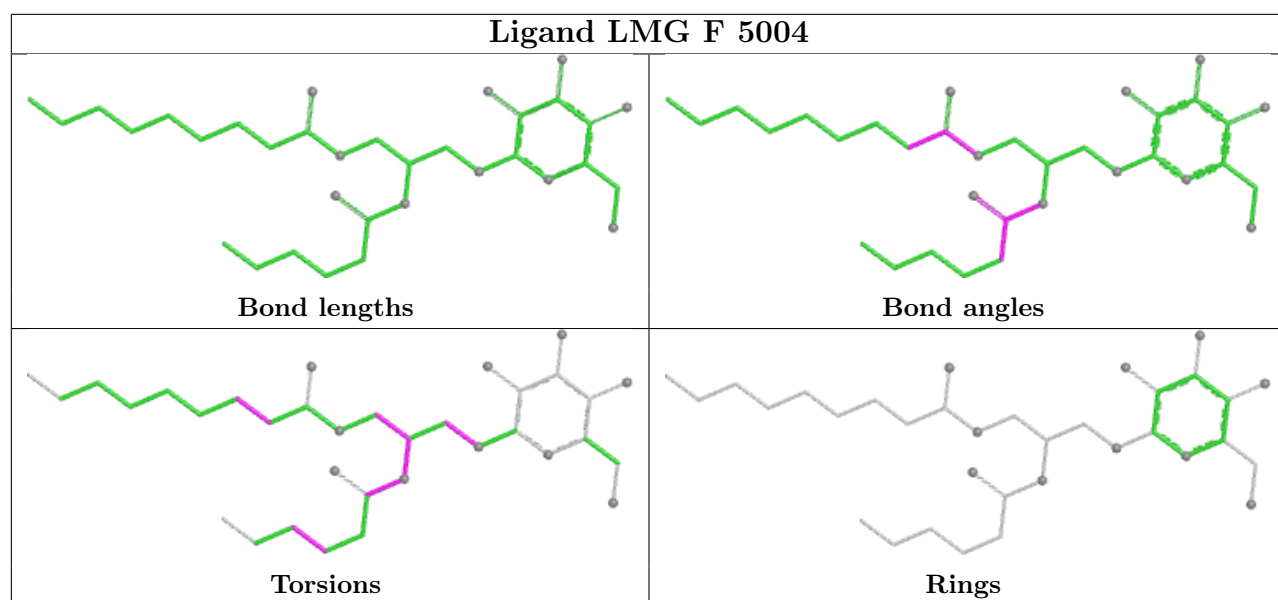
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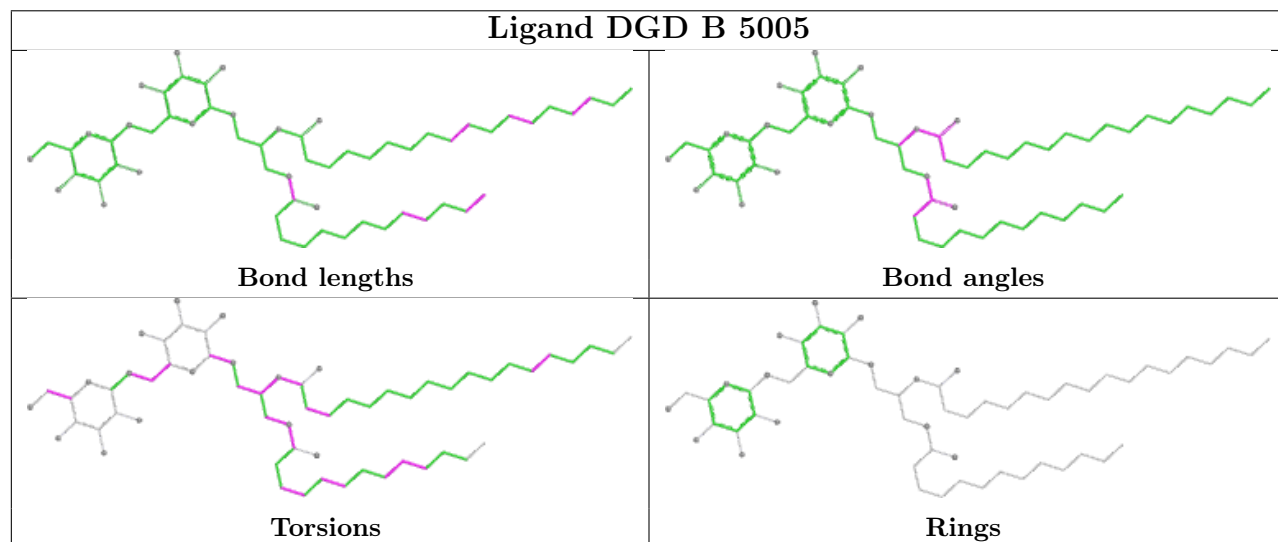
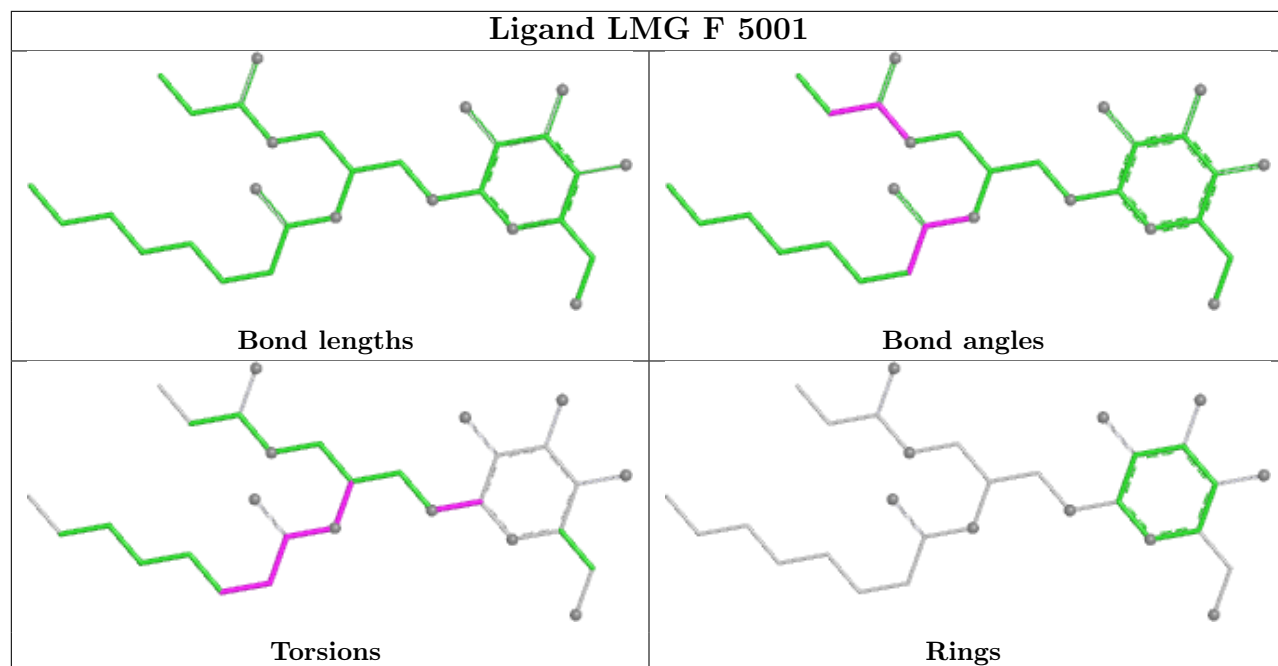


Ligand LMG G 5001

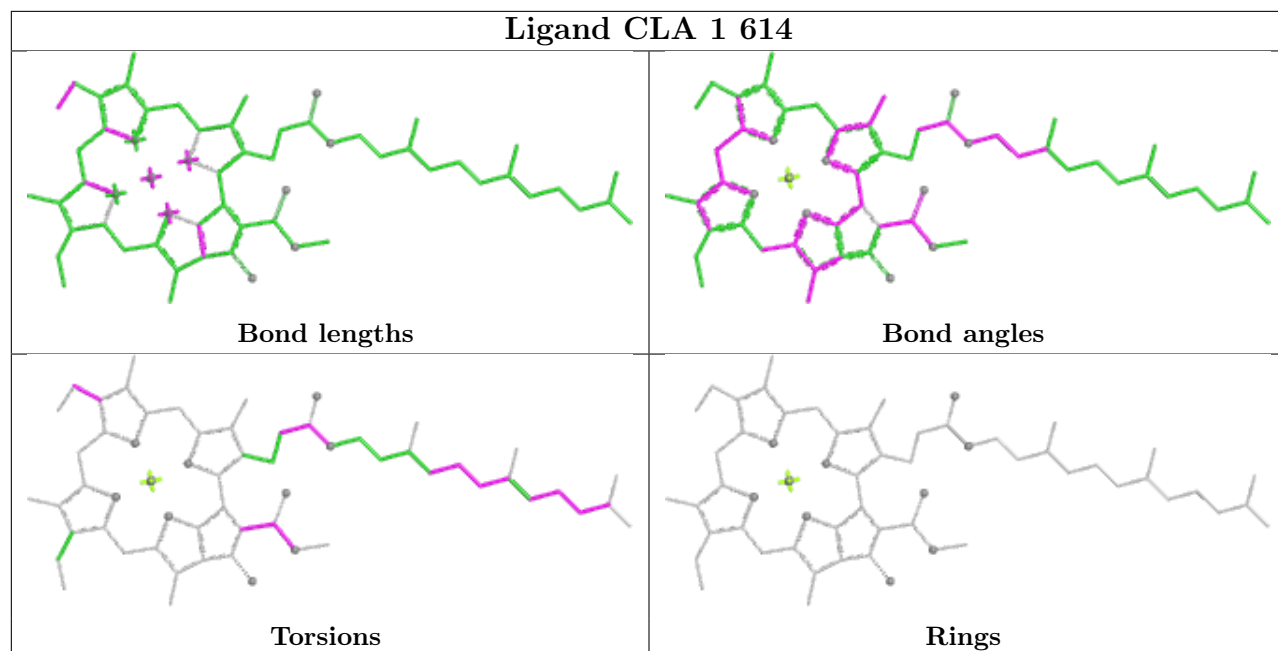


Ligand CLA 1 603**Ligand CLA 3 610**

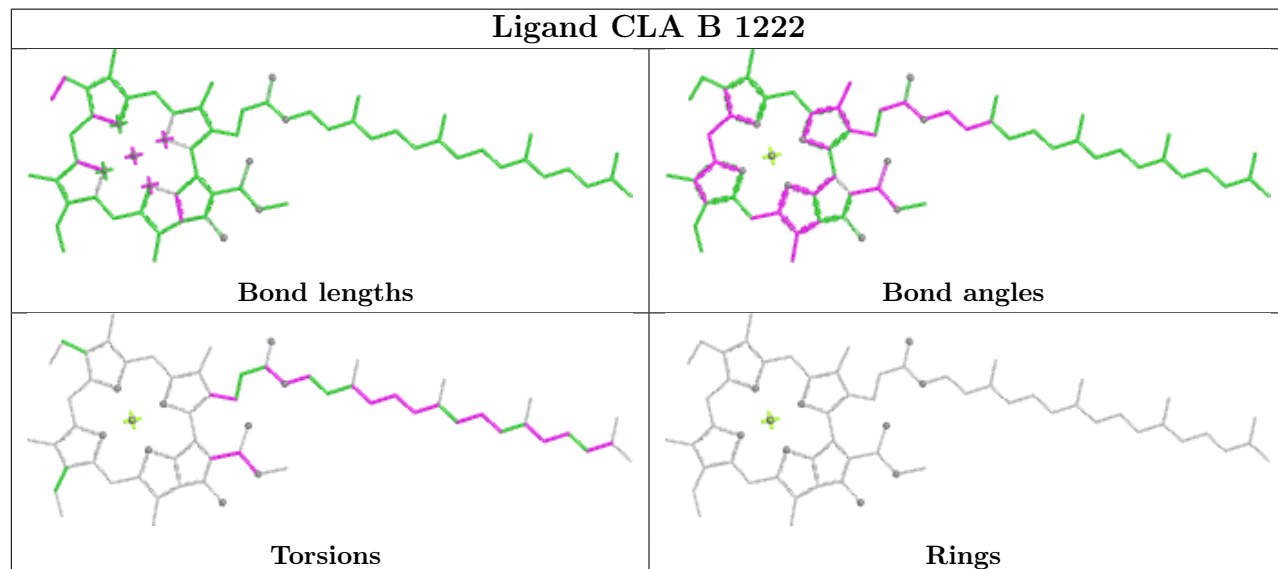


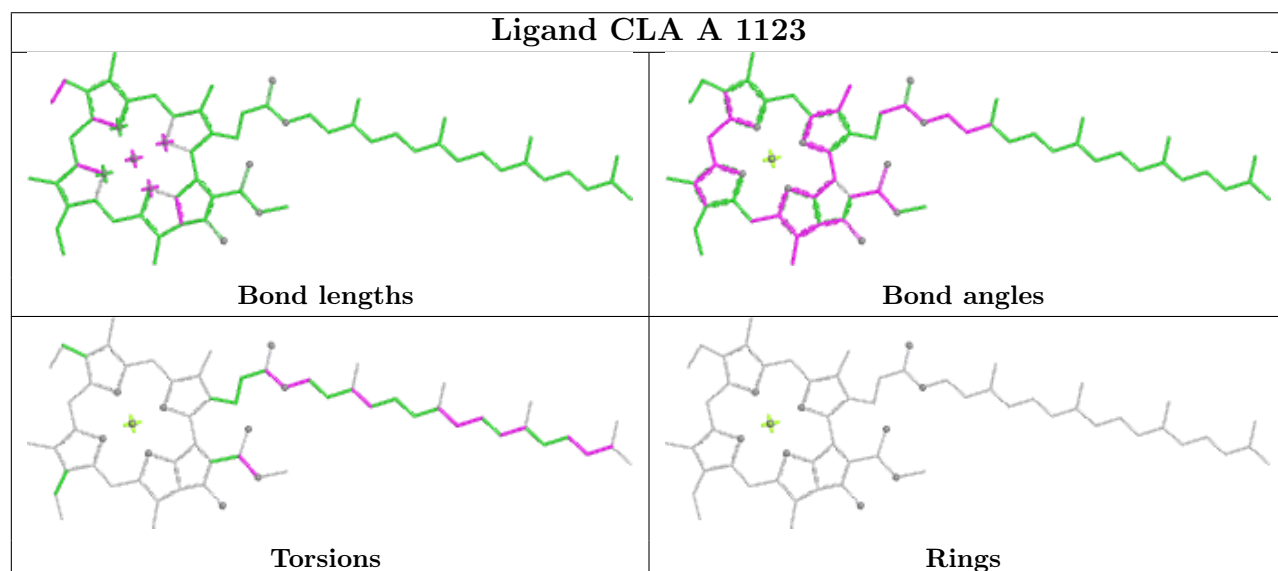
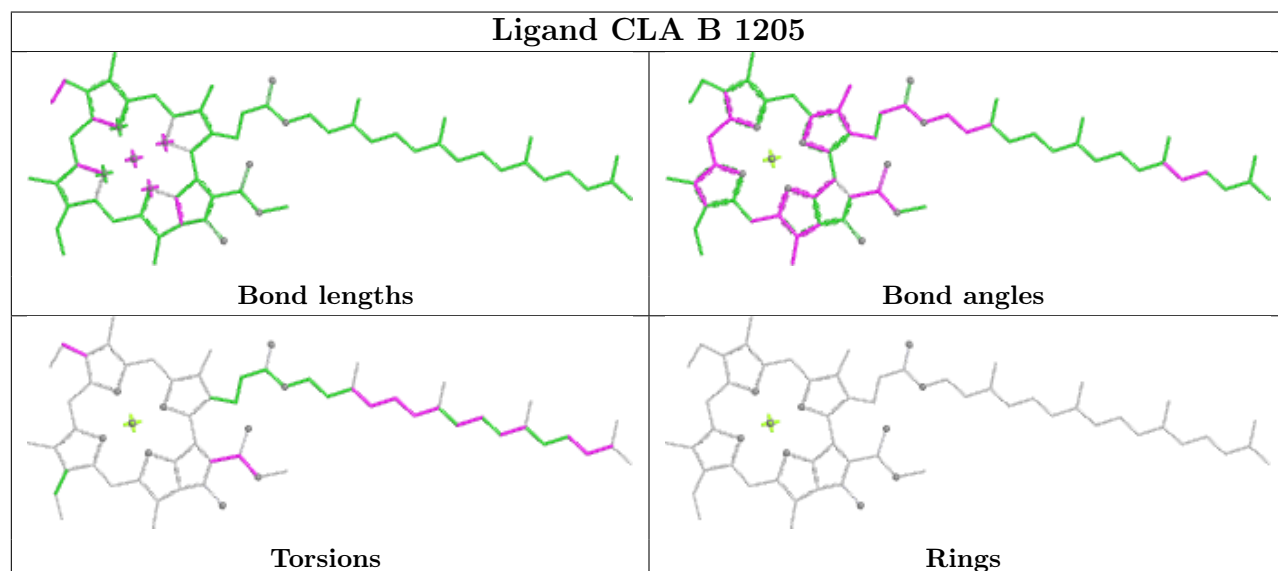
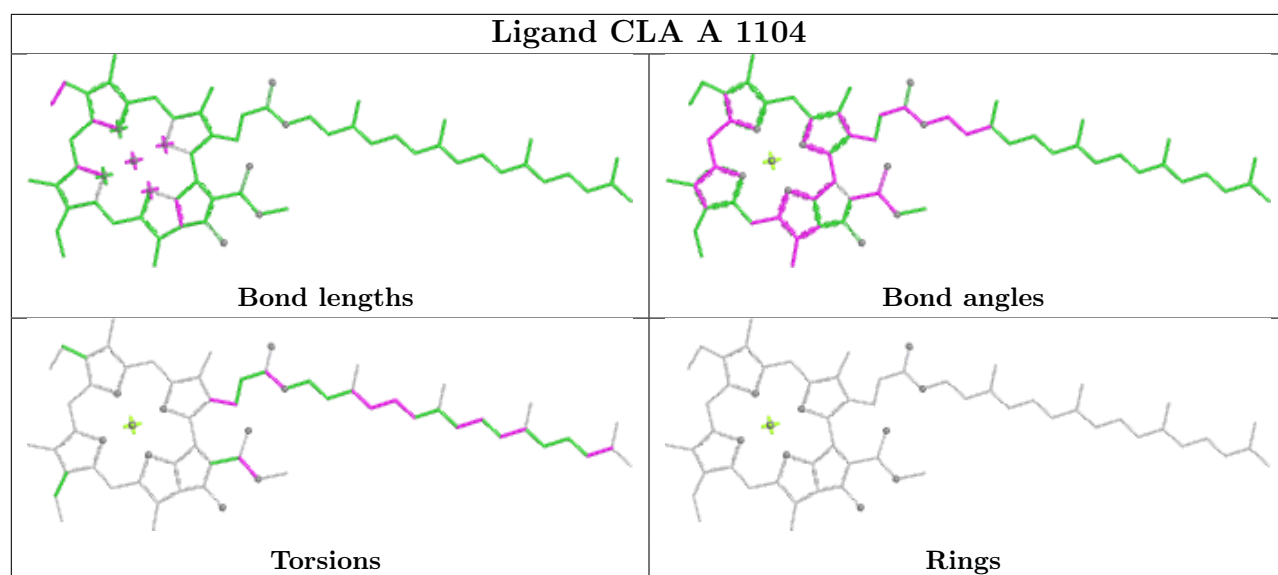


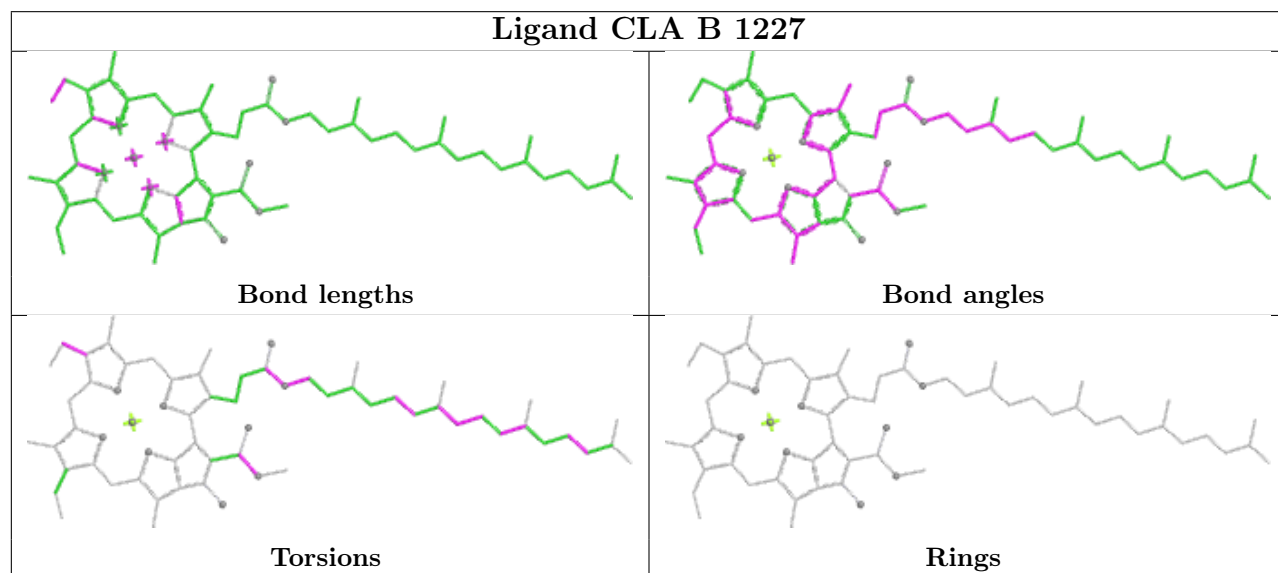
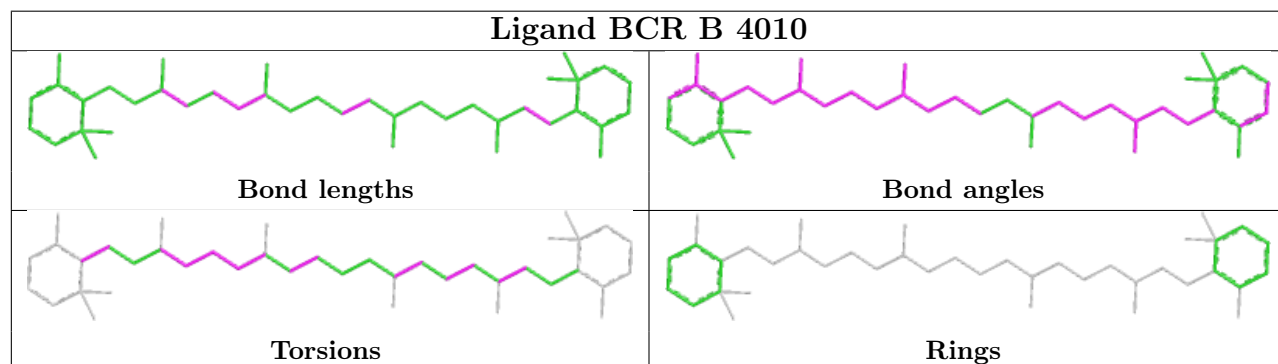
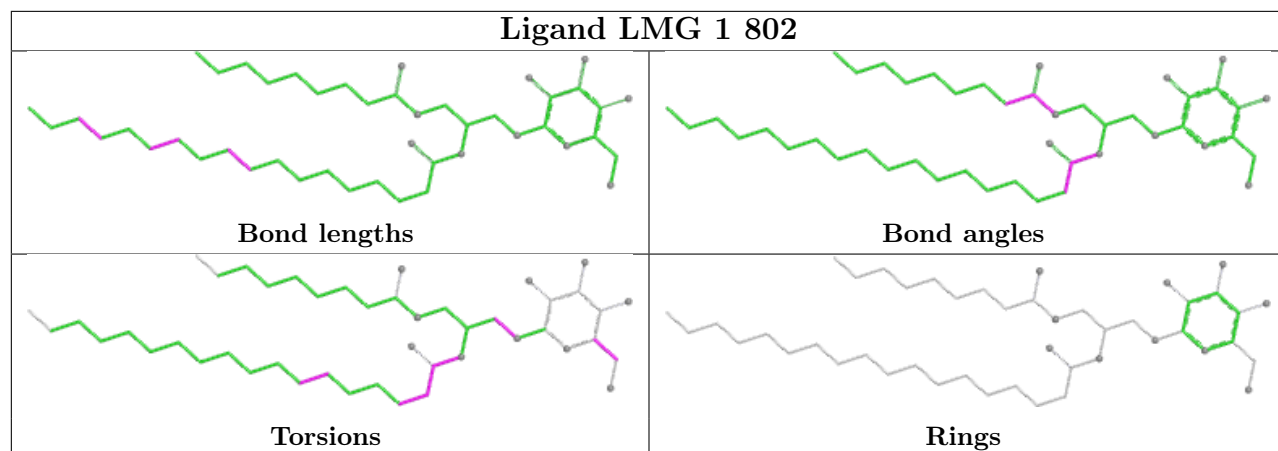
Ligand CLA 1 614



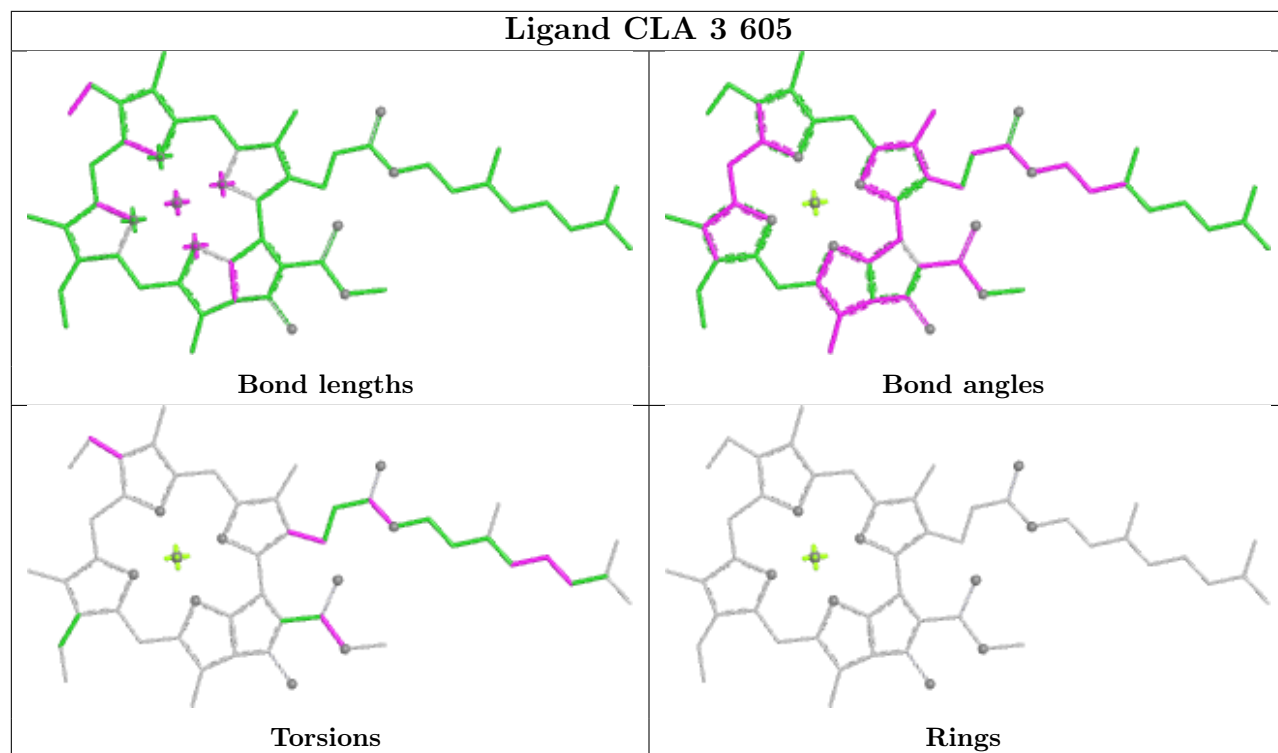
Ligand CLA B 1222



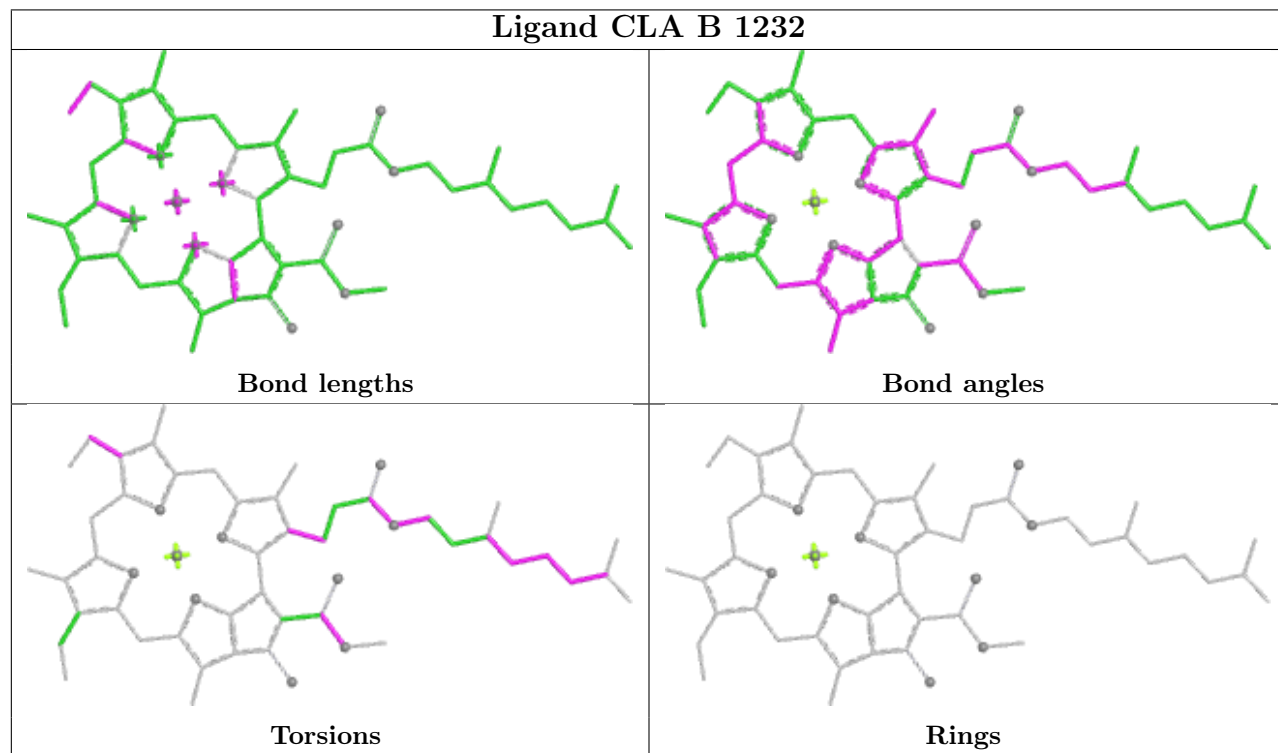


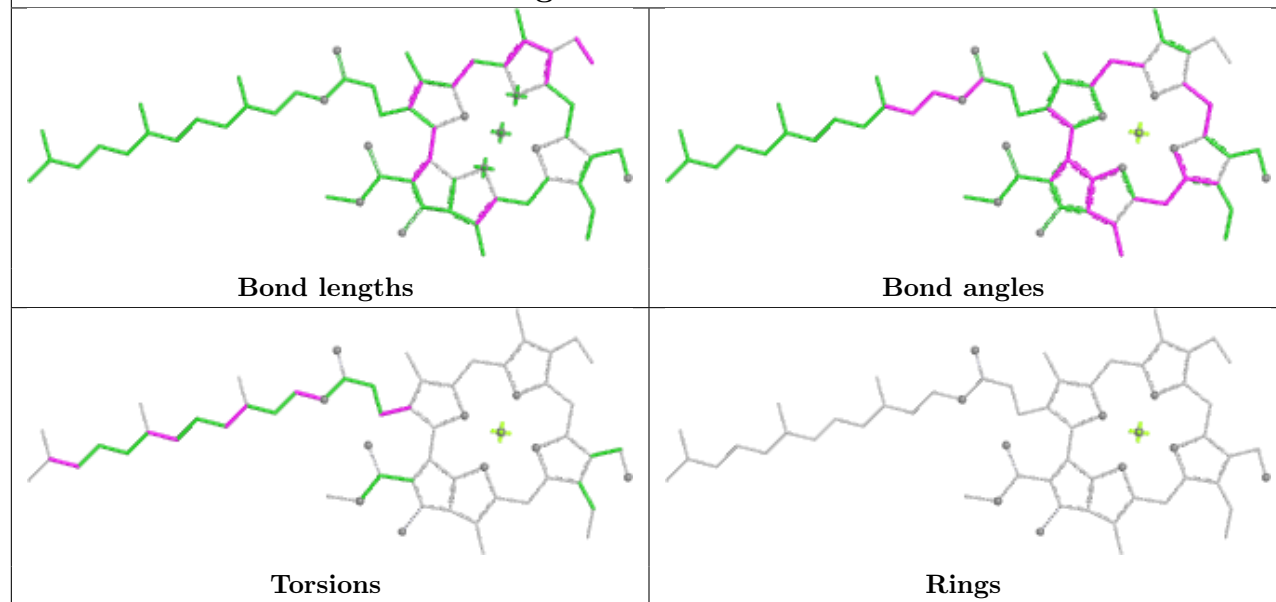
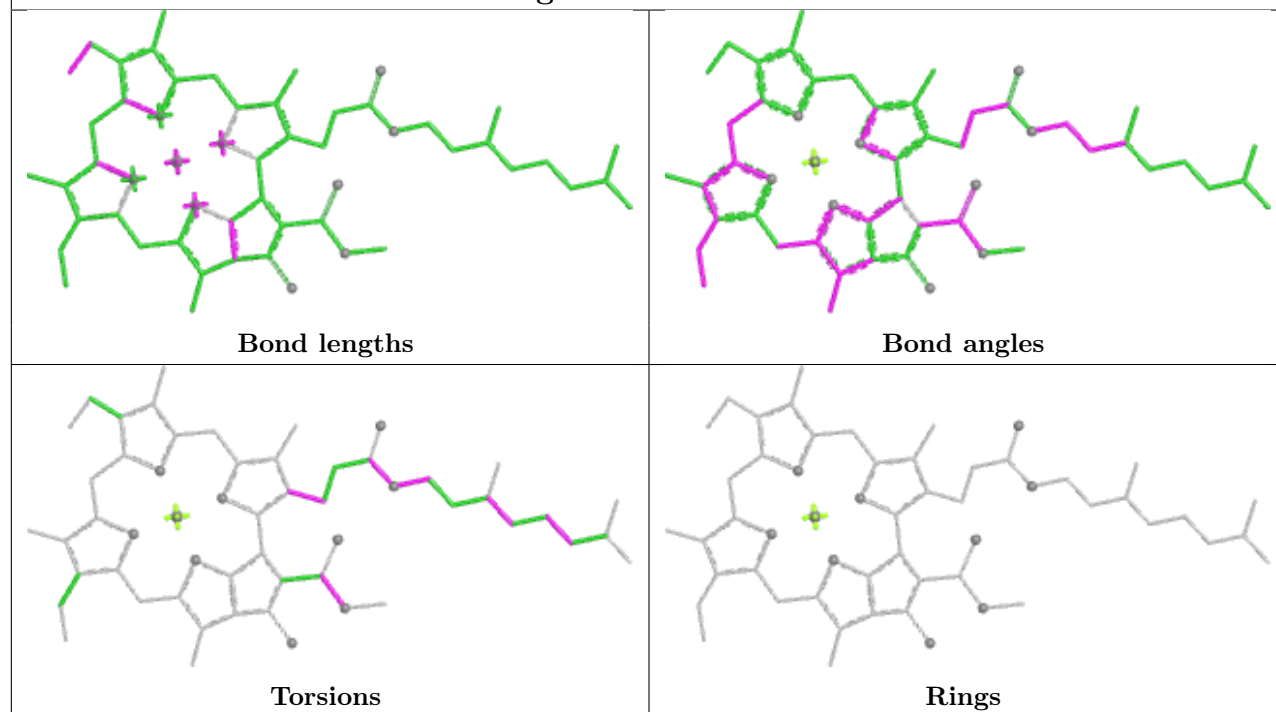


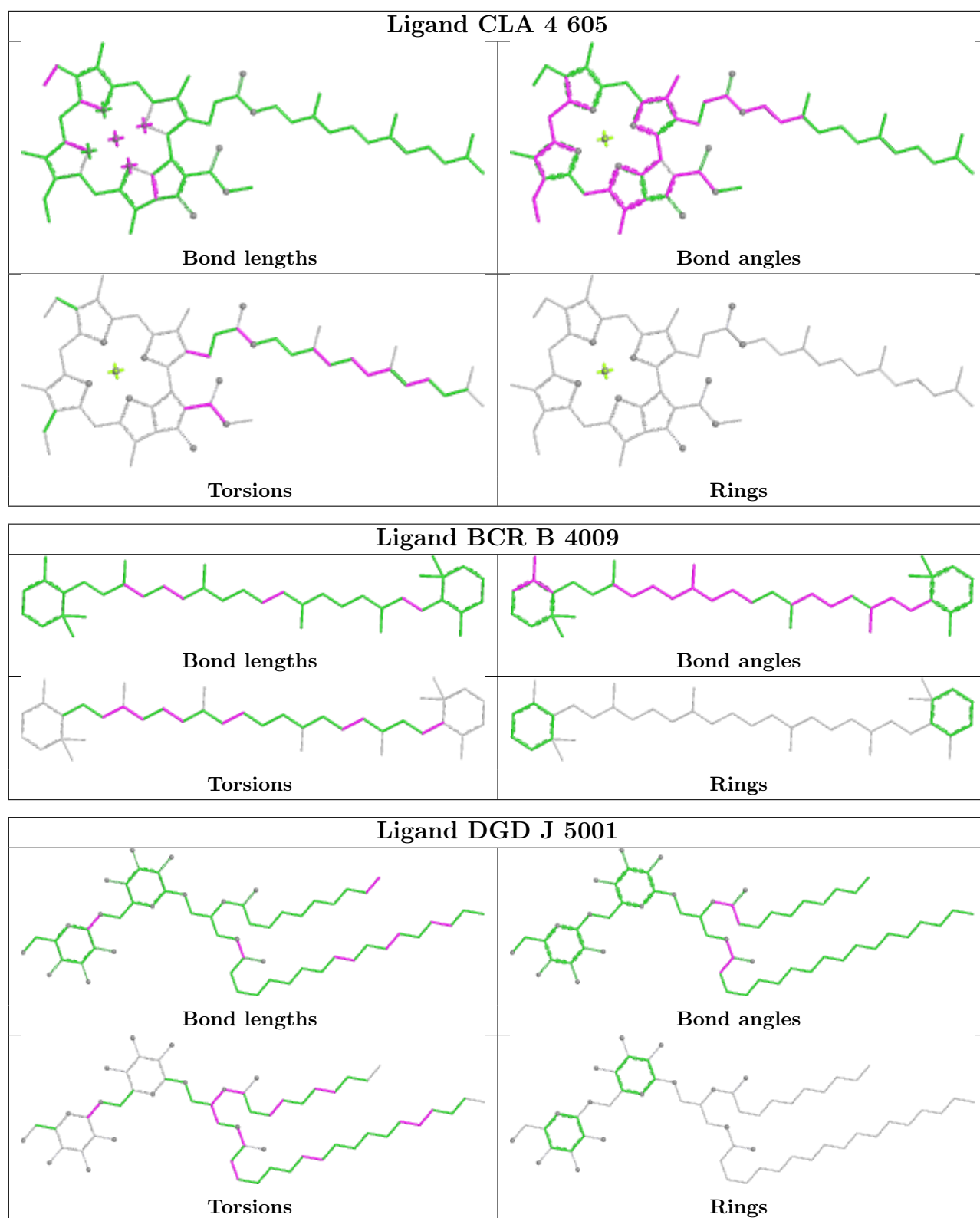
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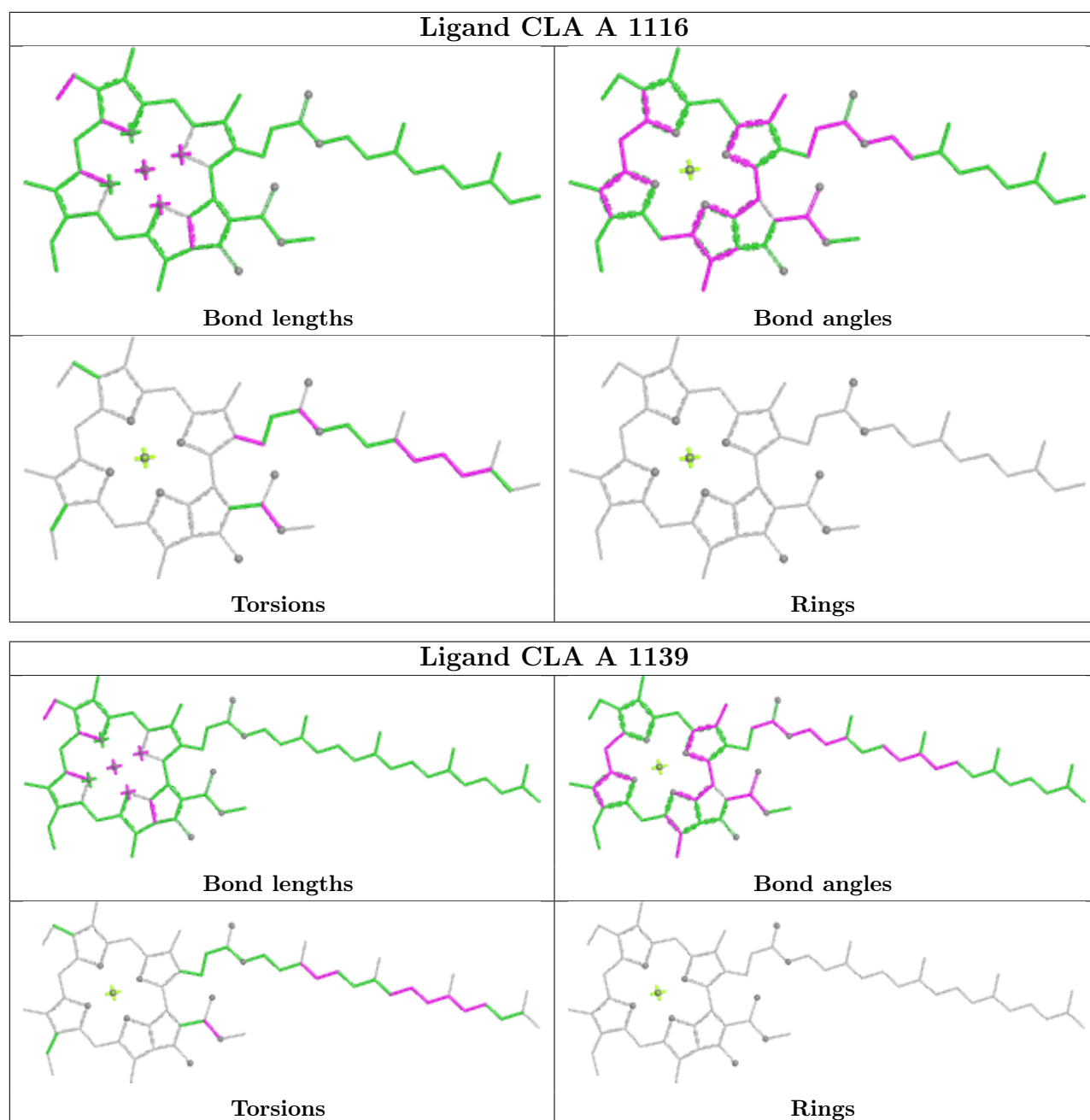


Ligand CLA B 1232

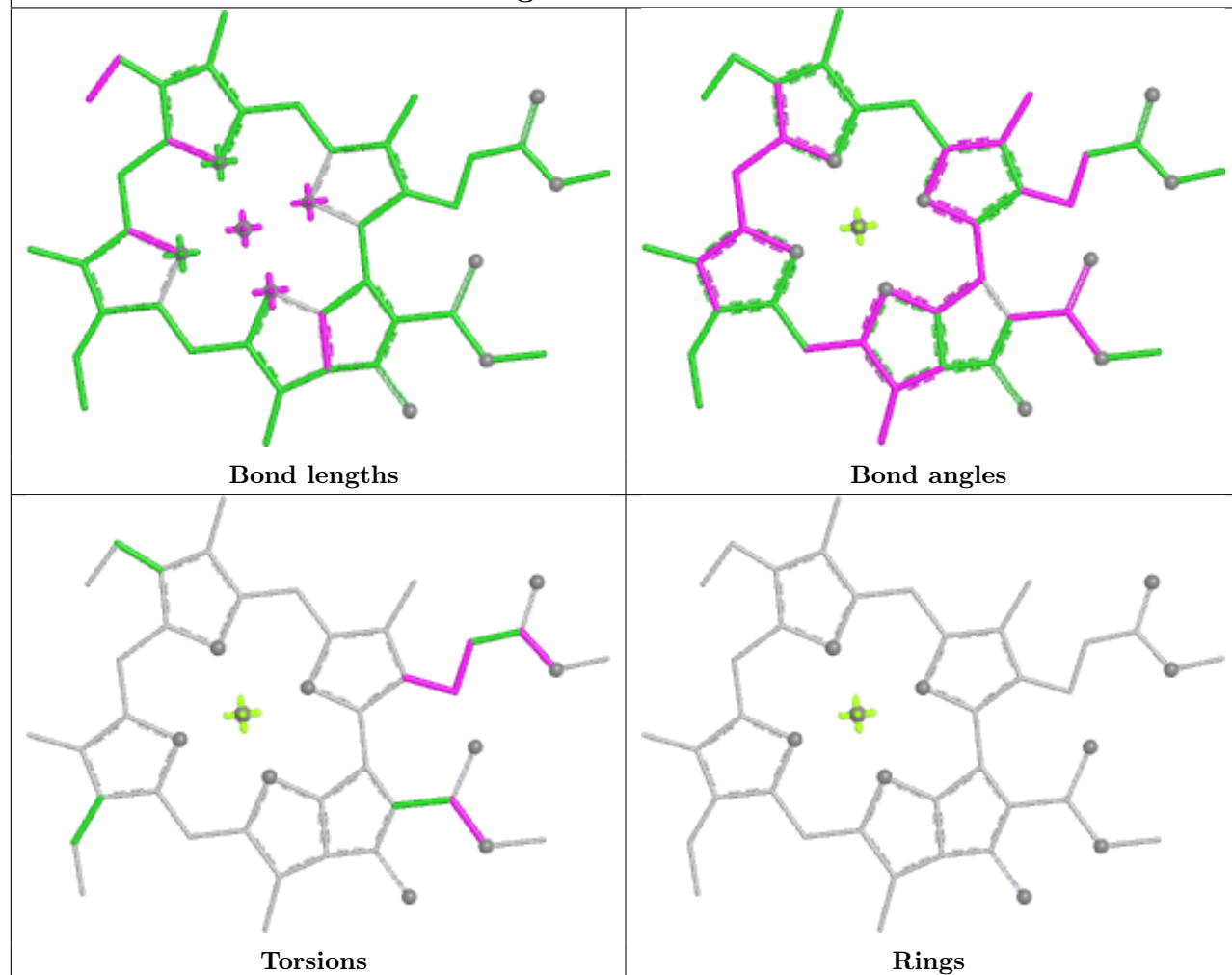


Ligand CHL 1 612**Ligand CLA 2 612**

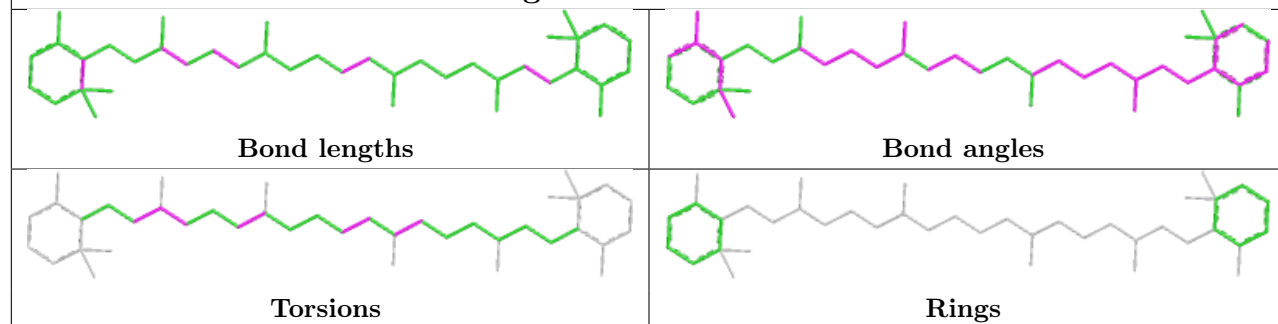




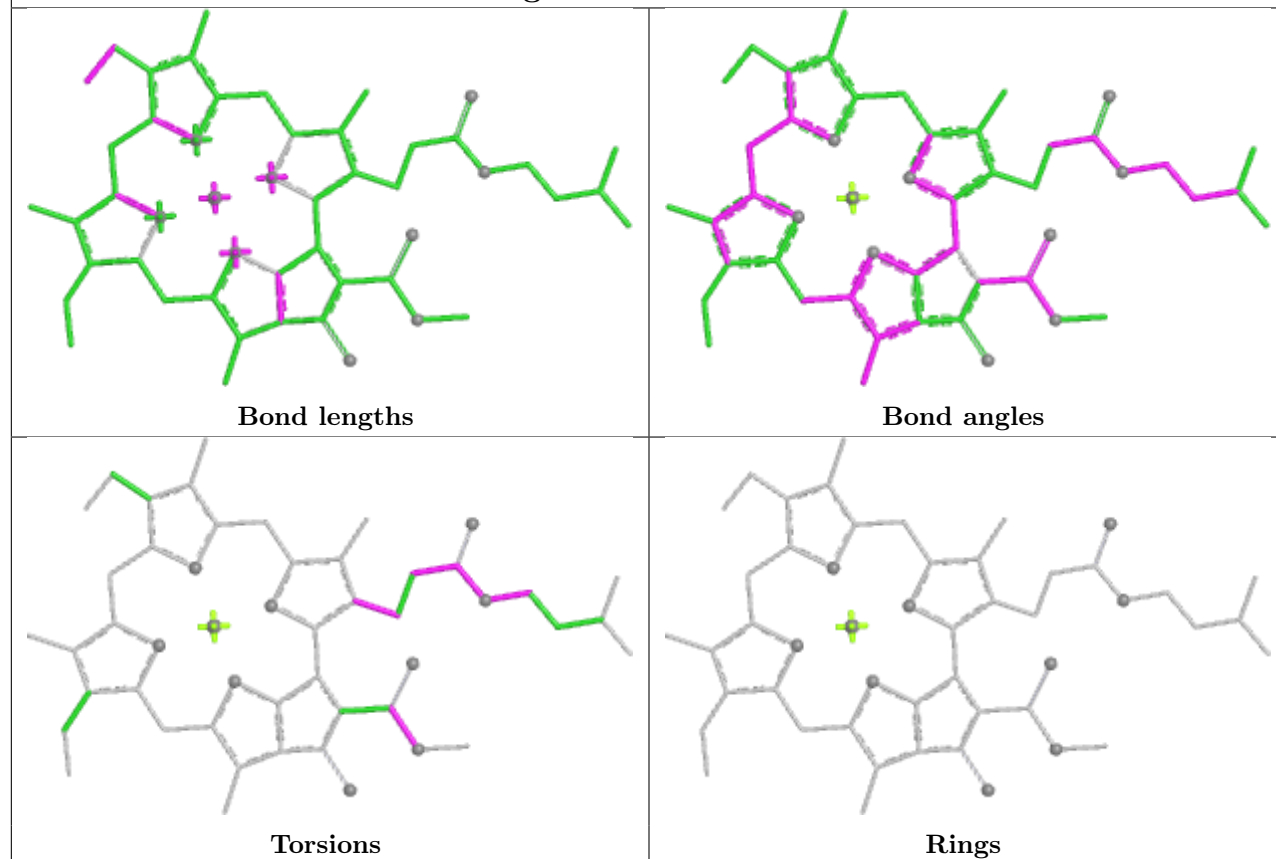
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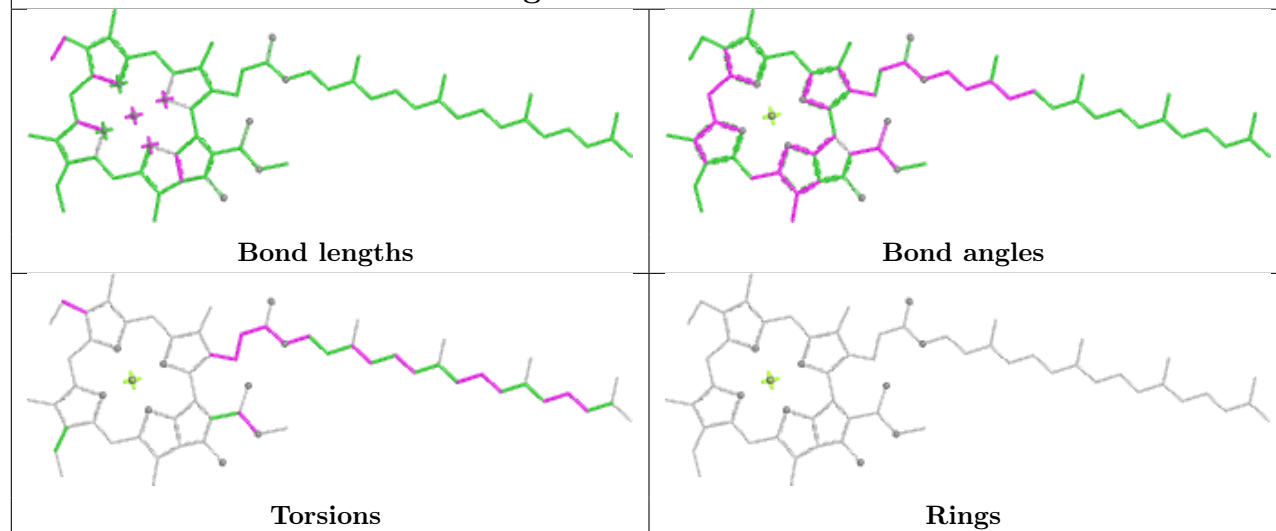
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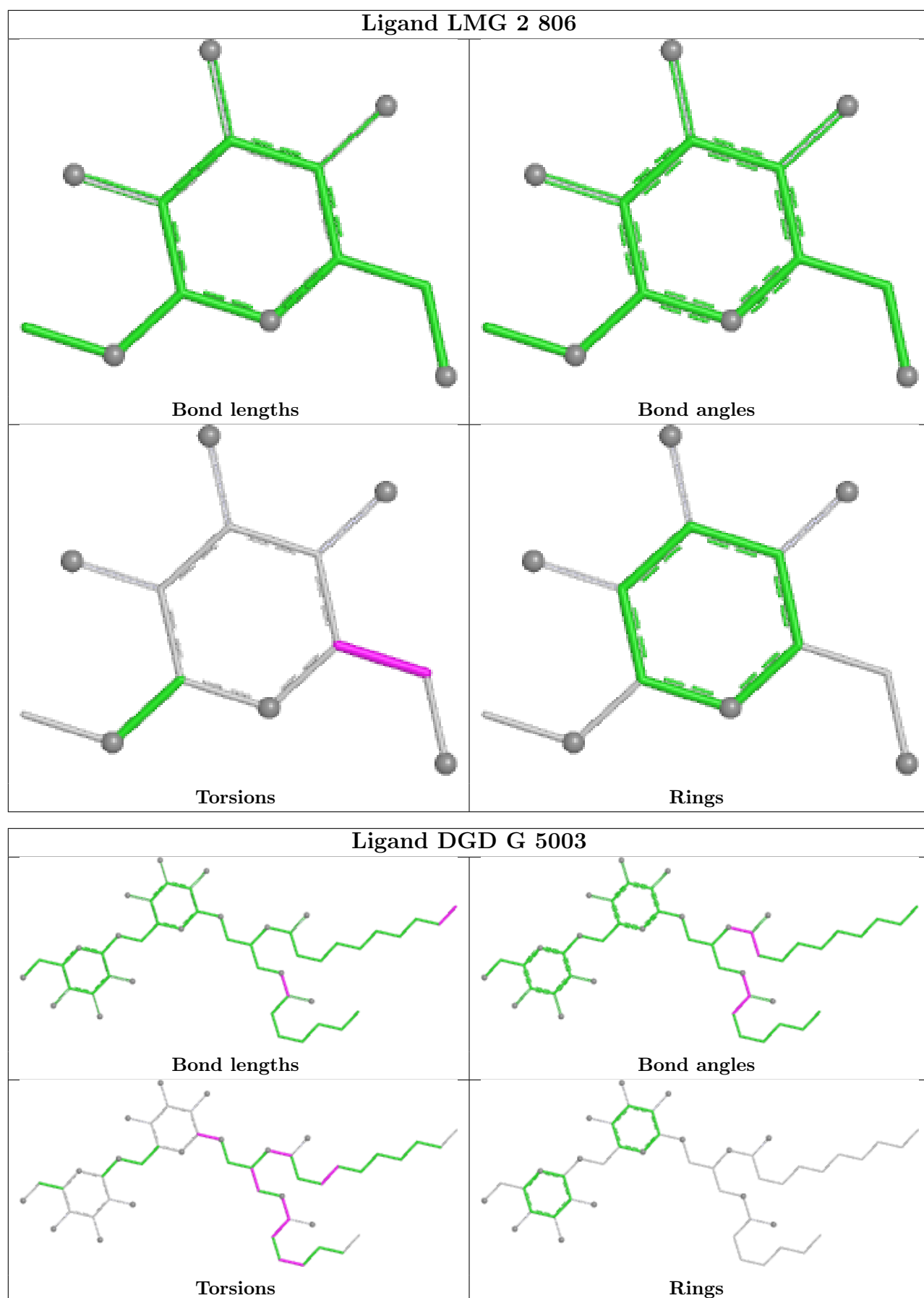


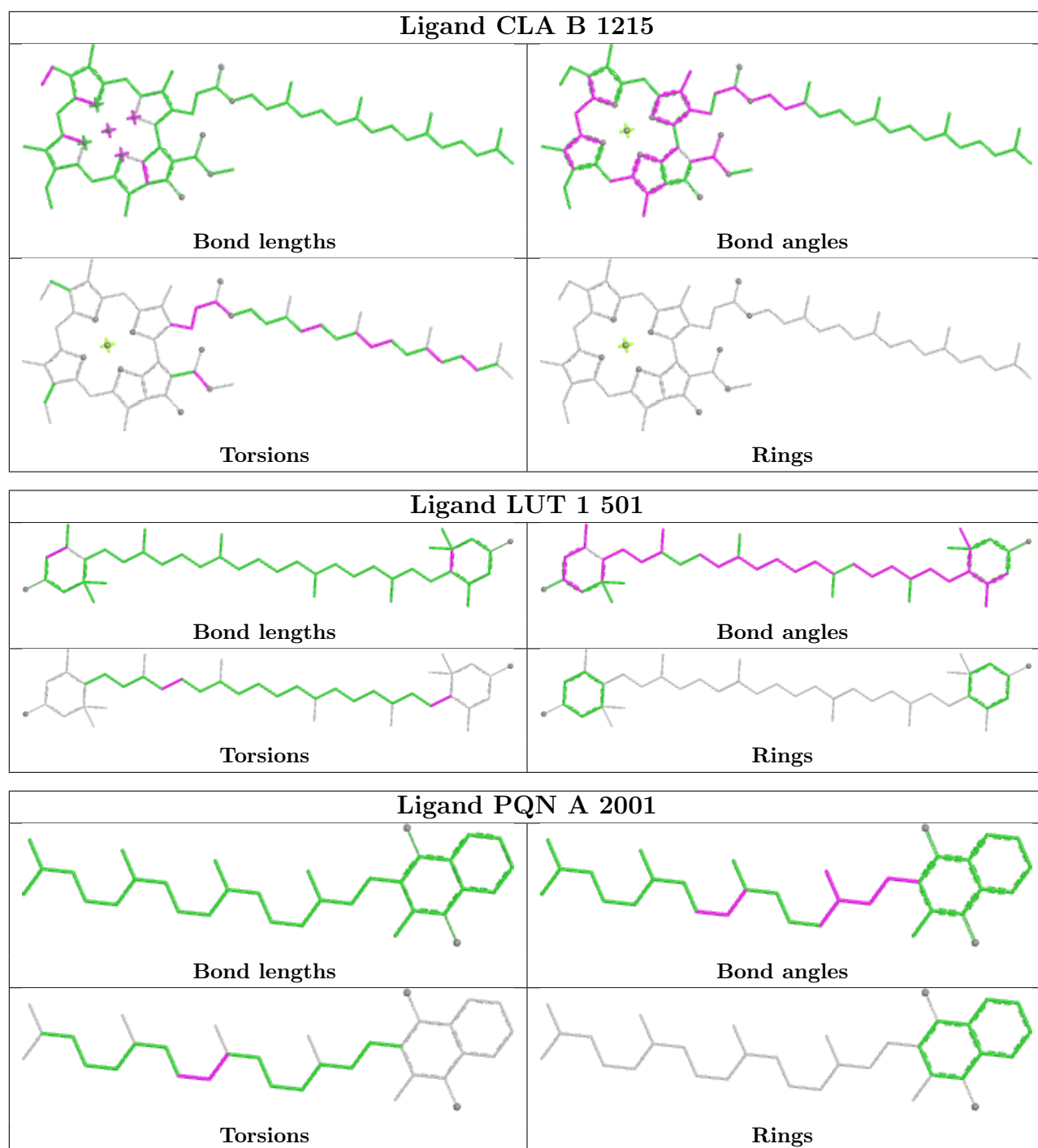
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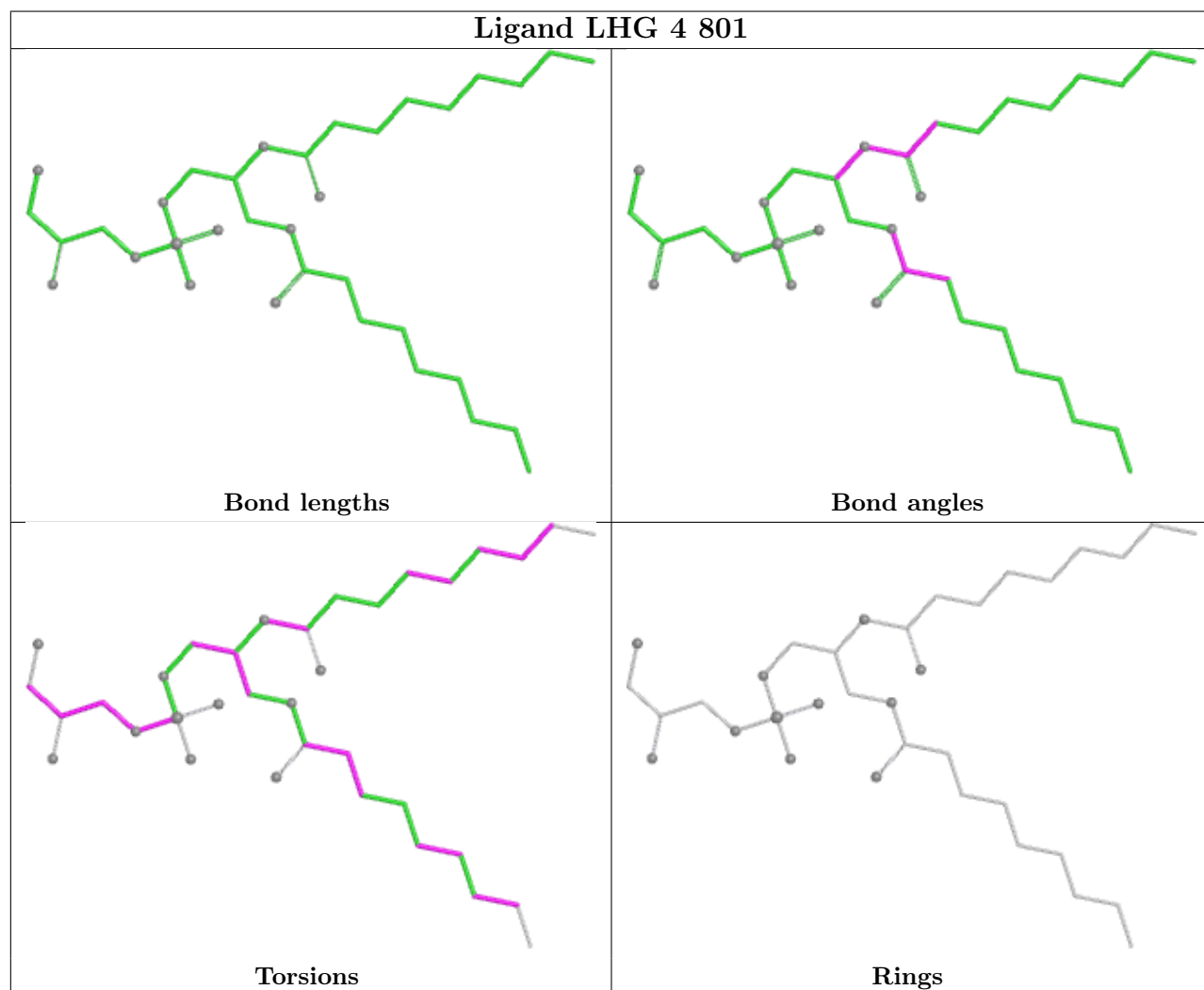
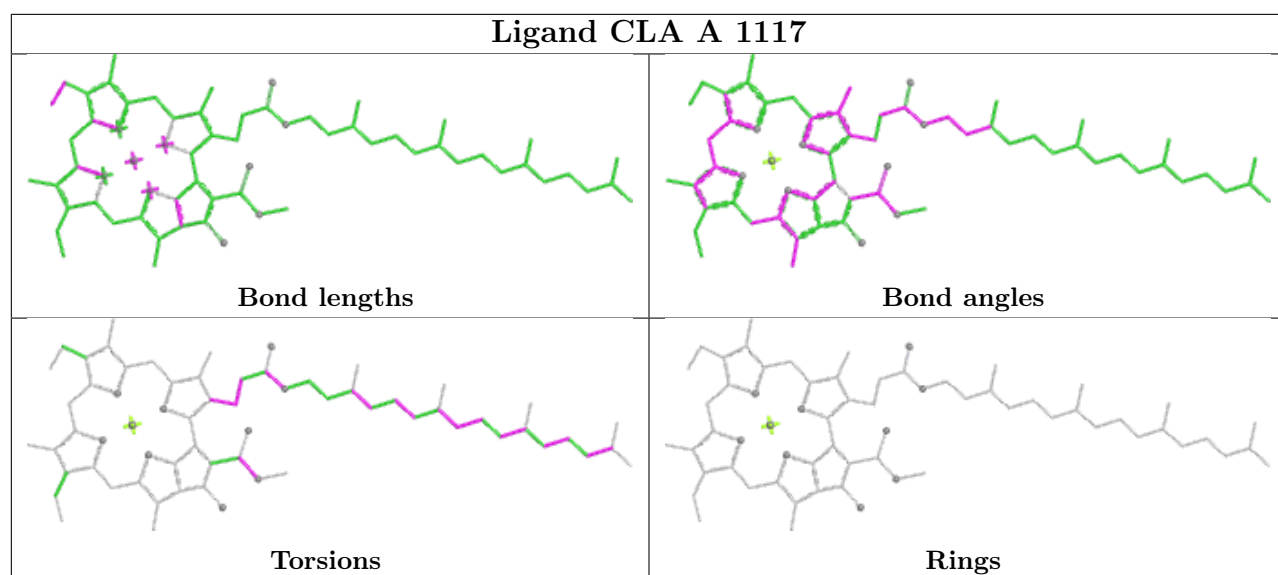


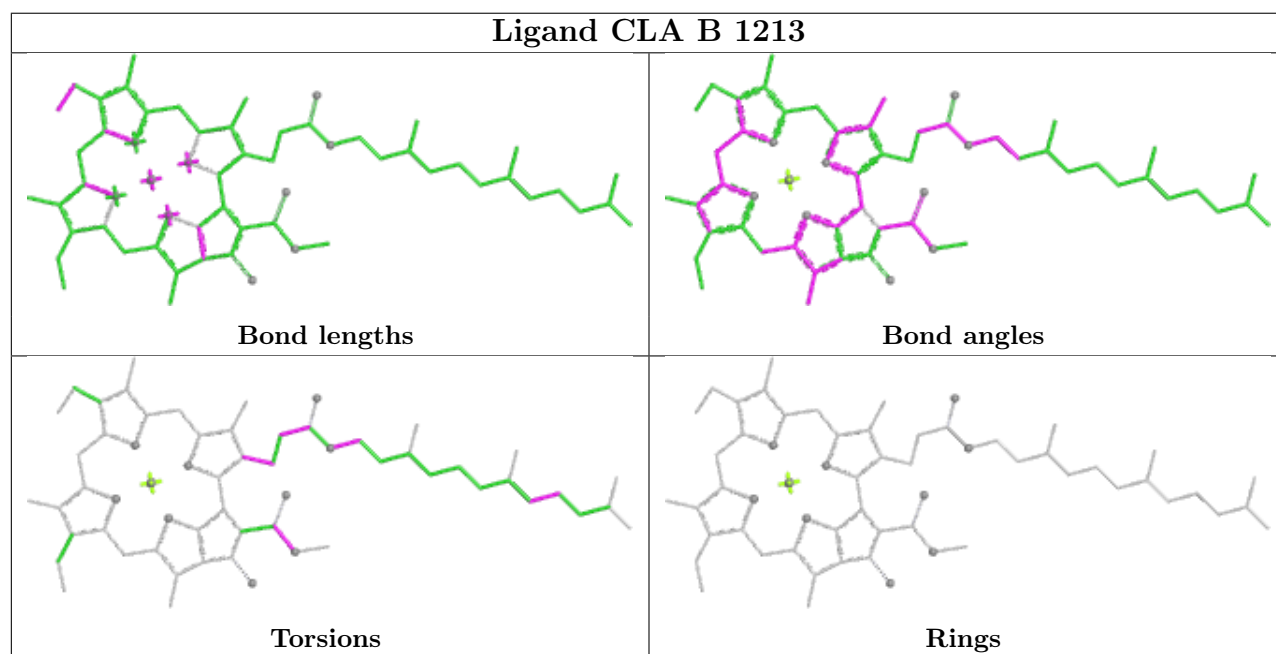
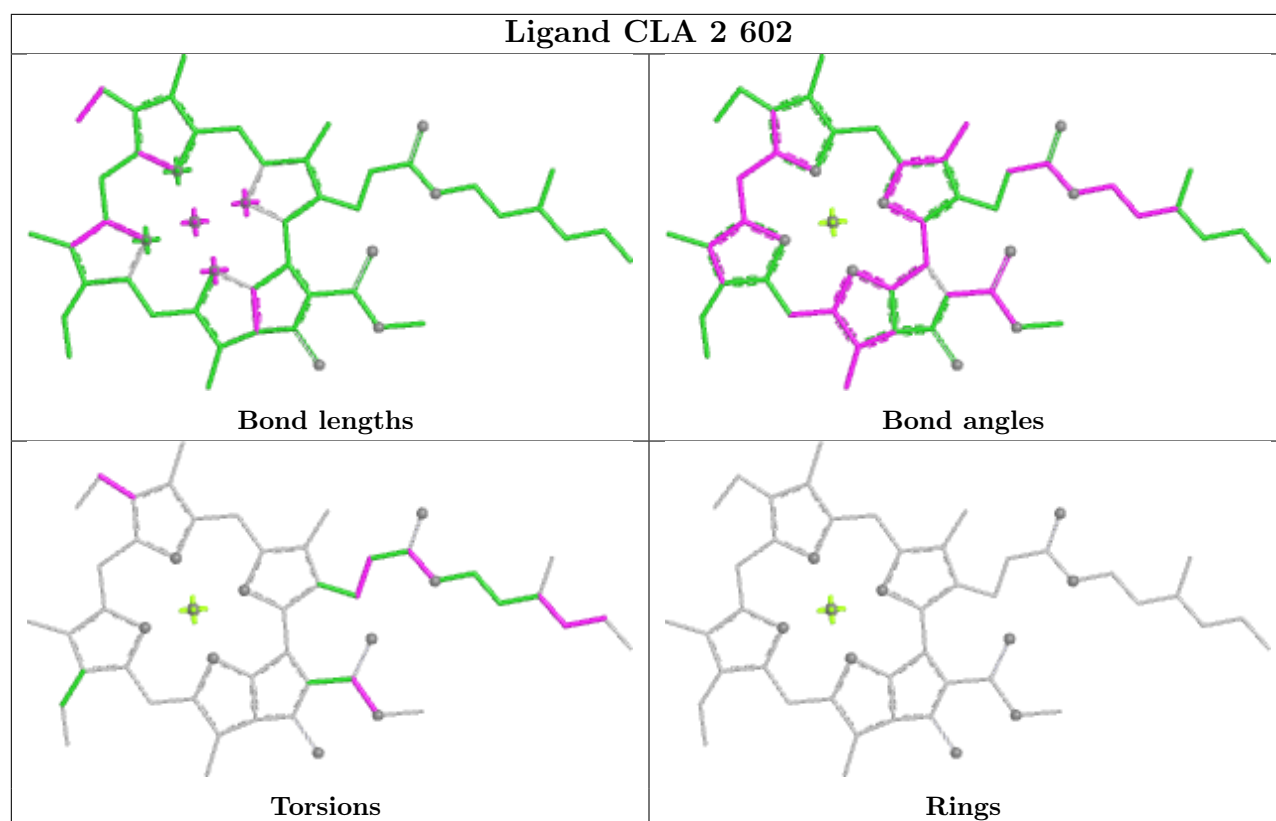
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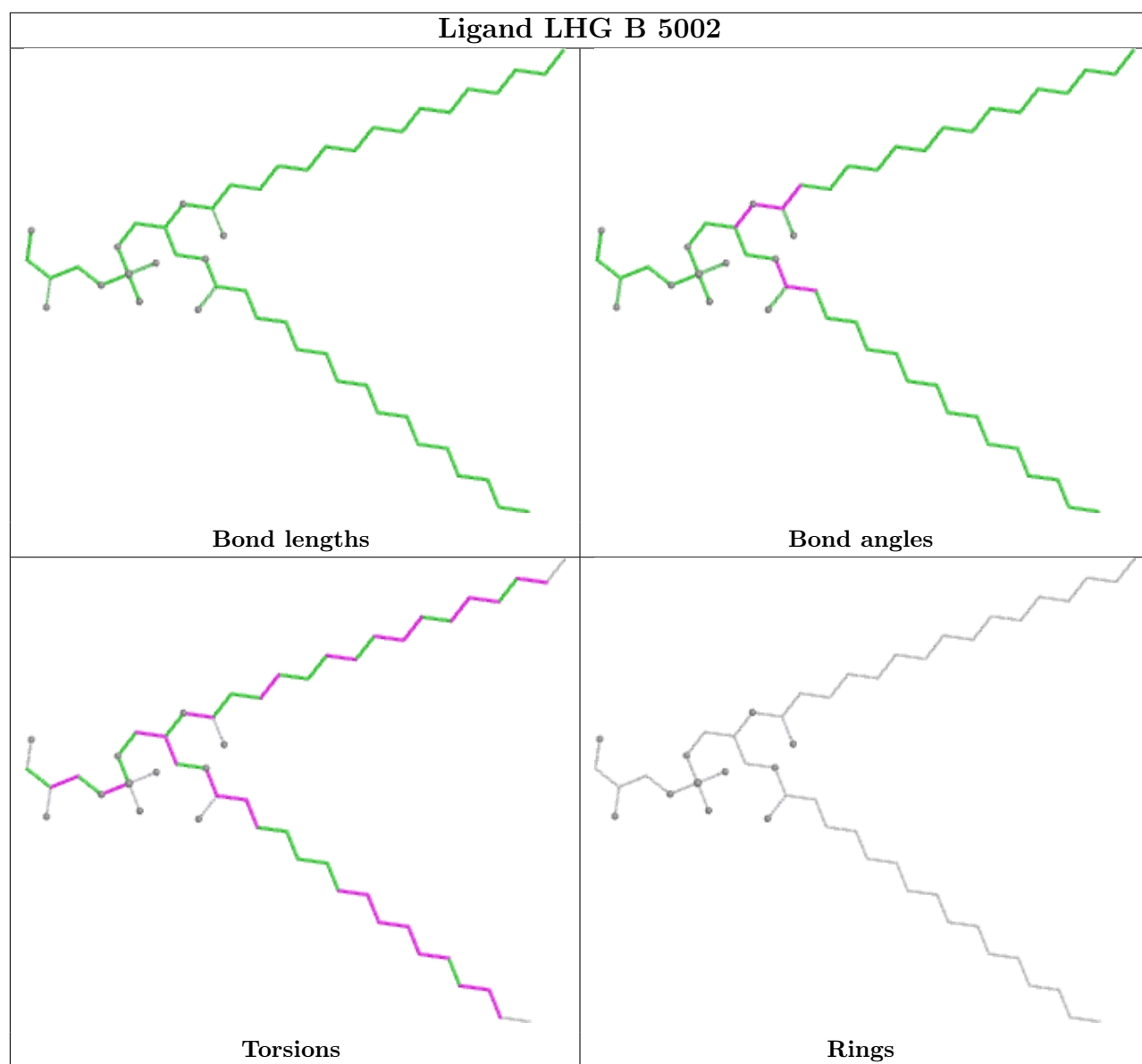


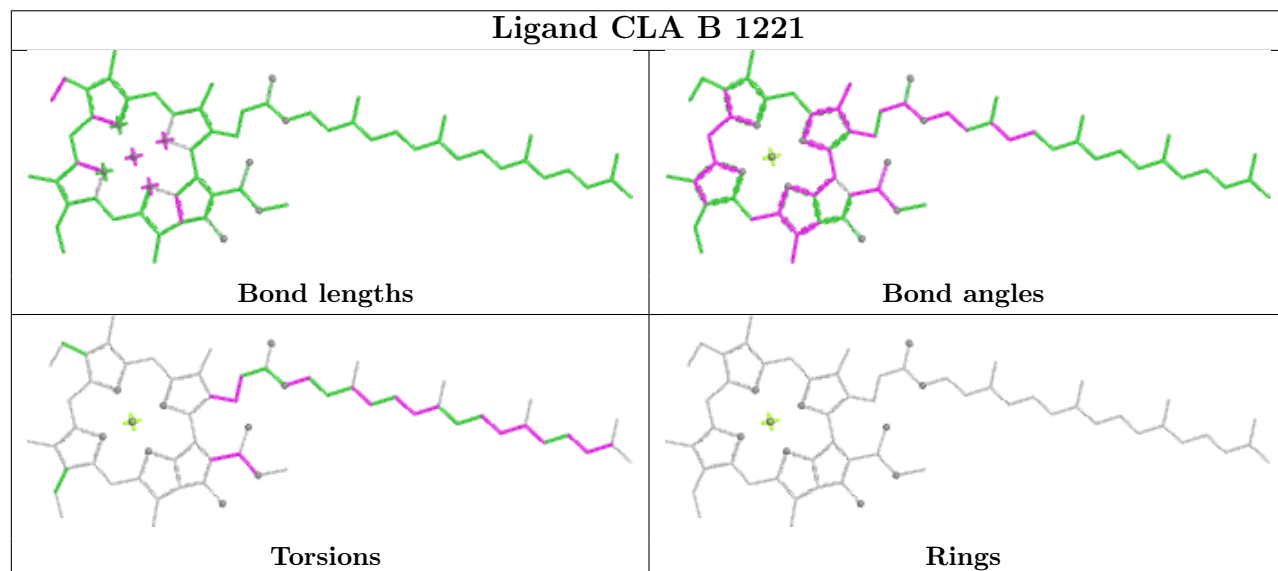
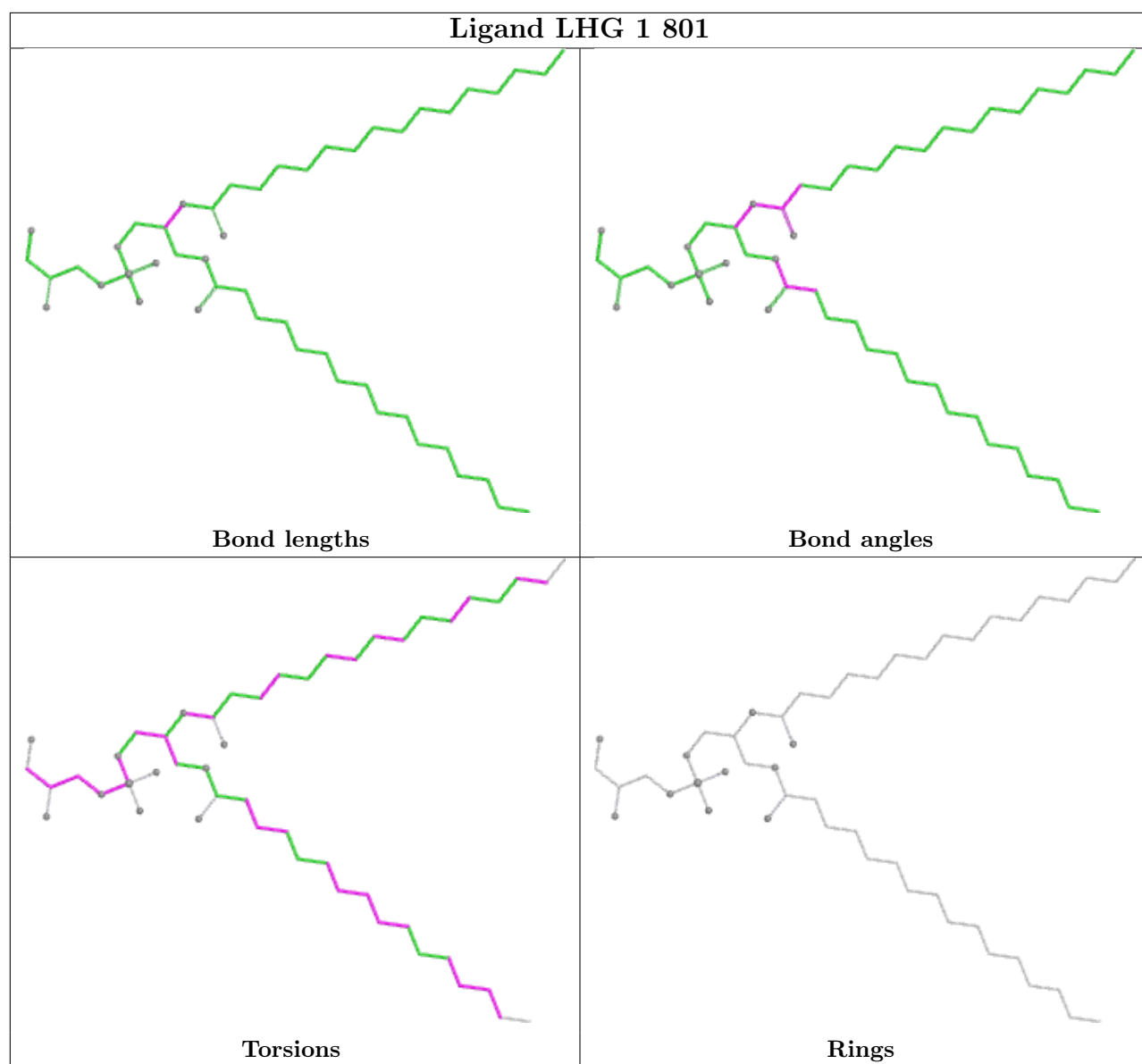


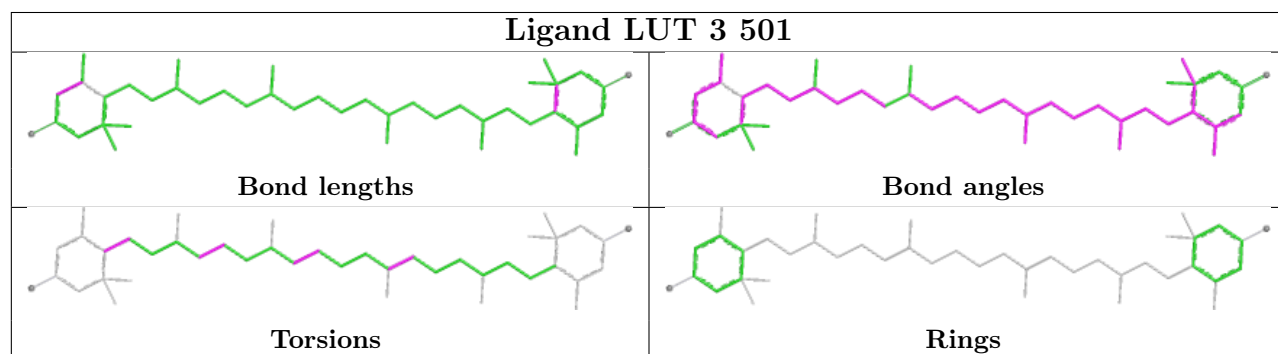
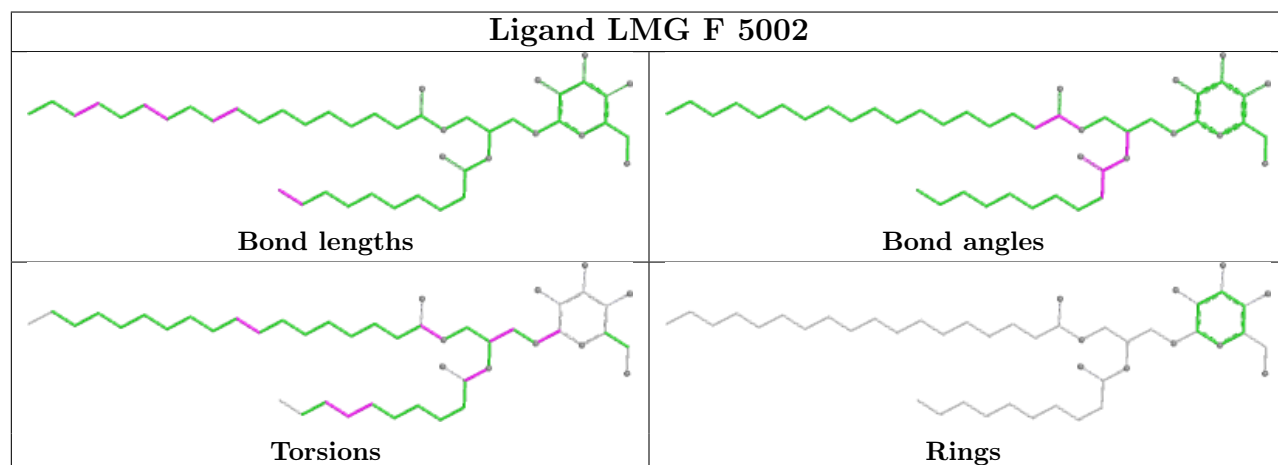
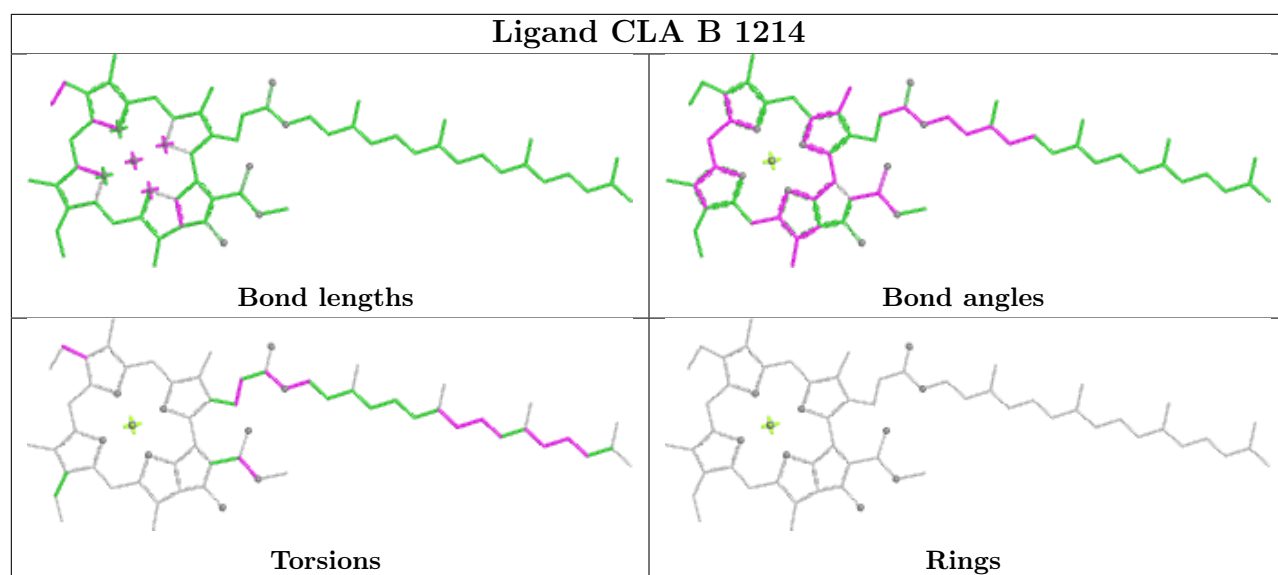


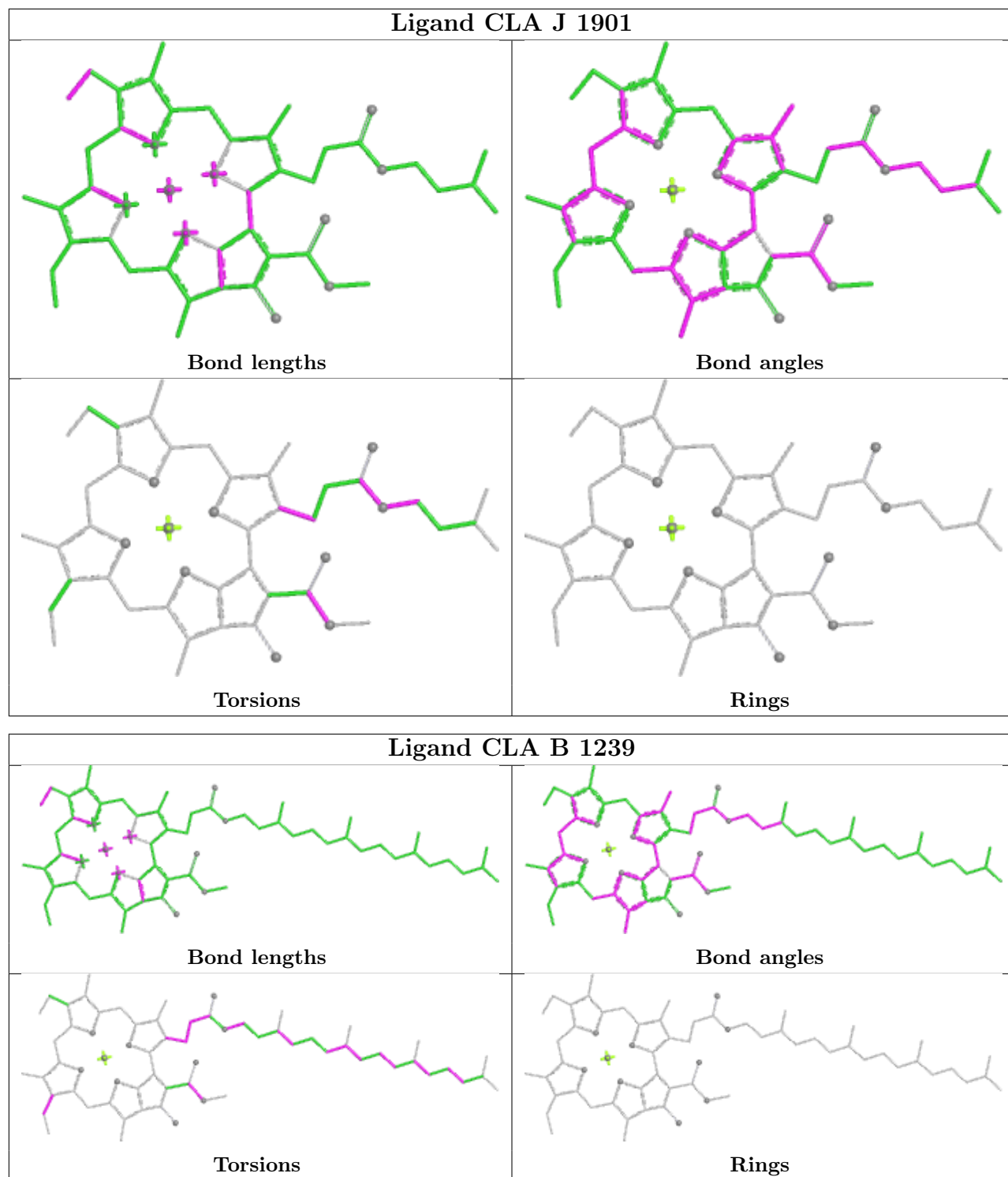


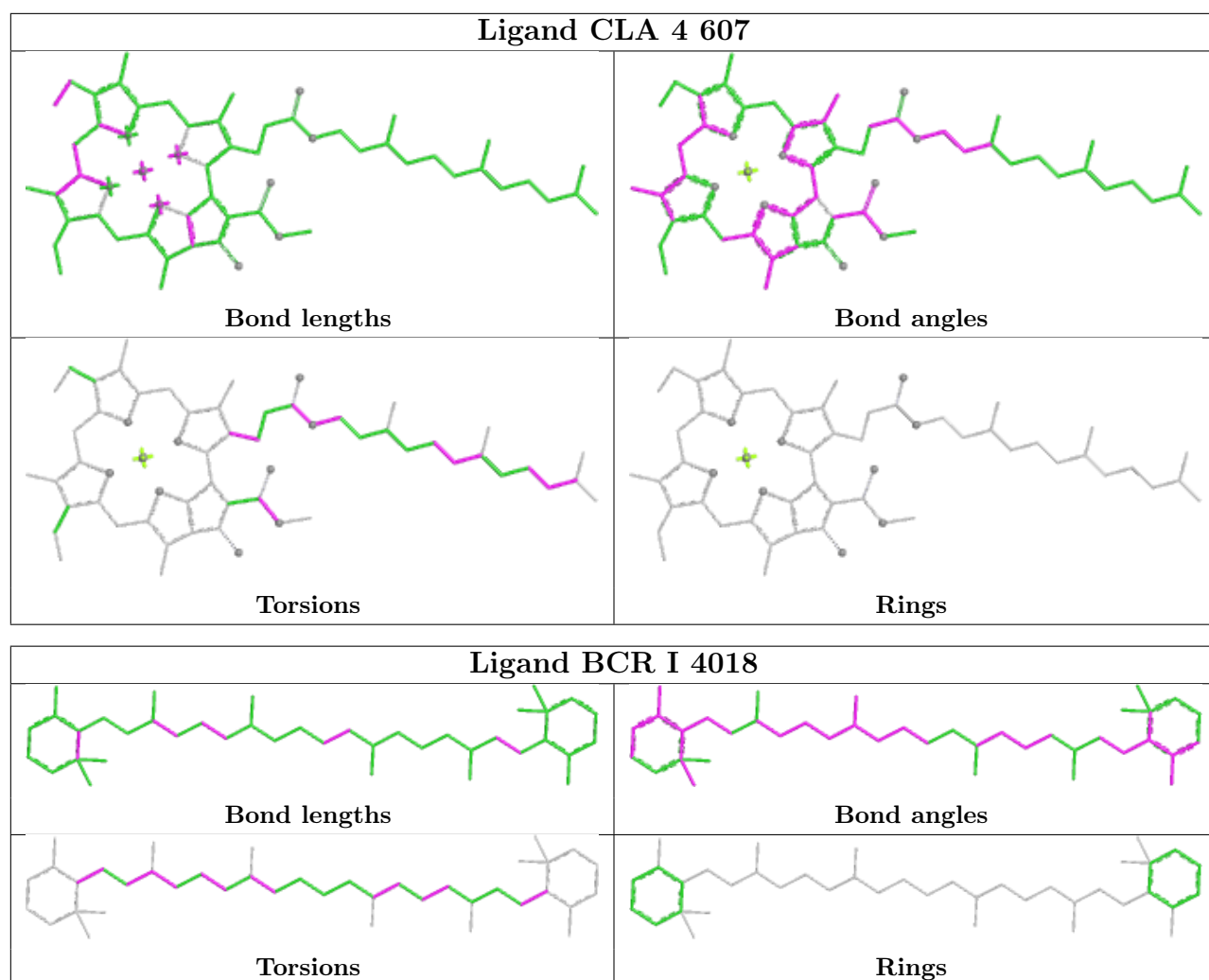


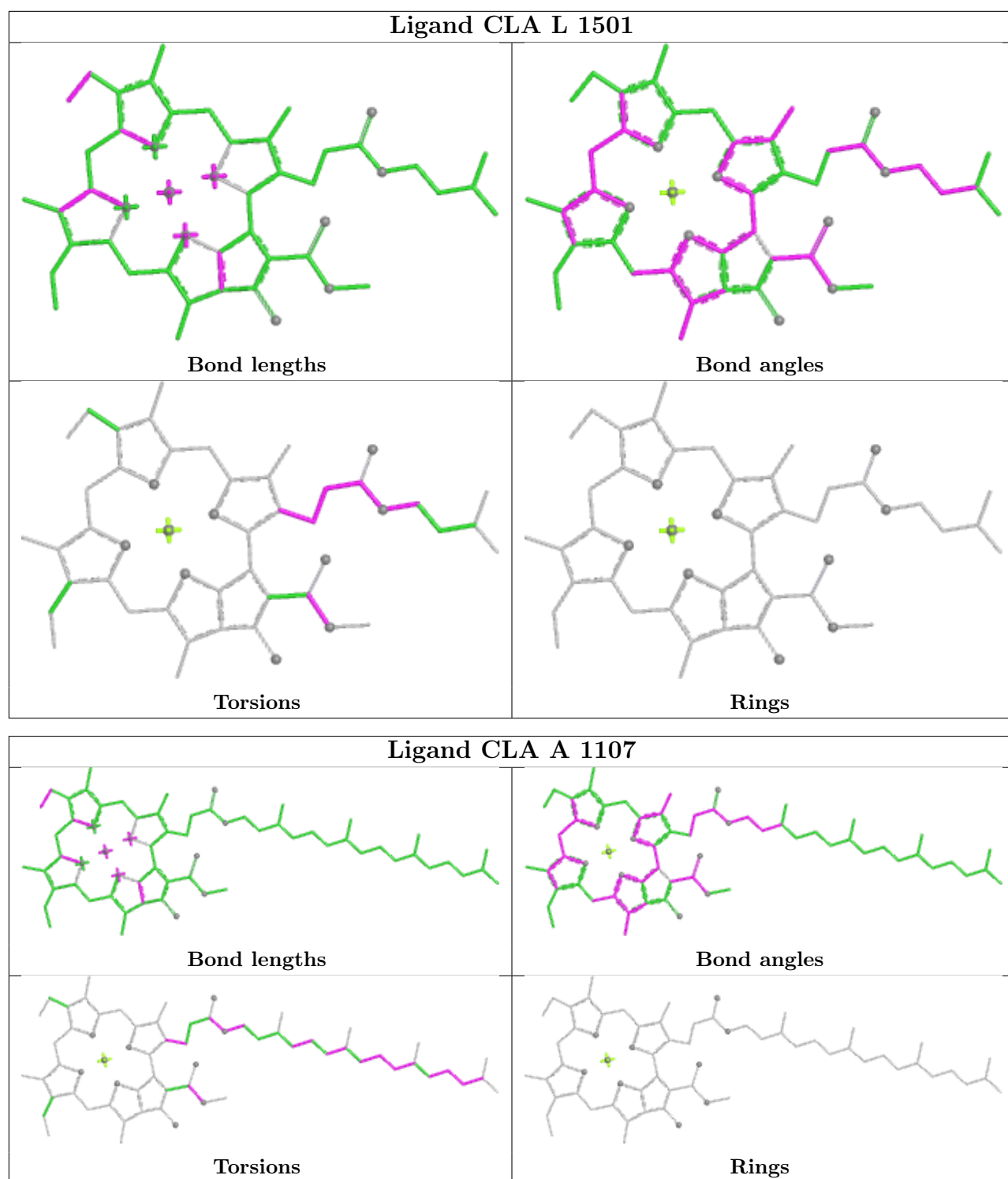




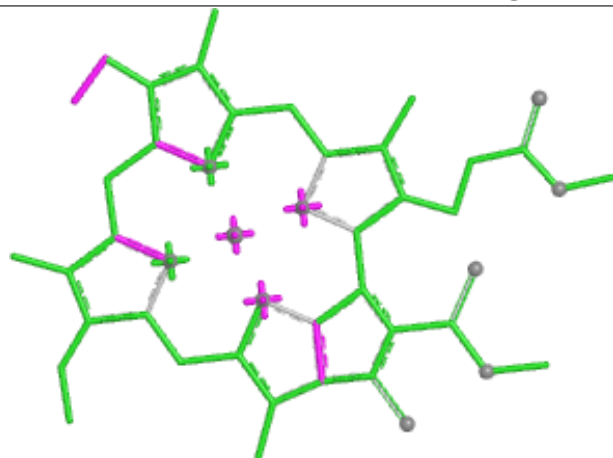




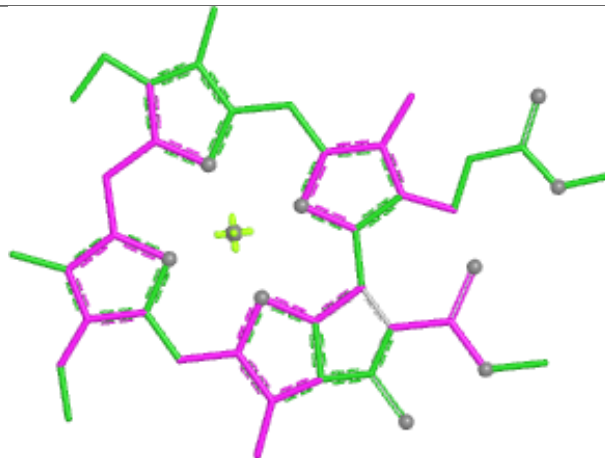




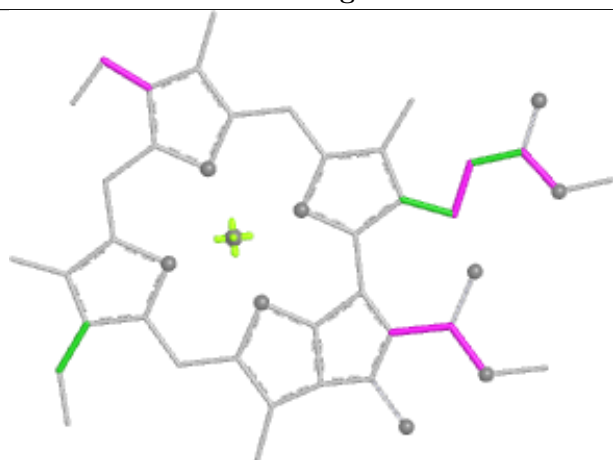
Ligand CLA B 1217



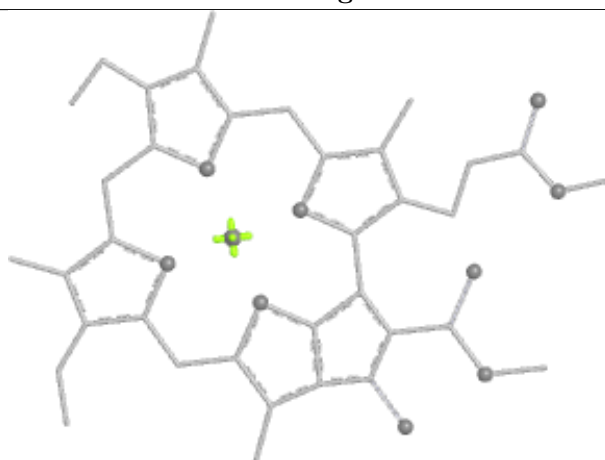
Bond lengths



Bond angles

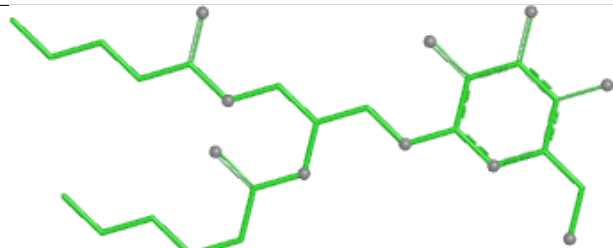


Torsions

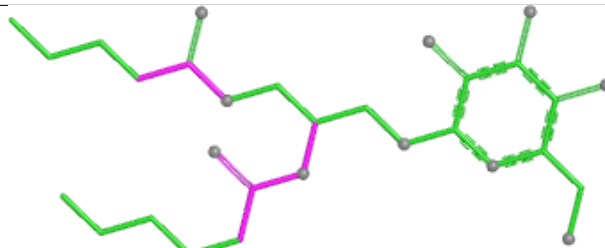


Rings

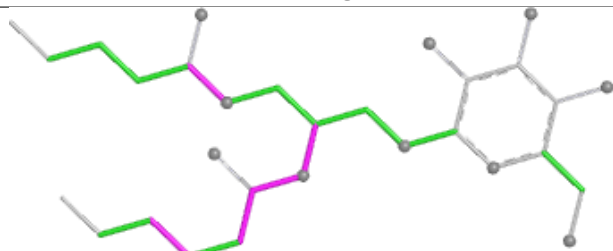
Ligand LMG 2 804



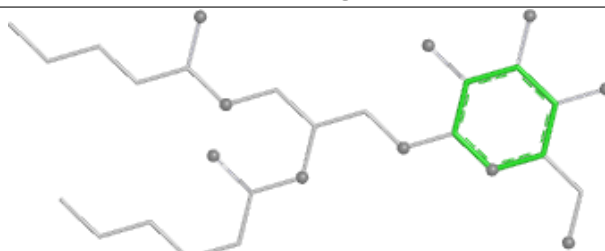
Bond lengths



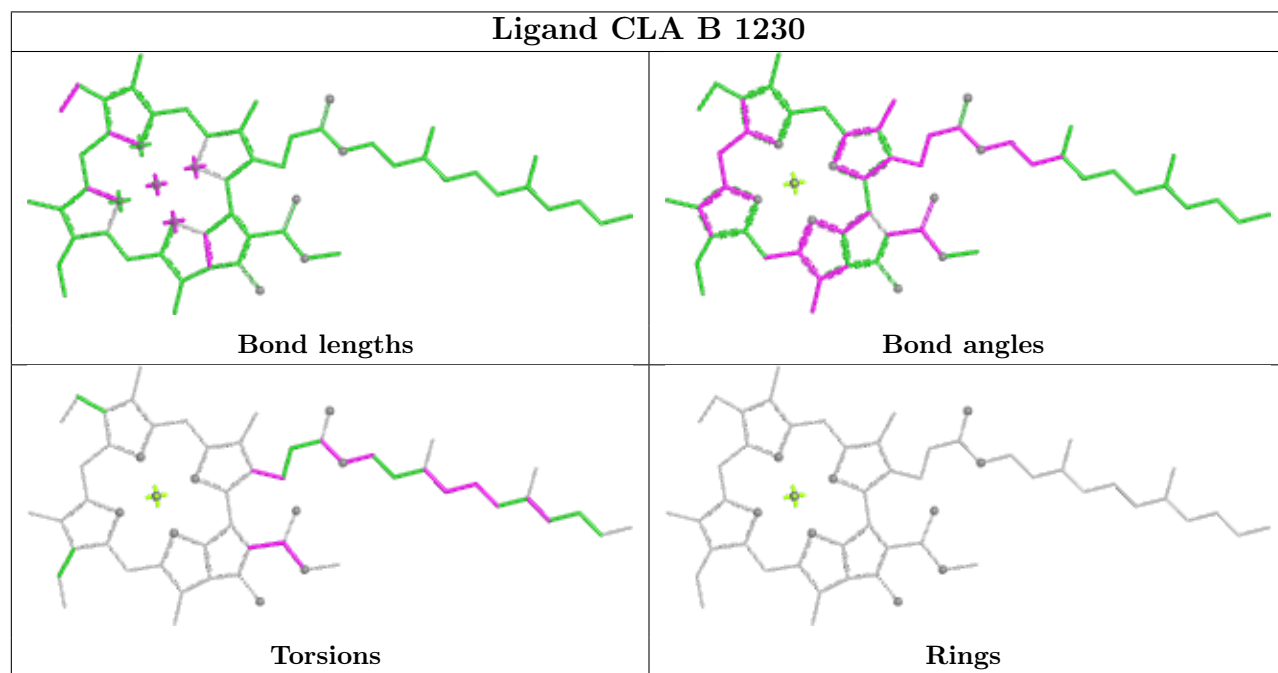
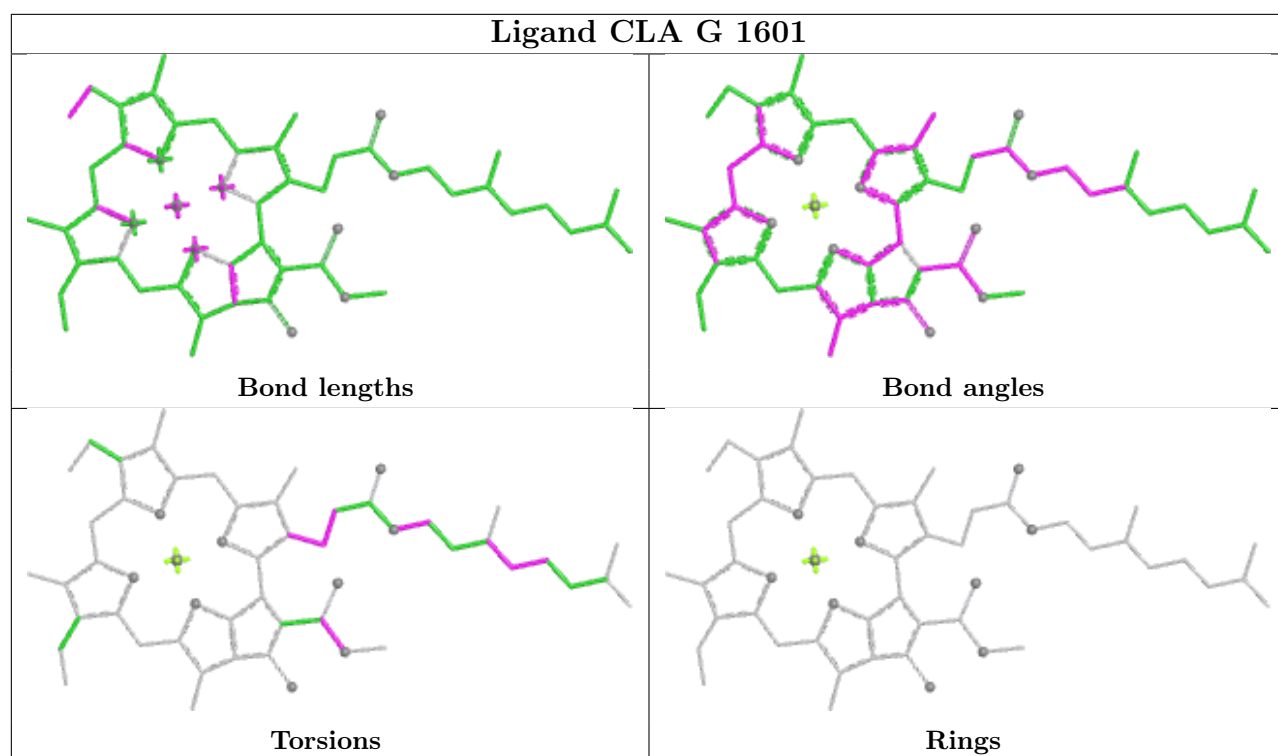
Bond angles

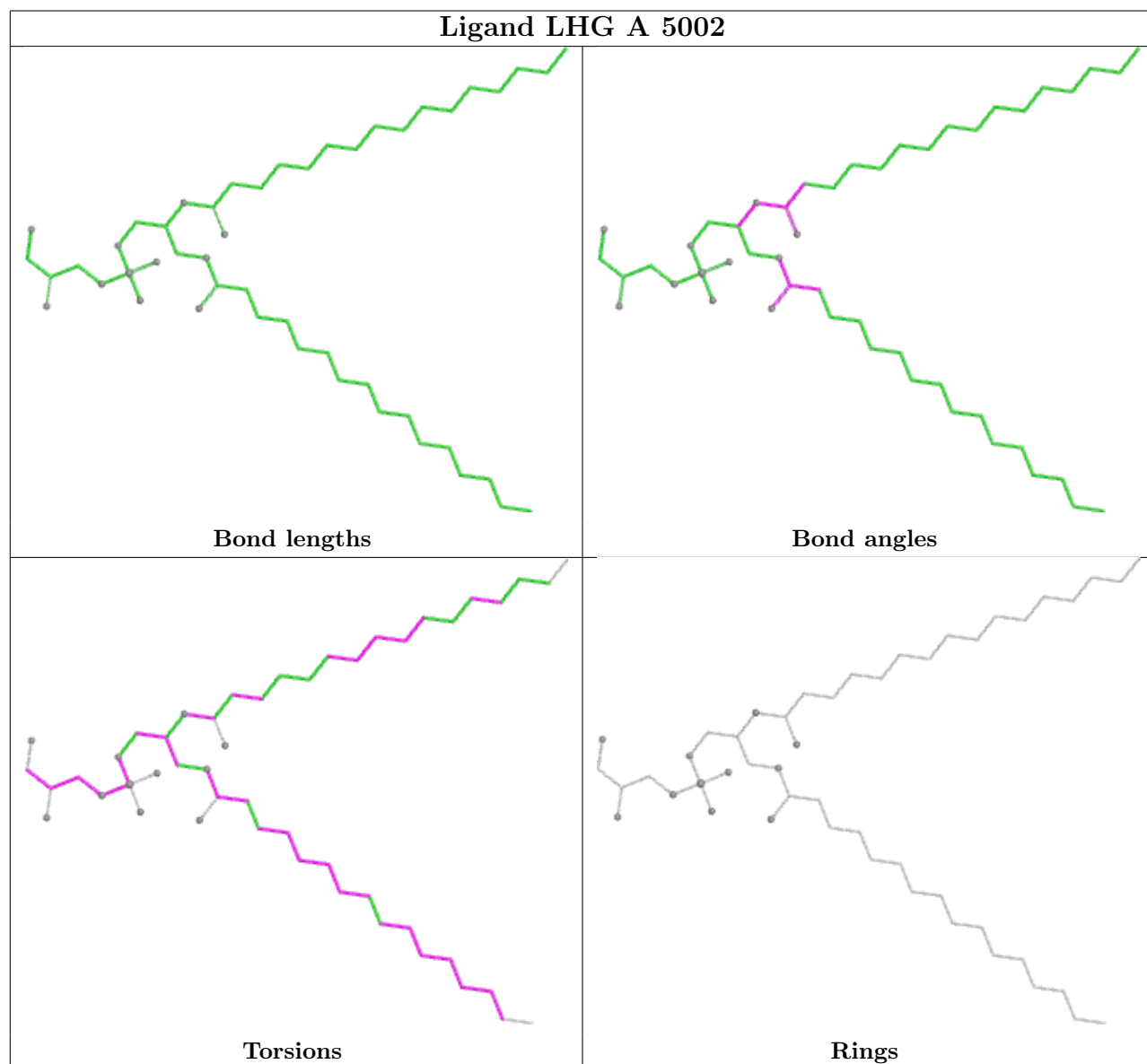
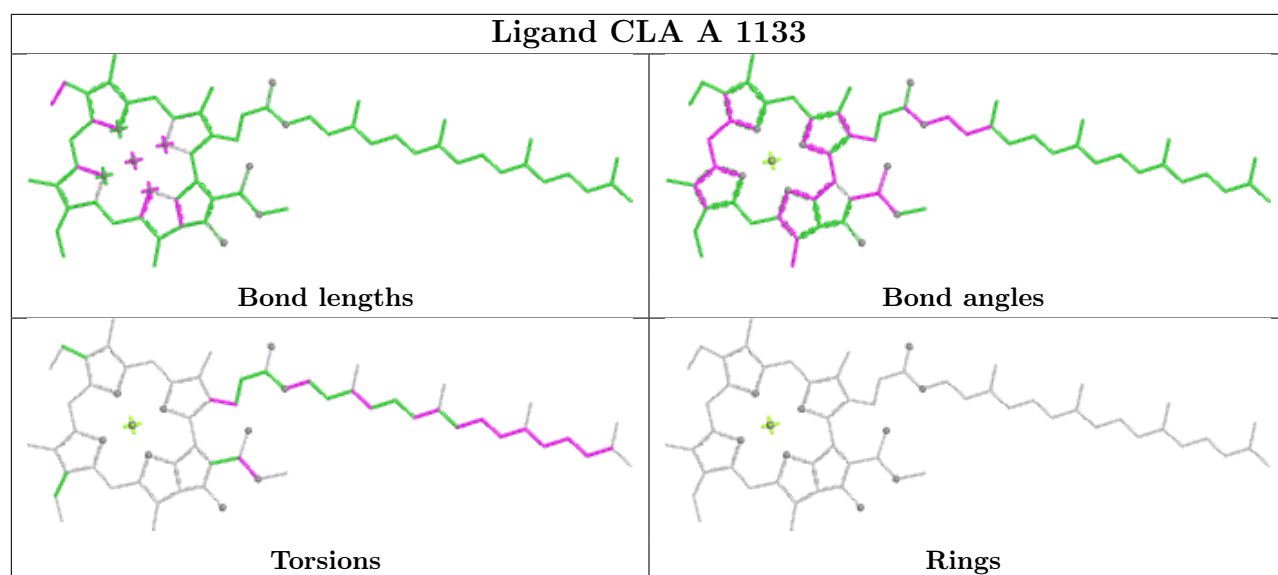


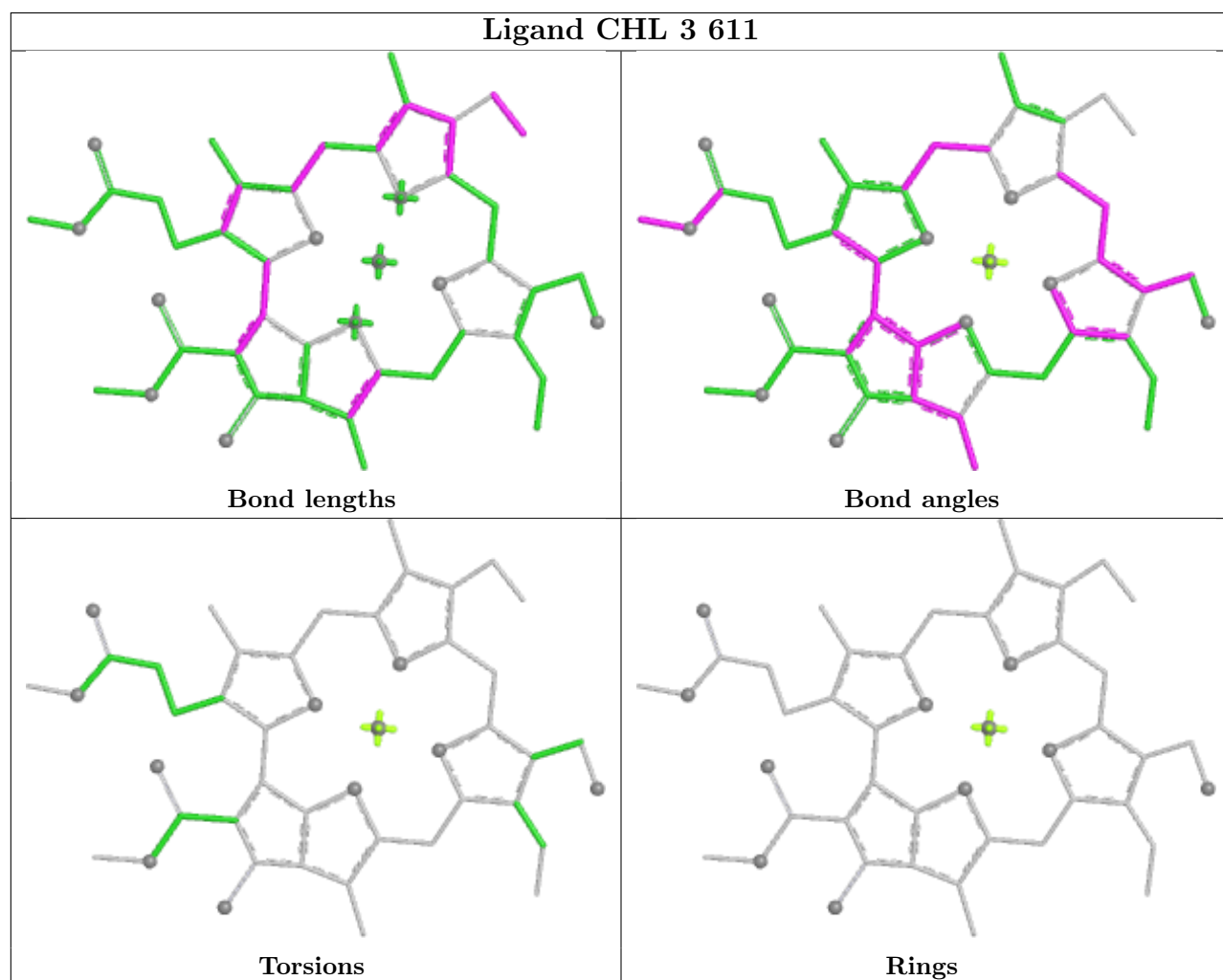
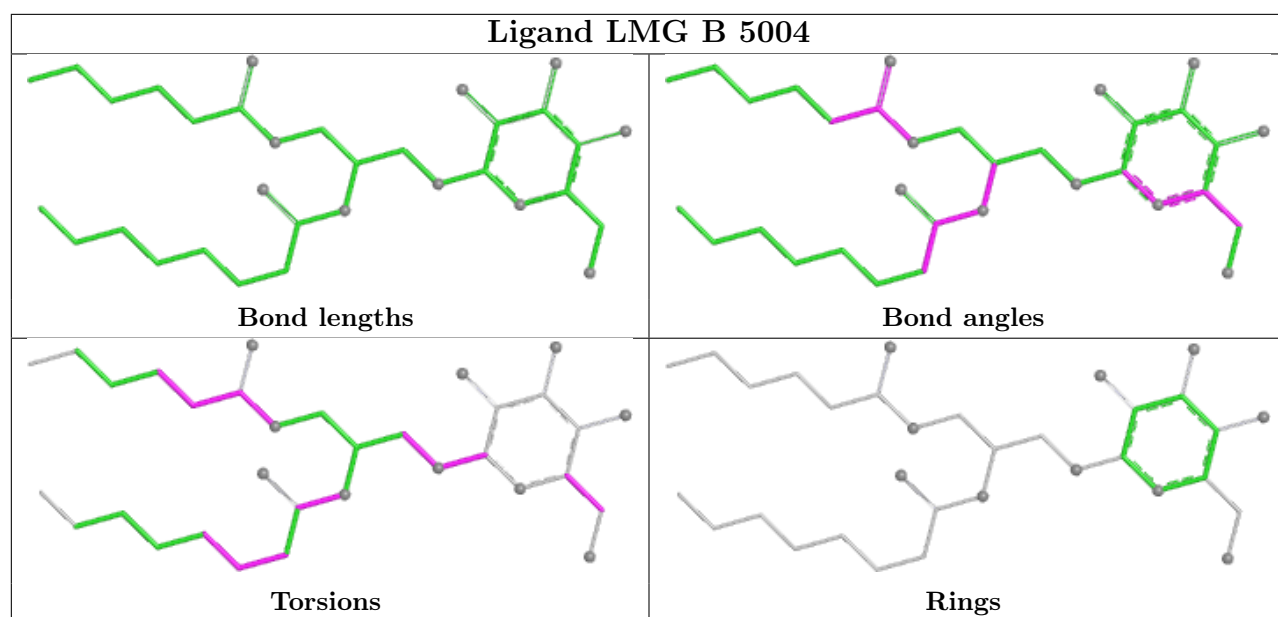
Torsions

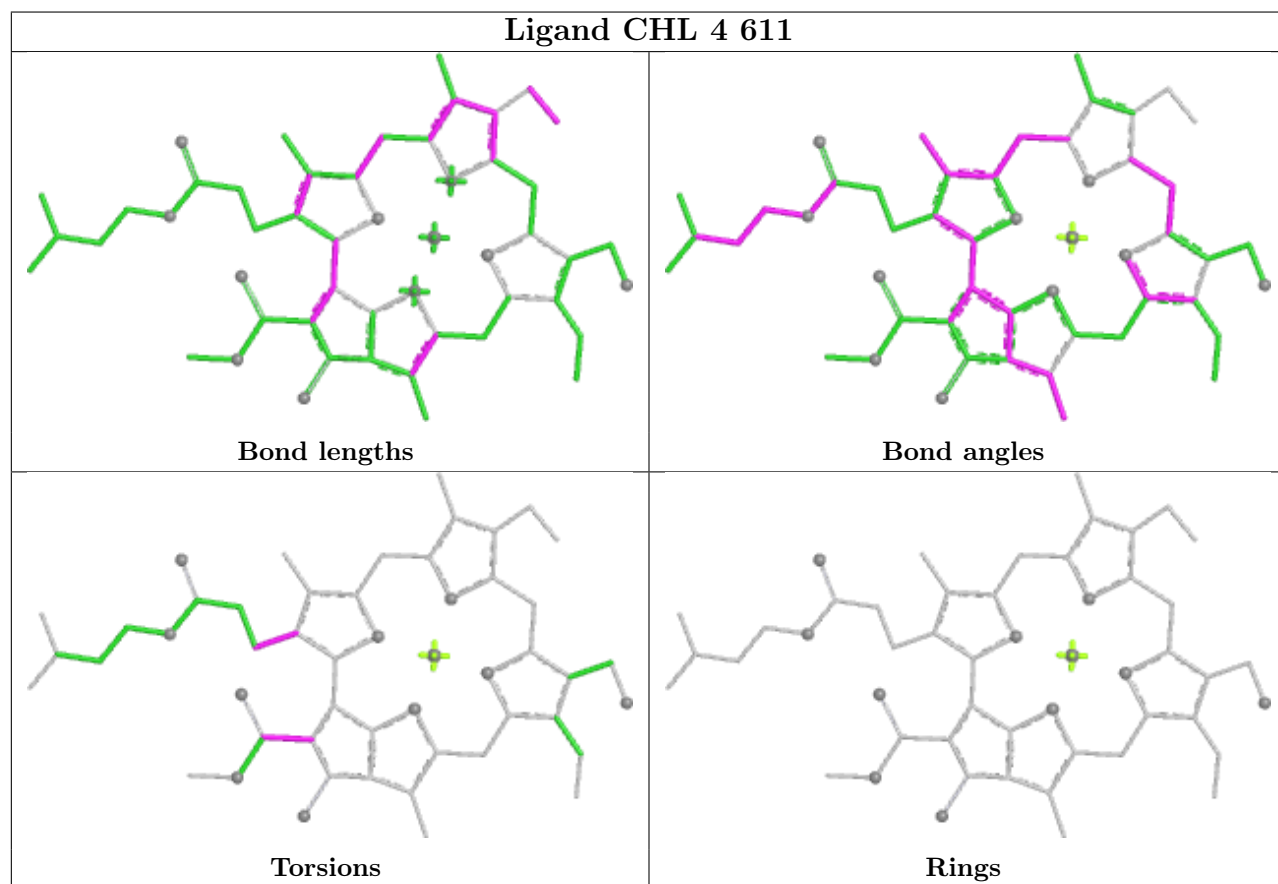
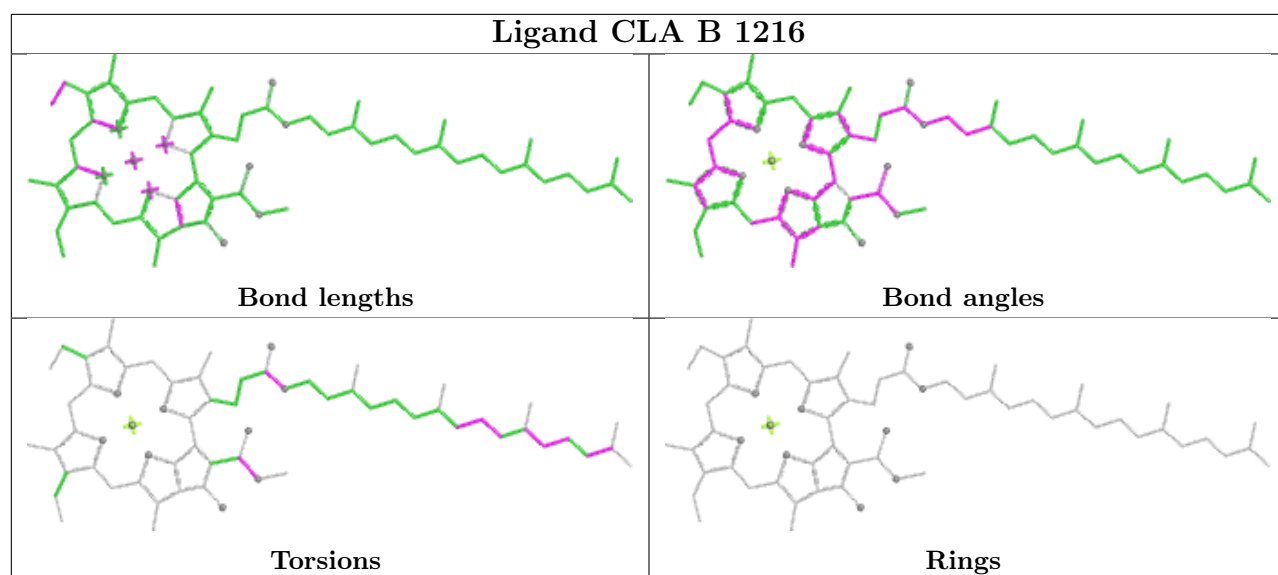


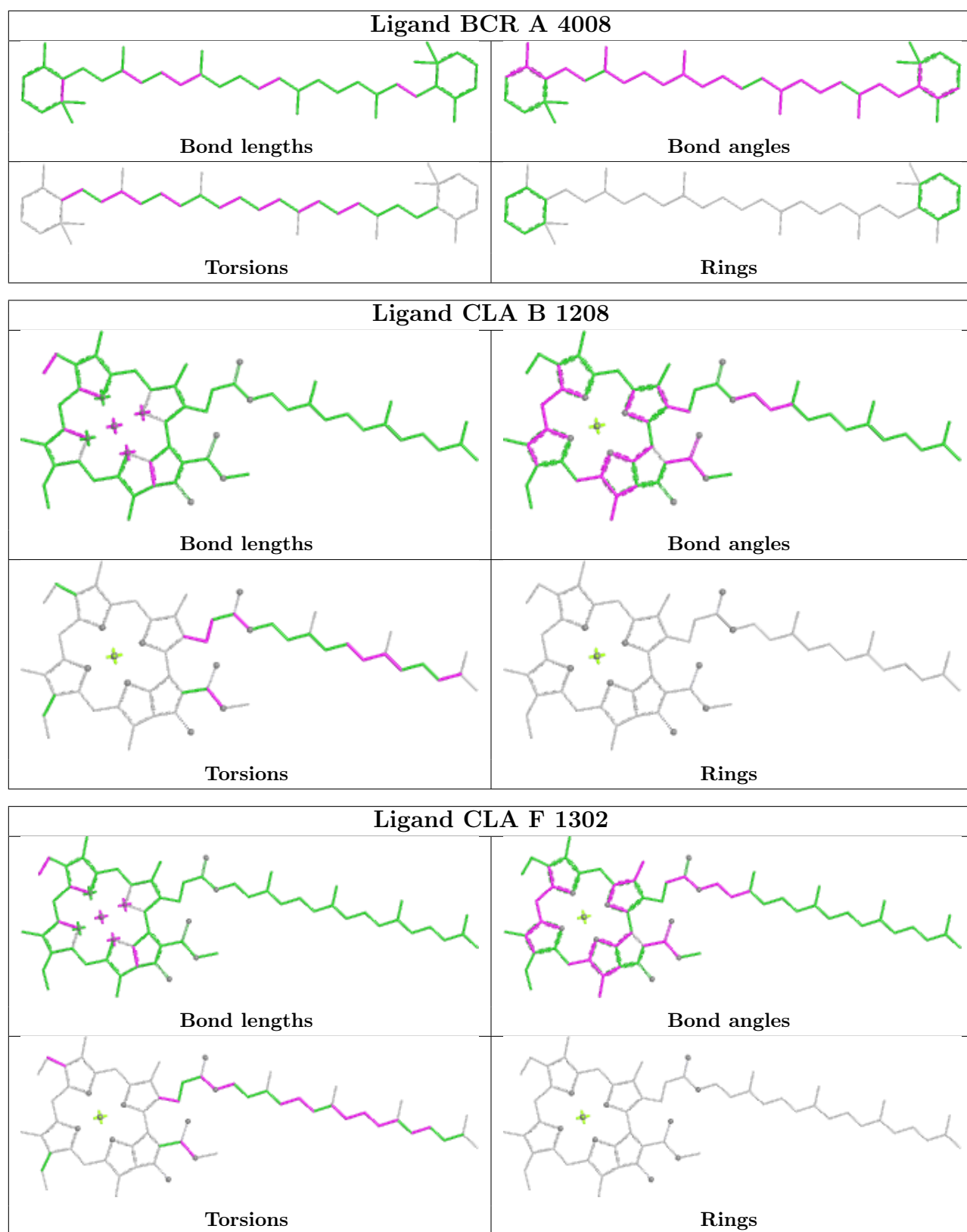
Rings

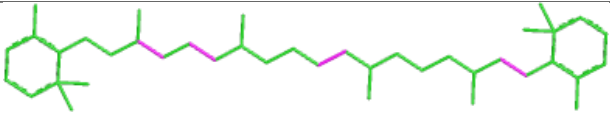
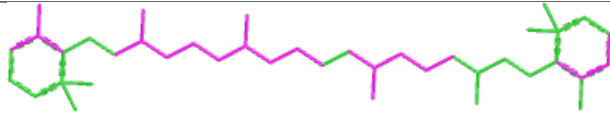
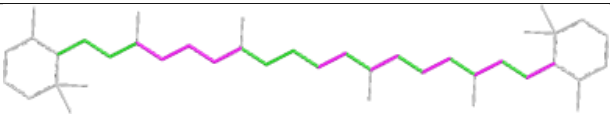
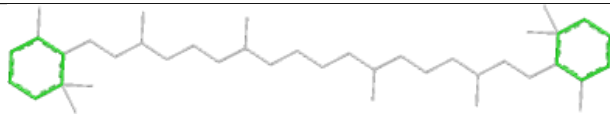
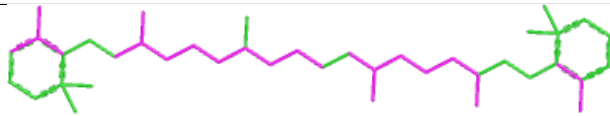
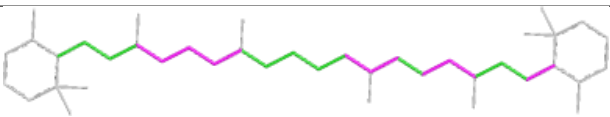
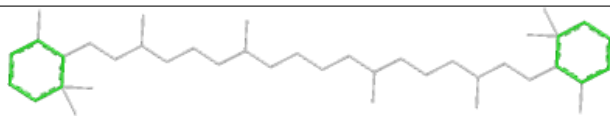
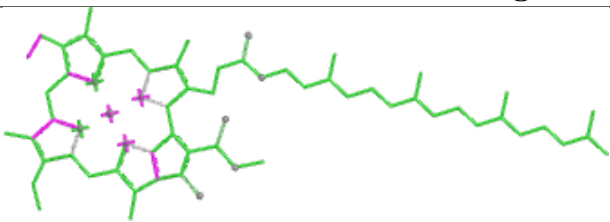
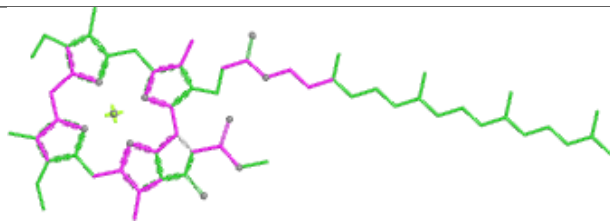
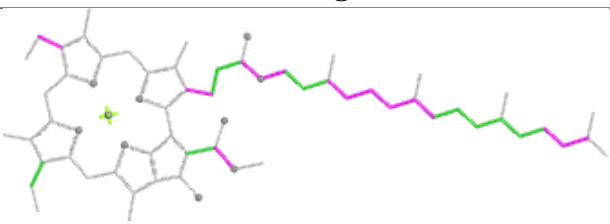
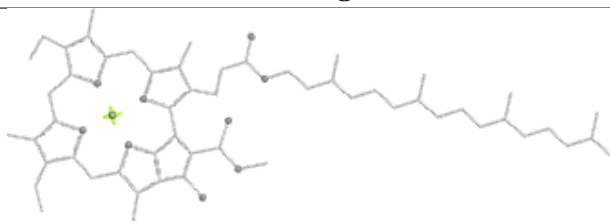


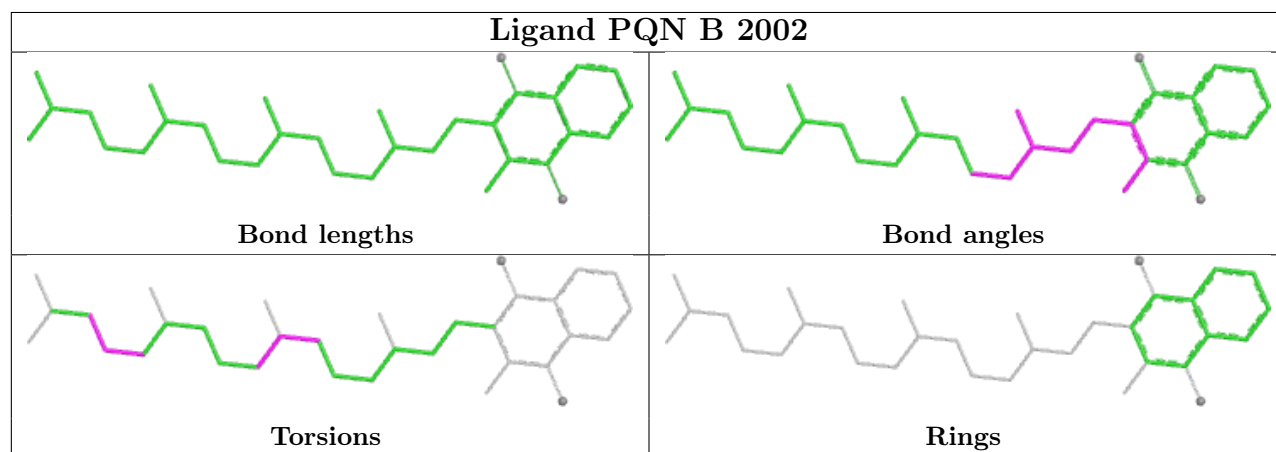
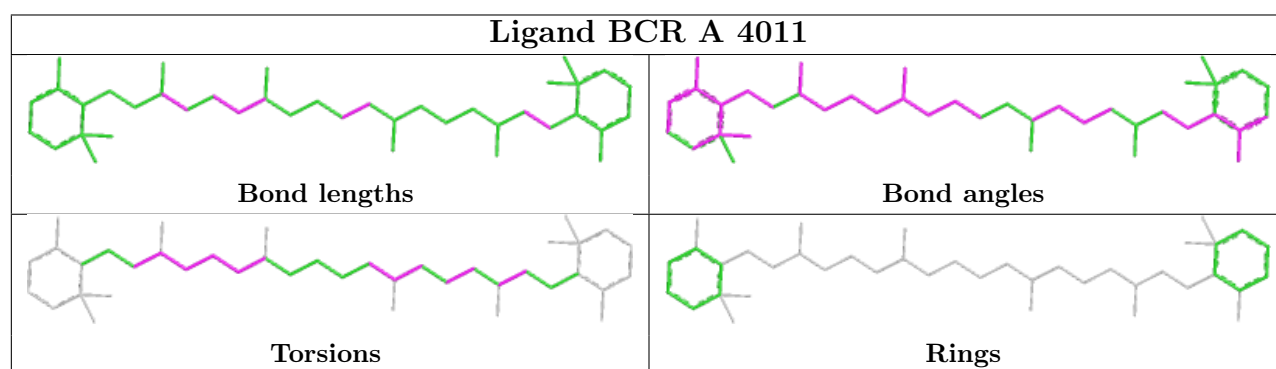
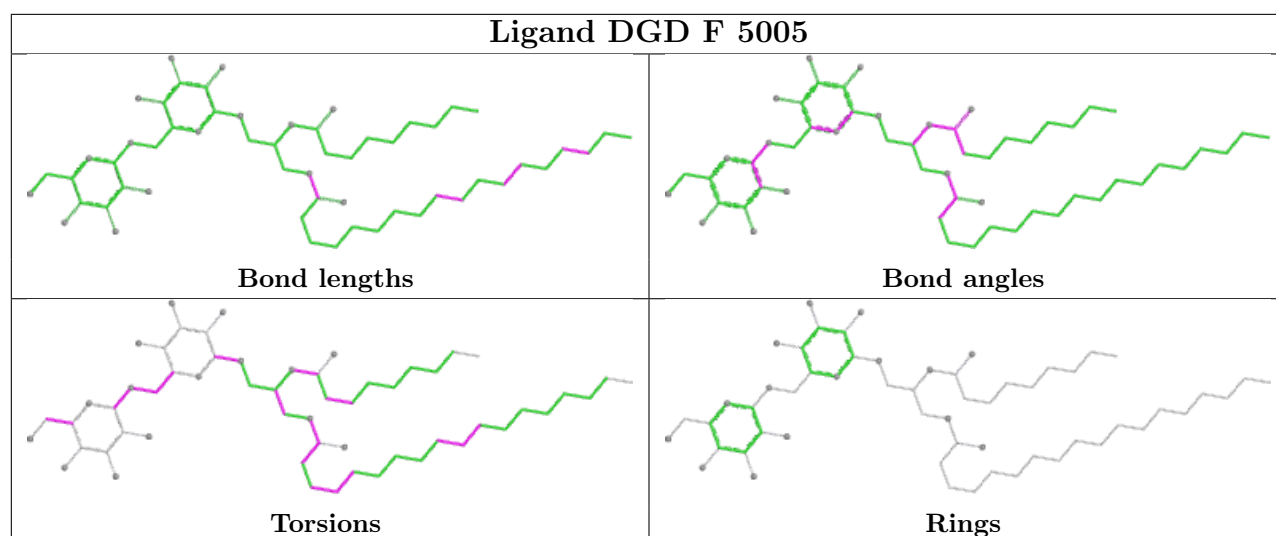


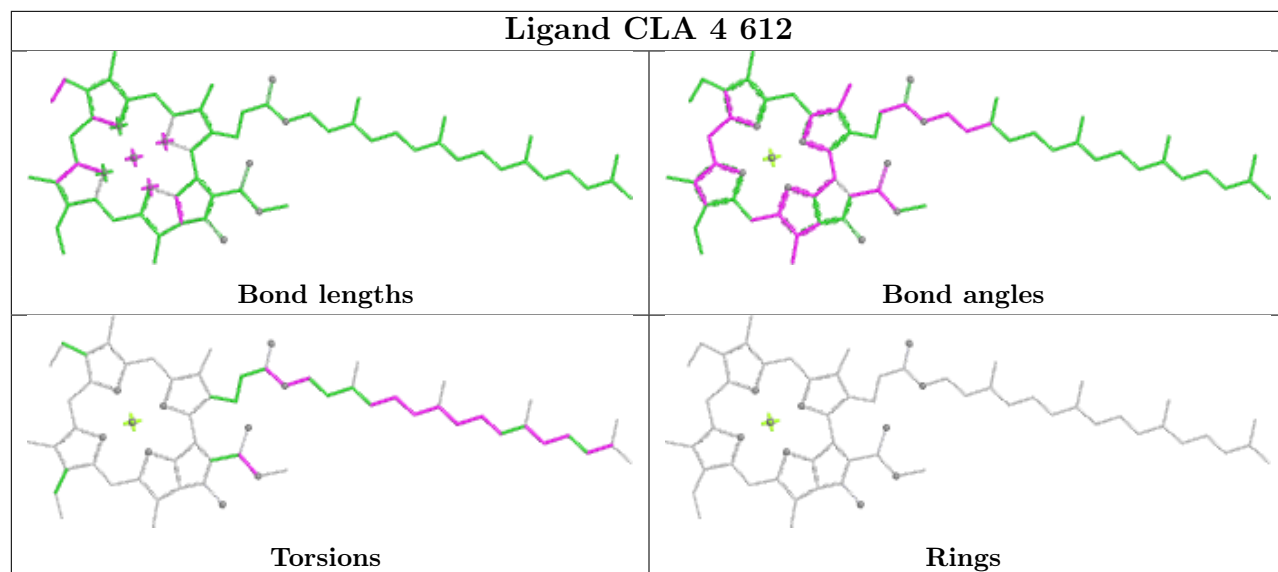
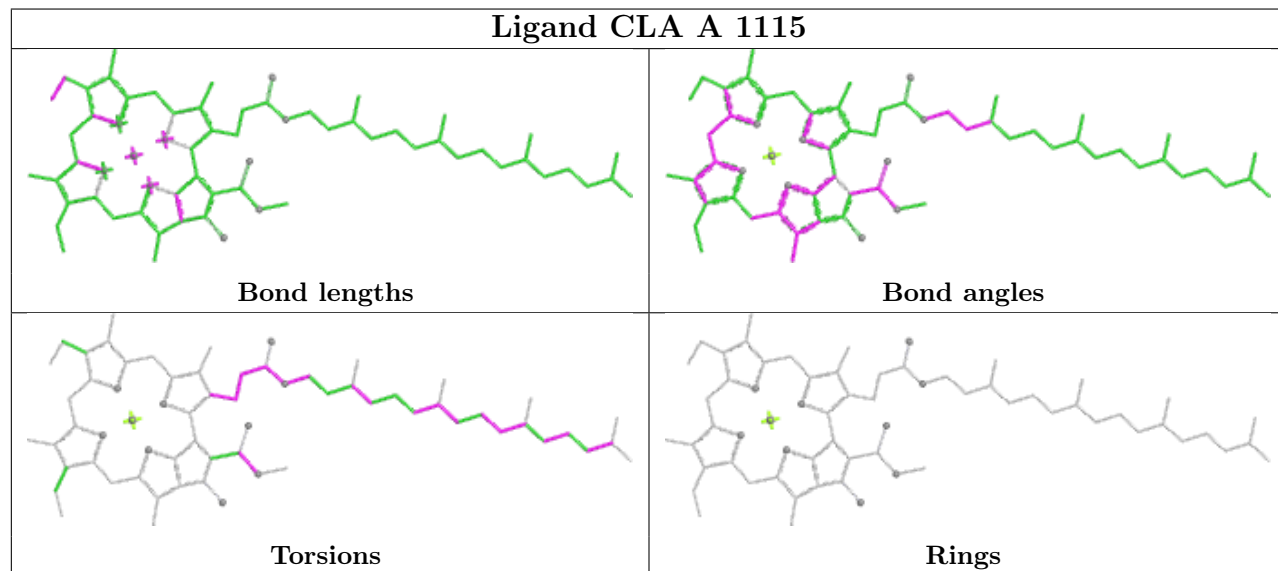


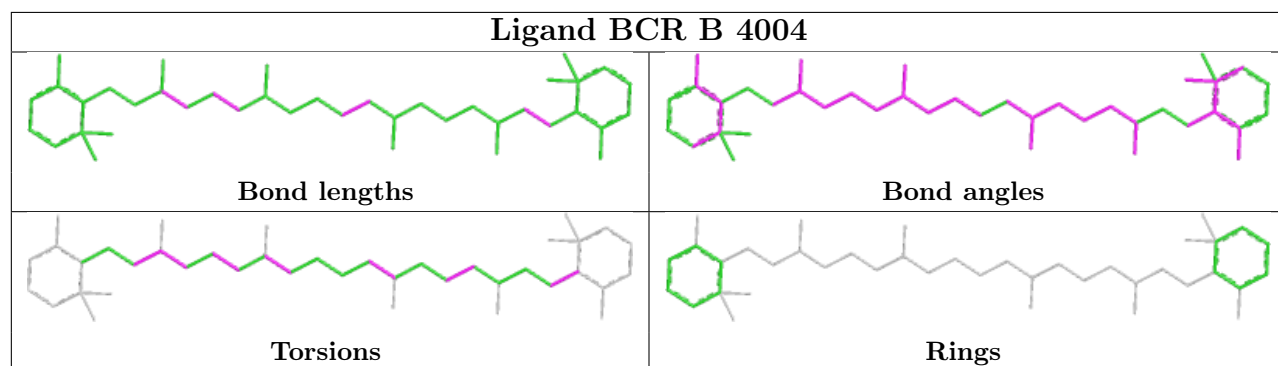
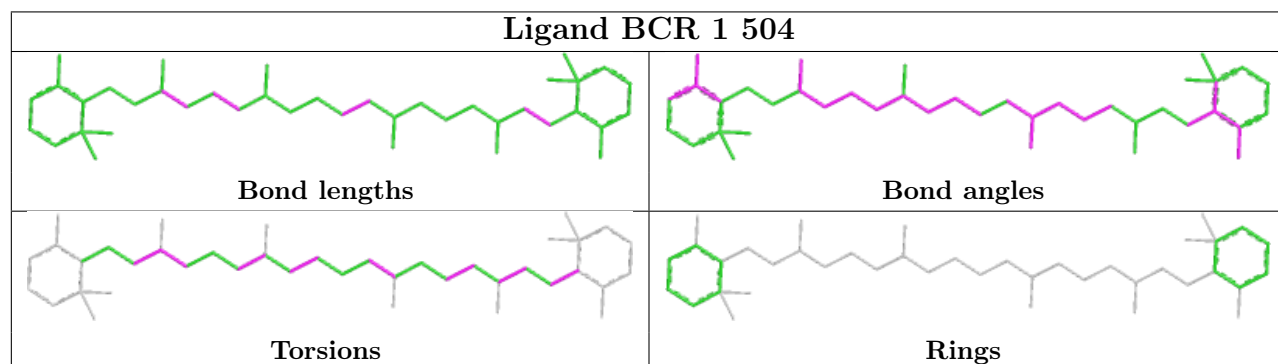
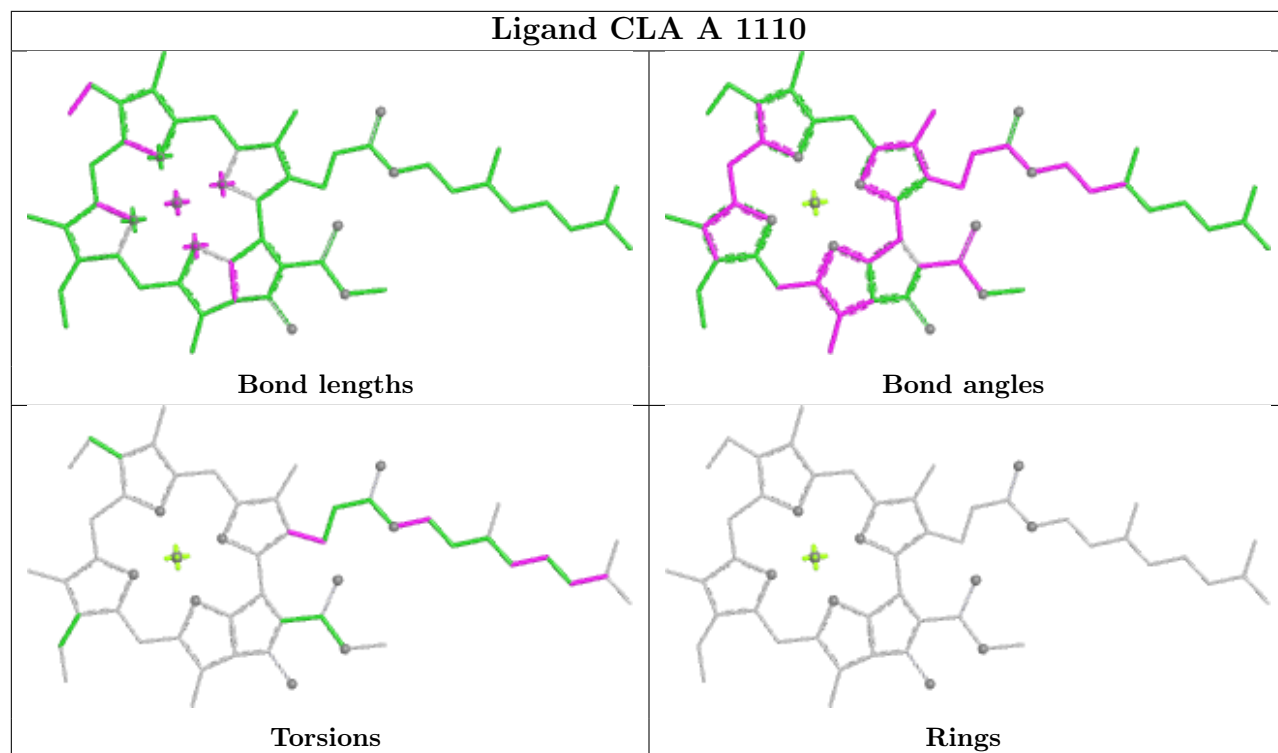


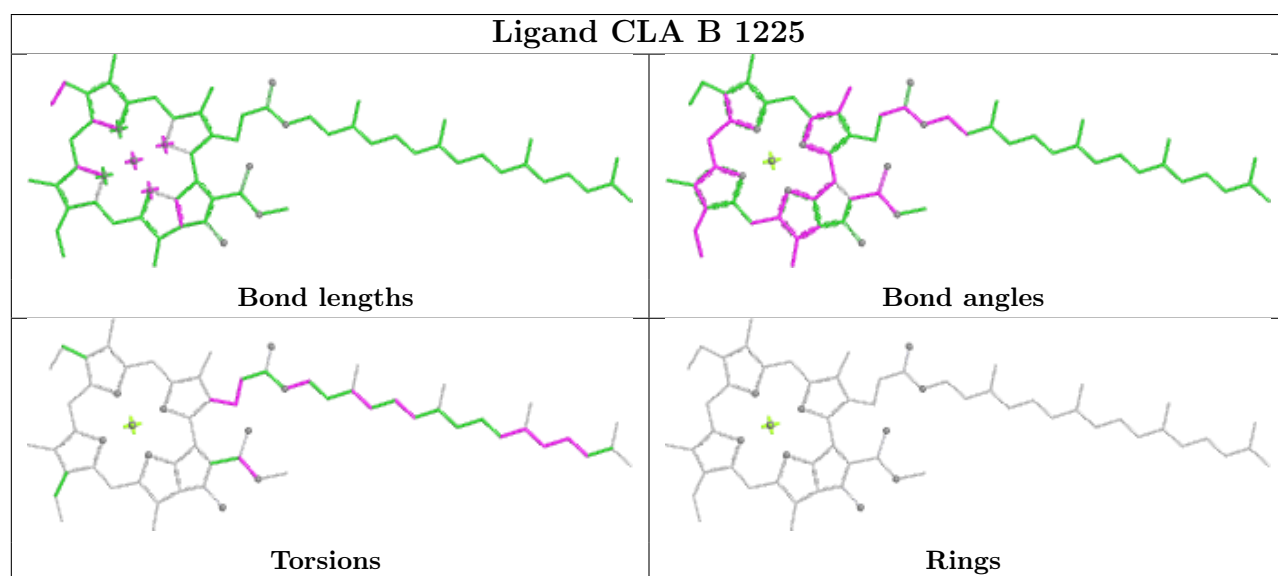
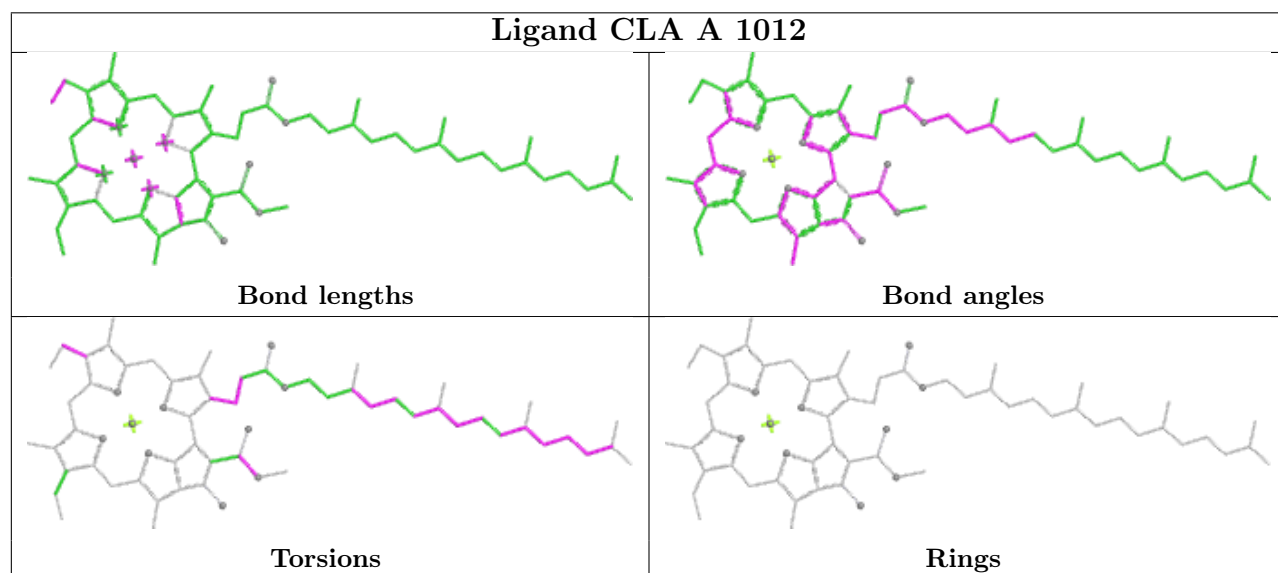
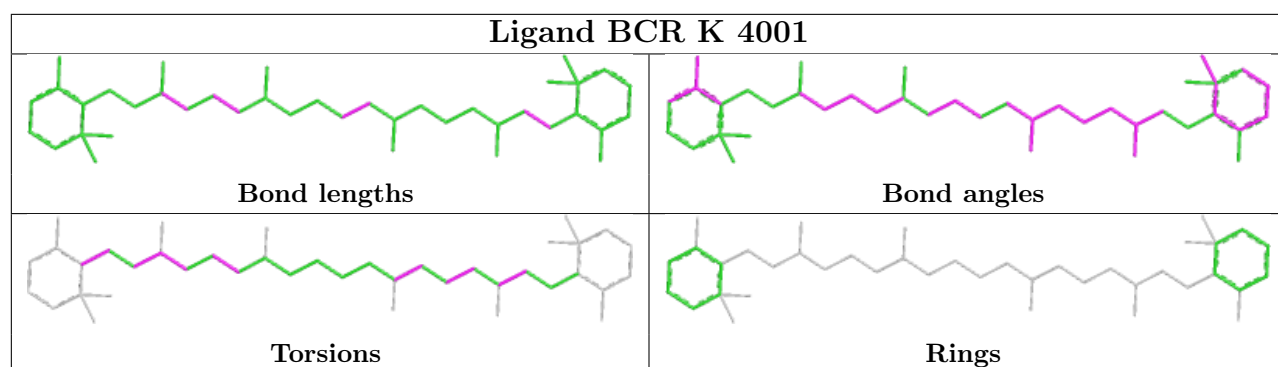


Ligand BCR L 4019	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR I 4020	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand CLA 2 604	
 Bond lengths	 Bond angles
 Torsions	 Rings

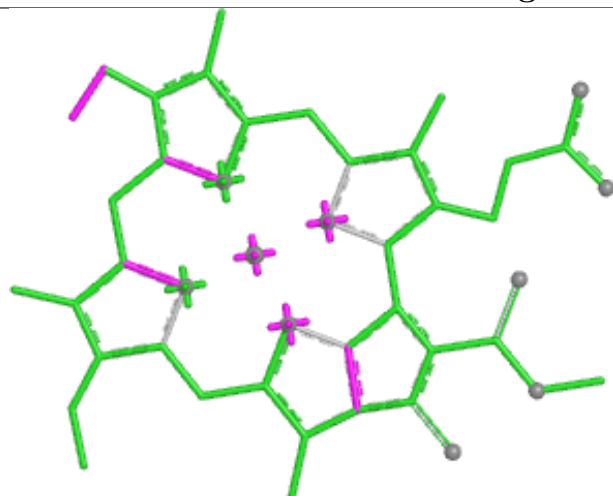


Ligand CLA 4 612**Ligand CLA A 1115**

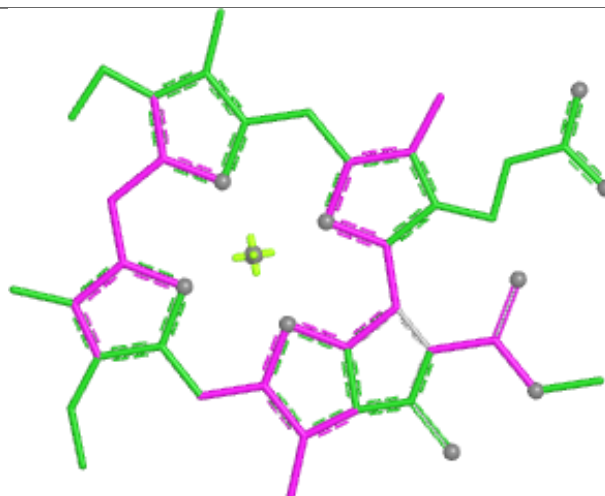




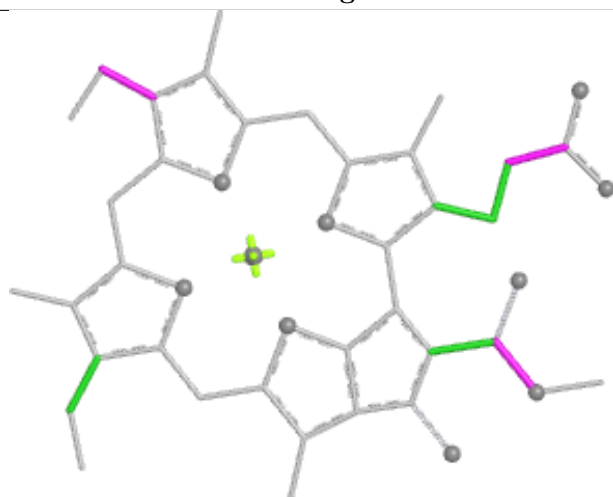
Ligand CLA 1 613



Bond lengths



Bond angles

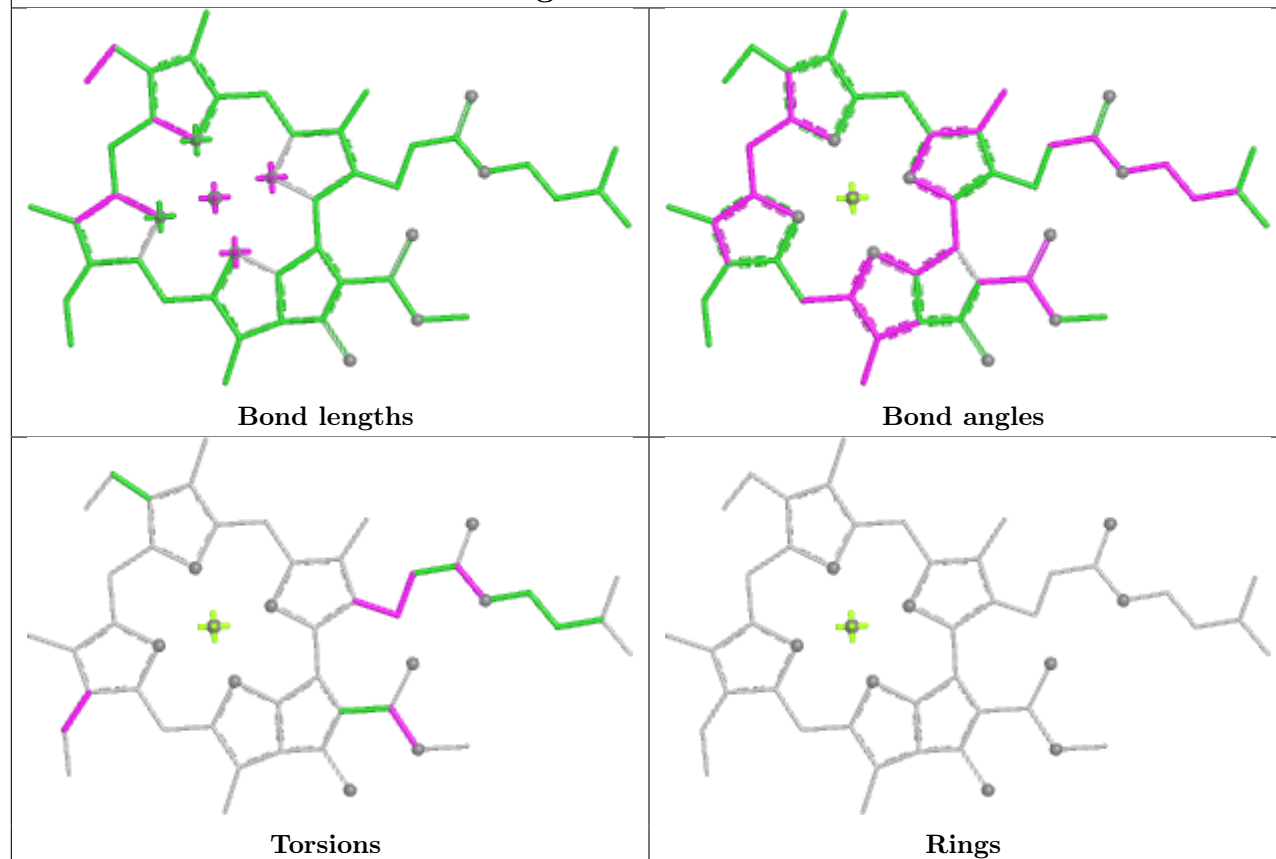


Torsions

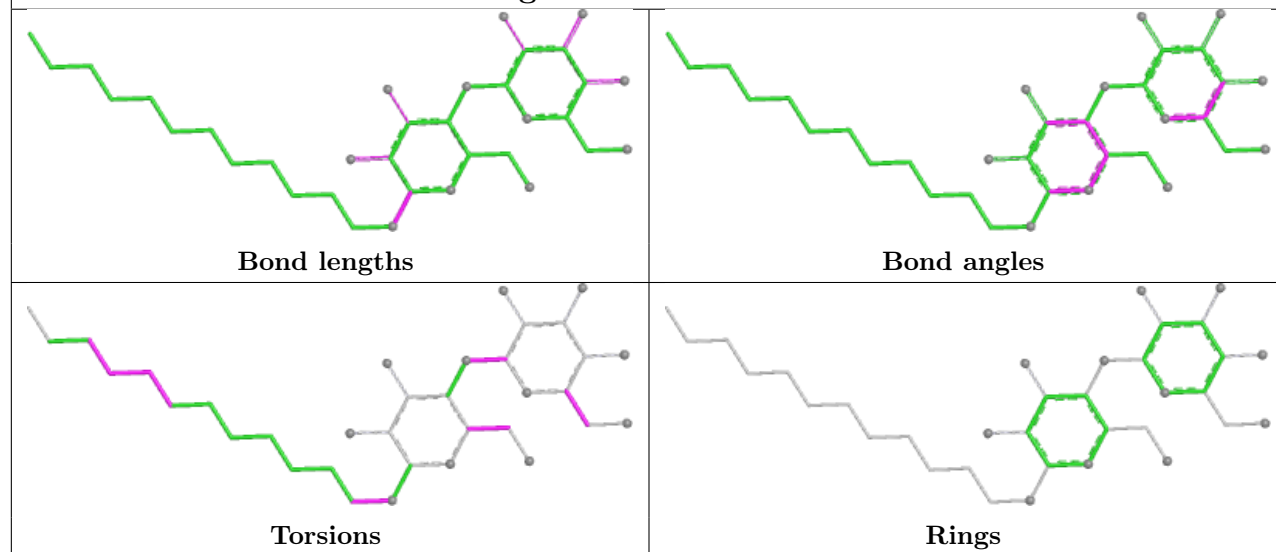


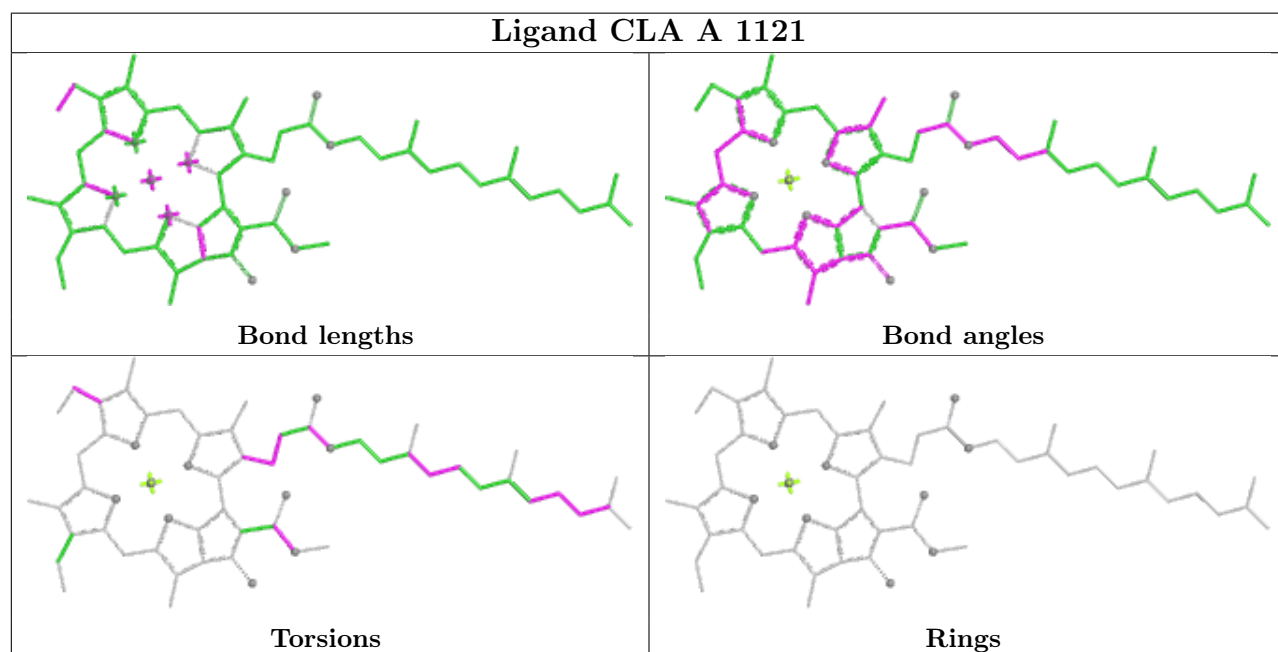
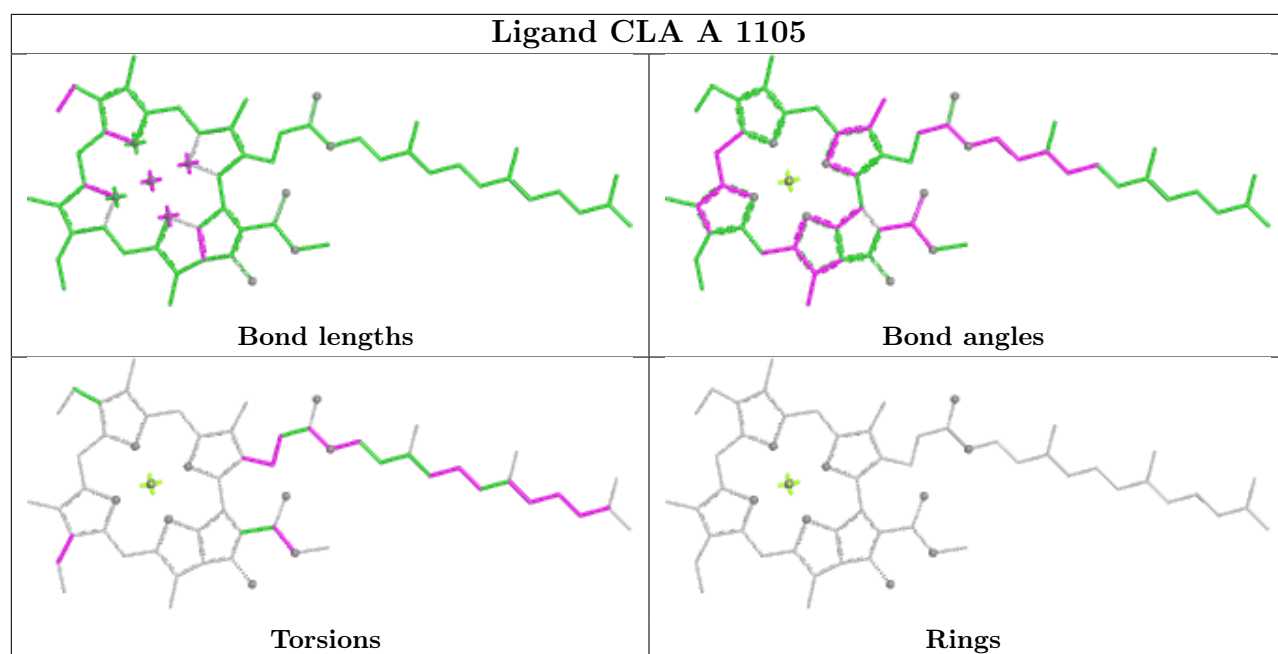
Rings

Ligand CLA 2 606

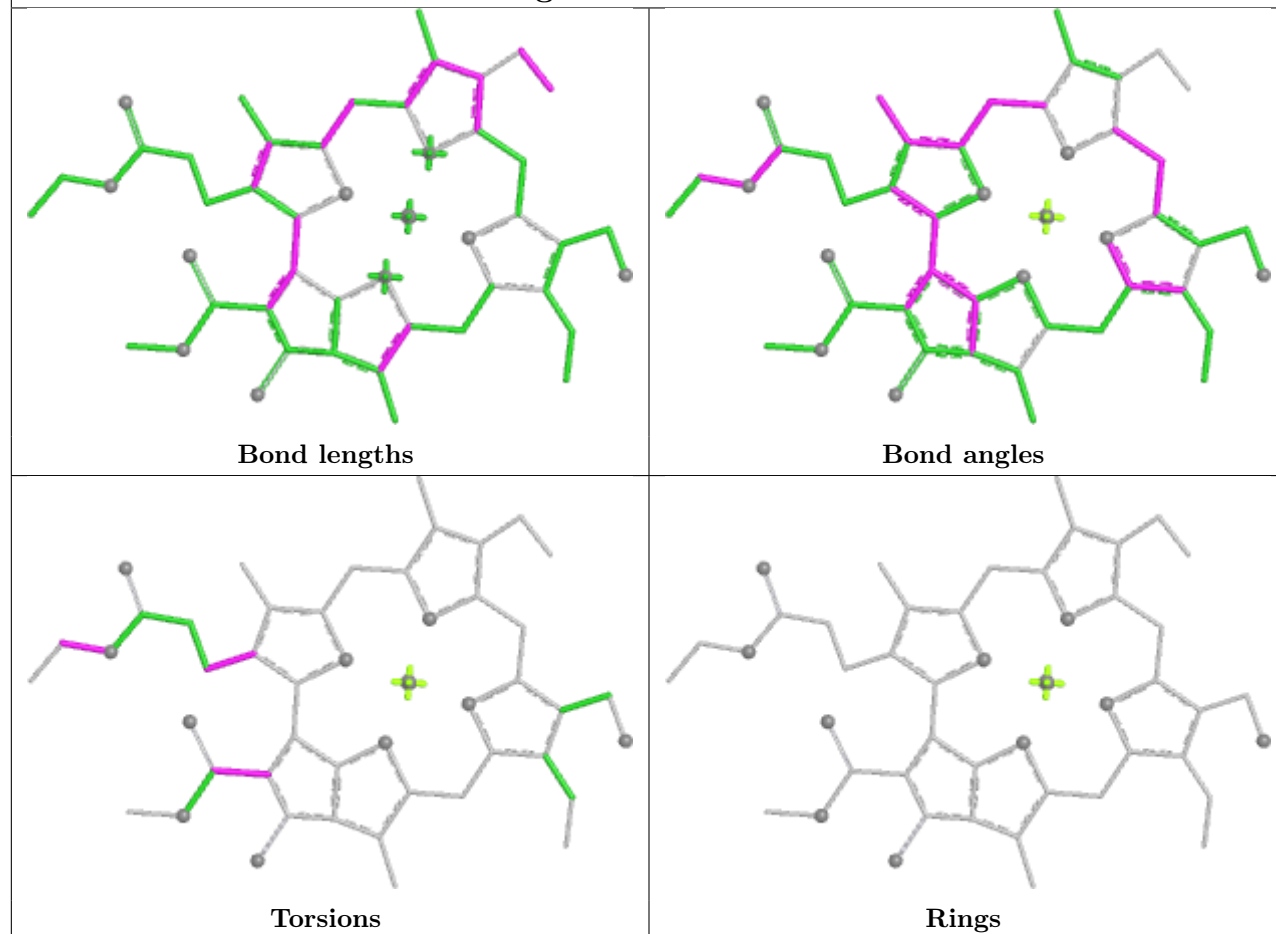


Ligand LMT G 5004

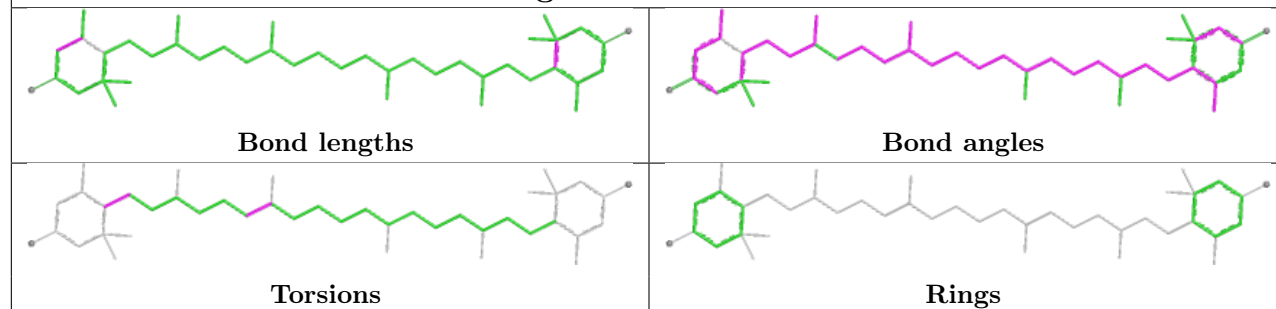




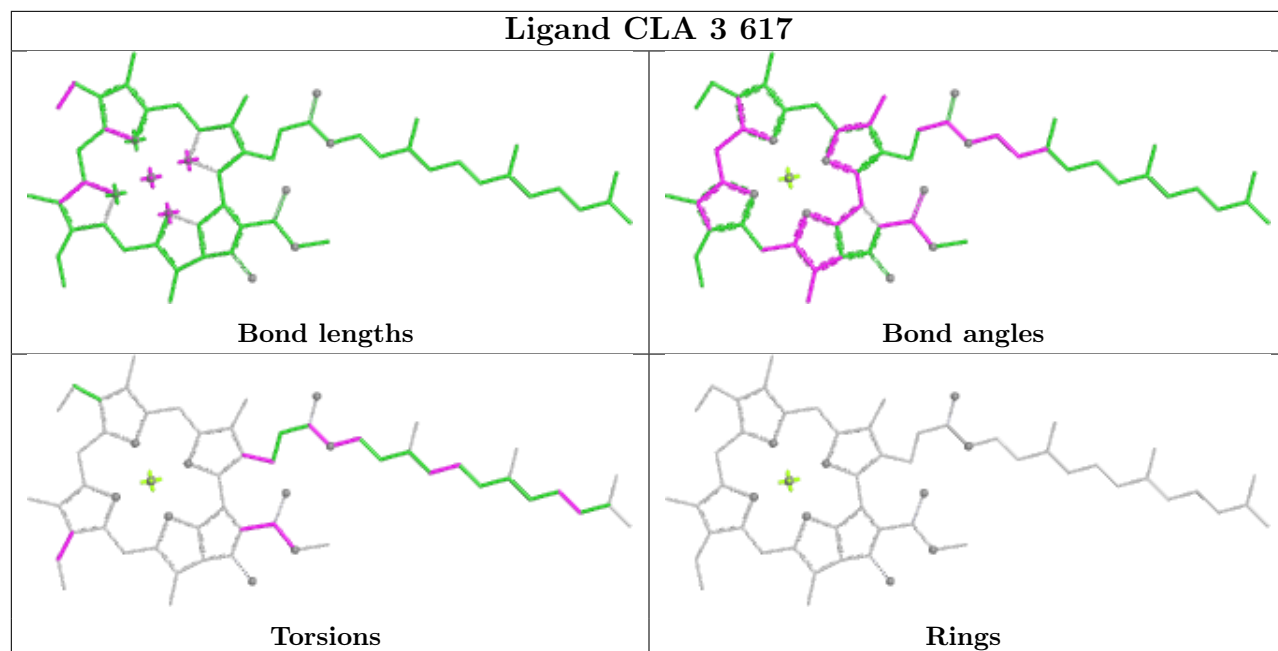
Ligand CHL 2 611



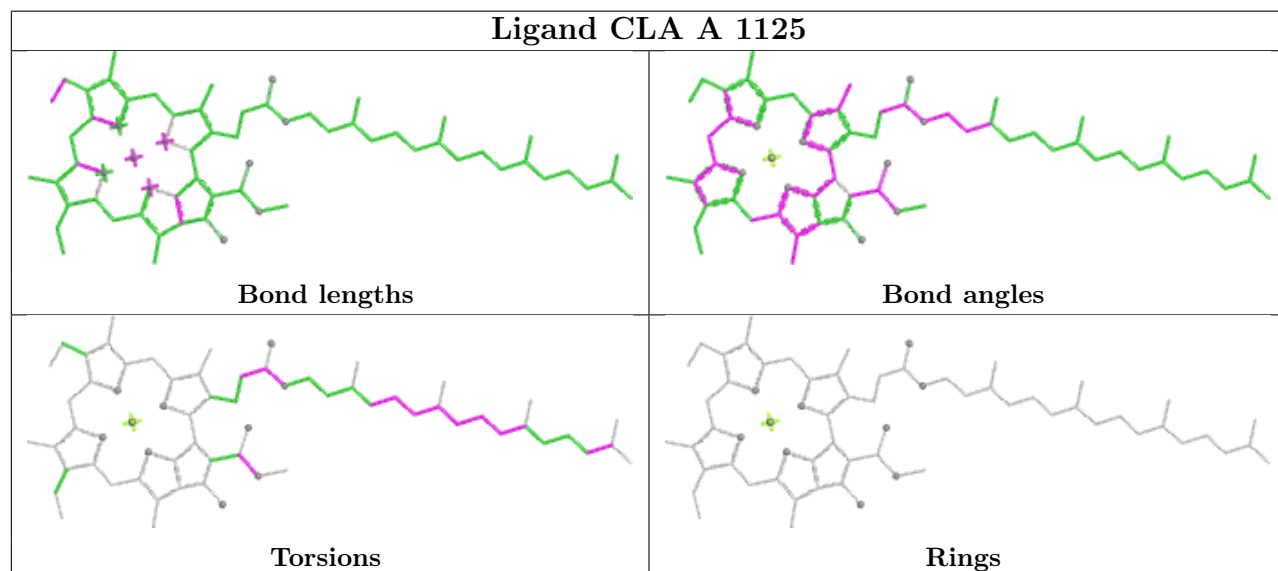
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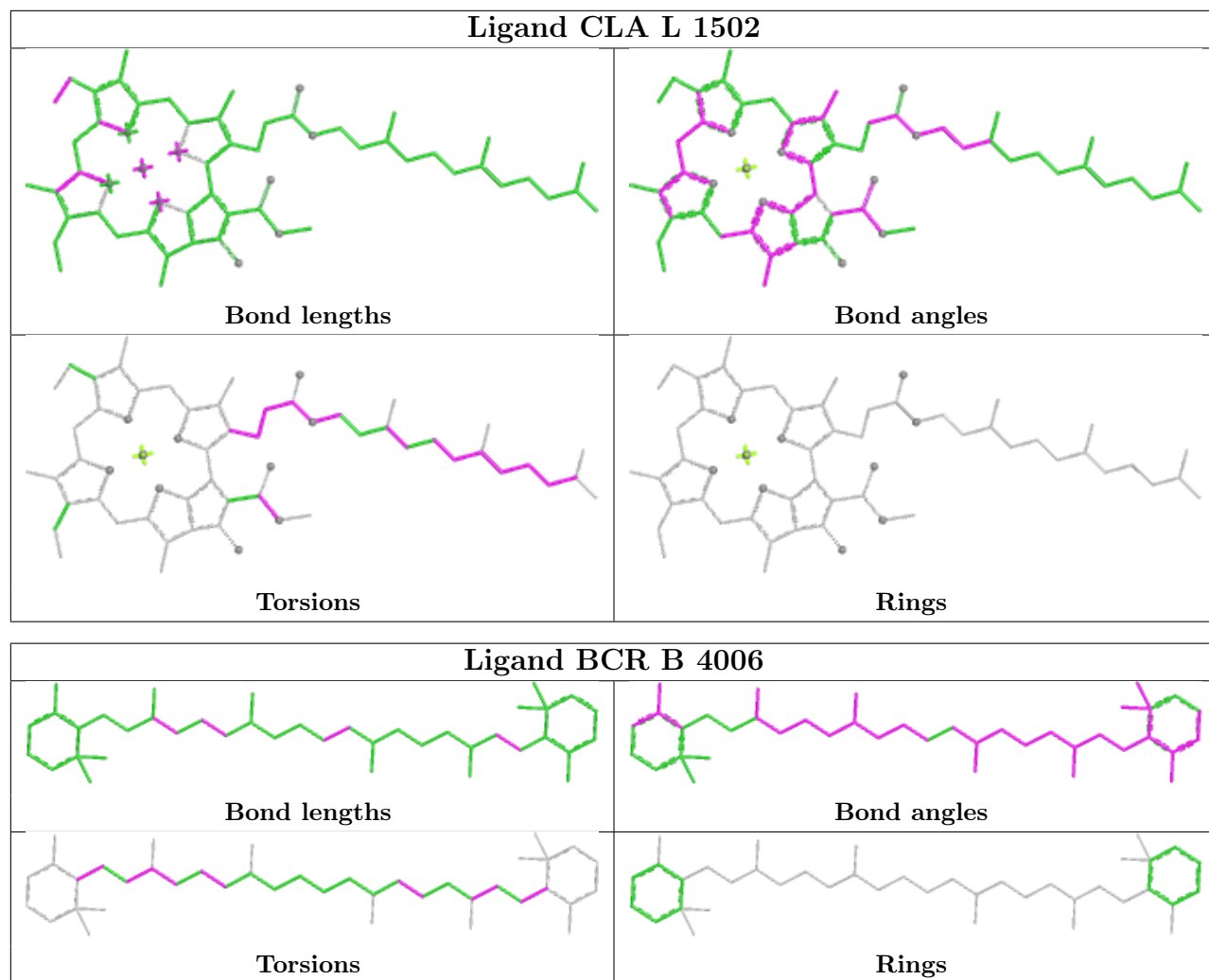


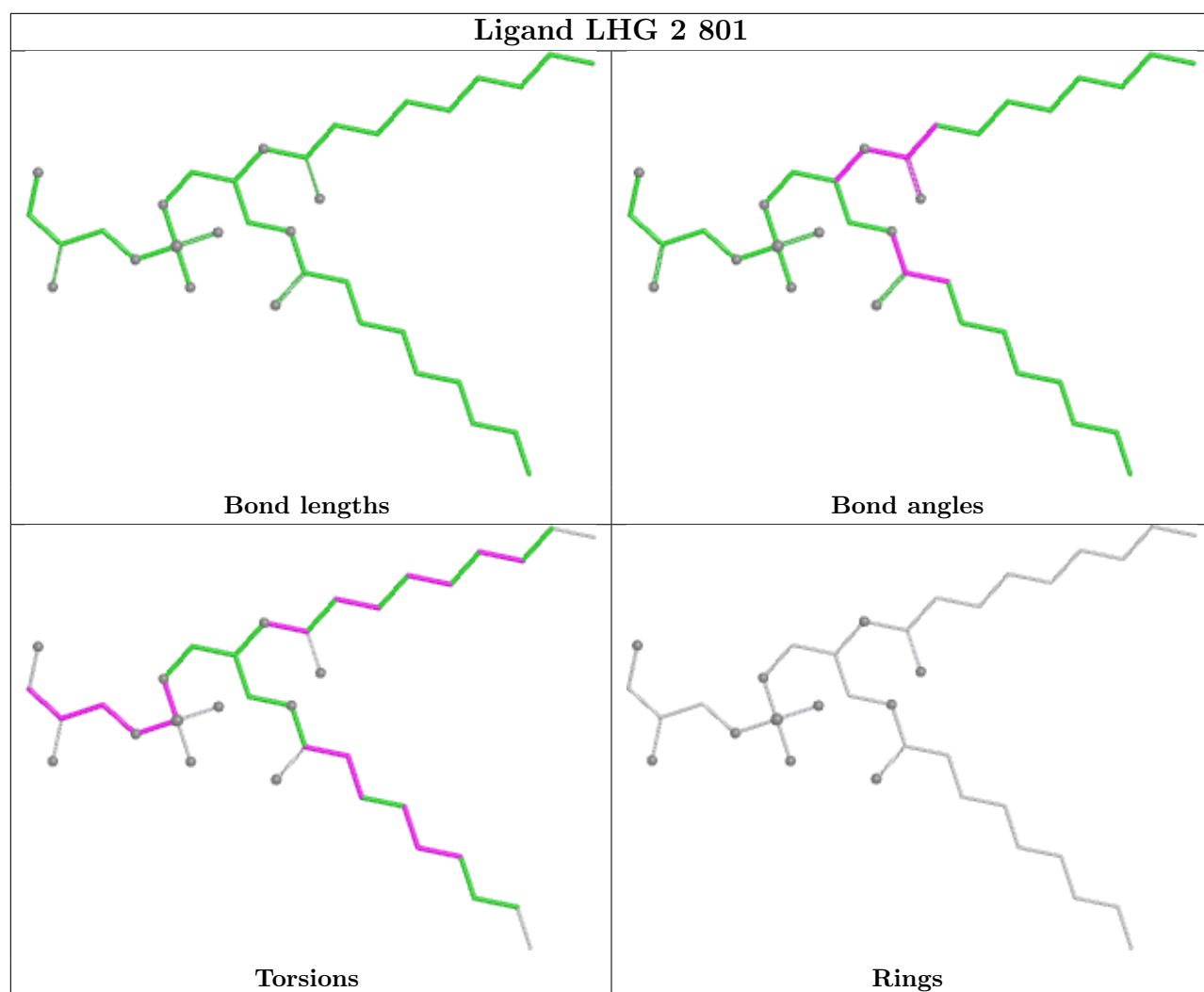
Ligand CLA 3 617



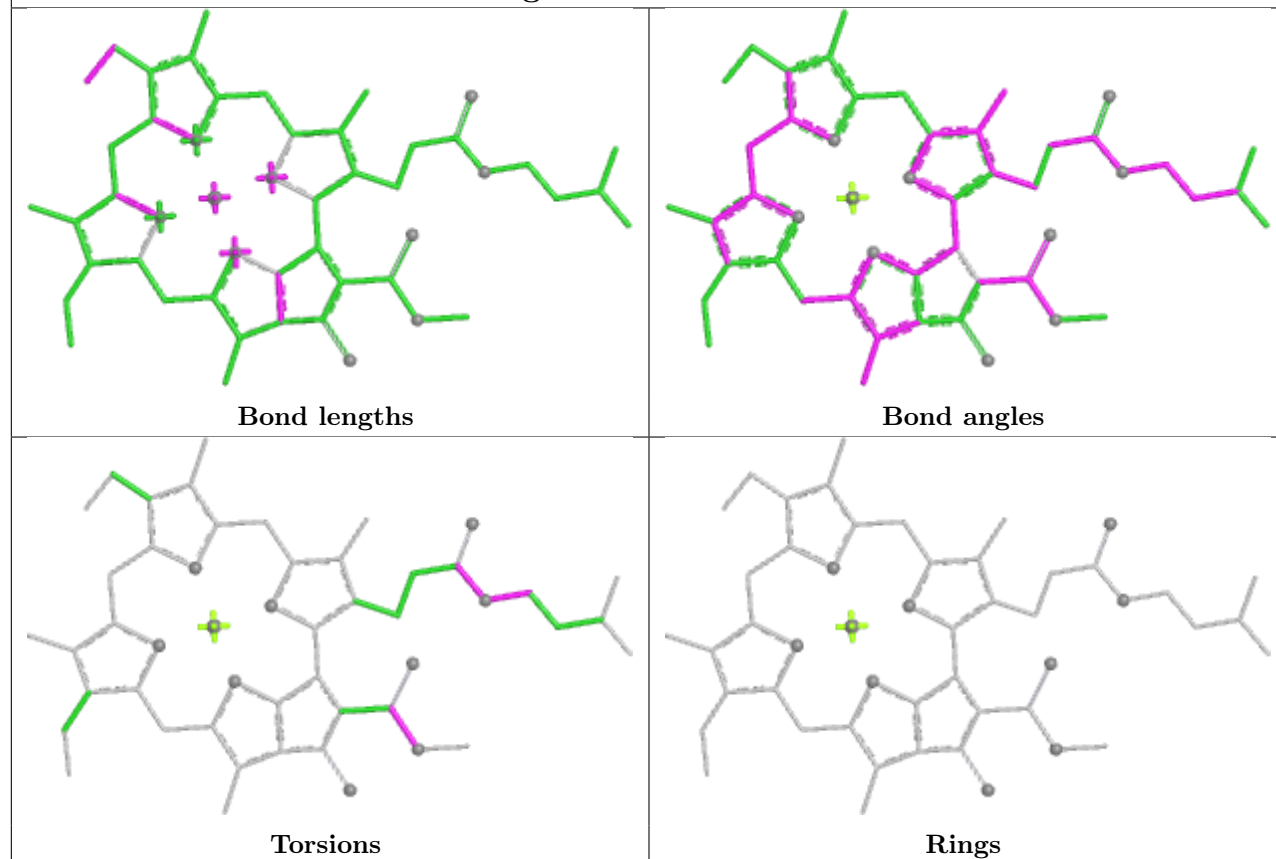
Ligand CLA A 1125



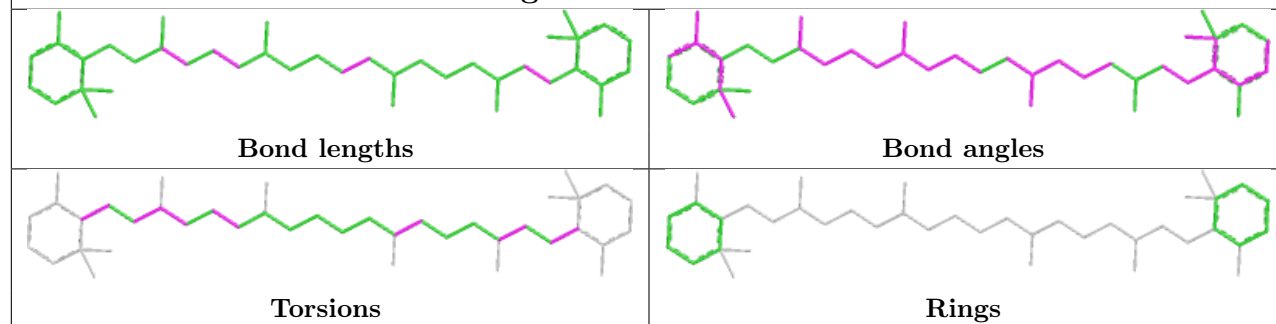


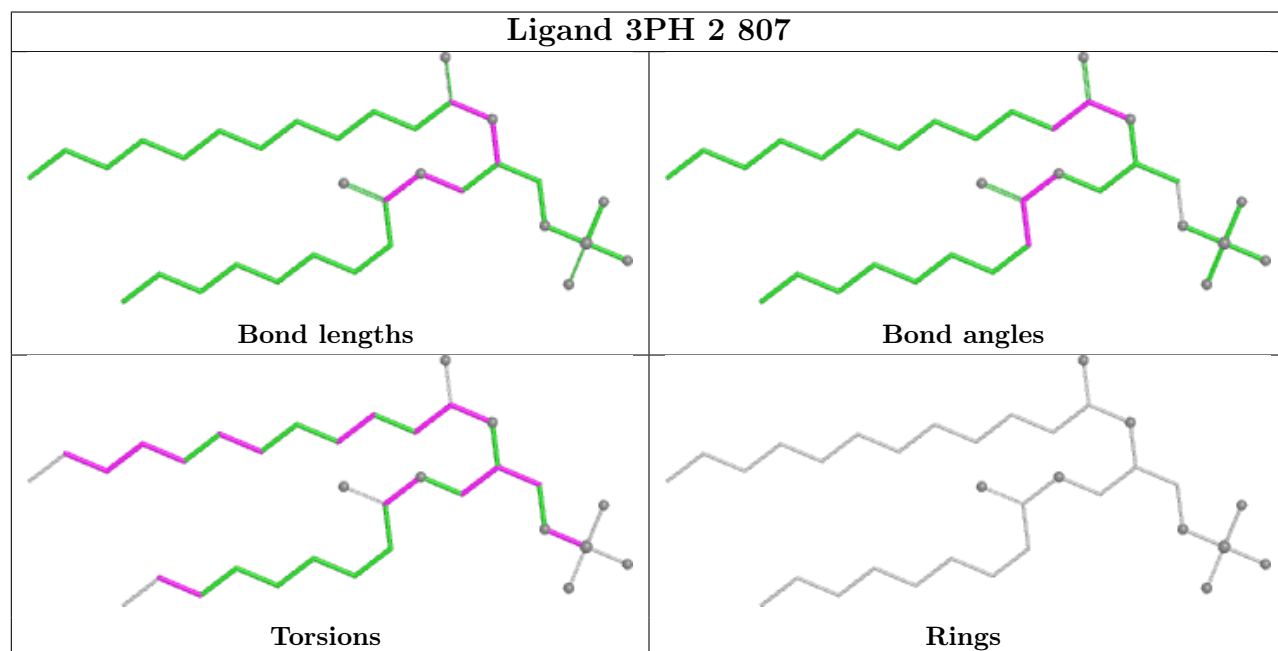
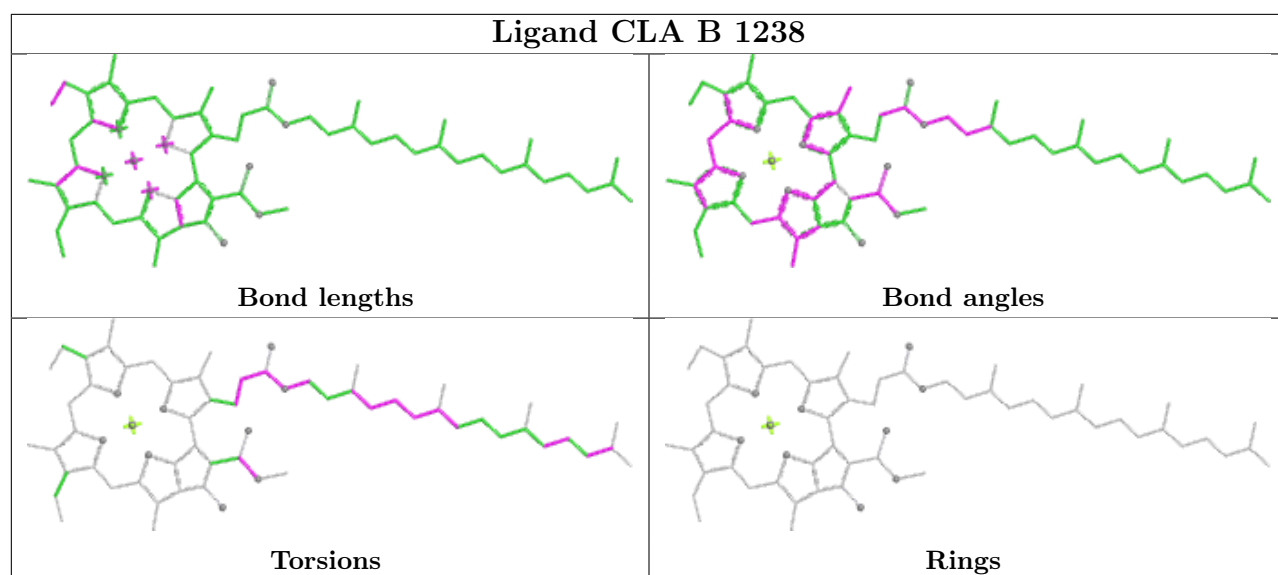


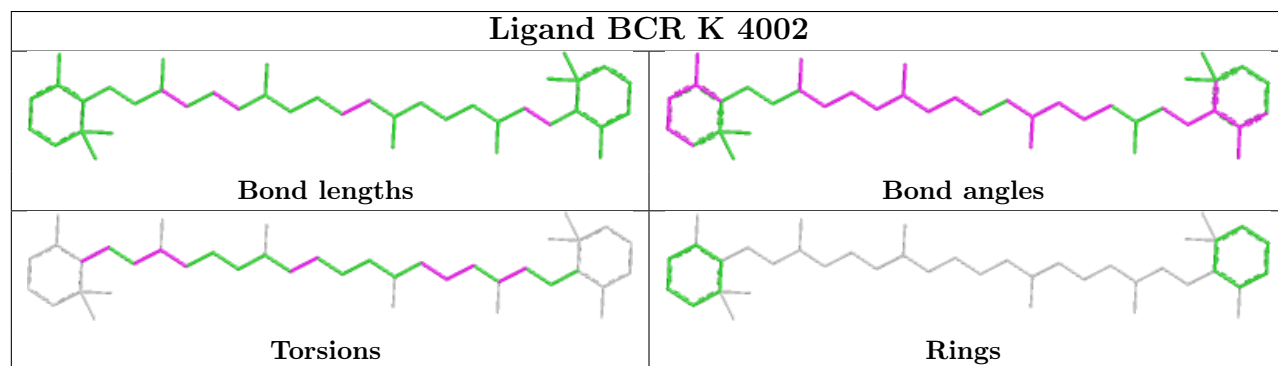
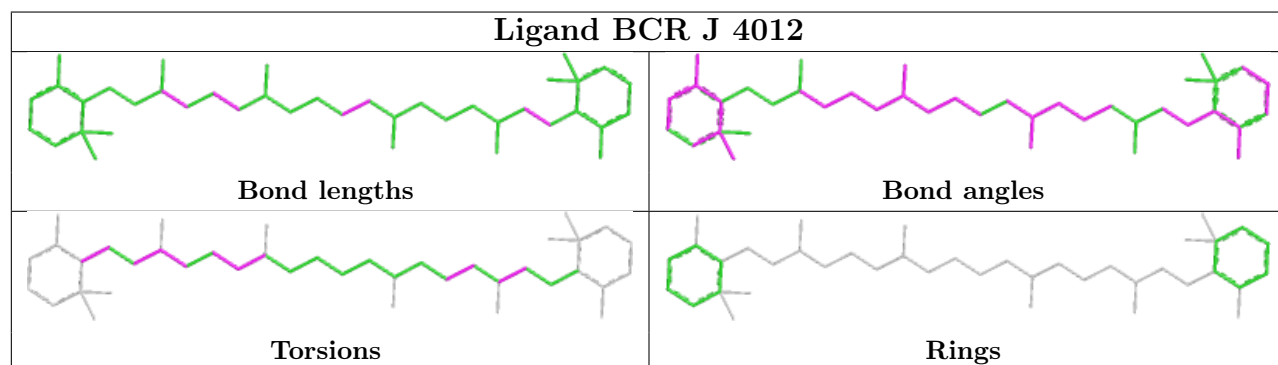
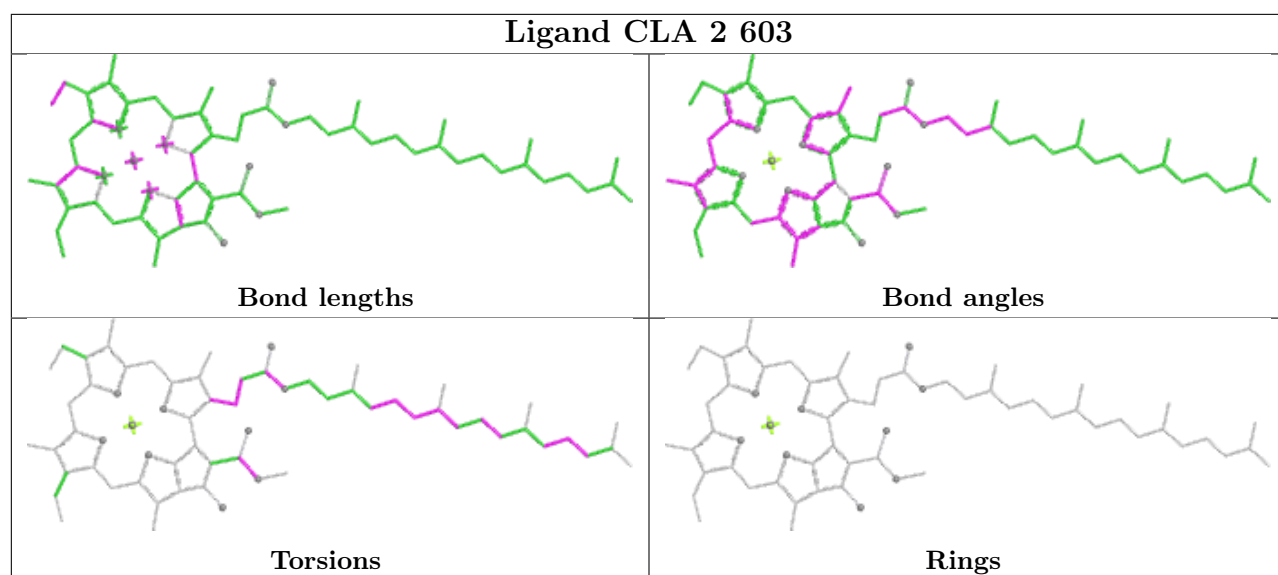
Ligand CLA A 1108

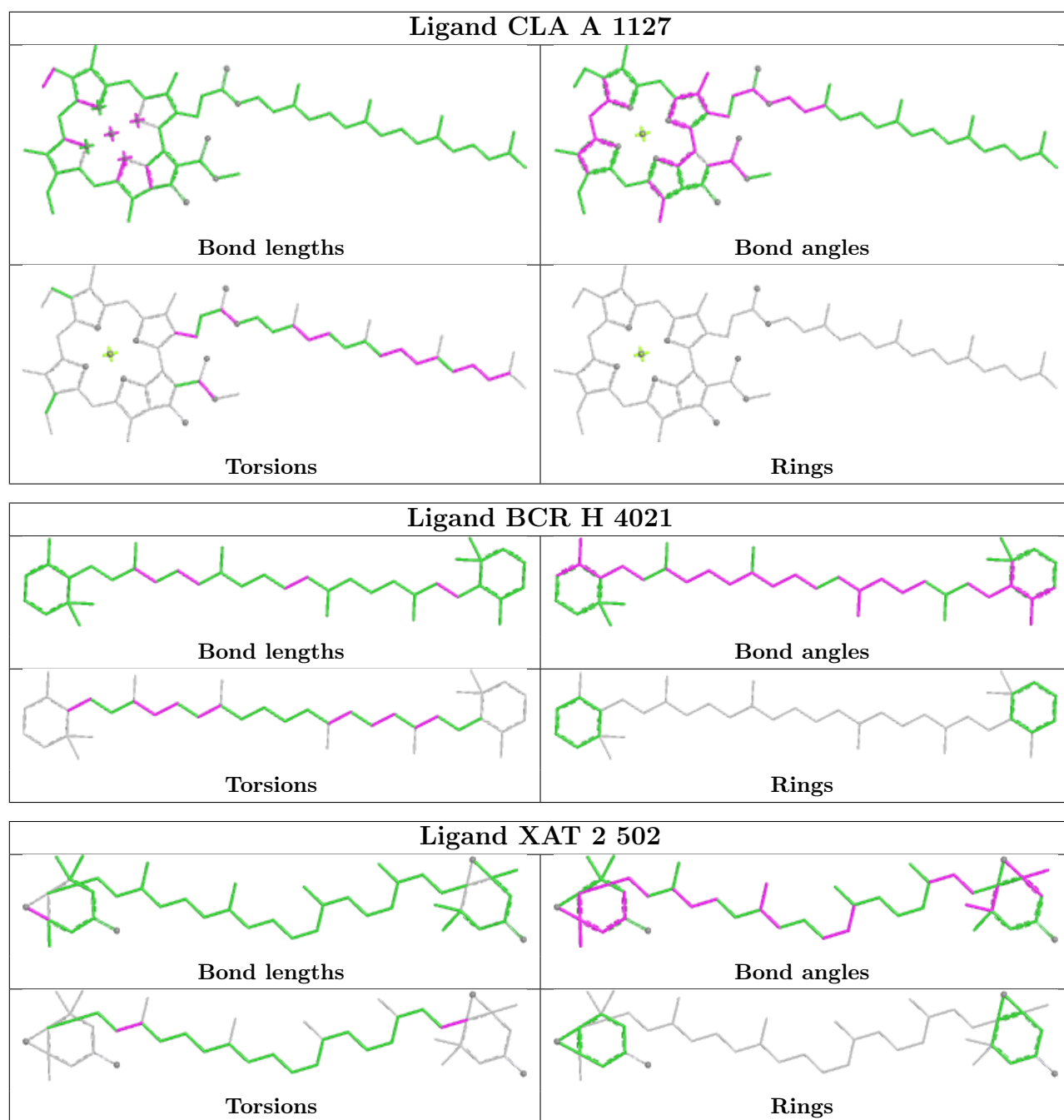


Ligand BCR A 4003

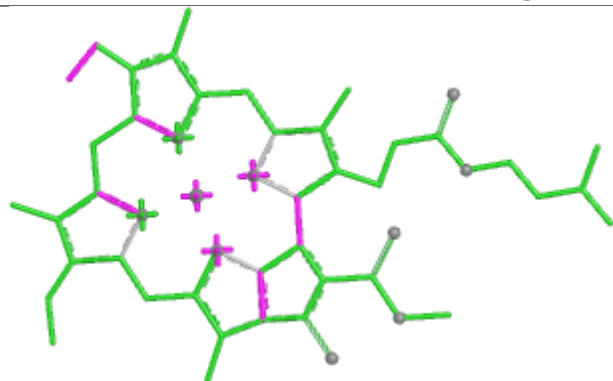




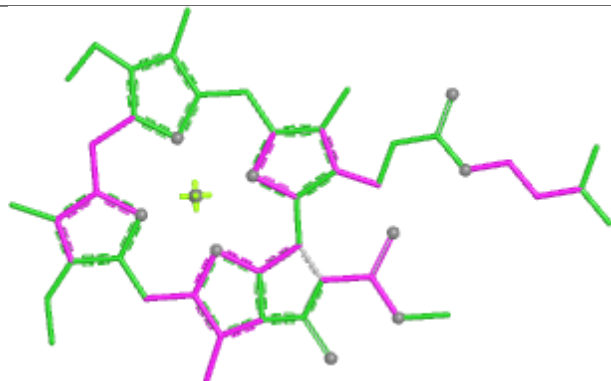




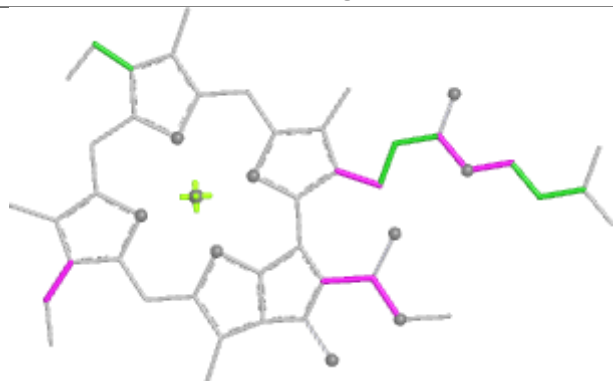
Ligand CLA 3 606



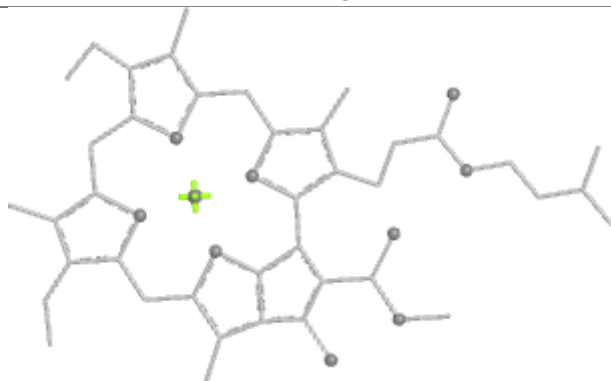
Bond lengths



Bond angles

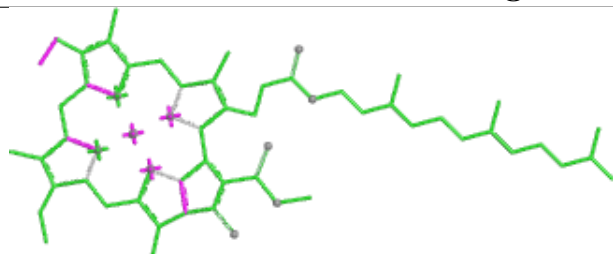


Torsions

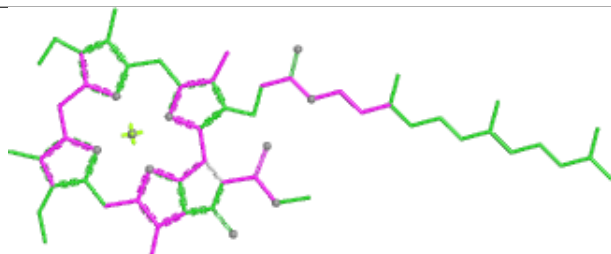


Rings

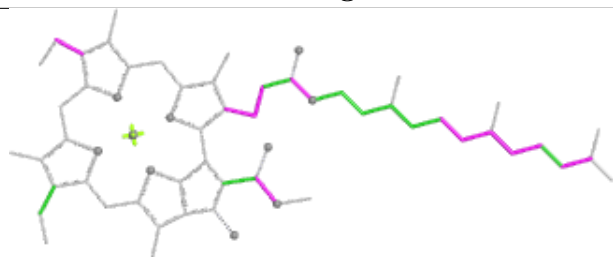
Ligand CLA A 1141



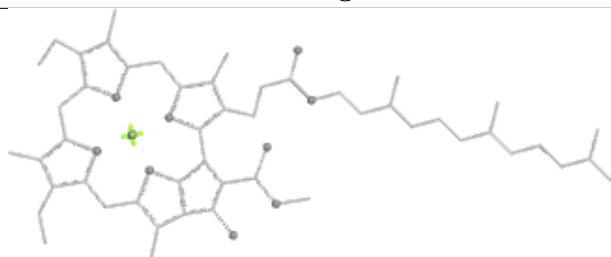
Bond lengths



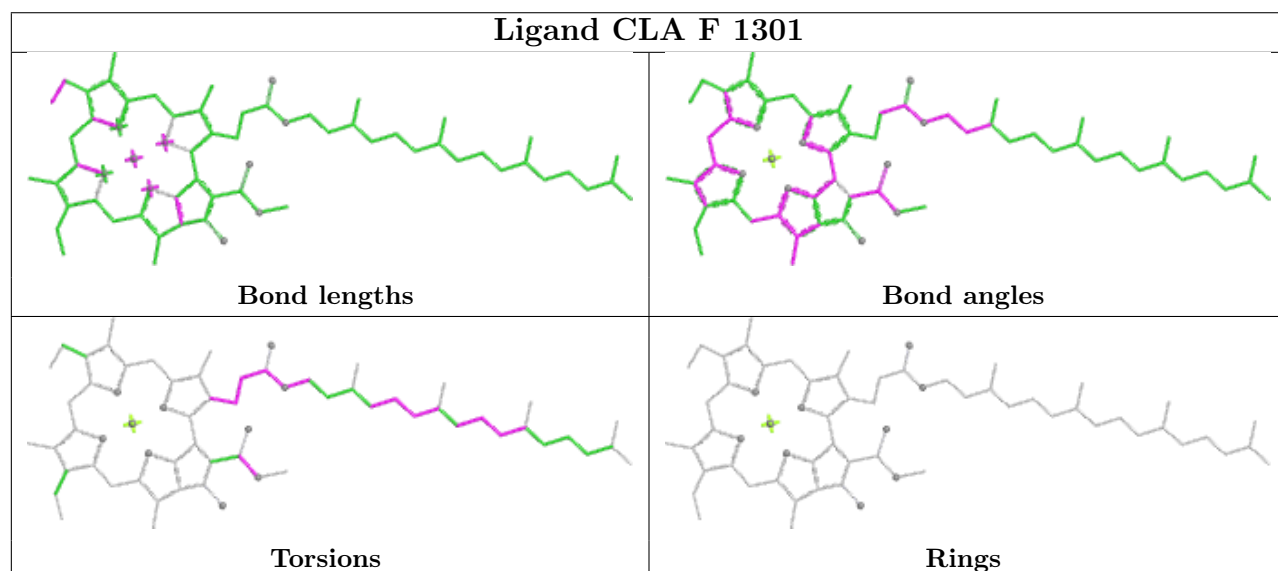
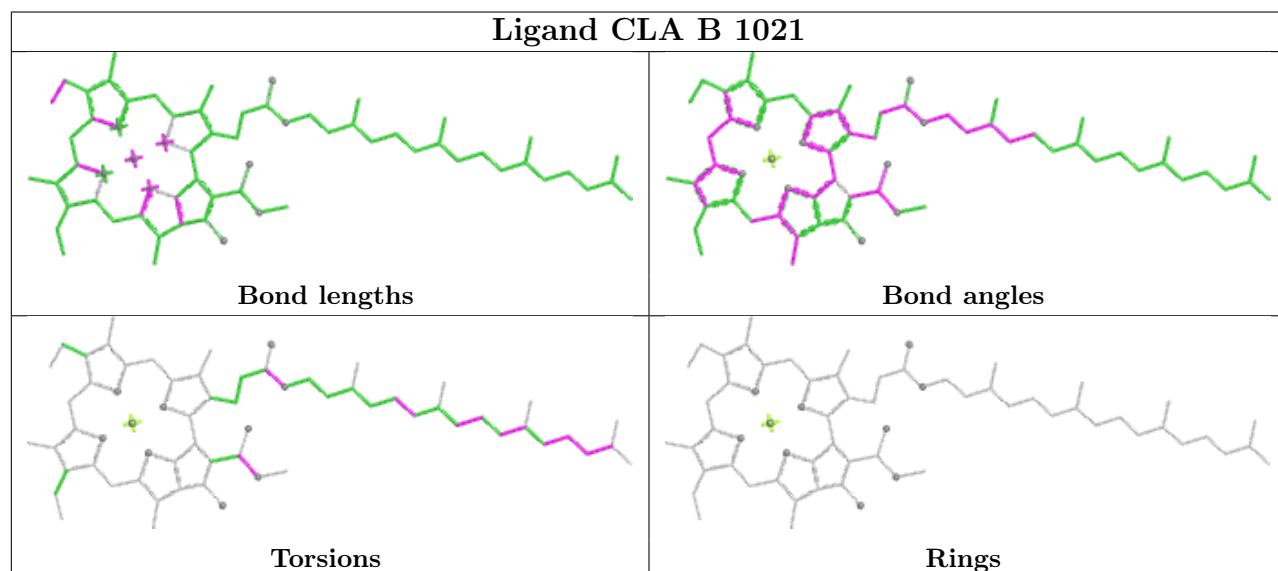
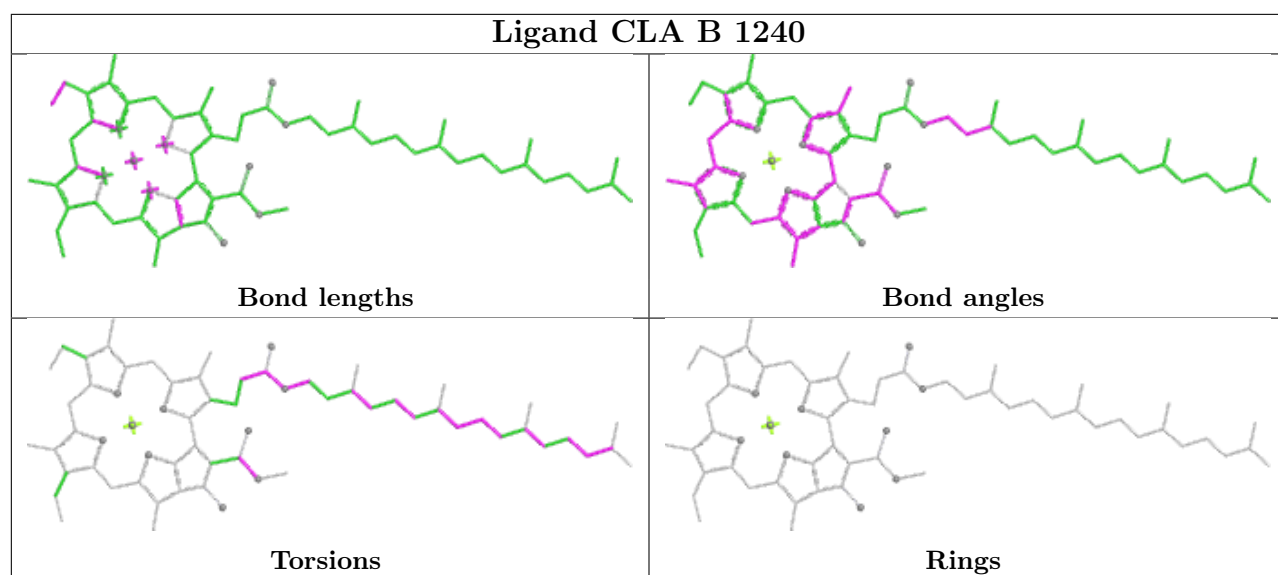
Bond angles



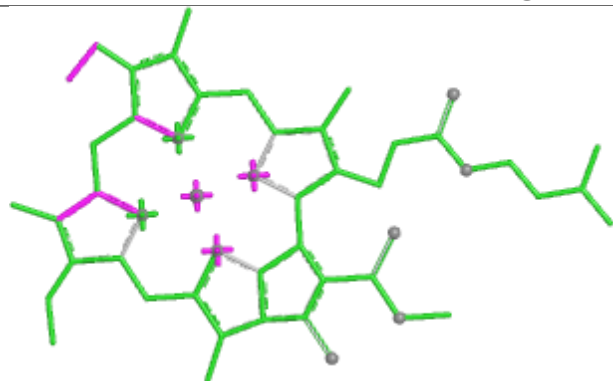
Torsions



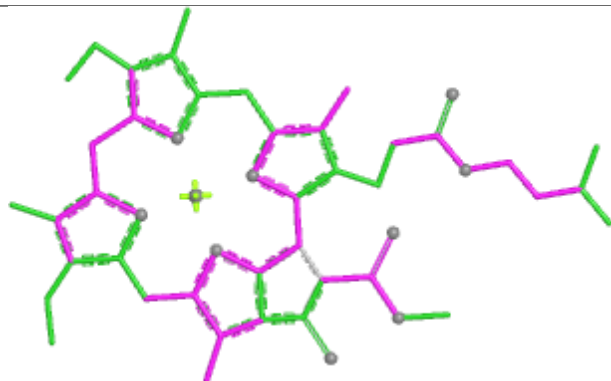
Rings



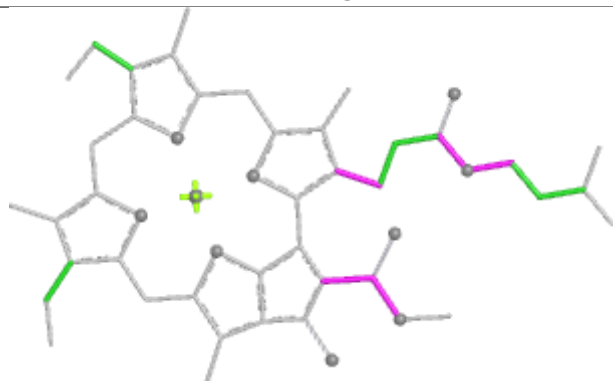
Ligand CLA 4 609



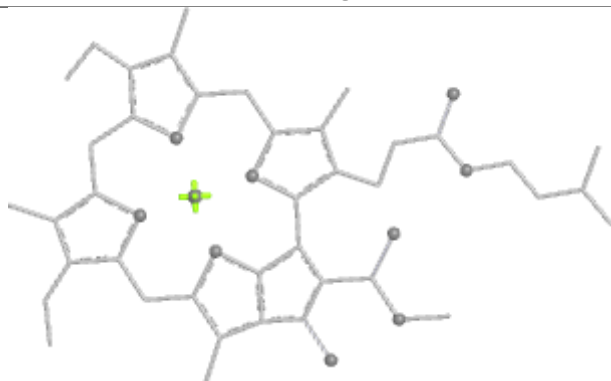
Bond lengths



Bond angles

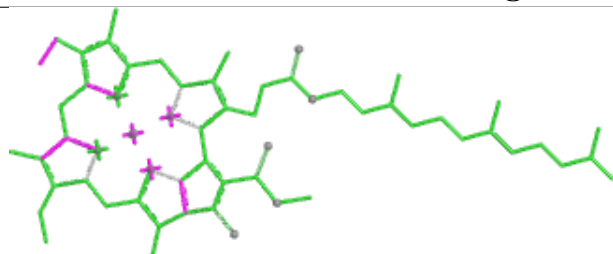


Torsions

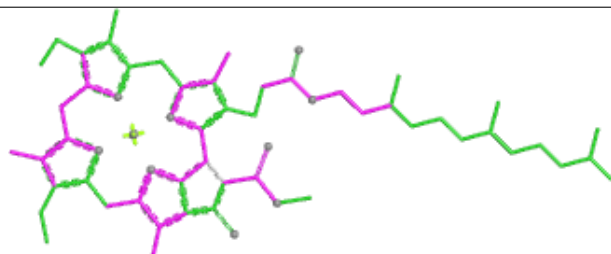


Rings

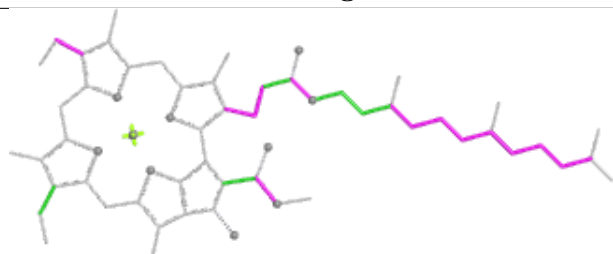
Ligand CLA K 1402



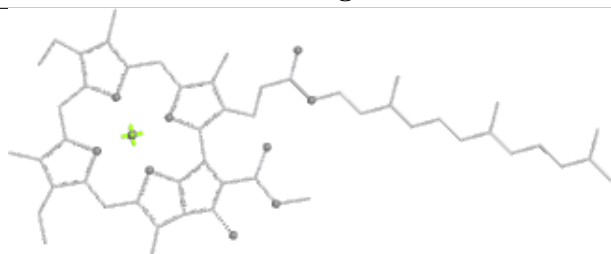
Bond lengths



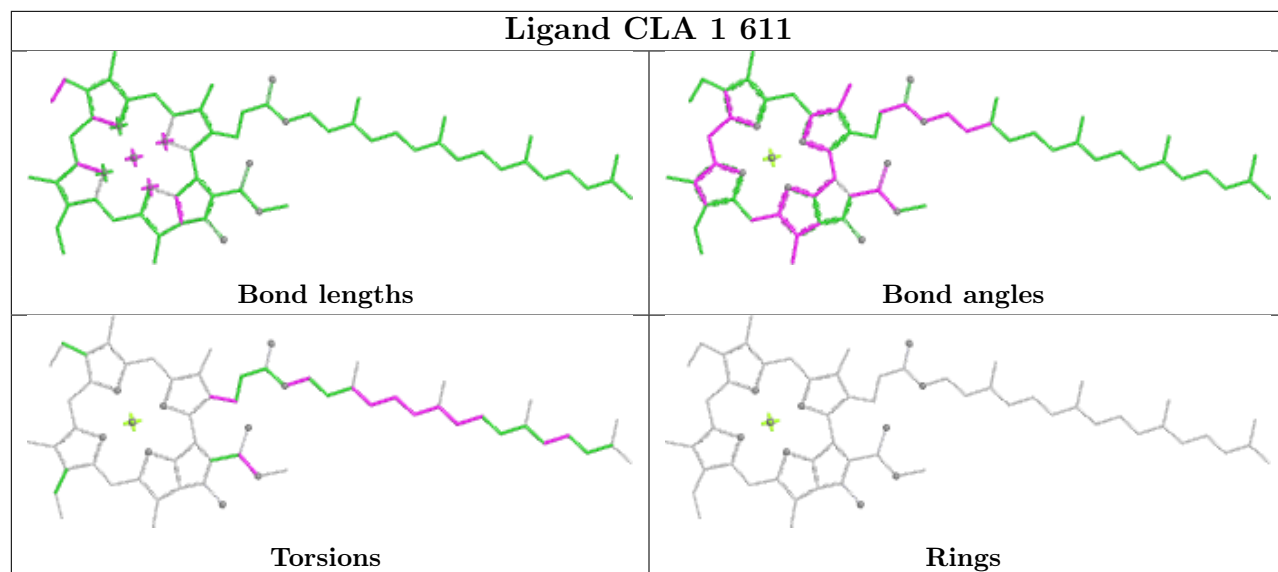
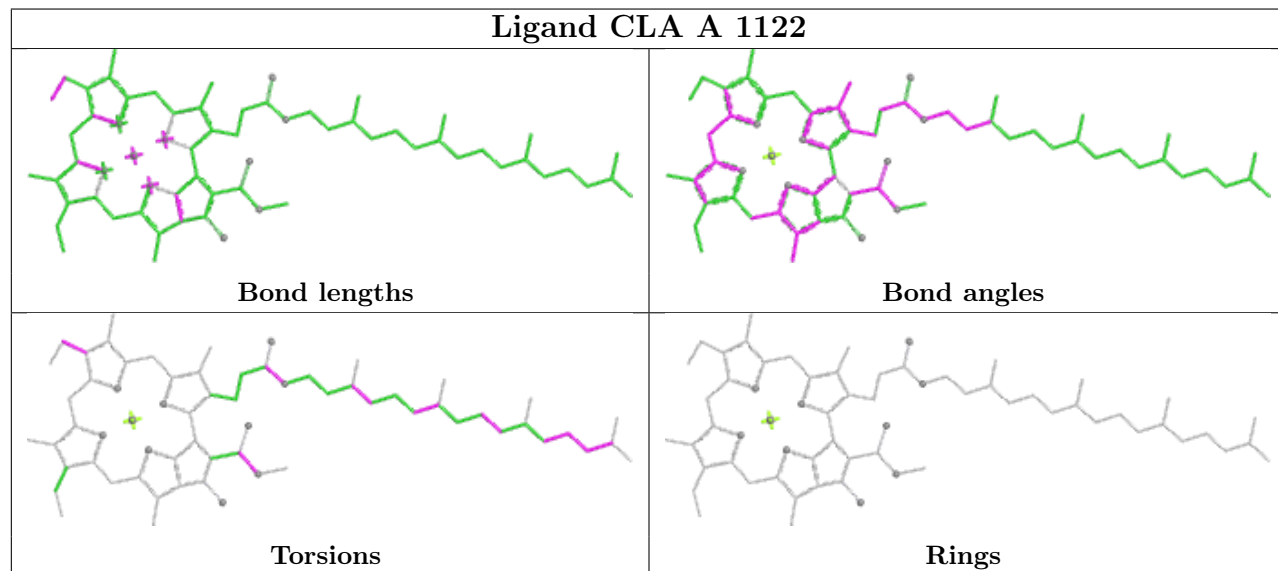
Bond angles

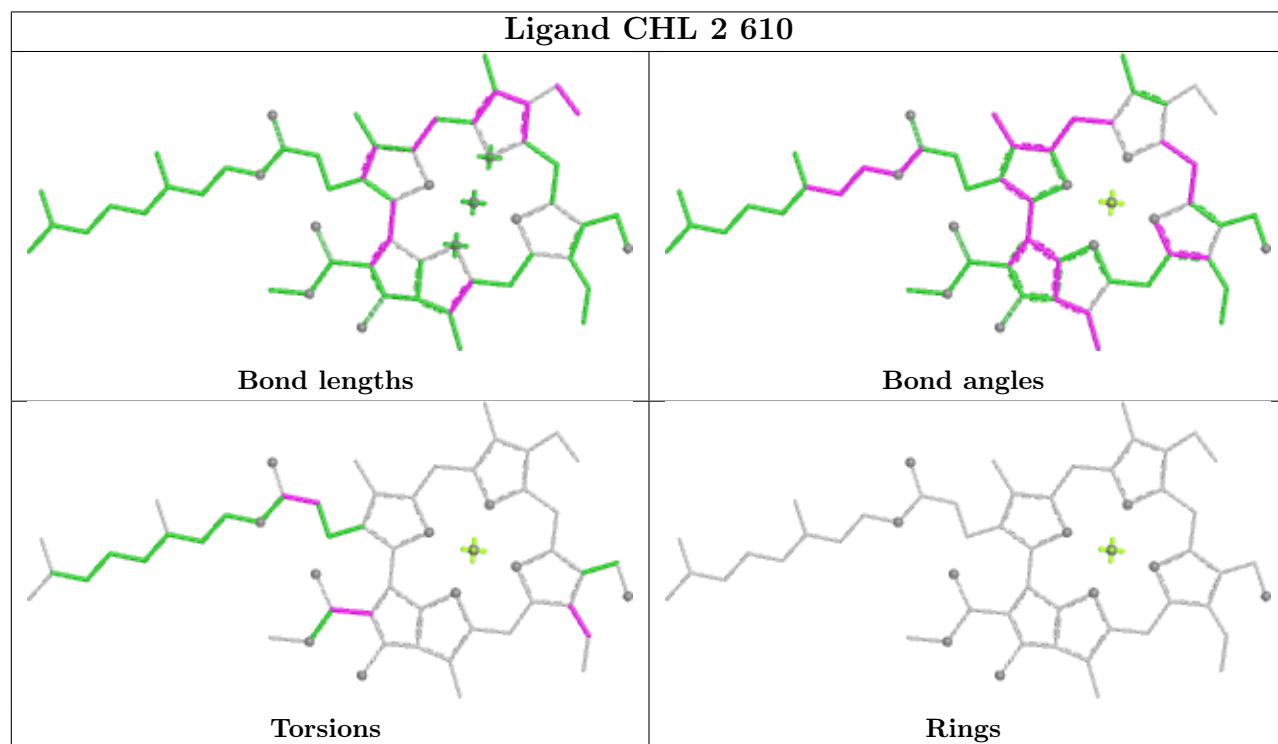
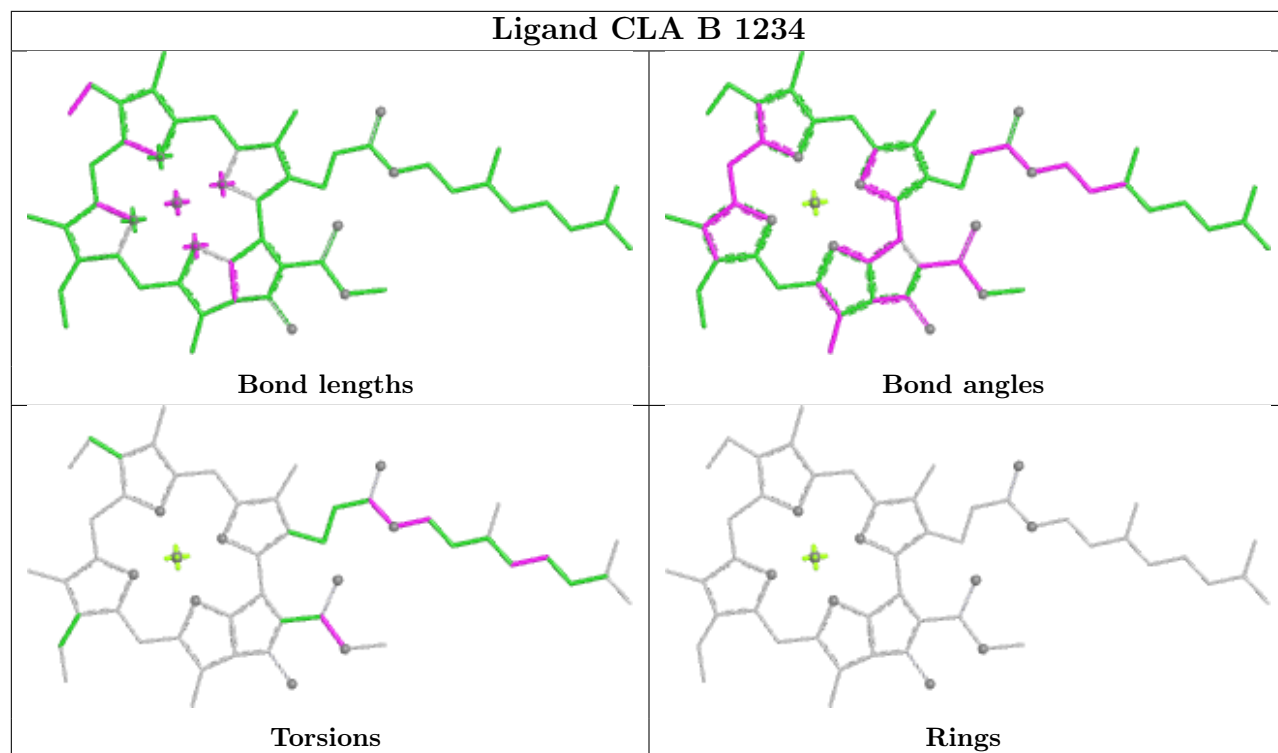


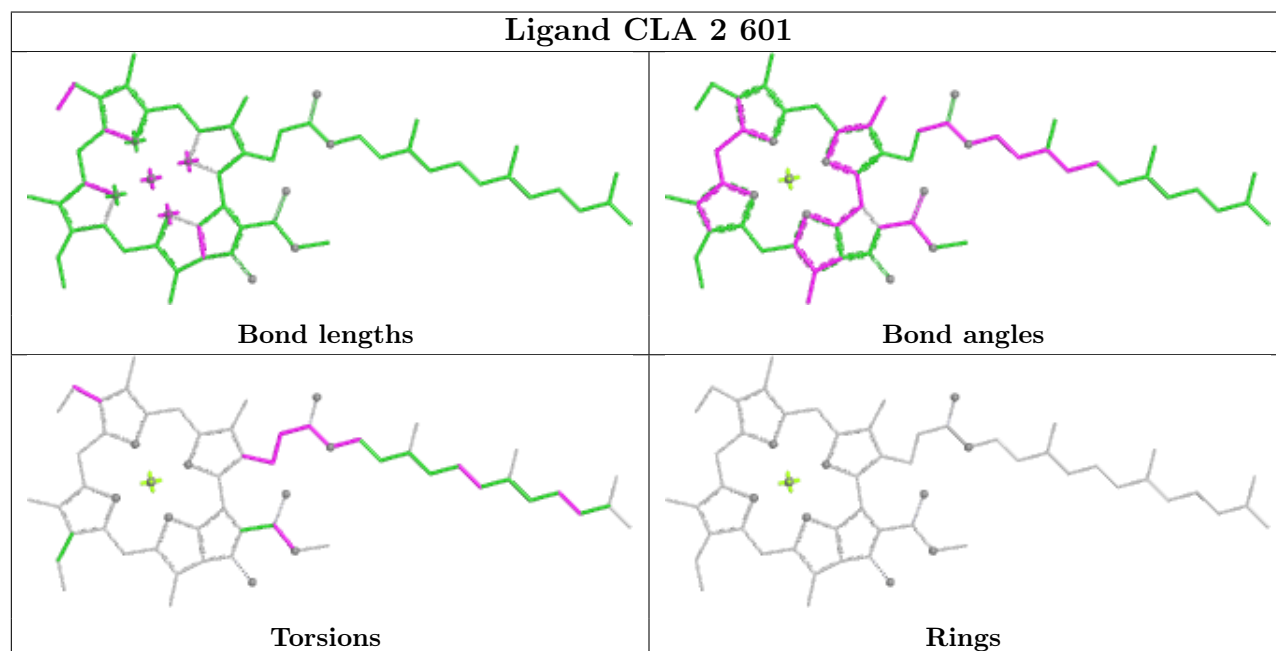
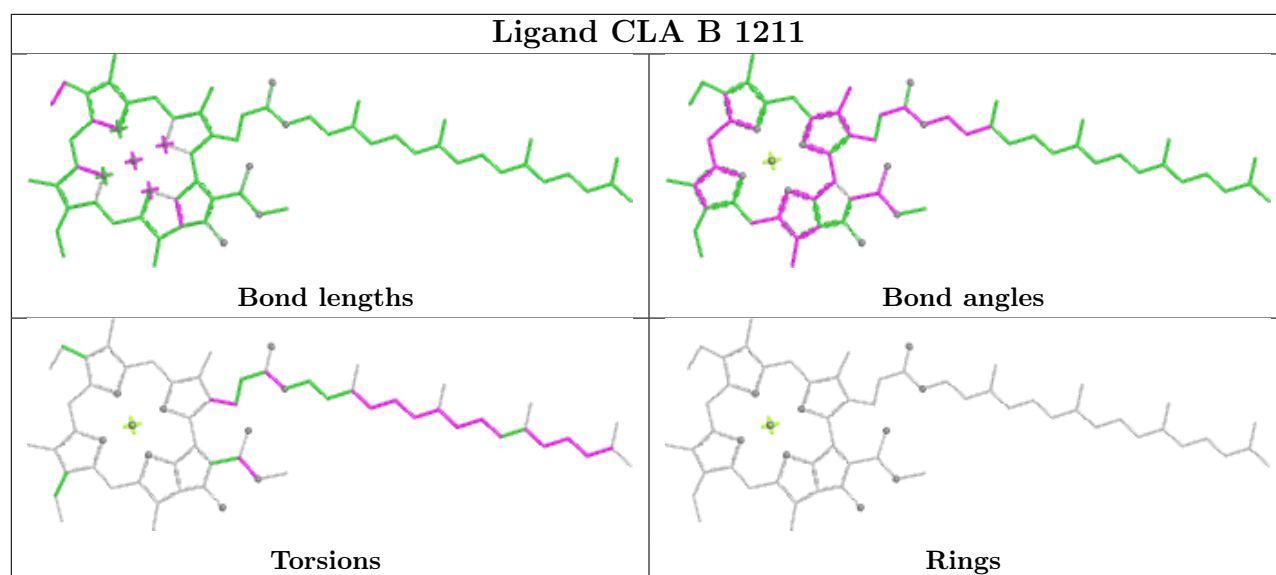
Torsions

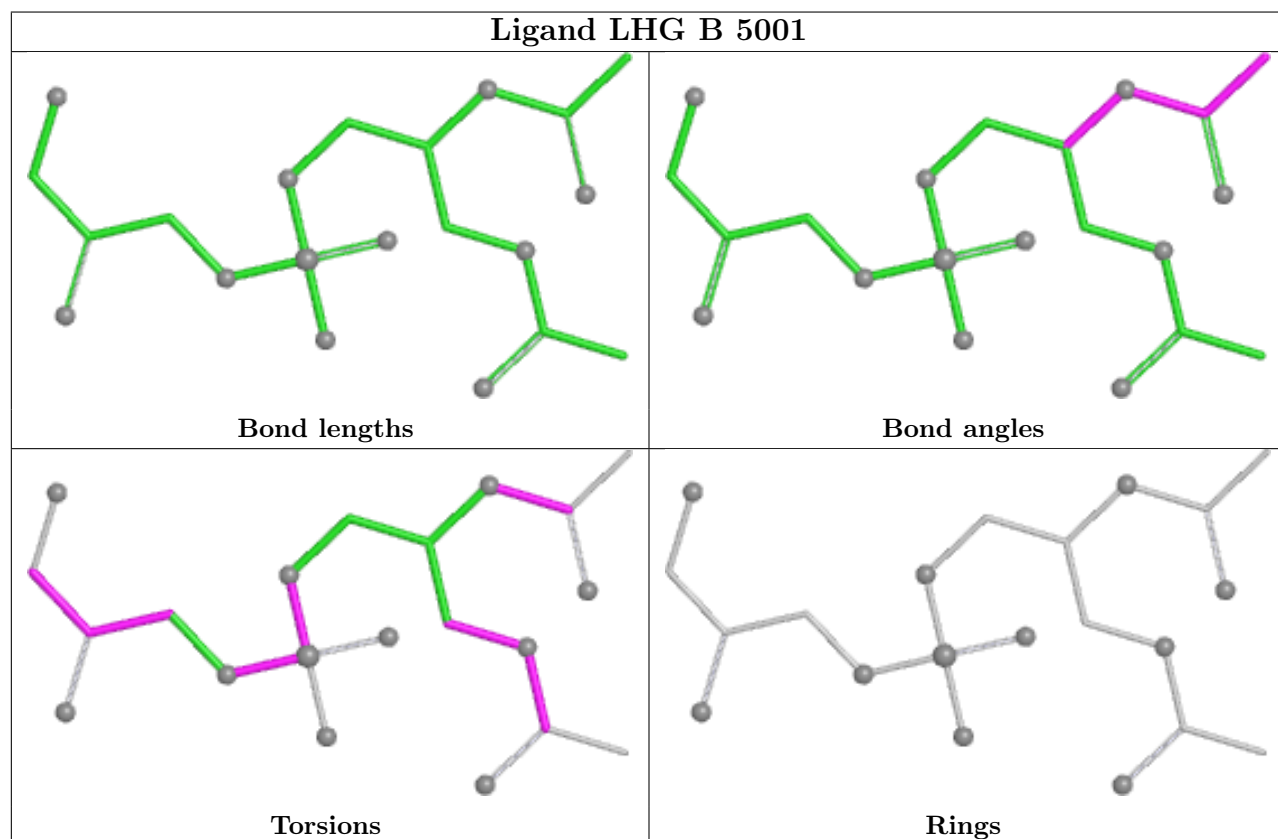
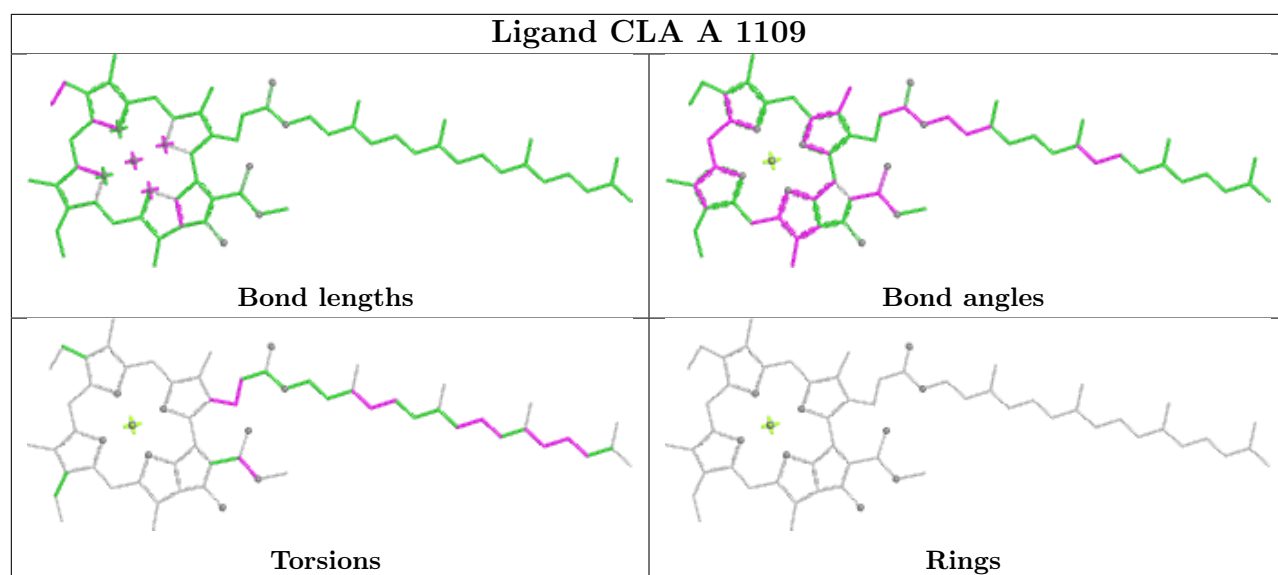


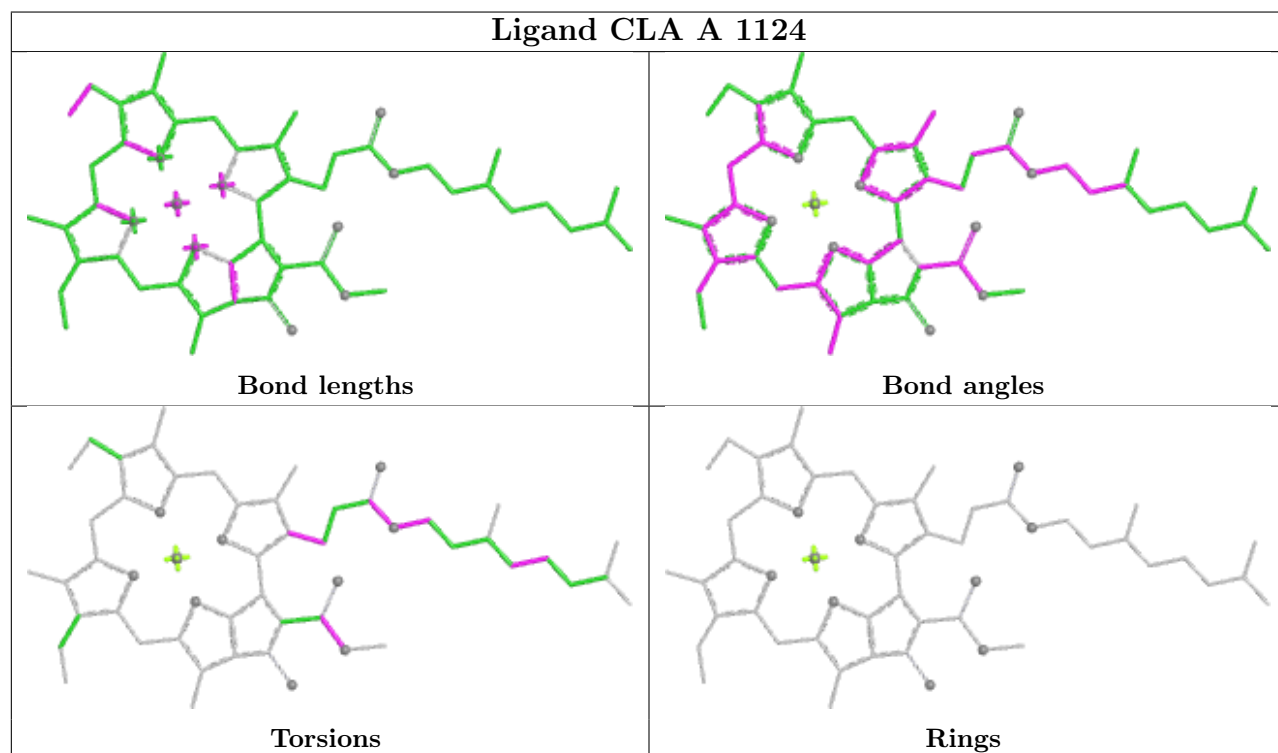
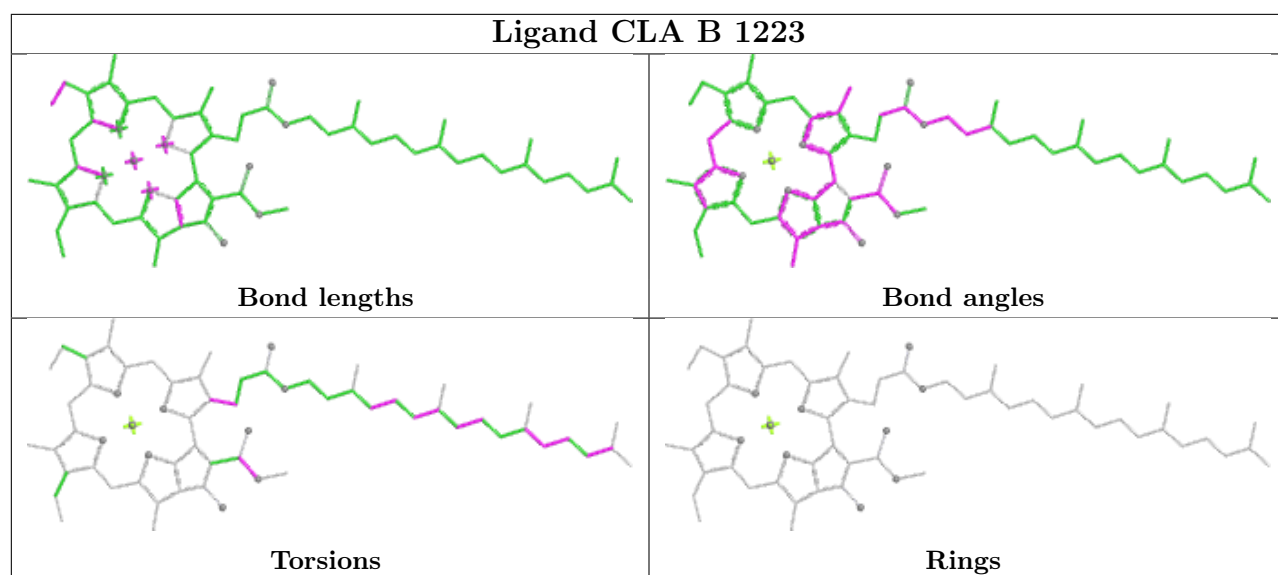
Rings

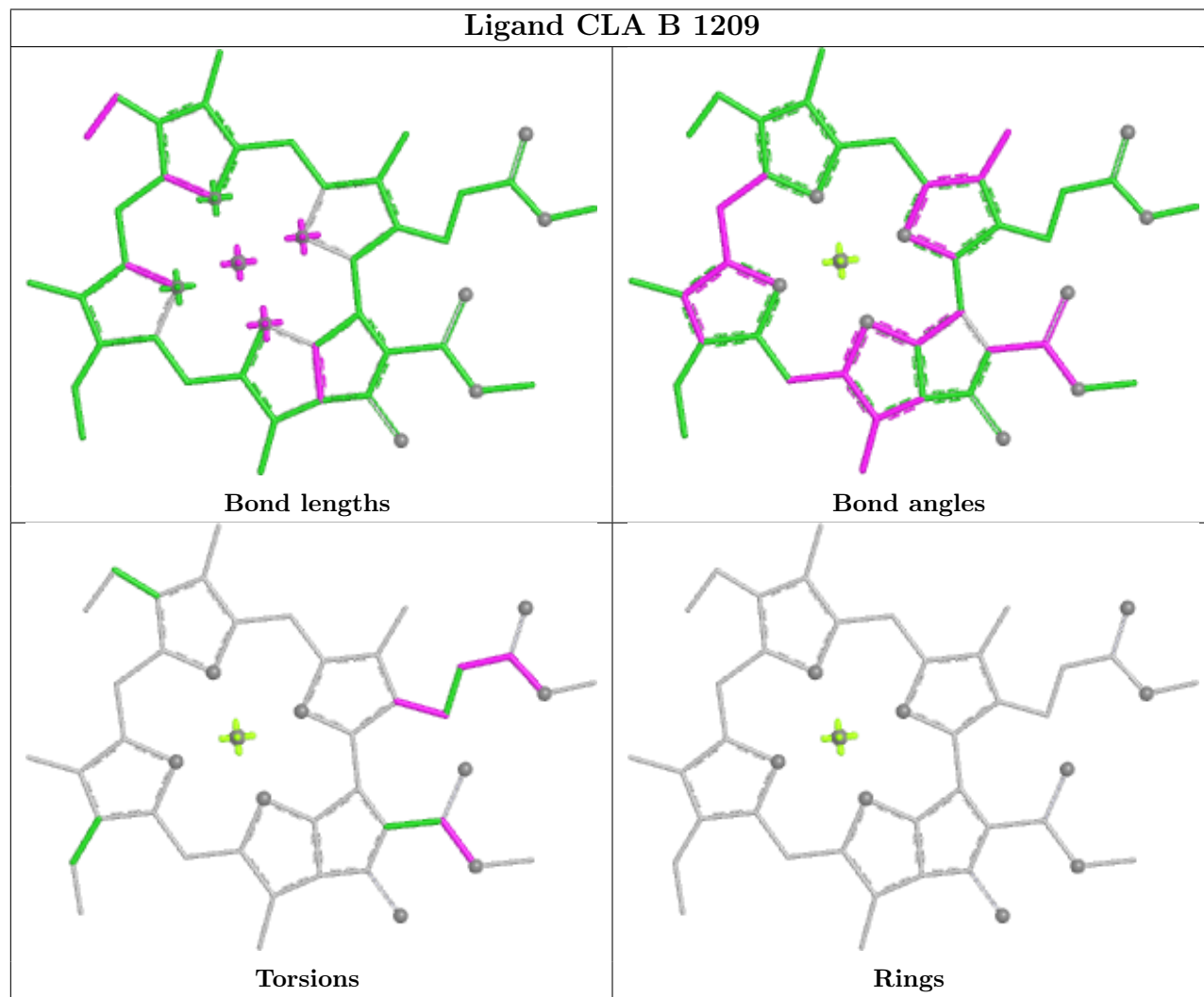
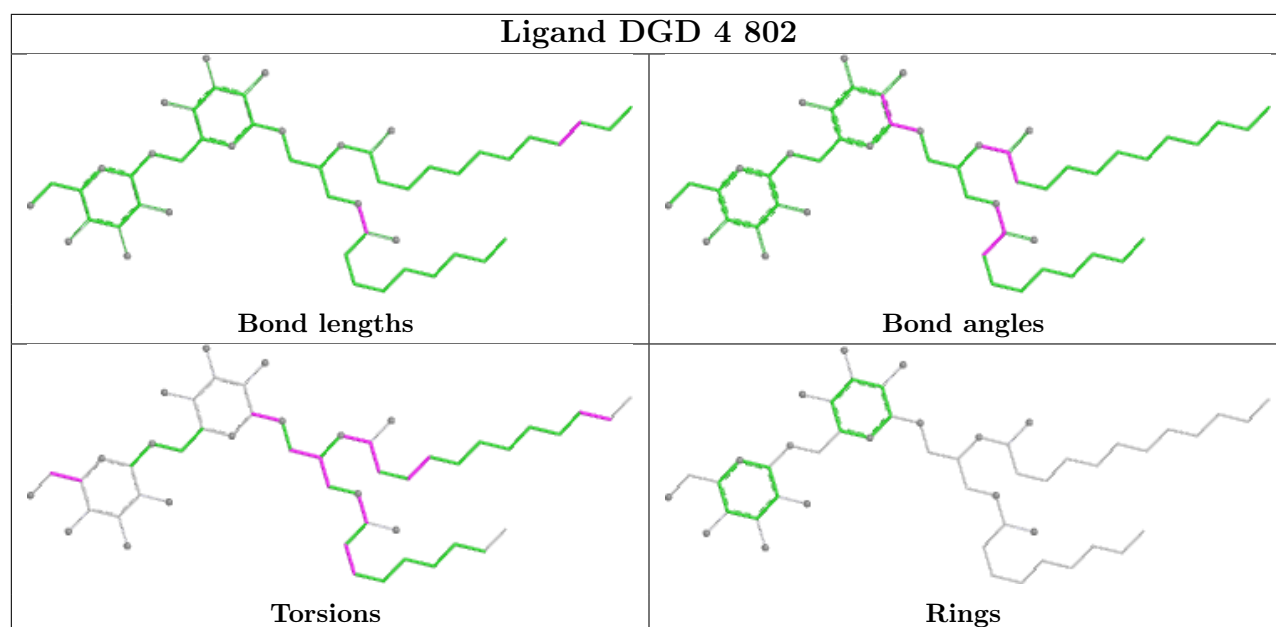
Ligand CLA 1 611**Ligand CLA A 1122**

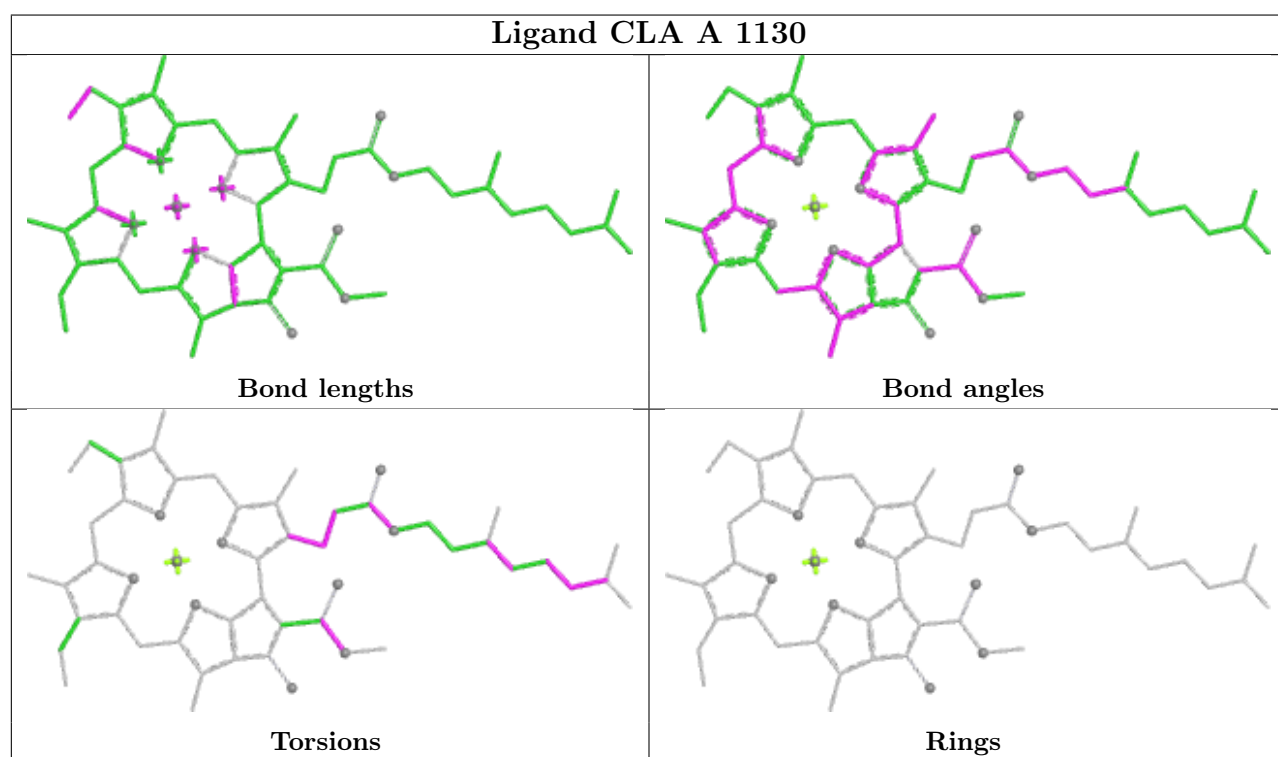
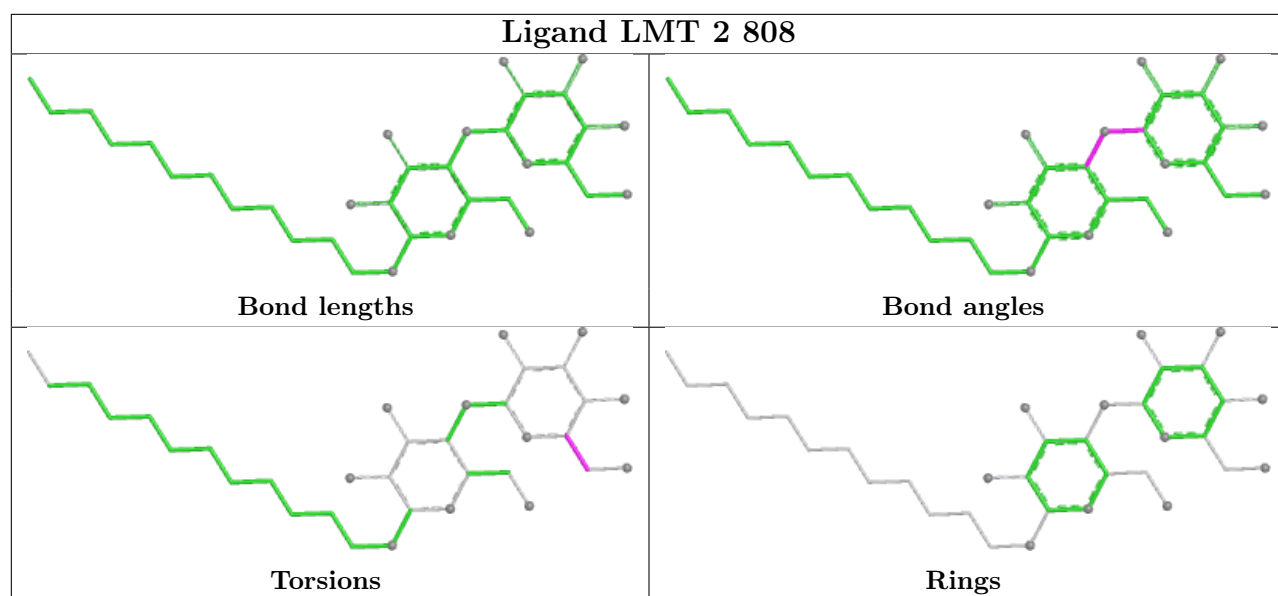




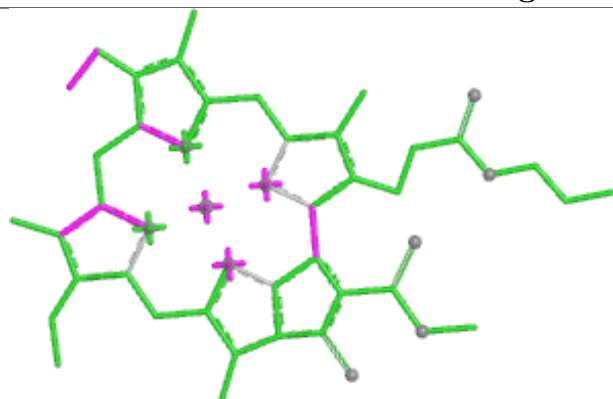




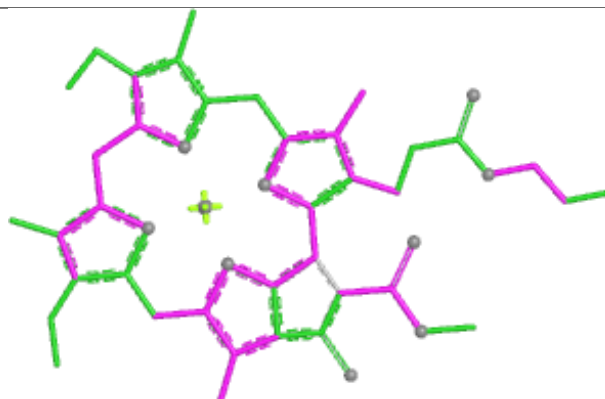




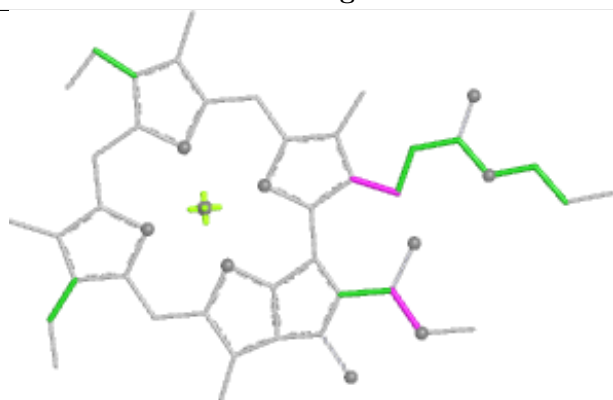
Ligand CLA 3 608



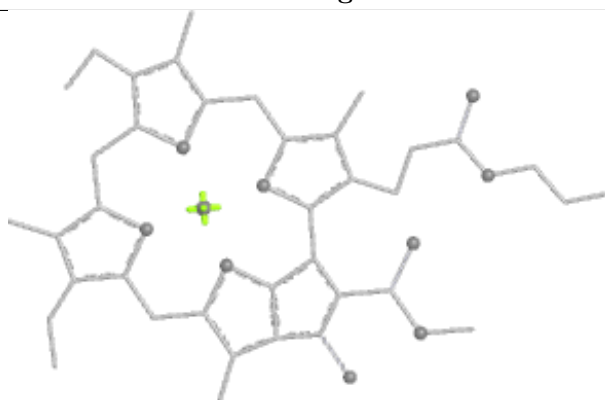
Bond lengths



Bond angles

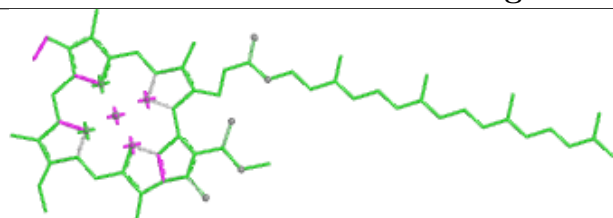


Torsions

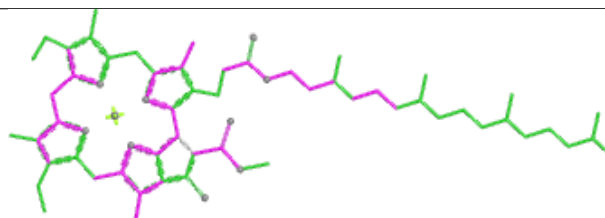


Rings

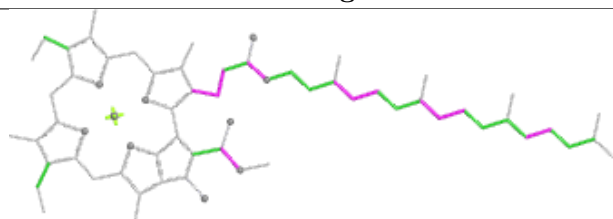
Ligand CLA A 1119



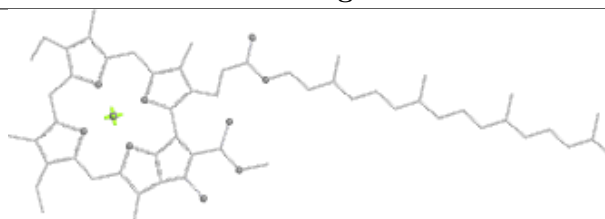
Bond lengths



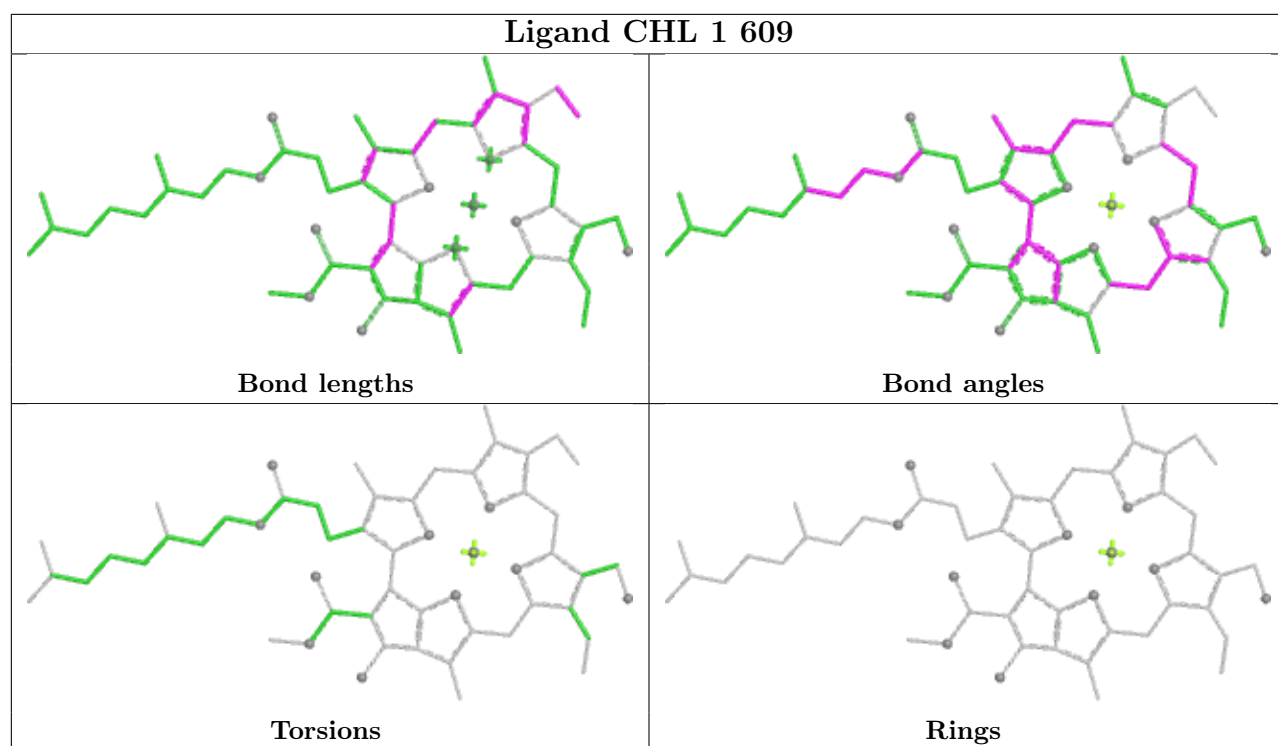
Bond angles



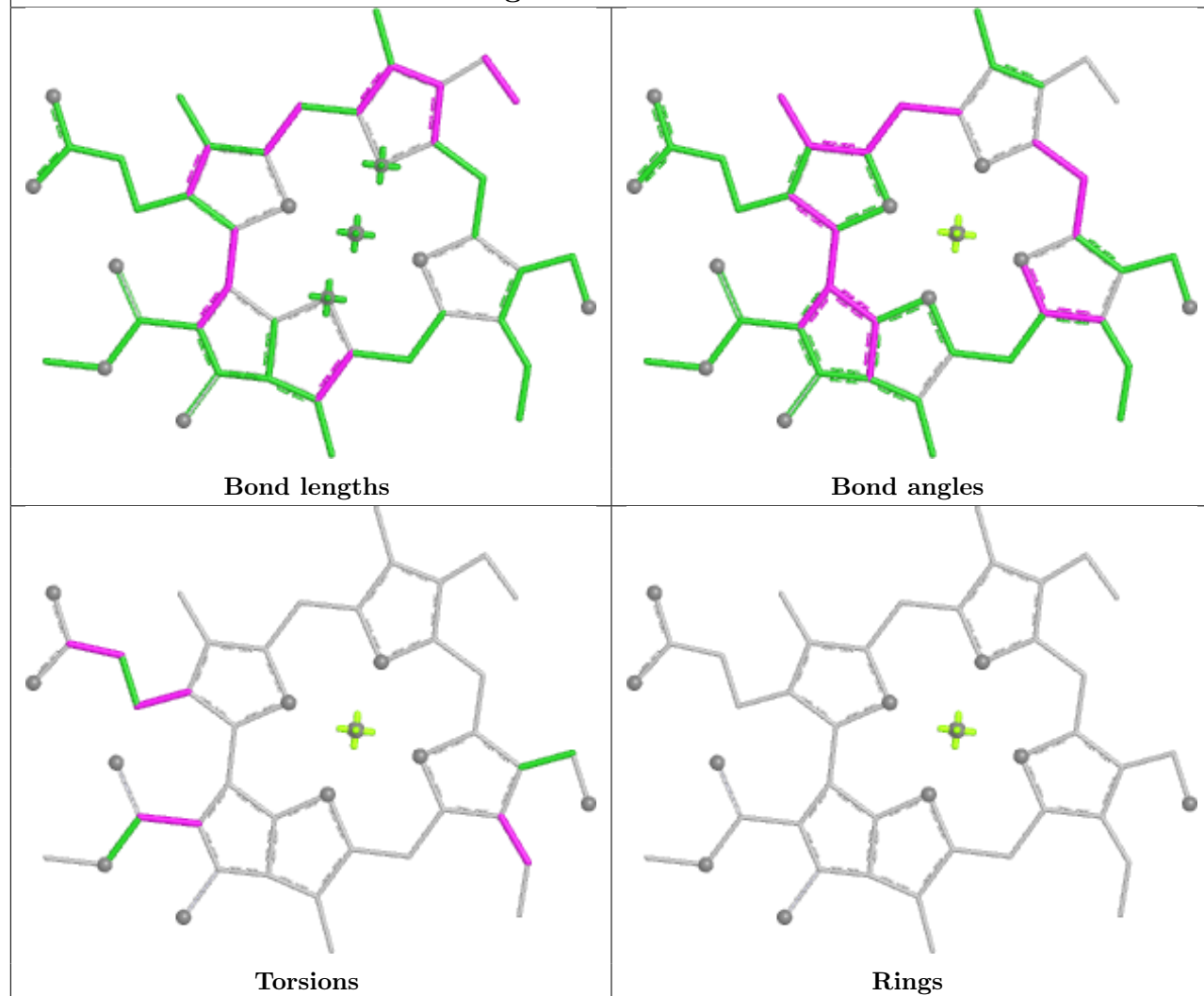
Torsions



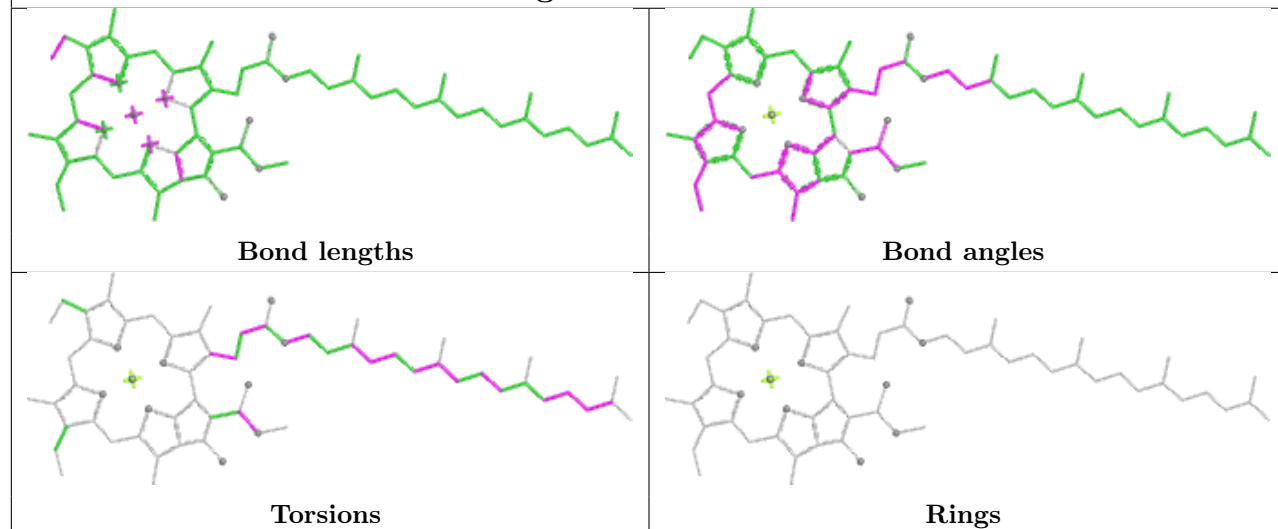
Rings



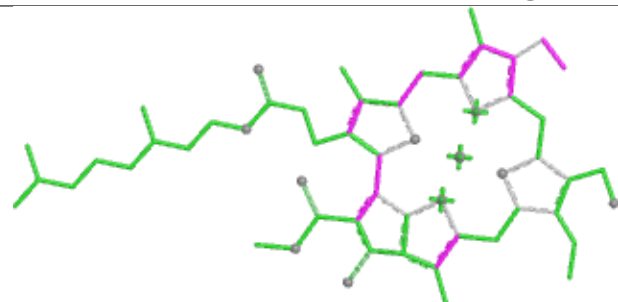
Ligand CHL 2 613



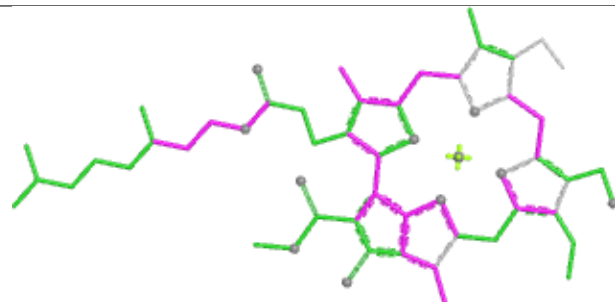
Ligand CLA 1 605



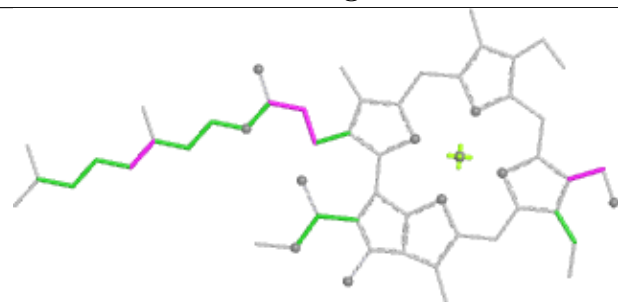
Ligand CHL 2 615



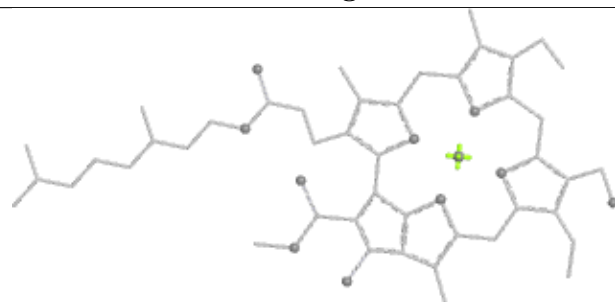
Bond lengths



Bond angles

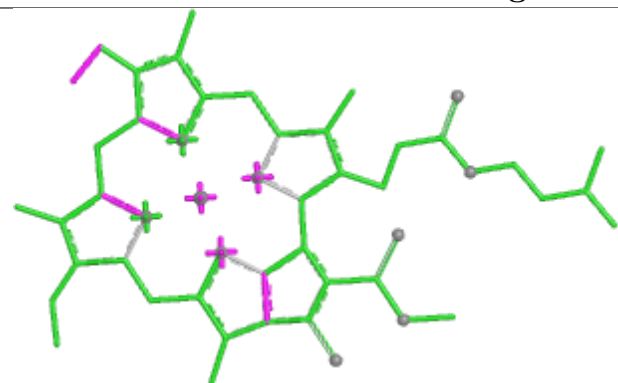


Torsions

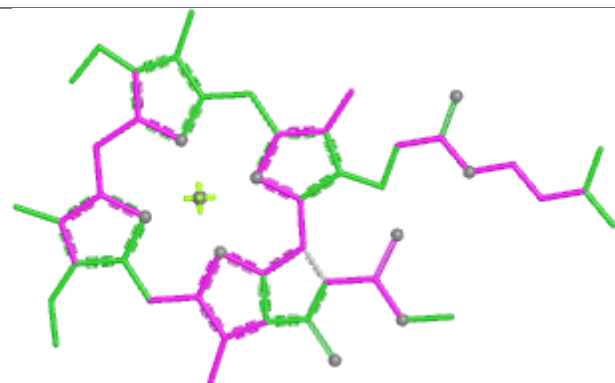


Rings

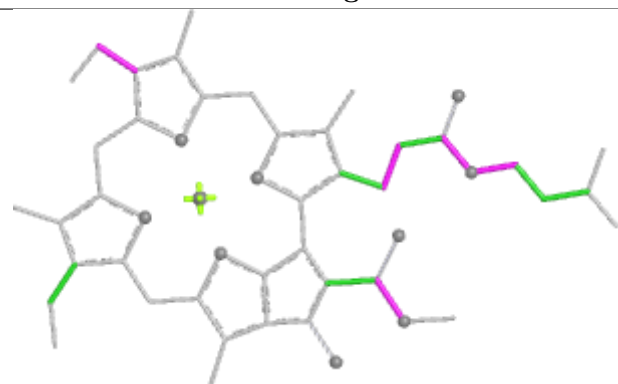
Ligand CLA A 1118



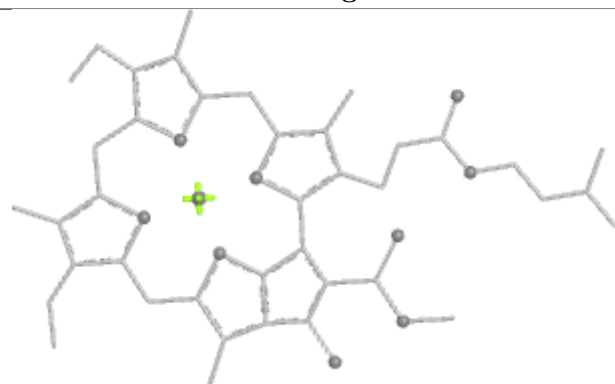
Bond lengths



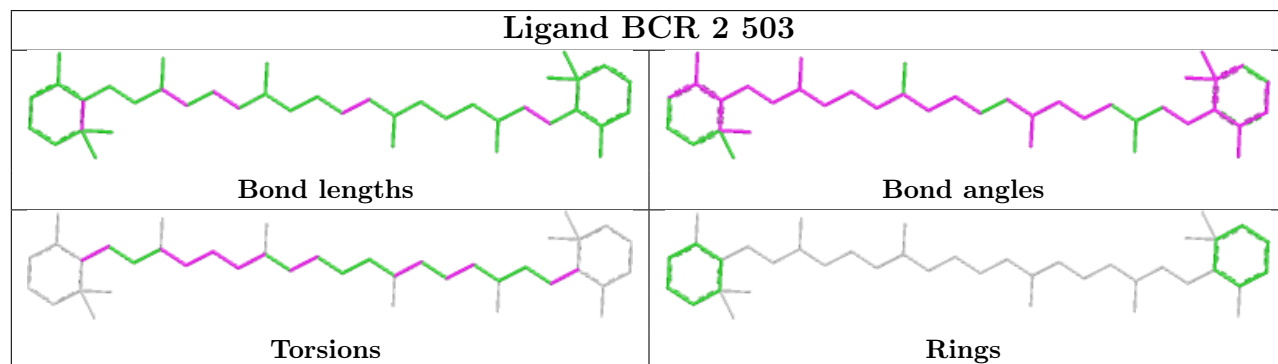
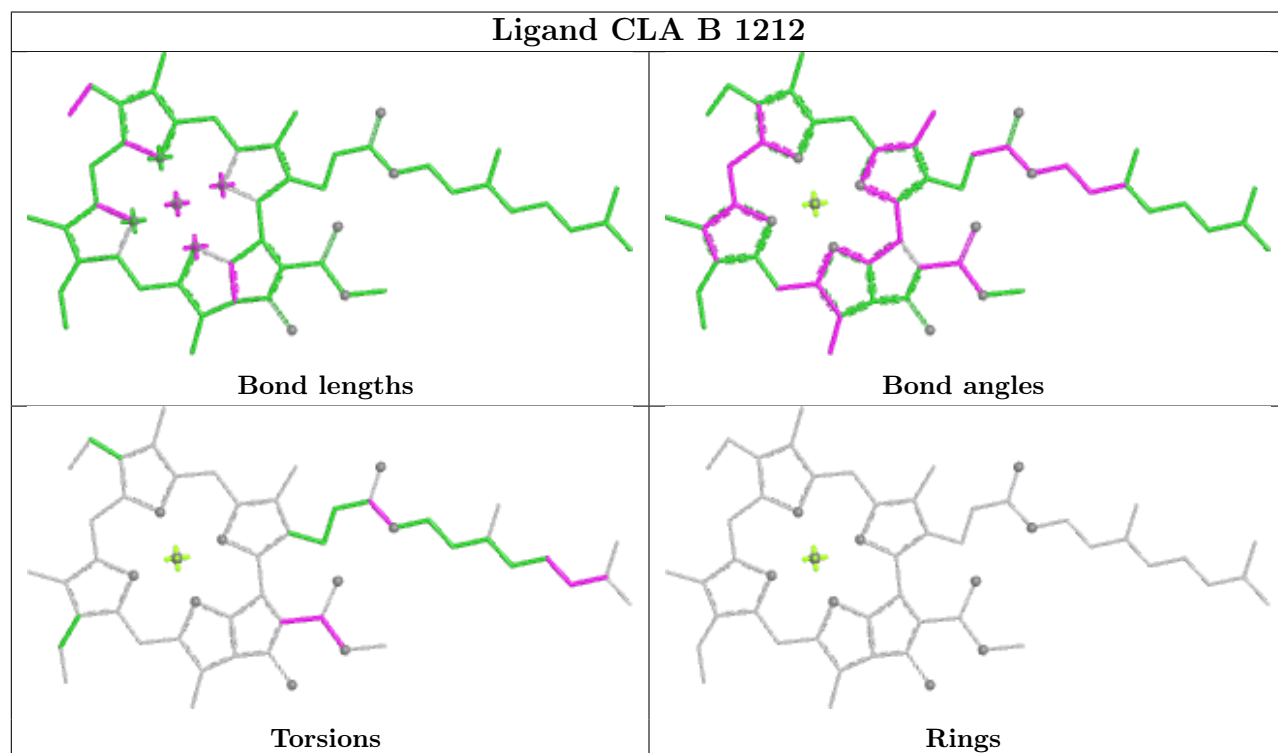
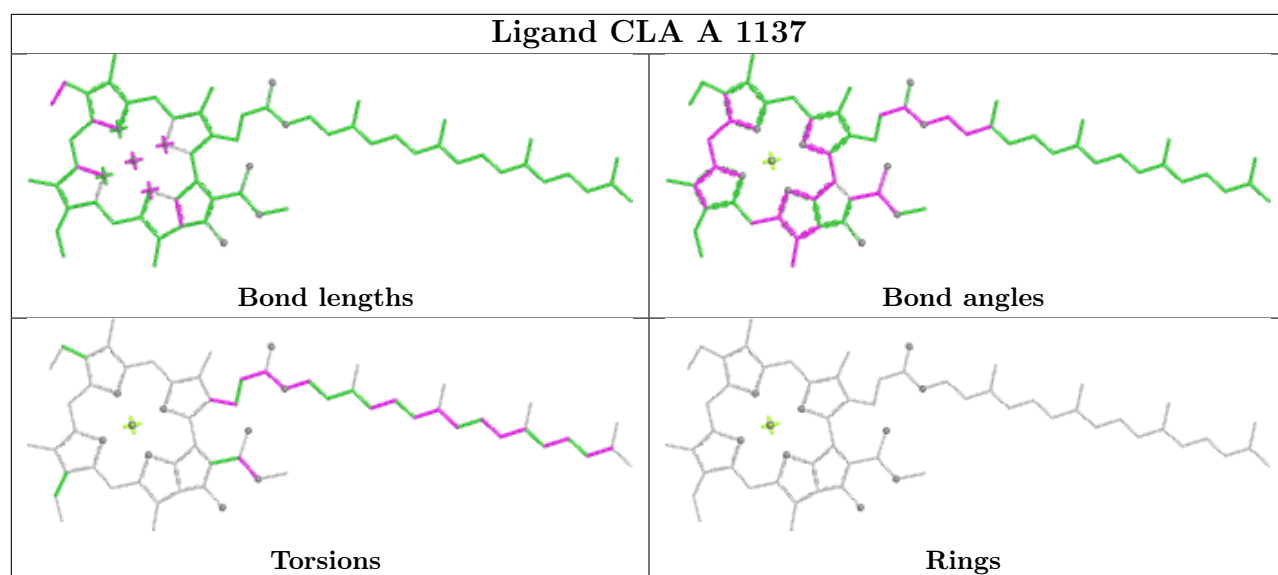
Bond angles

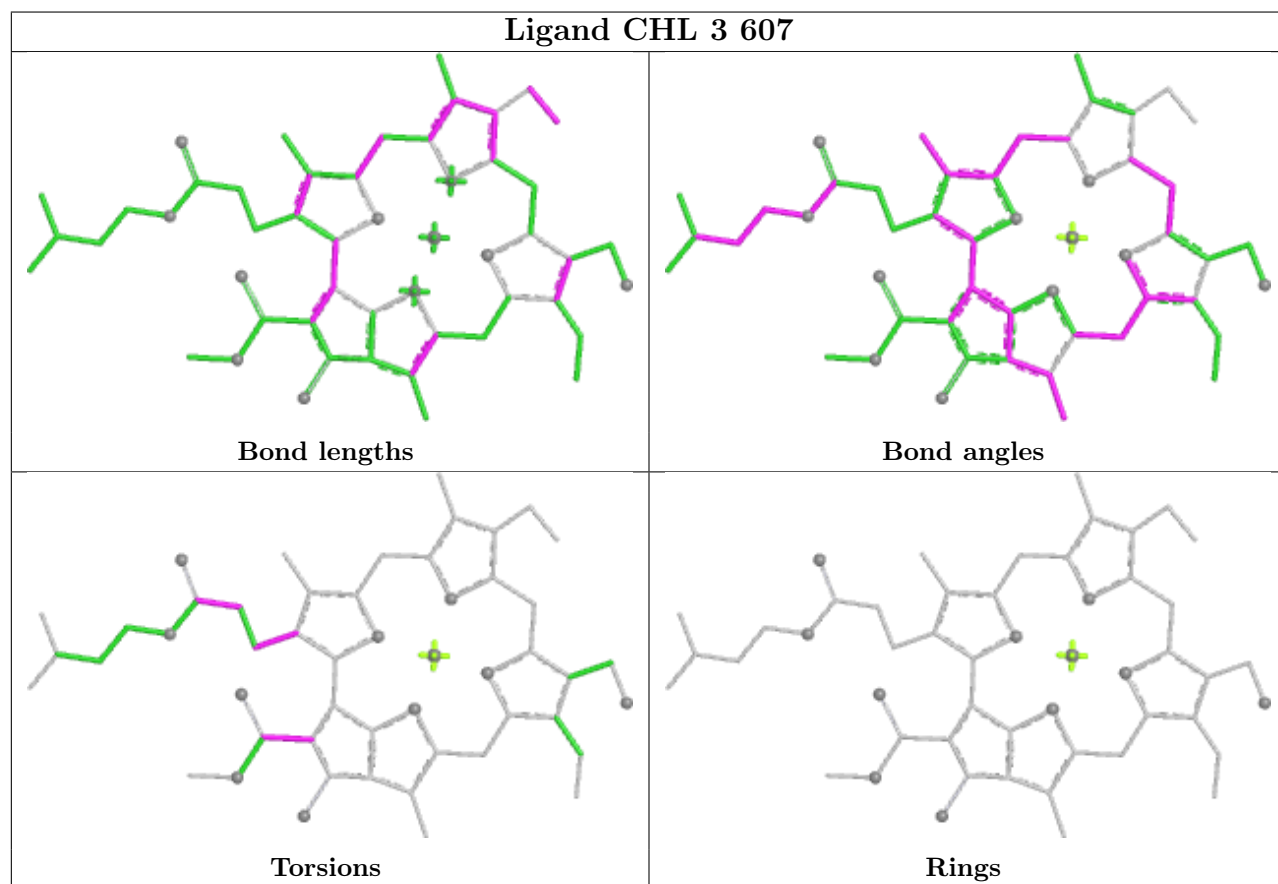
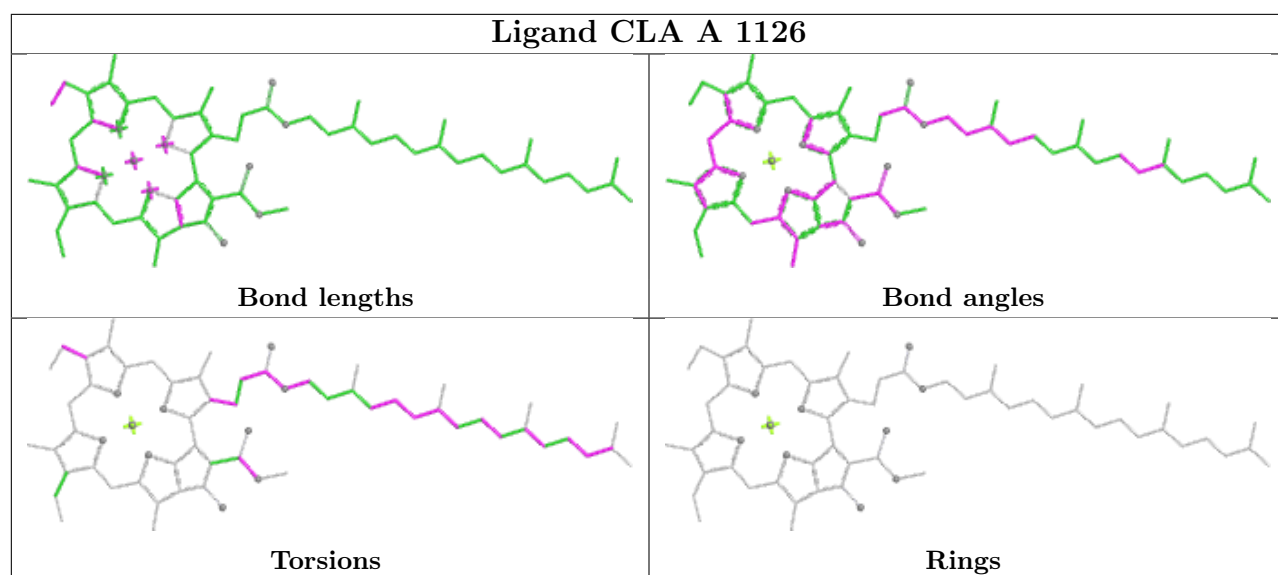


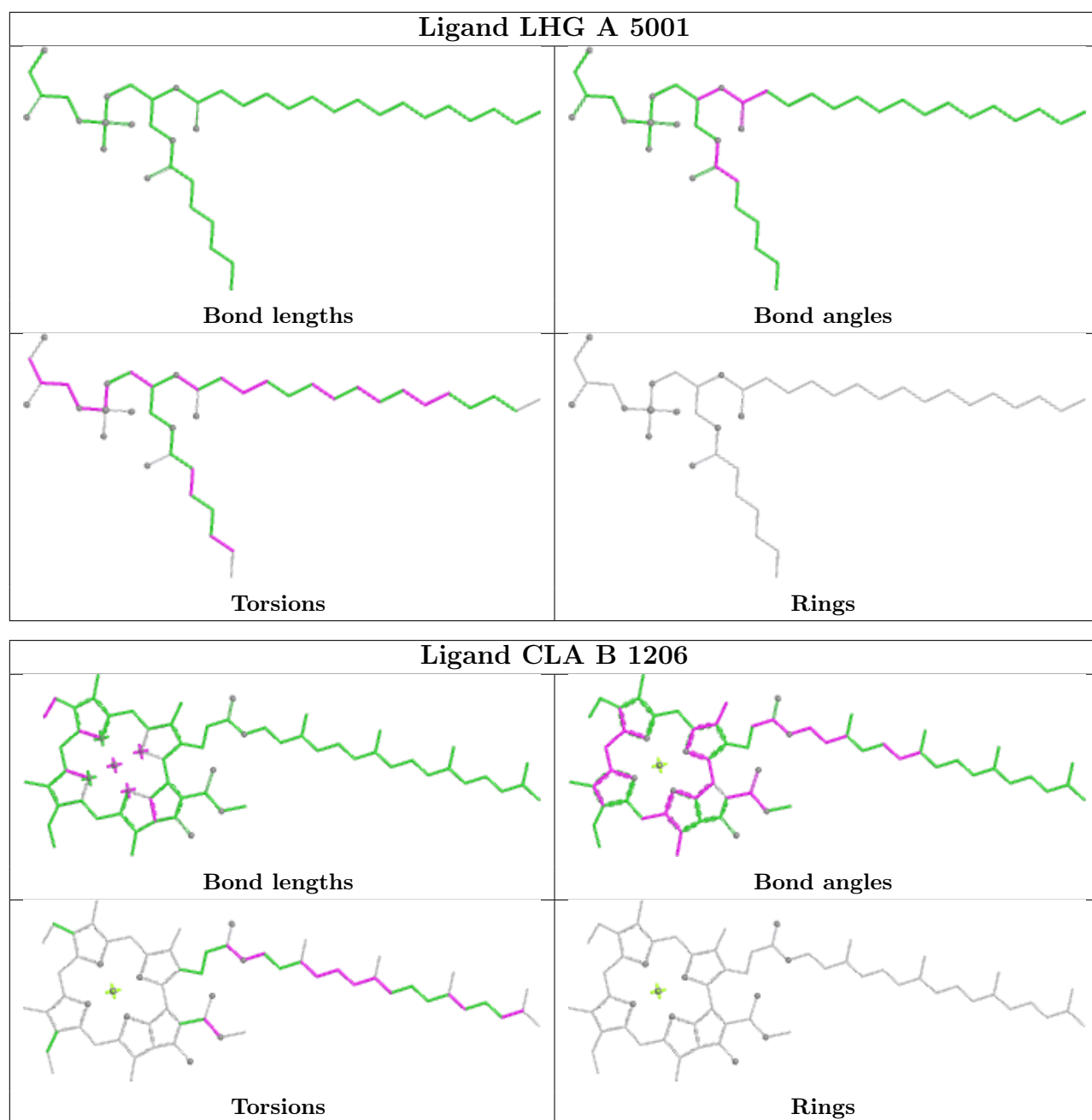
Torsions

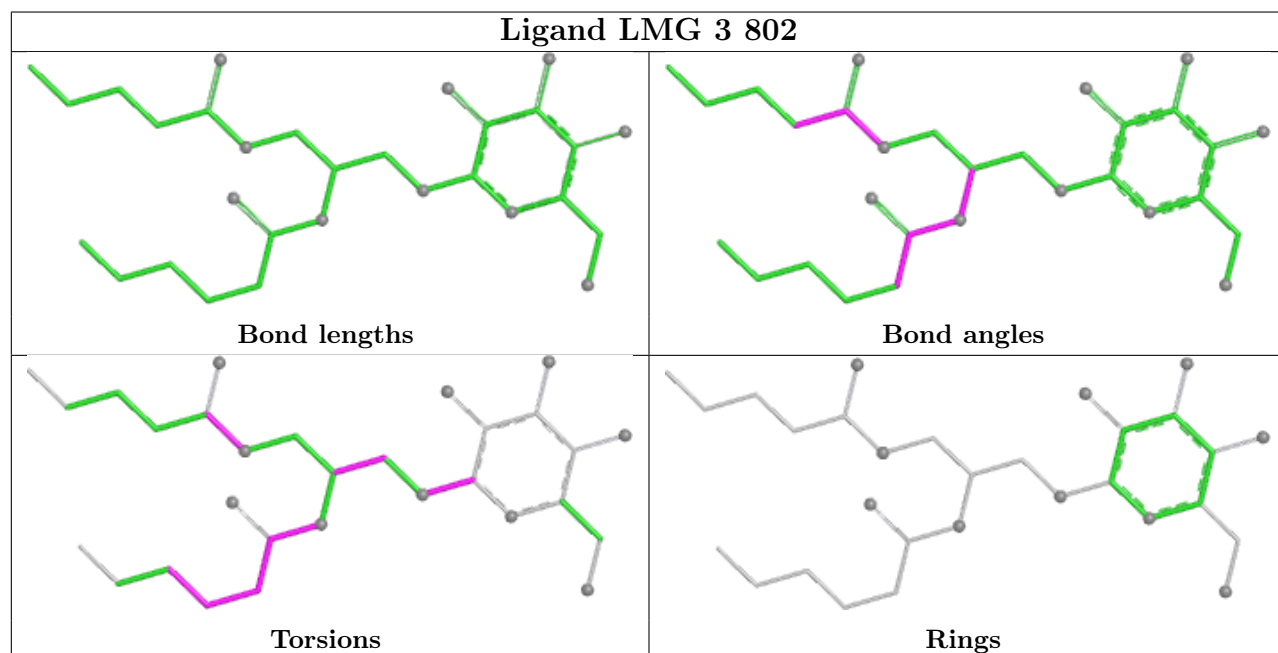
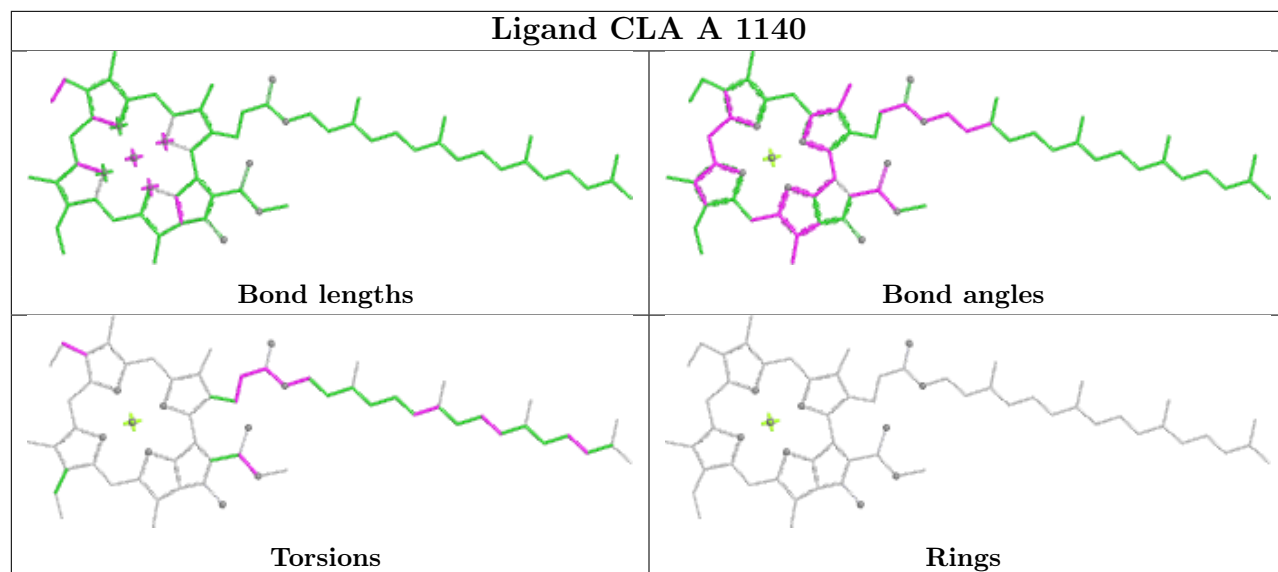


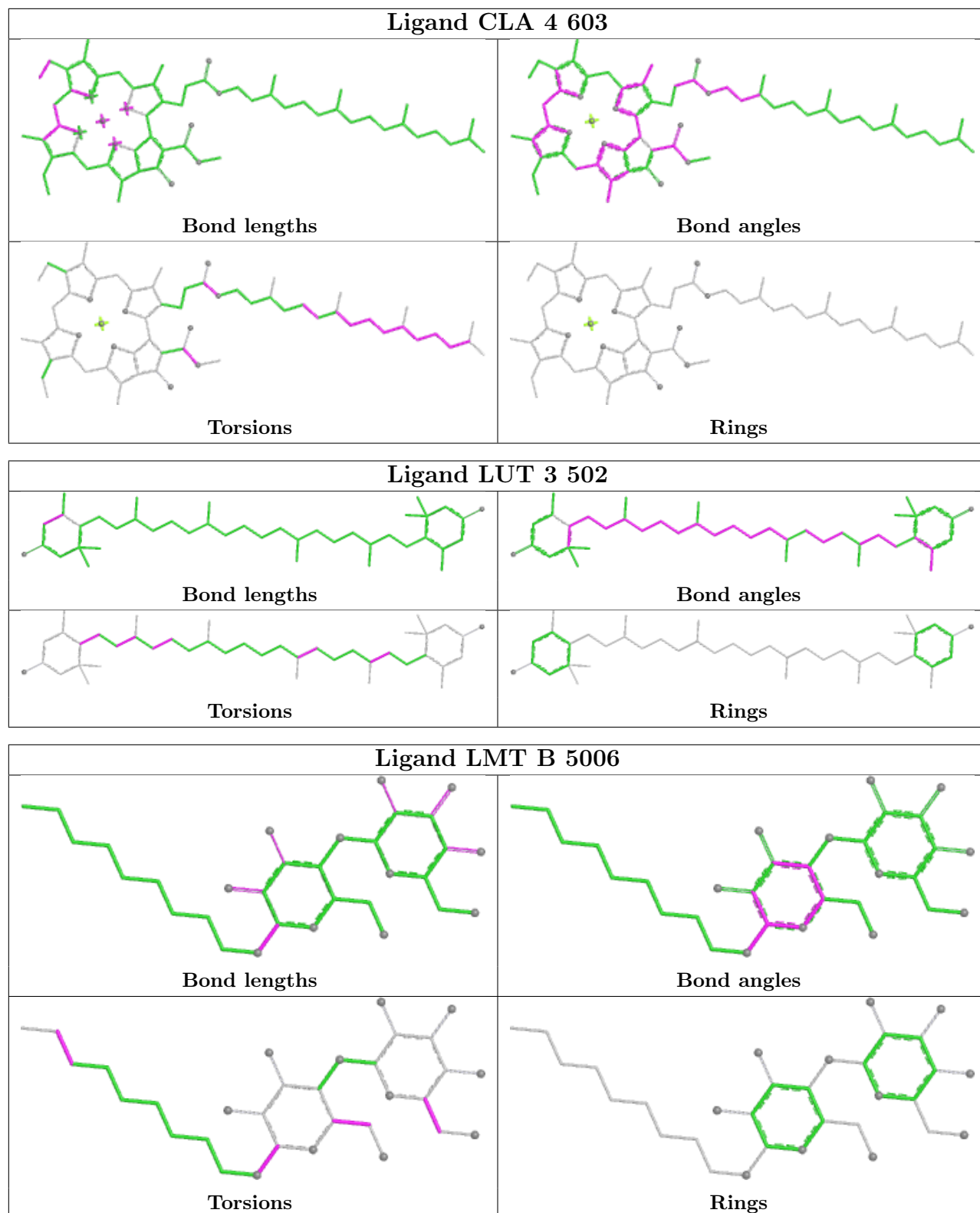
Rings

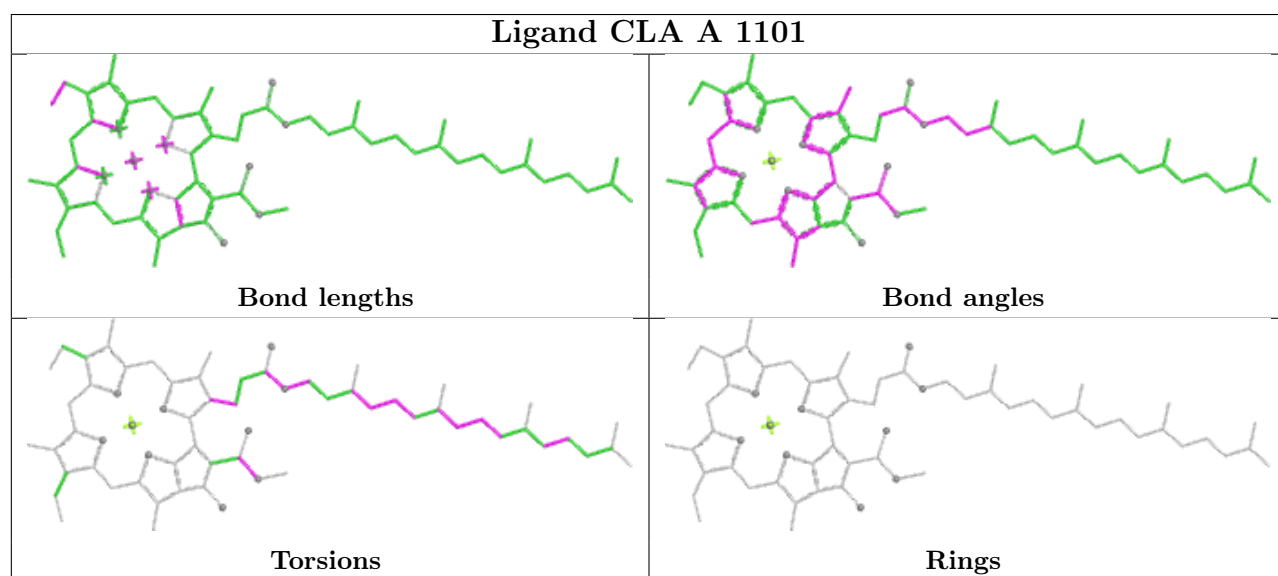
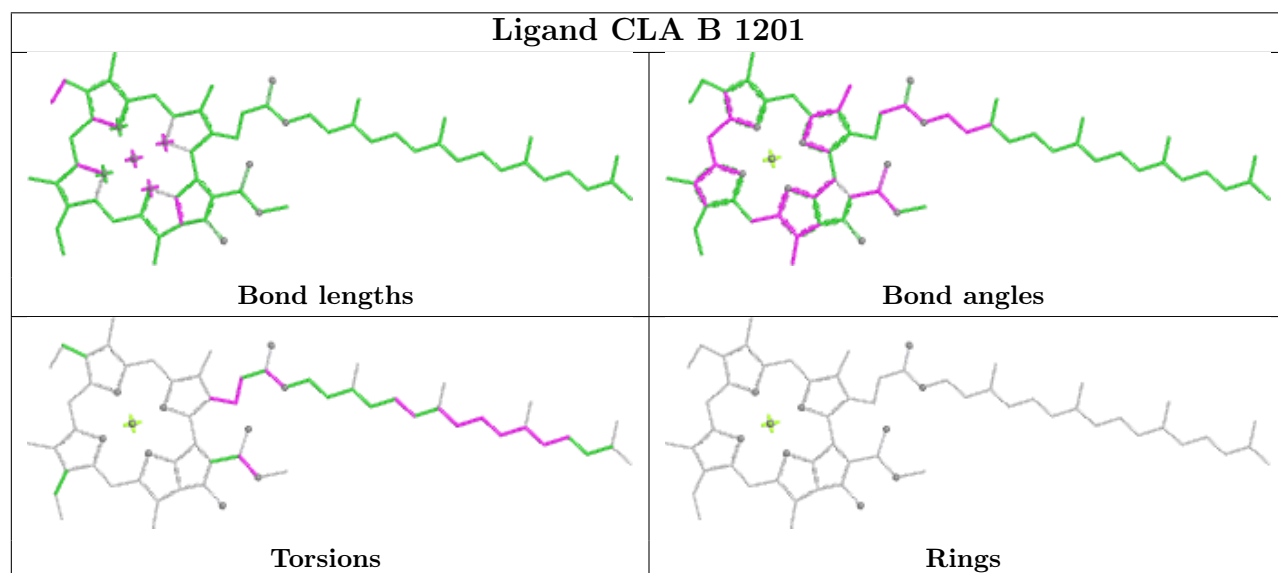
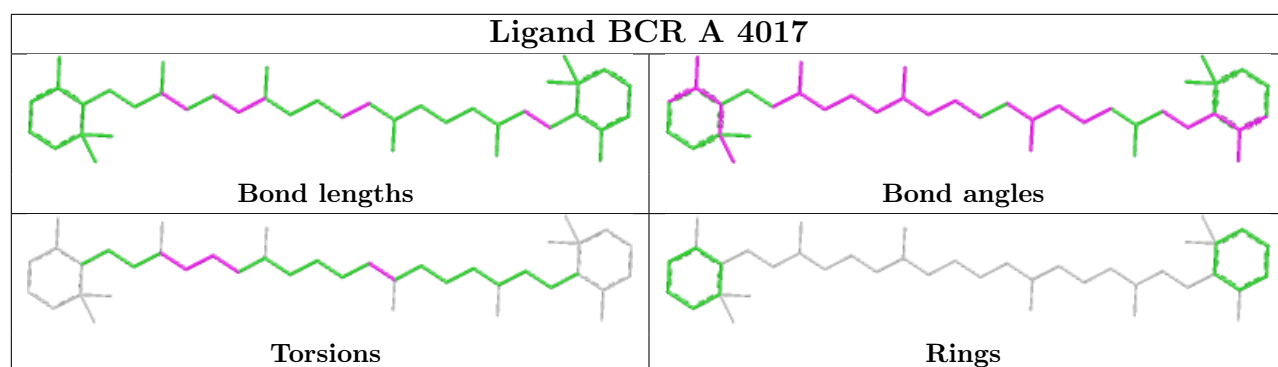


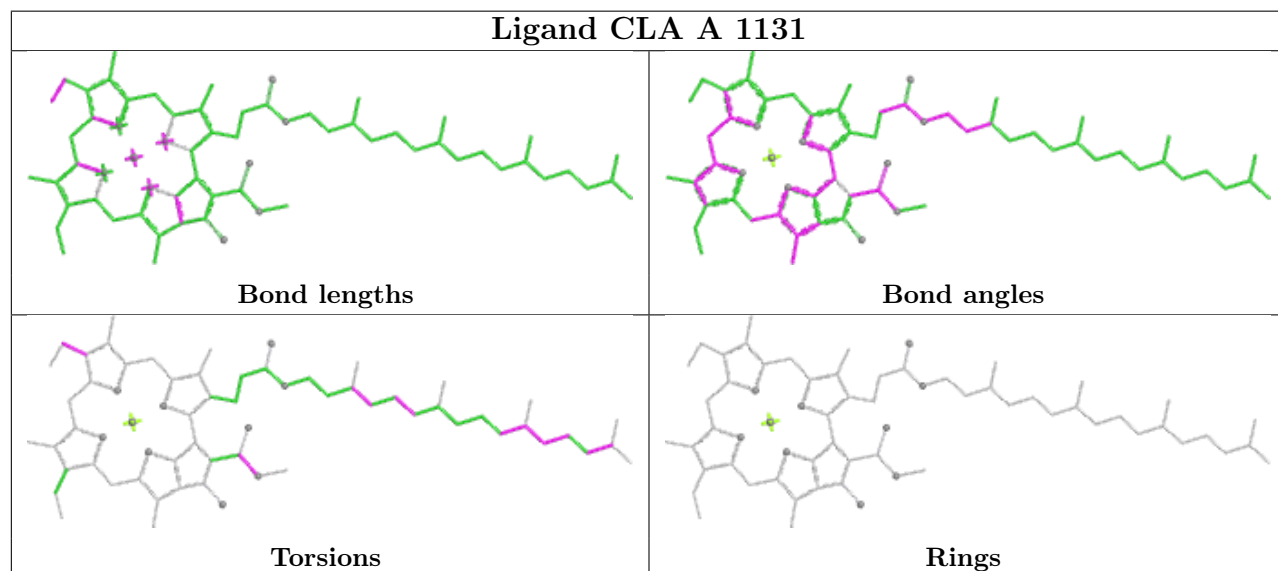
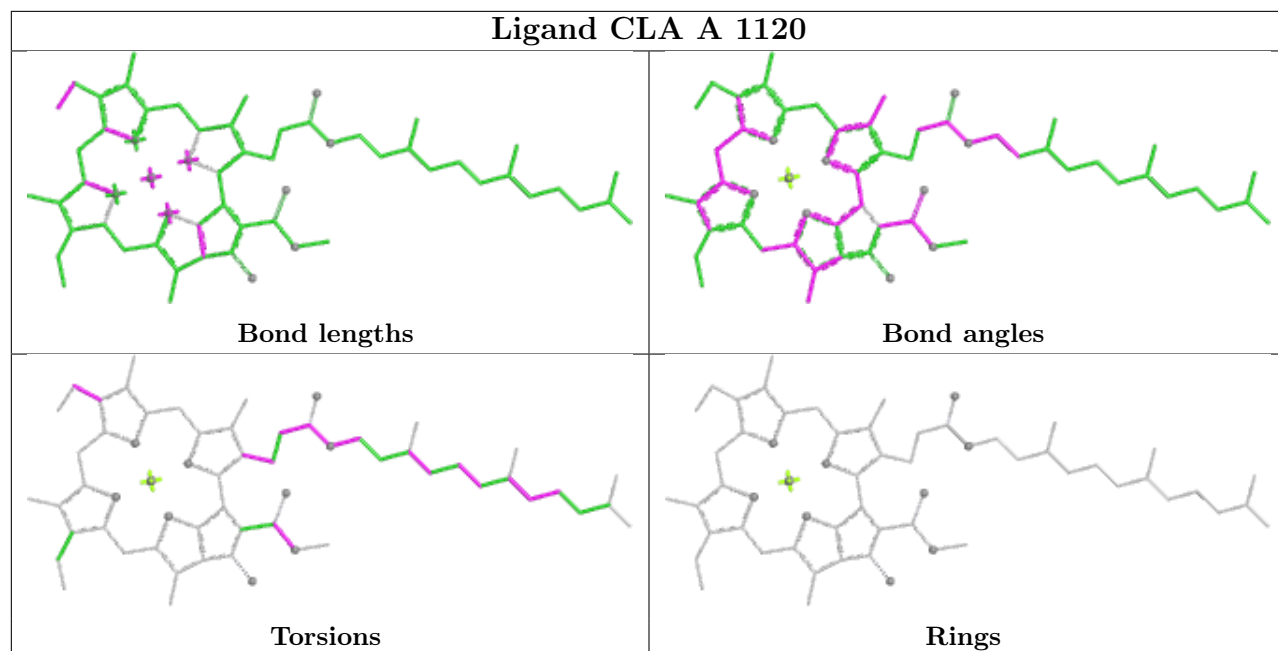


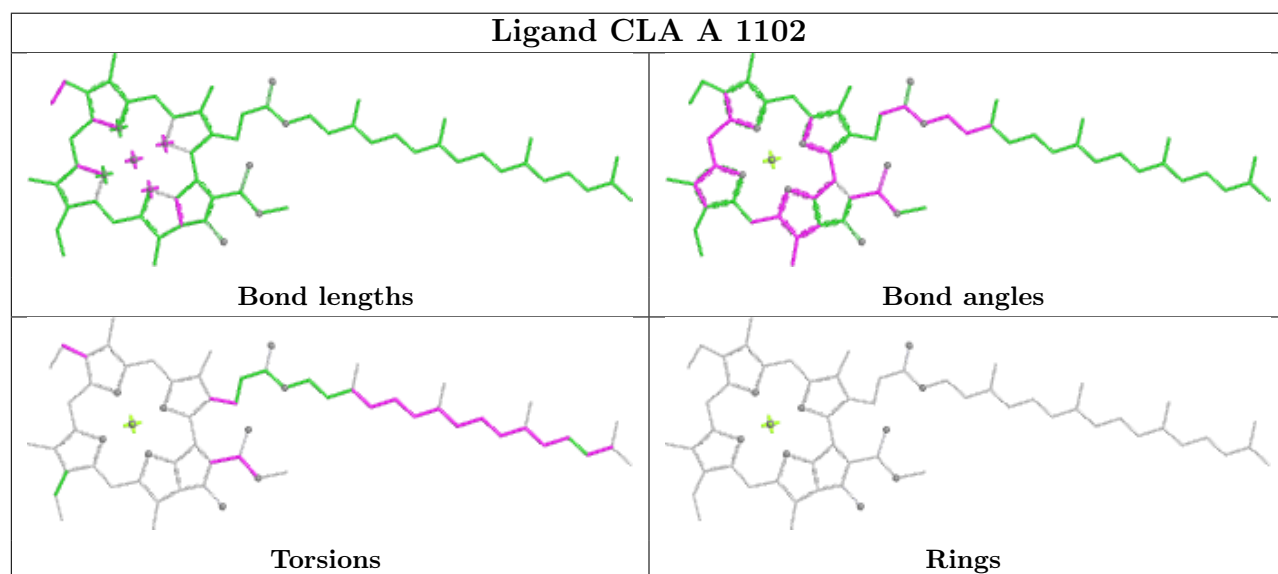
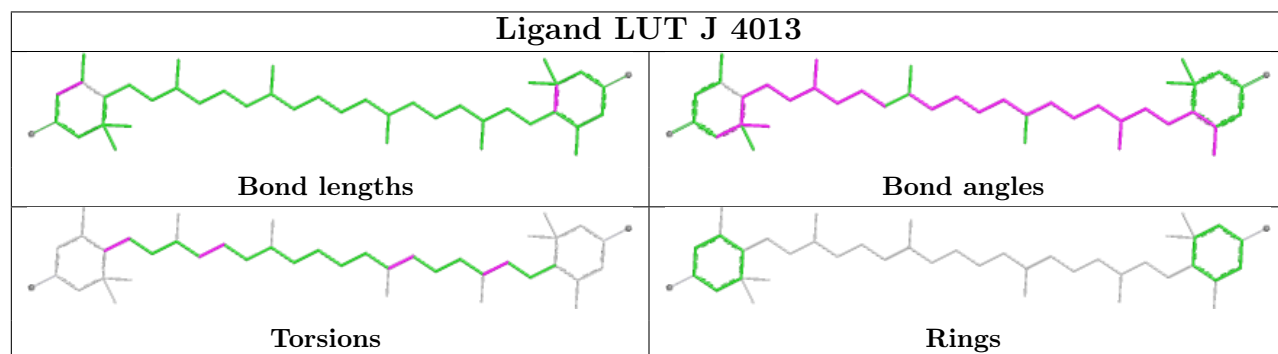
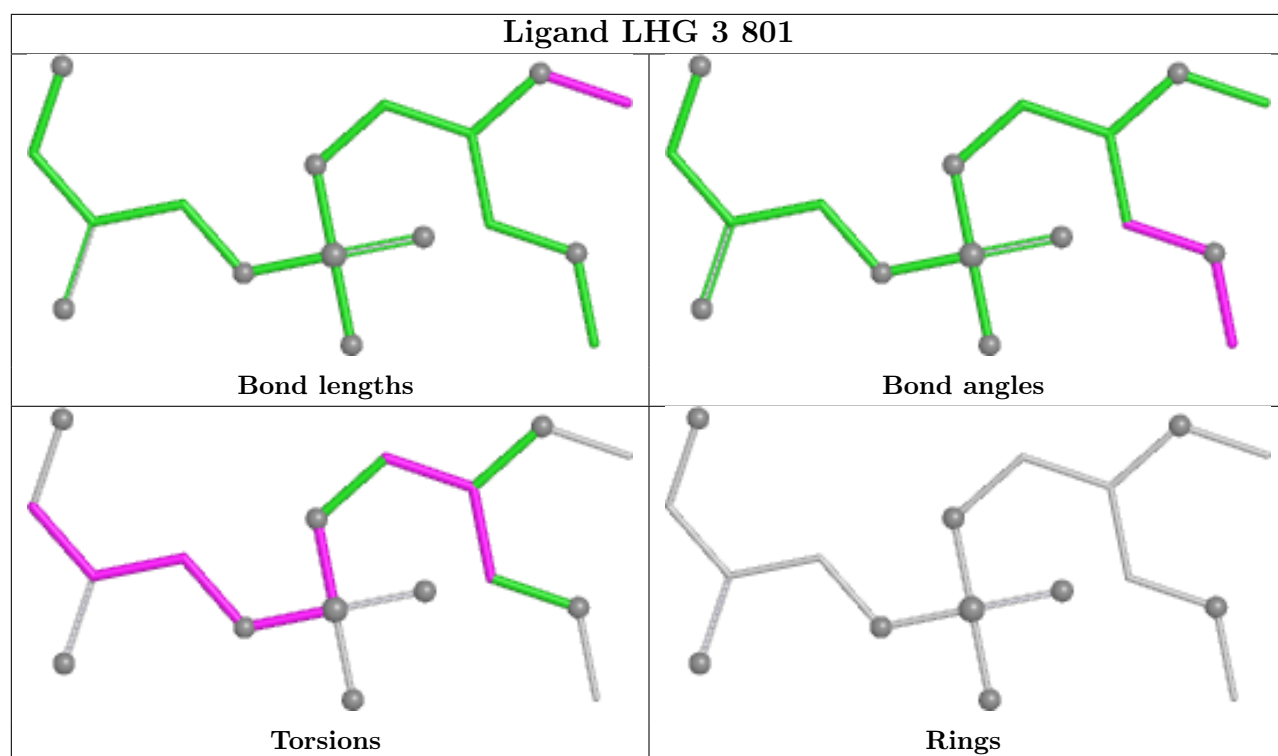




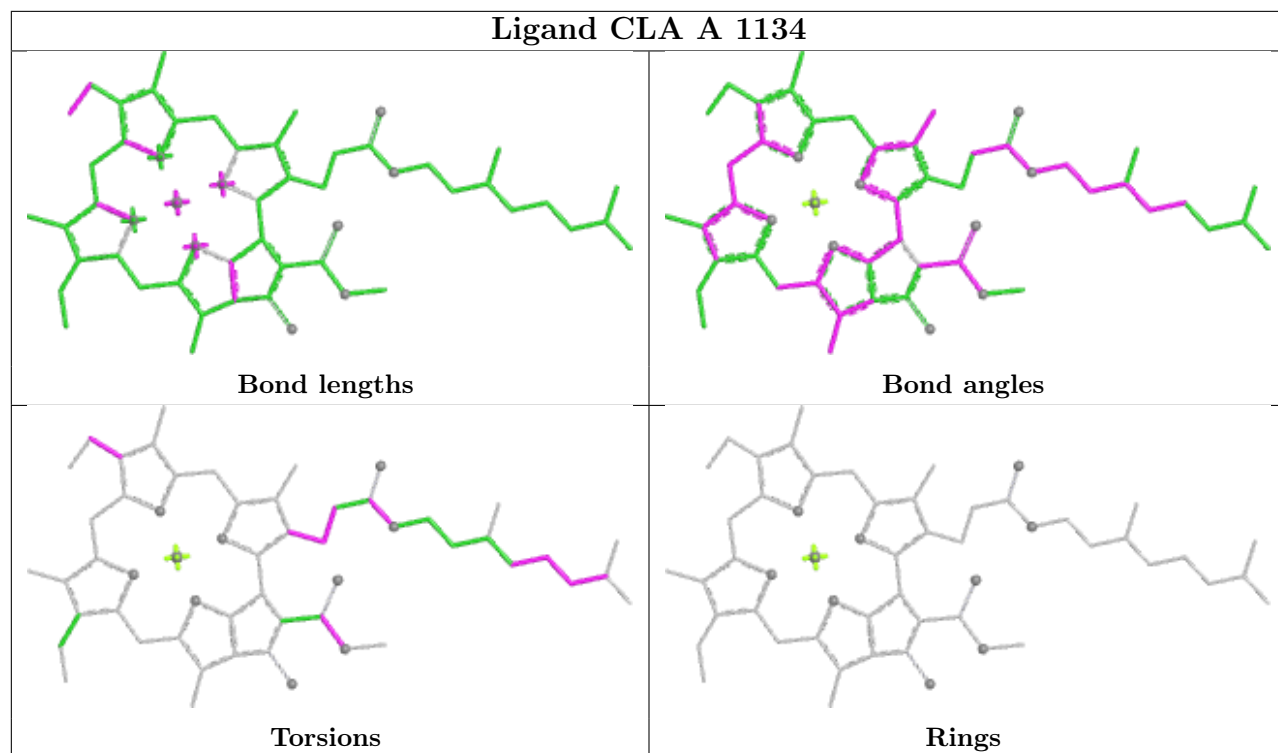




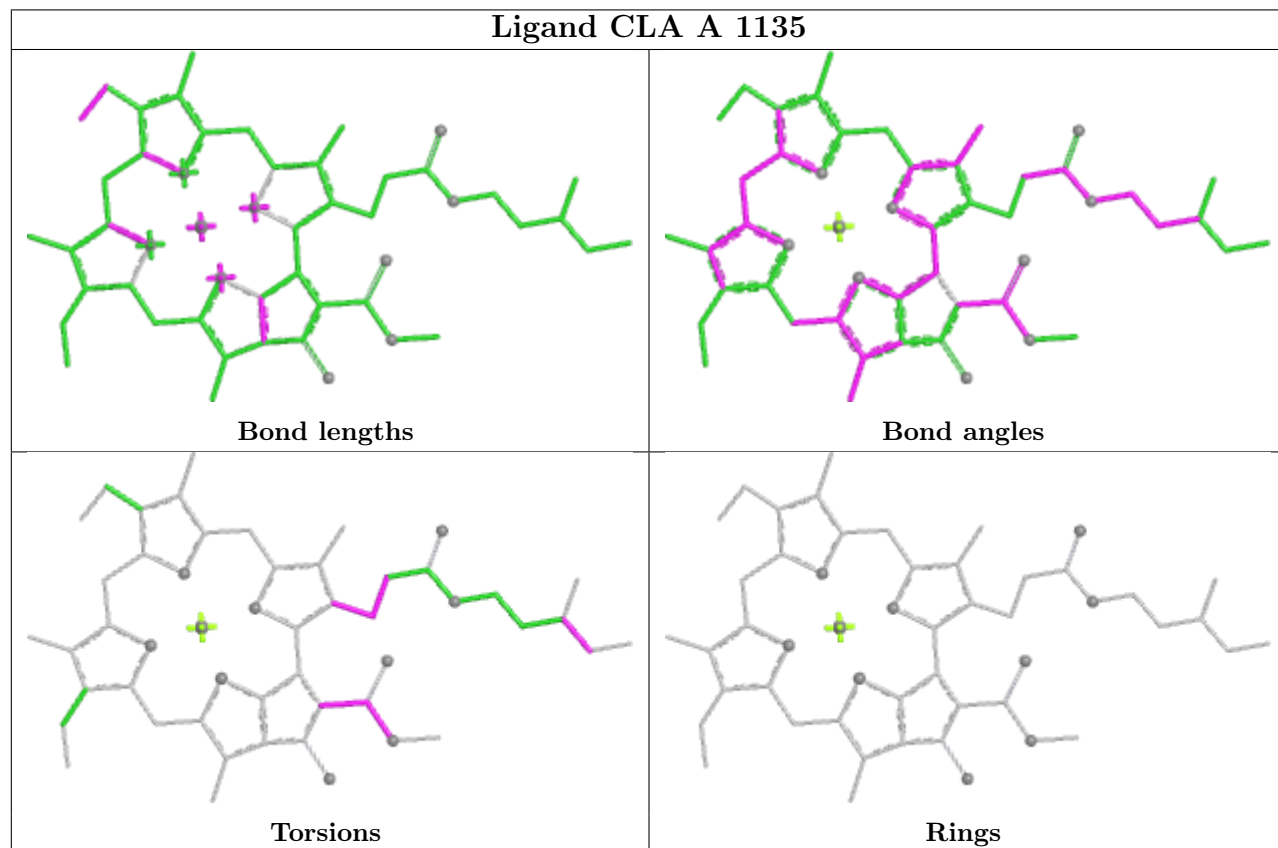


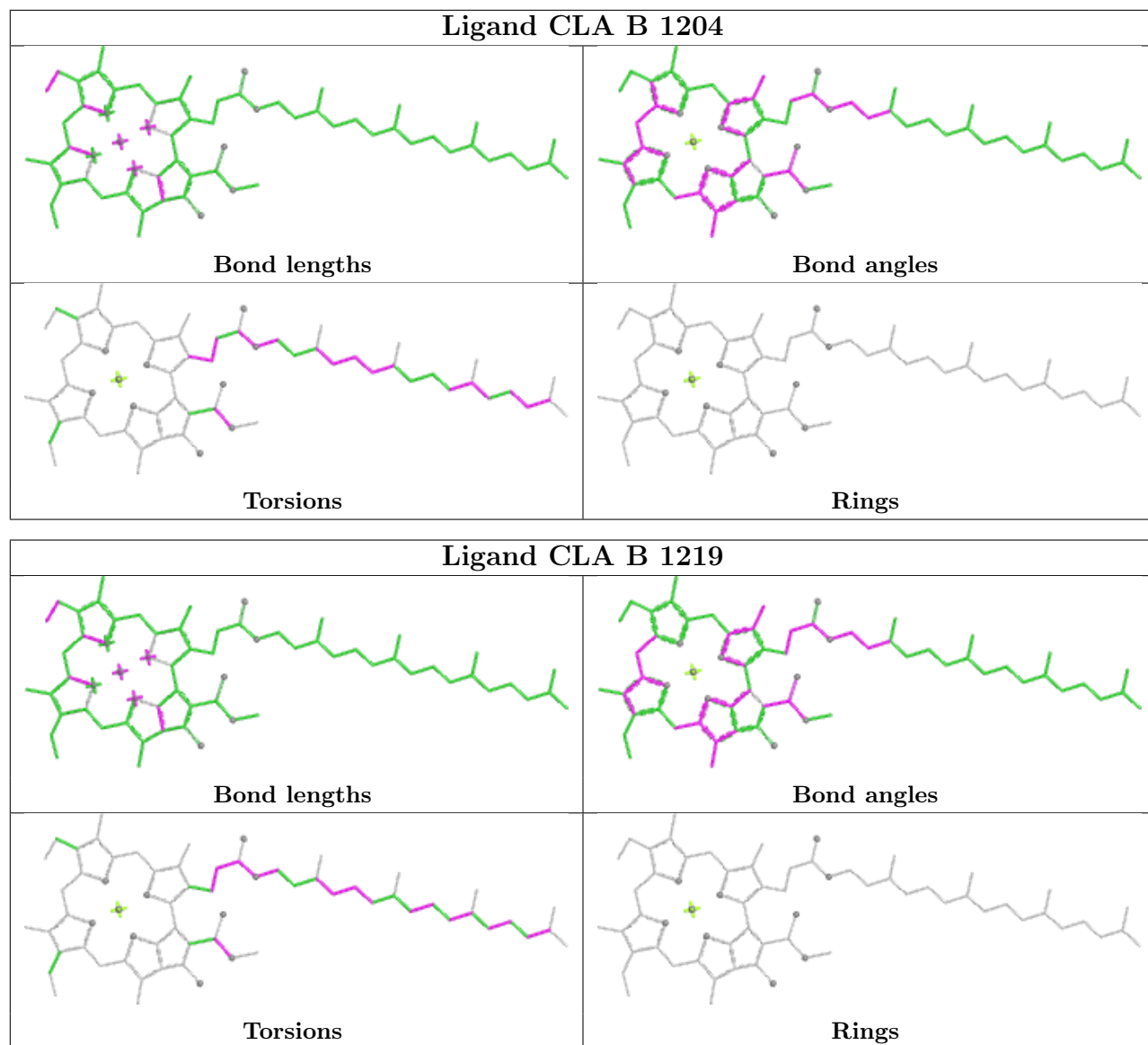


Ligand CLA A 1134

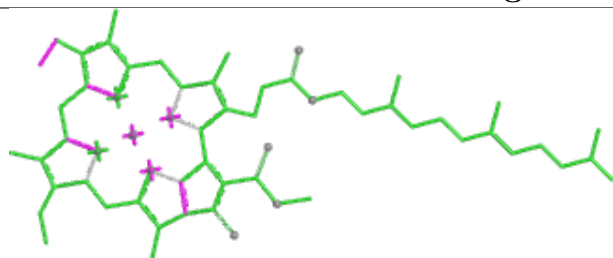


Ligand CLA A 1135

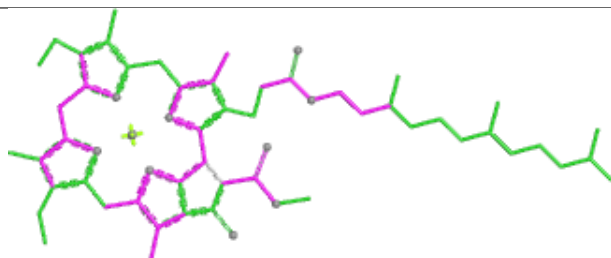




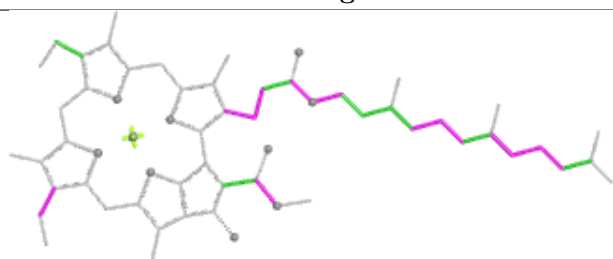
Ligand CLA H 1701



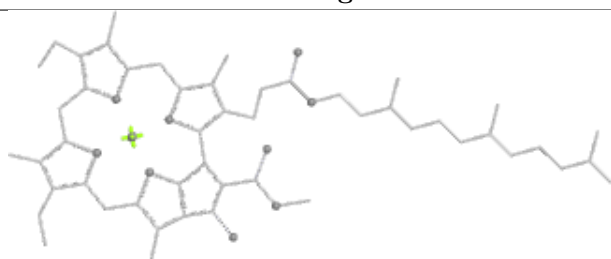
Bond lengths



Bond angles

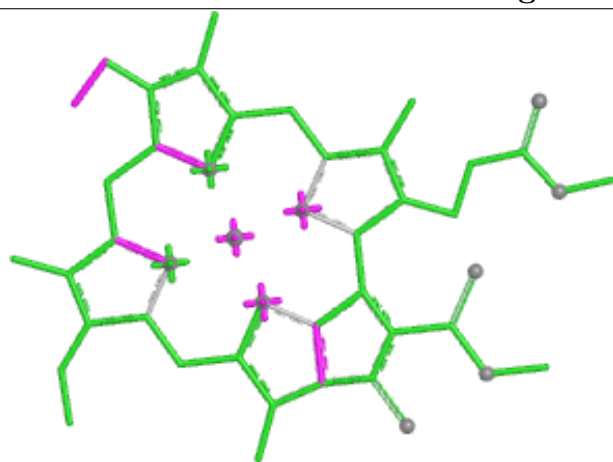


Torsions

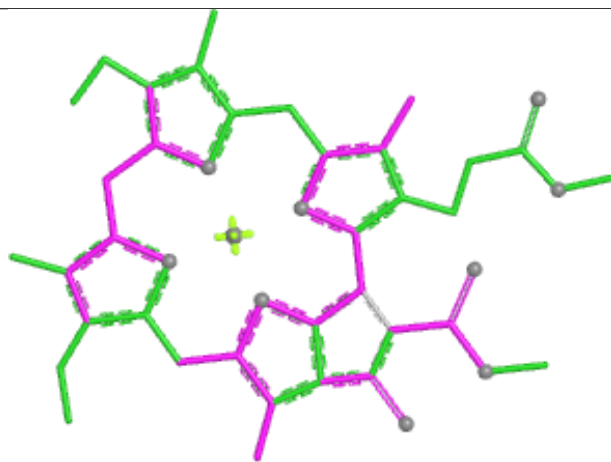


Rings

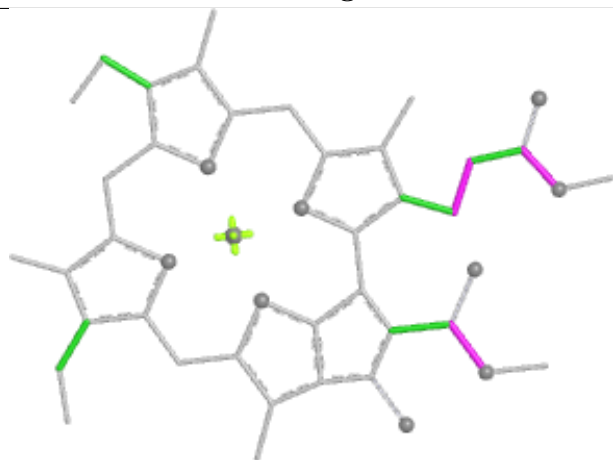
Ligand CLA 1 607



Bond lengths



Bond angles

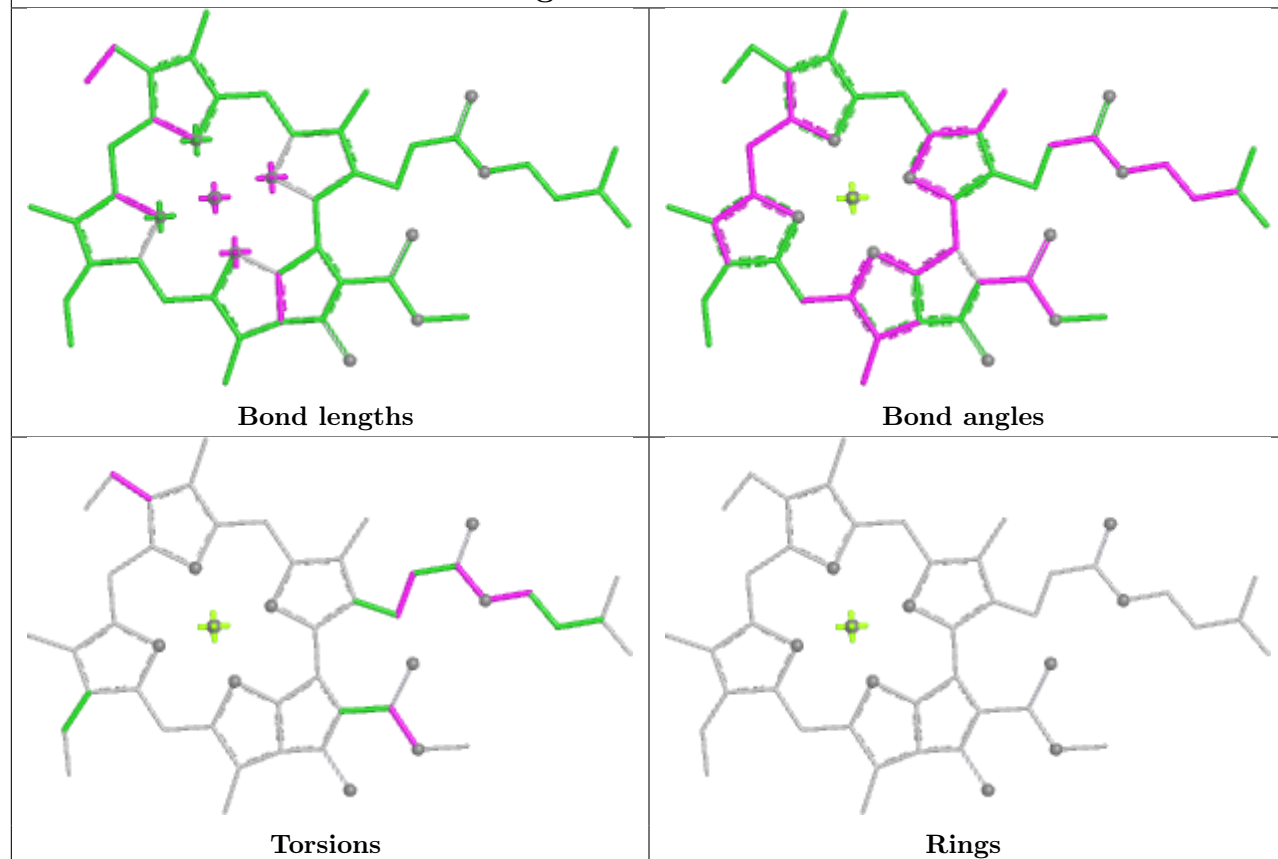


Torsions

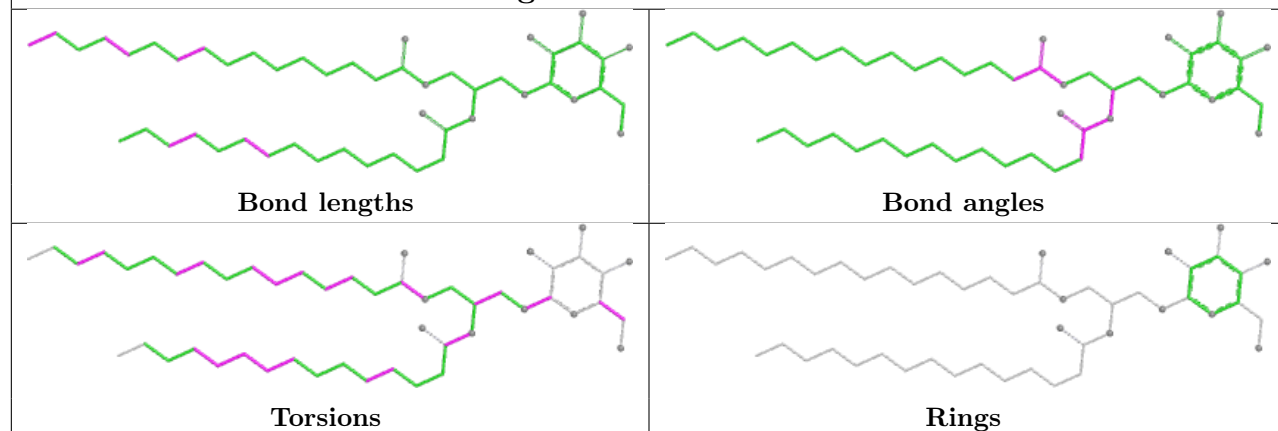


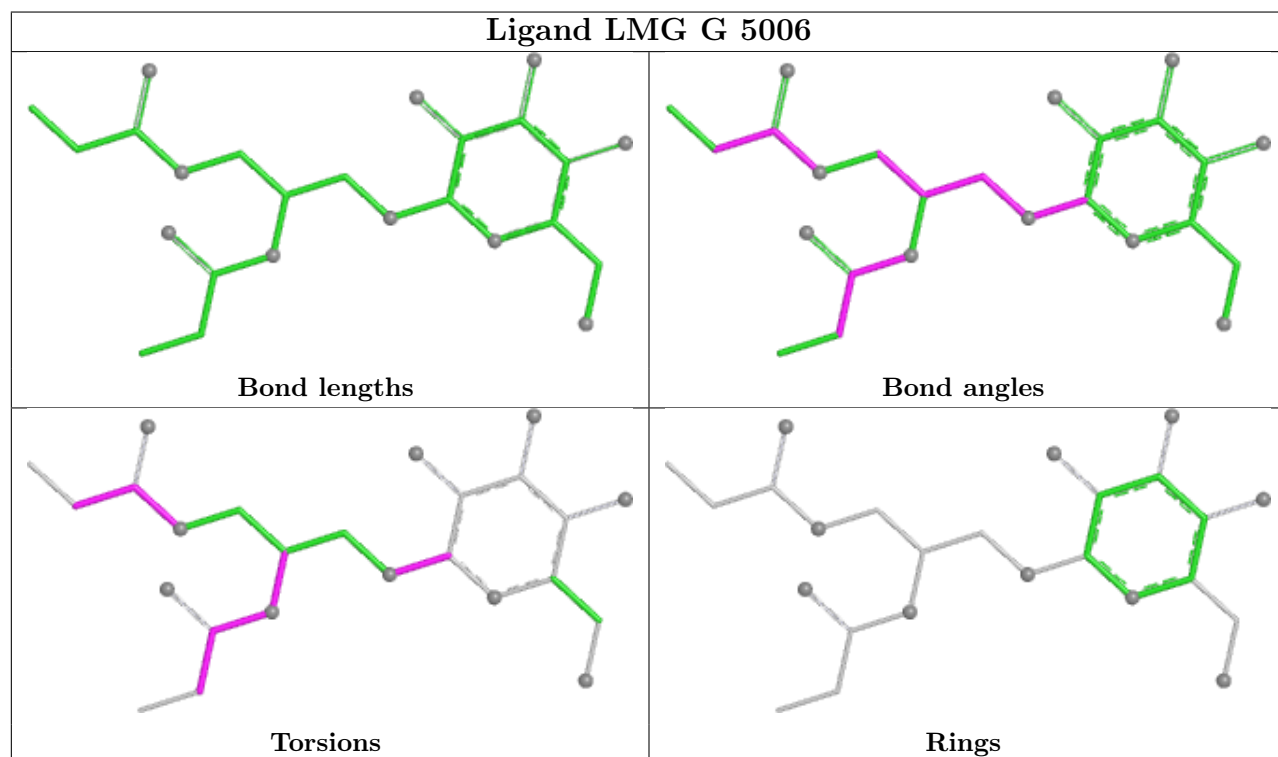
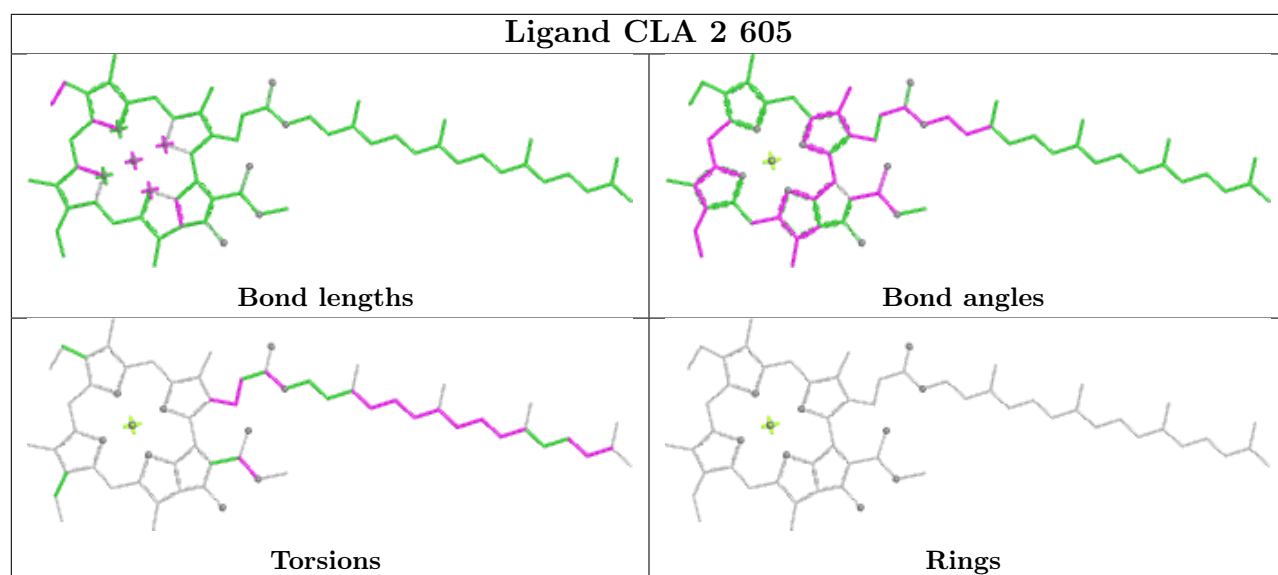
Rings

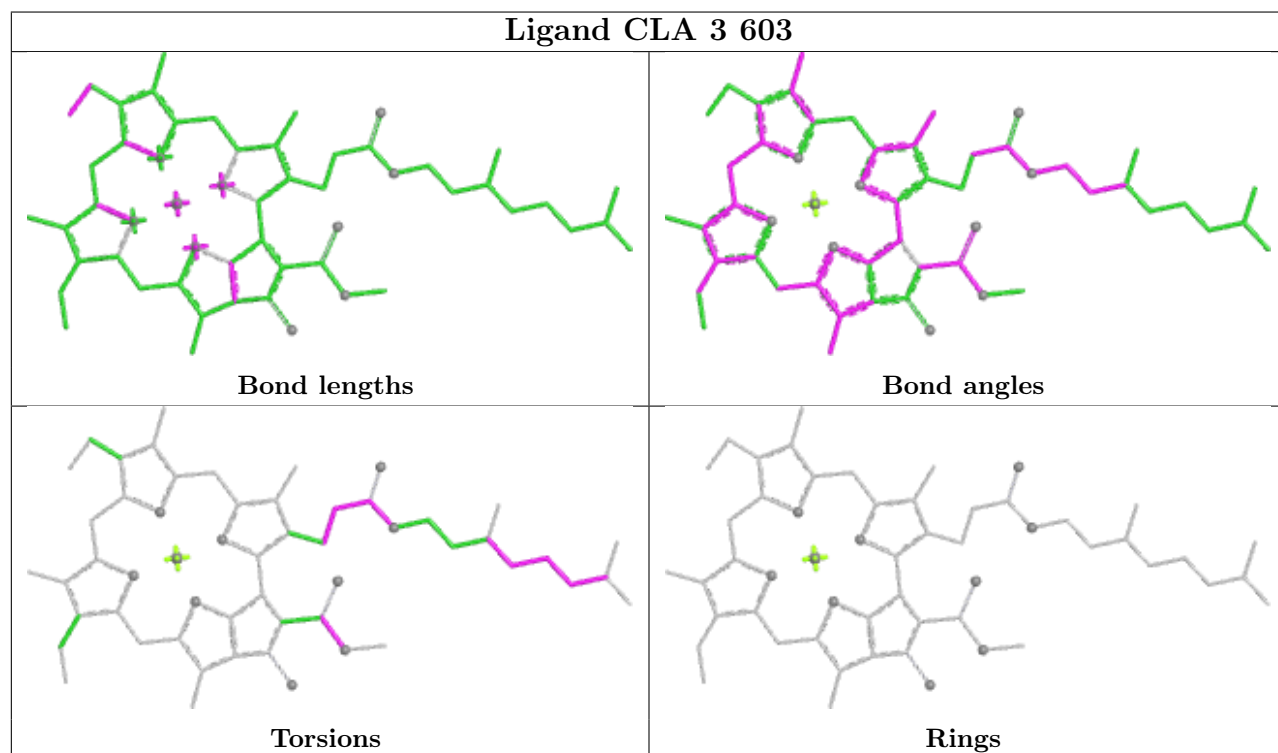
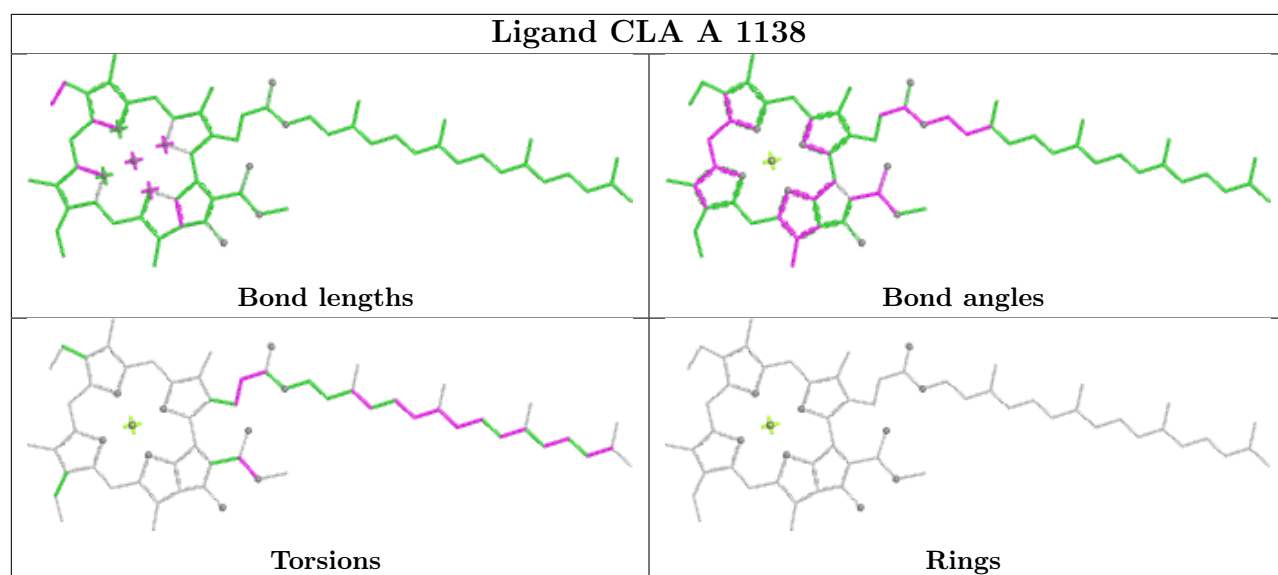
Ligand CLA 2 608

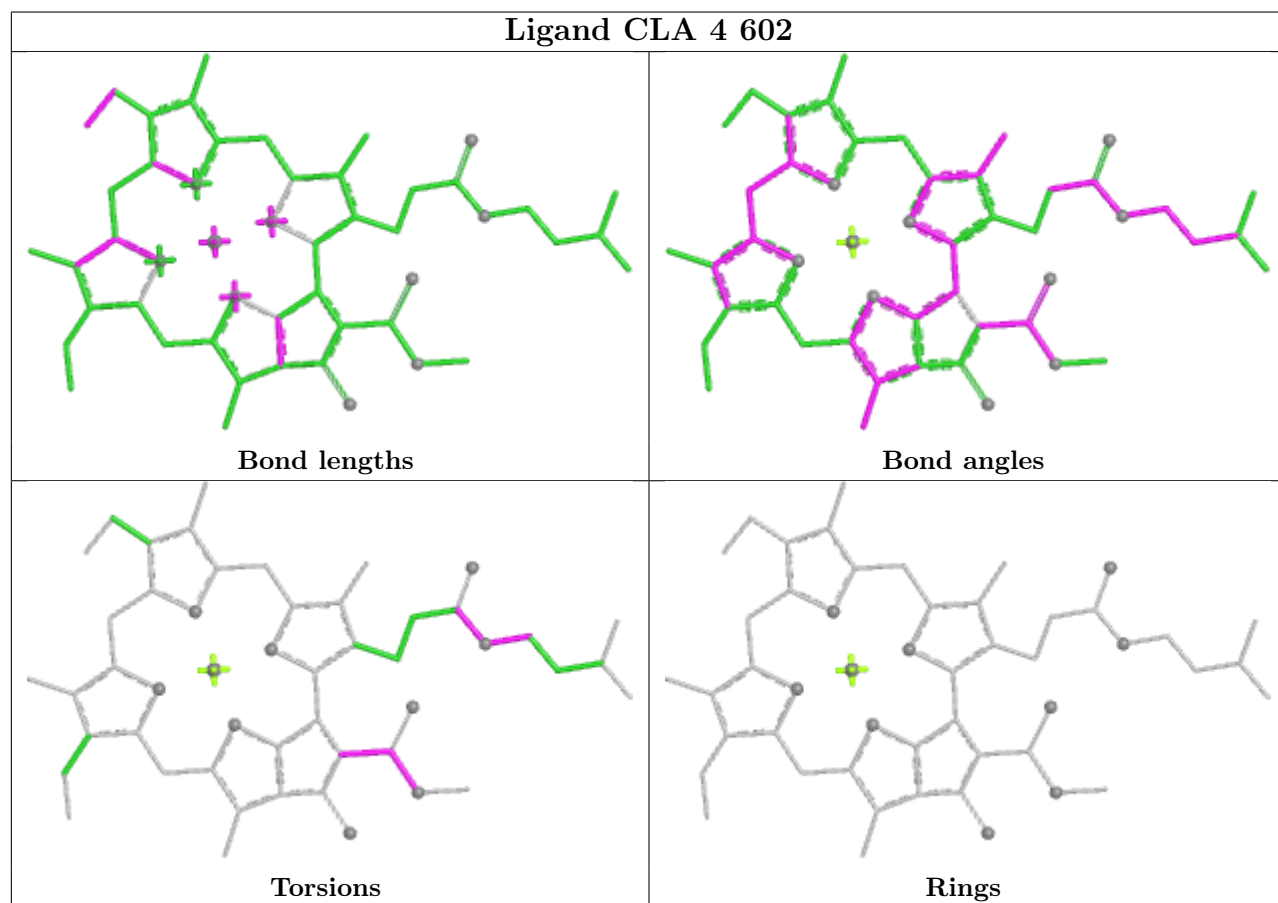
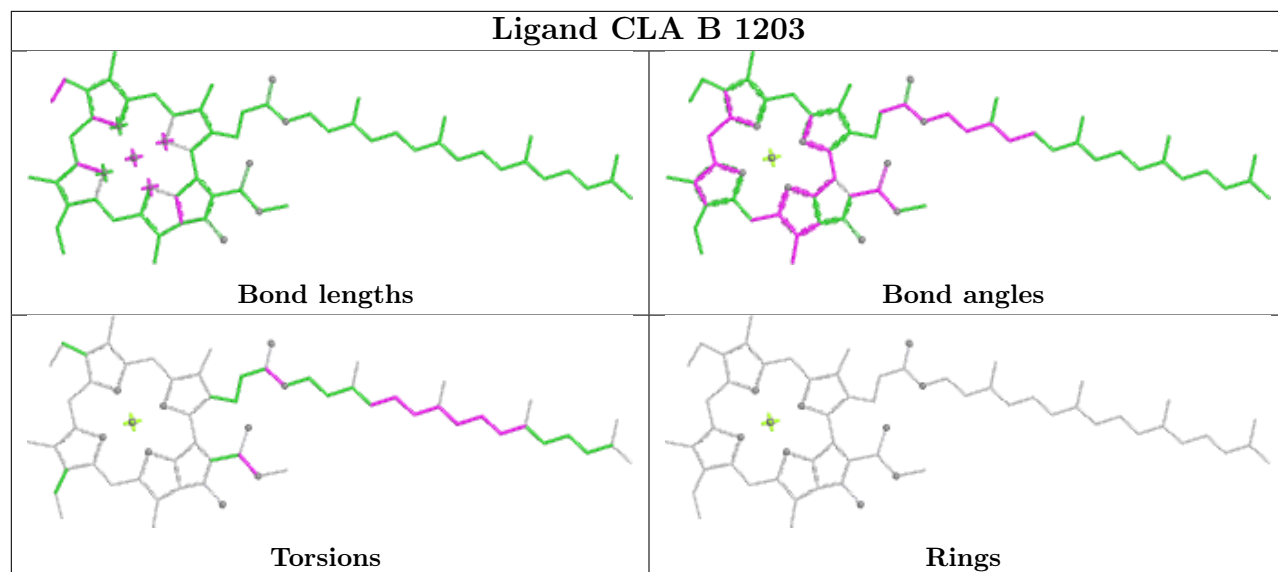


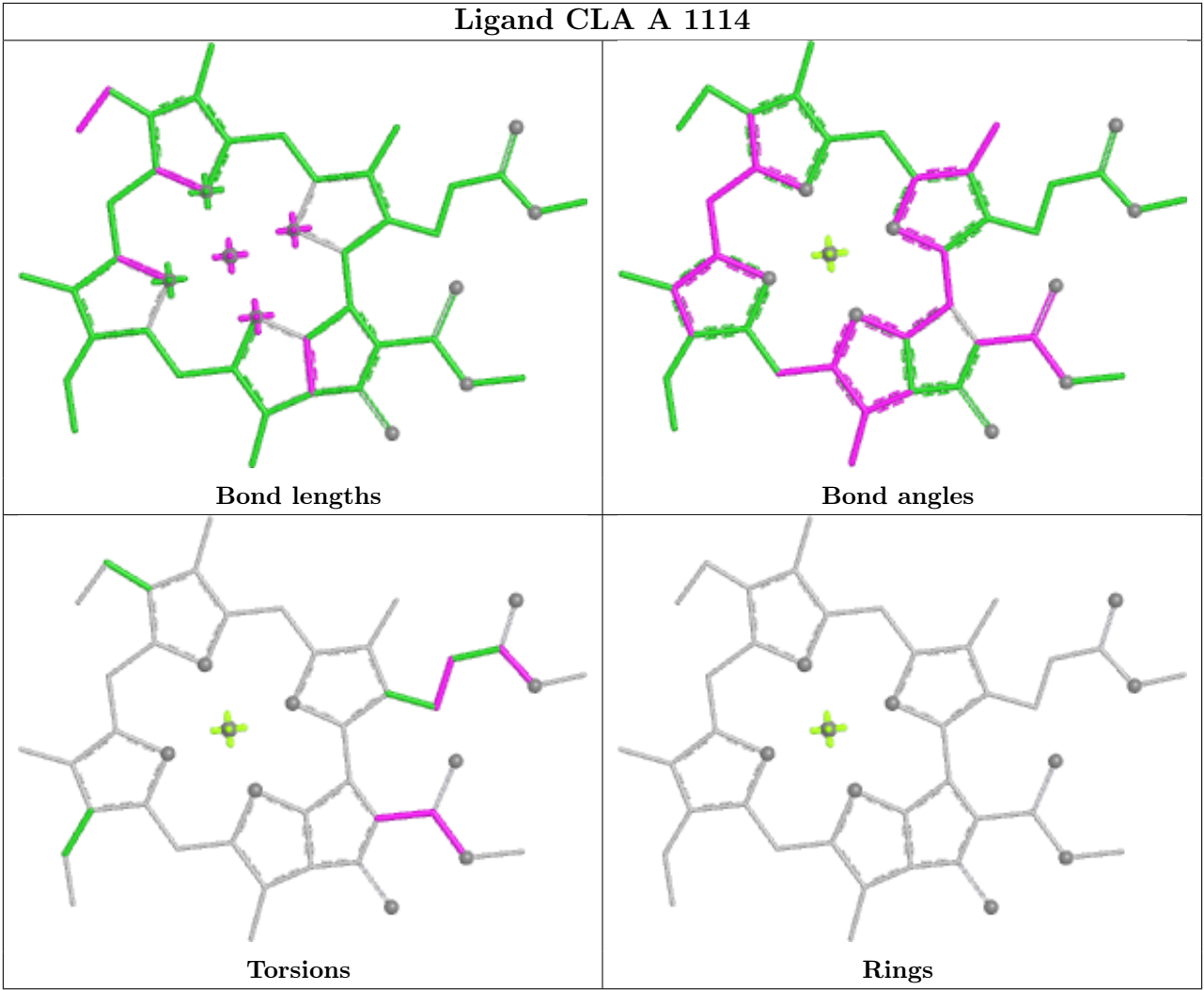
Ligand LMG G 5002











5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
17	N	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	N	35:LEU	C	36:PRO	N	1.19

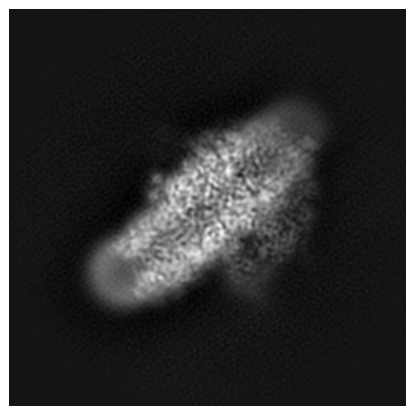
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-10798. These allow visual inspection of the internal detail of the map and identification of artifacts.

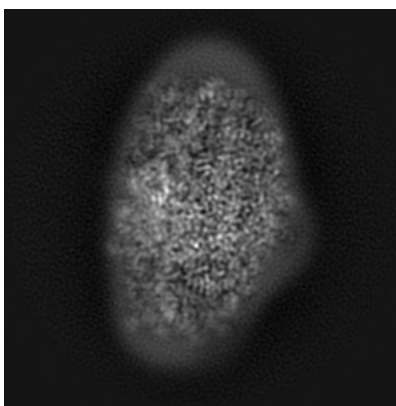
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

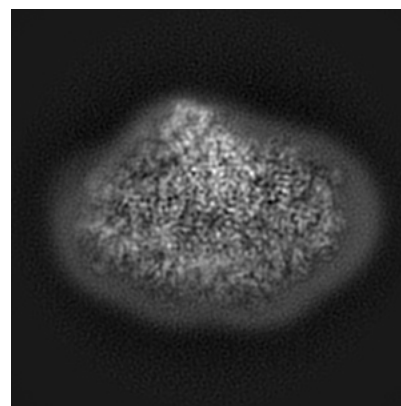
6.1.1 Primary map



X

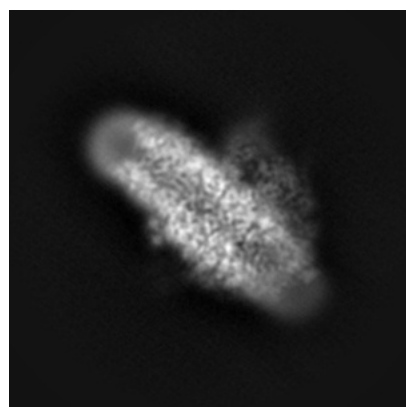


Y

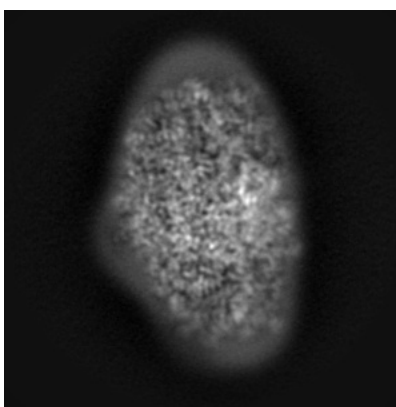


Z

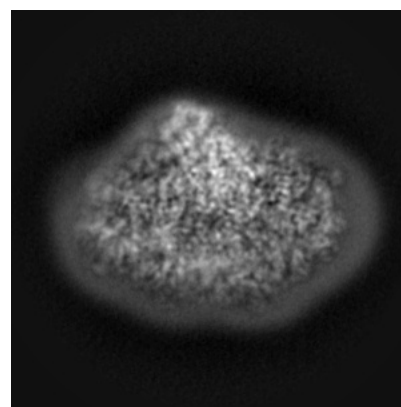
6.1.2 Raw map



X



Y

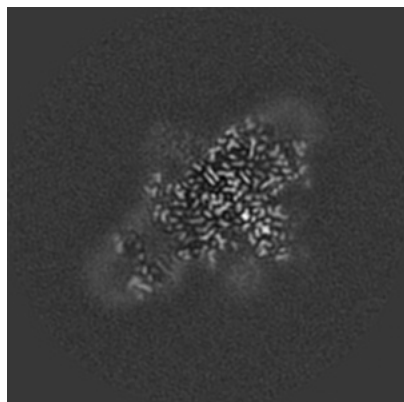


Z

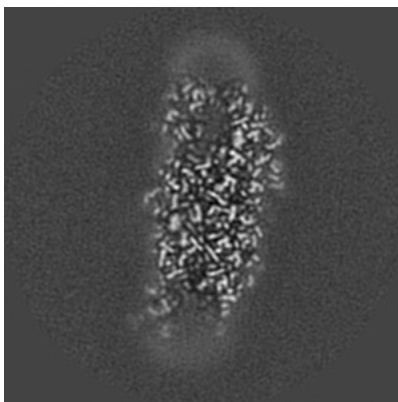
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

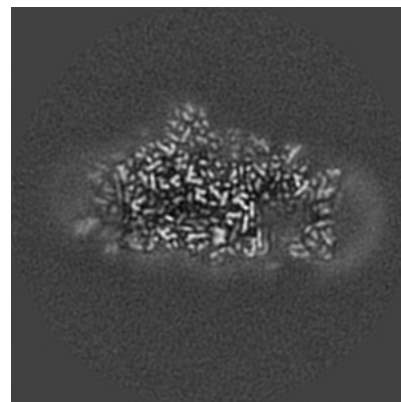
6.2.1 Primary map



X Index: 150

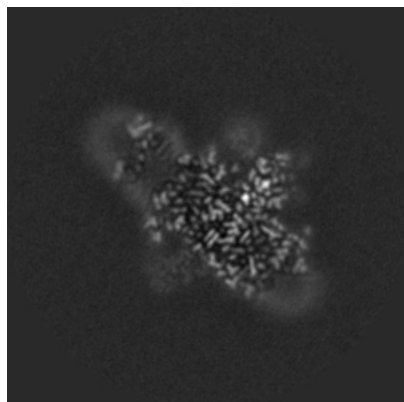


Y Index: 150

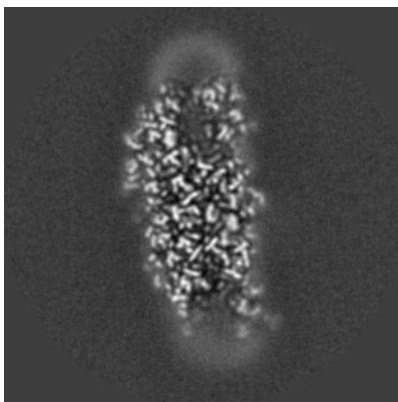


Z Index: 150

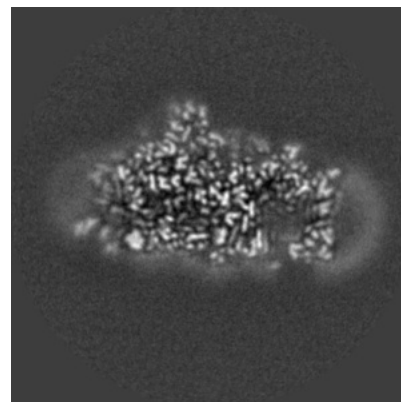
6.2.2 Raw map



X Index: 150



Y Index: 150

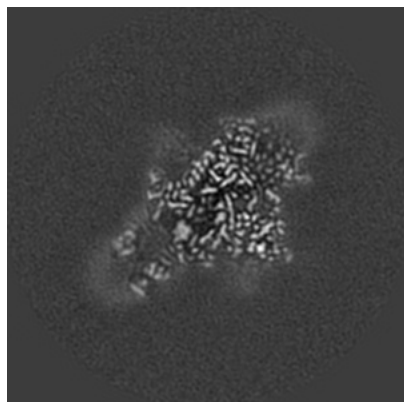


Z Index: 150

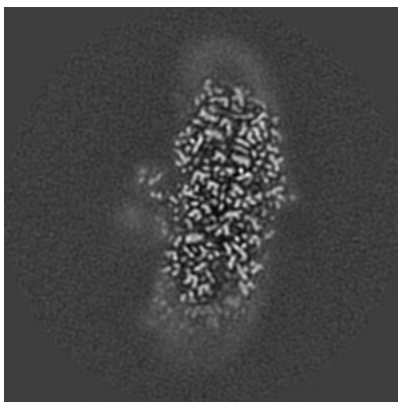
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

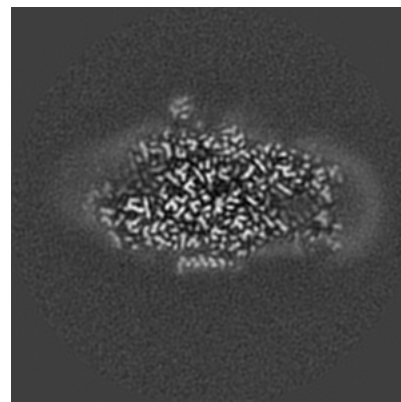
6.3.1 Primary map



X Index: 154

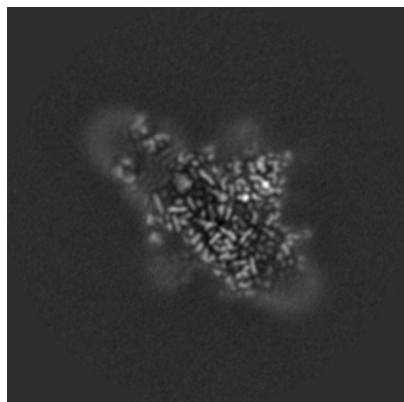


Y Index: 164

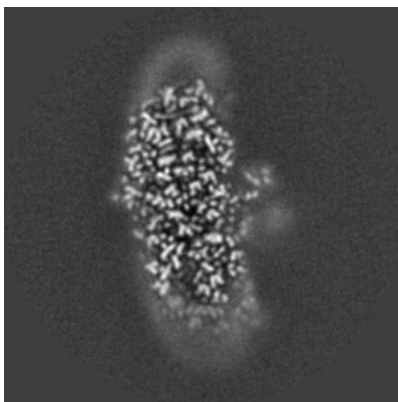


Z Index: 161

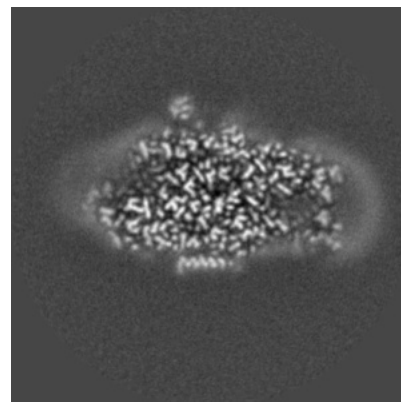
6.3.2 Raw map



X Index: 153



Y Index: 164

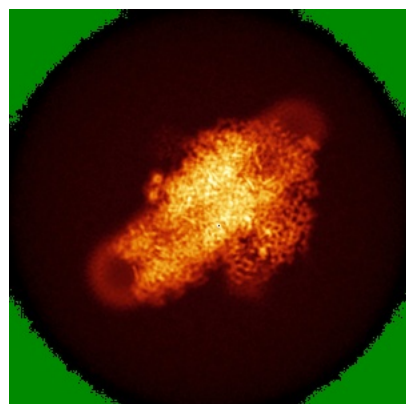


Z Index: 138

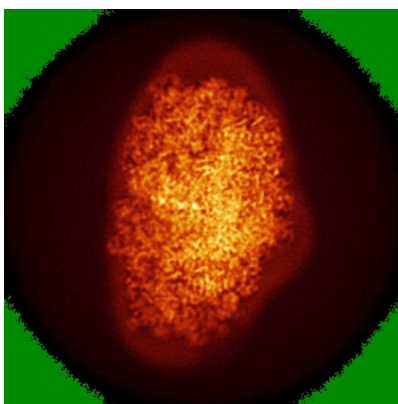
The images above show the largest variance slices of the map in three orthogonal directions.

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

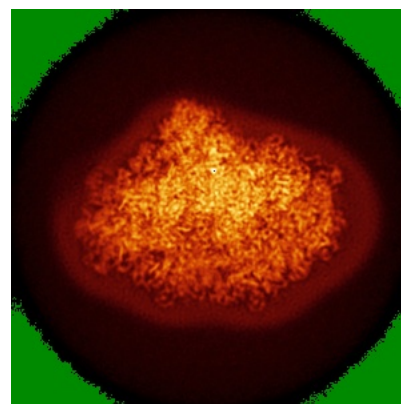
6.4.1 Primary map



X

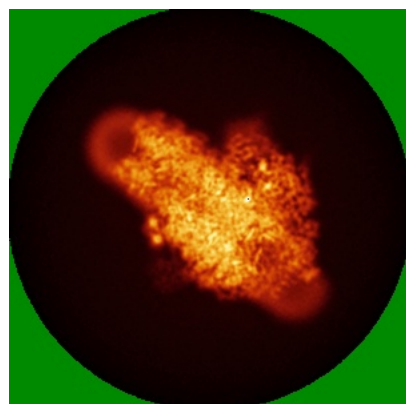


Y

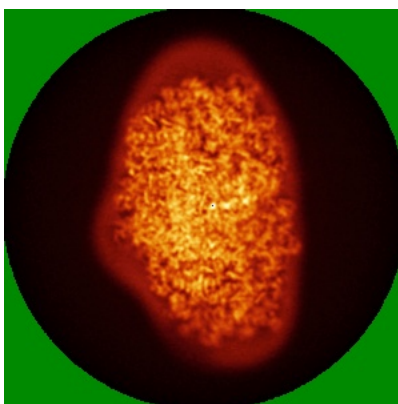


Z

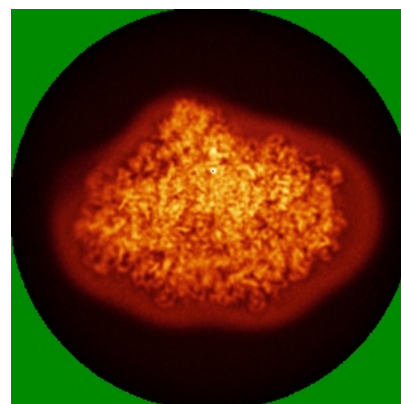
6.4.2 Raw map



X



Y

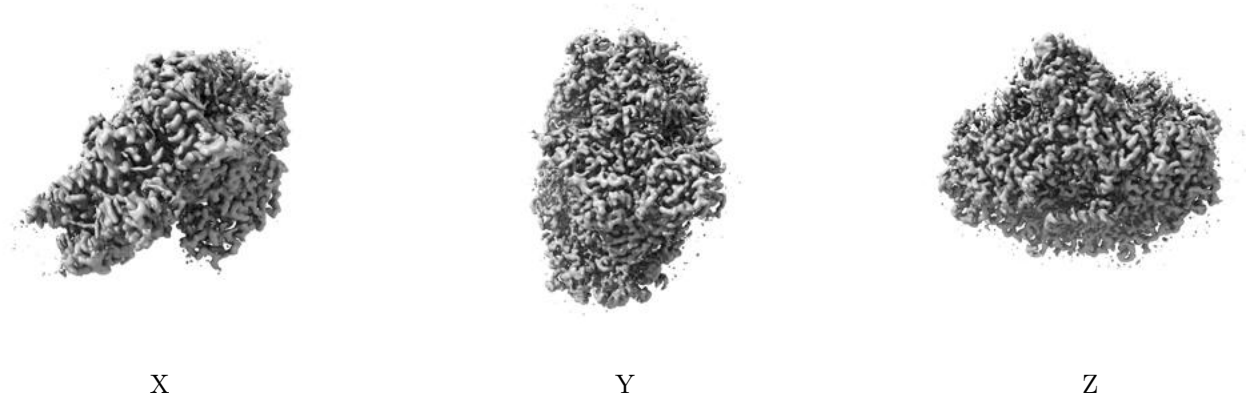


Z

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

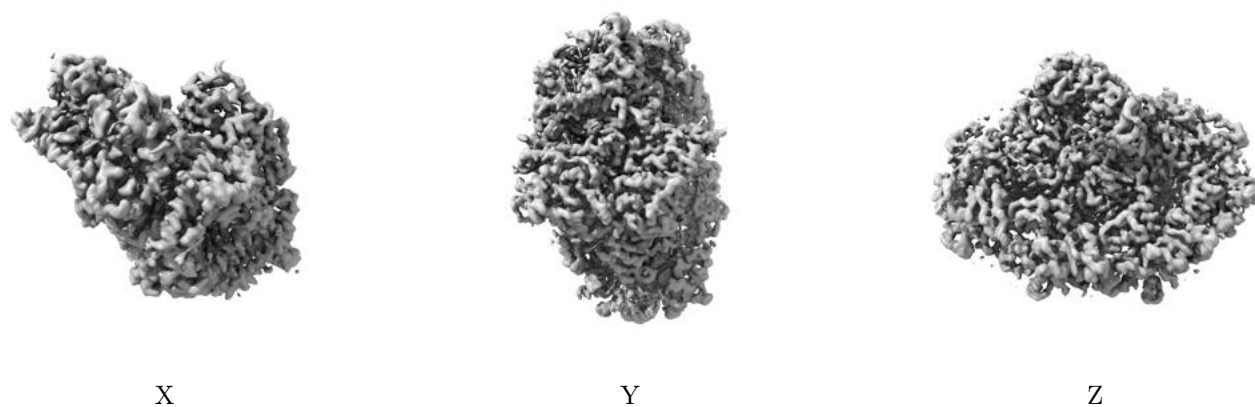
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.022. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

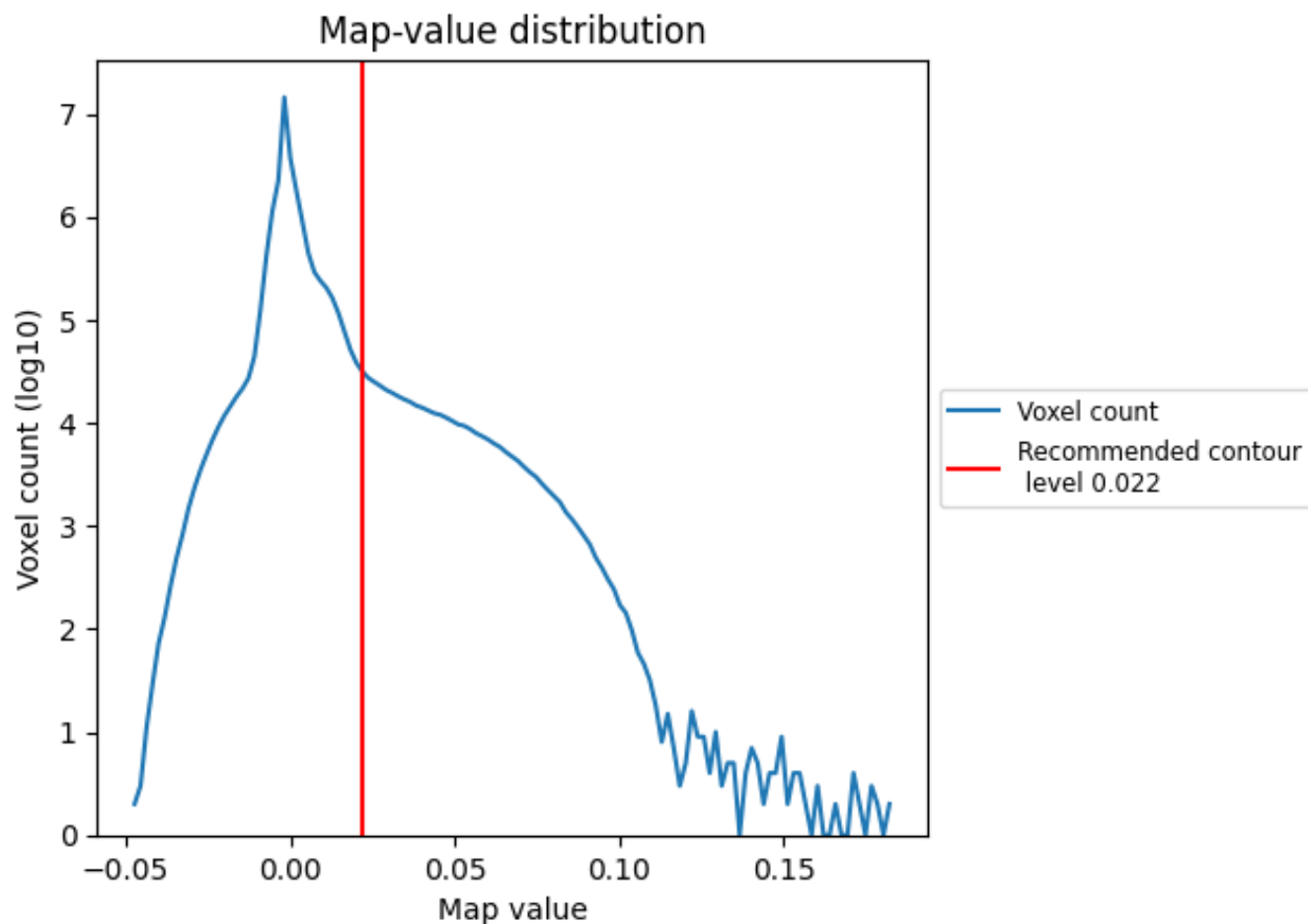
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

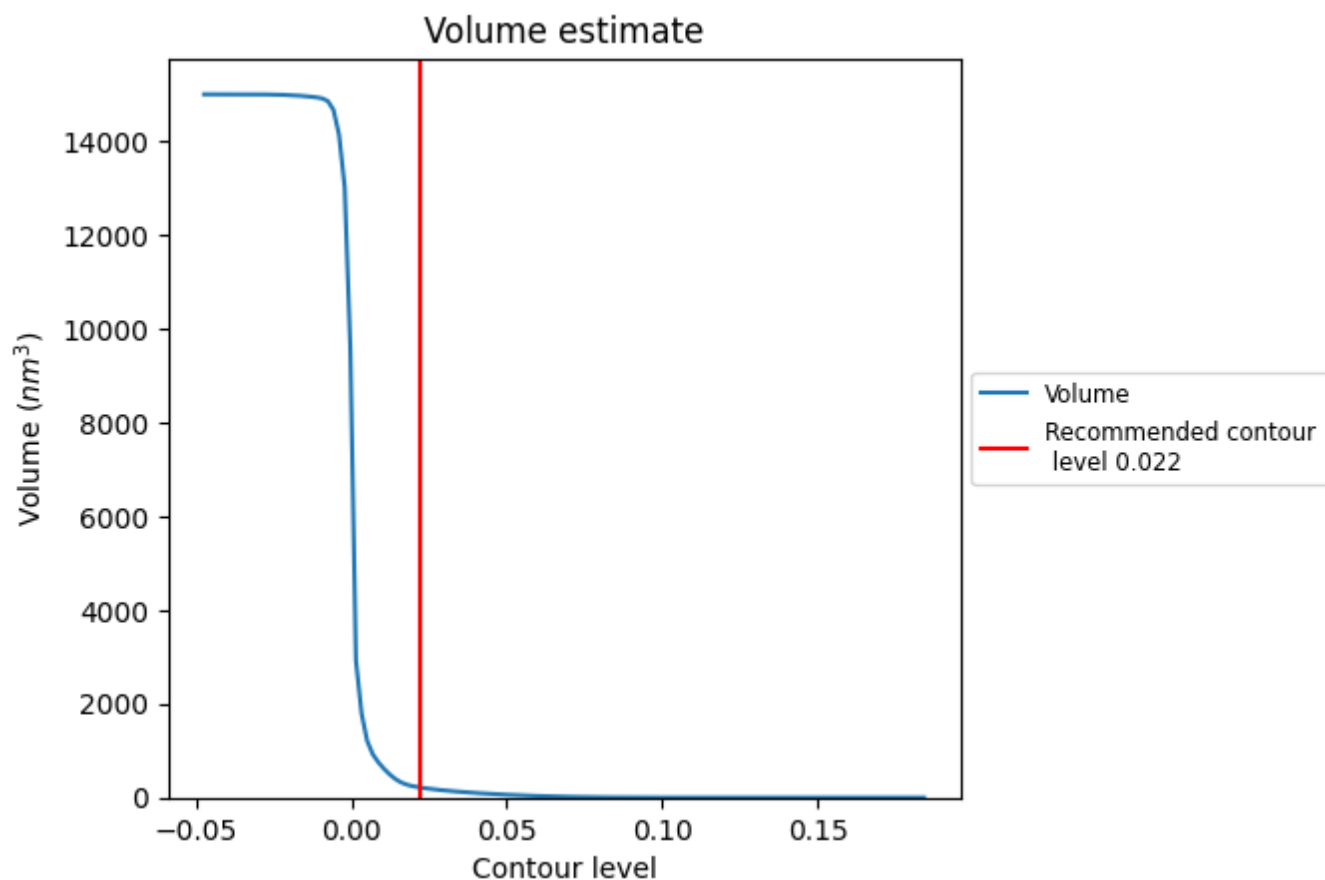
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

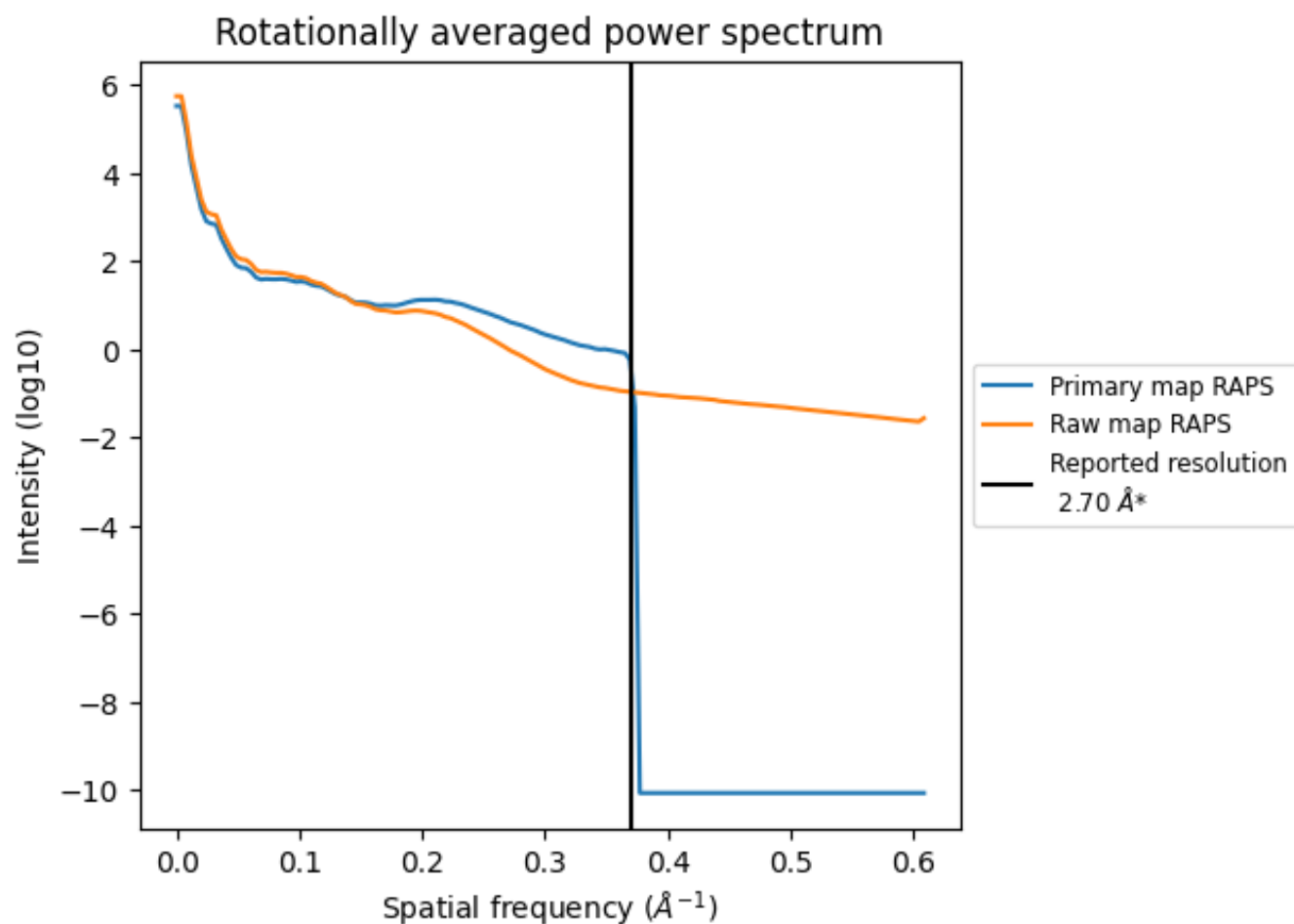
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 215 nm³; this corresponds to an approximate mass of 195 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 ⓘ

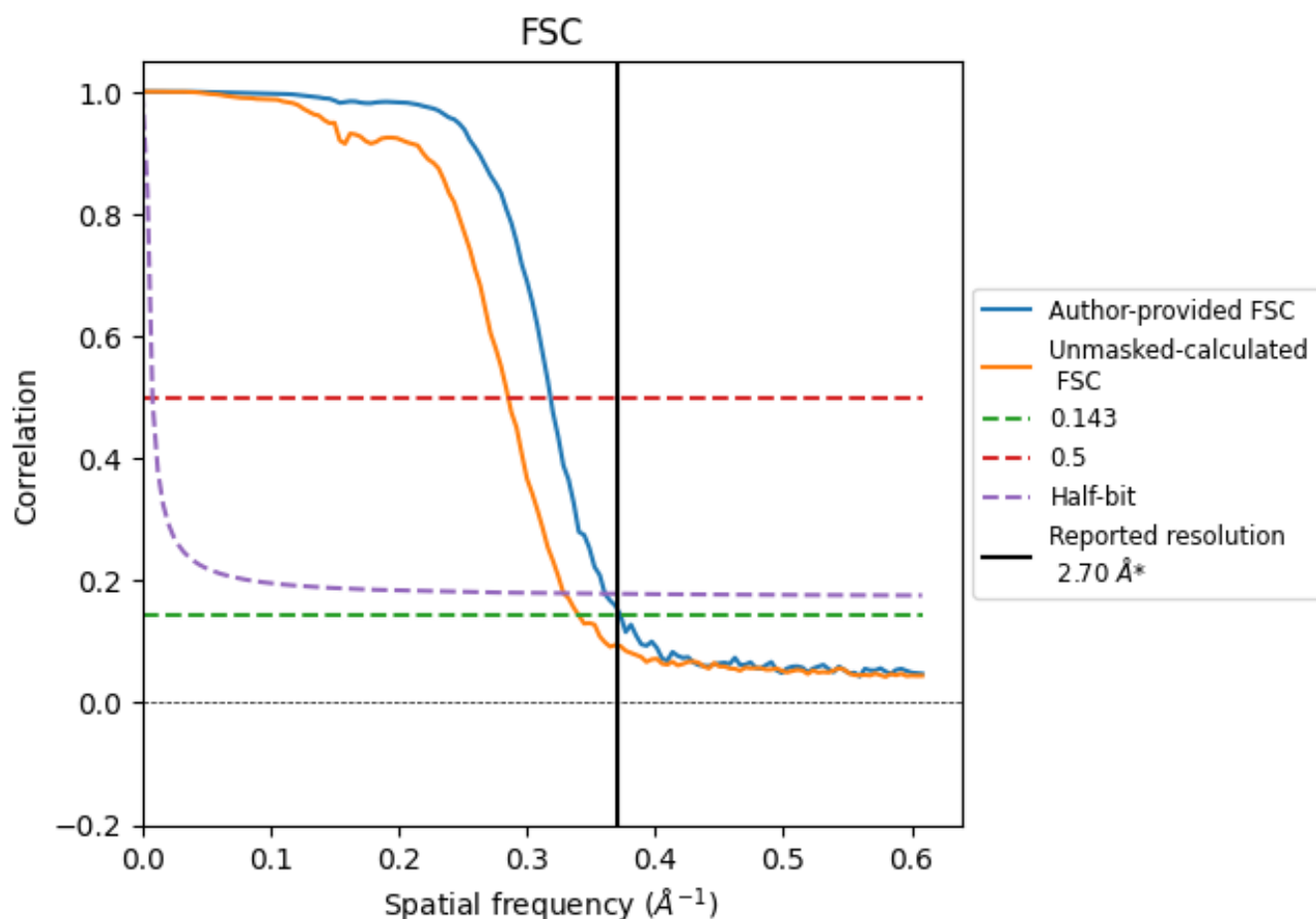


*Reported resolution corresponds to spatial frequency of 0.370 $\text{\AA}^{-1}$

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 0.370 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

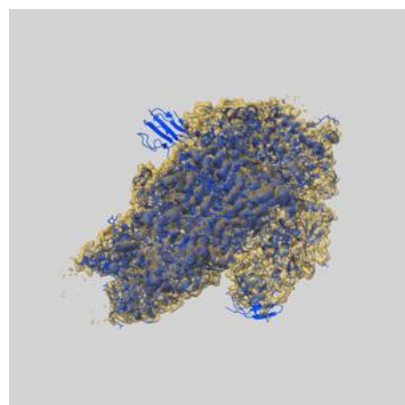
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.70	-	-
Author-provided FSC curve	2.68	3.14	2.77
Unmasked-calculated*	2.94	3.50	3.04

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

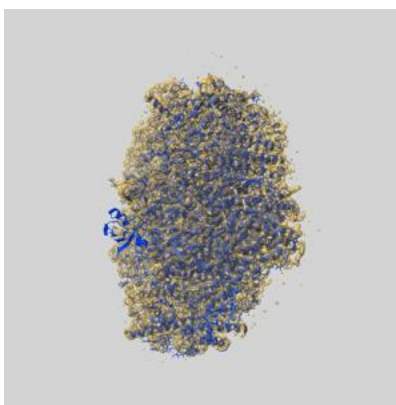
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-10798 and PDB model 6YEZ. Per-residue inclusion information can be found in section 3 on page 31.

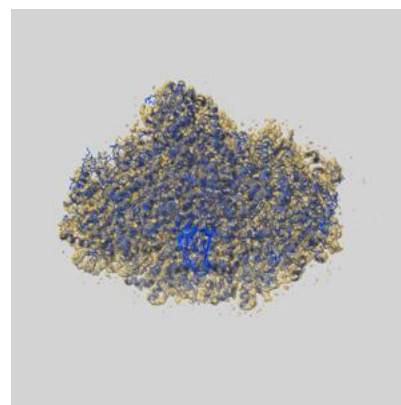
9.1 Map-model overlay [i](#)



X



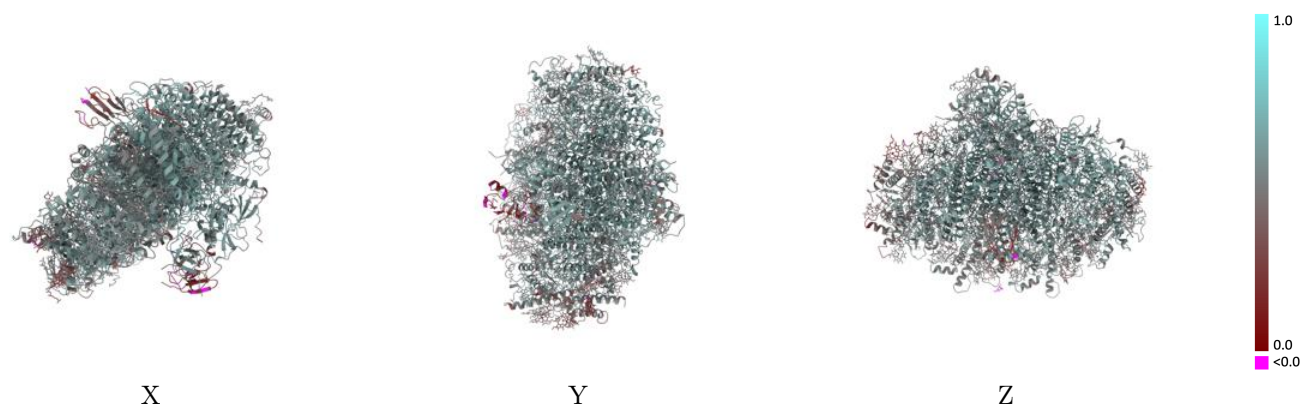
Y



Z

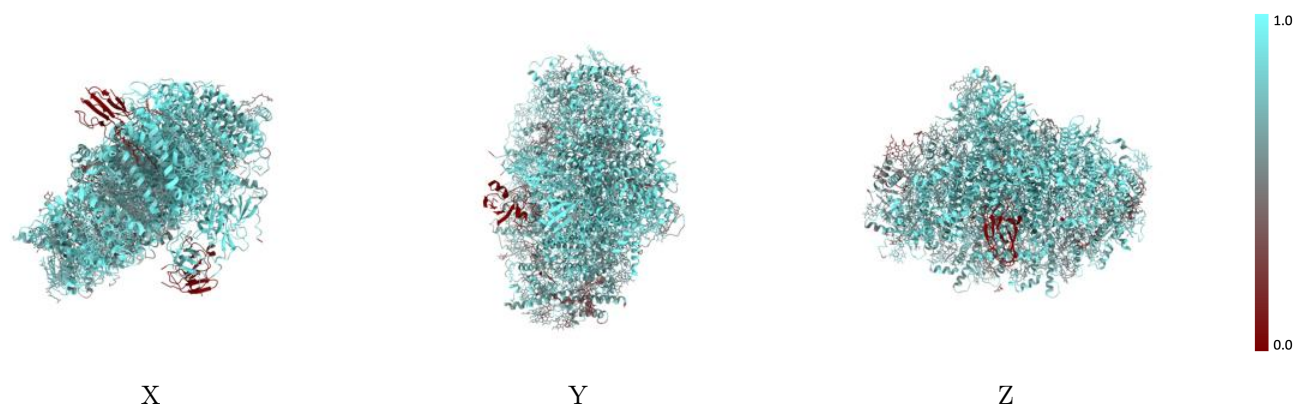
The images above show the 3D surface view of the map at the recommended contour level 0.022 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



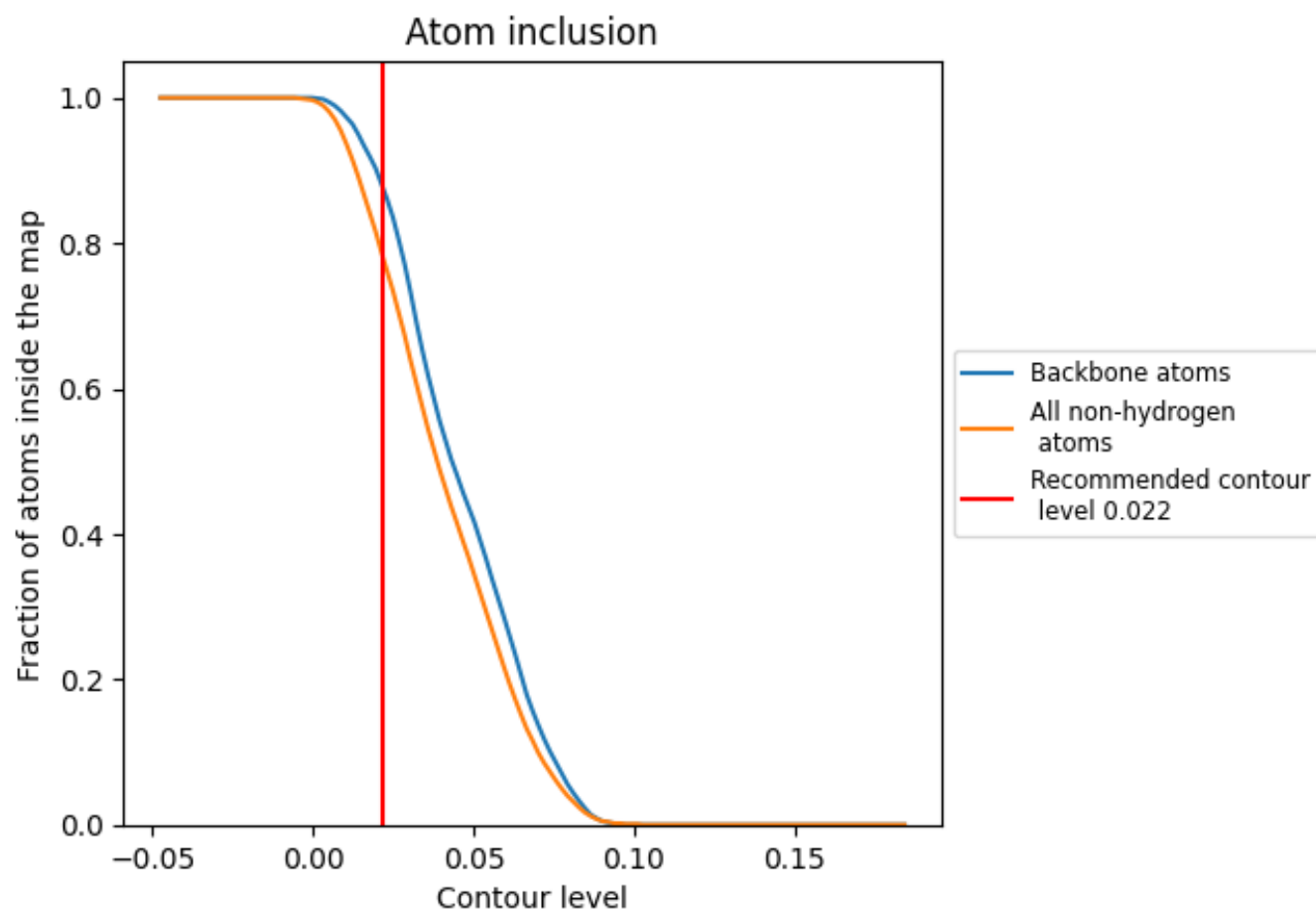
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.022).

9.4 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 78% 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 (0.022) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7780	0.5360
1	0.7920	0.5340
2	0.7140	0.4750
3	0.7210	0.4840
4	0.7870	0.5180
A	0.8470	0.5710
B	0.8780	0.5920
C	0.9270	0.5930
D	0.8900	0.5660
E	0.8310	0.5480
F	0.7670	0.5400
G	0.7330	0.5090
H	0.7480	0.4990
I	0.7890	0.5460
J	0.7540	0.5320
K	0.4650	0.4130
L	0.8330	0.5480
N	0.0570	0.2140
P	0.0040	0.3360

