



Full wwPDB EM Validation Report ⓘ

Mar 7, 2026 – 03:47 AM UTC

PDB ID : 6RHZ / pdb_00006rhz
EMDB ID : EMD-4883
Title : Structure of a minimal photosystem I from a green alga
Authors : Perez Boerema, A.; Klaiman, D.; Caspy, I.; Netzer-El, S.Y.; Amunts, A.;
Nelson, N.
Deposited on : 2019-04-23
Resolution : 3.20 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

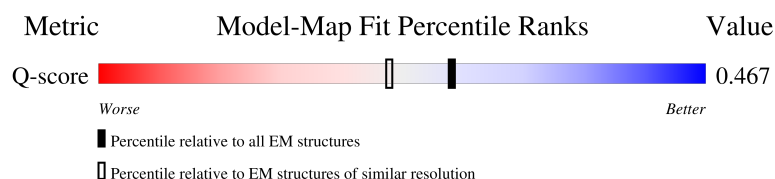
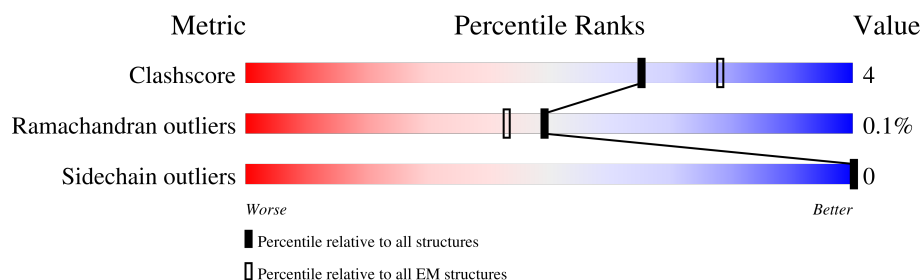
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

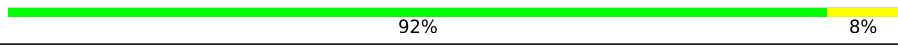
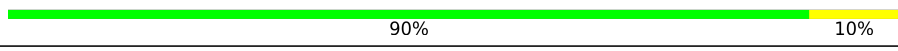
The reported resolution of this entry is 3.20 Å.

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



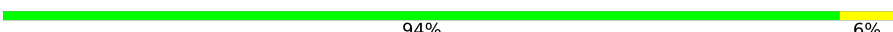
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	15020 (2.70 - 3.70)

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

Mol	Chain	Length	Quality of chain
1	1	197	 87%13%
2	2	208	 92%8%
3	3	210	 90%10%
4	4	211	 86%14%

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Mol	Chain	Length	Quality of chain
5	A	739	 92% 8%
6	B	730	 94% 5%
7	C	80	 94% 6%
8	D	141	 88% 12%
9	E	64	 91% 9%
10	F	163	 98% .
11	J	40	 100%

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
12	LUT	1	501	X	-	-	-
12	LUT	2	501	X	-	-	-
12	LUT	3	501	X	-	-	-
12	LUT	4	501	X	X	-	-
15	CLA	1	601	X	-	-	-
15	CLA	1	602	X	-	-	-
15	CLA	1	603	X	-	-	-
15	CLA	1	604	X	-	-	-
15	CLA	1	605	X	-	-	-
15	CLA	1	606	X	-	-	-
15	CLA	1	607	X	-	-	-
15	CLA	1	608	X	-	-	-
15	CLA	1	611	X	-	-	-
15	CLA	1	612	X	-	-	-
15	CLA	1	613	X	-	-	-
15	CLA	1	615	X	-	-	-
15	CLA	2	601	X	-	-	-
15	CLA	2	602	X	-	-	-
15	CLA	2	603	X	-	-	-
15	CLA	2	604	X	-	-	-
15	CLA	2	605	X	-	-	-
15	CLA	2	606	X	-	-	-
15	CLA	2	607	X	-	-	-
15	CLA	2	608	X	-	-	-
15	CLA	2	612	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
15	CLA	3	601	X	-	-	-
15	CLA	3	603	X	-	-	-
15	CLA	3	605	X	-	-	-
15	CLA	3	606	X	-	-	-
15	CLA	3	607	X	-	-	-
15	CLA	3	608	X	-	-	-
15	CLA	3	609	X	-	-	-
15	CLA	3	610	X	-	-	-
15	CLA	3	611	X	-	-	-
15	CLA	3	612	X	-	-	-
15	CLA	3	613	X	-	-	-
15	CLA	3	614	X	-	-	-
15	CLA	3	615	X	-	-	-
15	CLA	4	601	X	-	-	-
15	CLA	4	602	X	-	-	-
15	CLA	4	603	X	-	-	-
15	CLA	4	604	X	-	-	-
15	CLA	4	605	X	-	-	-
15	CLA	4	606	X	-	-	-
15	CLA	4	607	X	-	-	-
15	CLA	4	608	X	-	-	-
15	CLA	4	609	X	-	-	-
15	CLA	4	612	X	-	-	-
15	CLA	4	616	X	-	-	-
15	CLA	A	1012	X	-	-	-
15	CLA	A	1013	X	-	-	-
15	CLA	A	1101	X	-	-	-
15	CLA	A	1102	X	-	-	-
15	CLA	A	1103	X	-	-	-
15	CLA	A	1104	X	-	-	-
15	CLA	A	1105	X	-	-	-
15	CLA	A	1106	X	-	-	-
15	CLA	A	1107	X	-	-	-
15	CLA	A	1108	X	-	-	-
15	CLA	A	1109	X	-	-	-
15	CLA	A	1110	X	-	-	-
15	CLA	A	1112	X	-	-	-
15	CLA	A	1113	X	-	-	-
15	CLA	A	1114	X	-	-	-
15	CLA	A	1115	X	-	-	-
15	CLA	A	1116	X	-	-	-
15	CLA	A	1117	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
15	CLA	A	1118	X	-	-	-
15	CLA	A	1119	X	-	-	-
15	CLA	A	1120	X	-	-	-
15	CLA	A	1121	X	-	-	-
15	CLA	A	1122	X	-	-	-
15	CLA	A	1123	X	-	-	-
15	CLA	A	1124	X	-	-	-
15	CLA	A	1126	X	-	-	-
15	CLA	A	1127	X	-	-	-
15	CLA	A	1128	X	-	-	-
15	CLA	A	1129	X	-	-	-
15	CLA	A	1130	X	-	-	-
15	CLA	A	1131	X	-	-	-
15	CLA	A	1132	X	-	-	-
15	CLA	A	1133	X	-	-	-
15	CLA	A	1134	X	-	-	-
15	CLA	A	1135	X	-	-	-
15	CLA	A	1136	X	-	-	-
15	CLA	A	1137	X	-	-	-
15	CLA	A	1138	X	-	-	-
15	CLA	A	1139	X	-	-	-
15	CLA	A	1140	X	-	-	-
15	CLA	A	1141	X	-	-	-
15	CLA	B	1021	X	-	-	-
15	CLA	B	1022	X	-	-	-
15	CLA	B	1023	X	-	-	-
15	CLA	B	1201	X	-	-	-
15	CLA	B	1202	X	-	-	-
15	CLA	B	1203	X	-	-	-
15	CLA	B	1204	X	-	-	-
15	CLA	B	1205	X	-	-	-
15	CLA	B	1206	X	-	-	-
15	CLA	B	1208	X	-	-	-
15	CLA	B	1209	X	-	-	-
15	CLA	B	1211	X	-	-	-
15	CLA	B	1212	X	-	-	-
15	CLA	B	1213	X	-	-	-
15	CLA	B	1214	X	-	-	-
15	CLA	B	1215	X	-	-	-
15	CLA	B	1216	X	-	-	-
15	CLA	B	1217	X	-	-	-
15	CLA	B	1218	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
15	CLA	B	1220	X	-	-	-
15	CLA	B	1221	X	-	-	-
15	CLA	B	1222	X	-	-	-
15	CLA	B	1223	X	-	-	-
15	CLA	B	1224	X	-	-	-
15	CLA	B	1225	X	-	-	-
15	CLA	B	1226	X	-	-	-
15	CLA	B	1227	X	-	-	-
15	CLA	B	1228	X	-	-	-
15	CLA	B	1229	X	-	-	-
15	CLA	B	1230	X	-	-	-
15	CLA	B	1231	X	-	-	-
15	CLA	B	1232	X	-	-	-
15	CLA	B	1234	X	-	-	-
15	CLA	B	1235	X	-	-	-
15	CLA	B	1236	X	-	-	-
15	CLA	B	1237	X	-	-	-
15	CLA	B	1238	X	-	-	-
15	CLA	B	1239	X	-	-	-
15	CLA	B	1240	X	-	-	-
15	CLA	F	1301	X	-	-	-
15	CLA	F	1302	X	-	-	-
15	CLA	J	1302	X	-	-	-
16	CHL	1	609	X	-	-	-
16	CHL	1	610	X	-	-	-
16	CHL	2	609	X	-	-	-
16	CHL	2	610	X	-	-	-
16	CHL	2	611	X	-	-	-
16	CHL	2	613	X	-	-	-
16	CHL	3	604	X	-	-	-
16	CHL	4	610	X	-	-	-
16	CHL	4	611	X	-	-	-
16	CHL	4	613	X	-	-	-
19	CL0	A	1011	X	-	-	-

2 Entry composition [i](#)

There are 22 unique types of molecules in this entry. The entry contains 63437 atoms, of which 31549 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 Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	1	197	Total	C	H	N	O	S	0	0
			2970	963	1469	255	276	7		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	204	ALA	GLU	conflict	UNP C1K003

- Molecule 2 is a protein called Chlorophyll a-b binding protein, Lhca2.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	2	208	Total	C	H	N	O	S	0	0
			3164	1033	1555	272	297	7		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
3	3	210	Total	C	H	N	O	S	0	0
			3176	1050	1567	263	291	5		

- Molecule 4 is a protein called Chlorophyll a-b binding protein, Lhca4.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	4	211	Total	C	H	N	O	S	0	0
			3216	1058	1579	272	303	4		

- Molecule 5 is a protein called Photosystem I P700 chlorophyll a apoprotein A1.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	A	739	Total	C	H	N	O	S	0	0
			11429	3789	5630	991	1001	18		

- Molecule 6 is a protein called Photosystem I P700 chlorophyll a apoprotein A2.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	B	730	Total	C	H	N	O	S	0	0
			11312	3799	5528	970	1002	13		

- Molecule 7 is a protein called Photosystem I iron-sulfur center.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	C	80	Total	C	H	N	O	S	0	0
			1184	370	584	104	115	11		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
8	D	141	Total	C	H	N	O	S	0	0
			2242	714	1126	195	201	6		

- Molecule 9 is a protein called Photosystem I reaction center subunit IV, PsaE.

Mol	Chain	Residues	Atoms						AltConf	Trace
9	E	64	Total	C	H	N	O	S	0	0
			1021	327	506	89	99			

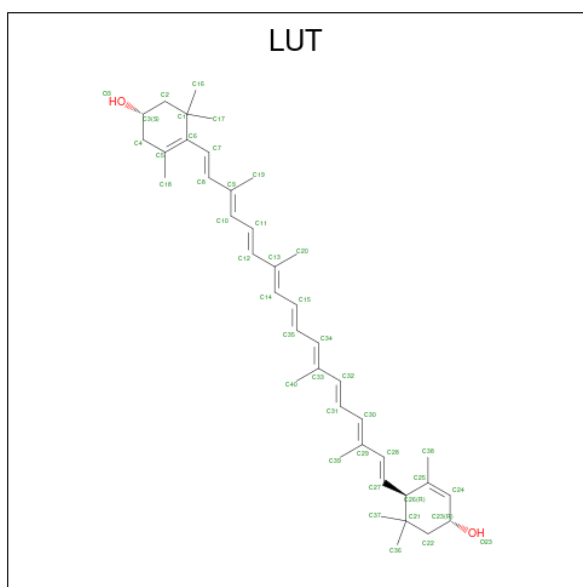
- Molecule 10 is a protein called Photosystem I reaction center subunit III, PsaF.

Mol	Chain	Residues	Atoms						AltConf	Trace
10	F	163	Total	C	H	N	O	S	0	0
			2589	828	1304	218	237	2		

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

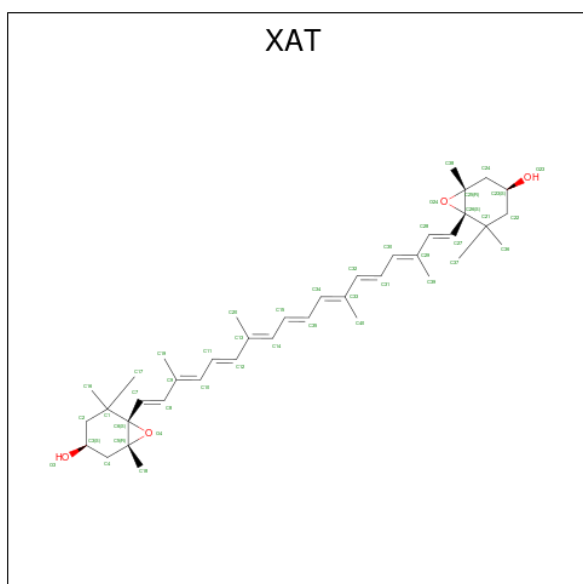
Mol	Chain	Residues	Atoms						AltConf	Trace
11	J	40	Total	C	H	N	O	S	0	0
			635	214	319	46	55	1		

- Molecule 12 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (CCD ID: LUT) (formula: C₄₀H₅₆O₂).



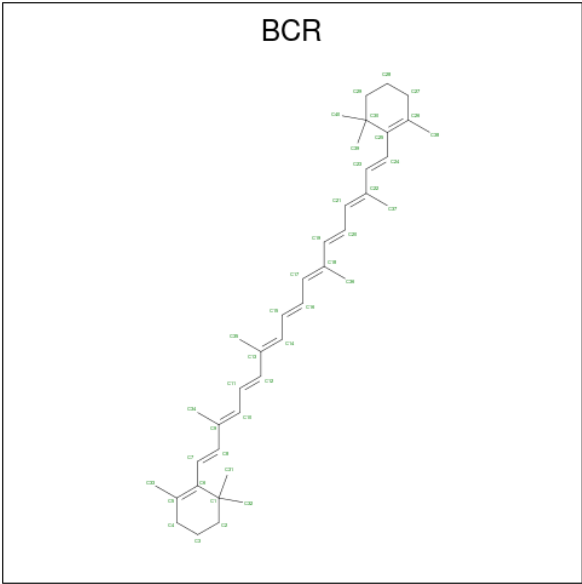
Mol	Chain	Residues	Atoms				AltConf
12	1	1	Total	C	H	O	0
			98	40	56	2	
12	2	1	Total	C	H	O	0
			98	40	56	2	
12	3	1	Total	C	H	O	0
			98	40	56	2	
12	4	1	Total	C	H	O	0
			98	40	56	2	

- Molecule 13 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
13	1	1	Total	C	H	O	0
			100	40	56	4	
13	2	1	Total	C	H	O	0
			100	40	56	4	
13	3	1	Total	C	H	O	0
			100	40	56	4	
13	4	1	Total	C	H	O	0
			100	40	56	4	

- Molecule 14 is BETA-CAROTENE (CCD ID: BCR) (formula: C₄₀H₅₆).



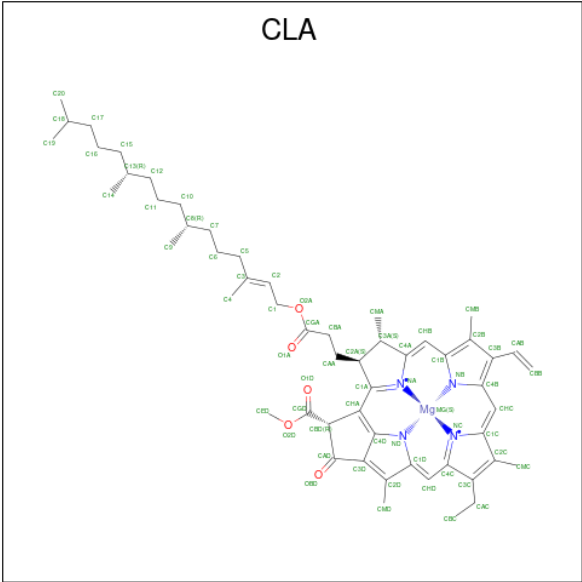
Mol	Chain	Residues	Atoms				AltConf
14	1	1	Total	C	H		0
			92	40	52		
14	2	1	Total	C	H		0
			93	40	53		
14	3	1	Total	C	H		0
			93	40	53		
14	3	1	Total	C	H		0
			92	40	52		
14	3	1	Total	C	H		0
			93	40	53		
14	4	1	Total	C	H		0
			93	40	53		
14	A	1	Total	C	H		0
			93	40	53		
14	A	1	Total	C	H		0
			93	40	53		

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Mol	Chain	Residues	Atoms			AltConf
14	A	1	Total	C	H	0
			92	40	52	
14	A	1	Total	C	H	0
			92	40	52	
14	A	1	Total	C	H	0
			92	40	52	
14	A	1	Total	C	H	0
			92	40	52	
14	A	1	Total	C	H	0
			93	40	53	
14	B	1	Total	C	H	0
			93	40	53	
14	B	1	Total	C	H	0
			92	40	52	
14	B	1	Total	C	H	0
			93	40	53	
14	B	1	Total	C	H	0
			92	40	52	
14	B	1	Total	C	H	0
			91	40	51	
14	B	1	Total	C	H	0
			92	40	52	
14	F	1	Total	C	H	0
			92	40	52	
14	F	1	Total	C	H	0
			90	40	50	
14	J	1	Total	C	H	0
			92	40	52	
14	J	1	Total	C	H	0
			92	40	52	

- Molecule 15 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



Mol	Chain	Residues	Atoms						AltConf
15	1	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
15	1	1	Total	C	H	Mg	N	O	0
			79	36	33	1	4	5	
15	1	1	Total	C	H	Mg	N	O	0
			116	50	56	1	4	5	
15	1	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
15	1	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
15	1	1	Total	C	H	Mg	N	O	0
			88	40	38	1	4	5	
15	1	1	Total	C	H	Mg	N	O	0
			79	36	33	1	4	5	
15	1	1	Total	C	H	Mg	N	O	0
			104	45	49	1	4	5	
15	1	1	Total	C	H	Mg	N	O	0
			84	38	36	1	4	5	
15	1	1	Total	C	H	Mg	N	O	0
			68	32	28	1	4	3	
15	1	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
15	1	1	Total	C	H	Mg	N	O	0
			79	38	31	1	4	5	
15	2	1	Total	C	H	Mg	N	O	0
			136	55	71	1	4	5	
15	2	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	

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Mol	Chain	Residues	Atoms						AltConf
15	2	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
15	2	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
15	2	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
15	2	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
15	2	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
15	2	1	Total	C	H	Mg	N	O	0
			89	40	39	1	4	5	
15	2	1	Total	C	H	Mg	N	O	0
			104	45	49	1	4	5	
15	2	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
15	3	1	Total	C	H	Mg	N	O	0
			116	50	56	1	4	5	
15	3	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
15	3	1	Total	C	H	Mg	N	O	0
			136	55	71	1	4	5	
15	3	1	Total	C	H	Mg	N	O	0
			104	45	49	1	4	5	
15	3	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
15	3	1	Total	C	H	Mg	N	O	0
			136	55	71	1	4	5	
15	3	1	Total	C	H	Mg	N	O	0
			74	34	32	1	4	3	
15	3	1	Total	C	H	Mg	N	O	0
			89	40	39	1	4	5	
15	3	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
15	3	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
15	3	1	Total	C	H	Mg	N	O	0
			79	36	33	1	4	5	
15	3	1	Total	C	H	Mg	N	O	0
			95	42	43	1	4	5	
15	3	1	Total	C	H	Mg	N	O	0
			73	34	31	1	4	3	

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Mol	Chain	Residues	Atoms						AltConf
15	4	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
15	4	1	Total	C	H	Mg	N	O	0
			89	40	39	1	4	5	
15	4	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
15	4	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
15	4	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
15	4	1	Total	C	H	Mg	N	O	0
			89	40	39	1	4	5	
15	4	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
15	4	1	Total	C	H	Mg	N	O	0
			77	36	31	1	4	5	
15	4	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
15	4	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
15	4	1	Total	C	H	Mg	N	O	0
			91	41	40	1	4	5	
15	A	1	Total	C	H	Mg	N	O	0
			136	55	71	1	4	5	
15	A	1	Total	C	H	Mg	N	O	0
			136	55	71	1	4	5	
15	A	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
15	A	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
15	A	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
15	A	1	Total	C	H	Mg	N	O	0
			118	50	58	1	4	5	
15	A	1	Total	C	H	Mg	N	O	0
			136	55	71	1	4	5	
15	A	1	Total	C	H	Mg	N	O	0
			91	41	40	1	4	5	
15	A	1	Total	C	H	Mg	N	O	0
			104	45	49	1	4	5	

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Mol	Chain	Residues	Atoms						AltConf
15	A	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
15	A	1	Total	C	H	Mg	N	O	0
			104	45	49	1	4	5	
15	A	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
15	A	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
15	A	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
15	A	1	Total	C	H	Mg	N	O	0
			103	45	48	1	4	5	
15	A	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
15	A	1	Total	C	H	Mg	N	O	0
			107	46	51	1	4	5	
15	A	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
15	A	1	Total	C	H	Mg	N	O	0
			73	34	31	1	4	3	
15	A	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
15	A	1	Total	C	H	Mg	N	O	0
			73	34	31	1	4	3	
15	A	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
15	A	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
15	A	1	Total	C	H	Mg	N	O	0
			136	55	71	1	4	5	
15	A	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
15	A	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
15	A	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
15	A	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
15	A	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
15	A	1	Total	C	H	Mg	N	O	0
			104	45	49	1	4	5	

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Mol	Chain	Residues	Atoms						AltConf
15	A	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
15	A	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
15	A	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
15	A	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
15	A	1	Total	C	H	Mg	N	O	0
			73	34	31	1	4	3	
15	A	1	Total	C	H	Mg	N	O	0
			92	41	41	1	4	5	
15	A	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
15	A	1	Total	C	H	Mg	N	O	0
			122	51	61	1	4	5	
15	A	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
15	A	1	Total	C	H	Mg	N	O	0
			136	55	71	1	4	5	
15	A	1	Total	C	H	Mg	N	O	0
			122	51	61	1	4	5	
15	A	1	Total	C	H	Mg	N	O	0
			70	33	29	1	4	3	
15	B	1	Total	C	H	Mg	N	O	0
			136	55	71	1	4	5	
15	B	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
15	B	1	Total	C	H	Mg	N	O	0
			136	55	71	1	4	5	
15	B	1	Total	C	H	Mg	N	O	0
			76	35	33	1	4	3	
15	B	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
15	B	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
15	B	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
15	B	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
15	B	1	Total	C	H	Mg	N	O	0
			77	35	32	1	4	5	

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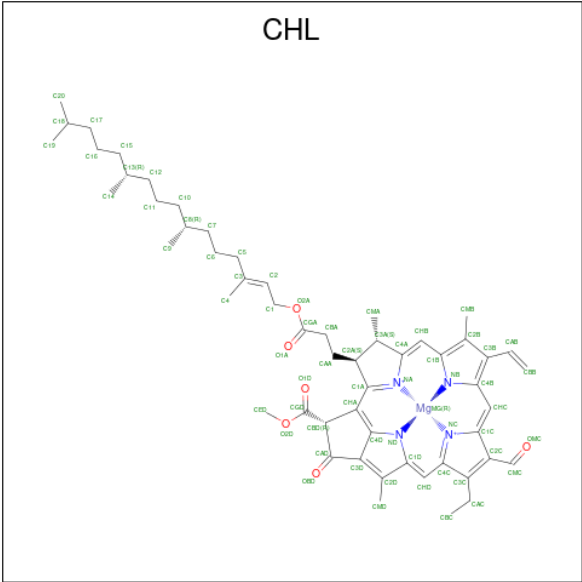
Mol	Chain	Residues	Atoms						AltConf
15	B	1	Total	C	H	Mg	N	O	0
			78	36	32	1	4	5	
15	B	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
15	B	1	Total	C	H	Mg	N	O	0
			79	36	33	1	4	5	
15	B	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
15	B	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
15	B	1	Total	C	H	Mg	N	O	0
			104	45	49	1	4	5	
15	B	1	Total	C	H	Mg	N	O	0
			104	45	49	1	4	5	
15	B	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
15	B	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
15	B	1	Total	C	H	Mg	N	O	0
			117	49	58	1	4	5	
15	B	1	Total	C	H	Mg	N	O	0
			79	36	33	1	4	5	
15	B	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
15	B	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
15	B	1	Total	C	H	Mg	N	O	0
			92	41	41	1	4	5	
15	B	1	Total	C	H	Mg	N	O	0
			136	55	71	1	4	5	
15	B	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
15	B	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
15	B	1	Total	C	H	Mg	N	O	0
			122	51	61	1	4	5	
15	B	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
15	B	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
15	B	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	

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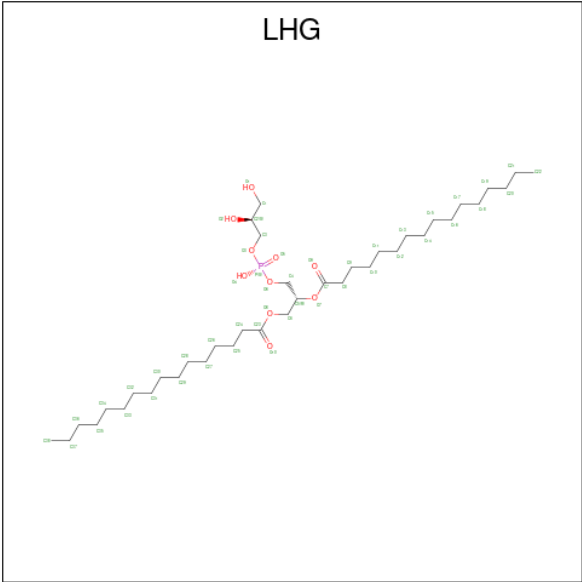
Mol	Chain	Residues	Atoms						AltConf
15	B	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
15	B	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
15	B	1	Total	C	H	Mg	N	O	0
			104	45	49	1	4	5	
15	B	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
15	B	1	Total	C	H	Mg	N	O	0
			78	36	32	1	4	5	
15	B	1	Total	C	H	Mg	N	O	0
			104	45	49	1	4	5	
15	B	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
15	B	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
15	B	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
15	B	1	Total	C	H	Mg	N	O	0
			102	44	50	1	4	3	
15	B	1	Total	C	H	Mg	N	O	0
			73	34	31	1	4	3	
15	B	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
15	F	1	Total	C	H	Mg	N	O	0
			79	36	33	1	4	5	
15	F	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
15	J	1	Total	C	H	Mg	N	O	0
			73	34	31	1	4	3	

- Molecule 16 is CHLOROPHYLL B (CCD ID: CHL) (formula: $C_{55}H_{70}MgN_4O_6$).



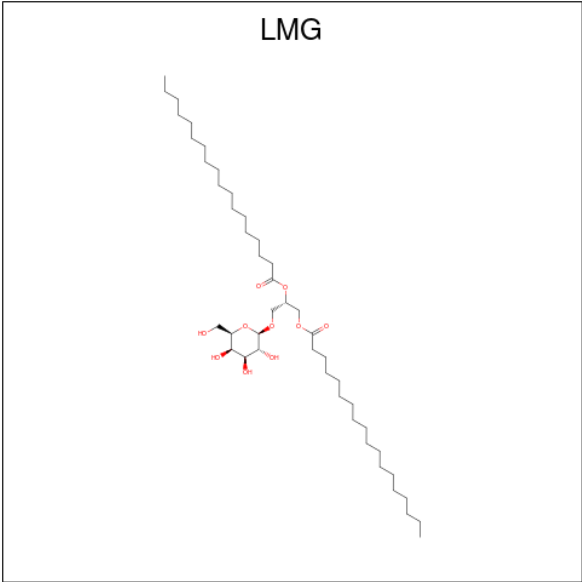
Mol	Chain	Residues	Atoms						AltConf
16	1	1	Total	C	H	Mg	N	O	0
			136	55	70	1	4	6	
16	1	1	Total	C	H	Mg	N	O	0
			80	36	33	1	4	6	
16	2	1	Total	C	H	Mg	N	O	0
			136	55	70	1	4	6	
16	2	1	Total	C	H	Mg	N	O	0
			75	35	31	1	4	4	
16	2	1	Total	C	H	Mg	N	O	0
			82	37	34	1	4	6	
16	2	1	Total	C	H	Mg	N	O	0
			77	35	31	1	4	6	
16	3	1	Total	C	H	Mg	N	O	0
			120	50	59	1	4	6	
16	4	1	Total	C	H	Mg	N	O	0
			80	36	33	1	4	6	
16	4	1	Total	C	H	Mg	N	O	0
			90	40	39	1	4	6	
16	4	1	Total	C	H	Mg	N	O	0
			120	50	59	1	4	6	

- Molecule 17 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).



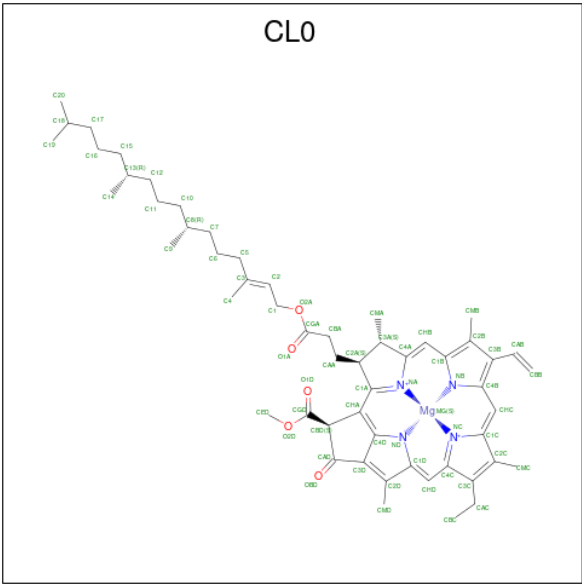
Mol	Chain	Residues	Atoms					AltConf
17	1	1	Total	C	H	O	P	0
			123	38	74	10	1	
17	2	1	Total	C	H	O	P	0
			75	24	40	10	1	
17	3	1	Total	C	H	O	P	0
			116	37	68	10	1	
17	A	1	Total	C	H	O	P	0
			123	38	74	10	1	
17	A	1	Total	C	H	O	P	0
			123	38	74	10	1	
17	B	1	Total	C	H	O	P	0
			99	31	57	10	1	

- Molecule 18 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: C₄₅H₈₆O₁₀).



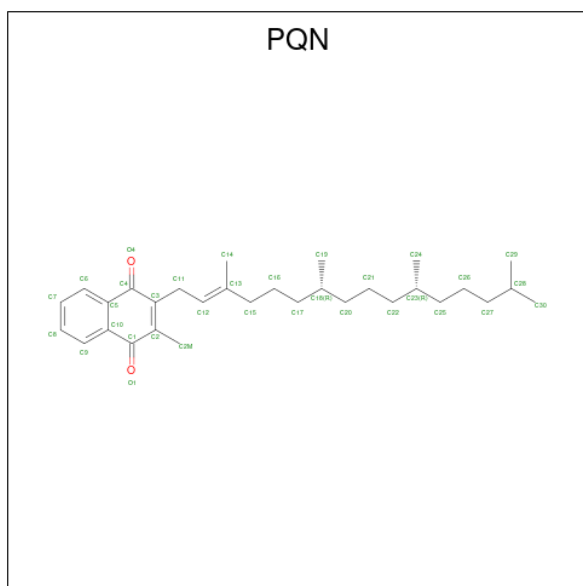
Mol	Chain	Residues	Atoms				AltConf
18	2	1	Total	C	H	O	0
			123	40	73	10	
18	2	1	Total	C	H	O	0
			90	30	50	10	
18	2	1	Total	C	H	O	0
			123	40	73	10	
18	4	1	Total	C	H	O	0
			80	27	43	10	
18	B	1	Total	C	H	O	0
			87	29	48	10	

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



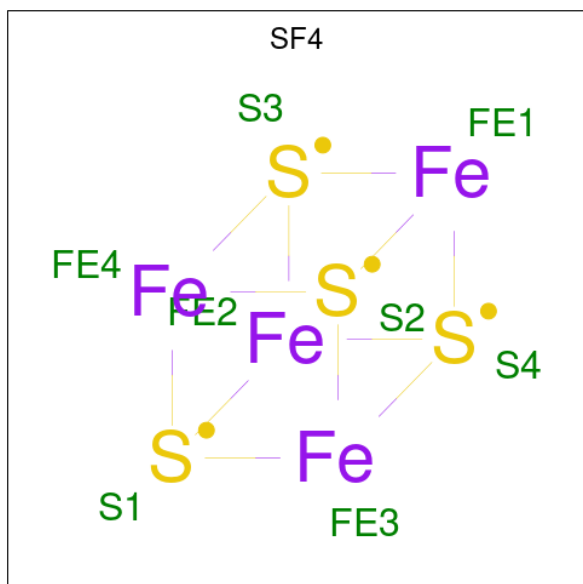
Mol	Chain	Residues	Atoms						AltConf
19	A	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	

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



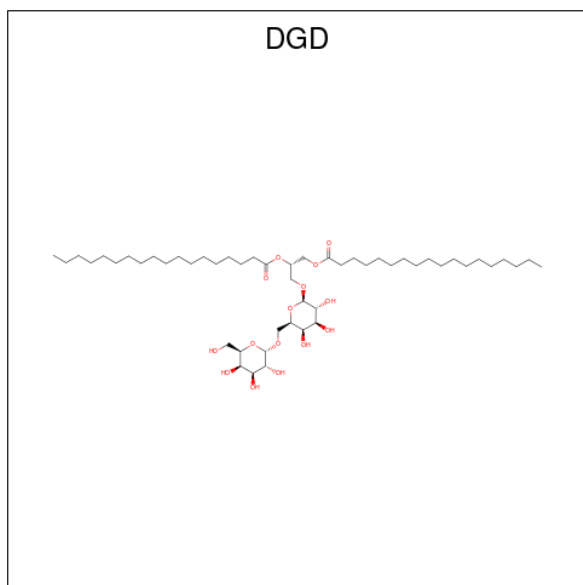
Mol	Chain	Residues	Atoms				AltConf
20	A	1	Total	C	H	O	0
			79	31	46	2	
20	B	1	Total	C	H	O	0
			79	31	46	2	

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



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

- Molecule 22 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).

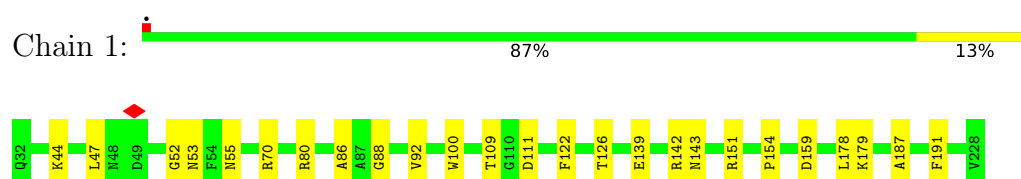


Mol	Chain	Residues	Atoms				AltConf
22	B	1	Total	C	H	O	0
			144	46	83	15	

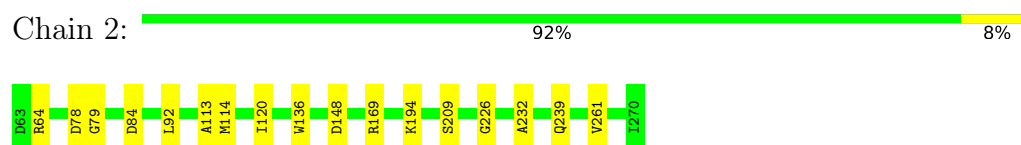
3 Residue-property plots

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.

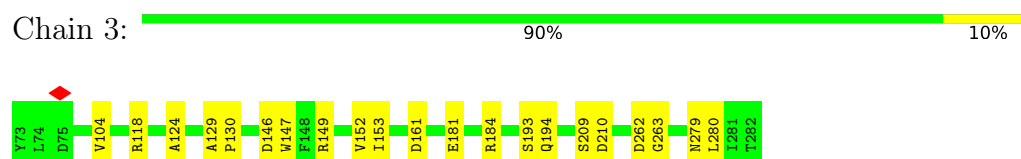
- Molecule 1: Chlorophyll a-b binding protein, chloroplastic



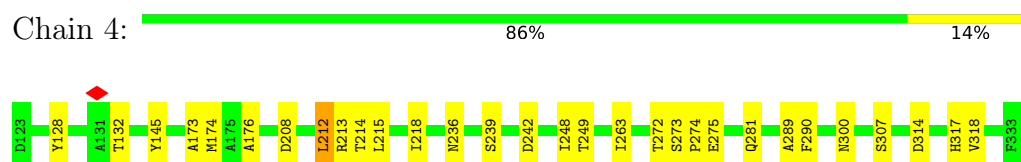
- Molecule 2: Chlorophyll a-b binding protein, Lhca2



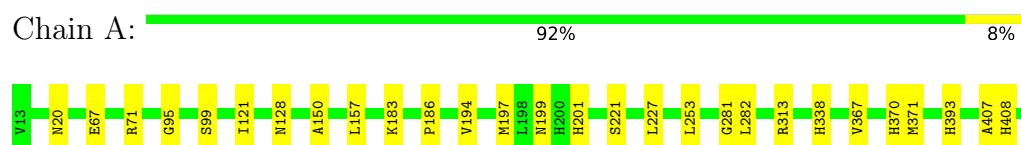
- Molecule 3: Chlorophyll a-b binding protein, chloroplastic

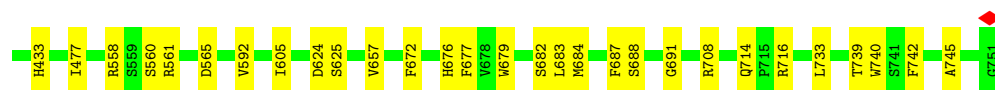


- Molecule 4: Chlorophyll a-b binding protein, Lhca4



- Molecule 5: Photosystem I P700 chlorophyll a apoprotein A1





- Molecule 6: Photosystem I P700 chlorophyll a apoprotein A2

Chain B: 94% 5%



- Molecule 7: Photosystem I iron-sulfur center

Chain C: 94% 6%



- Molecule 8: Photosystem I reaction center subunit II, PsaD

Chain D: 88% 12%



- Molecule 9: Photosystem I reaction center subunit IV, PsaE

Chain E: 91% 9%



- Molecule 10: Photosystem I reaction center subunit III, PsaF

Chain F: 98% 2%



- Molecule 11: Photosystem I reaction center subunit IX

Chain J: 100%

There are no outlier residues recorded for this chain.

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	132017	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	41.6	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	14.299	Depositor
Minimum map value	-4.307	Depositor
Average map value	0.010	Depositor
Map value standard deviation	0.186	Depositor
Recommended contour level	1	Depositor
Map size ($\text{\AA}$)	426.00003, 426.00003, 426.00003	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.065, 1.065, 1.065	Depositor

5 Model quality

5.1 Standard geometry

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

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	1	0.24	0/1540	0.42	0/2088
2	2	0.28	0/1656	0.43	0/2243
3	3	0.28	0/1657	0.43	0/2253
4	4	0.28	0/1687	0.49	0/2300
5	A	0.31	0/5995	0.40	0/8179
6	B	0.31	0/5997	0.40	1/8198 (0.0%)
7	C	0.33	0/610	0.41	0/828
8	D	0.27	0/1145	0.45	0/1546
9	E	0.26	0/525	0.42	0/712
10	F	0.24	0/1313	0.38	0/1776
11	J	0.29	0/326	0.37	0/445
All	All	0.29	0/22451	0.42	1/30568 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
4	4	0	2
5	A	0	1
All	All	0	3

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	571	ILE	CB-CA-C	-6.21	105.59	111.06

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	4	213	ARG	Peptide
4	4	274	PRO	Peptide
5	A	313	ARG	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	1	1501	1469	1469	20	0
2	2	1609	1555	1555	14	0
3	3	1609	1567	1566	13	0
4	4	1637	1579	1579	21	0
5	A	5799	5630	5628	50	0
6	B	5784	5528	5527	37	0
7	C	600	584	581	4	0
8	D	1116	1126	1126	11	0
9	E	515	506	508	4	0
10	F	1285	1304	1304	5	0
11	J	316	319	319	0	0
12	1	42	56	56	12	0
12	2	42	56	56	3	0
12	3	42	56	56	7	0
12	4	42	56	56	7	0
13	1	44	56	56	3	0
13	2	44	56	56	2	0
13	3	44	56	56	2	0
13	4	44	56	56	5	0
14	1	40	52	56	0	0
14	2	40	53	56	0	0
14	3	120	158	168	5	0
14	4	40	53	56	0	0
14	A	280	367	392	11	0
14	B	240	313	336	10	0
14	F	80	102	112	2	0
14	J	80	104	112	5	0
15	1	633	553	562	13	0
15	2	580	572	573	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	3	732	700	704	14	0
15	4	632	601	604	6	0
15	A	2487	2465	2473	37	0
15	B	2411	2358	2359	29	0
15	F	95	72	72	0	0
15	J	42	31	31	0	0
16	1	113	103	101	1	0
16	2	204	166	165	0	0
16	3	61	59	57	0	0
16	4	159	131	125	1	0
17	1	49	74	74	1	0
17	2	35	40	40	0	0
17	3	48	68	68	0	0
17	A	98	148	148	2	0
17	B	42	57	57	0	0
18	2	140	196	196	0	0
18	4	37	43	44	1	0
18	B	39	48	48	2	0
19	A	65	72	71	3	0
20	A	33	46	46	0	0
20	B	33	46	46	0	0
21	A	8	0	0	0	0
21	C	16	0	0	1	0
22	B	61	83	83	2	0
All	All	31888	31549	31645	253	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 4.

All (253) 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)
15:B:1214:CLA:H43	15:B:1231:CLA:HED3	1.61	0.82
7:C:7:ILE:HG22	7:C:65:VAL:HG22	1.67	0.77
5:A:71:ARG:NH1	5:A:186:PRO:O	2.19	0.76
3:3:181:GLU:OE1	3:3:184:ARG:NH1	2.20	0.74
2:2:169:ARG:NH2	15:2:612:CLA:O1D	2.21	0.73
1:1:139:GLU:OE2	1:1:142:ARG:NH2	2.24	0.71
5:A:95:GLY:O	5:A:99:SER:OG	2.06	0.70
6:B:616:TYR:OH	6:B:622:ARG:NH2	2.25	0.69
5:A:157:LEU:HD22	15:A:1114:CLA:HED1	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:100:TRP:O	13:1:502:XAT:O3	2.11	0.69
3:3:147:TRP:O	13:3:502:XAT:O3	2.11	0.69
5:A:714:GLN:OE1	9:E:82:TYR:OH	2.11	0.68
12:3:501:LUT:H192	15:3:601:CLA:H71	1.76	0.67
2:2:239:GLN:OE1	15:2:603:CLA:ND	2.28	0.67
5:A:121:ILE:HD11	15:A:1107:CLA:HMA2	1.75	0.66
2:2:113:ALA:HB2	13:2:502:XAT:H203	1.76	0.65
4:4:289:ALA:HB2	12:4:501:LUT:H392	1.79	0.64
3:3:193:SER:OG	3:3:194:GLN:OE1	2.13	0.64
4:4:289:ALA:HB2	12:4:501:LUT:C39	2.28	0.63
15:A:1126:CLA:C19	14:J:4001:BCR:H12C	2.29	0.63
8:D:134:ARG:NH2	8:D:136:GLU:OE1	2.31	0.63
5:A:708:ARG:NH1	10:F:229:SER:O	2.33	0.62
1:1:147:LEU:O	1:1:53:ASN:ND2	2.33	0.62
15:2:616:CLA:H192	15:2:616:CLA:H141	1.82	0.61
2:2:194:LYS:NZ	2:2:209:SER:O	2.33	0.61
5:A:367:VAL:HG12	5:A:371:MET:HE2	1.82	0.61
2:2:64:ARG:NH1	2:2:84:ASP:OD2	2.34	0.61
4:4:236:ASN:O	4:4:239:SER:OG	2.14	0.61
1:1:187:ALA:HB3	12:1:501:LUT:H393	1.83	0.61
3:3:279:ASN:OD1	3:3:280:LEU:N	2.34	0.61
12:3:501:LUT:H391	15:3:614:CLA:HMC2	1.83	0.60
1:1:179:LYS:NZ	17:1:801:LHG:O5	2.24	0.59
2:2:92:LEU:HD13	15:2:604:CLA:H42	1.84	0.59
15:3:605:CLA:HBC3	15:3:605:CLA:HHD	1.86	0.58
16:4:610:CHL:HBC3	16:4:610:CHL:HHD	1.85	0.58
15:B:1234:CLA:HBC2	15:B:1234:CLA:HHD	1.85	0.58
4:4:173:ALA:CB	13:4:502:XAT:H203	2.34	0.57
5:A:150:ALA:O	5:A:221:SER:OG	2.20	0.57
15:A:1126:CLA:H193	14:J:4001:BCR:H12C	1.87	0.57
6:B:701:LEU:HD22	6:B:705:GLN:NE2	2.20	0.57
6:B:494:TRP:NE1	15:B:1231:CLA:HED1	2.20	0.57
2:2:113:ALA:CB	13:2:502:XAT:H203	2.35	0.56
5:A:227:LEU:CD1	5:A:253:LEU:HD21	2.35	0.56
12:1:501:LUT:H383	15:1:603:CLA:HMB2	1.87	0.56
8:D:146:ARG:NH2	8:D:176:GLU:OE2	2.38	0.56
6:B:124:TRP:CZ2	15:B:1210:CLA:H191	2.40	0.56
1:1:109:THR:OG1	1:1:111:ASP:OD1	2.21	0.55
6:B:59:PHE:HD2	6:B:143:LEU:HD22	1.71	0.55
6:B:657:VAL:HG12	6:B:713:HIS:O	2.06	0.55
1:1:191:PHE:CZ	12:1:501:LUT:H392	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:657:VAL:HG22	5:A:745:ALA:HB3	1.88	0.55
15:B:1240:CLA:H2A	15:B:1240:CLA:HED3	1.87	0.55
4:4:300:ASN:ND2	4:4:307:SER:OG	2.40	0.55
8:D:171:ASP:OD2	8:D:179:ASN:ND2	2.40	0.54
4:4:145:TYR:OH	4:4:281:GLN:NE2	2.40	0.54
12:4:501:LUT:H30	12:4:501:LUT:H402	1.90	0.54
7:C:24:ASP:OD2	8:D:168:HIS:ND1	2.22	0.53
15:A:1141:CLA:NB	17:A:5001:LHG:O5	2.42	0.53
5:A:733:LEU:HD11	14:A:4006:BCR:HC8	1.89	0.53
5:A:739:THR:HG23	19:A:1011:CL0:O2D	2.09	0.53
6:B:494:TRP:CD1	15:B:1231:CLA:HED1	2.44	0.53
7:C:14:CYS:N	21:C:3003:SF4:S3	2.81	0.53
15:A:1012:CLA:H122	14:A:4006:BCR:H19C	1.91	0.53
6:B:143:LEU:HD11	14:B:4003:BCR:H402	1.89	0.53
4:4:128:TYR:CD2	4:4:132:THR:HG21	2.44	0.52
5:A:676:HIS:HB3	15:A:1012:CLA:HBD	1.89	0.52
6:B:340:ALA:HB2	14:B:4005:BCR:H372	1.91	0.52
5:A:367:VAL:CG1	5:A:371:MET:HE2	2.40	0.52
14:3:504:BCR:H343	15:3:605:CLA:HBC2	1.92	0.52
12:4:501:LUT:H203	15:4:601:CLA:HMC1	1.92	0.52
4:4:273:SER:O	4:4:275:GLU:N	2.43	0.51
4:4:314:ASP:O	4:4:318:VAL:HG22	2.10	0.51
15:B:1220:CLA:O1A	14:B:4004:BCR:H12C	2.09	0.51
5:A:197:MET:HG3	15:A:1111:CLA:HBC2	1.93	0.51
15:A:1012:CLA:C12	14:A:4006:BCR:H19C	2.40	0.51
6:B:465:GLN:NE2	15:B:1234:CLA:OBD	2.43	0.51
8:D:177:LYS:O	8:D:182:ARG:NH2	2.44	0.51
2:2:148:ASP:O	4:4:317:HIS:NE2	2.44	0.51
9:E:86:GLN:CD	10:F:237:ILE:HD11	2.35	0.51
5:A:561:ARG:O	8:D:134:ARG:NH1	2.43	0.51
4:4:173:ALA:HB2	13:4:502:XAT:H203	1.94	0.50
12:4:501:LUT:H202	15:4:601:CLA:HAB	1.93	0.50
5:A:625:SER:O	5:A:625:SER:OG	2.28	0.50
5:A:714:GLN:OE1	5:A:716:ARG:NH2	2.43	0.50
18:4:801:LMG:O5	18:4:801:LMG:O4	2.13	0.50
3:3:209:SER:OG	3:3:210:ASP:N	2.45	0.49
1:1:143:ASN:OD1	1:1:151:ARG:NH1	2.44	0.49
4:4:242:ASP:O	4:4:249:THR:HG21	2.13	0.49
13:4:502:XAT:H31	15:4:604:CLA:HMC2	1.94	0.49
4:4:176:ALA:CB	13:4:502:XAT:H193	2.43	0.49
1:1:159:ASP:OD1	1:1:159:ASP:N	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:3:501:LUT:H401	15:3:614:CLA:CBB	2.43	0.49
14:3:504:BCR:H10C	15:3:612:CLA:H91	1.94	0.49
1:1:44:LYS:N	1:1:55:ASN:OD1	2.43	0.49
5:A:20:ASN:N	5:A:183:LYS:O	2.42	0.49
15:A:1012:CLA:H201	15:A:1013:CLA:H202	1.94	0.49
12:3:501:LUT:H11	15:3:601:CLA:HMC2	1.94	0.49
5:A:560:SER:OG	5:A:561:ARG:N	2.45	0.48
5:A:657:VAL:HG21	5:A:742:PHE:HA	1.95	0.48
5:A:691:GLY:HA3	6:B:571:ILE:HG23	1.95	0.48
5:A:672:PHE:O	5:A:676:HIS:ND1	2.43	0.48
15:A:1141:CLA:CBB	14:A:4004:BCR:H20C	2.43	0.48
6:B:526:LEU:O	6:B:530:THR:HG22	2.14	0.48
5:A:67:GLU:OE2	5:A:71:ARG:NH2	2.47	0.48
8:D:157:ARG:HB2	8:D:167:LEU:HD11	1.96	0.48
15:B:1224:CLA:HBC3	22:B:5002:DGD:HBC3	1.96	0.48
1:1:179:LYS:NZ	15:1:607:CLA:O1D	2.39	0.48
12:1:501:LUT:H383	15:1:603:CLA:CMB	2.44	0.48
12:2:501:LUT:H10	12:2:501:LUT:H203	1.94	0.47
6:B:432:PHE:CZ	14:B:4006:BCR:H11C	2.49	0.47
5:A:679:TRP:CD2	19:A:1011:CL0:H5	2.49	0.47
6:B:374:THR:HG22	6:B:592:THR:HG23	1.95	0.47
15:A:1117:CLA:H143	15:A:1125:CLA:C9	2.45	0.47
15:A:1125:CLA:H122	15:A:1125:CLA:H91	1.97	0.47
2:2:114:MET:HE3	2:2:226:GLY:CA	2.45	0.47
15:A:1012:CLA:H42	6:B:439:VAL:HG22	1.97	0.47
1:1:70:ARG:NE	15:1:605:CLA:O1A	2.48	0.47
15:3:608:CLA:HBC3	15:3:608:CLA:HMC1	1.96	0.47
12:4:501:LUT:H383	15:4:603:CLA:C2B	2.45	0.47
5:A:624:ASP:OD1	5:A:625:SER:N	2.48	0.47
5:A:740:TRP:NE1	15:A:1126:CLA:O1A	2.43	0.47
5:A:407:ALA:HB2	5:A:592:VAL:HG21	1.97	0.47
15:A:1108:CLA:H92	15:A:1112:CLA:H191	1.96	0.47
6:B:529:HIS:CD2	15:B:1236:CLA:NB	2.83	0.46
5:A:561:ARG:NH2	8:D:88:THR:O	2.48	0.46
14:A:4002:BCR:H331	14:A:4002:BCR:C8	2.44	0.46
6:B:708:LEU:HD23	22:B:5002:DGD:HA22	1.96	0.46
1:1:187:ALA:CB	12:1:501:LUT:H393	2.45	0.46
5:A:194:VAL:HG13	15:A:1123:CLA:HMD1	1.97	0.46
10:F:163:GLU:O	14:F:4001:BCR:H362	2.16	0.46
15:3:605:CLA:H71	15:A:1111:CLA:H201	1.97	0.46
4:4:212:LEU:O	4:4:214:THR:N	2.43	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:281:GLY:C	5:A:282:LEU:HD12	2.41	0.46
15:A:1012:CLA:C4	14:A:4006:BCR:H362	2.46	0.46
8:D:129:LEU:C	8:D:130:LEU:HD12	2.41	0.46
4:4:248:ILE:HG22	4:4:248:ILE:O	2.16	0.46
6:B:475:PHE:HB3	6:B:477:LEU:HD23	1.97	0.45
2:2:232:ALA:HB1	12:2:501:LUT:H381	1.97	0.45
1:1:86:ALA:HB1	12:1:501:LUT:H391	1.97	0.45
15:A:1104:CLA:H193	15:A:1104:CLA:HED1	1.98	0.45
15:B:1208:CLA:HBC3	18:B:5003:LMG:H362	1.99	0.45
3:3:146:ASP:OD2	3:3:149:ARG:NH1	2.50	0.45
5:A:677:PHE:CD2	14:A:4006:BCR:H363	2.52	0.45
3:3:118:ARG:NH1	15:3:611:CLA:OBD	2.46	0.45
14:A:4007:BCR:H361	14:A:4007:BCR:H20C	1.81	0.45
15:1:603:CLA:H143	16:1:609:CHL:H92	1.98	0.45
15:3:605:CLA:HBC1	15:3:612:CLA:HBC2	1.98	0.45
5:A:157:LEU:HD23	5:A:157:LEU:O	2.17	0.45
15:B:1214:CLA:C4	15:B:1231:CLA:HED3	2.39	0.45
3:3:161:ASP:OD1	3:3:161:ASP:N	2.47	0.44
6:B:266:THR:O	6:B:268:SER:N	2.50	0.44
5:A:679:TRP:O	5:A:682:SER:OG	2.34	0.44
15:A:1012:CLA:C20	15:A:1013:CLA:H202	2.47	0.44
12:1:501:LUT:H383	15:1:603:CLA:C2B	2.47	0.44
15:4:608:CLA:HHD	15:4:608:CLA:HBC2	1.99	0.44
5:A:429:ARG:NH1	15:A:1129:CLA:O2D	2.51	0.44
5:A:433:HIS:CE1	15:A:1129:CLA:ND	2.85	0.44
12:3:501:LUT:C17	15:3:601:CLA:H72	2.48	0.44
5:A:684:MET:O	5:A:688:SER:OG	2.23	0.44
1:1:52:GLY:HA3	1:1:178:LEU:HD23	1.99	0.44
6:B:44:TYR:CZ	6:B:331:LEU:HD21	2.52	0.44
6:B:390:HIS:CE1	15:B:1226:CLA:NA	2.85	0.44
6:B:331:LEU:HD22	15:B:1202:CLA:H201	2.00	0.44
6:B:479:LEU:HD11	6:B:495:LEU:HD21	1.99	0.44
14:J:4001:BCR:C8	14:J:4001:BCR:H321	2.47	0.44
12:3:501:LUT:C20	14:3:506:BCR:H373	2.48	0.43
8:D:75:LEU:HD11	8:D:102:VAL:HG21	2.00	0.43
1:1:122:PHE:HD2	1:1:126:THR:HG21	1.83	0.43
13:1:502:XAT:H402	15:1:605:CLA:C3B	2.48	0.43
3:3:129:ALA:HB3	3:3:130:PRO:HD3	2.00	0.43
5:A:414:VAL:O	5:A:558:ARG:NH2	2.51	0.43
15:B:1216:CLA:HBC2	15:B:1221:CLA:H172	2.01	0.43
3:3:262:ASP:OD1	3:3:263:GLY:N	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:A:1117:CLA:H151	15:A:1125:CLA:H92	2.00	0.43
15:A:1122:CLA:CBB	15:A:1122:CLA:H191	2.48	0.43
6:B:44:TYR:CE1	6:B:331:LEU:HD21	2.54	0.43
2:2:261:VAL:HG23	2:2:261:VAL:O	2.17	0.43
4:4:215:LEU:HA	4:4:218:ILE:HG22	2.01	0.43
5:A:128:ASN:O	10:F:105:ARG:NH2	2.52	0.43
4:4:263:ILE:HG21	15:4:601:CLA:HMD2	1.99	0.43
4:4:290:PHE:CE1	13:4:502:XAT:H192	2.53	0.43
15:1:603:CLA:H51	15:1:603:CLA:H93	2.00	0.43
2:2:232:ALA:CB	12:2:501:LUT:H381	2.49	0.43
4:4:174:MET:SD	12:4:501:LUT:H201	2.58	0.43
2:2:120:ILE:HG23	2:2:136:TRP:HB3	1.99	0.43
5:A:201:HIS:CD2	15:A:1111:CLA:NB	2.87	0.43
5:A:687:PHE:CD2	6:B:665:LEU:HD23	2.54	0.43
9:E:110:ASN:OD1	9:E:114:VAL:N	2.49	0.43
2:2:78:ASP:OD2	2:2:79:GLY:N	2.52	0.43
14:A:4007:BCR:H15C	15:B:1023:CLA:H161	2.01	0.42
14:3:506:BCR:H20C	14:3:506:BCR:H361	1.75	0.42
4:4:272:THR:HG23	4:4:272:THR:O	2.20	0.42
15:B:1223:CLA:H13	14:B:4005:BCR:H15C	2.00	0.42
15:B:1240:CLA:CED	14:B:4004:BCR:H353	2.48	0.42
5:A:408:HIS:CE1	15:A:1128:CLA:NA	2.88	0.42
15:A:1105:CLA:HMC1	15:A:1105:CLA:HBC3	2.02	0.42
6:B:657:VAL:HG22	15:B:1239:CLA:HMB2	2.00	0.42
6:B:320:HIS:CD2	15:B:1220:CLA:ND	2.87	0.42
12:1:501:LUT:H203	15:1:601:CLA:HMC3	2.02	0.42
6:B:561:ASP:OD1	7:C:52:LYS:NZ	2.52	0.42
15:B:1208:CLA:HBC2	15:B:1208:CLA:HHD	2.02	0.42
15:A:1013:CLA:H41	15:A:1013:CLA:H62	1.87	0.42
14:A:4006:BCR:H20C	14:A:4006:BCR:H361	1.82	0.42
6:B:432:PHE:HZ	14:B:4006:BCR:H11C	1.84	0.42
14:B:4002:BCR:H20C	14:B:4002:BCR:H361	1.88	0.42
1:1:86:ALA:HB1	12:1:501:LUT:H30	2.02	0.42
6:B:546:LYS:NZ	10:F:237:ILE:HG21	2.35	0.41
15:B:1202:CLA:HBC2	15:B:1226:CLA:HMA1	2.02	0.41
3:3:124:ALA:HB3	12:3:501:LUT:H32	2.01	0.41
15:A:1104:CLA:H42	17:A:5002:LHG:H261	2.02	0.41
6:B:437:LEU:CD1	14:F:4001:BCR:H383	2.50	0.41
5:A:121:ILE:HG21	14:J:4002:BCR:H332	2.03	0.41
18:B:5003:LMG:O5	18:B:5003:LMG:O4	2.20	0.41
3:3:104:VAL:HG23	3:3:104:VAL:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:338:HIS:H	5:A:426:LEU:HD12	1.85	0.41
5:A:393:HIS:HE2	15:A:1127:CLA:C2B	2.33	0.41
5:A:565:ASP:OD1	5:A:565:ASP:N	2.52	0.41
1:1:154:PRO:O	15:1:601:CLA:HED2	2.21	0.41
13:3:502:XAT:H202	15:3:605:CLA:HMC1	2.03	0.41
15:B:1236:CLA:H11	14:B:4005:BCR:H352	2.02	0.41
8:D:82:PRO:HG2	8:D:130:LEU:HD11	2.02	0.41
12:1:501:LUT:H10	12:1:501:LUT:H202	2.01	0.41
13:1:502:XAT:H401	13:1:502:XAT:C15	2.49	0.41
14:3:504:BCR:H15C	14:3:504:BCR:H351	1.92	0.41
4:4:208:ASP:OD1	4:4:208:ASP:N	2.53	0.41
5:A:683:LEU:HB2	15:A:1013:CLA:HMC2	2.03	0.41
6:B:179:HIS:CD2	15:B:1210:CLA:NB	2.89	0.41
1:1:80:ARG:NH1	15:1:611:CLA:OBD	2.48	0.41
15:1:615:CLA:O1A	15:1:615:CLA:H2A	2.20	0.41
15:3:603:CLA:HMB2	15:3:608:CLA:HBC1	2.02	0.41
15:A:1012:CLA:H42	6:B:439:VAL:CG2	2.49	0.41
15:B:1224:CLA:O1D	15:B:1225:CLA:HMA1	2.21	0.41
12:1:501:LUT:H202	12:1:501:LUT:C10	2.50	0.41
5:A:199:ASN:HB3	15:A:1118:CLA:HMD1	2.02	0.41
5:A:370:HIS:CD2	15:A:1125:CLA:NC	2.89	0.41
15:A:1126:CLA:H141	15:A:1126:CLA:H202	2.03	0.41
9:E:73:LEU:HB2	9:E:127:VAL:HG11	2.02	0.41
1:1:88:GLY:O	1:1:92:VAL:HG23	2.21	0.41
14:A:4008:BCR:H11C	14:A:4008:BCR:H341	1.91	0.41
12:1:501:LUT:H203	15:1:601:CLA:CMC	2.50	0.40
14:B:4001:BCR:H20C	14:B:4001:BCR:H361	1.91	0.40
14:J:4002:BCR:H20C	14:J:4002:BCR:H361	1.96	0.40
15:2:608:CLA:HBC2	15:2:608:CLA:HHD	2.03	0.40
15:A:1125:CLA:H91	15:A:1125:CLA:C12	2.52	0.40
6:B:333:PHE:CE2	6:B:337:LEU:HD11	2.56	0.40
6:B:617:LEU:HD21	15:B:1021:CLA:H151	2.02	0.40
15:2:616:CLA:H121	15:2:616:CLA:H91	2.03	0.40
3:3:152:VAL:HG12	3:3:153:ILE:HG13	2.03	0.40
6:B:442:ASP:OD1	6:B:617:LEU:N	2.50	0.40
5:A:605:ILE:HD11	19:A:1011:CL0:H69	2.04	0.40
6:B:352:HIS:CD2	15:B:1223:CLA:NC	2.89	0.40
15:B:1223:CLA:CHC	15:B:1231:CLA:HMA2	2.51	0.40
15:B:1238:CLA:HHD	15:B:1238:CLA:HBC2	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1	195/197 (99%)	188 (96%)	7 (4%)	0	100	100
2	2	206/208 (99%)	200 (97%)	6 (3%)	0	100	100
3	3	208/210 (99%)	196 (94%)	12 (6%)	0	100	100
4	4	209/211 (99%)	192 (92%)	16 (8%)	1 (0%)	24	59
5	A	737/739 (100%)	706 (96%)	30 (4%)	1 (0%)	48	79
6	B	728/730 (100%)	713 (98%)	15 (2%)	0	100	100
7	C	78/80 (98%)	77 (99%)	1 (1%)	0	100	100
8	D	139/141 (99%)	130 (94%)	9 (6%)	0	100	100
9	E	62/64 (97%)	61 (98%)	1 (2%)	0	100	100
10	F	161/163 (99%)	159 (99%)	2 (1%)	0	100	100
11	J	38/40 (95%)	34 (90%)	4 (10%)	0	100	100
All	All	2761/2783 (99%)	2656 (96%)	103 (4%)	2 (0%)	49	79

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	4	212	LEU
5	A	477	ILE

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1	152/152 (100%)	152 (100%)	0	100	100
2	2	167/167 (100%)	167 (100%)	0	100	100
3	3	160/160 (100%)	160 (100%)	0	100	100
4	4	169/169 (100%)	169 (100%)	0	100	100
5	A	598/598 (100%)	598 (100%)	0	100	100
6	B	590/590 (100%)	590 (100%)	0	100	100
7	C	68/68 (100%)	68 (100%)	0	100	100
8	D	121/121 (100%)	121 (100%)	0	100	100
9	E	57/57 (100%)	57 (100%)	0	100	100
10	F	136/136 (100%)	136 (100%)	0	100	100
11	J	35/35 (100%)	35 (100%)	0	100	100
All	All	2253/2253 (100%)	2253 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
2	2	109	HIS
3	3	224	ASN
4	4	155	ASN
4	4	281	GLN
4	4	300	ASN
5	A	478	GLN
6	B	300	HIS
9	E	86	GLN
10	F	223	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

193 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
12	LUT	2	501	-	42,43,43	6.40	31 (73%)	51,60,60	2.41	18 (35%)
15	CLA	A	1113	-	49,53,73	1.36	8 (16%)	58,89,113	1.43	4 (6%)
15	CLA	1	611	-	52,56,73	1.34	9 (17%)	61,92,113	1.35	4 (6%)
15	CLA	A	1101	-	69,73,73	1.16	8 (11%)	82,113,113	1.31	7 (8%)
15	CLA	4	608	-	50,54,73	1.35	9 (18%)	59,90,113	1.60	8 (13%)
15	CLA	A	1117	-	69,73,73	1.14	9 (13%)	82,113,113	1.37	8 (9%)
15	CLA	A	1105	-	64,68,73	1.22	8 (12%)	76,107,113	1.47	13 (17%)
15	CLA	B	1227	-	69,73,73	1.17	7 (10%)	82,113,113	1.30	5 (6%)
14	BCR	B	4004	-	41,41,41	1.18	2 (4%)	56,56,56	1.34	8 (14%)
15	CLA	2	616	-	69,73,73	1.16	9 (13%)	82,113,113	1.46	10 (12%)
14	BCR	F	4002	-	41,41,41	1.26	3 (7%)	56,56,56	1.36	8 (14%)
15	CLA	B	1229	-	64,68,73	1.20	7 (10%)	76,107,113	1.37	6 (7%)
15	CLA	B	1231	-	64,68,73	1.22	9 (14%)	76,107,113	1.39	6 (7%)
15	CLA	A	1136	-	69,73,73	1.16	8 (11%)	82,113,113	1.27	4 (4%)
15	CLA	B	1221	-	69,73,73	1.17	10 (14%)	82,113,113	1.36	6 (7%)
15	CLA	B	1215	-	69,73,73	1.15	8 (11%)	82,113,113	1.31	8 (9%)
15	CLA	4	612	4	69,73,73	1.15	9 (13%)	82,113,113	1.24	5 (6%)
15	CLA	A	1139	-	69,73,73	1.16	8 (11%)	82,113,113	1.32	8 (9%)
15	CLA	B	1240	17	69,73,73	1.17	9 (13%)	82,113,113	1.36	8 (9%)
14	BCR	4	503	-	41,41,41	1.28	3 (7%)	56,56,56	1.36	9 (16%)
18	LMG	2	804	-	50,50,55	0.71	0	58,58,63	1.28	7 (12%)
15	CLA	2	605	-	69,73,73	1.16	8 (11%)	82,113,113	1.31	5 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
16	CHL	1	610	-	41,55,74	1.95	9 (21%)	35,91,114	2.18	10 (28%)
15	CLA	A	1107	5	55,59,73	1.32	8 (14%)	64,96,113	1.50	8 (12%)
15	CLA	2	604	2	69,73,73	1.14	9 (13%)	82,113,113	1.26	7 (8%)
15	CLA	1	612	1	44,48,73	1.43	8 (18%)	51,82,113	1.42	5 (9%)
20	PQN	B	2002	-	34,34,34	0.71	0	43,45,45	0.92	1 (2%)
17	LHG	A	5002	-	48,48,48	0.70	1 (2%)	51,54,54	1.20	4 (7%)
14	BCR	A	4004	-	41,41,41	1.19	3 (7%)	56,56,56	1.44	7 (12%)
15	CLA	A	1126	-	69,73,73	1.15	8 (11%)	82,113,113	1.23	8 (9%)
15	CLA	F	1301	-	50,54,73	1.36	7 (14%)	59,90,113	1.41	4 (6%)
15	CLA	A	1114	-	59,63,73	1.27	8 (13%)	70,101,113	1.45	5 (7%)
15	CLA	B	1209	-	50,54,73	1.34	8 (16%)	59,90,113	1.41	4 (6%)
15	CLA	A	1140	-	65,69,73	1.18	9 (13%)	77,108,113	1.37	5 (6%)
15	CLA	F	1302	10	53,57,73	1.30	8 (15%)	61,93,113	1.44	6 (9%)
13	XAT	2	502	-	41,47,47	2.72	19 (46%)	54,74,74	9.15	29 (53%)
15	CLA	A	1122	-	69,73,73	1.17	8 (11%)	82,113,113	1.40	7 (8%)
15	CLA	B	1216	-	63,67,73	1.21	9 (14%)	74,105,113	1.34	7 (9%)
15	CLA	B	1224	-	65,69,73	1.18	8 (12%)	77,108,113	1.21	4 (5%)
15	CLA	3	608	-	69,73,73	1.16	8 (11%)	82,113,113	1.23	5 (6%)
14	BCR	3	503	-	41,41,41	1.22	3 (7%)	56,56,56	1.22	7 (12%)
15	CLA	2	612	2	59,63,73	1.24	8 (13%)	70,101,113	1.33	5 (7%)
14	BCR	2	503	-	41,41,41	1.21	3 (7%)	56,56,56	1.21	8 (14%)
15	CLA	4	605	-	69,73,73	1.16	8 (11%)	82,113,113	1.33	6 (7%)
14	BCR	J	4001	-	41,41,41	1.09	3 (7%)	56,56,56	1.39	8 (14%)
15	CLA	B	1205	-	69,73,73	1.14	9 (13%)	82,113,113	1.26	6 (7%)
14	BCR	J	4002	-	41,41,41	1.26	4 (9%)	56,56,56	1.27	6 (10%)
15	CLA	4	609	4	64,68,73	1.19	7 (10%)	76,107,113	1.40	6 (7%)
15	CLA	B	1210	-	69,73,73	1.17	9 (13%)	82,113,113	1.28	9 (10%)
15	CLA	B	1239	-	46,50,73	1.39	7 (15%)	53,85,113	1.58	6 (11%)
16	CHL	4	611	-	45,59,74	1.99	8 (17%)	40,96,114	2.04	10 (25%)
15	CLA	B	1213	-	59,63,73	1.24	8 (13%)	70,101,113	1.37	5 (7%)
15	CLA	B	1203	-	69,73,73	1.18	8 (11%)	82,113,113	1.30	4 (4%)
15	CLA	1	605	-	69,73,73	1.17	8 (11%)	82,113,113	1.27	3 (3%)
15	CLA	B	1214	-	69,73,73	1.17	9 (13%)	82,113,113	1.37	8 (9%)
17	LHG	B	5001	15	41,41,48	0.74	1 (2%)	44,47,54	1.27	3 (6%)
15	CLA	A	1111	-	69,73,73	1.16	8 (11%)	82,113,113	1.33	7 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	DGD	B	5002	-	62,62,67	0.86	2 (3%)	76,76,81	1.40	12 (15%)
15	CLA	1	603	-	64,68,73	1.18	9 (14%)	76,107,113	1.41	10 (13%)
15	CLA	A	1102	-	69,73,73	1.14	9 (13%)	82,113,113	1.33	6 (7%)
16	CHL	2	613	-	40,54,74	1.72	9 (22%)	34,90,114	2.12	9 (26%)
17	LHG	3	801	-	46,46,48	0.67	1 (2%)	48,51,54	1.21	6 (12%)
14	BCR	3	504	-	41,41,41	1.31	4 (9%)	56,56,56	1.33	8 (14%)
15	CLA	3	615	3	46,50,73	1.38	8 (17%)	53,85,113	1.44	5 (9%)
15	CLA	A	1132	-	49,53,73	1.35	9 (18%)	58,89,113	1.67	8 (13%)
15	CLA	B	1219	-	69,73,73	1.17	9 (13%)	82,113,113	1.17	5 (6%)
15	CLA	A	1133	-	69,73,73	1.15	9 (13%)	82,113,113	1.32	4 (4%)
19	CL0	A	1011	-	58,73,73	6.22	25 (43%)	60,113,113	4.98	28 (46%)
15	CLA	3	613	-	50,54,73	1.34	8 (16%)	59,90,113	1.44	4 (6%)
15	CLA	4	602	-	54,58,73	1.32	7 (12%)	64,95,113	1.41	5 (7%)
15	CLA	A	1128	-	69,73,73	1.16	8 (11%)	82,113,113	1.30	5 (6%)
16	CHL	4	610	-	41,55,74	2.09	9 (21%)	35,91,114	2.10	9 (25%)
21	SF4	A	3001	5,6	0,12,12	-	-	-	-	-
15	CLA	B	1217	-	50,54,73	1.34	8 (16%)	59,90,113	1.38	4 (6%)
16	CHL	2	611	-	42,56,74	2.08	9 (21%)	36,92,114	2.11	9 (25%)
14	BCR	A	4006	-	41,41,41	1.27	3 (7%)	56,56,56	1.30	9 (16%)
15	CLA	3	603	-	69,73,73	1.16	7 (10%)	82,113,113	1.31	7 (8%)
15	CLA	1	607	17	50,54,73	1.34	9 (18%)	59,90,113	1.38	5 (8%)
15	CLA	B	1235	-	64,68,73	1.19	8 (12%)	76,107,113	1.37	4 (5%)
15	CLA	2	603	2	69,73,73	1.17	8 (11%)	82,113,113	1.26	6 (7%)
15	CLA	1	608	-	59,63,73	1.25	8 (13%)	70,101,113	1.37	6 (8%)
15	CLA	B	1218	-	49,53,73	1.39	7 (14%)	58,89,113	1.47	5 (8%)
15	CLA	1	602	-	50,54,73	1.35	8 (16%)	59,90,113	1.35	4 (6%)
15	CLA	B	1226	-	69,73,73	1.13	6 (8%)	82,113,113	1.45	6 (7%)
15	CLA	A	1124	-	64,68,73	1.21	9 (14%)	76,107,113	1.45	7 (9%)
14	BCR	3	506	-	41,41,41	1.24	3 (7%)	56,56,56	1.28	8 (14%)
15	CLA	B	1211	-	69,73,73	1.17	10 (14%)	82,113,113	1.35	8 (9%)
15	CLA	1	615	1	51,55,73	1.43	10 (19%)	59,90,113	1.49	6 (10%)
15	CLA	B	1207	-	50,54,73	1.34	8 (16%)	59,90,113	1.37	4 (6%)
15	CLA	3	606	-	59,63,73	1.24	9 (15%)	70,101,113	1.33	5 (7%)
14	BCR	B	4001	-	41,41,41	1.21	3 (7%)	56,56,56	1.40	10 (17%)
15	CLA	A	1112	-	69,73,73	1.18	8 (11%)	82,113,113	1.27	5 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	CLA	3	607	-	64,68,73	1.21	8 (12%)	76,107,113	1.33	5 (6%)
15	CLA	B	1204	-	49,53,73	1.36	9 (18%)	58,89,113	1.51	7 (12%)
15	CLA	A	1116	-	60,64,73	1.23	9 (15%)	71,102,113	1.43	7 (9%)
15	CLA	A	1012	-	69,73,73	1.16	9 (13%)	82,113,113	1.28	9 (10%)
15	CLA	2	607	17	64,68,73	1.21	9 (14%)	76,107,113	1.33	5 (6%)
15	CLA	A	1137	-	65,69,73	1.19	6 (9%)	77,108,113	1.47	10 (12%)
15	CLA	A	1141	17	45,49,73	1.39	8 (17%)	54,84,113	1.44	6 (11%)
15	CLA	3	610	-	54,58,73	1.29	9 (16%)	64,95,113	1.39	7 (10%)
15	CLA	B	1208	-	64,68,73	1.21	6 (9%)	76,107,113	1.25	5 (6%)
15	CLA	A	1109	-	69,73,73	1.15	7 (10%)	82,113,113	1.30	4 (4%)
15	CLA	A	1121	-	49,53,73	1.38	9 (18%)	58,89,113	1.43	4 (6%)
15	CLA	B	1236	-	53,57,73	1.32	9 (16%)	61,93,113	1.40	5 (8%)
16	CHL	2	609	2	60,74,74	1.87	9 (15%)	58,114,114	1.76	10 (17%)
17	LHG	1	801	15	48,48,48	0.62	0	51,54,54	1.20	4 (7%)
15	CLA	A	1119	-	69,73,73	1.15	8 (11%)	82,113,113	1.28	5 (6%)
12	LUT	3	501	-	42,43,43	6.41	28 (66%)	51,60,60	3.06	22 (43%)
15	CLA	1	613	-	49,53,73	1.37	8 (16%)	58,89,113	1.40	4 (6%)
15	CLA	3	609	-	46,50,73	1.40	8 (17%)	53,85,113	1.49	5 (9%)
14	BCR	B	4002	-	41,41,41	1.19	2 (4%)	56,56,56	1.43	7 (12%)
16	CHL	1	609	1	60,74,74	1.87	8 (13%)	58,114,114	1.69	10 (17%)
14	BCR	B	4003	-	41,41,41	1.17	2 (4%)	56,56,56	1.47	10 (17%)
15	CLA	A	1129	-	59,63,73	1.27	10 (16%)	70,101,113	1.36	6 (8%)
15	CLA	A	1134	5	46,50,73	1.38	9 (19%)	53,85,113	1.53	5 (9%)
15	CLA	A	1104	-	69,73,73	1.17	8 (11%)	82,113,113	1.31	7 (8%)
15	CLA	2	608	-	54,58,73	1.30	8 (14%)	64,95,113	1.42	5 (7%)
14	BCR	B	4005	-	41,41,41	1.26	3 (7%)	56,56,56	1.37	9 (16%)
15	CLA	A	1118	-	46,50,73	1.38	8 (17%)	53,85,113	1.46	4 (7%)
15	CLA	A	1138	-	69,73,73	1.15	7 (10%)	82,113,113	1.38	8 (9%)
13	XAT	4	502	-	41,47,47	2.67	19 (46%)	54,74,74	9.43	30 (55%)
15	CLA	3	601	3	64,68,73	1.20	9 (14%)	76,107,113	1.36	5 (6%)
15	CLA	4	604	-	64,68,73	1.19	9 (14%)	76,107,113	1.39	7 (9%)
15	CLA	A	1125	-	69,73,73	1.16	9 (13%)	82,113,113	1.22	6 (7%)
18	LMG	B	5003	-	39,39,55	0.86	1 (2%)	47,47,63	1.25	5 (10%)
15	CLA	B	1021	-	69,73,73	1.14	8 (11%)	82,113,113	1.27	5 (6%)
15	CLA	3	605	-	69,73,73	1.17	9 (13%)	82,113,113	1.33	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	LMG	2	803	-	40,40,55	0.88	1 (2%)	48,48,63	1.20	6 (12%)
15	CLA	A	1103	-	69,73,73	1.14	8 (11%)	82,113,113	1.32	5 (6%)
14	BCR	A	4007	-	41,41,41	1.26	3 (7%)	56,56,56	1.30	8 (14%)
15	CLA	A	1013	-	69,73,73	1.14	9 (13%)	82,113,113	1.34	7 (8%)
13	XAT	1	502	-	41,47,47	2.67	20 (48%)	54,74,74	9.50	24 (44%)
15	CLA	1	604	1	69,73,73	1.14	10 (14%)	82,113,113	1.27	6 (7%)
15	CLA	2	602	-	49,53,73	1.38	7 (14%)	58,89,113	1.43	5 (8%)
17	LHG	A	5001	15	48,48,48	0.65	0	51,54,54	1.14	3 (5%)
15	CLA	B	1022	-	69,73,73	1.16	9 (13%)	82,113,113	1.23	5 (6%)
15	CLA	B	1222	-	69,73,73	1.15	8 (11%)	82,113,113	1.33	8 (9%)
15	CLA	3	611	-	69,73,73	1.15	9 (13%)	82,113,113	1.27	4 (4%)
16	CHL	4	613	-	55,69,74	1.60	9 (16%)	52,108,114	1.94	10 (19%)
15	CLA	A	1108	-	59,63,73	1.26	8 (13%)	70,101,113	1.41	5 (7%)
15	CLA	A	1110	-	59,63,73	1.27	9 (15%)	70,101,113	1.52	11 (15%)
15	CLA	A	1130	-	49,53,73	1.36	8 (16%)	58,89,113	1.46	6 (10%)
15	CLA	B	1023	-	69,73,73	1.16	9 (13%)	82,113,113	1.33	5 (6%)
20	PQN	A	2001	-	34,34,34	0.66	0	43,45,45	0.92	1 (2%)
15	CLA	J	1302	11	46,50,73	1.38	8 (17%)	53,85,113	1.50	4 (7%)
21	SF4	C	3003	7	0,12,12	-	-	-	-	-
15	CLA	A	1106	5	69,73,73	1.15	8 (11%)	82,113,113	1.33	7 (8%)
15	CLA	4	616	4	55,59,73	1.29	9 (16%)	64,96,113	1.35	5 (7%)
17	LHG	2	801	15	34,34,48	0.82	2 (5%)	37,40,54	1.25	3 (8%)
16	CHL	3	604	3	55,69,74	1.48	8 (14%)	52,108,114	1.89	13 (25%)
15	CLA	B	1234	-	59,63,73	1.26	9 (15%)	70,101,113	1.37	5 (7%)
15	CLA	B	1237	-	49,53,73	1.37	9 (18%)	58,89,113	1.45	4 (6%)
14	BCR	A	4005	-	41,41,41	1.24	3 (7%)	56,56,56	1.26	9 (16%)
14	BCR	F	4001	-	41,41,41	1.20	3 (7%)	56,56,56	1.34	8 (14%)
15	CLA	4	606	-	54,58,73	1.30	9 (16%)	64,95,113	1.45	6 (9%)
15	CLA	B	1201	-	47,51,73	1.38	9 (19%)	55,86,113	1.40	4 (7%)
12	LUT	1	501	-	42,43,43	6.26	27 (64%)	51,60,60	2.26	17 (33%)
15	CLA	B	1232	-	50,54,73	1.34	9 (18%)	59,90,113	1.42	5 (8%)
15	CLA	B	1202	-	69,73,73	1.17	9 (13%)	82,113,113	1.28	6 (7%)
15	CLA	4	601	4	64,68,73	1.20	10 (15%)	76,107,113	1.36	8 (10%)
14	BCR	A	4003	-	41,41,41	1.17	2 (4%)	56,56,56	1.44	9 (16%)
15	CLA	A	1120	-	46,50,73	1.38	8 (17%)	53,85,113	1.48	5 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	CLA	4	603	-	69,73,73	1.17	8 (11%)	82,113,113	1.38	7 (8%)
14	BCR	A	4002	-	41,41,41	1.30	4 (9%)	56,56,56	1.34	8 (14%)
15	CLA	B	1220	-	55,59,73	1.31	9 (16%)	64,96,113	1.39	6 (9%)
15	CLA	B	1228	-	64,68,73	1.21	8 (12%)	76,107,113	1.29	6 (7%)
15	CLA	1	606	-	54,58,73	1.30	8 (14%)	64,95,113	1.40	6 (9%)
15	CLA	B	1225	-	69,73,73	1.15	8 (11%)	82,113,113	1.29	5 (6%)
15	CLA	B	1223	-	69,73,73	1.16	9 (13%)	82,113,113	1.37	6 (7%)
15	CLA	B	1238	-	55,59,73	1.55	10 (18%)	62,95,113	1.82	11 (17%)
15	CLA	1	601	-	69,73,73	1.15	9 (13%)	82,113,113	1.25	6 (7%)
12	LUT	4	501	-	42,43,43	6.30	29 (69%)	51,60,60	2.81	21 (41%)
15	CLA	2	606	-	49,53,73	1.37	9 (18%)	58,89,113	1.43	5 (8%)
15	CLA	B	1230	-	59,63,73	1.23	9 (15%)	70,101,113	1.41	10 (14%)
15	CLA	4	607	-	64,68,73	1.21	9 (14%)	76,107,113	1.34	7 (9%)
14	BCR	B	4006	-	41,41,41	1.27	3 (7%)	56,56,56	1.26	6 (10%)
15	CLA	A	1123	-	69,73,73	1.18	9 (13%)	82,113,113	1.32	6 (7%)
16	CHL	2	610	-	38,52,74	2.07	9 (23%)	31,87,114	2.23	9 (29%)
15	CLA	3	612	3	69,73,73	1.16	8 (11%)	82,113,113	1.26	5 (6%)
15	CLA	A	1115	-	49,53,73	1.36	9 (18%)	58,89,113	1.47	5 (8%)
18	LMG	2	802	-	50,50,55	0.70	0	58,58,63	1.26	5 (8%)
14	BCR	1	503	-	41,41,41	1.16	3 (7%)	56,56,56	1.37	11 (19%)
15	CLA	A	1127	-	69,73,73	1.15	9 (13%)	82,113,113	1.24	4 (4%)
15	CLA	B	1206	6	49,53,73	1.36	8 (16%)	58,89,113	1.43	5 (8%)
14	BCR	A	4008	-	41,41,41	1.19	3 (7%)	56,56,56	1.33	9 (16%)
15	CLA	2	601	-	69,73,73	1.16	9 (13%)	82,113,113	1.20	6 (7%)
15	CLA	3	614	-	56,60,73	1.31	8 (14%)	65,97,113	1.45	5 (7%)
15	CLA	A	1135	-	55,59,73	1.29	7 (12%)	64,96,113	1.45	5 (7%)
15	CLA	A	1131	-	49,53,73	1.38	8 (16%)	58,89,113	1.34	4 (6%)
21	SF4	C	3002	7	0,12,12	-	-	-	-	-
13	XAT	3	502	-	41,47,47	2.79	22 (53%)	54,74,74	9.72	29 (53%)
15	CLA	B	1212	-	59,63,73	1.25	8 (13%)	70,101,113	1.34	5 (7%)
18	LMG	4	801	-	37,37,55	1.02	3 (8%)	45,45,63	1.30	3 (6%)

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
12	LUT	2	501	-	1/1/27/27	18/29/67/67	0/2/2/2
15	CLA	A	1113	-	1/1/15/20	5/15/91/115	-
15	CLA	1	611	-	1/1/16/20	5/19/95/115	-
15	CLA	A	1101	-	1/1/20/20	18/39/115/115	-
15	CLA	4	608	-	1/1/15/20	6/17/93/115	-
15	CLA	A	1117	-	1/1/20/20	10/39/115/115	-
15	CLA	A	1105	-	1/1/19/20	15/33/109/115	-
15	CLA	B	1227	-	1/1/20/20	15/39/115/115	-
14	BCR	B	4004	-	-	11/29/63/63	0/2/2/2
15	CLA	2	616	-	-	16/39/115/115	-
14	BCR	F	4002	-	-	16/29/63/63	0/2/2/2
15	CLA	B	1229	-	1/1/19/20	6/33/109/115	-
15	CLA	B	1231	-	1/1/19/20	6/33/109/115	-
15	CLA	A	1136	-	1/1/20/20	14/39/115/115	-
15	CLA	B	1221	-	1/1/20/20	16/39/115/115	-
15	CLA	B	1215	-	1/1/20/20	10/39/115/115	-
15	CLA	4	612	4	1/1/20/20	8/39/115/115	-
15	CLA	A	1139	-	1/1/20/20	14/39/115/115	-
15	CLA	B	1240	17	1/1/20/20	11/39/115/115	-
14	BCR	4	503	-	-	16/29/63/63	0/2/2/2
18	LMG	2	804	-	-	24/45/65/70	0/1/1/1
15	CLA	2	605	-	1/1/20/20	13/39/115/115	-
16	CHL	1	610	-	3/3/21/26	2/17/115/137	-
15	CLA	A	1107	5	1/1/17/20	3/23/99/115	-
15	CLA	2	604	2	1/1/20/20	15/39/115/115	-
15	CLA	1	612	1	1/1/14/20	4/10/82/115	-
20	PQN	B	2002	-	-	4/23/43/43	0/2/2/2
17	LHG	A	5002	-	-	23/53/53/53	-
14	BCR	A	4004	-	-	16/29/63/63	0/2/2/2
15	CLA	A	1126	-	1/1/20/20	13/39/115/115	-
15	CLA	F	1301	-	1/1/15/20	8/17/93/115	-
15	CLA	A	1114	-	1/1/18/20	8/27/103/115	-
15	CLA	B	1209	-	1/1/15/20	5/17/93/115	-
15	CLA	A	1140	-	1/1/19/20	8/35/111/115	-
15	CLA	F	1302	10	1/1/16/20	7/20/96/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	XAT	2	502	-	-	12/31/93/93	0/4/4/4
15	CLA	A	1122	-	1/1/20/20	12/39/115/115	-
15	CLA	B	1216	-	1/1/18/20	10/32/108/115	-
15	CLA	B	1224	-	1/1/19/20	13/35/111/115	-
15	CLA	3	608	-	1/1/20/20	17/39/115/115	-
14	BCR	3	503	-	-	17/29/63/63	0/2/2/2
15	CLA	2	612	2	1/1/18/20	3/27/103/115	-
15	CLA	4	605	-	1/1/20/20	11/39/115/115	-
14	BCR	2	503	-	-	20/29/63/63	0/2/2/2
15	CLA	B	1205	-	1/1/20/20	9/39/115/115	-
14	BCR	J	4001	-	-	18/29/63/63	0/2/2/2
14	BCR	J	4002	-	-	17/29/63/63	0/2/2/2
15	CLA	4	609	4	1/1/19/20	10/33/109/115	-
15	CLA	B	1239	-	1/1/14/20	5/12/88/115	-
16	CHL	4	611	-	3/3/23/26	0/21/119/137	-
15	CLA	B	1210	-	-	5/39/115/115	-
15	CLA	B	1213	-	1/1/18/20	3/27/103/115	-
15	CLA	B	1203	-	1/1/20/20	10/39/115/115	-
15	CLA	1	605	-	1/1/20/20	14/39/115/115	-
15	CLA	B	1214	-	1/1/20/20	8/39/115/115	-
17	LHG	B	5001	15	-	25/46/46/53	-
15	CLA	A	1111	-	-	13/39/115/115	-
22	DGD	B	5002	-	-	17/50/90/95	0/2/2/2
15	CLA	1	603	-	1/1/19/20	13/33/109/115	-
15	CLA	A	1102	-	1/1/20/20	14/39/115/115	-
16	CHL	2	613	-	3/3/21/26	6/15/113/137	-
17	LHG	3	801	-	-	21/49/49/53	-
15	CLA	3	615	3	1/1/14/20	6/12/88/115	-
14	BCR	3	504	-	-	16/29/63/63	0/2/2/2
15	CLA	A	1132	-	1/1/15/20	9/15/91/115	-
15	CLA	B	1219	-	-	12/39/115/115	-
15	CLA	A	1133	-	1/1/20/20	19/39/115/115	-
19	CL0	A	1011	-	3/3/25/25	19/37/135/135	-
15	CLA	3	613	-	1/1/15/20	2/17/93/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CLA	4	602	-	1/1/17/20	9/21/97/115	-
15	CLA	A	1128	-	1/1/20/20	12/39/115/115	-
16	CHL	4	610	-	3/3/21/26	4/17/115/137	-
21	SF4	A	3001	5,6	-	-	0/6/5/5
15	CLA	B	1217	-	1/1/15/20	8/17/93/115	-
16	CHL	2	611	-	3/3/21/26	2/18/116/137	-
15	CLA	3	603	-	1/1/20/20	12/39/115/115	-
14	BCR	A	4006	-	-	16/29/63/63	0/2/2/2
15	CLA	1	607	17	1/1/15/20	8/17/93/115	-
15	CLA	B	1235	-	1/1/19/20	11/33/109/115	-
15	CLA	2	603	2	1/1/20/20	6/39/115/115	-
15	CLA	1	608	-	1/1/18/20	11/27/103/115	-
15	CLA	B	1218	-	1/1/15/20	5/15/91/115	-
15	CLA	1	602	-	1/1/15/20	6/17/93/115	-
15	CLA	B	1226	-	1/1/20/20	10/39/115/115	-
15	CLA	A	1124	-	1/1/19/20	6/33/109/115	-
15	CLA	B	1211	-	1/1/20/20	13/39/115/115	-
14	BCR	3	506	-	-	14/29/63/63	0/2/2/2
15	CLA	1	615	1	1/1/15/20	13/15/91/115	-
15	CLA	B	1207	-	-	11/17/93/115	-
15	CLA	3	606	-	1/1/18/20	6/27/103/115	-
14	BCR	B	4001	-	-	17/29/63/63	0/2/2/2
15	CLA	A	1112	-	1/1/20/20	10/39/115/115	-
15	CLA	3	607	-	1/1/19/20	10/33/109/115	-
15	CLA	B	1204	-	1/1/15/20	6/15/91/115	-
15	CLA	A	1116	-	1/1/18/20	8/29/105/115	-
15	CLA	A	1012	-	1/1/20/20	19/39/115/115	-
15	CLA	2	607	17	1/1/19/20	9/33/109/115	-
15	CLA	A	1137	-	1/1/19/20	10/35/111/115	-
15	CLA	A	1141	17	1/1/14/20	4/10/86/115	-
15	CLA	3	610	-	1/1/17/20	6/21/97/115	-
15	CLA	B	1208	-	1/1/19/20	11/33/109/115	-
15	CLA	A	1109	-	1/1/20/20	13/39/115/115	-
15	CLA	A	1121	-	1/1/15/20	6/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CLA	B	1236	-	1/1/16/20	9/20/96/115	-
16	CHL	2	609	2	4/4/26/26	11/39/137/137	-
17	LHG	1	801	15	-	22/53/53/53	-
15	CLA	A	1119	-	1/1/20/20	7/39/115/115	-
12	LUT	3	501	-	1/1/27/27	18/29/67/67	0/2/2/2
15	CLA	1	613	-	1/1/15/20	6/15/91/115	-
15	CLA	3	609	-	1/1/14/20	4/12/88/115	-
14	BCR	B	4002	-	-	14/29/63/63	0/2/2/2
16	CHL	1	609	1	4/4/26/26	12/39/137/137	-
14	BCR	B	4003	-	-	22/29/63/63	0/2/2/2
15	CLA	A	1129	-	1/1/18/20	8/27/103/115	-
15	CLA	A	1134	5	1/1/14/20	4/12/88/115	-
15	CLA	A	1104	-	1/1/20/20	12/39/115/115	-
15	CLA	2	608	-	1/1/17/20	3/21/97/115	-
15	CLA	A	1118	-	1/1/14/20	5/12/88/115	-
14	BCR	B	4005	-	-	17/29/63/63	0/2/2/2
15	CLA	A	1138	-	1/1/20/20	8/39/115/115	-
13	XAT	4	502	-	-	15/31/93/93	0/4/4/4
15	CLA	3	601	3	1/1/19/20	11/33/109/115	-
15	CLA	4	604	-	1/1/19/20	15/33/109/115	-
15	CLA	A	1125	-	-	14/39/115/115	-
18	LMG	B	5003	-	-	14/34/54/70	0/1/1/1
15	CLA	B	1021	-	1/1/20/20	14/39/115/115	-
15	CLA	3	605	-	1/1/20/20	16/39/115/115	-
18	LMG	2	803	-	-	20/35/55/70	0/1/1/1
15	CLA	A	1103	-	1/1/20/20	12/39/115/115	-
14	BCR	A	4007	-	-	14/29/63/63	0/2/2/2
15	CLA	A	1013	-	1/1/20/20	13/39/115/115	-
13	XAT	1	502	-	-	12/31/93/93	0/4/4/4
15	CLA	1	604	1	1/1/20/20	6/39/115/115	-
15	CLA	2	602	-	1/1/15/20	7/15/91/115	-
17	LHG	A	5001	15	-	16/53/53/53	-
15	CLA	B	1022	-	1/1/20/20	10/39/115/115	-
15	CLA	B	1222	-	1/1/20/20	11/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CLA	3	611	-	1/1/20/20	8/39/115/115	-
16	CHL	4	613	-	4/4/25/26	2/33/131/137	-
15	CLA	A	1108	-	1/1/18/20	7/27/103/115	-
15	CLA	A	1110	-	1/1/18/20	9/27/103/115	-
15	CLA	A	1130	-	1/1/15/20	7/15/91/115	-
15	CLA	B	1023	-	1/1/20/20	15/39/115/115	-
20	PQN	A	2001	-	-	1/23/43/43	0/2/2/2
15	CLA	J	1302	11	1/1/14/20	3/12/88/115	-
21	SF4	C	3003	7	-	-	0/6/5/5
15	CLA	A	1106	5	1/1/20/20	10/39/115/115	-
15	CLA	4	616	4	1/1/17/20	7/23/99/115	-
17	LHG	2	801	15	-	19/39/39/53	-
16	CHL	3	604	3	4/4/25/26	3/33/131/137	-
15	CLA	B	1234	-	1/1/18/20	12/27/103/115	-
15	CLA	B	1237	-	1/1/15/20	6/15/91/115	-
14	BCR	A	4005	-	-	16/29/63/63	0/2/2/2
15	CLA	4	606	-	1/1/17/20	7/21/97/115	-
14	BCR	F	4001	-	-	16/29/63/63	0/2/2/2
15	CLA	B	1201	-	1/1/14/20	1/13/89/115	-
12	LUT	1	501	-	1/1/27/27	22/29/67/67	0/2/2/2
15	CLA	B	1232	-	1/1/15/20	6/17/93/115	-
15	CLA	B	1202	-	1/1/20/20	14/39/115/115	-
15	CLA	4	601	4	1/1/19/20	9/33/109/115	-
15	CLA	A	1120	-	1/1/14/20	4/12/88/115	-
14	BCR	A	4003	-	-	16/29/63/63	0/2/2/2
15	CLA	4	603	-	1/1/20/20	13/39/115/115	-
14	BCR	A	4002	-	-	18/29/63/63	0/2/2/2
15	CLA	B	1220	-	1/1/17/20	7/23/99/115	-
15	CLA	B	1228	-	1/1/19/20	6/33/109/115	-
15	CLA	1	606	-	1/1/17/20	4/21/97/115	-
15	CLA	B	1225	-	1/1/20/20	16/39/115/115	-
15	CLA	B	1223	-	1/1/20/20	5/39/115/115	-
15	CLA	B	1238	-	2/2/17/20	9/20/96/115	-
15	CLA	1	601	-	1/1/20/20	7/39/115/115	-
12	LUT	4	501	-	1/1/27/27	20/29/67/67	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CLA	2	606	-	1/1/15/20	7/15/91/115	-
15	CLA	B	1230	-	1/1/18/20	6/27/103/115	-
15	CLA	4	607	-	1/1/19/20	11/33/109/115	-
15	CLA	A	1123	-	1/1/20/20	15/39/115/115	-
14	BCR	B	4006	-	-	14/29/63/63	0/2/2/2
16	CHL	2	610	-	3/3/20/26	3/13/111/137	-
15	CLA	3	612	3	1/1/20/20	7/39/115/115	-
15	CLA	A	1115	-	1/1/15/20	3/15/91/115	-
18	LMG	2	802	-	-	20/45/65/70	0/1/1/1
14	BCR	1	503	-	-	19/29/63/63	0/2/2/2
15	CLA	A	1127	-	1/1/20/20	10/39/115/115	-
15	CLA	B	1206	6	1/1/15/20	4/15/91/115	-
15	CLA	2	601	-	1/1/20/20	13/39/115/115	-
14	BCR	A	4008	-	-	11/29/63/63	0/2/2/2
15	CLA	3	614	-	1/1/17/20	6/24/100/115	-
15	CLA	A	1135	-	1/1/17/20	4/23/99/115	-
15	CLA	A	1131	-	1/1/15/20	7/15/91/115	-
21	SF4	C	3002	7	-	-	0/6/5/5
13	XAT	3	502	-	-	15/31/93/93	0/4/4/4
15	CLA	B	1212	-	1/1/18/20	5/27/103/115	-
18	LMG	4	801	-	-	10/32/52/70	0/1/1/1

All (1510) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	1011	CL0	C1A-CHA	23.10	1.66	1.40
12	2	501	LUT	C24-C25	22.25	1.59	1.33
12	3	501	LUT	C24-C25	22.14	1.59	1.33
12	1	501	LUT	C24-C25	22.07	1.59	1.33
12	4	501	LUT	C24-C25	21.78	1.59	1.33
19	A	1011	CL0	CHB-C4A	18.20	1.60	1.38
19	A	1011	CL0	CHB-C1B	16.73	1.66	1.39
12	3	501	LUT	C22-C21	-16.29	1.34	1.54
12	2	501	LUT	C22-C21	-16.13	1.35	1.54
12	1	501	LUT	C5-C6	15.61	1.60	1.34
12	4	501	LUT	C5-C6	15.51	1.60	1.34
12	4	501	LUT	C22-C21	-15.50	1.35	1.54
12	2	501	LUT	C5-C6	15.44	1.60	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	1	501	LUT	C22-C21	-15.27	1.36	1.54
12	3	501	LUT	C5-C6	15.24	1.60	1.34
19	A	1011	CL0	CHC-C4B	15.24	1.64	1.39
19	A	1011	CL0	MG-NB	-14.08	1.77	2.05
12	3	501	LUT	C2-C3	-12.43	1.34	1.52
12	4	501	LUT	C2-C3	-12.06	1.35	1.52
12	2	501	LUT	C2-C3	-11.86	1.35	1.52
12	1	501	LUT	C2-C3	-11.83	1.35	1.52
12	1	501	LUT	C22-C23	11.62	1.66	1.52
12	4	501	LUT	C22-C23	11.21	1.65	1.52
12	2	501	LUT	C22-C23	10.99	1.65	1.52
12	3	501	LUT	C22-C23	10.61	1.64	1.52
19	A	1011	CL0	CHC-C1C	9.86	1.58	1.39
19	A	1011	CL0	MG-ND	-9.02	1.87	2.05
16	1	609	CHL	C3A-C2A	-8.69	1.47	1.54
19	A	1011	CL0	C1D-C2D	8.28	1.49	1.39
16	2	609	CHL	C3A-C2A	-8.23	1.47	1.54
16	2	611	CHL	C3A-C2A	-8.16	1.47	1.54
19	A	1011	CL0	CHD-C1D	7.99	1.52	1.39
19	A	1011	CL0	CHD-C4C	7.94	1.54	1.39
16	2	610	CHL	C3A-C2A	-7.87	1.47	1.54
16	4	611	CHL	C3A-C2A	-7.80	1.48	1.54
16	4	610	CHL	C3A-C2A	-7.63	1.48	1.54
19	A	1011	CL0	C3D-CAD	7.57	1.62	1.47
12	4	501	LUT	C4-C3	7.40	1.65	1.52
12	1	501	LUT	C4-C3	7.36	1.65	1.52
12	2	501	LUT	C4-C3	7.35	1.65	1.52
12	3	501	LUT	C8-C9	7.13	1.61	1.46
12	3	501	LUT	C4-C3	7.07	1.64	1.52
16	1	609	CHL	C3B-C4B	6.99	1.48	1.41
16	4	611	CHL	C3B-C4B	6.91	1.48	1.41
16	3	604	CHL	C3B-C4B	6.85	1.48	1.41
16	4	613	CHL	C3B-C4B	6.85	1.48	1.41
16	2	609	CHL	C3B-C4B	6.59	1.47	1.41
16	2	611	CHL	C3B-C4B	6.56	1.47	1.41
16	1	610	CHL	C3B-C4B	6.55	1.47	1.41
16	1	610	CHL	C3A-C2A	-6.43	1.49	1.54
15	B	1238	CLA	C2-C3	6.34	1.53	1.33
16	4	610	CHL	C3B-C4B	6.26	1.47	1.41
16	2	613	CHL	C3B-C4B	6.17	1.47	1.41
19	A	1011	CL0	C3A-C2A	-6.14	1.49	1.54
12	3	501	LUT	C28-C29	5.94	1.58	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	2	610	CHL	C3B-C4B	5.93	1.47	1.41
12	2	501	LUT	C28-C29	5.78	1.58	1.46
12	2	501	LUT	C8-C9	5.74	1.58	1.46
12	4	501	LUT	C8-C9	5.70	1.58	1.46
12	2	501	LUT	C1-C6	-5.66	1.46	1.53
12	4	501	LUT	C1-C6	-5.64	1.46	1.53
12	1	501	LUT	C8-C9	5.64	1.58	1.46
12	1	501	LUT	C1-C6	-5.60	1.46	1.53
19	A	1011	CL0	CBD-CGD	-5.50	1.45	1.52
12	2	501	LUT	C32-C33	5.43	1.57	1.46
16	2	609	CHL	C1A-CHA	-5.36	1.33	1.40
19	A	1011	CL0	CMA-C3A	-5.30	1.44	1.53
13	4	502	XAT	C22-C23	-5.27	1.44	1.52
13	4	502	XAT	C8-C9	5.23	1.57	1.46
12	4	501	LUT	C23-C24	-5.19	1.43	1.50
13	3	502	XAT	C8-C9	5.18	1.57	1.46
12	3	501	LUT	C15-C14	5.17	1.59	1.43
13	3	502	XAT	C28-C29	5.16	1.57	1.46
13	3	502	XAT	C22-C23	-5.15	1.45	1.52
12	2	501	LUT	C15-C14	5.14	1.59	1.43
12	4	501	LUT	C32-C33	5.13	1.56	1.46
16	4	613	CHL	C3A-C2A	-5.12	1.50	1.54
12	4	501	LUT	C15-C14	5.09	1.59	1.43
12	1	501	LUT	C15-C14	5.01	1.58	1.43
12	3	501	LUT	C23-C24	-4.99	1.43	1.50
12	2	501	LUT	C4-C5	-4.98	1.43	1.51
13	1	502	XAT	C8-C9	4.98	1.56	1.46
13	1	502	XAT	C22-C23	-4.97	1.45	1.52
12	3	501	LUT	C4-C5	-4.96	1.43	1.51
13	1	502	XAT	C32-C33	4.95	1.56	1.46
13	3	502	XAT	C12-C13	4.94	1.56	1.46
13	2	502	XAT	C22-C23	-4.91	1.45	1.52
13	2	502	XAT	C28-C29	4.87	1.56	1.46
12	4	501	LUT	C28-C29	4.82	1.56	1.46
13	2	502	XAT	C8-C9	4.79	1.56	1.46
13	1	502	XAT	C28-C29	4.77	1.56	1.46
12	3	501	LUT	C40-C33	4.75	1.60	1.50
12	1	501	LUT	C28-C29	4.74	1.56	1.46
13	1	502	XAT	C12-C13	4.73	1.56	1.46
16	1	609	CHL	C1A-CHA	-4.70	1.34	1.40
13	4	502	XAT	C12-C13	4.69	1.56	1.46
13	2	502	XAT	C32-C33	4.69	1.56	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	2	502	XAT	C12-C13	4.68	1.56	1.46
13	1	502	XAT	C4-C5	4.64	1.58	1.52
12	1	501	LUT	C4-C5	-4.62	1.43	1.51
13	4	502	XAT	C32-C33	4.62	1.55	1.46
13	3	502	XAT	C26-C27	4.61	1.58	1.50
12	4	501	LUT	C11-C10	4.55	1.57	1.43
12	1	501	LUT	C11-C10	4.55	1.57	1.43
12	2	501	LUT	C40-C33	4.53	1.60	1.50
12	2	501	LUT	C11-C10	4.53	1.57	1.43
13	3	502	XAT	C32-C33	4.52	1.55	1.46
12	2	501	LUT	C23-C24	-4.52	1.44	1.50
12	3	501	LUT	C19-C9	4.50	1.59	1.50
12	4	501	LUT	C40-C33	4.48	1.59	1.50
13	3	502	XAT	C4-C5	4.45	1.58	1.52
19	A	1011	CL0	C4A-C3A	4.45	1.59	1.51
12	3	501	LUT	C32-C33	4.40	1.55	1.46
12	1	501	LUT	C23-C24	-4.38	1.44	1.50
14	B	4001	BCR	C1-C6	-4.37	1.48	1.53
12	4	501	LUT	C4-C5	-4.36	1.44	1.51
13	2	502	XAT	C4-C5	4.36	1.58	1.52
13	3	502	XAT	C11-C10	4.33	1.56	1.43
13	4	502	XAT	C28-C29	4.30	1.55	1.46
13	4	502	XAT	C11-C10	4.29	1.56	1.43
12	4	501	LUT	C21-C26	4.27	1.68	1.56
12	1	501	LUT	C40-C33	4.27	1.59	1.50
12	3	501	LUT	C1-C6	-4.27	1.48	1.53
12	3	501	LUT	C21-C26	4.25	1.68	1.56
13	2	502	XAT	C35-C34	4.25	1.56	1.43
12	3	501	LUT	C11-C10	4.23	1.56	1.43
13	4	502	XAT	C15-C14	4.22	1.56	1.43
14	F	4002	BCR	C1-C6	-4.21	1.48	1.53
14	3	506	BCR	C1-C6	-4.20	1.48	1.53
13	3	502	XAT	C15-C14	4.20	1.56	1.43
13	1	502	XAT	C35-C34	4.19	1.56	1.43
13	2	502	XAT	C15-C14	4.17	1.56	1.43
13	4	502	XAT	C4-C5	4.16	1.58	1.52
14	F	4001	BCR	C1-C6	-4.16	1.48	1.53
14	A	4002	BCR	C30-C25	-4.15	1.48	1.53
14	3	504	BCR	C30-C25	-4.15	1.48	1.53
13	4	502	XAT	C35-C34	4.10	1.55	1.43
12	2	501	LUT	C21-C26	4.08	1.67	1.56
14	A	4007	BCR	C1-C6	-4.08	1.48	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	2	502	XAT	C11-C10	4.08	1.55	1.43
12	3	501	LUT	C28-C27	4.06	1.41	1.32
14	3	504	BCR	C1-C6	-4.04	1.48	1.53
12	3	501	LUT	C35-C34	4.04	1.55	1.43
14	2	503	BCR	C1-C6	-4.03	1.48	1.53
12	1	501	LUT	C32-C33	4.02	1.54	1.46
14	4	503	BCR	C1-C6	-4.02	1.48	1.53
13	1	502	XAT	C31-C30	4.02	1.55	1.43
12	2	501	LUT	C19-C9	4.01	1.59	1.50
12	2	501	LUT	C2-C1	4.01	1.66	1.54
12	1	501	LUT	C2-C1	4.00	1.66	1.54
13	3	502	XAT	C31-C30	3.97	1.55	1.43
12	1	501	LUT	C35-C34	3.96	1.55	1.43
13	1	502	XAT	C11-C10	3.96	1.55	1.43
14	B	4006	BCR	C1-C6	-3.96	1.48	1.53
12	4	501	LUT	C19-C9	3.95	1.58	1.50
14	B	4002	BCR	C30-C25	-3.94	1.48	1.53
12	1	501	LUT	C19-C9	3.93	1.58	1.50
12	4	501	LUT	C35-C34	3.93	1.55	1.43
14	J	4002	BCR	C1-C6	-3.92	1.48	1.53
13	1	502	XAT	C15-C14	3.92	1.55	1.43
14	J	4002	BCR	C30-C25	-3.92	1.48	1.53
12	1	501	LUT	C21-C26	3.92	1.67	1.56
12	2	501	LUT	C35-C34	3.91	1.55	1.43
14	A	4002	BCR	C1-C6	-3.91	1.48	1.53
14	A	4006	BCR	C1-C6	-3.91	1.48	1.53
14	A	4005	BCR	C1-C6	-3.91	1.48	1.53
14	B	4005	BCR	C1-C6	-3.90	1.48	1.53
14	B	4006	BCR	C30-C25	-3.87	1.48	1.53
14	A	4008	BCR	C1-C6	-3.87	1.48	1.53
12	3	501	LUT	C2-C1	3.87	1.66	1.54
12	4	501	LUT	C12-C13	3.85	1.54	1.46
14	4	503	BCR	C30-C25	-3.85	1.48	1.53
12	4	501	LUT	C2-C1	3.85	1.66	1.54
13	4	502	XAT	C31-C30	3.83	1.55	1.43
12	2	501	LUT	C28-C27	3.82	1.41	1.32
16	2	609	CHL	C2C-C3C	3.82	1.40	1.36
13	2	502	XAT	C31-C30	3.81	1.55	1.43
14	1	503	BCR	C30-C25	-3.81	1.48	1.53
13	3	502	XAT	C35-C34	3.80	1.55	1.43
13	4	502	XAT	C6-C7	3.78	1.57	1.50
13	2	502	XAT	C26-C27	3.77	1.57	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	2	502	XAT	C24-C23	3.76	1.57	1.52
12	2	501	LUT	C12-C13	3.75	1.54	1.46
19	A	1011	CL0	C3B-C2B	-3.75	1.35	1.40
14	3	506	BCR	C30-C25	-3.74	1.49	1.53
16	1	610	CHL	C1A-CHA	-3.73	1.35	1.40
12	1	501	LUT	C12-C13	3.73	1.53	1.46
13	2	502	XAT	C6-C7	3.71	1.57	1.50
14	B	4005	BCR	C30-C25	-3.70	1.49	1.53
16	2	611	CHL	C1A-CHA	-3.69	1.35	1.40
16	4	610	CHL	C2C-C3C	3.67	1.39	1.36
14	3	503	BCR	C1-C6	-3.66	1.49	1.53
14	3	503	BCR	C30-C25	-3.65	1.49	1.53
12	3	501	LUT	C8-C7	3.63	1.43	1.33
16	4	611	CHL	C1A-CHA	-3.62	1.35	1.40
14	A	4003	BCR	C1-C6	-3.62	1.49	1.53
12	2	501	LUT	C31-C30	3.60	1.54	1.43
13	3	502	XAT	C2-C1	-3.60	1.49	1.54
16	1	610	CHL	CBB-CAB	3.60	1.51	1.29
12	3	501	LUT	C12-C13	3.60	1.53	1.46
14	A	4004	BCR	C30-C25	-3.59	1.49	1.53
16	4	610	CHL	CBB-CAB	3.59	1.51	1.29
13	1	502	XAT	C6-C7	3.54	1.56	1.50
13	4	502	XAT	C26-C27	3.54	1.56	1.50
15	1	615	CLA	C2-C3	3.53	1.51	1.29
16	4	611	CHL	CBB-CAB	3.52	1.51	1.29
14	A	4006	BCR	C30-C25	-3.52	1.49	1.53
13	2	502	XAT	C2-C1	-3.51	1.49	1.54
14	A	4004	BCR	C1-C6	-3.51	1.49	1.53
13	1	502	XAT	C2-C1	-3.51	1.49	1.54
16	2	613	CHL	C1A-CHA	-3.49	1.36	1.40
16	2	613	CHL	CBB-CAB	3.49	1.51	1.29
16	2	611	CHL	CBB-CAB	3.48	1.51	1.29
13	1	502	XAT	C26-C27	3.47	1.56	1.50
16	4	613	CHL	CBB-CAB	3.47	1.51	1.29
15	A	1126	CLA	C1D-ND	3.46	1.42	1.37
14	B	4003	BCR	C30-C25	-3.46	1.49	1.53
14	B	4004	BCR	C30-C25	-3.46	1.49	1.53
14	F	4002	BCR	C30-C25	-3.46	1.49	1.53
15	B	1218	CLA	C4B-NB	3.45	1.42	1.37
16	4	610	CHL	C1A-CHA	-3.44	1.36	1.40
14	A	4007	BCR	C30-C25	-3.43	1.49	1.53
14	A	4005	BCR	C30-C25	-3.42	1.49	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	1011	CL0	C1B-C2B	3.41	1.43	1.39
13	4	502	XAT	C2-C1	-3.40	1.49	1.54
16	3	604	CHL	CBB-CAB	3.40	1.50	1.29
16	1	609	CHL	CBB-CAB	3.39	1.50	1.29
15	1	611	CLA	C1D-ND	3.38	1.42	1.37
13	3	502	XAT	C6-C7	3.38	1.56	1.50
16	3	604	CHL	C1A-CHA	-3.36	1.36	1.40
15	B	1226	CLA	C1B-C2B	3.35	1.51	1.43
16	2	609	CHL	CBB-CAB	3.34	1.50	1.29
15	B	1214	CLA	C1D-ND	3.34	1.42	1.37
12	3	501	LUT	C7-C6	3.33	1.56	1.45
15	A	1116	CLA	C1D-ND	3.32	1.42	1.37
15	1	615	CLA	C1D-ND	3.30	1.42	1.37
14	B	4004	BCR	C1-C6	-3.29	1.49	1.53
15	3	607	CLA	C1D-ND	3.29	1.42	1.37
14	2	503	BCR	C30-C25	-3.29	1.49	1.53
15	3	614	CLA	C4B-NB	3.28	1.42	1.37
14	A	4008	BCR	C30-C25	-3.27	1.49	1.53
12	4	501	LUT	C31-C30	3.26	1.53	1.43
15	B	1223	CLA	C1D-ND	3.25	1.42	1.37
15	4	603	CLA	C1D-ND	3.24	1.42	1.37
15	2	616	CLA	C1D-ND	3.24	1.42	1.37
16	2	610	CHL	CBB-CAB	3.23	1.49	1.29
15	B	1224	CLA	C1D-ND	3.22	1.42	1.37
12	3	501	LUT	C31-C30	3.22	1.53	1.43
15	3	615	CLA	C1D-ND	3.22	1.42	1.37
15	B	1229	CLA	C1D-ND	3.22	1.42	1.37
16	2	613	CHL	C3A-C2A	-3.22	1.51	1.54
14	B	4002	BCR	C1-C6	-3.22	1.49	1.53
15	A	1114	CLA	C1D-ND	3.21	1.42	1.37
15	A	1123	CLA	C1D-ND	3.21	1.42	1.37
15	F	1301	CLA	C1D-ND	3.21	1.42	1.37
15	1	613	CLA	C1D-ND	3.21	1.42	1.37
15	3	609	CLA	C1D-ND	3.20	1.42	1.37
14	1	503	BCR	C1-C6	-3.20	1.49	1.53
15	F	1302	CLA	C1D-ND	3.20	1.42	1.37
16	3	604	CHL	CHB-C4A	-3.19	1.34	1.38
15	A	1135	CLA	C1D-ND	3.19	1.42	1.37
15	A	1134	CLA	C1D-ND	3.19	1.42	1.37
15	B	1219	CLA	C4B-NB	3.19	1.42	1.37
15	1	605	CLA	C1D-ND	3.19	1.42	1.37
15	B	1239	CLA	C1D-ND	3.18	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	2	610	CHL	C1A-CHA	-3.18	1.36	1.40
15	A	1137	CLA	C1D-ND	3.17	1.42	1.37
14	F	4001	BCR	C30-C25	-3.16	1.49	1.53
15	A	1121	CLA	C1D-ND	3.16	1.42	1.37
15	A	1130	CLA	C1D-ND	3.16	1.42	1.37
15	3	610	CLA	C1D-ND	3.16	1.42	1.37
15	1	612	CLA	C1D-ND	3.15	1.42	1.37
15	A	1131	CLA	C1D-ND	3.15	1.42	1.37
15	B	1235	CLA	C1D-ND	3.15	1.42	1.37
15	1	602	CLA	C1D-ND	3.15	1.42	1.37
15	2	608	CLA	C1D-ND	3.15	1.42	1.37
15	B	1232	CLA	C4B-NB	3.15	1.42	1.37
15	2	602	CLA	C1D-ND	3.15	1.42	1.37
15	4	607	CLA	C1D-ND	3.15	1.42	1.37
15	B	1202	CLA	C1D-ND	3.14	1.42	1.37
16	1	609	CHL	CHB-C4A	-3.14	1.34	1.38
16	4	613	CHL	C1A-CHA	-3.14	1.36	1.40
15	B	1231	CLA	CMD-C2D	-3.14	1.44	1.50
15	B	1207	CLA	C1D-ND	3.14	1.42	1.37
19	A	1011	CL0	O2A-CGA	3.14	1.42	1.33
15	B	1228	CLA	C1D-ND	3.14	1.42	1.37
15	B	1218	CLA	C1D-ND	3.13	1.42	1.37
16	2	610	CHL	CHB-C4A	-3.13	1.34	1.38
15	A	1107	CLA	C1D-ND	3.13	1.42	1.37
15	A	1124	CLA	C1D-ND	3.12	1.42	1.37
15	J	1302	CLA	C1D-ND	3.11	1.42	1.37
15	A	1122	CLA	C1D-ND	3.11	1.41	1.37
15	A	1109	CLA	C1D-ND	3.11	1.41	1.37
12	4	501	LUT	C8-C7	3.11	1.42	1.33
15	4	602	CLA	C1D-ND	3.11	1.41	1.37
15	1	606	CLA	C1D-ND	3.10	1.41	1.37
15	1	608	CLA	C1D-ND	3.10	1.41	1.37
12	2	501	LUT	C8-C7	3.09	1.42	1.33
16	2	609	CHL	CHB-C4A	-3.09	1.34	1.38
15	4	609	CLA	C1D-ND	3.09	1.41	1.37
15	A	1139	CLA	C1D-ND	3.09	1.41	1.37
15	A	1141	CLA	C1D-ND	3.09	1.41	1.37
15	B	1202	CLA	C4B-NB	3.09	1.41	1.37
15	3	614	CLA	C1D-ND	3.09	1.41	1.37
15	4	606	CLA	C1D-ND	3.09	1.41	1.37
15	2	603	CLA	C1D-ND	3.08	1.41	1.37
15	A	1119	CLA	C1D-ND	3.08	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	2	602	CLA	C4B-NB	3.08	1.41	1.37
15	B	1215	CLA	C1D-ND	3.07	1.41	1.37
15	A	1138	CLA	C1D-ND	3.07	1.41	1.37
12	2	501	LUT	C7-C6	3.07	1.55	1.45
15	4	616	CLA	C1D-ND	3.07	1.41	1.37
12	4	501	LUT	C7-C6	3.07	1.55	1.45
13	2	502	XAT	C38-C25	3.06	1.56	1.51
12	4	501	LUT	C28-C27	3.06	1.39	1.32
15	2	612	CLA	C1D-ND	3.06	1.41	1.37
15	B	1232	CLA	C1D-ND	3.06	1.41	1.37
15	B	1204	CLA	C1D-ND	3.06	1.41	1.37
15	B	1209	CLA	C1D-ND	3.06	1.41	1.37
15	2	606	CLA	C1D-ND	3.06	1.41	1.37
15	3	613	CLA	C1D-ND	3.06	1.41	1.37
15	B	1210	CLA	C1D-ND	3.06	1.41	1.37
15	B	1213	CLA	C1D-ND	3.06	1.41	1.37
15	B	1219	CLA	C1D-ND	3.05	1.41	1.37
15	A	1112	CLA	C1D-ND	3.05	1.41	1.37
15	B	1225	CLA	C1D-ND	3.05	1.41	1.37
15	A	1101	CLA	C1D-ND	3.05	1.41	1.37
15	2	603	CLA	C4B-NB	3.05	1.41	1.37
15	B	1212	CLA	C1D-ND	3.05	1.41	1.37
15	B	1239	CLA	C1B-C2B	3.04	1.50	1.43
19	A	1011	CL0	O2D-CGD	3.04	1.40	1.33
15	4	605	CLA	C1D-ND	3.04	1.41	1.37
12	1	501	LUT	C7-C6	3.04	1.55	1.45
15	A	1108	CLA	C1D-ND	3.04	1.41	1.37
15	2	601	CLA	C1D-ND	3.04	1.41	1.37
15	4	603	CLA	C4B-NB	3.03	1.41	1.37
15	A	1128	CLA	C1D-ND	3.03	1.41	1.37
15	B	1237	CLA	C1D-ND	3.03	1.41	1.37
15	B	1201	CLA	C1D-ND	3.03	1.41	1.37
15	1	607	CLA	C1D-ND	3.03	1.41	1.37
15	4	602	CLA	C4B-NB	3.02	1.41	1.37
15	1	601	CLA	C1D-ND	3.02	1.41	1.37
15	3	606	CLA	C1D-ND	3.02	1.41	1.37
15	A	1114	CLA	C4B-NB	3.02	1.41	1.37
15	4	601	CLA	C1D-ND	3.02	1.41	1.37
15	A	1125	CLA	C1D-ND	3.02	1.41	1.37
15	A	1133	CLA	C1D-ND	3.02	1.41	1.37
15	B	1217	CLA	C1D-ND	3.02	1.41	1.37
16	2	613	CHL	CHB-C4A	-3.01	1.35	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	3	501	LUT	O23-C23	-3.01	1.38	1.43
12	2	501	LUT	O23-C23	-3.01	1.38	1.43
15	A	1136	CLA	C1D-ND	3.01	1.41	1.37
15	B	1220	CLA	C1D-ND	3.01	1.41	1.37
15	A	1113	CLA	C1D-ND	3.00	1.41	1.37
15	A	1118	CLA	C1D-ND	2.99	1.41	1.37
15	1	602	CLA	C4B-NB	2.99	1.41	1.37
16	4	611	CHL	CHB-C4A	-2.99	1.35	1.38
15	A	1103	CLA	C1D-ND	2.99	1.41	1.37
15	B	1230	CLA	C1D-ND	2.99	1.41	1.37
15	B	1208	CLA	C1D-ND	2.98	1.41	1.37
15	3	608	CLA	C1D-ND	2.98	1.41	1.37
15	B	1203	CLA	C1D-ND	2.98	1.41	1.37
15	A	1106	CLA	C1D-ND	2.98	1.41	1.37
16	4	613	CHL	CHB-C4A	-2.98	1.35	1.38
15	B	1236	CLA	C4B-NB	2.97	1.41	1.37
15	1	603	CLA	C1D-ND	2.97	1.41	1.37
15	3	603	CLA	C1D-ND	2.97	1.41	1.37
15	3	611	CLA	C1D-ND	2.96	1.41	1.37
12	1	501	LUT	C8-C7	2.96	1.41	1.33
15	B	1221	CLA	C1D-ND	2.96	1.41	1.37
15	B	1240	CLA	C1D-ND	2.96	1.41	1.37
15	B	1206	CLA	C1D-ND	2.96	1.41	1.37
15	4	612	CLA	C1D-ND	2.96	1.41	1.37
15	A	1110	CLA	C4B-NB	2.96	1.41	1.37
15	A	1111	CLA	C1D-ND	2.96	1.41	1.37
15	B	1022	CLA	C1D-ND	2.96	1.41	1.37
14	B	4003	BCR	C1-C6	-2.96	1.50	1.53
15	A	1127	CLA	C1D-ND	2.96	1.41	1.37
15	B	1224	CLA	C4B-NB	2.96	1.41	1.37
15	2	605	CLA	C1D-ND	2.95	1.41	1.37
15	B	1227	CLA	C1D-ND	2.95	1.41	1.37
15	3	603	CLA	C1B-C2B	2.95	1.50	1.43
15	B	1205	CLA	C1D-ND	2.95	1.41	1.37
15	1	605	CLA	C1B-C2B	2.95	1.50	1.43
17	A	5002	LHG	O7-C5	-2.95	1.39	1.46
15	B	1207	CLA	C4B-NB	2.94	1.41	1.37
15	A	1117	CLA	C1D-ND	2.94	1.41	1.37
12	4	501	LUT	O23-C23	-2.94	1.38	1.43
15	A	1110	CLA	C1D-ND	2.94	1.41	1.37
14	J	4001	BCR	C30-C25	-2.94	1.50	1.53
15	2	607	CLA	C1D-ND	2.93	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	4	604	CLA	C1D-ND	2.93	1.41	1.37
12	1	501	LUT	O23-C23	-2.92	1.38	1.43
15	B	1236	CLA	C1D-ND	2.92	1.41	1.37
14	B	4001	BCR	C30-C25	-2.92	1.50	1.53
15	B	1226	CLA	C1D-ND	2.92	1.41	1.37
15	A	1104	CLA	C1D-ND	2.91	1.41	1.37
15	A	1102	CLA	C1D-ND	2.91	1.41	1.37
15	A	1120	CLA	C1D-ND	2.91	1.41	1.37
16	1	609	CHL	C2C-C3C	2.91	1.39	1.36
15	3	607	CLA	C4B-NB	2.91	1.41	1.37
15	A	1131	CLA	C4B-NB	2.91	1.41	1.37
15	B	1222	CLA	C1D-ND	2.90	1.41	1.37
12	1	501	LUT	C28-C27	2.90	1.38	1.32
15	A	1140	CLA	C1D-ND	2.90	1.41	1.37
16	2	611	CHL	CHB-C4A	-2.90	1.35	1.38
16	4	610	CHL	CHB-C4A	-2.90	1.35	1.38
15	3	615	CLA	C1B-C2B	2.90	1.49	1.43
15	B	1211	CLA	C1D-ND	2.90	1.41	1.37
15	A	1129	CLA	C1D-ND	2.89	1.41	1.37
15	B	1218	CLA	C3B-C4B	2.89	1.51	1.42
12	1	501	LUT	C31-C30	2.89	1.52	1.43
15	3	601	CLA	C1D-ND	2.88	1.41	1.37
15	1	612	CLA	C1B-C2B	2.88	1.49	1.43
15	B	1023	CLA	C1D-ND	2.88	1.41	1.37
15	A	1115	CLA	C1D-ND	2.87	1.41	1.37
15	A	1135	CLA	C1B-C2B	2.86	1.49	1.43
15	B	1022	CLA	C4B-NB	2.86	1.41	1.37
15	B	1216	CLA	CMD-C2D	-2.86	1.44	1.50
15	B	1234	CLA	C1D-ND	2.86	1.41	1.37
15	3	609	CLA	C1B-C2B	2.86	1.49	1.43
15	3	612	CLA	C1D-ND	2.85	1.41	1.37
15	1	612	CLA	C4B-NB	2.85	1.41	1.37
15	A	1121	CLA	C4B-NB	2.85	1.41	1.37
15	A	1132	CLA	C1B-C2B	2.84	1.49	1.43
16	1	610	CHL	CHB-C4A	-2.84	1.35	1.38
15	A	1124	CLA	C1B-C2B	2.84	1.49	1.43
15	1	613	CLA	C4B-NB	2.84	1.41	1.37
15	1	605	CLA	C4B-NB	2.84	1.41	1.37
15	1	603	CLA	C4B-NB	2.83	1.41	1.37
15	A	1140	CLA	C4B-NB	2.83	1.41	1.37
15	4	607	CLA	C4B-NB	2.83	1.41	1.37
15	B	1021	CLA	CMD-C2D	-2.83	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	4	502	XAT	C8-C7	2.82	1.38	1.32
15	F	1302	CLA	C4B-NB	2.82	1.41	1.37
15	A	1132	CLA	C1D-ND	2.82	1.41	1.37
15	A	1126	CLA	C4B-NB	2.82	1.41	1.37
17	2	801	LHG	O7-C5	-2.81	1.40	1.46
15	A	1012	CLA	C1D-ND	2.81	1.41	1.37
19	A	1011	CL0	CMC-C2C	2.81	1.54	1.50
15	2	608	CLA	C4B-NB	2.81	1.41	1.37
15	B	1218	CLA	C1B-C2B	2.81	1.49	1.43
15	2	604	CLA	C1D-ND	2.81	1.41	1.37
15	A	1105	CLA	C1D-ND	2.80	1.41	1.37
16	2	611	CHL	C1D-C2D	2.80	1.42	1.39
15	3	615	CLA	C4B-NB	2.80	1.41	1.37
15	3	609	CLA	C4B-NB	2.80	1.41	1.37
16	4	613	CHL	C1B-C2B	2.80	1.42	1.39
15	1	608	CLA	C4B-NB	2.79	1.41	1.37
15	1	611	CLA	C4B-NB	2.79	1.41	1.37
15	4	616	CLA	C4B-NB	2.79	1.41	1.37
15	2	602	CLA	C1B-C2B	2.78	1.49	1.43
15	B	1205	CLA	C4B-NB	2.78	1.41	1.37
15	B	1239	CLA	C4B-NB	2.78	1.41	1.37
15	A	1112	CLA	C1B-C2B	2.78	1.49	1.43
15	3	605	CLA	C1D-ND	2.78	1.41	1.37
15	4	607	CLA	C1B-C2B	2.78	1.49	1.43
15	B	1228	CLA	C4B-NB	2.78	1.41	1.37
16	2	613	CHL	C1D-C2D	2.78	1.42	1.39
15	A	1113	CLA	C1B-C2B	2.77	1.49	1.43
15	4	609	CLA	C1B-C2B	2.77	1.49	1.43
14	A	4003	BCR	C30-C25	-2.77	1.50	1.53
15	3	608	CLA	C1B-C2B	2.77	1.49	1.43
15	B	1209	CLA	C1B-C2B	2.77	1.49	1.43
16	4	613	CHL	C1D-C2D	2.76	1.42	1.39
15	B	1212	CLA	C1B-C2B	2.76	1.49	1.43
15	A	1114	CLA	C1B-C2B	2.76	1.49	1.43
15	B	1021	CLA	C1B-C2B	2.76	1.49	1.43
15	B	1021	CLA	C1D-ND	2.76	1.41	1.37
15	2	606	CLA	C4B-NB	2.75	1.41	1.37
15	A	1101	CLA	C4B-NB	2.75	1.41	1.37
15	3	613	CLA	C1B-C2B	2.75	1.49	1.43
15	A	1101	CLA	C1B-C2B	2.75	1.49	1.43
15	A	1113	CLA	C4B-NB	2.75	1.41	1.37
16	2	609	CHL	C1D-C2D	2.75	1.42	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	1	610	CHL	C1D-C2D	2.75	1.42	1.39
15	B	1208	CLA	C4B-NB	2.74	1.41	1.37
15	A	1013	CLA	C1D-ND	2.74	1.41	1.37
13	3	502	XAT	C39-C29	2.74	1.56	1.50
15	2	601	CLA	C4B-NB	2.74	1.41	1.37
15	A	1129	CLA	CMD-C2D	-2.74	1.45	1.50
15	1	613	CLA	C1B-C2B	2.74	1.49	1.43
15	A	1128	CLA	C1B-C2B	2.74	1.49	1.43
15	A	1109	CLA	C1B-C2B	2.73	1.49	1.43
15	3	607	CLA	C1B-C2B	2.73	1.49	1.43
15	B	1236	CLA	C1B-C2B	2.73	1.49	1.43
12	3	501	LUT	C10-C9	2.73	1.42	1.35
13	3	502	XAT	C8-C7	2.73	1.38	1.32
15	B	1204	CLA	C4B-NB	2.73	1.41	1.37
15	A	1120	CLA	C4B-NB	2.73	1.41	1.37
15	B	1206	CLA	C1B-C2B	2.73	1.49	1.43
12	3	501	LUT	C26-C27	2.72	1.54	1.50
15	B	1230	CLA	C1B-C2B	2.72	1.49	1.43
19	A	1011	CL0	C3D-C4D	2.72	1.45	1.41
15	1	607	CLA	C4B-NB	2.72	1.41	1.37
15	B	1238	CLA	C4B-NB	2.72	1.41	1.37
15	B	1236	CLA	CMD-C2D	-2.71	1.45	1.50
15	F	1302	CLA	C1B-C2B	2.71	1.49	1.43
15	A	1108	CLA	C4B-NB	2.71	1.41	1.37
15	1	606	CLA	C4B-NB	2.71	1.41	1.37
15	B	1220	CLA	C4B-NB	2.71	1.41	1.37
15	B	1222	CLA	C4B-NB	2.71	1.41	1.37
15	B	1204	CLA	C1B-C2B	2.70	1.49	1.43
15	3	603	CLA	C4B-NB	2.70	1.41	1.37
15	1	606	CLA	C1B-C2B	2.70	1.49	1.43
15	A	1130	CLA	C1B-C2B	2.70	1.49	1.43
15	B	1214	CLA	C4B-NB	2.70	1.41	1.37
15	B	1201	CLA	C4B-NB	2.70	1.41	1.37
15	B	1210	CLA	C4B-NB	2.70	1.41	1.37
16	4	610	CHL	C1B-C2B	2.70	1.42	1.39
15	B	1237	CLA	C4B-NB	2.70	1.41	1.37
15	4	606	CLA	C4B-NB	2.70	1.41	1.37
15	B	1215	CLA	C4B-NB	2.69	1.41	1.37
15	4	606	CLA	C1B-C2B	2.69	1.49	1.43
15	1	603	CLA	C3B-C4B	2.69	1.50	1.42
15	B	1212	CLA	C4B-NB	2.69	1.41	1.37
15	B	1238	CLA	C1D-ND	2.69	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	3	606	CLA	C4B-NB	2.69	1.41	1.37
15	3	606	CLA	C1B-C2B	2.68	1.49	1.43
15	A	1141	CLA	C1B-C2B	2.68	1.49	1.43
15	3	612	CLA	C4B-NB	2.68	1.41	1.37
15	3	608	CLA	C4B-NB	2.68	1.41	1.37
15	2	606	CLA	C1B-C2B	2.68	1.49	1.43
15	B	1229	CLA	C1B-C2B	2.68	1.49	1.43
15	B	1216	CLA	C1D-ND	2.68	1.41	1.37
19	A	1011	CL0	CBD-CAD	2.68	1.62	1.53
15	B	1217	CLA	C1B-C2B	2.68	1.49	1.43
15	3	610	CLA	C1B-C2B	2.68	1.49	1.43
15	A	1141	CLA	C4B-NB	2.67	1.41	1.37
15	A	1137	CLA	C1B-C2B	2.67	1.49	1.43
17	B	5001	LHG	O7-C5	-2.67	1.40	1.46
13	2	502	XAT	C8-C7	2.67	1.38	1.32
15	2	605	CLA	C1B-C2B	2.67	1.49	1.43
15	B	1222	CLA	C1B-C2B	2.67	1.49	1.43
22	B	5002	DGD	O2G-C2G	-2.67	1.40	1.46
15	3	611	CLA	C1B-C2B	2.67	1.49	1.43
15	A	1118	CLA	C1B-C2B	2.67	1.49	1.43
15	A	1134	CLA	C4B-NB	2.66	1.41	1.37
15	B	1211	CLA	C4B-NB	2.66	1.41	1.37
15	4	608	CLA	C1B-C2B	2.66	1.49	1.43
15	B	1217	CLA	C4B-NB	2.66	1.41	1.37
15	A	1117	CLA	C4B-NB	2.66	1.41	1.37
15	A	1129	CLA	C4B-NB	2.66	1.41	1.37
16	1	610	CHL	C1B-C2B	2.66	1.42	1.39
16	2	610	CHL	C1D-C2D	2.66	1.42	1.39
16	4	610	CHL	C1D-C2D	2.66	1.42	1.39
15	A	1122	CLA	C4B-NB	2.66	1.41	1.37
15	A	1133	CLA	C4B-NB	2.66	1.41	1.37
15	B	1237	CLA	C1B-C2B	2.66	1.49	1.43
15	B	1226	CLA	CMD-C2D	-2.65	1.45	1.50
15	A	1104	CLA	C4B-NB	2.65	1.41	1.37
15	4	608	CLA	C1D-ND	2.65	1.41	1.37
15	3	613	CLA	C4B-NB	2.65	1.41	1.37
12	1	501	LUT	C17-C1	2.65	1.58	1.53
15	1	604	CLA	C1D-ND	2.65	1.41	1.37
15	3	614	CLA	C3B-C4B	2.65	1.50	1.42
19	A	1011	CL0	OBD-CAD	-2.64	1.18	1.22
15	B	1216	CLA	MG-NB	-2.64	2.00	2.05
16	4	611	CHL	C1B-C2B	2.64	1.42	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	A	1112	CLA	C4B-NB	2.64	1.41	1.37
15	2	607	CLA	C4B-NB	2.63	1.41	1.37
15	B	1209	CLA	C4B-NB	2.63	1.41	1.37
15	1	608	CLA	C1B-C2B	2.63	1.49	1.43
15	1	604	CLA	C1B-C2B	2.63	1.49	1.43
15	4	616	CLA	C1B-C2B	2.63	1.49	1.43
15	2	616	CLA	C4B-NB	2.63	1.41	1.37
16	2	611	CHL	C1B-C2B	2.63	1.42	1.39
15	B	1213	CLA	C1B-C2B	2.63	1.49	1.43
15	4	612	CLA	C4B-NB	2.63	1.41	1.37
15	B	1235	CLA	C1B-C2B	2.63	1.49	1.43
15	A	1130	CLA	C4B-NB	2.63	1.41	1.37
15	3	611	CLA	C4B-NB	2.62	1.41	1.37
15	B	1206	CLA	C4B-NB	2.62	1.41	1.37
15	A	1131	CLA	C1B-C2B	2.62	1.49	1.43
15	A	1136	CLA	C4B-NB	2.62	1.41	1.37
15	3	610	CLA	C4B-NB	2.62	1.41	1.37
15	A	1115	CLA	C4B-NB	2.62	1.41	1.37
15	F	1301	CLA	C4B-NB	2.62	1.41	1.37
15	B	1021	CLA	MG-NB	-2.61	2.00	2.05
15	A	1102	CLA	C4B-NB	2.61	1.41	1.37
15	A	1118	CLA	C4B-NB	2.61	1.41	1.37
15	A	1134	CLA	C1B-C2B	2.60	1.49	1.43
16	4	611	CHL	C1D-C2D	2.60	1.42	1.39
15	2	612	CLA	CMD-C2D	-2.60	1.45	1.50
15	A	1120	CLA	C1B-C2B	2.60	1.49	1.43
15	B	1223	CLA	C4B-NB	2.60	1.41	1.37
16	3	604	CHL	C1B-C2B	2.60	1.42	1.39
15	A	1112	CLA	CMD-C2D	-2.60	1.45	1.50
15	A	1115	CLA	C1B-C2B	2.60	1.49	1.43
15	A	1128	CLA	C4B-NB	2.60	1.41	1.37
15	2	605	CLA	C4B-NB	2.59	1.41	1.37
15	B	1208	CLA	C1B-C2B	2.59	1.49	1.43
15	B	1227	CLA	C4B-NB	2.59	1.41	1.37
15	1	611	CLA	C1B-C2B	2.59	1.49	1.43
15	1	602	CLA	C3B-C4B	2.58	1.50	1.42
15	B	1231	CLA	C4B-NB	2.58	1.41	1.37
15	B	1215	CLA	C1B-C2B	2.58	1.49	1.43
15	2	608	CLA	C1B-C2B	2.58	1.49	1.43
15	B	1240	CLA	C4B-NB	2.58	1.41	1.37
15	B	1203	CLA	C1B-C2B	2.58	1.49	1.43
15	4	612	CLA	C1B-C2B	2.58	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	B	1213	CLA	C4B-NB	2.58	1.41	1.37
15	B	1231	CLA	C1D-ND	2.58	1.41	1.37
15	A	1138	CLA	C4B-NB	2.58	1.41	1.37
15	J	1302	CLA	C4B-NB	2.58	1.41	1.37
13	3	502	XAT	C20-C13	2.57	1.56	1.50
16	2	609	CHL	C1B-C2B	2.57	1.42	1.39
15	4	608	CLA	CMD-C2D	-2.57	1.45	1.50
15	B	1232	CLA	C1B-C2B	2.57	1.49	1.43
15	A	1111	CLA	C4B-NB	2.57	1.41	1.37
15	B	1221	CLA	C4B-NB	2.57	1.41	1.37
16	2	610	CHL	C1B-C2B	2.56	1.42	1.39
15	A	1121	CLA	C1B-C2B	2.56	1.49	1.43
15	B	1227	CLA	CMD-C2D	-2.56	1.45	1.50
15	A	1136	CLA	C1B-C2B	2.56	1.49	1.43
15	A	1123	CLA	CMD-C2D	-2.56	1.45	1.50
15	A	1138	CLA	C1B-C2B	2.56	1.49	1.43
15	A	1012	CLA	C1B-C2B	2.56	1.49	1.43
15	B	1234	CLA	C1B-C2B	2.56	1.49	1.43
12	2	501	LUT	C17-C1	2.56	1.58	1.53
15	A	1111	CLA	C1B-C2B	2.56	1.49	1.43
15	B	1224	CLA	C1B-C2B	2.56	1.49	1.43
15	4	605	CLA	C1B-C2B	2.56	1.49	1.43
15	A	1126	CLA	C1B-C2B	2.55	1.49	1.43
15	A	1133	CLA	CMB-C2B	-2.55	1.45	1.50
15	1	607	CLA	C1B-C2B	2.55	1.49	1.43
13	1	502	XAT	C24-C23	2.55	1.55	1.52
15	B	1229	CLA	C4B-NB	2.55	1.41	1.37
15	B	1207	CLA	C1B-C2B	2.55	1.49	1.43
15	4	601	CLA	C4B-NB	2.55	1.41	1.37
15	A	1124	CLA	C4B-NB	2.55	1.41	1.37
15	B	1235	CLA	C4B-NB	2.55	1.41	1.37
15	A	1107	CLA	C1B-C2B	2.55	1.49	1.43
15	B	1214	CLA	CMB-C2B	-2.55	1.45	1.50
15	1	604	CLA	C4B-NB	2.55	1.41	1.37
16	1	609	CHL	C1D-C2D	2.55	1.42	1.39
15	J	1302	CLA	C1B-C2B	2.55	1.49	1.43
15	3	612	CLA	C1B-C2B	2.55	1.49	1.43
15	A	1013	CLA	C1B-C2B	2.55	1.49	1.43
15	4	608	CLA	C4B-NB	2.55	1.41	1.37
16	2	613	CHL	C1B-C2B	2.54	1.42	1.39
15	A	1106	CLA	CMD-C2D	-2.54	1.45	1.50
15	A	1106	CLA	C4B-NB	2.54	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	2	616	CLA	C1B-C2B	2.54	1.49	1.43
15	B	1240	CLA	C1B-C2B	2.54	1.49	1.43
15	A	1123	CLA	C4B-NB	2.54	1.41	1.37
15	A	1135	CLA	C4B-NB	2.54	1.41	1.37
15	4	605	CLA	C4B-NB	2.53	1.41	1.37
16	1	609	CHL	C1B-C2B	2.53	1.42	1.39
16	3	604	CHL	C1D-C2D	2.53	1.42	1.39
15	B	1225	CLA	C4B-NB	2.53	1.41	1.37
15	A	1127	CLA	C1B-C2B	2.53	1.49	1.43
15	B	1230	CLA	C4B-NB	2.53	1.41	1.37
15	B	1229	CLA	CMD-C2D	-2.53	1.45	1.50
15	A	1137	CLA	C4B-NB	2.53	1.41	1.37
15	B	1221	CLA	CMD-C2D	-2.53	1.45	1.50
14	3	504	BCR	C33-C5	-2.52	1.46	1.50
15	2	604	CLA	C1B-C2B	2.52	1.49	1.43
15	2	612	CLA	C1B-C2B	2.52	1.49	1.43
15	1	615	CLA	C1B-C2B	2.52	1.49	1.43
15	A	1124	CLA	CMD-C2D	-2.52	1.45	1.50
15	A	1138	CLA	CMB-C2B	-2.52	1.45	1.50
15	A	1127	CLA	C4B-NB	2.52	1.41	1.37
15	A	1103	CLA	C1B-C2B	2.52	1.49	1.43
15	A	1123	CLA	CMB-C2B	-2.52	1.45	1.50
15	B	1227	CLA	CMB-C2B	-2.51	1.45	1.50
15	A	1119	CLA	C1B-C2B	2.51	1.49	1.43
15	B	1237	CLA	CMD-C2D	-2.51	1.45	1.50
15	A	1139	CLA	C1B-C2B	2.51	1.49	1.43
15	B	1022	CLA	C1B-C2B	2.51	1.49	1.43
15	B	1210	CLA	C1B-C2B	2.51	1.49	1.43
15	B	1023	CLA	CMD-C2D	-2.51	1.45	1.50
15	A	1136	CLA	CMB-C2B	-2.51	1.45	1.50
15	B	1023	CLA	C4B-NB	2.51	1.41	1.37
15	2	603	CLA	C1B-C2B	2.51	1.49	1.43
15	A	1107	CLA	C4B-NB	2.50	1.41	1.37
15	A	1139	CLA	C4B-NB	2.50	1.41	1.37
15	B	1231	CLA	C1B-C2B	2.50	1.49	1.43
15	4	602	CLA	C3B-C4B	2.50	1.50	1.42
15	A	1128	CLA	CMB-C2B	-2.50	1.45	1.50
15	A	1125	CLA	CMD-C2D	-2.50	1.45	1.50
15	B	1232	CLA	C3B-C4B	2.50	1.50	1.42
15	B	1219	CLA	C1B-C2B	2.50	1.49	1.43
15	B	1023	CLA	C1B-C2B	2.50	1.49	1.43
15	B	1211	CLA	CMD-C2D	-2.50	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	A	1109	CLA	C4B-NB	2.50	1.41	1.37
15	A	1133	CLA	CMD-C2D	-2.50	1.45	1.50
15	2	607	CLA	C1B-C2B	2.49	1.49	1.43
15	F	1301	CLA	C1B-C2B	2.49	1.49	1.43
15	2	612	CLA	C4B-NB	2.49	1.41	1.37
15	A	1107	CLA	CMD-C2D	-2.49	1.45	1.50
15	A	1125	CLA	MG-NB	-2.49	2.00	2.05
15	A	1104	CLA	C1B-C2B	2.49	1.49	1.43
13	3	502	XAT	C18-C5	2.49	1.55	1.51
18	4	801	LMG	O8-C9	-2.49	1.39	1.45
15	3	603	CLA	CMD-C2D	-2.49	1.45	1.50
15	A	1140	CLA	CMB-C2B	-2.49	1.45	1.50
15	1	604	CLA	CMD-C2D	-2.49	1.45	1.50
15	A	1104	CLA	CMD-C2D	-2.49	1.45	1.50
15	A	1110	CLA	CMB-C2B	-2.49	1.45	1.50
15	A	1108	CLA	C1B-C2B	2.49	1.49	1.43
15	A	1105	CLA	CMD-C2D	-2.48	1.45	1.50
15	1	601	CLA	C1B-C2B	2.48	1.49	1.43
15	B	1203	CLA	C4B-NB	2.48	1.41	1.37
15	B	1226	CLA	C4B-NB	2.48	1.41	1.37
15	B	1227	CLA	C1B-C2B	2.48	1.48	1.43
18	2	803	LMG	O7-C8	-2.48	1.40	1.46
15	A	1121	CLA	CMD-C2D	-2.47	1.45	1.50
15	A	1131	CLA	CMD-C2D	-2.47	1.45	1.50
15	B	1235	CLA	CMB-C2B	-2.47	1.45	1.50
15	3	612	CLA	CMD-C2D	-2.47	1.45	1.50
15	B	1202	CLA	C1B-C2B	2.47	1.48	1.43
15	4	605	CLA	CMD-C2D	-2.47	1.45	1.50
15	A	1118	CLA	CMD-C2D	-2.47	1.45	1.50
15	A	1101	CLA	CMD-C2D	-2.47	1.45	1.50
15	A	1108	CLA	CMB-C2B	-2.47	1.45	1.50
15	A	1112	CLA	MG-NB	-2.47	2.00	2.05
13	1	502	XAT	C18-C5	2.47	1.55	1.51
15	3	601	CLA	C4B-NB	2.47	1.41	1.37
15	A	1138	CLA	MG-NB	-2.47	2.00	2.05
15	2	604	CLA	CMD-C2D	-2.47	1.45	1.50
15	A	1119	CLA	CMD-C2D	-2.47	1.45	1.50
15	A	1105	CLA	C4B-NB	2.46	1.41	1.37
15	4	602	CLA	C1B-C2B	2.46	1.48	1.43
15	3	612	CLA	CMB-C2B	-2.46	1.45	1.50
15	B	1205	CLA	CMD-C2D	-2.46	1.45	1.50
15	B	1238	CLA	CMD-C2D	-2.46	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	A	1122	CLA	CMB-C2B	-2.46	1.45	1.50
15	B	1203	CLA	CMD-C2D	-2.46	1.45	1.50
15	3	605	CLA	C1B-C2B	2.46	1.48	1.43
15	4	616	CLA	CMD-C2D	-2.46	1.45	1.50
15	4	601	CLA	CMB-C2B	-2.46	1.45	1.50
15	A	1105	CLA	MG-NB	-2.46	2.00	2.05
15	B	1225	CLA	C1B-C2B	2.46	1.48	1.43
15	A	1117	CLA	C1B-C2B	2.46	1.48	1.43
15	4	604	CLA	C4B-NB	2.46	1.41	1.37
15	A	1136	CLA	CMD-C2D	-2.46	1.45	1.50
15	B	1219	CLA	CMB-C2B	-2.46	1.45	1.50
15	B	1231	CLA	MG-NB	-2.46	2.00	2.05
15	A	1132	CLA	C4B-NB	2.45	1.41	1.37
15	B	1231	CLA	CMB-C2B	-2.45	1.45	1.50
15	B	1209	CLA	CMD-C2D	-2.45	1.45	1.50
15	B	1218	CLA	CMD-C2D	-2.45	1.45	1.50
15	B	1202	CLA	CMD-C2D	-2.45	1.45	1.50
15	B	1240	CLA	MG-NB	-2.45	2.00	2.05
14	A	4002	BCR	C33-C5	-2.45	1.47	1.50
15	B	1222	CLA	CMD-C2D	-2.45	1.45	1.50
15	4	601	CLA	CMD-C2D	-2.44	1.45	1.50
15	3	609	CLA	CMB-C2B	-2.44	1.45	1.50
15	B	1239	CLA	CMD-C2D	-2.44	1.45	1.50
18	4	801	LMG	O7-C8	-2.44	1.40	1.46
15	B	1215	CLA	CMD-C2D	-2.44	1.45	1.50
15	B	1238	CLA	C3B-C4B	2.44	1.49	1.42
15	4	603	CLA	CMB-C2B	-2.44	1.45	1.50
15	A	1111	CLA	CMD-C2D	-2.44	1.45	1.50
15	1	615	CLA	C4B-NB	2.44	1.41	1.37
15	A	1110	CLA	CMD-C2D	-2.44	1.45	1.50
15	2	603	CLA	C3B-C4B	2.44	1.49	1.42
15	4	604	CLA	CMD-C2D	-2.44	1.45	1.50
15	A	1013	CLA	CMD-C2D	-2.44	1.45	1.50
15	3	601	CLA	CHC-C1C	2.44	1.43	1.38
15	B	1240	CLA	CMD-C2D	-2.43	1.45	1.50
13	1	502	XAT	C19-C9	2.43	1.55	1.50
15	A	1116	CLA	CMD-C2D	-2.43	1.45	1.50
15	B	1234	CLA	CMD-C2D	-2.43	1.45	1.50
15	B	1228	CLA	C1B-C2B	2.43	1.48	1.43
15	A	1129	CLA	C1B-C2B	2.43	1.48	1.43
15	A	1115	CLA	CMD-C2D	-2.43	1.45	1.50
15	B	1208	CLA	CMB-C2B	-2.43	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	B	1230	CLA	CMD-C2D	-2.43	1.45	1.50
15	3	601	CLA	CMD-C2D	-2.43	1.45	1.50
15	3	611	CLA	CMD-C2D	-2.43	1.45	1.50
13	4	502	XAT	C19-C9	2.43	1.55	1.50
15	B	1220	CLA	CMD-C2D	-2.43	1.45	1.50
15	B	1221	CLA	C1B-C2B	2.42	1.48	1.43
15	A	1122	CLA	C1B-C2B	2.42	1.48	1.43
15	A	1137	CLA	MG-NB	-2.42	2.01	2.05
15	3	613	CLA	CMC-C2C	-2.42	1.45	1.50
15	B	1216	CLA	C4B-NB	2.42	1.41	1.37
15	1	602	CLA	C1B-C2B	2.42	1.48	1.43
15	B	1201	CLA	CMD-C2D	-2.42	1.45	1.50
15	4	605	CLA	MG-NB	-2.42	2.01	2.05
15	B	1202	CLA	CMB-C2B	-2.42	1.45	1.50
15	4	602	CLA	CMD-C2D	-2.42	1.45	1.50
15	B	1205	CLA	C3B-C4B	2.42	1.49	1.42
15	4	604	CLA	C1B-C2B	2.42	1.48	1.43
15	A	1140	CLA	C1B-C2B	2.42	1.48	1.43
15	4	609	CLA	C4B-NB	2.42	1.41	1.37
15	2	607	CLA	CMD-C2D	-2.42	1.45	1.50
15	1	603	CLA	C1B-C2B	2.42	1.48	1.43
15	4	612	CLA	CMD-C2D	-2.42	1.45	1.50
15	A	1137	CLA	CMD-C2D	-2.42	1.45	1.50
15	B	1023	CLA	CMC-C2C	-2.42	1.45	1.50
15	B	1208	CLA	CMD-C2D	-2.42	1.45	1.50
15	A	1120	CLA	CMD-C2D	-2.42	1.45	1.50
15	3	601	CLA	C3B-C4B	2.42	1.49	1.42
15	1	602	CLA	CMD-C2D	-2.42	1.45	1.50
15	B	1223	CLA	C1B-C2B	2.42	1.48	1.43
15	3	603	CLA	CMB-C2B	-2.41	1.45	1.50
15	A	1102	CLA	CMD-C2D	-2.41	1.45	1.50
13	3	502	XAT	C38-C25	2.41	1.55	1.51
15	3	605	CLA	CMD-C2D	-2.41	1.45	1.50
15	B	1207	CLA	C3B-C4B	2.41	1.49	1.42
15	B	1211	CLA	C1B-C2B	2.41	1.48	1.43
15	4	609	CLA	CMD-C2D	-2.41	1.45	1.50
15	J	1302	CLA	CMD-C2D	-2.41	1.45	1.50
15	A	1103	CLA	CMD-C2D	-2.41	1.45	1.50
15	4	603	CLA	C3B-C4B	2.41	1.49	1.42
15	B	1210	CLA	CMD-C2D	-2.41	1.45	1.50
15	B	1225	CLA	CMD-C2D	-2.41	1.45	1.50
15	B	1202	CLA	CHC-C1C	2.40	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	A	1138	CLA	CMD-C2D	-2.40	1.45	1.50
15	3	601	CLA	C1B-C2B	2.40	1.48	1.43
15	A	1123	CLA	C1B-C2B	2.40	1.48	1.43
15	A	1114	CLA	CMD-C2D	-2.40	1.45	1.50
16	1	610	CHL	C2C-C3C	2.40	1.38	1.36
15	A	1126	CLA	C3B-C4B	2.40	1.49	1.42
15	2	604	CLA	C4B-NB	2.40	1.41	1.37
15	A	1012	CLA	C4B-NB	2.40	1.41	1.37
15	2	605	CLA	CMB-C2B	-2.40	1.45	1.50
15	B	1216	CLA	CMB-C2B	-2.40	1.45	1.50
15	1	604	CLA	MG-NB	-2.40	2.01	2.05
15	A	1109	CLA	CMD-C2D	-2.40	1.45	1.50
12	4	501	LUT	C17-C1	2.40	1.58	1.53
15	A	1119	CLA	C4B-NB	2.40	1.41	1.37
15	2	603	CLA	CMD-C2D	-2.39	1.45	1.50
15	A	1113	CLA	CMD-C2D	-2.39	1.45	1.50
15	B	1220	CLA	C1B-C2B	2.39	1.48	1.43
15	4	607	CLA	CMD-C2D	-2.39	1.45	1.50
15	1	606	CLA	CMD-C2D	-2.39	1.45	1.50
15	3	608	CLA	CMD-C2D	-2.39	1.45	1.50
15	B	1228	CLA	CMB-C2B	-2.39	1.45	1.50
15	2	601	CLA	C3B-C4B	2.39	1.49	1.42
15	A	1129	CLA	CMB-C2B	-2.39	1.45	1.50
15	A	1107	CLA	MG-NB	-2.39	2.01	2.05
15	4	608	CLA	MG-NB	-2.39	2.01	2.05
15	A	1012	CLA	MG-NB	-2.39	2.01	2.05
15	A	1126	CLA	CMC-C2C	-2.39	1.45	1.50
15	B	1201	CLA	MG-NB	-2.39	2.01	2.05
15	A	1140	CLA	CMD-C2D	-2.39	1.45	1.50
15	1	608	CLA	CMD-C2D	-2.39	1.45	1.50
15	B	1224	CLA	CMD-C2D	-2.38	1.45	1.50
15	A	1132	CLA	CMD-C2D	-2.38	1.45	1.50
15	F	1301	CLA	CMB-C2B	-2.38	1.45	1.50
15	A	1013	CLA	C4B-NB	2.38	1.41	1.37
15	F	1301	CLA	CMD-C2D	-2.38	1.45	1.50
15	B	1215	CLA	C3B-C4B	2.38	1.49	1.42
15	A	1135	CLA	CMD-C2D	-2.38	1.45	1.50
15	A	1103	CLA	C4B-NB	2.38	1.41	1.37
15	B	1235	CLA	MG-NB	-2.38	2.01	2.05
15	A	1117	CLA	CMD-C2D	-2.38	1.45	1.50
15	A	1139	CLA	MG-NB	-2.38	2.01	2.05
15	4	603	CLA	C1B-C2B	2.38	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	B	1205	CLA	C1B-C2B	2.38	1.48	1.43
15	A	1119	CLA	MG-NB	-2.38	2.01	2.05
13	3	502	XAT	C28-C27	2.38	1.37	1.32
15	B	1022	CLA	CMD-C2D	-2.38	1.45	1.50
15	A	1102	CLA	C1B-C2B	2.38	1.48	1.43
13	4	502	XAT	C38-C25	2.38	1.55	1.51
15	2	602	CLA	CMD-C2D	-2.38	1.45	1.50
13	3	502	XAT	C24-C23	2.38	1.55	1.52
15	A	1114	CLA	CMB-C2B	-2.37	1.45	1.50
15	B	1217	CLA	CMD-C2D	-2.37	1.45	1.50
15	2	601	CLA	C1B-C2B	2.37	1.48	1.43
15	B	1227	CLA	MG-NB	-2.37	2.01	2.05
15	4	605	CLA	CMB-C2B	-2.37	1.45	1.50
15	2	605	CLA	MG-NB	-2.37	2.01	2.05
15	A	1140	CLA	MG-NB	-2.37	2.01	2.05
15	2	602	CLA	C3B-C4B	2.37	1.49	1.42
15	A	1120	CLA	CMB-C2B	-2.37	1.45	1.50
13	4	502	XAT	C24-C23	2.37	1.55	1.52
15	4	606	CLA	MG-NB	-2.37	2.01	2.05
15	A	1130	CLA	CMD-C2D	-2.37	1.45	1.50
15	2	607	CLA	MG-NB	-2.37	2.01	2.05
15	B	1216	CLA	CMC-C2C	-2.36	1.45	1.50
15	B	1228	CLA	MG-NB	-2.36	2.01	2.05
15	2	607	CLA	CMB-C2B	-2.36	1.45	1.50
15	B	1228	CLA	CMD-C2D	-2.36	1.45	1.50
15	A	1109	CLA	CMB-C2B	-2.36	1.45	1.50
15	B	1216	CLA	C1B-C2B	2.36	1.48	1.43
15	3	614	CLA	CMB-C2B	-2.36	1.45	1.50
15	A	1106	CLA	C1B-C2B	2.36	1.48	1.43
15	B	1234	CLA	C4B-NB	2.36	1.41	1.37
12	2	501	LUT	C31-C32	2.36	1.40	1.34
15	A	1127	CLA	CMD-C2D	-2.36	1.45	1.50
15	B	1201	CLA	CMB-C2B	-2.36	1.45	1.50
15	1	608	CLA	MG-NB	-2.36	2.01	2.05
15	B	1220	CLA	CMB-C2B	-2.35	1.45	1.50
15	A	1108	CLA	MG-NB	-2.35	2.01	2.05
15	A	1105	CLA	CHC-C1C	2.35	1.43	1.38
12	2	501	LUT	C20-C13	2.35	1.55	1.50
15	A	1128	CLA	CMC-C2C	-2.35	1.45	1.50
15	B	1238	CLA	C1B-C2B	2.35	1.48	1.43
15	3	612	CLA	MG-NB	-2.35	2.01	2.05
15	B	1210	CLA	MG-NB	-2.35	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	A	1115	CLA	MG-NB	-2.35	2.01	2.05
15	3	614	CLA	CMC-C2C	-2.35	1.46	1.50
16	4	613	CHL	C2C-C3C	2.35	1.38	1.36
15	A	1122	CLA	CMD-C2D	-2.35	1.46	1.50
15	A	1013	CLA	MG-NB	-2.35	2.01	2.05
15	A	1110	CLA	C3B-C4B	2.35	1.49	1.42
15	B	1232	CLA	CMD-C2D	-2.35	1.46	1.50
15	2	616	CLA	MG-NB	-2.34	2.01	2.05
15	A	1128	CLA	CMD-C2D	-2.34	1.46	1.50
15	A	1125	CLA	C4B-NB	2.34	1.40	1.37
15	B	1211	CLA	CMB-C2B	-2.34	1.46	1.50
15	B	1235	CLA	CMD-C2D	-2.34	1.46	1.50
15	A	1139	CLA	CMD-C2D	-2.34	1.46	1.50
15	B	1234	CLA	MG-NB	-2.34	2.01	2.05
15	4	601	CLA	C3B-C4B	2.34	1.49	1.42
15	B	1211	CLA	MG-NB	-2.34	2.01	2.05
15	J	1302	CLA	MG-NB	-2.34	2.01	2.05
15	B	1214	CLA	CMD-C2D	-2.34	1.46	1.50
15	A	1141	CLA	MG-NB	-2.34	2.01	2.05
15	F	1301	CLA	MG-NB	-2.34	2.01	2.05
15	B	1212	CLA	CMB-C2B	-2.34	1.46	1.50
15	B	1023	CLA	MG-NB	-2.34	2.01	2.05
15	B	1221	CLA	MG-NB	-2.34	2.01	2.05
15	A	1012	CLA	CHC-C1C	2.34	1.43	1.38
15	1	601	CLA	MG-NB	-2.33	2.01	2.05
15	1	605	CLA	CMD-C2D	-2.33	1.46	1.50
15	A	1113	CLA	MG-NB	-2.33	2.01	2.05
15	3	613	CLA	CMD-C2D	-2.33	1.46	1.50
15	A	1104	CLA	MG-NB	-2.33	2.01	2.05
13	1	502	XAT	C38-C25	2.33	1.55	1.51
15	A	1133	CLA	C1B-C2B	2.33	1.48	1.43
15	A	1105	CLA	CMB-C2B	-2.33	1.46	1.50
15	B	1219	CLA	CMD-C2D	-2.33	1.46	1.50
15	F	1302	CLA	CMD-C2D	-2.33	1.46	1.50
15	B	1208	CLA	MG-NB	-2.33	2.01	2.05
15	A	1125	CLA	C1B-C2B	2.33	1.48	1.43
13	3	502	XAT	C19-C9	2.33	1.55	1.50
15	A	1123	CLA	MG-NB	-2.32	2.01	2.05
15	A	1134	CLA	CMD-C2D	-2.32	1.46	1.50
12	4	501	LUT	C11-C12	2.32	1.40	1.34
15	B	1204	CLA	CMD-C2D	-2.32	1.46	1.50
15	1	601	CLA	C4B-NB	2.32	1.40	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	B	1022	CLA	CMC-C2C	-2.32	1.46	1.50
15	B	1212	CLA	CMD-C2D	-2.32	1.46	1.50
15	B	1223	CLA	CMC-C2C	-2.32	1.46	1.50
15	A	1104	CLA	CMB-C2B	-2.32	1.46	1.50
15	A	1105	CLA	C1B-C2B	2.32	1.48	1.43
15	B	1221	CLA	C3B-C4B	2.32	1.49	1.42
15	3	610	CLA	CMD-C2D	-2.32	1.46	1.50
15	A	1102	CLA	CMB-C2B	-2.32	1.46	1.50
15	A	1136	CLA	MG-NB	-2.32	2.01	2.05
15	A	1141	CLA	CMB-C2B	-2.32	1.46	1.50
15	A	1129	CLA	CMC-C2C	-2.31	1.46	1.50
15	A	1129	CLA	MG-NB	-2.31	2.01	2.05
15	A	1125	CLA	CMB-C2B	-2.31	1.46	1.50
15	A	1124	CLA	CMB-C2B	-2.31	1.46	1.50
15	B	1223	CLA	CMD-C2D	-2.31	1.46	1.50
15	1	601	CLA	CMD-C2D	-2.31	1.46	1.50
15	4	601	CLA	MG-NB	-2.31	2.01	2.05
15	A	1012	CLA	CMD-C2D	-2.31	1.46	1.50
15	A	1140	CLA	CMC-C2C	-2.31	1.46	1.50
15	B	1225	CLA	MG-NB	-2.31	2.01	2.05
15	B	1201	CLA	C3B-C4B	2.31	1.49	1.42
15	1	612	CLA	C3B-C4B	2.31	1.49	1.42
15	B	1217	CLA	CMB-C2B	-2.31	1.46	1.50
15	A	1108	CLA	CMD-C2D	-2.31	1.46	1.50
15	B	1240	CLA	CMB-C2B	-2.31	1.46	1.50
15	B	1234	CLA	CMB-C2B	-2.31	1.46	1.50
15	A	1111	CLA	CMC-C2C	-2.30	1.46	1.50
15	A	1116	CLA	CMB-C2B	-2.30	1.46	1.50
15	B	1227	CLA	CMC-C2C	-2.30	1.46	1.50
15	1	603	CLA	CMD-C2D	-2.30	1.46	1.50
15	B	1203	CLA	MG-NB	-2.30	2.01	2.05
15	A	1103	CLA	CMB-C2B	-2.30	1.46	1.50
15	1	607	CLA	MG-NB	-2.30	2.01	2.05
15	B	1213	CLA	MG-NB	-2.30	2.01	2.05
15	B	1224	CLA	C3B-C4B	2.30	1.49	1.42
15	1	615	CLA	MG-NB	-2.30	2.01	2.05
15	2	606	CLA	CMD-C2D	-2.30	1.46	1.50
15	A	1130	CLA	CMB-C2B	-2.30	1.46	1.50
15	3	606	CLA	C3B-C4B	2.30	1.49	1.42
15	4	606	CLA	CMC-C2C	-2.30	1.46	1.50
15	B	1230	CLA	CMC-C2C	-2.30	1.46	1.50
15	B	1237	CLA	MG-NB	-2.30	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	2	603	CLA	CMB-C2B	-2.30	1.46	1.50
14	2	503	BCR	C33-C5	-2.29	1.47	1.50
12	3	501	LUT	C20-C13	2.29	1.55	1.50
15	3	615	CLA	CMD-C2D	-2.29	1.46	1.50
15	B	1237	CLA	CMB-C2B	-2.29	1.46	1.50
15	A	1120	CLA	MG-NB	-2.29	2.01	2.05
15	2	601	CLA	CMB-C2B	-2.29	1.46	1.50
15	A	1137	CLA	CMB-C2B	-2.29	1.46	1.50
19	A	1011	CL0	C1-C2	2.29	1.55	1.49
15	2	604	CLA	MG-NB	-2.29	2.01	2.05
15	A	1141	CLA	CMD-C2D	-2.29	1.46	1.50
15	B	1203	CLA	CMC-C2C	-2.29	1.46	1.50
15	3	607	CLA	CMD-C2D	-2.29	1.46	1.50
16	2	610	CHL	C2C-C3C	2.29	1.38	1.36
15	B	1219	CLA	C3B-C4B	2.29	1.49	1.42
15	2	601	CLA	CMD-C2D	-2.29	1.46	1.50
15	A	1124	CLA	MG-NB	-2.29	2.01	2.05
15	2	616	CLA	CMD-C2D	-2.29	1.46	1.50
15	4	603	CLA	CMC-C2C	-2.29	1.46	1.50
15	4	606	CLA	CMD-C2D	-2.29	1.46	1.50
15	A	1116	CLA	MG-NB	-2.29	2.01	2.05
15	A	1117	CLA	MG-NB	-2.29	2.01	2.05
15	B	1201	CLA	C1B-C2B	2.29	1.48	1.43
15	B	1205	CLA	CMB-C2B	-2.29	1.46	1.50
15	2	601	CLA	MG-NB	-2.29	2.01	2.05
17	3	801	LHG	P-O6	2.29	1.68	1.59
15	1	611	CLA	C3B-C4B	2.29	1.49	1.42
15	A	1012	CLA	CMB-C2B	-2.29	1.46	1.50
15	A	1141	CLA	CMC-C2C	-2.28	1.46	1.50
15	A	1117	CLA	C3B-C4B	2.28	1.49	1.42
15	B	1226	CLA	CMC-C2C	-2.28	1.46	1.50
15	A	1101	CLA	CMC-C2C	-2.28	1.46	1.50
15	4	604	CLA	CMC-C2C	-2.28	1.46	1.50
15	A	1127	CLA	C3B-C4B	2.28	1.49	1.42
15	A	1139	CLA	CMB-C2B	-2.28	1.46	1.50
15	B	1210	CLA	CMB-C2B	-2.28	1.46	1.50
15	B	1022	CLA	C3B-C4B	2.28	1.49	1.42
15	1	613	CLA	C3B-C4B	2.28	1.49	1.42
15	B	1225	CLA	CMB-C2B	-2.28	1.46	1.50
15	3	613	CLA	MG-NB	-2.28	2.01	2.05
15	2	601	CLA	CHC-C1C	2.28	1.43	1.38
15	B	1203	CLA	CMB-C2B	-2.28	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	2	612	CLA	MG-NB	-2.28	2.01	2.05
15	A	1126	CLA	CMD-C2D	-2.28	1.46	1.50
15	B	1201	CLA	CHC-C1C	2.28	1.43	1.38
15	B	1229	CLA	C3B-C4B	2.28	1.49	1.42
15	1	604	CLA	CMB-C2B	-2.28	1.46	1.50
15	2	608	CLA	CMD-C2D	-2.27	1.46	1.50
15	A	1108	CLA	CMC-C2C	-2.27	1.46	1.50
15	2	608	CLA	C3B-C4B	2.27	1.49	1.42
15	A	1112	CLA	CMB-C2B	-2.27	1.46	1.50
15	B	1238	CLA	CMB-C2B	-2.27	1.46	1.50
15	B	1209	CLA	MG-NB	-2.27	2.01	2.05
15	A	1121	CLA	CMB-C2B	-2.27	1.46	1.50
15	A	1113	CLA	CMB-C2B	-2.27	1.46	1.50
15	B	1220	CLA	MG-NB	-2.27	2.01	2.05
15	3	606	CLA	MG-NB	-2.27	2.01	2.05
15	1	601	CLA	C3B-C4B	2.27	1.49	1.42
15	3	601	CLA	CMB-C2B	-2.27	1.46	1.50
15	A	1118	CLA	CMC-C2C	-2.27	1.46	1.50
15	1	601	CLA	CHC-C1C	2.27	1.43	1.38
15	B	1236	CLA	C3B-C4B	2.27	1.49	1.42
15	A	1130	CLA	MG-NB	-2.27	2.01	2.05
15	2	604	CLA	CMB-C2B	-2.27	1.46	1.50
15	B	1202	CLA	C3B-C4B	2.27	1.49	1.42
15	4	609	CLA	MG-NB	-2.27	2.01	2.05
15	4	616	CLA	MG-NB	-2.27	2.01	2.05
15	A	1127	CLA	MG-NB	-2.26	2.01	2.05
15	3	601	CLA	MG-NB	-2.26	2.01	2.05
15	A	1106	CLA	MG-NB	-2.26	2.01	2.05
15	4	607	CLA	CMC-C2C	-2.26	1.46	1.50
15	B	1236	CLA	CMC-C2C	-2.26	1.46	1.50
15	A	1128	CLA	MG-NB	-2.26	2.01	2.05
15	B	1238	CLA	MG-NB	-2.26	2.01	2.05
15	1	613	CLA	CHC-C1C	2.26	1.43	1.38
15	A	1125	CLA	CHC-C1C	2.26	1.43	1.38
15	4	602	CLA	CMB-C2B	-2.26	1.46	1.50
15	1	607	CLA	CMD-C2D	-2.26	1.46	1.50
15	1	607	CLA	C3B-C4B	2.26	1.49	1.42
15	A	1132	CLA	MG-NB	-2.26	2.01	2.05
15	2	605	CLA	CMD-C2D	-2.26	1.46	1.50
15	B	1217	CLA	MG-NB	-2.26	2.01	2.05
15	A	1135	CLA	C3B-C4B	2.26	1.49	1.42
15	3	605	CLA	MG-NB	-2.25	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	B	1234	CLA	C3B-C4B	2.25	1.49	1.42
15	3	606	CLA	CMD-C2D	-2.25	1.46	1.50
15	3	614	CLA	C1B-C2B	2.25	1.48	1.43
15	A	1110	CLA	MG-NB	-2.25	2.01	2.05
14	A	4005	BCR	C33-C5	-2.25	1.47	1.50
15	3	605	CLA	CMB-C2B	-2.25	1.46	1.50
15	A	1134	CLA	CMB-C2B	-2.25	1.46	1.50
15	4	612	CLA	C3B-C4B	2.24	1.49	1.42
15	3	611	CLA	CMB-C2B	-2.24	1.46	1.50
15	3	611	CLA	CMC-C2C	-2.24	1.46	1.50
15	4	601	CLA	CMC-C2C	-2.24	1.46	1.50
15	3	611	CLA	MG-NB	-2.24	2.01	2.05
15	3	613	CLA	CMB-C2B	-2.24	1.46	1.50
16	2	613	CHL	C2C-C3C	2.24	1.38	1.36
15	B	1232	CLA	CMB-C2B	-2.24	1.46	1.50
15	3	614	CLA	CMD-C2D	-2.24	1.46	1.50
15	B	1204	CLA	MG-NB	-2.24	2.01	2.05
15	3	609	CLA	CMD-C2D	-2.24	1.46	1.50
15	A	1106	CLA	CMB-C2B	-2.24	1.46	1.50
15	A	1118	CLA	MG-NB	-2.24	2.01	2.05
15	B	1022	CLA	MG-NB	-2.24	2.01	2.05
15	3	605	CLA	C4B-NB	2.24	1.40	1.37
15	1	606	CLA	MG-NB	-2.24	2.01	2.05
15	B	1210	CLA	CMC-C2C	-2.23	1.46	1.50
15	B	1206	CLA	MG-NB	-2.23	2.01	2.05
15	B	1211	CLA	CHC-C1C	2.23	1.43	1.38
15	4	604	CLA	MG-NB	-2.23	2.01	2.05
15	2	612	CLA	CHC-C1C	2.23	1.43	1.38
15	A	1114	CLA	C3B-C4B	2.23	1.49	1.42
15	A	1110	CLA	C1B-C2B	2.23	1.48	1.43
15	3	608	CLA	MG-NB	-2.23	2.01	2.05
15	A	1101	CLA	CMB-C2B	-2.23	1.46	1.50
15	A	1119	CLA	CMB-C2B	-2.23	1.46	1.50
15	A	1134	CLA	C3B-C4B	2.23	1.49	1.42
15	B	1236	CLA	MG-NB	-2.23	2.01	2.05
15	4	608	CLA	CMB-C2B	-2.23	1.46	1.50
15	3	606	CLA	CHC-C1C	2.23	1.42	1.38
15	2	601	CLA	CMC-C2C	-2.23	1.46	1.50
15	1	606	CLA	C3B-C4B	2.23	1.49	1.42
15	A	1117	CLA	CMC-C2C	-2.23	1.46	1.50
15	B	1220	CLA	CMC-C2C	-2.23	1.46	1.50
15	A	1116	CLA	C1B-C2B	2.23	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	3	610	CLA	MG-NB	-2.23	2.01	2.05
15	B	1021	CLA	C4B-NB	2.23	1.40	1.37
15	B	1204	CLA	CMB-C2B	-2.22	1.46	1.50
15	B	1239	CLA	CMB-C2B	-2.22	1.46	1.50
15	3	609	CLA	MG-NB	-2.22	2.01	2.05
15	B	1213	CLA	CMD-C2D	-2.22	1.46	1.50
15	2	616	CLA	CMB-C2B	-2.22	1.46	1.50
15	B	1231	CLA	MG-ND	-2.22	2.01	2.05
14	F	4001	BCR	C33-C5	-2.22	1.47	1.50
15	A	1135	CLA	CMC-C2C	-2.22	1.46	1.50
15	A	1131	CLA	MG-NB	-2.22	2.01	2.05
15	B	1205	CLA	CMC-C2C	-2.22	1.46	1.50
15	A	1104	CLA	CMC-C2C	-2.22	1.46	1.50
15	A	1101	CLA	MG-NB	-2.22	2.01	2.05
15	B	1216	CLA	MG-ND	-2.22	2.01	2.05
15	1	611	CLA	MG-NB	-2.22	2.01	2.05
15	A	1121	CLA	C3B-C4B	2.22	1.49	1.42
15	B	1206	CLA	CMD-C2D	-2.22	1.46	1.50
15	B	1222	CLA	CMC-C2C	-2.22	1.46	1.50
15	4	612	CLA	MG-NB	-2.22	2.01	2.05
15	A	1116	CLA	C4B-NB	2.22	1.40	1.37
15	4	604	CLA	C3B-C4B	2.22	1.49	1.42
15	A	1102	CLA	CMC-C2C	-2.22	1.46	1.50
15	B	1213	CLA	CMB-C2B	-2.21	1.46	1.50
15	A	1111	CLA	MG-NB	-2.21	2.01	2.05
15	A	1132	CLA	CHC-C1C	2.21	1.42	1.38
15	1	608	CLA	CMB-C2B	-2.21	1.46	1.50
15	1	607	CLA	CMB-C2B	-2.21	1.46	1.50
15	A	1118	CLA	CMB-C2B	-2.21	1.46	1.50
15	A	1115	CLA	CMB-C2B	-2.21	1.46	1.50
15	B	1206	CLA	CMB-C2B	-2.21	1.46	1.50
15	2	606	CLA	MG-NB	-2.21	2.01	2.05
12	1	501	LUT	C11-C12	2.21	1.40	1.34
15	A	1136	CLA	CMC-C2C	-2.21	1.46	1.50
15	4	603	CLA	CMD-C2D	-2.21	1.46	1.50
15	A	1102	CLA	MG-NB	-2.21	2.01	2.05
15	B	1210	CLA	C3B-C4B	2.21	1.49	1.42
15	2	606	CLA	C3B-C4B	2.21	1.49	1.42
15	1	606	CLA	CHC-C1C	2.21	1.42	1.38
15	A	1102	CLA	CHC-C1C	2.21	1.42	1.38
15	A	1013	CLA	CMB-C2B	-2.21	1.46	1.50
15	B	1223	CLA	C3B-C4B	2.20	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	B	1212	CLA	CMC-C2C	-2.20	1.46	1.50
15	B	1214	CLA	C1B-C2B	2.20	1.48	1.43
13	1	502	XAT	C8-C7	2.20	1.37	1.32
15	A	1121	CLA	MG-NB	-2.20	2.01	2.05
15	2	602	CLA	CMB-C2B	-2.20	1.46	1.50
15	B	1206	CLA	CMC-C2C	-2.20	1.46	1.50
15	A	1104	CLA	C3B-C4B	2.20	1.49	1.42
15	F	1302	CLA	C3B-C4B	2.20	1.49	1.42
15	B	1215	CLA	MG-NB	-2.20	2.01	2.05
15	B	1220	CLA	C3B-C4B	2.20	1.49	1.42
15	B	1220	CLA	CHC-C1C	2.20	1.42	1.38
15	A	1109	CLA	MG-NB	-2.20	2.01	2.05
15	B	1223	CLA	MG-NB	-2.20	2.01	2.05
15	3	608	CLA	C3B-C4B	2.20	1.49	1.42
15	B	1225	CLA	C3B-C4B	2.20	1.49	1.42
18	B	5003	LMG	O1-C1	2.20	1.43	1.40
15	2	608	CLA	CHC-C1C	2.20	1.42	1.38
15	4	604	CLA	CHC-C1C	2.20	1.42	1.38
15	B	1219	CLA	MG-NB	-2.20	2.01	2.05
15	A	1115	CLA	C3B-C4B	2.20	1.49	1.42
14	A	4007	BCR	C33-C5	-2.20	1.47	1.50
15	B	1209	CLA	CMB-C2B	-2.20	1.46	1.50
15	B	1215	CLA	CMC-C2C	-2.20	1.46	1.50
15	B	1214	CLA	CMC-C2C	-2.20	1.46	1.50
15	A	1131	CLA	CMB-C2B	-2.19	1.46	1.50
15	A	1013	CLA	C3B-C4B	2.19	1.49	1.42
15	1	613	CLA	MG-NB	-2.19	2.01	2.05
15	4	609	CLA	CMC-C2C	-2.19	1.46	1.50
15	A	1119	CLA	CHC-C1C	2.19	1.42	1.38
15	B	1237	CLA	C3B-C4B	2.19	1.49	1.42
14	A	4002	BCR	C38-C26	-2.19	1.47	1.50
15	4	607	CLA	C3B-C4B	2.19	1.49	1.42
15	B	1023	CLA	CMB-C2B	-2.19	1.46	1.50
15	A	1107	CLA	CMB-C2B	-2.19	1.46	1.50
15	B	1232	CLA	CMC-C2C	-2.19	1.46	1.50
15	B	1023	CLA	C3B-C4B	2.19	1.49	1.42
15	4	602	CLA	MG-NB	-2.19	2.01	2.05
15	B	1229	CLA	MG-NB	-2.19	2.01	2.05
15	1	603	CLA	CHC-C1C	2.19	1.42	1.38
15	B	1228	CLA	C3B-C4B	2.18	1.49	1.42
15	B	1236	CLA	CMB-C2B	-2.18	1.46	1.50
15	A	1111	CLA	C3B-C4B	2.18	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	B	1230	CLA	CMB-C2B	-2.18	1.46	1.50
15	1	611	CLA	CMD-C2D	-2.18	1.46	1.50
15	A	1140	CLA	C3B-C4B	2.18	1.49	1.42
15	A	1110	CLA	CMC-C2C	-2.18	1.46	1.50
15	A	1131	CLA	C3B-C4B	2.18	1.49	1.42
15	B	1225	CLA	CMC-C2C	-2.18	1.46	1.50
14	3	504	BCR	C38-C26	-2.18	1.47	1.50
15	A	1101	CLA	C3B-C4B	2.18	1.49	1.42
15	B	1217	CLA	CMC-C2C	-2.18	1.46	1.50
15	F	1302	CLA	MG-NB	-2.18	2.01	2.05
15	A	1119	CLA	C3B-C4B	2.17	1.49	1.42
15	4	616	CLA	C3B-C4B	2.17	1.49	1.42
15	1	613	CLA	CMB-C2B	-2.17	1.46	1.50
14	B	4005	BCR	C33-C5	-2.17	1.47	1.50
15	3	603	CLA	MG-NB	-2.17	2.01	2.05
15	B	1211	CLA	C3B-C4B	2.17	1.49	1.42
15	B	1222	CLA	C3B-C4B	2.17	1.49	1.42
15	B	1207	CLA	CHC-C1C	2.17	1.42	1.38
15	2	603	CLA	CMC-C2C	-2.17	1.46	1.50
15	B	1226	CLA	C3B-C4B	2.17	1.49	1.42
15	3	607	CLA	C3B-C4B	2.17	1.49	1.42
15	2	608	CLA	MG-NB	-2.17	2.01	2.05
15	3	612	CLA	CMC-C2C	-2.17	1.46	1.50
15	A	1112	CLA	CMC-C2C	-2.17	1.46	1.50
15	B	1214	CLA	C3B-C4B	2.17	1.49	1.42
15	B	1023	CLA	CHC-C1C	2.17	1.42	1.38
14	3	506	BCR	C33-C5	-2.17	1.47	1.50
15	A	1130	CLA	CMC-C2C	-2.17	1.46	1.50
15	J	1302	CLA	CMB-C2B	-2.17	1.46	1.50
15	3	615	CLA	CHC-C1C	2.17	1.42	1.38
15	1	611	CLA	CMB-C2B	-2.17	1.46	1.50
15	B	1222	CLA	CMB-C2B	-2.17	1.46	1.50
15	3	607	CLA	MG-NB	-2.17	2.01	2.05
15	A	1122	CLA	MG-NB	-2.17	2.01	2.05
15	1	611	CLA	CHC-C1C	2.17	1.42	1.38
15	A	1013	CLA	CHC-C1C	2.17	1.42	1.38
15	3	605	CLA	C3B-C4B	2.17	1.49	1.42
15	J	1302	CLA	C3B-C4B	2.17	1.49	1.42
15	4	601	CLA	CHC-C1C	2.16	1.42	1.38
15	A	1109	CLA	CMC-C2C	-2.16	1.46	1.50
15	4	607	CLA	MG-NB	-2.16	2.01	2.05
15	A	1105	CLA	C3B-C4B	2.16	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	A	1133	CLA	C3B-C4B	2.16	1.49	1.42
15	1	605	CLA	CMB-C2B	-2.16	1.46	1.50
15	B	1239	CLA	CMC-C2C	-2.16	1.46	1.50
15	A	1121	CLA	CHC-C1C	2.16	1.42	1.38
15	A	1117	CLA	CMB-C2B	-2.16	1.46	1.50
15	4	601	CLA	C1B-C2B	2.16	1.48	1.43
15	2	607	CLA	CMC-C2C	-2.16	1.46	1.50
15	3	615	CLA	C3B-C4B	2.16	1.49	1.42
15	4	603	CLA	MG-NB	-2.16	2.01	2.05
13	2	502	XAT	C39-C29	2.16	1.55	1.50
15	B	1240	CLA	C3B-C4B	2.16	1.49	1.42
16	4	610	CHL	CHA-CBD	2.16	1.54	1.51
15	A	1113	CLA	CMC-C2C	-2.16	1.46	1.50
15	2	612	CLA	CMB-C2B	-2.16	1.46	1.50
15	A	1114	CLA	CMC-C2C	-2.16	1.46	1.50
15	B	1022	CLA	CMB-C2B	-2.15	1.46	1.50
15	A	1106	CLA	CHC-C1C	2.15	1.42	1.38
15	1	605	CLA	MG-NB	-2.15	2.01	2.05
15	4	612	CLA	CHC-C1C	2.15	1.42	1.38
15	4	604	CLA	CMB-C2B	-2.15	1.46	1.50
15	A	1103	CLA	C3B-C4B	2.15	1.49	1.42
15	B	1212	CLA	MG-NB	-2.15	2.01	2.05
15	B	1206	CLA	C3B-C4B	2.15	1.49	1.42
15	A	1114	CLA	MG-NB	-2.15	2.01	2.05
15	B	1222	CLA	MG-NB	-2.15	2.01	2.05
15	B	1221	CLA	CMB-C2B	-2.15	1.46	1.50
15	B	1223	CLA	CMB-C2B	-2.15	1.46	1.50
15	4	607	CLA	CMB-C2B	-2.15	1.46	1.50
15	B	1221	CLA	CMC-C2C	-2.15	1.46	1.50
15	2	608	CLA	CMB-C2B	-2.15	1.46	1.50
15	A	1107	CLA	CMC-C2C	-2.15	1.46	1.50
15	3	610	CLA	C3B-C4B	2.15	1.49	1.42
15	2	604	CLA	C3B-C4B	2.15	1.49	1.42
15	B	1021	CLA	MG-ND	-2.15	2.01	2.05
15	A	1121	CLA	CMC-C2C	-2.15	1.46	1.50
15	F	1302	CLA	CMC-C2C	-2.15	1.46	1.50
15	B	1213	CLA	C3B-C4B	2.15	1.49	1.42
15	B	1223	CLA	CHC-C1C	2.15	1.42	1.38
15	B	1224	CLA	CMB-C2B	-2.15	1.46	1.50
15	B	1201	CLA	CMC-C2C	-2.15	1.46	1.50
15	B	1207	CLA	CMB-C2B	-2.15	1.46	1.50
15	A	1129	CLA	MG-ND	-2.14	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	A	1106	CLA	C3B-C4B	2.14	1.49	1.42
15	4	612	CLA	CMB-C2B	-2.14	1.46	1.50
16	2	610	CHL	CHA-CBD	2.14	1.54	1.51
15	3	608	CLA	CMB-C2B	-2.14	1.46	1.50
15	B	1211	CLA	CMC-C2C	-2.14	1.46	1.50
15	F	1302	CLA	CMB-C2B	-2.14	1.46	1.50
15	A	1120	CLA	CMC-C2C	-2.14	1.46	1.50
15	3	610	CLA	CMB-C2B	-2.14	1.46	1.50
14	A	4008	BCR	C33-C5	-2.14	1.47	1.50
15	A	1012	CLA	C3B-C4B	2.14	1.49	1.42
15	3	603	CLA	CMC-C2C	-2.14	1.46	1.50
15	A	1127	CLA	CMB-C2B	-2.14	1.46	1.50
15	3	608	CLA	CHC-C1C	2.14	1.42	1.38
15	B	1209	CLA	CMC-C2C	-2.14	1.46	1.50
12	4	501	LUT	C26-C27	2.14	1.53	1.50
14	F	4002	BCR	C33-C5	-2.14	1.47	1.50
15	A	1103	CLA	MG-NB	-2.14	2.01	2.05
15	4	606	CLA	CMB-C2B	-2.14	1.46	1.50
15	1	601	CLA	CMB-C2B	-2.14	1.46	1.50
15	4	616	CLA	CMB-C2B	-2.14	1.46	1.50
15	B	1240	CLA	CHC-C1C	2.14	1.42	1.38
15	2	607	CLA	C3B-C4B	2.14	1.49	1.42
15	A	1134	CLA	CMC-C2C	-2.13	1.46	1.50
15	2	616	CLA	C3B-C4B	2.13	1.49	1.42
15	1	602	CLA	CMB-C2B	-2.13	1.46	1.50
15	1	615	CLA	CHC-C1C	2.13	1.42	1.38
15	1	602	CLA	MG-NB	-2.13	2.01	2.05
15	B	1203	CLA	C3B-C4B	2.13	1.49	1.42
15	4	608	CLA	CHC-C1C	2.13	1.42	1.38
15	B	1210	CLA	CHC-C1C	2.13	1.42	1.38
14	J	4002	BCR	C33-C5	-2.13	1.47	1.50
15	A	1133	CLA	MG-NB	-2.13	2.01	2.05
15	A	1108	CLA	C3B-C4B	2.13	1.48	1.42
15	B	1231	CLA	CMC-C2C	-2.13	1.46	1.50
15	A	1139	CLA	CMC-C2C	-2.13	1.46	1.50
15	B	1224	CLA	MG-NB	-2.13	2.01	2.05
15	3	611	CLA	C3B-C4B	2.13	1.48	1.42
15	A	1129	CLA	C3B-C4B	2.13	1.48	1.42
15	2	606	CLA	CMB-C2B	-2.13	1.46	1.50
14	J	4001	BCR	C1-C6	-2.13	1.51	1.53
15	4	609	CLA	CMB-C2B	-2.13	1.46	1.50
15	1	603	CLA	CMB-C2B	-2.12	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	1	607	CLA	CHC-C1C	2.12	1.42	1.38
14	J	4002	BCR	C38-C26	-2.12	1.47	1.50
15	B	1237	CLA	CHC-C1C	2.12	1.42	1.38
15	B	1204	CLA	CMC-C2C	-2.12	1.46	1.50
15	B	1221	CLA	C1B-NB	-2.12	1.35	1.37
14	A	4006	BCR	C33-C5	-2.12	1.47	1.50
12	2	501	LUT	C10-C9	2.12	1.40	1.35
13	1	502	XAT	C40-C33	2.12	1.55	1.50
15	3	612	CLA	C3B-C4B	2.12	1.48	1.42
15	1	612	CLA	MG-NB	-2.12	2.01	2.05
15	1	615	CLA	C3B-C4B	2.12	1.48	1.42
15	1	607	CLA	CMC-C2C	-2.12	1.46	1.50
15	B	1224	CLA	CMC-C2C	-2.12	1.46	1.50
15	B	1228	CLA	CMC-C2C	-2.12	1.46	1.50
15	A	1127	CLA	CMC-C2C	-2.12	1.46	1.50
14	3	503	BCR	C33-C5	-2.11	1.47	1.50
15	A	1113	CLA	C3B-C4B	2.11	1.48	1.42
15	B	1229	CLA	CMB-C2B	-2.11	1.46	1.50
15	A	1131	CLA	CMC-C2C	-2.11	1.46	1.50
15	F	1301	CLA	C3B-C4B	2.11	1.48	1.42
15	A	1115	CLA	CMC-C2C	-2.11	1.46	1.50
15	B	1217	CLA	C3B-C4B	2.11	1.48	1.42
15	B	1218	CLA	CHC-C1C	2.11	1.42	1.38
15	B	1231	CLA	C3B-C4B	2.11	1.48	1.42
15	1	612	CLA	CMB-C2B	-2.11	1.46	1.50
15	1	612	CLA	CMD-C2D	-2.11	1.46	1.50
15	B	1212	CLA	C3B-C4B	2.11	1.48	1.42
15	B	1207	CLA	CMD-C2D	-2.11	1.46	1.50
15	1	605	CLA	C3B-C4B	2.11	1.48	1.42
15	A	1126	CLA	CHC-C1C	2.11	1.42	1.38
15	A	1116	CLA	CMC-C2C	-2.11	1.46	1.50
15	A	1102	CLA	C3B-C4B	2.11	1.48	1.42
15	1	606	CLA	CMB-C2B	-2.11	1.46	1.50
15	1	613	CLA	CMD-C2D	-2.11	1.46	1.50
15	2	604	CLA	CMC-C2C	-2.11	1.46	1.50
15	B	1202	CLA	CMC-C2C	-2.11	1.46	1.50
12	2	501	LUT	C11-C12	2.11	1.40	1.34
15	A	1122	CLA	C3B-C4B	2.10	1.48	1.42
15	B	1230	CLA	C3B-C4B	2.10	1.48	1.42
15	3	601	CLA	CMC-C2C	-2.10	1.46	1.50
15	A	1134	CLA	MG-NB	-2.10	2.01	2.05
15	A	1123	CLA	CMC-C2C	-2.10	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	4	613	CHL	CHA-CBD	2.10	1.54	1.51
15	4	616	CLA	CHC-C1C	2.10	1.42	1.38
15	3	607	CLA	CMB-C2B	-2.10	1.46	1.50
15	3	610	CLA	CMC-C2C	-2.10	1.46	1.50
15	A	1110	CLA	CHC-C1C	2.10	1.42	1.38
15	A	1120	CLA	C3B-C4B	2.10	1.48	1.42
15	2	606	CLA	CMC-C2C	-2.10	1.46	1.50
15	3	607	CLA	CHC-C1C	2.10	1.42	1.38
15	A	1103	CLA	CHC-C1C	2.10	1.42	1.38
15	A	1136	CLA	C3B-C4B	2.10	1.48	1.42
16	3	604	CHL	C3A-C2A	-2.10	1.52	1.54
15	3	615	CLA	MG-NB	-2.10	2.01	2.05
15	B	1021	CLA	CMB-C2B	-2.09	1.46	1.50
15	B	1215	CLA	CMB-C2B	-2.09	1.46	1.50
15	A	1115	CLA	CHC-C1C	2.09	1.42	1.38
14	A	4004	BCR	C33-C5	-2.09	1.47	1.50
16	4	611	CHL	CHA-CBD	2.09	1.54	1.51
15	A	1125	CLA	C3B-C4B	2.09	1.48	1.42
15	B	1021	CLA	CMC-C2C	-2.09	1.46	1.50
15	2	612	CLA	C3B-C4B	2.09	1.48	1.42
15	B	1214	CLA	MG-NB	-2.09	2.01	2.05
15	B	1235	CLA	CMC-C2C	-2.09	1.46	1.50
15	A	1126	CLA	CMB-C2B	-2.09	1.46	1.50
15	1	608	CLA	C3B-C4B	2.09	1.48	1.42
15	1	604	CLA	C3B-C4B	2.09	1.48	1.42
15	A	1122	CLA	CMC-C2C	-2.09	1.46	1.50
15	2	607	CLA	CHC-C1C	2.09	1.42	1.38
15	A	1107	CLA	C3B-C4B	2.09	1.48	1.42
15	A	1118	CLA	C3B-C4B	2.09	1.48	1.42
15	B	1214	CLA	CHC-C1C	2.09	1.42	1.38
15	B	1238	CLA	CHC-C1C	2.09	1.42	1.38
16	2	611	CHL	CHA-CBD	2.08	1.54	1.51
15	2	605	CLA	CMC-C2C	-2.08	1.46	1.50
15	1	605	CLA	CMC-C2C	-2.08	1.46	1.50
14	B	4006	BCR	C33-C5	-2.08	1.47	1.50
15	B	1209	CLA	C3B-C4B	2.08	1.48	1.42
15	A	1111	CLA	CMB-C2B	-2.08	1.46	1.50
12	4	501	LUT	C10-C9	2.08	1.40	1.35
15	2	604	CLA	CHC-C1C	2.08	1.42	1.38
15	A	1141	CLA	C3B-C4B	2.08	1.48	1.42
15	A	1124	CLA	MG-ND	-2.08	2.01	2.05
18	4	801	LMG	C7-C8	2.08	1.57	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	B	1218	CLA	CMC-C2C	-2.08	1.46	1.50
15	4	608	CLA	C3B-C4B	2.08	1.48	1.42
15	A	1139	CLA	C3B-C4B	2.08	1.48	1.42
15	4	608	CLA	MG-ND	-2.07	2.01	2.05
15	B	1239	CLA	C3B-C4B	2.07	1.48	1.42
15	4	612	CLA	CMC-C2C	-2.07	1.46	1.50
13	4	502	XAT	C20-C13	2.07	1.55	1.50
15	3	605	CLA	CHC-C1C	2.07	1.42	1.38
13	4	502	XAT	C40-C33	2.07	1.55	1.50
15	1	604	CLA	CHC-C1C	2.07	1.42	1.38
15	A	1012	CLA	CMC-C2C	-2.07	1.46	1.50
15	B	1232	CLA	MG-NB	-2.07	2.01	2.05
16	1	610	CHL	CHA-CBD	2.07	1.54	1.51
15	1	612	CLA	CHC-C1C	2.07	1.42	1.38
15	B	1216	CLA	C3B-C4B	2.07	1.48	1.42
15	B	1205	CLA	MG-NB	-2.07	2.01	2.05
15	2	616	CLA	CHC-C1C	2.07	1.42	1.38
15	1	601	CLA	CMC-C2C	-2.07	1.46	1.50
13	2	502	XAT	C18-C5	2.06	1.54	1.51
15	3	606	CLA	CMC-C2C	-2.06	1.46	1.50
14	4	503	BCR	C38-C26	-2.06	1.47	1.50
15	J	1302	CLA	CHC-C1C	2.06	1.42	1.38
15	2	602	CLA	CMC-C2C	-2.06	1.46	1.50
15	A	1138	CLA	CMC-C2C	-2.06	1.46	1.50
15	4	606	CLA	C3B-C4B	2.06	1.48	1.42
15	A	1013	CLA	CMC-C2C	-2.06	1.46	1.50
15	1	615	CLA	CMD-C2D	-2.06	1.46	1.50
15	A	1133	CLA	CHC-C1C	2.06	1.42	1.38
15	2	605	CLA	C3B-C4B	2.06	1.48	1.42
15	A	1132	CLA	CMB-C2B	-2.06	1.46	1.50
15	B	1240	CLA	CMC-C2C	-2.06	1.46	1.50
15	1	615	CLA	CMB-C2B	-2.06	1.46	1.50
15	B	1236	CLA	CHC-C1C	2.06	1.42	1.38
15	B	1204	CLA	C3B-C4B	2.05	1.48	1.42
15	3	614	CLA	MG-NB	-2.05	2.01	2.05
15	A	1123	CLA	C3B-C4B	2.05	1.48	1.42
15	B	1022	CLA	MG-ND	-2.05	2.01	2.05
15	4	605	CLA	CMC-C2C	-2.05	1.46	1.50
15	4	606	CLA	CHC-C1C	2.05	1.42	1.38
15	A	1135	CLA	CMB-C2B	-2.05	1.46	1.50
15	B	1237	CLA	CMC-C2C	-2.05	1.46	1.50
15	B	1238	CLA	MG-ND	-2.05	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	1011	CL0	C5-C3	2.05	1.55	1.51
15	3	611	CLA	CHC-C1C	2.05	1.42	1.38
15	4	607	CLA	CHC-C1C	2.05	1.42	1.38
15	1	608	CLA	CHC-C1C	2.05	1.42	1.38
15	B	1232	CLA	CHC-C1C	2.05	1.42	1.38
15	B	1219	CLA	CMC-C2C	-2.05	1.46	1.50
13	2	502	XAT	C40-C33	2.04	1.55	1.50
13	1	502	XAT	C39-C29	2.04	1.55	1.50
15	A	1112	CLA	C3B-C4B	2.04	1.48	1.42
22	B	5002	DGD	O6D-C5D	-2.04	1.39	1.44
15	3	610	CLA	CHC-C1C	2.04	1.42	1.38
15	A	1123	CLA	MG-ND	-2.04	2.01	2.05
15	1	604	CLA	CMC-C2C	-2.04	1.46	1.50
15	B	1205	CLA	CHC-C1C	2.04	1.42	1.38
15	3	609	CLA	C3B-C4B	2.04	1.48	1.42
15	B	1211	CLA	MG-ND	-2.04	2.01	2.05
15	A	1124	CLA	CMC-C2C	-2.04	1.46	1.50
15	2	606	CLA	CHC-C1C	2.04	1.42	1.38
15	B	1204	CLA	CHC-C1C	2.04	1.42	1.38
16	3	604	CHL	CHA-CBD	2.04	1.54	1.51
15	B	1221	CLA	CHC-C1C	2.04	1.42	1.38
15	A	1133	CLA	CMC-C2C	-2.04	1.46	1.50
15	1	611	CLA	CMC-C2C	-2.04	1.46	1.50
15	A	1130	CLA	C3B-C4B	2.04	1.48	1.42
15	3	615	CLA	CMB-C2B	-2.03	1.46	1.50
15	2	603	CLA	MG-NB	-2.03	2.01	2.05
15	A	1124	CLA	C3B-C4B	2.03	1.48	1.42
16	2	613	CHL	CHA-CBD	2.03	1.54	1.51
15	B	1219	CLA	CHC-C1C	2.03	1.42	1.38
15	B	1202	CLA	MG-NB	-2.03	2.01	2.05
15	A	1116	CLA	CHC-C1C	2.03	1.42	1.38
15	1	602	CLA	CHC-C1C	2.03	1.42	1.38
15	B	1230	CLA	MG-NB	-2.03	2.01	2.05
15	1	615	CLA	CMC-C2C	-2.03	1.46	1.50
15	B	1213	CLA	CMC-C2C	-2.03	1.46	1.50
13	3	502	XAT	C40-C33	2.03	1.54	1.50
15	3	609	CLA	CMC-C2C	-2.03	1.46	1.50
15	4	616	CLA	CMC-C2C	-2.03	1.46	1.50
15	A	1127	CLA	CHC-C1C	2.03	1.42	1.38
15	1	603	CLA	CMC-C2C	-2.03	1.46	1.50
16	2	611	CHL	C2C-C3C	2.03	1.38	1.36
15	2	616	CLA	CMC-C2C	-2.03	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	4	605	CLA	C3B-C4B	2.03	1.48	1.42
15	A	1132	CLA	C3C-C2C	2.02	1.41	1.36
15	A	1129	CLA	CHC-C1C	2.02	1.42	1.38
15	B	1234	CLA	MG-ND	-2.02	2.01	2.05
15	A	1117	CLA	CHC-C1C	2.02	1.42	1.38
15	B	1234	CLA	CHC-C1C	2.02	1.42	1.38
15	B	1230	CLA	MG-ND	-2.02	2.01	2.05
15	3	613	CLA	C3B-C4B	2.02	1.48	1.42
15	A	1132	CLA	C3B-C4B	2.02	1.48	1.42
15	3	606	CLA	CMB-C2B	-2.02	1.46	1.50
15	A	1140	CLA	CHC-C1C	2.02	1.42	1.38
15	3	605	CLA	MG-ND	-2.02	2.01	2.05
17	2	801	LHG	P-O6	2.02	1.67	1.59
15	A	1116	CLA	C3B-C4B	2.02	1.48	1.42
15	A	1134	CLA	CHC-C1C	2.01	1.42	1.38
15	1	604	CLA	MG-ND	-2.01	2.01	2.05
15	1	603	CLA	MG-NB	-2.01	2.01	2.05
15	A	1125	CLA	MG-ND	-2.01	2.01	2.05
15	B	1235	CLA	C3B-C4B	2.01	1.48	1.42
14	B	4001	BCR	C33-C5	-2.01	1.47	1.50
16	2	609	CHL	CHA-CBD	2.01	1.54	1.51
15	B	1207	CLA	MG-NB	-2.01	2.01	2.05
12	2	501	LUT	C26-C27	2.00	1.53	1.50
15	A	1128	CLA	C3B-C4B	2.00	1.48	1.42
14	J	4001	BCR	C38-C26	-2.00	1.47	1.50
14	1	503	BCR	C38-C26	-2.00	1.47	1.50
15	4	601	CLA	MG-ND	-2.00	2.01	2.05

All (1362) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	3	502	XAT	O4-C5-C4	46.40	156.98	113.49
13	1	502	XAT	O4-C5-C4	45.82	156.43	113.49
13	1	502	XAT	O24-C25-C24	44.10	154.82	113.49
13	4	502	XAT	O4-C5-C4	43.37	154.14	113.49
13	2	502	XAT	O4-C5-C4	43.36	154.13	113.49
13	4	502	XAT	O24-C25-C24	42.55	153.37	113.49
13	3	502	XAT	O24-C25-C24	41.81	152.68	113.49
13	2	502	XAT	O24-C25-C24	40.19	151.16	113.49
19	A	1011	CL0	C4D-ND-C1D	-22.19	88.38	105.22
19	A	1011	CL0	C1B-CHB-C4A	-21.54	107.47	121.32
13	2	502	XAT	O24-C25-C38	-13.79	99.63	115.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	1	502	XAT	O24-C25-C38	-13.54	99.91	115.05
13	3	502	XAT	O24-C25-C38	-12.64	100.93	115.05
13	3	502	XAT	O4-C5-C18	-12.46	101.12	115.05
13	1	502	XAT	O4-C5-C18	-12.36	101.23	115.05
13	4	502	XAT	C18-C5-C4	-12.06	100.69	114.24
13	2	502	XAT	C18-C5-C4	-11.74	101.06	114.24
13	4	502	XAT	O24-C25-C38	-11.36	102.35	115.05
13	1	502	XAT	C38-C25-C24	-11.06	101.81	114.24
13	3	502	XAT	C18-C5-C4	-10.99	101.90	114.24
13	1	502	XAT	C18-C5-C4	-10.63	102.30	114.24
13	4	502	XAT	C38-C25-C24	-10.23	102.75	114.24
13	3	502	XAT	C38-C25-C24	-10.06	102.94	114.24
19	A	1011	CL0	CHA-C1A-C2A	-9.80	110.30	133.31
13	3	502	XAT	C15-C14-C13	-9.71	113.66	127.28
13	2	502	XAT	O4-C5-C18	-9.68	104.23	115.05
13	4	502	XAT	O4-C5-C18	-9.33	104.62	115.05
16	4	613	CHL	C1B-CHB-C4A	9.30	127.30	121.32
13	4	502	XAT	C11-C10-C9	-9.20	114.38	127.28
15	B	1226	CLA	C4A-NA-C1A	8.52	110.57	106.68
12	4	501	LUT	C20-C13-C14	-8.25	109.45	122.82
16	2	609	CHL	C1B-CHB-C4A	8.20	126.60	121.32
13	3	502	XAT	C32-C33-C34	8.20	131.90	119.01
15	A	1138	CLA	C4A-NA-C1A	8.11	110.38	106.68
13	4	502	XAT	C15-C14-C13	-8.10	115.91	127.28
13	2	502	XAT	C11-C10-C9	-8.08	115.95	127.28
15	A	1114	CLA	C4A-NA-C1A	8.03	110.34	106.68
15	A	1128	CLA	C4A-NA-C1A	7.95	110.31	106.68
16	1	610	CHL	C1B-CHB-C4A	7.95	126.44	121.32
16	4	611	CHL	C1B-CHB-C4A	7.87	126.39	121.32
15	A	1135	CLA	C4A-NA-C1A	7.83	110.25	106.68
13	2	502	XAT	C38-C25-C24	-7.82	105.46	114.24
13	3	502	XAT	C11-C10-C9	-7.79	116.35	127.28
15	A	1132	CLA	C4A-NA-C1A	7.74	110.21	106.68
15	3	611	CLA	C4A-NA-C1A	7.73	110.20	106.68
15	B	1239	CLA	C4A-NA-C1A	7.72	110.20	106.68
15	A	1124	CLA	C4A-NA-C1A	7.63	110.16	106.68
15	A	1109	CLA	C4A-NA-C1A	7.56	110.13	106.68
12	3	501	LUT	C1-C6-C5	-7.48	112.42	122.64
16	2	611	CHL	C1B-CHB-C4A	7.45	126.12	121.32
13	3	502	XAT	C31-C30-C29	-7.44	116.85	127.28
15	4	603	CLA	C4A-NA-C1A	7.41	110.06	106.68
12	3	501	LUT	C12-C13-C14	7.40	130.64	119.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	4	609	CLA	C4A-NA-C1A	7.36	110.04	106.68
15	2	605	CLA	C4A-NA-C1A	7.34	110.03	106.68
15	3	603	CLA	C4A-NA-C1A	7.33	110.02	106.68
15	A	1112	CLA	C4A-NA-C1A	7.32	110.02	106.68
15	B	1237	CLA	C4A-NA-C1A	7.31	110.01	106.68
15	F	1302	CLA	C4A-NA-C1A	7.31	110.01	106.68
15	A	1136	CLA	C4A-NA-C1A	7.29	110.01	106.68
15	3	613	CLA	C4A-NA-C1A	7.29	110.00	106.68
15	B	1235	CLA	C4A-NA-C1A	7.28	110.00	106.68
15	3	609	CLA	C4A-NA-C1A	7.26	109.99	106.68
15	A	1108	CLA	C4A-NA-C1A	7.23	109.98	106.68
15	B	1212	CLA	C4A-NA-C1A	7.23	109.98	106.68
12	4	501	LUT	C28-C29-C30	7.22	130.37	119.01
16	2	610	CHL	C1B-CHB-C4A	7.20	125.96	121.32
15	A	1103	CLA	C4A-NA-C1A	7.19	109.96	106.68
15	A	1104	CLA	C4A-NA-C1A	7.19	109.96	106.68
15	A	1133	CLA	C4A-NA-C1A	7.18	109.95	106.68
15	B	1221	CLA	C4A-NA-C1A	7.18	109.95	106.68
15	B	1236	CLA	C4A-NA-C1A	7.18	109.95	106.68
12	3	501	LUT	C8-C9-C10	7.18	130.30	119.01
13	3	502	XAT	C12-C13-C14	7.16	130.27	119.01
12	3	501	LUT	C19-C9-C10	-7.16	111.22	122.82
16	2	613	CHL	C1B-CHB-C4A	7.15	125.92	121.32
15	A	1113	CLA	C4A-NA-C1A	7.13	109.93	106.68
15	B	1023	CLA	C4A-NA-C1A	7.13	109.93	106.68
15	B	1204	CLA	C4A-NA-C1A	7.07	109.91	106.68
15	3	612	CLA	C4A-NA-C1A	7.06	109.90	106.68
15	B	1021	CLA	C4A-NA-C1A	7.06	109.90	106.68
15	2	603	CLA	C4A-NA-C1A	7.06	109.90	106.68
15	B	1213	CLA	C4A-NA-C1A	7.05	109.90	106.68
15	4	606	CLA	C4A-NA-C1A	7.03	109.88	106.68
15	2	602	CLA	C4A-NA-C1A	7.02	109.88	106.68
15	B	1222	CLA	C4A-NA-C1A	7.01	109.88	106.68
15	1	608	CLA	C4A-NA-C1A	7.01	109.88	106.68
15	A	1137	CLA	C4A-NA-C1A	7.00	109.87	106.68
15	B	1203	CLA	C4A-NA-C1A	6.99	109.87	106.68
15	A	1140	CLA	C4A-NA-C1A	6.99	109.87	106.68
15	1	605	CLA	C4A-NA-C1A	6.97	109.86	106.68
15	B	1231	CLA	C4A-NA-C1A	6.97	109.86	106.68
15	A	1134	CLA	C4A-NA-C1A	6.96	109.86	106.68
15	1	603	CLA	C4A-NA-C1A	6.96	109.85	106.68
15	A	1101	CLA	C4A-NA-C1A	6.94	109.85	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	A	1122	CLA	C4A-NA-C1A	6.93	109.84	106.68
15	A	1120	CLA	C4A-NA-C1A	6.91	109.83	106.68
15	4	605	CLA	C4A-NA-C1A	6.91	109.83	106.68
15	B	1209	CLA	C4A-NA-C1A	6.90	109.83	106.68
15	4	602	CLA	C4A-NA-C1A	6.89	109.82	106.68
15	A	1117	CLA	C4A-NA-C1A	6.87	109.81	106.68
15	J	1302	CLA	C4A-NA-C1A	6.86	109.81	106.68
15	A	1111	CLA	C4A-NA-C1A	6.85	109.80	106.68
15	A	1115	CLA	C4A-NA-C1A	6.85	109.80	106.68
15	A	1013	CLA	C4A-NA-C1A	6.85	109.80	106.68
19	A	1011	CL0	C1A-CHA-C4D	-6.84	107.57	118.98
15	3	607	CLA	C4A-NA-C1A	6.84	109.80	106.68
15	B	1229	CLA	C4A-NA-C1A	6.82	109.79	106.68
15	3	614	CLA	C4A-NA-C1A	6.81	109.79	106.68
15	B	1202	CLA	C4A-NA-C1A	6.81	109.78	106.68
13	4	502	XAT	C12-C13-C14	6.80	129.71	119.01
15	A	1139	CLA	C4A-NA-C1A	6.78	109.77	106.68
15	A	1118	CLA	C4A-NA-C1A	6.78	109.77	106.68
15	B	1227	CLA	C4A-NA-C1A	6.78	109.77	106.68
19	A	1011	CL0	O2D-CGD-CBD	6.78	118.39	110.95
15	B	1228	CLA	C4A-NA-C1A	6.75	109.76	106.68
15	4	612	CLA	C4A-NA-C1A	6.74	109.75	106.68
15	B	1211	CLA	C4A-NA-C1A	6.74	109.75	106.68
15	B	1217	CLA	C4A-NA-C1A	6.72	109.75	106.68
13	2	502	XAT	C18-C5-C6	-6.72	111.24	122.30
15	2	607	CLA	C4A-NA-C1A	6.71	109.74	106.68
15	B	1240	CLA	C4A-NA-C1A	6.71	109.74	106.68
15	B	1223	CLA	C4A-NA-C1A	6.70	109.74	106.68
15	B	1232	CLA	C4A-NA-C1A	6.69	109.73	106.68
15	A	1130	CLA	C4A-NA-C1A	6.66	109.72	106.68
15	A	1106	CLA	C4A-NA-C1A	6.66	109.72	106.68
15	B	1220	CLA	C4A-NA-C1A	6.62	109.70	106.68
15	3	615	CLA	C4A-NA-C1A	6.60	109.69	106.68
15	4	604	CLA	C4A-NA-C1A	6.60	109.69	106.68
15	A	1121	CLA	C4A-NA-C1A	6.59	109.69	106.68
16	3	604	CHL	C1B-CHB-C4A	6.59	125.56	121.32
15	3	606	CLA	C4A-NA-C1A	6.57	109.68	106.68
16	1	609	CHL	C1B-CHB-C4A	6.57	125.55	121.32
15	2	612	CLA	C4A-NA-C1A	6.57	109.67	106.68
15	A	1123	CLA	C4A-NA-C1A	6.55	109.67	106.68
13	3	502	XAT	C40-C33-C34	-6.55	112.21	122.82
13	3	502	XAT	O24-C26-C27	-6.55	98.12	116.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	1	606	CLA	C4A-NA-C1A	6.54	109.66	106.68
15	A	1119	CLA	C4A-NA-C1A	6.53	109.66	106.68
13	2	502	XAT	C15-C14-C13	-6.52	118.13	127.28
15	F	1301	CLA	C4A-NA-C1A	6.52	109.65	106.68
15	B	1215	CLA	C4A-NA-C1A	6.51	109.65	106.68
15	B	1206	CLA	C4A-NA-C1A	6.50	109.64	106.68
15	1	604	CLA	C4A-NA-C1A	6.49	109.64	106.68
15	2	606	CLA	C4A-NA-C1A	6.48	109.64	106.68
15	B	1225	CLA	C4A-NA-C1A	6.48	109.64	106.68
15	2	616	CLA	C4A-NA-C1A	6.47	109.63	106.68
15	B	1234	CLA	C4A-NA-C1A	6.47	109.63	106.68
15	B	1214	CLA	C4A-NA-C1A	6.46	109.63	106.68
15	A	1110	CLA	C4A-NA-C1A	6.46	109.62	106.68
15	A	1131	CLA	C4A-NA-C1A	6.45	109.62	106.68
15	A	1107	CLA	C4A-NA-C1A	6.44	109.62	106.68
15	3	601	CLA	C4A-NA-C1A	6.42	109.61	106.68
13	2	502	XAT	C7-C8-C9	-6.41	115.58	125.53
15	A	1105	CLA	C4A-NA-C1A	6.41	109.61	106.68
13	4	502	XAT	O24-C26-C27	-6.41	98.52	116.88
15	4	607	CLA	C4A-NA-C1A	6.40	109.60	106.68
15	B	1224	CLA	C4A-NA-C1A	6.39	109.59	106.68
15	A	1141	CLA	C4A-NA-C1A	6.36	109.58	106.68
15	2	604	CLA	C4A-NA-C1A	6.35	109.58	106.68
15	A	1102	CLA	C4A-NA-C1A	6.34	109.57	106.68
15	3	610	CLA	C4A-NA-C1A	6.33	109.57	106.68
19	A	1011	CL0	C3D-CAD-CBD	-6.31	99.29	107.61
15	B	1218	CLA	C4A-NA-C1A	6.31	109.56	106.68
13	2	502	XAT	C11-C12-C13	-6.31	109.06	126.36
12	1	501	LUT	C20-C13-C14	-6.29	112.63	122.82
15	1	607	CLA	C4A-NA-C1A	6.28	109.55	106.68
12	2	501	LUT	C28-C29-C30	6.26	128.86	119.01
15	B	1205	CLA	C4A-NA-C1A	6.25	109.53	106.68
15	B	1230	CLA	C4A-NA-C1A	6.23	109.52	106.68
15	3	605	CLA	C4A-NA-C1A	6.22	109.52	106.68
12	4	501	LUT	C40-C33-C34	-6.21	112.75	122.82
15	A	1129	CLA	C4A-NA-C1A	6.21	109.51	106.68
13	4	502	XAT	C18-C5-C6	-6.18	112.13	122.30
15	1	601	CLA	C4A-NA-C1A	6.18	109.50	106.68
15	B	1022	CLA	C4A-NA-C1A	6.17	109.50	106.68
13	4	502	XAT	C40-C33-C34	-6.16	112.83	122.82
15	B	1216	CLA	C4A-NA-C1A	6.15	109.48	106.68
15	1	602	CLA	C4A-NA-C1A	6.13	109.48	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	4	610	CHL	C1B-CHB-C4A	6.12	125.26	121.32
15	1	613	CLA	C4A-NA-C1A	6.12	109.47	106.68
15	3	608	CLA	C4A-NA-C1A	6.11	109.47	106.68
15	B	1208	CLA	C4A-NA-C1A	6.08	109.45	106.68
15	A	1127	CLA	C4A-NA-C1A	6.08	109.45	106.68
15	1	615	CLA	C4A-NA-C1A	6.07	109.45	106.68
15	B	1207	CLA	C4A-NA-C1A	6.05	109.44	106.68
15	1	611	CLA	C4A-NA-C1A	5.99	109.41	106.68
15	4	616	CLA	C4A-NA-C1A	5.98	109.41	106.68
15	2	608	CLA	C4A-NA-C1A	5.98	109.41	106.68
15	B	1219	CLA	C4A-NA-C1A	5.98	109.41	106.68
15	B	1210	CLA	C4A-NA-C1A	5.94	109.39	106.68
15	B	1201	CLA	C4A-NA-C1A	5.93	109.38	106.68
12	3	501	LUT	C28-C29-C30	5.92	128.32	119.01
13	4	502	XAT	C32-C33-C34	5.90	128.30	119.01
15	1	612	CLA	C4A-NA-C1A	5.90	109.37	106.68
13	4	502	XAT	C11-C12-C13	-5.89	110.22	126.36
15	4	601	CLA	C4A-NA-C1A	5.85	109.35	106.68
15	2	601	CLA	C4A-NA-C1A	5.82	109.33	106.68
13	1	502	XAT	C18-C5-C6	-5.81	112.74	122.30
15	A	1116	CLA	C4A-NA-C1A	5.81	109.33	106.68
16	4	610	CHL	C1C-CHC-C4B	5.80	136.83	116.07
15	B	1238	CLA	C1-C2-C3	-5.76	113.32	126.44
15	B	1238	CLA	CAC-C3C-C4C	5.74	132.26	124.79
15	4	608	CLA	C4A-NA-C1A	5.72	109.29	106.68
15	4	608	CLA	CAC-C3C-C4C	5.66	132.16	124.79
13	2	502	XAT	C32-C33-C34	5.64	127.88	119.01
15	A	1012	CLA	C4A-NA-C1A	5.61	109.24	106.68
15	A	1126	CLA	C4A-NA-C1A	5.60	109.23	106.68
15	B	1238	CLA	C4A-NA-C1A	5.59	109.23	106.68
15	A	1125	CLA	C4A-NA-C1A	5.57	109.22	106.68
13	1	502	XAT	C11-C10-C9	-5.56	119.48	127.28
12	3	501	LUT	C38-C25-C24	-5.51	110.32	123.36
13	4	502	XAT	C15-C35-C34	-5.50	112.26	123.52
12	1	501	LUT	C1-C6-C5	-5.45	115.19	122.64
12	2	501	LUT	C40-C33-C34	-5.43	114.01	122.82
13	2	502	XAT	C40-C33-C34	-5.42	114.03	122.82
16	1	609	CHL	C1C-CHC-C4B	5.37	135.29	116.07
12	2	501	LUT	C1-C6-C5	-5.35	115.32	122.64
16	3	604	CHL	C1C-CHC-C4B	5.33	135.14	116.07
12	4	501	LUT	C12-C13-C14	5.32	127.38	119.01
13	3	502	XAT	C18-C5-C6	-5.30	113.58	122.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	4	501	LUT	C27-C28-C29	-5.25	115.04	126.32
16	2	611	CHL	C1C-CHC-C4B	5.24	134.82	116.07
16	4	611	CHL	C1C-CHC-C4B	5.15	134.48	116.07
16	1	610	CHL	C1C-CHC-C4B	5.13	134.44	116.07
16	2	613	CHL	C1C-CHC-C4B	5.13	134.43	116.07
19	A	1011	CL0	C4D-CHA-CBD	5.13	114.13	108.97
16	2	610	CHL	C1C-CHC-C4B	5.12	134.40	116.07
16	4	613	CHL	C1C-CHC-C4B	5.11	134.34	116.07
13	3	502	XAT	C15-C35-C34	-5.11	113.07	123.52
19	A	1011	CL0	C4C-CHD-C1D	-5.08	97.88	116.07
13	2	502	XAT	O24-C26-C27	-5.08	102.32	116.88
13	2	502	XAT	C31-C30-C29	-5.08	120.16	127.28
13	2	502	XAT	C15-C35-C34	-5.06	113.17	123.52
13	4	502	XAT	C20-C13-C12	-5.04	110.40	118.09
12	4	501	LUT	C18-C5-C6	-5.03	119.00	124.48
13	4	502	XAT	C8-C9-C10	5.01	126.89	119.01
12	3	501	LUT	C39-C29-C30	-5.01	114.70	122.82
16	2	609	CHL	C1C-CHC-C4B	4.97	133.84	116.07
13	3	502	XAT	C20-C13-C12	-4.95	110.53	118.09
13	1	502	XAT	O24-C26-C27	-4.95	102.71	116.88
19	A	1011	CL0	C3D-C4D-ND	4.89	120.78	112.94
13	3	502	XAT	C35-C34-C33	4.89	134.13	127.28
12	1	501	LUT	C18-C5-C6	-4.88	119.16	124.48
13	4	502	XAT	C7-C8-C9	-4.86	117.99	125.53
12	1	501	LUT	C28-C29-C30	4.85	126.64	119.01
12	2	501	LUT	C38-C25-C24	-4.84	111.91	123.36
12	2	501	LUT	C20-C13-C14	-4.79	115.06	122.82
13	3	502	XAT	C7-C8-C9	-4.74	118.18	125.53
13	2	502	XAT	C12-C13-C14	4.71	126.41	119.01
12	3	501	LUT	C18-C5-C6	-4.67	119.39	124.48
13	4	502	XAT	C31-C30-C29	-4.59	120.84	127.28
13	3	502	XAT	C8-C9-C10	4.58	126.22	119.01
17	B	5001	LHG	O4-P-O5	4.49	133.34	112.44
17	1	801	LHG	O4-P-O5	4.48	133.30	112.44
12	2	501	LUT	C39-C29-C30	-4.48	115.56	122.82
12	1	501	LUT	C12-C13-C14	4.47	126.04	119.01
17	A	5002	LHG	O4-P-O5	4.46	133.18	112.44
17	A	5001	LHG	O4-P-O5	4.45	133.16	112.44
13	4	502	XAT	C26-C27-C28	-4.44	116.60	125.99
13	1	502	XAT	C15-C14-C13	-4.42	121.07	127.28
15	A	1110	CLA	CAA-C2A-C3A	-4.42	101.06	113.00
17	2	801	LHG	O4-P-O5	4.40	132.90	112.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	3	801	LHG	O4-P-O5	4.36	132.71	112.44
15	A	1107	CLA	CAA-C2A-C3A	-4.28	101.43	113.00
13	2	502	XAT	C38-C25-C26	-4.20	115.38	122.30
14	A	4004	BCR	C15-C16-C17	-4.14	115.04	123.52
13	1	502	XAT	C31-C30-C29	-4.14	121.47	127.28
13	2	502	XAT	C35-C15-C14	4.12	131.96	123.52
14	A	4002	BCR	C30-C25-C26	-4.12	117.01	122.64
12	2	501	LUT	C19-C9-C10	-4.11	116.15	122.82
19	A	1011	CL0	CBC-CAC-C3C	-4.10	107.00	112.87
19	A	1011	CL0	CMA-C3A-C4A	-4.07	105.84	114.61
16	2	610	CHL	C3D-C4D-CHA	4.05	114.69	108.54
16	3	604	CHL	C3D-C4D-CHA	4.04	114.67	108.54
16	4	613	CHL	C3D-C4D-CHA	4.02	114.65	108.54
19	A	1011	CL0	CED-O2D-CGD	-4.00	106.84	115.92
12	1	501	LUT	C27-C28-C29	-4.00	117.72	126.32
19	A	1011	CL0	C1C-CHC-C4B	-3.99	101.80	116.07
12	4	501	LUT	C39-C29-C28	-3.98	112.00	118.09
12	3	501	LUT	C32-C33-C34	3.96	125.23	119.01
16	4	611	CHL	C3D-C4D-CHA	3.96	114.56	108.54
14	B	4003	BCR	C3-C4-C5	-3.93	107.04	114.06
16	4	610	CHL	C3D-C4D-CHA	3.92	114.50	108.54
16	1	610	CHL	C3D-C4D-CHA	3.92	114.49	108.54
16	1	609	CHL	C3D-C4D-CHA	3.91	114.49	108.54
12	3	501	LUT	C7-C8-C9	-3.89	120.48	126.23
15	4	607	CLA	CAA-C2A-C3A	-3.89	102.49	113.00
16	2	613	CHL	C3D-C4D-CHA	3.88	114.44	108.54
13	1	502	XAT	C38-C25-C26	-3.86	115.94	122.30
15	A	1140	CLA	C4-C3-C5	3.86	121.93	115.23
12	4	501	LUT	C1-C6-C5	-3.86	117.37	122.64
13	2	502	XAT	C8-C9-C10	3.86	125.07	119.01
12	1	501	LUT	C39-C29-C30	-3.85	116.58	122.82
14	A	4006	BCR	C24-C23-C22	-3.85	120.54	126.23
13	4	502	XAT	C38-C25-C26	-3.84	115.97	122.30
16	2	611	CHL	C3D-C4D-CHA	3.82	114.35	108.54
19	A	1011	CL0	CAA-C2A-C3A	-3.81	102.69	113.00
12	4	501	LUT	C19-C9-C10	-3.81	116.65	122.82
13	3	502	XAT	C11-C12-C13	-3.79	115.96	126.36
12	1	501	LUT	C19-C9-C10	-3.79	116.67	122.82
16	2	609	CHL	C3D-C4D-CHA	3.79	114.30	108.54
15	B	1218	CLA	CAA-C2A-C3A	-3.78	102.78	113.00
14	A	4004	BCR	C15-C14-C13	-3.76	122.00	127.28
13	4	502	XAT	C35-C15-C14	3.73	131.15	123.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B	4002	BCR	C30-C25-C26	-3.73	117.54	122.64
12	4	501	LUT	C38-C25-C24	-3.70	114.60	123.36
15	A	1124	CLA	O2D-CGD-CBD	3.70	117.70	111.23
12	3	501	LUT	C20-C13-C12	-3.70	112.44	118.09
15	A	1124	CLA	O2D-CGD-O1D	-3.67	116.71	123.85
12	3	501	LUT	C20-C13-C14	-3.65	116.89	122.82
13	3	502	XAT	C31-C32-C33	-3.65	116.34	126.36
14	J	4002	BCR	C15-C14-C13	-3.65	122.16	127.28
15	A	1105	CLA	CAA-C2A-C3A	-3.63	103.19	113.00
19	A	1011	CL0	O2D-CGD-O1D	-3.62	116.81	123.85
15	B	1232	CLA	O2D-CGD-O1D	-3.61	116.82	123.85
14	B	4005	BCR	C15-C16-C17	-3.60	116.16	123.52
16	4	610	CHL	CHA-C1A-C2A	-3.58	124.89	133.31
16	1	609	CHL	C1-O2A-CGA	3.57	125.29	116.65
12	2	501	LUT	C27-C28-C29	-3.57	118.65	126.32
16	2	613	CHL	CHA-C1A-C2A	-3.56	124.96	133.31
14	B	4004	BCR	C2-C1-C6	3.55	115.59	110.44
15	3	605	CLA	CHB-C4A-NA	3.54	129.51	124.40
15	4	601	CLA	C3B-C4B-NB	-3.54	107.37	110.53
15	B	1201	CLA	C3B-C4B-NB	-3.54	107.37	110.53
15	4	601	CLA	CAA-C2A-C1A	-3.52	100.43	111.97
15	2	608	CLA	CAA-C2A-C3A	-3.52	103.48	113.00
15	2	616	CLA	C1-O2A-CGA	3.49	125.11	116.65
15	4	603	CLA	O2D-CGD-O1D	-3.49	117.06	123.85
14	A	4004	BCR	C24-C23-C22	-3.48	121.09	126.23
12	2	501	LUT	C21-C26-C27	-3.46	108.85	112.83
14	B	4004	BCR	C3-C4-C5	-3.46	107.89	114.06
14	B	4003	BCR	C2-C1-C6	3.44	115.44	110.44
15	B	1229	CLA	O2D-CGD-O1D	-3.44	117.16	123.85
15	A	1137	CLA	O2D-CGD-O1D	-3.41	117.20	123.85
15	3	615	CLA	O2D-CGD-O1D	-3.41	117.21	123.85
15	B	1238	CLA	C5-C3-C2	-3.40	112.82	120.36
15	A	1134	CLA	O2D-CGD-O1D	-3.40	117.23	123.85
15	3	605	CLA	CAC-C3C-C4C	3.40	129.21	124.79
16	1	610	CHL	CHA-C1A-C2A	-3.40	125.33	133.31
19	A	1011	CL0	CAC-C3C-C4C	3.40	132.76	124.03
16	2	611	CHL	CHA-C1A-C2A	-3.39	125.34	133.31
13	1	502	XAT	C36-C21-C26	3.38	119.18	110.05
15	3	609	CLA	O2D-CGD-O1D	-3.38	117.26	123.85
15	2	601	CLA	C3B-C4B-NB	-3.38	107.51	110.53
15	B	1223	CLA	O2D-CGD-O1D	-3.38	117.27	123.85
15	A	1012	CLA	O2D-CGD-O1D	-3.37	117.28	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	B	1240	CLA	C5-C3-C2	3.37	128.74	121.17
14	3	506	BCR	C35-C13-C14	-3.37	117.35	122.82
15	A	1125	CLA	C3B-C4B-NB	-3.37	107.52	110.53
12	4	501	LUT	C37-C21-C26	-3.37	104.44	109.55
16	4	613	CHL	C1-O2A-CGA	3.36	124.78	116.65
18	4	801	LMG	C1-C2-C3	-3.36	102.94	110.01
16	3	604	CHL	C1A-CHA-C4D	3.36	124.58	118.98
14	J	4002	BCR	C27-C26-C25	3.35	127.23	122.70
16	3	604	CHL	CAA-C2A-C3A	3.35	122.04	113.00
15	A	1117	CLA	O2D-CGD-O1D	-3.35	117.33	123.85
15	B	1202	CLA	O2D-CGD-O1D	-3.34	117.34	123.85
14	A	4003	BCR	C1-C6-C5	-3.33	118.08	122.64
14	A	4002	BCR	C27-C26-C25	3.33	127.21	122.70
14	3	504	BCR	C15-C16-C17	-3.33	116.70	123.52
15	B	1229	CLA	O2D-CGD-CBD	3.33	117.05	111.23
12	4	501	LUT	C20-C13-C12	3.33	123.17	118.09
16	4	611	CHL	CHA-C1A-C2A	-3.33	125.50	133.31
15	4	605	CLA	O2D-CGD-O1D	-3.32	117.38	123.85
15	A	1012	CLA	C3B-C4B-NB	-3.32	107.56	110.53
22	B	5002	DGD	O6D-C1D-O3G	-3.32	102.20	110.04
15	B	1239	CLA	O2D-CGD-O1D	-3.31	117.40	123.85
15	B	1204	CLA	O2D-CGD-O1D	-3.31	117.40	123.85
15	1	601	CLA	C3B-C4B-NB	-3.31	107.58	110.53
14	B	4002	BCR	C1-C6-C5	-3.31	118.11	122.64
18	4	801	LMG	O6-C1-O1	-3.29	102.28	110.04
16	3	604	CHL	CHA-C1A-C2A	-3.28	125.60	133.31
14	A	4007	BCR	C24-C23-C22	-3.28	121.38	126.23
15	1	613	CLA	O2D-CGD-O1D	-3.28	117.47	123.85
15	B	1226	CLA	CAA-C2A-C3A	-3.28	104.15	113.00
12	4	501	LUT	C32-C33-C34	3.27	124.16	119.01
12	4	501	LUT	C40-C33-C32	3.27	123.08	118.09
15	A	1101	CLA	O2D-CGD-O1D	-3.27	117.49	123.85
13	2	502	XAT	C10-C11-C12	3.26	132.64	123.20
14	F	4002	BCR	C28-C27-C26	-3.25	108.25	114.06
15	A	1123	CLA	O2D-CGD-O1D	-3.25	117.52	123.85
15	B	1220	CLA	C3B-C4B-NB	-3.24	107.63	110.53
19	A	1011	CL0	CGD-CBD-CAD	3.24	121.33	110.85
15	B	1216	CLA	C3B-C4B-NB	-3.23	107.64	110.53
15	4	608	CLA	CAC-C3C-C2C	-3.22	121.64	127.56
19	A	1011	CL0	C1-C2-C3	-3.22	120.92	126.20
15	B	1232	CLA	C3B-C4B-NB	-3.22	107.66	110.53
15	A	1122	CLA	C5-C3-C2	3.22	128.39	121.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	1	503	BCR	C15-C14-C13	-3.22	122.77	127.28
14	4	503	BCR	C27-C26-C25	3.22	127.05	122.70
22	B	5002	DGD	O3G-C3G-C2G	-3.21	103.01	110.82
15	A	1132	CLA	O2D-CGD-O1D	-3.21	117.61	123.85
15	A	1116	CLA	C3B-C4B-NB	-3.20	107.67	110.53
15	A	1132	CLA	CHB-C4A-NA	3.20	129.02	124.40
12	4	501	LUT	C39-C29-C30	-3.20	117.63	122.82
12	3	501	LUT	C11-C10-C9	3.20	131.77	127.28
13	1	502	XAT	C6-C7-C8	-3.20	119.23	125.99
15	A	1013	CLA	C3B-C4B-NB	-3.19	107.68	110.53
16	4	610	CHL	C3C-C4C-NC	-3.18	106.87	114.65
15	A	1013	CLA	C6-C5-C3	3.18	121.22	113.47
14	A	4003	BCR	C2-C1-C6	3.18	115.06	110.44
15	B	1238	CLA	CAC-C3C-C2C	-3.17	121.73	127.56
14	J	4001	BCR	C3-C4-C5	-3.17	108.41	114.06
16	3	604	CHL	C1-C2-C3	-3.16	121.02	126.20
14	J	4002	BCR	C15-C16-C17	-3.16	117.06	123.52
12	3	501	LUT	C4-C5-C6	-3.16	114.27	120.76
15	A	1106	CLA	O2D-CGD-O1D	-3.15	117.72	123.85
15	B	1214	CLA	O2D-CGD-O1D	-3.15	117.73	123.85
15	1	612	CLA	C3A-C2A-C1A	-3.14	103.08	106.30
19	A	1011	CL0	C3C-C4C-NC	3.14	122.33	114.65
15	B	1203	CLA	CHB-C4A-NA	3.14	128.93	124.40
15	A	1138	CLA	O2D-CGD-O1D	-3.14	117.74	123.85
15	B	1215	CLA	O2D-CGD-O1D	-3.14	117.74	123.85
15	A	1124	CLA	CHB-C4A-NA	3.14	128.93	124.40
16	2	610	CHL	C3C-C4C-NC	-3.14	106.98	114.65
14	B	4002	BCR	C3-C4-C5	-3.13	108.47	114.06
15	B	1223	CLA	C3B-C4B-NB	-3.13	107.74	110.53
13	4	502	XAT	C35-C34-C33	3.13	131.67	127.28
14	B	4003	BCR	C15-C14-C13	-3.12	122.90	127.28
16	2	609	CHL	CHA-C1A-C2A	-3.12	125.98	133.31
15	4	606	CLA	C3B-C4B-NB	-3.12	107.74	110.53
15	B	1240	CLA	C3B-C4B-NB	-3.12	107.75	110.53
15	B	1218	CLA	O2D-CGD-O1D	-3.12	117.78	123.85
15	1	602	CLA	C3B-C4B-NB	-3.12	107.75	110.53
16	2	613	CHL	C1A-CHA-C4D	3.11	124.17	118.98
15	1	603	CLA	O2D-CGD-O1D	-3.11	117.80	123.85
15	1	606	CLA	O2D-CGD-O1D	-3.10	117.81	123.85
14	A	4004	BCR	C27-C26-C25	3.10	126.89	122.70
15	B	1202	CLA	C3B-C4B-NB	-3.10	107.77	110.53
16	2	613	CHL	C3C-C4C-NC	-3.10	107.08	114.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	A	1102	CLA	O2D-CGD-O1D	-3.10	117.82	123.85
15	A	1110	CLA	O2D-CGD-O1D	-3.09	117.84	123.85
16	1	610	CHL	C3C-C4C-NC	-3.09	107.11	114.65
15	1	612	CLA	C3B-C4B-NB	-3.08	107.78	110.53
14	A	4008	BCR	C2-C1-C6	3.08	114.92	110.44
16	4	611	CHL	C3C-C4C-NC	-3.08	107.12	114.65
15	A	1137	CLA	CAA-CBA-CGA	-3.08	104.47	113.21
14	F	4001	BCR	C8-C7-C6	-3.08	118.78	127.00
12	3	501	LUT	C21-C26-C27	-3.07	109.29	112.83
15	2	608	CLA	O2D-CGD-O1D	-3.07	117.87	123.85
15	A	1103	CLA	O2D-CGD-O1D	-3.07	117.87	123.85
15	3	607	CLA	O2D-CGD-O1D	-3.07	117.88	123.85
16	3	604	CHL	C3C-C4C-NC	-3.06	107.16	114.65
15	2	616	CLA	O2A-CGA-O1A	-3.06	115.97	123.63
14	4	503	BCR	C15-C16-C17	-3.06	117.25	123.52
15	4	609	CLA	O2D-CGD-O1D	-3.06	117.89	123.85
15	2	607	CLA	C3B-C4B-NB	-3.06	107.80	110.53
13	2	502	XAT	C20-C13-C12	-3.05	113.42	118.09
16	2	611	CHL	C3C-C4C-NC	-3.05	107.20	114.65
22	B	5002	DGD	C1E-O6E-C5E	3.05	119.67	113.72
15	B	1206	CLA	CHB-C4A-NA	3.05	128.80	124.40
15	B	1205	CLA	O2D-CGD-O1D	-3.04	117.93	123.85
15	B	1023	CLA	C3B-C4B-NB	-3.04	107.82	110.53
15	2	602	CLA	O2D-CGD-O1D	-3.04	117.93	123.85
15	4	604	CLA	CHB-C4A-NA	3.04	128.78	124.40
14	J	4001	BCR	C2-C1-C6	3.03	114.85	110.44
15	A	1141	CLA	O2D-CGD-O1D	-3.03	117.95	123.85
13	1	502	XAT	C27-C28-C29	-3.03	120.83	125.53
16	2	610	CHL	CHA-C1A-C2A	-3.03	126.20	133.31
15	A	1136	CLA	O2D-CGD-O1D	-3.02	117.96	123.85
15	B	1206	CLA	O2D-CGD-O1D	-3.02	117.96	123.85
14	3	504	BCR	C27-C26-C25	3.02	126.79	122.70
15	1	615	CLA	O2D-CGD-O1D	-3.02	117.97	123.85
14	B	4006	BCR	C15-C14-C13	-3.02	123.04	127.28
15	B	1210	CLA	C3B-C4B-NB	-3.02	107.83	110.53
14	A	4007	BCR	C15-C14-C13	-3.02	123.05	127.28
16	4	613	CHL	CHA-C1A-C2A	-3.02	126.22	133.31
15	4	604	CLA	O2D-CGD-O1D	-3.02	117.98	123.85
15	B	1221	CLA	O2D-CGD-O1D	-3.01	117.98	123.85
14	A	4003	BCR	C27-C26-C25	3.01	126.78	122.70
15	2	612	CLA	O2D-CGD-O1D	-3.01	117.99	123.85
15	A	1121	CLA	O2D-CGD-O1D	-3.01	117.99	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	B	1214	CLA	CHB-C4A-NA	3.01	128.74	124.40
17	A	5002	LHG	O8-C23-C24	3.01	121.00	111.83
12	3	501	LUT	C40-C33-C34	-3.01	117.95	122.82
16	1	609	CHL	C3C-C4C-NC	-3.00	107.31	114.65
15	A	1117	CLA	C3B-C4B-NB	-3.00	107.85	110.53
14	J	4001	BCR	C15-C16-C17	-3.00	117.37	123.52
15	B	1239	CLA	CHB-C4A-NA	3.00	128.73	124.40
13	2	502	XAT	C26-C27-C28	-3.00	119.65	125.99
15	B	1207	CLA	O2D-CGD-O1D	-3.00	118.01	123.85
15	B	1236	CLA	C3B-C4B-NB	-3.00	107.86	110.53
15	A	1119	CLA	C3B-C4B-NB	-2.99	107.86	110.53
14	3	506	BCR	C1-C6-C5	-2.99	118.55	122.64
15	A	1111	CLA	O2D-CGD-O1D	-2.99	118.03	123.85
15	B	1234	CLA	O2D-CGD-O1D	-2.99	118.03	123.85
15	B	1209	CLA	O2D-CGD-O1D	-2.99	118.03	123.85
15	A	1106	CLA	CHB-C4A-NA	2.99	128.72	124.40
15	2	607	CLA	O2D-CGD-O1D	-2.99	118.03	123.85
15	1	611	CLA	C3B-C4B-NB	-2.99	107.86	110.53
15	A	1102	CLA	CAA-C2A-C1A	-2.99	102.19	111.97
15	4	602	CLA	O2D-CGD-O1D	-2.98	118.04	123.85
14	B	4005	BCR	C15-C14-C13	-2.98	123.10	127.28
15	1	604	CLA	C3B-C4B-NB	-2.98	107.87	110.53
15	4	603	CLA	O2D-CGD-CBD	2.98	116.43	111.23
15	3	601	CLA	C3B-C4B-NB	-2.98	107.87	110.53
15	A	1107	CLA	O2D-CGD-O1D	-2.98	118.06	123.85
16	2	609	CHL	C3C-C4C-NC	-2.97	107.38	114.65
15	A	1133	CLA	O2D-CGD-O1D	-2.97	118.07	123.85
16	2	609	CHL	C1-O2A-CGA	2.97	123.84	116.65
15	J	1302	CLA	O2D-CGD-O1D	-2.97	118.07	123.85
15	A	1118	CLA	O2D-CGD-O1D	-2.97	118.07	123.85
13	4	502	XAT	C31-C32-C33	-2.97	118.23	126.36
15	B	1210	CLA	O2D-CGD-O1D	-2.97	118.07	123.85
15	3	603	CLA	O2D-CGD-O1D	-2.97	118.08	123.85
15	A	1109	CLA	O2D-CGD-O1D	-2.97	118.08	123.85
15	A	1013	CLA	O2D-CGD-O1D	-2.96	118.08	123.85
13	2	502	XAT	C31-C32-C33	-2.96	118.24	126.36
12	2	501	LUT	C26-C27-C28	2.96	129.18	124.58
15	A	1105	CLA	O2D-CGD-O1D	-2.96	118.09	123.85
14	B	4001	BCR	C15-C14-C13	-2.96	123.13	127.28
15	A	1116	CLA	O2D-CGD-O1D	-2.95	118.10	123.85
14	F	4001	BCR	C33-C5-C6	-2.95	121.26	124.48
15	4	603	CLA	C3B-C4B-NB	-2.95	107.89	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	3	614	CLA	CHB-C4A-NA	2.95	128.65	124.40
15	3	611	CLA	O2D-CGD-O1D	-2.95	118.11	123.85
15	B	1223	CLA	O2D-CGD-CBD	2.95	116.38	111.23
15	B	1216	CLA	O2D-CGD-O1D	-2.94	118.12	123.85
15	A	1115	CLA	O2D-CGD-O1D	-2.94	118.12	123.85
15	B	1221	CLA	C3B-C4B-NB	-2.94	107.90	110.53
15	4	612	CLA	C3B-C4B-NB	-2.93	107.91	110.53
16	1	609	CHL	CHA-C1A-C2A	-2.93	126.42	133.31
15	A	1130	CLA	CHB-C4A-NA	2.93	128.63	124.40
15	1	608	CLA	O2D-CGD-O1D	-2.93	118.14	123.85
15	4	603	CLA	CHB-C4A-NA	2.93	128.63	124.40
14	A	4007	BCR	C15-C16-C17	-2.93	117.52	123.52
15	A	1135	CLA	CHB-C4A-NA	2.93	128.62	124.40
15	A	1113	CLA	O2D-CGD-O1D	-2.92	118.16	123.85
18	2	803	LMG	O6-C1-O1	-2.92	103.13	110.04
15	B	1218	CLA	CHB-C4A-NA	2.92	128.62	124.40
15	A	1103	CLA	CHB-C4A-NA	2.92	128.61	124.40
15	B	1226	CLA	CHB-C4A-NA	2.92	128.61	124.40
15	2	605	CLA	O2D-CGD-O1D	-2.92	118.17	123.85
15	3	605	CLA	O2D-CGD-O1D	-2.92	118.17	123.85
15	1	604	CLA	O2D-CGD-O1D	-2.92	118.17	123.85
15	A	1126	CLA	O2D-CGD-O1D	-2.92	118.17	123.85
15	B	1222	CLA	O2A-CGA-O1A	-2.92	116.33	123.63
15	A	1110	CLA	C3B-C4B-NB	-2.92	107.93	110.53
14	J	4002	BCR	C35-C13-C14	-2.92	118.09	122.82
15	B	1236	CLA	O2D-CGD-O1D	-2.91	118.17	123.85
15	4	616	CLA	O2D-CGD-O1D	-2.91	118.18	123.85
14	1	503	BCR	C24-C23-C22	-2.91	121.92	126.23
15	A	1130	CLA	O2D-CGD-O1D	-2.91	118.18	123.85
15	A	1107	CLA	C3B-C4B-NB	-2.91	107.93	110.53
15	A	1127	CLA	C3B-C4B-NB	-2.91	107.93	110.53
15	1	605	CLA	CHB-C4A-NA	2.91	128.60	124.40
15	2	606	CLA	O2D-CGD-O1D	-2.91	118.18	123.85
15	A	1117	CLA	CHB-C4A-NA	2.91	128.60	124.40
15	4	608	CLA	O2D-CGD-O1D	-2.91	118.19	123.85
15	A	1129	CLA	O2D-CGD-O1D	-2.91	118.19	123.85
15	1	615	CLA	C4-C3-C2	-2.90	110.13	125.12
12	2	501	LUT	C40-C33-C32	2.90	122.52	118.09
15	2	604	CLA	CHB-C4A-NA	2.90	128.59	124.40
16	4	613	CHL	C3C-C4C-NC	-2.90	107.56	114.65
15	1	603	CLA	CHB-C4A-NA	2.90	128.58	124.40
13	4	502	XAT	C10-C11-C12	2.90	131.59	123.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	B	1226	CLA	O2D-CGD-O1D	-2.89	118.21	123.85
12	3	501	LUT	C26-C27-C28	2.89	129.08	124.58
15	A	1125	CLA	O2D-CGD-O1D	-2.89	118.22	123.85
15	B	1211	CLA	CHB-C4A-NA	2.89	128.58	124.40
15	2	616	CLA	C3B-C4B-NB	-2.89	107.95	110.53
15	3	610	CLA	C3B-C4B-NB	-2.89	107.95	110.53
12	4	501	LUT	C21-C26-C27	2.89	116.15	112.83
15	A	1133	CLA	C3B-C4B-NB	-2.89	107.95	110.53
15	B	1201	CLA	O2D-CGD-O1D	-2.89	118.22	123.85
12	1	501	LUT	C32-C33-C34	2.89	123.55	119.01
15	B	1207	CLA	C3B-C4B-NB	-2.89	107.95	110.53
15	F	1301	CLA	O2D-CGD-O1D	-2.89	118.23	123.85
14	A	4008	BCR	C15-C16-C17	-2.88	117.62	123.52
15	A	1112	CLA	C3B-C4B-NB	-2.88	107.96	110.53
15	A	1134	CLA	CHB-C4A-NA	2.88	128.55	124.40
15	3	615	CLA	CHB-C4A-NA	2.88	128.55	124.40
15	B	1211	CLA	C3B-C4B-NB	-2.88	107.96	110.53
15	1	607	CLA	C3B-C4B-NB	-2.87	107.96	110.53
15	B	1218	CLA	C3B-C4B-NB	-2.87	107.96	110.53
15	2	603	CLA	O2D-CGD-O1D	-2.87	118.26	123.85
15	A	1013	CLA	CHB-C4A-NA	2.87	128.54	124.40
13	3	502	XAT	C36-C21-C26	2.87	117.80	110.05
15	B	1224	CLA	O2D-CGD-O1D	-2.87	118.26	123.85
14	F	4002	BCR	C15-C16-C17	-2.87	117.65	123.52
15	A	1119	CLA	O2D-CGD-O1D	-2.87	118.27	123.85
15	A	1120	CLA	O2D-CGD-O1D	-2.87	118.27	123.85
15	B	1237	CLA	O2D-CGD-O1D	-2.86	118.28	123.85
15	1	607	CLA	O2D-CGD-O1D	-2.86	118.28	123.85
16	1	610	CHL	C1A-CHA-C4D	2.86	123.76	118.98
15	2	602	CLA	CHB-C4A-NA	2.86	128.53	124.40
15	B	1225	CLA	C3B-C4B-NB	-2.86	107.98	110.53
15	4	602	CLA	CHB-C4A-NA	2.85	128.52	124.40
15	A	1101	CLA	C3B-C4B-NB	-2.85	107.98	110.53
14	B	4001	BCR	C33-C5-C6	-2.85	121.37	124.48
15	3	613	CLA	O2D-CGD-O1D	-2.85	118.30	123.85
15	2	616	CLA	C1-C2-C3	-2.85	121.53	126.20
15	B	1235	CLA	O2D-CGD-O1D	-2.85	118.30	123.85
15	B	1203	CLA	O2D-CGD-O1D	-2.85	118.31	123.85
15	A	1111	CLA	CHB-C4A-NA	2.85	128.51	124.40
15	4	609	CLA	CHB-C4A-NA	2.84	128.50	124.40
15	A	1110	CLA	CHB-C4A-NA	2.84	128.50	124.40
12	3	501	LUT	C27-C28-C29	-2.84	120.22	126.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	A	1140	CLA	C3B-C4B-NB	-2.84	108.00	110.53
15	A	1114	CLA	O2D-CGD-O1D	-2.84	118.32	123.85
18	2	802	LMG	O6-C1-O1	-2.84	103.34	110.04
15	4	606	CLA	C1-C2-C3	-2.84	122.17	126.76
15	3	613	CLA	CHB-C4A-NA	2.84	128.49	124.40
12	2	501	LUT	C32-C33-C34	2.83	123.46	119.01
15	A	1141	CLA	C3B-C4B-NB	-2.83	108.01	110.53
15	B	1227	CLA	O2D-CGD-O1D	-2.82	118.35	123.85
16	3	604	CHL	C4D-CHA-CBD	-2.82	106.12	108.97
16	2	611	CHL	C1A-CHA-C4D	2.82	123.69	118.98
19	A	1011	CL0	CMA-C3A-C2A	-2.82	103.23	114.13
15	B	1208	CLA	O2D-CGD-O1D	-2.82	118.36	123.85
15	1	603	CLA	CMB-C2B-C1B	-2.82	121.12	125.42
15	3	601	CLA	O2D-CGD-O1D	-2.82	118.36	123.85
15	A	1137	CLA	C6-C5-C3	2.82	120.34	113.47
15	2	616	CLA	O2D-CGD-O1D	-2.82	118.36	123.85
15	3	610	CLA	O2D-CGD-O1D	-2.82	118.36	123.85
15	B	1219	CLA	O2D-CGD-O1D	-2.82	118.36	123.85
15	A	1128	CLA	O2D-CGD-O1D	-2.82	118.37	123.85
15	A	1104	CLA	C3B-C4B-NB	-2.81	108.02	110.53
14	A	4004	BCR	C30-C25-C26	-2.81	118.79	122.64
15	B	1211	CLA	O2D-CGD-O1D	-2.81	118.37	123.85
15	3	611	CLA	C3B-C4B-NB	-2.81	108.02	110.53
15	B	1238	CLA	C3B-C4B-NB	-2.81	108.02	110.53
15	B	1022	CLA	O2D-CGD-O1D	-2.81	118.38	123.85
15	A	1121	CLA	C3B-C4B-NB	-2.81	108.02	110.53
15	B	1023	CLA	O2D-CGD-O1D	-2.81	118.39	123.85
13	1	502	XAT	C37-C21-C36	-2.80	103.30	107.37
15	B	1231	CLA	C3B-C4B-NB	-2.80	108.03	110.53
13	1	502	XAT	C11-C12-C13	-2.80	118.69	126.36
14	A	4004	BCR	C2-C1-C6	2.80	114.50	110.44
14	B	4002	BCR	C2-C1-C6	2.80	114.50	110.44
15	2	612	CLA	CHB-C4A-NA	2.80	128.44	124.40
15	B	1201	CLA	CHB-C4A-NA	2.80	128.44	124.40
15	A	1133	CLA	CHB-C4A-NA	2.80	128.44	124.40
15	B	1231	CLA	CHB-C4A-NA	2.80	128.44	124.40
15	B	1230	CLA	O2D-CGD-O1D	-2.80	118.41	123.85
15	A	1101	CLA	CHB-C4A-NA	2.79	128.43	124.40
15	B	1212	CLA	CHB-C4A-NA	2.79	128.43	124.40
15	A	1129	CLA	C3B-C4B-NB	-2.79	108.04	110.53
15	4	612	CLA	O2D-CGD-O1D	-2.79	118.42	123.85
15	B	1230	CLA	CAA-C2A-C1A	-2.79	102.83	111.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	2	610	CHL	C1A-CHA-C4D	2.79	123.64	118.98
17	3	801	LHG	O8-C23-C24	2.79	120.34	111.83
18	2	804	LMG	O6-C1-O1	-2.79	103.45	110.04
15	B	1238	CLA	CBC-CAC-C3C	2.78	119.96	112.42
15	B	1228	CLA	O2D-CGD-O1D	-2.78	118.43	123.85
15	B	1238	CLA	O2D-CGD-O1D	-2.78	118.43	123.85
15	1	615	CLA	C3B-C4B-NB	-2.78	108.05	110.53
14	F	4001	BCR	C15-C16-C17	-2.78	117.83	123.52
15	1	606	CLA	C3B-C4B-NB	-2.78	108.05	110.53
15	3	609	CLA	O2D-CGD-CBD	2.78	116.09	111.23
15	A	1110	CLA	O2A-CGA-O1A	-2.78	116.68	123.63
15	B	1215	CLA	CHB-C4A-NA	2.78	128.41	124.40
15	1	605	CLA	O2D-CGD-O1D	-2.78	118.44	123.85
15	4	606	CLA	CHB-C4A-NA	2.78	128.41	124.40
14	F	4002	BCR	C30-C25-C26	-2.78	118.84	122.64
16	2	610	CHL	C4D-CHA-CBD	-2.77	106.17	108.97
19	A	1011	CL0	O2A-CGA-CBA	2.77	120.29	111.83
15	A	1107	CLA	CHB-C4A-NA	2.77	128.40	124.40
15	B	1217	CLA	C3B-C4B-NB	-2.77	108.06	110.53
17	B	5001	LHG	O8-C23-C24	2.77	120.28	111.83
15	3	608	CLA	O2D-CGD-O1D	-2.77	118.46	123.85
15	F	1302	CLA	CHB-C4A-NA	2.77	128.40	124.40
15	2	603	CLA	C3B-C4B-NB	-2.77	108.06	110.53
15	B	1226	CLA	C3B-C4B-NB	-2.77	108.06	110.53
14	B	4005	BCR	C33-C5-C6	-2.77	121.47	124.48
15	A	1132	CLA	CAC-C3C-C2C	2.77	132.64	127.56
15	A	1102	CLA	C3B-C4B-NB	-2.76	108.06	110.53
15	A	1117	CLA	O2D-CGD-CBD	2.76	116.06	111.23
15	4	607	CLA	C3B-C4B-NB	-2.76	108.06	110.53
15	B	1234	CLA	CAC-C3C-C4C	2.76	128.38	124.79
15	2	605	CLA	CHB-C4A-NA	2.76	128.38	124.40
15	A	1106	CLA	C3B-C4B-NB	-2.76	108.07	110.53
15	A	1114	CLA	CHB-C4A-NA	2.76	128.38	124.40
15	3	606	CLA	C3B-C4B-NB	-2.76	108.07	110.53
15	A	1130	CLA	C3B-C4B-NB	-2.76	108.07	110.53
15	A	1104	CLA	CHB-C4A-NA	2.76	128.38	124.40
15	2	612	CLA	C3B-C4B-NB	-2.76	108.07	110.53
14	A	4007	BCR	C33-C5-C6	-2.75	121.48	124.48
15	A	1132	CLA	CAC-C3C-C4C	-2.75	121.20	124.79
16	4	611	CHL	C1A-CHA-C4D	2.75	123.58	118.98
15	A	1122	CLA	CHB-C4A-NA	2.75	128.38	124.40
16	2	611	CHL	C1-O2A-CGA	2.75	124.49	116.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	A	1138	CLA	CHB-C4A-NA	2.75	128.37	124.40
15	B	1229	CLA	CHB-C4A-NA	2.75	128.37	124.40
15	B	1223	CLA	CHB-C4A-NA	2.75	128.37	124.40
15	B	1237	CLA	CHB-C4A-NA	2.75	128.36	124.40
12	1	501	LUT	C35-C34-C33	-2.74	123.44	127.28
15	2	616	CLA	CHB-C4A-NA	2.74	128.35	124.40
14	B	4006	BCR	C2-C1-C6	2.74	114.42	110.44
13	2	502	XAT	C36-C21-C22	-2.74	104.16	108.97
16	4	610	CHL	C1A-CHA-C4D	2.74	123.55	118.98
14	F	4001	BCR	C11-C10-C9	-2.73	123.44	127.28
15	A	1118	CLA	CHB-C4A-NA	2.73	128.34	124.40
15	1	601	CLA	O2D-CGD-O1D	-2.73	118.53	123.85
15	A	1105	CLA	C3B-C4B-NB	-2.73	108.09	110.53
15	A	1114	CLA	C3B-C4B-NB	-2.73	108.09	110.53
15	B	1217	CLA	O2D-CGD-O1D	-2.72	118.55	123.85
15	A	1111	CLA	C3B-C4B-NB	-2.72	108.10	110.53
15	1	602	CLA	O2D-CGD-O1D	-2.72	118.55	123.85
15	B	1237	CLA	C3B-C4B-NB	-2.72	108.10	110.53
15	A	1108	CLA	O2D-CGD-O1D	-2.72	118.56	123.85
15	4	612	CLA	CHB-C4A-NA	2.72	128.32	124.40
14	A	4008	BCR	C15-C14-C13	-2.72	123.47	127.28
19	A	1011	CL0	C4-C3-C5	2.71	119.94	115.23
14	3	506	BCR	C15-C16-C17	-2.71	117.97	123.52
16	2	611	CHL	C4D-CHA-CBD	-2.71	106.23	108.97
16	4	611	CHL	C4D-CHA-CBD	-2.71	106.23	108.97
14	B	4001	BCR	C30-C25-C26	-2.71	118.93	122.64
15	A	1138	CLA	C1-C2-C3	-2.71	121.76	126.20
15	3	601	CLA	CHB-C4A-NA	2.71	128.31	124.40
15	B	1238	CLA	C4-C3-C5	-2.71	110.53	115.23
15	B	1240	CLA	O2D-CGD-O1D	-2.70	118.58	123.85
15	4	604	CLA	C3B-C4B-NB	-2.70	108.12	110.53
15	A	1118	CLA	C3B-C4B-NB	-2.70	108.12	110.53
15	B	1214	CLA	C3B-C4B-NB	-2.70	108.12	110.53
14	B	4006	BCR	C33-C5-C6	-2.70	121.54	124.48
15	4	601	CLA	O2D-CGD-O1D	-2.70	118.59	123.85
15	A	1139	CLA	O2D-CGD-O1D	-2.70	118.59	123.85
14	B	4003	BCR	C7-C8-C9	-2.70	122.24	126.23
14	B	4005	BCR	C27-C26-C25	2.70	126.35	122.70
15	1	608	CLA	C3B-C4B-NB	-2.70	108.12	110.53
15	2	606	CLA	C3B-C4B-NB	-2.69	108.12	110.53
15	A	1132	CLA	C3B-C4B-NB	-2.69	108.12	110.53
14	1	503	BCR	C33-C5-C6	-2.69	121.55	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	4	607	CLA	CHB-C4A-NA	2.69	128.28	124.40
16	4	610	CHL	C4C-CHD-C1D	2.69	125.69	116.07
15	2	604	CLA	C3B-C4B-NB	-2.69	108.13	110.53
15	3	615	CLA	C3B-C4B-NB	-2.69	108.13	110.53
14	B	4005	BCR	C8-C7-C6	-2.69	119.82	127.00
15	B	1215	CLA	C1-C2-C3	-2.69	121.80	126.20
12	2	501	LUT	C12-C13-C14	2.69	123.23	119.01
15	A	1135	CLA	O2D-CGD-O1D	-2.69	118.62	123.85
14	A	4008	BCR	C33-C5-C6	-2.68	121.56	124.48
15	3	607	CLA	C3B-C4B-NB	-2.68	108.14	110.53
14	3	504	BCR	C33-C5-C6	-2.68	121.56	124.48
14	F	4002	BCR	C33-C5-C6	-2.68	121.56	124.48
15	A	1136	CLA	C3B-C4B-NB	-2.68	108.14	110.53
14	A	4008	BCR	C27-C26-C25	2.67	126.32	122.70
15	3	615	CLA	O2D-CGD-CBD	2.67	115.90	111.23
15	A	1102	CLA	CHB-C4A-NA	2.67	128.26	124.40
15	A	1137	CLA	O2D-CGD-CBD	2.67	115.90	111.23
15	A	1140	CLA	O2D-CGD-O1D	-2.67	118.66	123.85
15	B	1227	CLA	CHB-C4A-NA	2.67	128.25	124.40
15	B	1205	CLA	O2A-CGA-O1A	-2.66	116.97	123.63
15	A	1139	CLA	CAA-CBA-CGA	-2.66	105.65	113.21
15	A	1115	CLA	CAC-C3C-C4C	2.66	128.25	124.79
15	A	1116	CLA	CHB-C4A-NA	2.66	128.24	124.40
15	3	606	CLA	CHB-C4A-NA	2.66	128.24	124.40
15	3	606	CLA	O2D-CGD-O1D	-2.66	118.68	123.85
14	3	504	BCR	C11-C10-C9	-2.66	123.55	127.28
15	1	601	CLA	CHB-C4A-NA	2.66	128.23	124.40
15	3	611	CLA	CHB-C4A-NA	2.65	128.23	124.40
15	J	1302	CLA	CHB-C4A-NA	2.65	128.23	124.40
14	F	4001	BCR	C15-C14-C13	-2.65	123.56	127.28
14	A	4005	BCR	C15-C16-C17	-2.65	118.09	123.52
15	4	606	CLA	O2D-CGD-O1D	-2.65	118.69	123.85
13	4	502	XAT	C36-C21-C22	-2.65	104.31	108.97
15	B	1209	CLA	C3B-C4B-NB	-2.65	108.17	110.53
16	4	613	CHL	C4D-CHA-CBD	-2.65	106.30	108.97
12	1	501	LUT	C40-C33-C34	-2.65	118.53	122.82
15	A	1132	CLA	O2D-CGD-CBD	2.65	115.86	111.23
17	2	801	LHG	O8-C23-C24	2.65	119.91	111.83
15	2	608	CLA	C3B-C4B-NB	-2.65	108.17	110.53
15	B	1222	CLA	CHB-C4A-NA	2.65	128.22	124.40
15	A	1012	CLA	O2A-CGA-O1A	-2.65	117.01	123.63
15	2	607	CLA	CHB-C4A-NA	2.65	128.22	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	B	1206	CLA	C3B-C4B-NB	-2.64	108.17	110.53
15	B	1223	CLA	C1-C2-C3	-2.64	121.87	126.20
15	A	1137	CLA	C3B-C4B-NB	-2.64	108.17	110.53
15	B	1209	CLA	CHB-C4A-NA	2.64	128.21	124.40
14	3	506	BCR	C27-C26-C25	2.64	126.27	122.70
15	4	608	CLA	C3B-C4B-NB	-2.64	108.17	110.53
15	F	1301	CLA	C3B-C4B-NB	-2.64	108.18	110.53
15	1	602	CLA	CHB-C4A-NA	2.63	128.20	124.40
13	3	502	XAT	C39-C29-C30	-2.63	118.55	122.82
14	B	4006	BCR	C15-C16-C17	-2.63	118.13	123.52
15	B	1236	CLA	CHB-C4A-NA	2.63	128.20	124.40
14	2	503	BCR	C33-C5-C6	-2.63	121.61	124.48
15	A	1122	CLA	O2D-CGD-O1D	-2.63	118.73	123.85
15	3	612	CLA	O2D-CGD-O1D	-2.63	118.73	123.85
15	4	608	CLA	CBC-CAC-C3C	2.63	119.54	112.42
14	A	4005	BCR	C33-C5-C6	-2.62	121.62	124.48
15	B	1213	CLA	C3B-C4B-NB	-2.62	108.19	110.53
14	B	4004	BCR	C15-C16-C17	-2.62	118.15	123.52
15	A	1115	CLA	C3B-C4B-NB	-2.62	108.19	110.53
12	4	501	LUT	C7-C6-C5	-2.62	115.53	121.56
13	4	502	XAT	C36-C21-C26	2.61	117.10	110.05
15	A	1123	CLA	CHB-C4A-NA	2.61	128.17	124.40
15	3	614	CLA	O2D-CGD-O1D	-2.61	118.76	123.85
14	A	4003	BCR	C38-C26-C27	-2.61	108.03	113.60
22	B	5002	DGD	C6D-O5D-C1E	2.61	119.39	113.80
15	A	1116	CLA	C5-C3-C2	2.61	127.02	121.17
15	A	1109	CLA	CHB-C4A-NA	2.61	128.16	124.40
15	A	1137	CLA	CHB-C4A-NA	2.61	128.16	124.40
15	1	604	CLA	CHB-C4A-NA	2.61	128.16	124.40
15	1	611	CLA	O2D-CGD-O1D	-2.61	118.78	123.85
15	B	1225	CLA	CHB-C4A-NA	2.60	128.16	124.40
19	A	1011	CL0	C4C-C3C-C2C	-2.60	103.09	113.37
15	4	605	CLA	CHB-C4A-NA	2.60	128.16	124.40
14	4	503	BCR	C8-C7-C6	-2.60	120.05	127.00
15	B	1205	CLA	C3B-C4B-NB	-2.60	108.21	110.53
15	B	1202	CLA	CHB-C4A-NA	2.60	128.15	124.40
15	A	1139	CLA	C3B-C4B-NB	-2.60	108.21	110.53
15	B	1240	CLA	O2A-CGA-O1A	-2.59	117.14	123.63
15	B	1213	CLA	CHB-C4A-NA	2.59	128.14	124.40
15	F	1302	CLA	O2D-CGD-O1D	-2.59	118.80	123.85
15	J	1302	CLA	C3B-C4B-NB	-2.59	108.22	110.53
15	4	609	CLA	C3B-C4B-NB	-2.59	108.22	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	B	1235	CLA	CHB-C4A-NA	2.59	128.14	124.40
13	1	502	XAT	C39-C29-C28	2.59	122.04	118.09
15	2	606	CLA	CHB-C4A-NA	2.59	128.13	124.40
15	B	1227	CLA	C3B-C4B-NB	-2.59	108.22	110.53
15	4	616	CLA	C3B-C4B-NB	-2.59	108.22	110.53
15	4	605	CLA	C5-C3-C2	2.58	126.97	121.17
16	4	613	CHL	C4C-CHD-C1D	2.58	125.32	116.07
15	B	1219	CLA	C3B-C4B-NB	-2.58	108.22	110.53
15	2	603	CLA	CHB-C4A-NA	2.58	128.13	124.40
15	1	608	CLA	CHB-C4A-NA	2.58	128.12	124.40
15	B	1204	CLA	CHB-C4A-NA	2.58	128.12	124.40
15	B	1213	CLA	O2D-CGD-O1D	-2.58	118.83	123.85
15	F	1301	CLA	CHB-C4A-NA	2.58	128.12	124.40
15	B	1023	CLA	CHB-C4A-NA	2.57	128.12	124.40
15	B	1240	CLA	C4-C3-C2	-2.57	117.01	123.63
15	1	612	CLA	O2D-CGD-O1D	-2.57	118.84	123.85
15	A	1119	CLA	CHB-C4A-NA	2.57	128.11	124.40
15	2	604	CLA	O2D-CGD-O1D	-2.57	118.84	123.85
15	A	1134	CLA	O2D-CGD-CBD	2.57	115.72	111.23
15	A	1122	CLA	C4-C3-C2	-2.57	117.03	123.63
15	3	609	CLA	CHB-C4A-NA	2.57	128.11	124.40
15	B	1212	CLA	O2D-CGD-O1D	-2.57	118.85	123.85
14	B	4006	BCR	C27-C26-C25	2.57	126.17	122.70
13	1	502	XAT	C37-C21-C26	-2.57	103.11	110.05
15	B	1229	CLA	C3B-C4B-NB	-2.57	108.24	110.53
13	2	502	XAT	C35-C34-C33	2.57	130.88	127.28
15	B	1230	CLA	CHB-C4A-NA	2.57	128.10	124.40
16	2	609	CHL	C4C-CHD-C1D	2.56	125.24	116.07
15	3	610	CLA	CHB-C4A-NA	2.56	128.10	124.40
16	4	610	CHL	C4D-CHA-CBD	-2.56	106.38	108.97
15	B	1225	CLA	O2D-CGD-O1D	-2.56	118.87	123.85
15	A	1108	CLA	CHB-C4A-NA	2.56	128.09	124.40
15	2	602	CLA	C3B-C4B-NB	-2.56	108.25	110.53
15	B	1240	CLA	CHB-C4A-NA	2.55	128.08	124.40
16	4	613	CHL	C1A-CHA-C4D	2.55	123.24	118.98
14	A	4006	BCR	C15-C16-C17	-2.55	118.30	123.52
15	B	1214	CLA	CMB-C2B-C1B	-2.55	121.54	125.42
12	2	501	LUT	C37-C21-C26	-2.55	105.69	109.55
15	A	1105	CLA	CAC-C3C-C2C	2.55	132.24	127.56
14	3	506	BCR	C33-C5-C6	-2.55	121.71	124.48
15	B	1221	CLA	CHB-C4A-NA	2.55	128.07	124.40
15	B	1230	CLA	C1-C2-C3	-2.55	122.03	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	B	1021	CLA	O2D-CGD-O1D	-2.54	118.90	123.85
15	A	1137	CLA	CAA-C2A-C1A	-2.54	103.64	111.97
15	1	606	CLA	CHB-C4A-NA	2.54	128.07	124.40
15	B	1021	CLA	C3B-C4B-NB	-2.54	108.26	110.53
13	3	502	XAT	C37-C21-C36	-2.54	103.68	107.37
15	B	1022	CLA	CHB-C4A-NA	2.54	128.06	124.40
15	4	605	CLA	C3B-C4B-NB	-2.54	108.27	110.53
15	2	601	CLA	O2A-CGA-O1A	-2.54	117.28	123.63
13	2	502	XAT	C39-C29-C28	2.54	121.96	118.09
15	A	1103	CLA	C3B-C4B-NB	-2.53	108.27	110.53
12	3	501	LUT	C37-C21-C26	-2.53	105.71	109.55
14	4	503	BCR	C11-C10-C9	-2.53	123.73	127.28
15	A	1012	CLA	CHB-C4A-NA	2.53	128.05	124.40
15	B	1224	CLA	CHB-C4A-NA	2.53	128.05	124.40
15	A	1105	CLA	CHB-C4A-NA	2.53	128.04	124.40
15	2	607	CLA	C1-O2A-CGA	2.53	122.76	116.65
15	1	606	CLA	C1-C2-C3	-2.52	122.68	126.76
15	4	607	CLA	O2A-CGA-O1A	-2.52	117.31	123.63
18	2	803	LMG	O1-C7-C8	-2.52	104.68	110.82
14	B	4001	BCR	C8-C7-C6	-2.52	120.26	127.00
17	A	5001	LHG	O8-C23-C24	2.52	119.52	111.83
15	B	1217	CLA	CHB-C4A-NA	2.52	128.04	124.40
19	A	1011	CL0	C2C-C1C-NC	2.52	117.59	110.46
15	A	1116	CLA	C1-O2A-CGA	2.52	122.75	116.65
15	1	613	CLA	CHB-C4A-NA	2.52	128.04	124.40
15	A	1124	CLA	C3B-C4B-NB	-2.52	108.28	110.53
13	4	502	XAT	C19-C9-C10	-2.52	118.73	122.82
15	B	1235	CLA	C3B-C4B-NB	-2.52	108.28	110.53
17	A	5001	LHG	C11-C10-C9	-2.52	101.64	114.37
14	3	503	BCR	C33-C5-C6	-2.51	121.74	124.48
14	A	4006	BCR	C33-C5-C6	-2.51	121.74	124.48
15	2	601	CLA	CHB-C4A-NA	2.51	128.02	124.40
15	B	1215	CLA	C3B-C4B-NB	-2.51	108.29	110.53
15	B	1203	CLA	C3B-C4B-NB	-2.51	108.29	110.53
15	4	601	CLA	CHB-C4A-NA	2.51	128.02	124.40
14	A	4002	BCR	C2-C1-C6	2.51	114.08	110.44
15	B	1230	CLA	C3B-C4B-NB	-2.51	108.29	110.53
15	3	608	CLA	C3B-C4B-NB	-2.50	108.29	110.53
19	A	1011	CL0	C1A-NA-C4A	-2.50	95.31	107.39
15	B	1207	CLA	CHB-C4A-NA	2.50	128.01	124.40
15	3	607	CLA	CHB-C4A-NA	2.50	128.01	124.40
14	4	503	BCR	C2-C1-C6	2.50	114.07	110.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	B	1227	CLA	O2A-CGA-O1A	-2.50	117.38	123.63
14	F	4002	BCR	C29-C30-C25	2.50	114.06	110.44
15	B	1204	CLA	O2D-CGD-CBD	2.49	115.59	111.23
15	A	1112	CLA	CHB-C4A-NA	2.49	128.00	124.40
15	3	614	CLA	CMB-C2B-C1B	-2.49	121.62	125.42
15	3	612	CLA	CHB-C4A-NA	2.49	128.00	124.40
15	A	1105	CLA	CAC-C3C-C4C	-2.49	121.55	124.79
15	A	1134	CLA	C3B-C4B-NB	-2.49	108.31	110.53
14	A	4002	BCR	C34-C9-C8	-2.49	114.29	118.09
15	A	1129	CLA	CHB-C4A-NA	2.49	127.99	124.40
12	4	501	LUT	C18-C5-C4	2.49	118.99	114.42
14	B	4001	BCR	C15-C16-C17	-2.48	118.44	123.52
16	1	610	CHL	C4D-CHA-CBD	-2.48	106.47	108.97
14	B	4001	BCR	C35-C13-C14	-2.48	118.80	122.82
15	B	1238	CLA	CHB-C4A-NA	2.48	127.98	124.40
22	B	5002	DGD	O5D-C6D-C5D	-2.48	103.84	109.42
15	B	1234	CLA	CHB-C4A-NA	2.48	127.97	124.40
15	B	1204	CLA	C3B-C4B-NB	-2.47	108.32	110.53
14	1	503	BCR	C27-C26-C25	2.47	126.04	122.70
15	A	1012	CLA	O2D-CGD-CBD	2.47	115.55	111.23
15	4	612	CLA	O2A-CGA-O1A	-2.47	117.45	123.63
14	3	504	BCR	C2-C1-C6	2.47	114.02	110.44
16	1	609	CHL	C1A-CHA-C4D	2.47	123.10	118.98
14	B	4005	BCR	C2-C1-C6	2.47	114.02	110.44
15	2	601	CLA	O2D-CGD-O1D	-2.46	119.05	123.85
15	1	613	CLA	C3B-C4B-NB	-2.46	108.33	110.53
18	2	802	LMG	O1-C7-C8	-2.46	104.84	110.82
17	1	801	LHG	O8-C23-C24	2.46	119.33	111.83
15	A	1110	CLA	C2A-C1A-CHA	2.46	128.13	123.87
15	A	1131	CLA	O2D-CGD-O1D	-2.46	119.07	123.85
15	B	1208	CLA	CHB-C4A-NA	2.45	127.94	124.40
14	3	503	BCR	C27-C26-C25	2.45	126.02	122.70
15	A	1139	CLA	CHB-C4A-NA	2.45	127.94	124.40
16	1	610	CHL	C4C-CHD-C1D	2.45	124.83	116.07
16	2	613	CHL	C4D-CHA-CBD	-2.45	106.50	108.97
13	1	502	XAT	C35-C34-C33	-2.45	123.84	127.28
15	A	1013	CLA	C4-C3-C5	2.45	119.48	115.23
14	4	503	BCR	C33-C5-C6	-2.45	121.81	124.48
13	3	502	XAT	C27-C28-C29	-2.45	121.74	125.53
15	B	1222	CLA	CAA-C2A-C1A	-2.44	103.97	111.97
15	A	1101	CLA	O2D-CGD-CBD	2.44	115.50	111.23
14	3	504	BCR	C24-C23-C22	-2.44	122.62	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	A	1112	CLA	O2D-CGD-O1D	-2.44	119.09	123.85
16	2	610	CHL	C4C-CHD-C1D	2.44	124.81	116.07
15	3	612	CLA	C3B-C4B-NB	-2.44	108.35	110.53
15	B	1208	CLA	O2A-CGA-O1A	-2.43	117.54	123.63
15	1	615	CLA	CHB-C4A-NA	2.43	127.91	124.40
13	4	502	XAT	C19-C9-C8	-2.43	114.37	118.09
15	B	1205	CLA	CHB-C4A-NA	2.43	127.91	124.40
15	A	1126	CLA	CAC-C3C-C4C	2.43	127.95	124.79
16	2	611	CHL	C4C-CHD-C1D	2.43	124.77	116.07
15	2	608	CLA	CHB-C4A-NA	2.43	127.91	124.40
15	A	1121	CLA	CHB-C4A-NA	2.43	127.91	124.40
12	2	501	LUT	C18-C5-C6	-2.43	121.83	124.48
15	A	1141	CLA	CHB-C4A-NA	2.42	127.90	124.40
16	4	611	CHL	C1-O2A-CGA	2.42	122.52	116.65
14	F	4001	BCR	C24-C23-C22	-2.42	122.65	126.23
15	A	1012	CLA	C6-C5-C3	2.42	119.37	113.47
15	A	1111	CLA	CAC-C3C-C4C	2.42	127.94	124.79
18	2	804	LMG	O1-C7-C8	-2.42	104.94	110.82
12	3	501	LUT	C7-C6-C5	-2.42	115.98	121.56
15	4	607	CLA	O2D-CGD-O1D	-2.42	119.14	123.85
15	3	608	CLA	O2A-CGA-O1A	-2.41	117.59	123.63
14	B	4003	BCR	C15-C16-C17	-2.41	118.58	123.52
15	B	1216	CLA	C1-C2-C3	-2.41	122.25	126.20
15	B	1232	CLA	CHB-C4A-NA	2.41	127.88	124.40
15	B	1210	CLA	C1-C2-C3	-2.41	122.25	126.20
15	B	1228	CLA	CHB-C4A-NA	2.41	127.88	124.40
15	A	1105	CLA	CMB-C2B-C1B	-2.41	121.75	125.42
16	1	609	CHL	C4D-CHA-CBD	-2.41	106.54	108.97
15	1	601	CLA	C1-C2-C3	-2.41	122.25	126.20
15	A	1106	CLA	CAA-C2A-C1A	-2.40	104.10	111.97
15	B	1239	CLA	C3B-C4B-NB	-2.40	108.39	110.53
14	F	4002	BCR	C8-C7-C6	-2.40	120.58	127.00
16	2	613	CHL	C4C-CHD-C1D	2.40	124.65	116.07
15	3	603	CLA	C4-C3-C5	2.40	119.39	115.23
19	A	1011	CL0	C6-C5-C3	-2.39	107.64	113.47
15	2	616	CLA	C4-C3-C5	2.39	119.38	115.23
15	B	1220	CLA	CHB-C4A-NA	2.39	127.85	124.40
15	A	1122	CLA	C3B-C4B-NB	-2.39	108.40	110.53
15	A	1127	CLA	O2D-CGD-O1D	-2.39	119.20	123.85
15	A	1131	CLA	CHB-C4A-NA	2.39	127.85	124.40
15	1	603	CLA	C3B-C4B-NB	-2.39	108.40	110.53
15	B	1221	CLA	O2A-CGA-O1A	-2.39	117.66	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	4005	BCR	C8-C7-C6	-2.39	120.62	127.00
14	J	4001	BCR	C24-C23-C22	-2.39	122.71	126.23
15	B	1230	CLA	O2A-CGA-O1A	-2.38	117.67	123.63
15	4	604	CLA	O2A-CGA-O1A	-2.38	117.67	123.63
14	3	504	BCR	C15-C14-C13	-2.38	123.94	127.28
15	B	1228	CLA	C3B-C4B-NB	-2.38	108.40	110.53
14	A	4007	BCR	C38-C26-C25	-2.38	121.89	124.48
15	A	1105	CLA	C1-C2-C3	-2.38	122.30	126.20
15	A	1120	CLA	CHB-C4A-NA	2.38	127.83	124.40
14	3	504	BCR	C38-C26-C25	-2.38	121.89	124.48
13	2	502	XAT	C36-C21-C26	2.38	116.47	110.05
13	1	502	XAT	C26-C27-C28	-2.38	120.97	125.99
15	F	1302	CLA	C3B-C4B-NB	-2.38	108.41	110.53
15	A	1138	CLA	O2D-CGD-CBD	2.38	115.39	111.23
15	A	1120	CLA	C3B-C4B-NB	-2.38	108.41	110.53
14	2	503	BCR	C38-C26-C25	-2.38	121.89	124.48
16	3	604	CHL	C1-O2A-CGA	2.38	122.40	116.65
14	1	503	BCR	C15-C16-C17	-2.37	118.67	123.52
15	4	602	CLA	O2D-CGD-CBD	2.37	115.38	111.23
12	1	501	LUT	C26-C27-C28	-2.37	120.89	124.58
15	4	609	CLA	C4-C3-C2	-2.37	117.55	123.63
15	A	1107	CLA	C2A-C1A-CHA	2.37	127.97	123.87
14	B	4004	BCR	C27-C26-C25	2.37	125.90	122.70
16	2	609	CHL	CBA-CAA-C2A	2.36	120.74	113.78
12	2	501	LUT	C19-C9-C8	2.36	121.70	118.09
15	A	1140	CLA	CHB-C4A-NA	2.36	127.81	124.40
15	3	601	CLA	O2A-CGA-O1A	-2.36	117.72	123.63
12	2	501	LUT	C20-C13-C12	2.36	121.69	118.09
15	B	1215	CLA	O2A-CGA-O1A	-2.35	117.75	123.63
14	3	503	BCR	C2-C1-C6	2.35	113.85	110.44
15	1	611	CLA	CHB-C4A-NA	2.35	127.79	124.40
15	4	616	CLA	CHB-C4A-NA	2.34	127.78	124.40
16	4	611	CHL	C4C-CHD-C1D	2.34	124.44	116.07
15	4	605	CLA	C4-C3-C2	-2.34	117.62	123.63
14	B	4005	BCR	C38-C26-C25	-2.34	121.93	124.48
14	B	4001	BCR	C1-C6-C5	-2.34	119.44	122.64
15	2	605	CLA	C3B-C4B-NB	-2.34	108.44	110.53
15	A	1132	CLA	CBC-CAC-C3C	2.34	118.76	112.42
15	1	603	CLA	CBA-CAA-C2A	2.34	120.75	113.79
15	B	1231	CLA	CAC-C3C-C4C	2.34	127.83	124.79
15	A	1128	CLA	CHB-C4A-NA	2.34	127.77	124.40
15	4	602	CLA	C3B-C4B-NB	-2.34	108.44	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	A	1115	CLA	CHB-C4A-NA	2.34	127.77	124.40
19	A	1011	CL0	C9-C8-C10	2.33	119.59	111.27
15	4	601	CLA	CBA-CAA-C2A	2.33	120.73	113.79
14	A	4006	BCR	C8-C7-C6	-2.33	120.77	127.00
14	B	4003	BCR	C35-C13-C14	-2.33	119.05	122.82
15	4	604	CLA	CBA-CAA-C2A	2.32	120.71	113.79
14	J	4001	BCR	C27-C26-C25	2.32	125.84	122.70
14	B	4004	BCR	C8-C7-C6	-2.32	120.79	127.00
13	3	502	XAT	C19-C9-C8	-2.32	114.54	118.09
14	F	4002	BCR	C24-C23-C22	-2.32	122.80	126.23
18	B	5003	LMG	O3-C3-C2	-2.32	104.91	110.38
15	A	1138	CLA	O2A-CGA-O1A	-2.32	117.83	123.63
15	4	603	CLA	C3A-C2A-C1A	2.32	104.81	101.34
15	B	1212	CLA	O2A-CGA-O1A	-2.32	117.83	123.63
13	1	502	XAT	C19-C9-C8	2.32	121.63	118.09
15	4	606	CLA	O2A-CGA-O1A	-2.31	117.84	123.63
15	B	1212	CLA	C3B-C4B-NB	-2.31	108.46	110.53
15	B	1224	CLA	O2A-CGA-O1A	-2.31	117.84	123.63
15	A	1127	CLA	CHB-C4A-NA	2.31	127.74	124.40
15	A	1131	CLA	C3B-C4B-NB	-2.31	108.47	110.53
15	A	1125	CLA	CHB-C4A-NA	2.31	127.74	124.40
19	A	1011	CL0	C1A-CHA-CBD	2.31	138.28	132.36
15	A	1104	CLA	C5-C3-C2	2.31	126.35	121.17
17	B	5001	LHG	C11-C10-C9	-2.31	102.70	114.37
15	A	1113	CLA	C3B-C4B-NB	-2.31	108.47	110.53
16	1	609	CHL	C4C-CHD-C1D	2.31	124.32	116.07
15	1	604	CLA	CAC-C3C-C4C	2.31	127.79	124.79
14	A	4007	BCR	C2-C1-C6	2.30	113.79	110.44
15	A	1136	CLA	CHB-C4A-NA	2.30	127.72	124.40
15	B	1222	CLA	C1-O2A-CGA	2.30	122.22	116.65
14	1	503	BCR	C7-C8-C9	-2.30	122.83	126.23
15	3	613	CLA	C3B-C4B-NB	-2.30	108.48	110.53
15	A	1105	CLA	CBC-CAC-C3C	2.30	118.64	112.42
14	J	4002	BCR	C2-C1-C6	2.29	113.77	110.44
14	A	4004	BCR	C33-C5-C6	-2.29	121.99	124.48
14	A	4002	BCR	C1-C6-C5	-2.29	119.51	122.64
15	A	1139	CLA	C5-C3-C2	2.28	126.30	121.17
15	3	603	CLA	CHB-C4A-NA	2.28	127.69	124.40
15	1	607	CLA	CHB-C4A-NA	2.28	127.69	124.40
14	B	4003	BCR	C1-C6-C5	-2.28	119.52	122.64
14	4	503	BCR	C15-C14-C13	-2.28	124.08	127.28
15	A	1126	CLA	O2A-CGA-O1A	-2.28	117.93	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	A	1109	CLA	C3B-C4B-NB	-2.28	108.50	110.53
15	B	1231	CLA	C4-C3-C2	-2.28	117.78	123.63
15	A	1110	CLA	C5-C3-C2	2.27	126.27	121.17
15	1	612	CLA	CHB-C4A-NA	2.27	127.68	124.40
15	2	601	CLA	CBA-CAA-C2A	2.27	120.55	113.79
15	B	1239	CLA	CAC-C3C-C4C	2.27	127.75	124.79
15	4	608	CLA	CHD-C4C-C3C	2.27	128.09	124.77
13	3	502	XAT	C38-C25-C26	-2.27	118.56	122.30
15	A	1126	CLA	CHB-C4A-NA	2.27	127.67	124.40
14	F	4001	BCR	C27-C26-C25	2.27	125.77	122.70
15	B	1238	CLA	CHD-C4C-C3C	2.27	128.08	124.77
15	F	1302	CLA	CBA-CAA-C2A	2.26	120.53	113.79
15	4	616	CLA	O2A-CGA-O1A	-2.26	117.97	123.63
15	1	601	CLA	O2A-CGA-O1A	-2.26	117.97	123.63
22	B	5002	DGD	O6E-C5E-C4E	2.26	113.77	109.70
16	2	609	CHL	C4D-CHA-CBD	-2.26	106.69	108.97
14	1	503	BCR	C16-C15-C14	-2.26	118.90	123.52
15	B	1210	CLA	CHB-C4A-NA	2.26	127.66	124.40
14	J	4001	BCR	C33-C5-C6	-2.26	122.02	124.48
15	B	1216	CLA	O2A-CGA-O1A	-2.26	117.98	123.63
14	3	503	BCR	C37-C22-C21	-2.26	119.16	122.82
15	3	612	CLA	CAC-C3C-C4C	2.26	127.72	124.79
15	B	1202	CLA	O2D-CGD-CBD	2.25	115.17	111.23
15	B	1022	CLA	C4-C3-C5	2.25	119.14	115.23
16	3	604	CHL	C4C-CHD-C1D	2.25	124.12	116.07
14	A	4005	BCR	C11-C10-C9	-2.25	124.12	127.28
14	B	4005	BCR	C35-C13-C14	-2.25	119.17	122.82
22	B	5002	DGD	CFB-CEB-CDB	-2.24	103.02	114.37
14	A	4007	BCR	C27-C26-C25	2.24	125.73	122.70
14	3	503	BCR	C15-C16-C17	-2.24	118.94	123.52
15	A	1106	CLA	C5-C3-C2	2.24	126.19	121.17
17	1	801	LHG	C20-C19-C18	-2.24	103.06	114.37
15	B	1219	CLA	CHB-C4A-NA	2.24	127.63	124.40
13	3	502	XAT	C20-C13-C14	-2.24	119.19	122.82
15	1	615	CLA	CAC-C3C-C4C	2.24	127.70	124.79
15	B	1211	CLA	CMB-C2B-C1B	-2.23	122.02	125.42
14	A	4005	BCR	C16-C15-C14	-2.23	118.95	123.52
14	A	4008	BCR	C35-C13-C14	-2.23	119.20	122.82
15	B	1222	CLA	O2D-CGD-O1D	-2.23	119.50	123.85
14	1	503	BCR	C2-C1-C6	2.23	113.68	110.44
15	A	1129	CLA	CAC-C3C-C4C	2.23	127.69	124.79
14	A	4006	BCR	C2-C1-C6	2.23	113.68	110.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	4005	BCR	C27-C26-C25	2.23	125.72	122.70
15	B	1204	CLA	O2A-CGA-O1A	-2.23	117.60	123.33
18	B	5003	LMG	C7-O1-C1	2.23	118.57	113.80
15	A	1139	CLA	CMB-C2B-C1B	-2.23	122.03	125.42
14	4	503	BCR	C16-C15-C14	-2.23	118.96	123.52
14	J	4002	BCR	C38-C26-C25	-2.23	122.06	124.48
13	1	502	XAT	C40-C33-C32	2.23	121.49	118.09
15	B	1231	CLA	O2A-CGA-O1A	-2.23	118.06	123.63
15	B	1214	CLA	O2A-CGA-O1A	-2.22	118.06	123.63
16	3	604	CHL	CBA-CAA-C2A	2.22	120.33	113.78
14	B	4001	BCR	C2-C3-C4	2.22	116.17	111.28
15	B	1226	CLA	CBA-CAA-C2A	2.22	120.41	113.79
15	4	608	CLA	CHB-C4A-NA	2.22	127.61	124.40
14	J	4001	BCR	C10-C11-C12	-2.22	116.76	123.20
16	4	610	CHL	C1-O2A-CGA	2.22	123.18	116.07
15	4	601	CLA	O2A-CGA-O1A	-2.22	118.08	123.63
13	3	502	XAT	C19-C9-C10	-2.21	119.23	122.82
15	3	608	CLA	CHB-C4A-NA	2.21	127.59	124.40
14	2	503	BCR	C15-C16-C17	-2.21	119.00	123.52
15	A	1102	CLA	O2A-CGA-O1A	-2.21	118.10	123.63
22	B	5002	DGD	CDB-CCB-CBB	-2.21	103.22	114.37
14	A	4003	BCR	C7-C8-C9	-2.21	122.97	126.23
14	3	503	BCR	C7-C8-C9	-2.21	122.97	126.23
14	B	4002	BCR	C15-C16-C17	-2.21	119.01	123.52
15	B	1219	CLA	O2A-CGA-O1A	-2.20	118.11	123.63
14	1	503	BCR	C11-C10-C9	-2.20	124.19	127.28
15	A	1110	CLA	C4-C3-C2	-2.20	117.97	123.63
15	2	604	CLA	CBA-CAA-C2A	2.20	120.34	113.79
14	A	4003	BCR	C16-C15-C14	-2.20	119.02	123.52
15	B	1222	CLA	CAA-CBA-CGA	-2.20	106.96	113.21
14	3	503	BCR	C20-C21-C22	-2.20	124.19	127.28
15	A	1138	CLA	C3A-C2A-C1A	2.20	104.63	101.34
15	1	603	CLA	CAC-C3C-C4C	2.20	127.65	124.79
12	1	501	LUT	C7-C6-C5	-2.20	116.50	121.56
14	A	4002	BCR	C38-C26-C27	-2.20	108.91	113.60
15	A	1108	CLA	C3B-C4B-NB	-2.19	108.57	110.53
15	3	606	CLA	C1-O2A-CGA	2.19	121.96	116.65
17	2	801	LHG	C5-O7-C7	-2.19	112.55	117.80
20	B	2002	PQN	C21-C20-C18	-2.19	108.67	115.97
15	B	1230	CLA	CAC-C3C-C4C	2.19	127.64	124.79
15	A	1126	CLA	C3B-C4B-NB	-2.19	108.57	110.53
15	B	1222	CLA	C3B-C4B-NB	-2.19	108.57	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	2	804	LMG	O2-C2-C1	-2.19	104.86	110.08
12	1	501	LUT	C19-C9-C8	2.19	121.43	118.09
15	A	1126	CLA	CBA-CAA-C2A	2.19	120.31	113.79
14	J	4001	BCR	C16-C15-C14	-2.19	119.04	123.52
15	2	604	CLA	CAC-C3C-C4C	2.19	127.63	124.79
15	A	1106	CLA	O2D-CGD-CBD	2.19	115.05	111.23
14	A	4006	BCR	C38-C26-C25	-2.18	122.10	124.48
15	1	603	CLA	CMB-C2B-C3B	2.18	131.69	126.55
15	B	1211	CLA	O2A-CGA-O1A	-2.18	118.17	123.63
18	2	803	LMG	O2-C2-C1	-2.18	104.88	110.08
14	2	503	BCR	C4-C5-C6	2.18	125.65	122.70
15	A	1137	CLA	C4-C3-C2	-2.18	118.03	123.63
15	F	1302	CLA	O2A-CGA-O1A	-2.18	118.18	123.63
15	B	1021	CLA	CHB-C4A-NA	2.18	127.54	124.40
14	B	4003	BCR	C24-C23-C22	-2.18	123.02	126.23
15	A	1130	CLA	O2D-CGD-CBD	2.17	115.03	111.23
15	A	1013	CLA	C4-C3-C2	-2.17	118.05	123.63
15	B	1210	CLA	O2D-CGD-CBD	2.17	115.03	111.23
15	B	1202	CLA	O2A-CGA-O1A	-2.17	118.19	123.63
18	2	802	LMG	O2-C2-C1	-2.17	104.90	110.08
16	2	609	CHL	C1A-CHA-C4D	2.17	122.60	118.98
14	A	4005	BCR	C7-C8-C9	-2.17	123.03	126.23
15	3	607	CLA	O2A-CGA-O1A	-2.17	118.21	123.63
17	1	801	LHG	O8-C23-O10	-2.17	118.21	123.63
14	A	4003	BCR	C24-C23-C22	-2.17	123.03	126.23
15	A	1111	CLA	C1-C2-C3	-2.16	122.65	126.20
15	B	1021	CLA	O2A-CGA-O1A	-2.16	118.22	123.63
14	1	503	BCR	C38-C26-C25	-2.16	122.13	124.48
14	B	4005	BCR	C11-C10-C9	-2.16	124.25	127.28
15	2	616	CLA	C14-C13-C12	-2.16	103.58	111.27
14	B	4003	BCR	C28-C27-C26	-2.16	110.21	114.06
15	A	1135	CLA	CBA-CAA-C2A	-2.16	107.38	113.79
13	4	502	XAT	C24-C23-C22	-2.16	106.76	110.79
15	A	1105	CLA	O2A-CGA-O1A	-2.16	118.23	123.63
15	2	604	CLA	O2A-CGA-O1A	-2.16	118.24	123.63
14	B	4002	BCR	C11-C10-C9	-2.15	124.26	127.28
15	3	610	CLA	O2A-CGA-O1A	-2.15	118.24	123.63
15	B	1215	CLA	O2D-CGD-CBD	2.15	114.99	111.23
15	B	1228	CLA	CMB-C2B-C1B	-2.15	122.14	125.42
15	A	1124	CLA	C2A-C1A-CHA	2.15	127.60	123.87
15	3	605	CLA	O1D-CGD-CBD	2.15	128.76	124.52
17	3	801	LHG	C20-C19-C18	-2.15	103.50	114.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	3	506	BCR	C16-C15-C14	-2.15	119.12	123.52
15	B	1213	CLA	O2A-CGA-O1A	-2.15	118.25	123.63
18	2	802	LMG	O3-C3-C2	-2.15	105.31	110.38
15	B	1236	CLA	O2A-CGA-O1A	-2.15	118.26	123.63
15	3	603	CLA	C3B-C4B-NB	-2.15	108.61	110.53
15	A	1117	CLA	C3A-C2A-C1A	2.15	104.55	101.34
15	A	1117	CLA	C11-C12-C13	-2.14	108.84	115.97
14	B	4006	BCR	C8-C7-C6	-2.14	121.28	127.00
18	2	803	LMG	C1-C2-C3	-2.14	105.51	110.01
15	A	1113	CLA	CHB-C4A-NA	2.14	127.49	124.40
15	2	602	CLA	C2A-C1A-CHA	2.14	127.58	123.87
15	A	1101	CLA	C1-C2-C3	-2.14	122.69	126.20
14	B	4004	BCR	C11-C10-C9	-2.14	124.28	127.28
14	2	503	BCR	C8-C7-C6	-2.14	121.29	127.00
14	A	4007	BCR	C35-C13-C14	-2.14	119.36	122.82
15	B	1234	CLA	O2A-CGA-O1A	-2.14	118.28	123.63
15	A	1123	CLA	C2A-C1A-CHA	2.13	127.57	123.87
15	A	1120	CLA	CAC-C3C-C4C	2.13	127.56	124.79
15	A	1116	CLA	CBA-CAA-C2A	2.13	120.13	113.79
15	4	603	CLA	O2A-CGA-O1A	-2.13	118.31	123.63
14	F	4001	BCR	C4-C5-C6	2.13	125.58	122.70
15	1	607	CLA	CAC-C3C-C4C	2.12	127.55	124.79
15	A	1141	CLA	CMA-C3A-C2A	-2.12	111.36	116.23
15	B	1215	CLA	CAA-C2A-C1A	-2.12	105.02	111.97
15	B	1239	CLA	O1D-CGD-CBD	2.12	128.70	124.52
15	1	603	CLA	O2A-CGA-O1A	-2.12	118.32	123.63
16	1	610	CHL	C1-O2A-CGA	2.12	122.86	116.07
12	1	501	LUT	C20-C13-C12	2.12	121.33	118.09
15	B	1225	CLA	CBA-CAA-C2A	2.12	120.10	113.79
15	B	1216	CLA	CMB-C2B-C1B	-2.12	122.19	125.42
18	B	5003	LMG	C1-C2-C3	-2.12	105.55	110.01
18	2	804	LMG	O7-C10-O9	-2.12	118.76	123.70
15	A	1128	CLA	C1-C2-C3	-2.11	122.73	126.20
15	3	614	CLA	C3B-C4B-NB	-2.11	108.64	110.53
15	B	1229	CLA	C6-C5-C3	2.11	118.61	113.47
15	B	1211	CLA	C1-C2-C3	-2.11	122.74	126.20
15	A	1103	CLA	O1D-CGD-CBD	2.11	128.67	124.52
15	A	1105	CLA	CMB-C2B-C3B	2.11	131.50	126.55
15	3	603	CLA	O2A-CGA-O1A	-2.10	118.36	123.63
15	B	1221	CLA	C2A-C1A-CHA	2.10	127.51	123.87
17	A	5002	LHG	C11-C10-C9	-2.10	103.75	114.37
15	2	612	CLA	C1-O2A-CGA	2.10	121.73	116.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	3	801	LHG	O8-C23-O10	-2.10	118.38	123.63
14	A	4003	BCR	C40-C30-C25	2.10	113.53	110.24
14	2	503	BCR	C16-C15-C14	-2.10	119.22	123.52
14	A	4002	BCR	C4-C5-C6	2.10	125.54	122.70
15	A	1125	CLA	O2A-CGA-O1A	-2.10	118.38	123.63
20	A	2001	PQN	C2M-C2-C3	-2.09	121.01	124.45
12	4	501	LUT	C8-C9-C10	2.09	122.30	119.01
15	A	1137	CLA	C4-C3-C5	2.09	118.86	115.23
15	2	606	CLA	CAC-C3C-C4C	2.09	127.51	124.79
14	A	4008	BCR	C24-C23-C22	-2.09	123.14	126.23
15	4	609	CLA	O2A-CGA-O1A	-2.09	118.40	123.63
15	A	1139	CLA	C4-C3-C2	-2.09	118.26	123.63
12	1	501	LUT	C4-C5-C6	-2.09	116.46	120.76
15	B	1220	CLA	O2D-CGD-O1D	-2.09	119.78	123.85
15	A	1130	CLA	CBA-CAA-C2A	2.08	120.00	113.79
15	A	1126	CLA	C6-C5-C3	-2.08	108.39	113.47
14	A	4006	BCR	C7-C8-C9	-2.08	123.15	126.23
15	A	1135	CLA	CMB-C2B-C1B	-2.08	122.25	125.42
18	2	803	LMG	O3-C3-C2	-2.08	105.47	110.38
18	4	801	LMG	O5-C6-C5	-2.08	104.24	111.33
22	B	5002	DGD	C3D-C4D-C5D	-2.08	106.46	110.23
14	A	4005	BCR	C37-C22-C23	2.08	121.27	118.09
15	B	1216	CLA	CHB-C4A-NA	2.08	127.40	124.40
15	B	1210	CLA	O2A-CGA-O1A	-2.08	118.42	123.63
14	B	4001	BCR	C35-C13-C12	2.08	121.27	118.09
12	4	501	LUT	C36-C21-C26	2.08	112.69	109.55
14	A	4008	BCR	C11-C10-C9	-2.08	124.36	127.28
17	3	801	LHG	C11-C10-C9	-2.08	103.86	114.37
15	4	604	CLA	CMC-C2C-C1C	2.08	128.28	125.03
15	A	1105	CLA	C3A-C2A-C1A	2.07	104.44	101.34
15	A	1114	CLA	C2A-C1A-CHA	2.07	127.46	123.87
15	A	1110	CLA	CBA-CAA-C2A	2.07	119.95	113.79
18	2	804	LMG	O3-C3-C2	-2.07	105.50	110.38
14	3	506	BCR	C8-C7-C6	-2.07	121.47	127.00
15	A	1107	CLA	O2A-CGA-O1A	-2.07	118.45	123.63
15	A	1101	CLA	C5-C3-C2	2.07	125.81	121.17
15	B	1220	CLA	O1D-CGD-CBD	2.07	128.60	124.52
14	3	506	BCR	C38-C26-C25	-2.07	122.23	124.48
15	B	1210	CLA	CAC-C3C-C4C	2.07	127.48	124.79
15	A	1129	CLA	O2A-CGA-O1A	-2.07	118.46	123.63
15	B	1228	CLA	O2A-CGA-O1A	-2.07	118.46	123.63
15	A	1110	CLA	O2D-CGD-CBD	2.06	114.84	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	5002	DGD	O6E-C1E-O5D	-2.06	105.17	110.04
15	A	1119	CLA	O2A-CGA-O1A	-2.06	118.47	123.63
16	3	604	CHL	CMD-C2D-C3D	2.06	128.80	124.68
15	A	1128	CLA	C3B-C4B-NB	-2.06	108.69	110.53
14	B	4001	BCR	C28-C27-C26	-2.06	110.38	114.06
15	3	603	CLA	C6-C5-C3	2.06	118.48	113.47
18	2	803	LMG	O7-C10-O9	-2.06	118.89	123.70
15	2	605	CLA	O2A-CGA-O1A	-2.06	118.48	123.63
15	1	608	CLA	O2A-CGA-O1A	-2.06	118.48	123.63
15	2	616	CLA	C16-C15-C13	2.06	122.80	115.97
14	4	503	BCR	C38-C26-C25	-2.06	122.24	124.48
16	4	611	CHL	CMD-C2D-C3D	2.06	128.79	124.68
15	A	1117	CLA	C2A-C1A-CHA	2.06	127.44	123.87
16	4	613	CHL	CMD-C2D-C3D	2.06	128.79	124.68
15	A	1107	CLA	CHA-C1A-NA	-2.06	121.74	126.39
15	A	1104	CLA	O2A-CGA-O1A	-2.05	118.49	123.63
15	4	607	CLA	C2A-C1A-CHA	2.05	127.43	123.87
15	B	1210	CLA	C6-C5-C3	2.05	118.47	113.47
15	A	1138	CLA	C3B-C4B-NB	-2.05	108.70	110.53
15	A	1104	CLA	C7-C6-C5	-2.05	107.79	113.26
12	3	501	LUT	C1-C6-C7	2.05	121.21	115.65
15	1	606	CLA	O2A-CGA-O1A	-2.05	118.51	123.63
14	A	4005	BCR	C2-C1-C6	2.05	113.41	110.44
15	B	1230	CLA	O1D-CGD-CBD	2.05	128.55	124.52
15	A	1012	CLA	C4-C3-C5	2.05	118.78	115.23
15	A	1112	CLA	O1D-CGD-CBD	2.05	128.55	124.52
15	A	1104	CLA	O2D-CGD-O1D	-2.04	119.87	123.85
15	B	1220	CLA	O2A-CGA-O1A	-2.04	118.52	123.63
15	3	605	CLA	CHD-C4C-C3C	2.04	127.75	124.77
18	B	5003	LMG	O2-C2-C1	-2.04	105.21	110.08
15	A	1124	CLA	O2A-CGA-O1A	-2.04	118.52	123.63
14	1	503	BCR	C8-C7-C6	-2.04	121.55	127.00
22	B	5002	DGD	O2D-C2D-C1D	-2.04	105.22	110.08
15	3	610	CLA	CBA-CAA-C2A	2.04	119.86	113.79
15	B	1232	CLA	O1D-CGD-CBD	2.04	128.53	124.52
15	A	1123	CLA	O1D-CGD-CBD	2.03	128.53	124.52
15	B	1206	CLA	O1D-CGD-CBD	2.03	128.53	124.52
12	3	501	LUT	C36-C21-C26	2.03	112.62	109.55
17	3	801	LHG	C27-C26-C25	-2.03	104.09	114.37
18	B	5003	LMG	O7-C10-O9	-2.03	118.95	123.70
15	1	604	CLA	CMC-C2C-C1C	2.03	128.21	125.03
14	B	4002	BCR	C37-C22-C23	2.03	121.19	118.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	3	610	CLA	O2D-CGD-CBD	2.03	114.78	111.23
15	B	1214	CLA	CMB-C2B-C3B	2.03	131.32	126.55
15	B	1205	CLA	O1D-CGD-CBD	2.03	128.52	124.52
15	A	1012	CLA	C11-C12-C13	-2.03	109.22	115.97
15	B	1240	CLA	C1-C2-C3	2.03	129.52	126.20
15	3	609	CLA	C3B-C4B-NB	-2.03	108.72	110.53
14	B	4004	BCR	C1-C6-C5	-2.02	119.87	122.64
15	A	1141	CLA	CAA-C2A-C3A	-2.02	111.59	116.23
15	B	1230	CLA	CBA-CAA-C2A	2.02	119.81	113.79
14	A	4003	BCR	C11-C10-C9	-2.02	124.44	127.28
15	1	608	CLA	C5-C3-C2	2.02	125.71	121.17
14	B	4004	BCR	C38-C26-C25	-2.02	122.28	124.48
16	2	613	CHL	CMD-C2D-C3D	2.02	128.72	124.68
15	2	603	CLA	C3A-C2A-C1A	2.02	104.37	101.34
12	2	501	LUT	C4-C5-C6	-2.02	116.61	120.76
12	4	501	LUT	C1-C6-C7	2.02	121.13	115.65
14	A	4008	BCR	C34-C9-C10	-2.02	119.54	122.82
15	A	1108	CLA	CMB-C2B-C1B	-2.02	122.34	125.42
18	2	804	LMG	C38-C37-C36	-2.02	104.16	114.37
15	B	1214	CLA	C4-C3-C2	-2.02	118.45	123.63
15	B	1023	CLA	C4-C3-C5	2.02	118.73	115.23
14	B	4003	BCR	C8-C7-C6	-2.01	121.62	127.00
14	A	4006	BCR	C27-C26-C25	2.01	125.42	122.70
15	1	603	CLA	O1D-CGD-CBD	2.01	128.49	124.52
13	1	502	XAT	C39-C29-C30	-2.01	119.56	122.82
14	2	503	BCR	C20-C21-C22	-2.01	124.46	127.28
14	F	4002	BCR	C2-C1-C6	2.01	113.36	110.44
18	2	804	LMG	C18-C17-C16	-2.01	104.20	114.37
16	2	610	CHL	CMD-C2D-C3D	2.01	128.70	124.68
15	4	601	CLA	C4-C3-C5	2.01	118.72	115.23
16	1	610	CHL	CMD-C2D-C3D	2.01	128.70	124.68
14	A	4002	BCR	C16-C15-C14	-2.01	119.41	123.52
15	B	1022	CLA	C3B-C4B-NB	-2.01	108.74	110.53
15	A	1111	CLA	O2A-CGA-O1A	-2.01	118.60	123.63
15	A	1125	CLA	CAA-C2A-C3A	-2.01	107.57	113.00
13	2	502	XAT	O23-C23-C22	-2.01	105.64	109.75
22	B	5002	DGD	O3E-C3E-C2E	-2.01	105.64	110.38
14	A	4006	BCR	C16-C15-C14	-2.01	119.41	123.52
16	1	609	CHL	CMD-C2D-C3D	2.01	128.69	124.68
15	B	1208	CLA	CAA-CBA-CGA	-2.01	107.51	113.21
12	1	501	LUT	C37-C21-C26	-2.01	106.51	109.55
15	B	1204	CLA	CAA-C2A-C1A	-2.01	105.40	111.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	A	1123	CLA	C1-C2-C3	-2.00	122.91	126.20
17	A	5002	LHG	C18-C17-C16	-2.00	104.24	114.37
18	2	802	LMG	O1-C1-C2	-2.00	105.23	108.27
14	2	503	BCR	C27-C26-C25	2.00	125.41	122.70
15	A	1122	CLA	C16-C15-C13	-2.00	109.31	115.97
15	2	603	CLA	O2A-CGA-O1A	-2.00	118.62	123.63
15	B	1211	CLA	CMB-C2B-C3B	2.00	131.26	126.55

All (170) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
12	1	501	LUT	C26
12	2	501	LUT	C26
12	3	501	LUT	C26
12	4	501	LUT	C26
15	1	601	CLA	ND
15	1	602	CLA	ND
15	1	603	CLA	ND
15	1	604	CLA	ND
15	1	605	CLA	ND
15	1	606	CLA	ND
15	1	607	CLA	ND
15	1	608	CLA	ND
15	1	611	CLA	ND
15	1	612	CLA	ND
15	1	613	CLA	ND
15	1	615	CLA	ND
15	2	601	CLA	ND
15	2	602	CLA	ND
15	2	603	CLA	ND
15	2	604	CLA	ND
15	2	605	CLA	ND
15	2	606	CLA	ND
15	2	607	CLA	ND
15	2	608	CLA	ND
15	2	612	CLA	ND
15	3	601	CLA	ND
15	3	603	CLA	ND
15	3	605	CLA	ND
15	3	606	CLA	ND
15	3	607	CLA	ND
15	3	608	CLA	ND

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Mol	Chain	Res	Type	Atom
15	3	609	CLA	ND
15	3	610	CLA	ND
15	3	611	CLA	ND
15	3	612	CLA	ND
15	3	613	CLA	ND
15	3	614	CLA	ND
15	3	615	CLA	ND
15	4	601	CLA	ND
15	4	602	CLA	ND
15	4	603	CLA	ND
15	4	604	CLA	ND
15	4	605	CLA	ND
15	4	606	CLA	ND
15	4	607	CLA	ND
15	4	608	CLA	ND
15	4	609	CLA	ND
15	4	612	CLA	ND
15	4	616	CLA	ND
15	A	1012	CLA	ND
15	A	1013	CLA	ND
15	A	1101	CLA	ND
15	A	1102	CLA	ND
15	A	1103	CLA	ND
15	A	1104	CLA	ND
15	A	1105	CLA	ND
15	A	1106	CLA	ND
15	A	1107	CLA	ND
15	A	1108	CLA	ND
15	A	1109	CLA	ND
15	A	1110	CLA	ND
15	A	1112	CLA	ND
15	A	1113	CLA	ND
15	A	1114	CLA	ND
15	A	1115	CLA	ND
15	A	1116	CLA	ND
15	A	1117	CLA	ND
15	A	1118	CLA	ND
15	A	1119	CLA	ND
15	A	1120	CLA	ND
15	A	1121	CLA	ND
15	A	1122	CLA	ND
15	A	1123	CLA	ND

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Mol	Chain	Res	Type	Atom
15	A	1124	CLA	ND
15	A	1126	CLA	ND
15	A	1127	CLA	ND
15	A	1128	CLA	ND
15	A	1129	CLA	ND
15	A	1130	CLA	ND
15	A	1131	CLA	ND
15	A	1132	CLA	ND
15	A	1133	CLA	ND
15	A	1134	CLA	ND
15	A	1135	CLA	ND
15	A	1136	CLA	ND
15	A	1137	CLA	ND
15	A	1138	CLA	ND
15	A	1139	CLA	ND
15	A	1140	CLA	ND
15	A	1141	CLA	ND
15	B	1021	CLA	ND
15	B	1022	CLA	ND
15	B	1023	CLA	ND
15	B	1201	CLA	ND
15	B	1202	CLA	ND
15	B	1203	CLA	ND
15	B	1204	CLA	ND
15	B	1205	CLA	ND
15	B	1206	CLA	ND
15	B	1208	CLA	ND
15	B	1209	CLA	ND
15	B	1211	CLA	ND
15	B	1212	CLA	ND
15	B	1213	CLA	ND
15	B	1214	CLA	ND
15	B	1215	CLA	ND
15	B	1216	CLA	ND
15	B	1217	CLA	ND
15	B	1218	CLA	ND
15	B	1220	CLA	ND
15	B	1221	CLA	ND
15	B	1222	CLA	ND
15	B	1223	CLA	ND
15	B	1224	CLA	ND
15	B	1225	CLA	ND

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Mol	Chain	Res	Type	Atom
15	B	1226	CLA	ND
15	B	1227	CLA	ND
15	B	1228	CLA	ND
15	B	1229	CLA	ND
15	B	1230	CLA	ND
15	B	1231	CLA	ND
15	B	1232	CLA	ND
15	B	1234	CLA	ND
15	B	1235	CLA	ND
15	B	1236	CLA	ND
15	B	1237	CLA	ND
15	B	1238	CLA	C8
15	B	1238	CLA	ND
15	B	1239	CLA	ND
15	B	1240	CLA	ND
15	F	1301	CLA	ND
15	F	1302	CLA	ND
15	J	1302	CLA	ND
16	1	609	CHL	NA
16	1	609	CHL	C8
16	1	609	CHL	ND
16	1	609	CHL	NC
16	1	610	CHL	NA
16	1	610	CHL	ND
16	1	610	CHL	NC
16	2	609	CHL	NA
16	2	609	CHL	C8
16	2	609	CHL	ND
16	2	609	CHL	NC
16	2	610	CHL	NA
16	2	610	CHL	ND
16	2	610	CHL	NC
16	2	611	CHL	NA
16	2	611	CHL	ND
16	2	611	CHL	NC
16	2	613	CHL	NA
16	2	613	CHL	ND
16	2	613	CHL	NC
16	3	604	CHL	NA
16	3	604	CHL	C8
16	3	604	CHL	ND
16	3	604	CHL	NC

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Mol	Chain	Res	Type	Atom
16	4	610	CHL	NA
16	4	610	CHL	ND
16	4	610	CHL	NC
16	4	611	CHL	NA
16	4	611	CHL	ND
16	4	611	CHL	NC
16	4	613	CHL	NA
16	4	613	CHL	C8
16	4	613	CHL	ND
16	4	613	CHL	NC
19	A	1011	CL0	NA
19	A	1011	CL0	C8
19	A	1011	CL0	CBD

All (2024) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	1	501	LUT	C11-C12-C13-C14
12	2	501	LUT	C25-C26-C27-C28
12	3	501	LUT	C25-C26-C27-C28
12	4	501	LUT	C11-C12-C13-C14
12	4	501	LUT	C21-C26-C27-C28
12	4	501	LUT	C25-C26-C27-C28
12	4	501	LUT	C31-C32-C33-C34
13	1	502	XAT	O4-C6-C7-C8
13	2	502	XAT	C31-C32-C33-C34
13	3	502	XAT	O4-C6-C7-C8
13	3	502	XAT	C7-C8-C9-C10
13	3	502	XAT	C7-C8-C9-C19
13	3	502	XAT	C25-C26-C27-C28
13	3	502	XAT	C29-C30-C31-C32
13	3	502	XAT	C31-C32-C33-C34
13	3	502	XAT	C31-C32-C33-C40
13	4	502	XAT	C7-C8-C9-C19
13	4	502	XAT	C13-C14-C15-C35
13	4	502	XAT	O24-C26-C27-C28
13	4	502	XAT	C27-C28-C29-C30
13	4	502	XAT	C27-C28-C29-C39
13	4	502	XAT	C31-C32-C33-C34
13	4	502	XAT	C31-C32-C33-C40
14	1	503	BCR	C7-C8-C9-C10
14	1	503	BCR	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
14	1	503	BCR	C11-C10-C9-C34
14	1	503	BCR	C10-C11-C12-C13
14	1	503	BCR	C11-C12-C13-C35
14	1	503	BCR	C16-C17-C18-C19
14	1	503	BCR	C16-C17-C18-C36
14	1	503	BCR	C18-C19-C20-C21
14	1	503	BCR	C21-C22-C23-C24
14	1	503	BCR	C37-C22-C23-C24
14	2	503	BCR	C7-C8-C9-C34
14	2	503	BCR	C11-C10-C9-C8
14	2	503	BCR	C10-C11-C12-C13
14	2	503	BCR	C11-C12-C13-C35
14	2	503	BCR	C36-C18-C19-C20
14	2	503	BCR	C20-C21-C22-C37
14	3	503	BCR	C7-C8-C9-C10
14	3	503	BCR	C7-C8-C9-C34
14	3	503	BCR	C11-C10-C9-C8
14	3	503	BCR	C11-C10-C9-C34
14	3	503	BCR	C11-C12-C13-C14
14	3	503	BCR	C16-C17-C18-C36
14	3	504	BCR	C7-C8-C9-C34
14	3	504	BCR	C11-C10-C9-C34
14	3	504	BCR	C11-C12-C13-C14
14	3	504	BCR	C11-C12-C13-C35
14	3	504	BCR	C16-C17-C18-C36
14	3	504	BCR	C37-C22-C23-C24
14	3	506	BCR	C6-C7-C8-C9
14	3	506	BCR	C10-C11-C12-C13
14	3	506	BCR	C11-C12-C13-C14
14	3	506	BCR	C12-C13-C14-C15
14	3	506	BCR	C15-C16-C17-C18
14	3	506	BCR	C16-C17-C18-C19
14	3	506	BCR	C16-C17-C18-C36
14	3	506	BCR	C20-C21-C22-C37
14	4	503	BCR	C7-C8-C9-C34
14	4	503	BCR	C11-C10-C9-C8
14	4	503	BCR	C11-C10-C9-C34
14	4	503	BCR	C11-C12-C13-C35
14	4	503	BCR	C16-C17-C18-C19
14	4	503	BCR	C16-C17-C18-C36
14	4	503	BCR	C18-C19-C20-C21
14	4	503	BCR	C20-C21-C22-C37

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Mol	Chain	Res	Type	Atoms
14	4	503	BCR	C37-C22-C23-C24
14	4	503	BCR	C23-C24-C25-C26
14	4	503	BCR	C23-C24-C25-C30
14	A	4002	BCR	C6-C7-C8-C9
14	A	4002	BCR	C7-C8-C9-C34
14	A	4002	BCR	C11-C10-C9-C34
14	A	4002	BCR	C10-C11-C12-C13
14	A	4002	BCR	C18-C19-C20-C21
14	A	4002	BCR	C20-C21-C22-C23
14	A	4002	BCR	C20-C21-C22-C37
14	A	4003	BCR	C7-C8-C9-C10
14	A	4003	BCR	C11-C12-C13-C35
14	A	4003	BCR	C36-C18-C19-C20
14	A	4003	BCR	C18-C19-C20-C21
14	A	4003	BCR	C22-C23-C24-C25
14	A	4003	BCR	C23-C24-C25-C26
14	A	4004	BCR	C10-C11-C12-C13
14	A	4004	BCR	C14-C15-C16-C17
14	A	4004	BCR	C16-C17-C18-C19
14	A	4004	BCR	C17-C18-C19-C20
14	A	4004	BCR	C18-C19-C20-C21
14	A	4004	BCR	C19-C20-C21-C22
14	A	4004	BCR	C20-C21-C22-C23
14	A	4004	BCR	C20-C21-C22-C37
14	A	4004	BCR	C37-C22-C23-C24
14	A	4005	BCR	C7-C8-C9-C10
14	A	4005	BCR	C7-C8-C9-C34
14	A	4005	BCR	C10-C11-C12-C13
14	A	4005	BCR	C11-C12-C13-C14
14	A	4005	BCR	C20-C21-C22-C23
14	A	4005	BCR	C20-C21-C22-C37
14	A	4006	BCR	C7-C8-C9-C34
14	A	4006	BCR	C11-C10-C9-C34
14	A	4006	BCR	C10-C11-C12-C13
14	A	4006	BCR	C12-C13-C14-C15
14	A	4006	BCR	C35-C13-C14-C15
14	A	4006	BCR	C16-C17-C18-C19
14	A	4006	BCR	C16-C17-C18-C36
14	A	4006	BCR	C21-C22-C23-C24
14	A	4007	BCR	C7-C8-C9-C10
14	A	4007	BCR	C10-C11-C12-C13
14	A	4007	BCR	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
14	A	4007	BCR	C12-C13-C14-C15
14	A	4007	BCR	C35-C13-C14-C15
14	A	4007	BCR	C14-C15-C16-C17
14	A	4007	BCR	C16-C17-C18-C36
14	A	4007	BCR	C21-C22-C23-C24
14	A	4008	BCR	C7-C8-C9-C10
14	A	4008	BCR	C11-C12-C13-C14
14	A	4008	BCR	C11-C12-C13-C35
14	B	4001	BCR	C7-C8-C9-C10
14	B	4001	BCR	C16-C17-C18-C19
14	B	4001	BCR	C23-C24-C25-C26
14	B	4001	BCR	C23-C24-C25-C30
14	B	4002	BCR	C1-C6-C7-C8
14	B	4002	BCR	C5-C6-C7-C8
14	B	4002	BCR	C11-C10-C9-C34
14	B	4002	BCR	C10-C11-C12-C13
14	B	4002	BCR	C16-C17-C18-C36
14	B	4002	BCR	C20-C21-C22-C23
14	B	4002	BCR	C22-C23-C24-C25
14	B	4003	BCR	C6-C7-C8-C9
14	B	4003	BCR	C7-C8-C9-C10
14	B	4003	BCR	C11-C10-C9-C8
14	B	4003	BCR	C11-C10-C9-C34
14	B	4003	BCR	C10-C11-C12-C13
14	B	4003	BCR	C11-C12-C13-C14
14	B	4003	BCR	C11-C12-C13-C35
14	B	4003	BCR	C12-C13-C14-C15
14	B	4003	BCR	C35-C13-C14-C15
14	B	4003	BCR	C14-C15-C16-C17
14	B	4003	BCR	C16-C17-C18-C36
14	B	4004	BCR	C7-C8-C9-C34
14	B	4004	BCR	C11-C10-C9-C34
14	B	4004	BCR	C10-C11-C12-C13
14	B	4004	BCR	C11-C12-C13-C14
14	B	4004	BCR	C20-C21-C22-C37
14	B	4005	BCR	C11-C10-C9-C34
14	B	4005	BCR	C11-C12-C13-C35
14	B	4005	BCR	C16-C17-C18-C36
14	B	4005	BCR	C18-C19-C20-C21
14	B	4005	BCR	C20-C21-C22-C37
14	B	4006	BCR	C7-C8-C9-C34
14	B	4006	BCR	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
14	B	4006	BCR	C11-C12-C13-C35
14	B	4006	BCR	C35-C13-C14-C15
14	B	4006	BCR	C20-C21-C22-C37
14	B	4006	BCR	C37-C22-C23-C24
14	F	4001	BCR	C11-C10-C9-C8
14	F	4001	BCR	C11-C10-C9-C34
14	F	4001	BCR	C9-C10-C11-C12
14	F	4001	BCR	C10-C11-C12-C13
14	F	4001	BCR	C20-C21-C22-C37
14	F	4001	BCR	C23-C24-C25-C26
14	F	4002	BCR	C7-C8-C9-C10
14	F	4002	BCR	C12-C13-C14-C15
14	F	4002	BCR	C35-C13-C14-C15
14	F	4002	BCR	C14-C15-C16-C17
14	F	4002	BCR	C16-C17-C18-C36
14	F	4002	BCR	C18-C19-C20-C21
14	F	4002	BCR	C20-C21-C22-C37
14	F	4002	BCR	C21-C22-C23-C24
14	F	4002	BCR	C22-C23-C24-C25
14	J	4001	BCR	C1-C6-C7-C8
14	J	4001	BCR	C5-C6-C7-C8
14	J	4001	BCR	C6-C7-C8-C9
14	J	4001	BCR	C11-C12-C13-C14
14	J	4001	BCR	C11-C12-C13-C35
14	J	4001	BCR	C16-C17-C18-C36
14	J	4001	BCR	C17-C18-C19-C20
14	J	4001	BCR	C20-C21-C22-C37
14	J	4001	BCR	C21-C22-C23-C24
14	J	4001	BCR	C37-C22-C23-C24
14	J	4002	BCR	C6-C7-C8-C9
14	J	4002	BCR	C10-C11-C12-C13
14	J	4002	BCR	C11-C12-C13-C14
14	J	4002	BCR	C12-C13-C14-C15
14	J	4002	BCR	C35-C13-C14-C15
14	J	4002	BCR	C16-C17-C18-C36
14	J	4002	BCR	C23-C24-C25-C26
14	J	4002	BCR	C23-C24-C25-C30
15	1	601	CLA	CBD-CGD-O2D-CED
15	1	602	CLA	CBA-CGA-O2A-C1
15	1	603	CLA	C1A-C2A-CAA-CBA
15	1	603	CLA	CBD-CGD-O2D-CED
15	1	604	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
15	1	604	CLA	CHA-CBD-CGD-O2D
15	1	607	CLA	CBD-CGD-O2D-CED
15	1	612	CLA	CBD-CGD-O2D-CED
15	1	615	CLA	CBD-CGD-O2D-CED
15	2	601	CLA	C1A-C2A-CAA-CBA
15	2	601	CLA	C3A-C2A-CAA-CBA
15	2	601	CLA	CBD-CGD-O2D-CED
15	2	602	CLA	CBD-CGD-O2D-CED
15	2	603	CLA	CBD-CGD-O2D-CED
15	2	604	CLA	C1A-C2A-CAA-CBA
15	2	604	CLA	C3A-C2A-CAA-CBA
15	2	605	CLA	CBD-CGD-O2D-CED
15	2	606	CLA	CBD-CGD-O2D-CED
15	2	616	CLA	C1A-C2A-CAA-CBA
15	2	616	CLA	C3A-C2A-CAA-CBA
15	2	616	CLA	CBD-CGD-O2D-CED
15	3	601	CLA	CBD-CGD-O2D-CED
15	3	605	CLA	CBD-CGD-O2D-CED
15	3	606	CLA	CBD-CGD-O2D-CED
15	3	607	CLA	C2B-C3B-CAB-CBB
15	3	607	CLA	C4B-C3B-CAB-CBB
15	3	608	CLA	C3A-C2A-CAA-CBA
15	3	608	CLA	CBD-CGD-O2D-CED
15	3	609	CLA	CHA-CBD-CGD-O1D
15	3	609	CLA	CHA-CBD-CGD-O2D
15	3	611	CLA	CBD-CGD-O2D-CED
15	3	613	CLA	C1A-C2A-CAA-CBA
15	3	615	CLA	C1A-C2A-CAA-CBA
15	3	615	CLA	CHA-CBD-CGD-O1D
15	3	615	CLA	CHA-CBD-CGD-O2D
15	4	601	CLA	C1A-C2A-CAA-CBA
15	4	601	CLA	C3A-C2A-CAA-CBA
15	4	602	CLA	CHA-CBD-CGD-O1D
15	4	602	CLA	CHA-CBD-CGD-O2D
15	4	602	CLA	CBD-CGD-O2D-CED
15	4	604	CLA	C3A-C2A-CAA-CBA
15	4	604	CLA	CHA-CBD-CGD-O1D
15	4	604	CLA	CHA-CBD-CGD-O2D
15	4	606	CLA	CBD-CGD-O2D-CED
15	4	608	CLA	C2B-C3B-CAB-CBB
15	4	608	CLA	C4B-C3B-CAB-CBB
15	4	608	CLA	C2C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
15	4	608	CLA	C4C-C3C-CAC-CBC
15	4	616	CLA	C1A-C2A-CAA-CBA
15	4	616	CLA	C3A-C2A-CAA-CBA
15	4	616	CLA	CBD-CGD-O2D-CED
15	A	1012	CLA	CAD-CBD-CGD-O1D
15	A	1012	CLA	CAD-CBD-CGD-O2D
15	A	1012	CLA	C2-C3-C5-C6
15	A	1012	CLA	C4-C3-C5-C6
15	A	1101	CLA	CHA-CBD-CGD-O1D
15	A	1101	CLA	CHA-CBD-CGD-O2D
15	A	1102	CLA	C1A-C2A-CAA-CBA
15	A	1102	CLA	C3A-C2A-CAA-CBA
15	A	1102	CLA	CHA-CBD-CGD-O2D
15	A	1105	CLA	C1A-C2A-CAA-CBA
15	A	1106	CLA	C1A-C2A-CAA-CBA
15	A	1106	CLA	C3A-C2A-CAA-CBA
15	A	1106	CLA	CHA-CBD-CGD-O1D
15	A	1106	CLA	CHA-CBD-CGD-O2D
15	A	1112	CLA	CBD-CGD-O2D-CED
15	A	1112	CLA	O1D-CGD-O2D-CED
15	A	1114	CLA	CBD-CGD-O2D-CED
15	A	1116	CLA	C1A-C2A-CAA-CBA
15	A	1116	CLA	C3A-C2A-CAA-CBA
15	A	1117	CLA	CHA-CBD-CGD-O1D
15	A	1117	CLA	CHA-CBD-CGD-O2D
15	A	1118	CLA	CHA-CBD-CGD-O2D
15	A	1119	CLA	CBD-CGD-O2D-CED
15	A	1121	CLA	CBD-CGD-O2D-CED
15	A	1121	CLA	O1D-CGD-O2D-CED
15	A	1123	CLA	CHA-CBD-CGD-O1D
15	A	1123	CLA	CHA-CBD-CGD-O2D
15	A	1126	CLA	CBD-CGD-O2D-CED
15	A	1128	CLA	CHA-CBD-CGD-O1D
15	A	1128	CLA	CHA-CBD-CGD-O2D
15	A	1129	CLA	CBD-CGD-O2D-CED
15	A	1130	CLA	CHA-CBD-CGD-O1D
15	A	1130	CLA	CHA-CBD-CGD-O2D
15	A	1132	CLA	C2B-C3B-CAB-CBB
15	A	1132	CLA	C4B-C3B-CAB-CBB
15	A	1132	CLA	CBD-CGD-O2D-CED
15	A	1134	CLA	CHA-CBD-CGD-O1D
15	A	1134	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
15	A	1136	CLA	C2B-C3B-CAB-CBB
15	A	1136	CLA	C4B-C3B-CAB-CBB
15	A	1137	CLA	CHA-CBD-CGD-O1D
15	A	1137	CLA	CHA-CBD-CGD-O2D
15	A	1139	CLA	CBD-CGD-O2D-CED
15	A	1141	CLA	CAD-CBD-CGD-O1D
15	A	1141	CLA	CAD-CBD-CGD-O2D
15	B	1021	CLA	CBD-CGD-O2D-CED
15	B	1022	CLA	CBD-CGD-O2D-CED
15	B	1023	CLA	CBD-CGD-O2D-CED
15	B	1202	CLA	C1A-C2A-CAA-CBA
15	B	1202	CLA	C3A-C2A-CAA-CBA
15	B	1203	CLA	CBD-CGD-O2D-CED
15	B	1204	CLA	C1A-C2A-CAA-CBA
15	B	1204	CLA	C3A-C2A-CAA-CBA
15	B	1204	CLA	CHA-CBD-CGD-O1D
15	B	1204	CLA	CHA-CBD-CGD-O2D
15	B	1207	CLA	CBA-CGA-O2A-C1
15	B	1207	CLA	CAD-CBD-CGD-O1D
15	B	1207	CLA	CAD-CBD-CGD-O2D
15	B	1210	CLA	C1A-C2A-CAA-CBA
15	B	1211	CLA	CHA-CBD-CGD-O1D
15	B	1211	CLA	CHA-CBD-CGD-O2D
15	B	1212	CLA	CHA-CBD-CGD-O2D
15	B	1214	CLA	C2B-C3B-CAB-CBB
15	B	1214	CLA	C4B-C3B-CAB-CBB
15	B	1217	CLA	CBA-CGA-O2A-C1
15	B	1217	CLA	O1A-CGA-O2A-C1
15	B	1217	CLA	C2B-C3B-CAB-CBB
15	B	1217	CLA	C4B-C3B-CAB-CBB
15	B	1218	CLA	CHA-CBD-CGD-O1D
15	B	1218	CLA	CHA-CBD-CGD-O2D
15	B	1220	CLA	C2B-C3B-CAB-CBB
15	B	1220	CLA	C4B-C3B-CAB-CBB
15	B	1221	CLA	CHA-CBD-CGD-O1D
15	B	1221	CLA	CHA-CBD-CGD-O2D
15	B	1226	CLA	C11-C12-C13-C14
15	B	1227	CLA	CAD-CBD-CGD-O2D
15	B	1227	CLA	CBD-CGD-O2D-CED
15	B	1228	CLA	CBD-CGD-O2D-CED
15	B	1229	CLA	CHA-CBD-CGD-O1D
15	B	1229	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
15	B	1232	CLA	CAD-CBD-CGD-O1D
15	B	1232	CLA	CAD-CBD-CGD-O2D
15	B	1234	CLA	CHA-CBD-CGD-O1D
15	B	1234	CLA	CHA-CBD-CGD-O2D
15	B	1236	CLA	CHA-CBD-CGD-O1D
15	B	1236	CLA	CHA-CBD-CGD-O2D
15	B	1238	CLA	C1A-C2A-CAA-CBA
15	B	1238	CLA	C2C-C3C-CAC-CBC
15	B	1238	CLA	C4C-C3C-CAC-CBC
15	B	1238	CLA	C1-C2-C3-C5
15	B	1240	CLA	CBD-CGD-O2D-CED
15	F	1301	CLA	CBA-CGA-O2A-C1
16	2	613	CHL	C1A-C2A-CAA-CBA
16	2	613	CHL	C3A-C2A-CAA-CBA
16	2	613	CHL	CHA-CBD-CGD-O1D
16	2	613	CHL	CHA-CBD-CGD-O2D
16	3	604	CHL	C3A-C2A-CAA-CBA
16	4	610	CHL	C4C-C3C-CAC-CBC
17	1	801	LHG	C3-O3-P-O4
17	2	801	LHG	C3-O3-P-O6
17	2	801	LHG	C4-O6-P-O3
17	2	801	LHG	C4-O6-P-O4
17	2	801	LHG	C4-O6-P-O5
17	3	801	LHG	O2-C2-C3-O3
17	3	801	LHG	C3-O3-P-O6
17	3	801	LHG	O9-C7-O7-C5
17	A	5001	LHG	O1-C1-C2-C3
17	A	5001	LHG	C4-O6-P-O4
17	A	5002	LHG	C1-C2-C3-O3
17	A	5002	LHG	O2-C2-C3-O3
17	A	5002	LHG	C3-O3-P-O4
17	B	5001	LHG	C1-C2-C3-O3
17	B	5001	LHG	O2-C2-C3-O3
17	B	5001	LHG	C3-O3-P-O5
17	B	5001	LHG	C3-O3-P-O6
17	B	5001	LHG	C4-O6-P-O3
17	B	5001	LHG	C4-O6-P-O5
17	B	5001	LHG	C8-C7-O7-C5
18	2	803	LMG	C11-C10-O7-C8
18	2	804	LMG	O9-C10-O7-C8
18	2	804	LMG	C11-C10-O7-C8
19	A	1011	CL0	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
19	A	1011	CL0	CAD-CBD-CGD-O2D
19	A	1011	CL0	CBD-CGD-O2D-CED
22	B	5002	DGD	C2B-C1B-O2G-C2G
15	3	608	CLA	C4C-C3C-CAC-CBC
15	1	612	CLA	O1D-CGD-O2D-CED
15	1	615	CLA	O1D-CGD-O2D-CED
15	A	1126	CLA	O1D-CGD-O2D-CED
15	A	1138	CLA	O1D-CGD-O2D-CED
15	A	1139	CLA	O1D-CGD-O2D-CED
15	B	1021	CLA	O1D-CGD-O2D-CED
19	A	1011	CL0	O1D-CGD-O2D-CED
15	3	608	CLA	C2C-C3C-CAC-CBC
15	1	613	CLA	O1D-CGD-O2D-CED
15	2	602	CLA	O1D-CGD-O2D-CED
15	2	606	CLA	O1D-CGD-O2D-CED
15	A	1109	CLA	O1D-CGD-O2D-CED
15	A	1129	CLA	O1D-CGD-O2D-CED
15	B	1205	CLA	O1D-CGD-O2D-CED
15	1	608	CLA	CBD-CGD-O2D-CED
15	1	611	CLA	CBD-CGD-O2D-CED
15	1	613	CLA	CBD-CGD-O2D-CED
15	2	604	CLA	CBD-CGD-O2D-CED
15	3	603	CLA	CBD-CGD-O2D-CED
15	3	607	CLA	CBD-CGD-O2D-CED
15	4	603	CLA	CBD-CGD-O2D-CED
15	4	609	CLA	CBD-CGD-O2D-CED
15	A	1013	CLA	CBD-CGD-O2D-CED
15	A	1107	CLA	CBD-CGD-O2D-CED
15	A	1109	CLA	CBD-CGD-O2D-CED
15	A	1118	CLA	CBD-CGD-O2D-CED
15	A	1123	CLA	CBD-CGD-O2D-CED
15	A	1125	CLA	CBD-CGD-O2D-CED
15	A	1127	CLA	CBD-CGD-O2D-CED
15	A	1133	CLA	CBD-CGD-O2D-CED
15	A	1138	CLA	CBD-CGD-O2D-CED
15	A	1140	CLA	CBD-CGD-O2D-CED
15	A	1141	CLA	CBD-CGD-O2D-CED
15	B	1205	CLA	CBD-CGD-O2D-CED
15	B	1206	CLA	CBD-CGD-O2D-CED
15	B	1216	CLA	CBD-CGD-O2D-CED
15	B	1217	CLA	CBD-CGD-O2D-CED
15	B	1236	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
15	J	1302	CLA	CBD-CGD-O2D-CED
15	B	1222	CLA	O1A-CGA-O2A-C1
15	1	602	CLA	O1A-CGA-O2A-C1
15	B	1207	CLA	O1A-CGA-O2A-C1
16	4	610	CHL	C2C-C3C-CAC-CBC
15	A	1105	CLA	C2C-C3C-CAC-CBC
15	A	1132	CLA	C2C-C3C-CAC-CBC
15	1	603	CLA	O1D-CGD-O2D-CED
15	2	605	CLA	O1D-CGD-O2D-CED
15	3	605	CLA	O1D-CGD-O2D-CED
15	B	1023	CLA	O1D-CGD-O2D-CED
15	B	1203	CLA	O1D-CGD-O2D-CED
15	2	616	CLA	C13-C15-C16-C17
15	4	608	CLA	CBA-CGA-O2A-C1
15	A	1105	CLA	C4C-C3C-CAC-CBC
15	A	1132	CLA	C4C-C3C-CAC-CBC
15	A	1107	CLA	O1D-CGD-O2D-CED
15	B	1206	CLA	O1D-CGD-O2D-CED
15	B	1216	CLA	O1D-CGD-O2D-CED
15	J	1302	CLA	O1D-CGD-O2D-CED
15	B	1227	CLA	CBA-CGA-O2A-C1
15	B	1219	CLA	CBD-CGD-O2D-CED
15	2	605	CLA	O1A-CGA-O2A-C1
15	2	616	CLA	O1A-CGA-O2A-C1
15	3	603	CLA	O1A-CGA-O2A-C1
15	3	614	CLA	O1A-CGA-O2A-C1
15	4	605	CLA	O1A-CGA-O2A-C1
15	4	606	CLA	O1A-CGA-O2A-C1
15	4	607	CLA	O1A-CGA-O2A-C1
15	4	612	CLA	O1A-CGA-O2A-C1
15	4	616	CLA	O1A-CGA-O2A-C1
15	A	1012	CLA	O1A-CGA-O2A-C1
15	A	1104	CLA	O1A-CGA-O2A-C1
15	B	1021	CLA	O1A-CGA-O2A-C1
15	B	1208	CLA	O1A-CGA-O2A-C1
15	B	1213	CLA	O1A-CGA-O2A-C1
15	B	1214	CLA	O1A-CGA-O2A-C1
15	B	1227	CLA	O1A-CGA-O2A-C1
15	B	1230	CLA	O1A-CGA-O2A-C1
15	F	1302	CLA	O1A-CGA-O2A-C1
18	2	803	LMG	O10-C28-O8-C9
18	B	5003	LMG	O10-C28-O8-C9

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Mol	Chain	Res	Type	Atoms
15	4	608	CLA	O1A-CGA-O2A-C1
15	F	1301	CLA	O1A-CGA-O2A-C1
15	3	605	CLA	C2C-C3C-CAC-CBC
15	1	607	CLA	O1D-CGD-O2D-CED
15	3	603	CLA	O1D-CGD-O2D-CED
15	3	608	CLA	O1D-CGD-O2D-CED
15	3	611	CLA	O1D-CGD-O2D-CED
15	4	616	CLA	O1D-CGD-O2D-CED
15	A	1119	CLA	O1D-CGD-O2D-CED
15	A	1125	CLA	O1D-CGD-O2D-CED
15	B	1228	CLA	O1D-CGD-O2D-CED
15	1	601	CLA	O1D-CGD-O2D-CED
15	4	602	CLA	O1D-CGD-O2D-CED
15	A	1114	CLA	O1D-CGD-O2D-CED
15	A	1132	CLA	O1D-CGD-O2D-CED
15	B	1022	CLA	O1D-CGD-O2D-CED
15	B	1227	CLA	O1D-CGD-O2D-CED
15	B	1225	CLA	CBD-CGD-O2D-CED
15	3	601	CLA	O1A-CGA-O2A-C1
17	B	5001	LHG	O9-C7-O7-C5
18	2	803	LMG	O9-C10-O7-C8
22	B	5002	DGD	O1B-C1B-O2G-C2G
15	B	1209	CLA	CBA-CGA-O2A-C1
15	B	1209	CLA	O1A-CGA-O2A-C1
18	B	5003	LMG	C4-C5-C6-O5
15	2	601	CLA	C3-C5-C6-C7
15	2	605	CLA	C3-C5-C6-C7
15	A	1111	CLA	C3-C5-C6-C7
15	B	1205	CLA	C3-C5-C6-C7
15	B	1240	CLA	O1D-CGD-O2D-CED
15	4	606	CLA	CBA-CGA-O2A-C1
15	4	607	CLA	CBA-CGA-O2A-C1
15	4	612	CLA	CBA-CGA-O2A-C1
15	A	1102	CLA	CBA-CGA-O2A-C1
15	B	1214	CLA	CBA-CGA-O2A-C1
15	B	1222	CLA	CBA-CGA-O2A-C1
18	2	803	LMG	C29-C28-O8-C9
18	B	5003	LMG	C29-C28-O8-C9
15	1	602	CLA	CBD-CGD-O2D-CED
15	2	607	CLA	CBD-CGD-O2D-CED
15	3	612	CLA	CBD-CGD-O2D-CED
15	3	614	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
15	4	604	CLA	CBD-CGD-O2D-CED
15	A	1110	CLA	CBD-CGD-O2D-CED
15	A	1120	CLA	CBD-CGD-O2D-CED
15	B	1221	CLA	CBD-CGD-O2D-CED
15	B	1224	CLA	CBD-CGD-O2D-CED
15	B	1232	CLA	CBD-CGD-O2D-CED
15	B	1238	CLA	CBD-CGD-O2D-CED
15	F	1302	CLA	CBD-CGD-O2D-CED
17	3	801	LHG	C8-C7-O7-C5
15	1	611	CLA	O1D-CGD-O2D-CED
15	2	601	CLA	O1D-CGD-O2D-CED
15	2	603	CLA	O1D-CGD-O2D-CED
15	2	616	CLA	O1D-CGD-O2D-CED
15	3	601	CLA	O1D-CGD-O2D-CED
15	3	606	CLA	O1D-CGD-O2D-CED
15	4	603	CLA	O1D-CGD-O2D-CED
15	4	606	CLA	O1D-CGD-O2D-CED
15	A	1133	CLA	O1D-CGD-O2D-CED
15	1	612	CLA	C2C-C3C-CAC-CBC
15	B	1234	CLA	C2C-C3C-CAC-CBC
15	1	603	CLA	C4-C3-C5-C6
15	3	606	CLA	C4-C3-C5-C6
15	A	1013	CLA	C4-C3-C5-C6
15	A	1108	CLA	C4-C3-C5-C6
15	A	1112	CLA	C4-C3-C5-C6
15	A	1133	CLA	C4-C3-C5-C6
15	A	1137	CLA	C4-C3-C5-C6
15	A	1140	CLA	C4-C3-C5-C6
15	B	1225	CLA	C4-C3-C5-C6
15	B	1235	CLA	C4-C3-C5-C6
15	3	606	CLA	C2-C3-C5-C6
15	A	1013	CLA	C2-C3-C5-C6
15	A	1108	CLA	C2-C3-C5-C6
15	A	1133	CLA	C2-C3-C5-C6
15	A	1137	CLA	C2-C3-C5-C6
15	A	1140	CLA	C2-C3-C5-C6
15	B	1225	CLA	C2-C3-C5-C6
15	B	1235	CLA	C2-C3-C5-C6
15	B	1209	CLA	CBD-CGD-O2D-CED
15	B	1222	CLA	CBD-CGD-O2D-CED
15	B	1237	CLA	CBD-CGD-O2D-CED
15	2	604	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
15	A	1122	CLA	C2A-CAA-CBA-CGA
15	3	611	CLA	C3-C5-C6-C7
15	4	603	CLA	C3-C5-C6-C7
15	4	609	CLA	C3-C5-C6-C7
15	A	1116	CLA	C3-C5-C6-C7
15	A	1137	CLA	C3-C5-C6-C7
20	B	2002	PQN	C13-C15-C16-C17
15	1	603	CLA	CBA-CGA-O2A-C1
15	1	606	CLA	CBA-CGA-O2A-C1
15	1	608	CLA	CBA-CGA-O2A-C1
15	2	605	CLA	CBA-CGA-O2A-C1
15	2	616	CLA	CBA-CGA-O2A-C1
15	3	601	CLA	CBA-CGA-O2A-C1
15	3	603	CLA	CBA-CGA-O2A-C1
15	3	614	CLA	CBA-CGA-O2A-C1
15	4	605	CLA	CBA-CGA-O2A-C1
15	4	616	CLA	CBA-CGA-O2A-C1
15	A	1012	CLA	CBA-CGA-O2A-C1
15	A	1101	CLA	CBA-CGA-O2A-C1
15	A	1104	CLA	CBA-CGA-O2A-C1
15	B	1021	CLA	CBA-CGA-O2A-C1
15	B	1208	CLA	CBA-CGA-O2A-C1
15	B	1213	CLA	CBA-CGA-O2A-C1
15	B	1229	CLA	CBA-CGA-O2A-C1
15	B	1230	CLA	CBA-CGA-O2A-C1
15	F	1302	CLA	CBA-CGA-O2A-C1
17	1	801	LHG	C24-C23-O8-C6
17	3	801	LHG	C24-C23-O8-C6
18	B	5003	LMG	O6-C5-C6-O5
13	1	502	XAT	C9-C10-C11-C12
13	1	502	XAT	C33-C34-C35-C15
13	2	502	XAT	C9-C10-C11-C12
13	3	502	XAT	C9-C10-C11-C12
13	3	502	XAT	C13-C14-C15-C35
13	4	502	XAT	C9-C10-C11-C12
14	A	4002	BCR	C9-C10-C11-C12
14	A	4003	BCR	C19-C20-C21-C22
14	A	4007	BCR	C13-C14-C15-C16
14	B	4001	BCR	C19-C20-C21-C22
15	1	603	CLA	O1A-CGA-O2A-C1
15	1	605	CLA	O1A-CGA-O2A-C1
15	1	606	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
15	1	608	CLA	O1A-CGA-O2A-C1
15	3	610	CLA	O1A-CGA-O2A-C1
15	4	603	CLA	O1A-CGA-O2A-C1
15	A	1101	CLA	O1A-CGA-O2A-C1
15	A	1102	CLA	O1A-CGA-O2A-C1
15	A	1111	CLA	O1A-CGA-O2A-C1
15	A	1119	CLA	O1A-CGA-O2A-C1
15	B	1211	CLA	O1A-CGA-O2A-C1
15	B	1221	CLA	O1A-CGA-O2A-C1
17	3	801	LHG	O10-C23-O8-C6
15	A	1127	CLA	O1D-CGD-O2D-CED
15	3	605	CLA	C4C-C3C-CAC-CBC
15	A	1140	CLA	O1D-CGD-O2D-CED
15	3	608	CLA	C3-C5-C6-C7
15	A	1012	CLA	C3-C5-C6-C7
15	A	1106	CLA	C3-C5-C6-C7
15	A	1110	CLA	C3-C5-C6-C7
15	B	1227	CLA	C3-C5-C6-C7
15	3	609	CLA	CBD-CGD-O2D-CED
15	A	1113	CLA	CBD-CGD-O2D-CED
17	1	801	LHG	O2-C2-C3-O3
15	1	608	CLA	O1D-CGD-O2D-CED
15	3	607	CLA	O1D-CGD-O2D-CED
15	A	1123	CLA	O1D-CGD-O2D-CED
15	B	1236	CLA	O1D-CGD-O2D-CED
15	1	605	CLA	CBA-CGA-O2A-C1
15	2	601	CLA	CBA-CGA-O2A-C1
15	2	603	CLA	CBA-CGA-O2A-C1
15	2	604	CLA	CBA-CGA-O2A-C1
15	3	610	CLA	CBA-CGA-O2A-C1
15	A	1111	CLA	CBA-CGA-O2A-C1
15	A	1126	CLA	CBA-CGA-O2A-C1
15	B	1211	CLA	CBA-CGA-O2A-C1
15	B	1219	CLA	CBA-CGA-O2A-C1
15	B	1231	CLA	CBA-CGA-O2A-C1
19	A	1011	CL0	CBA-CGA-O2A-C1
15	A	1126	CLA	O1A-CGA-O2A-C1
15	B	1207	CLA	C2C-C3C-CAC-CBC
15	B	1207	CLA	CBD-CGD-O2D-CED
15	B	1229	CLA	O1A-CGA-O2A-C1
15	A	1118	CLA	O1D-CGD-O2D-CED
15	A	1125	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
15	B	1230	CLA	C3-C5-C6-C7
15	B	1234	CLA	C4C-C3C-CAC-CBC
15	4	609	CLA	O1D-CGD-O2D-CED
15	4	603	CLA	CBA-CGA-O2A-C1
15	A	1119	CLA	CBA-CGA-O2A-C1
15	B	1221	CLA	CBA-CGA-O2A-C1
15	3	603	CLA	C4-C3-C5-C6
15	4	601	CLA	C4-C3-C5-C6
15	A	1109	CLA	C4-C3-C5-C6
15	1	605	CLA	C2-C3-C5-C6
15	3	603	CLA	C2-C3-C5-C6
15	4	601	CLA	C2-C3-C5-C6
15	A	1109	CLA	C2-C3-C5-C6
15	B	1238	CLA	C2-C3-C5-C6
15	2	601	CLA	O1A-CGA-O2A-C1
15	2	603	CLA	O1A-CGA-O2A-C1
17	B	5001	LHG	O10-C23-O8-C6
19	A	1011	CL0	O1A-CGA-O2A-C1
15	B	1217	CLA	O1D-CGD-O2D-CED
15	1	608	CLA	C2A-CAA-CBA-CGA
15	A	1132	CLA	C2A-CAA-CBA-CGA
15	B	1228	CLA	C2A-CAA-CBA-CGA
15	B	1229	CLA	C2A-CAA-CBA-CGA
15	2	604	CLA	O1A-CGA-O2A-C1
15	B	1219	CLA	O1A-CGA-O2A-C1
15	B	1231	CLA	O1A-CGA-O2A-C1
18	2	804	LMG	O6-C1-O1-C7
15	A	1141	CLA	O1D-CGD-O2D-CED
15	A	1105	CLA	CBA-CGA-O2A-C1
15	4	601	CLA	CBD-CGD-O2D-CED
15	B	1211	CLA	CBD-CGD-O2D-CED
15	B	1231	CLA	CBD-CGD-O2D-CED
15	F	1301	CLA	CBD-CGD-O2D-CED
15	B	1232	CLA	CBA-CGA-O2A-C1
17	1	801	LHG	O10-C23-O8-C6
15	B	1225	CLA	O1D-CGD-O2D-CED
15	1	612	CLA	C4C-C3C-CAC-CBC
15	3	607	CLA	C3-C5-C6-C7
15	A	1013	CLA	O1D-CGD-O2D-CED
14	1	503	BCR	C13-C14-C15-C16
14	4	503	BCR	C9-C10-C11-C12
14	F	4001	BCR	C19-C20-C21-C22

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Mol	Chain	Res	Type	Atoms
15	A	1105	CLA	O1A-CGA-O2A-C1
17	1	801	LHG	O9-C7-O7-C5
15	3	607	CLA	CBA-CGA-O2A-C1
15	3	608	CLA	CBA-CGA-O2A-C1
15	4	604	CLA	CBA-CGA-O2A-C1
15	A	1110	CLA	CBA-CGA-O2A-C1
15	A	1125	CLA	CBA-CGA-O2A-C1
15	A	1128	CLA	CBA-CGA-O2A-C1
15	A	1135	CLA	CBA-CGA-O2A-C1
15	A	1139	CLA	CBA-CGA-O2A-C1
15	B	1215	CLA	CBA-CGA-O2A-C1
15	B	1220	CLA	CBA-CGA-O2A-C1
15	B	1225	CLA	CBA-CGA-O2A-C1
17	B	5001	LHG	C24-C23-O8-C6
18	2	804	LMG	C29-C28-O8-C9
15	B	1234	CLA	CBD-CGD-O2D-CED
15	1	615	CLA	C2C-C3C-CAC-CBC
15	1	602	CLA	O1D-CGD-O2D-CED
15	B	1219	CLA	O1D-CGD-O2D-CED
15	1	605	CLA	C4-C3-C5-C6
15	1	603	CLA	C2-C3-C5-C6
15	A	1112	CLA	C2-C3-C5-C6
15	1	608	CLA	C3-C5-C6-C7
15	1	603	CLA	C6-C7-C8-C9
15	2	607	CLA	C11-C10-C8-C9
15	3	605	CLA	C14-C13-C15-C16
15	A	1102	CLA	C11-C10-C8-C9
15	A	1104	CLA	C14-C13-C15-C16
15	A	1106	CLA	C11-C12-C13-C14
15	A	1133	CLA	C11-C10-C8-C9
15	B	1023	CLA	C6-C7-C8-C9
15	B	1222	CLA	C11-C10-C8-C9
16	1	609	CHL	C11-C10-C8-C9
19	A	1011	CL0	C11-C10-C8-C9
15	A	1110	CLA	O1D-CGD-O2D-CED
18	2	804	LMG	C2-C1-O1-C7
17	2	801	LHG	O2-C2-C3-O3
15	3	612	CLA	O1D-CGD-O2D-CED
15	B	1224	CLA	O1D-CGD-O2D-CED
15	A	1125	CLA	O1A-CGA-O2A-C1
12	1	501	LUT	C11-C12-C13-C20
12	1	501	LUT	C27-C28-C29-C39

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Mol	Chain	Res	Type	Atoms
12	1	501	LUT	C31-C32-C33-C40
12	3	501	LUT	C31-C32-C33-C40
12	4	501	LUT	C11-C12-C13-C20
12	4	501	LUT	C31-C32-C33-C40
13	2	502	XAT	C7-C8-C9-C19
13	2	502	XAT	C31-C32-C33-C40
13	3	502	XAT	C11-C12-C13-C20
14	1	503	BCR	C7-C8-C9-C34
14	3	503	BCR	C11-C12-C13-C35
14	3	503	BCR	C37-C22-C23-C24
14	3	506	BCR	C7-C8-C9-C34
14	4	503	BCR	C36-C18-C19-C20
14	A	4002	BCR	C36-C18-C19-C20
14	A	4003	BCR	C7-C8-C9-C34
14	A	4003	BCR	C37-C22-C23-C24
14	A	4004	BCR	C36-C18-C19-C20
14	A	4005	BCR	C11-C12-C13-C35
14	A	4005	BCR	C36-C18-C19-C20
14	A	4006	BCR	C11-C12-C13-C35
14	A	4007	BCR	C7-C8-C9-C34
14	A	4007	BCR	C11-C12-C13-C35
14	A	4007	BCR	C37-C22-C23-C24
14	A	4008	BCR	C7-C8-C9-C34
14	A	4008	BCR	C36-C18-C19-C20
14	A	4008	BCR	C37-C22-C23-C24
14	B	4001	BCR	C7-C8-C9-C34
14	B	4001	BCR	C11-C12-C13-C35
14	B	4002	BCR	C7-C8-C9-C34
14	B	4002	BCR	C11-C12-C13-C35
14	B	4003	BCR	C7-C8-C9-C34
14	B	4004	BCR	C11-C12-C13-C35
14	B	4005	BCR	C7-C8-C9-C34
14	F	4001	BCR	C7-C8-C9-C34
14	F	4002	BCR	C7-C8-C9-C34
14	F	4002	BCR	C36-C18-C19-C20
14	J	4002	BCR	C11-C12-C13-C35
12	1	501	LUT	C27-C28-C29-C30
12	1	501	LUT	C31-C32-C33-C34
12	3	501	LUT	C31-C32-C33-C34
13	2	502	XAT	C7-C8-C9-C10
13	2	502	XAT	C11-C12-C13-C14
13	3	502	XAT	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
13	4	502	XAT	C7-C8-C9-C10
13	4	502	XAT	C11-C12-C13-C14
14	1	503	BCR	C11-C12-C13-C14
14	4	503	BCR	C11-C12-C13-C14
14	A	4002	BCR	C7-C8-C9-C10
14	A	4002	BCR	C11-C12-C13-C14
14	A	4004	BCR	C11-C12-C13-C14
14	A	4006	BCR	C11-C12-C13-C14
14	A	4008	BCR	C21-C22-C23-C24
14	B	4003	BCR	C21-C22-C23-C24
15	A	1105	CLA	C2A-CAA-CBA-CGA
15	A	1111	CLA	C2A-CAA-CBA-CGA
15	B	1220	CLA	C2A-CAA-CBA-CGA
15	3	608	CLA	O1A-CGA-O2A-C1
15	A	1110	CLA	O1A-CGA-O2A-C1
15	A	1135	CLA	O1A-CGA-O2A-C1
15	A	1139	CLA	O1A-CGA-O2A-C1
15	B	1215	CLA	O1A-CGA-O2A-C1
22	B	5002	DGD	O2G-C2G-C3G-O3G
17	2	801	LHG	C24-C23-O8-C6
15	1	603	CLA	C8-C10-C11-C12
15	2	606	CLA	C2C-C3C-CAC-CBC
15	2	616	CLA	C2-C1-O2A-CGA
15	B	1221	CLA	O1D-CGD-O2D-CED
15	F	1302	CLA	O1D-CGD-O2D-CED
15	4	603	CLA	C10-C11-C12-C13
15	B	1227	CLA	C10-C11-C12-C13
17	A	5001	LHG	O1-C1-C2-O2
15	4	612	CLA	C3-C5-C6-C7
15	B	1232	CLA	O1D-CGD-O2D-CED
15	B	1225	CLA	O1A-CGA-O2A-C1
15	B	1202	CLA	CBD-CGD-O2D-CED
18	2	804	LMG	O6-C5-C6-O5
15	B	1240	CLA	CBA-CGA-O2A-C1
18	4	801	LMG	C28-C29-C30-C31
12	4	501	LUT	C9-C10-C11-C12
13	1	502	XAT	C13-C14-C15-C35
13	2	502	XAT	C29-C30-C31-C32
14	A	4002	BCR	C19-C20-C21-C22
14	A	4007	BCR	C15-C16-C17-C18
14	B	4001	BCR	C13-C14-C15-C16
14	B	4003	BCR	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
15	2	607	CLA	O1D-CGD-O2D-CED
15	3	614	CLA	O1D-CGD-O2D-CED
15	A	1120	CLA	O1D-CGD-O2D-CED
15	B	1222	CLA	O1D-CGD-O2D-CED
15	B	1201	CLA	C2A-CAA-CBA-CGA
15	B	1211	CLA	C13-C15-C16-C17
15	3	607	CLA	O1A-CGA-O2A-C1
15	4	604	CLA	O1A-CGA-O2A-C1
15	B	1220	CLA	O1A-CGA-O2A-C1
15	B	1238	CLA	O1D-CGD-O2D-CED
15	1	605	CLA	C8-C10-C11-C12
15	4	607	CLA	C5-C6-C7-C8
15	4	612	CLA	C5-C6-C7-C8
15	A	1101	CLA	C5-C6-C7-C8
15	A	1109	CLA	C15-C16-C17-C18
15	A	1128	CLA	C15-C16-C17-C18
15	A	1138	CLA	C5-C6-C7-C8
15	A	1138	CLA	C8-C10-C11-C12
15	B	1227	CLA	C15-C16-C17-C18
16	4	613	CHL	C8-C10-C11-C12
15	1	615	CLA	C2A-CAA-CBA-CGA
15	A	1012	CLA	C2A-CAA-CBA-CGA
15	A	1119	CLA	C2A-CAA-CBA-CGA
15	A	1127	CLA	C2A-CAA-CBA-CGA
15	B	1207	CLA	C2A-CAA-CBA-CGA
15	B	1225	CLA	C2A-CAA-CBA-CGA
16	1	610	CHL	C2A-CAA-CBA-CGA
16	4	610	CHL	C2A-CAA-CBA-CGA
14	A	4005	BCR	C18-C19-C20-C21
15	A	1114	CLA	C5-C6-C7-C8
15	A	1123	CLA	C8-C10-C11-C12
17	1	801	LHG	C23-C24-C25-C26
17	2	801	LHG	C23-C24-C25-C26
17	3	801	LHG	C23-C24-C25-C26
18	B	5003	LMG	C28-C29-C30-C31
14	J	4001	BCR	C22-C23-C24-C25
15	3	606	CLA	C5-C6-C7-C8
15	A	1102	CLA	C10-C11-C12-C13
15	A	1122	CLA	C5-C6-C7-C8
15	A	1123	CLA	C10-C11-C12-C13
15	A	1128	CLA	O1A-CGA-O2A-C1
17	A	5002	LHG	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
15	4	605	CLA	C13-C15-C16-C17
15	B	1022	CLA	C13-C15-C16-C17
15	B	1207	CLA	C4C-C3C-CAC-CBC
15	4	604	CLA	O1D-CGD-O2D-CED
15	B	1209	CLA	O1D-CGD-O2D-CED
15	A	1119	CLA	C5-C6-C7-C8
15	A	1139	CLA	C8-C10-C11-C12
15	B	1203	CLA	C5-C6-C7-C8
15	B	1238	CLA	C5-C6-C7-C8
15	1	607	CLA	C2C-C3C-CAC-CBC
15	3	609	CLA	O1D-CGD-O2D-CED
15	A	1113	CLA	O1D-CGD-O2D-CED
15	B	1237	CLA	O1D-CGD-O2D-CED
15	A	1133	CLA	C13-C15-C16-C17
15	B	1021	CLA	C13-C15-C16-C17
16	1	609	CHL	C13-C15-C16-C17
15	3	605	CLA	CBA-CGA-O2A-C1
15	B	1234	CLA	CBA-CGA-O2A-C1
15	1	611	CLA	O2A-C1-C2-C3
15	3	601	CLA	C3-C5-C6-C7
15	B	1221	CLA	C3-C5-C6-C7
12	1	501	LUT	C29-C30-C31-C32
13	1	502	XAT	C29-C30-C31-C32
13	2	502	XAT	C13-C14-C15-C35
14	1	503	BCR	C19-C20-C21-C22
14	A	4006	BCR	C9-C10-C11-C12
14	B	4003	BCR	C13-C14-C15-C16
14	J	4002	BCR	C13-C14-C15-C16
15	4	604	CLA	C10-C11-C12-C13
15	A	1106	CLA	C5-C6-C7-C8
15	A	1122	CLA	C10-C11-C12-C13
16	1	609	CHL	C5-C6-C7-C8
20	A	2001	PQN	C23-C25-C26-C27
17	2	801	LHG	O9-C7-O7-C5
17	2	801	LHG	C1-C2-C3-O3
17	3	801	LHG	C1-C2-C3-O3
15	2	602	CLA	C2A-CAA-CBA-CGA
15	A	1130	CLA	C2A-CAA-CBA-CGA
15	A	1108	CLA	CBA-CGA-O2A-C1
15	A	1109	CLA	CBA-CGA-O2A-C1
15	A	1114	CLA	CBA-CGA-O2A-C1
15	B	1022	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
15	B	1216	CLA	CBA-CGA-O2A-C1
15	B	1228	CLA	CBA-CGA-O2A-C1
15	3	603	CLA	C13-C15-C16-C17
15	A	1101	CLA	C13-C15-C16-C17
15	A	1123	CLA	C13-C15-C16-C17
15	B	1219	CLA	C8-C10-C11-C12
15	B	1219	CLA	C13-C15-C16-C17
15	B	1226	CLA	C15-C16-C17-C18
16	2	609	CHL	C13-C15-C16-C17
20	B	2002	PQN	C20-C21-C22-C23
15	2	605	CLA	C10-C11-C12-C13
15	2	607	CLA	C10-C11-C12-C13
15	2	616	CLA	C15-C16-C17-C18
15	3	603	CLA	C5-C6-C7-C8
15	A	1117	CLA	C15-C16-C17-C18
15	A	1126	CLA	C15-C16-C17-C18
19	A	1011	CL0	C5-C6-C7-C8
15	3	615	CLA	CBD-CGD-O2D-CED
15	A	1101	CLA	CBD-CGD-O2D-CED
15	4	607	CLA	C8-C10-C11-C12
15	A	1129	CLA	C5-C6-C7-C8
15	B	1222	CLA	C5-C6-C7-C8
15	B	1225	CLA	C5-C6-C7-C8
16	2	609	CHL	C5-C6-C7-C8
16	2	609	CHL	C10-C11-C12-C13
15	4	609	CLA	CBA-CGA-O2A-C1
16	2	610	CHL	C2A-CAA-CBA-CGA
15	A	1140	CLA	C10-C11-C12-C13
15	A	1013	CLA	C3-C5-C6-C7
15	A	1105	CLA	C3-C5-C6-C7
15	B	1240	CLA	O1A-CGA-O2A-C1
15	B	1227	CLA	C13-C15-C16-C17
15	B	1207	CLA	O1D-CGD-O2D-CED
15	A	1103	CLA	CBA-CGA-O2A-C1
15	B	1236	CLA	CBA-CGA-O2A-C1
14	2	503	BCR	C11-C10-C9-C34
14	3	503	BCR	C35-C13-C14-C15
14	3	504	BCR	C20-C21-C22-C37
14	3	506	BCR	C35-C13-C14-C15
14	A	4004	BCR	C16-C17-C18-C36
14	A	4005	BCR	C11-C10-C9-C34
14	A	4005	BCR	C16-C17-C18-C36

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Mol	Chain	Res	Type	Atoms
14	A	4008	BCR	C35-C13-C14-C15
14	B	4001	BCR	C16-C17-C18-C36
14	B	4001	BCR	C20-C21-C22-C37
14	B	4002	BCR	C20-C21-C22-C37
14	B	4006	BCR	C11-C10-C9-C34
14	F	4001	BCR	C16-C17-C18-C36
14	J	4002	BCR	C20-C21-C22-C37
15	A	1109	CLA	C10-C11-C12-C13
15	A	1111	CLA	C15-C16-C17-C18
15	B	1021	CLA	C8-C10-C11-C12
12	1	501	LUT	C7-C8-C9-C19
12	2	501	LUT	C27-C28-C29-C39
12	3	501	LUT	C11-C12-C13-C20
12	4	501	LUT	C27-C28-C29-C39
13	2	502	XAT	C11-C12-C13-C20
13	4	502	XAT	C11-C12-C13-C20
14	2	503	BCR	C37-C22-C23-C24
14	A	4002	BCR	C11-C12-C13-C35
14	A	4004	BCR	C11-C12-C13-C35
14	A	4006	BCR	C37-C22-C23-C24
14	F	4001	BCR	C36-C18-C19-C20
17	3	801	LHG	C2-C3-O3-P
12	3	501	LUT	C11-C12-C13-C14
12	4	501	LUT	C27-C28-C29-C30
14	2	503	BCR	C17-C18-C19-C20
14	A	4003	BCR	C21-C22-C23-C24
14	A	4005	BCR	C17-C18-C19-C20
14	F	4001	BCR	C7-C8-C9-C10
15	A	1108	CLA	O1A-CGA-O2A-C1
15	A	1109	CLA	O1A-CGA-O2A-C1
15	B	1234	CLA	O1A-CGA-O2A-C1
15	3	605	CLA	C2A-CAA-CBA-CGA
15	3	607	CLA	C2A-CAA-CBA-CGA
15	B	1021	CLA	C2A-CAA-CBA-CGA
15	B	1213	CLA	C2A-CAA-CBA-CGA
15	B	1215	CLA	C2A-CAA-CBA-CGA
15	4	605	CLA	C10-C11-C12-C13
17	1	801	LHG	O1-C1-C2-C3
17	A	5002	LHG	O1-C1-C2-C3
17	B	5001	LHG	O1-C1-C2-C3
15	2	601	CLA	C16-C17-C18-C19
15	A	1124	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
15	3	605	CLA	O1A-CGA-O2A-C1
15	A	1105	CLA	C10-C11-C12-C13
14	2	503	BCR	C20-C21-C22-C23
14	3	506	BCR	C11-C10-C9-C8
14	3	506	BCR	C20-C21-C22-C23
14	A	4003	BCR	C11-C10-C9-C8
14	A	4006	BCR	C11-C10-C9-C8
14	A	4007	BCR	C16-C17-C18-C19
14	B	4001	BCR	C12-C13-C14-C15
14	B	4002	BCR	C11-C10-C9-C8
14	B	4002	BCR	C16-C17-C18-C19
14	B	4003	BCR	C16-C17-C18-C19
14	B	4004	BCR	C11-C10-C9-C8
14	B	4004	BCR	C20-C21-C22-C23
14	B	4005	BCR	C11-C10-C9-C8
14	B	4005	BCR	C20-C21-C22-C23
14	B	4006	BCR	C12-C13-C14-C15
14	F	4001	BCR	C20-C21-C22-C23
14	F	4002	BCR	C11-C10-C9-C8
14	F	4002	BCR	C16-C17-C18-C19
14	J	4001	BCR	C11-C10-C9-C8
14	J	4001	BCR	C20-C21-C22-C23
14	J	4002	BCR	C16-C17-C18-C19
18	2	803	LMG	O6-C1-O1-C7
15	2	605	CLA	C5-C6-C7-C8
15	4	603	CLA	C5-C6-C7-C8
15	A	1109	CLA	C13-C15-C16-C17
15	A	1108	CLA	CBD-CGD-O2D-CED
15	B	1226	CLA	CBD-CGD-O2D-CED
15	A	1126	CLA	C2-C1-O2A-CGA
15	1	605	CLA	C16-C17-C18-C19
15	2	601	CLA	C16-C17-C18-C20
15	4	607	CLA	C11-C12-C13-C15
15	A	1110	CLA	C6-C7-C8-C9
15	A	1112	CLA	C16-C17-C18-C20
15	B	1211	CLA	C16-C17-C18-C19
15	B	1022	CLA	O1A-CGA-O2A-C1
15	B	1228	CLA	O1A-CGA-O2A-C1
16	1	609	CHL	C10-C11-C12-C13
17	A	5001	LHG	C30-C31-C32-C33
14	3	506	BCR	C14-C15-C16-C17
18	2	803	LMG	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
17	A	5001	LHG	C23-C24-C25-C26
15	3	611	CLA	C8-C10-C11-C12
18	2	804	LMG	C29-C30-C31-C32
17	1	801	LHG	O1-C1-C2-O2
17	1	801	LHG	C12-C13-C14-C15
15	4	601	CLA	O1D-CGD-O2D-CED
15	B	1231	CLA	O1D-CGD-O2D-CED
15	4	601	CLA	C4B-C3B-CAB-CBB
15	A	1012	CLA	C4B-C3B-CAB-CBB
15	A	1122	CLA	C4B-C3B-CAB-CBB
15	B	1227	CLA	C4B-C3B-CAB-CBB
15	1	605	CLA	C16-C17-C18-C20
15	4	607	CLA	C11-C12-C13-C14
15	A	1124	CLA	C11-C12-C13-C15
15	A	1128	CLA	C16-C17-C18-C20
15	B	1023	CLA	C2A-CAA-CBA-CGA
15	2	603	CLA	C5-C6-C7-C8
15	A	1013	CLA	C10-C11-C12-C13
15	B	1021	CLA	C15-C16-C17-C18
15	A	1104	CLA	CBD-CGD-O2D-CED
15	A	1131	CLA	CBD-CGD-O2D-CED
18	2	802	LMG	C11-C10-O7-C8
18	2	802	LMG	C38-C39-C40-C41
15	1	602	CLA	C3A-C2A-CAA-CBA
15	1	613	CLA	C3A-C2A-CAA-CBA
15	1	615	CLA	C3A-C2A-CAA-CBA
15	3	613	CLA	C3A-C2A-CAA-CBA
15	4	605	CLA	C3A-C2A-CAA-CBA
15	A	1101	CLA	C3A-C2A-CAA-CBA
15	A	1103	CLA	C3A-C2A-CAA-CBA
15	A	1104	CLA	C3A-C2A-CAA-CBA
15	B	1207	CLA	C3A-C2A-CAA-CBA
15	B	1210	CLA	C3A-C2A-CAA-CBA
15	A	1110	CLA	C6-C7-C8-C10
15	A	1128	CLA	C16-C17-C18-C19
15	A	1114	CLA	O1A-CGA-O2A-C1
15	B	1232	CLA	O1A-CGA-O2A-C1
17	1	801	LHG	C29-C30-C31-C32
15	1	615	CLA	C4C-C3C-CAC-CBC
17	A	5002	LHG	C17-C18-C19-C20
18	B	5003	LMG	C30-C31-C32-C33
15	B	1222	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
17	B	5001	LHG	C16-C17-C18-C19
15	4	609	CLA	O1A-CGA-O2A-C1
15	A	1103	CLA	O1A-CGA-O2A-C1
18	2	804	LMG	O10-C28-O8-C9
17	B	5001	LHG	C13-C14-C15-C16
15	F	1301	CLA	O1D-CGD-O2D-CED
15	1	604	CLA	C16-C17-C18-C19
15	B	1236	CLA	O1A-CGA-O2A-C1
14	1	503	BCR	C23-C24-C25-C26
14	1	503	BCR	C23-C24-C25-C30
14	2	503	BCR	C1-C6-C7-C8
14	2	503	BCR	C5-C6-C7-C8
14	A	4003	BCR	C23-C24-C25-C30
14	B	4001	BCR	C1-C6-C7-C8
14	B	4001	BCR	C5-C6-C7-C8
14	B	4003	BCR	C1-C6-C7-C8
14	B	4003	BCR	C23-C24-C25-C26
14	B	4003	BCR	C23-C24-C25-C30
14	B	4005	BCR	C23-C24-C25-C26
14	B	4005	BCR	C23-C24-C25-C30
14	F	4001	BCR	C23-C24-C25-C30
14	J	4001	BCR	C23-C24-C25-C26
14	J	4001	BCR	C23-C24-C25-C30
15	A	1012	CLA	C2B-C3B-CAB-CBB
18	4	801	LMG	C33-C34-C35-C36
15	A	1112	CLA	C8-C10-C11-C12
17	3	801	LHG	C5-C4-O6-P
15	2	603	CLA	C2A-CAA-CBA-CGA
15	B	1214	CLA	C2A-CAA-CBA-CGA
18	2	802	LMG	C10-C11-C12-C13
15	B	1216	CLA	O1A-CGA-O2A-C1
14	2	503	BCR	C18-C19-C20-C21
14	3	503	BCR	C10-C11-C12-C13
14	3	503	BCR	C18-C19-C20-C21
14	3	504	BCR	C18-C19-C20-C21
14	B	4001	BCR	C10-C11-C12-C13
14	B	4006	BCR	C18-C19-C20-C21
15	A	1112	CLA	C16-C17-C18-C19
15	A	1126	CLA	C4C-C3C-CAC-CBC
15	A	1126	CLA	C2C-C3C-CAC-CBC
15	A	1122	CLA	CBA-CGA-O2A-C1
15	3	608	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
17	3	801	LHG	C12-C13-C14-C15
22	B	5002	DGD	CAB-CBB-CCB-CDB
14	A	4002	BCR	C22-C23-C24-C25
14	J	4002	BCR	C22-C23-C24-C25
15	2	605	CLA	C8-C10-C11-C12
15	3	603	CLA	C15-C16-C17-C18
15	4	601	CLA	C5-C6-C7-C8
15	A	1137	CLA	C8-C10-C11-C12
17	A	5001	LHG	O10-C23-O8-C6
17	B	5001	LHG	C27-C28-C29-C30
17	A	5001	LHG	C10-C11-C12-C13
15	B	1023	CLA	CBA-CGA-O2A-C1
12	1	501	LUT	C9-C10-C11-C12
12	3	501	LUT	C29-C30-C31-C32
13	3	502	XAT	C33-C34-C35-C15
14	J	4002	BCR	C9-C10-C11-C12
15	B	1220	CLA	CBD-CGD-O2D-CED
17	1	801	LHG	C8-C7-O7-C5
17	2	801	LHG	C8-C7-O7-C5
17	2	801	LHG	C28-C29-C30-C31
15	B	1223	CLA	C10-C11-C12-C13
15	B	1240	CLA	C13-C15-C16-C17
18	2	802	LMG	O9-C10-O7-C8
17	1	801	LHG	C26-C27-C28-C29
17	1	801	LHG	C28-C29-C30-C31
12	2	501	LUT	C11-C12-C13-C20
13	1	502	XAT	C7-C8-C9-C19
14	B	4003	BCR	C36-C18-C19-C20
14	F	4001	BCR	C11-C12-C13-C35
14	3	503	BCR	C21-C22-C23-C24
14	A	4002	BCR	C17-C18-C19-C20
14	A	4002	BCR	C21-C22-C23-C24
14	A	4003	BCR	C11-C12-C13-C14
15	A	1110	CLA	C2A-CAA-CBA-CGA
15	1	604	CLA	C16-C17-C18-C20
15	2	604	CLA	C16-C17-C18-C19
15	2	604	CLA	C16-C17-C18-C20
15	B	1211	CLA	C16-C17-C18-C20
19	A	1011	CL0	C16-C17-C18-C20
17	A	5001	LHG	C32-C33-C34-C35
15	A	1138	CLA	C4-C3-C5-C6
15	B	1212	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
15	B	1221	CLA	C15-C16-C17-C18
15	B	1208	CLA	C2C-C3C-CAC-CBC
15	B	1211	CLA	O1D-CGD-O2D-CED
15	A	1114	CLA	C3-C5-C6-C7
15	2	612	CLA	C5-C6-C7-C8
15	3	611	CLA	C10-C11-C12-C13
15	4	607	CLA	C10-C11-C12-C13
15	A	1013	CLA	C15-C16-C17-C18
15	A	1106	CLA	C15-C16-C17-C18
15	A	1123	CLA	C5-C6-C7-C8
15	B	1208	CLA	C8-C10-C11-C12
15	B	1228	CLA	C10-C11-C12-C13
17	A	5002	LHG	C11-C10-C9-C8
15	2	606	CLA	C4C-C3C-CAC-CBC
18	2	803	LMG	C14-C15-C16-C17
15	B	1230	CLA	C5-C6-C7-C8
15	B	1231	CLA	C8-C10-C11-C12
15	3	601	CLA	C5-C6-C7-C8
15	B	1212	CLA	C3-C5-C6-C7
17	A	5002	LHG	O7-C5-C6-O8
17	A	5002	LHG	C13-C14-C15-C16
15	A	1012	CLA	C2-C1-O2A-CGA
15	1	601	CLA	C10-C11-C12-C13
15	A	1138	CLA	C2-C3-C5-C6
15	B	1210	CLA	C2-C3-C5-C6
15	A	1115	CLA	C2A-CAA-CBA-CGA
15	A	1134	CLA	CBD-CGD-O2D-CED
18	2	803	LMG	C29-C30-C31-C32
15	A	1104	CLA	C10-C11-C12-C13
15	A	1112	CLA	C5-C6-C7-C8
15	B	1231	CLA	C5-C6-C7-C8
18	B	5003	LMG	C11-C10-O7-C8
17	A	5002	LHG	O1-C1-C2-O2
15	B	1023	CLA	O1A-CGA-O2A-C1
18	4	801	LMG	O10-C28-O8-C9
15	1	602	CLA	C1A-C2A-CAA-CBA
15	1	613	CLA	C1A-C2A-CAA-CBA
15	1	615	CLA	C1A-C2A-CAA-CBA
15	3	606	CLA	C1A-C2A-CAA-CBA
15	3	608	CLA	C1A-C2A-CAA-CBA
15	4	604	CLA	C1A-C2A-CAA-CBA
15	4	605	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
15	A	1101	CLA	C1A-C2A-CAA-CBA
15	A	1103	CLA	C1A-C2A-CAA-CBA
15	A	1104	CLA	C1A-C2A-CAA-CBA
15	A	1112	CLA	C1A-C2A-CAA-CBA
15	A	1130	CLA	C1A-C2A-CAA-CBA
15	A	1133	CLA	C1A-C2A-CAA-CBA
15	B	1207	CLA	C1A-C2A-CAA-CBA
15	B	1224	CLA	C1A-C2A-CAA-CBA
15	B	1202	CLA	C15-C16-C17-C18
17	A	5002	LHG	C28-C29-C30-C31
15	4	605	CLA	C5-C6-C7-C8
15	A	1133	CLA	C10-C11-C12-C13
15	1	605	CLA	C12-C13-C15-C16
15	3	611	CLA	C12-C13-C15-C16
15	A	1116	CLA	C6-C7-C8-C10
15	A	1123	CLA	C11-C12-C13-C15
15	A	1126	CLA	C11-C12-C13-C15
15	A	1127	CLA	C12-C13-C15-C16
15	A	1133	CLA	C11-C10-C8-C7
15	A	1139	CLA	C6-C7-C8-C10
15	B	1021	CLA	C6-C7-C8-C10
15	B	1203	CLA	C12-C13-C15-C16
15	B	1023	CLA	C16-C17-C18-C19
19	A	1011	CL0	C16-C17-C18-C19
17	A	5001	LHG	C14-C15-C16-C17
15	3	615	CLA	C3A-C2A-CAA-CBA
15	B	1238	CLA	C3A-C2A-CAA-CBA
17	3	801	LHG	C14-C15-C16-C17
15	B	1234	CLA	O1D-CGD-O2D-CED
15	A	1103	CLA	C4-C3-C5-C6
15	A	1117	CLA	C4-C3-C5-C6
15	A	1125	CLA	C4-C3-C5-C6
15	A	1103	CLA	C2-C3-C5-C6
15	A	1125	CLA	C2-C3-C5-C6
15	B	1215	CLA	C5-C6-C7-C8
15	A	1137	CLA	CBD-CGD-O2D-CED
15	3	603	CLA	C2A-CAA-CBA-CGA
15	A	1104	CLA	C2A-CAA-CBA-CGA
15	2	601	CLA	C11-C12-C13-C14
15	2	605	CLA	C6-C7-C8-C9
15	A	1101	CLA	C6-C7-C8-C9
15	A	1105	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
15	A	1109	CLA	C6-C7-C8-C9
15	A	1123	CLA	C11-C12-C13-C14
15	B	1023	CLA	C14-C13-C15-C16
15	B	1227	CLA	C11-C10-C8-C9
15	B	1235	CLA	C6-C7-C8-C9
15	B	1202	CLA	CBA-CGA-O2A-C1
16	2	609	CHL	CBA-CGA-O2A-C1
17	3	801	LHG	C11-C12-C13-C14
15	1	607	CLA	C4C-C3C-CAC-CBC
17	2	801	LHG	C4-C5-C6-O8
18	2	803	LMG	C7-C8-C9-O8
22	B	5002	DGD	O1G-C1G-C2G-C3G
18	2	803	LMG	O6-C5-C6-O5
15	1	605	CLA	C5-C6-C7-C8
15	2	604	CLA	C10-C11-C12-C13
15	B	1225	CLA	C16-C17-C18-C19
15	B	1225	CLA	C16-C17-C18-C20
17	A	5002	LHG	C10-C11-C12-C13
14	2	503	BCR	C16-C17-C18-C36
15	A	1122	CLA	O1A-CGA-O2A-C1
15	B	1210	CLA	C4-C3-C5-C6
15	A	1117	CLA	C2-C3-C5-C6
15	4	609	CLA	C5-C6-C7-C8
15	A	1139	CLA	C10-C11-C12-C13
14	A	4002	BCR	C37-C22-C23-C24
17	3	801	LHG	C15-C16-C17-C18
15	A	1133	CLA	C16-C17-C18-C20
18	2	802	LMG	C15-C16-C17-C18
14	F	4001	BCR	C11-C12-C13-C14
15	B	1202	CLA	O1A-CGA-O2A-C1
17	1	801	LHG	C11-C10-C9-C8
15	4	605	CLA	C8-C10-C11-C12
15	4	616	CLA	O2A-C1-C2-C3
15	A	1012	CLA	O2A-C1-C2-C3
15	A	1103	CLA	O2A-C1-C2-C3
15	A	1125	CLA	O2A-C1-C2-C3
15	A	1126	CLA	O2A-C1-C2-C3
17	A	5002	LHG	C25-C26-C27-C28
14	A	4006	BCR	C18-C19-C20-C21
15	A	1104	CLA	O1D-CGD-O2D-CED
15	A	1133	CLA	C16-C17-C18-C19
15	B	1205	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
15	B	1202	CLA	C3-C5-C6-C7
14	A	4005	BCR	C16-C17-C18-C19
22	B	5002	DGD	C2A-C3A-C4A-C5A
18	2	804	LMG	C31-C32-C33-C34
22	B	5002	DGD	C5A-C6A-C7A-C8A
15	4	602	CLA	CBA-CGA-O2A-C1
15	B	1235	CLA	CBA-CGA-O2A-C1
18	2	802	LMG	C29-C30-C31-C32
15	A	1111	CLA	C2C-C3C-CAC-CBC
15	B	1023	CLA	C16-C17-C18-C20
15	B	1208	CLA	CBD-CGD-O2D-CED
15	A	1124	CLA	CBA-CGA-O2A-C1
17	A	5001	LHG	C19-C20-C21-C22
18	2	802	LMG	C32-C33-C34-C35
18	2	802	LMG	C41-C42-C43-C44
15	2	607	CLA	C2C-C3C-CAC-CBC
15	A	1124	CLA	C3-C5-C6-C7
15	A	1012	CLA	C8-C10-C11-C12
15	A	1103	CLA	C15-C16-C17-C18
15	B	1205	CLA	C16-C17-C18-C20
15	3	601	CLA	C4-C3-C5-C6
15	B	1021	CLA	C4-C3-C5-C6
15	B	1211	CLA	C4-C3-C5-C6
15	B	1224	CLA	C4-C3-C5-C6
15	A	1123	CLA	CBA-CGA-O2A-C1
15	A	1136	CLA	CBA-CGA-O2A-C1
17	A	5002	LHG	C34-C35-C36-C37
17	A	5001	LHG	C29-C30-C31-C32
17	B	5001	LHG	O1-C1-C2-O2
15	1	605	CLA	C14-C13-C15-C16
15	3	605	CLA	C6-C7-C8-C9
15	3	611	CLA	C14-C13-C15-C16
15	A	1126	CLA	C11-C12-C13-C14
15	A	1127	CLA	C14-C13-C15-C16
15	A	1128	CLA	C11-C10-C8-C9
15	A	1133	CLA	C11-C12-C13-C14
15	A	1136	CLA	C11-C10-C8-C9
15	A	1139	CLA	C6-C7-C8-C9
15	B	1021	CLA	C6-C7-C8-C9
15	B	1216	CLA	C6-C7-C8-C9
15	B	1219	CLA	C11-C12-C13-C14
19	A	1011	CL0	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
18	4	801	LMG	C12-C13-C14-C15
15	B	1210	CLA	C5-C6-C7-C8
15	1	615	CLA	C4B-C3B-CAB-CBB
15	4	607	CLA	C4B-C3B-CAB-CBB
15	A	1109	CLA	C4B-C3B-CAB-CBB
15	B	1208	CLA	C4B-C3B-CAB-CBB
18	2	802	LMG	C18-C19-C20-C21
15	3	605	CLA	C10-C11-C12-C13
15	3	611	CLA	C2A-CAA-CBA-CGA
15	A	1106	CLA	C2A-CAA-CBA-CGA
18	2	802	LMG	C34-C35-C36-C37
18	2	804	LMG	C22-C23-C24-C25
18	B	5003	LMG	C2-C1-O1-C7
15	A	1105	CLA	C5-C6-C7-C8
15	A	1136	CLA	C13-C15-C16-C17
15	B	1225	CLA	C13-C15-C16-C17
22	B	5002	DGD	C7B-C8B-C9B-CAB
15	4	604	CLA	C3-C5-C6-C7
15	B	1226	CLA	C3-C5-C6-C7
17	1	801	LHG	C30-C31-C32-C33
15	A	1131	CLA	O1D-CGD-O2D-CED
15	1	604	CLA	C11-C12-C13-C15
15	2	601	CLA	C11-C12-C13-C15
15	2	604	CLA	C11-C10-C8-C7
15	2	605	CLA	C6-C7-C8-C10
15	3	605	CLA	C6-C7-C8-C10
15	3	605	CLA	C11-C12-C13-C15
15	A	1101	CLA	C6-C7-C8-C10
15	A	1105	CLA	C11-C10-C8-C7
15	A	1109	CLA	C6-C7-C8-C10
15	A	1117	CLA	C12-C13-C15-C16
15	A	1123	CLA	C6-C7-C8-C10
15	A	1128	CLA	C11-C10-C8-C7
15	A	1133	CLA	C11-C12-C13-C15
15	A	1136	CLA	C11-C10-C8-C7
15	B	1023	CLA	C12-C13-C15-C16
15	B	1202	CLA	C11-C10-C8-C7
15	B	1216	CLA	C6-C7-C8-C10
15	B	1219	CLA	C11-C12-C13-C15
15	B	1227	CLA	C11-C10-C8-C7
15	B	1235	CLA	C6-C7-C8-C10
22	B	5002	DGD	C4B-C5B-C6B-C7B

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Mol	Chain	Res	Type	Atoms
15	A	1130	CLA	C3A-C2A-CAA-CBA
15	B	1215	CLA	C3A-C2A-CAA-CBA
15	B	1224	CLA	C3A-C2A-CAA-CBA
15	B	1230	CLA	C3A-C2A-CAA-CBA
15	1	601	CLA	C5-C6-C7-C8
15	B	1240	CLA	CAA-CBA-CGA-O2A
17	3	801	LHG	C11-C10-C9-C8
18	B	5003	LMG	C13-C14-C15-C16
15	B	1205	CLA	C15-C16-C17-C18
15	B	1202	CLA	O1D-CGD-O2D-CED
15	1	601	CLA	CBA-CGA-O2A-C1
12	3	501	LUT	C33-C34-C35-C15
14	3	503	BCR	C19-C20-C21-C22
14	3	504	BCR	C9-C10-C11-C12
14	A	4004	BCR	C13-C14-C15-C16
14	B	4005	BCR	C9-C10-C11-C12
14	B	4005	BCR	C13-C14-C15-C16
14	J	4002	BCR	C19-C20-C21-C22
15	A	1139	CLA	C16-C17-C18-C19
14	B	4003	BCR	C37-C22-C23-C24
15	B	1235	CLA	O1A-CGA-O2A-C1
15	3	615	CLA	O1D-CGD-O2D-CED
18	2	804	LMG	C21-C22-C23-C24
17	A	5002	LHG	C4-C5-C6-O8
18	2	802	LMG	O1-C7-C8-C9
22	B	5002	DGD	C1G-C2G-C3G-O3G
18	2	803	LMG	C15-C16-C17-C18
16	1	609	CHL	C16-C17-C18-C19
15	A	1101	CLA	O1D-CGD-O2D-CED
15	3	607	CLA	C10-C11-C12-C13
15	B	1216	CLA	C8-C10-C11-C12
15	B	1021	CLA	C2-C3-C5-C6
15	B	1211	CLA	C2-C3-C5-C6
15	A	1112	CLA	C15-C16-C17-C18
15	A	1139	CLA	C16-C17-C18-C20
14	2	503	BCR	C23-C24-C25-C30
14	3	503	BCR	C1-C6-C7-C8
15	4	607	CLA	C2B-C3B-CAB-CBB
17	A	5001	LHG	C27-C28-C29-C30
15	B	1215	CLA	C15-C16-C17-C18
15	4	609	CLA	C2A-CAA-CBA-CGA
15	A	1108	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
15	A	1110	CLA	C5-C6-C7-C8
18	2	802	LMG	O1-C7-C8-O7
17	B	5001	LHG	C11-C12-C13-C14
15	B	1205	CLA	C4-C3-C5-C6
18	2	804	LMG	C30-C31-C32-C33
15	B	1224	CLA	C2-C3-C5-C6
18	2	802	LMG	C13-C14-C15-C16
18	2	803	LMG	C19-C20-C21-C22
18	B	5003	LMG	C12-C13-C14-C15
15	3	605	CLA	C11-C12-C13-C14
15	A	1125	CLA	C11-C12-C13-C14
15	B	1202	CLA	C11-C10-C8-C9
15	B	1203	CLA	C14-C13-C15-C16
15	B	1235	CLA	C11-C10-C8-C9
15	A	1127	CLA	C15-C16-C17-C18
18	2	804	LMG	C4-C5-C6-O5
14	4	503	BCR	C6-C7-C8-C9
14	A	4004	BCR	C22-C23-C24-C25
14	A	4005	BCR	C6-C7-C8-C9
14	A	4008	BCR	C22-C23-C24-C25
14	J	4002	BCR	C14-C15-C16-C17
15	A	1129	CLA	C3-C5-C6-C7
15	B	1223	CLA	CBA-CGA-O2A-C1
18	2	803	LMG	C17-C18-C19-C20
15	A	1120	CLA	C1A-C2A-CAA-CBA
15	J	1302	CLA	C1A-C2A-CAA-CBA
15	B	1220	CLA	O1D-CGD-O2D-CED
15	B	1214	CLA	C8-C10-C11-C12
14	B	4002	BCR	C19-C20-C21-C22
15	4	602	CLA	O1A-CGA-O2A-C1
15	1	601	CLA	C13-C15-C16-C17
17	1	801	LHG	C1-C2-C3-O3
14	A	4008	BCR	C20-C21-C22-C37
14	B	4002	BCR	C35-C13-C14-C15
14	J	4002	BCR	C11-C10-C9-C34
18	2	804	LMG	C37-C38-C39-C40
15	B	1223	CLA	C13-C15-C16-C17
16	1	609	CHL	C16-C17-C18-C20
15	B	1226	CLA	O1D-CGD-O2D-CED
15	4	603	CLA	C13-C15-C16-C17
13	1	502	XAT	C11-C12-C13-C20
14	F	4002	BCR	C37-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
15	A	1013	CLA	C6-C7-C8-C10
15	A	1102	CLA	C12-C13-C15-C16
15	B	1226	CLA	C11-C12-C13-C15
15	B	1235	CLA	C11-C10-C8-C7
16	1	609	CHL	C6-C7-C8-C10
18	2	802	LMG	C42-C43-C44-C45
15	A	1126	CLA	C13-C15-C16-C17
12	1	501	LUT	C7-C8-C9-C10
12	2	501	LUT	C27-C28-C29-C30
13	1	502	XAT	C11-C12-C13-C14
13	1	502	XAT	C27-C28-C29-C30
14	2	503	BCR	C7-C8-C9-C10
14	2	503	BCR	C21-C22-C23-C24
14	A	4003	BCR	C17-C18-C19-C20
14	B	4001	BCR	C17-C18-C19-C20
14	B	4005	BCR	C11-C12-C13-C14
14	B	4006	BCR	C11-C12-C13-C14
15	A	1123	CLA	O1A-CGA-O2A-C1
15	A	1124	CLA	O1A-CGA-O2A-C1
15	B	1223	CLA	O1A-CGA-O2A-C1
17	2	801	LHG	O10-C23-O8-C6
15	B	1226	CLA	C10-C11-C12-C13
15	B	1204	CLA	C2A-CAA-CBA-CGA
15	A	1134	CLA	O1D-CGD-O2D-CED
15	1	601	CLA	O1A-CGA-O2A-C1
15	A	1136	CLA	O1A-CGA-O2A-C1
15	2	601	CLA	C5-C6-C7-C8
17	3	801	LHG	C26-C27-C28-C29
15	B	1219	CLA	C10-C11-C12-C13
15	B	1221	CLA	O2A-C1-C2-C3
18	2	802	LMG	C9-C8-O7-C10
16	2	609	CHL	O1A-CGA-O2A-C1
18	2	802	LMG	C36-C37-C38-C39
14	1	503	BCR	C12-C13-C14-C15
14	3	503	BCR	C16-C17-C18-C19
14	3	504	BCR	C16-C17-C18-C19
14	B	4005	BCR	C12-C13-C14-C15
14	F	4002	BCR	C20-C21-C22-C23
15	A	1137	CLA	O1D-CGD-O2D-CED
17	B	5001	LHG	C4-C5-C6-O8
15	B	1203	CLA	C13-C15-C16-C17
15	4	605	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
15	2	612	CLA	C4-C3-C5-C6
15	B	1022	CLA	C2A-CAA-CBA-CGA
15	B	1205	CLA	C2-C3-C5-C6
19	A	1011	CL0	C3-C5-C6-C7
17	B	5001	LHG	O7-C5-C6-O8
15	A	1122	CLA	C11-C12-C13-C14
15	B	1221	CLA	C6-C7-C8-C9
18	B	5003	LMG	C33-C34-C35-C36
15	3	612	CLA	C10-C11-C12-C13
15	A	1139	CLA	C4-C3-C5-C6
16	2	609	CHL	C3-C5-C6-C7
15	A	1101	CLA	C2A-CAA-CBA-CGA
17	A	5002	LHG	C24-C23-O8-C6
14	B	4001	BCR	C14-C15-C16-C17
18	4	801	LMG	C4-C5-C6-O5
15	1	607	CLA	C4B-C3B-CAB-CBB
15	2	602	CLA	C1A-C2A-CAA-CBA
15	3	608	CLA	C4B-C3B-CAB-CBB
15	A	1101	CLA	C4B-C3B-CAB-CBB
15	A	1104	CLA	C4B-C3B-CAB-CBB
15	A	1121	CLA	C4B-C3B-CAB-CBB
15	A	1131	CLA	C4B-C3B-CAB-CBB
15	A	1133	CLA	C4B-C3B-CAB-CBB
15	A	1140	CLA	C4B-C3B-CAB-CBB
15	B	1215	CLA	C1A-C2A-CAA-CBA
15	B	1230	CLA	C1A-C2A-CAA-CBA
15	B	1234	CLA	C1A-C2A-CAA-CBA
15	B	1237	CLA	C4B-C3B-CAB-CBB
15	B	1239	CLA	C4B-C3B-CAB-CBB
15	F	1301	CLA	C4B-C3B-CAB-CBB
15	2	616	CLA	C4-C3-C5-C6
14	2	503	BCR	C11-C12-C13-C14
14	A	4004	BCR	C21-C22-C23-C24
14	B	4006	BCR	C7-C8-C9-C10
14	B	4006	BCR	C21-C22-C23-C24
16	4	613	CHL	C11-C12-C13-C15
15	B	1021	CLA	C3-C5-C6-C7
15	A	1013	CLA	C2A-CAA-CBA-CGA
15	A	1136	CLA	C8-C10-C11-C12
15	A	1135	CLA	C2-C3-C5-C6
15	B	1208	CLA	O1D-CGD-O2D-CED
15	4	603	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
15	4	609	CLA	C6-C7-C8-C10
15	A	1012	CLA	C11-C12-C13-C15
15	A	1102	CLA	C6-C7-C8-C10
15	A	1106	CLA	C11-C12-C13-C15
15	A	1111	CLA	C11-C10-C8-C7
15	A	1133	CLA	C6-C7-C8-C10
15	B	1023	CLA	C11-C10-C8-C7
19	A	1011	CL0	C11-C10-C8-C7
17	3	801	LHG	C16-C17-C18-C19
18	2	804	LMG	C33-C34-C35-C36
15	B	1219	CLA	C16-C17-C18-C20
15	A	1013	CLA	C6-C7-C8-C9
15	A	1116	CLA	C6-C7-C8-C9
15	A	1117	CLA	C14-C13-C15-C16
15	A	1123	CLA	C6-C7-C8-C9
14	A	4006	BCR	C19-C20-C21-C22
14	F	4002	BCR	C19-C20-C21-C22
15	A	1102	CLA	C8-C10-C11-C12
15	B	1236	CLA	C1-C2-C3-C4
18	2	803	LMG	O7-C8-C9-O8
18	4	801	LMG	O1-C7-C8-O7
22	B	5002	DGD	O1G-C1G-C2G-O2G
15	F	1302	CLA	O2A-C1-C2-C3
18	2	803	LMG	C2-C1-O1-C7
15	2	612	CLA	C2-C3-C5-C6
15	1	603	CLA	CAD-CBD-CGD-O2D
15	1	615	CLA	CAD-CBD-CGD-O2D
15	2	602	CLA	CAD-CBD-CGD-O2D
15	4	606	CLA	CAD-CBD-CGD-O2D
15	A	1103	CLA	CAD-CBD-CGD-O2D
15	B	1217	CLA	CAD-CBD-CGD-O2D
15	B	1239	CLA	CAD-CBD-CGD-O2D
16	1	609	CHL	CAD-CBD-CGD-O2D
16	2	609	CHL	CAD-CBD-CGD-O2D
17	B	5001	LHG	C15-C16-C17-C18
15	B	1023	CLA	C3-C5-C6-C7
15	B	1203	CLA	C3-C5-C6-C7
15	B	1234	CLA	C3-C5-C6-C7
15	3	614	CLA	C3-C5-C6-C7
15	A	1013	CLA	C5-C6-C7-C8
12	1	501	LUT	C33-C34-C35-C15
12	2	501	LUT	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
14	3	503	BCR	C9-C10-C11-C12
14	A	4002	BCR	C16-C17-C18-C36
15	1	603	CLA	CAD-CBD-CGD-O1D
15	1	615	CLA	CAD-CBD-CGD-O1D
15	2	602	CLA	CAD-CBD-CGD-O1D
15	2	608	CLA	CHA-CBD-CGD-O1D
15	4	603	CLA	CHA-CBD-CGD-O1D
15	4	603	CLA	CHA-CBD-CGD-O2D
15	4	606	CLA	CAD-CBD-CGD-O1D
15	A	1102	CLA	CHA-CBD-CGD-O1D
15	A	1103	CLA	CAD-CBD-CGD-O1D
15	A	1118	CLA	CHA-CBD-CGD-O1D
15	A	1131	CLA	CHA-CBD-CGD-O1D
15	B	1202	CLA	CHA-CBD-CGD-O1D
15	B	1202	CLA	CHA-CBD-CGD-O2D
15	B	1212	CLA	CHA-CBD-CGD-O1D
15	B	1217	CLA	CAD-CBD-CGD-O1D
15	B	1222	CLA	CHA-CBD-CGD-O1D
15	B	1222	CLA	CHA-CBD-CGD-O2D
15	B	1224	CLA	CHA-CBD-CGD-O1D
15	B	1227	CLA	CAD-CBD-CGD-O1D
15	B	1239	CLA	CAD-CBD-CGD-O1D
16	1	609	CHL	CAD-CBD-CGD-O1D
16	2	609	CHL	CAD-CBD-CGD-O1D
17	2	801	LHG	C3-O3-P-O5
17	3	801	LHG	C3-O3-P-O5
17	B	5001	LHG	C3-O3-P-O4
17	B	5001	LHG	C4-O6-P-O4
15	2	608	CLA	C2C-C3C-CAC-CBC
22	B	5002	DGD	C3B-C4B-C5B-C6B
15	1	607	CLA	C2B-C3B-CAB-CBB
15	4	601	CLA	C2B-C3B-CAB-CBB
15	A	1101	CLA	C2B-C3B-CAB-CBB
15	A	1104	CLA	C2B-C3B-CAB-CBB
15	A	1122	CLA	C2B-C3B-CAB-CBB
15	B	1227	CLA	C2B-C3B-CAB-CBB
15	F	1301	CLA	C2B-C3B-CAB-CBB
15	3	601	CLA	C2-C3-C5-C6
15	B	1224	CLA	C8-C10-C11-C12
17	A	5002	LHG	C2-C3-O3-P
15	A	1136	CLA	C10-C11-C12-C13
15	4	612	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
15	B	1219	CLA	C16-C17-C18-C19
15	A	1105	CLA	O1D-CGD-O2D-CED
15	2	607	CLA	C4C-C3C-CAC-CBC
18	2	804	LMG	C24-C25-C26-C27
17	1	801	LHG	C4-C5-O7-C7
18	2	804	LMG	C9-C8-O7-C10
17	A	5001	LHG	C25-C26-C27-C28
12	1	501	LUT	C10-C11-C12-C13
12	1	501	LUT	C30-C31-C32-C33
12	2	501	LUT	C10-C11-C12-C13
12	2	501	LUT	C30-C31-C32-C33
12	3	501	LUT	C10-C11-C12-C13
12	3	501	LUT	C30-C31-C32-C33
12	4	501	LUT	C10-C11-C12-C13
12	4	501	LUT	C30-C31-C32-C33
15	4	605	CLA	C16-C17-C18-C19
20	B	2002	PQN	C26-C27-C28-C29
15	1	604	CLA	C11-C12-C13-C14
15	4	603	CLA	C6-C7-C8-C9
15	A	1111	CLA	C11-C12-C13-C14
15	A	1122	CLA	C6-C7-C8-C9
15	3	605	CLA	C12-C13-C15-C16
15	A	1111	CLA	C11-C12-C13-C15
15	A	1122	CLA	C6-C7-C8-C10
17	2	801	LHG	C10-C11-C12-C13
18	2	802	LMG	C39-C40-C41-C42
15	A	1012	CLA	C15-C16-C17-C18
15	B	1211	CLA	C15-C16-C17-C18
15	A	1124	CLA	C10-C11-C12-C13
17	2	801	LHG	O7-C5-C6-O8
15	A	1126	CLA	CAA-CBA-CGA-O2A
20	B	2002	PQN	C26-C27-C28-C30
22	B	5002	DGD	CAA-CBA-CCA-CDA
15	1	611	CLA	O1A-CGA-O2A-C1
15	B	1022	CLA	C4-C3-C5-C6
15	B	1224	CLA	CAA-CBA-CGA-O2A
14	B	4004	BCR	C36-C18-C19-C20
15	3	601	CLA	C11-C12-C13-C15
15	A	1128	CLA	C3-C5-C6-C7
15	A	1012	CLA	C13-C15-C16-C17
15	A	1138	CLA	C2A-CAA-CBA-CGA
15	A	1136	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
17	A	5002	LHG	C31-C32-C33-C34
15	B	1219	CLA	C5-C6-C7-C8
15	A	1111	CLA	C4C-C3C-CAC-CBC
17	3	801	LHG	C28-C29-C30-C31
15	2	604	CLA	C11-C10-C8-C9
15	4	609	CLA	C6-C7-C8-C9
15	A	1111	CLA	C11-C10-C8-C9
15	A	1139	CLA	C14-C13-C15-C16
15	1	608	CLA	C4B-C3B-CAB-CBB
15	B	1202	CLA	C4B-C3B-CAB-CBB
15	B	1214	CLA	C15-C16-C17-C18
22	B	5002	DGD	C7A-C8A-C9A-CAA
15	1	611	CLA	CBA-CGA-O2A-C1
19	A	1011	CL0	CAA-CBA-CGA-O2A
18	2	804	LMG	C36-C37-C38-C39
15	B	1022	CLA	C2-C3-C5-C6
15	B	1236	CLA	O2A-C1-C2-C3
15	B	1021	CLA	C5-C6-C7-C8
15	3	610	CLA	O1D-CGD-O2D-CED
15	2	616	CLA	C11-C12-C13-C15
15	3	608	CLA	C12-C13-C15-C16
15	A	1125	CLA	C12-C13-C15-C16
15	A	1139	CLA	C12-C13-C15-C16
15	B	1023	CLA	C6-C7-C8-C10
19	A	1011	CL0	C6-C7-C8-C10
15	A	1133	CLA	CBA-CGA-O2A-C1
15	A	1133	CLA	O1A-CGA-O2A-C1
22	B	5002	DGD	C9B-CAB-CBB-CCB
17	2	801	LHG	C9-C10-C11-C12
15	2	602	CLA	C3A-C2A-CAA-CBA
15	A	1105	CLA	C3A-C2A-CAA-CBA
15	A	1114	CLA	C3A-C2A-CAA-CBA
15	B	1221	CLA	C4-C3-C5-C6
15	B	1234	CLA	C3A-C2A-CAA-CBA
12	1	501	LUT	C11-C10-C9-C19
12	1	501	LUT	C20-C13-C14-C15
12	1	501	LUT	C39-C29-C30-C31
12	1	501	LUT	C40-C33-C34-C35
12	2	501	LUT	C11-C10-C9-C19
12	2	501	LUT	C20-C13-C14-C15
12	2	501	LUT	C39-C29-C30-C31
12	2	501	LUT	C40-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
12	3	501	LUT	C11-C10-C9-C19
12	3	501	LUT	C20-C13-C14-C15
12	3	501	LUT	C39-C29-C30-C31
12	3	501	LUT	C40-C33-C34-C35
12	4	501	LUT	C11-C10-C9-C19
12	4	501	LUT	C20-C13-C14-C15
12	4	501	LUT	C39-C29-C30-C31
12	4	501	LUT	C40-C33-C34-C35
13	2	502	XAT	C40-C33-C34-C35
13	3	502	XAT	C40-C33-C34-C35
13	4	502	XAT	C40-C33-C34-C35
14	A	4003	BCR	C16-C17-C18-C36
14	A	4005	BCR	C35-C13-C14-C15
15	A	1136	CLA	O1D-CGD-O2D-CED
12	2	501	LUT	C13-C14-C15-C35
12	2	501	LUT	C33-C34-C35-C15
13	4	502	XAT	C29-C30-C31-C32
13	4	502	XAT	C33-C34-C35-C15
14	3	506	BCR	C9-C10-C11-C12
14	A	4005	BCR	C9-C10-C11-C12
15	B	1208	CLA	C2-C1-O2A-CGA
15	A	1135	CLA	C4-C3-C5-C6
18	2	803	LMG	C30-C31-C32-C33
15	A	1116	CLA	O1D-CGD-O2D-CED
15	3	608	CLA	CAA-CBA-CGA-O2A
15	2	616	CLA	C2-C3-C5-C6
15	3	601	CLA	C11-C12-C13-C14
16	2	613	CHL	CAA-CBA-CGA-O2A
15	3	608	CLA	C14-C13-C15-C16
15	3	612	CLA	C14-C13-C15-C16
15	A	1140	CLA	C6-C7-C8-C9
15	B	1240	CLA	C14-C13-C15-C16
15	A	1111	CLA	C10-C11-C12-C13
15	3	610	CLA	CBD-CGD-O2D-CED
15	A	1105	CLA	CBD-CGD-O2D-CED
15	A	1129	CLA	C2C-C3C-CAC-CBC
15	A	1136	CLA	C2A-CAA-CBA-CGA
18	2	802	LMG	C30-C31-C32-C33
12	1	501	LUT	C11-C10-C9-C8
12	1	501	LUT	C12-C13-C14-C15
12	1	501	LUT	C28-C29-C30-C31
12	1	501	LUT	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
12	2	501	LUT	C11-C10-C9-C8
12	2	501	LUT	C12-C13-C14-C15
12	2	501	LUT	C28-C29-C30-C31
12	2	501	LUT	C32-C33-C34-C35
12	3	501	LUT	C11-C10-C9-C8
12	3	501	LUT	C12-C13-C14-C15
12	3	501	LUT	C28-C29-C30-C31
12	3	501	LUT	C32-C33-C34-C35
12	4	501	LUT	C11-C10-C9-C8
12	4	501	LUT	C12-C13-C14-C15
12	4	501	LUT	C28-C29-C30-C31
12	4	501	LUT	C32-C33-C34-C35
13	2	502	XAT	C32-C33-C34-C35
13	3	502	XAT	C32-C33-C34-C35
13	4	502	XAT	C32-C33-C34-C35
15	1	607	CLA	C1A-C2A-CAA-CBA
15	A	1113	CLA	C1A-C2A-CAA-CBA
15	A	1114	CLA	C1A-C2A-CAA-CBA
15	B	1209	CLA	C1A-C2A-CAA-CBA
15	B	1216	CLA	C1A-C2A-CAA-CBA
15	B	1240	CLA	C1A-C2A-CAA-CBA
12	1	501	LUT	C5-C6-C7-C8
12	3	501	LUT	C5-C6-C7-C8
14	1	503	BCR	C1-C6-C7-C8
14	2	503	BCR	C23-C24-C25-C26
14	3	503	BCR	C5-C6-C7-C8
14	3	504	BCR	C1-C6-C7-C8
14	3	504	BCR	C23-C24-C25-C30
14	B	4003	BCR	C5-C6-C7-C8
14	B	4005	BCR	C1-C6-C7-C8
14	B	4006	BCR	C23-C24-C25-C30
15	1	608	CLA	C2B-C3B-CAB-CBB
15	1	615	CLA	C2B-C3B-CAB-CBB
15	3	608	CLA	C2B-C3B-CAB-CBB
15	A	1109	CLA	C2B-C3B-CAB-CBB
15	A	1121	CLA	C2B-C3B-CAB-CBB
15	A	1131	CLA	C2B-C3B-CAB-CBB
15	A	1133	CLA	C2B-C3B-CAB-CBB
15	A	1140	CLA	C2B-C3B-CAB-CBB
15	B	1208	CLA	C2B-C3B-CAB-CBB
15	B	1237	CLA	C2B-C3B-CAB-CBB
15	B	1239	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
15	A	1130	CLA	CAA-CBA-CGA-O1A
15	B	1240	CLA	C16-C17-C18-C19
16	2	613	CHL	CAA-CBA-CGA-O1A
15	4	607	CLA	C4-C3-C5-C6
15	A	1119	CLA	C4-C3-C5-C6
15	A	1127	CLA	C4-C3-C5-C6
14	J	4001	BCR	C13-C14-C15-C16
15	1	603	CLA	C6-C7-C8-C10
15	3	612	CLA	C12-C13-C15-C16
15	4	604	CLA	C11-C10-C8-C7
15	4	612	CLA	C11-C12-C13-C15
15	A	1125	CLA	C11-C10-C8-C7
15	A	1136	CLA	C12-C13-C15-C16
15	A	1137	CLA	C6-C7-C8-C10
15	B	1222	CLA	C11-C10-C8-C7
15	B	1225	CLA	C6-C7-C8-C10
15	B	1226	CLA	C11-C10-C8-C7
15	2	605	CLA	C16-C17-C18-C19
15	3	614	CLA	C2A-CAA-CBA-CGA
15	4	604	CLA	C2A-CAA-CBA-CGA
17	A	5002	LHG	C11-C12-C13-C14
17	A	5001	LHG	C34-C35-C36-C37
17	A	5002	LHG	O9-C7-O7-C5
13	1	502	XAT	C27-C28-C29-C39
14	B	4005	BCR	C37-C22-C23-C24
14	F	4001	BCR	C37-C22-C23-C24
22	B	5002	DGD	O1A-C1A-O1G-C1G
15	3	605	CLA	C16-C17-C18-C20
15	B	1229	CLA	C10-C11-C12-C13
18	2	803	LMG	C31-C32-C33-C34
14	A	4008	BCR	C13-C14-C15-C16
15	2	604	CLA	C15-C16-C17-C18
15	A	1125	CLA	C8-C10-C11-C12
14	A	4003	BCR	C6-C7-C8-C9
15	B	1227	CLA	C4-C3-C5-C6
17	1	801	LHG	C2-C3-O3-P
15	A	1121	CLA	CAA-CBA-CGA-O2A
15	A	1131	CLA	CAA-CBA-CGA-O2A
22	B	5002	DGD	C2B-C3B-C4B-C5B
18	B	5003	LMG	C14-C15-C16-C17
15	B	1215	CLA	C8-C10-C11-C12
15	1	613	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
15	A	1113	CLA	CAA-CBA-CGA-O2A
15	A	1130	CLA	CAA-CBA-CGA-O2A
15	A	1118	CLA	C1A-C2A-CAA-CBA
15	A	1116	CLA	CAA-CBA-CGA-O2A
15	B	1203	CLA	C4-C3-C5-C6
15	B	1212	CLA	C4-C3-C5-C6
15	A	1115	CLA	CAA-CBA-CGA-O2A
15	1	606	CLA	O1D-CGD-O2D-CED
17	1	801	LHG	C15-C16-C17-C18
17	A	5002	LHG	C30-C31-C32-C33
15	1	607	CLA	CAA-CBA-CGA-O2A
15	B	1240	CLA	CAA-CBA-CGA-O1A
15	B	1224	CLA	C10-C11-C12-C13
15	A	1117	CLA	O1D-CGD-O2D-CED
15	A	1116	CLA	CBD-CGD-O2D-CED
16	2	610	CHL	CHA-CBD-CGD-O1D
16	2	610	CHL	CHA-CBD-CGD-O2D
16	2	611	CHL	CHA-CBD-CGD-O1D
16	2	611	CHL	CHA-CBD-CGD-O2D
16	3	604	CHL	CHA-CBD-CGD-O1D
16	3	604	CHL	CHA-CBD-CGD-O2D
16	4	610	CHL	CHA-CBD-CGD-O2D
15	A	1128	CLA	C13-C15-C16-C17
17	A	5001	LHG	C24-C23-O8-C6
18	2	804	LMG	C19-C20-C21-C22
18	4	801	LMG	C30-C31-C32-C33
18	2	804	LMG	C34-C35-C36-C37
15	A	1101	CLA	C3-C5-C6-C7
15	2	607	CLA	C11-C10-C8-C7
15	B	1211	CLA	C11-C12-C13-C15
15	A	1012	CLA	C11-C12-C13-C14
15	A	1122	CLA	C14-C13-C15-C16
17	A	5001	LHG	C24-C25-C26-C27
15	A	1115	CLA	CAA-CBA-CGA-O1A
15	2	605	CLA	C2A-CAA-CBA-CGA
15	B	1224	CLA	C2A-CAA-CBA-CGA
19	A	1011	CL0	C2A-CAA-CBA-CGA
15	B	1215	CLA	C2-C1-O2A-CGA
15	B	1216	CLA	C10-C11-C12-C13
15	1	603	CLA	C3A-C2A-CAA-CBA
15	4	612	CLA	C3A-C2A-CAA-CBA
15	B	1225	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
15	1	615	CLA	CAA-CBA-CGA-O1A
15	1	615	CLA	CAA-CBA-CGA-O2A
15	B	1203	CLA	O1A-CGA-O2A-C1
15	A	1139	CLA	C2-C3-C5-C6
14	J	4001	BCR	C18-C19-C20-C21
15	B	1240	CLA	C16-C17-C18-C20
15	A	1121	CLA	CAA-CBA-CGA-O1A
15	4	606	CLA	C2A-CAA-CBA-CGA
15	1	613	CLA	CAA-CBA-CGA-O1A
15	A	1131	CLA	CAA-CBA-CGA-O1A
15	A	1132	CLA	CAA-CBA-CGA-O2A
15	B	1237	CLA	CAA-CBA-CGA-O2A
15	B	1203	CLA	CBA-CGA-O2A-C1
15	B	1221	CLA	C16-C17-C18-C19
13	1	502	XAT	O24-C26-C27-C28
13	2	502	XAT	O4-C6-C7-C8
13	3	502	XAT	O24-C26-C27-C28
14	J	4001	BCR	C16-C17-C18-C19
15	A	1113	CLA	CAA-CBA-CGA-O1A
18	2	804	LMG	O1-C7-C8-C9
18	2	804	LMG	C7-C8-C9-O8
18	B	5003	LMG	O1-C7-C8-C9
15	B	1202	CLA	C13-C15-C16-C17
15	A	1117	CLA	CBD-CGD-O2D-CED
18	2	802	LMG	C28-C29-C30-C31
15	B	1239	CLA	O1D-CGD-O2D-CED
15	A	1132	CLA	CAA-CBA-CGA-O1A
15	B	1221	CLA	C5-C6-C7-C8
15	A	1104	CLA	C6-C7-C8-C9
15	A	1133	CLA	C6-C7-C8-C9
15	B	1023	CLA	C11-C10-C8-C9
15	B	1223	CLA	C11-C10-C8-C9
19	A	1011	CL0	C14-C13-C15-C16
15	B	1221	CLA	C16-C17-C18-C20
16	2	609	CHL	CAA-CBA-CGA-O2A
12	2	501	LUT	C11-C12-C13-C14
15	3	612	CLA	C3-C5-C6-C7
15	A	1012	CLA	CAA-CBA-CGA-O2A
15	2	606	CLA	C2A-CAA-CBA-CGA
15	A	1108	CLA	C2A-CAA-CBA-CGA
15	A	1128	CLA	C2A-CAA-CBA-CGA
15	A	1102	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
15	B	1225	CLA	C12-C13-C15-C16
12	4	501	LUT	C5-C6-C7-C8
14	1	503	BCR	C5-C6-C7-C8
14	3	504	BCR	C5-C6-C7-C8
14	3	504	BCR	C23-C24-C25-C26
14	B	4005	BCR	C5-C6-C7-C8
14	B	4006	BCR	C23-C24-C25-C26
15	2	607	CLA	C2B-C3B-CAB-CBB
15	2	616	CLA	C2B-C3B-CAB-CBB
15	1	605	CLA	C2-C1-O2A-CGA
15	2	601	CLA	C2-C1-O2A-CGA
15	B	1221	CLA	C2-C1-O2A-CGA
19	A	1011	CL0	C2-C1-O2A-CGA
15	1	605	CLA	CAA-CBA-CGA-O2A
15	A	1129	CLA	CAA-CBA-CGA-O2A
17	1	801	LHG	C9-C10-C11-C12
15	3	605	CLA	C16-C17-C18-C19
15	B	1237	CLA	CAA-CBA-CGA-O1A
15	3	608	CLA	C10-C11-C12-C13
15	B	1022	CLA	CAA-CBA-CGA-O2A
15	B	1234	CLA	C4-C3-C5-C6
19	A	1011	CL0	C4-C3-C5-C6
17	B	5001	LHG	C23-C24-C25-C26
15	A	1013	CLA	CAA-CBA-CGA-O2A
17	2	801	LHG	C11-C12-C13-C14
15	B	1235	CLA	CAA-CBA-CGA-O2A
15	A	1122	CLA	C3-C5-C6-C7
15	A	1136	CLA	C14-C13-C15-C16
15	B	1208	CLA	C6-C7-C8-C9
15	B	1224	CLA	C11-C10-C8-C9
15	B	1225	CLA	C6-C7-C8-C9
15	B	1226	CLA	C11-C10-C8-C9
15	B	1023	CLA	CAA-CBA-CGA-O2A
18	B	5003	LMG	C7-C8-C9-O8
15	2	607	CLA	C4B-C3B-CAB-CBB
15	2	616	CLA	C4B-C3B-CAB-CBB
15	A	1138	CLA	C4B-C3B-CAB-CBB
15	B	1225	CLA	C1A-C2A-CAA-CBA
15	B	1236	CLA	C1A-C2A-CAA-CBA
15	B	1218	CLA	CAA-CBA-CGA-O1A
15	2	604	CLA	CAA-CBA-CGA-O2A
15	4	602	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
15	F	1302	CLA	CAA-CBA-CGA-O2A
16	1	609	CHL	CAA-CBA-CGA-O2A
17	B	5001	LHG	O7-C7-C8-C9
18	2	802	LMG	C33-C34-C35-C36
13	1	502	XAT	C7-C8-C9-C10
14	3	504	BCR	C21-C22-C23-C24
14	A	4006	BCR	C7-C8-C9-C10
14	B	4004	BCR	C7-C8-C9-C10
15	A	1120	CLA	C2C-C3C-CAC-CBC
14	2	503	BCR	C19-C20-C21-C22
15	1	606	CLA	CBD-CGD-O2D-CED
15	B	1218	CLA	CAA-CBA-CGA-O2A
15	1	608	CLA	CAA-CBA-CGA-O2A
17	3	801	LHG	O7-C7-C8-C9
17	A	5002	LHG	O8-C23-C24-C25
15	4	609	CLA	C11-C12-C13-C15
18	2	804	LMG	C23-C24-C25-C26
15	2	604	CLA	C2-C1-O2A-CGA
15	3	610	CLA	C2-C1-O2A-CGA
15	A	1105	CLA	C2-C1-O2A-CGA
15	B	1235	CLA	C2-C1-O2A-CGA
15	2	616	CLA	C11-C10-C8-C7
15	A	1101	CLA	C11-C10-C8-C7
15	A	1127	CLA	C11-C12-C13-C15
15	A	1137	CLA	C11-C12-C13-C15
15	B	1215	CLA	C11-C10-C8-C7
15	B	1224	CLA	C11-C10-C8-C7
18	2	804	LMG	C7-C8-O7-C10
15	2	616	CLA	C8-C10-C11-C12
15	A	1103	CLA	C5-C6-C7-C8
14	B	4004	BCR	C9-C10-C11-C12
15	3	601	CLA	C2A-CAA-CBA-CGA
15	4	603	CLA	C2A-CAA-CBA-CGA
15	A	1117	CLA	C2A-CAA-CBA-CGA
15	B	1206	CLA	CAA-CBA-CGA-O2A
15	A	1125	CLA	C5-C6-C7-C8
15	F	1301	CLA	C2C-C3C-CAC-CBC
15	2	608	CLA	C3A-C2A-CAA-CBA
15	4	607	CLA	C3A-C2A-CAA-CBA
15	A	1107	CLA	C3A-C2A-CAA-CBA
15	B	1218	CLA	C3A-C2A-CAA-CBA
15	B	1226	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
17	B	5001	LHG	O9-C7-C8-C9
15	1	608	CLA	C5-C6-C7-C8
15	A	1101	CLA	C15-C16-C17-C18
18	2	803	LMG	O7-C10-C11-C12
15	B	1221	CLA	C2-C3-C5-C6
15	B	1208	CLA	C4C-C3C-CAC-CBC
14	4	503	BCR	C20-C21-C22-C23
14	B	4001	BCR	C11-C10-C9-C8
18	2	803	LMG	C16-C17-C18-C19
16	1	609	CHL	CAA-CBA-CGA-O1A
15	B	1205	CLA	C10-C11-C12-C13
15	4	602	CLA	C2A-CAA-CBA-CGA
15	A	1103	CLA	C2A-CAA-CBA-CGA
15	2	606	CLA	CAA-CBA-CGA-O2A
15	4	604	CLA	C11-C10-C8-C9
15	4	612	CLA	C11-C12-C13-C14
15	A	1102	CLA	C6-C7-C8-C9
15	A	1102	CLA	C14-C13-C15-C16
15	A	1127	CLA	C11-C12-C13-C14
15	B	1214	CLA	C14-C13-C15-C16
15	3	603	CLA	CAA-CBA-CGA-O2A
15	4	604	CLA	CAA-CBA-CGA-O2A
15	B	1022	CLA	CAA-CBA-CGA-O1A
17	B	5001	LHG	O10-C23-C24-C25
17	A	5002	LHG	C12-C13-C14-C15
15	A	1012	CLA	CAA-CBA-CGA-O1A
15	A	1127	CLA	C2-C3-C5-C6
15	4	602	CLA	CAA-CBA-CGA-O1A
18	4	801	LMG	O10-C28-C29-C30
15	1	605	CLA	CAA-CBA-CGA-O1A
15	3	603	CLA	C8-C10-C11-C12
16	2	609	CHL	C8-C10-C11-C12
18	4	801	LMG	C8-C7-O1-C1
18	2	803	LMG	O1-C7-C8-O7
15	A	1013	CLA	CAA-CBA-CGA-O1A
16	2	609	CHL	CAA-CBA-CGA-O1A
18	4	801	LMG	C14-C15-C16-C17
15	2	604	CLA	CAA-CBA-CGA-O1A
17	1	801	LHG	O9-C7-C8-C9
15	A	1123	CLA	CAA-CBA-CGA-O2A
14	3	504	BCR	C13-C14-C15-C16
15	A	1129	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
15	A	1129	CLA	C4C-C3C-CAC-CBC
15	2	605	CLA	C16-C17-C18-C20
15	1	605	CLA	CAD-CBD-CGD-O2D
15	3	607	CLA	CAD-CBD-CGD-O2D
15	3	608	CLA	CAD-CBD-CGD-O2D
15	4	605	CLA	CAD-CBD-CGD-O2D
15	A	1125	CLA	CAD-CBD-CGD-O2D
15	B	1216	CLA	CAD-CBD-CGD-O2D
15	3	612	CLA	C5-C6-C7-C8
15	F	1301	CLA	CAA-CBA-CGA-O2A
16	1	610	CHL	CAA-CBA-CGA-O2A
15	B	1204	CLA	CAA-CBA-CGA-O1A
15	A	1111	CLA	C2-C1-O2A-CGA
15	B	1222	CLA	C2-C1-O2A-CGA
16	1	609	CHL	C2-C1-O2A-CGA
15	1	608	CLA	CAA-CBA-CGA-O1A
15	F	1302	CLA	CAA-CBA-CGA-O1A
15	3	610	CLA	CAA-CBA-CGA-O2A
15	B	1206	CLA	CAA-CBA-CGA-O1A
17	1	801	LHG	C13-C14-C15-C16
17	2	801	LHG	O8-C23-C24-C25
15	2	606	CLA	CAA-CBA-CGA-O1A
15	4	604	CLA	CAA-CBA-CGA-O1A
15	B	1235	CLA	CAA-CBA-CGA-O1A
17	3	801	LHG	O9-C7-C8-C9

There are no ring outliers.

94 monomers are involved in 157 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	2	501	LUT	3	0
15	1	611	CLA	1	0
15	4	608	CLA	1	0
15	A	1117	CLA	2	0
15	A	1105	CLA	1	0
14	B	4004	BCR	2	0
15	2	616	CLA	2	0
15	B	1231	CLA	5	0
15	B	1221	CLA	1	0
15	B	1240	CLA	2	0
15	A	1107	CLA	1	0
15	2	604	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	A	5002	LHG	1	0
14	A	4004	BCR	1	0
15	A	1126	CLA	4	0
15	A	1114	CLA	1	0
13	2	502	XAT	2	0
15	A	1122	CLA	1	0
15	B	1216	CLA	1	0
15	B	1224	CLA	2	0
15	3	608	CLA	2	0
15	2	612	CLA	1	0
14	J	4001	BCR	3	0
14	J	4002	BCR	2	0
15	B	1210	CLA	2	0
15	B	1239	CLA	1	0
15	1	605	CLA	2	0
15	B	1214	CLA	2	0
15	A	1111	CLA	3	0
22	B	5002	DGD	2	0
15	1	603	CLA	5	0
14	3	504	BCR	3	0
19	A	1011	CL0	3	0
15	A	1128	CLA	1	0
16	4	610	CHL	1	0
14	A	4006	BCR	6	0
15	3	603	CLA	1	0
15	1	607	CLA	1	0
15	2	603	CLA	1	0
15	B	1226	CLA	2	0
14	3	506	BCR	2	0
15	1	615	CLA	1	0
14	B	4001	BCR	1	0
15	A	1112	CLA	1	0
15	A	1012	CLA	8	0
15	A	1141	CLA	2	0
15	B	1208	CLA	2	0
15	B	1236	CLA	2	0
17	1	801	LHG	1	0
12	3	501	LUT	7	0
14	B	4002	BCR	1	0
16	1	609	CHL	1	0
14	B	4003	BCR	1	0
15	A	1129	CLA	2	0

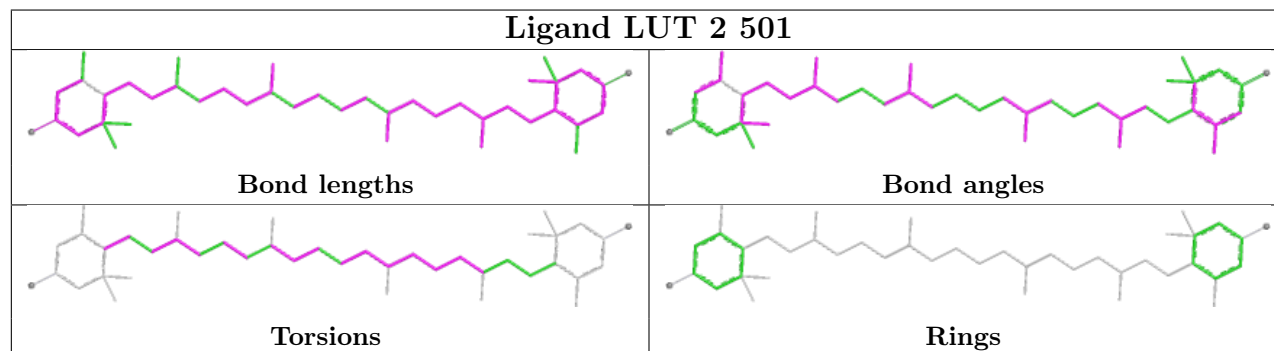
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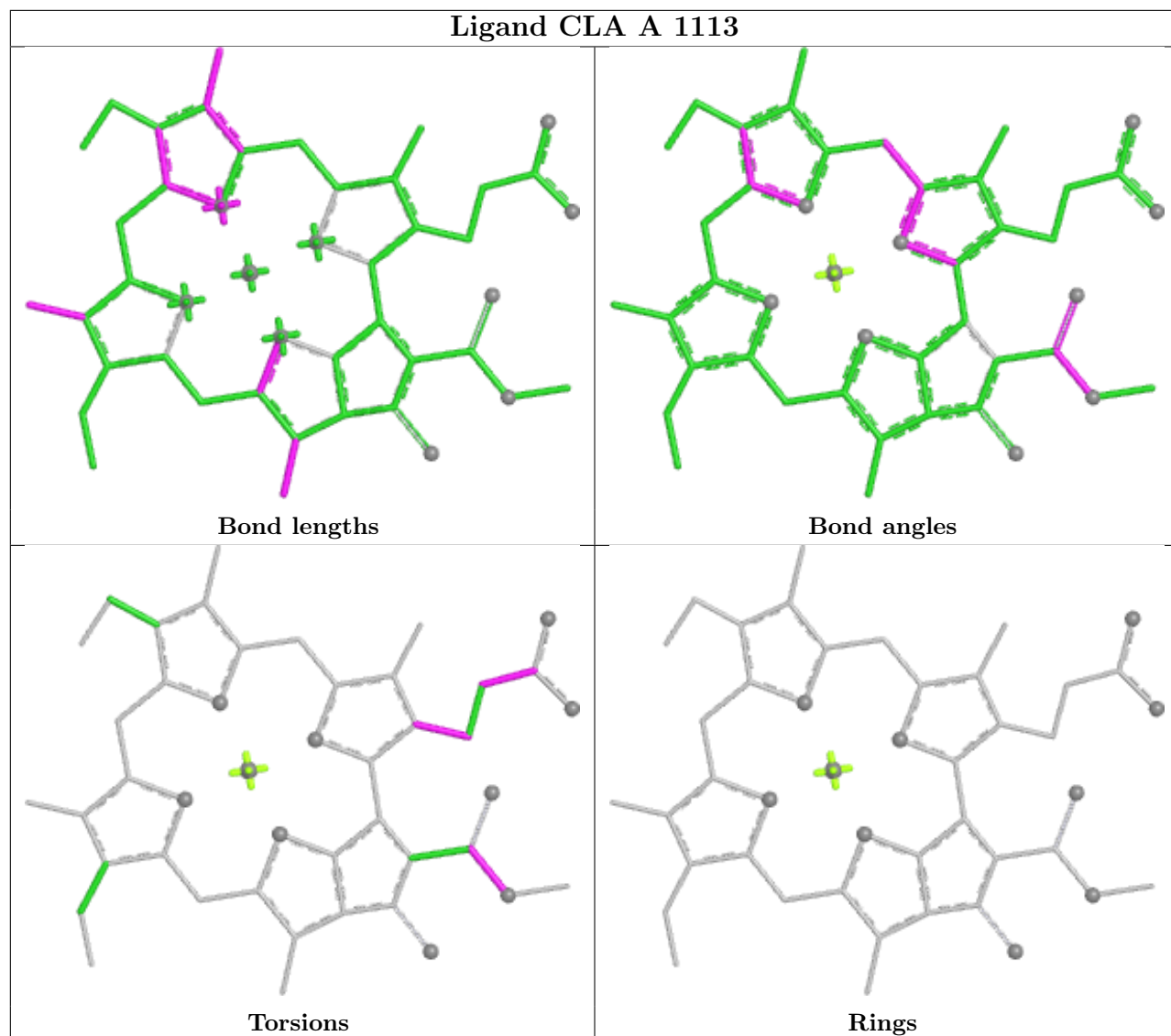
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	A	1104	CLA	2	0
15	2	608	CLA	1	0
14	B	4005	BCR	3	0
15	A	1118	CLA	1	0
13	4	502	XAT	5	0
15	3	601	CLA	3	0
15	4	604	CLA	1	0
15	A	1125	CLA	5	0
18	B	5003	LMG	2	0
15	B	1021	CLA	1	0
15	3	605	CLA	5	0
14	A	4007	BCR	2	0
15	A	1013	CLA	4	0
13	1	502	XAT	3	0
17	A	5001	LHG	1	0
15	3	611	CLA	1	0
15	A	1108	CLA	1	0
15	B	1023	CLA	1	0
21	C	3003	SF4	1	0
15	B	1234	CLA	2	0
14	F	4001	BCR	2	0
12	1	501	LUT	12	0
15	B	1202	CLA	2	0
15	4	601	CLA	3	0
15	4	603	CLA	1	0
14	A	4002	BCR	1	0
15	B	1220	CLA	2	0
15	B	1225	CLA	1	0
15	B	1223	CLA	3	0
15	B	1238	CLA	1	0
15	1	601	CLA	3	0
12	4	501	LUT	7	0
14	B	4006	BCR	2	0
15	A	1123	CLA	1	0
15	3	612	CLA	2	0
15	A	1127	CLA	1	0
14	A	4008	BCR	1	0
15	3	614	CLA	2	0
13	3	502	XAT	2	0
18	4	801	LMG	1	0

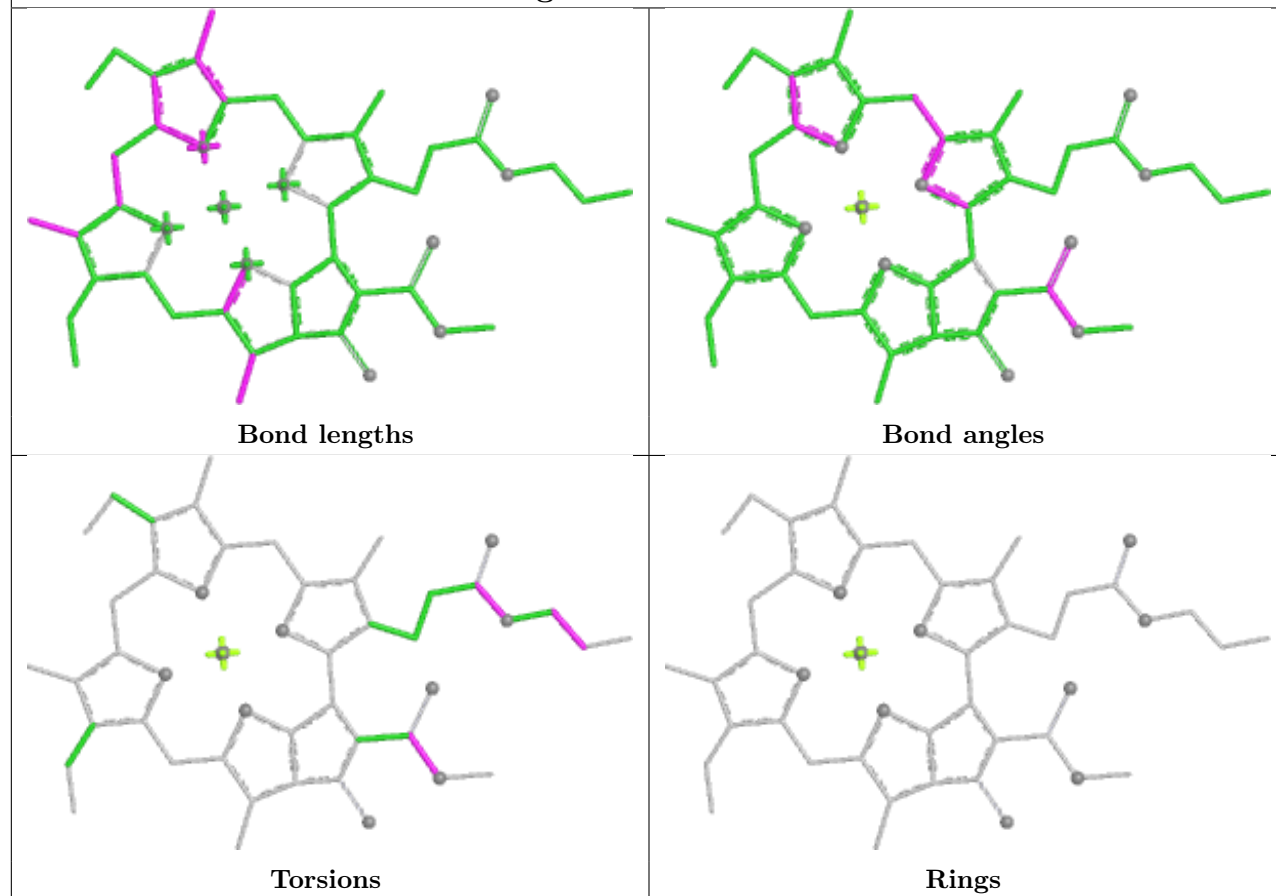
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

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

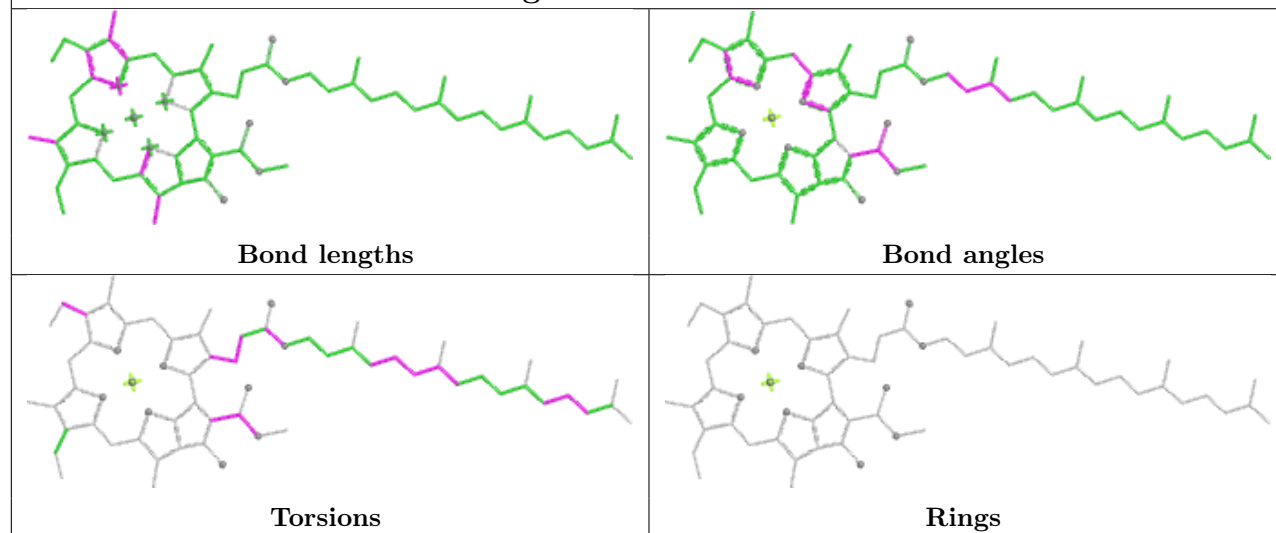




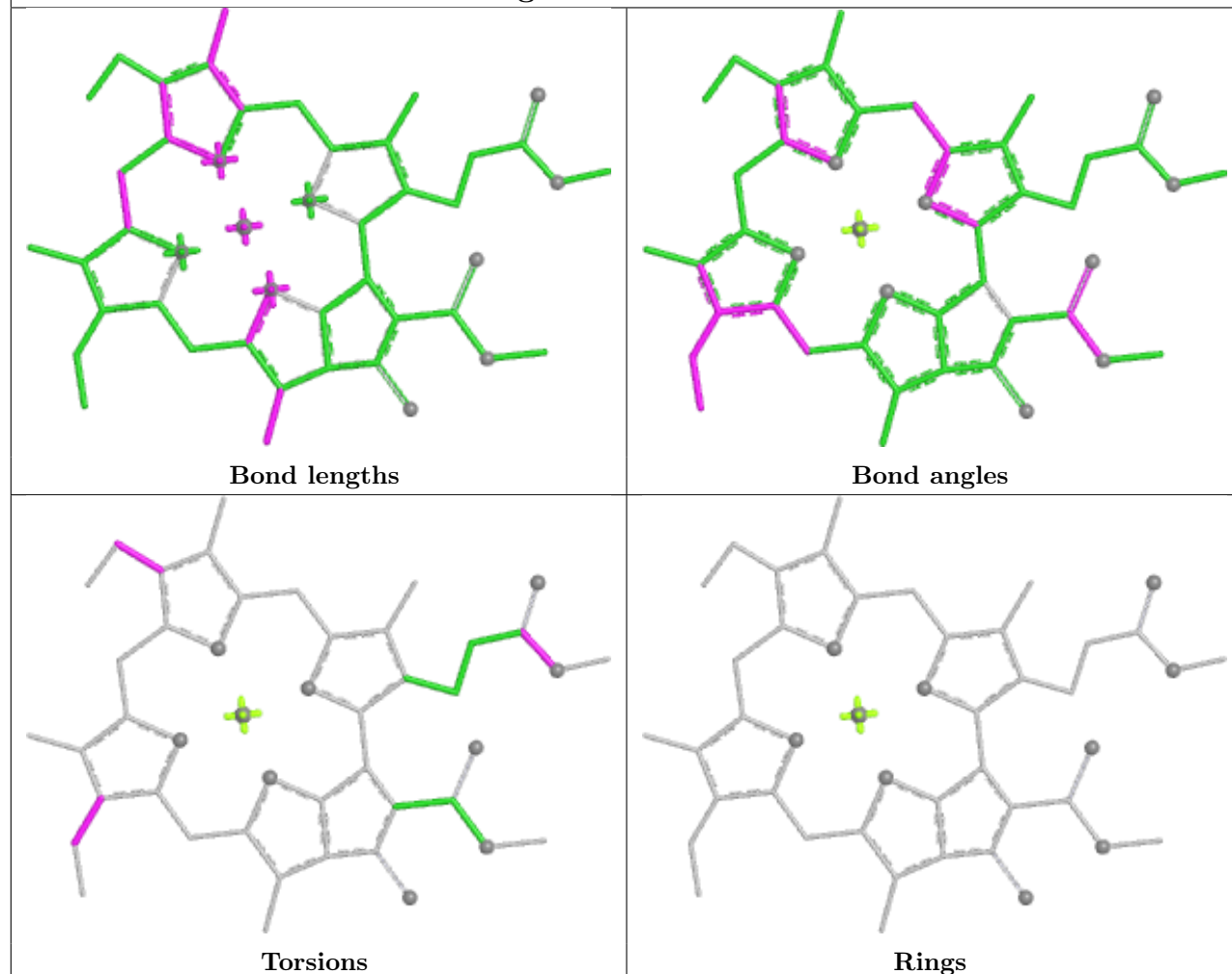
Ligand CLA 1 611



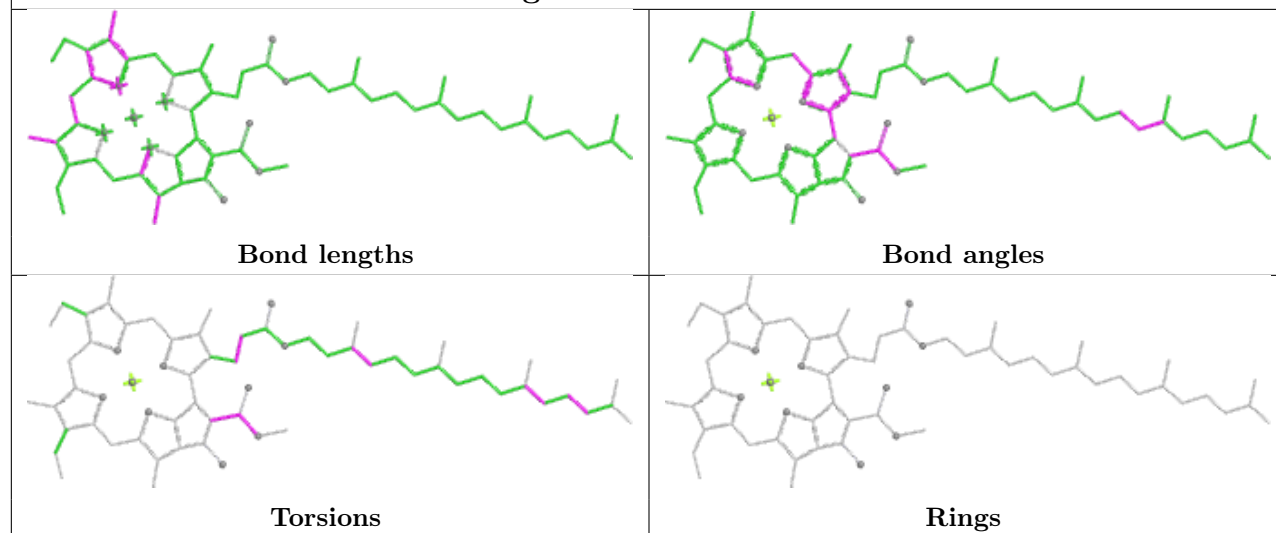
Ligand CLA A 1101

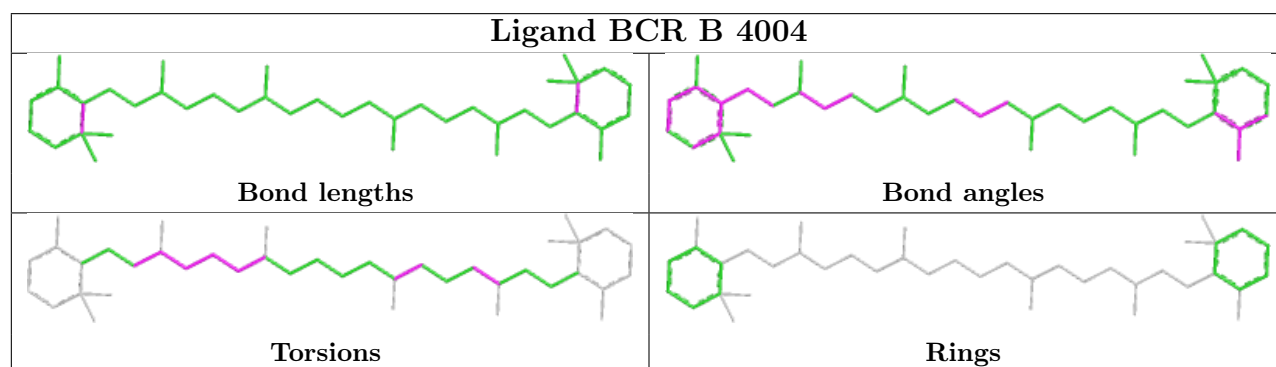
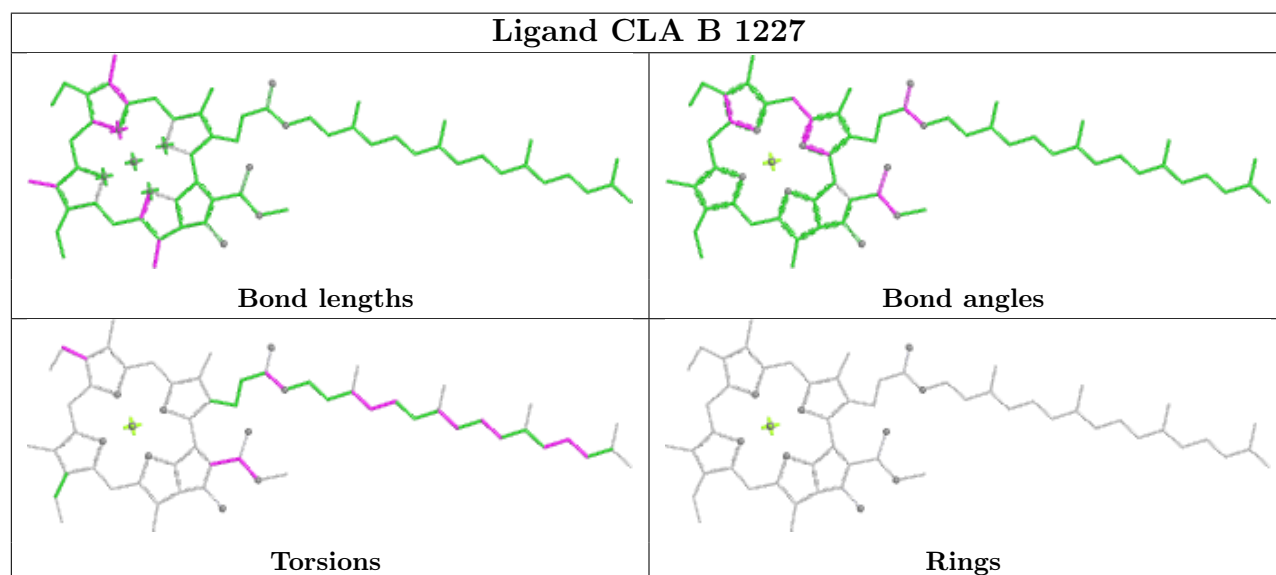
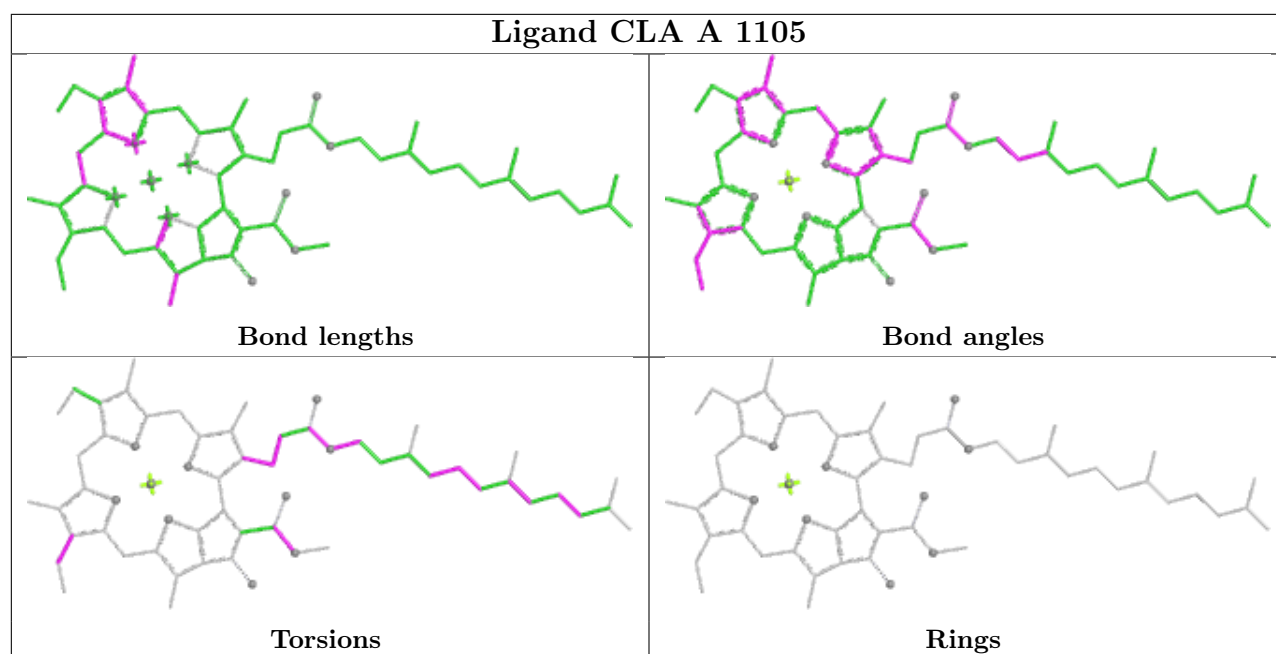


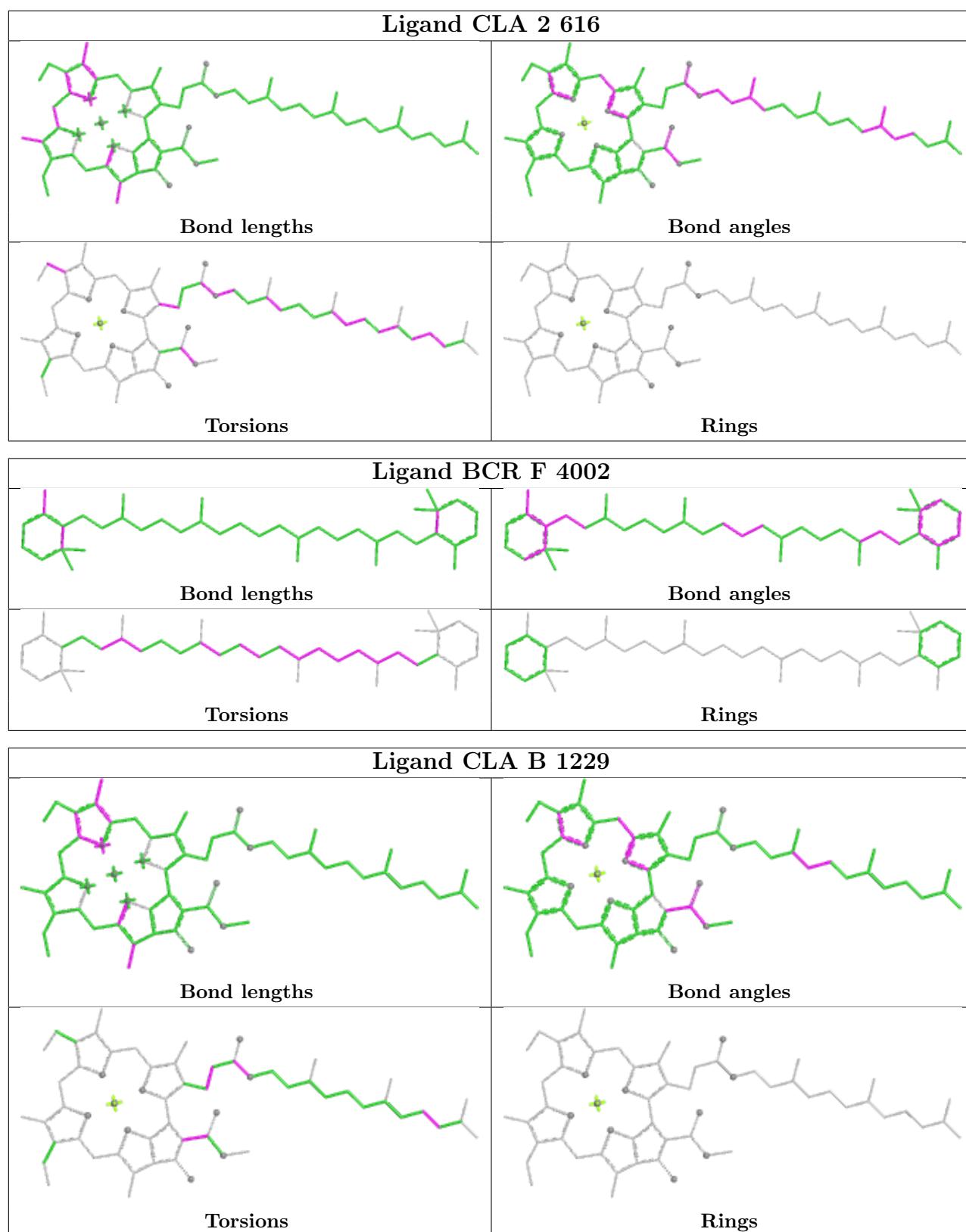
Ligand CLA 4 608

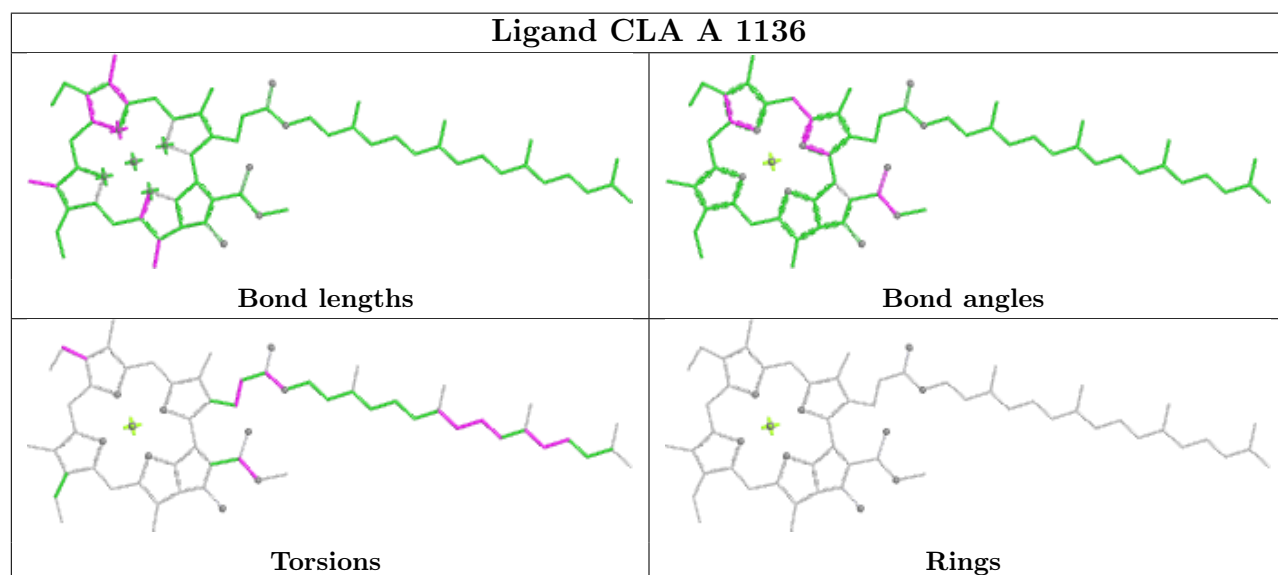
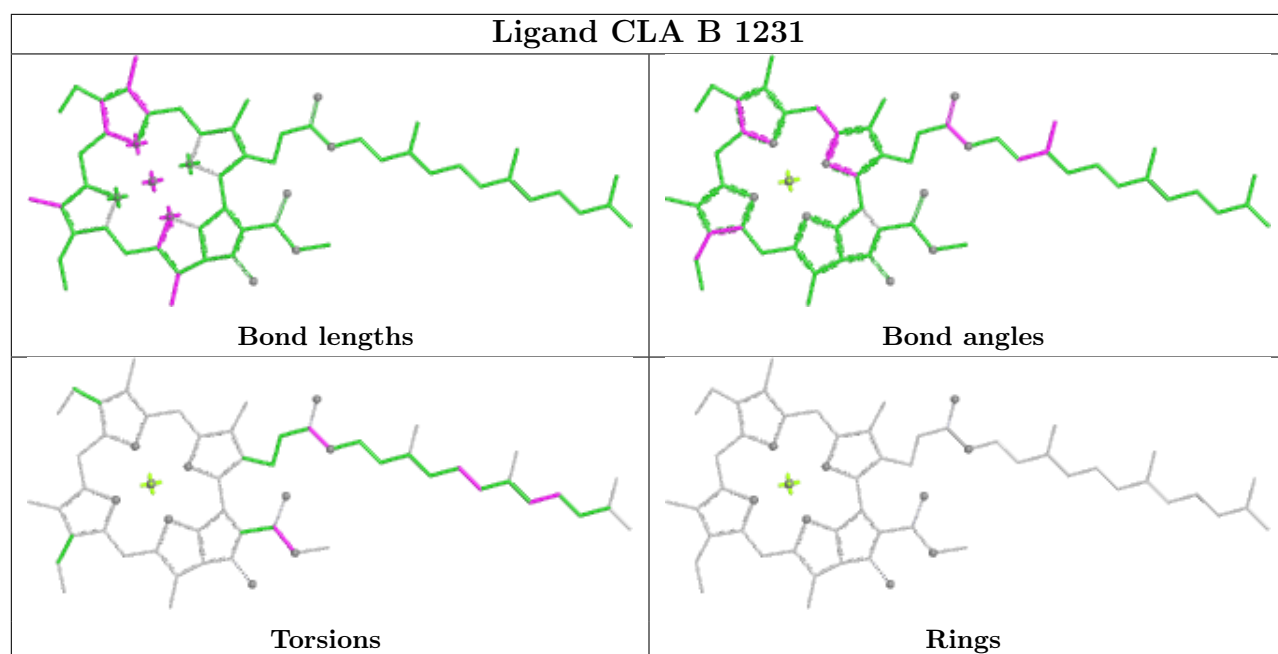


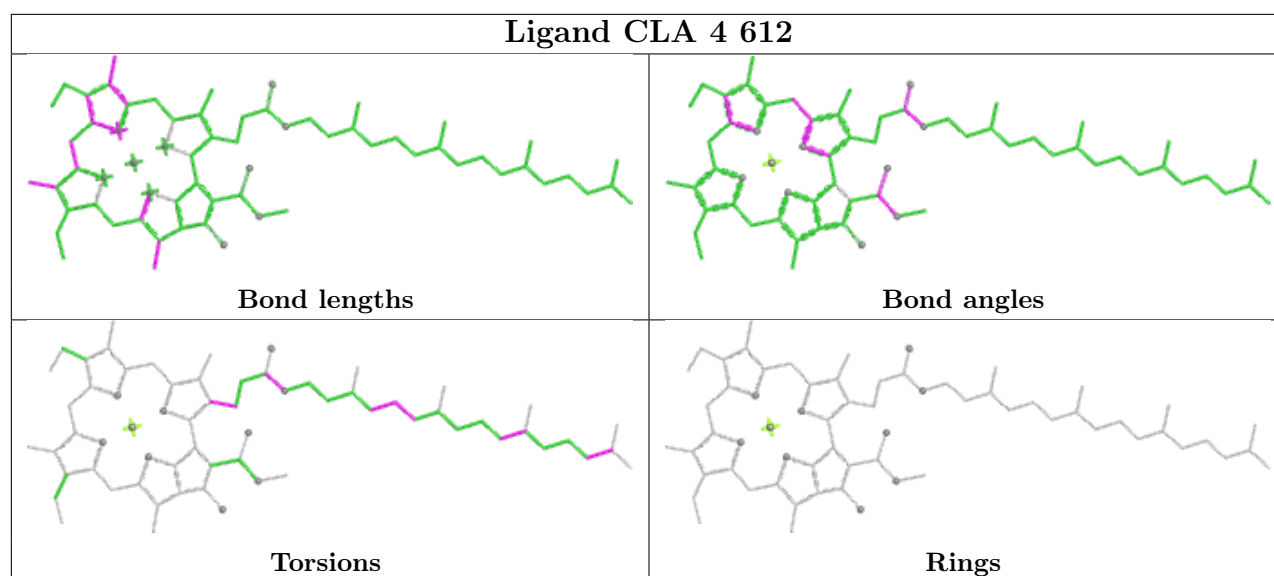
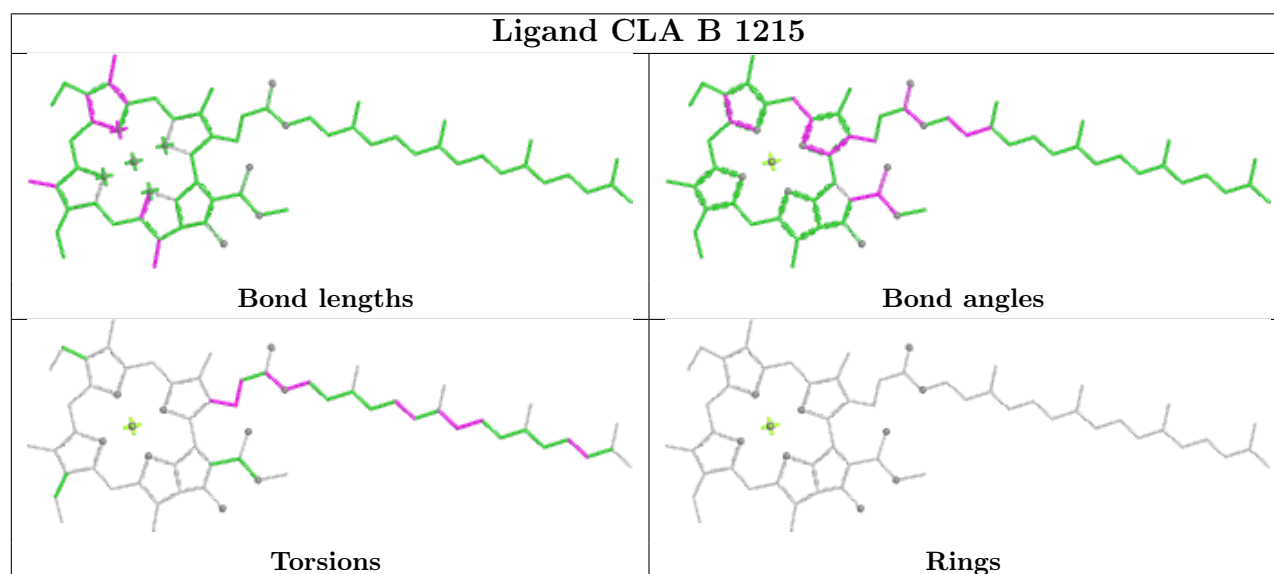
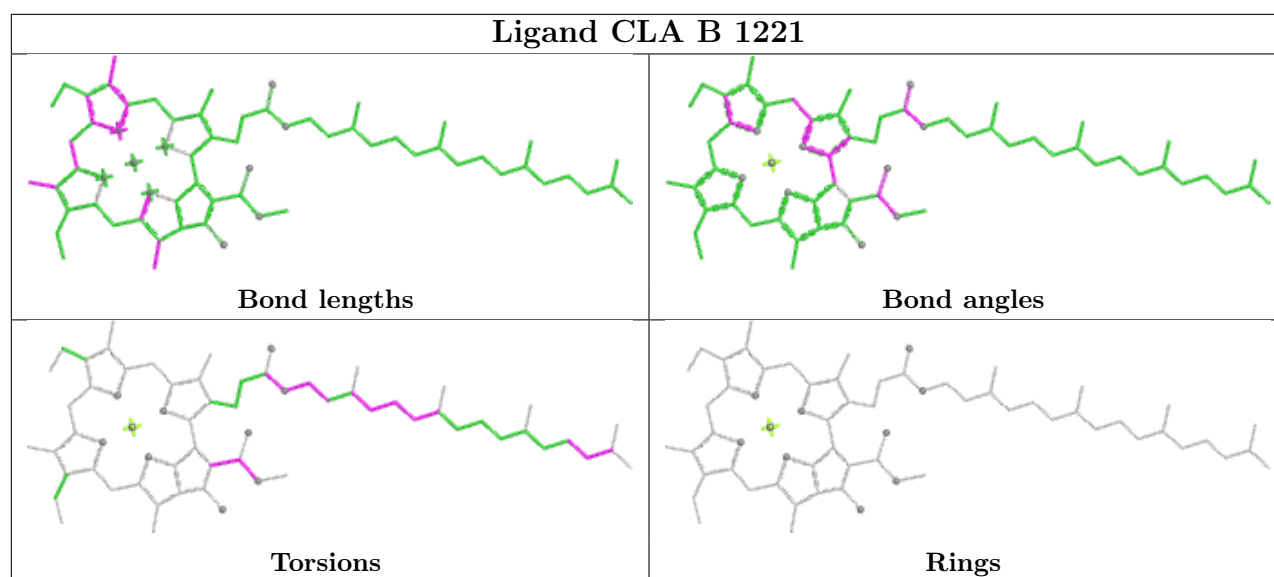
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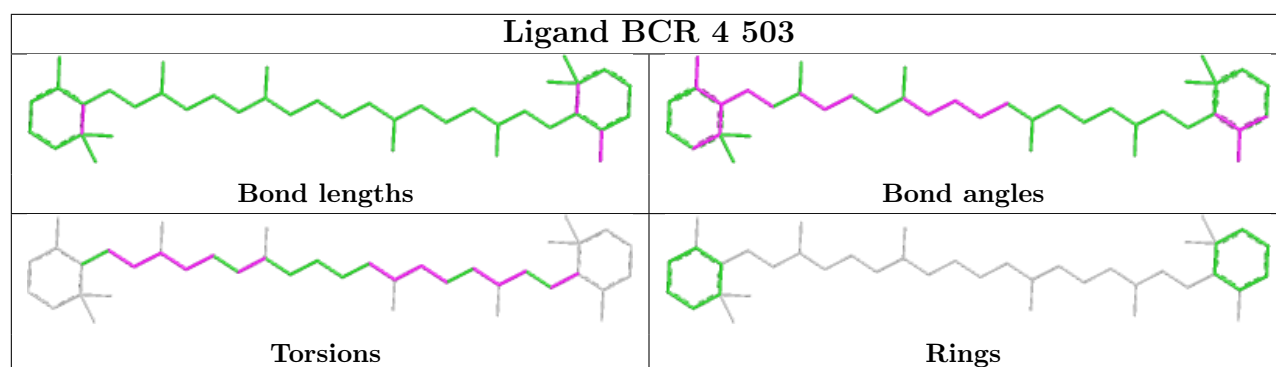
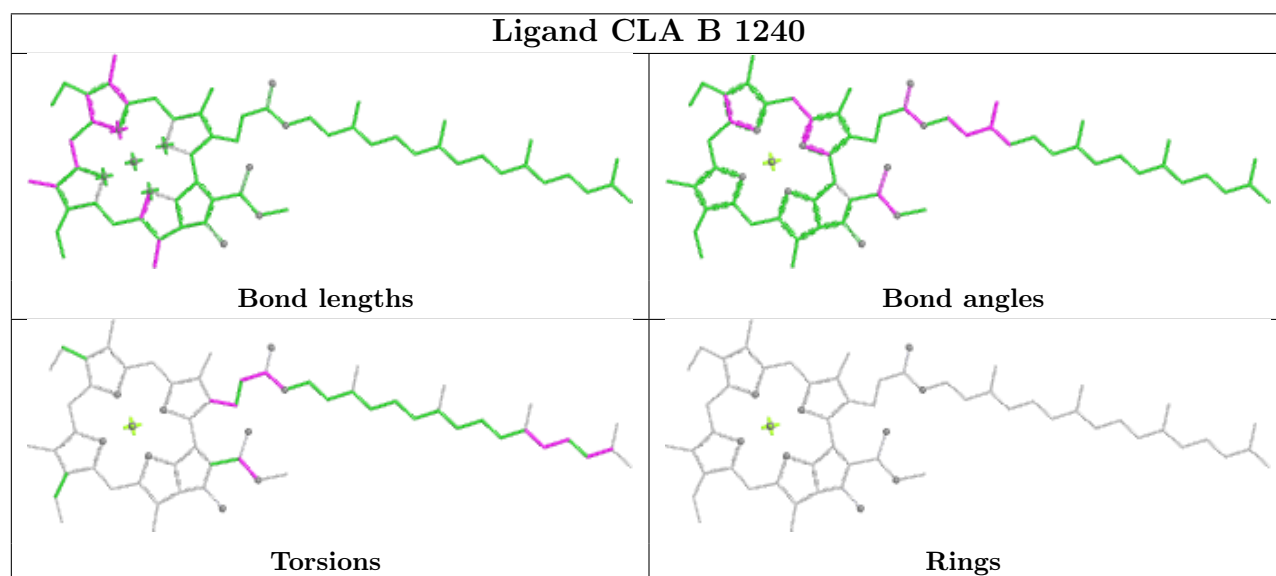
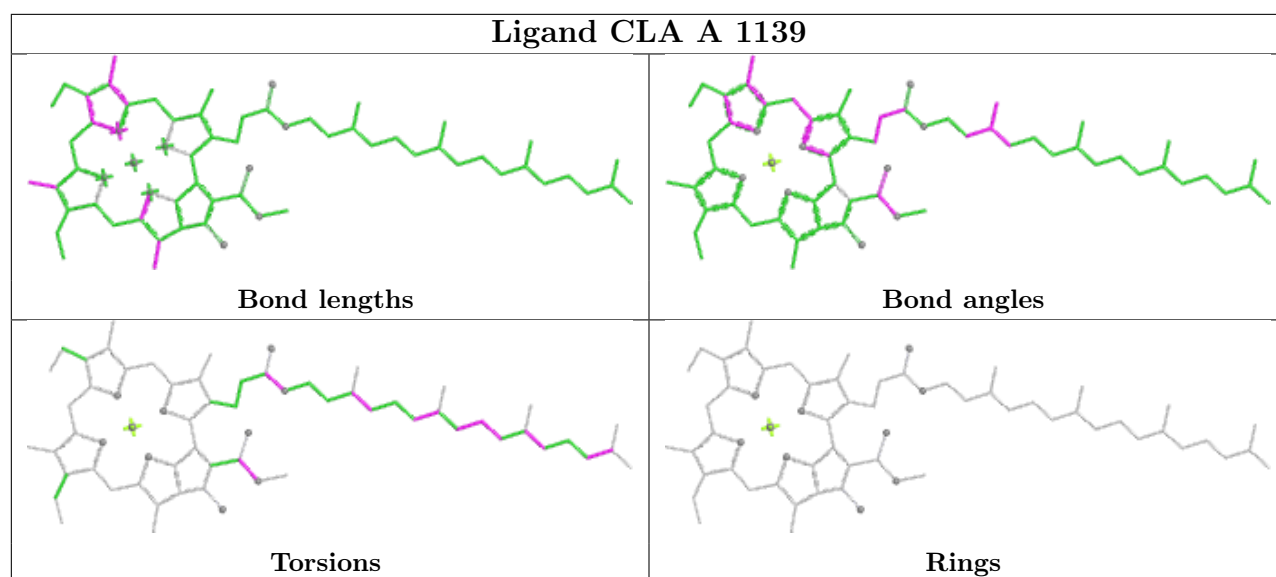


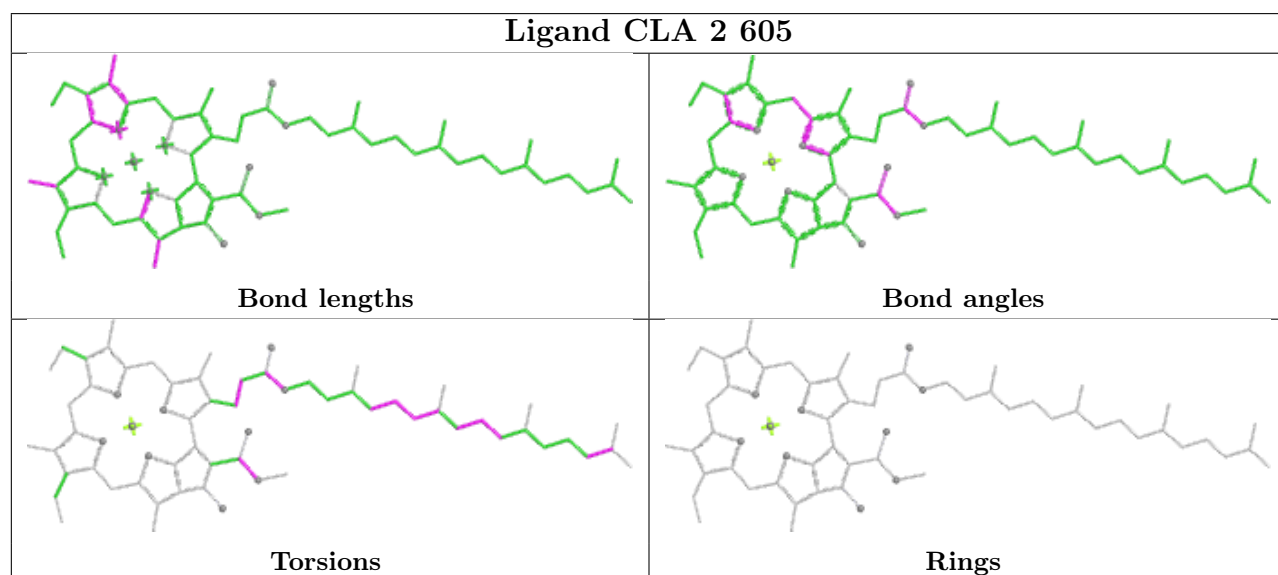
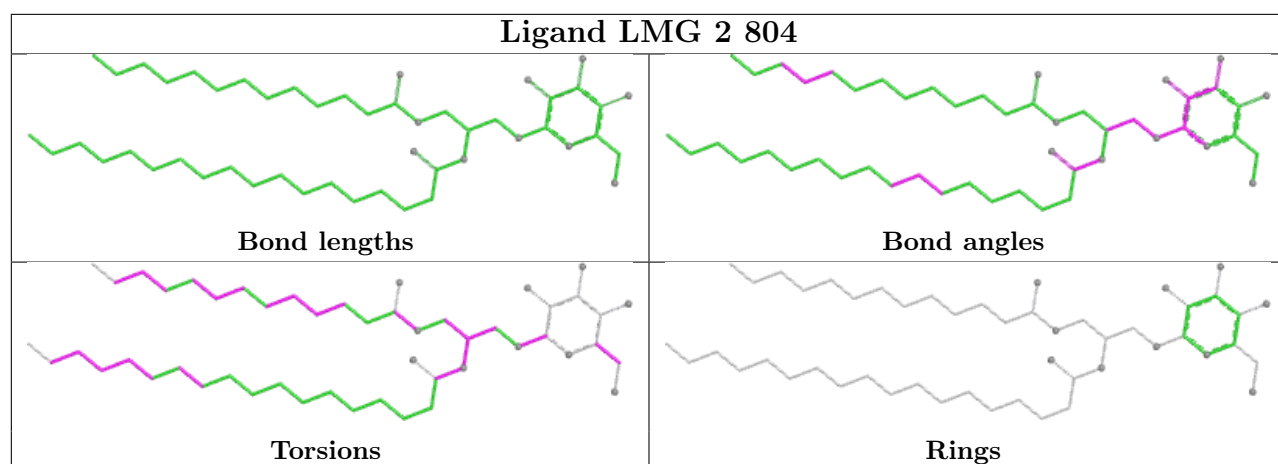


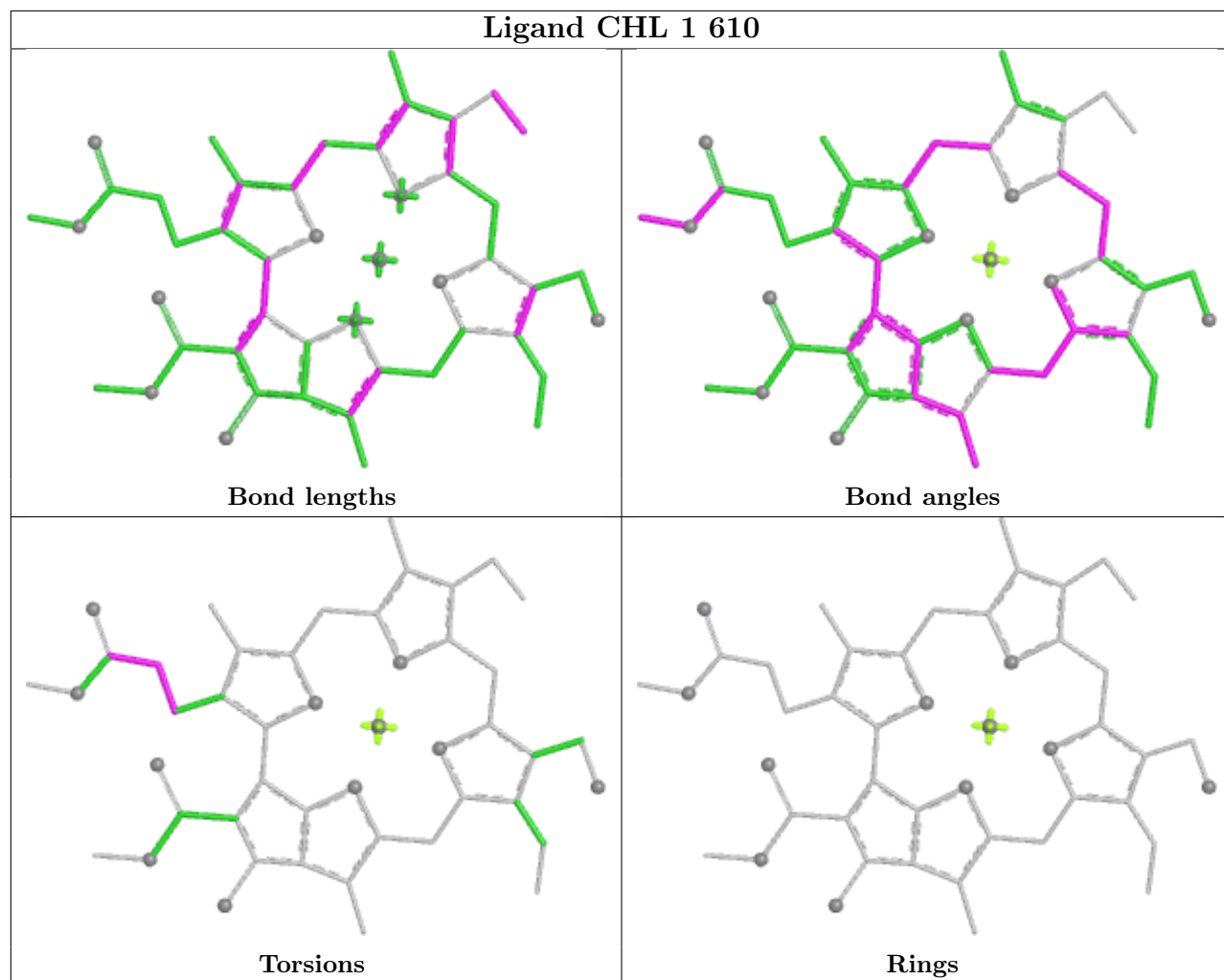




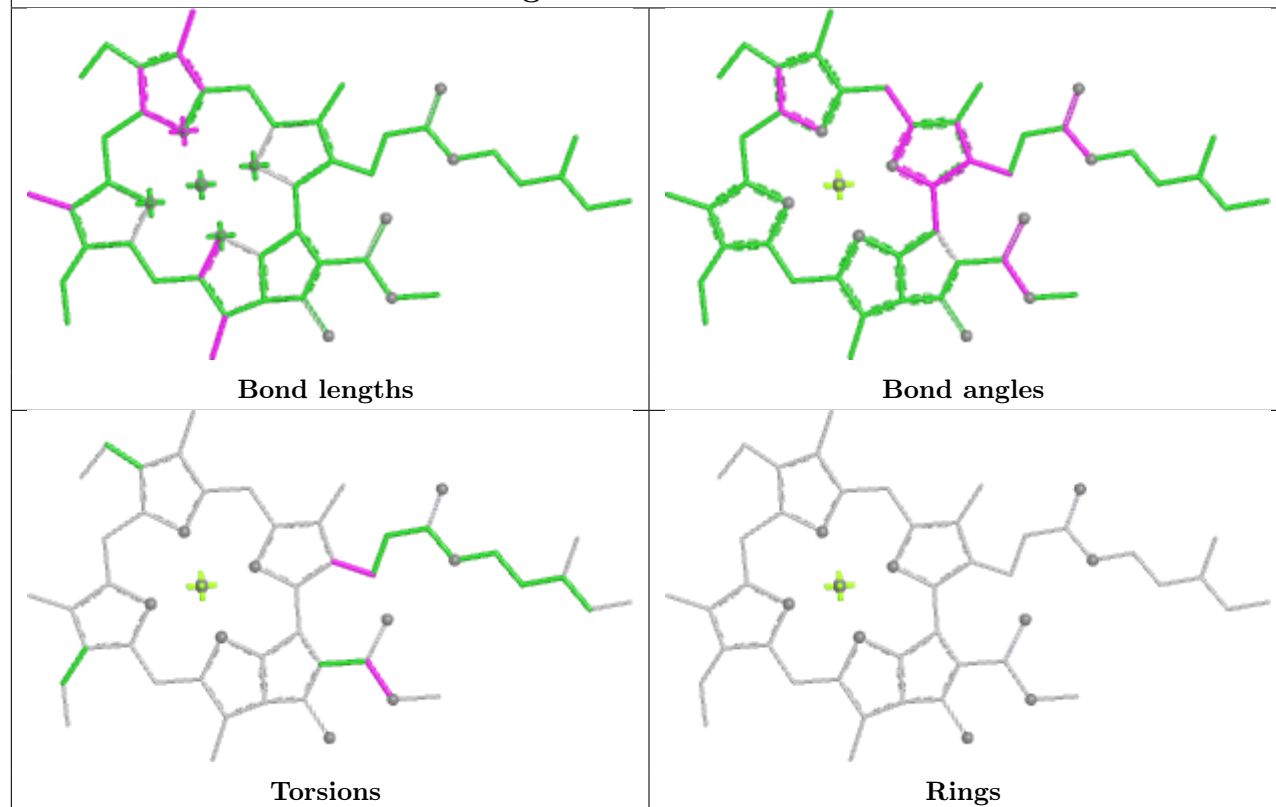




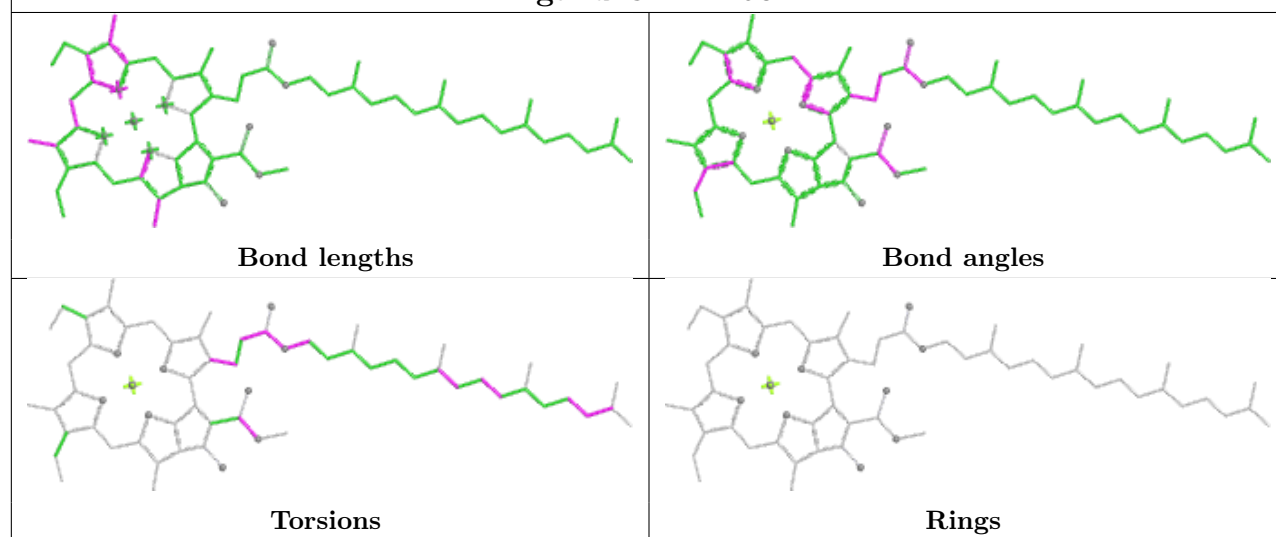




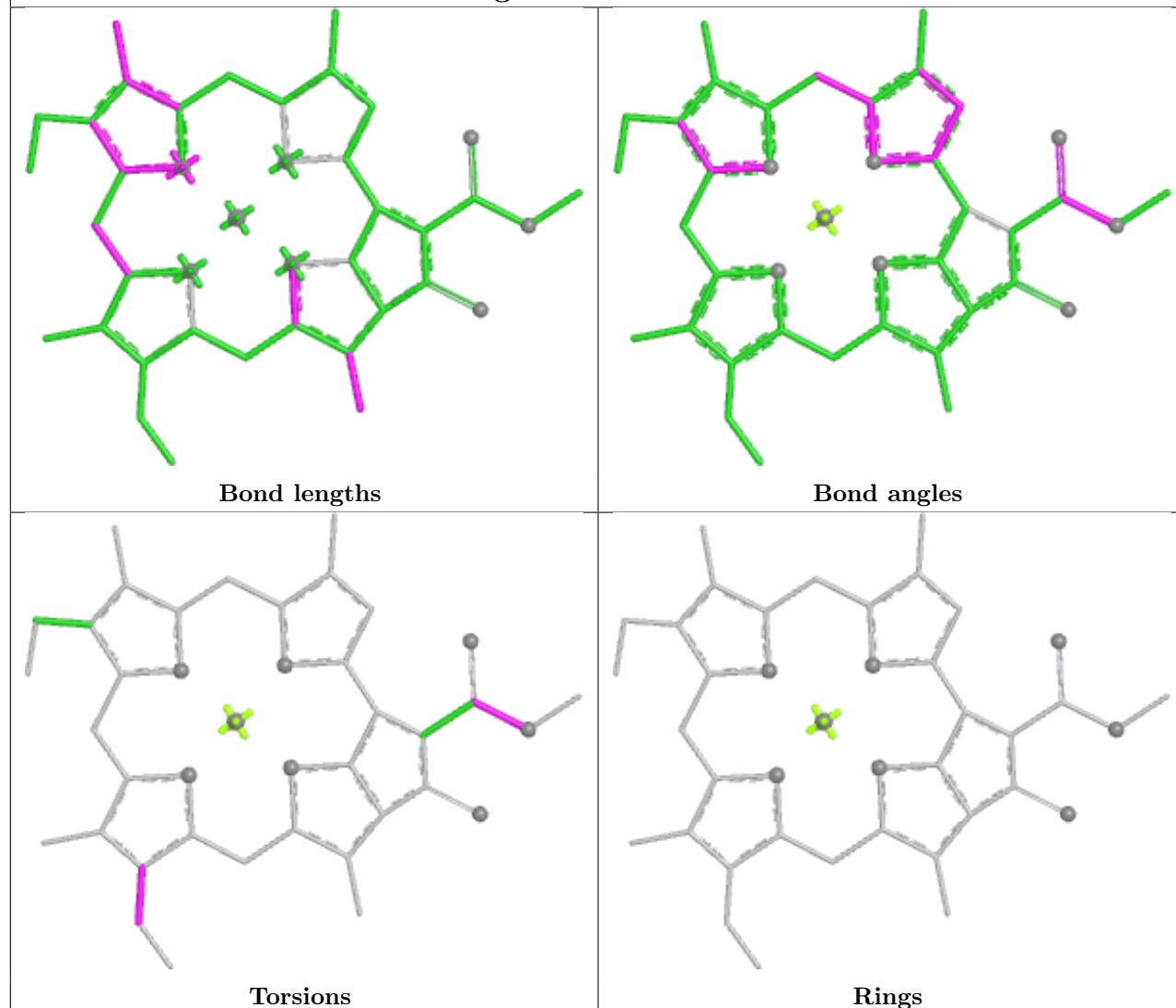
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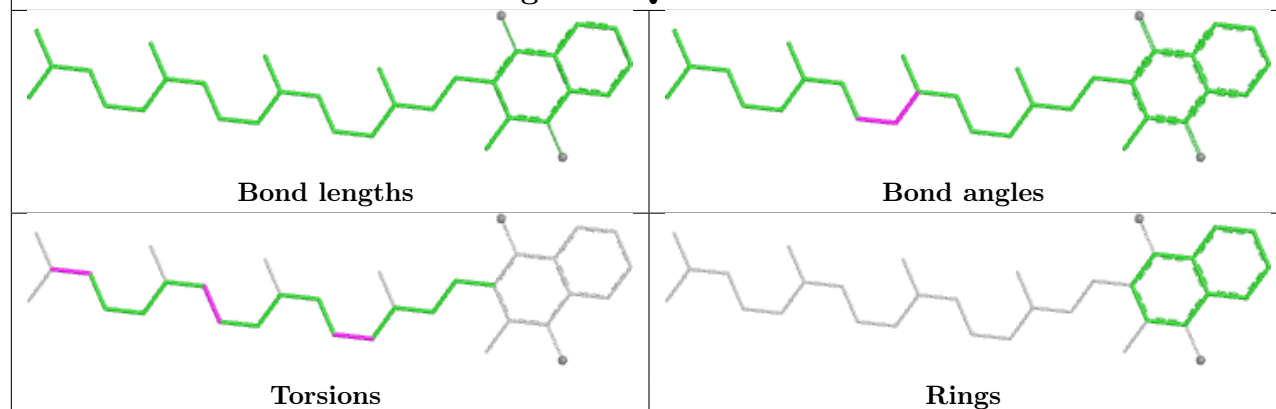
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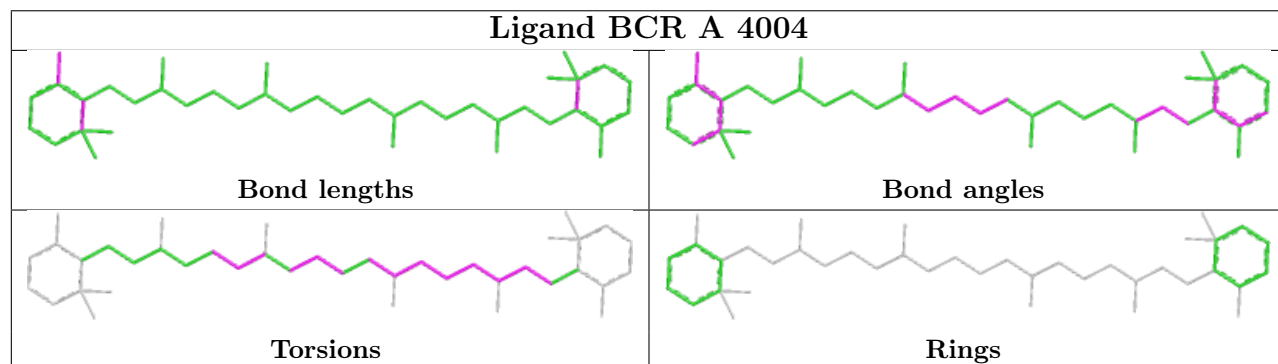
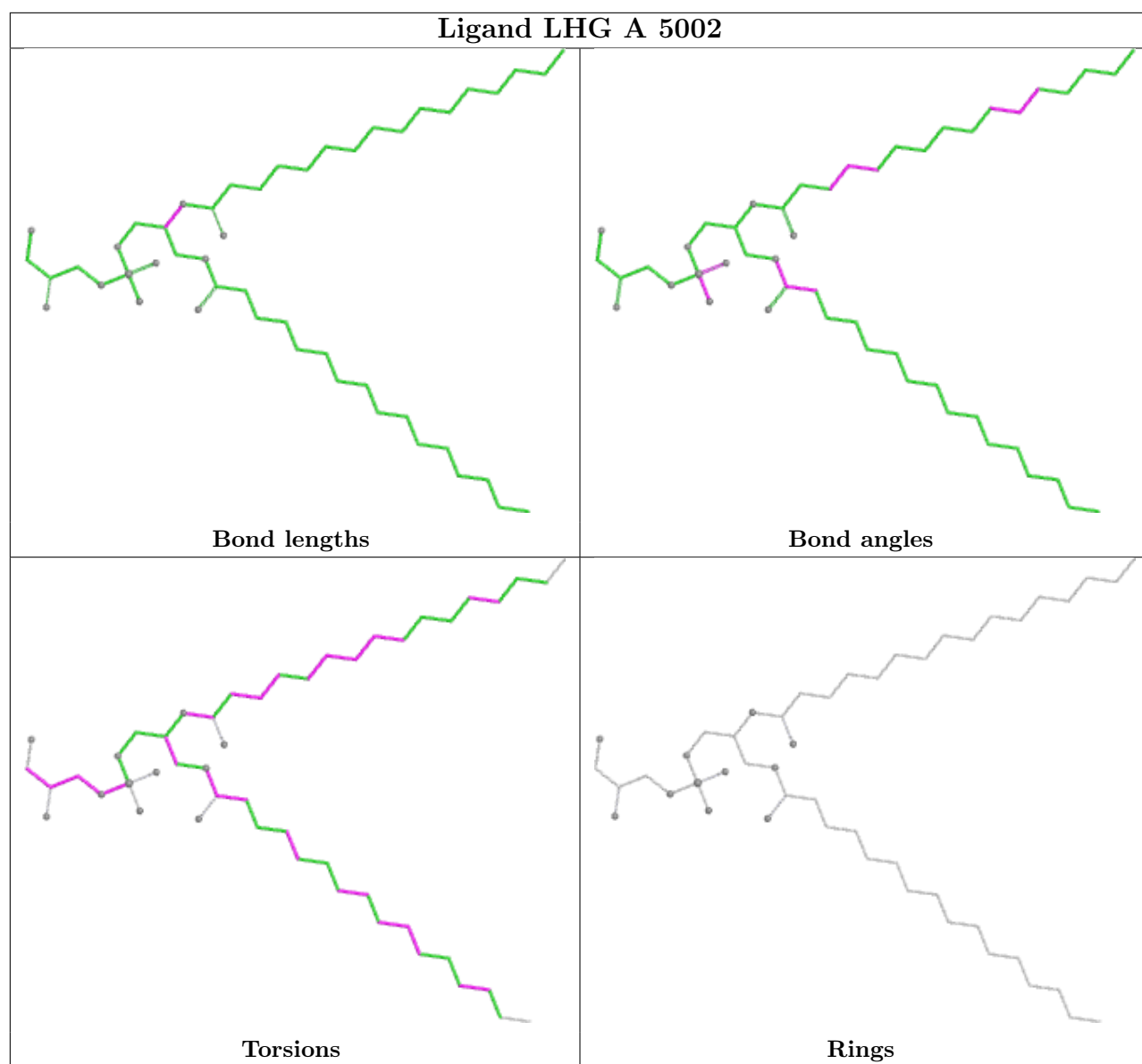


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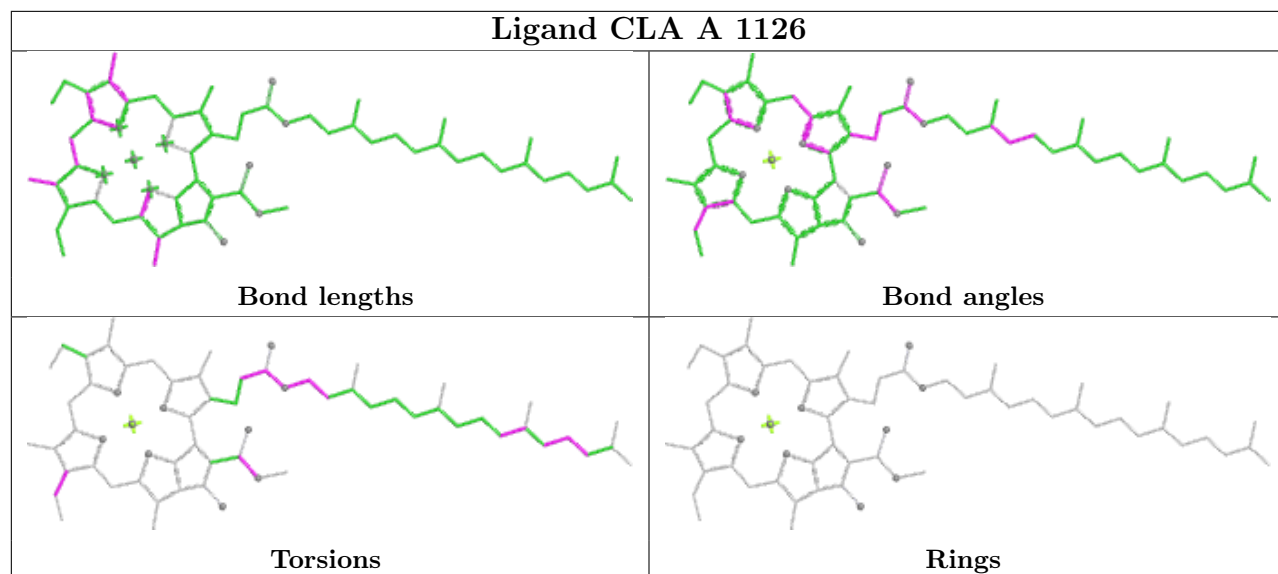


Ligand PQN B 2002

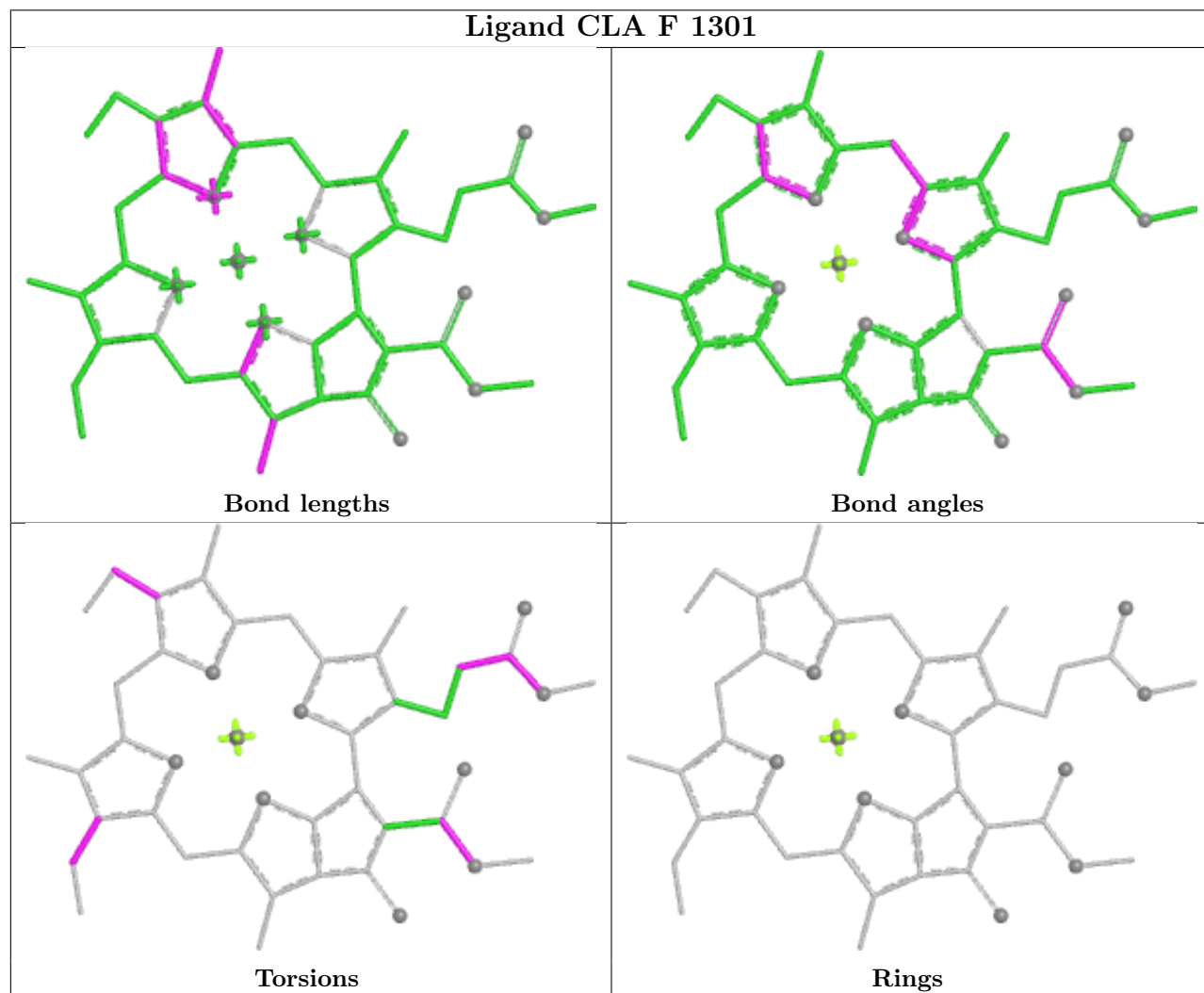


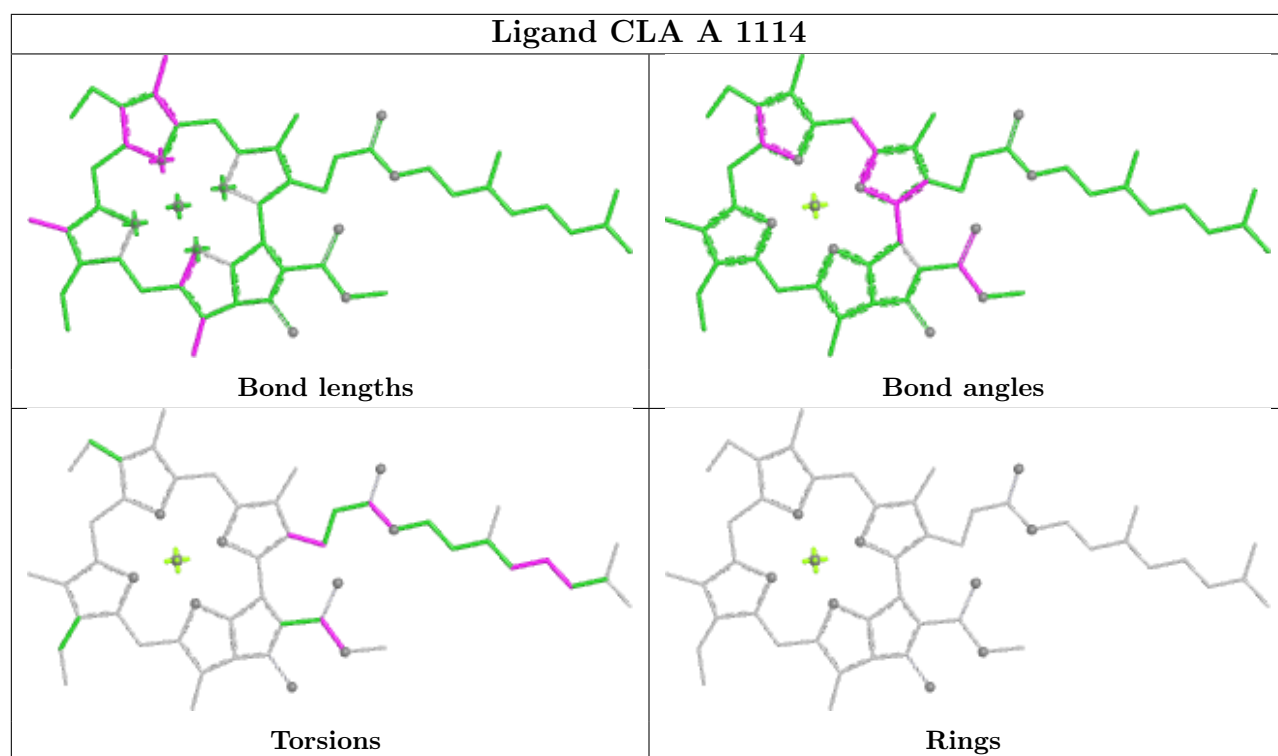


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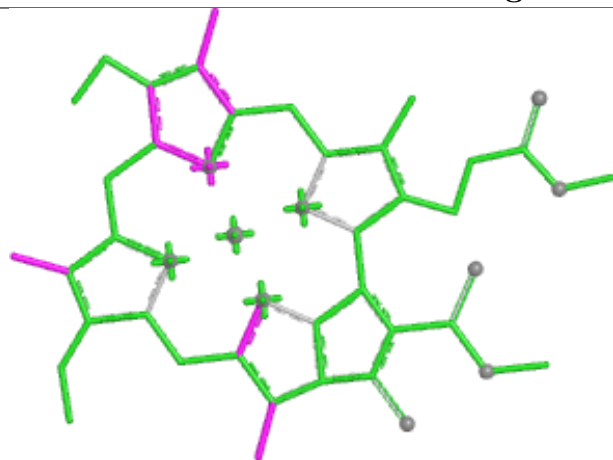


Ligand CLA F 1301

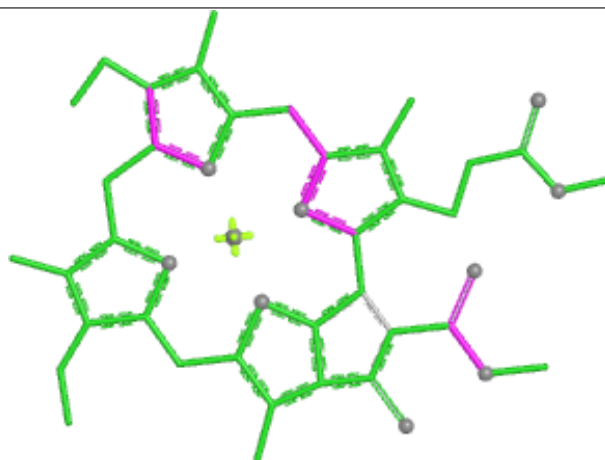




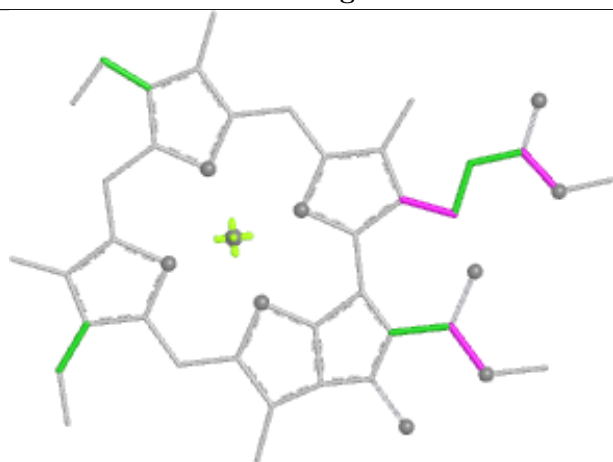
Ligand CLA B 1209



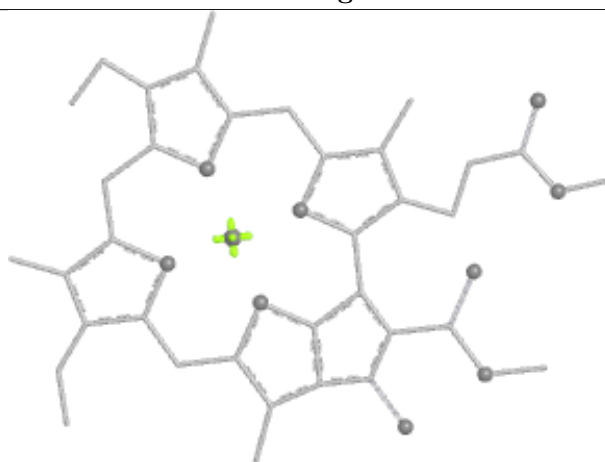
Bond lengths



Bond angles

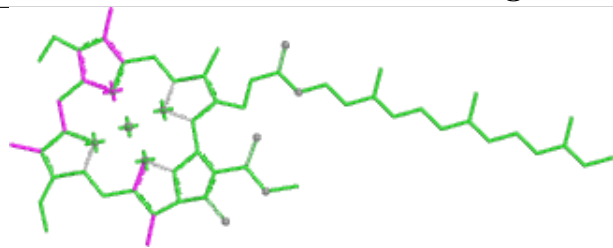


Torsions

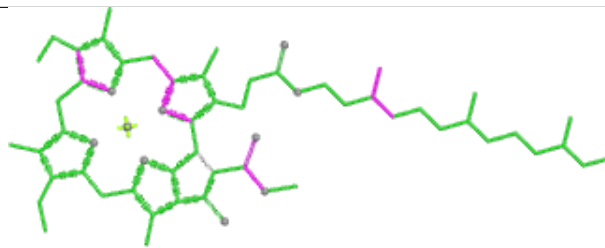


Rings

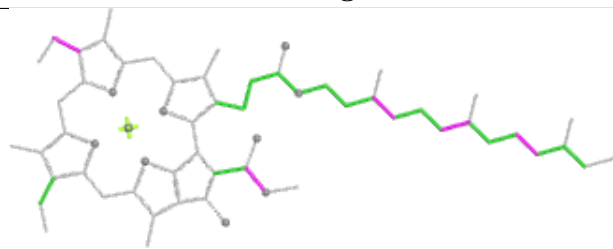
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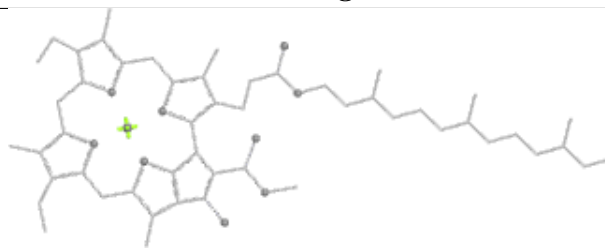
Bond lengths



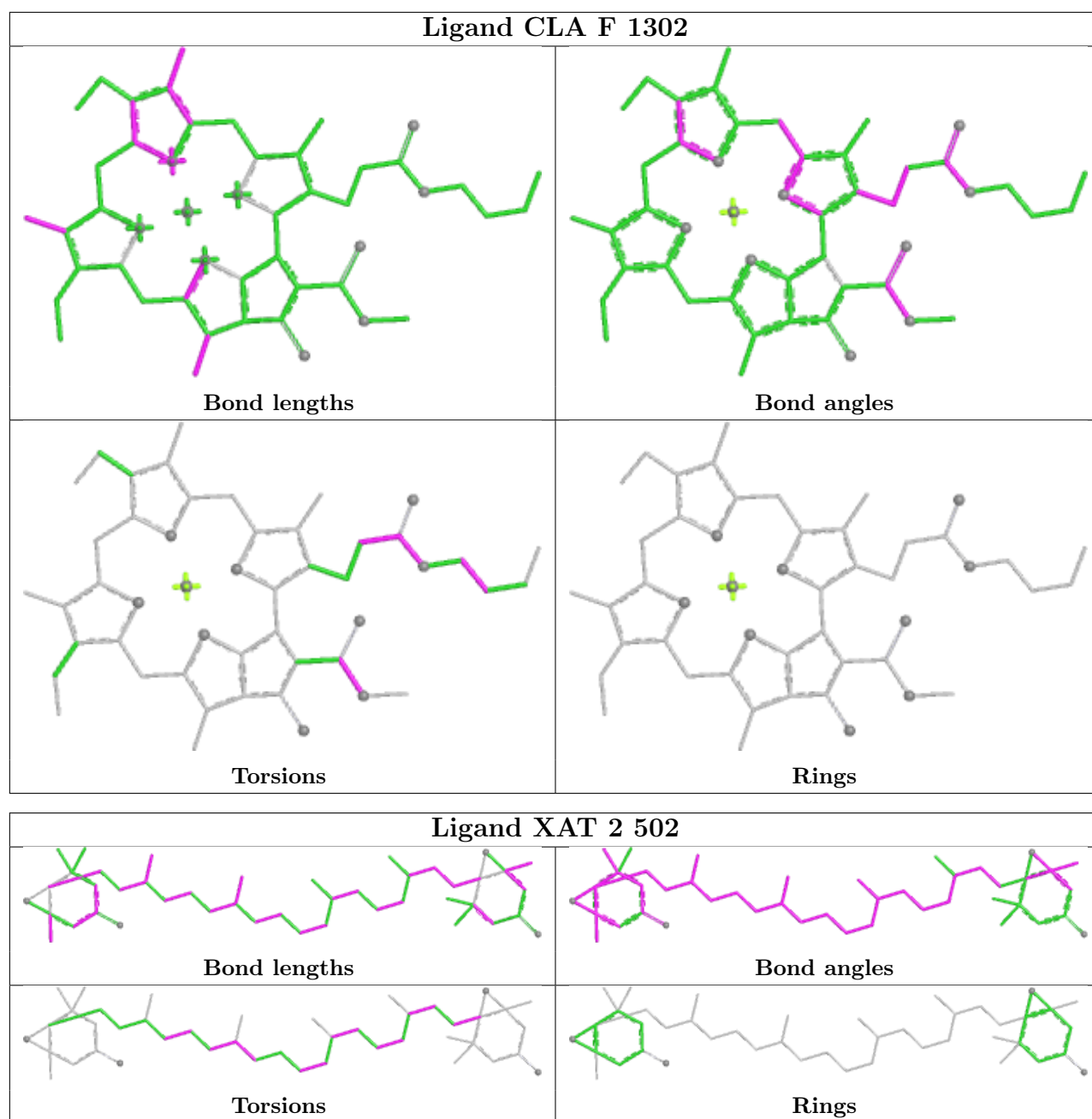
Bond angles

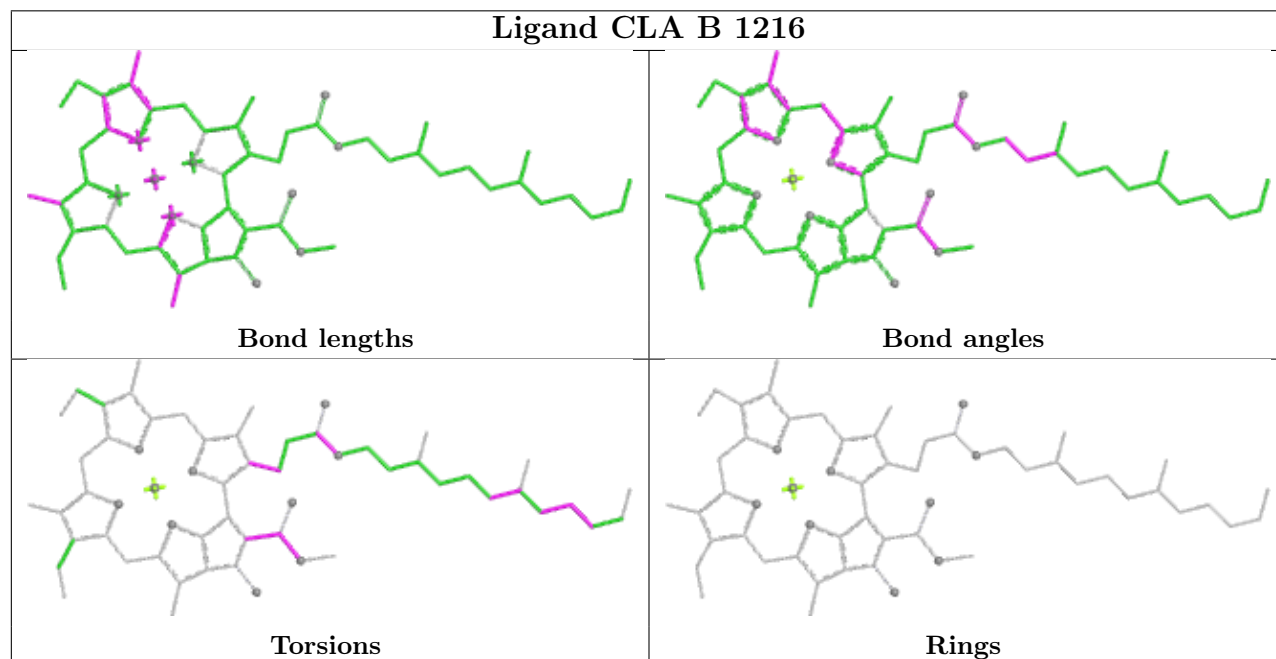
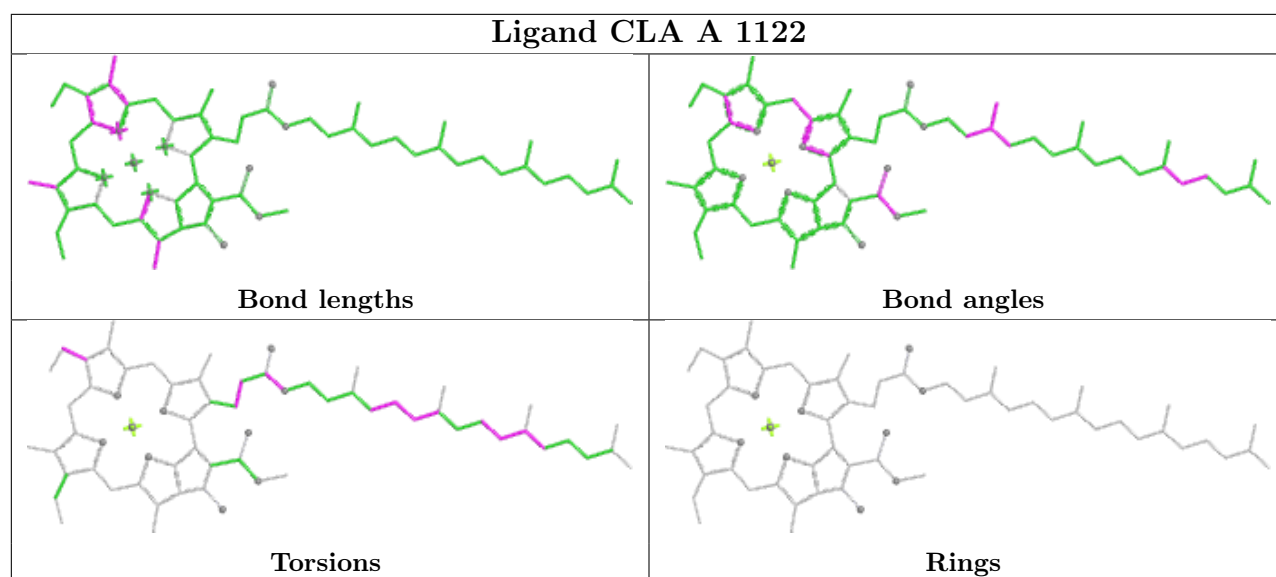


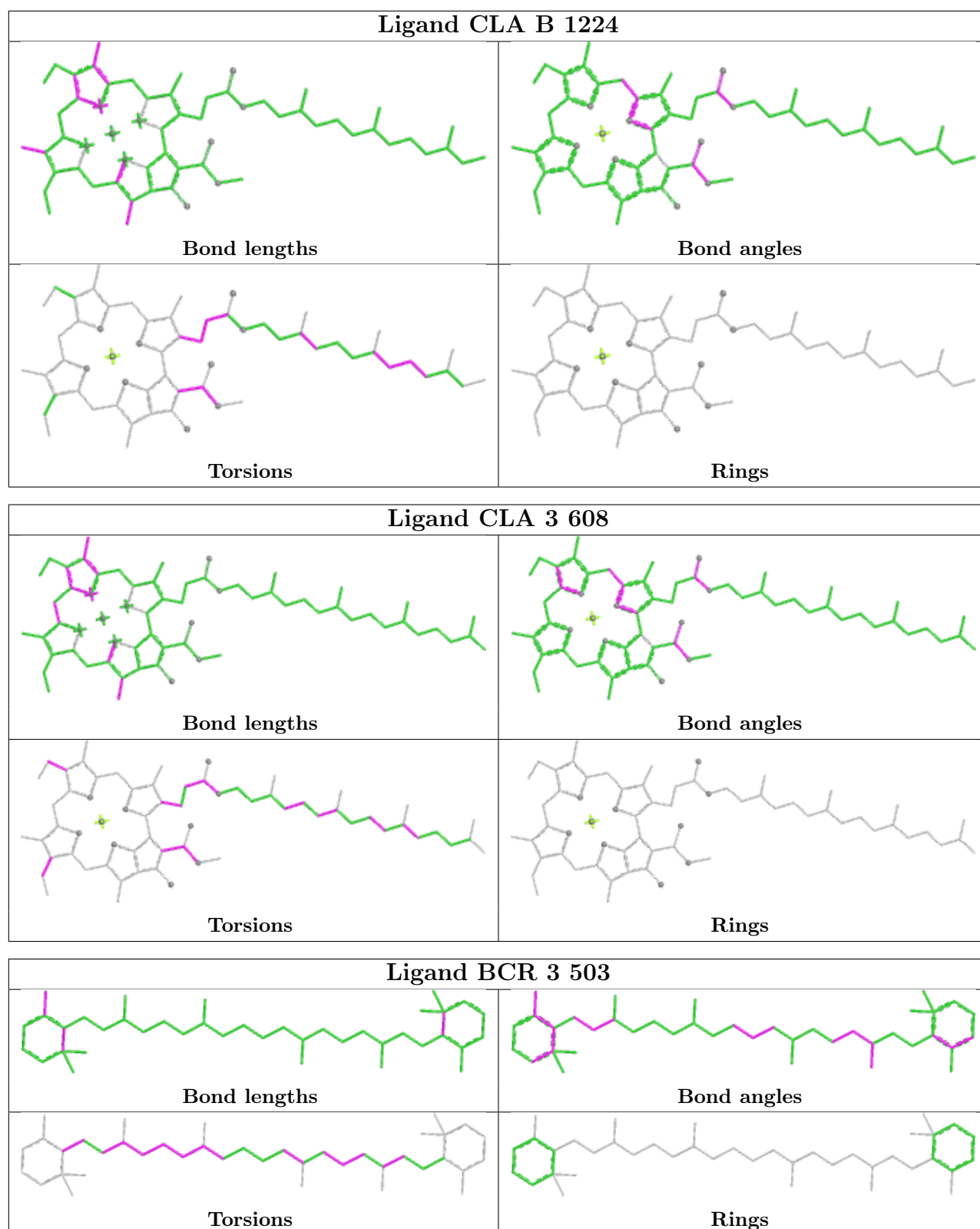
Torsions



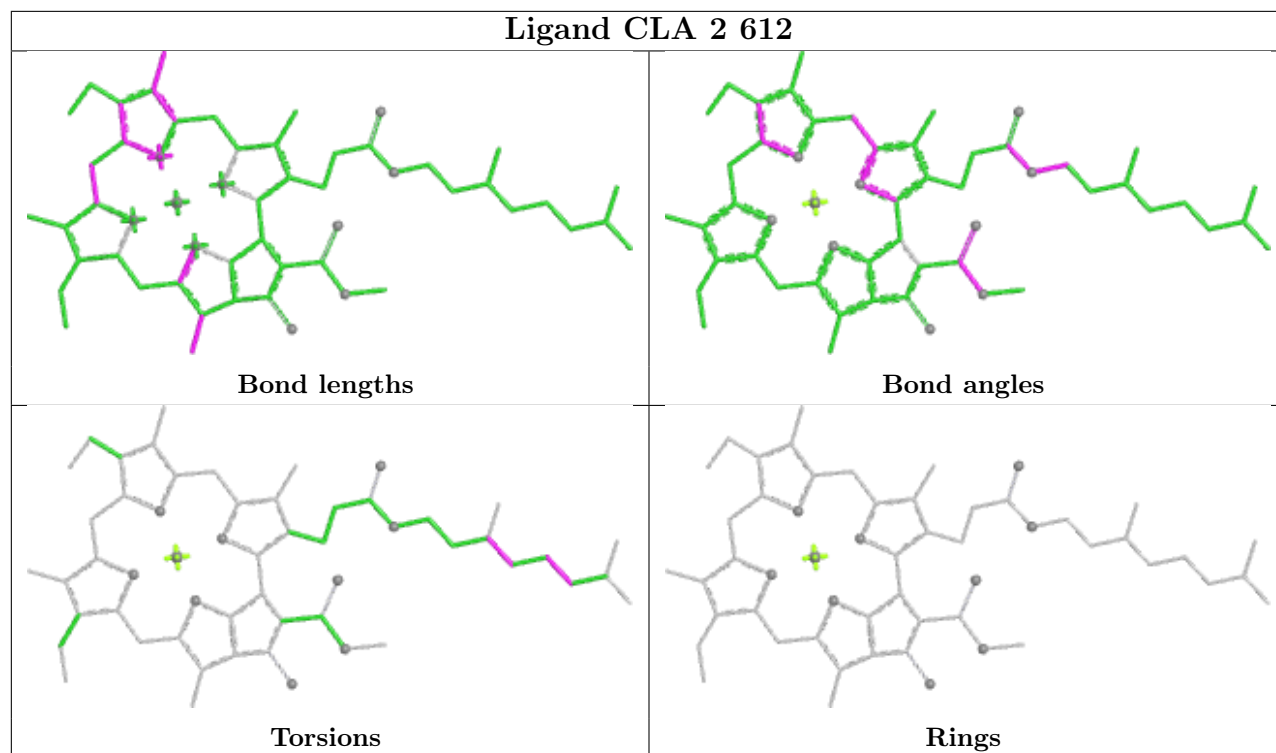
Rings



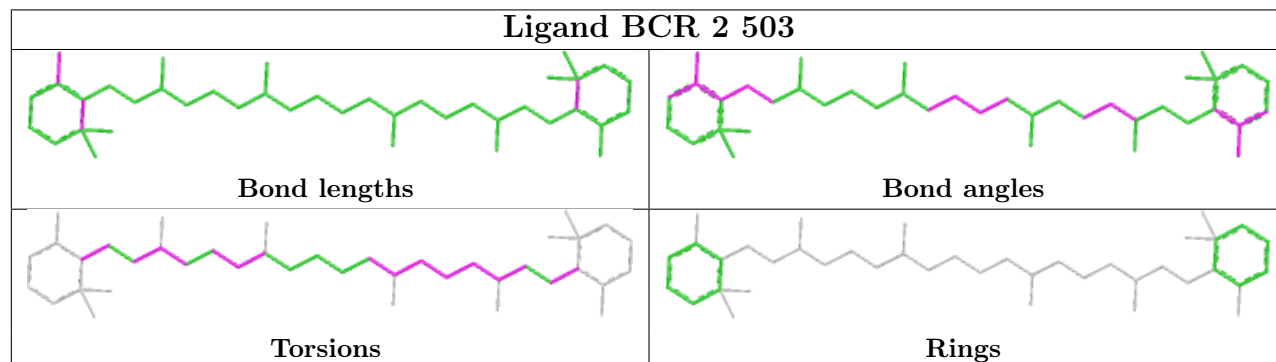




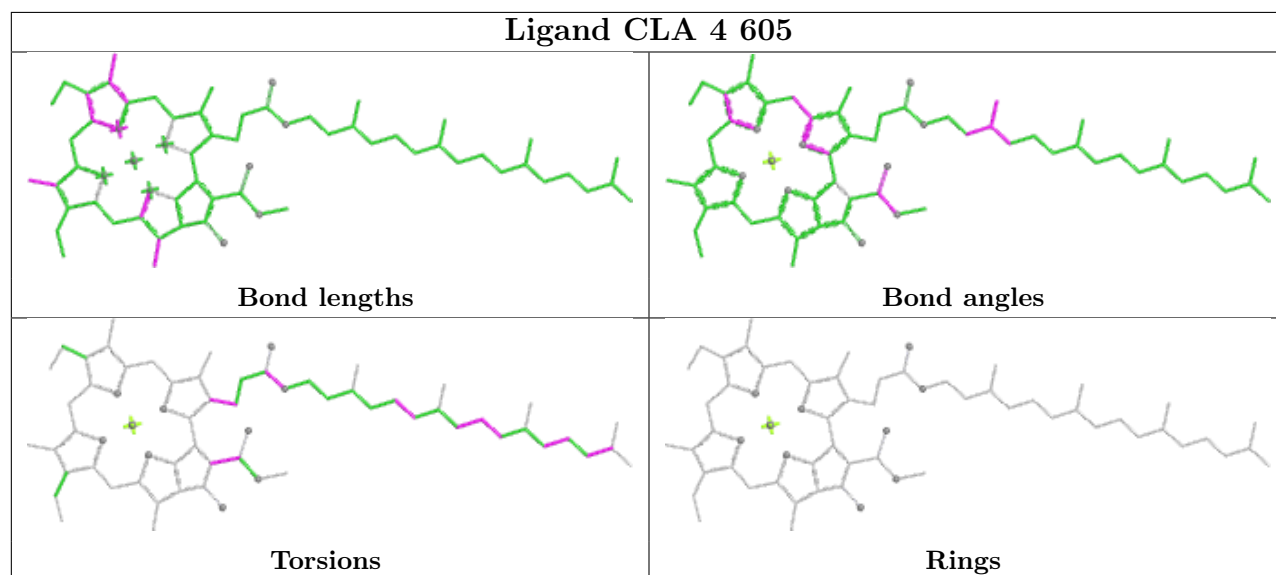
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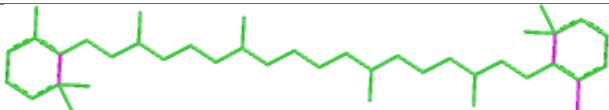
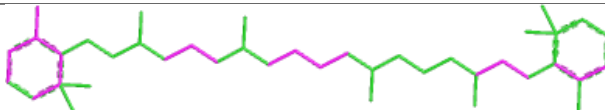
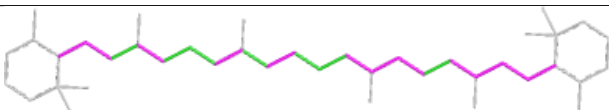
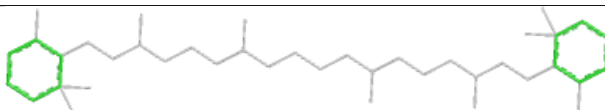


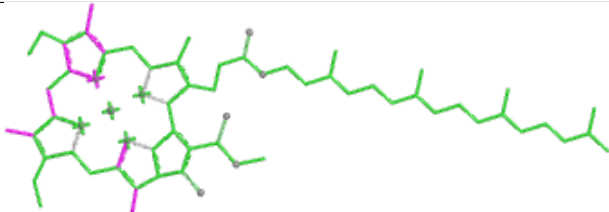
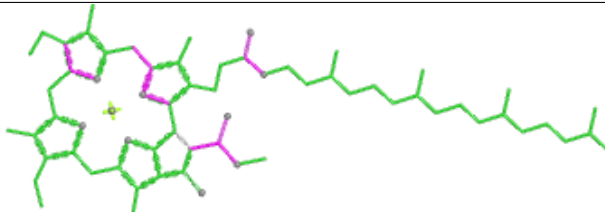
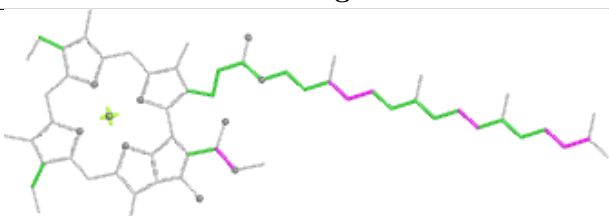
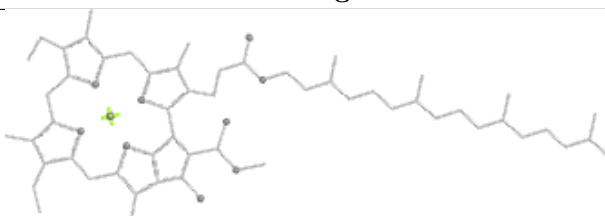
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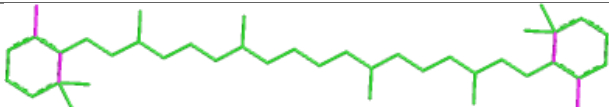
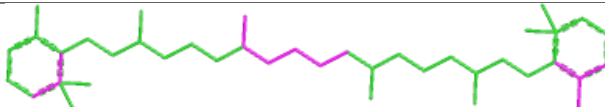
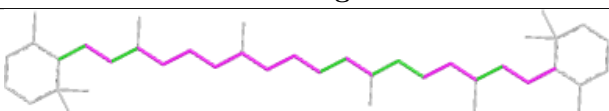
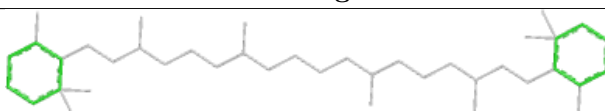


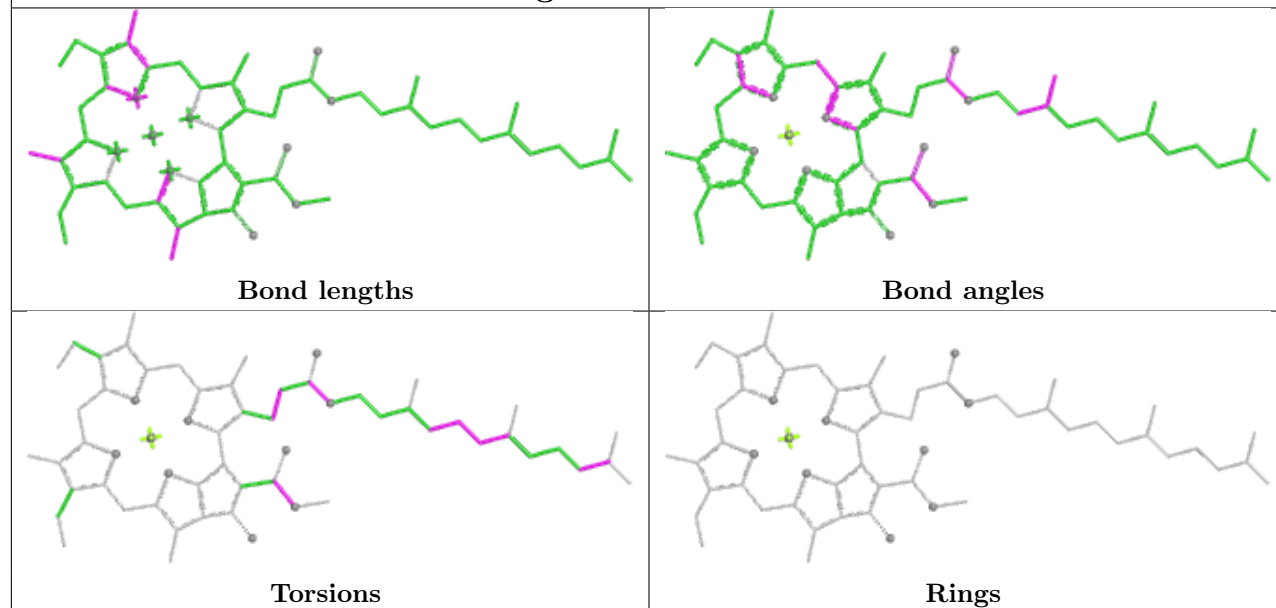
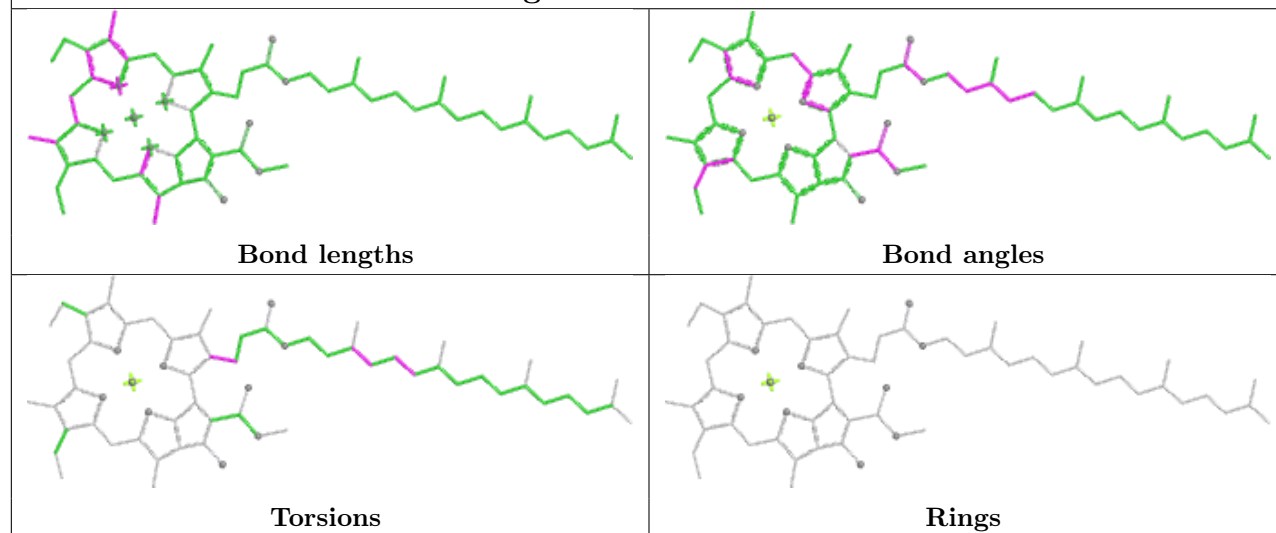
Ligand CLA 4 605

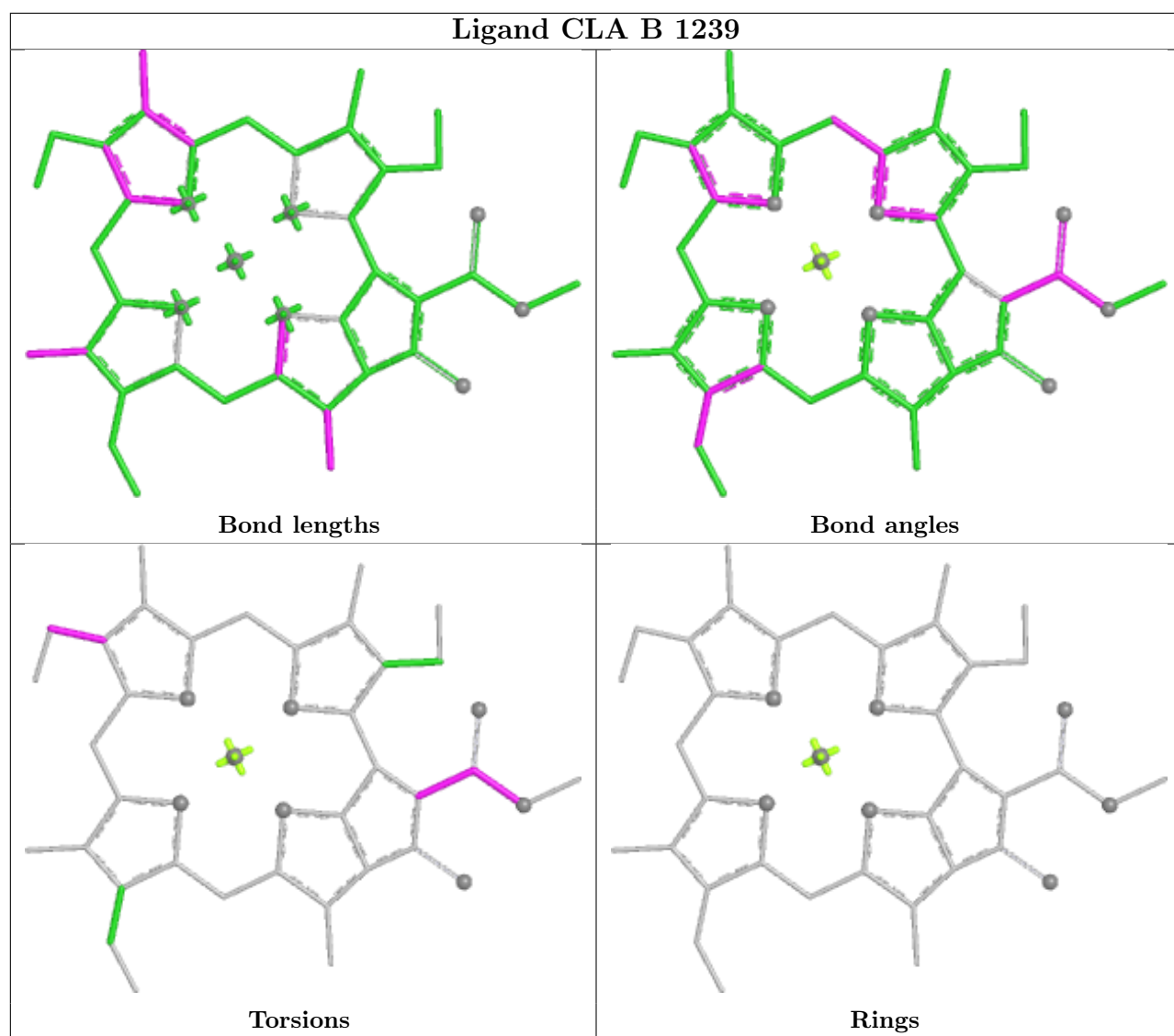


Ligand BCR J 4001	
	
Bond lengths	Bond angles
	
Torsions	Rings

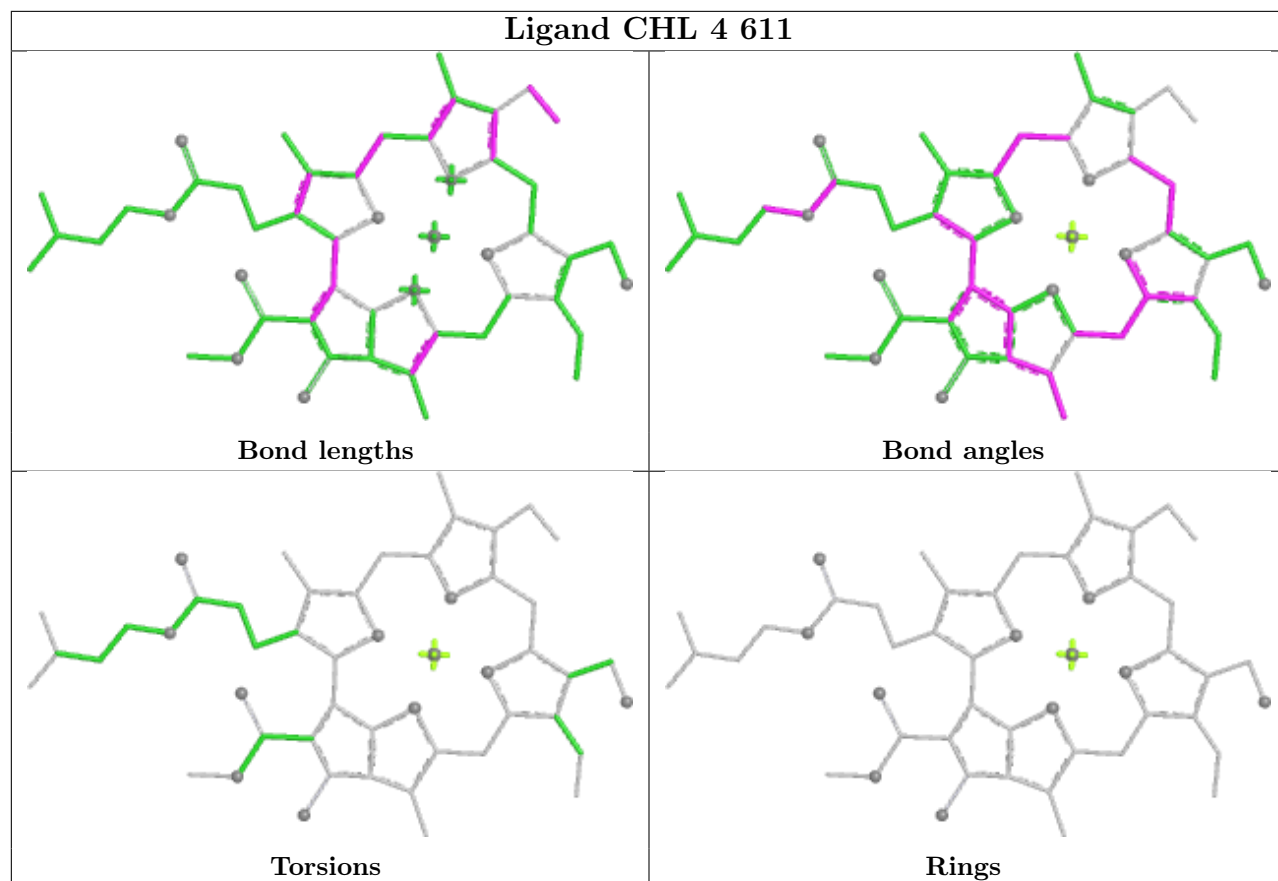
Ligand CLA B 1205	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR J 4002	
	
Bond lengths	Bond angles
	
Torsions	Rings

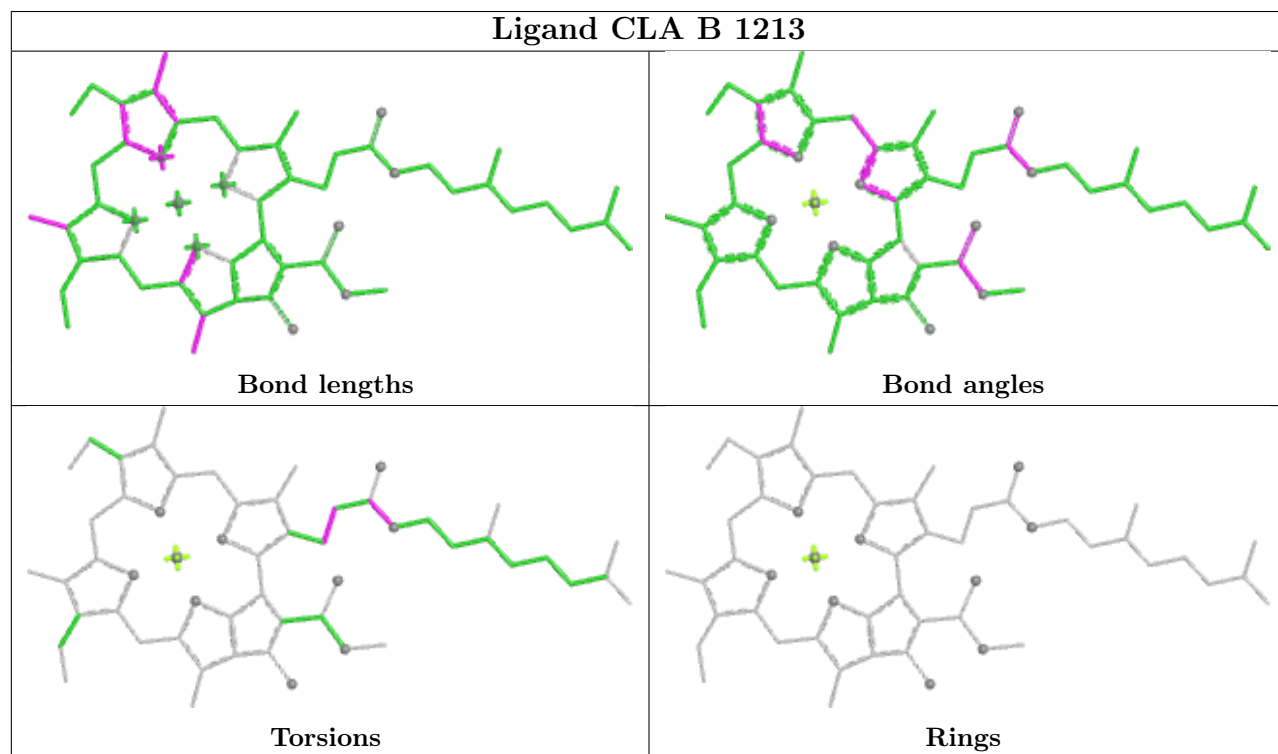
Ligand CLA 4 609**Ligand CLA B 1210**

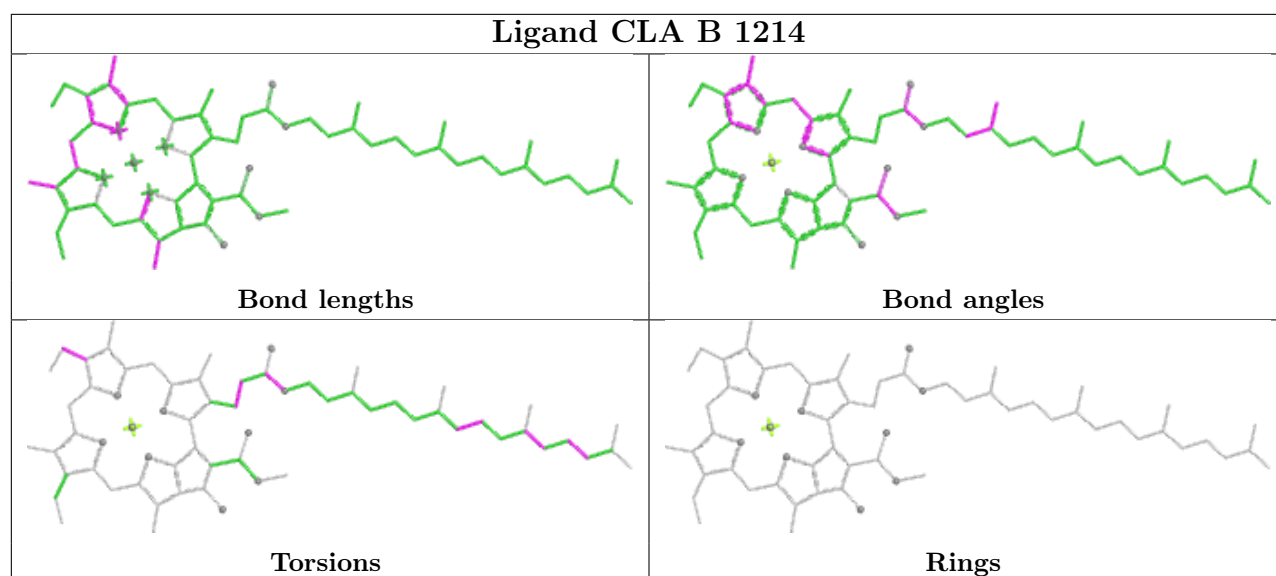
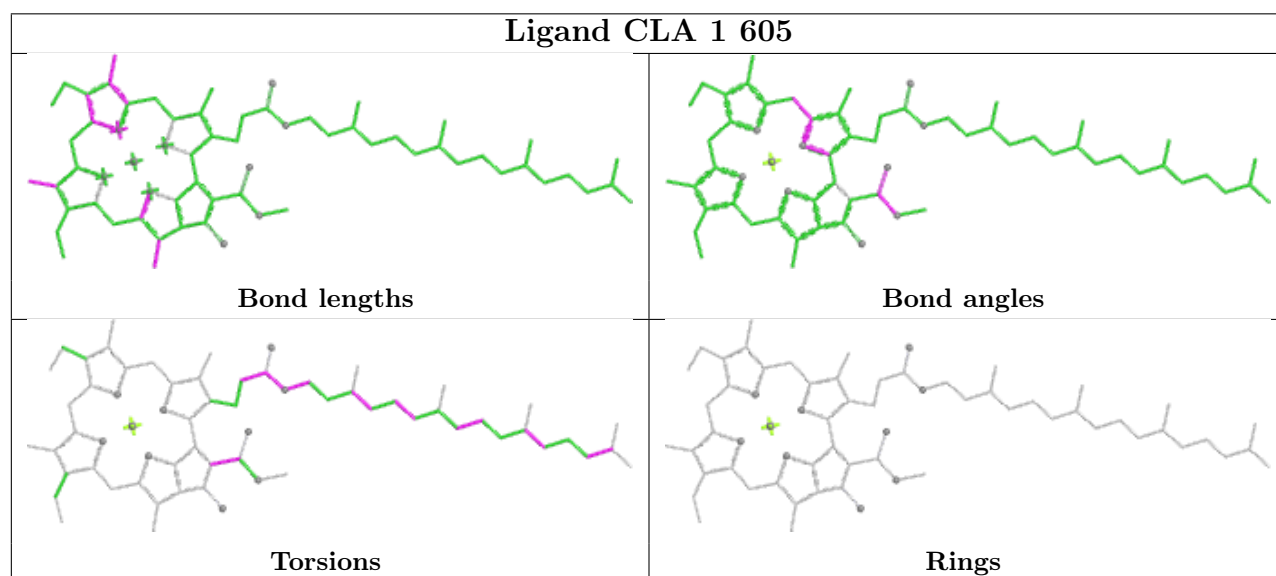
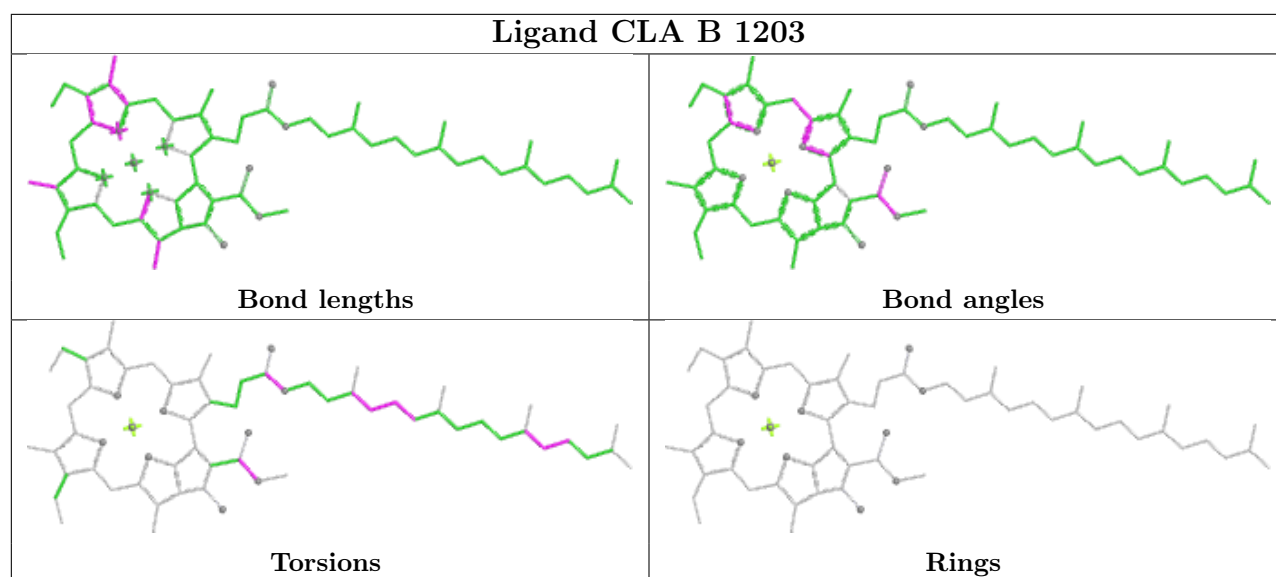


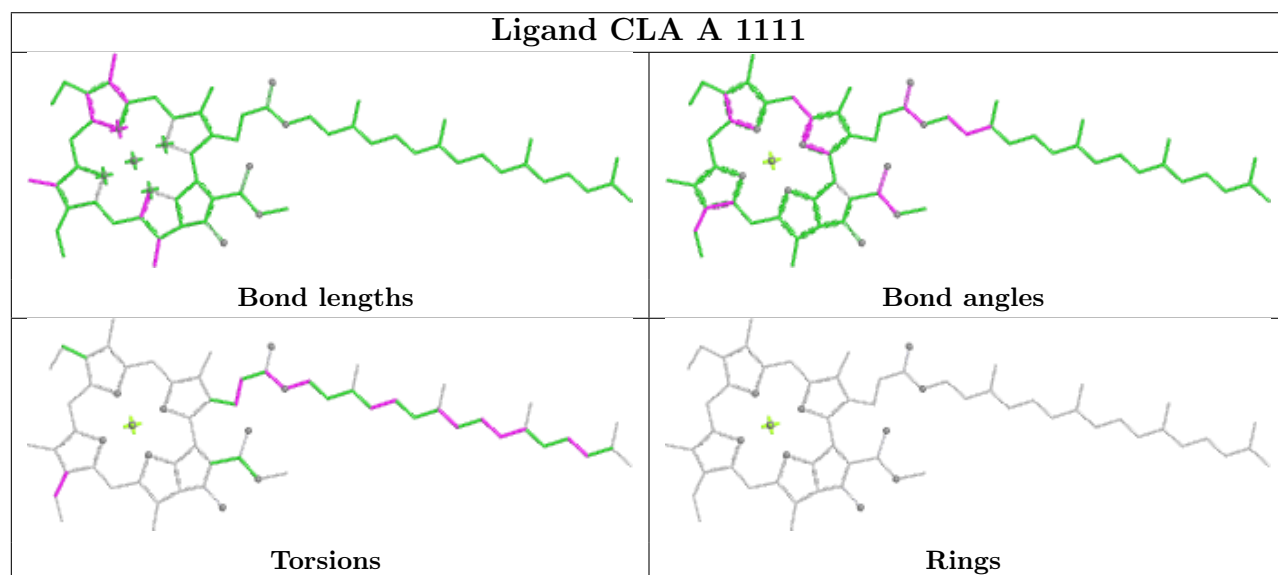
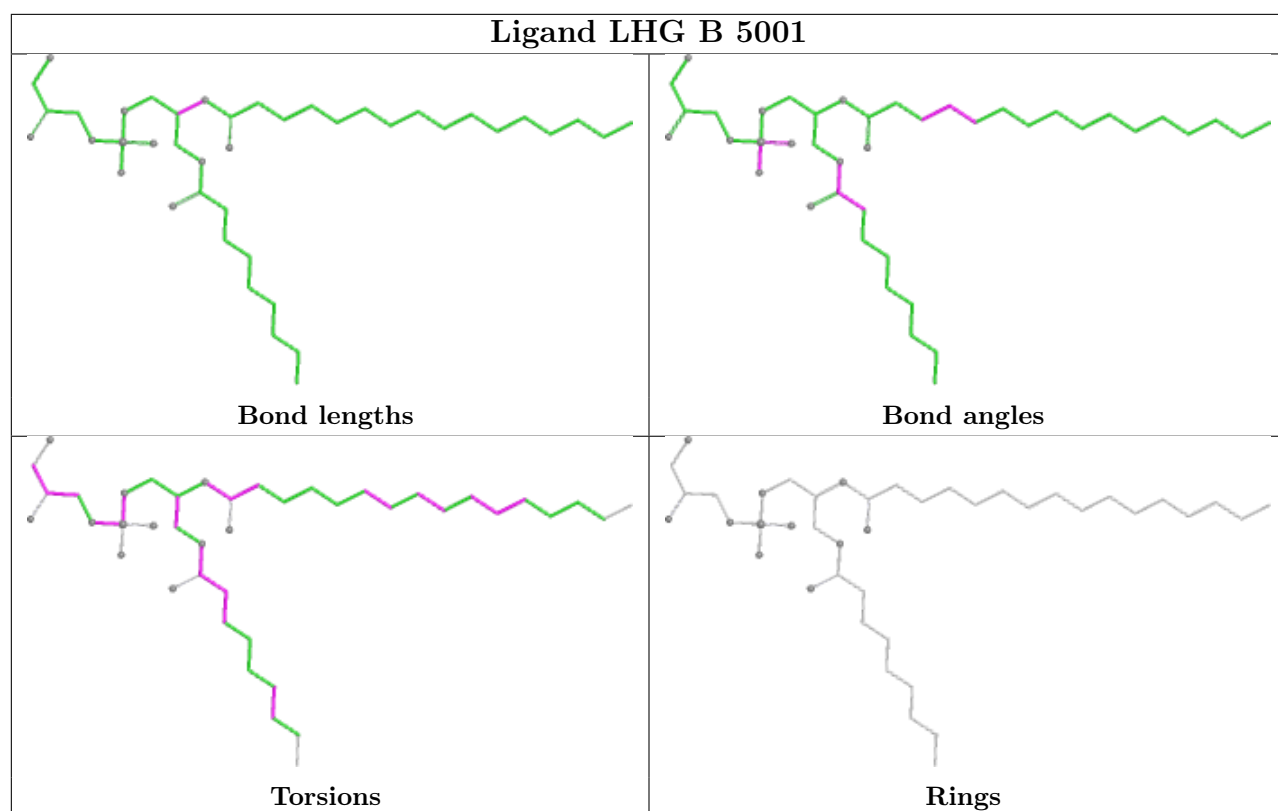
Ligand CHL 4 611

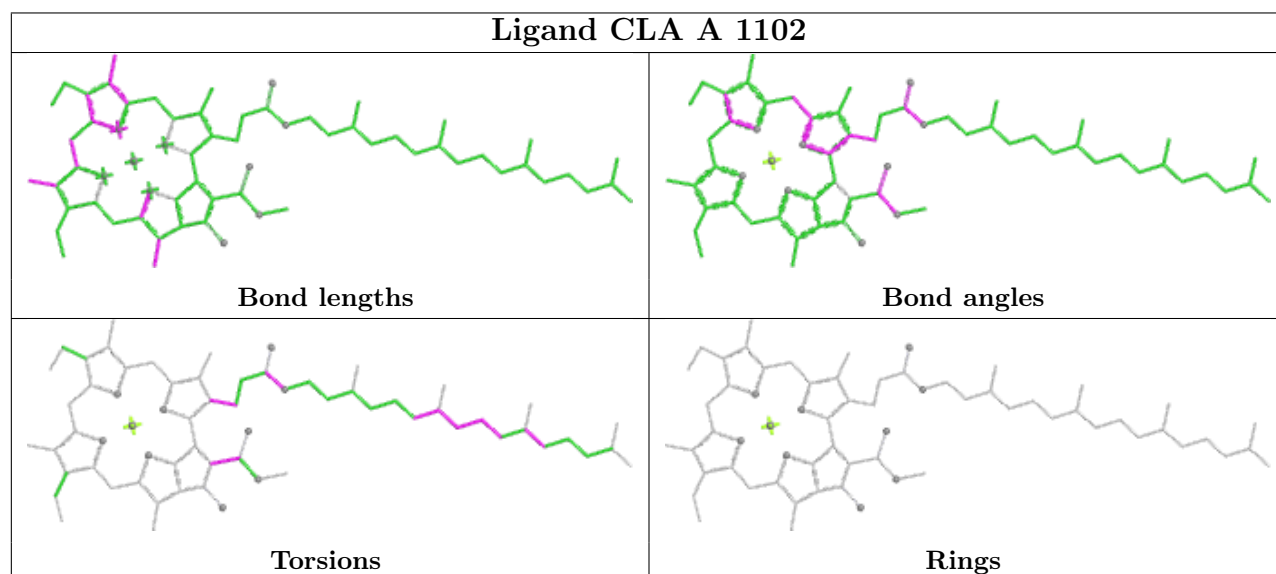
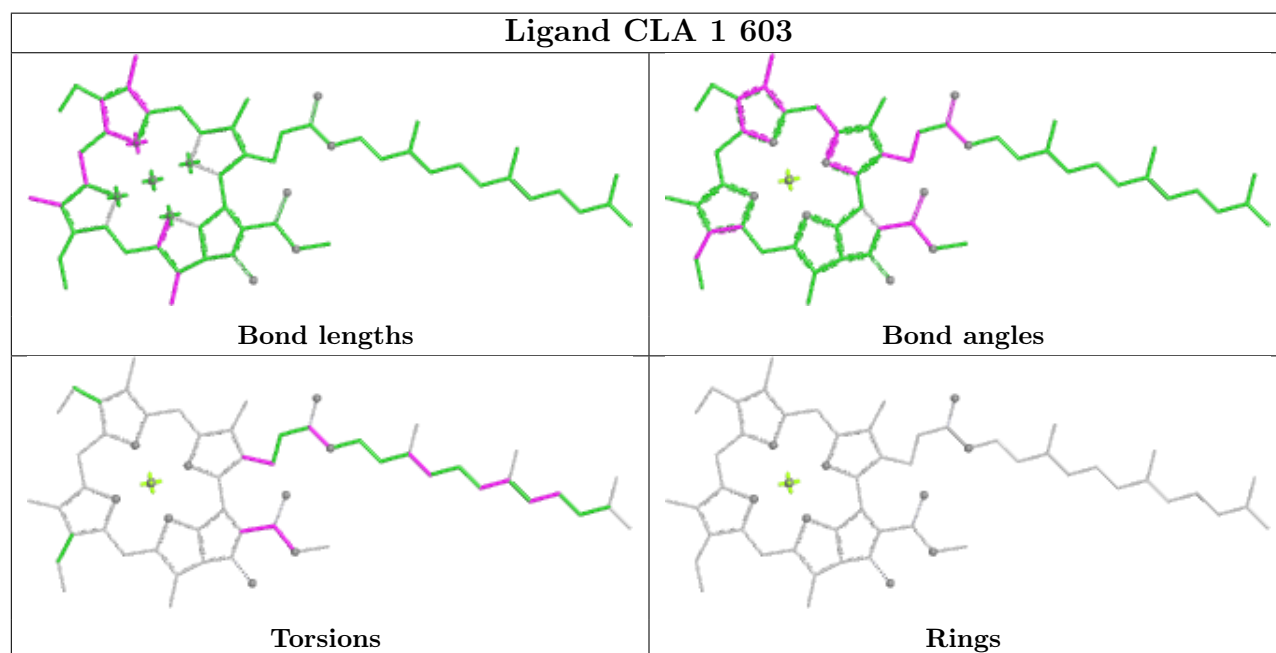
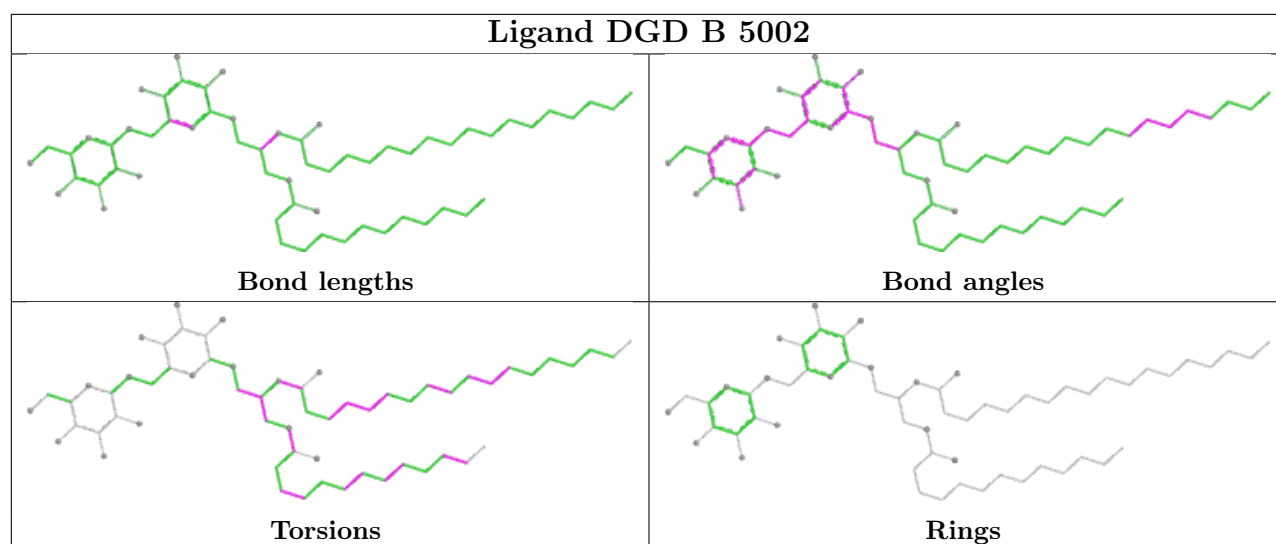


Ligand CLA B 1213

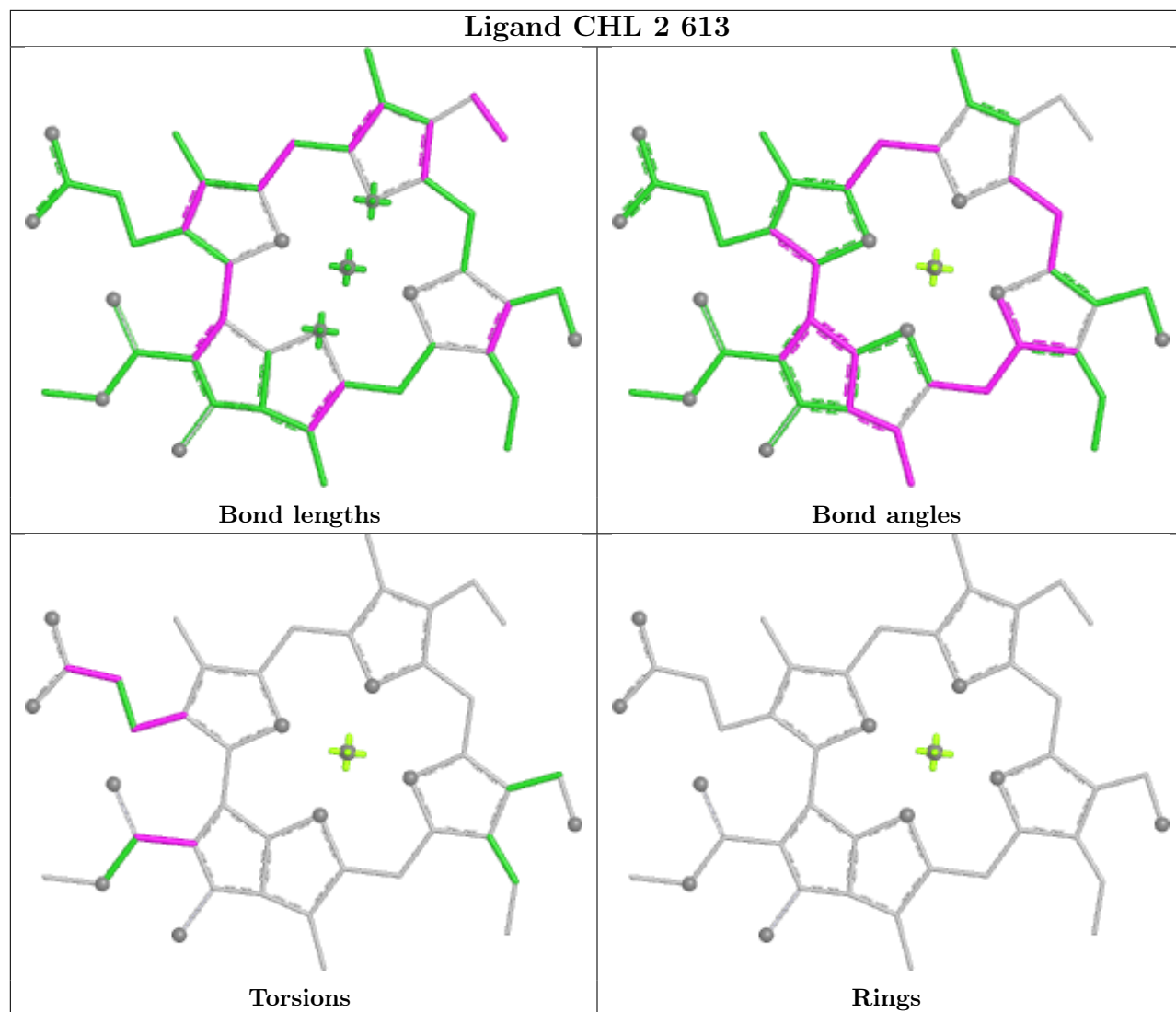


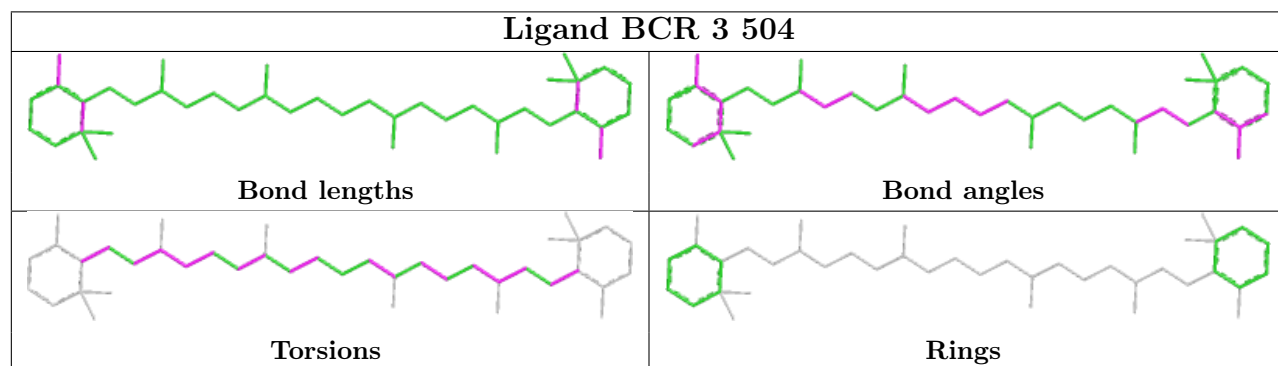
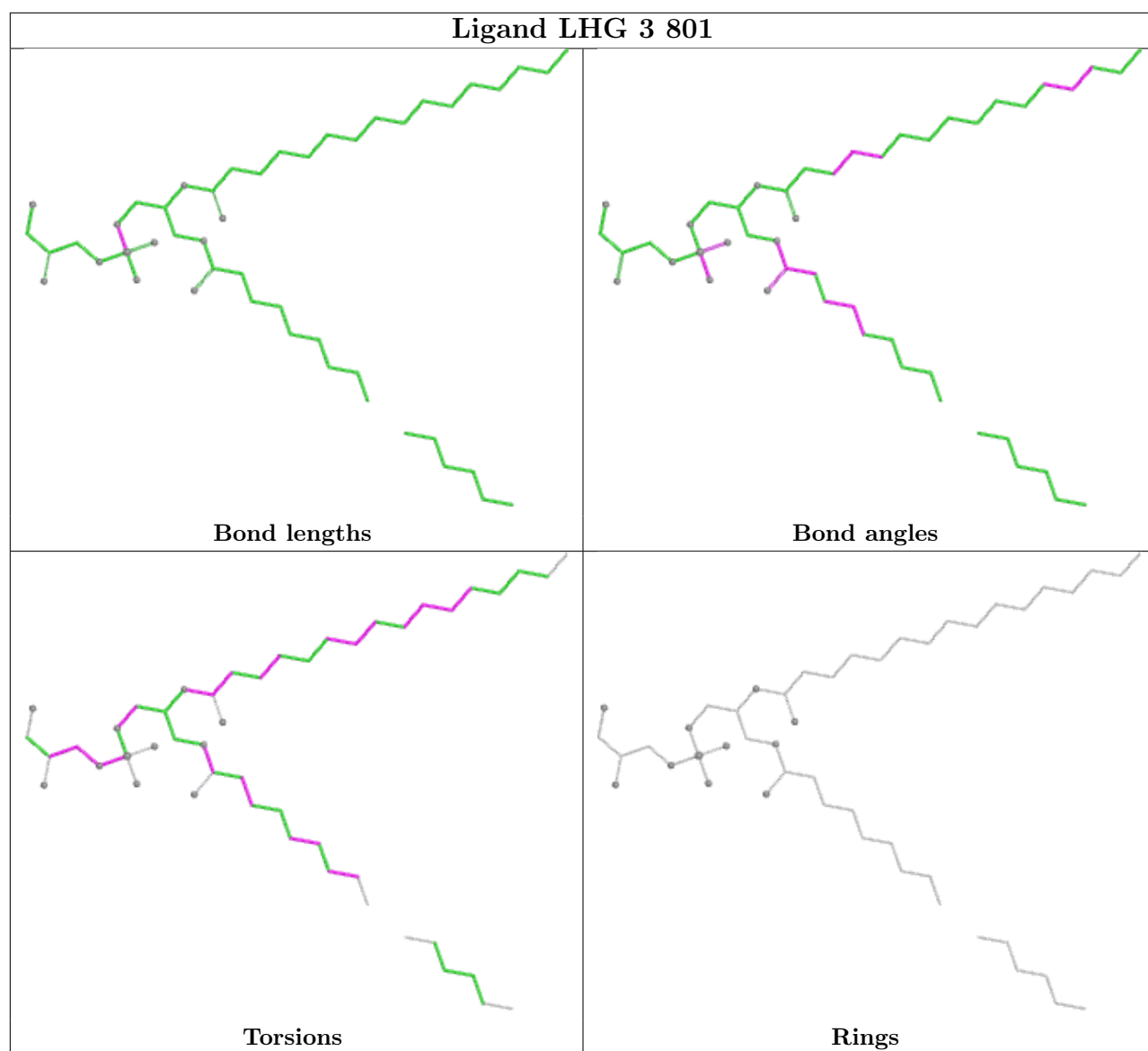




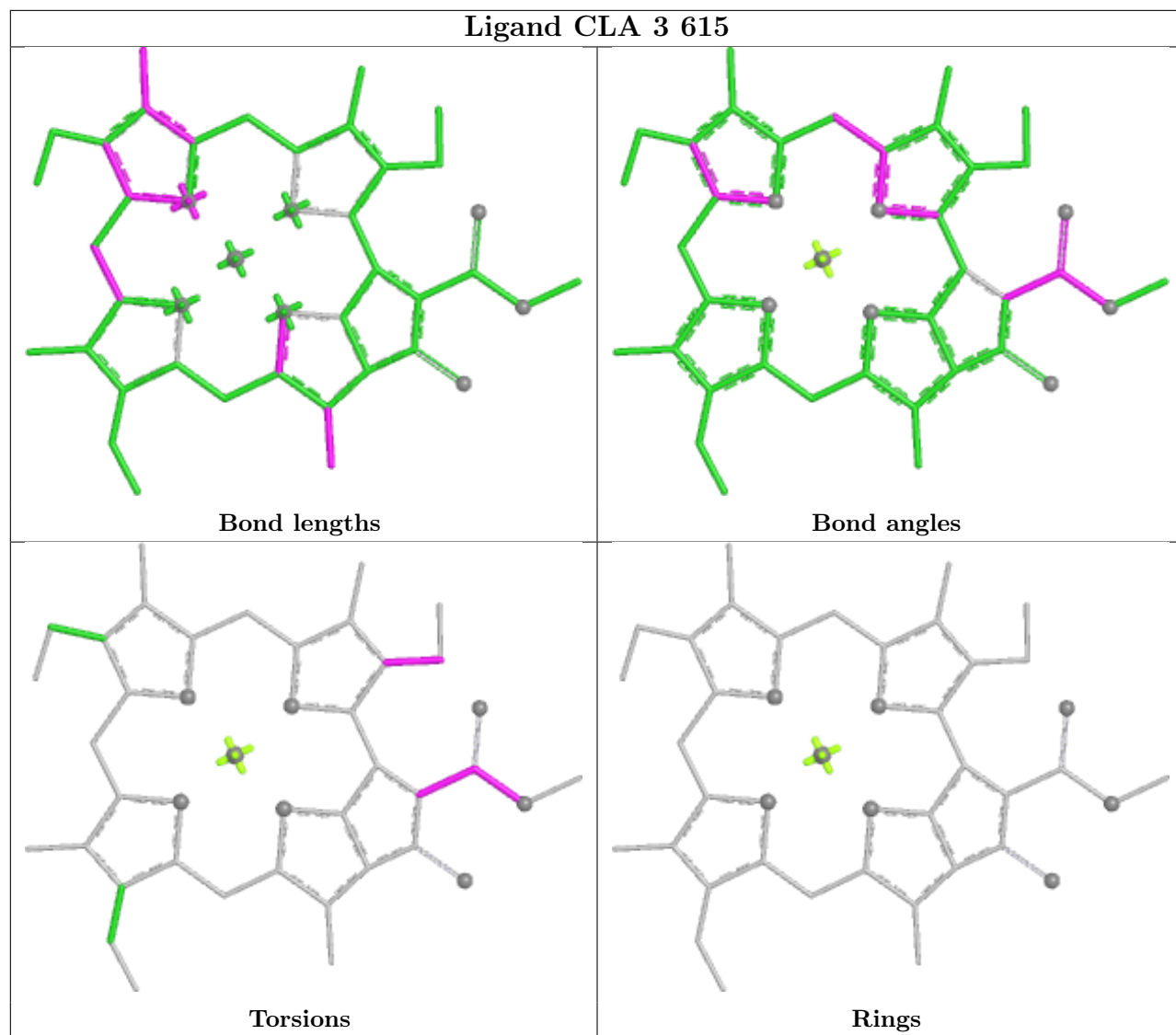


Ligand CHL 2 613

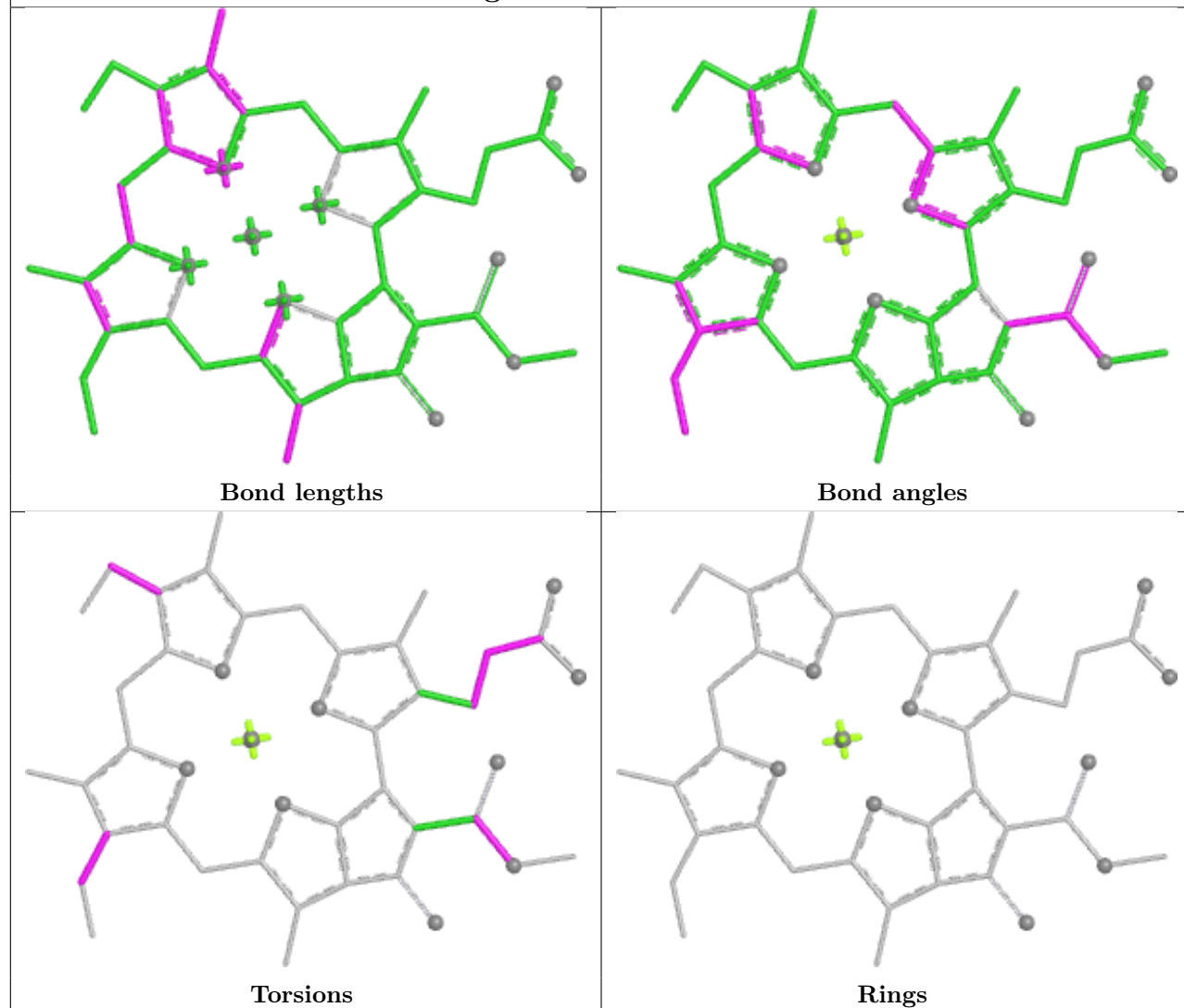




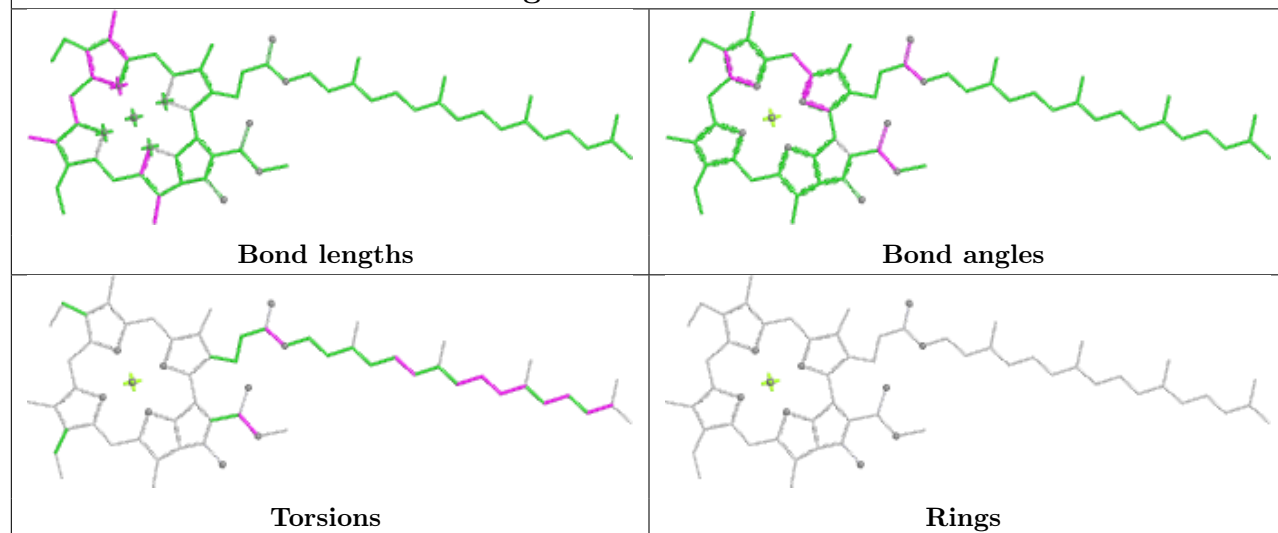
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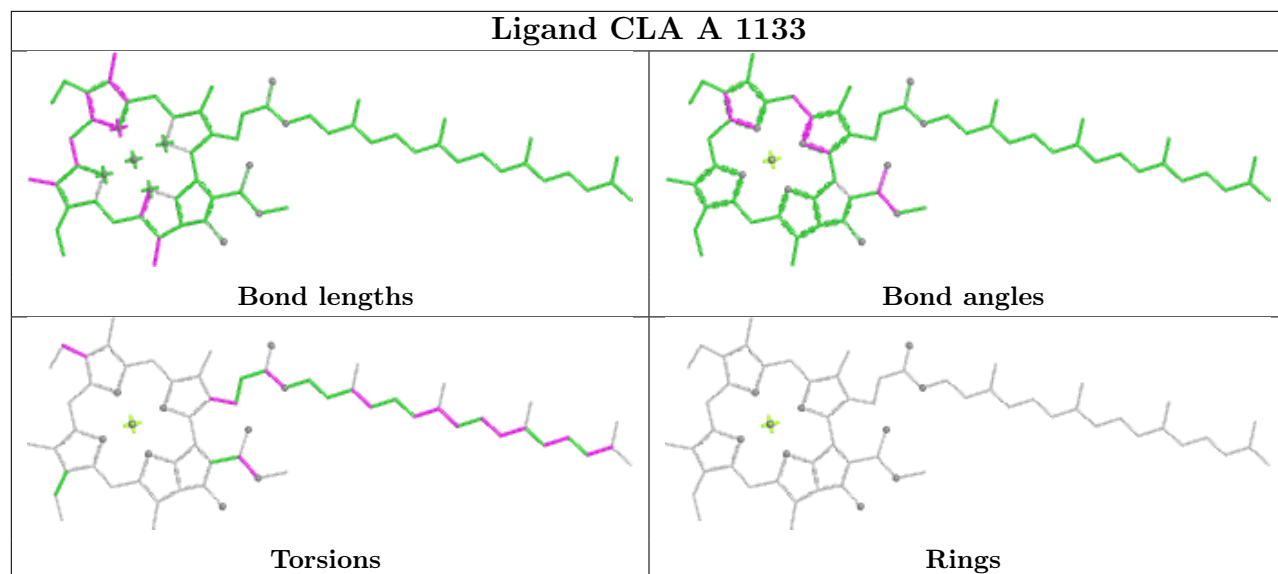
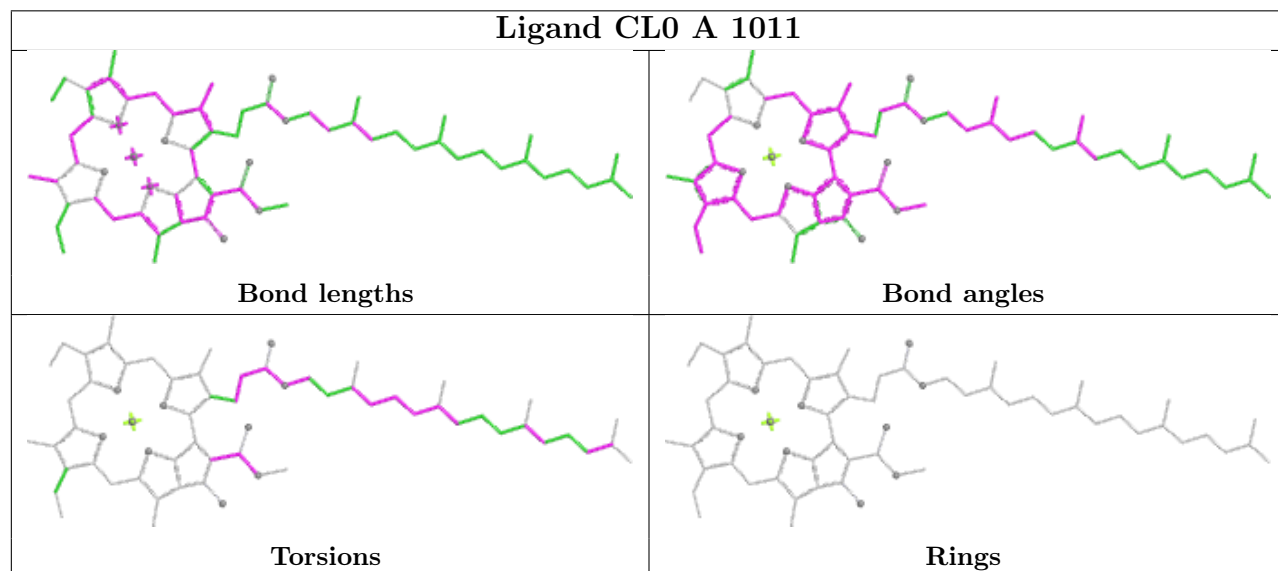


Ligand CLA A 1132

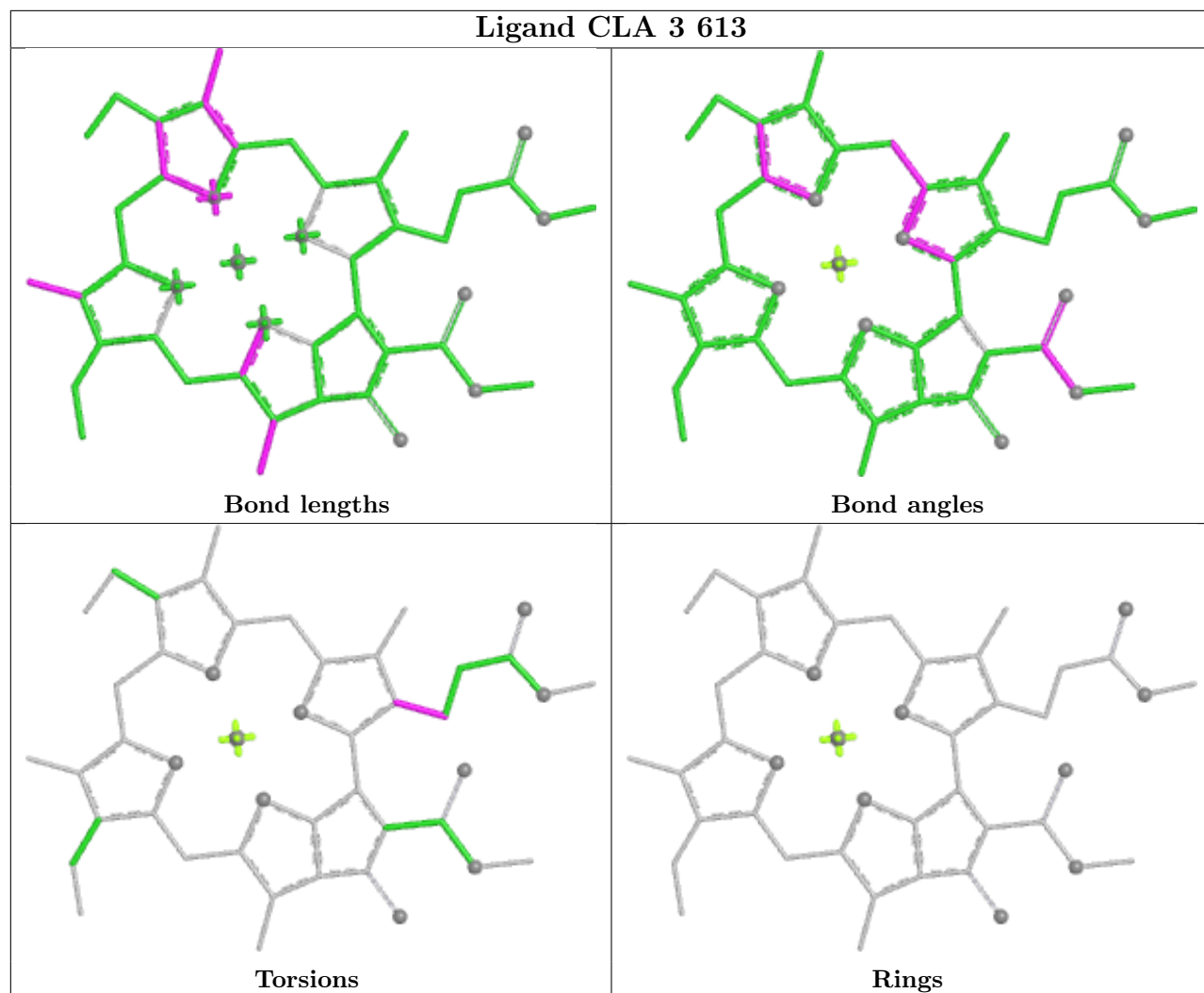


Ligand CLA B 1219

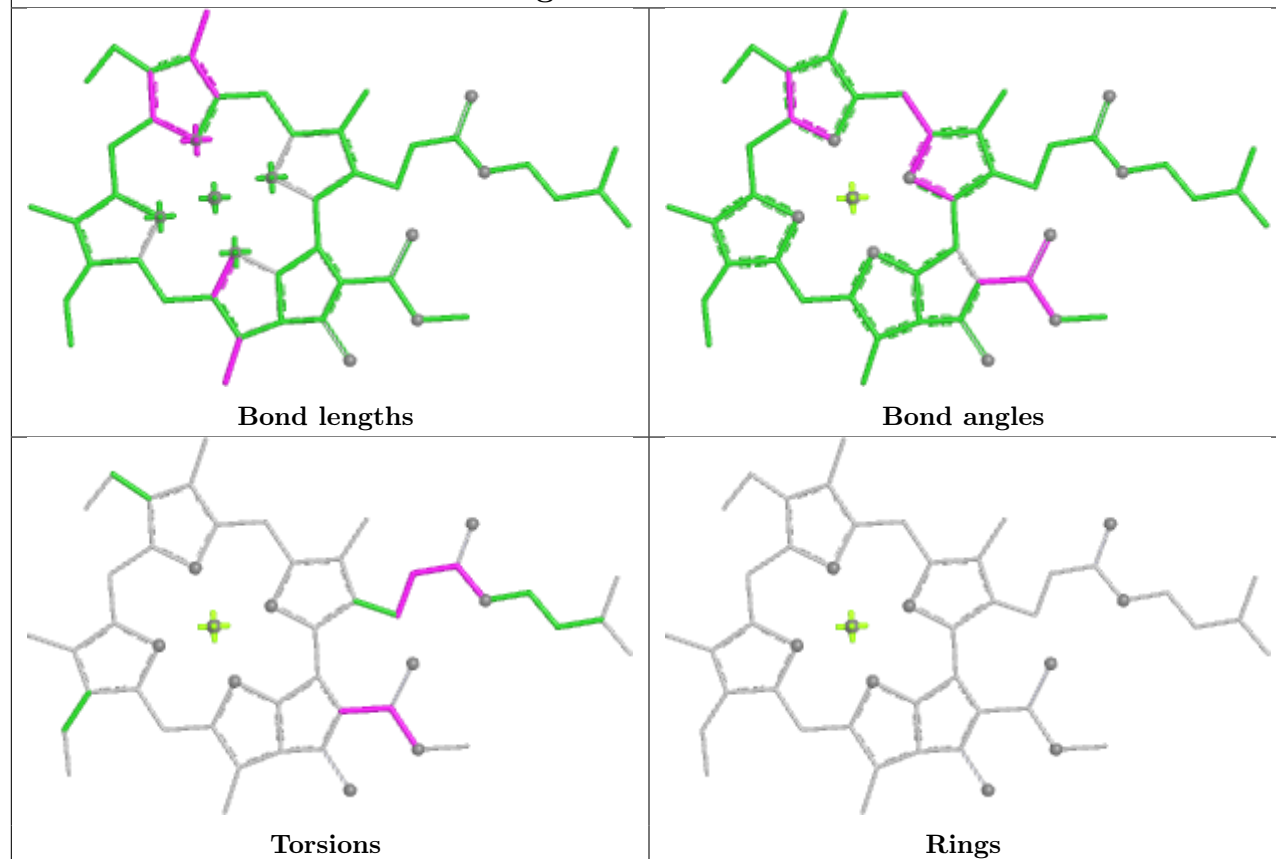


Ligand CLA A 1133**Ligand CL0 A 1011**

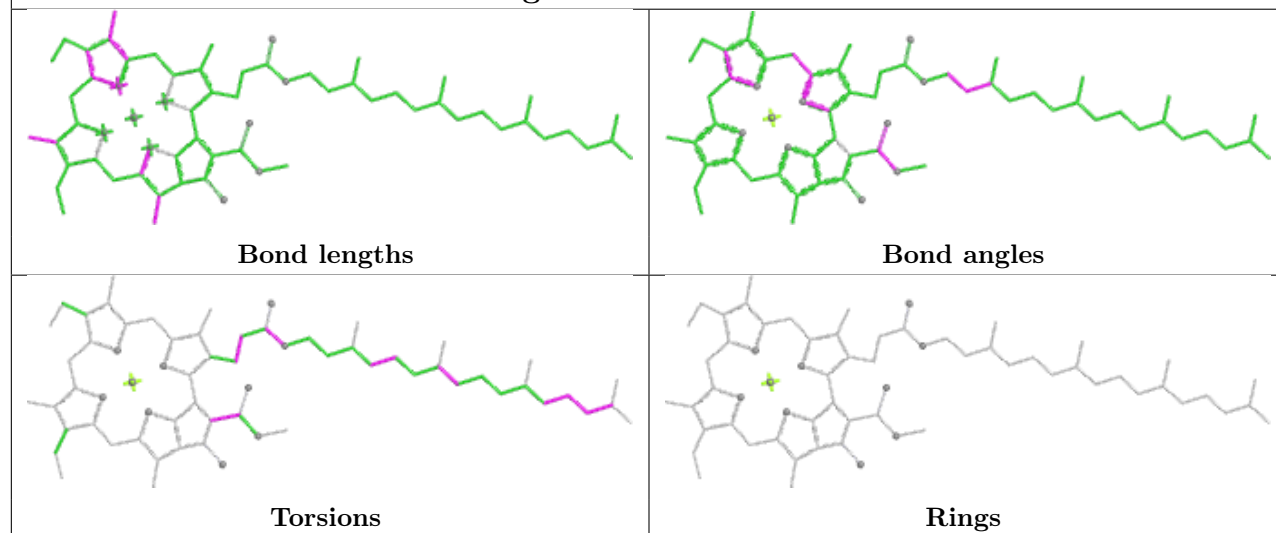
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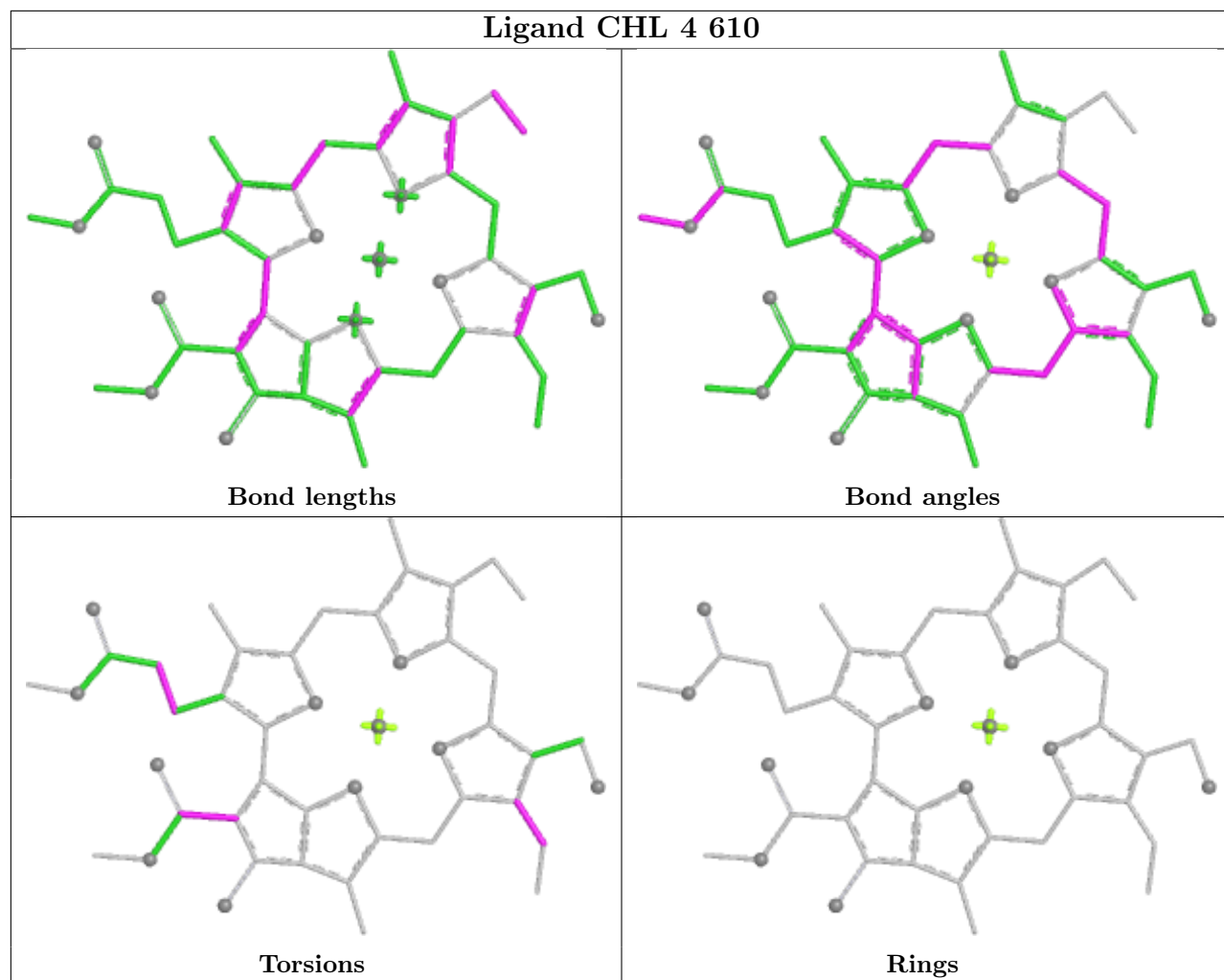
Ligand CLA 4 602

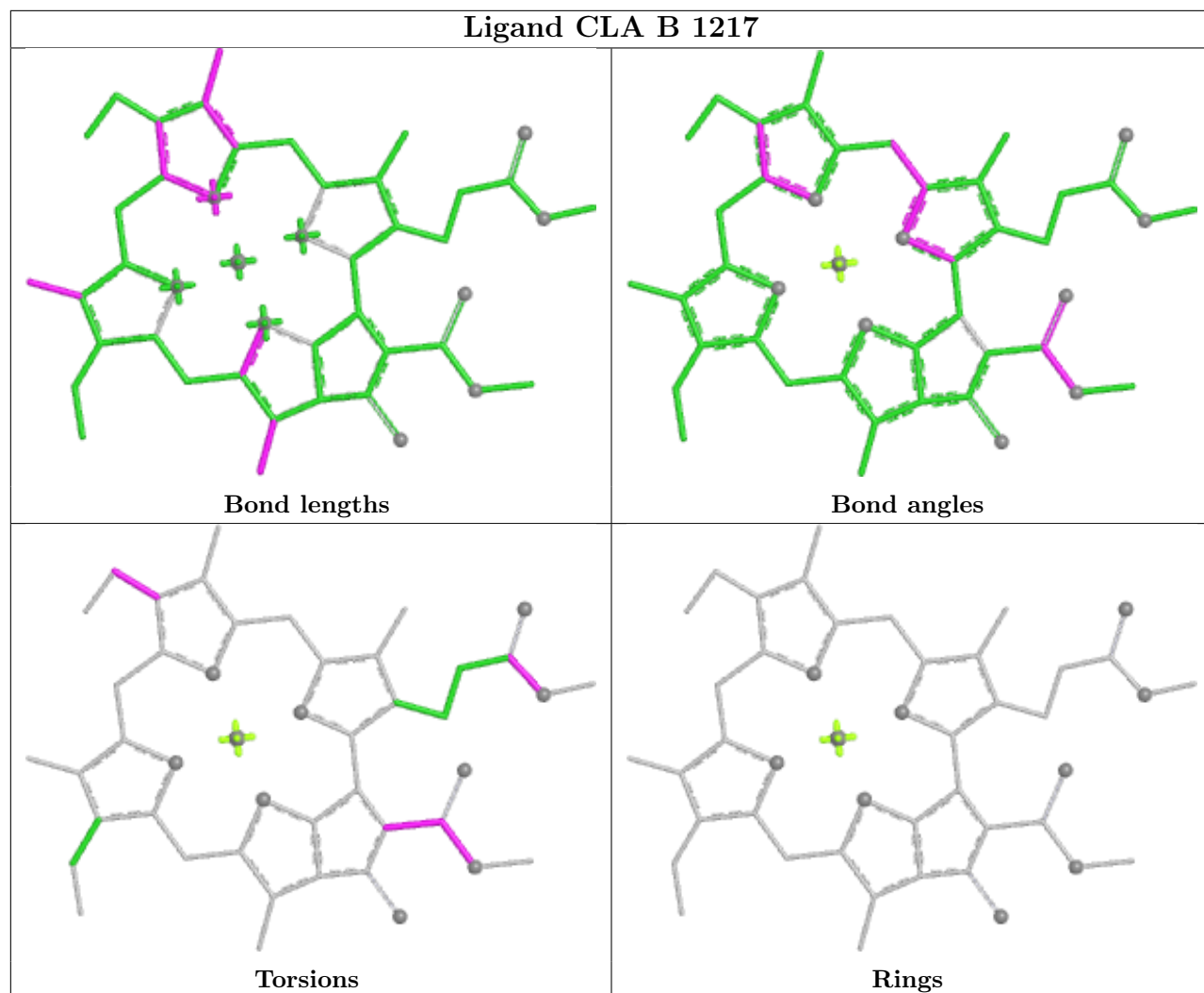


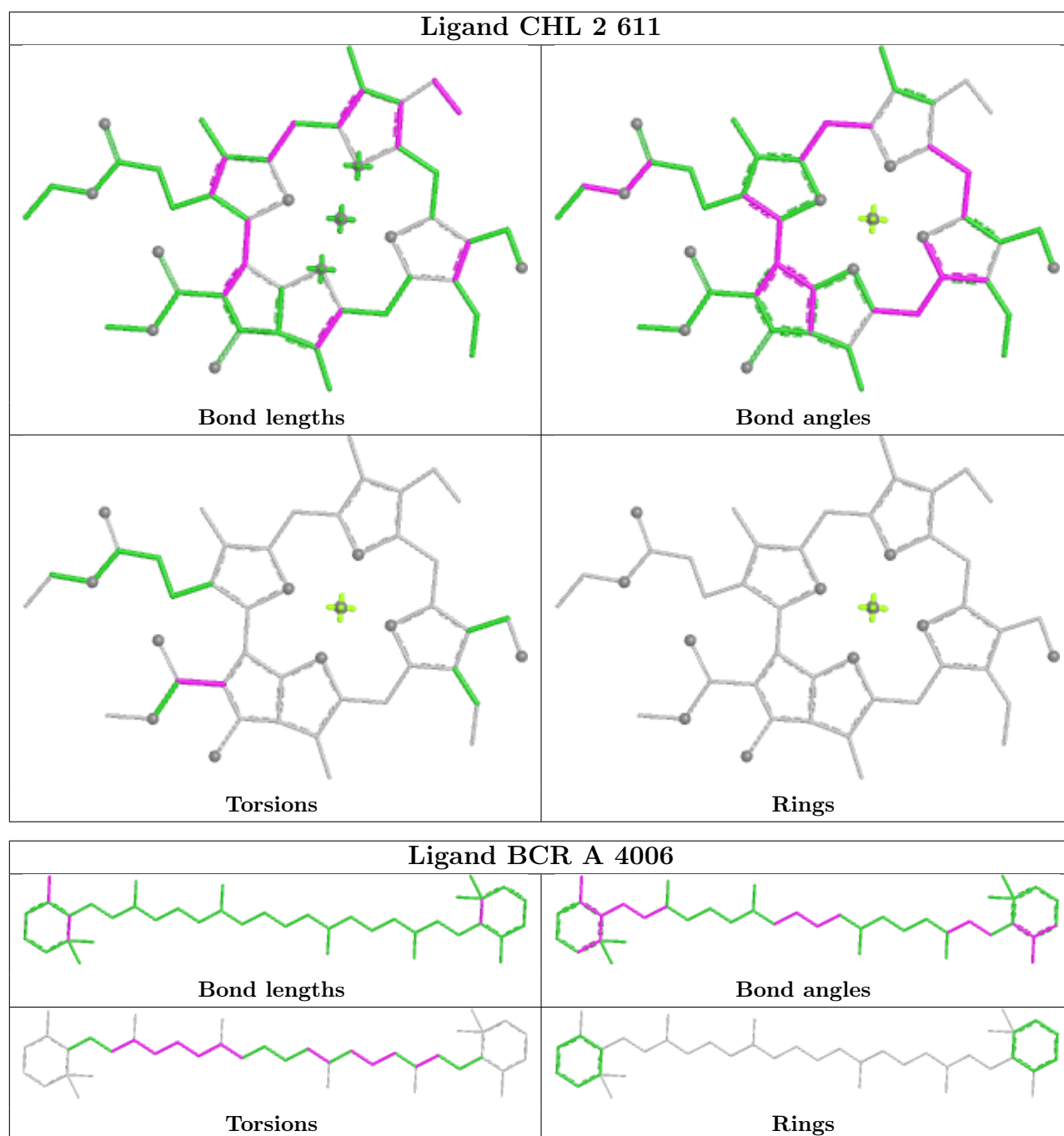
Ligand CLA A 1128



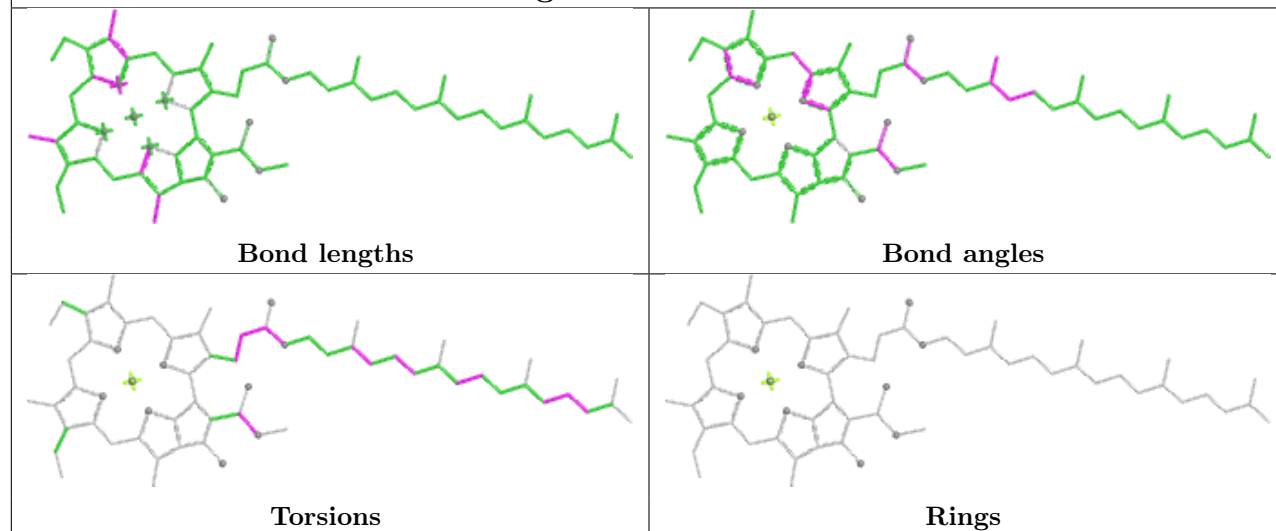
Ligand CHL 4 610



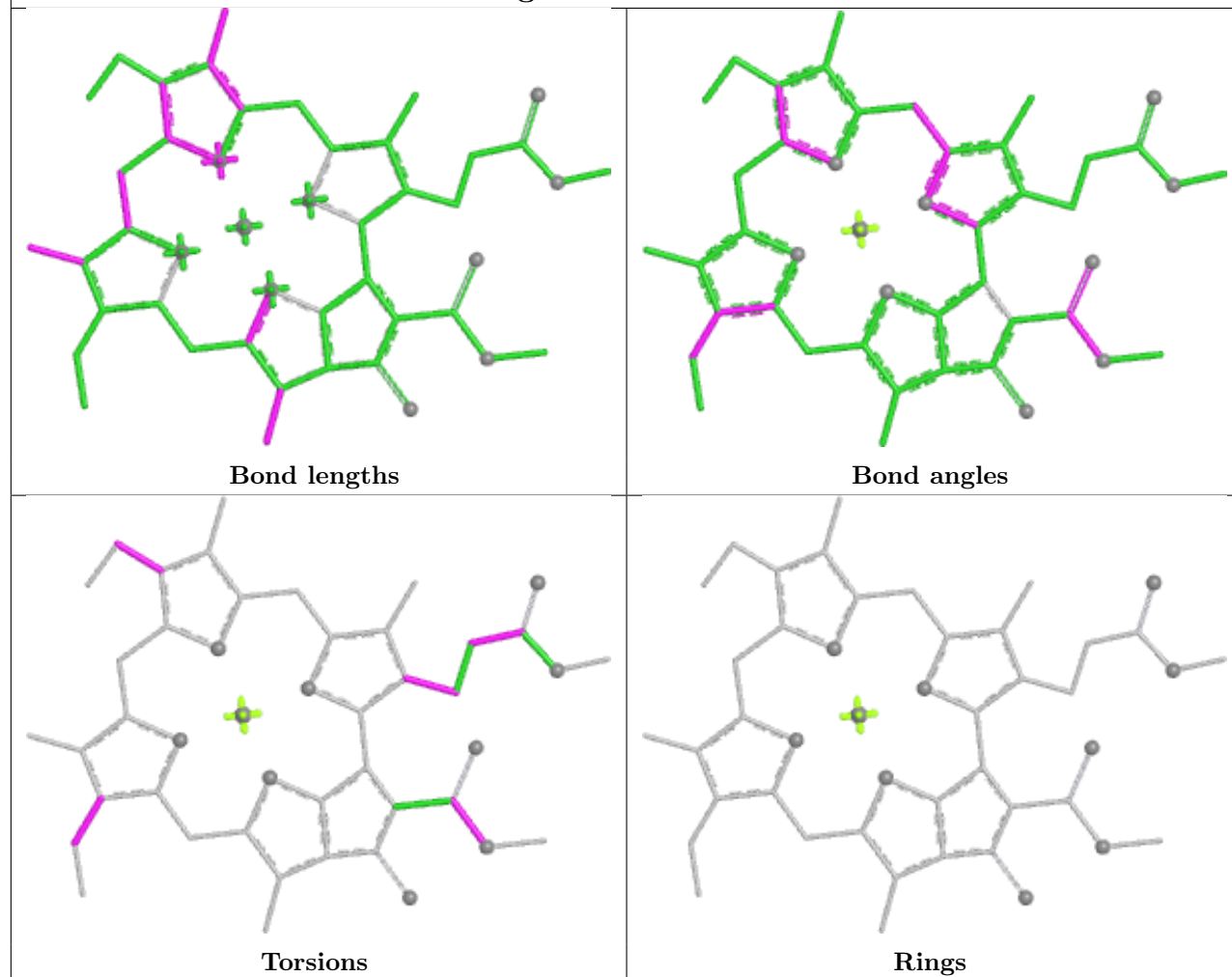


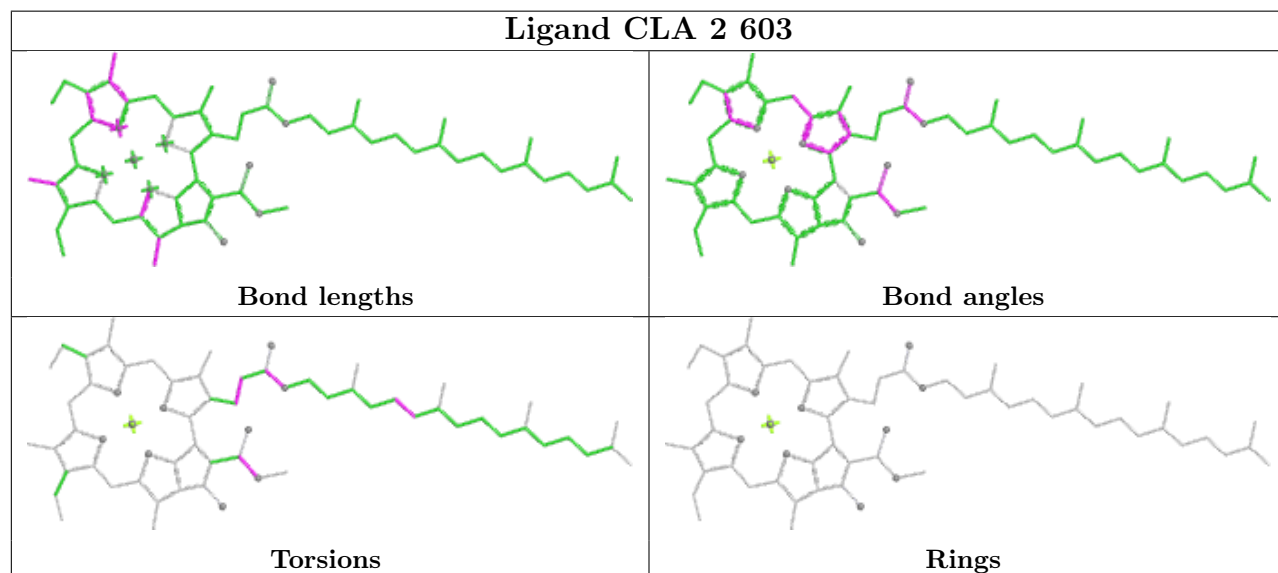
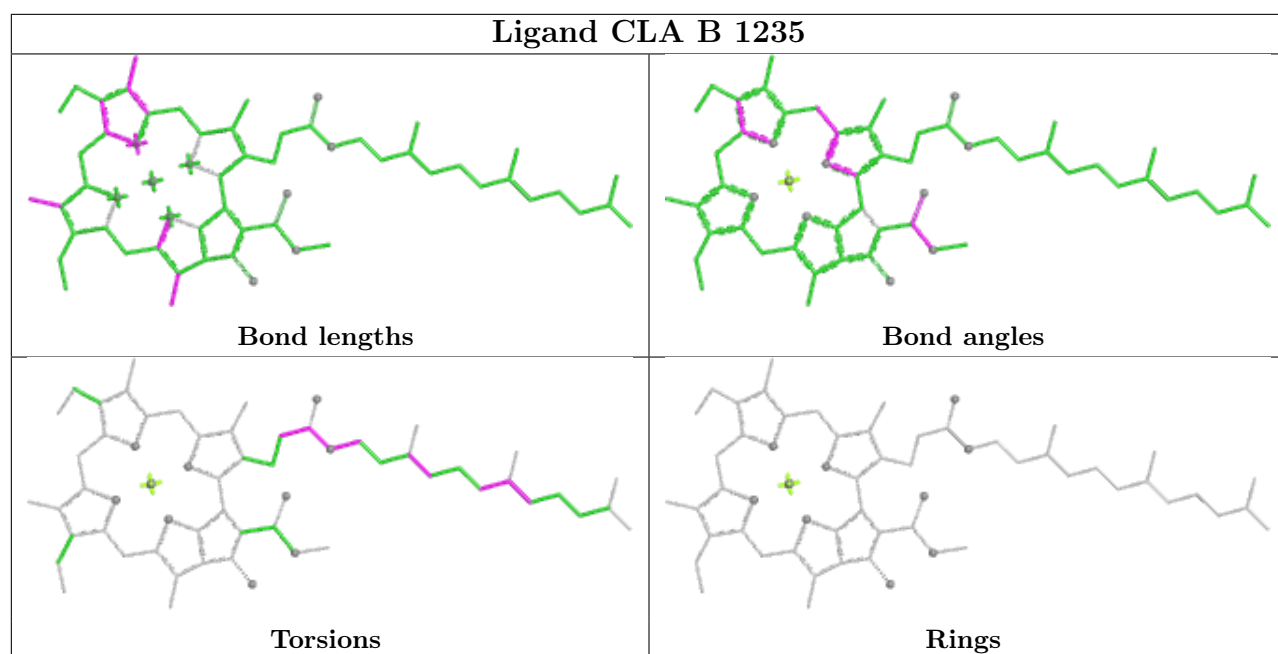


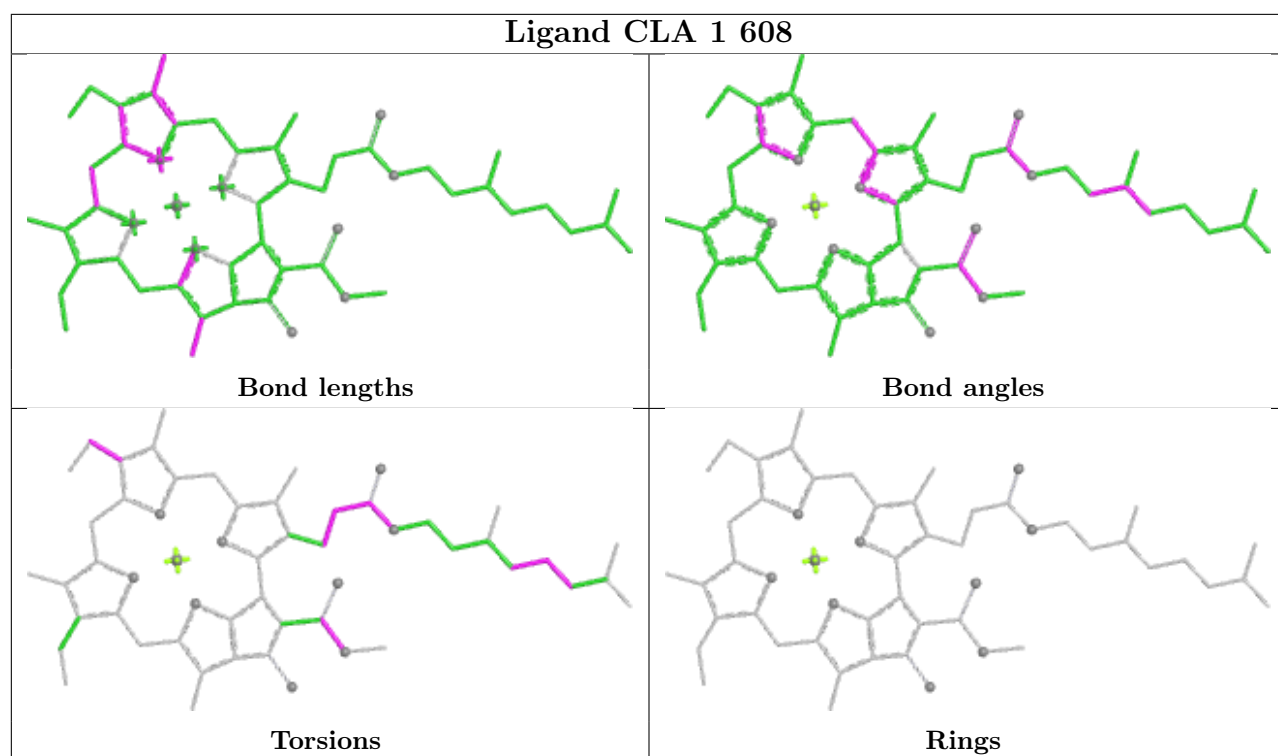
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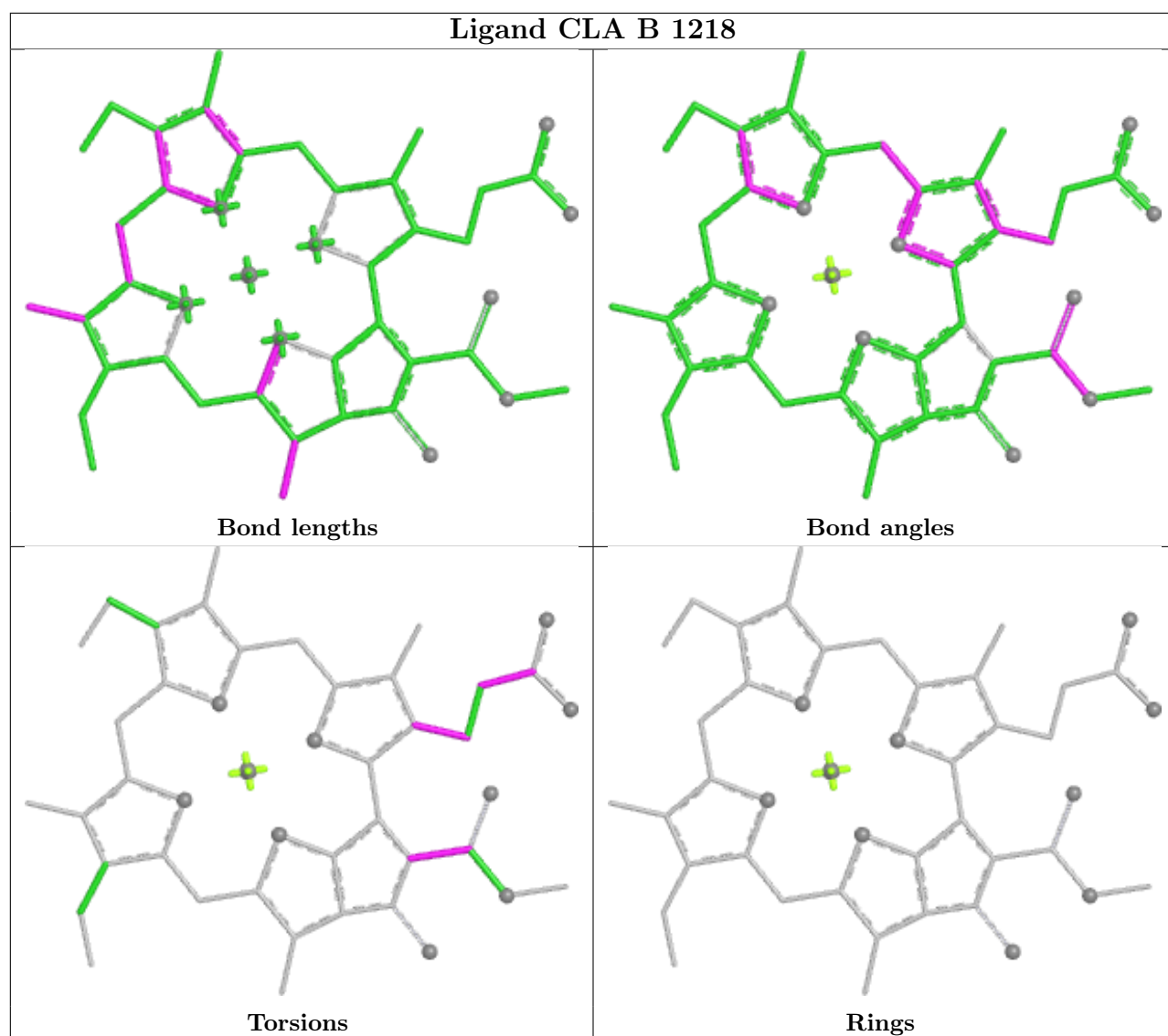


Ligand CLA 1 607

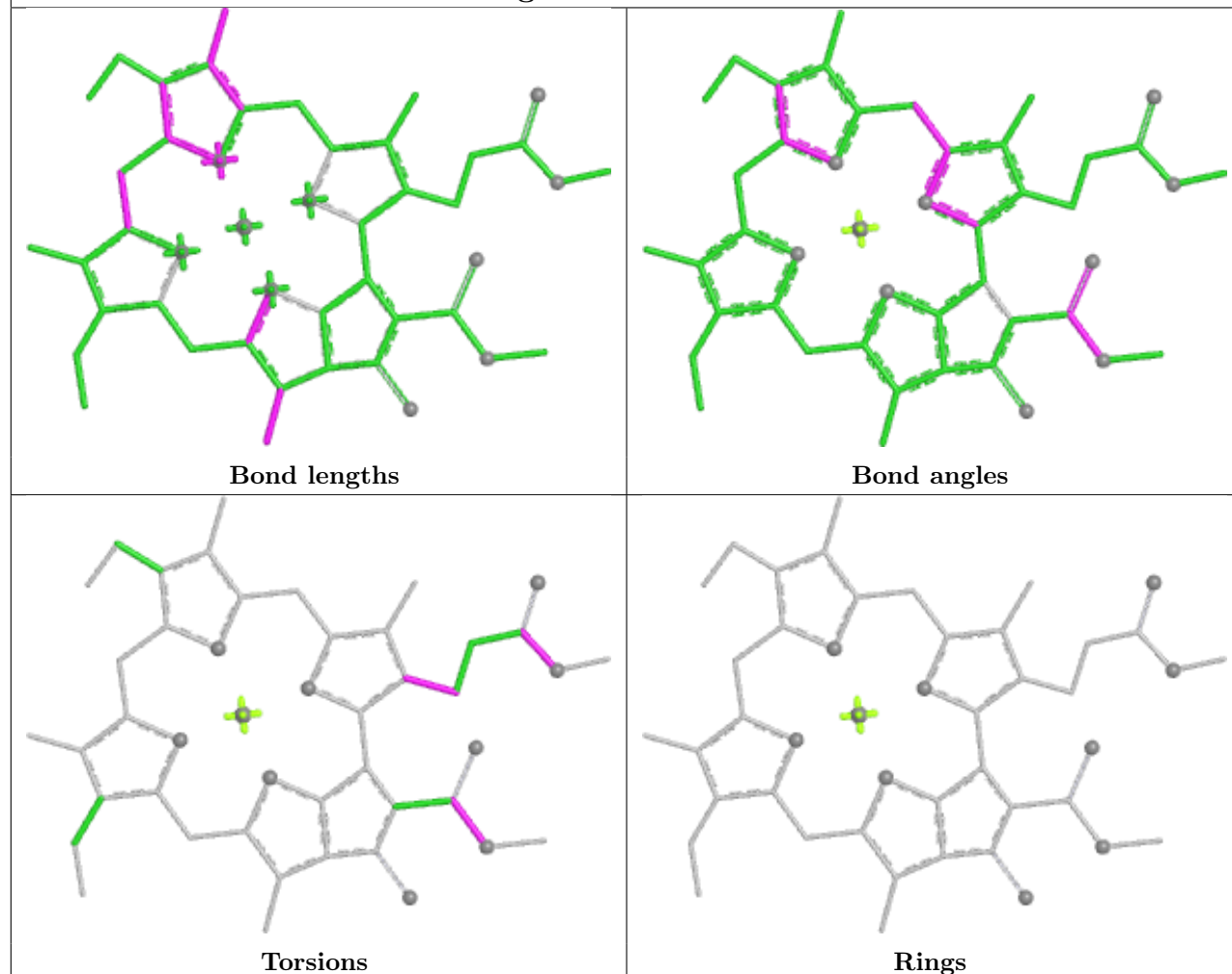




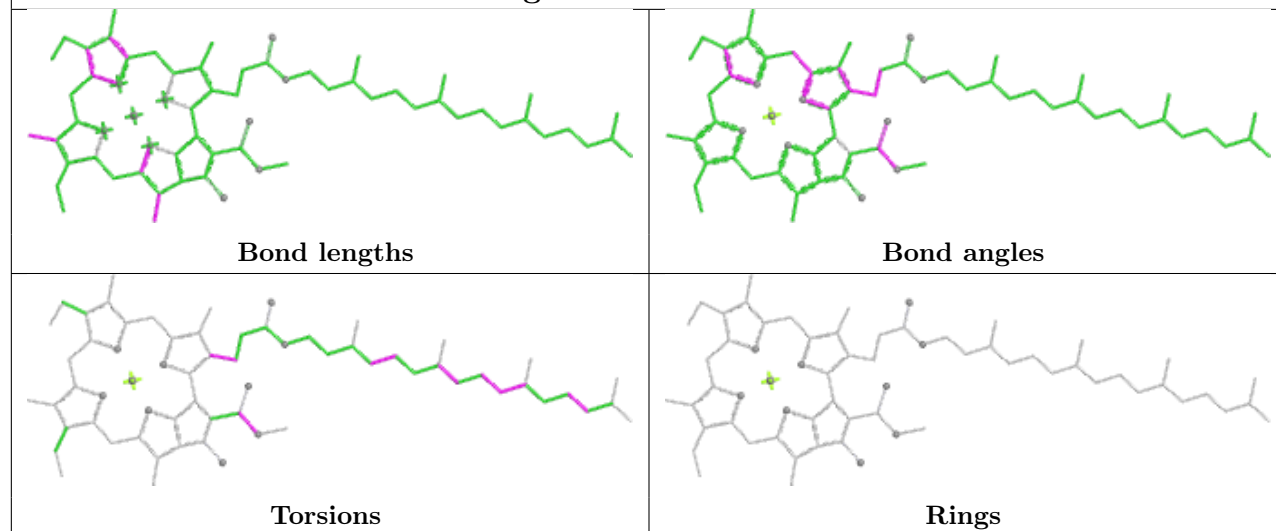


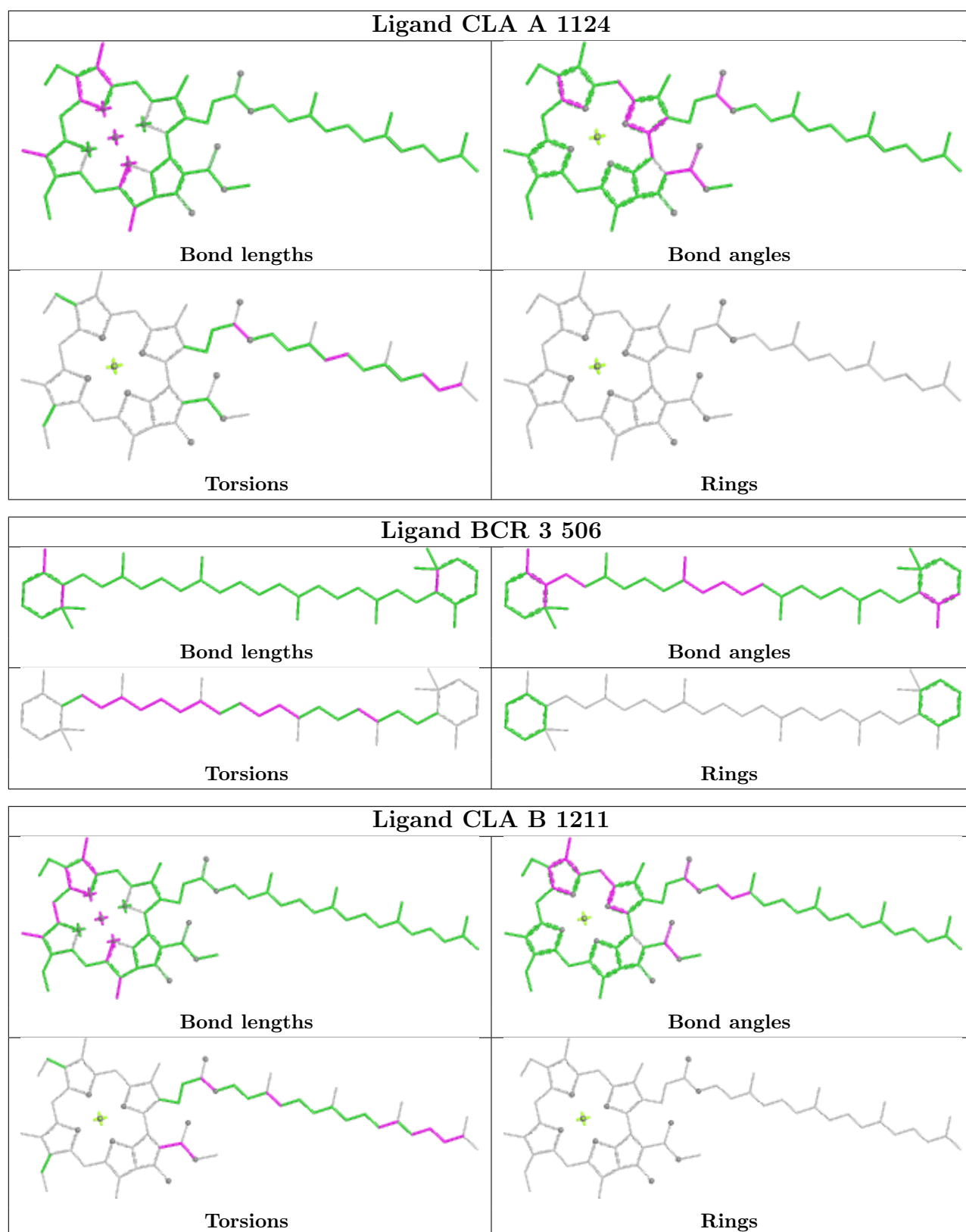


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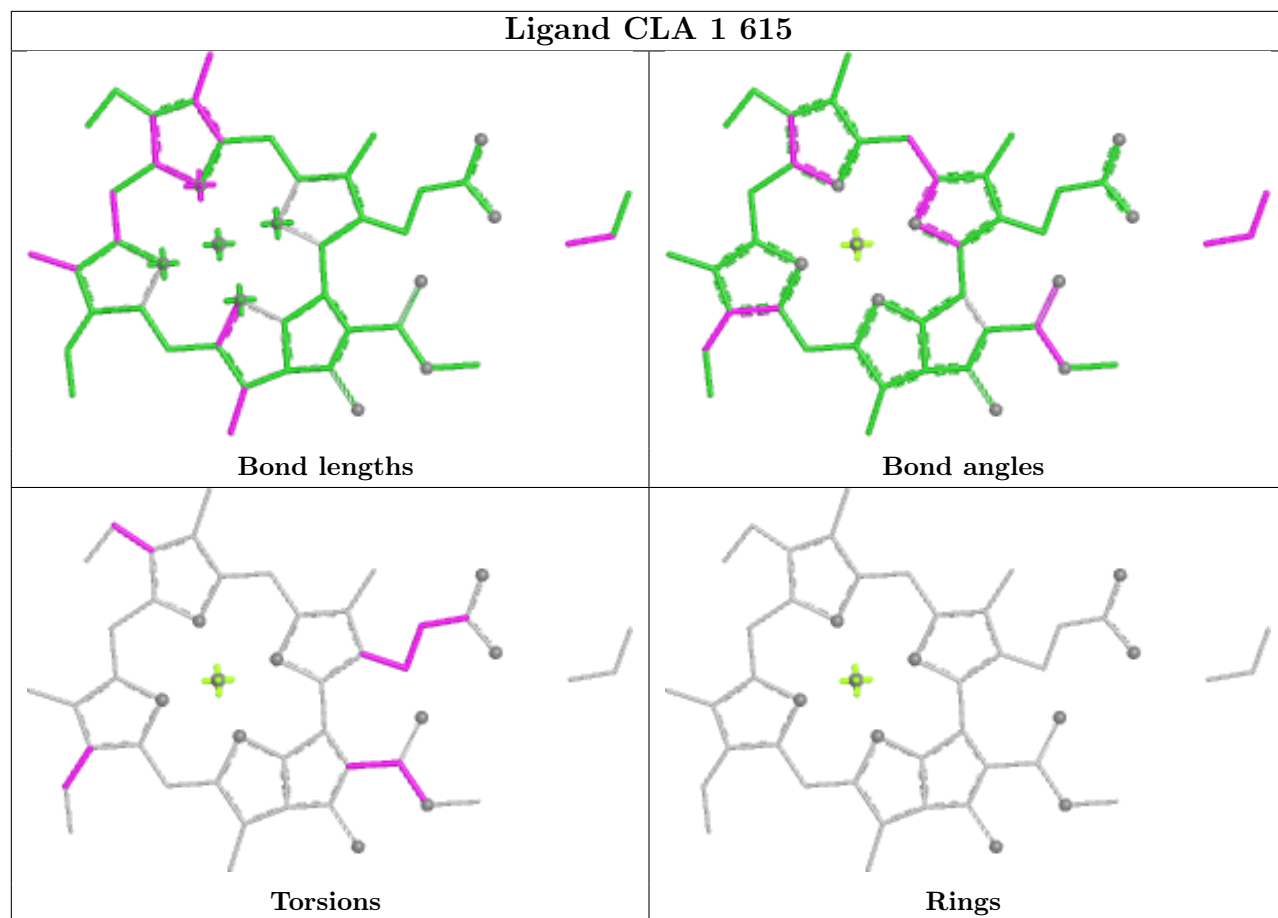


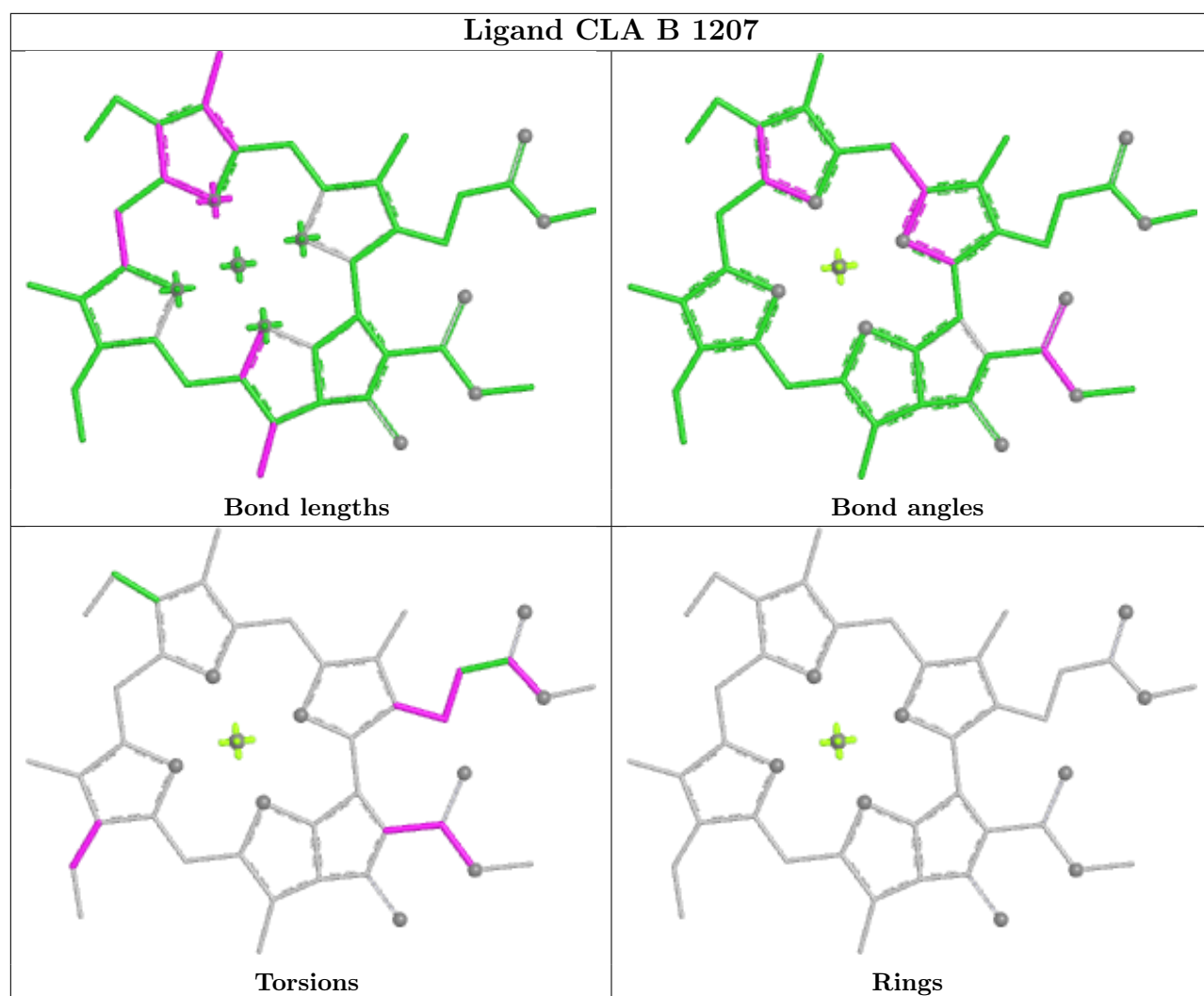
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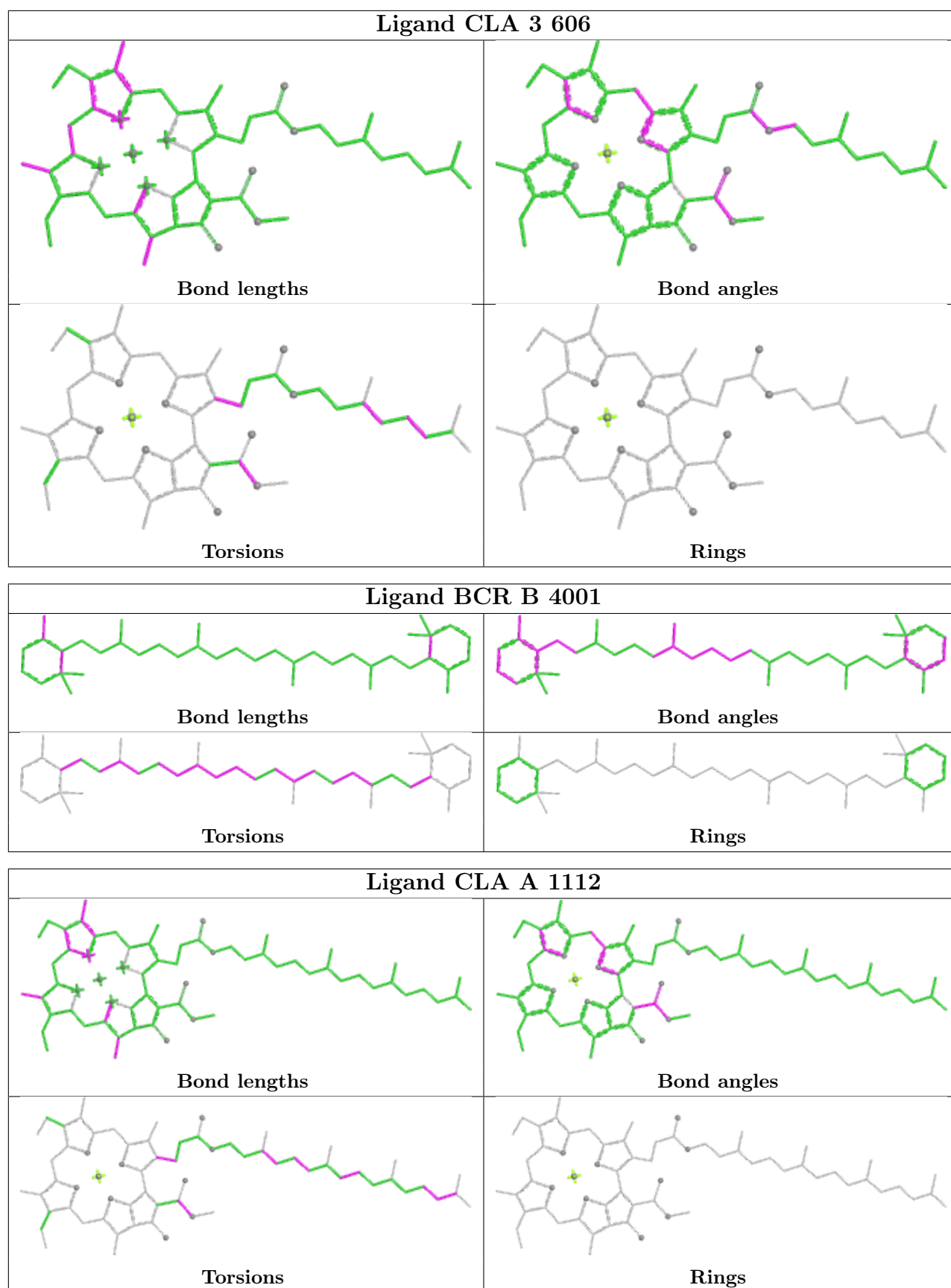




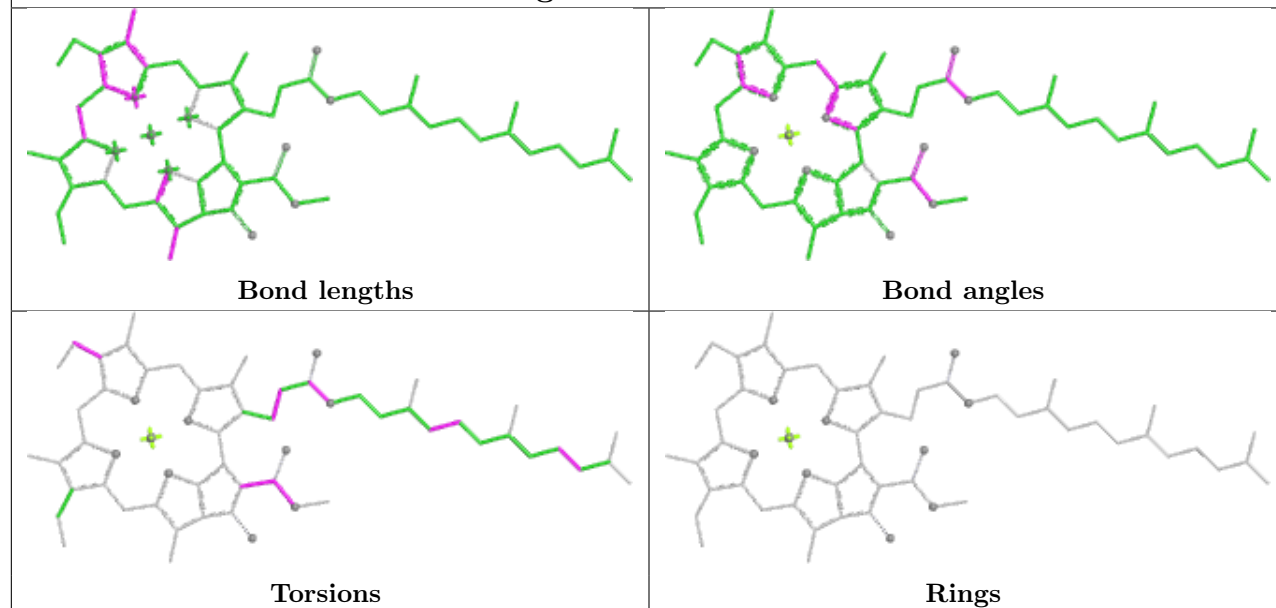
Ligand CLA 1 615



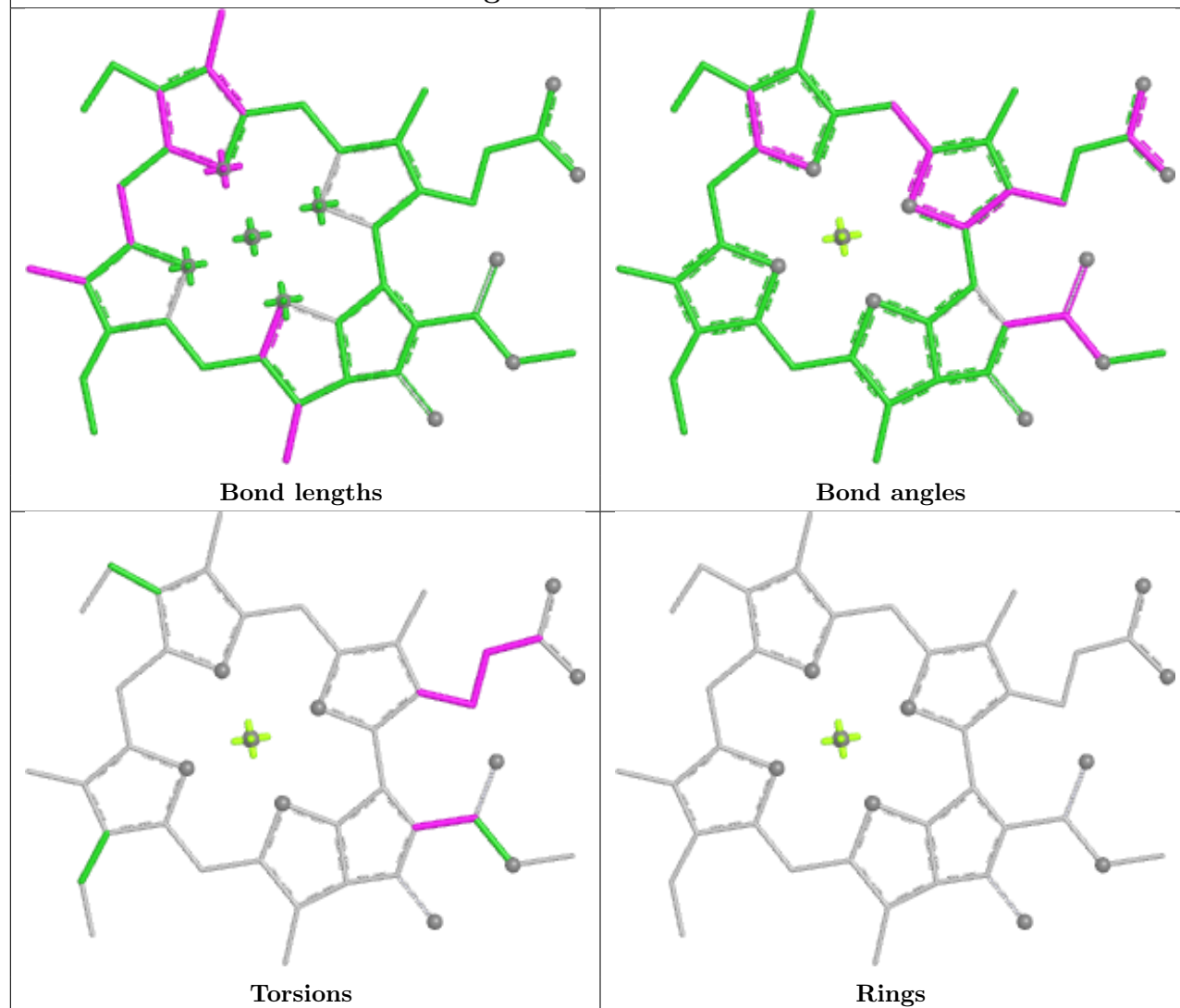


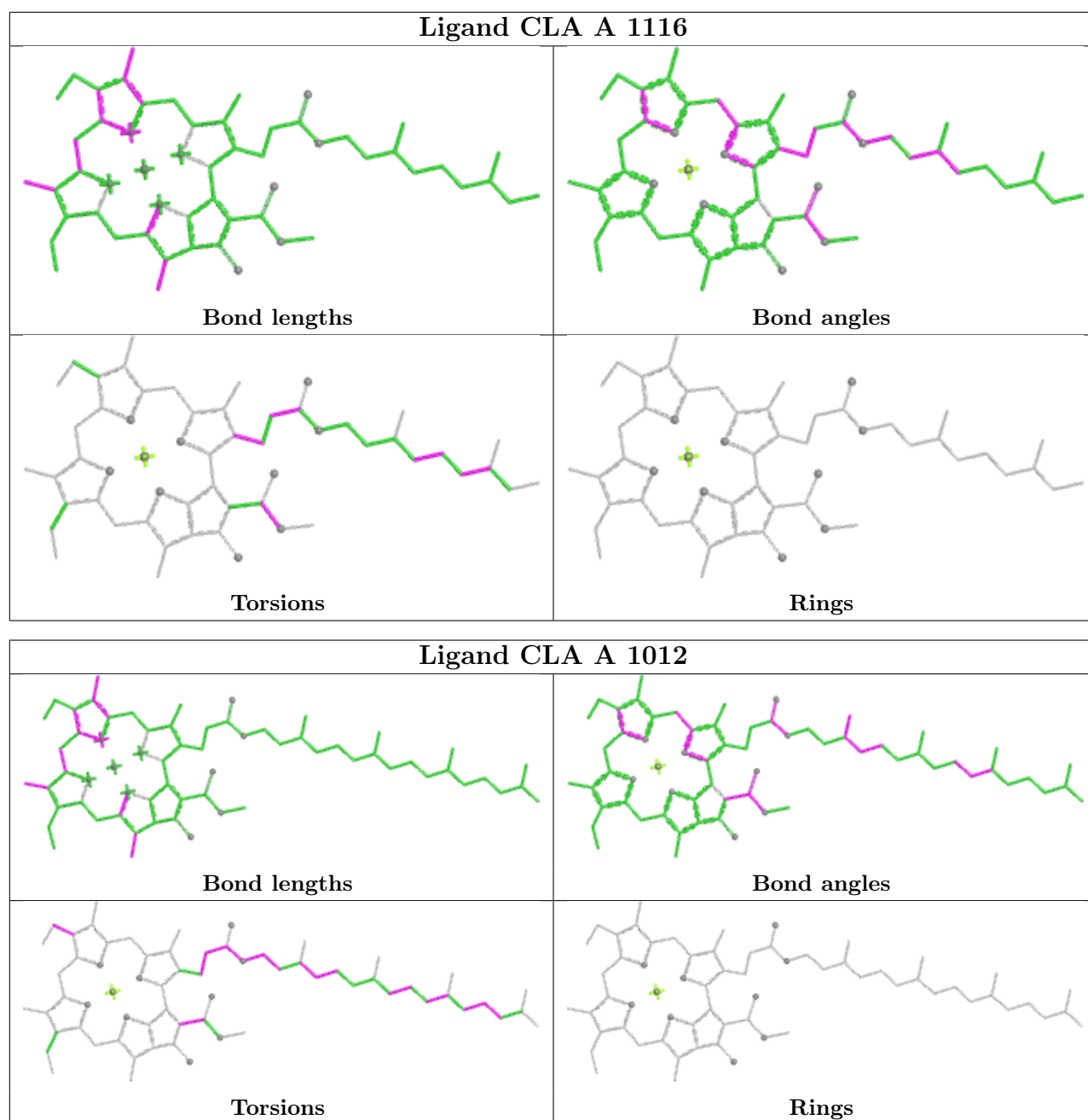


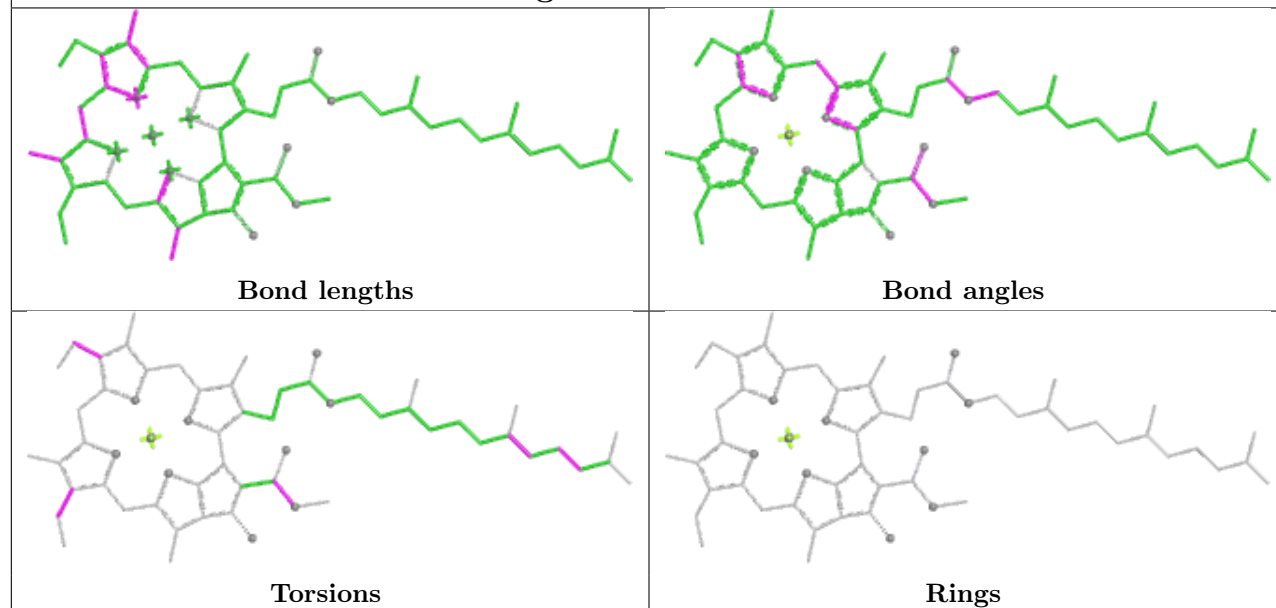
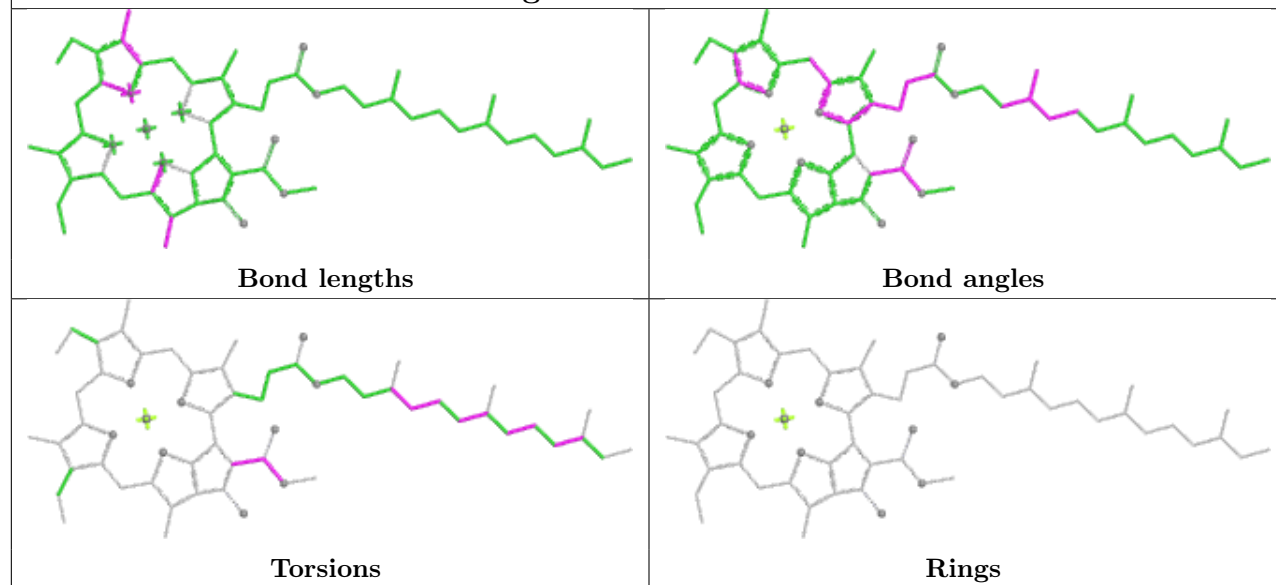
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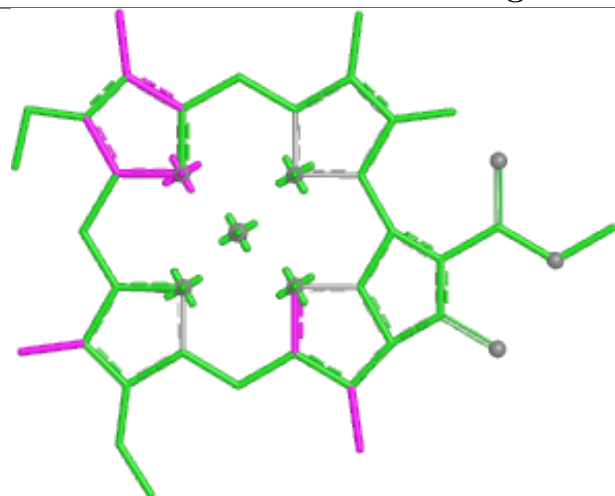
Ligand CLA B 1204



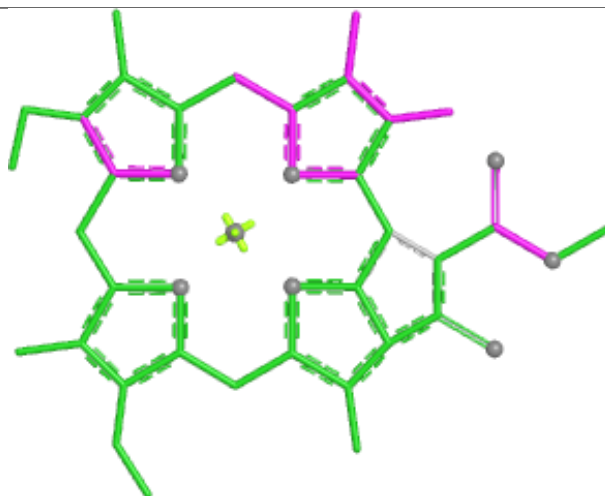


Ligand CLA 2 607**Ligand CLA A 1137**

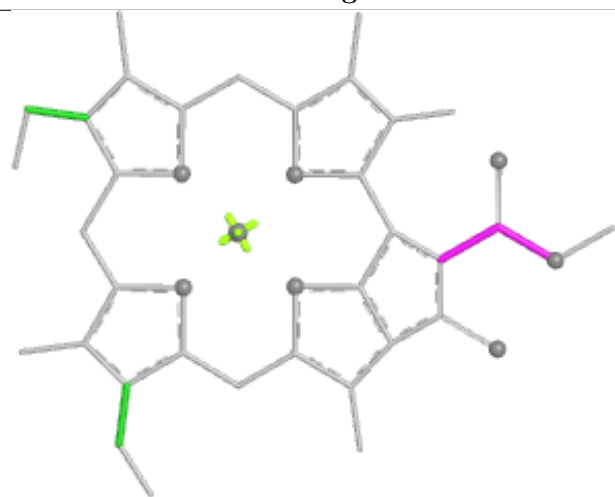
Ligand CLA A 1141



Bond lengths



Bond angles

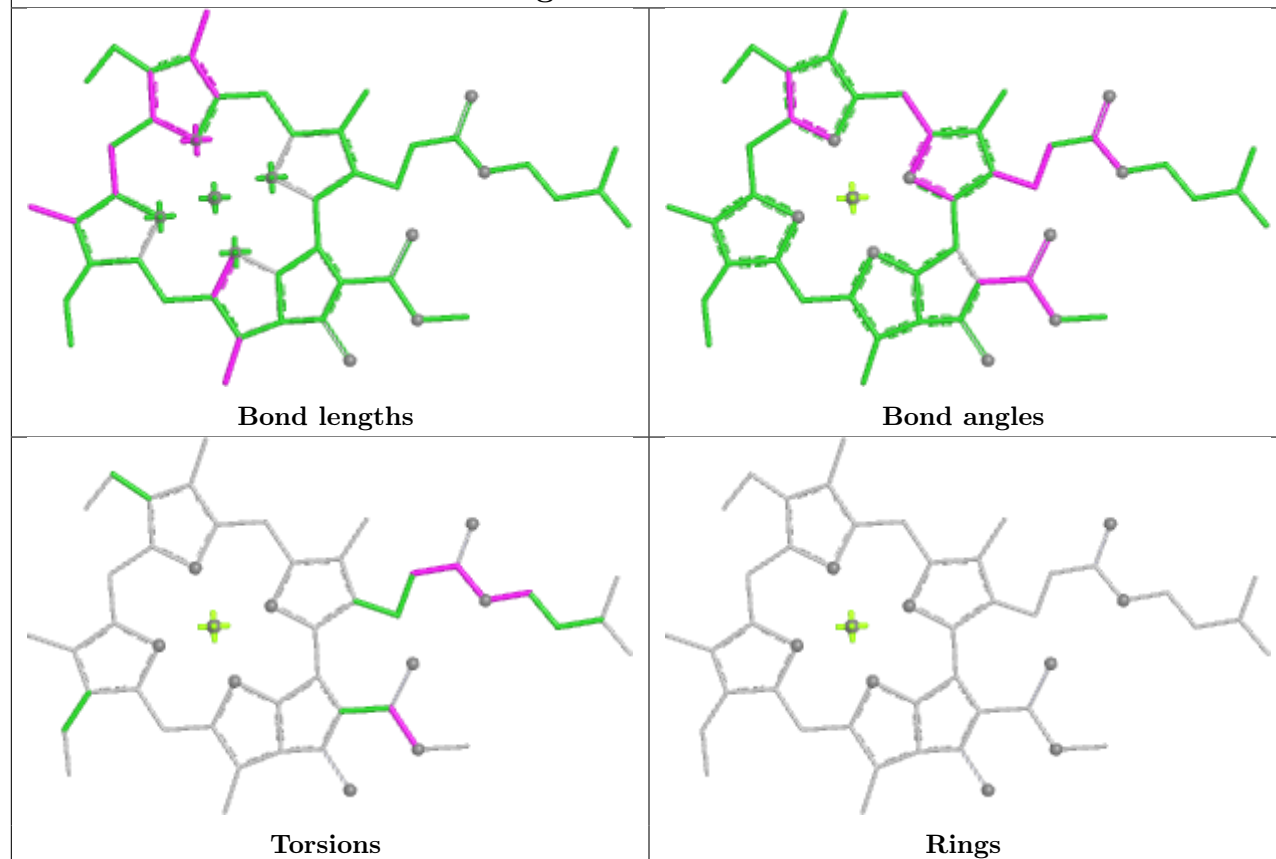


Torsions

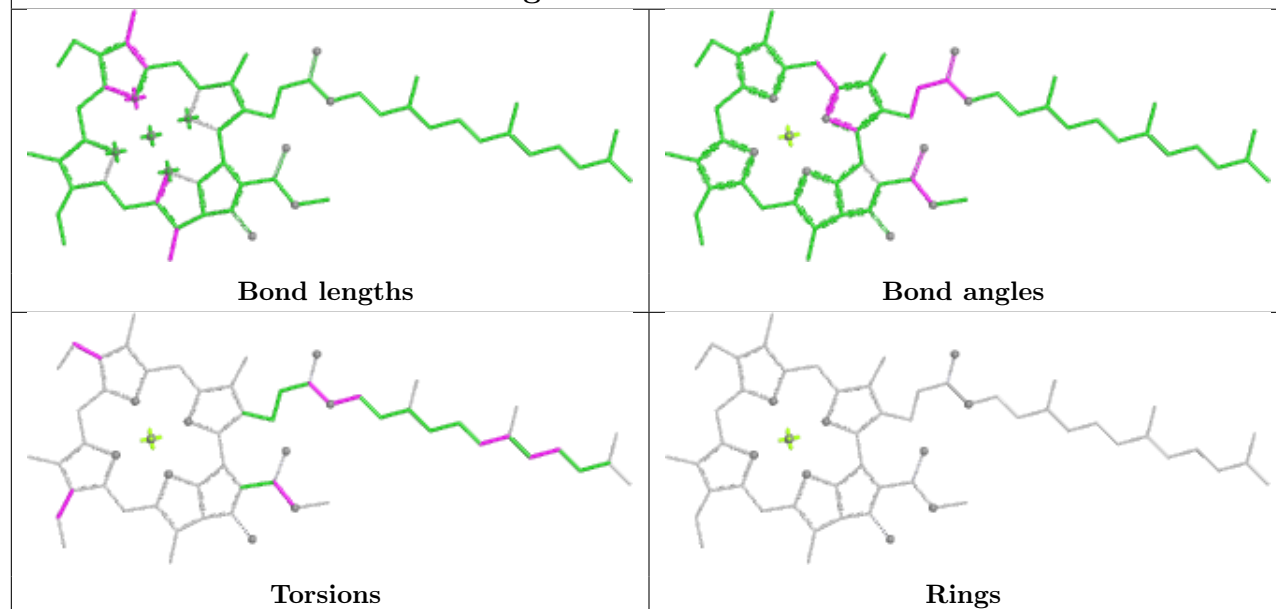


Rings

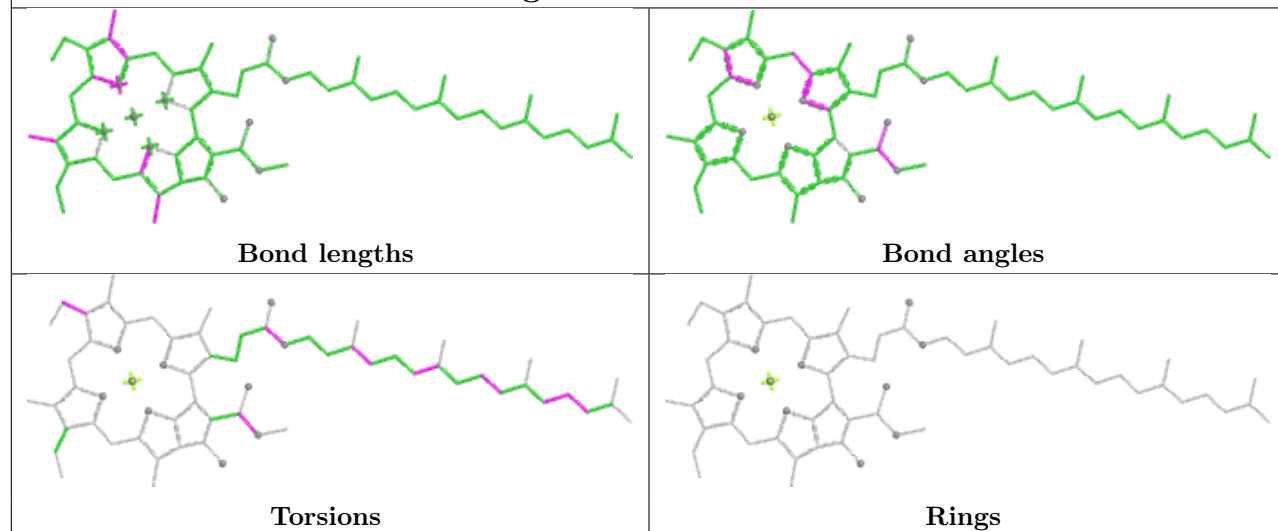
Ligand CLA 3 610



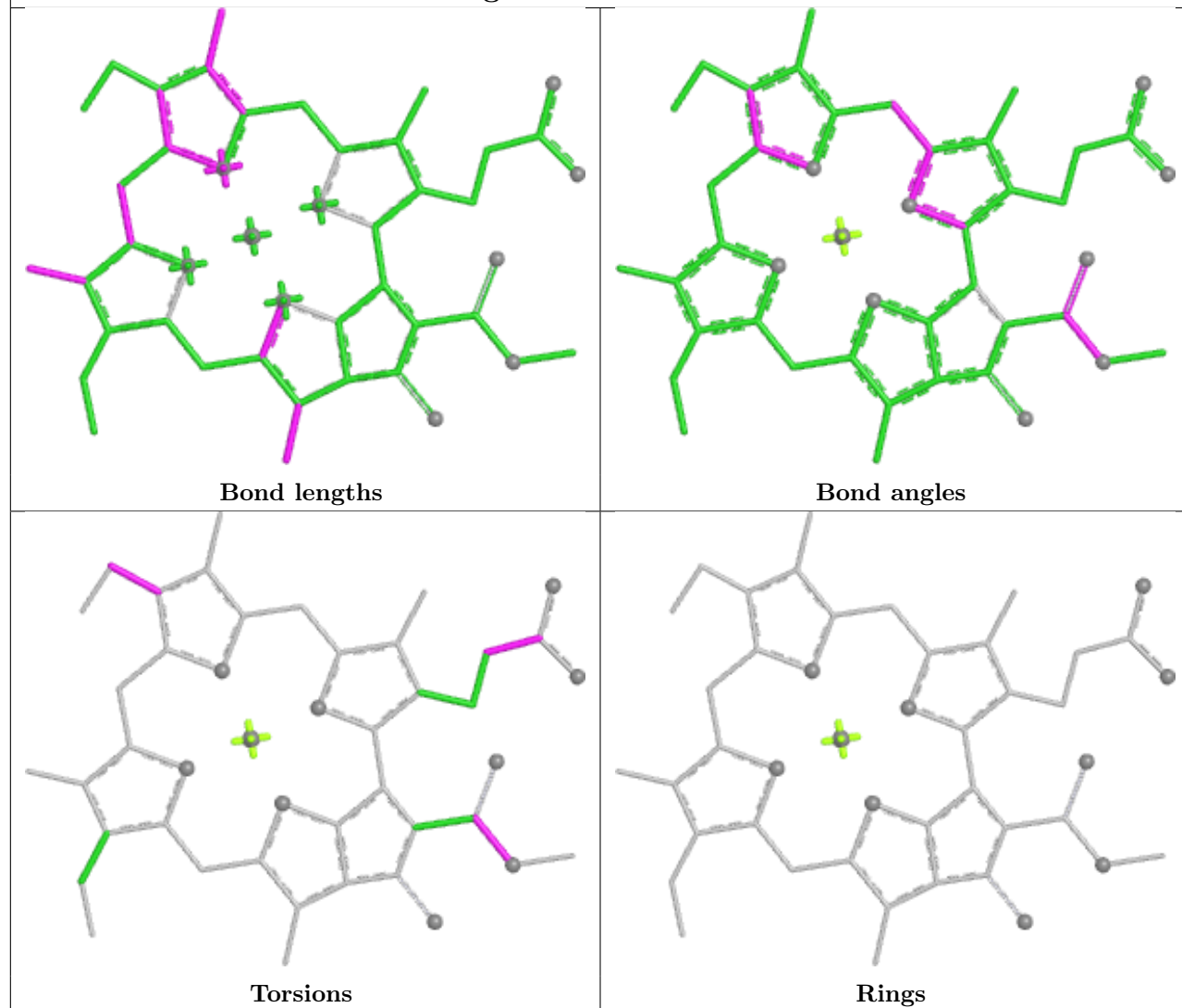
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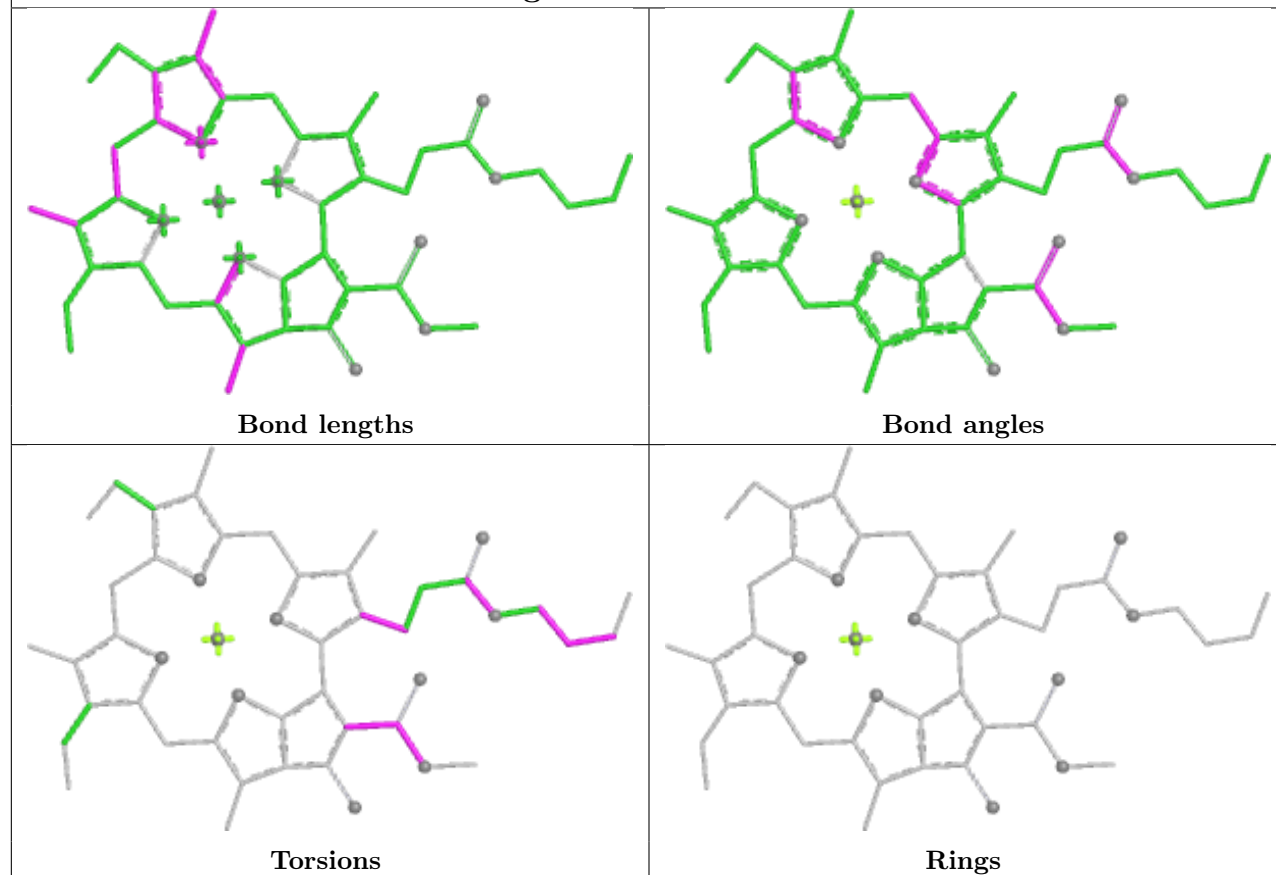
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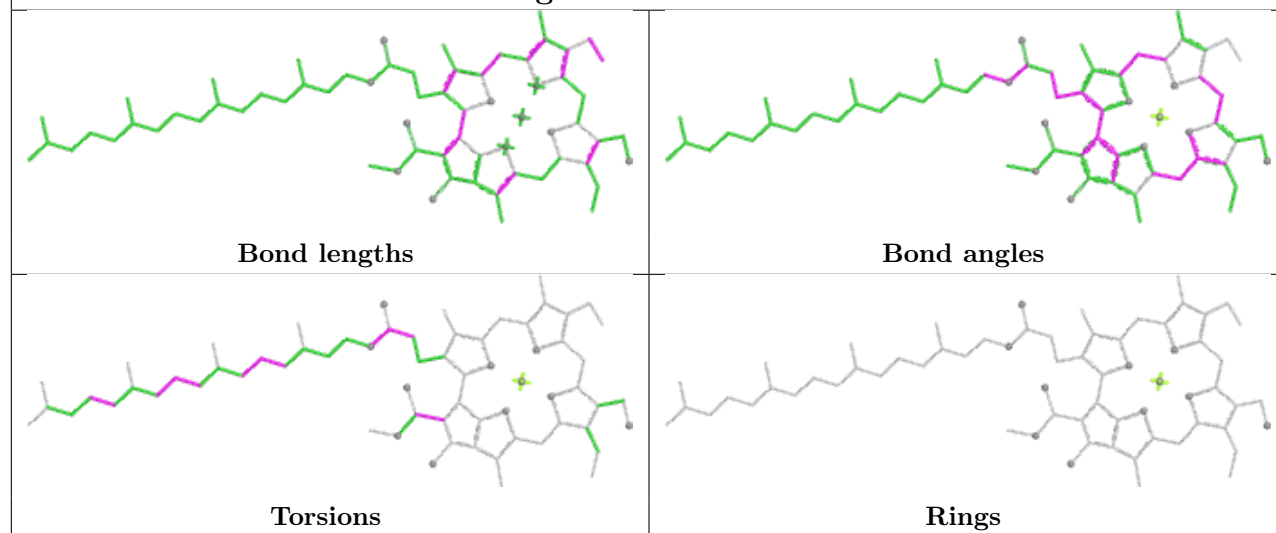
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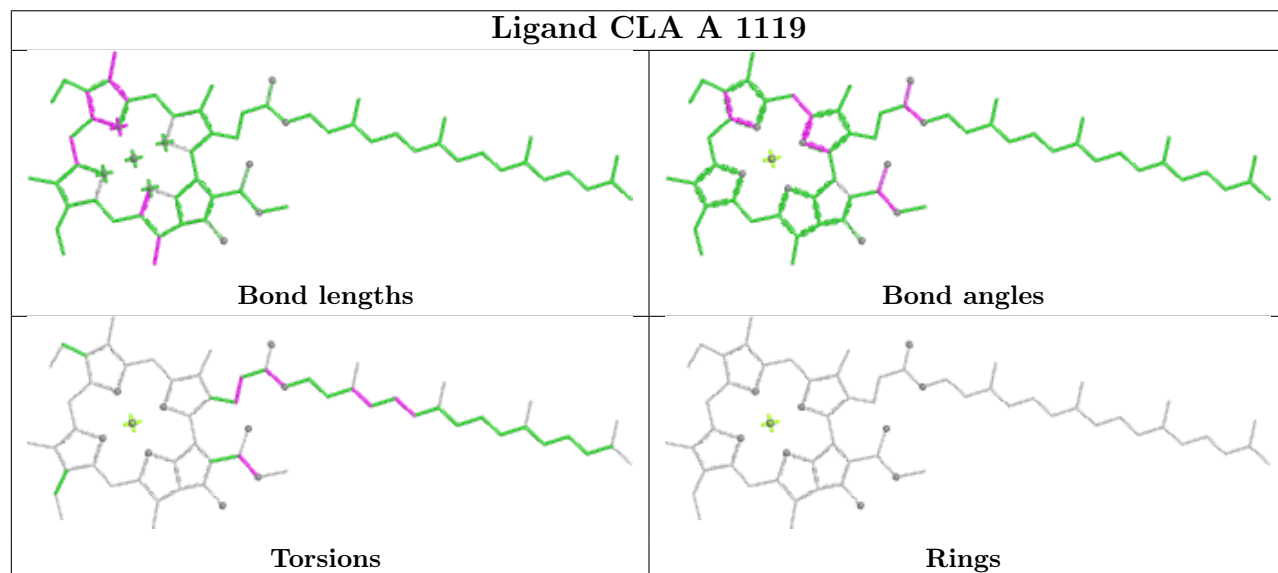
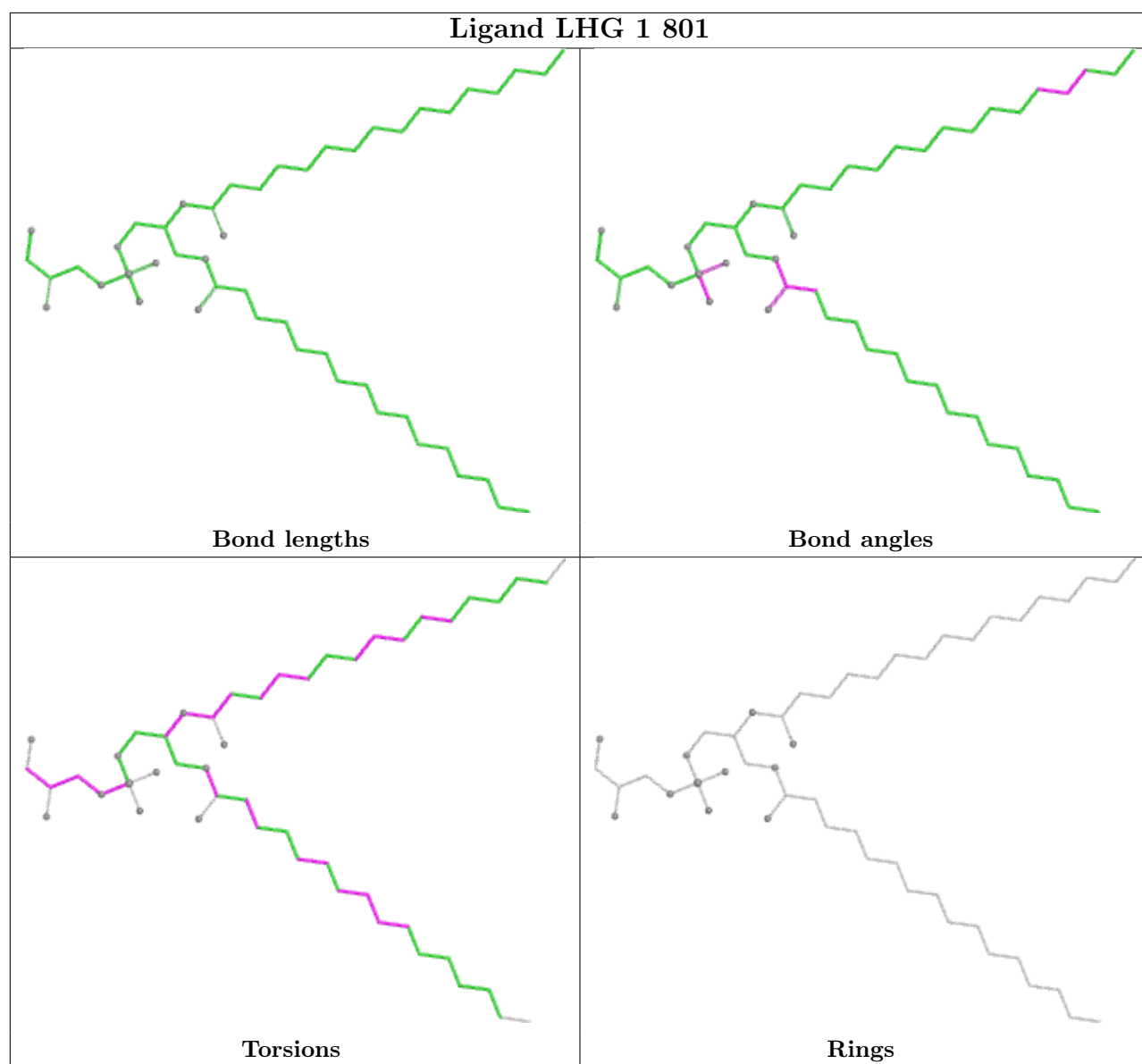


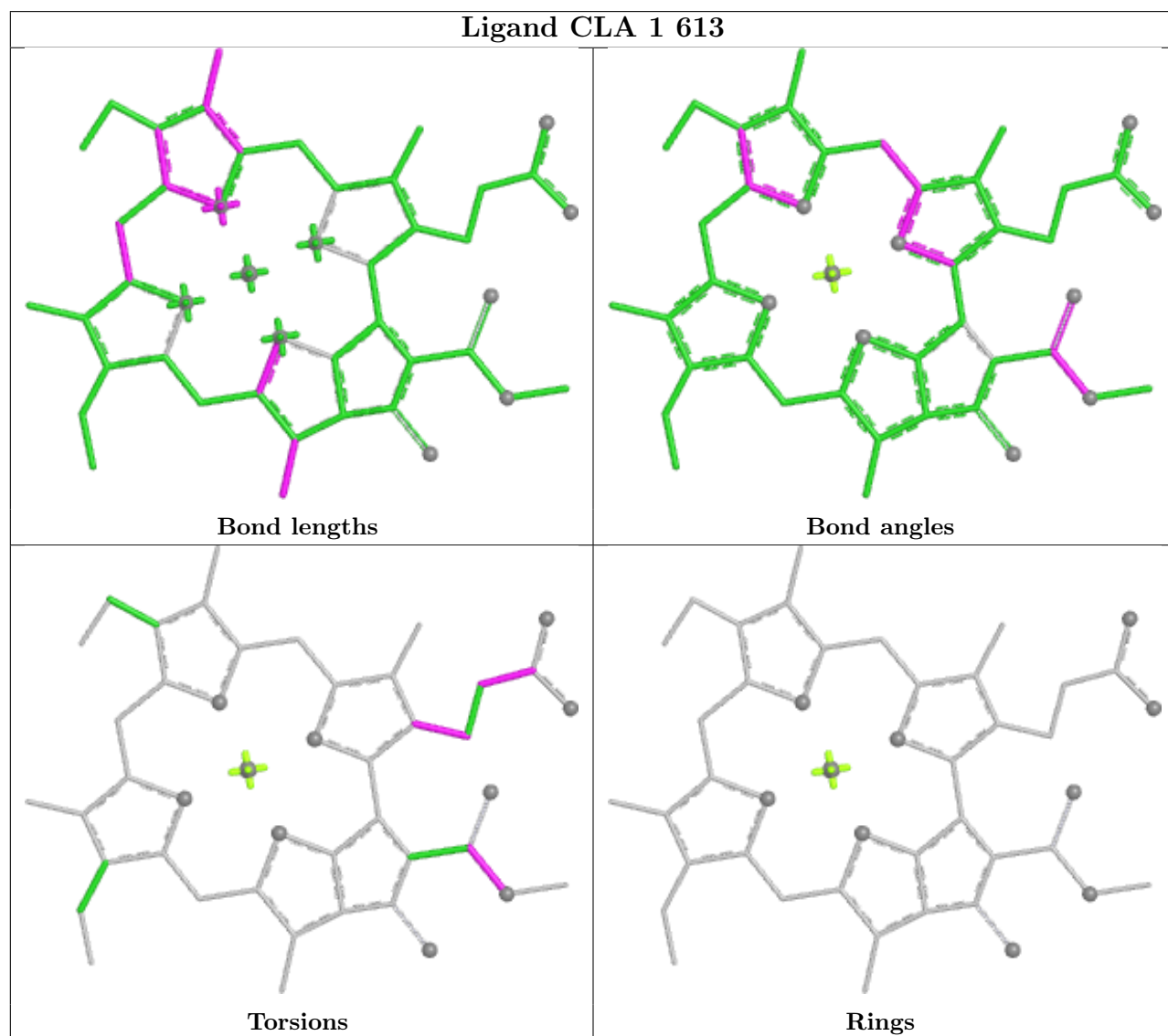
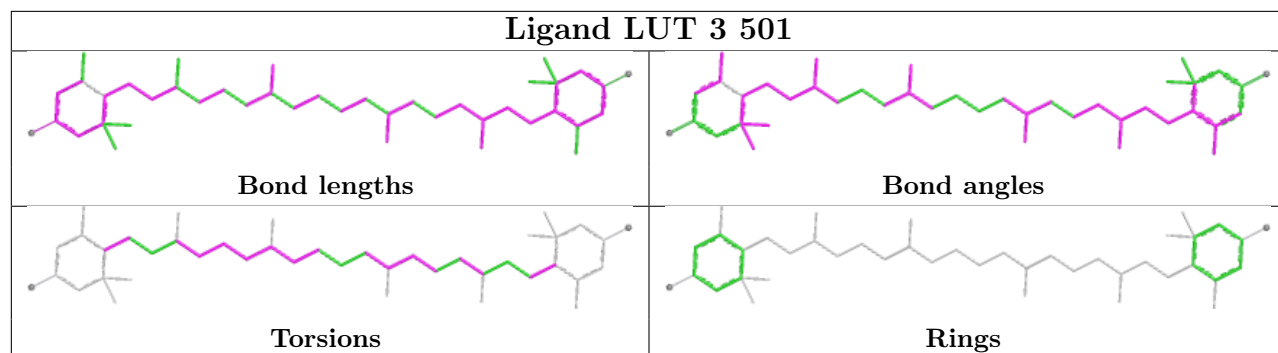
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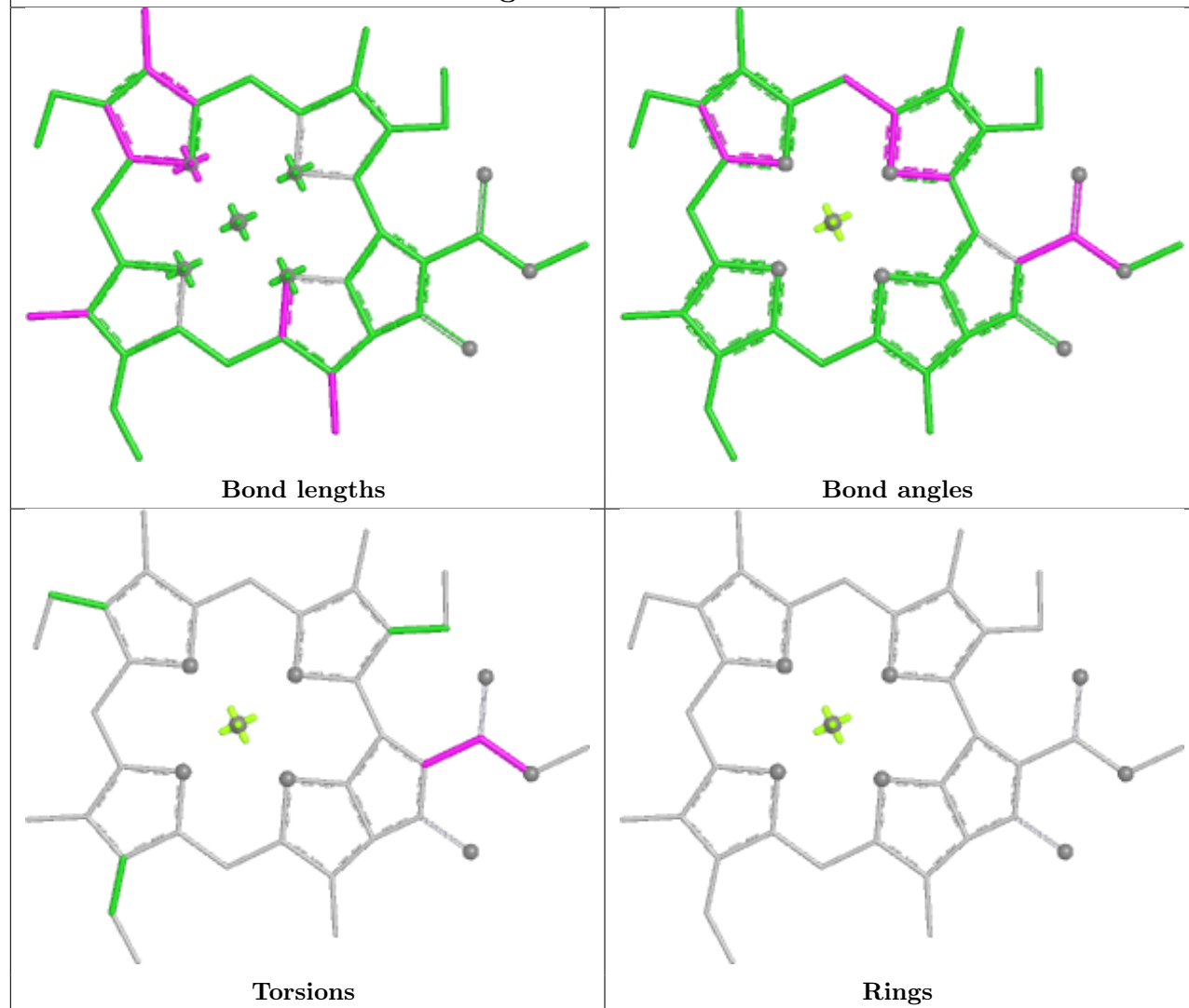
Ligand CHL 2 609



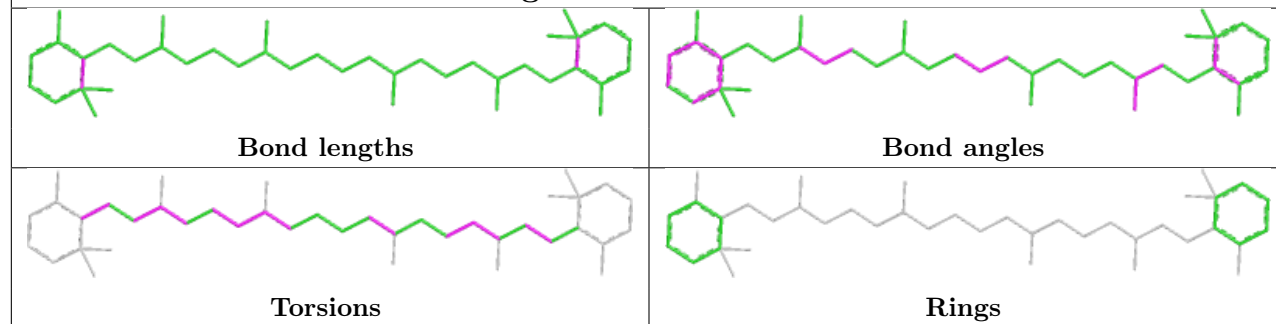


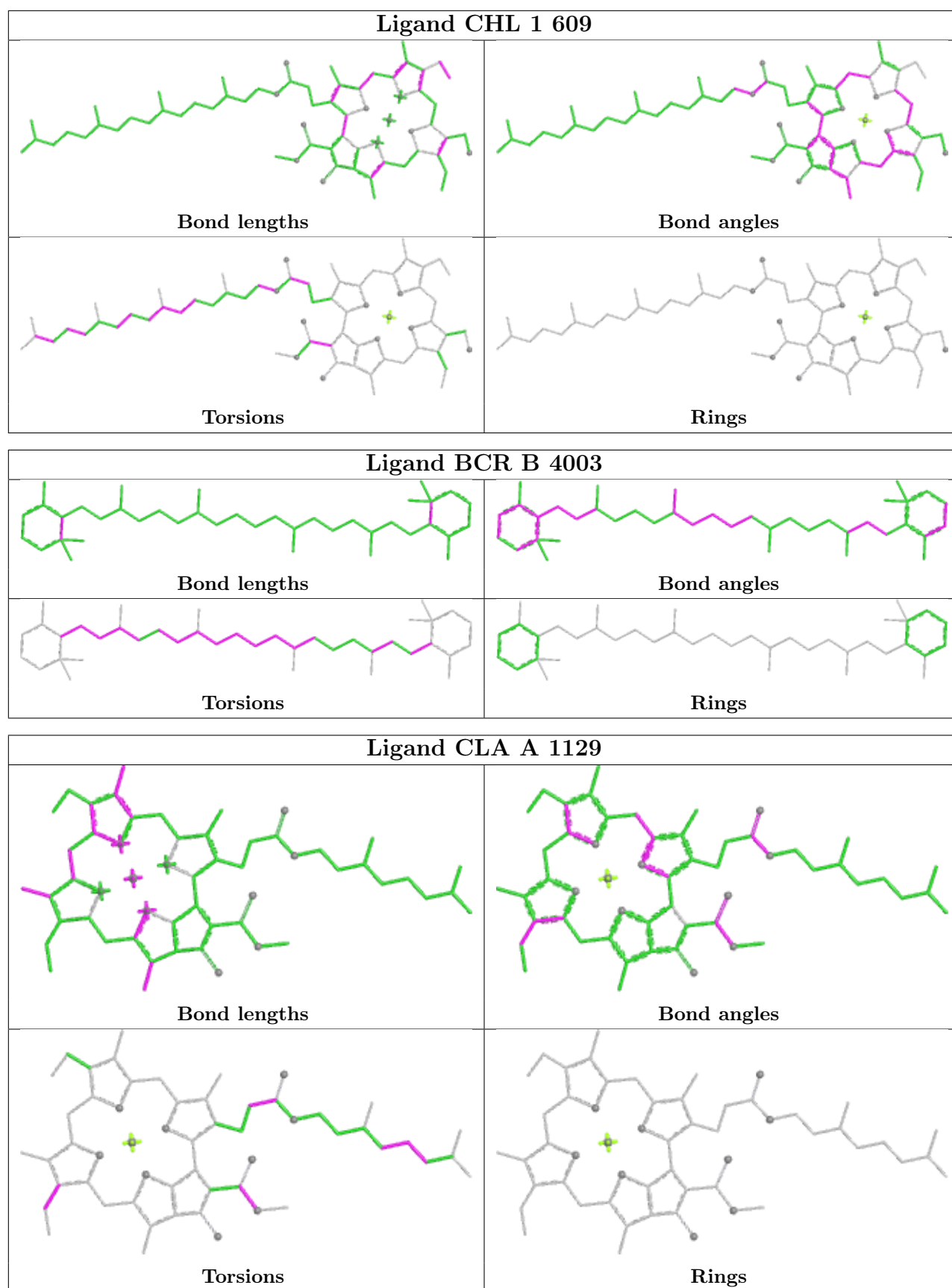


Ligand CLA 3 609

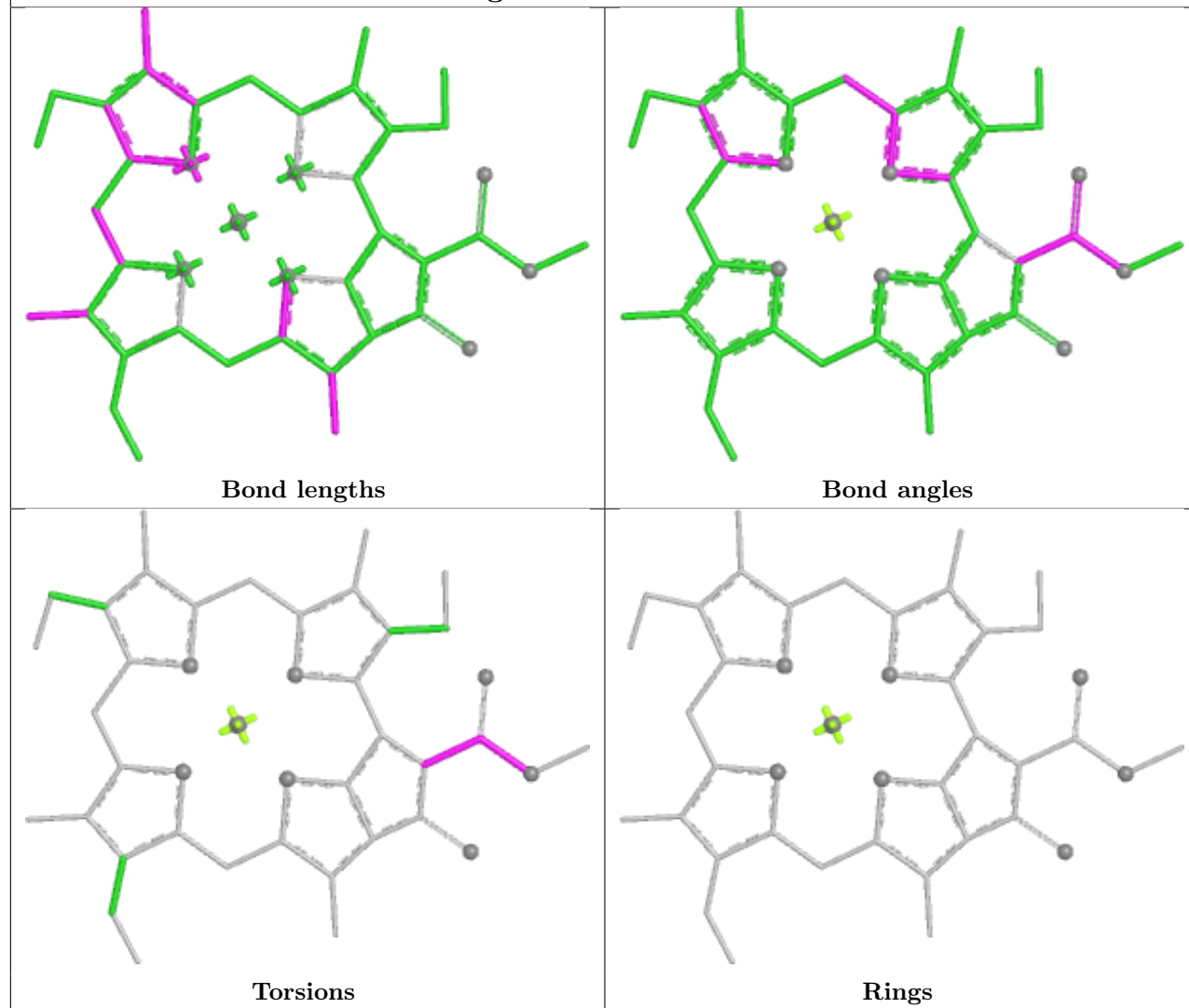


Ligand BCR B 4002

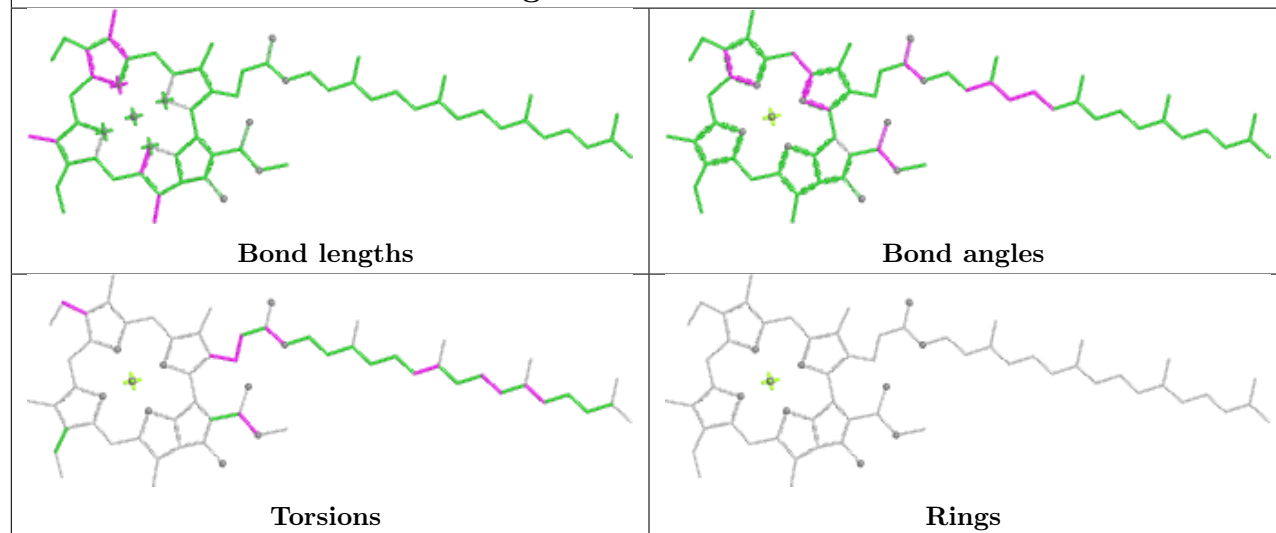




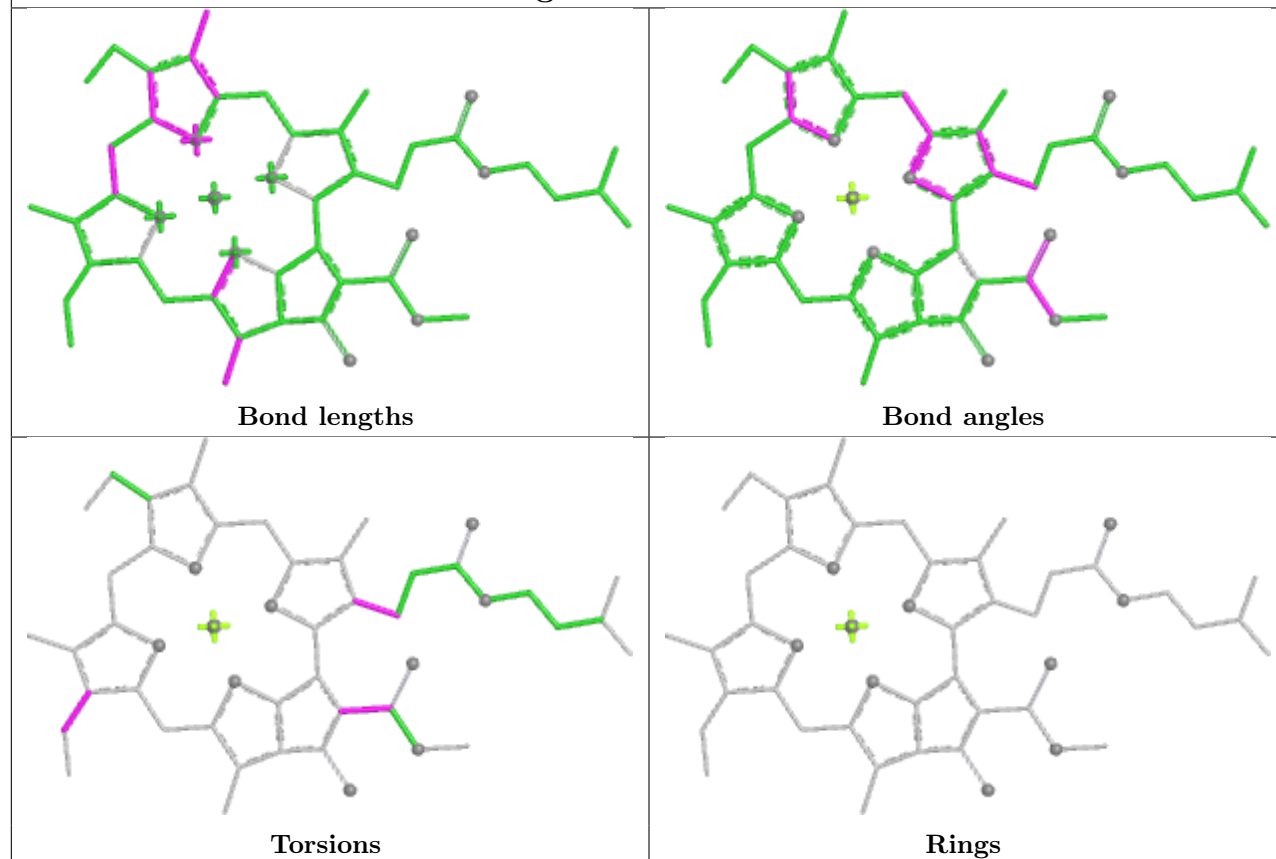
Ligand CLA A 1134



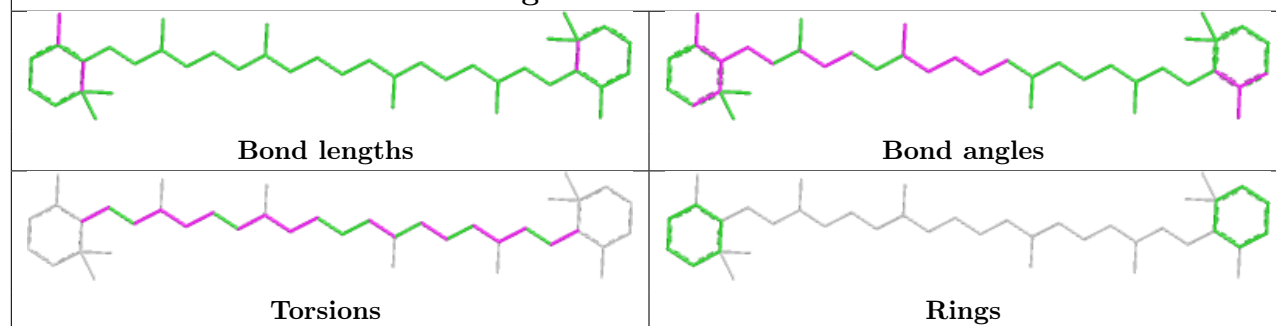
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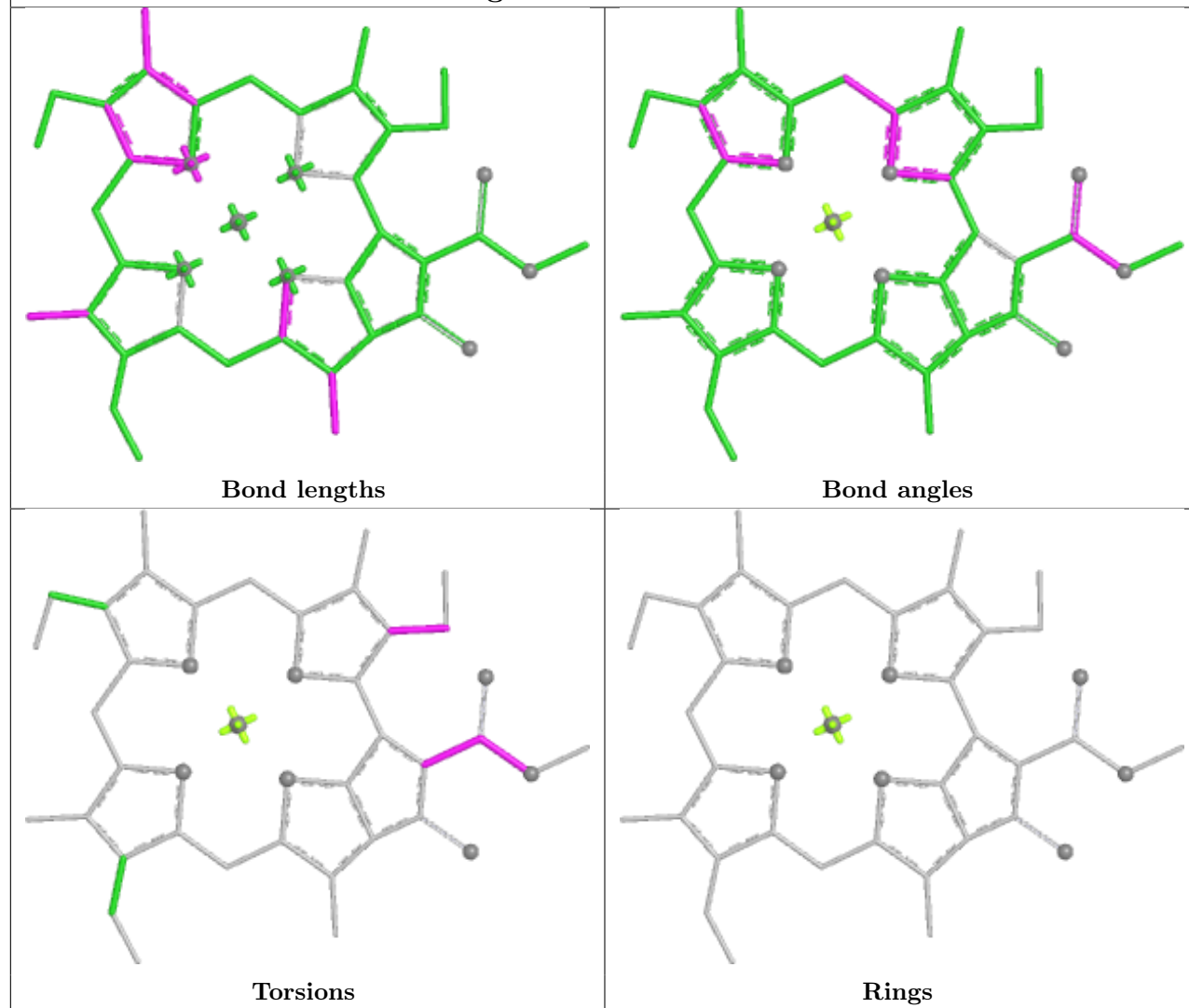
Ligand CLA 2 608



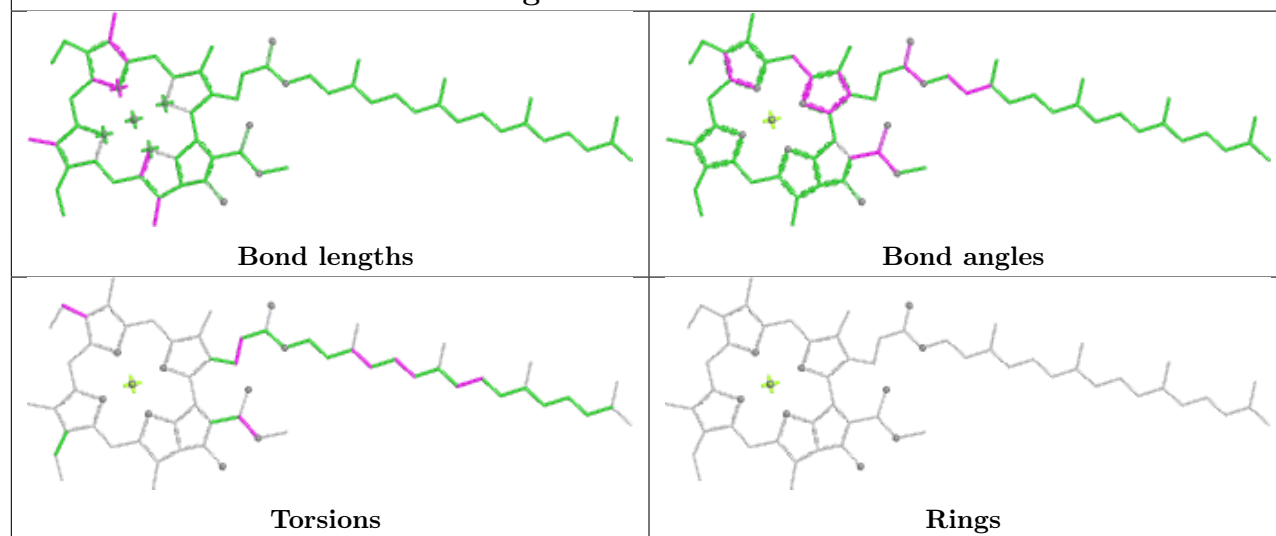
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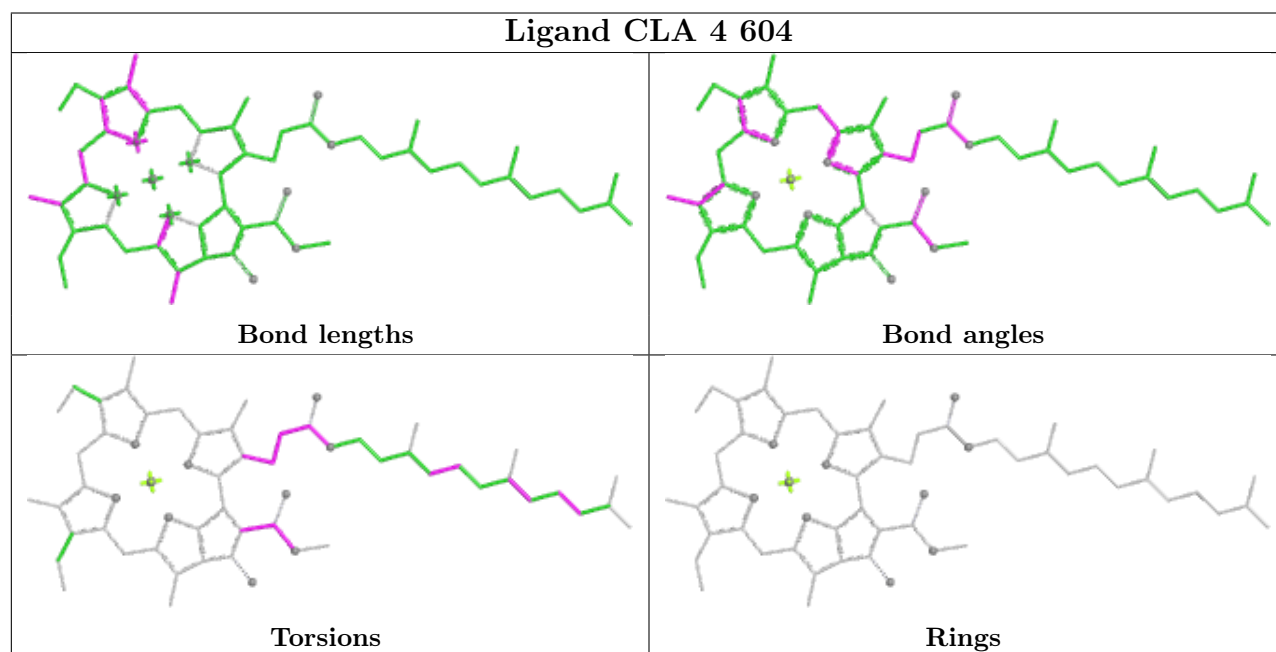
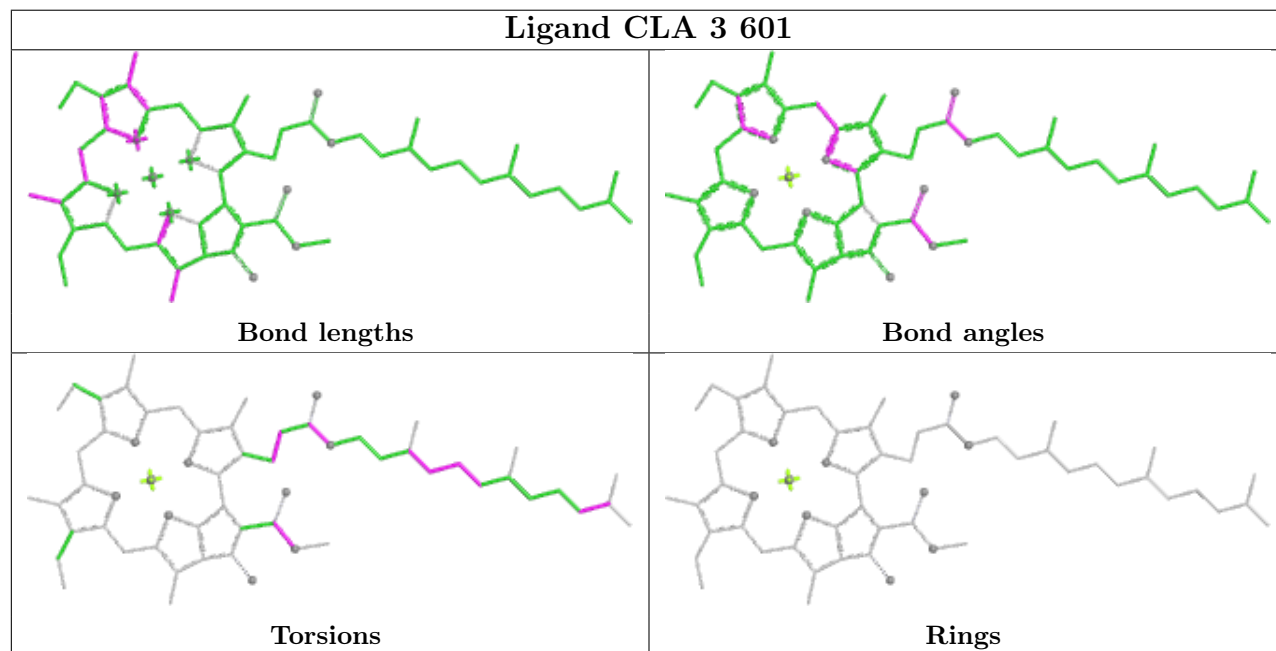
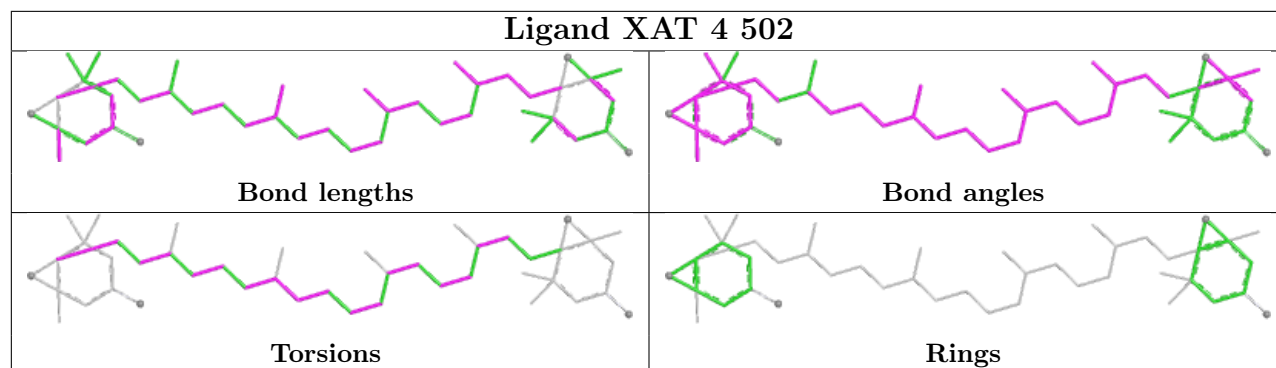


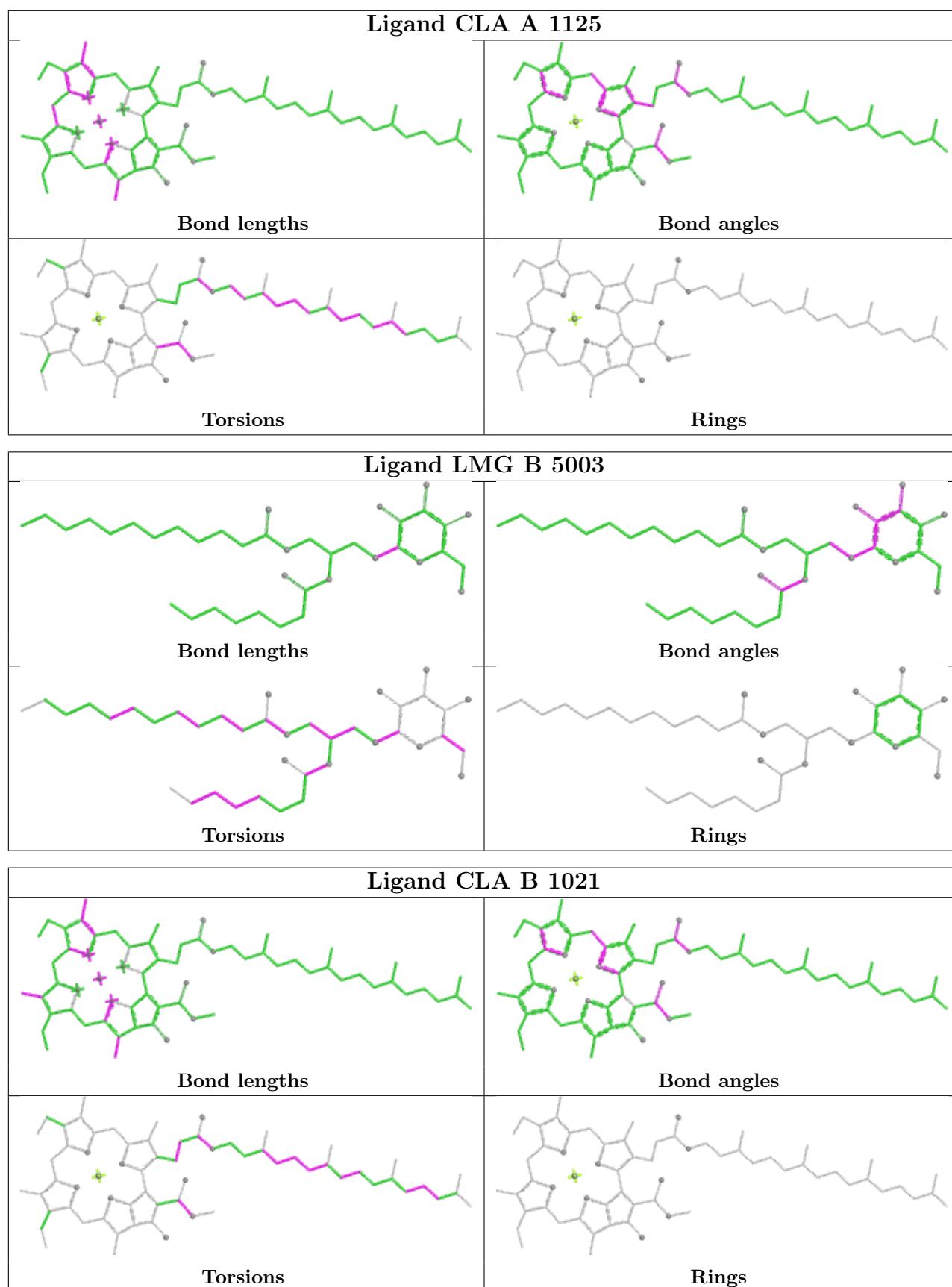
Ligand CLA A 1118



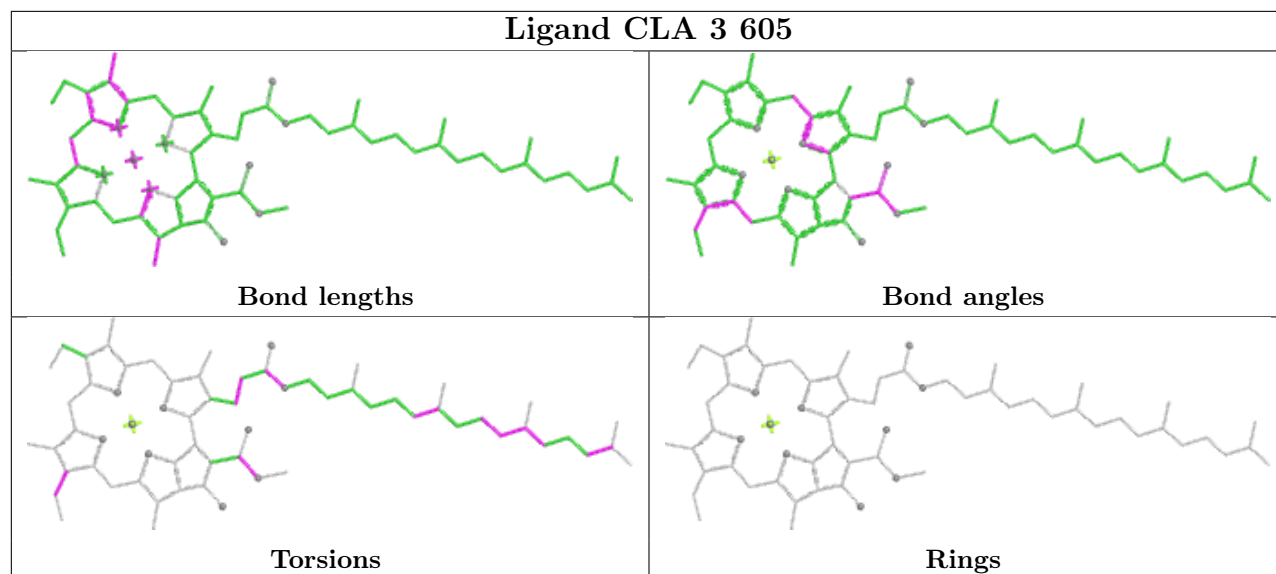
Ligand CLA A 1138



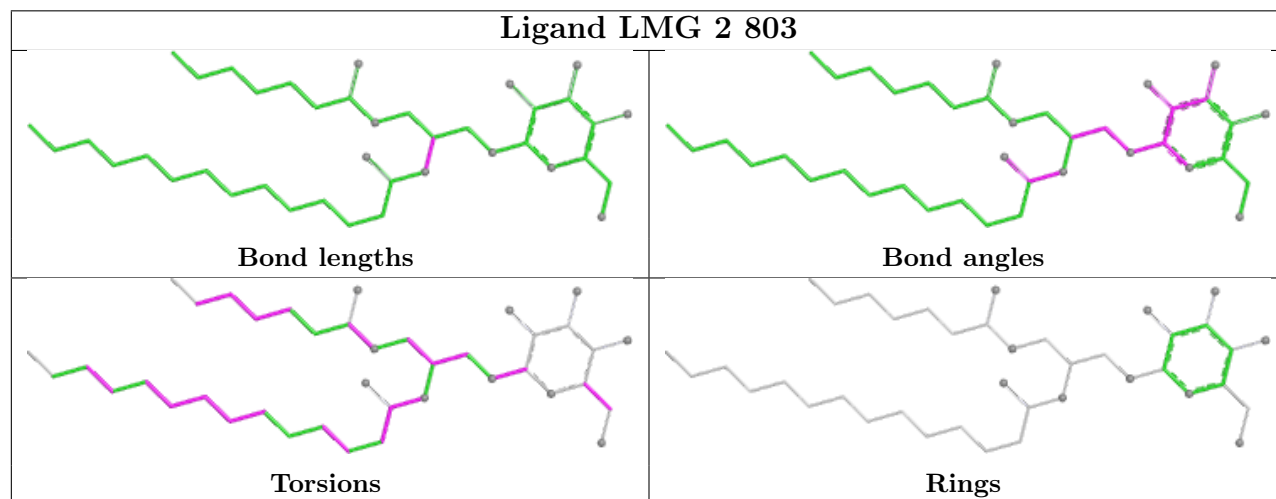




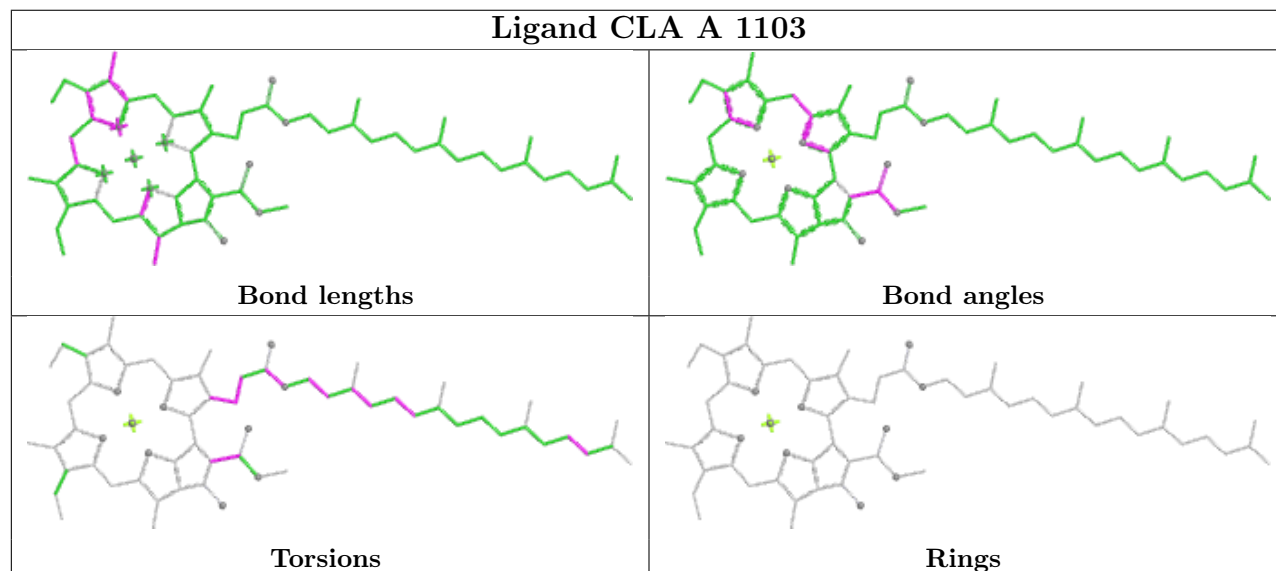
Ligand CLA 3 605

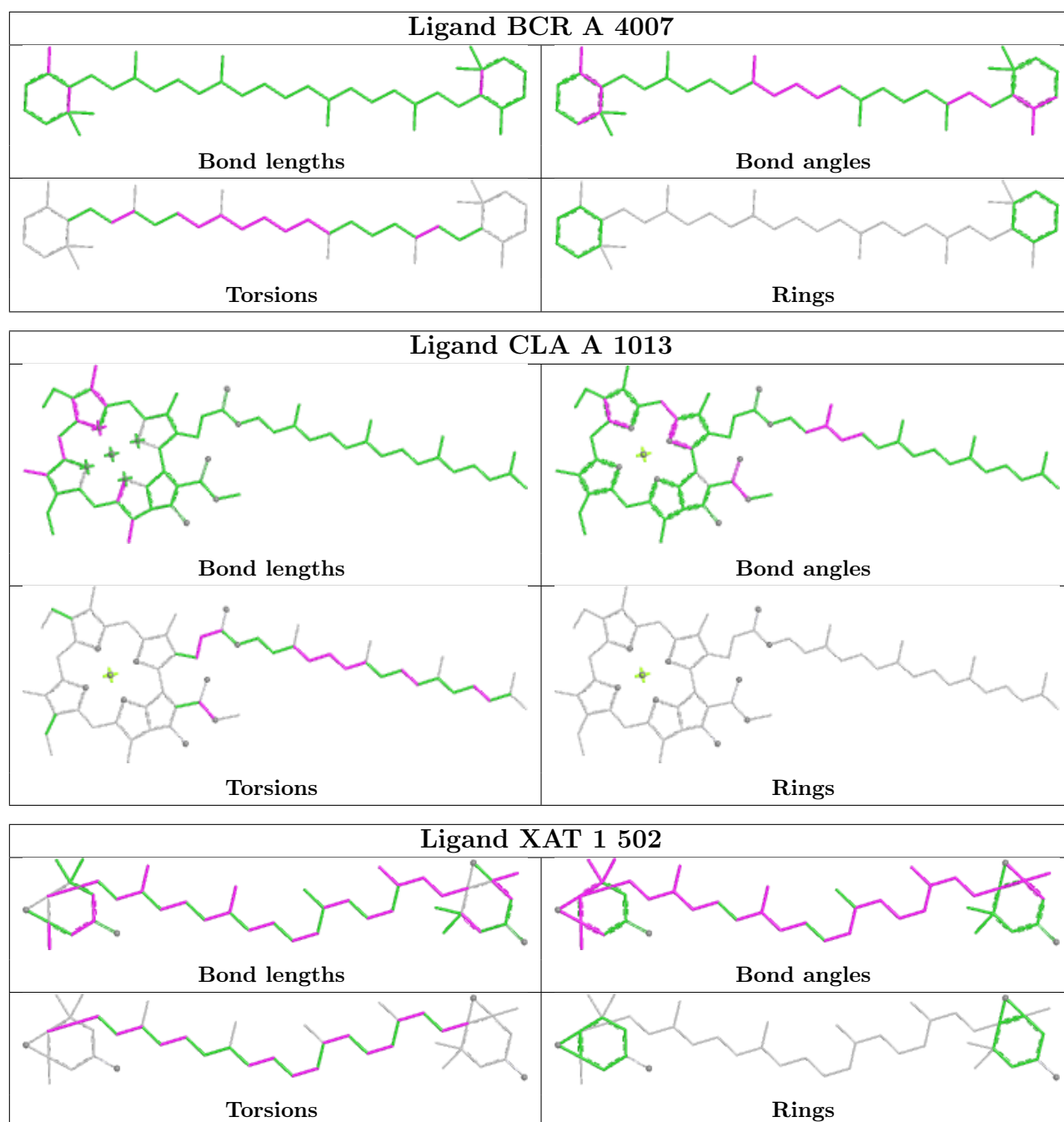


Ligand LMG 2 803

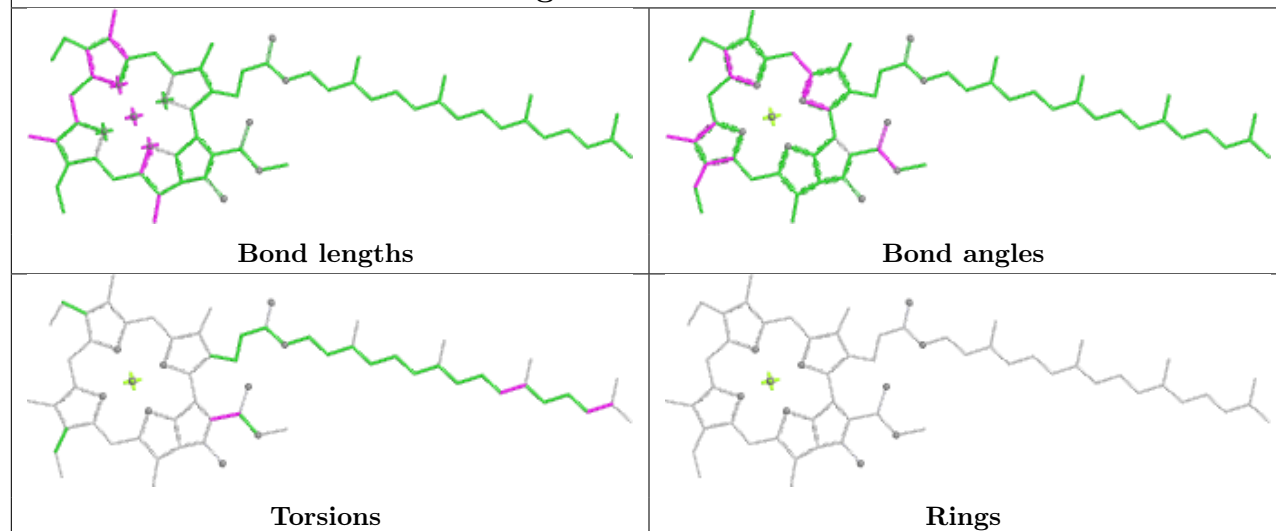


Ligand CLA A 1103

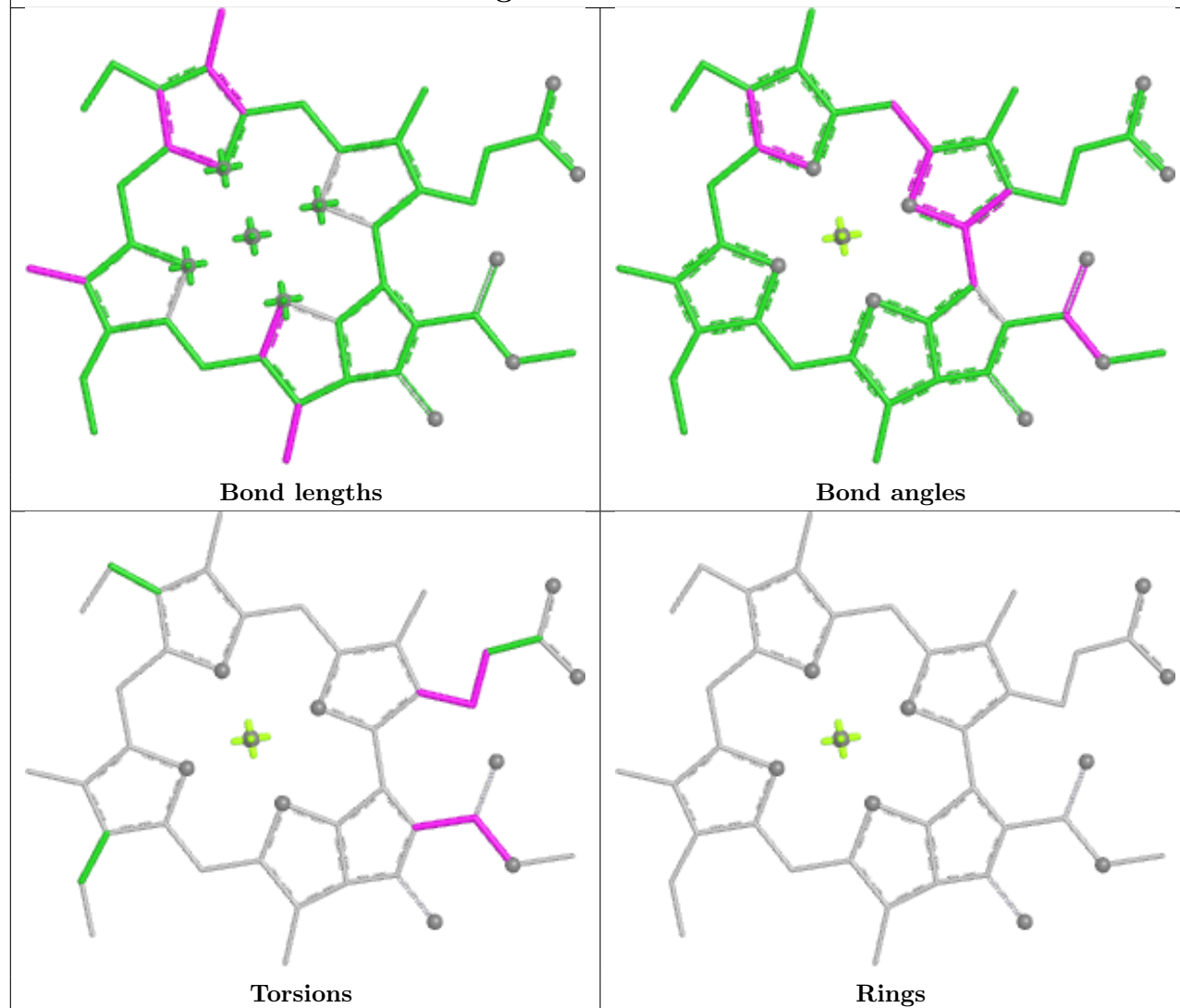


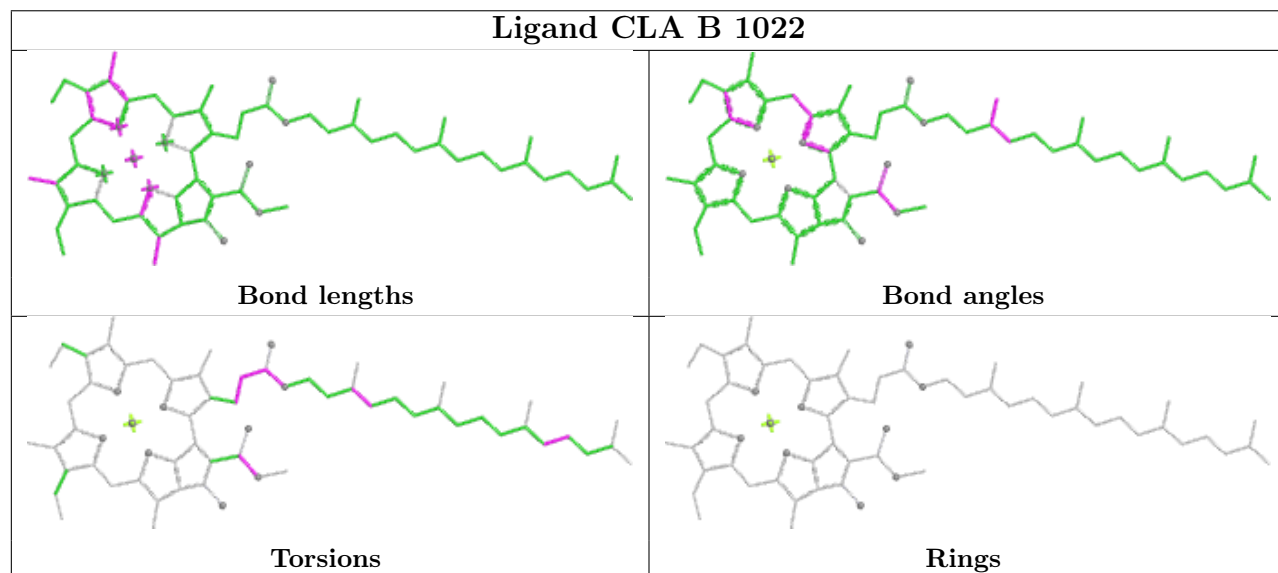
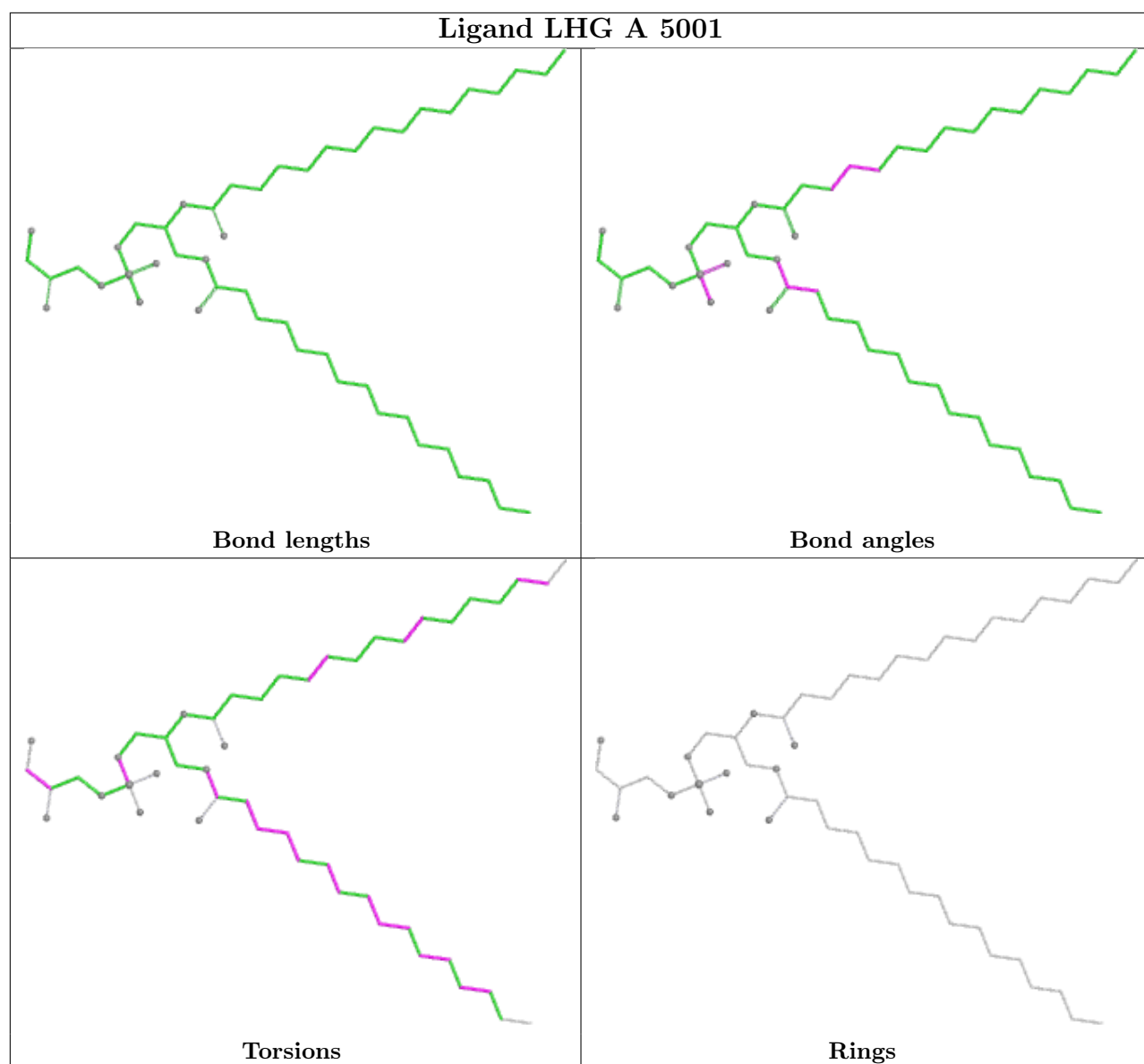


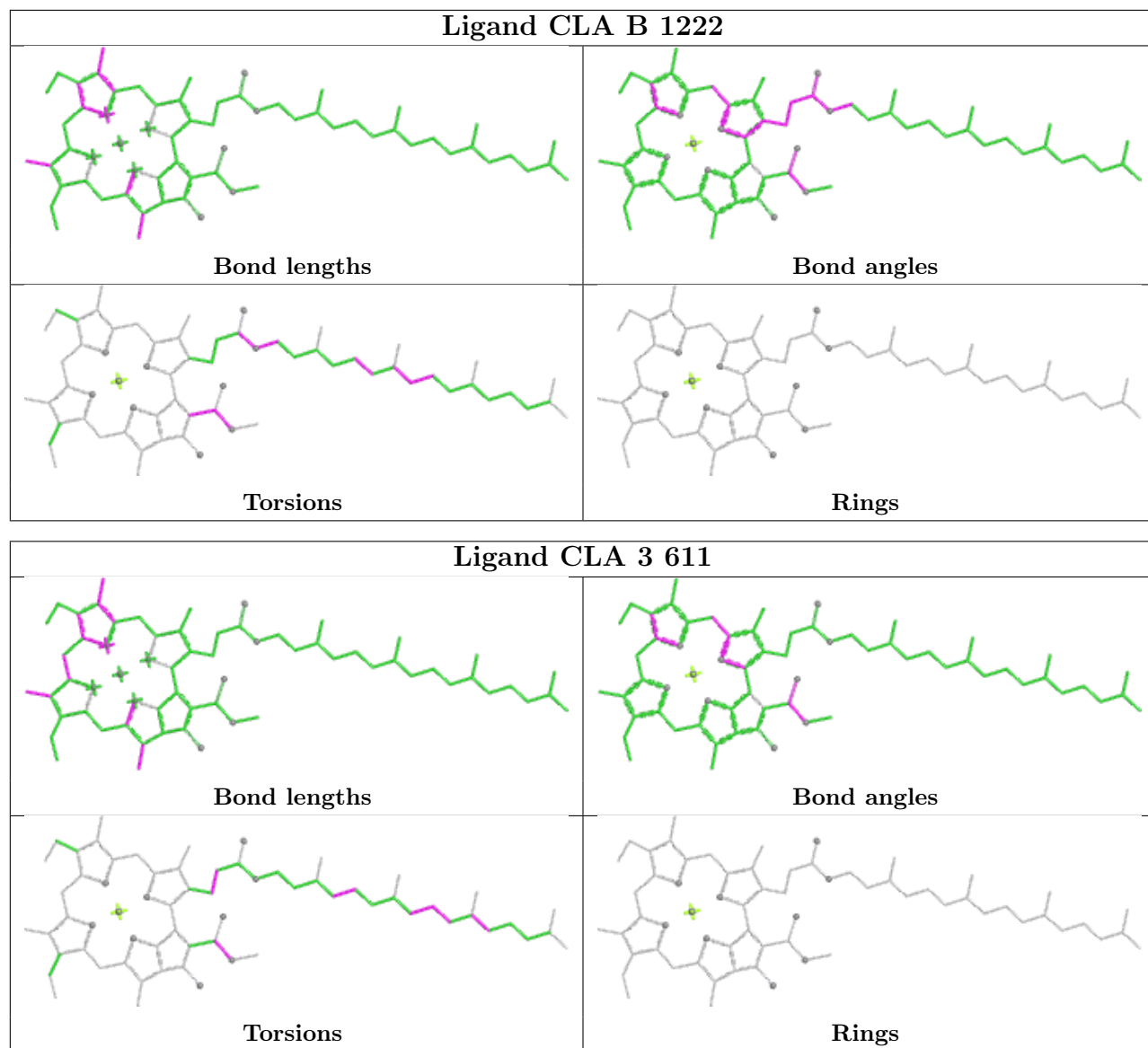
Ligand CLA 1 604

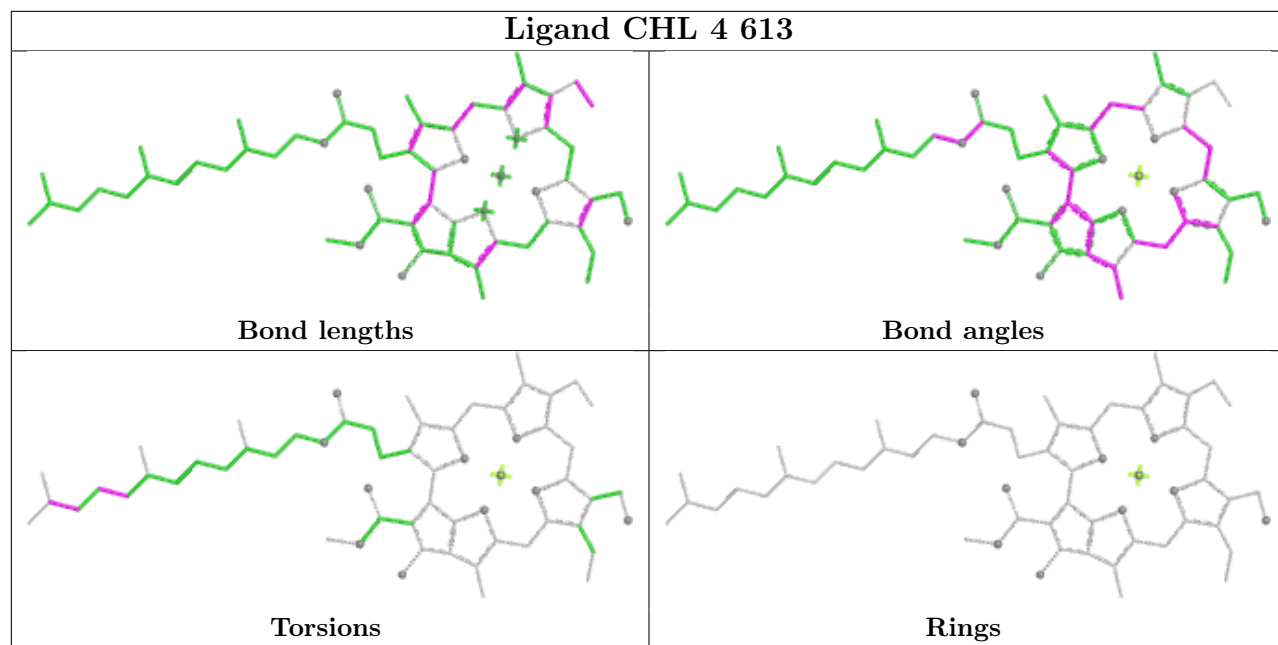
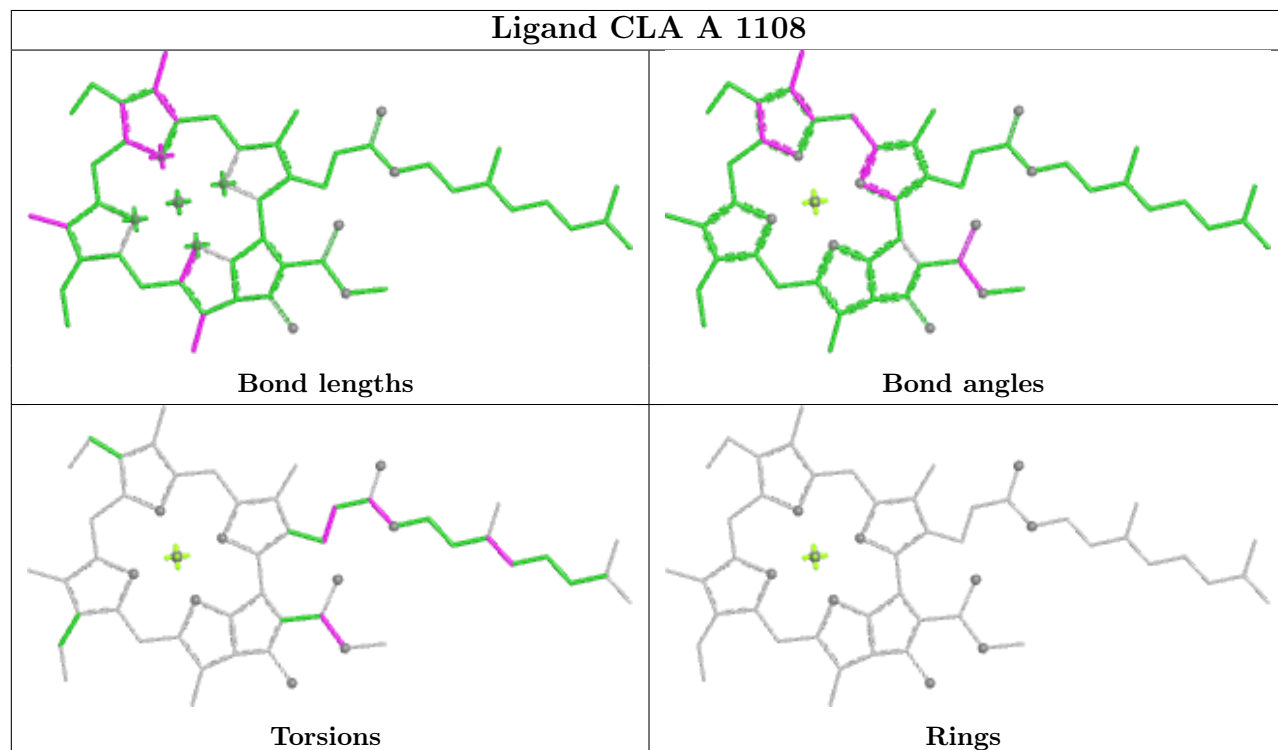


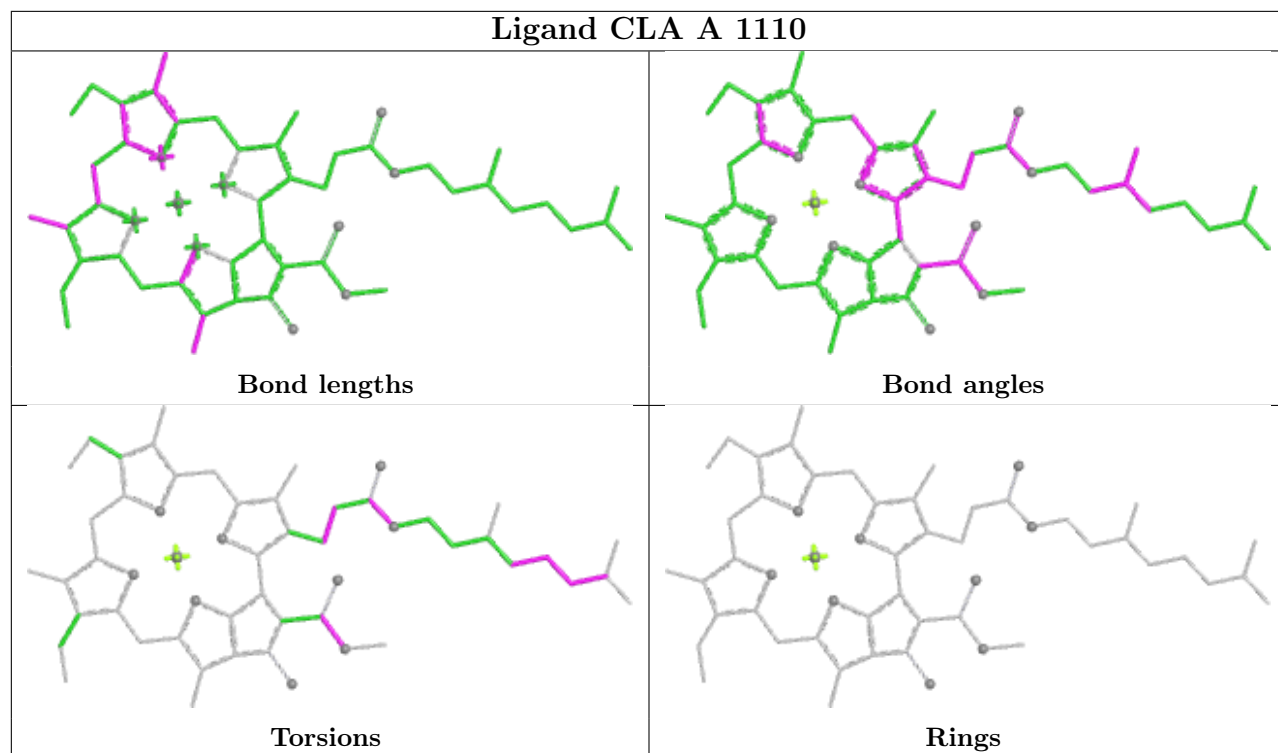
Ligand CLA 2 602



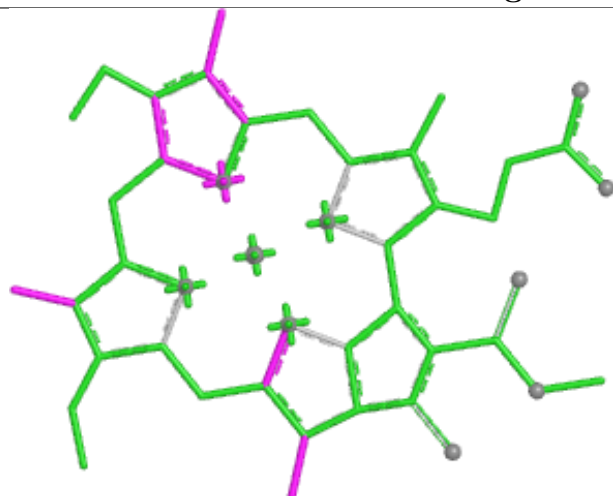




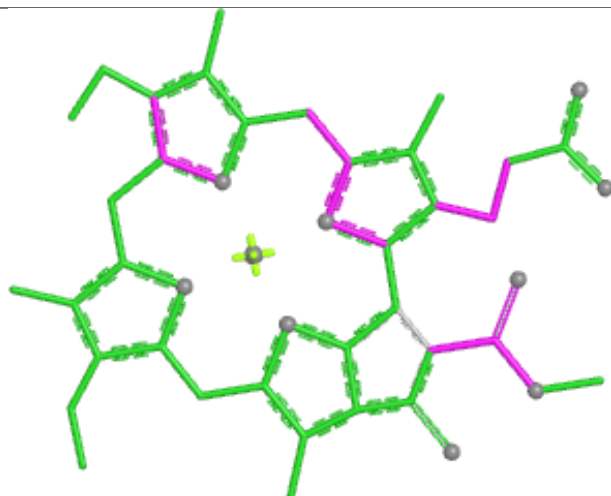
Ligand CHL 4 613**Ligand CLA A 1108**



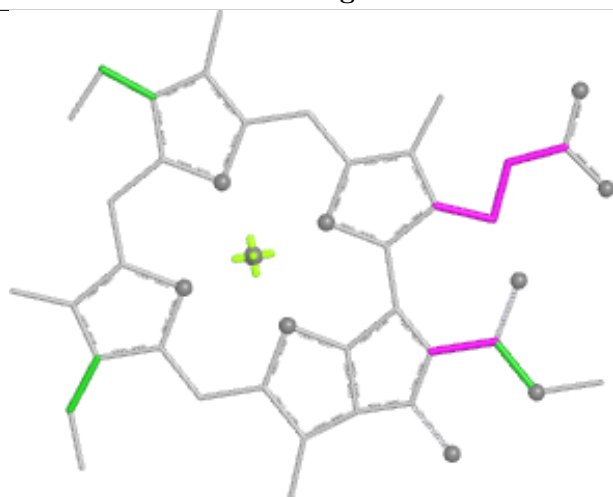
Ligand CLA A 1130



Bond lengths



Bond angles

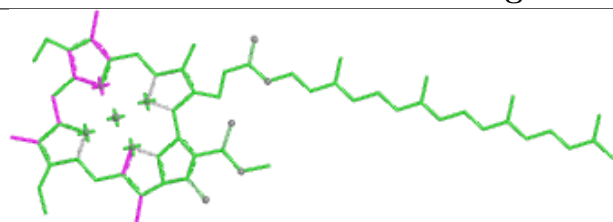


Torsions

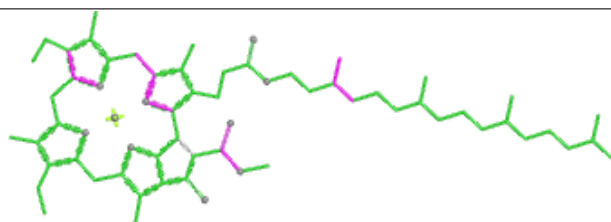


Rings

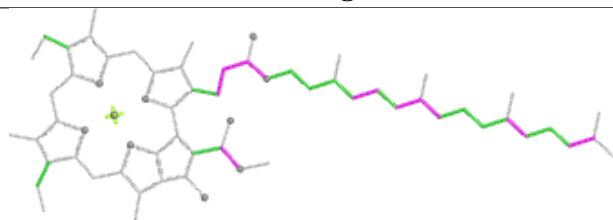
Ligand CLA B 1023



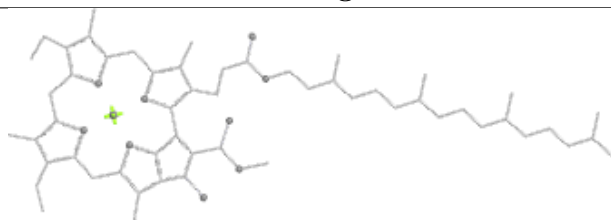
Bond lengths



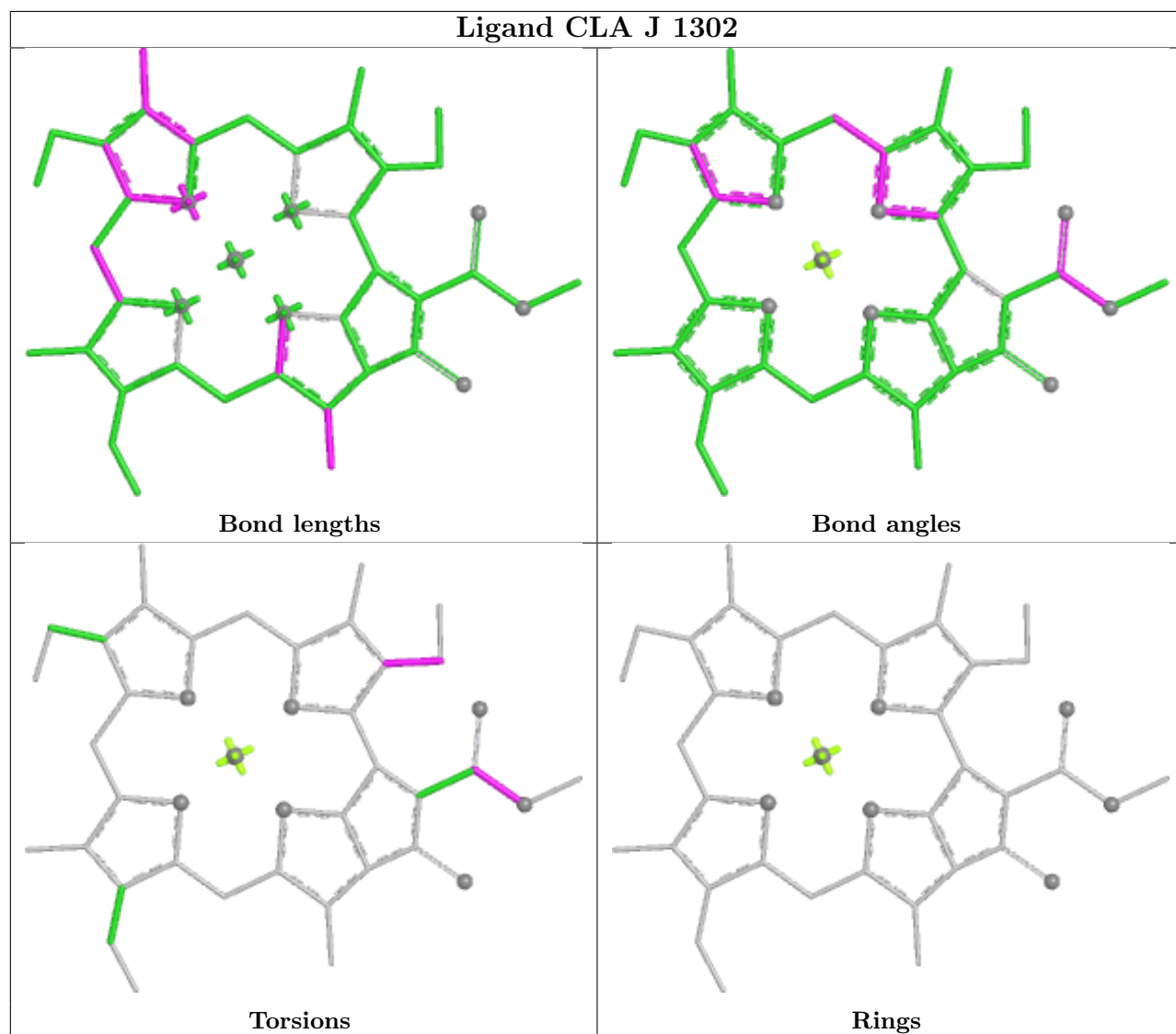
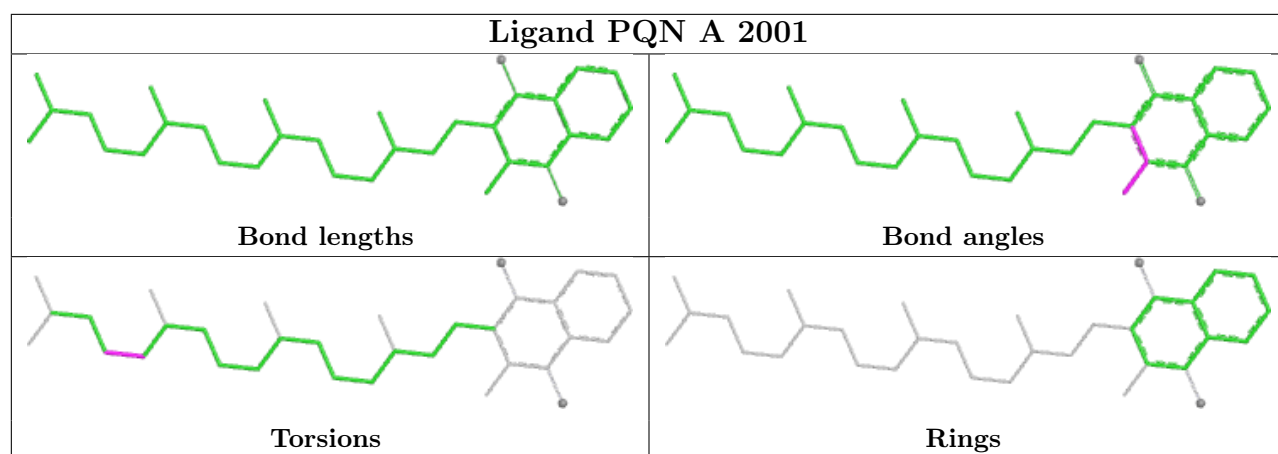
Bond angles



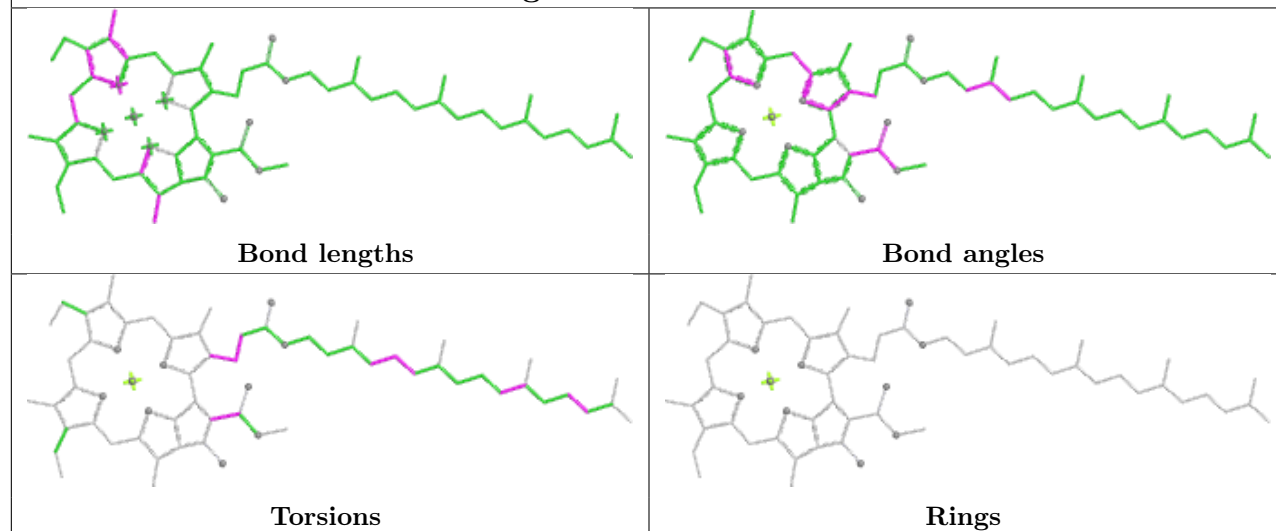
Torsions



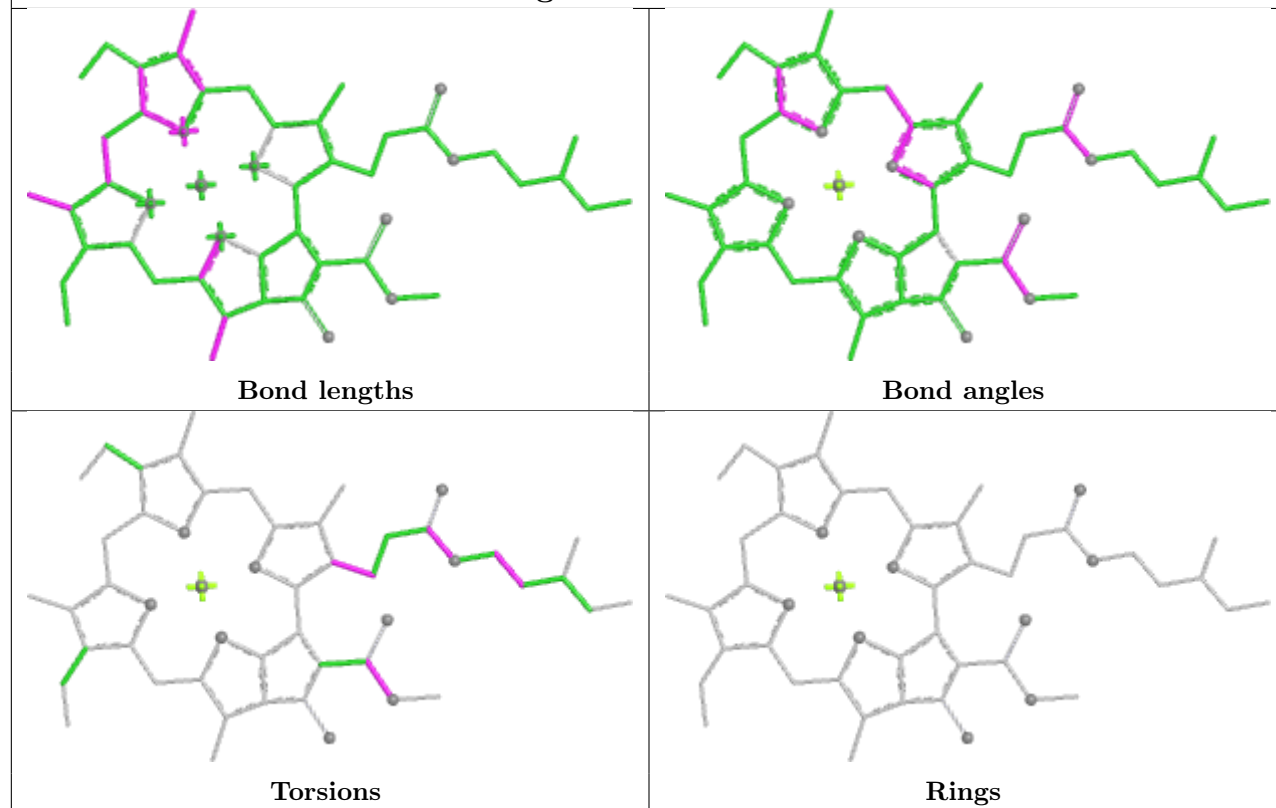
Rings

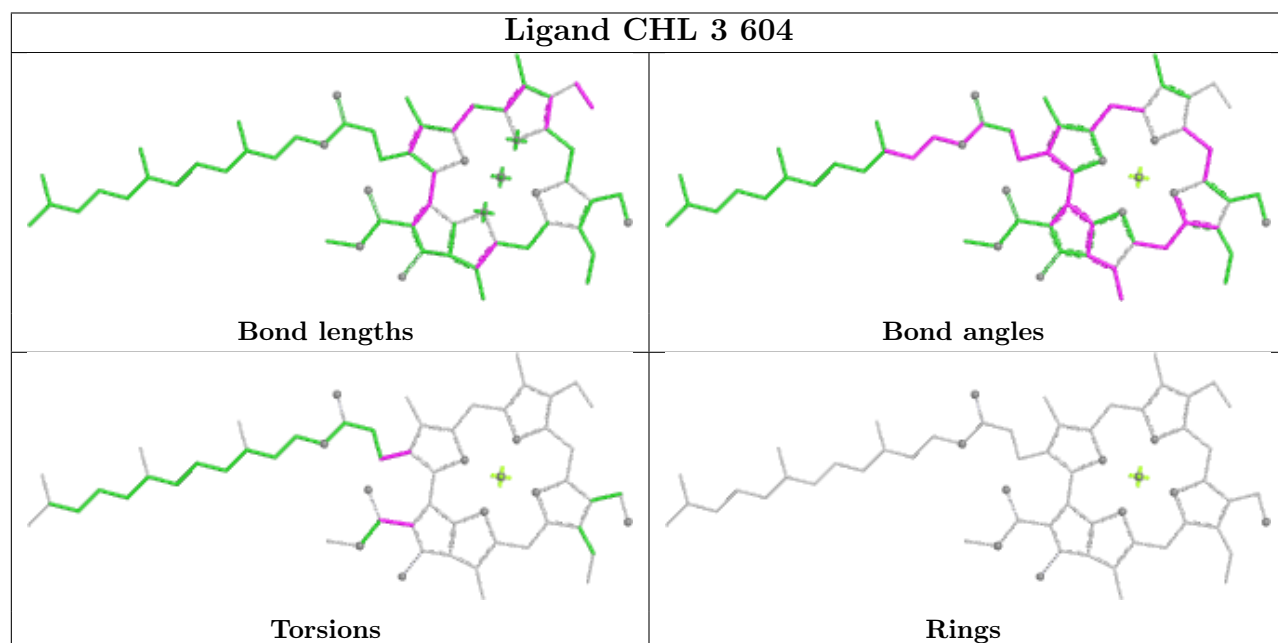
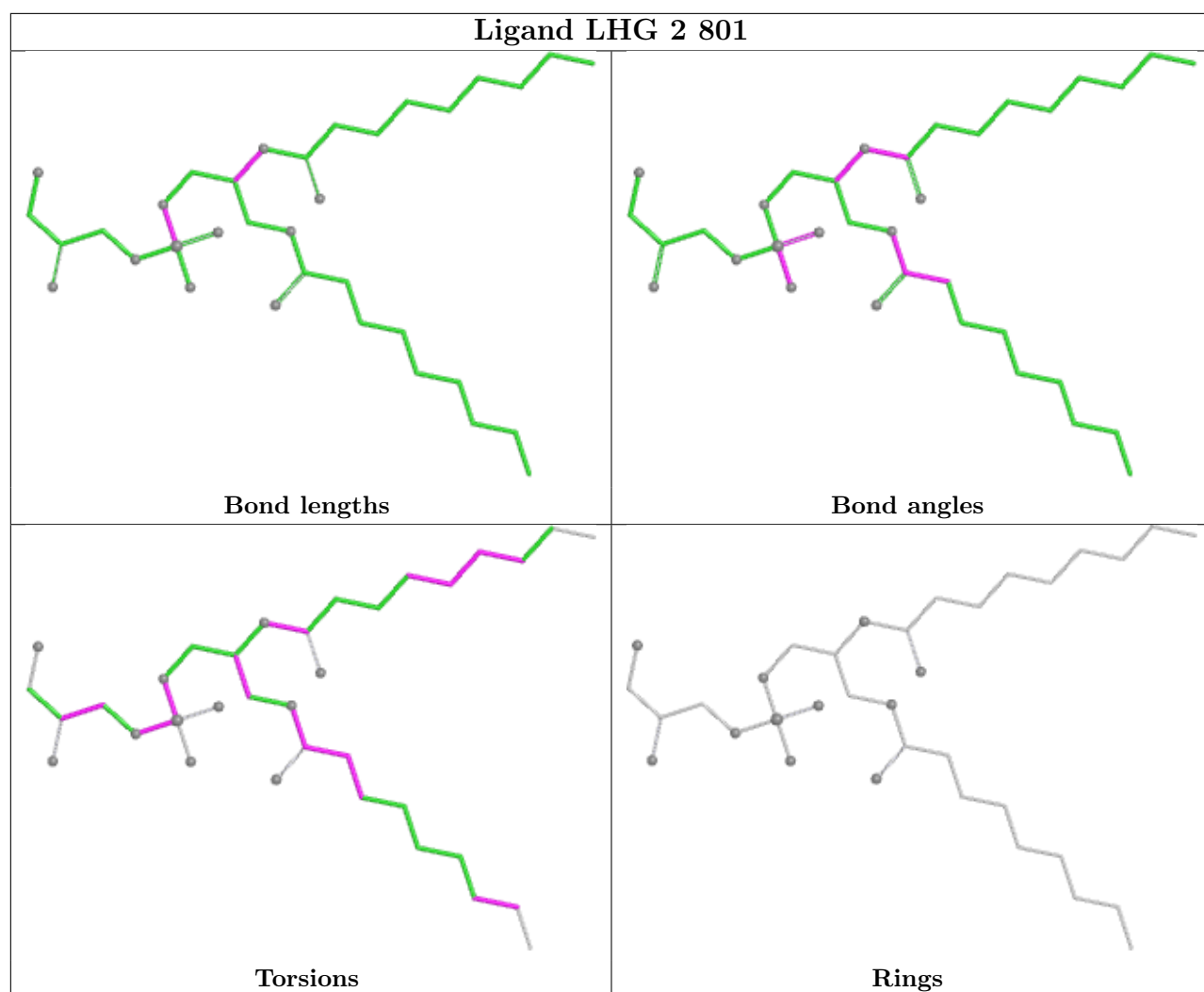


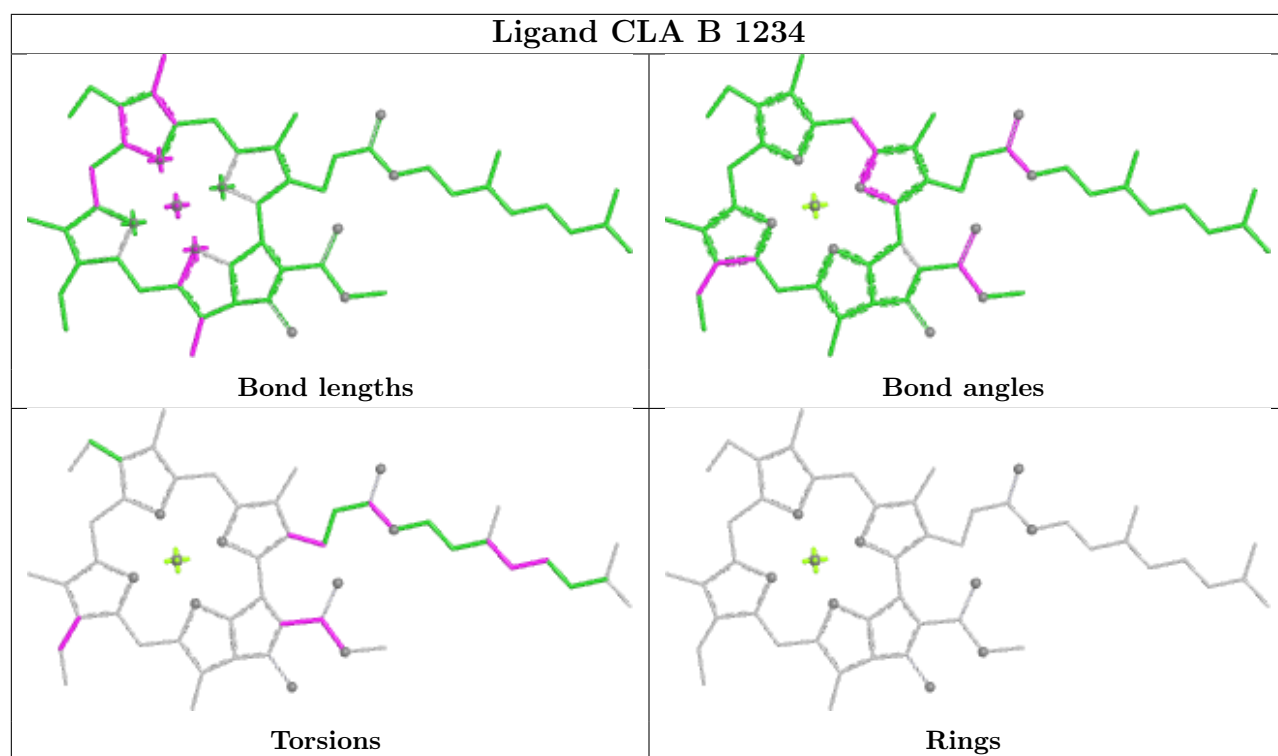
Ligand CLA A 1106



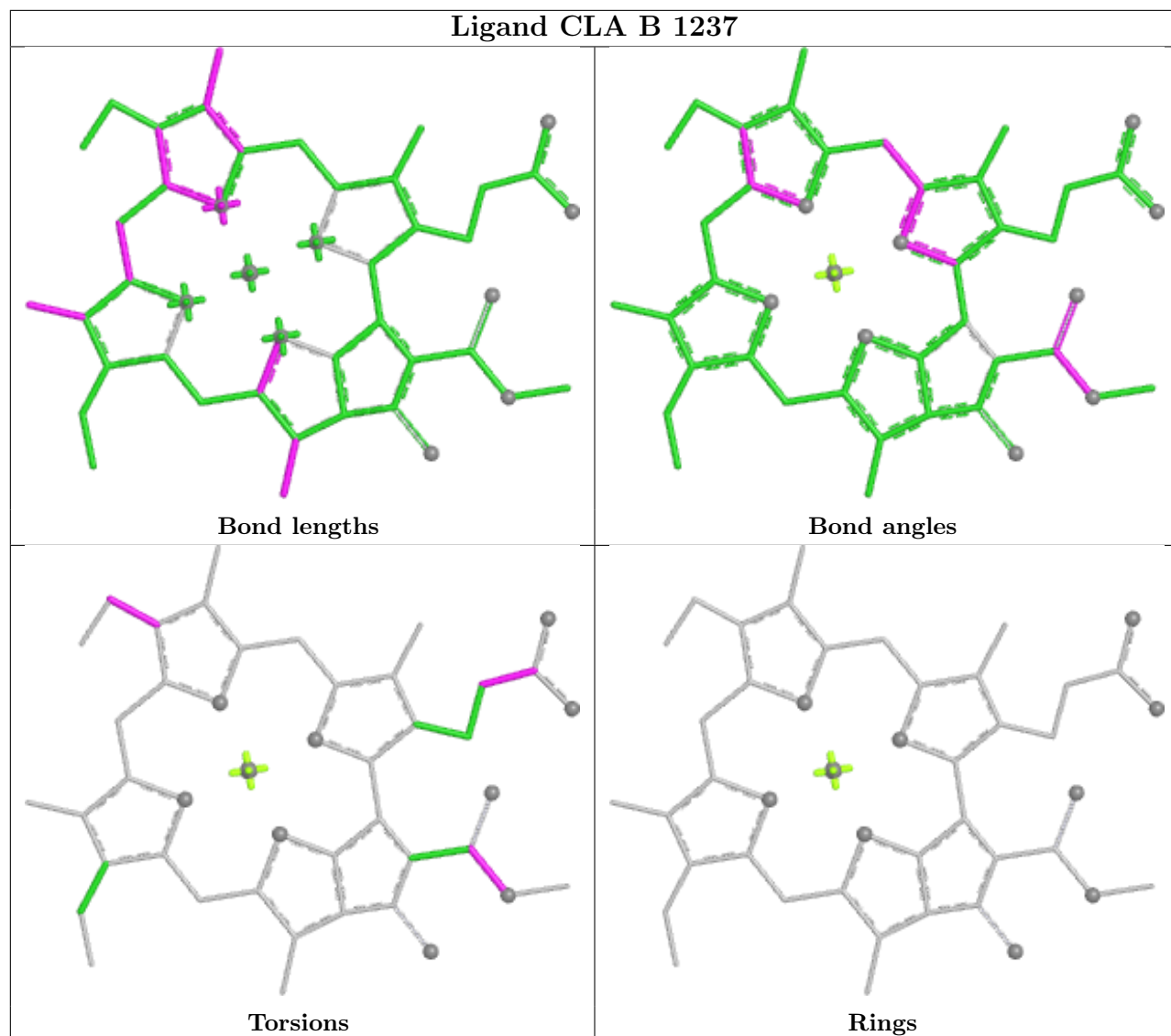
Ligand CLA 4 616



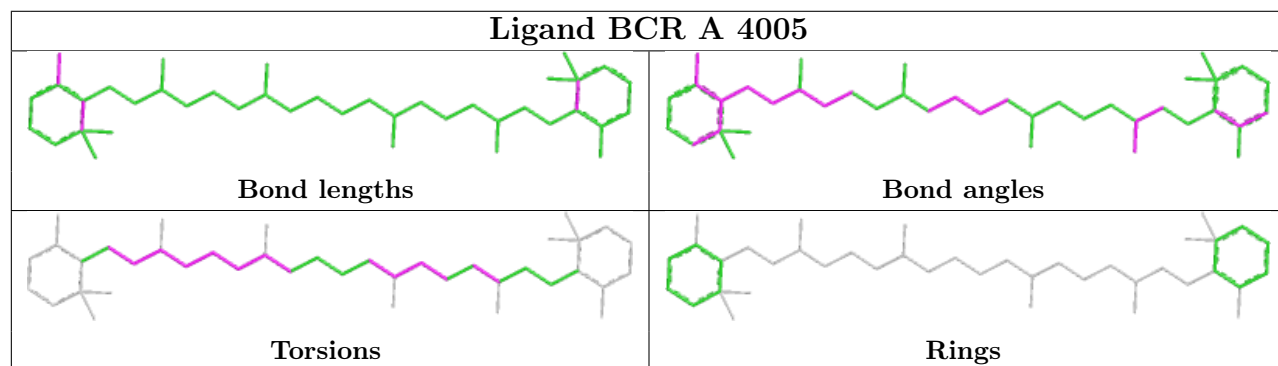


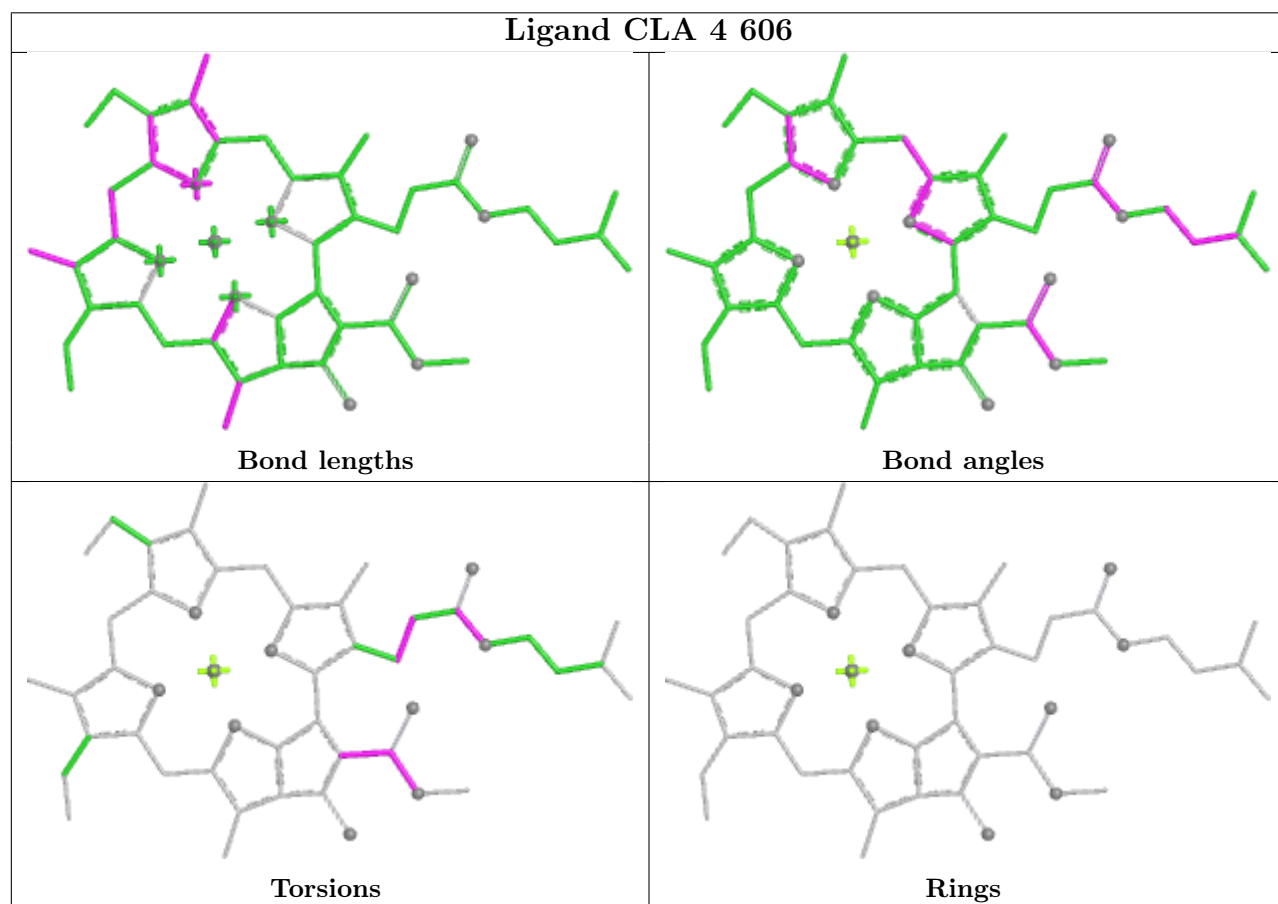
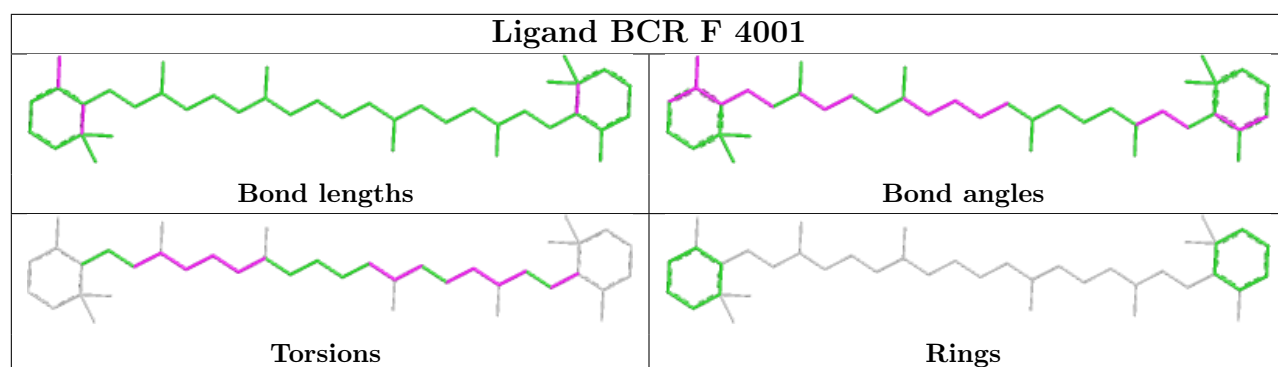


Ligand CLA B 1237

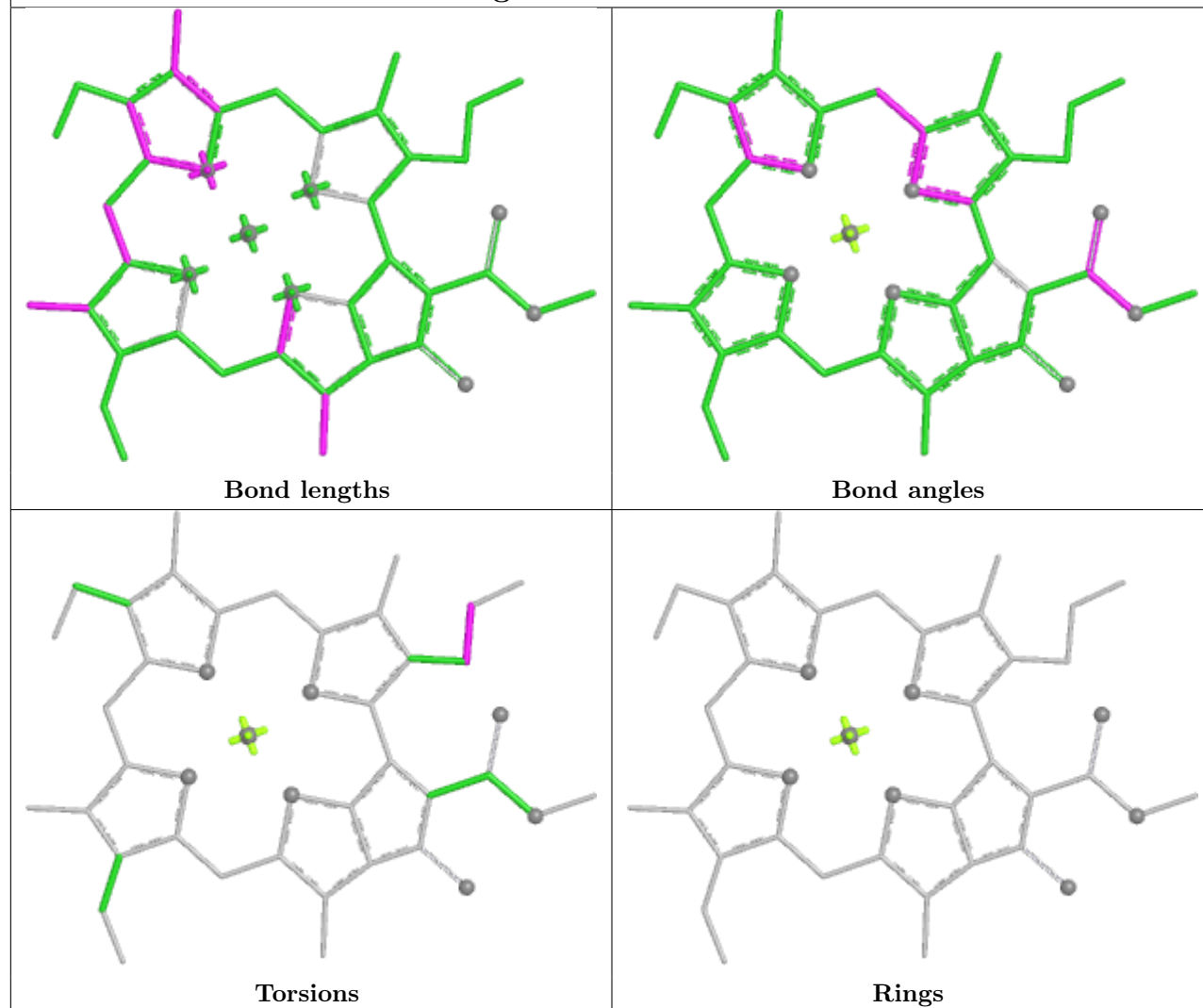


Ligand BCR A 4005

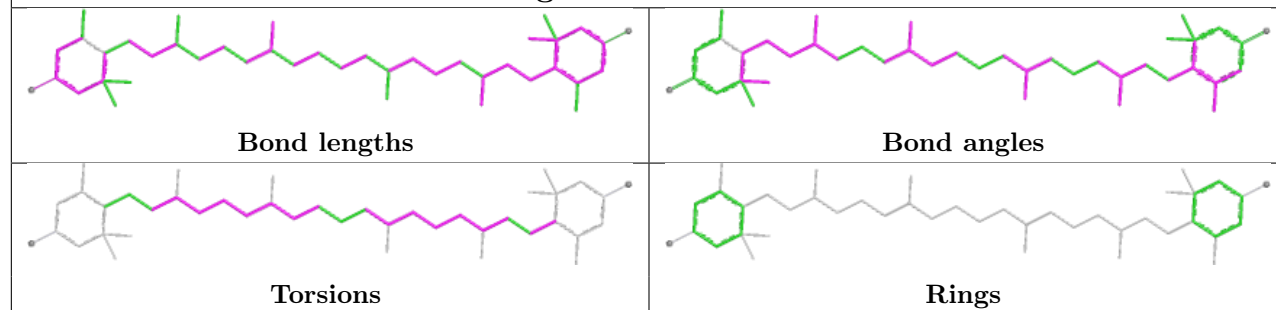




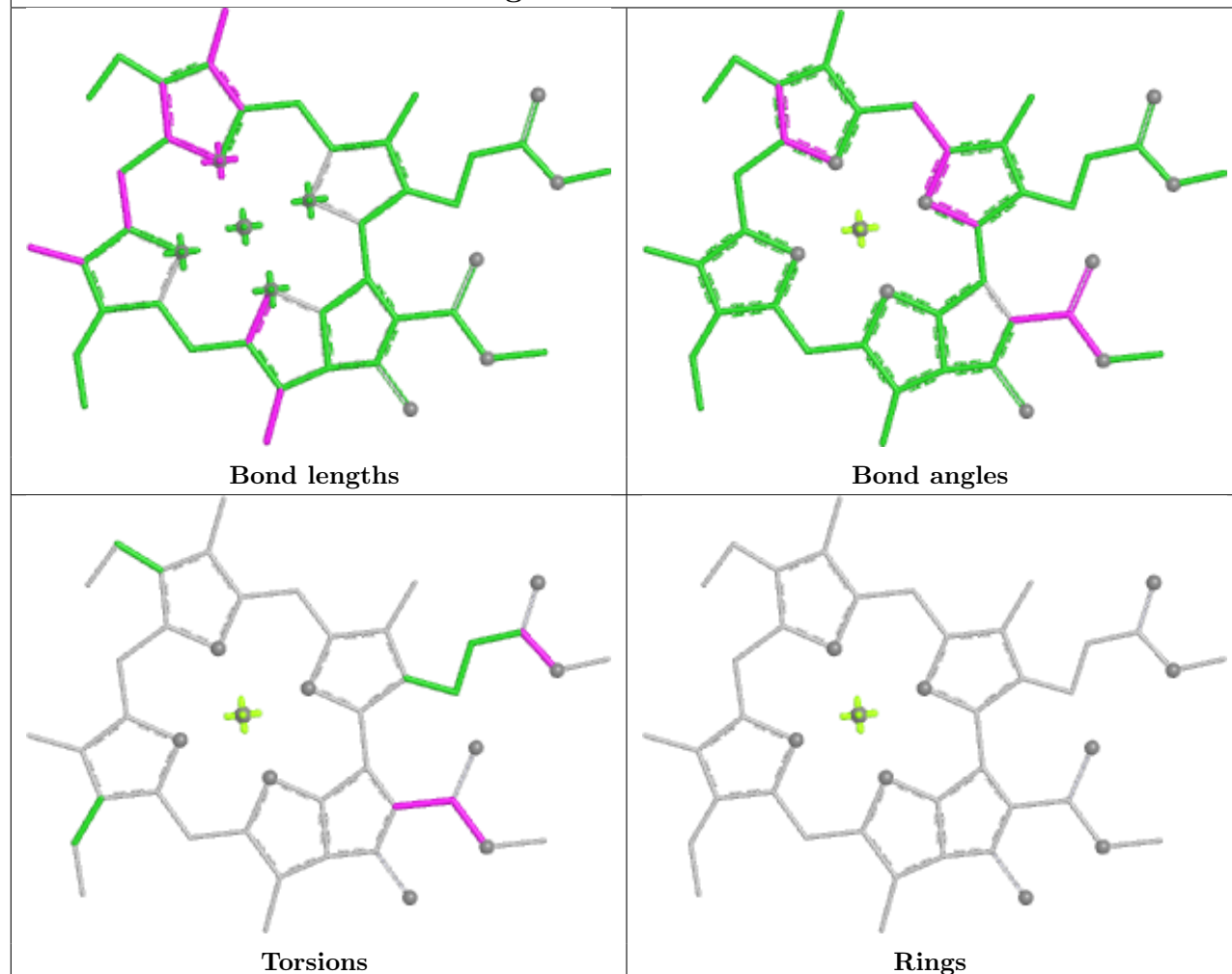
Ligand CLA B 1201



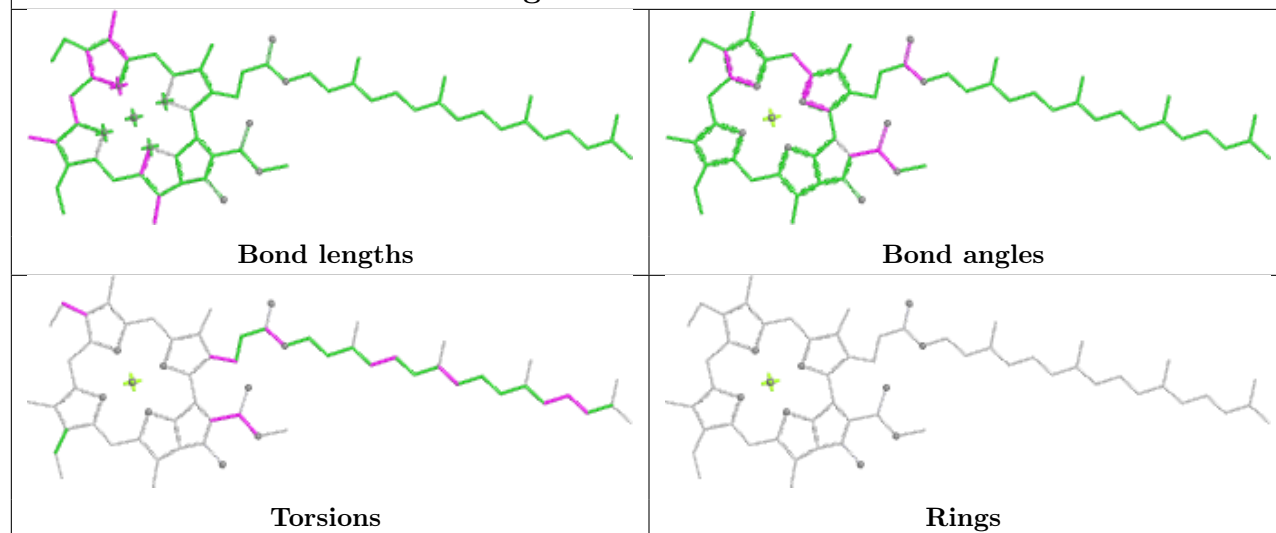
Ligand LUT 1 501

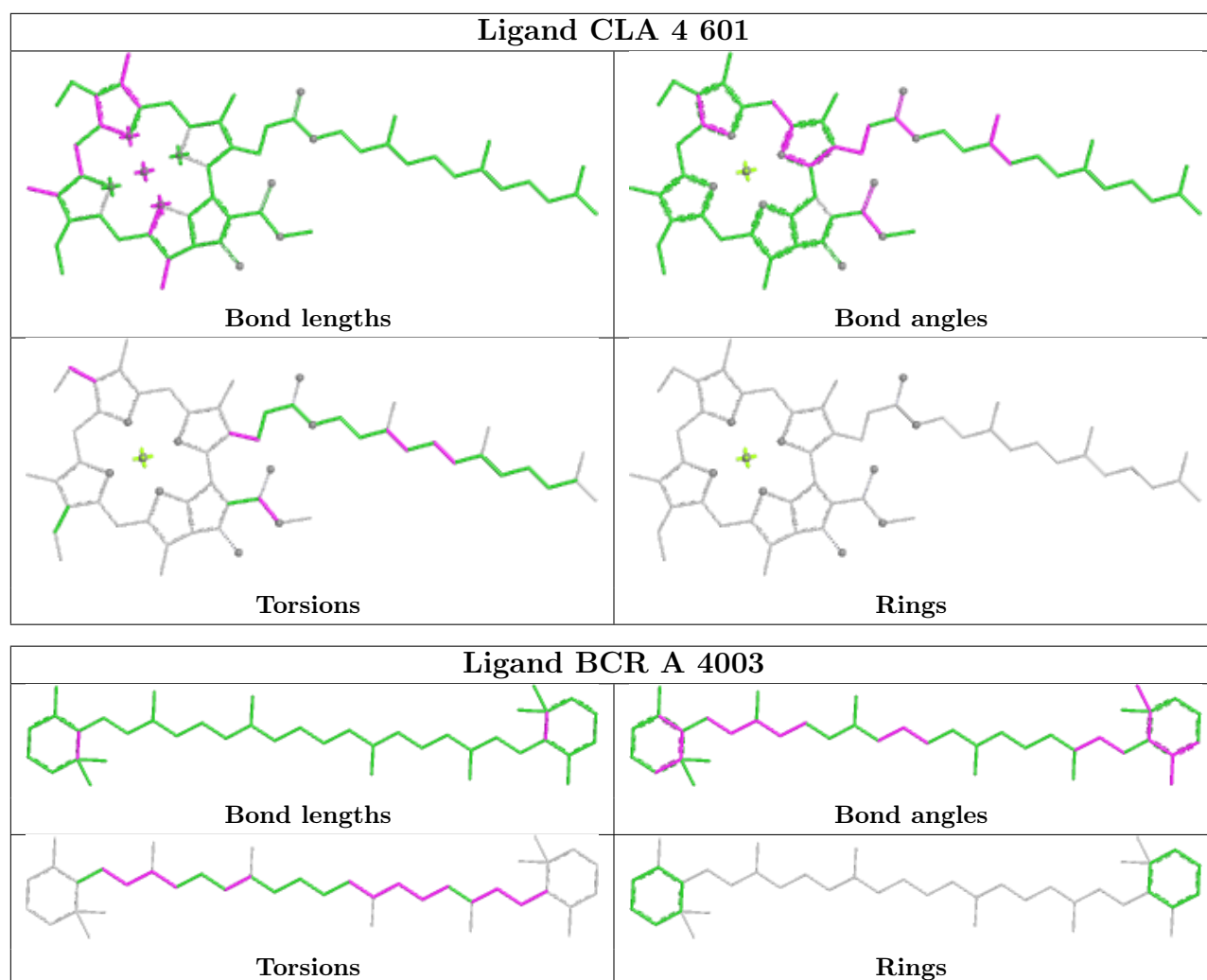


Ligand CLA B 1232

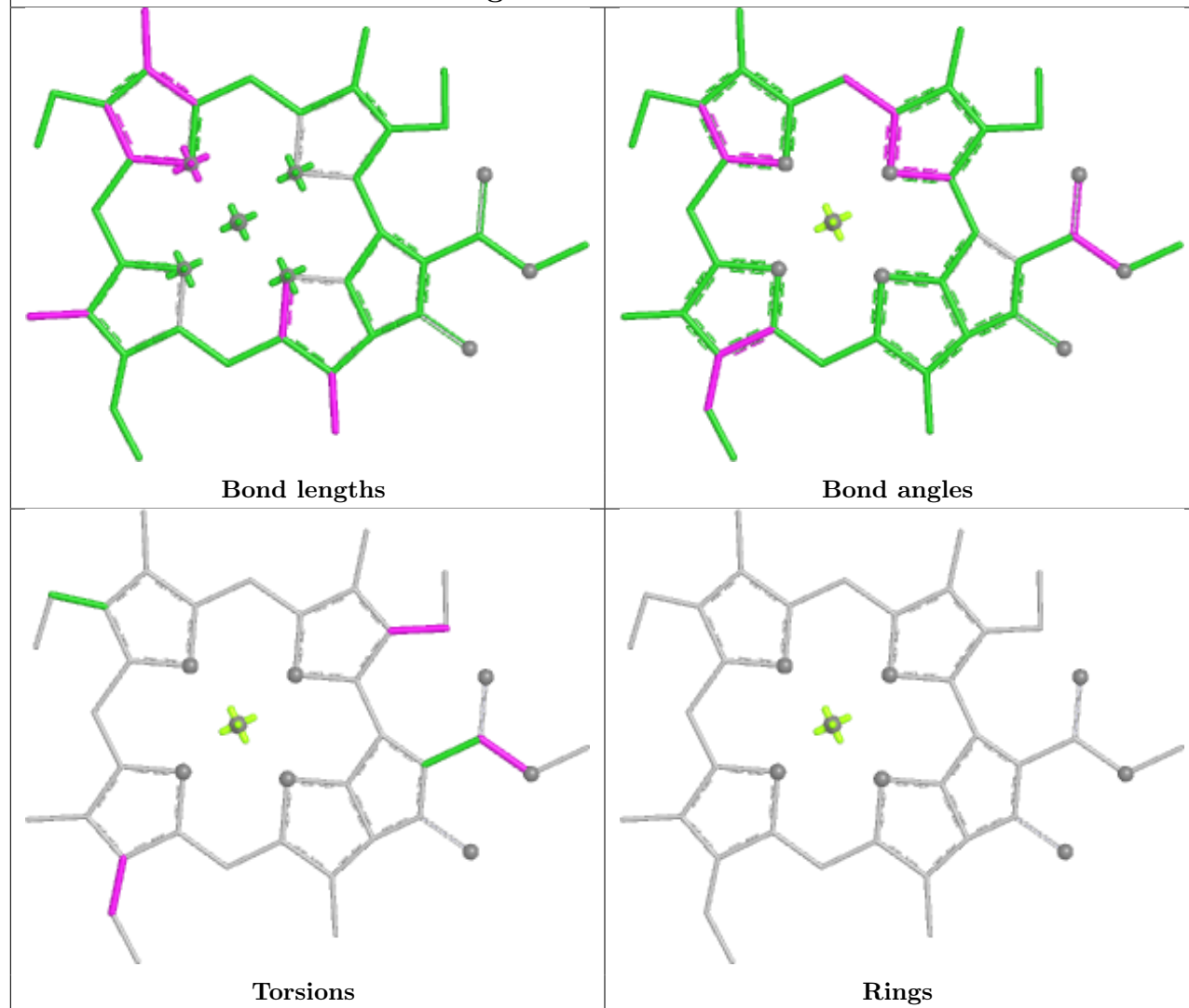


Ligand CLA B 1202

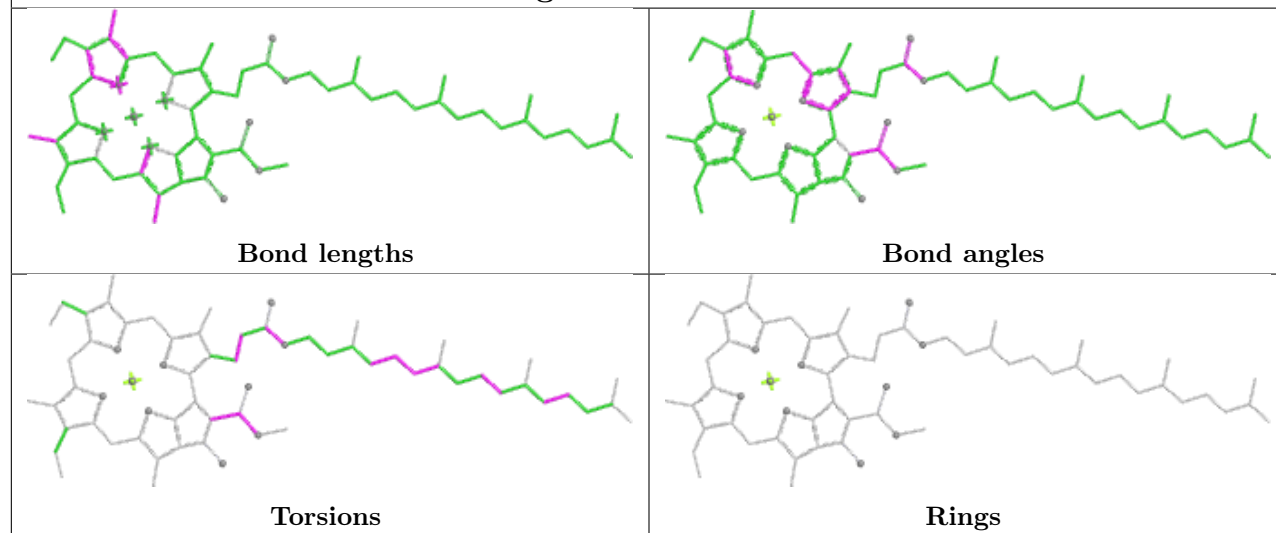


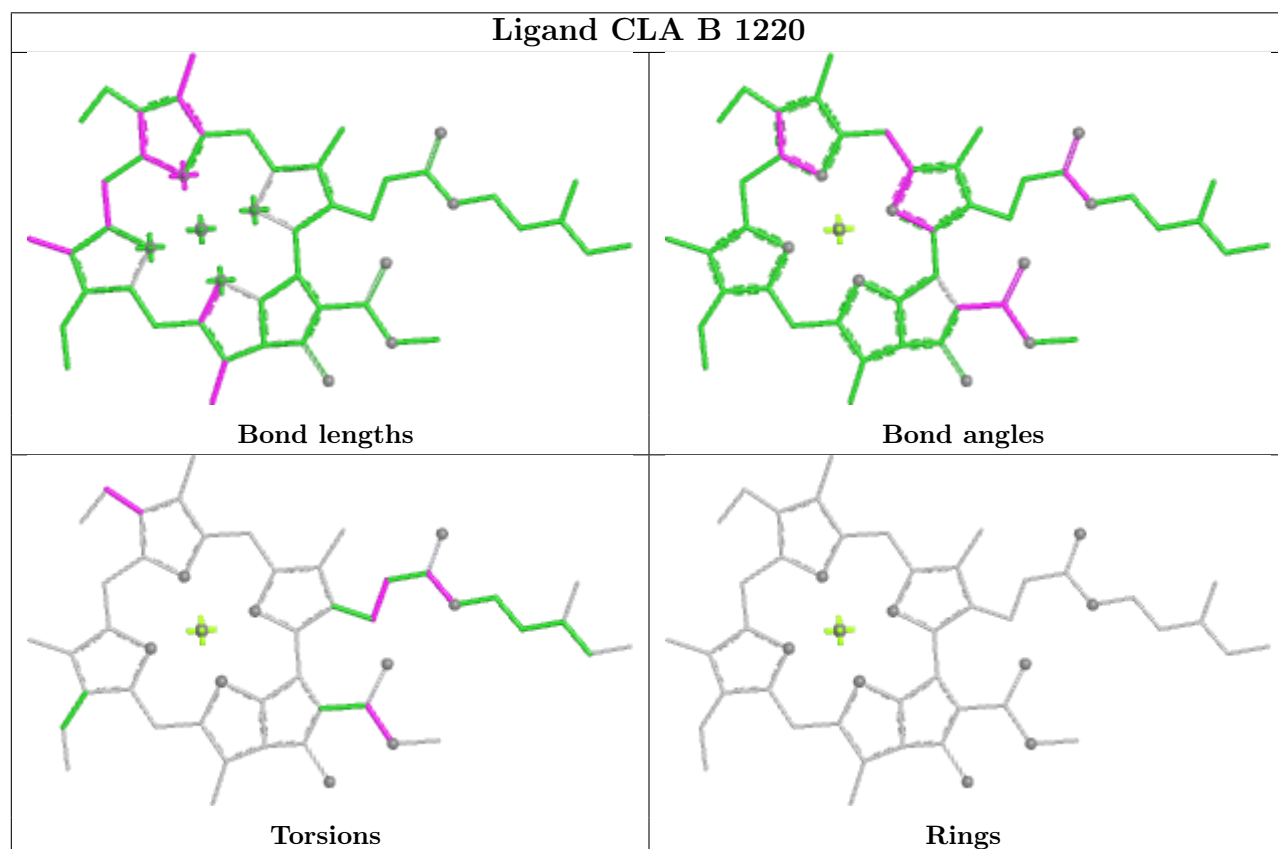
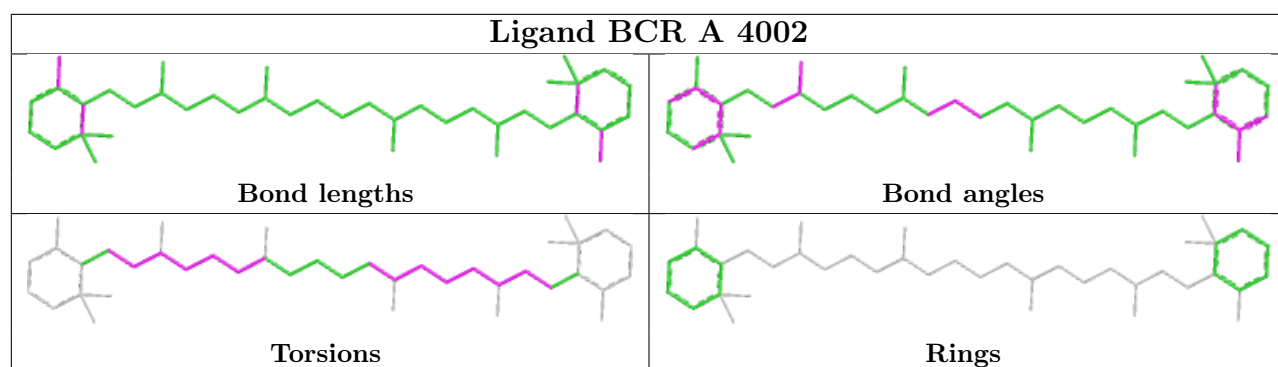


Ligand CLA A 1120

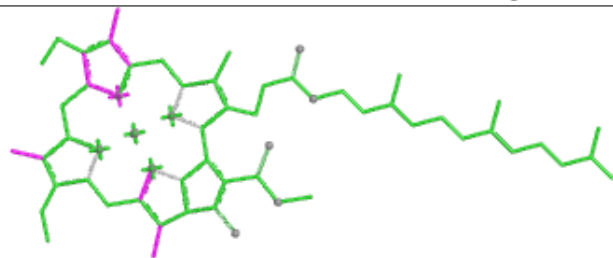


Ligand CLA 4 603

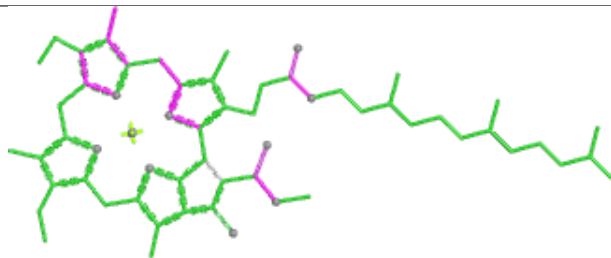




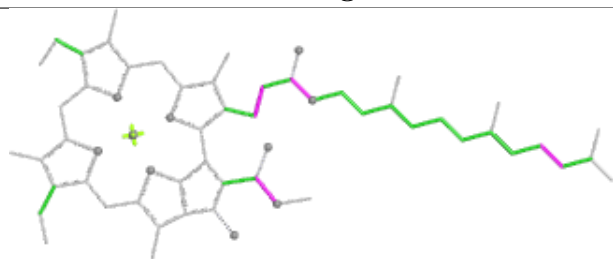
Ligand CLA B 1228



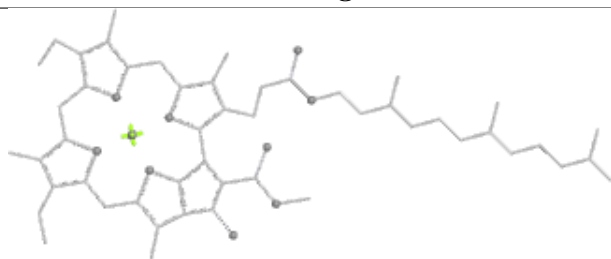
Bond lengths



Bond angles

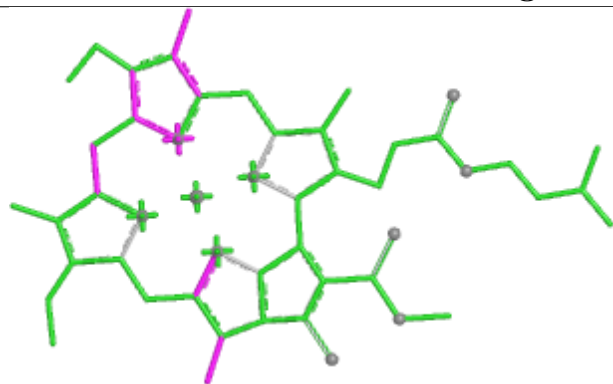


Torsions

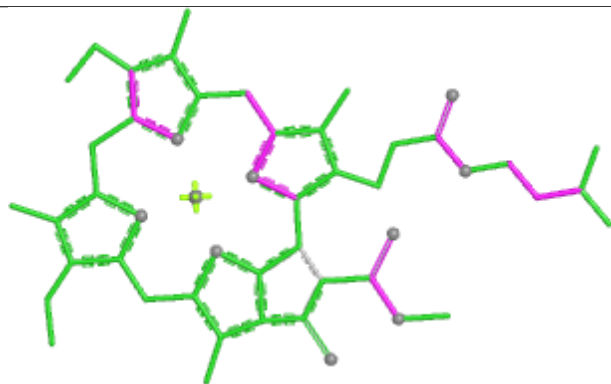


Rings

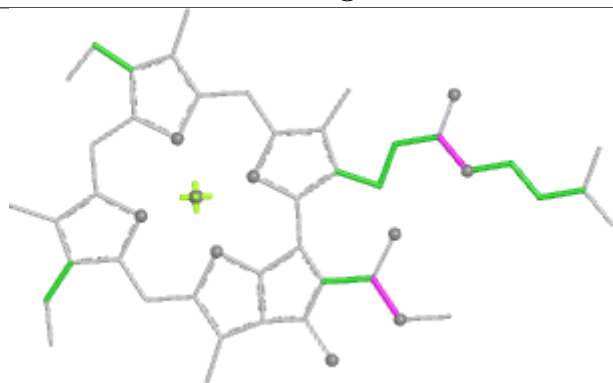
Ligand CLA 1 606



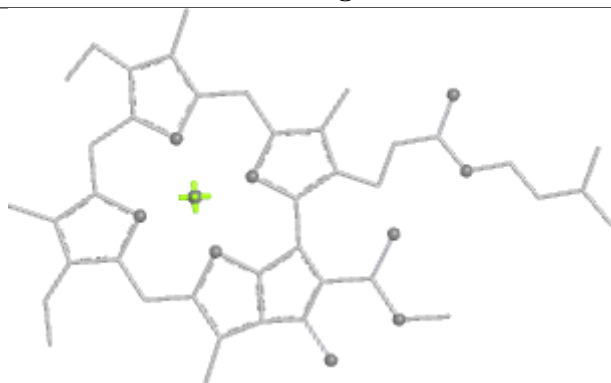
Bond lengths



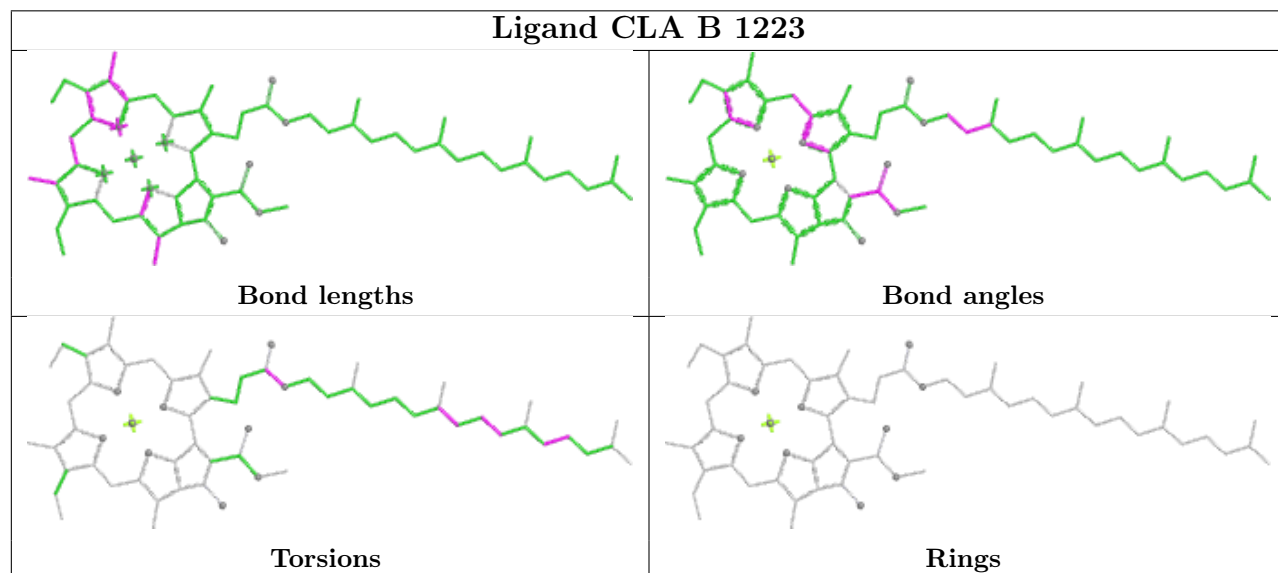
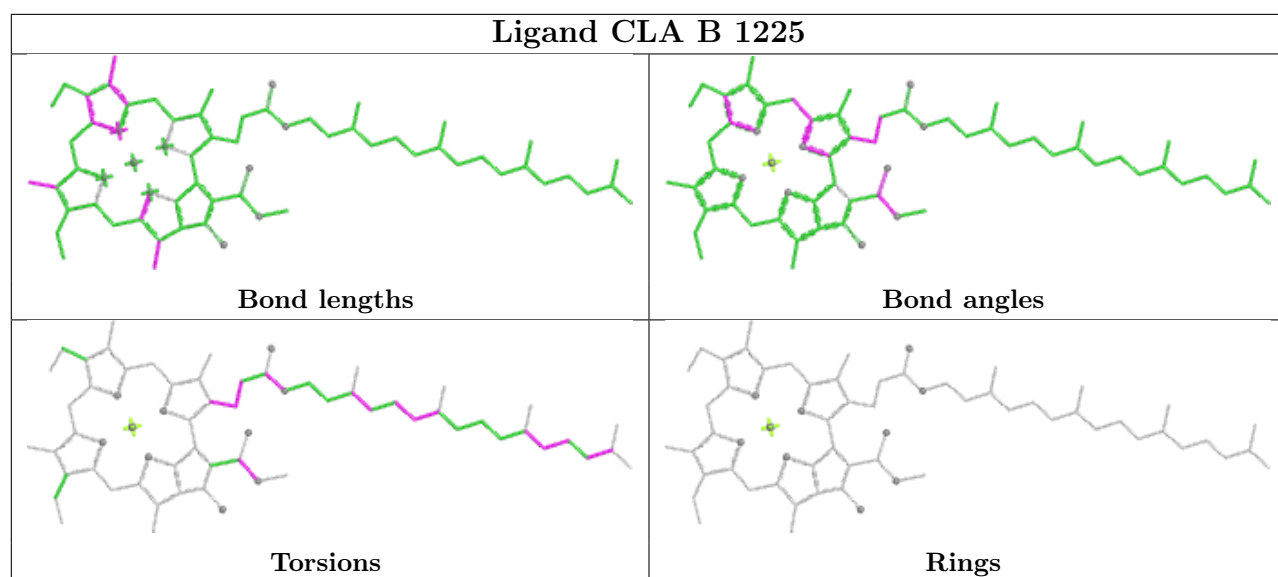
Bond angles

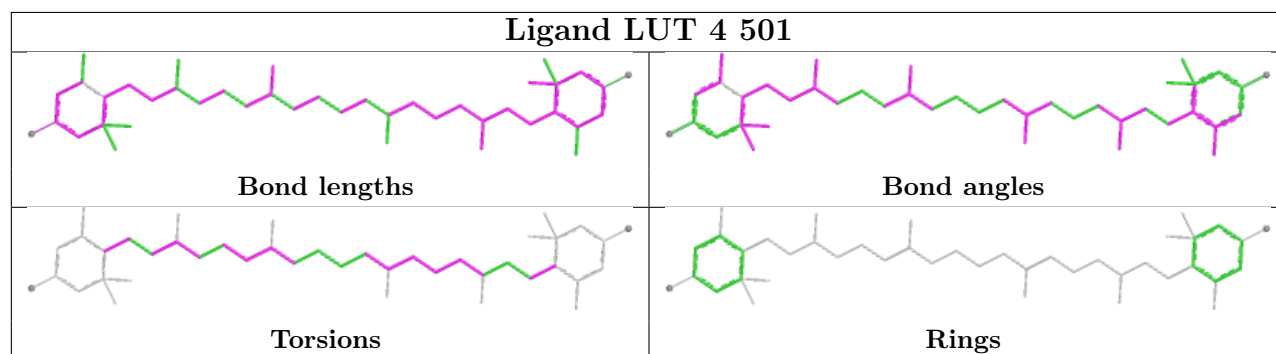
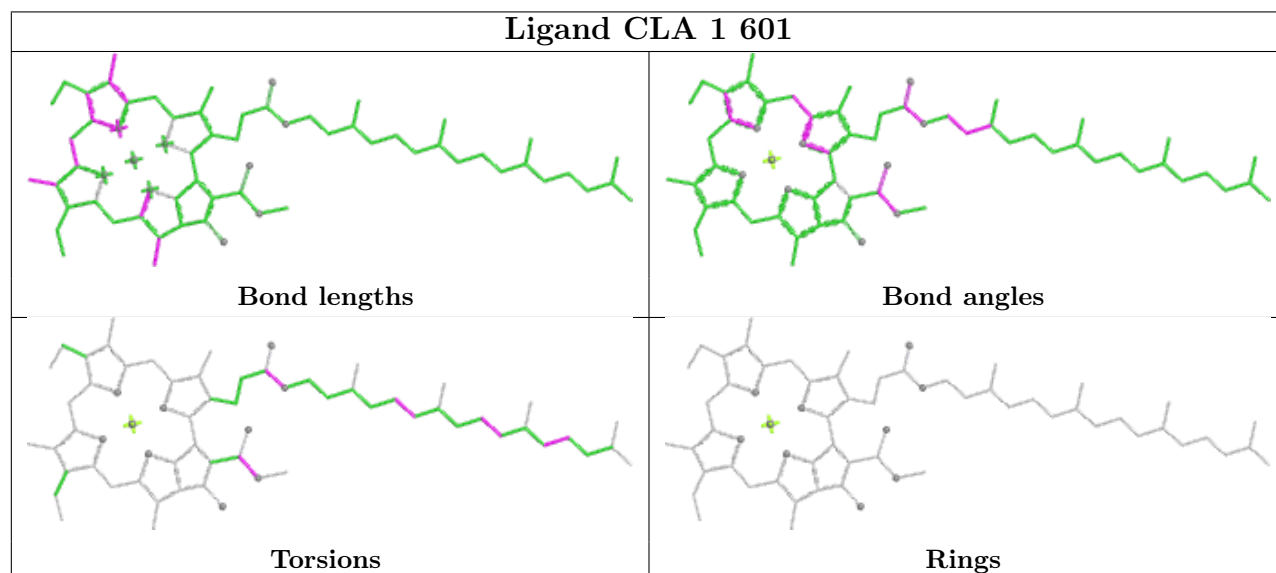
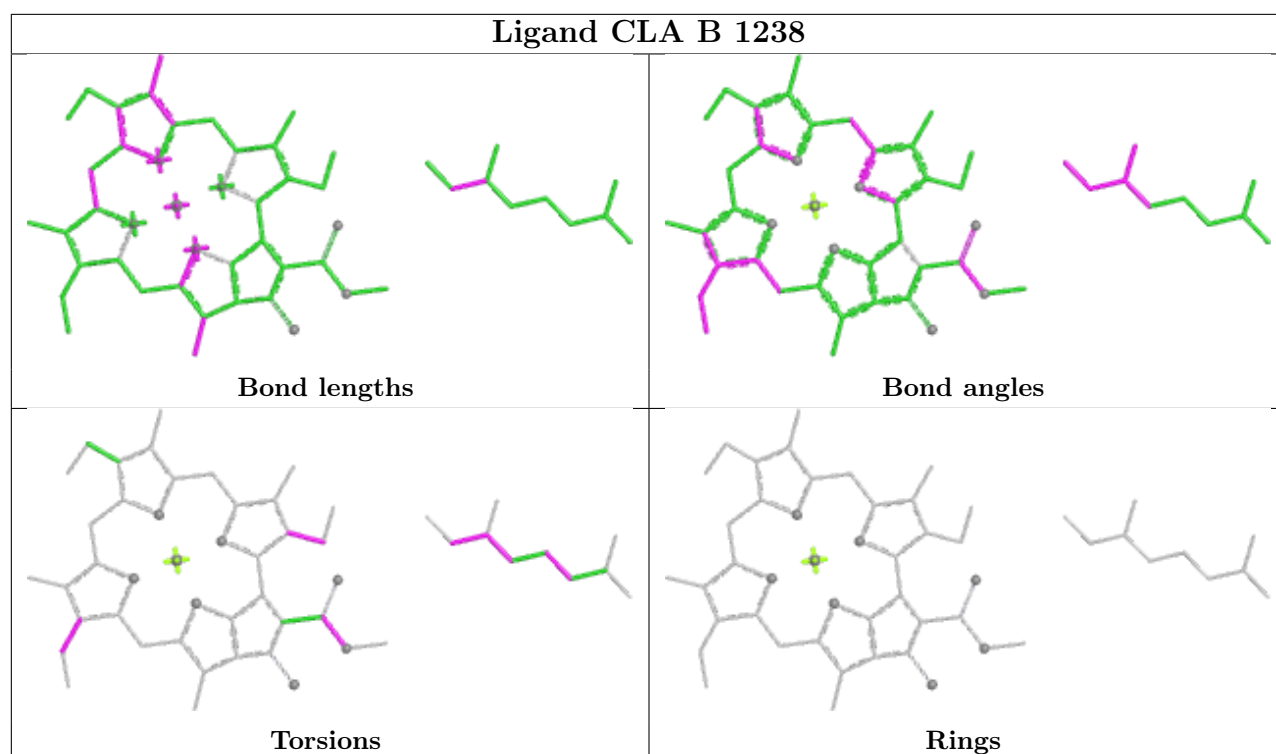


Torsions

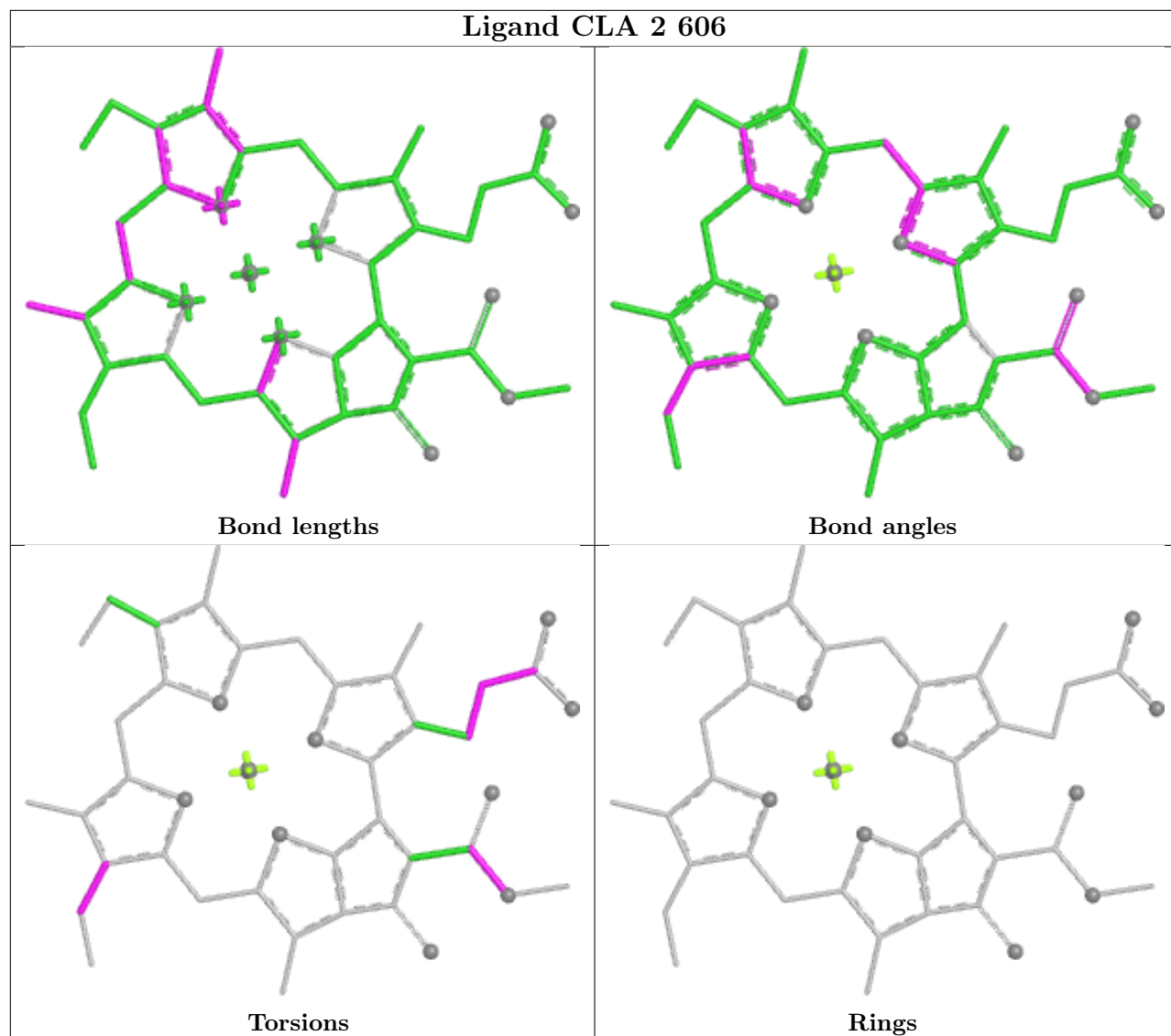


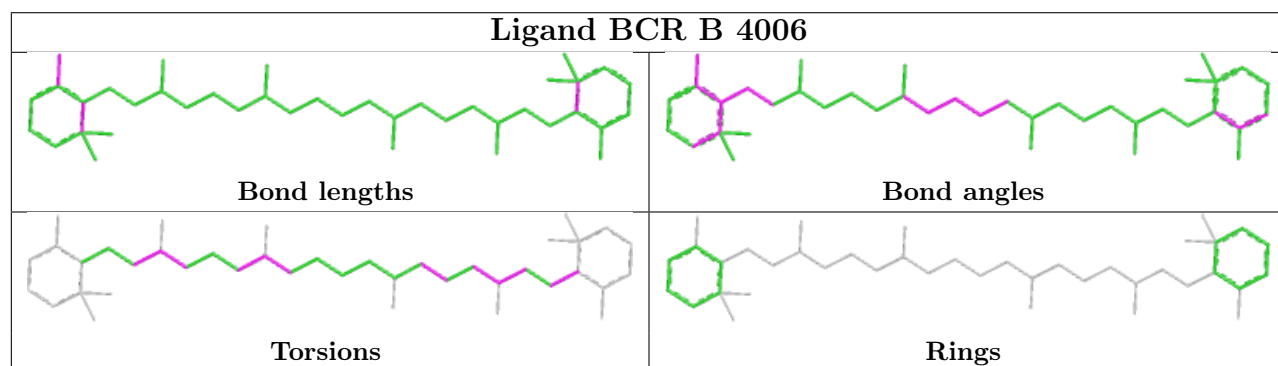
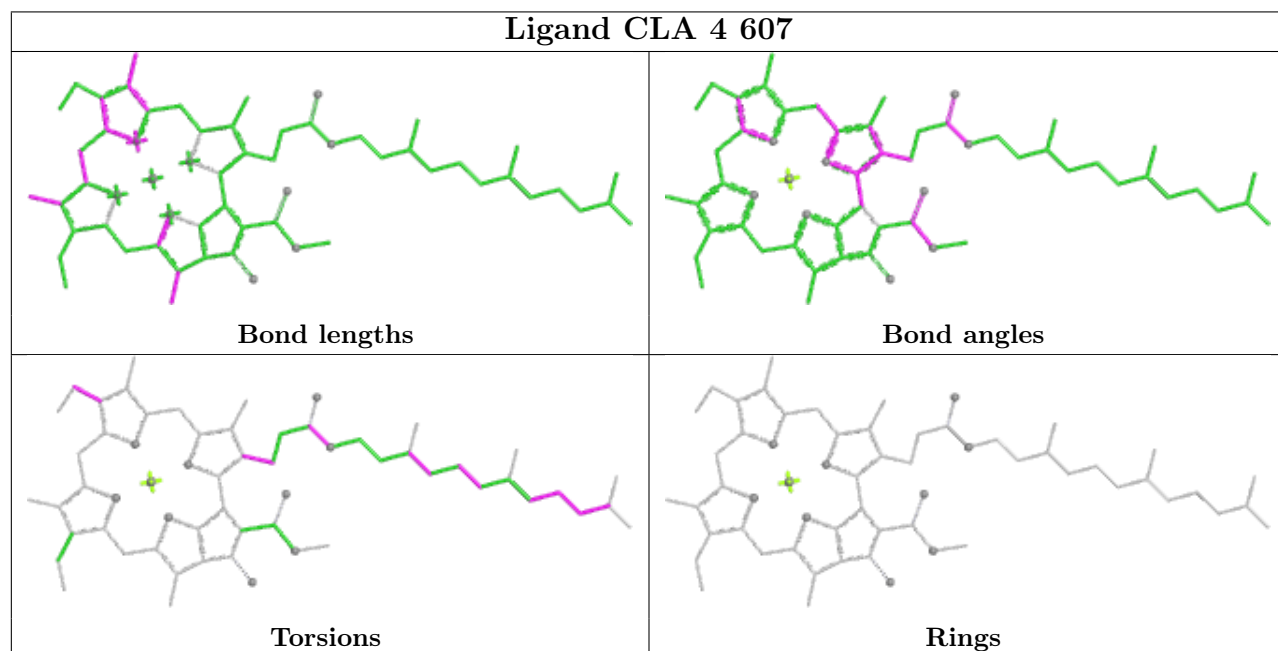
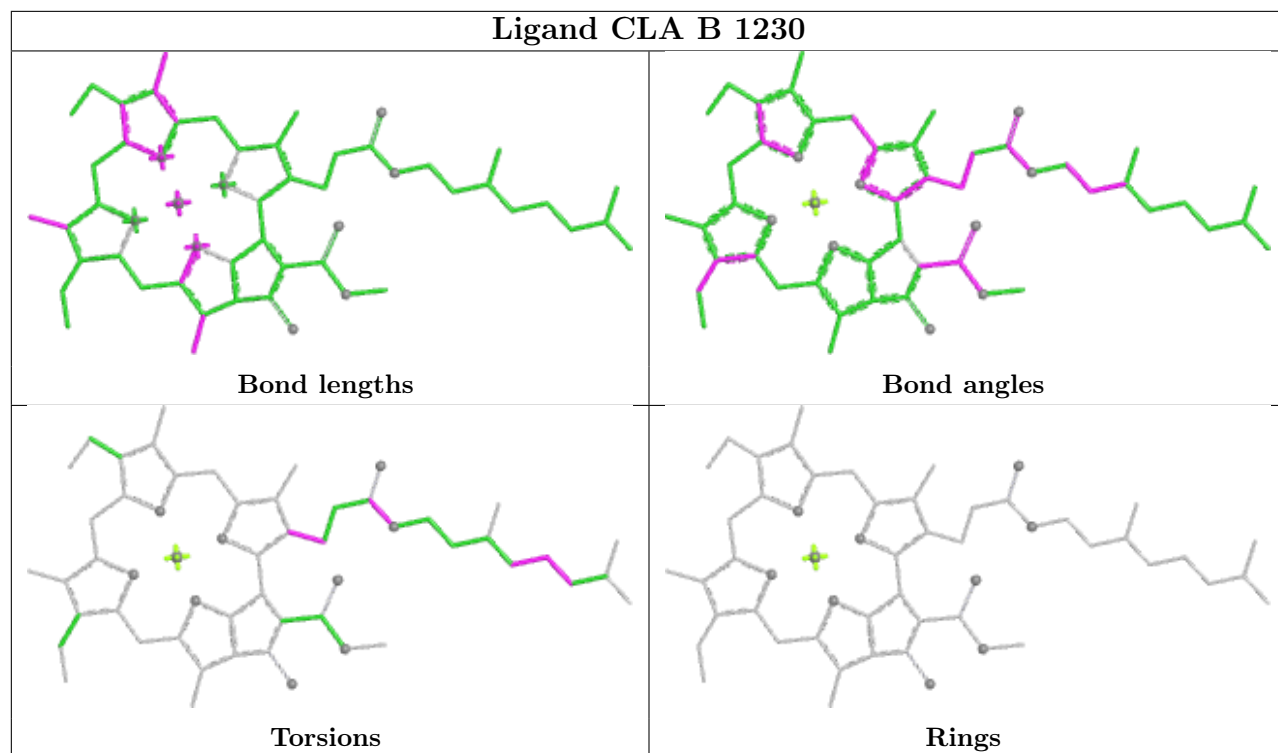
Rings



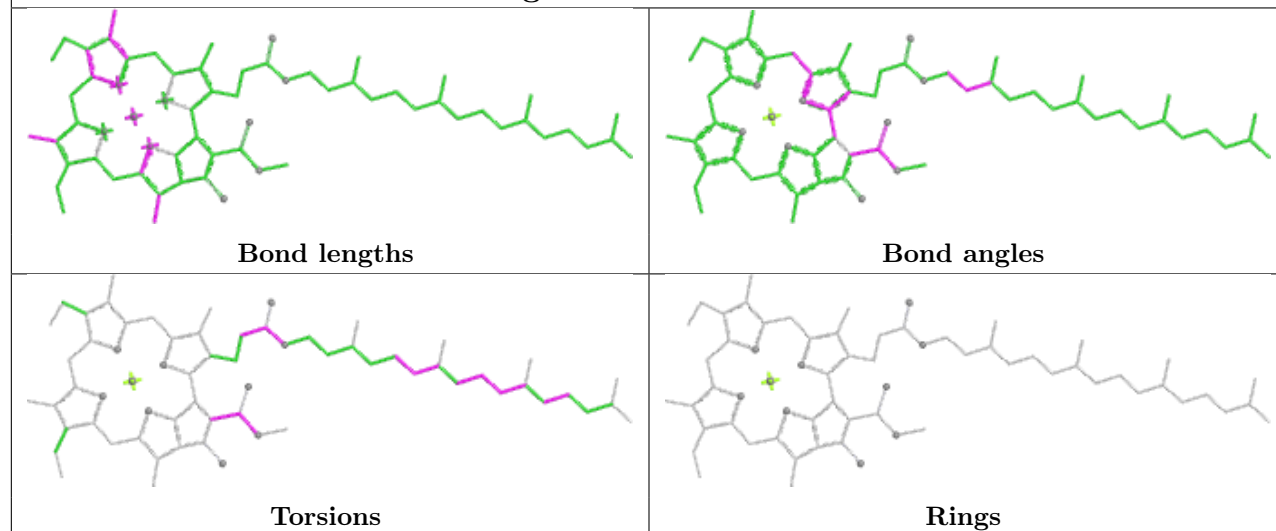


Ligand CLA 2 606

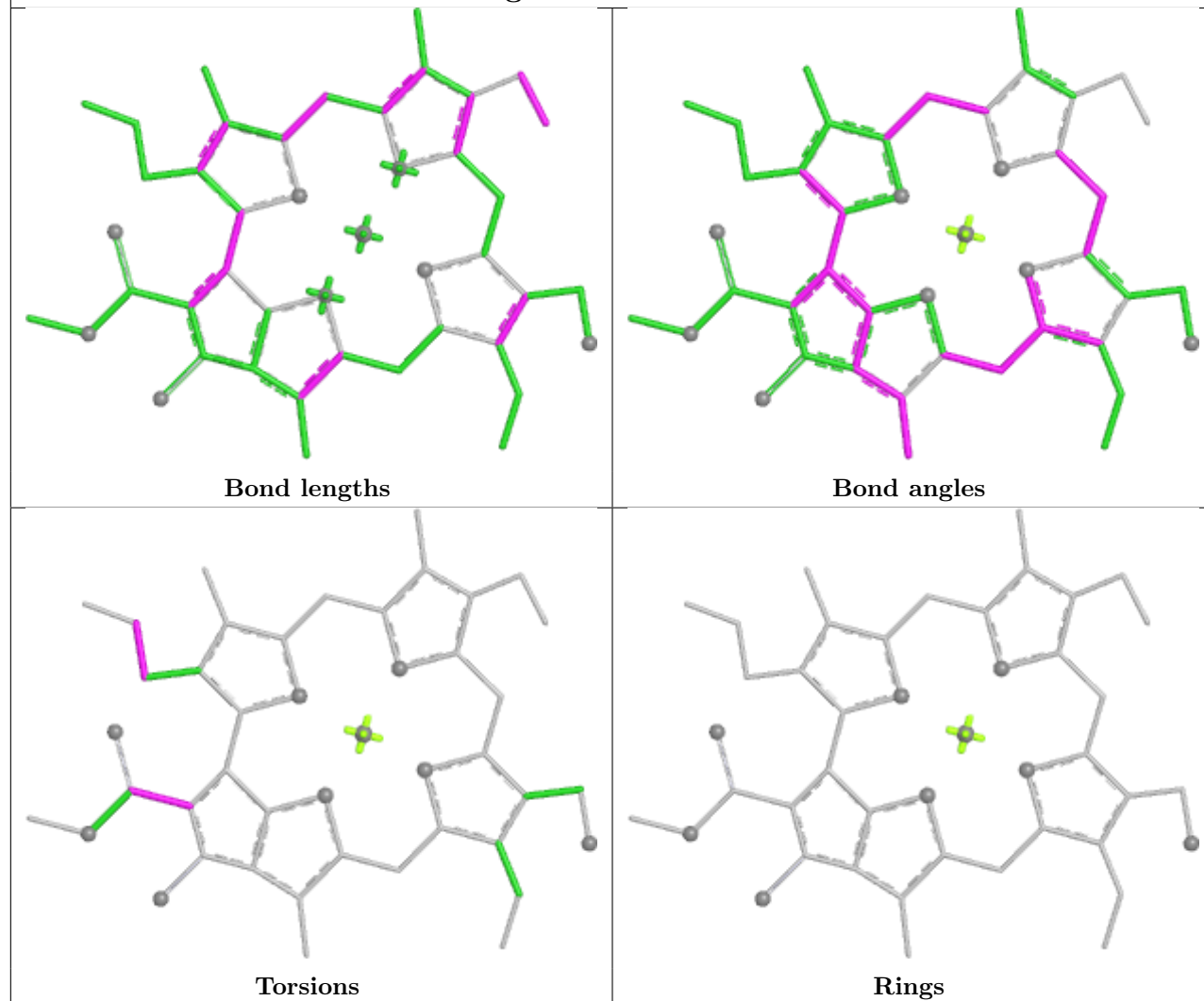




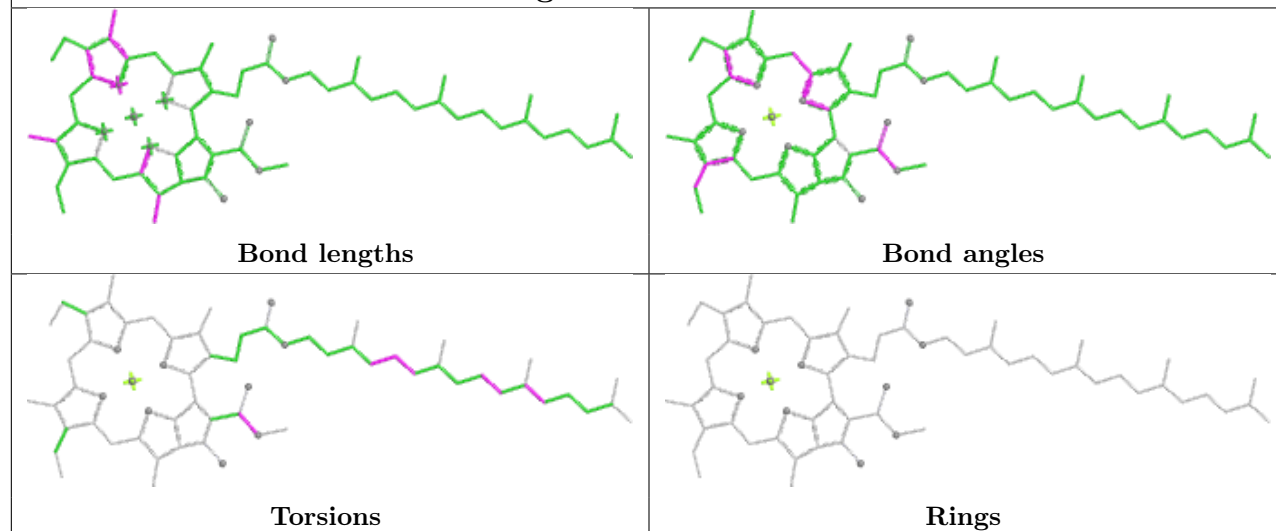
Ligand CLA A 1123



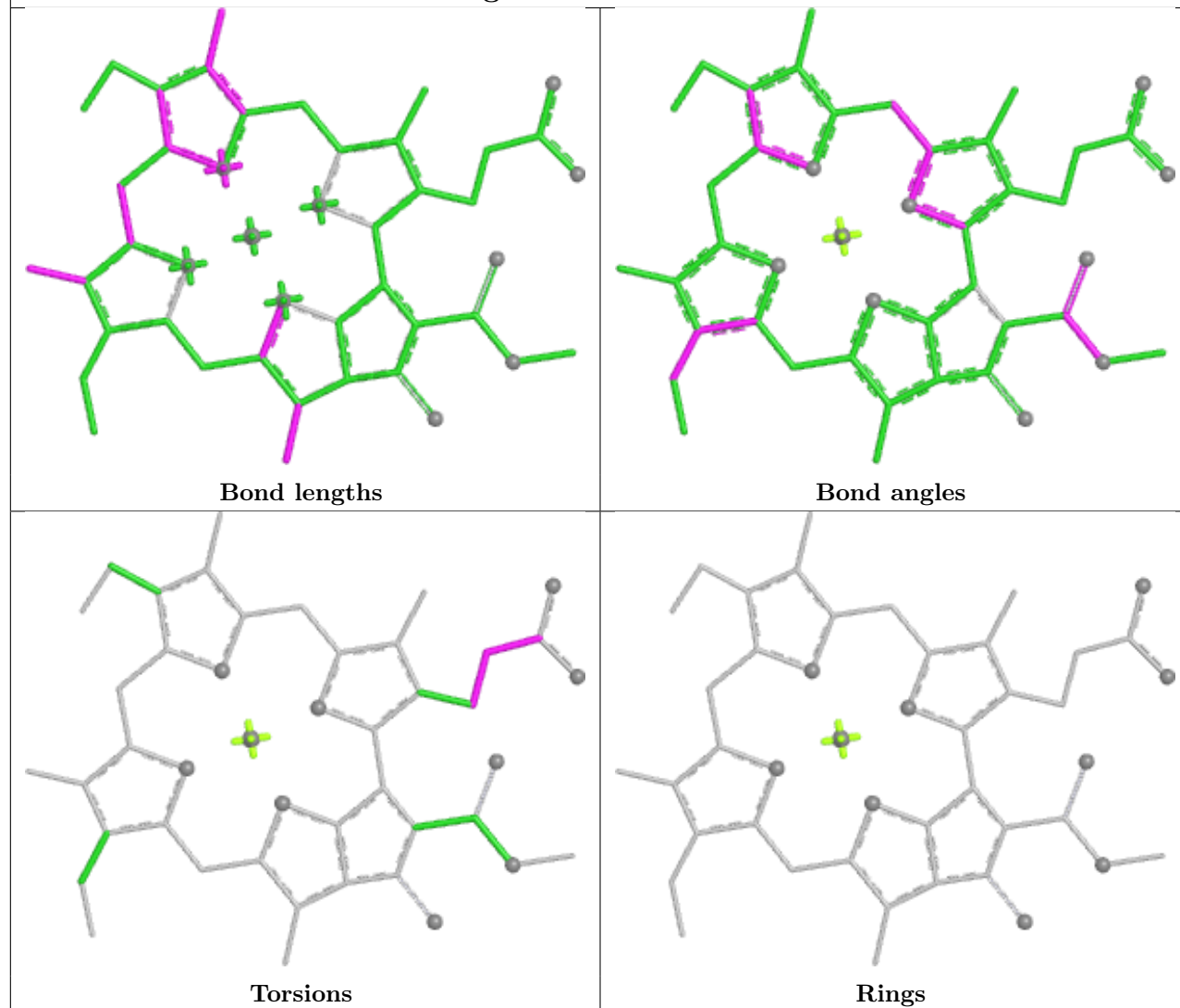
Ligand CHL 2 610

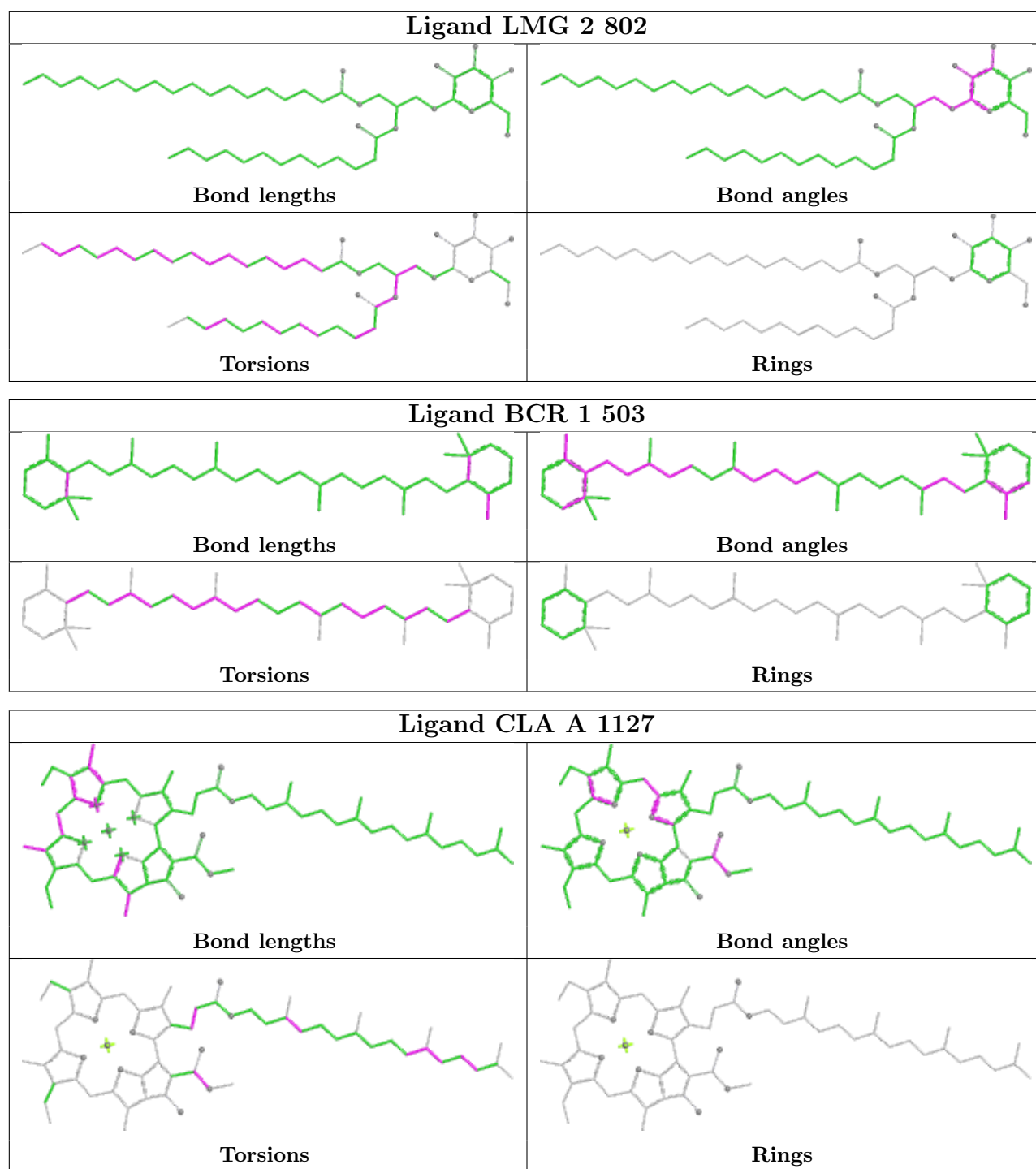


Ligand CLA 3 612

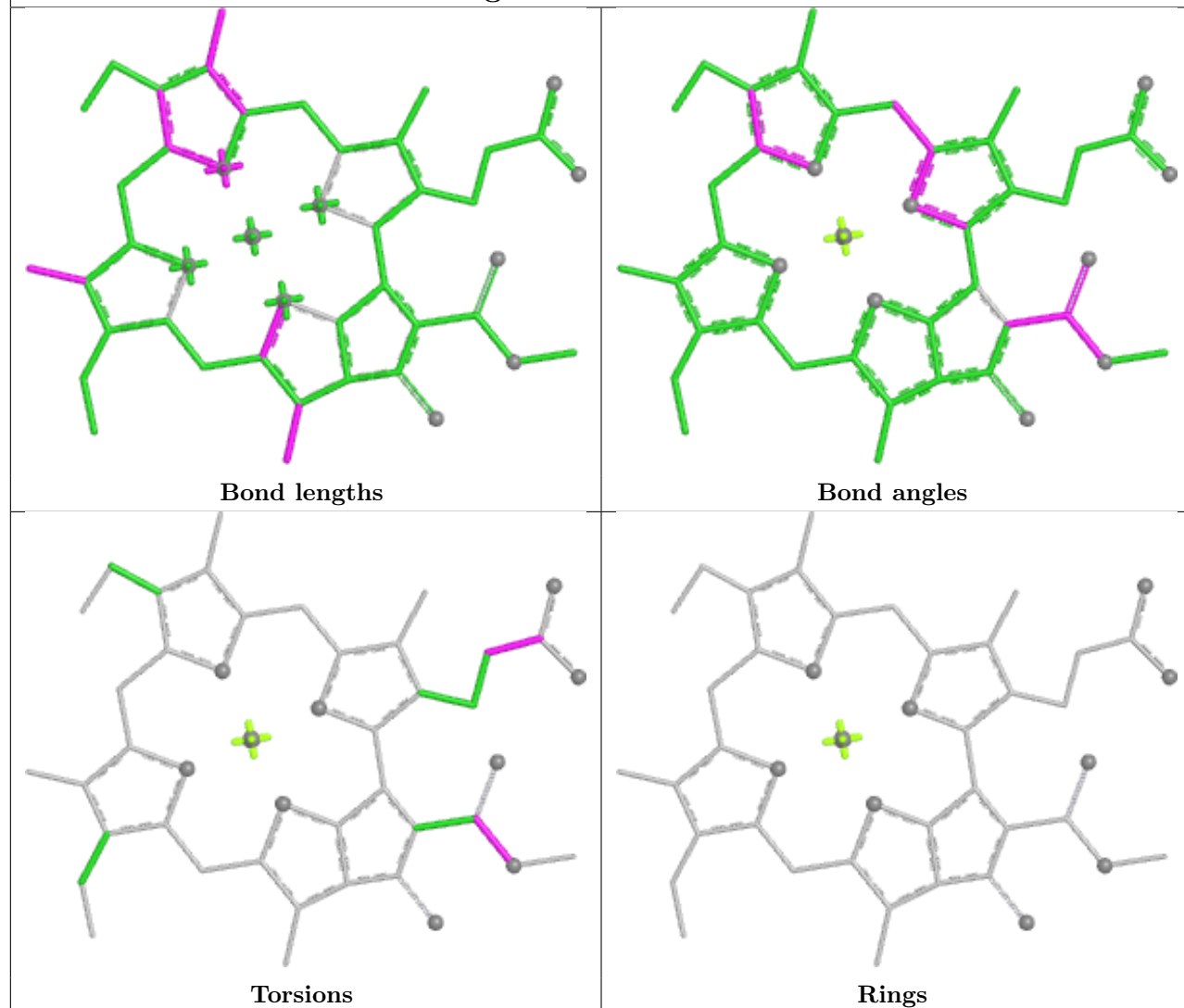


Ligand CLA A 1115

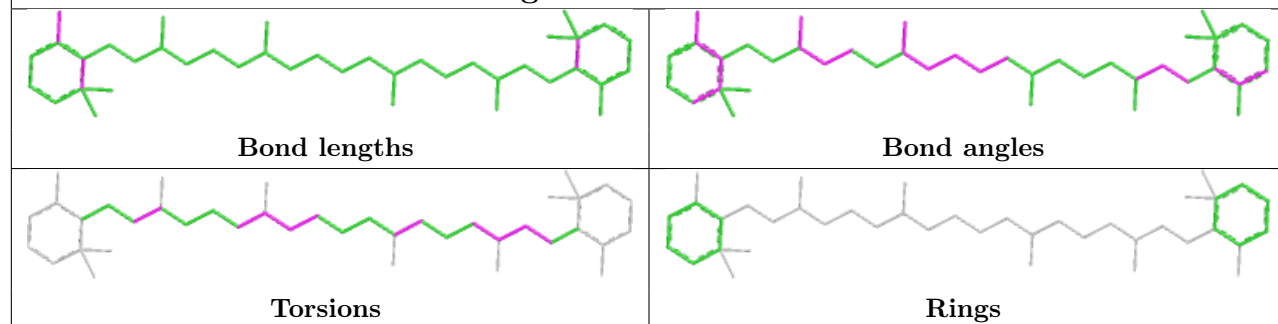


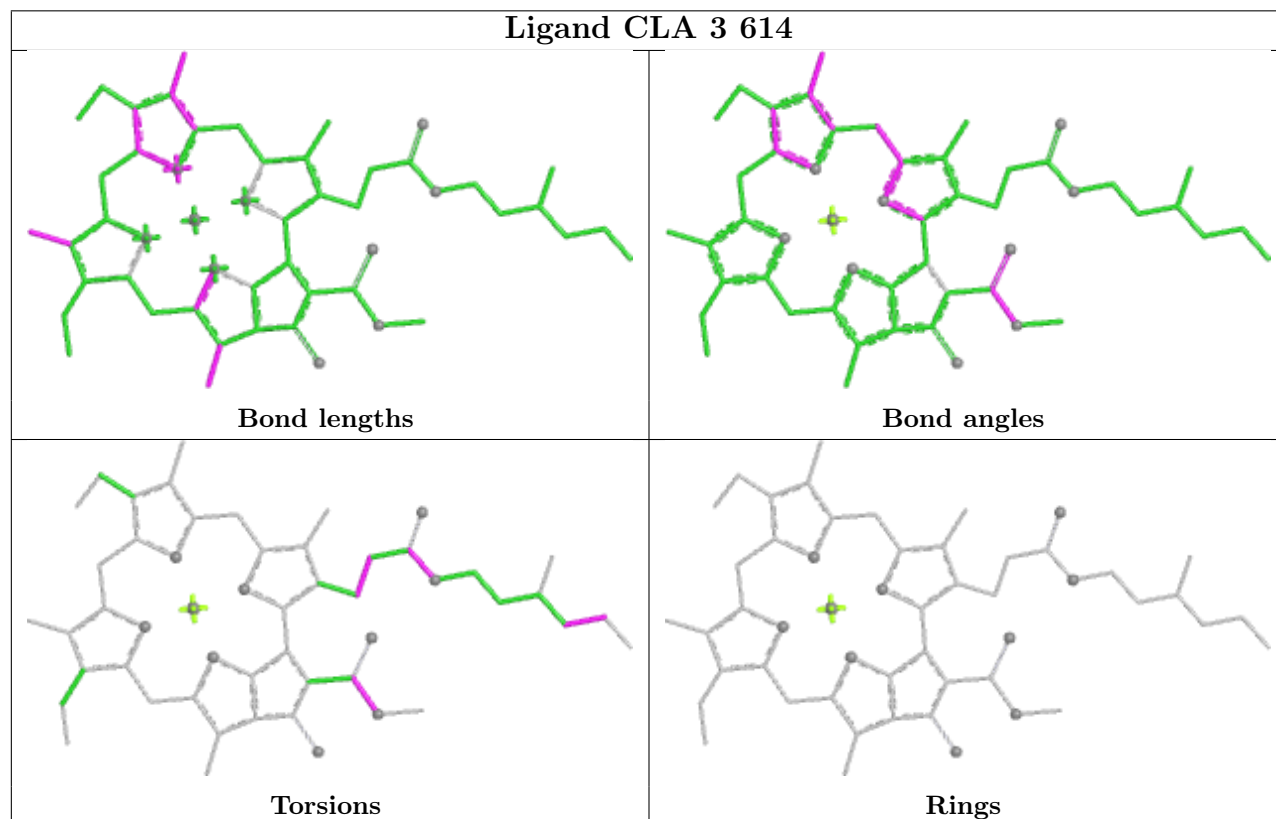
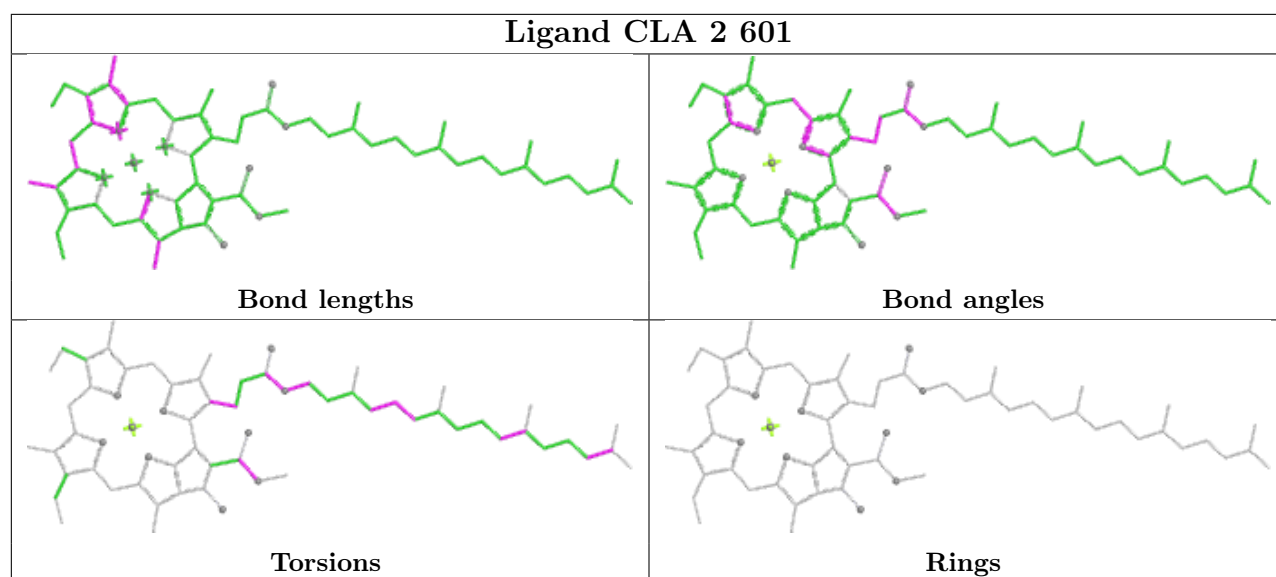


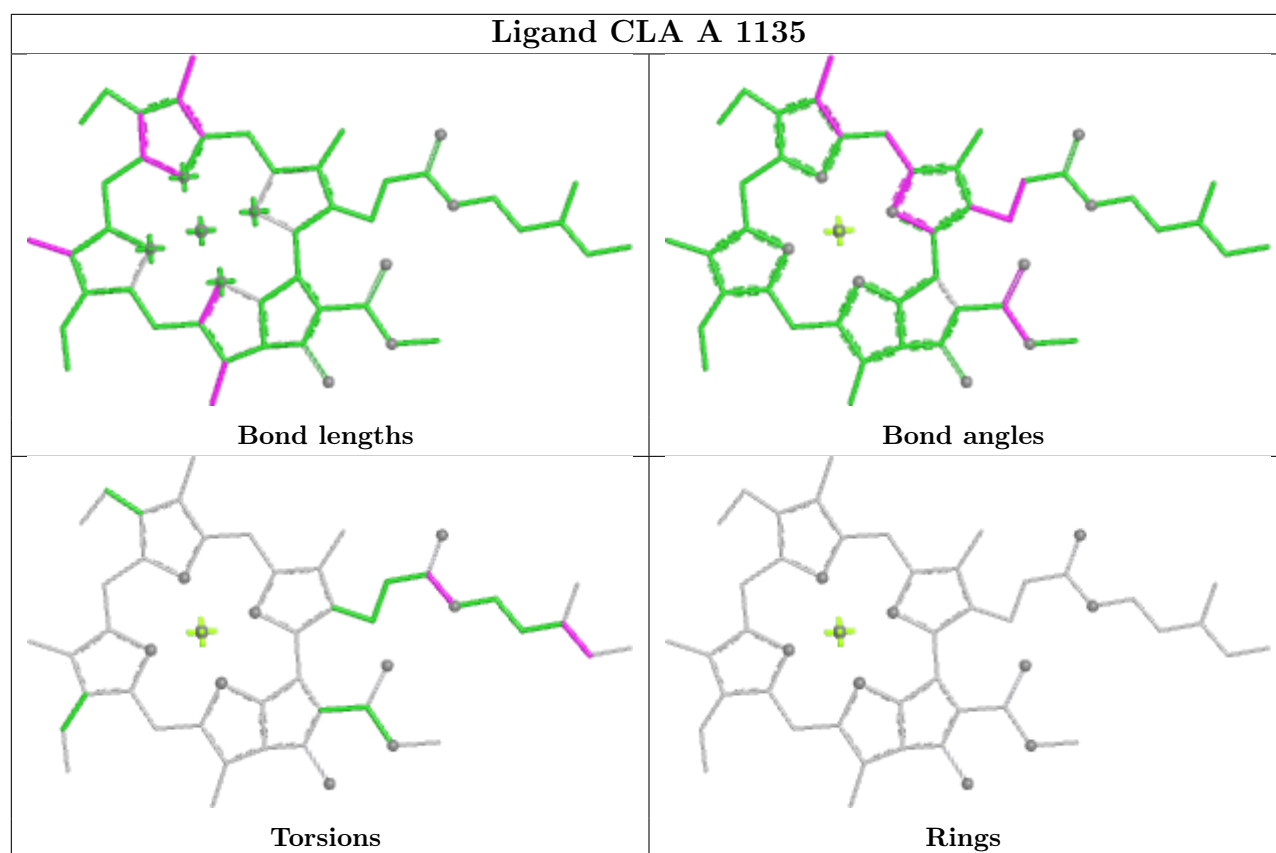
Ligand CLA B 1206



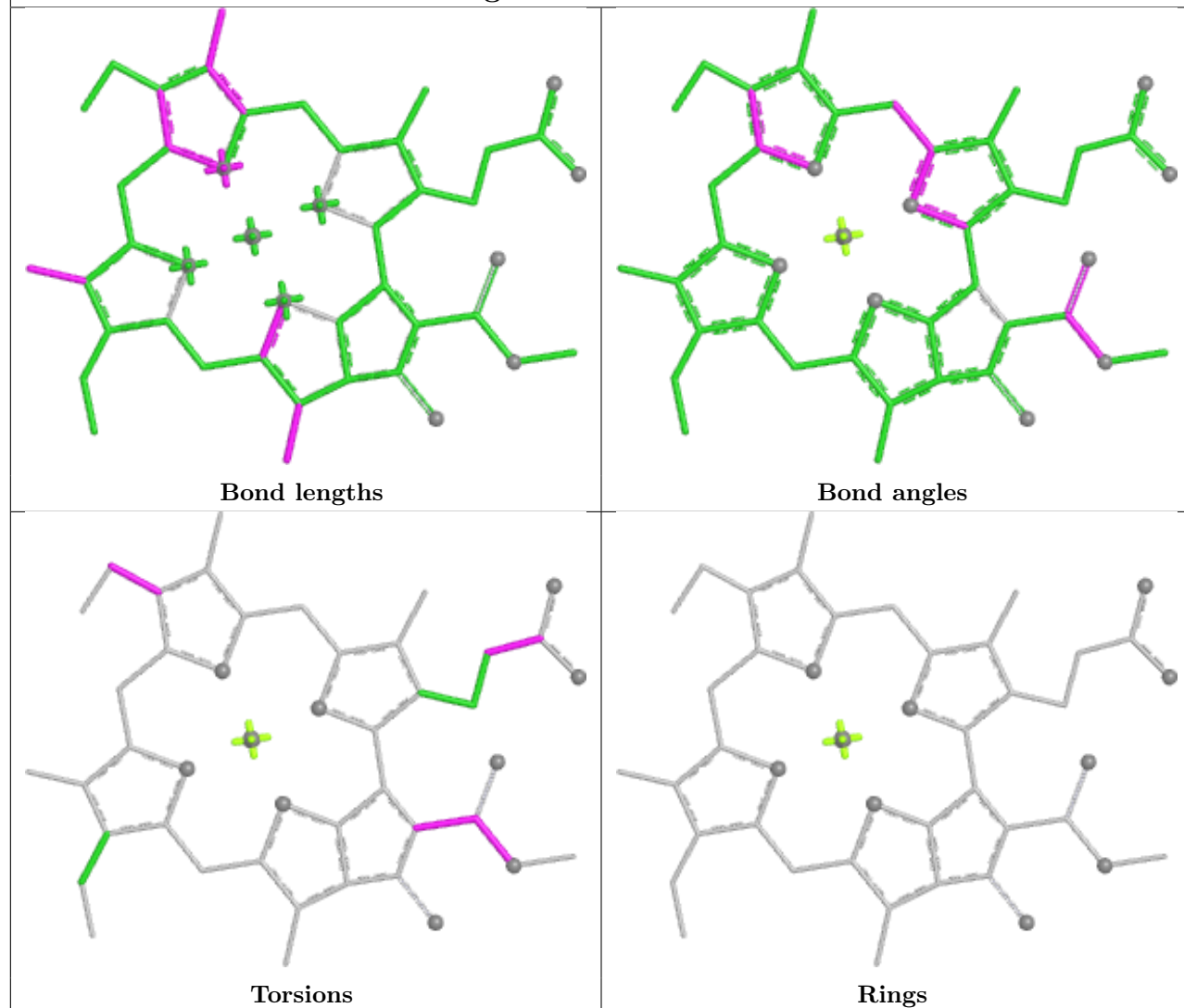
Ligand BCR A 4008



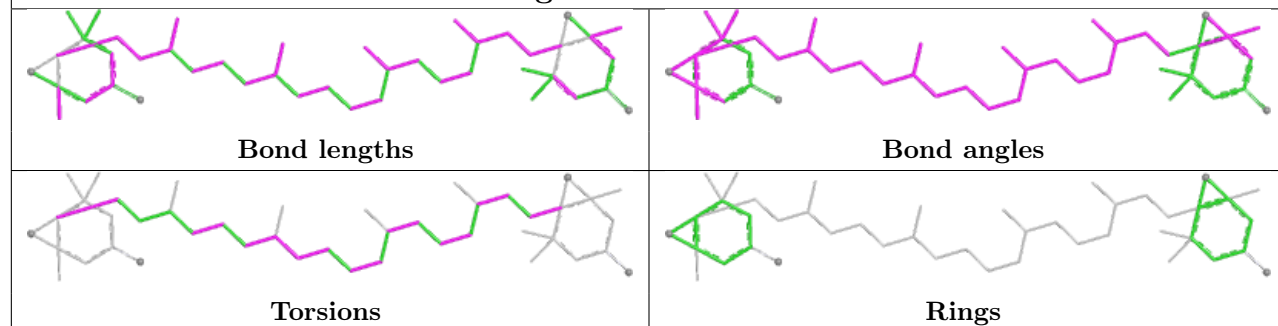


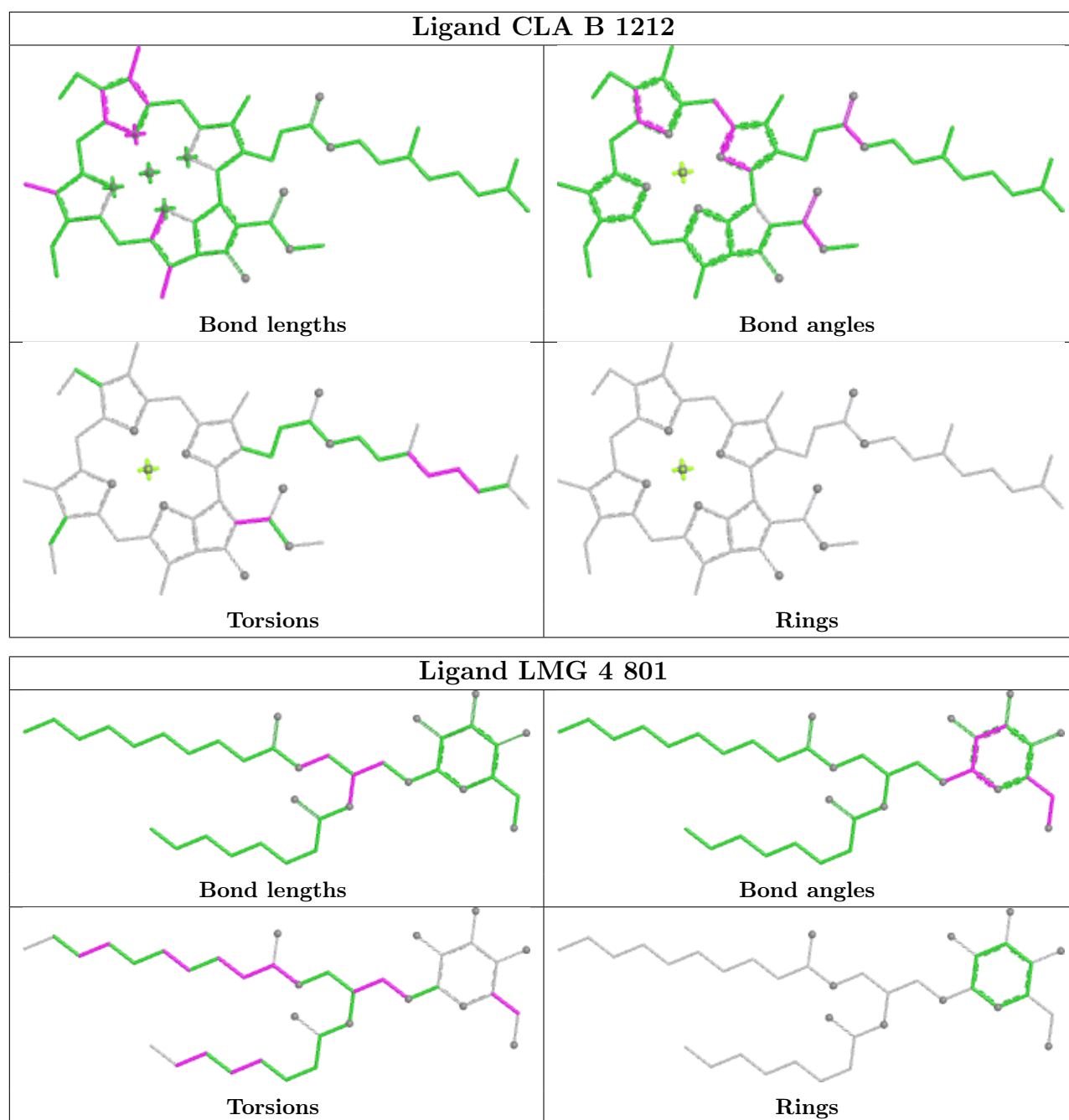


Ligand CLA A 1131



Ligand XAT 3 502





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

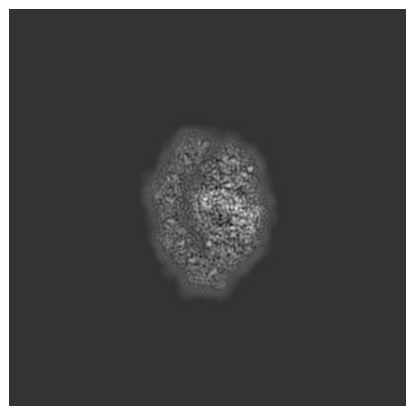
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4883. These allow visual inspection of the internal detail of the map and identification of artifacts.

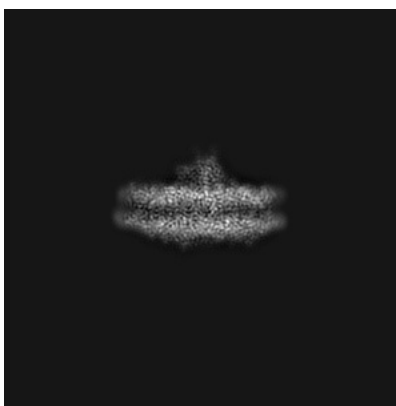
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

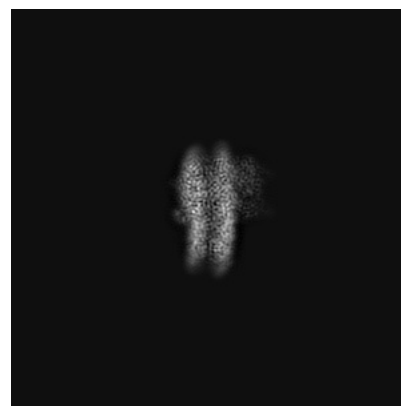
6.1.1 Primary map



X

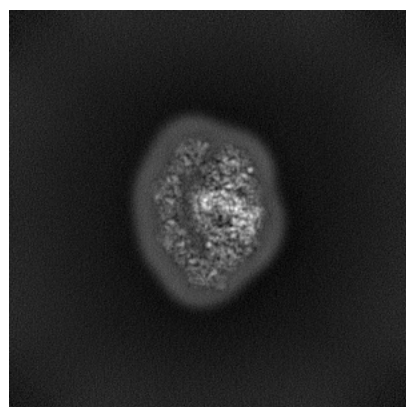


Y

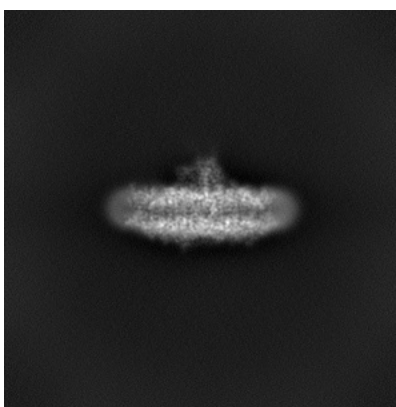


Z

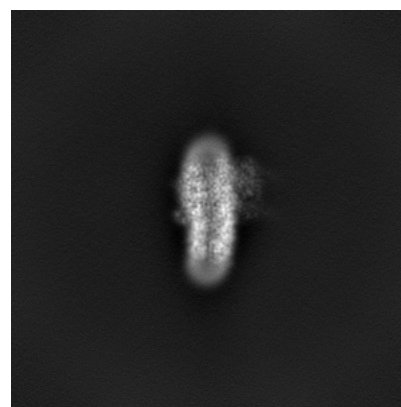
6.1.2 Raw map



X



Y

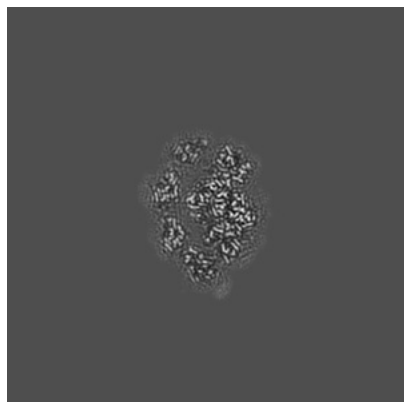


Z

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

6.2 Central slices [i](#)

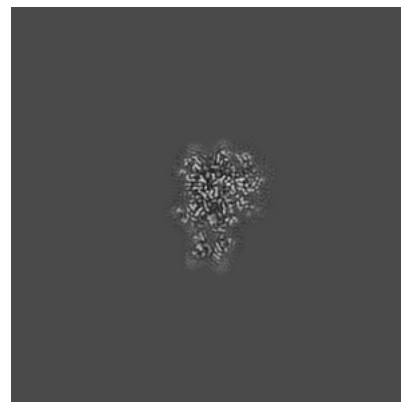
6.2.1 Primary map



X Index: 200

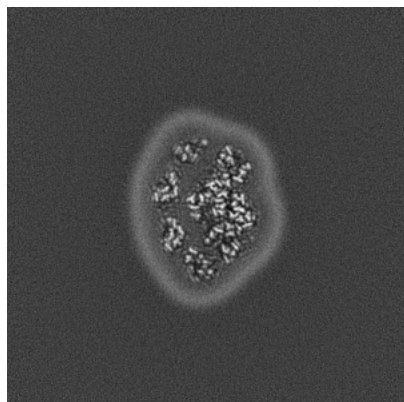


Y Index: 200

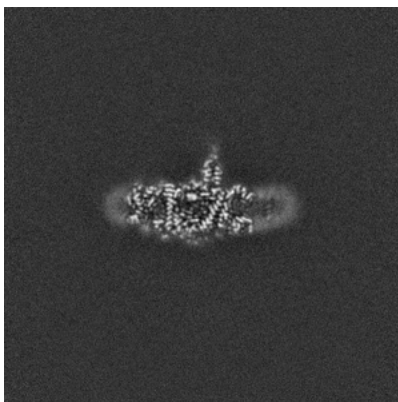


Z Index: 200

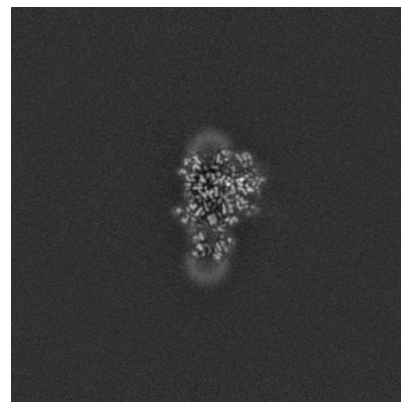
6.2.2 Raw map



X Index: 200



Y Index: 200

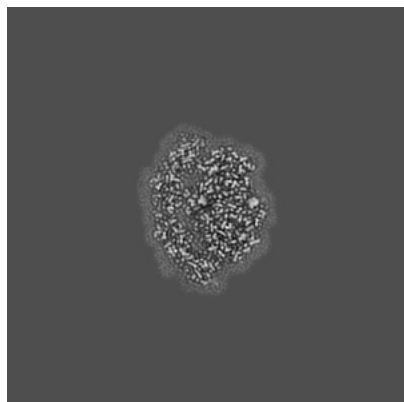


Z Index: 200

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

6.3 Largest variance slices [i](#)

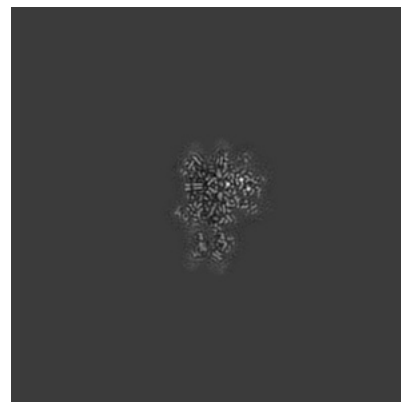
6.3.1 Primary map



X Index: 210

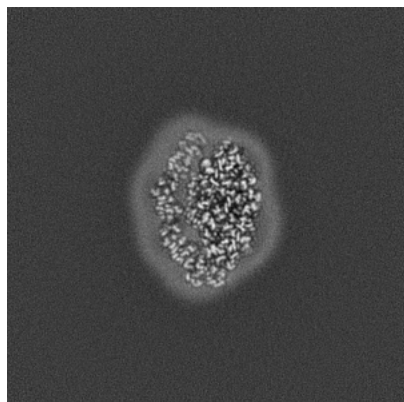


Y Index: 222

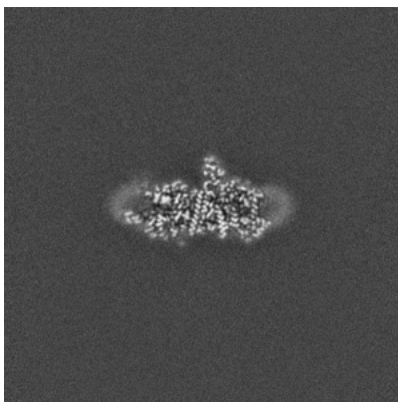


Z Index: 202

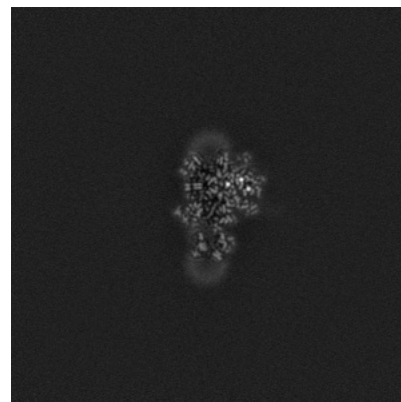
6.3.2 Raw map



X Index: 186



Y Index: 214

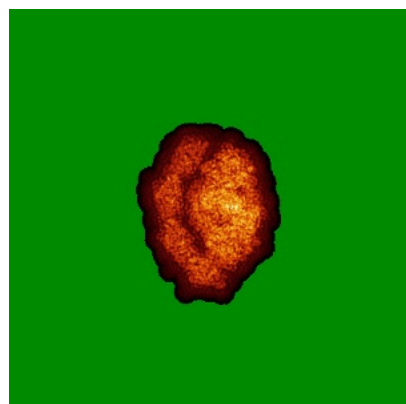


Z Index: 202

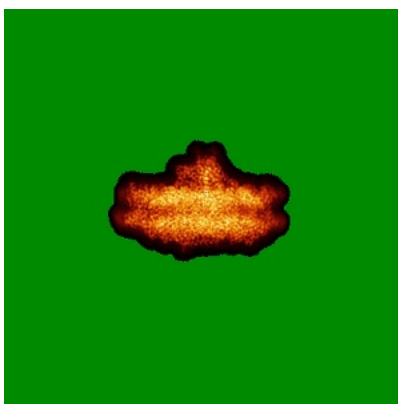
The images above show the largest variance slices of the map in three orthogonal directions.

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

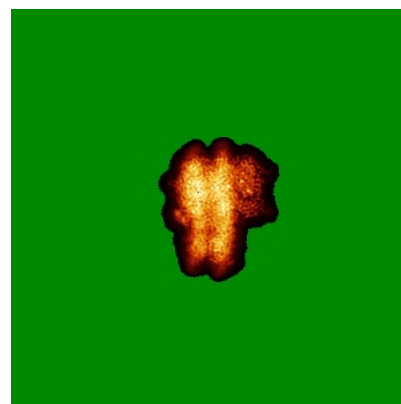
6.4.1 Primary map



X

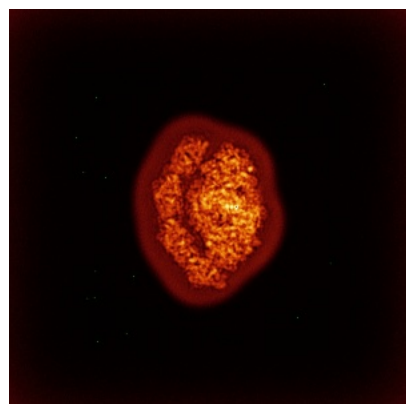


Y

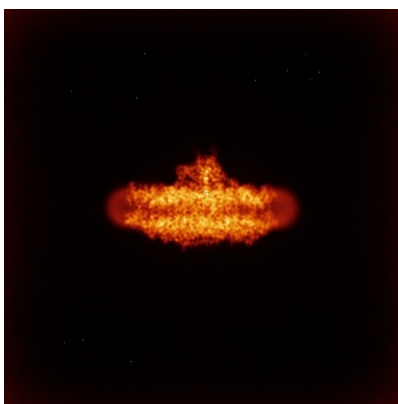


Z

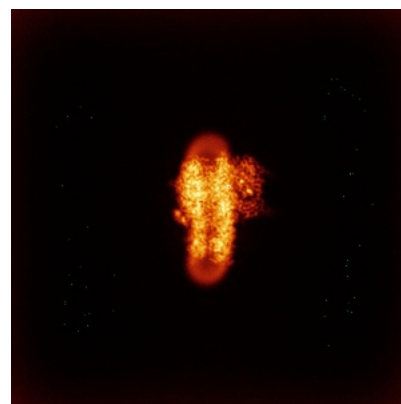
6.4.2 Raw map



X



Y

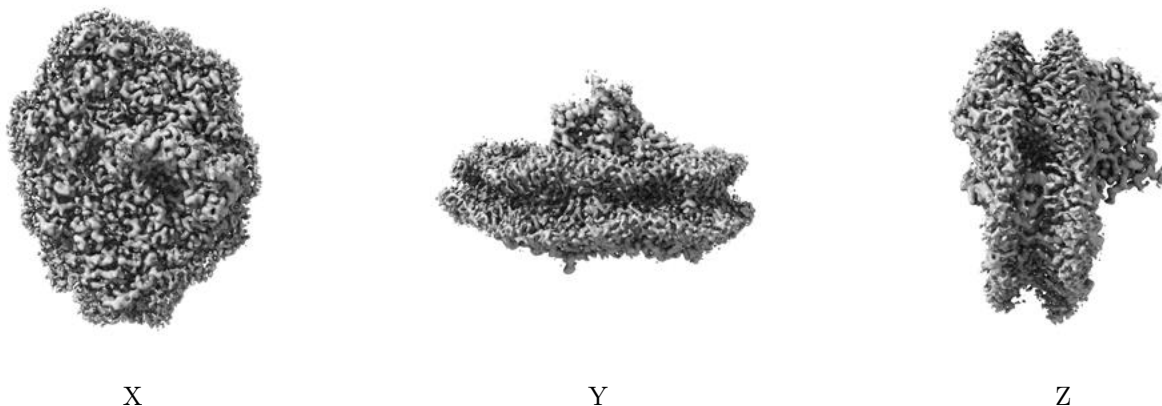


Z

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.

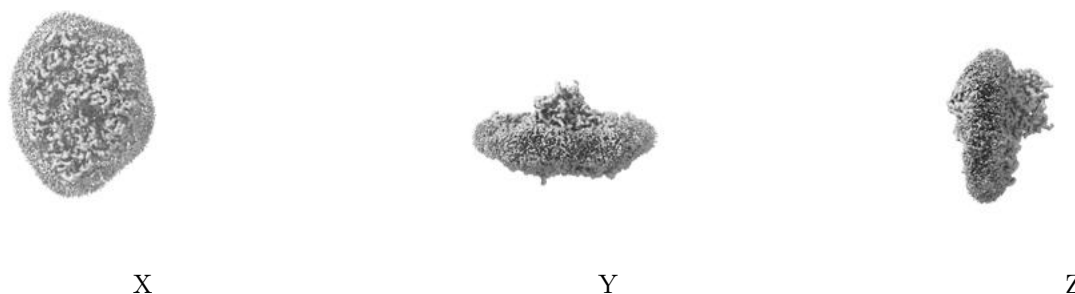
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 1.0. 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.

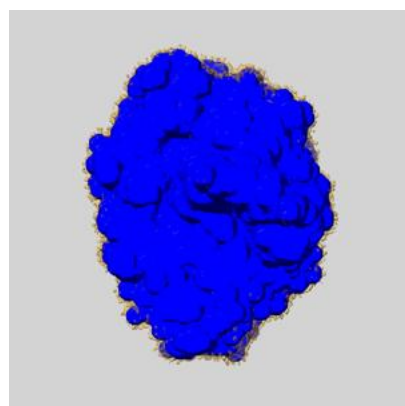
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

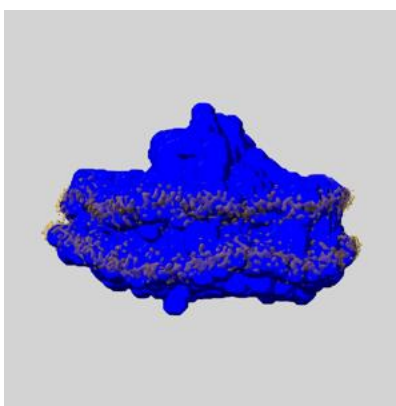
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

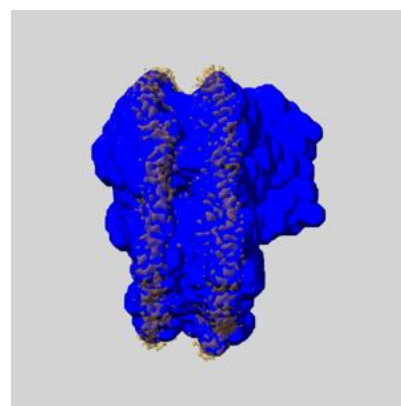
6.6.1 emd_4883_msk_1.map [i](#)



X



Y

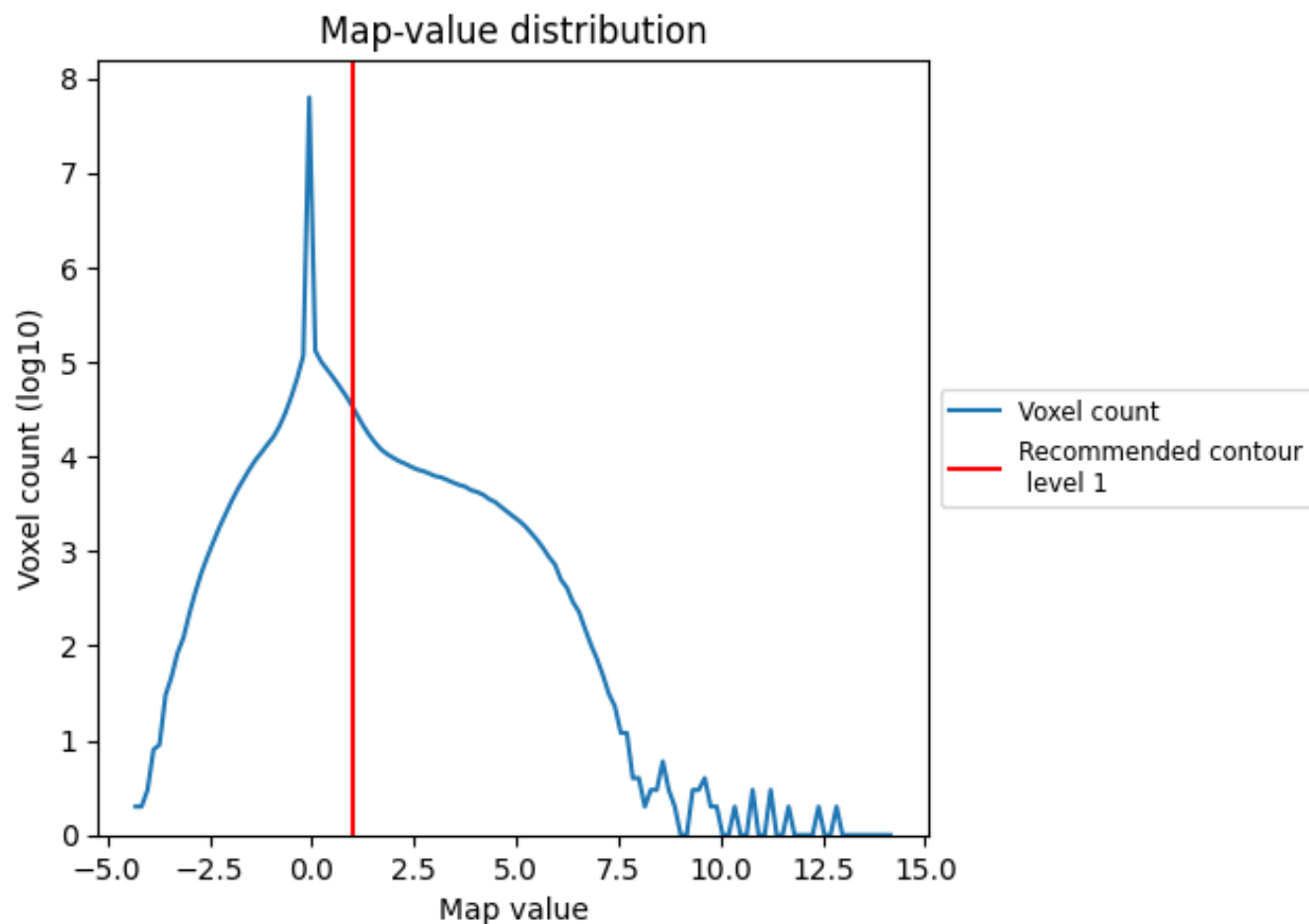


Z

7 Map analysis [i](#)

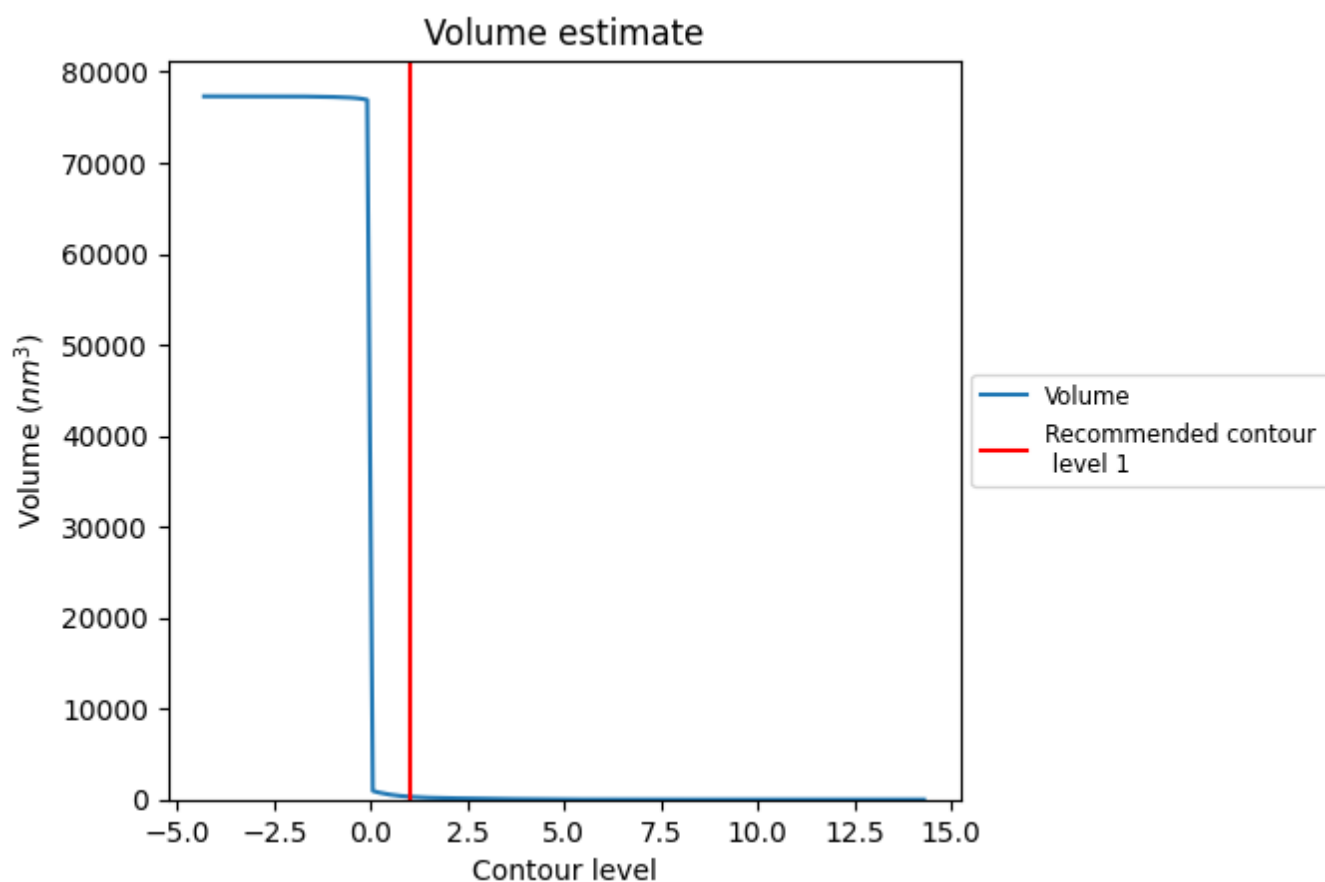
This section contains the results of statistical analysis of the map.

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.

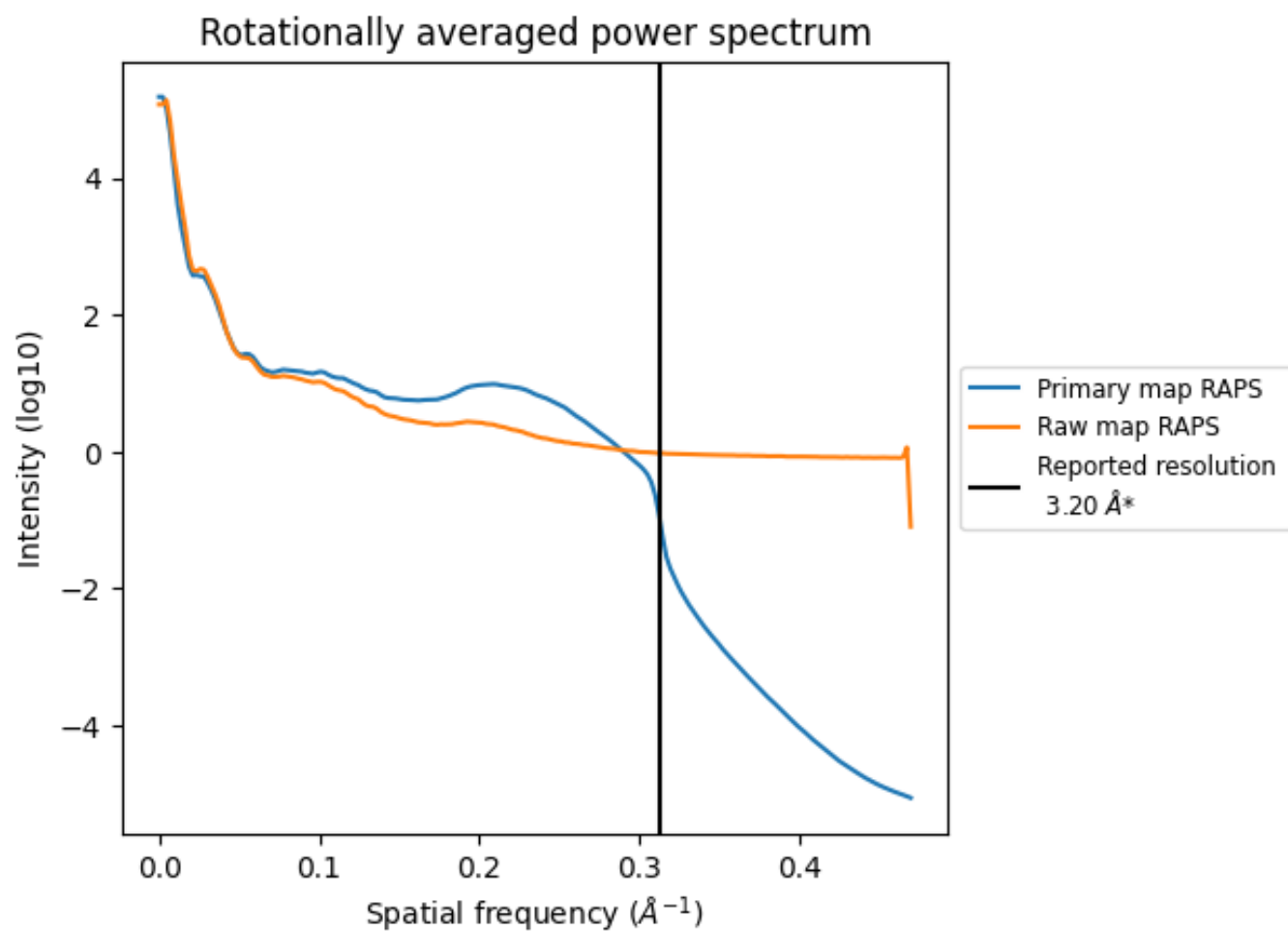
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 312 nm³; this corresponds to an approximate mass of 282 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 ⓘ

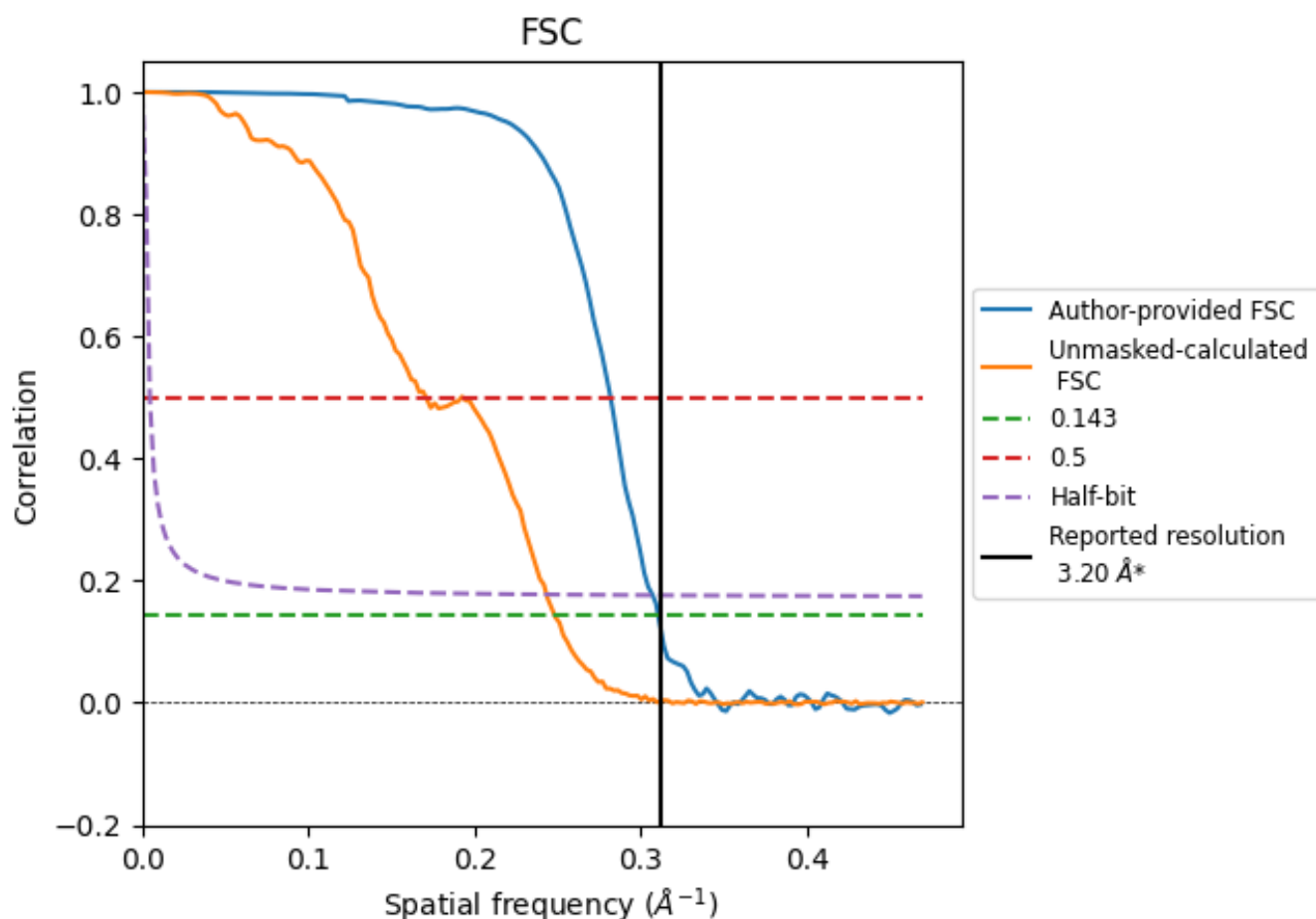


*Reported resolution corresponds to spatial frequency of 0.312 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.312 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

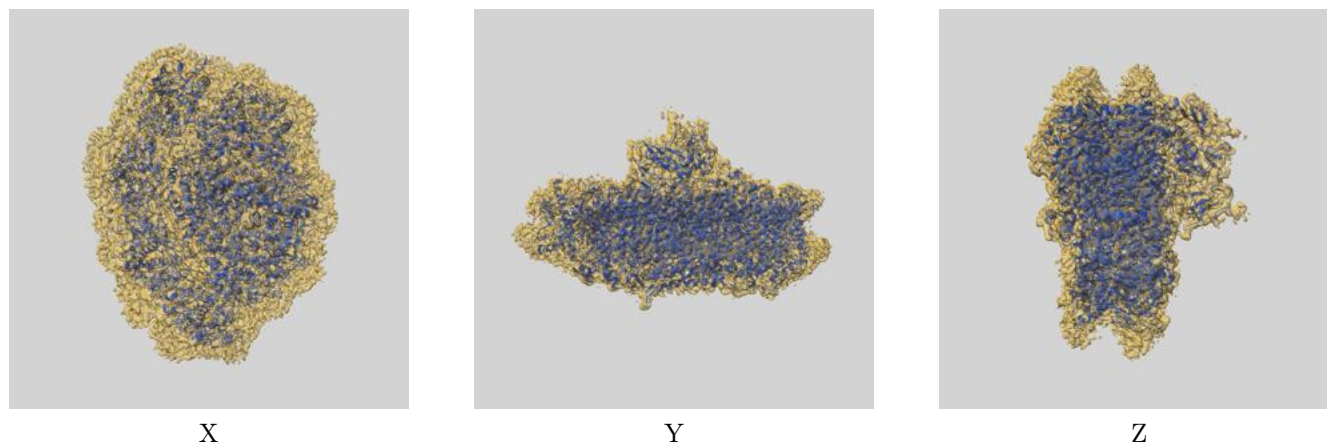
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	3.22	3.55	3.25
Unmasked-calculated*	4.03	5.85	4.11

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.03 differs from the reported value 3.2 by more than 10 %

9 Map-model fit [i](#)

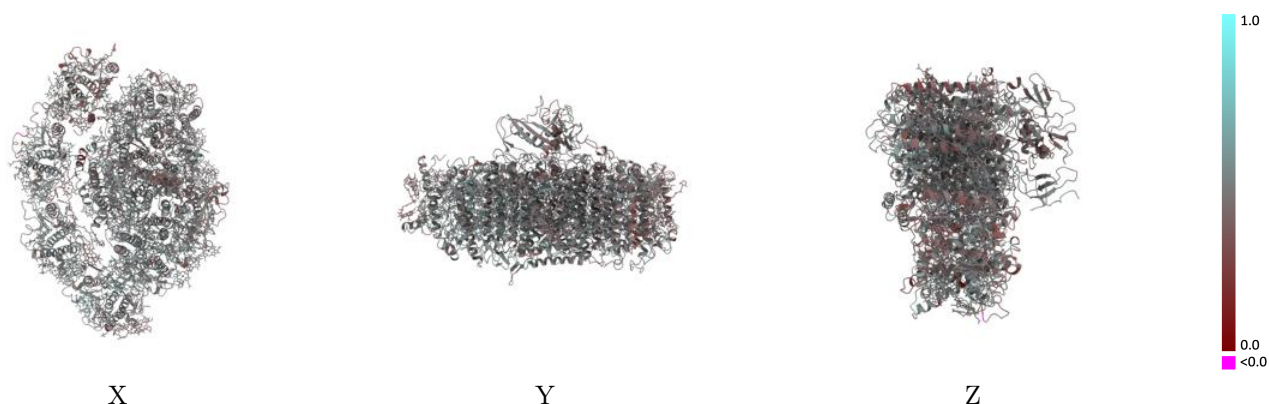
This section contains information regarding the fit between EMDB map EMD-4883 and PDB model 6RHZ. Per-residue inclusion information can be found in section 3 on page 24.

9.1 Map-model overlay [i](#)



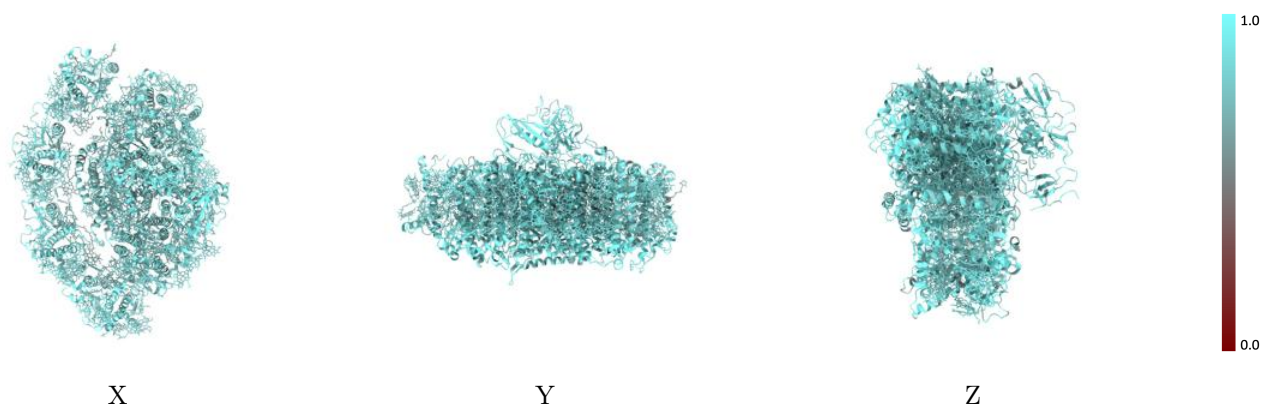
The images above show the 3D surface view of the map at the recommended contour level 1.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



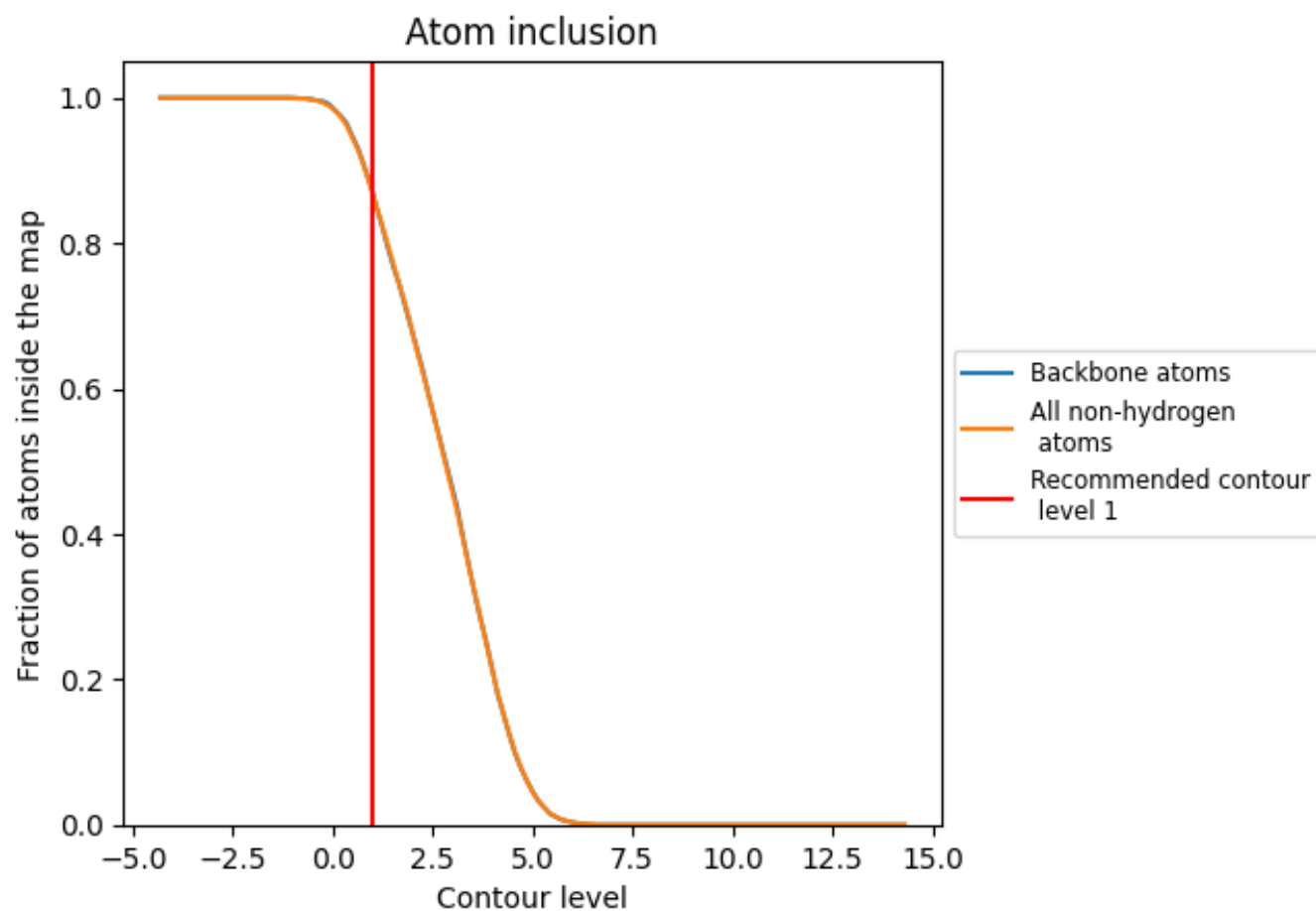
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (1).

9.4 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 87% 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 (1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8680	0.4670
1	0.8400	0.4240
2	0.8680	0.4760
3	0.8630	0.4740
4	0.8460	0.4470
A	0.8830	0.4870
B	0.8730	0.4650
C	0.8900	0.4440
D	0.8610	0.4330
E	0.8840	0.4690
F	0.8370	0.4540
J	0.8860	0.4880

1.0

0.0

<0.0