



Full wwPDB EM Validation Report ⓘ

Apr 2, 2025 – 03:27 am BST

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.dev117
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.42

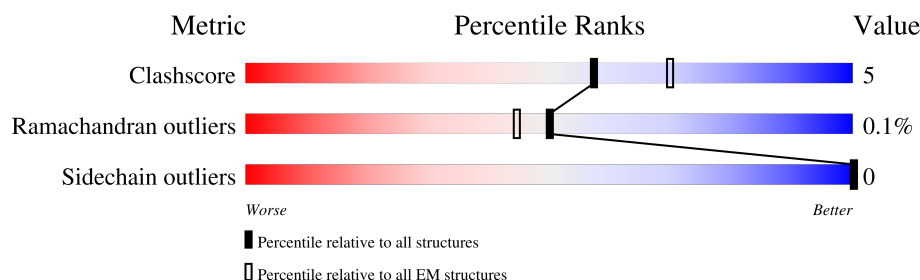
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 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.




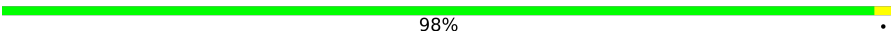
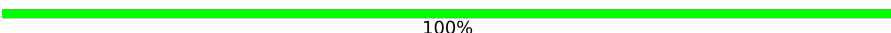
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	
2	2	208	
3	3	210	
4	4	211	
5	A	739	
6	B	730	
7	C	80	
8	D	141	

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Mol	Chain	Length	Quality of chain
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	-	-	-
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	-	-	-

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

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

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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	CLO	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			

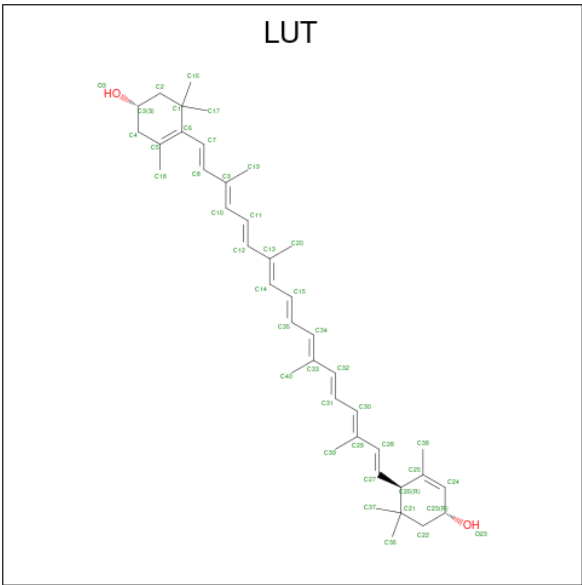
- Molecule 10 is a protein called Photosystem I reaction center subunit III, PsaF.

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.

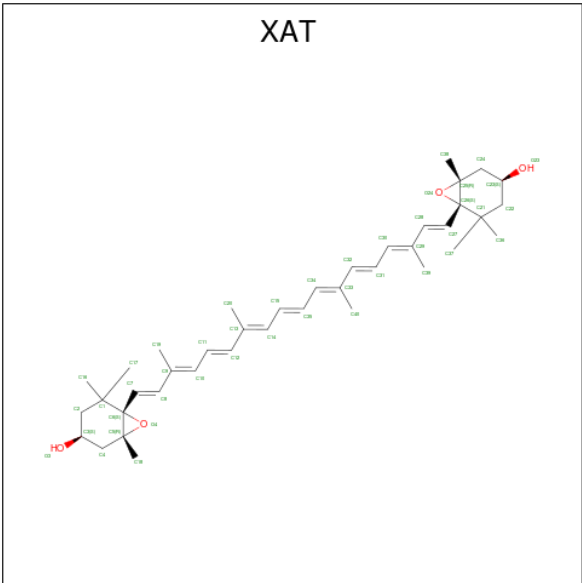
Mol	Chain	Residues	Atoms						AltConf	Trace
11	J	40	Total	C	H	N	O	S	0	0
			635	214	319	46	55	1		

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



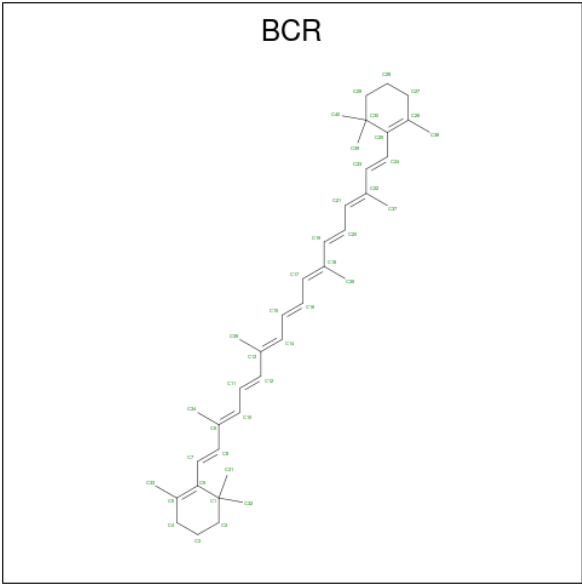
Mol	Chain	Residues	Atoms				AltConf
12	1	1	Total	C	H	O	0
			98	40	56	2	
12	2	1	Total	C	H	O	0
			98	40	56	2	
12	3	1	Total	C	H	O	0
			98	40	56	2	
12	4	1	Total	C	H	O	0
			98	40	56	2	

- 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: $C_{55}H_{72}MgN_4O_5$).



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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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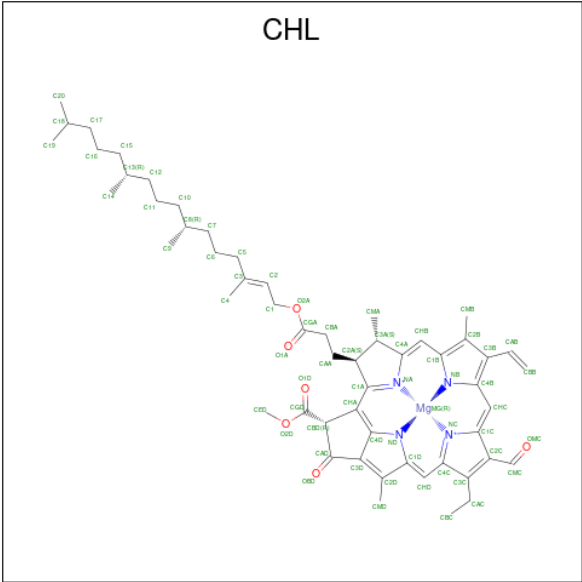
Mol	Chain	Residues	Atoms						AltConf
15	B	1	Total	C	H	Mg	N	O	0
			78	36	32	1	4	5	
15	B	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
15	B	1	Total	C	H	Mg	N	O	0
			79	36	33	1	4	5	
15	B	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
15	B	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
15	B	1	Total	C	H	Mg	N	O	0
			104	45	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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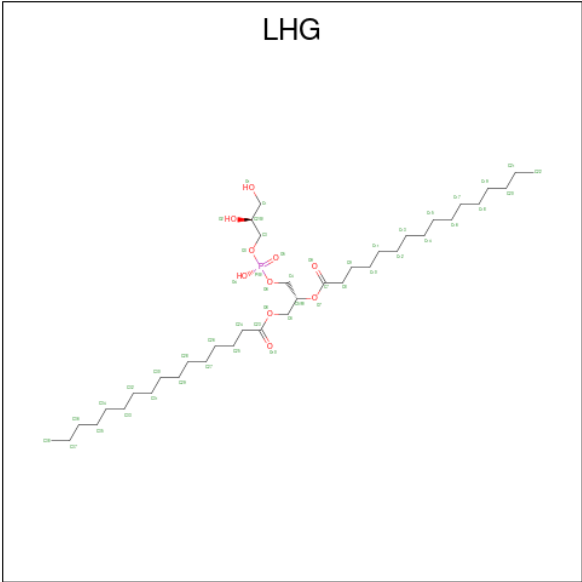
Mol	Chain	Residues	Atoms						AltConf
15	B	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
15	B	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
15	B	1	Total	C	H	Mg	N	O	0
			104	45	49	1	4	5	
15	B	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
15	B	1	Total	C	H	Mg	N	O	0
			78	36	32	1	4	5	
15	B	1	Total	C	H	Mg	N	O	0
			104	45	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: $C_{55}H_{70}MgN_4O_6$).



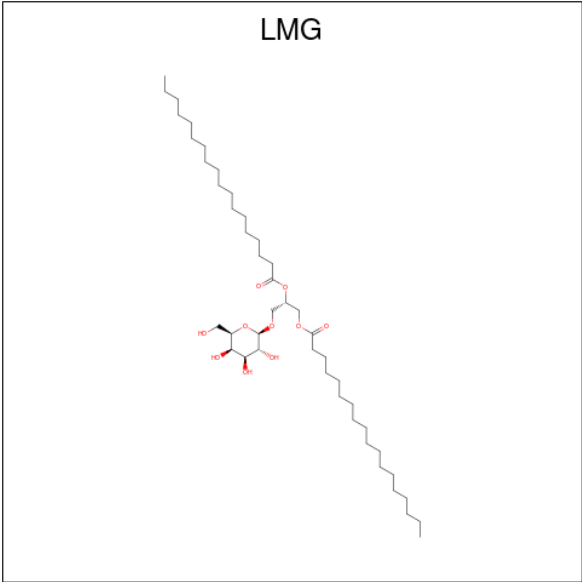
Mol	Chain	Residues	Atoms						AltConf
16	1	1	Total	C	H	Mg	N	O	0
			136	55	70	1	4	6	
16	1	1	Total	C	H	Mg	N	O	0
			80	36	33	1	4	6	
16	2	1	Total	C	H	Mg	N	O	0
			136	55	70	1	4	6	
16	2	1	Total	C	H	Mg	N	O	0
			75	35	31	1	4	4	
16	2	1	Total	C	H	Mg	N	O	0
			82	37	34	1	4	6	
16	2	1	Total	C	H	Mg	N	O	0
			77	35	31	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).



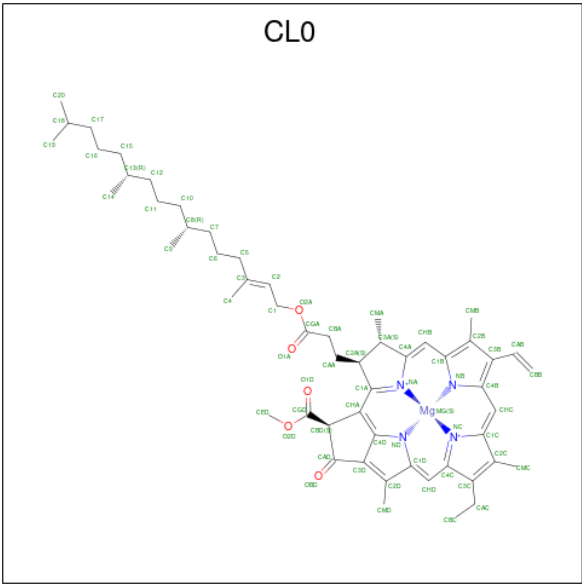
Mol	Chain	Residues	Atoms					AltConf
17	1	1	Total	C	H	O	P	0
			123	38	74	10	1	
17	2	1	Total	C	H	O	P	0
			75	24	40	10	1	
17	3	1	Total	C	H	O	P	0
			116	37	68	10	1	
17	A	1	Total	C	H	O	P	0
			123	38	74	10	1	
17	A	1	Total	C	H	O	P	0
			123	38	74	10	1	
17	B	1	Total	C	H	O	P	0
			99	31	57	10	1	

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



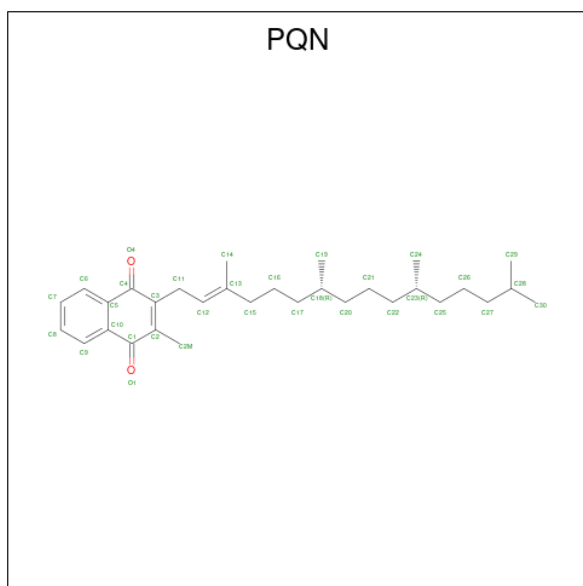
Mol	Chain	Residues	Atoms				AltConf
18	2	1	Total	C	H	O	0
			123	40	73	10	
18	2	1	Total	C	H	O	0
			90	30	50	10	
18	2	1	Total	C	H	O	0
			123	40	73	10	
18	4	1	Total	C	H	O	0
			80	27	43	10	
18	B	1	Total	C	H	O	0
			87	29	48	10	

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



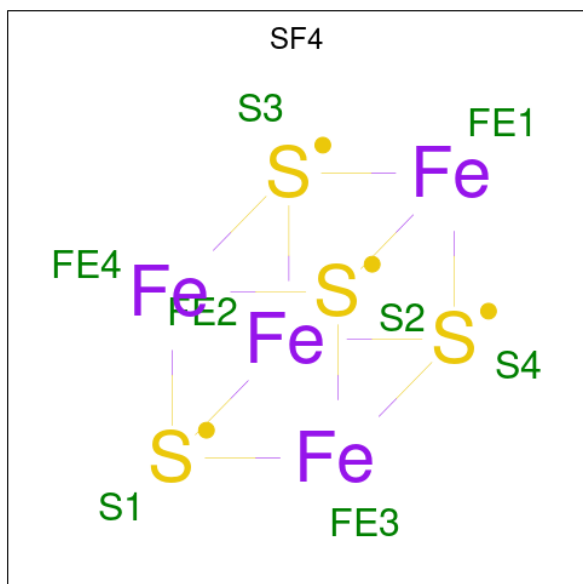
Mol	Chain	Residues	Atoms						AltConf
19	A	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	

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



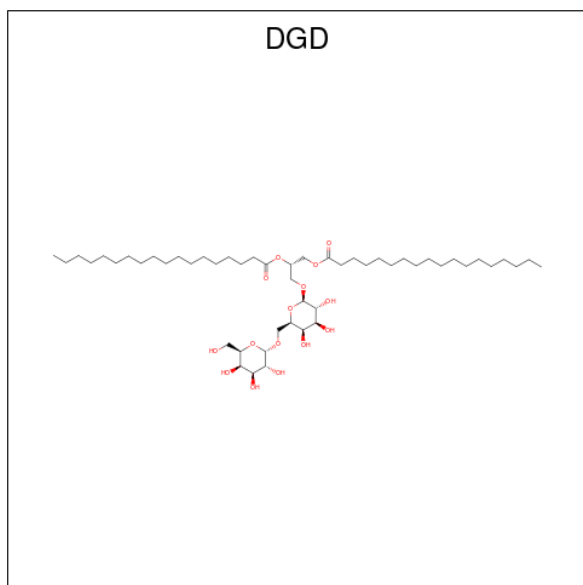
Mol	Chain	Residues	Atoms				AltConf
20	A	1	Total	C	H	O	0
			79	31	46	2	
20	B	1	Total	C	H	O	0
			79	31	46	2	

- 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: $C_{51}H_{96}O_{15}$).

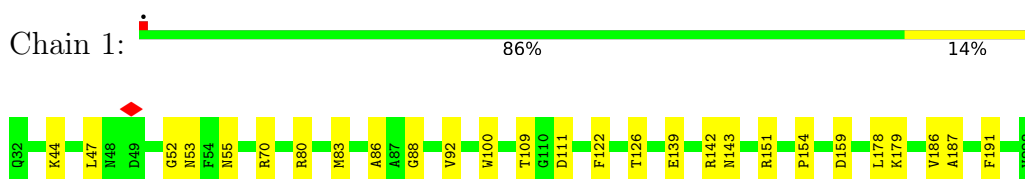


Mol	Chain	Residues	Atoms				AltConf
22	B	1	Total	C	H	O	0
			144	46	83	15	

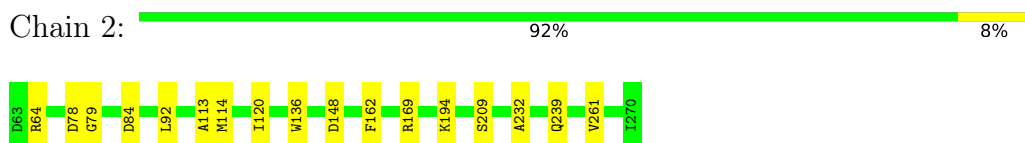
3 Residue-property plots

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.

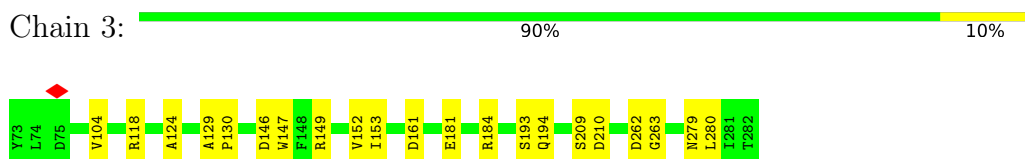
- Molecule 1: Chlorophyll a-b binding protein, chloroplastic



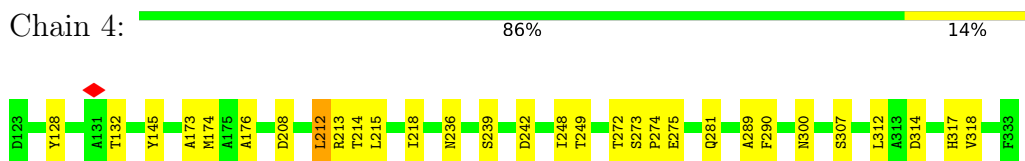
- Molecule 2: Chlorophyll a-b binding protein, Lhca2



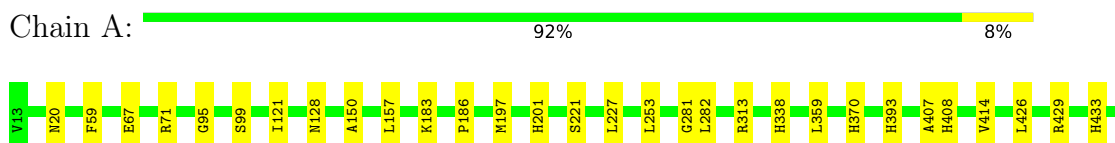
- Molecule 3: Chlorophyll a-b binding protein, chloroplastic



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



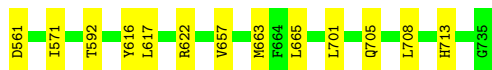
- Molecule 5: Photosystem I P700 chlorophyll a apoprotein A1





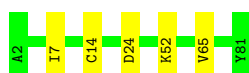
- Molecule 6: Photosystem I P700 chlorophyll a apoprotein A2

Chain B: 94% 6%



- Molecule 7: Photosystem I iron-sulfur center

Chain C: 94% 6%



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

Chain D: 87% 13%



- 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 (\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 (\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: BCR, SF4, LHG, PQN, CL0, LMG, DGD, LUT, XAT, CLA, CHL

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	0.31	0/1540	0.46	0/2088
2	2	0.34	0/1656	0.50	0/2243
3	3	0.36	0/1657	0.48	0/2253
4	4	0.33	0/1687	0.53	0/2300
5	A	0.37	0/5995	0.46	0/8179
6	B	0.38	0/5997	0.46	0/8198
7	C	0.39	0/610	0.53	0/828
8	D	0.36	0/1145	0.55	0/1546
9	E	0.37	0/525	0.50	0/712
10	F	0.32	0/1313	0.48	0/1776
11	J	0.36	0/326	0.46	0/445
All	All	0.36	0/22451	0.48	0/30568

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.

There are no bond angle outliers.

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

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	24	0
2	2	1609	1555	1555	15	0
3	3	1609	1567	1566	13	0
4	4	1637	1579	1579	22	0
5	A	5799	5630	5628	46	0
6	B	5784	5528	5527	39	0
7	C	600	584	581	4	0
8	D	1116	1126	1126	12	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	11	0
12	2	42	56	56	5	0
12	3	42	56	56	8	0
12	4	42	56	56	6	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	6	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	14	0
14	B	240	313	336	11	0
14	F	80	102	112	2	0
14	J	80	104	112	5	0
15	1	633	553	562	21	0
15	2	580	572	573	11	0
15	3	732	700	704	17	0
15	4	632	601	604	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	A	2487	2465	2473	50	0
15	B	2411	2358	2359	43	0
15	F	95	72	72	0	0
15	J	42	31	31	0	0
16	1	113	103	101	2	0
16	2	204	166	165	2	0
16	3	61	59	57	1	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	0	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	293	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 5.

All (293) 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
15:3:603:CLA:HMB2	15:3:608:CLA:HBC1	1.69	0.71
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
1:1:100:TRP:O	13:1:502:XAT:O3	2.11	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:147:TRP:O	13:3:502:XAT:O3	2.11	0.69
15:1:612:CLA:HBC2	15:1:612:CLA:HMC1	1.75	0.68
5:A:714:GLN:OE1	9:E:82:TYR:OH	2.11	0.68
15:3:608:CLA:HBC3	15:3:608:CLA:HMC1	1.74	0.68
12:3:501:LUT:H192	15:3:601:CLA:H71	1.76	0.67
6:B:663:MET:HE3	15:B:1023:CLA:NB	2.09	0.67
2:2:239:GLN:OE1	15:2:603:CLA:ND	2.28	0.67
12:1:501:LUT:H203	15:1:601:CLA:HMC2	1.78	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
12:3:501:LUT:H26	15:3:603:CLA:HMB3	1.81	0.62
5:A:708:ARG:NH1	10:F:229:SER:O	2.33	0.62
1:1:47: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
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
2:2:114:MET:SD	15:2:601:CLA:HMC3	2.42	0.59
1:1:179:LYS:NZ	17:1:801:LHG:O5	2.24	0.59
12:3:501:LUT:H11	15:3:601:CLA:HMC2	1.85	0.59
13:4:502:XAT:H31	15:4:604:CLA:HMC2	1.84	0.59
2:2:92:LEU:HD13	15:2:604:CLA:H42	1.84	0.59
16:2:610:CHL:HBB1	16:2:610:CHL:HMB1	1.85	0.58
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
13:3:502:XAT:H202	15:3:605:CLA:HMC2	1.86	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
15:B:1229:CLA:HAB	15:B:1230:CLA:HMB2	1.87	0.56
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:D:146:ARG:NH2	8:D:176:GLU:OE2	2.38	0.56
16:3:604:CHL:HBB1	16:3:604:CHL:HMB1	1.87	0.56
6:B:124:TRP:CZ2	15:B:1210:CLA:H191	2.40	0.56
15:B:1207:CLA:HMC1	15:B:1207:CLA:HBC3	1.88	0.56
15:B:1021:CLA:HMB3	15:B:1022:CLA:OBD	2.05	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
15:1:603:CLA:HBB1	15:1:603:CLA:HMB1	1.88	0.55
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
16:2:609:CHL:HMB2	15:3:615:CLA:O1D	2.08	0.53
15:A:1105:CLA:HMC1	15:A:1105:CLA:HBC3	1.90	0.53
15:1:605:CLA:HBC1	15:1:612:CLA:HMB3	1.89	0.53
15:1:615:CLA:HMC1	15:1:615:CLA:HBC2	1.89	0.53
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
15:2:606:CLA:HMC1	15:2:606:CLA:HBC2	1.91	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
5:A:683:LEU:HB2	15:A:1013:CLA:HMC3	1.89	0.52
6:B:340:ALA:HB2	14:B:4005:BCR:H372	1.91	0.52
15:1:605:CLA:CBC	15:1:612:CLA:HMB3	2.39	0.52
14:3:504:BCR:H343	15:3:605:CLA:HBC2	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
1:1:186:VAL:O	15:1:603:CLA:HMC3	2.10	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
4:4:312:LEU:HD21	15:4:608:CLA:HMC3	1.93	0.51
5:A:561:ARG:O	8:D:134:ARG:NH1	2.43	0.51
1:1:154:PRO:CG	15:1:611:CLA:HMD2	2.41	0.50
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
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
5:A:498:THR:HG21	15:A:1133:CLA:HMD1	1.93	0.49
12:2:501:LUT:C11	15:2:601:CLA:HMC2	2.42	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
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
14:A:4007:BCR:C35	15:B:1239:CLA:HMB2	2.42	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
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
13:4:502:XAT:C31	15:4:604:CLA:HMC2	2.43	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
19:A:1011:CL0:H13	15:A:1012:CLA:OBD	2.13	0.48
15:B:1230:CLA:HMB1	15:B:1230:CLA:HBB1	1.96	0.48
5:A:67:GLU:OE2	5:A:71:ARG:NH2	2.47	0.48
15:B:1215:CLA:HMB1	15:B:1215:CLA:HBB1	1.96	0.48
8:D:157:ARG:HB2	8:D:167:LEU:HD11	1.96	0.48
12:2:501:LUT:H391	15:2:602:CLA:HMC2	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
15:B:1221:CLA:HMA2	15:B:1221:CLA:O2A	2.14	0.48
12:2:501:LUT:H10	12:2:501:LUT:H203	1.94	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:432:PHE:CZ	14:B:4006:BCR:H11C	2.49	0.47
6:B:374:THR:HG22	6:B:592:THR:HG23	1.95	0.47
15:1:607:CLA:HMC1	15:1:607:CLA:HBC2	1.97	0.47
15:A:1112:CLA:HMB2	14:A:4002:BCR:H343	1.96	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
15:A:1012:CLA:H42	6:B:439:VAL:HG22	1.97	0.47
15:A:1126:CLA:HMC1	15:A:1126:CLA:HBC3	1.95	0.47
1:1:70:ARG:NE	15:1:605:CLA:O1A	2.48	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
15:A:1119:CLA:HMD3	15:A:1121:CLA:HMC3	1.97	0.46
15:A:1132:CLA:HMC1	15:A:1132:CLA:HBC3	1.98	0.46
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
15:A:1126:CLA:HMB1	15:A:1126:CLA:HBB1	1.98	0.46
9:E:86:GLN:CD	10:F:237:ILE:HD11	2.35	0.46
15:A:1105:CLA:HMC1	15:A:1105:CLA:CBC	2.46	0.46
10:F:163:GLU:O	14:F:4001:BCR:H362	2.16	0.46
15:A:1112:CLA:HBA2	15:A:1114:CLA:HMB3	1.97	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
15:A:1012:CLA:C4	14:A:4006:BCR:H362	2.46	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
5:A:359:LEU:HD11	15:A:1123:CLA:HMB2	1.97	0.45
1:1:86:ALA:HB1	12:1:501:LUT:H391	1.97	0.45
15:B:1209:CLA:HMC2	14:B:4002:BCR:H331	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
2:2:162:PHE:CG	15:2:612:CLA:HMC3	2.52	0.45
3:3:118:ARG:NH1	15:3:611:CLA:OBD	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:1012:CLA:HMB3	15:B:1021:CLA:H191	1.99	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
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
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
1:1:83:MET:HE2	12:1:501:LUT:H201	1.99	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
4:4:128:TYR:CE1	15:4:609:CLA:HMA3	2.53	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
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
8:D:104:THR:HG1	8:D:154:CYS:HG	1.65	0.43
2:2:261:VAL:HG23	2:2:261:VAL:O	2.17	0.43
6:B:96:HIS:CE1	15:B:1206:CLA:HMB3	2.54	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
4:4:290: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:3:608:CLA:HMC1	15:3:608:CLA:CBC	2.46	0.43
4:4:174:MET:SD	12:4:501:LUT:H201	2.58	0.43
5:A:59:PHE:CD2	15:A:1103:CLA:HMC2	2.53	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
6:B:657:VAL:HG22	15:B:1239:CLA:HMB3	2.00	0.42
1:1:154:PRO:HG3	15:1:611:CLA:HMD2	2.00	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:1117:CLA:HMB1	15:A:1117:CLA:HBB1	2.01	0.42
15:B:1022:CLA:HBB1	15:B:1022:CLA:HMB1	2.02	0.42
15:B:1206:CLA:HMB1	15:B:1206:CLA:HBB1	2.01	0.42
6:B:320:HIS:CD2	15:B:1220:CLA:ND	2.87	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
4:4:208:ASP:N	4:4:208:ASP:OD1	2.53	0.42
14:A:4007:BCR:H353	15:B:1239:CLA:HMB2	2.02	0.41
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
5:A:547:VAL:HG11	15:A:1137:CLA:HMB3	2.02	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
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
15:A:1127:CLA:HBB1	15:A:1127:CLA:HMB1	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:154:PRO:O	15:1:601:CLA:HED2	2.21	0.41
5:A:281:GLY:C	5:A:282:LEU:HD12	2.41	0.41
6:B:561:ASP:OD1	7:C:52:LYS:NZ	2.52	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
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:A:1012:CLA:H42	6:B:439:VAL:CG2	2.49	0.41
15:A:1119:CLA:HMB3	15:A:1123:CLA:HED1	2.01	0.41
15:B:1224:CLA:O1D	15:B:1225:CLA:HMA1	2.21	0.41
8:D:129:LEU:C	8:D:130:LEU:HD12	2.41	0.41
12:1:501:LUT:H202	12:1:501:LUT:C10	2.50	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
16:1:610:CHL:C1C	15:1:613:CLA:HMC3	2.51	0.40
12:3:501:LUT:C11	15:3:601:CLA:HMC2	2.48	0.40
15:B:1229:CLA:HBB1	15:B:1229:CLA:HMB1	2.03	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: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%)	25	60
5	A	737/739 (100%)	706 (96%)	30 (4%)	1 (0%)	48	80
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%)	50	80

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 (11) such sidechains are listed below:

Mol	Chain	Res	Type
2	2	109	HIS
4	4	155	ASN
4	4	281	GLN
4	4	282	ASN
4	4	300	ASN
6	B	300	HIS
6	B	586	ASN
6	B	713	HIS
9	E	86	GLN
9	E	117	ASN
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$
17	LHG	A	5001	15	48,48,48	0.64	0	51,54,54	1.12	3 (5%)
15	CLA	1	605	-	65,73,73	1.47	8 (12%)	76,113,113	1.36	4 (5%)
15	CLA	3	614	-	52,60,73	1.69	8 (15%)	60,97,113	1.61	7 (11%)
14	BCR	3	506	-	41,41,41	1.21	3 (7%)	56,56,56	1.30	8 (14%)
15	CLA	B	1207	-	46,54,73	1.74	6 (13%)	53,90,113	1.50	6 (11%)
16	CHL	4	610	-	47,55,74	1.07	3 (6%)	50,91,114	1.49	10 (20%)
15	CLA	B	1238	-	51,59,73	1.85	9 (17%)	58,95,113	2.15	14 (24%)
15	CLA	F	1302	10	49,57,73	1.66	7 (14%)	55,93,113	1.58	8 (14%)
15	CLA	B	1217	-	46,54,73	1.71	8 (17%)	53,90,113	1.51	6 (11%)
15	CLA	B	1206	6	45,53,73	1.72	7 (15%)	52,89,113	1.57	7 (13%)
15	CLA	A	1140	-	61,69,73	1.52	8 (13%)	71,108,113	1.48	8 (11%)
15	CLA	A	1122	-	65,73,73	1.49	9 (13%)	76,113,113	1.54	12 (15%)
21	SF4	A	3001	5,6	0,12,12	-	-	-	-	-
16	CHL	2	613	-	46,54,74	1.01	2 (4%)	49,90,114	1.32	8 (16%)
14	BCR	3	504	-	41,41,41	1.28	4 (9%)	56,56,56	1.32	9 (16%)
15	CLA	B	1215	-	65,73,73	1.44	7 (10%)	76,113,113	1.42	11 (14%)
15	CLA	1	604	1	65,73,73	1.43	9 (13%)	76,113,113	1.35	8 (10%)
15	CLA	3	609	-	42,50,73	1.80	7 (16%)	48,85,113	1.61	6 (12%)
15	CLA	A	1102	-	65,73,73	1.45	9 (13%)	76,113,113	1.48	10 (13%)
13	XAT	1	502	-	39,47,47	2.59	17 (43%)	54,74,74	11.46	25 (46%)
15	CLA	B	1232	-	46,54,73	1.76	8 (17%)	53,90,113	1.51	5 (9%)
15	CLA	A	1124	-	60,68,73	1.50	8 (13%)	70,107,113	1.52	6 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	BCR	B	4004	-	41,41,41	1.16	2 (4%)	56,56,56	1.32	7 (12%)
15	CLA	B	1216	-	59,67,73	1.50	9 (15%)	68,105,113	1.45	9 (13%)
15	CLA	A	1118	-	42,50,73	1.76	7 (16%)	48,85,113	1.63	6 (12%)
15	CLA	2	607	17	60,68,73	1.51	9 (15%)	70,107,113	1.43	7 (10%)
12	LUT	1	501	-	42,43,43	5.97	30 (71%)	51,60,60	2.29	15 (29%)
15	CLA	A	1126	-	65,73,73	1.49	7 (10%)	76,113,113	1.35	10 (13%)
20	PQN	B	2002	-	34,34,34	0.69	0	42,45,45	0.90	1 (2%)
15	CLA	B	1203	-	65,73,73	1.45	9 (13%)	76,113,113	1.41	6 (7%)
15	CLA	1	615	1	47,55,73	1.76	8 (17%)	53,90,113	1.66	9 (16%)
15	CLA	4	605	-	65,73,73	1.44	6 (9%)	76,113,113	1.46	9 (11%)
13	XAT	2	502	-	39,47,47	2.63	15 (38%)	54,74,74	10.93	32 (59%)
14	BCR	J	4001	-	41,41,41	1.10	1 (2%)	56,56,56	1.37	8 (14%)
15	CLA	A	1113	-	45,53,73	1.72	7 (15%)	52,89,113	1.58	5 (9%)
15	CLA	B	1226	-	65,73,73	1.42	7 (10%)	76,113,113	1.52	8 (10%)
15	CLA	A	1104	-	65,73,73	1.47	9 (13%)	76,113,113	1.42	10 (13%)
15	CLA	4	612	4	65,73,73	1.45	8 (12%)	76,113,113	1.34	7 (9%)
18	LMG	4	801	-	37,37,55	1.02	3 (8%)	45,45,63	1.30	3 (6%)
15	CLA	3	615	3	42,50,73	1.77	6 (14%)	48,85,113	1.54	6 (12%)
15	CLA	F	1301	-	46,54,73	1.72	7 (15%)	53,90,113	1.55	6 (11%)
15	CLA	A	1129	-	55,63,73	1.60	10 (18%)	64,101,113	1.49	9 (14%)
21	SF4	C	3003	7	0,12,12	-	-	-	-	-
15	CLA	2	604	2	65,73,73	1.42	9 (13%)	76,113,113	1.38	10 (13%)
15	CLA	4	602	-	50,58,73	1.68	7 (14%)	58,95,113	1.56	7 (12%)
14	BCR	B	4002	-	41,41,41	1.17	2 (4%)	56,56,56	1.40	7 (12%)
16	CHL	3	604	3	61,69,74	0.90	3 (4%)	67,108,114	1.33	12 (17%)
15	CLA	A	1136	-	65,73,73	1.46	8 (12%)	76,113,113	1.37	6 (7%)
15	CLA	A	1133	-	65,73,73	1.47	8 (12%)	76,113,113	1.44	7 (9%)
15	CLA	A	1119	-	65,73,73	1.44	8 (12%)	76,113,113	1.38	8 (10%)
14	BCR	A	4005	-	41,41,41	1.22	3 (7%)	56,56,56	1.25	8 (14%)
15	CLA	A	1110	-	55,63,73	1.63	8 (14%)	64,101,113	1.65	13 (20%)
15	CLA	B	1214	-	65,73,73	1.49	9 (13%)	76,113,113	1.52	10 (13%)
14	BCR	3	503	-	41,41,41	1.19	3 (7%)	56,56,56	1.22	7 (12%)
14	BCR	A	4007	-	41,41,41	1.22	3 (7%)	56,56,56	1.30	9 (16%)
15	CLA	B	1208	-	60,68,73	1.54	8 (13%)	70,107,113	1.37	8 (11%)
14	BCR	F	4002	-	41,41,41	1.24	3 (7%)	56,56,56	1.34	7 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	BCR	4	503	-	41,41,41	1.26	2 (4%)	56,56,56	1.34	9 (16%)
16	CHL	2	611	-	48,56,74	1.05	3 (6%)	51,92,114	1.33	10 (19%)
14	BCR	A	4006	-	41,41,41	1.25	3 (7%)	56,56,56	1.29	8 (14%)
14	BCR	A	4004	-	41,41,41	1.17	3 (7%)	56,56,56	1.43	8 (14%)
15	CLA	B	1240	17	65,73,73	1.46	9 (13%)	76,113,113	1.45	10 (13%)
15	CLA	2	602	-	45,53,73	1.80	8 (17%)	52,89,113	1.49	5 (9%)
15	CLA	A	1013	-	65,73,73	1.42	9 (13%)	76,113,113	1.41	9 (11%)
15	CLA	3	608	-	65,73,73	1.45	8 (12%)	76,113,113	1.32	8 (10%)
15	CLA	B	1201	-	43,51,73	1.78	9 (20%)	49,86,113	1.52	7 (14%)
15	CLA	B	1225	-	65,73,73	1.44	7 (10%)	76,113,113	1.41	8 (10%)
15	CLA	3	611	-	65,73,73	1.45	8 (12%)	76,113,113	1.34	6 (7%)
15	CLA	2	616	-	65,73,73	1.45	7 (10%)	76,113,113	1.56	12 (15%)
15	CLA	A	1103	-	65,73,73	1.42	6 (9%)	76,113,113	1.45	8 (10%)
15	CLA	B	1210	-	65,73,73	1.47	8 (12%)	76,113,113	1.37	10 (13%)
15	CLA	1	611	-	48,56,73	1.70	6 (12%)	55,92,113	1.50	7 (12%)
16	CHL	4	611	-	51,59,74	1.04	3 (5%)	55,96,114	1.22	8 (14%)
15	CLA	A	1135	-	51,59,73	1.60	7 (13%)	59,96,113	1.62	6 (10%)
15	CLA	B	1234	-	55,63,73	1.55	7 (12%)	64,101,113	1.52	8 (12%)
14	BCR	B	4001	-	41,41,41	1.19	2 (4%)	56,56,56	1.39	10 (17%)
15	CLA	3	612	3	65,73,73	1.45	7 (10%)	76,113,113	1.39	7 (9%)
15	CLA	A	1130	-	45,53,73	1.74	8 (17%)	52,89,113	1.57	8 (15%)
15	CLA	A	1121	-	45,53,73	1.78	8 (17%)	52,89,113	1.58	6 (11%)
14	BCR	J	4002	-	41,41,41	1.22	4 (9%)	56,56,56	1.27	6 (10%)
15	CLA	B	1022	-	65,73,73	1.48	9 (13%)	76,113,113	1.37	7 (9%)
15	CLA	A	1114	-	55,63,73	1.62	8 (14%)	64,101,113	1.51	4 (6%)
15	CLA	1	603	-	60,68,73	1.48	6 (10%)	70,107,113	1.58	10 (14%)
15	CLA	A	1101	-	65,73,73	1.46	8 (12%)	76,113,113	1.38	7 (9%)
15	CLA	B	1209	-	46,54,73	1.70	7 (15%)	53,90,113	1.54	6 (11%)
16	CHL	1	609	1	66,74,74	0.95	5 (7%)	73,114,114	1.20	8 (10%)
15	CLA	4	601	4	60,68,73	1.54	10 (16%)	70,107,113	1.48	11 (15%)
15	CLA	A	1116	-	56,64,73	1.56	9 (16%)	65,102,113	1.58	10 (15%)
15	CLA	A	1138	-	65,73,73	1.45	10 (15%)	76,113,113	1.47	10 (13%)
15	CLA	A	1125	-	65,73,73	1.44	9 (13%)	76,113,113	1.30	7 (9%)
14	BCR	B	4003	-	41,41,41	1.15	2 (4%)	56,56,56	1.46	9 (16%)
15	CLA	B	1222	-	65,73,73	1.44	8 (12%)	76,113,113	1.43	10 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	CLA	A	1131	-	45,53,73	1.79	8 (17%)	52,89,113	1.49	7 (13%)
15	CLA	A	1120	-	42,50,73	1.77	7 (16%)	48,85,113	1.66	7 (14%)
14	BCR	2	503	-	41,41,41	1.18	3 (7%)	56,56,56	1.20	7 (12%)
16	CHL	2	610	-	44,52,74	1.04	3 (6%)	46,87,114	1.39	7 (15%)
16	CHL	1	610	-	47,55,74	1.01	2 (4%)	50,91,114	1.31	8 (16%)
15	CLA	B	1213	-	55,63,73	1.55	6 (10%)	64,101,113	1.49	8 (12%)
15	CLA	2	603	2	65,73,73	1.49	8 (12%)	76,113,113	1.35	8 (10%)
13	XAT	3	502	-	39,47,47	2.69	19 (48%)	54,74,74	11.58	28 (51%)
15	CLA	B	1205	-	65,73,73	1.46	8 (12%)	76,113,113	1.37	7 (9%)
15	CLA	A	1112	-	65,73,73	1.46	7 (10%)	76,113,113	1.34	6 (7%)
21	SF4	C	3002	7	0,12,12	-	-	-	-	-
14	BCR	F	4001	-	41,41,41	1.17	3 (7%)	56,56,56	1.32	7 (12%)
15	CLA	1	608	-	55,63,73	1.59	7 (12%)	64,101,113	1.48	8 (12%)
14	BCR	B	4006	-	41,41,41	1.24	3 (7%)	56,56,56	1.24	7 (12%)
15	CLA	3	606	-	55,63,73	1.57	7 (12%)	64,101,113	1.46	8 (12%)
15	CLA	B	1235	-	60,68,73	1.51	9 (15%)	70,107,113	1.48	7 (10%)
15	CLA	B	1219	-	65,73,73	1.52	7 (10%)	76,113,113	1.26	7 (9%)
15	CLA	B	1231	-	60,68,73	1.51	8 (13%)	70,107,113	1.51	10 (14%)
15	CLA	3	607	-	60,68,73	1.53	6 (10%)	70,107,113	1.45	8 (11%)
18	LMG	B	5003	-	39,39,55	0.86	1 (2%)	47,47,63	1.25	3 (6%)
15	CLA	1	601	-	65,73,73	1.43	9 (13%)	76,113,113	1.34	8 (10%)
15	CLA	3	610	-	50,58,73	1.64	7 (14%)	58,95,113	1.52	9 (15%)
17	LHG	1	801	15	48,48,48	0.61	0	51,54,54	1.18	4 (7%)
15	CLA	A	1127	-	65,73,73	1.43	7 (10%)	76,113,113	1.35	6 (7%)
15	CLA	A	1123	-	65,73,73	1.46	10 (15%)	76,113,113	1.47	9 (11%)
15	CLA	A	1108	-	55,63,73	1.59	8 (14%)	64,101,113	1.58	7 (10%)
15	CLA	A	1109	-	65,73,73	1.45	10 (15%)	76,113,113	1.39	7 (9%)
14	BCR	A	4003	-	41,41,41	1.15	2 (4%)	56,56,56	1.43	10 (17%)
15	CLA	B	1236	-	49,57,73	1.71	8 (16%)	55,93,113	1.48	6 (10%)
15	CLA	A	1141	17	41,49,73	1.80	9 (21%)	47,84,113	1.57	7 (14%)
15	CLA	2	605	-	65,73,73	1.44	8 (12%)	76,113,113	1.41	8 (10%)
15	CLA	A	1107	5	51,59,73	1.64	8 (15%)	59,96,113	1.60	10 (16%)
16	CHL	2	609	2	66,74,74	0.96	5 (7%)	73,114,114	1.22	10 (13%)
15	CLA	B	1227	-	65,73,73	1.48	9 (13%)	76,113,113	1.38	7 (9%)
17	LHG	B	5001	15	41,41,48	0.72	1 (2%)	44,47,54	1.25	3 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	CLA	3	613	-	46,54,73	1.71	7 (15%)	53,90,113	1.59	6 (11%)
15	CLA	A	1134	5	42,50,73	1.77	7 (16%)	48,85,113	1.72	8 (16%)
20	PQN	A	2001	-	34,34,34	0.64	0	42,45,45	0.89	1 (2%)
15	CLA	A	1139	-	65,73,73	1.44	7 (10%)	76,113,113	1.46	10 (13%)
15	CLA	B	1220	-	51,59,73	1.68	9 (17%)	59,96,113	1.50	9 (15%)
17	LHG	2	801	15	34,34,48	0.80	1 (2%)	37,40,54	1.22	3 (8%)
15	CLA	B	1212	-	55,63,73	1.58	8 (14%)	64,101,113	1.46	7 (10%)
14	BCR	B	4005	-	41,41,41	1.24	3 (7%)	56,56,56	1.36	10 (17%)
15	CLA	4	606	-	50,58,73	1.65	8 (16%)	58,95,113	1.55	8 (13%)
15	CLA	4	616	4	51,59,73	1.64	6 (11%)	59,96,113	1.48	7 (11%)
15	CLA	B	1230	-	55,63,73	1.56	9 (16%)	64,101,113	1.51	9 (14%)
15	CLA	3	603	-	65,73,73	1.45	8 (12%)	76,113,113	1.37	5 (6%)
15	CLA	B	1239	-	42,50,73	1.80	8 (19%)	48,85,113	1.67	6 (12%)
15	CLA	B	1237	-	45,53,73	1.75	7 (15%)	52,89,113	1.58	6 (11%)
15	CLA	A	1111	-	65,73,73	1.44	8 (12%)	76,113,113	1.44	7 (9%)
15	CLA	B	1023	-	65,73,73	1.45	8 (12%)	76,113,113	1.44	7 (9%)
15	CLA	A	1012	-	65,73,73	1.45	9 (13%)	76,113,113	1.33	10 (13%)
15	CLA	1	613	-	45,53,73	1.74	6 (13%)	52,89,113	1.57	8 (15%)
15	CLA	B	1221	-	65,73,73	1.44	9 (13%)	76,113,113	1.47	7 (9%)
14	BCR	A	4008	-	41,41,41	1.17	3 (7%)	56,56,56	1.33	9 (16%)
15	CLA	B	1021	-	65,73,73	1.38	8 (12%)	76,113,113	1.34	6 (7%)
15	CLA	2	608	-	50,58,73	1.66	6 (12%)	58,95,113	1.57	8 (13%)
15	CLA	A	1106	5	65,73,73	1.44	8 (12%)	76,113,113	1.46	9 (11%)
15	CLA	3	605	-	65,73,73	1.43	9 (13%)	76,113,113	1.48	12 (15%)
15	CLA	B	1218	-	45,53,73	1.81	7 (15%)	52,89,113	1.54	4 (7%)
13	XAT	4	502	-	39,47,47	2.58	17 (43%)	54,74,74	11.25	31 (57%)
14	BCR	A	4002	-	41,41,41	1.25	4 (9%)	56,56,56	1.33	6 (10%)
15	CLA	B	1204	-	45,53,73	1.74	8 (17%)	52,89,113	1.65	9 (17%)
15	CLA	B	1211	-	65,73,73	1.46	10 (15%)	76,113,113	1.48	10 (13%)
18	LMG	2	803	-	40,40,55	0.87	1 (2%)	48,48,63	1.19	5 (10%)
15	CLA	4	603	-	65,73,73	1.49	8 (12%)	76,113,113	1.48	9 (11%)
15	CLA	1	607	17	46,54,73	1.72	7 (15%)	53,90,113	1.52	7 (13%)
15	CLA	2	601	-	65,73,73	1.47	8 (12%)	76,113,113	1.26	8 (10%)
15	CLA	J	1302	11	42,50,73	1.76	6 (14%)	48,85,113	1.70	6 (12%)
22	DGD	B	5002	-	62,62,67	0.86	2 (3%)	76,76,81	1.41	11 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	CLA	B	1224	-	61,69,73	1.54	8 (13%)	71,108,113	1.35	8 (11%)
15	CLA	4	608	-	46,54,73	1.71	9 (19%)	53,90,113	1.74	10 (18%)
15	CLA	A	1105	-	60,68,73	1.52	9 (15%)	70,107,113	1.61	14 (20%)
18	LMG	2	802	-	50,50,55	0.71	0	58,58,63	1.26	4 (6%)
15	CLA	A	1132	-	45,53,73	1.71	9 (20%)	52,89,113	1.75	9 (17%)
12	LUT	3	501	-	42,43,43	6.16	29 (69%)	51,60,60	3.18	20 (39%)
15	CLA	1	606	-	50,58,73	1.65	6 (12%)	58,95,113	1.53	8 (13%)
15	CLA	B	1228	-	60,68,73	1.54	8 (13%)	70,107,113	1.44	7 (10%)
15	CLA	A	1115	-	45,53,73	1.72	7 (15%)	52,89,113	1.63	7 (13%)
15	CLA	A	1137	-	61,69,73	1.48	7 (11%)	71,108,113	1.56	12 (16%)
18	LMG	2	804	-	50,50,55	0.72	1 (2%)	58,58,63	1.28	7 (12%)
12	LUT	2	501	-	42,43,43	6.13	31 (73%)	51,60,60	2.49	17 (33%)
15	CLA	3	601	3	60,68,73	1.49	9 (15%)	70,107,113	1.49	7 (10%)
16	CHL	4	613	-	61,69,74	0.87	2 (3%)	67,108,114	1.16	8 (11%)
17	LHG	3	801	-	46,46,48	0.66	1 (2%)	48,51,54	1.19	6 (12%)
19	CL0	A	1011	-	65,73,73	5.00	27 (41%)	76,113,113	6.07	36 (47%)
15	CLA	4	604	-	60,68,73	1.49	9 (15%)	70,107,113	1.53	10 (14%)
15	CLA	1	602	-	46,54,73	1.75	7 (15%)	53,90,113	1.48	6 (11%)
15	CLA	1	612	1	39,48,73	1.87	7 (17%)	45,82,113	1.46	5 (11%)
15	CLA	2	612	2	55,63,73	1.55	6 (10%)	64,101,113	1.48	7 (10%)
15	CLA	B	1229	-	60,68,73	1.48	6 (10%)	70,107,113	1.49	8 (11%)
15	CLA	4	609	4	60,68,73	1.49	9 (15%)	70,107,113	1.50	8 (11%)
15	CLA	A	1117	-	65,73,73	1.43	7 (10%)	76,113,113	1.47	10 (13%)
15	CLA	4	607	-	60,68,73	1.54	8 (13%)	70,107,113	1.41	8 (11%)
12	LUT	4	501	-	42,43,43	6.03	31 (73%)	51,60,60	2.90	19 (37%)
14	BCR	1	503	-	41,41,41	1.14	2 (4%)	56,56,56	1.37	13 (23%)
15	CLA	A	1128	-	65,73,73	1.45	8 (12%)	76,113,113	1.41	6 (7%)
15	CLA	B	1202	-	65,73,73	1.50	8 (12%)	76,113,113	1.37	8 (10%)
15	CLA	B	1223	-	65,73,73	1.47	8 (12%)	76,113,113	1.49	9 (11%)
17	LHG	A	5002	-	48,48,48	0.68	1 (2%)	51,54,54	1.18	4 (7%)
15	CLA	2	606	-	45,53,73	1.75	8 (17%)	52,89,113	1.57	7 (13%)

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
17	LHG	A	5001	15	-	17/53/53/53	-
15	CLA	1	605	-	1/1/20/20	14/37/115/115	-
15	CLA	3	614	-	1/1/17/20	6/22/100/115	-
14	BCR	3	506	-	-	14/29/63/63	0/2/2/2
15	CLA	B	1207	-	-	11/15/93/115	-
16	CHL	4	610	-	3/3/21/26	3/17/115/137	-
15	CLA	B	1238	-	2/2/17/20	10/18/96/115	-
15	CLA	F	1302	10	1/1/16/20	10/18/96/115	-
15	CLA	B	1217	-	1/1/15/20	7/15/93/115	-
15	CLA	B	1206	6	1/1/15/20	4/13/91/115	-
15	CLA	A	1140	-	1/1/19/20	6/33/111/115	-
15	CLA	A	1122	-	1/1/20/20	14/37/115/115	-
21	SF4	A	3001	5,6	-	-	0/6/5/5
16	CHL	2	613	-	3/3/21/26	4/15/113/137	-
14	BCR	3	504	-	-	16/29/63/63	0/2/2/2
15	CLA	B	1215	-	1/1/20/20	15/37/115/115	-
15	CLA	1	604	1	1/1/20/20	6/37/115/115	-
15	CLA	3	609	-	1/1/14/20	4/10/88/115	-
15	CLA	A	1102	-	1/1/20/20	13/37/115/115	-
13	XAT	1	502	-	-	12/31/93/93	0/4/4/4
15	CLA	B	1232	-	1/1/15/20	8/15/93/115	-
15	CLA	A	1124	-	1/1/19/20	6/31/109/115	-
15	CLA	B	1216	-	1/1/18/20	10/30/108/115	-
14	BCR	B	4004	-	-	11/29/63/63	0/2/2/2
15	CLA	A	1118	-	1/1/14/20	3/10/88/115	-
15	CLA	2	607	17	1/1/19/20	7/31/109/115	-
12	LUT	1	501	-	1/1/27/27	22/29/67/67	0/2/2/2
15	CLA	A	1126	-	1/1/20/20	13/37/115/115	-
20	PQN	B	2002	-	-	4/23/43/43	0/2/2/2
15	CLA	B	1203	-	1/1/20/20	11/37/115/115	-
15	CLA	1	615	1	1/1/15/20	12/13/91/115	-
15	CLA	4	605	-	1/1/20/20	11/37/115/115	-
15	CLA	A	1113	-	1/1/15/20	5/13/91/115	-
15	CLA	B	1226	-	1/1/20/20	10/37/115/115	-
13	XAT	2	502	-	-	12/31/93/93	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	BCR	J	4001	-	-	19/29/63/63	0/2/2/2
15	CLA	A	1104	-	1/1/20/20	11/37/115/115	-
15	CLA	4	612	4	1/1/20/20	9/37/115/115	-
18	LMG	4	801	-	-	10/32/52/70	0/1/1/1
15	CLA	3	615	3	1/1/14/20	6/10/88/115	-
15	CLA	F	1301	-	1/1/15/20	7/15/93/115	-
15	CLA	A	1129	-	1/1/18/20	9/25/103/115	-
21	SF4	C	3003	7	-	-	0/6/5/5
15	CLA	2	604	2	1/1/20/20	15/37/115/115	-
15	CLA	4	602	-	1/1/17/20	9/19/97/115	-
14	BCR	B	4002	-	-	14/29/63/63	0/2/2/2
16	CHL	3	604	3	4/4/25/26	2/33/131/137	-
15	CLA	A	1136	-	1/1/20/20	14/37/115/115	-
15	CLA	A	1133	-	1/1/20/20	18/37/115/115	-
15	CLA	A	1119	-	1/1/20/20	8/37/115/115	-
15	CLA	B	1214	-	1/1/20/20	7/37/115/115	-
15	CLA	A	1110	-	1/1/18/20	9/25/103/115	-
14	BCR	A	4005	-	-	16/29/63/63	0/2/2/2
14	BCR	3	503	-	-	17/29/63/63	0/2/2/2
14	BCR	A	4007	-	-	14/29/63/63	0/2/2/2
15	CLA	B	1208	-	1/1/19/20	10/31/109/115	-
14	BCR	F	4002	-	-	17/29/63/63	0/2/2/2
14	BCR	4	503	-	-	16/29/63/63	0/2/2/2
16	CHL	2	611	-	3/3/21/26	1/18/116/137	-
15	CLA	B	1240	17	1/1/20/20	11/37/115/115	-
14	BCR	A	4004	-	-	16/29/63/63	0/2/2/2
14	BCR	A	4006	-	-	16/29/63/63	0/2/2/2
15	CLA	2	602	-	1/1/15/20	6/13/91/115	-
15	CLA	A	1013	-	1/1/20/20	13/37/115/115	-
15	CLA	3	608	-	1/1/20/20	16/37/115/115	-
15	CLA	B	1201	-	1/1/14/20	3/11/89/115	-
15	CLA	B	1225	-	1/1/20/20	18/37/115/115	-
15	CLA	3	611	-	1/1/20/20	8/37/115/115	-
15	CLA	A	1103	-	1/1/20/20	13/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CLA	2	616	-	-	16/37/115/115	-
15	CLA	B	1210	-	-	8/37/115/115	-
15	CLA	1	611	-	1/1/16/20	7/17/95/115	-
16	CHL	4	611	-	3/3/23/26	0/21/119/137	-
15	CLA	A	1135	-	1/1/17/20	4/21/99/115	-
15	CLA	B	1234	-	1/1/18/20	12/25/103/115	-
15	CLA	3	612	3	1/1/20/20	8/37/115/115	-
14	BCR	B	4001	-	-	16/29/63/63	0/2/2/2
15	CLA	A	1130	-	1/1/15/20	7/13/91/115	-
15	CLA	A	1121	-	1/1/15/20	4/13/91/115	-
14	BCR	J	4002	-	-	17/29/63/63	0/2/2/2
15	CLA	B	1022	-	1/1/20/20	12/37/115/115	-
15	CLA	A	1114	-	1/1/18/20	11/25/103/115	-
15	CLA	1	603	-	1/1/19/20	12/31/109/115	-
15	CLA	A	1101	-	1/1/20/20	16/37/115/115	-
15	CLA	B	1209	-	1/1/15/20	6/15/93/115	-
16	CHL	1	609	1	4/4/26/26	14/39/137/137	-
15	CLA	4	601	4	1/1/19/20	7/31/109/115	-
15	CLA	A	1116	-	1/1/18/20	8/27/105/115	-
15	CLA	A	1138	-	1/1/20/20	8/37/115/115	-
15	CLA	A	1125	-	-	14/37/115/115	-
14	BCR	B	4003	-	-	22/29/63/63	0/2/2/2
15	CLA	B	1222	-	1/1/20/20	11/37/115/115	-
15	CLA	A	1131	-	1/1/15/20	4/13/91/115	-
15	CLA	A	1120	-	1/1/14/20	5/10/88/115	-
16	CHL	2	610	-	3/3/20/26	2/13/111/137	-
14	BCR	2	503	-	-	20/29/63/63	0/2/2/2
16	CHL	1	610	-	3/3/21/26	5/17/115/137	-
15	CLA	B	1213	-	1/1/18/20	5/25/103/115	-
15	CLA	2	603	2	1/1/20/20	9/37/115/115	-
13	XAT	3	502	-	-	15/31/93/93	0/4/4/4
15	CLA	B	1205	-	1/1/20/20	9/37/115/115	-
15	CLA	A	1112	-	1/1/20/20	10/37/115/115	-
21	SF4	C	3002	7	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CLA	1	608	-	1/1/18/20	9/25/103/115	-
14	BCR	F	4001	-	-	17/29/63/63	0/2/2/2
14	BCR	B	4006	-	-	15/29/63/63	0/2/2/2
15	CLA	3	606	-	1/1/18/20	8/25/103/115	-
15	CLA	B	1235	-	1/1/19/20	11/31/109/115	-
15	CLA	B	1219	-	-	15/37/115/115	-
15	CLA	B	1231	-	1/1/19/20	6/31/109/115	-
15	CLA	3	607	-	1/1/19/20	10/31/109/115	-
18	LMG	B	5003	-	-	14/34/54/70	0/1/1/1
15	CLA	1	601	-	1/1/20/20	9/37/115/115	-
15	CLA	3	610	-	1/1/17/20	9/19/97/115	-
17	LHG	1	801	15	-	22/53/53/53	-
15	CLA	A	1127	-	1/1/20/20	11/37/115/115	-
15	CLA	A	1123	-	1/1/20/20	16/37/115/115	-
15	CLA	A	1108	-	1/1/18/20	9/25/103/115	-
15	CLA	A	1109	-	1/1/20/20	13/37/115/115	-
15	CLA	B	1236	-	1/1/16/20	9/18/96/115	-
14	BCR	A	4003	-	-	16/29/63/63	0/2/2/2
15	CLA	A	1141	17	1/1/14/20	6/8/86/115	-
15	CLA	2	605	-	1/1/20/20	13/37/115/115	-
15	CLA	A	1107	5	1/1/17/20	4/21/99/115	-
16	CHL	2	609	2	4/4/26/26	13/39/137/137	-
15	CLA	B	1227	-	1/1/20/20	14/37/115/115	-
17	LHG	B	5001	15	-	26/46/46/53	-
15	CLA	3	613	-	1/1/15/20	2/15/93/115	-
15	CLA	A	1134	5	1/1/14/20	4/10/88/115	-
20	PQN	A	2001	-	-	1/23/43/43	0/2/2/2
15	CLA	A	1139	-	1/1/20/20	16/37/115/115	-
15	CLA	B	1220	-	1/1/17/20	7/21/99/115	-
17	LHG	2	801	15	-	18/39/39/53	-
15	CLA	B	1212	-	1/1/18/20	4/25/103/115	-
14	BCR	B	4005	-	-	17/29/63/63	0/2/2/2
15	CLA	4	606	-	1/1/17/20	8/19/97/115	-
15	CLA	4	616	4	1/1/17/20	9/21/99/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CLA	B	1230	-	1/1/18/20	7/25/103/115	-
15	CLA	3	603	-	1/1/20/20	15/37/115/115	-
15	CLA	B	1239	-	1/1/14/20	2/10/88/115	-
15	CLA	B	1237	-	1/1/15/20	4/13/91/115	-
15	CLA	A	1111	-	-	13/37/115/115	-
15	CLA	B	1023	-	1/1/20/20	18/37/115/115	-
15	CLA	A	1012	-	1/1/20/20	19/37/115/115	-
15	CLA	1	613	-	1/1/15/20	8/13/91/115	-
15	CLA	B	1221	-	1/1/20/20	17/37/115/115	-
15	CLA	B	1021	-	1/1/20/20	16/37/115/115	-
14	BCR	A	4008	-	-	11/29/63/63	0/2/2/2
15	CLA	2	608	-	1/1/17/20	2/19/97/115	-
15	CLA	A	1106	5	1/1/20/20	10/37/115/115	-
15	CLA	3	605	-	1/1/20/20	16/37/115/115	-
15	CLA	B	1218	-	1/1/15/20	5/13/91/115	-
13	XAT	4	502	-	-	15/31/93/93	0/4/4/4
14	BCR	A	4002	-	-	18/29/63/63	0/2/2/2
15	CLA	B	1204	-	1/1/15/20	7/13/91/115	-
15	CLA	B	1211	-	1/1/20/20	14/37/115/115	-
18	LMG	2	803	-	-	19/35/55/70	0/1/1/1
15	CLA	4	603	-	1/1/20/20	11/37/115/115	-
15	CLA	1	607	17	1/1/15/20	7/15/93/115	-
15	CLA	2	601	-	1/1/20/20	17/37/115/115	-
15	CLA	J	1302	11	1/1/14/20	5/10/88/115	-
22	DGD	B	5002	-	-	17/50/90/95	0/2/2/2
15	CLA	B	1224	-	1/1/19/20	14/33/111/115	-
15	CLA	4	608	-	1/1/15/20	6/15/93/115	-
15	CLA	A	1105	-	1/1/19/20	16/31/109/115	-
18	LMG	2	802	-	-	20/45/65/70	0/1/1/1
15	CLA	A	1132	-	1/1/15/20	7/13/91/115	-
12	LUT	3	501	-	1/1/27/27	18/29/67/67	0/2/2/2
15	CLA	1	606	-	1/1/17/20	4/19/97/115	-
15	CLA	B	1228	-	1/1/19/20	7/31/109/115	-
15	CLA	A	1115	-	1/1/15/20	3/13/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CLA	A	1137	-	1/1/19/20	11/33/111/115	-
18	LMG	2	804	-	-	24/45/65/70	0/1/1/1
12	LUT	2	501	-	1/1/27/27	18/29/67/67	0/2/2/2
15	CLA	3	601	3	1/1/19/20	13/31/109/115	-
16	CHL	4	613	-	4/4/25/26	2/33/131/137	-
17	LHG	3	801	-	-	21/49/49/53	-
19	CL0	A	1011	-	3/3/25/25	21/37/135/135	-
15	CLA	4	604	-	1/1/19/20	16/31/109/115	-
15	CLA	1	602	-	1/1/15/20	7/15/93/115	-
15	CLA	1	612	1	1/1/14/20	6/8/82/115	-
15	CLA	2	612	2	1/1/18/20	3/25/103/115	-
15	CLA	B	1229	-	1/1/19/20	7/31/109/115	-
15	CLA	4	609	4	1/1/19/20	12/31/109/115	-
15	CLA	A	1117	-	1/1/20/20	13/37/115/115	-
15	CLA	4	607	-	1/1/19/20	9/31/109/115	-
12	LUT	4	501	-	1/1/27/27	21/29/67/67	0/2/2/2
15	CLA	A	1128	-	1/1/20/20	13/37/115/115	-
14	BCR	1	503	-	-	19/29/63/63	0/2/2/2
15	CLA	B	1202	-	1/1/20/20	13/37/115/115	-
15	CLA	B	1223	-	1/1/20/20	7/37/115/115	-
17	LHG	A	5002	-	-	25/53/53/53	-
15	CLA	2	606	-	1/1/15/20	7/13/91/115	-

All (1373) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	2	501	LUT	C24-C25	21.20	1.59	1.33
12	3	501	LUT	C24-C25	21.11	1.59	1.33
12	1	501	LUT	C24-C25	21.03	1.59	1.33
12	4	501	LUT	C24-C25	20.76	1.59	1.33
19	A	1011	CL0	C1D-ND	19.62	1.61	1.37
12	3	501	LUT	C22-C21	-15.87	1.34	1.54
12	2	501	LUT	C22-C21	-15.71	1.35	1.54
12	1	501	LUT	C5-C6	15.15	1.60	1.34
12	4	501	LUT	C22-C21	-15.10	1.35	1.54
12	4	501	LUT	C5-C6	15.05	1.60	1.34
12	2	501	LUT	C5-C6	14.99	1.60	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	1	501	LUT	C22-C21	-14.87	1.36	1.54
12	3	501	LUT	C5-C6	14.79	1.60	1.34
19	A	1011	CL0	C4D-ND	13.98	1.56	1.37
12	3	501	LUT	C2-C3	-12.24	1.34	1.52
12	4	501	LUT	C2-C3	-11.88	1.35	1.52
12	2	501	LUT	C2-C3	-11.68	1.35	1.52
12	1	501	LUT	C2-C3	-11.65	1.35	1.52
19	A	1011	CL0	C1C-NC	11.62	1.55	1.37
19	A	1011	CL0	MG-NC	-9.99	1.82	2.06
19	A	1011	CL0	MG-NA	-9.91	1.82	2.06
19	A	1011	CL0	C1B-CHB	9.24	1.66	1.41
19	A	1011	CL0	CHC-C1C	9.13	1.58	1.35
19	A	1011	CL0	MG-ND	-9.02	1.87	2.05
19	A	1011	CL0	C4B-CHC	8.37	1.64	1.41
15	B	1218	CLA	C4B-NB	8.06	1.42	1.35
12	1	501	LUT	C22-C23	7.83	1.66	1.53
15	3	614	CLA	C4B-NB	7.80	1.42	1.35
15	B	1219	CLA	C4B-NB	7.67	1.42	1.35
15	B	1232	CLA	C4B-NB	7.61	1.42	1.35
12	4	501	LUT	C22-C23	7.54	1.65	1.53
15	B	1202	CLA	C4B-NB	7.52	1.41	1.35
15	2	602	CLA	C4B-NB	7.50	1.41	1.35
12	4	501	LUT	C4-C3	7.47	1.65	1.52
15	2	603	CLA	C4B-NB	7.46	1.41	1.35
15	4	603	CLA	C4B-NB	7.44	1.41	1.35
12	1	501	LUT	C4-C3	7.43	1.65	1.52
15	4	602	CLA	C4B-NB	7.43	1.41	1.35
15	A	1114	CLA	C4B-NB	7.42	1.41	1.35
12	2	501	LUT	C4-C3	7.42	1.65	1.52
12	2	501	LUT	C22-C23	7.40	1.65	1.53
15	1	602	CLA	C4B-NB	7.38	1.41	1.35
15	B	1236	CLA	C4B-NB	7.35	1.41	1.35
15	A	1110	CLA	C4B-NB	7.33	1.41	1.35
15	B	1224	CLA	C4B-NB	7.33	1.41	1.35
15	B	1207	CLA	C4B-NB	7.31	1.41	1.35
19	A	1011	CL0	CHD-C1D	7.29	1.52	1.38
15	3	607	CLA	C4B-NB	7.25	1.41	1.35
15	A	1131	CLA	C4B-NB	7.25	1.41	1.35
15	B	1022	CLA	C4B-NB	7.19	1.41	1.35
15	1	612	CLA	C4B-NB	7.17	1.41	1.35
15	A	1121	CLA	C4B-NB	7.17	1.41	1.35
15	1	613	CLA	C4B-NB	7.16	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	1	605	CLA	C4B-NB	7.16	1.41	1.35
15	1	603	CLA	C4B-NB	7.15	1.41	1.35
15	A	1140	CLA	C4B-NB	7.14	1.41	1.35
15	4	607	CLA	C4B-NB	7.14	1.41	1.35
12	3	501	LUT	C4-C3	7.14	1.64	1.52
12	3	501	LUT	C22-C23	7.13	1.64	1.53
15	F	1302	CLA	C4B-NB	7.13	1.41	1.35
15	A	1126	CLA	C4B-NB	7.12	1.41	1.35
15	2	608	CLA	C4B-NB	7.11	1.41	1.35
12	3	501	LUT	C8-C9	7.10	1.61	1.45
15	3	615	CLA	C4B-NB	7.10	1.41	1.35
15	3	609	CLA	C4B-NB	7.09	1.41	1.35
15	1	608	CLA	C4B-NB	7.09	1.41	1.35
15	1	611	CLA	C4B-NB	7.09	1.41	1.35
15	4	616	CLA	C4B-NB	7.09	1.41	1.35
15	B	1205	CLA	C4B-NB	7.07	1.41	1.35
15	B	1239	CLA	C4B-NB	7.07	1.41	1.35
15	B	1228	CLA	C4B-NB	7.06	1.41	1.35
15	2	606	CLA	C4B-NB	7.03	1.41	1.35
15	A	1101	CLA	C4B-NB	7.03	1.41	1.35
15	A	1113	CLA	C4B-NB	7.02	1.41	1.35
15	B	1208	CLA	C4B-NB	7.02	1.41	1.35
15	2	601	CLA	C4B-NB	7.01	1.41	1.35
15	B	1204	CLA	C4B-NB	6.99	1.41	1.35
15	A	1120	CLA	C4B-NB	6.99	1.41	1.35
15	1	607	CLA	C4B-NB	6.98	1.41	1.35
15	B	1238	CLA	C4B-NB	6.98	1.41	1.35
15	A	1108	CLA	C4B-NB	6.96	1.41	1.35
15	1	606	CLA	C4B-NB	6.96	1.41	1.35
15	B	1220	CLA	C4B-NB	6.96	1.41	1.35
15	B	1222	CLA	C4B-NB	6.96	1.41	1.35
15	3	603	CLA	C4B-NB	6.95	1.41	1.35
15	B	1214	CLA	C4B-NB	6.95	1.41	1.35
15	B	1201	CLA	C4B-NB	6.95	1.41	1.35
15	B	1210	CLA	C4B-NB	6.95	1.41	1.35
15	B	1237	CLA	C4B-NB	6.94	1.41	1.35
15	4	606	CLA	C4B-NB	6.94	1.41	1.35
15	B	1215	CLA	C4B-NB	6.94	1.41	1.35
15	B	1212	CLA	C4B-NB	6.93	1.41	1.35
15	3	606	CLA	C4B-NB	6.93	1.41	1.35
15	3	612	CLA	C4B-NB	6.93	1.41	1.35
15	3	608	CLA	C4B-NB	6.92	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	A	1141	CLA	C4B-NB	6.91	1.41	1.35
15	A	1134	CLA	C4B-NB	6.90	1.41	1.35
15	B	1211	CLA	C4B-NB	6.90	1.41	1.35
15	B	1217	CLA	C4B-NB	6.89	1.41	1.35
15	A	1117	CLA	C4B-NB	6.89	1.41	1.35
15	A	1129	CLA	C4B-NB	6.89	1.41	1.35
15	A	1122	CLA	C4B-NB	6.89	1.41	1.35
15	A	1133	CLA	C4B-NB	6.88	1.41	1.35
15	A	1104	CLA	C4B-NB	6.88	1.41	1.35
15	3	613	CLA	C4B-NB	6.87	1.41	1.35
15	A	1112	CLA	C4B-NB	6.86	1.41	1.35
15	2	607	CLA	C4B-NB	6.85	1.41	1.35
15	B	1209	CLA	C4B-NB	6.85	1.41	1.35
15	2	616	CLA	C4B-NB	6.85	1.41	1.35
15	4	612	CLA	C4B-NB	6.84	1.41	1.35
15	A	1130	CLA	C4B-NB	6.84	1.41	1.35
15	3	611	CLA	C4B-NB	6.84	1.41	1.35
15	B	1206	CLA	C4B-NB	6.83	1.41	1.35
15	A	1136	CLA	C4B-NB	6.83	1.41	1.35
15	3	610	CLA	C4B-NB	6.83	1.41	1.35
15	A	1115	CLA	C4B-NB	6.83	1.41	1.35
15	F	1301	CLA	C4B-NB	6.83	1.41	1.35
15	A	1102	CLA	C4B-NB	6.81	1.41	1.35
15	A	1118	CLA	C4B-NB	6.81	1.41	1.35
15	B	1223	CLA	C4B-NB	6.80	1.41	1.35
15	A	1128	CLA	C4B-NB	6.80	1.41	1.35
15	2	605	CLA	C4B-NB	6.79	1.41	1.35
15	B	1227	CLA	C4B-NB	6.79	1.41	1.35
15	B	1231	CLA	C4B-NB	6.78	1.41	1.35
15	B	1240	CLA	C4B-NB	6.78	1.41	1.35
15	B	1213	CLA	C4B-NB	6.77	1.41	1.35
15	A	1138	CLA	C4B-NB	6.77	1.41	1.35
15	J	1302	CLA	C4B-NB	6.77	1.41	1.35
19	A	1011	CL0	CHD-C4C	6.76	1.54	1.39
15	A	1111	CLA	C4B-NB	6.76	1.41	1.35
15	B	1221	CLA	C4B-NB	6.76	1.41	1.35
15	B	1229	CLA	C4B-NB	6.73	1.41	1.35
15	4	601	CLA	C4B-NB	6.73	1.41	1.35
15	A	1124	CLA	C4B-NB	6.73	1.41	1.35
15	B	1235	CLA	C4B-NB	6.73	1.41	1.35
15	1	604	CLA	C4B-NB	6.73	1.41	1.35
15	4	608	CLA	C4B-NB	6.72	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	A	1106	CLA	C4B-NB	6.72	1.41	1.35
15	A	1123	CLA	C4B-NB	6.71	1.41	1.35
15	A	1135	CLA	C4B-NB	6.71	1.41	1.35
15	4	605	CLA	C4B-NB	6.71	1.41	1.35
15	B	1225	CLA	C4B-NB	6.70	1.41	1.35
15	B	1230	CLA	C4B-NB	6.70	1.41	1.35
15	A	1137	CLA	C4B-NB	6.69	1.41	1.35
15	A	1127	CLA	C4B-NB	6.68	1.41	1.35
15	B	1023	CLA	C4B-NB	6.67	1.41	1.35
15	A	1107	CLA	C4B-NB	6.66	1.41	1.35
15	A	1139	CLA	C4B-NB	6.66	1.41	1.35
15	A	1109	CLA	C4B-NB	6.65	1.41	1.35
15	2	612	CLA	C4B-NB	6.65	1.41	1.35
15	B	1203	CLA	C4B-NB	6.63	1.41	1.35
15	B	1226	CLA	C4B-NB	6.63	1.41	1.35
15	3	601	CLA	C4B-NB	6.61	1.41	1.35
15	A	1105	CLA	C4B-NB	6.60	1.41	1.35
15	4	604	CLA	C4B-NB	6.59	1.41	1.35
15	A	1132	CLA	C4B-NB	6.59	1.41	1.35
15	1	615	CLA	C4B-NB	6.57	1.41	1.35
15	B	1216	CLA	C4B-NB	6.54	1.41	1.35
15	4	609	CLA	C4B-NB	6.54	1.41	1.35
15	2	604	CLA	C4B-NB	6.50	1.41	1.35
15	A	1012	CLA	C4B-NB	6.50	1.41	1.35
15	A	1119	CLA	C4B-NB	6.50	1.41	1.35
15	A	1013	CLA	C4B-NB	6.48	1.41	1.35
15	A	1103	CLA	C4B-NB	6.48	1.41	1.35
15	B	1234	CLA	C4B-NB	6.45	1.41	1.35
15	A	1125	CLA	C4B-NB	6.42	1.40	1.35
15	1	601	CLA	C4B-NB	6.39	1.40	1.35
15	3	605	CLA	C4B-NB	6.27	1.40	1.35
15	B	1021	CLA	C4B-NB	6.25	1.40	1.35
15	A	1116	CLA	C4B-NB	6.24	1.40	1.35
19	A	1011	CL0	C4B-NB	6.13	1.40	1.35
15	B	1238	CLA	C2-C3	6.11	1.53	1.33
12	3	501	LUT	C28-C29	5.92	1.58	1.45
12	2	501	LUT	C28-C29	5.76	1.58	1.45
12	2	501	LUT	C8-C9	5.72	1.58	1.45
12	4	501	LUT	C8-C9	5.69	1.58	1.45
12	1	501	LUT	C8-C9	5.62	1.58	1.45
19	A	1011	CL0	C1A-CHA	5.58	1.66	1.43
12	2	501	LUT	C32-C33	5.41	1.57	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	2	501	LUT	C1-C6	-5.27	1.46	1.53
12	4	501	LUT	C1-C6	-5.25	1.46	1.53
13	4	502	XAT	C8-C9	5.22	1.57	1.45
12	1	501	LUT	C1-C6	-5.21	1.46	1.53
13	4	502	XAT	C22-C23	-5.19	1.44	1.52
19	A	1011	CL0	C1B-NB	5.19	1.39	1.35
13	3	502	XAT	C8-C9	5.17	1.57	1.45
13	3	502	XAT	C28-C29	5.15	1.57	1.45
12	4	501	LUT	C32-C33	5.12	1.56	1.45
12	3	501	LUT	C15-C14	5.08	1.59	1.43
19	A	1011	CL0	C3D-CAD	5.08	1.62	1.45
13	3	502	XAT	C22-C23	-5.07	1.45	1.52
12	2	501	LUT	C15-C14	5.06	1.59	1.43
12	2	501	LUT	C4-C5	-5.01	1.43	1.51
12	4	501	LUT	C15-C14	5.01	1.59	1.43
12	3	501	LUT	C4-C5	-4.99	1.43	1.51
12	4	501	LUT	C23-C24	-4.98	1.43	1.50
13	1	502	XAT	C8-C9	4.96	1.56	1.45
13	1	502	XAT	C32-C33	4.93	1.56	1.45
12	1	501	LUT	C15-C14	4.93	1.58	1.43
13	3	502	XAT	C12-C13	4.93	1.56	1.45
13	1	502	XAT	C22-C23	-4.90	1.45	1.52
13	2	502	XAT	C28-C29	4.85	1.56	1.45
13	2	502	XAT	C22-C23	-4.84	1.45	1.52
12	4	501	LUT	C28-C29	4.81	1.56	1.45
12	3	501	LUT	C23-C24	-4.78	1.43	1.50
13	2	502	XAT	C8-C9	4.78	1.56	1.45
12	3	501	LUT	C10-C9	4.77	1.42	1.35
13	1	502	XAT	C28-C29	4.76	1.56	1.45
12	1	501	LUT	C28-C29	4.72	1.56	1.45
13	1	502	XAT	C12-C13	4.72	1.56	1.45
13	4	502	XAT	C12-C13	4.68	1.56	1.45
13	2	502	XAT	C32-C33	4.68	1.56	1.45
13	2	502	XAT	C12-C13	4.67	1.56	1.45
19	A	1011	CL0	C1C-C2C	4.66	1.53	1.44
12	1	501	LUT	C4-C5	-4.65	1.43	1.51
13	1	502	XAT	C4-C5	4.65	1.58	1.52
12	3	501	LUT	C40-C33	4.63	1.60	1.50
13	4	502	XAT	C32-C33	4.61	1.55	1.45
13	3	502	XAT	C32-C33	4.51	1.55	1.45
12	4	501	LUT	C11-C10	4.47	1.57	1.43
12	1	501	LUT	C11-C10	4.47	1.57	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	3	502	XAT	C4-C5	4.47	1.58	1.52
12	2	501	LUT	C11-C10	4.45	1.57	1.43
12	2	501	LUT	C40-C33	4.42	1.60	1.50
12	4	501	LUT	C4-C5	-4.40	1.44	1.51
12	3	501	LUT	C32-C33	4.39	1.55	1.45
12	3	501	LUT	C19-C9	4.39	1.59	1.50
13	2	502	XAT	C4-C5	4.37	1.58	1.52
12	4	501	LUT	C40-C33	4.37	1.59	1.50
12	2	501	LUT	C23-C24	-4.32	1.44	1.50
13	4	502	XAT	C28-C29	4.29	1.55	1.45
12	4	501	LUT	C21-C26	4.27	1.68	1.56
13	3	502	XAT	C11-C10	4.25	1.56	1.43
12	3	501	LUT	C21-C26	4.25	1.68	1.56
13	4	502	XAT	C11-C10	4.21	1.56	1.43
12	1	501	LUT	C23-C24	-4.18	1.44	1.50
13	4	502	XAT	C4-C5	4.17	1.58	1.52
13	2	502	XAT	C35-C34	4.17	1.56	1.43
12	1	501	LUT	C40-C33	4.16	1.59	1.50
12	3	501	LUT	C11-C10	4.15	1.56	1.43
13	4	502	XAT	C15-C14	4.14	1.56	1.43
13	3	502	XAT	C15-C14	4.12	1.56	1.43
13	1	502	XAT	C35-C34	4.11	1.56	1.43
19	A	1011	CL0	CMA-C3A	-4.10	1.44	1.53
13	2	502	XAT	C15-C14	4.09	1.56	1.43
12	2	501	LUT	C21-C26	4.08	1.67	1.56
14	B	4001	BCR	C1-C6	-4.06	1.48	1.53
13	4	502	XAT	C35-C34	4.02	1.55	1.43
12	1	501	LUT	C32-C33	4.01	1.54	1.45
13	2	502	XAT	C11-C10	4.00	1.55	1.43
12	3	501	LUT	C1-C6	-3.97	1.48	1.53
12	3	501	LUT	C35-C34	3.96	1.55	1.43
13	1	502	XAT	C31-C30	3.93	1.55	1.43
12	1	501	LUT	C21-C26	3.92	1.67	1.56
14	F	4002	BCR	C1-C6	-3.91	1.48	1.53
12	2	501	LUT	C19-C9	3.91	1.59	1.50
14	3	506	BCR	C1-C6	-3.91	1.48	1.53
12	3	501	LUT	C28-C27	3.90	1.41	1.32
19	A	1011	CL0	C4C-C3C	3.89	1.51	1.45
13	3	502	XAT	C31-C30	3.89	1.55	1.43
12	1	501	LUT	C35-C34	3.88	1.55	1.43
13	1	502	XAT	C11-C10	3.88	1.55	1.43
14	F	4001	BCR	C1-C6	-3.87	1.48	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	4002	BCR	C30-C25	-3.86	1.48	1.53
14	3	504	BCR	C30-C25	-3.86	1.48	1.53
12	4	501	LUT	C35-C34	3.85	1.55	1.43
12	4	501	LUT	C12-C13	3.84	1.54	1.45
12	4	501	LUT	C19-C9	3.84	1.58	1.50
13	1	502	XAT	C15-C14	3.84	1.55	1.43
12	1	501	LUT	C19-C9	3.83	1.58	1.50
12	2	501	LUT	C35-C34	3.83	1.55	1.43
12	2	501	LUT	C2-C1	3.83	1.66	1.54
12	1	501	LUT	C2-C1	3.82	1.66	1.54
14	A	4007	BCR	C1-C6	-3.79	1.48	1.53
15	A	1126	CLA	C1D-ND	3.76	1.42	1.37
14	3	504	BCR	C1-C6	-3.76	1.48	1.53
13	4	502	XAT	C31-C30	3.75	1.55	1.43
14	2	503	BCR	C1-C6	-3.74	1.48	1.53
12	2	501	LUT	C12-C13	3.74	1.54	1.45
14	4	503	BCR	C1-C6	-3.73	1.48	1.53
13	2	502	XAT	C31-C30	3.73	1.55	1.43
12	1	501	LUT	C12-C13	3.72	1.53	1.45
13	3	502	XAT	C35-C34	3.71	1.55	1.43
12	2	501	LUT	C10-C9	3.71	1.40	1.35
13	2	502	XAT	C24-C23	3.69	1.57	1.52
12	3	501	LUT	C2-C1	3.69	1.66	1.54
15	1	611	CLA	C1D-ND	3.68	1.42	1.37
14	B	4006	BCR	C1-C6	-3.68	1.48	1.53
12	4	501	LUT	C2-C1	3.67	1.66	1.54
12	2	501	LUT	C28-C27	3.67	1.41	1.32
14	B	4002	BCR	C30-C25	-3.66	1.48	1.53
19	A	1011	CL0	C3B-C2B	-3.66	1.35	1.40
14	J	4002	BCR	C1-C6	-3.65	1.48	1.53
12	4	501	LUT	C10-C9	3.64	1.40	1.35
14	J	4002	BCR	C30-C25	-3.64	1.48	1.53
14	A	4002	BCR	C1-C6	-3.63	1.48	1.53
14	A	4006	BCR	C1-C6	-3.63	1.48	1.53
14	A	4005	BCR	C1-C6	-3.63	1.48	1.53
14	B	4005	BCR	C1-C6	-3.63	1.48	1.53
15	B	1214	CLA	C1D-ND	3.63	1.42	1.37
15	A	1116	CLA	C1D-ND	3.61	1.42	1.37
14	B	4006	BCR	C30-C25	-3.60	1.48	1.53
15	1	615	CLA	C1D-ND	3.59	1.42	1.37
14	A	4008	BCR	C1-C6	-3.59	1.48	1.53
12	3	501	LUT	C12-C13	3.59	1.53	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	3	501	LUT	C8-C7	3.58	1.43	1.33
15	3	607	CLA	C1D-ND	3.58	1.42	1.37
14	4	503	BCR	C30-C25	-3.58	1.48	1.53
15	A	1116	CLA	C4D-ND	-3.55	1.32	1.37
14	1	503	BCR	C30-C25	-3.54	1.48	1.53
15	B	1223	CLA	C1D-ND	3.53	1.42	1.37
15	4	603	CLA	C1D-ND	3.53	1.42	1.37
15	2	616	CLA	C1D-ND	3.52	1.42	1.37
12	2	501	LUT	C31-C30	3.52	1.54	1.43
15	B	1224	CLA	C1D-ND	3.51	1.42	1.37
15	3	615	CLA	C1D-ND	3.50	1.42	1.37
15	B	1229	CLA	C1D-ND	3.50	1.42	1.37
13	3	502	XAT	C2-C1	-3.50	1.49	1.54
15	A	1114	CLA	C1D-ND	3.50	1.42	1.37
15	A	1123	CLA	C1D-ND	3.49	1.42	1.37
15	F	1301	CLA	C1D-ND	3.49	1.42	1.37
15	1	613	CLA	C1D-ND	3.49	1.42	1.37
15	3	609	CLA	C1D-ND	3.48	1.42	1.37
15	F	1302	CLA	C1D-ND	3.48	1.42	1.37
15	A	1135	CLA	C1D-ND	3.47	1.42	1.37
14	3	506	BCR	C30-C25	-3.47	1.49	1.53
15	A	1134	CLA	C1D-ND	3.47	1.42	1.37
15	1	605	CLA	C1D-ND	3.47	1.42	1.37
15	B	1239	CLA	C1D-ND	3.46	1.42	1.37
15	A	1126	CLA	C4D-ND	-3.46	1.32	1.37
15	1	615	CLA	C2-C3	3.45	1.51	1.28
15	B	1226	CLA	C4D-ND	-3.45	1.33	1.37
15	A	1137	CLA	C1D-ND	3.45	1.42	1.37
15	A	1105	CLA	C4D-ND	-3.45	1.33	1.37
15	A	1121	CLA	C1D-ND	3.44	1.42	1.37
14	B	4005	BCR	C30-C25	-3.44	1.49	1.53
15	A	1130	CLA	C1D-ND	3.44	1.42	1.37
15	3	610	CLA	C1D-ND	3.44	1.42	1.37
15	1	612	CLA	C1D-ND	3.43	1.42	1.37
15	A	1131	CLA	C1D-ND	3.43	1.42	1.37
15	B	1235	CLA	C1D-ND	3.43	1.42	1.37
15	1	602	CLA	C1D-ND	3.43	1.42	1.37
15	2	608	CLA	C1D-ND	3.43	1.42	1.37
15	2	602	CLA	C1D-ND	3.42	1.42	1.37
15	4	607	CLA	C1D-ND	3.42	1.42	1.37
15	A	1112	CLA	C4D-ND	-3.42	1.33	1.37
15	B	1202	CLA	C1D-ND	3.42	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	B	1207	CLA	C1D-ND	3.42	1.42	1.37
15	B	1228	CLA	C1D-ND	3.41	1.42	1.37
13	2	502	XAT	C2-C1	-3.41	1.49	1.54
15	B	1218	CLA	C1D-ND	3.41	1.42	1.37
13	1	502	XAT	C2-C1	-3.41	1.49	1.54
15	A	1107	CLA	C1D-ND	3.41	1.42	1.37
16	1	610	CHL	CBB-CAB	3.40	1.51	1.29
15	4	601	CLA	C4D-ND	-3.40	1.33	1.37
14	3	503	BCR	C1-C6	-3.40	1.49	1.53
15	A	1124	CLA	C1D-ND	3.40	1.42	1.37
16	4	610	CHL	CBB-CAB	3.40	1.51	1.29
14	3	503	BCR	C30-C25	-3.39	1.49	1.53
15	B	1022	CLA	C4D-ND	-3.39	1.33	1.37
15	J	1302	CLA	C1D-ND	3.39	1.42	1.37
15	A	1122	CLA	C1D-ND	3.38	1.41	1.37
15	A	1109	CLA	C1D-ND	3.38	1.41	1.37
15	4	602	CLA	C1D-ND	3.38	1.41	1.37
15	1	606	CLA	C1D-ND	3.38	1.41	1.37
15	A	1128	CLA	C4D-ND	-3.38	1.33	1.37
15	1	608	CLA	C1D-ND	3.37	1.41	1.37
15	4	609	CLA	C1D-ND	3.36	1.41	1.37
15	A	1139	CLA	C1D-ND	3.36	1.41	1.37
15	A	1141	CLA	C1D-ND	3.36	1.41	1.37
14	A	4003	BCR	C1-C6	-3.36	1.49	1.53
15	3	614	CLA	C1D-ND	3.36	1.41	1.37
15	4	606	CLA	C1D-ND	3.36	1.41	1.37
15	B	1220	CLA	C4D-ND	-3.36	1.33	1.37
15	2	603	CLA	C1D-ND	3.35	1.41	1.37
15	A	1119	CLA	C1D-ND	3.35	1.41	1.37
15	B	1210	CLA	C4D-ND	-3.35	1.33	1.37
15	B	1230	CLA	C4D-ND	-3.35	1.33	1.37
15	B	1215	CLA	C1D-ND	3.35	1.41	1.37
15	3	611	CLA	C4D-ND	-3.35	1.33	1.37
15	A	1138	CLA	C1D-ND	3.34	1.41	1.37
15	4	616	CLA	C1D-ND	3.34	1.41	1.37
14	A	4004	BCR	C30-C25	-3.34	1.49	1.53
15	2	612	CLA	C1D-ND	3.33	1.41	1.37
15	B	1232	CLA	C1D-ND	3.33	1.41	1.37
15	B	1204	CLA	C1D-ND	3.33	1.41	1.37
15	B	1209	CLA	C1D-ND	3.33	1.41	1.37
15	2	606	CLA	C1D-ND	3.33	1.41	1.37
15	B	1216	CLA	C4D-ND	-3.33	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	4	611	CHL	CBB-CAB	3.33	1.51	1.29
15	3	613	CLA	C1D-ND	3.33	1.41	1.37
15	B	1210	CLA	C1D-ND	3.33	1.41	1.37
15	B	1213	CLA	C1D-ND	3.33	1.41	1.37
15	A	1119	CLA	C4D-ND	-3.32	1.33	1.37
15	B	1215	CLA	C4D-ND	-3.32	1.33	1.37
15	B	1219	CLA	C1D-ND	3.32	1.41	1.37
15	2	604	CLA	C4D-ND	-3.32	1.33	1.37
15	A	1112	CLA	C1D-ND	3.32	1.41	1.37
15	B	1225	CLA	C1D-ND	3.32	1.41	1.37
15	A	1101	CLA	C1D-ND	3.32	1.41	1.37
15	B	1212	CLA	C1D-ND	3.32	1.41	1.37
15	A	1122	CLA	C4D-ND	-3.32	1.33	1.37
15	4	605	CLA	C1D-ND	3.31	1.41	1.37
15	3	613	CLA	C4D-ND	-3.31	1.33	1.37
15	A	1108	CLA	C1D-ND	3.31	1.41	1.37
15	B	1224	CLA	C4D-ND	-3.31	1.33	1.37
15	2	601	CLA	C1D-ND	3.31	1.41	1.37
15	B	1240	CLA	C4D-ND	-3.30	1.33	1.37
15	2	605	CLA	C4D-ND	-3.30	1.33	1.37
15	A	1128	CLA	C1D-ND	3.30	1.41	1.37
15	B	1237	CLA	C1D-ND	3.30	1.41	1.37
15	B	1201	CLA	C1D-ND	3.30	1.41	1.37
13	4	502	XAT	C2-C1	-3.30	1.49	1.54
15	A	1108	CLA	C4D-ND	-3.30	1.33	1.37
15	1	607	CLA	C1D-ND	3.30	1.41	1.37
16	2	613	CHL	CBB-CAB	3.30	1.51	1.29
15	1	601	CLA	C1D-ND	3.29	1.41	1.37
15	3	606	CLA	C4D-ND	-3.29	1.33	1.37
15	3	606	CLA	C1D-ND	3.29	1.41	1.37
15	4	601	CLA	C1D-ND	3.29	1.41	1.37
16	2	611	CHL	CBB-CAB	3.29	1.51	1.29
15	A	1125	CLA	C1D-ND	3.29	1.41	1.37
15	A	1133	CLA	C1D-ND	3.29	1.41	1.37
15	B	1217	CLA	C1D-ND	3.28	1.41	1.37
15	A	1125	CLA	C4D-ND	-3.28	1.33	1.37
15	1	601	CLA	C4D-ND	-3.28	1.33	1.37
12	1	501	LUT	C10-C9	3.28	1.40	1.35
16	4	613	CHL	CBB-CAB	3.28	1.51	1.29
15	3	601	CLA	CHC-C1C	3.28	1.43	1.35
15	4	605	CLA	C4D-ND	-3.28	1.33	1.37
15	A	1136	CLA	C1D-ND	3.27	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	B	1220	CLA	C1D-ND	3.27	1.41	1.37
15	A	1104	CLA	C4D-ND	-3.27	1.33	1.37
15	A	1113	CLA	C1D-ND	3.27	1.41	1.37
14	A	4006	BCR	C30-C25	-3.27	1.49	1.53
15	A	1139	CLA	C4D-ND	-3.26	1.33	1.37
15	A	1111	CLA	C4D-ND	-3.26	1.33	1.37
15	B	1023	CLA	C4D-ND	-3.26	1.33	1.37
15	A	1118	CLA	C1D-ND	3.26	1.41	1.37
14	A	4004	BCR	C1-C6	-3.26	1.49	1.53
15	A	1109	CLA	C4D-ND	-3.26	1.33	1.37
15	A	1136	CLA	C4D-ND	-3.26	1.33	1.37
15	A	1103	CLA	C1D-ND	3.25	1.41	1.37
15	B	1230	CLA	C1D-ND	3.25	1.41	1.37
15	B	1208	CLA	C1D-ND	3.25	1.41	1.37
15	B	1202	CLA	CHC-C1C	3.25	1.43	1.35
15	3	608	CLA	C1D-ND	3.25	1.41	1.37
15	B	1203	CLA	C1D-ND	3.25	1.41	1.37
15	B	1228	CLA	C4D-ND	-3.25	1.33	1.37
15	B	1238	CLA	C4D-ND	-3.25	1.33	1.37
15	4	609	CLA	C4D-ND	-3.25	1.33	1.37
15	A	1106	CLA	C1D-ND	3.25	1.41	1.37
15	B	1225	CLA	C4D-ND	-3.24	1.33	1.37
15	A	1107	CLA	C4D-ND	-3.24	1.33	1.37
15	A	1140	CLA	C4D-ND	-3.23	1.33	1.37
15	1	603	CLA	C1D-ND	3.23	1.41	1.37
15	A	1102	CLA	C4D-ND	-3.23	1.33	1.37
15	3	603	CLA	C1D-ND	3.23	1.41	1.37
15	B	1206	CLA	C4D-ND	-3.23	1.33	1.37
15	3	611	CLA	C1D-ND	3.23	1.41	1.37
15	B	1221	CLA	C1D-ND	3.23	1.41	1.37
15	B	1240	CLA	C1D-ND	3.23	1.41	1.37
15	B	1206	CLA	C1D-ND	3.23	1.41	1.37
15	4	612	CLA	C1D-ND	3.22	1.41	1.37
15	A	1111	CLA	C1D-ND	3.22	1.41	1.37
15	B	1022	CLA	C1D-ND	3.22	1.41	1.37
15	A	1127	CLA	C1D-ND	3.22	1.41	1.37
15	2	605	CLA	C1D-ND	3.22	1.41	1.37
15	B	1227	CLA	C1D-ND	3.22	1.41	1.37
16	3	604	CHL	CBB-CAB	3.21	1.50	1.29
15	B	1205	CLA	C1D-ND	3.21	1.41	1.37
15	4	606	CLA	C4D-ND	-3.21	1.33	1.37
15	A	1105	CLA	CHC-C1C	3.21	1.43	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	4003	BCR	C30-C25	-3.21	1.49	1.53
16	1	609	CHL	CBB-CAB	3.21	1.50	1.29
14	B	4004	BCR	C30-C25	-3.21	1.49	1.53
14	F	4002	BCR	C30-C25	-3.21	1.49	1.53
15	A	1110	CLA	C4D-ND	-3.21	1.33	1.37
15	B	1223	CLA	C4D-ND	-3.21	1.33	1.37
15	2	601	CLA	C4D-ND	-3.20	1.33	1.37
15	A	1117	CLA	C1D-ND	3.20	1.41	1.37
15	B	1227	CLA	C4D-ND	-3.20	1.33	1.37
15	B	1203	CLA	C4D-ND	-3.20	1.33	1.37
15	1	607	CLA	C4D-ND	-3.20	1.33	1.37
15	B	1209	CLA	C4D-ND	-3.20	1.33	1.37
15	B	1021	CLA	C4D-ND	-3.20	1.33	1.37
15	A	1110	CLA	C1D-ND	3.20	1.41	1.37
15	A	1012	CLA	CHC-C1C	3.20	1.43	1.35
15	B	1214	CLA	C4D-ND	-3.20	1.33	1.37
12	3	501	LUT	C7-C6	3.20	1.56	1.45
15	2	607	CLA	C1D-ND	3.20	1.41	1.37
15	4	604	CLA	C1D-ND	3.19	1.41	1.37
15	1	602	CLA	C4D-ND	-3.19	1.33	1.37
15	1	604	CLA	C4D-ND	-3.19	1.33	1.37
15	A	1129	CLA	C4D-ND	-3.19	1.33	1.37
15	4	604	CLA	C4D-ND	-3.19	1.33	1.37
15	B	1236	CLA	C1D-ND	3.18	1.41	1.37
14	A	4007	BCR	C30-C25	-3.18	1.49	1.53
15	B	1226	CLA	C1D-ND	3.18	1.41	1.37
15	B	1236	CLA	C4D-ND	-3.18	1.33	1.37
15	A	1137	CLA	C4D-ND	-3.18	1.33	1.37
12	4	501	LUT	C31-C30	3.18	1.53	1.43
15	A	1127	CLA	C4D-ND	-3.18	1.33	1.37
14	A	4005	BCR	C30-C25	-3.18	1.49	1.53
15	A	1120	CLA	C4D-ND	-3.18	1.33	1.37
15	F	1301	CLA	C4D-ND	-3.18	1.33	1.37
15	A	1104	CLA	C1D-ND	3.18	1.41	1.37
15	1	612	CLA	C4D-ND	-3.17	1.33	1.37
15	A	1102	CLA	C1D-ND	3.17	1.41	1.37
15	A	1120	CLA	C1D-ND	3.17	1.41	1.37
15	A	1141	CLA	C4D-ND	-3.17	1.33	1.37
15	B	1205	CLA	C4D-ND	-3.17	1.33	1.37
15	B	1237	CLA	C4D-ND	-3.17	1.33	1.37
15	B	1235	CLA	C4D-ND	-3.16	1.33	1.37
15	B	1212	CLA	C4D-ND	-3.16	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	2	609	CHL	CBB-CAB	3.16	1.50	1.29
15	4	616	CLA	C4D-ND	-3.16	1.33	1.37
15	A	1115	CLA	C4D-ND	-3.16	1.33	1.37
15	B	1222	CLA	C1D-ND	3.16	1.41	1.37
15	A	1140	CLA	C1D-ND	3.16	1.41	1.37
15	B	1213	CLA	C4D-ND	-3.16	1.33	1.37
15	B	1211	CLA	C1D-ND	3.16	1.41	1.37
15	4	612	CLA	C4D-ND	-3.15	1.33	1.37
15	2	601	CLA	CHC-C1C	3.15	1.43	1.35
15	B	1201	CLA	CHC-C1C	3.15	1.43	1.35
15	3	610	CLA	C4D-ND	-3.15	1.33	1.37
15	3	603	CLA	C4D-ND	-3.15	1.33	1.37
15	A	1129	CLA	C1D-ND	3.15	1.41	1.37
15	A	1121	CLA	C4D-ND	-3.15	1.33	1.37
15	B	1234	CLA	C4D-ND	-3.15	1.33	1.37
15	1	601	CLA	CHC-C1C	3.15	1.43	1.35
15	3	601	CLA	C1D-ND	3.14	1.41	1.37
15	1	615	CLA	C4D-ND	-3.14	1.33	1.37
15	A	1133	CLA	C4D-ND	-3.14	1.33	1.37
15	A	1118	CLA	C4D-ND	-3.14	1.33	1.37
12	3	501	LUT	C31-C30	3.14	1.53	1.43
15	1	613	CLA	CHC-C1C	3.14	1.43	1.35
15	A	1125	CLA	CHC-C1C	3.14	1.43	1.35
19	A	1011	CL0	O2A-CGA	3.14	1.42	1.33
15	4	608	CLA	C4D-ND	-3.13	1.33	1.37
15	B	1023	CLA	C1D-ND	3.13	1.41	1.37
15	A	1115	CLA	C1D-ND	3.13	1.41	1.37
15	2	606	CLA	C4D-ND	-3.13	1.33	1.37
15	B	1231	CLA	C4D-ND	-3.13	1.33	1.37
15	2	616	CLA	C4D-ND	-3.13	1.33	1.37
15	1	611	CLA	C4D-ND	-3.13	1.33	1.37
15	A	1130	CLA	C4D-ND	-3.12	1.33	1.37
15	J	1302	CLA	C4D-ND	-3.12	1.33	1.37
15	A	1135	CLA	C4D-ND	-3.12	1.33	1.37
15	4	607	CLA	C4D-ND	-3.12	1.33	1.37
15	B	1211	CLA	CHC-C1C	3.12	1.43	1.35
15	2	603	CLA	C4D-ND	-3.12	1.33	1.37
15	2	612	CLA	CHC-C1C	3.12	1.43	1.35
15	B	1217	CLA	C4D-ND	-3.12	1.33	1.37
15	B	1234	CLA	C1D-ND	3.11	1.41	1.37
15	3	606	CLA	CHC-C1C	3.11	1.42	1.35
15	A	1012	CLA	C4D-ND	-3.11	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	3	612	CLA	C1D-ND	3.11	1.41	1.37
15	B	1219	CLA	C4D-ND	-3.11	1.33	1.37
15	A	1132	CLA	CHC-C1C	3.10	1.42	1.35
15	2	607	CLA	C4D-ND	-3.10	1.33	1.37
15	1	606	CLA	CHC-C1C	3.10	1.42	1.35
15	A	1102	CLA	CHC-C1C	3.10	1.42	1.35
15	1	608	CLA	C4D-ND	-3.09	1.33	1.37
15	B	1220	CLA	CHC-C1C	3.09	1.42	1.35
15	2	608	CLA	CHC-C1C	3.09	1.42	1.35
15	4	604	CLA	CHC-C1C	3.09	1.42	1.35
15	2	608	CLA	C4D-ND	-3.09	1.33	1.37
15	A	1119	CLA	CHC-C1C	3.09	1.42	1.35
15	B	1211	CLA	C4D-ND	-3.09	1.33	1.37
15	B	1208	CLA	C4D-ND	-3.08	1.33	1.37
15	3	601	CLA	C4D-ND	-3.08	1.33	1.37
15	1	603	CLA	CHC-C1C	3.08	1.42	1.35
15	A	1131	CLA	C4D-ND	-3.08	1.33	1.37
19	A	1011	CL0	O2D-CGD	3.08	1.40	1.33
15	B	1222	CLA	C4D-ND	-3.08	1.33	1.37
15	A	1132	CLA	C1D-ND	3.08	1.41	1.37
15	B	1221	CLA	C4D-ND	-3.07	1.33	1.37
15	B	1207	CLA	CHC-C1C	3.07	1.42	1.35
15	1	606	CLA	C4D-ND	-3.07	1.33	1.37
12	4	501	LUT	C8-C7	3.07	1.42	1.33
15	B	1023	CLA	CHC-C1C	3.07	1.42	1.35
15	3	615	CLA	CHC-C1C	3.07	1.42	1.35
15	1	611	CLA	CHC-C1C	3.07	1.42	1.35
15	A	1013	CLA	CHC-C1C	3.07	1.42	1.35
15	3	608	CLA	C4D-ND	-3.07	1.33	1.37
15	A	1012	CLA	C1D-ND	3.07	1.41	1.37
15	A	1013	CLA	C4D-ND	-3.07	1.33	1.37
15	4	601	CLA	CHC-C1C	3.06	1.42	1.35
15	A	1121	CLA	CHC-C1C	3.06	1.42	1.35
15	B	1232	CLA	C4D-ND	-3.06	1.33	1.37
15	2	604	CLA	C1D-ND	3.06	1.41	1.37
15	A	1123	CLA	C4D-ND	-3.06	1.33	1.37
15	B	1218	CLA	C4D-ND	-3.06	1.33	1.37
15	A	1105	CLA	C1D-ND	3.06	1.41	1.37
15	A	1106	CLA	CHC-C1C	3.06	1.42	1.35
12	2	501	LUT	C8-C7	3.06	1.42	1.33
19	A	1011	CL0	C3B-CAB	3.06	1.54	1.47
15	4	612	CLA	CHC-C1C	3.06	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	A	1106	CLA	C4D-ND	-3.06	1.33	1.37
14	B	4004	BCR	C1-C6	-3.06	1.49	1.53
15	A	1134	CLA	C4D-ND	-3.05	1.33	1.37
16	2	610	CHL	CBB-CAB	3.05	1.49	1.29
14	2	503	BCR	C30-C25	-3.05	1.49	1.53
15	B	1231	CLA	CMD-C2D	-3.05	1.44	1.50
15	B	1223	CLA	CHC-C1C	3.05	1.42	1.35
15	3	614	CLA	C4D-ND	-3.05	1.33	1.37
15	3	608	CLA	CHC-C1C	3.05	1.42	1.35
15	B	1207	CLA	C4D-ND	-3.05	1.33	1.37
15	A	1113	CLA	C4D-ND	-3.04	1.33	1.37
15	B	1240	CLA	CHC-C1C	3.04	1.42	1.35
15	1	615	CLA	CHC-C1C	3.04	1.42	1.35
15	4	608	CLA	CHC-C1C	3.04	1.42	1.35
15	B	1210	CLA	CHC-C1C	3.04	1.42	1.35
15	F	1302	CLA	C4D-ND	-3.04	1.33	1.37
15	A	1114	CLA	C4D-ND	-3.04	1.33	1.37
15	3	605	CLA	C1D-ND	3.03	1.41	1.37
15	1	607	CLA	CHC-C1C	3.03	1.42	1.35
15	B	1237	CLA	CHC-C1C	3.03	1.42	1.35
14	A	4008	BCR	C30-C25	-3.03	1.49	1.53
15	2	612	CLA	C4D-ND	-3.02	1.33	1.37
15	3	607	CLA	C4D-ND	-3.02	1.33	1.37
15	B	1218	CLA	CHC-C1C	3.02	1.42	1.35
15	B	1201	CLA	C4D-ND	-3.02	1.33	1.37
15	A	1126	CLA	CHC-C1C	3.02	1.42	1.35
15	B	1204	CLA	C4D-ND	-3.02	1.33	1.37
15	4	616	CLA	CHC-C1C	3.02	1.42	1.35
15	A	1110	CLA	CHC-C1C	3.01	1.42	1.35
15	3	607	CLA	CHC-C1C	3.01	1.42	1.35
15	A	1103	CLA	CHC-C1C	3.01	1.42	1.35
15	B	1239	CLA	C4D-ND	-3.01	1.33	1.37
15	A	1115	CLA	CHC-C1C	3.01	1.42	1.35
15	A	1117	CLA	C4D-ND	-3.01	1.33	1.37
15	B	1021	CLA	C1D-ND	3.01	1.41	1.37
15	2	607	CLA	CHC-C1C	3.00	1.42	1.35
15	B	1214	CLA	CHC-C1C	3.00	1.42	1.35
15	B	1238	CLA	CHC-C1C	3.00	1.42	1.35
15	A	1101	CLA	C4D-ND	-3.00	1.33	1.37
15	A	1103	CLA	C4D-ND	-3.00	1.33	1.37
15	2	604	CLA	CHC-C1C	3.00	1.42	1.35
15	3	612	CLA	C4D-ND	-3.00	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	3	605	CLA	CHC-C1C	2.99	1.42	1.35
15	A	1013	CLA	C1D-ND	2.99	1.41	1.37
15	1	604	CLA	CHC-C1C	2.99	1.42	1.35
15	1	612	CLA	CHC-C1C	2.99	1.42	1.35
15	2	616	CLA	CHC-C1C	2.99	1.42	1.35
14	B	4002	BCR	C1-C6	-2.99	1.49	1.53
15	B	1229	CLA	C4D-ND	-2.99	1.33	1.37
15	J	1302	CLA	CHC-C1C	2.98	1.42	1.35
15	A	1133	CLA	CHC-C1C	2.98	1.42	1.35
15	4	603	CLA	C4D-ND	-2.98	1.33	1.37
15	B	1236	CLA	CHC-C1C	2.98	1.42	1.35
16	4	613	CHL	C4B-NB	2.98	1.37	1.35
15	4	606	CLA	CHC-C1C	2.98	1.42	1.35
15	3	611	CLA	CHC-C1C	2.97	1.42	1.35
15	4	607	CLA	CHC-C1C	2.97	1.42	1.35
15	1	608	CLA	CHC-C1C	2.97	1.42	1.35
15	B	1232	CLA	CHC-C1C	2.97	1.42	1.35
15	A	1124	CLA	C4D-ND	-2.97	1.33	1.37
15	3	610	CLA	CHC-C1C	2.97	1.42	1.35
15	B	1205	CLA	CHC-C1C	2.97	1.42	1.35
14	1	503	BCR	C1-C6	-2.97	1.49	1.53
15	1	613	CLA	C4D-ND	-2.97	1.33	1.37
15	2	606	CLA	CHC-C1C	2.97	1.42	1.35
15	B	1204	CLA	CHC-C1C	2.97	1.42	1.35
15	B	1221	CLA	CHC-C1C	2.97	1.42	1.35
15	1	603	CLA	C4D-ND	-2.96	1.33	1.37
15	A	1132	CLA	C4D-ND	-2.96	1.33	1.37
15	B	1219	CLA	CHC-C1C	2.96	1.42	1.35
15	4	602	CLA	C4D-ND	-2.96	1.33	1.37
15	A	1116	CLA	CHC-C1C	2.96	1.42	1.35
15	1	602	CLA	CHC-C1C	2.96	1.42	1.35
15	3	605	CLA	C4D-ND	-2.96	1.33	1.37
15	A	1127	CLA	CHC-C1C	2.96	1.42	1.35
16	1	610	CHL	C4B-NB	2.96	1.37	1.35
15	A	1129	CLA	CHC-C1C	2.95	1.42	1.35
15	A	1117	CLA	CHC-C1C	2.95	1.42	1.35
15	A	1138	CLA	C4D-ND	-2.95	1.33	1.37
15	B	1234	CLA	CHC-C1C	2.95	1.42	1.35
15	A	1140	CLA	CHC-C1C	2.95	1.42	1.35
12	4	501	LUT	C28-C27	2.95	1.39	1.32
12	2	501	LUT	C7-C6	2.95	1.55	1.45
15	A	1134	CLA	CHC-C1C	2.95	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	4	501	LUT	C7-C6	2.94	1.55	1.45
14	F	4001	BCR	C30-C25	-2.94	1.49	1.53
15	A	1133	CLA	CMB-C2B	-2.94	1.45	1.51
15	B	1228	CLA	CHC-C1C	2.94	1.42	1.35
15	B	1238	CLA	C1D-ND	2.93	1.41	1.37
15	4	603	CLA	CHC-C1C	2.93	1.42	1.35
15	B	1208	CLA	CHC-C1C	2.93	1.42	1.35
15	A	1112	CLA	CHC-C1C	2.93	1.42	1.35
15	B	1213	CLA	CHC-C1C	2.93	1.42	1.35
15	B	1224	CLA	CHC-C1C	2.93	1.42	1.35
12	1	501	LUT	C8-C7	2.93	1.41	1.33
15	B	1214	CLA	CMB-C2B	-2.93	1.45	1.51
15	B	1229	CLA	CHC-C1C	2.93	1.42	1.35
15	A	1107	CLA	CHC-C1C	2.93	1.42	1.35
15	F	1302	CLA	CHC-C1C	2.93	1.42	1.35
15	3	609	CLA	C4D-ND	-2.93	1.33	1.37
15	B	1216	CLA	C1D-ND	2.93	1.41	1.37
15	4	602	CLA	CHC-C1C	2.93	1.42	1.35
15	A	1101	CLA	CHC-C1C	2.93	1.42	1.35
15	B	1217	CLA	CHC-C1C	2.92	1.42	1.35
15	F	1301	CLA	CHC-C1C	2.92	1.42	1.35
15	B	1215	CLA	CHC-C1C	2.92	1.42	1.35
15	A	1111	CLA	CHC-C1C	2.92	1.42	1.35
12	1	501	LUT	C7-C6	2.92	1.55	1.45
15	3	614	CLA	CHC-C1C	2.92	1.42	1.35
15	B	1226	CLA	CHC-C1C	2.92	1.42	1.35
15	3	615	CLA	C4D-ND	-2.91	1.33	1.37
15	A	1130	CLA	CHC-C1C	2.91	1.42	1.35
15	B	1225	CLA	CHC-C1C	2.91	1.42	1.35
15	2	602	CLA	C4D-ND	-2.91	1.33	1.37
15	A	1138	CLA	CHC-C1C	2.90	1.42	1.35
15	4	605	CLA	CHC-C1C	2.90	1.42	1.35
15	2	602	CLA	CHC-C1C	2.90	1.42	1.35
15	2	603	CLA	CHC-C1C	2.90	1.42	1.35
13	2	502	XAT	C38-C25	2.90	1.56	1.51
15	A	1136	CLA	CHC-C1C	2.90	1.42	1.35
15	A	1138	CLA	CMB-C2B	-2.90	1.45	1.51
15	4	608	CLA	C1D-ND	2.90	1.41	1.37
15	A	1123	CLA	CMB-C2B	-2.90	1.45	1.51
15	B	1227	CLA	CMB-C2B	-2.90	1.45	1.51
16	2	613	CHL	C4B-NB	2.90	1.37	1.35
15	A	1104	CLA	CHC-C1C	2.90	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	4	502	XAT	C8-C7	2.89	1.38	1.32
15	A	1118	CLA	CHC-C1C	2.89	1.42	1.35
15	A	1136	CLA	CMB-C2B	-2.89	1.45	1.51
16	4	611	CHL	C4B-NB	2.89	1.37	1.35
15	1	604	CLA	C1D-ND	2.89	1.41	1.37
15	B	1203	CLA	CHC-C1C	2.89	1.42	1.35
15	A	1141	CLA	CHC-C1C	2.89	1.42	1.35
15	A	1131	CLA	CHC-C1C	2.88	1.42	1.35
15	A	1128	CLA	CMB-C2B	-2.88	1.45	1.51
15	1	605	CLA	C4D-ND	-2.88	1.33	1.37
15	A	1139	CLA	CHC-C1C	2.88	1.42	1.35
15	B	1231	CLA	CHC-C1C	2.88	1.42	1.35
15	B	1227	CLA	CHC-C1C	2.88	1.42	1.35
15	2	605	CLA	CHC-C1C	2.87	1.42	1.35
15	A	1140	CLA	CMB-C2B	-2.87	1.45	1.51
15	A	1110	CLA	CMB-C2B	-2.87	1.45	1.51
15	A	1108	CLA	CHC-C1C	2.87	1.42	1.35
15	B	1209	CLA	CHC-C1C	2.87	1.42	1.35
16	2	611	CHL	C4B-NB	2.86	1.37	1.35
15	B	1216	CLA	CHC-C1C	2.86	1.42	1.35
15	B	1235	CLA	CMB-C2B	-2.86	1.45	1.51
15	A	1108	CLA	CMB-C2B	-2.85	1.45	1.51
15	3	612	CLA	CMB-C2B	-2.85	1.45	1.51
15	A	1122	CLA	CMB-C2B	-2.84	1.45	1.51
15	4	601	CLA	CMB-C2B	-2.84	1.45	1.51
12	3	501	LUT	O23-C23	-2.84	1.38	1.43
15	3	613	CLA	CHC-C1C	2.84	1.42	1.35
15	B	1219	CLA	CMB-C2B	-2.84	1.45	1.51
15	3	612	CLA	CHC-C1C	2.84	1.42	1.35
15	B	1231	CLA	CMB-C2B	-2.84	1.45	1.51
12	2	501	LUT	O23-C23	-2.84	1.38	1.43
15	3	609	CLA	CMB-C2B	-2.83	1.45	1.51
15	4	603	CLA	CMB-C2B	-2.82	1.45	1.51
12	3	501	LUT	C26-C27	2.82	1.54	1.50
15	A	1120	CLA	CHC-C1C	2.82	1.42	1.35
15	1	605	CLA	CHC-C1C	2.82	1.42	1.35
15	B	1222	CLA	CHC-C1C	2.82	1.42	1.35
15	B	1231	CLA	C1D-ND	2.82	1.41	1.37
15	B	1208	CLA	CMB-C2B	-2.81	1.45	1.51
15	A	1122	CLA	CHC-C1C	2.81	1.42	1.35
15	B	1202	CLA	CMB-C2B	-2.81	1.45	1.51
12	1	501	LUT	C31-C30	2.80	1.52	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	A	1114	CLA	CHC-C1C	2.80	1.42	1.35
15	B	1230	CLA	CHC-C1C	2.80	1.42	1.35
15	B	1235	CLA	CHC-C1C	2.80	1.42	1.35
15	3	603	CLA	CMB-C2B	-2.80	1.45	1.51
12	1	501	LUT	C28-C27	2.80	1.38	1.32
15	B	1022	CLA	CHC-C1C	2.80	1.42	1.35
13	3	502	XAT	C8-C7	2.80	1.38	1.32
15	B	1202	CLA	C4D-ND	-2.79	1.33	1.37
15	B	1206	CLA	CHC-C1C	2.79	1.42	1.35
15	3	609	CLA	CHC-C1C	2.79	1.42	1.35
15	A	1124	CLA	CHC-C1C	2.78	1.42	1.35
15	B	1212	CLA	CHC-C1C	2.78	1.42	1.35
15	2	605	CLA	CMB-C2B	-2.78	1.45	1.51
15	B	1216	CLA	CMB-C2B	-2.78	1.45	1.51
15	B	1216	CLA	CMD-C2D	-2.78	1.44	1.50
16	2	609	CHL	C4B-NB	2.78	1.37	1.35
15	B	1228	CLA	CMB-C2B	-2.77	1.45	1.51
15	A	1129	CLA	CMB-C2B	-2.77	1.45	1.51
15	A	1137	CLA	CHC-C1C	2.77	1.42	1.35
12	4	501	LUT	O23-C23	-2.77	1.38	1.43
17	A	5002	LHG	O7-C5	-2.77	1.39	1.46
15	F	1301	CLA	CMB-C2B	-2.77	1.45	1.51
15	A	1135	CLA	CHC-C1C	2.76	1.42	1.35
15	A	1109	CLA	CHC-C1C	2.76	1.42	1.35
12	1	501	LUT	O23-C23	-2.76	1.38	1.43
15	A	1114	CLA	CMB-C2B	-2.76	1.45	1.51
15	4	605	CLA	CMB-C2B	-2.76	1.45	1.51
15	B	1239	CLA	CHC-C1C	2.75	1.42	1.35
15	4	609	CLA	CHC-C1C	2.75	1.42	1.35
15	A	1120	CLA	CMB-C2B	-2.75	1.45	1.51
15	B	1021	CLA	CMD-C2D	-2.75	1.45	1.50
15	2	607	CLA	CMB-C2B	-2.75	1.45	1.51
15	A	1109	CLA	CMB-C2B	-2.75	1.45	1.51
15	3	614	CLA	CMB-C2B	-2.74	1.45	1.51
14	B	4003	BCR	C1-C6	-2.74	1.50	1.53
15	B	1201	CLA	CMB-C2B	-2.74	1.45	1.51
15	A	1113	CLA	CHC-C1C	2.74	1.42	1.35
13	2	502	XAT	C8-C7	2.74	1.38	1.32
15	B	1220	CLA	CMB-C2B	-2.74	1.45	1.51
15	B	1211	CLA	CMB-C2B	-2.73	1.46	1.51
14	J	4001	BCR	C30-C25	-2.72	1.50	1.53
15	B	1212	CLA	CMB-C2B	-2.72	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	A	1105	CLA	CMB-C2B	-2.71	1.46	1.51
14	B	4001	BCR	C30-C25	-2.71	1.50	1.53
15	A	1104	CLA	CMB-C2B	-2.70	1.46	1.51
15	3	603	CLA	CHC-C1C	2.70	1.41	1.35
15	A	1102	CLA	CMB-C2B	-2.70	1.46	1.51
15	A	1141	CLA	CMB-C2B	-2.70	1.46	1.51
15	A	1125	CLA	CMB-C2B	-2.70	1.46	1.51
15	A	1124	CLA	CMB-C2B	-2.70	1.46	1.51
15	B	1217	CLA	CMB-C2B	-2.69	1.46	1.51
16	1	609	CHL	C4B-NB	2.69	1.37	1.35
15	A	1123	CLA	CHC-C1C	2.69	1.41	1.35
15	B	1240	CLA	CMB-C2B	-2.69	1.46	1.51
15	B	1234	CLA	CMB-C2B	-2.69	1.46	1.51
15	A	1116	CLA	CMB-C2B	-2.69	1.46	1.51
15	A	1103	CLA	CMB-C2B	-2.69	1.46	1.51
15	2	602	CLA	C3B-C2B	-2.69	1.36	1.40
15	A	1130	CLA	CMB-C2B	-2.68	1.46	1.51
15	2	603	CLA	CMB-C2B	-2.68	1.46	1.51
15	B	1237	CLA	CMB-C2B	-2.68	1.46	1.51
15	A	1128	CLA	CHC-C1C	2.68	1.41	1.35
15	2	601	CLA	CMB-C2B	-2.68	1.46	1.51
15	A	1137	CLA	CMB-C2B	-2.68	1.46	1.51
15	B	1205	CLA	CMB-C2B	-2.67	1.46	1.51
15	A	1012	CLA	CMB-C2B	-2.67	1.46	1.51
15	A	1139	CLA	CMB-C2B	-2.67	1.46	1.51
15	B	1210	CLA	CMB-C2B	-2.66	1.46	1.51
15	B	1225	CLA	CMB-C2B	-2.66	1.46	1.51
13	3	502	XAT	C39-C29	2.66	1.56	1.50
15	B	1203	CLA	CMB-C2B	-2.66	1.46	1.51
15	A	1129	CLA	CMD-C2D	-2.66	1.45	1.50
15	1	604	CLA	CMB-C2B	-2.66	1.46	1.51
15	A	1112	CLA	CMB-C2B	-2.66	1.46	1.51
15	B	1238	CLA	CMB-C2B	-2.66	1.46	1.51
15	A	1121	CLA	CMB-C2B	-2.66	1.46	1.51
15	A	1113	CLA	CMB-C2B	-2.66	1.46	1.51
15	3	601	CLA	CMB-C2B	-2.65	1.46	1.51
15	2	604	CLA	CMB-C2B	-2.65	1.46	1.51
15	4	602	CLA	CMB-C2B	-2.64	1.46	1.51
17	2	801	LHG	O7-C5	-2.64	1.40	1.46
15	A	1012	CLA	C3B-C2B	-2.64	1.36	1.40
15	B	1236	CLA	CMD-C2D	-2.64	1.45	1.50
15	3	605	CLA	CMB-C2B	-2.63	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	A	1134	CLA	CMB-C2B	-2.63	1.46	1.51
15	3	611	CLA	CMB-C2B	-2.63	1.46	1.51
15	3	613	CLA	CMB-C2B	-2.63	1.46	1.51
15	4	601	CLA	C3B-C2B	-2.63	1.36	1.40
15	B	1232	CLA	CMB-C2B	-2.63	1.46	1.51
15	A	1106	CLA	CMB-C2B	-2.62	1.46	1.51
15	B	1227	CLA	C3B-C2B	-2.62	1.36	1.40
15	A	1101	CLA	CMB-C2B	-2.62	1.46	1.51
15	A	1119	CLA	CMB-C2B	-2.62	1.46	1.51
15	4	608	CLA	CMB-C2B	-2.62	1.46	1.51
15	B	1204	CLA	CMB-C2B	-2.61	1.46	1.51
15	B	1239	CLA	CMB-C2B	-2.61	1.46	1.51
15	2	616	CLA	CMB-C2B	-2.61	1.46	1.51
16	3	604	CHL	C4B-NB	2.61	1.37	1.35
16	1	609	CHL	C3A-C2A	-2.60	1.47	1.54
15	B	1213	CLA	CMB-C2B	-2.60	1.46	1.51
15	1	608	CLA	CMB-C2B	-2.60	1.46	1.51
15	1	607	CLA	CMB-C2B	-2.60	1.46	1.51
15	A	1118	CLA	CMB-C2B	-2.60	1.46	1.51
15	A	1115	CLA	CMB-C2B	-2.60	1.46	1.51
15	B	1206	CLA	CMB-C2B	-2.60	1.46	1.51
15	A	1013	CLA	CMB-C2B	-2.59	1.46	1.51
15	2	602	CLA	CMB-C2B	-2.59	1.46	1.51
15	A	1138	CLA	C3B-C2B	-2.59	1.36	1.40
15	B	1209	CLA	CMB-C2B	-2.58	1.46	1.51
15	A	1131	CLA	CMB-C2B	-2.58	1.46	1.51
15	B	1226	CLA	CMD-C2D	-2.58	1.45	1.50
15	B	1023	CLA	CMB-C2B	-2.58	1.46	1.51
15	A	1107	CLA	CMB-C2B	-2.57	1.46	1.51
16	4	610	CHL	C4B-NB	2.57	1.37	1.35
15	B	1236	CLA	CMB-C2B	-2.57	1.46	1.51
15	B	1230	CLA	CMB-C2B	-2.57	1.46	1.51
14	A	4003	BCR	C30-C25	-2.57	1.50	1.53
15	1	613	CLA	CMB-C2B	-2.56	1.46	1.51
16	2	610	CHL	C4B-NB	2.56	1.37	1.35
15	J	1302	CLA	CMB-C2B	-2.55	1.46	1.51
15	1	611	CLA	CMB-C2B	-2.55	1.46	1.51
15	B	1222	CLA	CMB-C2B	-2.55	1.46	1.51
15	1	605	CLA	CMB-C2B	-2.55	1.46	1.51
15	A	1117	CLA	CMB-C2B	-2.55	1.46	1.51
15	2	612	CLA	CMB-C2B	-2.54	1.46	1.51
15	B	1022	CLA	CMB-C2B	-2.54	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	1	501	LUT	C17-C1	2.54	1.58	1.53
15	4	604	CLA	CMB-C2B	-2.54	1.46	1.51
15	B	1221	CLA	CMB-C2B	-2.54	1.46	1.51
15	B	1223	CLA	CMB-C2B	-2.54	1.46	1.51
15	4	607	CLA	CMB-C2B	-2.54	1.46	1.51
15	2	608	CLA	CMB-C2B	-2.54	1.46	1.51
15	B	1224	CLA	CMB-C2B	-2.53	1.46	1.51
15	B	1207	CLA	CMB-C2B	-2.53	1.46	1.51
15	4	612	CLA	CMB-C2B	-2.53	1.46	1.51
15	3	608	CLA	CMB-C2B	-2.53	1.46	1.51
15	2	612	CLA	CMD-C2D	-2.53	1.45	1.50
15	F	1302	CLA	CMB-C2B	-2.53	1.46	1.51
15	3	610	CLA	CMB-C2B	-2.53	1.46	1.51
15	A	1127	CLA	CMB-C2B	-2.53	1.46	1.51
15	A	1112	CLA	CMD-C2D	-2.53	1.45	1.50
15	4	606	CLA	CMB-C2B	-2.52	1.46	1.51
15	1	601	CLA	CMB-C2B	-2.52	1.46	1.51
15	4	616	CLA	CMB-C2B	-2.52	1.46	1.51
15	1	602	CLA	CMB-C2B	-2.52	1.46	1.51
15	2	606	CLA	CMB-C2B	-2.51	1.46	1.51
15	4	609	CLA	CMB-C2B	-2.51	1.46	1.51
15	1	603	CLA	CMB-C2B	-2.51	1.46	1.51
15	B	1219	CLA	C3B-C2B	-2.51	1.36	1.40
17	B	5001	LHG	O7-C5	-2.51	1.40	1.46
15	A	1110	CLA	C3B-C2B	-2.51	1.36	1.40
12	1	501	LUT	C34-C33	-2.51	1.32	1.35
22	B	5002	DGD	O2G-C2G	-2.51	1.40	1.46
13	3	502	XAT	C20-C13	2.50	1.56	1.50
13	1	502	XAT	C24-C23	2.50	1.55	1.52
15	B	1229	CLA	CMB-C2B	-2.50	1.46	1.51
15	4	608	CLA	CMD-C2D	-2.50	1.45	1.50
15	1	612	CLA	CMB-C2B	-2.50	1.46	1.51
15	B	1227	CLA	CMD-C2D	-2.49	1.45	1.50
15	1	606	CLA	CMB-C2B	-2.49	1.46	1.51
15	A	1123	CLA	CMD-C2D	-2.49	1.45	1.50
15	3	607	CLA	CMB-C2B	-2.49	1.46	1.51
15	B	1021	CLA	CMB-C2B	-2.48	1.46	1.51
15	B	1215	CLA	CMB-C2B	-2.48	1.46	1.51
15	1	612	CLA	C3B-C2B	-2.48	1.36	1.40
15	A	1126	CLA	CMB-C2B	-2.48	1.46	1.51
15	A	1106	CLA	CMD-C2D	-2.47	1.45	1.50
15	A	1111	CLA	CMB-C2B	-2.47	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	B	1239	CLA	C3B-C2B	-2.47	1.36	1.40
15	B	1201	CLA	C3B-C2B	-2.46	1.37	1.40
16	2	609	CHL	C3A-C2A	-2.46	1.47	1.54
15	B	1229	CLA	CMD-C2D	-2.46	1.45	1.50
15	2	601	CLA	C3B-C2B	-2.46	1.37	1.40
15	B	1221	CLA	CMD-C2D	-2.46	1.45	1.50
12	2	501	LUT	C17-C1	2.45	1.58	1.53
15	A	1133	CLA	C3B-C2B	-2.45	1.37	1.40
15	A	1124	CLA	CMD-C2D	-2.45	1.45	1.50
15	B	1237	CLA	CMD-C2D	-2.45	1.45	1.50
15	A	1132	CLA	CMB-C2B	-2.44	1.46	1.51
14	3	504	BCR	C33-C5	-2.44	1.46	1.50
15	1	615	CLA	CMB-C2B	-2.44	1.46	1.51
13	3	502	XAT	C28-C27	2.44	1.37	1.32
15	B	1023	CLA	CMD-C2D	-2.44	1.45	1.50
15	A	1135	CLA	CMB-C2B	-2.44	1.46	1.51
16	2	611	CHL	C3A-C2A	-2.44	1.47	1.54
15	A	1125	CLA	CMD-C2D	-2.43	1.45	1.50
18	4	801	LMG	O8-C9	-2.43	1.39	1.45
15	B	1211	CLA	CMD-C2D	-2.43	1.45	1.50
15	A	1132	CLA	C3B-C2B	-2.43	1.37	1.40
12	2	501	LUT	C31-C32	2.43	1.40	1.34
15	A	1133	CLA	CMD-C2D	-2.43	1.45	1.50
15	A	1114	CLA	C3B-C2B	-2.43	1.37	1.40
15	A	1107	CLA	CMD-C2D	-2.42	1.45	1.50
15	3	615	CLA	CMB-C2B	-2.42	1.46	1.51
15	3	603	CLA	CMD-C2D	-2.42	1.45	1.50
15	1	604	CLA	CMD-C2D	-2.42	1.45	1.50
15	A	1104	CLA	CMD-C2D	-2.42	1.45	1.50
15	A	1105	CLA	CMD-C2D	-2.42	1.45	1.50
15	4	601	CLA	C3B-CAB	-2.41	1.43	1.47
15	B	1208	CLA	C3B-C2B	-2.41	1.37	1.40
15	3	606	CLA	CMB-C2B	-2.41	1.46	1.51
15	A	1121	CLA	CMD-C2D	-2.41	1.45	1.50
15	A	1131	CLA	CMD-C2D	-2.41	1.45	1.50
15	A	1012	CLA	C3B-CAB	-2.41	1.43	1.47
15	3	612	CLA	CMD-C2D	-2.41	1.45	1.50
15	4	605	CLA	CMD-C2D	-2.41	1.45	1.50
15	A	1118	CLA	CMD-C2D	-2.40	1.45	1.50
15	A	1101	CLA	CMD-C2D	-2.40	1.45	1.50
19	A	1011	CL0	C3A-C4A	2.40	1.59	1.51
15	2	604	CLA	CMD-C2D	-2.40	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	A	1119	CLA	CMD-C2D	-2.40	1.45	1.50
15	B	1205	CLA	CMD-C2D	-2.40	1.45	1.50
15	B	1238	CLA	CMD-C2D	-2.39	1.45	1.50
15	B	1203	CLA	CMD-C2D	-2.39	1.45	1.50
15	4	616	CLA	CMD-C2D	-2.39	1.45	1.50
12	4	501	LUT	C11-C12	2.39	1.40	1.34
15	A	1136	CLA	CMD-C2D	-2.39	1.45	1.50
15	B	1209	CLA	CMD-C2D	-2.39	1.45	1.50
15	A	1116	CLA	C3B-CAB	-2.39	1.43	1.47
15	B	1218	CLA	CMD-C2D	-2.38	1.45	1.50
15	B	1202	CLA	CMD-C2D	-2.38	1.45	1.50
15	B	1021	CLA	CHC-C1C	2.38	1.41	1.35
15	B	1222	CLA	CMD-C2D	-2.38	1.45	1.50
15	4	601	CLA	CMD-C2D	-2.38	1.45	1.50
15	B	1239	CLA	CMD-C2D	-2.38	1.45	1.50
15	B	1215	CLA	CMD-C2D	-2.38	1.45	1.50
15	A	1111	CLA	CMD-C2D	-2.37	1.45	1.50
15	A	1110	CLA	CMD-C2D	-2.37	1.45	1.50
14	A	4002	BCR	C33-C5	-2.37	1.47	1.50
15	4	604	CLA	CMD-C2D	-2.37	1.45	1.50
15	A	1013	CLA	CMD-C2D	-2.37	1.45	1.50
15	A	1122	CLA	C3B-C2B	-2.37	1.37	1.40
15	B	1240	CLA	CMD-C2D	-2.37	1.45	1.50
15	A	1116	CLA	CMD-C2D	-2.37	1.45	1.50
15	B	1234	CLA	CMD-C2D	-2.37	1.45	1.50
13	1	502	XAT	C19-C9	2.36	1.55	1.50
15	A	1115	CLA	CMD-C2D	-2.36	1.45	1.50
15	B	1230	CLA	CMD-C2D	-2.36	1.45	1.50
15	3	601	CLA	CMD-C2D	-2.36	1.45	1.50
15	3	611	CLA	CMD-C2D	-2.36	1.45	1.50
15	B	1220	CLA	CMD-C2D	-2.36	1.45	1.50
13	4	502	XAT	C19-C9	2.36	1.55	1.50
15	3	613	CLA	CMC-C2C	-2.36	1.45	1.50
15	B	1201	CLA	CMD-C2D	-2.36	1.45	1.50
15	4	602	CLA	CMD-C2D	-2.36	1.45	1.50
13	3	502	XAT	C18-C5	2.35	1.55	1.51
15	2	607	CLA	CMD-C2D	-2.35	1.45	1.50
15	4	612	CLA	CMD-C2D	-2.35	1.45	1.50
12	1	501	LUT	C14-C13	-2.35	1.32	1.35
15	A	1137	CLA	CMD-C2D	-2.35	1.45	1.50
15	B	1023	CLA	CMC-C2C	-2.35	1.45	1.50
15	B	1208	CLA	CMD-C2D	-2.35	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	A	1120	CLA	CMD-C2D	-2.35	1.45	1.50
15	1	602	CLA	CMD-C2D	-2.35	1.45	1.50
15	A	1102	CLA	CMD-C2D	-2.35	1.45	1.50
16	2	610	CHL	C3A-C2A	-2.35	1.47	1.54
15	3	605	CLA	CMD-C2D	-2.35	1.45	1.50
15	4	609	CLA	CMD-C2D	-2.34	1.45	1.50
15	J	1302	CLA	CMD-C2D	-2.34	1.45	1.50
15	A	1103	CLA	CMD-C2D	-2.34	1.45	1.50
15	B	1210	CLA	CMD-C2D	-2.34	1.45	1.50
15	B	1225	CLA	CMD-C2D	-2.34	1.45	1.50
15	A	1138	CLA	CMD-C2D	-2.34	1.45	1.50
15	A	1114	CLA	CMD-C2D	-2.33	1.45	1.50
13	1	502	XAT	C18-C5	2.33	1.55	1.51
15	A	1109	CLA	CMD-C2D	-2.33	1.45	1.50
15	2	603	CLA	CMD-C2D	-2.33	1.45	1.50
15	A	1113	CLA	CMD-C2D	-2.33	1.45	1.50
18	2	803	LMG	O7-C8	-2.33	1.40	1.46
15	B	1235	CLA	C3B-C2B	-2.33	1.37	1.40
15	4	607	CLA	CMD-C2D	-2.33	1.45	1.50
13	3	502	XAT	C24-C23	2.33	1.55	1.52
15	1	606	CLA	CMD-C2D	-2.33	1.45	1.50
15	3	608	CLA	CMD-C2D	-2.33	1.45	1.50
16	4	611	CHL	C3A-C2A	-2.32	1.48	1.54
15	A	1126	CLA	CMC-C2C	-2.32	1.45	1.50
15	3	603	CLA	C3B-C2B	-2.32	1.37	1.40
15	A	1140	CLA	CMD-C2D	-2.32	1.45	1.50
15	1	608	CLA	CMD-C2D	-2.32	1.45	1.50
15	B	1224	CLA	CMD-C2D	-2.32	1.45	1.50
15	A	1132	CLA	CMD-C2D	-2.32	1.45	1.50
13	4	502	XAT	C24-C23	2.32	1.55	1.52
15	F	1301	CLA	CMD-C2D	-2.32	1.45	1.50
15	A	1135	CLA	CMD-C2D	-2.32	1.45	1.50
15	A	1117	CLA	CMD-C2D	-2.31	1.45	1.50
15	B	1220	CLA	C3B-C2B	-2.31	1.37	1.40
15	B	1022	CLA	CMD-C2D	-2.31	1.45	1.50
15	2	602	CLA	CMD-C2D	-2.31	1.45	1.50
15	B	1217	CLA	CMD-C2D	-2.31	1.45	1.50
15	A	1130	CLA	CMD-C2D	-2.30	1.45	1.50
15	B	1216	CLA	CMC-C2C	-2.30	1.45	1.50
15	B	1228	CLA	CMD-C2D	-2.30	1.45	1.50
12	4	501	LUT	C17-C1	2.30	1.58	1.53
15	B	1227	CLA	C3B-CAB	-2.30	1.43	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	4	801	LMG	O7-C8	-2.30	1.40	1.46
15	A	1127	CLA	CMD-C2D	-2.29	1.45	1.50
15	A	1128	CLA	CMC-C2C	-2.29	1.45	1.50
12	2	501	LUT	C20-C13	2.29	1.55	1.50
15	3	614	CLA	CMC-C2C	-2.28	1.46	1.50
15	A	1122	CLA	CMD-C2D	-2.28	1.46	1.50
15	B	1232	CLA	CMD-C2D	-2.28	1.46	1.50
13	3	502	XAT	C38-C25	2.28	1.55	1.51
15	3	609	CLA	C3B-C2B	-2.28	1.37	1.40
15	A	1125	CLA	C3B-CAB	-2.28	1.43	1.47
15	A	1128	CLA	CMD-C2D	-2.28	1.46	1.50
15	B	1235	CLA	CMD-C2D	-2.28	1.46	1.50
15	A	1139	CLA	CMD-C2D	-2.28	1.46	1.50
12	1	501	LUT	C11-C12	2.28	1.40	1.34
15	B	1214	CLA	CMD-C2D	-2.28	1.46	1.50
16	4	610	CHL	C3A-C2A	-2.27	1.48	1.54
15	1	605	CLA	CMD-C2D	-2.27	1.46	1.50
15	A	1109	CLA	C3B-C2B	-2.27	1.37	1.40
15	3	613	CLA	CMD-C2D	-2.27	1.46	1.50
13	1	502	XAT	C8-C7	2.27	1.37	1.32
15	B	1219	CLA	CMD-C2D	-2.27	1.46	1.50
15	F	1302	CLA	CMD-C2D	-2.26	1.46	1.50
15	A	1134	CLA	CMD-C2D	-2.26	1.46	1.50
15	B	1204	CLA	CMD-C2D	-2.26	1.46	1.50
13	3	502	XAT	C19-C9	2.26	1.55	1.50
12	4	501	LUT	C26-C27	2.26	1.53	1.50
15	B	1022	CLA	CMC-C2C	-2.26	1.46	1.50
15	B	1212	CLA	CMD-C2D	-2.26	1.46	1.50
15	B	1223	CLA	CMC-C2C	-2.26	1.46	1.50
15	A	1136	CLA	C3B-C2B	-2.26	1.37	1.40
15	3	610	CLA	CMD-C2D	-2.25	1.46	1.50
15	B	1236	CLA	C3B-C2B	-2.25	1.37	1.40
15	A	1129	CLA	CMC-C2C	-2.25	1.46	1.50
15	2	603	CLA	C3B-C2B	-2.25	1.37	1.40
15	4	603	CLA	C3B-C2B	-2.25	1.37	1.40
15	B	1223	CLA	CMD-C2D	-2.25	1.46	1.50
15	1	601	CLA	CMD-C2D	-2.25	1.46	1.50
15	A	1012	CLA	CMD-C2D	-2.25	1.46	1.50
15	A	1140	CLA	CMC-C2C	-2.25	1.46	1.50
15	A	1123	CLA	C3B-C2B	-2.25	1.37	1.40
15	A	1108	CLA	CMD-C2D	-2.25	1.46	1.50
13	4	502	XAT	C38-C25	2.25	1.55	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	B	1232	CLA	C3B-C2B	-2.24	1.37	1.40
15	B	1201	CLA	C3B-CAB	-2.24	1.43	1.47
15	A	1111	CLA	CMC-C2C	-2.24	1.46	1.50
15	B	1227	CLA	CMC-C2C	-2.24	1.46	1.50
15	1	603	CLA	CMD-C2D	-2.24	1.46	1.50
15	2	606	CLA	CMD-C2D	-2.24	1.46	1.50
15	A	1101	CLA	C3B-C2B	-2.24	1.37	1.40
15	4	606	CLA	CMC-C2C	-2.24	1.46	1.50
15	B	1230	CLA	CMC-C2C	-2.24	1.46	1.50
17	3	801	LHG	P-O6	2.23	1.68	1.59
15	4	609	CLA	C3B-CAB	-2.23	1.43	1.47
15	A	1124	CLA	C3B-C2B	-2.23	1.37	1.40
15	3	615	CLA	CMD-C2D	-2.23	1.46	1.50
15	A	1104	CLA	C3B-C2B	-2.23	1.37	1.40
15	A	1131	CLA	C3B-C2B	-2.23	1.37	1.40
15	A	1141	CLA	CMD-C2D	-2.23	1.46	1.50
15	B	1203	CLA	CMC-C2C	-2.23	1.46	1.50
12	3	501	LUT	C20-C13	2.23	1.55	1.50
15	3	607	CLA	CMD-C2D	-2.23	1.46	1.50
15	2	601	CLA	CMD-C2D	-2.23	1.46	1.50
15	A	1116	CLA	C3B-C2B	-2.23	1.37	1.40
15	2	616	CLA	CMD-C2D	-2.23	1.46	1.50
15	4	603	CLA	CMC-C2C	-2.23	1.46	1.50
15	4	606	CLA	CMD-C2D	-2.23	1.46	1.50
15	B	1237	CLA	C3B-C2B	-2.22	1.37	1.40
14	2	503	BCR	C33-C5	-2.22	1.47	1.50
15	B	1231	CLA	MG-ND	-2.22	2.01	2.05
15	A	1141	CLA	CMC-C2C	-2.22	1.46	1.50
15	B	1226	CLA	CMC-C2C	-2.22	1.46	1.50
15	A	1101	CLA	CMC-C2C	-2.22	1.46	1.50
15	4	604	CLA	CMC-C2C	-2.22	1.46	1.50
15	B	1216	CLA	MG-ND	-2.22	2.01	2.05
16	2	609	CHL	C1A-CHA	-2.22	1.33	1.43
15	1	602	CLA	C3B-C2B	-2.22	1.37	1.40
15	B	1205	CLA	C3B-C2B	-2.22	1.37	1.40
15	A	1126	CLA	CMD-C2D	-2.21	1.46	1.50
15	2	608	CLA	CMD-C2D	-2.21	1.46	1.50
15	A	1108	CLA	CMC-C2C	-2.21	1.46	1.50
15	B	1202	CLA	C3B-C2B	-2.21	1.37	1.40
15	A	1102	CLA	C3B-CAB	-2.21	1.43	1.47
15	A	1118	CLA	CMC-C2C	-2.21	1.46	1.50
19	A	1011	CL0	C1-C2	2.20	1.55	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	1	502	XAT	C38-C25	2.20	1.55	1.51
15	1	601	CLA	C3B-CAB	-2.20	1.43	1.47
15	4	607	CLA	CMC-C2C	-2.20	1.46	1.50
15	B	1236	CLA	CMC-C2C	-2.20	1.46	1.50
15	1	607	CLA	CMD-C2D	-2.20	1.46	1.50
15	2	605	CLA	CMD-C2D	-2.20	1.46	1.50
19	A	1011	CL0	CBD-CGD	-2.19	1.45	1.52
15	3	606	CLA	CMD-C2D	-2.19	1.46	1.50
16	3	604	CHL	C1D-ND	-2.19	1.35	1.37
15	3	605	CLA	C3B-C2B	-2.19	1.37	1.40
15	1	601	CLA	C3B-C2B	-2.19	1.37	1.40
15	B	1220	CLA	C3B-CAB	-2.19	1.43	1.47
15	3	611	CLA	CMC-C2C	-2.18	1.46	1.50
15	4	601	CLA	CMC-C2C	-2.18	1.46	1.50
15	A	1013	CLA	C3B-C2B	-2.18	1.37	1.40
15	3	614	CLA	CMD-C2D	-2.18	1.46	1.50
15	F	1301	CLA	C3B-C2B	-2.18	1.37	1.40
15	3	609	CLA	CMD-C2D	-2.18	1.46	1.50
14	A	4005	BCR	C33-C5	-2.18	1.47	1.50
15	B	1210	CLA	CMC-C2C	-2.17	1.46	1.50
15	B	1224	CLA	C3B-C2B	-2.17	1.37	1.40
12	2	501	LUT	C11-C12	2.17	1.40	1.34
15	2	601	CLA	CMC-C2C	-2.17	1.46	1.50
15	B	1022	CLA	C3B-C2B	-2.17	1.37	1.40
15	A	1117	CLA	CMC-C2C	-2.17	1.46	1.50
15	B	1220	CLA	CMC-C2C	-2.17	1.46	1.50
15	B	1213	CLA	CMD-C2D	-2.16	1.46	1.50
15	A	1135	CLA	CMC-C2C	-2.16	1.46	1.50
15	B	1205	CLA	CMC-C2C	-2.16	1.46	1.50
15	A	1104	CLA	CMC-C2C	-2.16	1.46	1.50
15	B	1206	CLA	CMD-C2D	-2.16	1.46	1.50
15	B	1222	CLA	CMC-C2C	-2.16	1.46	1.50
15	A	1102	CLA	CMC-C2C	-2.16	1.46	1.50
15	B	1208	CLA	C3B-CAB	-2.16	1.43	1.47
18	4	801	LMG	C7-C8	2.15	1.57	1.50
15	A	1138	CLA	C3B-CAB	-2.15	1.43	1.47
12	4	501	LUT	C34-C33	-2.15	1.32	1.35
18	B	5003	LMG	O1-C1	2.15	1.43	1.40
14	F	4001	BCR	C33-C5	-2.15	1.47	1.50
15	A	1013	CLA	C3B-CAB	-2.15	1.43	1.47
15	A	1136	CLA	CMC-C2C	-2.15	1.46	1.50
15	4	603	CLA	CMD-C2D	-2.15	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	A	1140	CLA	C3B-C2B	-2.15	1.37	1.40
15	B	1021	CLA	MG-ND	-2.15	2.01	2.05
15	A	1129	CLA	MG-ND	-2.14	2.01	2.05
15	B	1212	CLA	CMC-C2C	-2.14	1.46	1.50
15	B	1206	CLA	CMC-C2C	-2.14	1.46	1.50
15	A	1130	CLA	C3B-C2B	-2.14	1.37	1.40
15	2	616	CLA	C3B-CAB	-2.14	1.43	1.47
15	B	1214	CLA	C3B-CAB	-2.14	1.43	1.47
15	1	605	CLA	C3B-C2B	-2.14	1.37	1.40
15	B	1226	CLA	C3B-CAB	-2.14	1.43	1.47
15	B	1215	CLA	CMC-C2C	-2.14	1.46	1.50
15	B	1214	CLA	CMC-C2C	-2.14	1.46	1.50
15	B	1211	CLA	C3B-CAB	-2.14	1.43	1.47
19	A	1011	CL0	OBD-CAD	-2.13	1.18	1.22
15	4	609	CLA	CMC-C2C	-2.13	1.46	1.50
14	A	4007	BCR	C33-C5	-2.13	1.47	1.50
12	2	501	LUT	C26-C27	2.13	1.53	1.50
15	B	1232	CLA	CMC-C2C	-2.13	1.46	1.50
15	3	614	CLA	C3B-C2B	-2.12	1.37	1.40
15	B	1218	CLA	CMB-C2B	-2.12	1.47	1.51
15	1	611	CLA	CMD-C2D	-2.12	1.46	1.50
16	2	609	CHL	CHC-C1C	2.12	1.40	1.35
14	A	4002	BCR	C38-C26	-2.12	1.47	1.50
15	B	1238	CLA	C3B-C2B	-2.12	1.37	1.40
15	A	1102	CLA	C3B-C2B	-2.12	1.37	1.40
15	A	1110	CLA	CMC-C2C	-2.12	1.46	1.50
15	B	1225	CLA	CMC-C2C	-2.12	1.46	1.50
15	B	1228	CLA	C3B-C2B	-2.12	1.37	1.40
15	B	1230	CLA	C3B-C2B	-2.12	1.37	1.40
15	B	1217	CLA	CMC-C2C	-2.12	1.46	1.50
15	3	605	CLA	C4B-CHC	-2.12	1.35	1.41
15	2	603	CLA	CMC-C2C	-2.11	1.46	1.50
15	B	1214	CLA	C3B-C2B	-2.11	1.37	1.40
15	3	612	CLA	CMC-C2C	-2.11	1.46	1.50
15	A	1112	CLA	CMC-C2C	-2.11	1.46	1.50
15	A	1130	CLA	CMC-C2C	-2.11	1.46	1.50
14	3	504	BCR	C38-C26	-2.11	1.47	1.50
15	A	1121	CLA	C3B-C2B	-2.11	1.37	1.40
14	B	4005	BCR	C33-C5	-2.11	1.47	1.50
15	3	611	CLA	C3B-C2B	-2.11	1.37	1.40
15	4	607	CLA	C3B-C2B	-2.11	1.37	1.40
15	A	1106	CLA	C3B-CAB	-2.11	1.43	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	B	1223	CLA	C3B-CAB	-2.11	1.43	1.47
15	A	1109	CLA	CMC-C2C	-2.11	1.46	1.50
15	B	1204	CLA	C3B-C2B	-2.10	1.37	1.40
15	B	1239	CLA	CMC-C2C	-2.10	1.46	1.50
14	3	506	BCR	C33-C5	-2.10	1.47	1.50
15	2	607	CLA	CMC-C2C	-2.10	1.46	1.50
15	A	1113	CLA	CMC-C2C	-2.10	1.46	1.50
15	A	1114	CLA	CMC-C2C	-2.10	1.46	1.50
13	2	502	XAT	C39-C29	2.09	1.55	1.50
15	A	1108	CLA	C3B-C2B	-2.09	1.37	1.40
15	A	1132	CLA	C3B-CAB	-2.09	1.43	1.47
15	3	608	CLA	C3B-C2B	-2.09	1.37	1.40
15	B	1216	CLA	C3B-CAB	-2.09	1.43	1.47
15	B	1221	CLA	CMC-C2C	-2.09	1.46	1.50
15	A	1107	CLA	CMC-C2C	-2.09	1.46	1.50
15	A	1129	CLA	C3B-C2B	-2.09	1.37	1.40
15	4	604	CLA	C3B-CAB	-2.09	1.43	1.47
15	A	1121	CLA	CMC-C2C	-2.09	1.46	1.50
15	F	1302	CLA	CMC-C2C	-2.09	1.46	1.50
15	B	1201	CLA	CMC-C2C	-2.09	1.46	1.50
15	B	1235	CLA	C3B-CAB	-2.09	1.43	1.47
15	B	1211	CLA	CMC-C2C	-2.09	1.46	1.50
15	A	1120	CLA	CMC-C2C	-2.09	1.46	1.50
15	A	1132	CLA	C3C-C2C	2.09	1.41	1.36
15	3	603	CLA	CMC-C2C	-2.08	1.46	1.50
15	B	1240	CLA	C3B-C2B	-2.08	1.37	1.40
15	B	1209	CLA	CMC-C2C	-2.08	1.46	1.50
15	2	604	CLA	C3B-C2B	-2.08	1.37	1.40
15	A	1124	CLA	MG-ND	-2.08	2.01	2.05
15	2	607	CLA	C3B-C2B	-2.08	1.37	1.40
15	4	612	CLA	C3B-CAB	-2.08	1.43	1.47
15	4	609	CLA	C3B-C2B	-2.08	1.37	1.40
15	A	1134	CLA	CMC-C2C	-2.08	1.46	1.50
15	B	1240	CLA	C3B-CAB	-2.08	1.43	1.47
14	A	4008	BCR	C33-C5	-2.08	1.47	1.50
15	A	1125	CLA	C3B-C2B	-2.08	1.37	1.40
15	4	606	CLA	C3B-CAB	-2.07	1.43	1.47
15	4	608	CLA	MG-ND	-2.07	2.01	2.05
15	B	1231	CLA	CMC-C2C	-2.07	1.46	1.50
15	A	1139	CLA	CMC-C2C	-2.07	1.46	1.50
14	F	4002	BCR	C33-C5	-2.07	1.47	1.50
15	1	604	CLA	C3B-CAB	-2.07	1.43	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	1	604	CLA	C3B-C2B	-2.07	1.37	1.40
15	B	1204	CLA	CMC-C2C	-2.07	1.46	1.50
14	J	4002	BCR	C33-C5	-2.07	1.47	1.50
15	1	608	CLA	C3B-C2B	-2.06	1.37	1.40
15	2	605	CLA	C3B-C2B	-2.06	1.37	1.40
15	1	607	CLA	CMC-C2C	-2.06	1.46	1.50
15	B	1224	CLA	CMC-C2C	-2.06	1.46	1.50
15	B	1228	CLA	CMC-C2C	-2.06	1.46	1.50
15	A	1127	CLA	CMC-C2C	-2.06	1.46	1.50
15	2	604	CLA	C3B-CAB	-2.06	1.43	1.47
15	A	1105	CLA	C3B-CAB	-2.06	1.43	1.47
15	B	1217	CLA	C3B-C2B	-2.06	1.37	1.40
14	J	4002	BCR	C38-C26	-2.06	1.47	1.50
15	B	1221	CLA	C3B-C2B	-2.06	1.37	1.40
15	A	1131	CLA	CMC-C2C	-2.06	1.46	1.50
15	2	607	CLA	C3B-CAB	-2.06	1.43	1.47
15	A	1109	CLA	C3B-CAB	-2.06	1.43	1.47
14	A	4006	BCR	C33-C5	-2.06	1.47	1.50
13	1	502	XAT	C40-C33	2.06	1.55	1.50
15	A	1115	CLA	CMC-C2C	-2.06	1.46	1.50
15	2	606	CLA	C3B-C2B	-2.05	1.37	1.40
15	1	612	CLA	CMD-C2D	-2.05	1.46	1.50
15	A	1104	CLA	C3B-CAB	-2.05	1.43	1.47
15	B	1207	CLA	CMD-C2D	-2.05	1.46	1.50
15	B	1022	CLA	MG-ND	-2.05	2.01	2.05
15	A	1116	CLA	CMC-C2C	-2.05	1.46	1.50
15	B	1238	CLA	MG-ND	-2.05	2.01	2.05
15	A	1133	CLA	C3B-CAB	-2.05	1.43	1.47
14	3	503	BCR	C33-C5	-2.05	1.47	1.50
15	1	613	CLA	CMD-C2D	-2.05	1.46	1.50
15	2	604	CLA	CMC-C2C	-2.05	1.46	1.50
15	B	1202	CLA	CMC-C2C	-2.05	1.46	1.50
15	3	601	CLA	CMC-C2C	-2.05	1.46	1.50
15	A	1109	CLA	C4B-CHC	-2.05	1.35	1.41
15	A	1119	CLA	C3B-C2B	-2.05	1.37	1.40
15	A	1123	CLA	CMC-C2C	-2.05	1.46	1.50
15	3	610	CLA	CMC-C2C	-2.04	1.46	1.50
22	B	5002	DGD	O6D-C5D	-2.04	1.39	1.44
15	B	1203	CLA	C3B-C2B	-2.04	1.37	1.40
15	2	606	CLA	CMC-C2C	-2.04	1.46	1.50
15	A	1123	CLA	MG-ND	-2.04	2.01	2.05
15	1	615	CLA	C3B-CAB	-2.04	1.43	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	B	1211	CLA	MG-ND	-2.04	2.01	2.05
16	1	609	CHL	C1A-CHA	-2.04	1.34	1.43
12	3	501	LUT	C11-C12	2.04	1.39	1.34
15	B	1021	CLA	CMC-C2C	-2.03	1.46	1.50
19	A	1011	CL0	C5-C3	2.03	1.55	1.51
15	B	1235	CLA	CMC-C2C	-2.03	1.46	1.50
16	1	609	CHL	CHC-C1C	2.03	1.40	1.35
15	A	1106	CLA	C3B-C2B	-2.03	1.37	1.40
15	A	1122	CLA	C3B-CAB	-2.03	1.43	1.47
15	A	1122	CLA	CMC-C2C	-2.03	1.46	1.50
15	A	1105	CLA	C3B-C2B	-2.03	1.37	1.40
15	B	1221	CLA	C3B-CAB	-2.03	1.43	1.47
14	A	4004	BCR	C33-C5	-2.03	1.47	1.50
15	A	1129	CLA	C3B-CAB	-2.03	1.43	1.47
15	2	605	CLA	CMC-C2C	-2.03	1.46	1.50
15	A	1119	CLA	C3B-CAB	-2.03	1.43	1.47
15	A	1123	CLA	C4B-CHC	-2.03	1.35	1.41
15	A	1141	CLA	C3B-C2B	-2.03	1.37	1.40
15	B	1212	CLA	C3B-C2B	-2.03	1.37	1.40
15	1	605	CLA	CMC-C2C	-2.03	1.46	1.50
15	A	1137	CLA	C3B-C2B	-2.03	1.37	1.40
15	3	608	CLA	C3C-C2C	2.02	1.41	1.36
15	3	601	CLA	C3B-C2B	-2.02	1.37	1.40
15	A	1138	CLA	C4B-CHC	-2.02	1.35	1.41
15	4	602	CLA	C3B-C2B	-2.02	1.37	1.40
15	B	1211	CLA	C3B-C2B	-2.02	1.37	1.40
15	B	1218	CLA	CMC-C2C	-2.02	1.46	1.50
15	B	1234	CLA	MG-ND	-2.02	2.01	2.05
15	A	1111	CLA	C3B-CAB	-2.02	1.43	1.47
15	B	1230	CLA	MG-ND	-2.02	2.01	2.05
15	B	1222	CLA	C3B-C2B	-2.02	1.37	1.40
18	2	804	LMG	C7-C8	2.02	1.56	1.50
14	B	4006	BCR	C33-C5	-2.02	1.47	1.50
15	4	612	CLA	CMC-C2C	-2.02	1.46	1.50
15	3	605	CLA	MG-ND	-2.02	2.01	2.05
15	B	1203	CLA	C3B-CAB	-2.01	1.43	1.47
15	A	1012	CLA	CMC-C2C	-2.01	1.46	1.50
15	4	604	CLA	C3B-C2B	-2.01	1.37	1.40
15	1	604	CLA	MG-ND	-2.01	2.01	2.05
15	1	601	CLA	CMC-C2C	-2.01	1.46	1.50
15	A	1125	CLA	MG-ND	-2.01	2.01	2.05
13	4	502	XAT	C20-C13	2.01	1.55	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	4	502	XAT	C40-C33	2.01	1.55	1.50
15	A	1105	CLA	C3C-C2C	2.01	1.41	1.36
15	4	608	CLA	C3B-C2B	-2.01	1.37	1.40
15	3	606	CLA	CMC-C2C	-2.01	1.46	1.50
15	2	602	CLA	CMC-C2C	-2.01	1.46	1.50
15	A	1107	CLA	C3B-CAB	-2.01	1.43	1.47
15	A	1138	CLA	CMC-C2C	-2.01	1.46	1.50
15	A	1013	CLA	CMC-C2C	-2.01	1.46	1.50
15	1	615	CLA	CMD-C2D	-2.00	1.46	1.50
15	B	1210	CLA	C3B-CAB	-2.00	1.43	1.47
12	4	501	LUT	C14-C13	-2.00	1.33	1.35
15	4	601	CLA	MG-ND	-2.00	2.01	2.05
15	4	608	CLA	C3B-CAB	-2.00	1.43	1.47
15	B	1240	CLA	CMC-C2C	-2.00	1.46	1.50
15	A	1128	CLA	C3B-C2B	-2.00	1.37	1.40
15	3	601	CLA	C3B-CAB	-2.00	1.43	1.47
15	A	1141	CLA	C3B-CAB	-2.00	1.43	1.47
15	B	1023	CLA	C3B-CAB	-2.00	1.43	1.47

All (1617) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	3	502	XAT	O4-C5-C4	58.04	156.98	113.38
13	1	502	XAT	O4-C5-C4	57.31	156.43	113.38
13	1	502	XAT	O24-C25-C24	55.17	154.82	113.38
13	4	502	XAT	O4-C5-C4	54.25	154.14	113.38
13	2	502	XAT	O4-C5-C4	54.24	154.13	113.38
13	4	502	XAT	O24-C25-C24	53.23	153.37	113.38
13	3	502	XAT	O24-C25-C24	52.31	152.68	113.38
13	2	502	XAT	O24-C25-C24	50.29	151.16	113.38
19	A	1011	CL0	C4A-NA-C1A	-25.34	95.31	106.71
19	A	1011	CL0	C1D-ND-C4D	-25.27	88.38	106.33
19	A	1011	CL0	CHD-C4C-C3C	-15.81	101.60	124.84
19	A	1011	CL0	C1D-CHD-C4C	-13.07	97.88	126.06
13	2	502	XAT	O24-C25-C38	-12.87	99.63	115.06
13	1	502	XAT	O24-C25-C38	-12.64	99.91	115.06
13	4	502	XAT	C18-C5-C4	-12.08	100.69	114.28
13	3	502	XAT	O24-C25-C38	-11.79	100.93	115.06
13	2	502	XAT	C18-C5-C4	-11.75	101.06	114.28
13	3	502	XAT	O4-C5-C18	-11.63	101.12	115.06
13	1	502	XAT	O4-C5-C18	-11.54	101.23	115.06
19	A	1011	CL0	C1B-CHB-C4A	-11.44	107.47	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	1011	CL0	C2D-C1D-ND	11.43	118.53	110.10
19	A	1011	CL0	C4D-CHA-C1A	-11.24	107.57	121.25
13	1	502	XAT	C38-C25-C24	-11.08	101.81	114.28
13	3	502	XAT	C18-C5-C4	-11.01	101.90	114.28
13	1	502	XAT	C18-C5-C4	-10.65	102.30	114.28
13	4	502	XAT	O24-C25-C38	-10.61	102.35	115.06
19	A	1011	CL0	C3C-C4C-NC	10.48	122.33	110.57
13	4	502	XAT	C38-C25-C24	-10.24	102.75	114.28
13	3	502	XAT	C38-C25-C24	-10.08	102.94	114.28
12	4	501	LUT	C20-C13-C14	-9.62	109.45	122.92
13	3	502	XAT	C15-C14-C13	-9.57	113.66	127.31
13	4	502	XAT	C11-C10-C9	-9.06	114.38	127.31
13	2	502	XAT	O4-C5-C18	-9.03	104.23	115.06
13	4	502	XAT	O4-C5-C18	-8.71	104.62	115.06
15	B	1226	CLA	C4A-NA-C1A	8.59	110.57	106.71
13	3	502	XAT	C32-C33-C34	8.45	131.90	118.94
12	3	501	LUT	C19-C9-C10	-8.35	111.22	122.92
15	A	1138	CLA	C4A-NA-C1A	8.17	110.38	106.71
19	A	1011	CL0	C2C-C1C-NC	8.13	117.59	109.97
15	A	1114	CLA	C4A-NA-C1A	8.09	110.34	106.71
15	A	1128	CLA	C4A-NA-C1A	8.01	110.31	106.71
13	4	502	XAT	C15-C14-C13	-7.99	115.91	127.31
13	2	502	XAT	C11-C10-C9	-7.96	115.95	127.31
15	A	1135	CLA	C4A-NA-C1A	7.88	110.25	106.71
13	2	502	XAT	C38-C25-C24	-7.84	105.46	114.28
19	A	1011	CL0	C3B-C4B-NB	7.83	119.33	109.21
15	A	1132	CLA	C4A-NA-C1A	7.79	110.21	106.71
15	3	611	CLA	C4A-NA-C1A	7.78	110.20	106.71
15	B	1239	CLA	C4A-NA-C1A	7.77	110.20	106.71
19	A	1011	CL0	C2A-C1A-CHA	-7.75	110.30	123.86
13	3	502	XAT	C11-C10-C9	-7.68	116.35	127.31
15	A	1124	CLA	C4A-NA-C1A	7.68	110.16	106.71
13	3	502	XAT	C40-C33-C34	-7.65	112.21	122.92
12	3	501	LUT	C12-C13-C14	7.63	130.64	118.94
15	A	1109	CLA	C4A-NA-C1A	7.61	110.13	106.71
15	4	603	CLA	C4A-NA-C1A	7.46	110.06	106.71
12	4	501	LUT	C28-C29-C30	7.45	130.37	118.94
15	4	609	CLA	C4A-NA-C1A	7.41	110.04	106.71
12	3	501	LUT	C8-C9-C10	7.40	130.30	118.94
15	2	605	CLA	C4A-NA-C1A	7.39	110.03	106.71
13	3	502	XAT	C12-C13-C14	7.38	130.27	118.94
19	A	1011	CL0	CHD-C4C-NC	7.37	135.82	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	3	603	CLA	C4A-NA-C1A	7.37	110.02	106.71
15	A	1112	CLA	C4A-NA-C1A	7.36	110.02	106.71
15	B	1237	CLA	C4A-NA-C1A	7.36	110.01	106.71
15	F	1302	CLA	C4A-NA-C1A	7.35	110.01	106.71
12	1	501	LUT	C20-C13-C14	-7.35	112.63	122.92
15	A	1136	CLA	C4A-NA-C1A	7.34	110.01	106.71
15	3	613	CLA	C4A-NA-C1A	7.33	110.00	106.71
13	3	502	XAT	C31-C30-C29	-7.33	116.85	127.31
15	B	1235	CLA	C4A-NA-C1A	7.33	110.00	106.71
15	3	609	CLA	C4A-NA-C1A	7.30	109.99	106.71
15	A	1108	CLA	C4A-NA-C1A	7.28	109.98	106.71
15	B	1212	CLA	C4A-NA-C1A	7.28	109.98	106.71
12	4	501	LUT	C40-C33-C34	-7.26	112.75	122.92
12	3	501	LUT	C1-C6-C5	-7.24	112.42	122.61
15	A	1103	CLA	C4A-NA-C1A	7.24	109.96	106.71
15	A	1104	CLA	C4A-NA-C1A	7.23	109.96	106.71
15	A	1133	CLA	C4A-NA-C1A	7.23	109.95	106.71
15	B	1221	CLA	C4A-NA-C1A	7.22	109.95	106.71
15	B	1236	CLA	C4A-NA-C1A	7.22	109.95	106.71
13	4	502	XAT	C40-C33-C34	-7.20	112.83	122.92
15	A	1113	CLA	C4A-NA-C1A	7.17	109.93	106.71
15	B	1023	CLA	C4A-NA-C1A	7.17	109.93	106.71
15	B	1204	CLA	C4A-NA-C1A	7.12	109.91	106.71
15	3	612	CLA	C4A-NA-C1A	7.11	109.90	106.71
15	B	1021	CLA	C4A-NA-C1A	7.10	109.90	106.71
15	2	603	CLA	C4A-NA-C1A	7.10	109.90	106.71
15	B	1213	CLA	C4A-NA-C1A	7.10	109.90	106.71
15	4	606	CLA	C4A-NA-C1A	7.07	109.88	106.71
15	2	602	CLA	C4A-NA-C1A	7.06	109.88	106.71
15	B	1222	CLA	C4A-NA-C1A	7.05	109.88	106.71
15	1	608	CLA	C4A-NA-C1A	7.05	109.88	106.71
15	A	1137	CLA	C4A-NA-C1A	7.04	109.87	106.71
15	B	1203	CLA	C4A-NA-C1A	7.03	109.87	106.71
15	A	1140	CLA	C4A-NA-C1A	7.03	109.87	106.71
13	4	502	XAT	C12-C13-C14	7.02	129.71	118.94
15	1	605	CLA	C4A-NA-C1A	7.01	109.86	106.71
15	B	1231	CLA	C4A-NA-C1A	7.01	109.86	106.71
15	A	1134	CLA	C4A-NA-C1A	7.01	109.86	106.71
15	1	603	CLA	C4A-NA-C1A	7.00	109.85	106.71
15	B	1238	CLA	C4-C3-C2	-6.99	109.97	123.81
15	A	1101	CLA	C4A-NA-C1A	6.99	109.85	106.71
15	A	1122	CLA	C4A-NA-C1A	6.97	109.84	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	A	1120	CLA	C4A-NA-C1A	6.95	109.83	106.71
15	4	605	CLA	C4A-NA-C1A	6.95	109.83	106.71
15	B	1209	CLA	C4A-NA-C1A	6.94	109.83	106.71
15	4	602	CLA	C4A-NA-C1A	6.93	109.82	106.71
15	A	1117	CLA	C4A-NA-C1A	6.91	109.81	106.71
15	J	1302	CLA	C4A-NA-C1A	6.90	109.81	106.71
15	A	1111	CLA	C4A-NA-C1A	6.89	109.80	106.71
15	A	1115	CLA	C4A-NA-C1A	6.89	109.80	106.71
15	A	1013	CLA	C4A-NA-C1A	6.89	109.80	106.71
15	3	607	CLA	C4A-NA-C1A	6.88	109.80	106.71
15	B	1229	CLA	C4A-NA-C1A	6.86	109.79	106.71
15	3	614	CLA	C4A-NA-C1A	6.86	109.79	106.71
15	B	1202	CLA	C4A-NA-C1A	6.85	109.78	106.71
15	A	1139	CLA	C4A-NA-C1A	6.82	109.77	106.71
15	A	1118	CLA	C4A-NA-C1A	6.82	109.77	106.71
15	B	1227	CLA	C4A-NA-C1A	6.82	109.77	106.71
15	B	1228	CLA	C4A-NA-C1A	6.79	109.76	106.71
15	4	612	CLA	C4A-NA-C1A	6.78	109.75	106.71
15	B	1211	CLA	C4A-NA-C1A	6.78	109.75	106.71
15	B	1217	CLA	C4A-NA-C1A	6.76	109.75	106.71
15	2	607	CLA	C4A-NA-C1A	6.75	109.74	106.71
15	B	1240	CLA	C4A-NA-C1A	6.75	109.74	106.71
15	B	1223	CLA	C4A-NA-C1A	6.74	109.74	106.71
15	B	1232	CLA	C4A-NA-C1A	6.73	109.73	106.71
15	A	1130	CLA	C4A-NA-C1A	6.70	109.72	106.71
15	A	1106	CLA	C4A-NA-C1A	6.70	109.72	106.71
15	B	1220	CLA	C4A-NA-C1A	6.66	109.70	106.71
15	3	615	CLA	C4A-NA-C1A	6.64	109.69	106.71
15	4	604	CLA	C4A-NA-C1A	6.63	109.69	106.71
15	A	1121	CLA	C4A-NA-C1A	6.63	109.69	106.71
15	3	606	CLA	C4A-NA-C1A	6.61	109.68	106.71
15	2	612	CLA	C4A-NA-C1A	6.60	109.67	106.71
15	A	1123	CLA	C4A-NA-C1A	6.59	109.67	106.71
15	1	606	CLA	C4A-NA-C1A	6.58	109.66	106.71
13	2	502	XAT	C18-C5-C6	-6.58	111.24	122.26
15	A	1119	CLA	C4A-NA-C1A	6.57	109.66	106.71
15	F	1301	CLA	C4A-NA-C1A	6.56	109.65	106.71
15	B	1215	CLA	C4A-NA-C1A	6.55	109.65	106.71
15	B	1206	CLA	C4A-NA-C1A	6.54	109.64	106.71
15	1	604	CLA	C4A-NA-C1A	6.52	109.64	106.71
15	2	606	CLA	C4A-NA-C1A	6.52	109.64	106.71
15	B	1225	CLA	C4A-NA-C1A	6.52	109.64	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	1011	CL0	C3D-C4D-ND	6.52	120.78	110.24
15	2	616	CLA	C4A-NA-C1A	6.51	109.63	106.71
15	B	1234	CLA	C4A-NA-C1A	6.50	109.63	106.71
15	B	1214	CLA	C4A-NA-C1A	6.50	109.63	106.71
15	A	1110	CLA	C4A-NA-C1A	6.49	109.62	106.71
15	A	1131	CLA	C4A-NA-C1A	6.48	109.62	106.71
15	A	1107	CLA	C4A-NA-C1A	6.48	109.62	106.71
12	2	501	LUT	C28-C29-C30	6.46	128.86	118.94
15	3	601	CLA	C4A-NA-C1A	6.46	109.61	106.71
15	A	1105	CLA	C4A-NA-C1A	6.45	109.61	106.71
15	4	607	CLA	C4A-NA-C1A	6.43	109.60	106.71
13	2	502	XAT	C15-C14-C13	-6.43	118.13	127.31
15	B	1224	CLA	C4A-NA-C1A	6.42	109.59	106.71
13	2	502	XAT	C7-C8-C9	-6.41	115.58	125.53
15	A	1141	CLA	C4A-NA-C1A	6.39	109.58	106.71
15	2	604	CLA	C4A-NA-C1A	6.39	109.58	106.71
15	A	1102	CLA	C4A-NA-C1A	6.38	109.57	106.71
15	3	610	CLA	C4A-NA-C1A	6.36	109.57	106.71
12	2	501	LUT	C40-C33-C34	-6.36	114.01	122.92
13	2	502	XAT	C40-C33-C34	-6.35	114.03	122.92
15	B	1218	CLA	C4A-NA-C1A	6.34	109.56	106.71
15	1	607	CLA	C4A-NA-C1A	6.31	109.55	106.71
15	B	1205	CLA	C4A-NA-C1A	6.28	109.53	106.71
15	B	1230	CLA	C4A-NA-C1A	6.26	109.52	106.71
15	3	605	CLA	C4A-NA-C1A	6.25	109.52	106.71
15	A	1129	CLA	C4A-NA-C1A	6.24	109.51	106.71
15	1	601	CLA	C4A-NA-C1A	6.21	109.50	106.71
15	B	1022	CLA	C4A-NA-C1A	6.20	109.50	106.71
12	3	501	LUT	C38-C25-C24	-6.19	110.32	123.56
15	B	1216	CLA	C4A-NA-C1A	6.18	109.48	106.71
13	2	502	XAT	C11-C12-C13	-6.18	109.06	126.42
15	1	602	CLA	C4A-NA-C1A	6.16	109.48	106.71
15	1	613	CLA	C4A-NA-C1A	6.15	109.47	106.71
15	3	608	CLA	C4A-NA-C1A	6.14	109.47	106.71
19	A	1011	CL0	CAC-C3C-C4C	6.12	132.76	124.81
12	3	501	LUT	C28-C29-C30	6.11	128.32	118.94
15	B	1208	CLA	C4A-NA-C1A	6.11	109.45	106.71
15	A	1127	CLA	C4A-NA-C1A	6.11	109.45	106.71
13	4	502	XAT	C32-C33-C34	6.10	128.30	118.94
15	1	615	CLA	C4A-NA-C1A	6.10	109.45	106.71
15	B	1207	CLA	C4A-NA-C1A	6.08	109.44	106.71
13	4	502	XAT	C18-C5-C6	-6.04	112.13	122.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	1	611	CLA	C4A-NA-C1A	6.01	109.41	106.71
15	4	616	CLA	C4A-NA-C1A	6.01	109.41	106.71
15	2	608	CLA	C4A-NA-C1A	6.01	109.41	106.71
15	B	1219	CLA	C4A-NA-C1A	6.00	109.41	106.71
15	B	1210	CLA	C4A-NA-C1A	5.96	109.39	106.71
15	B	1201	CLA	C4A-NA-C1A	5.96	109.38	106.71
15	1	612	CLA	C4A-NA-C1A	5.93	109.37	106.71
15	4	601	CLA	C4A-NA-C1A	5.87	109.35	106.71
12	3	501	LUT	C39-C29-C30	-5.87	114.70	122.92
15	2	601	CLA	C4A-NA-C1A	5.84	109.33	106.71
15	A	1116	CLA	C4A-NA-C1A	5.83	109.33	106.71
13	2	502	XAT	C32-C33-C34	5.82	127.88	118.94
15	B	1238	CLA	C1-C2-C3	-5.77	113.32	126.57
13	4	502	XAT	C11-C12-C13	-5.77	110.22	126.42
15	4	608	CLA	C4A-NA-C1A	5.75	109.29	106.71
15	B	1238	CLA	CAC-C3C-C4C	5.74	132.26	124.81
13	1	502	XAT	C18-C5-C6	-5.68	112.74	122.26
15	4	608	CLA	CAC-C3C-C4C	5.66	132.16	124.81
15	A	1012	CLA	C4A-NA-C1A	5.63	109.24	106.71
15	A	1126	CLA	C4A-NA-C1A	5.62	109.23	106.71
12	2	501	LUT	C20-C13-C14	-5.61	115.06	122.92
15	B	1238	CLA	C4A-NA-C1A	5.61	109.23	106.71
15	A	1125	CLA	C4A-NA-C1A	5.59	109.22	106.71
12	4	501	LUT	C12-C13-C14	5.50	127.38	118.94
13	1	502	XAT	C11-C10-C9	-5.48	119.48	127.31
13	4	502	XAT	C15-C35-C34	-5.47	112.26	123.47
12	2	501	LUT	C38-C25-C24	-5.45	111.91	123.56
12	1	501	LUT	C1-C6-C5	-5.27	115.19	122.61
12	2	501	LUT	C39-C29-C30	-5.26	115.56	122.92
19	A	1011	CL0	CHC-C1C-C2C	-5.21	112.30	126.72
13	3	502	XAT	C18-C5-C6	-5.18	113.58	122.26
13	4	502	XAT	C8-C9-C10	5.18	126.89	118.94
12	2	501	LUT	C1-C6-C5	-5.18	115.32	122.61
16	4	610	CHL	CHD-C4C-C3C	5.09	132.33	124.84
13	3	502	XAT	C15-C35-C34	-5.08	113.07	123.47
13	2	502	XAT	C15-C35-C34	-5.03	113.17	123.47
12	1	501	LUT	C28-C29-C30	5.02	126.64	118.94
13	2	502	XAT	C31-C30-C29	-5.01	120.16	127.31
19	A	1011	CL0	C4D-C3D-CAD	4.94	113.92	108.10
12	4	501	LUT	C18-C5-C6	-4.93	119.00	124.53
19	A	1011	CL0	CHD-C1D-C2D	-4.89	115.22	125.48
13	4	502	XAT	C20-C13-C12	-4.87	110.40	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	2	502	XAT	C12-C13-C14	4.87	126.41	118.94
13	4	502	XAT	C7-C8-C9	-4.86	117.99	125.53
12	2	501	LUT	C19-C9-C10	-4.83	116.15	122.92
13	3	502	XAT	C20-C13-C12	-4.79	110.53	118.08
12	1	501	LUT	C18-C5-C6	-4.78	119.16	124.53
13	3	502	XAT	C35-C34-C33	4.78	134.13	127.31
15	1	603	CLA	CMB-C2B-C1B	-4.78	121.12	128.46
13	3	502	XAT	C8-C9-C10	4.74	126.22	118.94
13	3	502	XAT	C7-C8-C9	-4.74	118.18	125.53
12	1	501	LUT	C12-C13-C14	4.63	126.04	118.94
12	3	501	LUT	C18-C5-C6	-4.57	119.39	124.53
12	1	501	LUT	C39-C29-C30	-4.53	116.58	122.92
13	4	502	XAT	C31-C30-C29	-4.53	120.84	127.31
15	B	1214	CLA	CMB-C2B-C1B	-4.50	121.54	128.46
12	4	501	LUT	C19-C9-C10	-4.48	116.65	122.92
12	1	501	LUT	C19-C9-C10	-4.46	116.67	122.92
15	3	614	CLA	CMB-C2B-C1B	-4.45	121.62	128.46
13	4	502	XAT	C26-C27-C28	-4.44	116.60	125.99
13	1	502	XAT	C15-C14-C13	-4.37	121.07	127.31
15	A	1105	CLA	CMB-C2B-C1B	-4.37	121.75	128.46
16	2	609	CHL	CHD-C1D-ND	-4.36	120.45	124.45
12	3	501	LUT	C20-C13-C14	-4.30	116.89	122.92
15	A	1110	CLA	CAA-C2A-C3A	-4.28	101.06	112.78
17	B	5001	LHG	O4-P-O5	4.27	133.34	112.24
17	1	801	LHG	O4-P-O5	4.26	133.30	112.24
17	A	5002	LHG	O4-P-O5	4.23	133.18	112.24
17	A	5001	LHG	O4-P-O5	4.23	133.16	112.24
16	2	611	CHL	CHD-C1D-ND	-4.20	120.59	124.45
15	B	1211	CLA	CMB-C2B-C1B	-4.20	122.02	128.46
12	4	501	LUT	C38-C25-C24	-4.19	114.60	123.56
15	A	1139	CLA	CMB-C2B-C1B	-4.19	122.03	128.46
17	2	801	LHG	O4-P-O5	4.18	132.90	112.24
15	A	1107	CLA	CAA-C2A-C3A	-4.14	101.43	112.78
13	2	502	XAT	C35-C15-C14	4.14	131.96	123.47
17	3	801	LHG	O4-P-O5	4.14	132.71	112.24
14	A	4004	BCR	C15-C16-C17	-4.12	115.04	123.47
15	B	1228	CLA	CMB-C2B-C1B	-4.11	122.14	128.46
13	2	502	XAT	C38-C25-C26	-4.10	115.38	122.26
12	3	501	LUT	C32-C33-C34	4.10	125.23	118.94
13	1	502	XAT	C31-C30-C29	-4.09	121.47	127.31
15	B	1216	CLA	CMB-C2B-C1B	-4.08	122.19	128.46
15	A	1135	CLA	CMB-C2B-C1B	-4.05	122.25	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	1011	CL0	CED-O2D-CGD	-4.02	106.84	115.94
19	A	1011	CL0	O2D-CGD-CBD	4.01	118.39	111.27
13	2	502	XAT	C8-C9-C10	4.00	125.07	118.94
16	2	613	CHL	CHD-C1D-ND	-3.98	120.79	124.45
15	A	1108	CLA	CMB-C2B-C1B	-3.98	122.34	128.46
14	A	4002	BCR	C30-C25-C26	-3.98	117.01	122.61
14	3	506	BCR	C35-C13-C14	-3.98	117.35	122.92
15	A	1140	CLA	C4-C3-C5	3.96	121.93	115.27
15	J	1302	CLA	CMB-C2B-C1B	-3.95	122.39	128.46
15	A	1102	CLA	CMB-C2B-C1B	-3.95	122.39	128.46
14	B	4003	BCR	C3-C4-C5	-3.94	107.04	114.08
15	A	1116	CLA	CMB-C2B-C1B	-3.94	122.42	128.46
15	B	1223	CLA	CMB-C2B-C1B	-3.90	122.47	128.46
15	B	1234	CLA	CMB-C2B-C1B	-3.88	122.50	128.46
15	4	605	CLA	CMB-C2B-C1B	-3.86	122.53	128.46
12	4	501	LUT	C39-C29-C28	-3.85	112.00	118.08
19	A	1011	CL0	CHC-C1C-NC	3.84	130.03	124.20
15	3	612	CLA	CMB-C2B-C1B	-3.82	122.59	128.46
12	3	501	LUT	C7-C8-C9	-3.81	120.48	126.23
15	A	1106	CLA	CMB-C2B-C1B	-3.81	122.61	128.46
12	4	501	LUT	C39-C29-C30	-3.78	117.63	122.92
13	1	502	XAT	C38-C25-C26	-3.77	115.94	122.26
14	A	4006	BCR	C24-C23-C22	-3.77	120.54	126.23
15	B	1240	CLA	C5-C3-C2	3.77	128.74	121.12
15	1	615	CLA	CMB-C2B-C1B	-3.77	122.67	128.46
15	4	607	CLA	CAA-C2A-C3A	-3.76	102.49	112.78
13	4	502	XAT	C38-C25-C26	-3.75	115.97	122.26
13	4	502	XAT	C35-C15-C14	3.75	131.15	123.47
15	1	603	CLA	CMB-C2B-C3B	3.75	131.69	124.68
16	3	604	CHL	CHD-C1D-ND	-3.74	121.02	124.45
15	A	1129	CLA	CMB-C2B-C1B	-3.73	122.73	128.46
15	4	604	CLA	CMB-C2B-C1B	-3.73	122.73	128.46
12	4	501	LUT	C1-C6-C5	-3.73	117.37	122.61
15	B	1238	CLA	CMB-C2B-C1B	-3.72	122.74	128.46
13	3	502	XAT	C11-C12-C13	-3.72	115.96	126.42
14	A	4004	BCR	C15-C14-C13	-3.72	122.00	127.31
15	2	612	CLA	CMB-C2B-C1B	-3.70	122.77	128.46
15	3	601	CLA	CMB-C2B-C1B	-3.70	122.78	128.46
19	A	1011	CL0	CAA-C2A-C3A	-3.68	102.69	112.78
15	B	1210	CLA	CMB-C2B-C1B	-3.67	122.83	128.46
15	B	1218	CLA	CAA-C2A-C3A	-3.65	102.78	112.78
15	A	1105	CLA	CMB-C2B-C3B	3.65	131.50	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	A	1124	CLA	O2D-CGD-O1D	-3.65	116.71	123.84
15	3	605	CLA	CMB-C2B-C1B	-3.63	122.88	128.46
15	4	602	CLA	CMB-C2B-C1B	-3.63	122.89	128.46
15	A	1120	CLA	CMB-C2B-C1B	-3.62	122.90	128.46
15	B	1023	CLA	CMB-C2B-C1B	-3.62	122.90	128.46
15	A	1124	CLA	O2D-CGD-CBD	3.62	117.70	111.27
15	3	605	CLA	CHB-C4A-NA	3.62	129.51	124.51
14	J	4002	BCR	C15-C14-C13	-3.61	122.16	127.31
14	B	4002	BCR	C30-C25-C26	-3.60	117.54	122.61
19	A	1011	CL0	O2D-CGD-O1D	-3.60	116.81	123.84
15	A	1122	CLA	C5-C3-C2	3.59	128.39	121.12
15	B	1232	CLA	O2D-CGD-O1D	-3.59	116.82	123.84
13	3	502	XAT	C31-C32-C33	-3.58	116.34	126.42
15	A	1115	CLA	CMB-C2B-C1B	-3.58	122.96	128.46
12	3	501	LUT	C20-C13-C12	-3.58	112.44	118.08
15	B	1221	CLA	CMB-C2B-C1B	-3.58	122.97	128.46
14	B	4005	BCR	C15-C16-C17	-3.57	116.16	123.47
15	B	1225	CLA	CMB-C2B-C1B	-3.55	123.00	128.46
12	3	501	LUT	C40-C33-C34	-3.55	117.95	122.92
15	B	1214	CLA	CMB-C2B-C3B	3.55	131.32	124.68
16	1	610	CHL	CHD-C1D-ND	-3.55	121.19	124.45
15	B	1231	CLA	CMB-C2B-C1B	-3.55	123.01	128.46
15	A	1110	CLA	CMB-C2B-C1B	-3.53	123.04	128.46
15	4	601	CLA	CAA-C2A-C1A	-3.52	100.43	111.97
15	1	611	CLA	CMB-C2B-C1B	-3.52	123.05	128.46
15	B	1211	CLA	CMB-C2B-C3B	3.52	131.26	124.68
15	4	616	CLA	CMB-C2B-C1B	-3.50	123.08	128.46
15	A	1105	CLA	CAA-C2A-C3A	-3.50	103.19	112.78
15	A	1103	CLA	CMB-C2B-C1B	-3.47	123.12	128.46
15	2	608	CLA	CMB-C2B-C1B	-3.47	123.14	128.46
14	B	4004	BCR	C3-C4-C5	-3.47	107.89	114.08
15	4	603	CLA	O2D-CGD-O1D	-3.47	117.06	123.84
15	B	1205	CLA	CMB-C2B-C1B	-3.46	123.14	128.46
15	A	1116	CLA	CMB-C2B-C3B	3.46	131.15	124.68
15	A	1125	CLA	CMB-C2B-C1B	-3.45	123.16	128.46
16	4	613	CHL	CHD-C1D-ND	-3.45	121.28	124.45
14	J	4002	BCR	C35-C13-C14	-3.45	118.09	122.92
15	4	608	CLA	CAC-C3C-C2C	-3.44	121.64	127.53
15	2	616	CLA	CMB-C2B-C1B	-3.44	123.17	128.46
15	A	1123	CLA	CMB-C2B-C1B	-3.44	123.17	128.46
15	4	603	CLA	CMB-C2B-C1B	-3.44	123.17	128.46
15	A	1133	CLA	CMB-C2B-C1B	-3.44	123.18	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	1	609	CHL	CHD-C1D-ND	-3.44	121.30	124.45
15	A	1139	CLA	CMB-C2B-C3B	3.42	131.08	124.68
15	A	1135	CLA	CMB-C2B-C3B	3.42	131.07	124.68
15	B	1229	CLA	O2D-CGD-O1D	-3.42	117.16	123.84
14	A	4004	BCR	C24-C23-C22	-3.40	121.09	126.23
15	B	1220	CLA	CMB-C2B-C1B	-3.40	123.23	128.46
15	B	1215	CLA	CMB-C2B-C1B	-3.40	123.24	128.46
12	4	501	LUT	C32-C33-C34	3.40	124.16	118.94
15	3	605	CLA	CAC-C3C-C4C	3.39	129.21	124.81
15	A	1137	CLA	O2D-CGD-O1D	-3.39	117.20	123.84
15	2	608	CLA	CAA-C2A-C3A	-3.39	103.48	112.78
15	3	615	CLA	O2D-CGD-O1D	-3.39	117.21	123.84
15	B	1238	CLA	CAC-C3C-C2C	-3.39	121.73	127.53
18	4	801	LMG	C1-C2-C3	-3.39	102.94	110.00
13	1	502	XAT	C36-C21-C26	3.38	119.18	110.05
16	3	604	CHL	CAA-C2A-C3A	3.38	122.04	112.78
15	A	1134	CLA	O2D-CGD-O1D	-3.38	117.23	123.84
15	B	1229	CLA	CMB-C2B-C1B	-3.38	123.28	128.46
16	1	609	CHL	C1-O2A-CGA	3.37	125.29	116.44
15	B	1216	CLA	CMB-C2B-C3B	3.37	130.99	124.68
15	A	1102	CLA	CMB-C2B-C3B	3.37	130.98	124.68
15	1	615	CLA	CMB-C2B-C3B	3.37	130.98	124.68
12	4	501	LUT	C37-C21-C26	-3.37	104.44	109.55
15	3	609	CLA	O2D-CGD-O1D	-3.36	117.26	123.84
15	2	607	CLA	CMB-C2B-C1B	-3.36	123.30	128.46
15	B	1223	CLA	O2D-CGD-O1D	-3.36	117.27	123.84
16	2	610	CHL	CHD-C1D-ND	-3.36	121.37	124.45
16	4	611	CHL	CHD-C1D-ND	-3.36	121.37	124.45
15	A	1111	CLA	CMB-C2B-C1B	-3.36	123.31	128.46
15	A	1012	CLA	O2D-CGD-O1D	-3.35	117.28	123.84
15	A	1140	CLA	CMB-C2B-C1B	-3.35	123.32	128.46
15	A	1122	CLA	CMB-C2B-C1B	-3.34	123.33	128.46
15	1	607	CLA	CMB-C2B-C1B	-3.34	123.33	128.46
15	1	613	CLA	CMB-C2B-C1B	-3.33	123.34	128.46
15	A	1104	CLA	CMB-C2B-C1B	-3.33	123.35	128.46
15	A	1117	CLA	O2D-CGD-O1D	-3.33	117.33	123.84
14	B	4004	BCR	C2-C1-C6	3.32	115.59	110.48
15	B	1202	CLA	O2D-CGD-O1D	-3.32	117.34	123.84
15	B	1223	CLA	CMB-C2B-C3B	3.32	130.89	124.68
15	2	604	CLA	CMB-C2B-C1B	-3.31	123.37	128.46
15	2	605	CLA	CMB-C2B-C1B	-3.31	123.37	128.46
15	A	1127	CLA	CMB-C2B-C1B	-3.31	123.38	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	J	1302	CLA	CMB-C2B-C3B	3.31	130.87	124.68
15	4	601	CLA	CMB-C2B-C1B	-3.31	123.38	128.46
14	3	504	BCR	C15-C16-C17	-3.31	116.70	123.47
15	4	605	CLA	O2D-CGD-O1D	-3.31	117.38	123.84
15	B	1203	CLA	CMB-C2B-C1B	-3.30	123.39	128.46
15	2	616	CLA	C1-O2A-CGA	3.30	125.11	116.44
16	4	610	CHL	C3C-C4C-NC	-3.30	106.87	110.57
15	3	607	CLA	CMB-C2B-C1B	-3.29	123.40	128.46
15	B	1239	CLA	O2D-CGD-O1D	-3.29	117.40	123.84
15	B	1204	CLA	O2D-CGD-O1D	-3.29	117.40	123.84
15	3	614	CLA	CMB-C2B-C3B	3.29	130.83	124.68
15	B	1228	CLA	CMB-C2B-C3B	3.28	130.82	124.68
22	B	5002	DGD	O6D-C1D-O3G	-3.28	102.20	109.97
16	2	610	CHL	C2C-C3C-C4C	3.27	108.82	106.49
15	A	1106	CLA	CMB-C2B-C3B	3.27	130.80	124.68
19	A	1011	CL0	CGD-CBD-CAD	3.27	121.33	110.73
22	B	5002	DGD	O3G-C3G-C2G	-3.27	103.01	110.90
15	A	1134	CLA	CMB-C2B-C1B	-3.27	123.44	128.46
16	1	610	CHL	C2C-C3C-C4C	3.26	108.82	106.49
15	A	1132	CLA	CHB-C4A-NA	3.26	129.02	124.51
14	F	4002	BCR	C28-C27-C26	-3.26	108.25	114.08
15	B	1238	CLA	C5-C3-C2	-3.26	112.82	120.27
15	1	613	CLA	O2D-CGD-O1D	-3.26	117.47	123.84
15	B	1213	CLA	CMB-C2B-C1B	-3.26	123.46	128.46
15	B	1229	CLA	O2D-CGD-CBD	3.25	117.05	111.27
18	4	801	LMG	O6-C1-O1	-3.25	102.28	109.97
15	A	1101	CLA	O2D-CGD-O1D	-3.25	117.49	123.84
15	B	1221	CLA	CMB-C2B-C3B	3.25	130.75	124.68
15	4	604	CLA	CMB-C2B-C3B	3.24	130.75	124.68
15	1	606	CLA	CMB-C2B-C1B	-3.24	123.49	128.46
12	4	501	LUT	C20-C13-C12	3.23	123.17	118.08
15	B	1207	CLA	CMB-C2B-C1B	-3.23	123.50	128.46
15	A	1123	CLA	O2D-CGD-O1D	-3.23	117.52	123.84
14	B	4003	BCR	C2-C1-C6	3.22	115.44	110.48
14	A	4003	BCR	C1-C6-C5	-3.22	118.08	122.61
14	A	4007	BCR	C24-C23-C22	-3.21	121.38	126.23
15	A	1108	CLA	CMB-C2B-C3B	3.21	130.68	124.68
15	A	1107	CLA	CMB-C2B-C1B	-3.21	123.53	128.46
15	3	601	CLA	CMB-C2B-C3B	3.21	130.68	124.68
15	3	606	CLA	CMB-C2B-C1B	-3.20	123.54	128.46
16	2	610	CHL	C3C-C4C-NC	-3.20	106.98	110.57
15	B	1203	CLA	CHB-C4A-NA	3.20	128.93	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	1	502	XAT	C6-C7-C8	-3.20	119.23	125.99
14	B	4002	BCR	C1-C6-C5	-3.20	118.11	122.61
15	A	1124	CLA	CHB-C4A-NA	3.19	128.93	124.51
15	3	605	CLA	CMB-C2B-C3B	3.19	130.65	124.68
15	A	1118	CLA	CMB-C2B-C1B	-3.19	123.56	128.46
15	B	1234	CLA	CMB-C2B-C3B	3.19	130.64	124.68
15	A	1132	CLA	O2D-CGD-O1D	-3.19	117.61	123.84
15	A	1119	CLA	CMB-C2B-C1B	-3.19	123.57	128.46
14	1	503	BCR	C15-C14-C13	-3.18	122.77	127.31
16	4	613	CHL	C1-O2A-CGA	3.18	124.78	116.44
12	4	501	LUT	C40-C33-C32	3.17	123.08	118.08
14	J	4001	BCR	C3-C4-C5	-3.17	108.41	114.08
15	A	1121	CLA	CMB-C2B-C1B	-3.16	123.61	128.46
15	B	1226	CLA	CAA-C2A-C3A	-3.15	104.15	112.78
15	2	612	CLA	CMB-C2B-C3B	3.15	130.57	124.68
12	1	501	LUT	C40-C33-C34	-3.14	118.53	122.92
14	B	4002	BCR	C3-C4-C5	-3.14	108.47	114.08
15	1	601	CLA	CMB-C2B-C1B	-3.14	123.64	128.46
14	J	4002	BCR	C15-C16-C17	-3.13	117.06	123.47
15	A	1106	CLA	O2D-CGD-O1D	-3.13	117.72	123.84
15	B	1214	CLA	O2D-CGD-O1D	-3.13	117.73	123.84
13	3	502	XAT	C39-C29-C30	-3.12	118.55	122.92
12	3	501	LUT	C11-C10-C9	3.12	131.77	127.31
15	A	1138	CLA	O2D-CGD-O1D	-3.12	117.74	123.84
15	B	1215	CLA	O2D-CGD-O1D	-3.12	117.74	123.84
15	B	1023	CLA	CMB-C2B-C3B	3.12	130.51	124.68
15	1	602	CLA	CMB-C2B-C1B	-3.11	123.68	128.46
15	4	612	CLA	CMB-C2B-C1B	-3.11	123.68	128.46
16	2	613	CHL	C3C-C4C-NC	-3.11	107.08	110.57
15	A	1136	CLA	CMB-C2B-C1B	-3.10	123.69	128.46
15	B	1201	CLA	CMB-C2B-C1B	-3.10	123.70	128.46
14	J	4002	BCR	C27-C26-C25	3.10	127.23	122.73
15	B	1206	CLA	CHB-C4A-NA	3.10	128.80	124.51
15	B	1218	CLA	O2D-CGD-O1D	-3.10	117.78	123.84
15	4	605	CLA	CMB-C2B-C3B	3.09	130.46	124.68
14	B	4003	BCR	C15-C14-C13	-3.09	122.90	127.31
15	1	615	CLA	C4-C3-C2	-3.09	110.13	125.76
15	1	603	CLA	O2D-CGD-O1D	-3.09	117.80	123.84
15	F	1302	CLA	CMB-C2B-C1B	-3.09	123.72	128.46
15	4	604	CLA	CHB-C4A-NA	3.09	128.78	124.51
16	1	610	CHL	C3C-C4C-NC	-3.09	107.11	110.57
15	1	606	CLA	O2D-CGD-O1D	-3.09	117.81	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	4002	BCR	C27-C26-C25	3.08	127.21	122.73
16	2	610	CHL	CHB-C4A-NA	3.08	128.77	124.51
15	B	1021	CLA	CMB-C2B-C1B	-3.08	123.73	128.46
16	4	611	CHL	C3C-C4C-NC	-3.08	107.12	110.57
15	A	1102	CLA	O2D-CGD-O1D	-3.08	117.82	123.84
16	4	613	CHL	CHB-C4A-NA	3.07	128.76	124.51
15	A	1110	CLA	O2D-CGD-O1D	-3.07	117.84	123.84
15	B	1214	CLA	CHB-C4A-NA	3.06	128.74	124.51
15	B	1239	CLA	CHB-C4A-NA	3.05	128.73	124.51
13	4	502	XAT	C35-C34-C33	3.05	131.67	127.31
15	2	608	CLA	O2D-CGD-O1D	-3.05	117.87	123.84
15	A	1103	CLA	O2D-CGD-O1D	-3.05	117.87	123.84
22	B	5002	DGD	C1E-O6E-C5E	3.05	119.67	113.69
15	3	607	CLA	O2D-CGD-O1D	-3.05	117.88	123.84
12	2	501	LUT	C21-C26-C27	-3.05	108.85	112.70
16	2	613	CHL	C2C-C3C-C4C	3.05	108.66	106.49
15	4	609	CLA	O2D-CGD-O1D	-3.04	117.89	123.84
15	B	1022	CLA	CMB-C2B-C1B	-3.04	123.79	128.46
16	3	604	CHL	C3C-C4C-NC	-3.04	107.16	110.57
15	A	1106	CLA	CHB-C4A-NA	3.04	128.72	124.51
14	4	503	BCR	C15-C16-C17	-3.04	117.25	123.47
13	1	502	XAT	C27-C28-C29	-3.03	120.83	125.53
15	B	1202	CLA	CMB-C2B-C1B	-3.03	123.81	128.46
15	B	1205	CLA	O2D-CGD-O1D	-3.02	117.93	123.84
15	2	602	CLA	O2D-CGD-O1D	-3.02	117.93	123.84
15	2	616	CLA	O2A-CGA-O1A	-3.02	115.97	123.59
13	2	502	XAT	C10-C11-C12	3.02	132.64	123.22
15	A	1141	CLA	O2D-CGD-O1D	-3.01	117.95	123.84
15	A	1137	CLA	CAA-CBA-CGA	-3.01	104.47	113.25
12	1	501	LUT	C32-C33-C34	3.01	123.55	118.94
15	A	1136	CLA	O2D-CGD-O1D	-3.00	117.96	123.84
15	B	1206	CLA	O2D-CGD-O1D	-3.00	117.96	123.84
15	A	1128	CLA	CMB-C2B-C1B	-3.00	123.85	128.46
15	A	1125	CLA	CMB-C2B-C3B	3.00	130.30	124.68
15	A	1117	CLA	CMB-C2B-C1B	-3.00	123.85	128.46
16	2	611	CHL	C3C-C4C-NC	-3.00	107.20	110.57
15	1	615	CLA	O2D-CGD-O1D	-3.00	117.97	123.84
13	2	502	XAT	C26-C27-C28	-3.00	119.65	125.99
14	F	4001	BCR	C8-C7-C6	-3.00	118.78	127.20
15	A	1129	CLA	CMB-C2B-C3B	3.00	130.29	124.68
15	4	604	CLA	O2D-CGD-O1D	-3.00	117.98	123.84
15	B	1225	CLA	CMB-C2B-C3B	3.00	130.28	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	B	1221	CLA	O2D-CGD-O1D	-3.00	117.98	123.84
15	3	614	CLA	CHB-C4A-NA	2.99	128.65	124.51
15	2	612	CLA	O2D-CGD-O1D	-2.99	117.99	123.84
15	A	1121	CLA	O2D-CGD-O1D	-2.99	117.99	123.84
14	B	4006	BCR	C15-C14-C13	-2.99	123.04	127.31
13	4	502	XAT	C19-C9-C10	-2.99	118.73	122.92
15	4	601	CLA	C1B-CHB-C4A	-2.99	124.20	130.12
14	A	4007	BCR	C15-C14-C13	-2.99	123.05	127.31
15	A	1113	CLA	CMB-C2B-C1B	-2.99	123.87	128.46
15	A	1132	CLA	CAC-C3C-C2C	2.99	132.64	127.53
15	A	1102	CLA	CAA-C2A-C1A	-2.99	102.19	111.97
15	B	1224	CLA	CMB-C2B-C1B	-2.98	123.88	128.46
15	2	606	CLA	CMB-C2B-C1B	-2.98	123.88	128.46
15	A	1130	CLA	CHB-C4A-NA	2.98	128.63	124.51
15	B	1207	CLA	O2D-CGD-O1D	-2.98	118.01	123.84
15	4	603	CLA	CHB-C4A-NA	2.98	128.63	124.51
16	2	609	CHL	CHB-C4A-NA	2.98	128.63	124.51
15	B	1222	CLA	CMB-C2B-C1B	-2.98	123.89	128.46
14	J	4001	BCR	C15-C16-C17	-2.98	117.37	123.47
14	4	503	BCR	C27-C26-C25	2.97	127.05	122.73
14	A	4003	BCR	C2-C1-C6	2.97	115.06	110.48
15	A	1135	CLA	CHB-C4A-NA	2.97	128.62	124.51
15	A	1111	CLA	O2D-CGD-O1D	-2.97	118.03	123.84
15	B	1234	CLA	O2D-CGD-O1D	-2.97	118.03	123.84
15	B	1209	CLA	O2D-CGD-O1D	-2.97	118.03	123.84
15	2	607	CLA	O2D-CGD-O1D	-2.97	118.03	123.84
15	A	1115	CLA	CMB-C2B-C3B	2.97	130.23	124.68
16	2	609	CHL	CAA-C2A-C1A	-2.97	102.25	111.97
15	B	1218	CLA	CHB-C4A-NA	2.97	128.62	124.51
15	A	1103	CLA	CHB-C4A-NA	2.97	128.61	124.51
15	B	1226	CLA	CHB-C4A-NA	2.97	128.61	124.51
15	4	602	CLA	O2D-CGD-O1D	-2.97	118.04	123.84
19	A	1011	CL0	C1-C2-C3	-2.96	120.92	126.04
15	A	1013	CLA	C6-C5-C3	2.96	121.22	113.45
15	B	1210	CLA	CMB-C2B-C3B	2.96	130.22	124.68
15	A	1107	CLA	O2D-CGD-O1D	-2.96	118.06	123.84
15	1	605	CLA	CHB-C4A-NA	2.96	128.60	124.51
15	A	1111	CLA	CMB-C2B-C3B	2.96	130.21	124.68
15	A	1117	CLA	CHB-C4A-NA	2.95	128.60	124.51
15	3	612	CLA	CMB-C2B-C3B	2.95	130.21	124.68
15	B	1240	CLA	CMB-C2B-C1B	-2.95	123.92	128.46
13	2	502	XAT	C20-C13-C12	-2.95	113.42	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	A	1133	CLA	O2D-CGD-O1D	-2.95	118.07	123.84
14	B	4005	BCR	C15-C14-C13	-2.95	123.10	127.31
15	2	616	CLA	CMB-C2B-C3B	2.95	130.20	124.68
15	J	1302	CLA	O2D-CGD-O1D	-2.95	118.07	123.84
15	3	610	CLA	CMB-C2B-C1B	-2.95	123.93	128.46
12	3	501	LUT	C4-C5-C6	-2.95	114.27	120.85
15	A	1118	CLA	O2D-CGD-O1D	-2.95	118.07	123.84
15	B	1210	CLA	O2D-CGD-O1D	-2.95	118.07	123.84
15	3	603	CLA	O2D-CGD-O1D	-2.95	118.08	123.84
15	A	1109	CLA	O2D-CGD-O1D	-2.95	118.08	123.84
12	2	501	LUT	C32-C33-C34	2.95	123.46	118.94
15	2	604	CLA	CHB-C4A-NA	2.95	128.59	124.51
14	B	4001	BCR	C35-C13-C14	-2.94	118.80	122.92
15	A	1013	CLA	O2D-CGD-O1D	-2.94	118.08	123.84
15	1	603	CLA	CHB-C4A-NA	2.94	128.58	124.51
15	A	1103	CLA	CMB-C2B-C3B	2.94	130.18	124.68
15	A	1105	CLA	O2D-CGD-O1D	-2.94	118.09	123.84
15	B	1211	CLA	CHB-C4A-NA	2.94	128.58	124.51
15	F	1301	CLA	CMB-C2B-C1B	-2.94	123.95	128.46
15	3	613	CLA	CMB-C2B-C1B	-2.94	123.95	128.46
15	A	1116	CLA	O2D-CGD-O1D	-2.94	118.10	123.84
15	3	611	CLA	O2D-CGD-O1D	-2.93	118.11	123.84
14	B	4001	BCR	C15-C14-C13	-2.93	123.13	127.31
15	B	1216	CLA	O2D-CGD-O1D	-2.93	118.12	123.84
15	A	1115	CLA	O2D-CGD-O1D	-2.93	118.12	123.84
15	A	1134	CLA	CHB-C4A-NA	2.92	128.55	124.51
15	1	611	CLA	CMB-C2B-C3B	2.92	130.14	124.68
15	3	615	CLA	CHB-C4A-NA	2.92	128.55	124.51
15	A	1116	CLA	C5-C3-C2	2.92	127.02	121.12
15	4	608	CLA	CMB-C2B-C1B	-2.92	123.98	128.46
15	1	608	CLA	O2D-CGD-O1D	-2.92	118.14	123.84
15	A	1013	CLA	CHB-C4A-NA	2.92	128.54	124.51
15	4	616	CLA	CMB-C2B-C3B	2.91	130.13	124.68
13	4	502	XAT	C31-C32-C33	-2.91	118.23	126.42
16	1	609	CHL	C3C-C4C-NC	-2.91	107.31	110.57
14	F	4001	BCR	C33-C5-C6	-2.91	121.26	124.53
13	2	502	XAT	C31-C32-C33	-2.91	118.24	126.42
15	4	603	CLA	O2D-CGD-CBD	2.91	116.43	111.27
14	A	4003	BCR	C38-C26-C27	-2.91	108.03	113.62
15	A	1113	CLA	O2D-CGD-O1D	-2.91	118.16	123.84
14	A	4007	BCR	C15-C16-C17	-2.91	117.52	123.47
15	2	602	CLA	CHB-C4A-NA	2.90	128.53	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	3	604	CHL	C1-C2-C3	-2.90	121.02	126.04
15	2	605	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
15	3	605	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
15	1	604	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
15	A	1126	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
17	A	5002	LHG	O8-C23-C24	2.90	121.00	111.91
15	B	1217	CLA	CMB-C2B-C1B	-2.90	124.01	128.46
15	4	602	CLA	CHB-C4A-NA	2.90	128.52	124.51
15	B	1236	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
15	A	1137	CLA	CMB-C2B-C1B	-2.90	124.01	128.46
15	4	616	CLA	O2D-CGD-O1D	-2.90	118.18	123.84
15	A	1130	CLA	O2D-CGD-O1D	-2.89	118.18	123.84
15	2	606	CLA	O2D-CGD-O1D	-2.89	118.18	123.84
22	B	5002	DGD	C6D-O5D-C1E	2.89	119.39	113.74
15	4	605	CLA	C5-C3-C2	2.89	126.97	121.12
15	4	608	CLA	O2D-CGD-O1D	-2.89	118.19	123.84
15	A	1111	CLA	CHB-C4A-NA	2.89	128.51	124.51
18	2	803	LMG	O6-C1-O1	-2.89	103.13	109.97
15	2	608	CLA	CMB-C2B-C3B	2.89	130.08	124.68
15	A	1129	CLA	O2D-CGD-O1D	-2.89	118.19	123.84
14	3	506	BCR	C1-C6-C5	-2.89	118.55	122.61
15	A	1120	CLA	CMB-C2B-C3B	2.88	130.07	124.68
15	4	609	CLA	CHB-C4A-NA	2.88	128.50	124.51
15	A	1110	CLA	CHB-C4A-NA	2.88	128.50	124.51
14	A	4008	BCR	C2-C1-C6	2.88	114.92	110.48
15	3	613	CLA	CHB-C4A-NA	2.88	128.49	124.51
15	1	601	CLA	CMB-C2B-C3B	2.88	130.06	124.68
15	B	1226	CLA	O2D-CGD-O1D	-2.88	118.21	123.84
15	B	1223	CLA	O2D-CGD-CBD	2.88	116.38	111.27
15	B	1222	CLA	O2A-CGA-O1A	-2.88	116.33	123.59
15	A	1125	CLA	O2D-CGD-O1D	-2.88	118.22	123.84
15	B	1201	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
15	1	604	CLA	CMB-C2B-C1B	-2.87	124.05	128.46
13	3	502	XAT	C36-C21-C26	2.87	117.80	110.05
15	F	1301	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
14	A	4004	BCR	C27-C26-C25	2.87	126.89	122.73
16	2	611	CHL	C2C-C3C-C4C	2.87	108.53	106.49
15	2	603	CLA	CMB-C2B-C1B	-2.86	124.07	128.46
14	A	4008	BCR	C15-C16-C17	-2.86	117.62	123.47
15	4	601	CLA	CMB-C2B-C3B	2.86	130.02	124.68
16	3	604	CHL	C2C-C3C-C4C	2.85	108.52	106.49
15	2	603	CLA	O2D-CGD-O1D	-2.85	118.26	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	B	1224	CLA	O2D-CGD-O1D	-2.85	118.26	123.84
14	1	503	BCR	C24-C23-C22	-2.85	121.92	126.23
15	A	1127	CLA	CMB-C2B-C3B	2.85	130.01	124.68
15	A	1119	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
15	A	1120	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
16	2	609	CHL	C3C-C4C-NC	-2.85	107.38	110.57
15	B	1237	CLA	O2D-CGD-O1D	-2.85	118.28	123.84
15	1	607	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
14	F	4002	BCR	C15-C16-C17	-2.84	117.65	123.47
15	A	1126	CLA	CMB-C2B-C1B	-2.84	124.09	128.46
15	2	612	CLA	CHB-C4A-NA	2.84	128.44	124.51
15	B	1201	CLA	CHB-C4A-NA	2.84	128.44	124.51
15	A	1133	CLA	CHB-C4A-NA	2.84	128.44	124.51
15	B	1231	CLA	CHB-C4A-NA	2.84	128.44	124.51
14	J	4001	BCR	C2-C1-C6	2.84	114.85	110.48
15	3	613	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
15	A	1101	CLA	CHB-C4A-NA	2.83	128.43	124.51
15	B	1203	CLA	CMB-C2B-C3B	2.83	129.98	124.68
15	B	1212	CLA	CHB-C4A-NA	2.83	128.43	124.51
15	B	1235	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
15	2	604	CLA	CMB-C2B-C3B	2.83	129.97	124.68
15	4	606	CLA	C1-C2-C3	-2.83	122.17	126.75
15	B	1203	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
15	A	1131	CLA	CMB-C2B-C1B	-2.83	124.12	128.46
15	B	1219	CLA	CMB-C2B-C1B	-2.82	124.13	128.46
12	2	501	LUT	C40-C33-C32	2.82	122.52	118.08
15	A	1114	CLA	O2D-CGD-O1D	-2.82	118.32	123.84
16	2	609	CHL	C1-O2A-CGA	2.82	123.84	116.44
15	B	1229	CLA	CMB-C2B-C3B	2.82	129.95	124.68
15	B	1238	CLA	C4-C3-C5	-2.82	110.53	115.27
15	B	1215	CLA	CHB-C4A-NA	2.82	128.41	124.51
15	4	606	CLA	CHB-C4A-NA	2.82	128.41	124.51
22	B	5002	DGD	O5D-C6D-C5D	-2.82	103.84	109.05
15	A	1107	CLA	CHB-C4A-NA	2.81	128.40	124.51
15	1	608	CLA	CMB-C2B-C1B	-2.81	124.14	128.46
14	B	4001	BCR	C33-C5-C6	-2.81	121.37	124.53
15	B	1231	CLA	CMB-C2B-C3B	2.81	129.94	124.68
15	F	1302	CLA	CHB-C4A-NA	2.81	128.40	124.51
15	B	1227	CLA	O2D-CGD-O1D	-2.81	118.35	123.84
15	1	606	CLA	CMB-C2B-C3B	2.80	129.92	124.68
15	B	1208	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
15	3	601	CLA	O2D-CGD-O1D	-2.80	118.36	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	B	1022	CLA	CMB-C2B-C3B	2.80	129.92	124.68
15	2	616	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
15	3	610	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
15	B	1204	CLA	CMB-C2B-C1B	-2.80	124.16	128.46
18	2	802	LMG	O6-C1-O1	-2.80	103.34	109.97
15	B	1219	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
15	2	605	CLA	CHB-C4A-NA	2.80	128.38	124.51
15	A	1114	CLA	CHB-C4A-NA	2.80	128.38	124.51
15	A	1128	CLA	O2D-CGD-O1D	-2.80	118.37	123.84
15	B	1212	CLA	CMB-C2B-C1B	-2.80	124.16	128.46
12	2	501	LUT	C12-C13-C14	2.80	123.23	118.94
15	B	1238	CLA	CMB-C2B-C3B	2.80	129.91	124.68
15	A	1104	CLA	CHB-C4A-NA	2.80	128.38	124.51
15	B	1211	CLA	O2D-CGD-O1D	-2.80	118.37	123.84
14	3	504	BCR	C27-C26-C25	2.79	126.79	122.73
15	B	1022	CLA	O2D-CGD-O1D	-2.79	118.38	123.84
15	A	1122	CLA	CHB-C4A-NA	2.79	128.38	124.51
15	A	1138	CLA	CHB-C4A-NA	2.79	128.37	124.51
15	B	1229	CLA	CHB-C4A-NA	2.79	128.37	124.51
15	B	1230	CLA	CAA-C2A-C1A	-2.79	102.83	111.97
15	2	607	CLA	CMB-C2B-C3B	2.79	129.90	124.68
15	B	1223	CLA	CHB-C4A-NA	2.79	128.37	124.51
15	B	1023	CLA	O2D-CGD-O1D	-2.79	118.39	123.84
14	A	4003	BCR	C27-C26-C25	2.79	126.78	122.73
15	B	1237	CLA	CHB-C4A-NA	2.79	128.36	124.51
15	4	602	CLA	CMB-C2B-C3B	2.78	129.89	124.68
15	B	1227	CLA	CMB-C2B-C1B	-2.78	124.19	128.46
15	A	1132	CLA	CAC-C3C-C4C	-2.78	121.20	124.81
15	B	1230	CLA	O2D-CGD-O1D	-2.78	118.41	123.84
15	2	616	CLA	CHB-C4A-NA	2.78	128.35	124.51
19	A	1011	CL0	C4-C3-C5	2.78	119.94	115.27
13	2	502	XAT	C36-C21-C22	-2.78	104.16	108.98
15	4	612	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
15	A	1118	CLA	CHB-C4A-NA	2.77	128.34	124.51
14	B	4003	BCR	C35-C13-C14	-2.77	119.05	122.92
15	B	1220	CLA	CMB-C2B-C3B	2.77	129.85	124.68
15	B	1228	CLA	O2D-CGD-O1D	-2.76	118.43	123.84
15	B	1238	CLA	O2D-CGD-O1D	-2.76	118.43	123.84
15	A	1119	CLA	CMB-C2B-C3B	2.76	129.85	124.68
16	1	609	CHL	CHB-C4A-NA	2.76	128.33	124.51
13	1	502	XAT	C37-C21-C36	-2.76	103.30	107.37
15	1	605	CLA	O2D-CGD-O1D	-2.76	118.44	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	F	4001	BCR	C15-C16-C17	-2.76	117.83	123.47
15	4	612	CLA	CHB-C4A-NA	2.75	128.32	124.51
15	A	1107	CLA	CMB-C2B-C3B	2.75	129.83	124.68
15	B	1234	CLA	CAC-C3C-C4C	2.75	128.38	124.81
18	2	804	LMG	O6-C1-O1	-2.75	103.45	109.97
15	A	1105	CLA	CAC-C3C-C2C	2.75	132.24	127.53
15	A	1126	CLA	C1B-CHB-C4A	-2.75	124.67	130.12
13	1	502	XAT	C11-C12-C13	-2.75	118.69	126.42
15	3	608	CLA	O2D-CGD-O1D	-2.75	118.46	123.84
15	A	1110	CLA	CMB-C2B-C3B	2.75	129.82	124.68
15	4	606	CLA	CMB-C2B-C1B	-2.75	124.24	128.46
15	A	1123	CLA	CMB-C2B-C3B	2.74	129.81	124.68
15	3	601	CLA	CHB-C4A-NA	2.74	128.31	124.51
19	A	1011	CL0	CHB-C4A-NA	2.74	128.31	124.51
15	A	1110	CLA	O2A-CGA-O1A	-2.74	116.68	123.59
16	3	604	CHL	C4D-CHA-C1A	2.74	124.58	121.25
15	B	1215	CLA	CMB-C2B-C3B	2.74	129.80	124.68
15	B	1238	CLA	CBC-CAC-C3C	2.73	119.96	112.43
15	A	1134	CLA	CMB-C2B-C3B	2.73	129.79	124.68
15	1	613	CLA	CMB-C2B-C3B	2.73	129.79	124.68
14	B	4005	BCR	C33-C5-C6	-2.73	121.47	124.53
12	4	501	LUT	C21-C26-C27	2.73	116.15	112.70
15	4	607	CLA	CHB-C4A-NA	2.73	128.28	124.51
16	4	610	CHL	CHD-C1D-ND	-2.72	121.95	124.45
15	B	1213	CLA	CMB-C2B-C3B	2.72	129.77	124.68
14	A	4007	BCR	C33-C5-C6	-2.72	121.48	124.53
16	3	604	CHL	CHD-C4C-C3C	2.71	128.83	124.84
12	1	501	LUT	C35-C34-C33	-2.71	123.44	127.31
15	3	609	CLA	O2D-CGD-CBD	2.71	116.09	111.27
14	A	4004	BCR	C30-C25-C26	-2.71	118.79	122.61
15	1	601	CLA	O2D-CGD-O1D	-2.71	118.53	123.84
14	F	4001	BCR	C11-C10-C9	-2.71	123.44	127.31
15	A	1102	CLA	CHB-C4A-NA	2.71	128.26	124.51
15	1	607	CLA	CMB-C2B-C3B	2.71	129.74	124.68
15	B	1217	CLA	O2D-CGD-O1D	-2.71	118.55	123.84
15	1	602	CLA	O2D-CGD-O1D	-2.71	118.55	123.84
15	B	1227	CLA	CHB-C4A-NA	2.70	128.25	124.51
15	A	1108	CLA	O2D-CGD-O1D	-2.70	118.56	123.84
15	A	1117	CLA	O2D-CGD-CBD	2.70	116.06	111.27
15	B	1208	CLA	CMB-C2B-C1B	-2.70	124.32	128.46
12	3	501	LUT	C21-C26-C27	-2.70	109.29	112.70
15	A	1116	CLA	CHB-C4A-NA	2.69	128.24	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	3	606	CLA	CHB-C4A-NA	2.69	128.24	124.51
15	3	608	CLA	CMB-C2B-C1B	-2.69	124.33	128.46
14	A	4008	BCR	C15-C14-C13	-2.69	123.47	127.31
15	1	601	CLA	CHB-C4A-NA	2.69	128.23	124.51
15	3	607	CLA	CMB-C2B-C3B	2.69	129.71	124.68
15	A	1102	CLA	C1B-CHB-C4A	-2.69	124.79	130.12
13	4	502	XAT	C36-C21-C22	-2.69	104.31	108.98
15	3	611	CLA	CHB-C4A-NA	2.69	128.23	124.51
14	3	506	BCR	C15-C16-C17	-2.69	117.97	123.47
15	B	1240	CLA	O2D-CGD-O1D	-2.69	118.58	123.84
15	J	1302	CLA	CHB-C4A-NA	2.69	128.23	124.51
17	3	801	LHG	O8-C23-C24	2.69	120.34	111.91
14	3	503	BCR	C37-C22-C21	-2.69	119.16	122.92
15	4	601	CLA	O2D-CGD-O1D	-2.68	118.59	123.84
15	A	1139	CLA	O2D-CGD-O1D	-2.68	118.59	123.84
13	4	502	XAT	C10-C11-C12	2.68	131.59	123.22
15	B	1222	CLA	CHB-C4A-NA	2.68	128.22	124.51
16	4	613	CHL	C3C-C4C-NC	-2.68	107.56	110.57
15	2	607	CLA	CHB-C4A-NA	2.68	128.22	124.51
15	A	1133	CLA	CMB-C2B-C3B	2.68	129.69	124.68
14	F	4002	BCR	C30-C25-C26	-2.68	118.84	122.61
14	B	4005	BCR	C35-C13-C14	-2.68	119.17	122.92
16	4	611	CHL	CHB-C4A-NA	2.67	128.21	124.51
15	B	1209	CLA	CHB-C4A-NA	2.67	128.21	124.51
15	A	1118	CLA	CMB-C2B-C3B	2.67	129.68	124.68
16	2	611	CHL	C1-O2A-CGA	2.67	124.49	116.73
15	A	1138	CLA	CMB-C2B-C1B	-2.67	124.36	128.46
19	A	1011	CL0	O2A-CGA-CBA	2.67	120.29	111.91
15	B	1224	CLA	CMB-C2B-C3B	2.67	129.67	124.68
15	B	1206	CLA	CMB-C2B-C1B	-2.67	124.36	128.46
15	1	602	CLA	CHB-C4A-NA	2.67	128.20	124.51
15	A	1135	CLA	O2D-CGD-O1D	-2.67	118.62	123.84
17	B	5001	LHG	O8-C23-C24	2.67	120.28	111.91
15	B	1236	CLA	CHB-C4A-NA	2.67	128.20	124.51
15	A	1122	CLA	CMB-C2B-C3B	2.67	129.66	124.68
14	B	4006	BCR	C33-C5-C6	-2.66	121.54	124.53
15	A	1141	CLA	CMB-C2B-C1B	-2.66	124.37	128.46
13	3	502	XAT	C20-C13-C14	-2.66	119.19	122.92
14	A	4008	BCR	C35-C13-C14	-2.66	119.20	122.92
15	4	609	CLA	CMB-C2B-C1B	-2.66	124.38	128.46
19	A	1011	CL0	C3D-C4D-CHA	-2.66	106.64	112.72
15	4	612	CLA	CMB-C2B-C3B	2.66	129.65	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	A	1122	CLA	CHD-C1D-ND	-2.66	122.01	124.45
14	1	503	BCR	C33-C5-C6	-2.65	121.55	124.53
15	A	1115	CLA	CAC-C3C-C4C	2.65	128.25	124.81
15	A	1104	CLA	CMB-C2B-C3B	2.65	129.64	124.68
15	B	1237	CLA	CMB-C2B-C1B	-2.65	124.39	128.46
15	A	1140	CLA	O2D-CGD-O1D	-2.65	118.66	123.84
15	B	1209	CLA	CMB-C2B-C1B	-2.65	124.39	128.46
14	A	4008	BCR	C33-C5-C6	-2.65	121.56	124.53
15	A	1123	CLA	CHB-C4A-NA	2.65	128.17	124.51
15	3	606	CLA	CMB-C2B-C3B	2.65	129.63	124.68
14	B	4003	BCR	C7-C8-C9	-2.64	122.24	126.23
14	3	504	BCR	C33-C5-C6	-2.64	121.56	124.53
14	F	4002	BCR	C33-C5-C6	-2.64	121.56	124.53
15	A	1109	CLA	CHB-C4A-NA	2.64	128.16	124.51
15	3	606	CLA	O2D-CGD-O1D	-2.64	118.68	123.84
15	A	1137	CLA	CHB-C4A-NA	2.64	128.16	124.51
15	1	604	CLA	CHB-C4A-NA	2.64	128.16	124.51
13	3	502	XAT	C19-C9-C10	-2.64	119.23	122.92
15	B	1225	CLA	CHB-C4A-NA	2.64	128.16	124.51
15	4	605	CLA	CHB-C4A-NA	2.63	128.16	124.51
15	4	606	CLA	O2D-CGD-O1D	-2.63	118.69	123.84
14	3	504	BCR	C11-C10-C9	-2.63	123.55	127.31
15	B	1202	CLA	CHB-C4A-NA	2.63	128.15	124.51
14	F	4001	BCR	C15-C14-C13	-2.63	123.56	127.31
14	B	4005	BCR	C8-C7-C6	-2.63	119.82	127.20
15	B	1205	CLA	CMB-C2B-C3B	2.63	129.59	124.68
19	A	1011	CL0	CMA-C3A-C2A	-2.63	103.23	113.83
14	A	4005	BCR	C15-C16-C17	-2.63	118.09	123.47
15	B	1205	CLA	O2A-CGA-O1A	-2.63	116.97	123.59
15	A	1137	CLA	C6-C5-C3	2.63	120.34	113.45
15	B	1213	CLA	CHB-C4A-NA	2.63	128.14	124.51
15	A	1112	CLA	CMB-C2B-C1B	-2.62	124.43	128.46
15	B	1235	CLA	CHB-C4A-NA	2.62	128.14	124.51
15	2	606	CLA	CHB-C4A-NA	2.62	128.13	124.51
13	4	502	XAT	C36-C21-C26	2.61	117.10	110.05
14	A	4004	BCR	C2-C1-C6	2.61	114.50	110.48
19	A	1011	CL0	C4C-C3C-C2C	-2.61	103.09	106.90
15	2	603	CLA	CHB-C4A-NA	2.61	128.13	124.51
14	B	4002	BCR	C2-C1-C6	2.61	114.50	110.48
15	A	1122	CLA	O2D-CGD-O1D	-2.61	118.73	123.84
14	B	4001	BCR	C30-C25-C26	-2.61	118.93	122.61
15	2	616	CLA	C1-C2-C3	-2.61	121.53	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	1	608	CLA	CHB-C4A-NA	2.61	128.12	124.51
15	B	1204	CLA	CHB-C4A-NA	2.61	128.12	124.51
15	3	612	CLA	O2D-CGD-O1D	-2.61	118.73	123.84
15	4	603	CLA	CMB-C2B-C3B	2.61	129.56	124.68
15	3	615	CLA	O2D-CGD-CBD	2.61	115.90	111.27
15	A	1012	CLA	O2A-CGA-O1A	-2.61	117.01	123.59
14	B	4006	BCR	C15-C16-C17	-2.61	118.13	123.47
15	A	1137	CLA	O2D-CGD-CBD	2.61	115.90	111.27
15	F	1301	CLA	CHB-C4A-NA	2.61	128.12	124.51
15	B	1023	CLA	CHB-C4A-NA	2.61	128.12	124.51
15	A	1105	CLA	C1B-CHB-C4A	-2.60	124.96	130.12
15	A	1119	CLA	CHB-C4A-NA	2.60	128.11	124.51
15	A	1139	CLA	CAA-CBA-CGA	-2.60	105.65	113.25
15	3	609	CLA	CHB-C4A-NA	2.60	128.11	124.51
16	4	610	CHL	CHB-C4A-NA	2.60	128.11	124.51
15	2	605	CLA	CMB-C2B-C3B	2.60	129.54	124.68
15	B	1022	CLA	C1B-CHB-C4A	-2.60	124.97	130.12
15	B	1240	CLA	C4-C3-C2	-2.60	117.01	123.68
14	B	4004	BCR	C15-C16-C17	-2.60	118.15	123.47
15	3	614	CLA	O2D-CGD-O1D	-2.60	118.76	123.84
15	B	1230	CLA	CHB-C4A-NA	2.60	128.10	124.51
15	3	605	CLA	C1B-CHB-C4A	-2.60	124.98	130.12
14	2	503	BCR	C33-C5-C6	-2.59	121.61	124.53
15	3	610	CLA	CHB-C4A-NA	2.59	128.10	124.51
15	F	1302	CLA	CMB-C2B-C3B	2.59	129.53	124.68
15	A	1122	CLA	C4-C3-C2	-2.59	117.03	123.68
16	4	611	CHL	C2C-C3C-C4C	2.59	108.34	106.49
14	A	4005	BCR	C33-C5-C6	-2.59	121.62	124.53
15	3	610	CLA	CMB-C2B-C3B	2.59	129.52	124.68
15	1	611	CLA	O2D-CGD-O1D	-2.59	118.78	123.84
15	A	1108	CLA	CHB-C4A-NA	2.59	128.09	124.51
15	A	1104	CLA	C5-C3-C2	2.59	126.35	121.12
15	A	1121	CLA	CMB-C2B-C3B	2.58	129.51	124.68
15	A	1132	CLA	O2D-CGD-CBD	2.58	115.86	111.27
15	B	1240	CLA	CHB-C4A-NA	2.58	128.08	124.51
15	2	608	CLA	CHD-C1D-ND	-2.58	122.08	124.45
15	4	608	CLA	CBC-CAC-C3C	2.58	119.54	112.43
15	B	1201	CLA	CMB-C2B-C3B	2.58	129.50	124.68
15	B	1208	CLA	C1B-CHB-C4A	-2.58	125.01	130.12
18	2	803	LMG	O1-C7-C8	-2.58	104.68	110.90
15	F	1302	CLA	O2D-CGD-O1D	-2.58	118.80	123.84
15	B	1221	CLA	CHB-C4A-NA	2.58	128.07	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	A	1123	CLA	C2D-C1D-ND	-2.58	108.21	110.10
15	A	1140	CLA	CMB-C2B-C3B	2.57	129.49	124.68
15	1	606	CLA	CHB-C4A-NA	2.57	128.07	124.51
15	A	1126	CLA	CMB-C2B-C3B	2.57	129.49	124.68
15	B	1022	CLA	CHB-C4A-NA	2.57	128.06	124.51
15	1	611	CLA	CHD-C1D-ND	-2.57	122.09	124.45
15	A	1117	CLA	CMB-C2B-C3B	2.57	129.48	124.68
13	1	502	XAT	C37-C21-C26	-2.57	103.11	110.05
15	A	1110	CLA	C1B-CHB-C4A	-2.56	125.04	130.12
15	B	1213	CLA	O2D-CGD-O1D	-2.56	118.83	123.84
15	A	1139	CLA	C5-C3-C2	2.56	126.30	121.12
15	1	601	CLA	C1B-CHB-C4A	-2.56	125.05	130.12
15	A	1012	CLA	CHB-C4A-NA	2.56	128.05	124.51
15	B	1224	CLA	CHB-C4A-NA	2.56	128.05	124.51
15	1	612	CLA	O2D-CGD-O1D	-2.56	118.84	123.84
15	A	1108	CLA	C1B-CHB-C4A	-2.56	125.06	130.12
15	B	1240	CLA	O2A-CGA-O1A	-2.56	117.14	123.59
14	B	4006	BCR	C2-C1-C6	2.56	114.42	110.48
15	A	1105	CLA	CHB-C4A-NA	2.55	128.04	124.51
15	2	604	CLA	O2D-CGD-O1D	-2.55	118.84	123.84
15	B	1212	CLA	O2D-CGD-O1D	-2.55	118.85	123.84
16	4	613	CHL	C2C-C3C-C4C	2.55	108.31	106.49
15	2	606	CLA	CMB-C2B-C3B	2.55	129.45	124.68
15	B	1217	CLA	CHB-C4A-NA	2.55	128.04	124.51
17	2	801	LHG	O8-C23-C24	2.55	119.91	111.91
15	A	1110	CLA	C5-C3-C2	2.55	126.27	121.12
15	1	613	CLA	CHB-C4A-NA	2.55	128.04	124.51
12	2	501	LUT	C37-C21-C26	-2.55	105.69	109.55
14	A	4007	BCR	C35-C13-C14	-2.55	119.36	122.92
15	3	614	CLA	C1B-CHB-C4A	-2.55	125.07	130.12
15	B	1205	CLA	C1B-CHB-C4A	-2.55	125.07	130.12
14	4	503	BCR	C8-C7-C6	-2.55	120.05	127.20
15	A	1137	CLA	CAA-C2A-C1A	-2.54	103.64	111.97
15	B	1225	CLA	O2D-CGD-O1D	-2.54	118.87	123.84
15	2	601	CLA	CHB-C4A-NA	2.54	128.02	124.51
15	B	1235	CLA	CMB-C2B-C1B	-2.54	124.56	128.46
15	1	612	CLA	CBD-CHA-C1A	2.54	131.49	128.50
15	4	601	CLA	CHB-C4A-NA	2.54	128.02	124.51
15	A	1116	CLA	C1B-CHB-C4A	-2.54	125.10	130.12
12	3	501	LUT	C37-C21-C26	-2.53	105.71	109.55
15	B	1207	CLA	CHB-C4A-NA	2.53	128.01	124.51
15	3	607	CLA	CHB-C4A-NA	2.53	128.01	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	B	1021	CLA	O2D-CGD-O1D	-2.53	118.90	123.84
14	A	4006	BCR	C15-C16-C17	-2.52	118.30	123.47
15	A	1112	CLA	CHB-C4A-NA	2.52	128.00	124.51
15	3	612	CLA	CHB-C4A-NA	2.52	128.00	124.51
16	2	610	CHL	CHD-C4C-C3C	2.52	128.54	124.84
15	1	606	CLA	C1-C2-C3	-2.52	122.68	126.75
17	A	5001	LHG	C11-C10-C9	-2.52	101.64	114.42
13	1	502	XAT	C39-C29-C28	2.52	122.04	118.08
15	1	612	CLA	CHD-C1D-ND	-2.52	122.14	124.45
14	3	506	BCR	C33-C5-C6	-2.51	121.71	124.53
15	A	1129	CLA	CHB-C4A-NA	2.51	127.99	124.51
15	2	612	CLA	C1B-CHB-C4A	-2.51	125.14	130.12
15	A	1105	CLA	CAC-C3C-C4C	-2.51	121.55	124.81
18	2	802	LMG	O1-C7-C8	-2.51	104.84	110.90
15	B	1231	CLA	C2D-C1D-ND	-2.51	108.25	110.10
14	4	503	BCR	C11-C10-C9	-2.51	123.73	127.31
15	A	1106	CLA	C5-C3-C2	2.51	126.19	121.12
15	A	1134	CLA	O2D-CGD-CBD	2.51	115.72	111.27
15	B	1238	CLA	CHB-C4A-NA	2.51	127.98	124.51
13	3	502	XAT	C37-C21-C36	-2.50	103.68	107.37
15	B	1234	CLA	CHB-C4A-NA	2.50	127.97	124.51
12	4	501	LUT	C18-C5-C4	2.50	118.99	114.36
15	A	1138	CLA	C1B-CHB-C4A	-2.50	125.16	130.12
15	A	1109	CLA	C1B-CHB-C4A	-2.50	125.16	130.12
15	A	1013	CLA	C4-C3-C5	2.50	119.48	115.27
15	2	601	CLA	O2A-CGA-O1A	-2.50	117.28	123.59
13	2	502	XAT	C35-C34-C33	2.50	130.88	127.31
15	1	602	CLA	CMB-C2B-C3B	2.50	129.35	124.68
15	3	613	CLA	CMB-C2B-C3B	2.50	129.35	124.68
14	B	4005	BCR	C27-C26-C25	2.49	126.35	122.73
16	2	611	CHL	CHB-C4A-NA	2.49	127.96	124.51
16	1	610	CHL	CHB-C4A-NA	2.49	127.95	124.51
15	4	607	CLA	O2A-CGA-O1A	-2.49	117.31	123.59
14	3	503	BCR	C33-C5-C6	-2.48	121.74	124.53
15	A	1109	CLA	CMB-C2B-C1B	-2.48	124.65	128.46
15	B	1208	CLA	CHB-C4A-NA	2.48	127.94	124.51
14	A	4006	BCR	C33-C5-C6	-2.48	121.74	124.53
15	B	1207	CLA	CMB-C2B-C3B	2.48	129.32	124.68
15	A	1123	CLA	O2A-C1-C2	-2.48	102.12	108.64
15	A	1138	CLA	C1-C2-C3	-2.48	121.76	126.04
15	A	1139	CLA	CHB-C4A-NA	2.48	127.94	124.51
18	B	5003	LMG	C7-O1-C1	2.47	118.57	113.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B	4001	BCR	C8-C7-C6	-2.47	120.26	127.20
18	2	804	LMG	O1-C7-C8	-2.47	104.94	110.90
15	B	1228	CLA	C1B-CHB-C4A	-2.47	125.22	130.12
14	A	4008	BCR	C27-C26-C25	2.47	126.32	122.73
15	A	1012	CLA	C1B-CHB-C4A	-2.47	125.23	130.12
13	2	502	XAT	C39-C29-C28	2.47	121.96	118.08
15	A	1122	CLA	C1B-CHB-C4A	-2.46	125.24	130.12
15	B	1021	CLA	CMB-C2B-C3B	2.46	129.28	124.68
15	B	1227	CLA	O2A-CGA-O1A	-2.46	117.38	123.59
15	A	1131	CLA	C1B-CHB-C4A	-2.46	125.25	130.12
15	1	615	CLA	CHB-C4A-NA	2.46	127.91	124.51
14	B	4001	BCR	C15-C16-C17	-2.46	118.44	123.47
15	B	1205	CLA	CHB-C4A-NA	2.46	127.91	124.51
15	B	1222	CLA	CMB-C2B-C3B	2.46	129.28	124.68
15	2	608	CLA	CHB-C4A-NA	2.46	127.91	124.51
15	A	1121	CLA	CHB-C4A-NA	2.46	127.91	124.51
15	B	1215	CLA	C1-C2-C3	-2.46	121.80	126.04
16	4	610	CHL	C1B-CHB-C4A	-2.45	125.26	130.12
15	B	1240	CLA	CMB-C2B-C3B	2.45	129.26	124.68
12	4	501	LUT	C7-C6-C5	-2.45	115.53	121.46
15	A	1141	CLA	CHB-C4A-NA	2.45	127.90	124.51
16	2	613	CHL	CHB-C4A-NA	2.45	127.90	124.51
15	2	601	CLA	O2D-CGD-O1D	-2.45	119.05	123.84
14	A	4002	BCR	C38-C26-C27	-2.45	108.91	113.62
15	3	603	CLA	C4-C3-C5	2.45	119.39	115.27
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	2	616	CLA	C4-C3-C5	2.44	119.38	115.27
15	A	1110	CLA	C2A-C1A-CHA	2.44	128.13	123.86
15	4	609	CLA	CMB-C2B-C3B	2.44	129.24	124.68
15	A	1131	CLA	O2D-CGD-O1D	-2.44	119.07	123.84
15	1	602	CLA	C1B-CHB-C4A	-2.44	125.29	130.12
14	3	506	BCR	C27-C26-C25	2.44	126.27	122.73
15	4	606	CLA	CMB-C2B-C3B	2.44	129.24	124.68
15	A	1130	CLA	CMB-C2B-C1B	-2.44	124.72	128.46
15	B	1232	CLA	CHB-C4A-NA	2.43	127.88	124.51
15	B	1228	CLA	CHB-C4A-NA	2.43	127.88	124.51
15	4	612	CLA	O2A-CGA-O1A	-2.43	117.45	123.59
15	B	1204	CLA	O2D-CGD-CBD	2.43	115.59	111.27
13	1	502	XAT	C35-C34-C33	-2.43	123.84	127.31
17	A	5001	LHG	O8-C23-C24	2.43	119.52	111.91
15	A	1112	CLA	O2D-CGD-O1D	-2.43	119.09	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	A	1126	CLA	CAC-C3C-C4C	2.42	127.95	124.81
15	4	604	CLA	C1B-CHB-C4A	-2.42	125.32	130.12
15	A	1106	CLA	C1B-CHB-C4A	-2.42	125.32	130.12
15	B	1220	CLA	C1B-CHB-C4A	-2.42	125.32	130.12
15	B	1211	CLA	C1B-CHB-C4A	-2.42	125.33	130.12
14	4	503	BCR	C33-C5-C6	-2.42	121.81	124.53
15	B	1220	CLA	CHB-C4A-NA	2.41	127.85	124.51
15	B	1217	CLA	CMB-C2B-C3B	2.41	129.19	124.68
15	B	1223	CLA	C1-C2-C3	-2.41	121.87	126.04
14	A	4008	BCR	C34-C9-C10	-2.41	119.54	122.92
15	A	1131	CLA	CHB-C4A-NA	2.41	127.85	124.51
15	A	1111	CLA	CAC-C3C-C4C	2.41	127.94	124.81
15	B	1224	CLA	C1B-CHB-C4A	-2.41	125.34	130.12
15	A	1012	CLA	O2D-CGD-CBD	2.41	115.55	111.27
15	2	607	CLA	C1-O2A-CGA	2.41	122.76	116.44
15	3	605	CLA	C2D-C1D-ND	-2.41	108.33	110.10
15	4	608	CLA	CMB-C2B-C3B	2.41	129.18	124.68
14	A	4002	BCR	C34-C9-C8	-2.40	114.29	118.08
15	A	1106	CLA	CAA-C2A-C1A	-2.40	104.10	111.97
15	4	602	CLA	C1B-CHB-C4A	-2.40	125.36	130.12
15	A	1116	CLA	C1-O2A-CGA	2.40	122.75	116.44
13	1	502	XAT	C39-C29-C30	-2.40	119.56	122.92
15	A	1120	CLA	CHB-C4A-NA	2.40	127.83	124.51
15	4	612	CLA	C1B-CHB-C4A	-2.40	125.36	130.12
15	4	607	CLA	O2D-CGD-O1D	-2.40	119.14	123.84
16	2	613	CHL	C4D-CHA-C1A	2.40	124.17	121.25
15	B	1226	CLA	CMB-C2B-C3B	2.40	129.17	124.68
12	2	501	LUT	C18-C5-C6	-2.40	121.83	124.53
15	B	1208	CLA	O2A-CGA-O1A	-2.40	117.54	123.59
15	2	616	CLA	C1B-CHB-C4A	-2.40	125.37	130.12
15	A	1013	CLA	CMB-C2B-C1B	-2.40	124.78	128.46
14	3	504	BCR	C24-C23-C22	-2.39	122.62	126.23
15	2	601	CLA	C1B-CHB-C4A	-2.39	125.38	130.12
15	4	609	CLA	C4-C3-C2	-2.39	117.55	123.68
14	B	4003	BCR	C15-C16-C17	-2.39	118.58	123.47
15	1	604	CLA	CMB-C2B-C3B	2.39	129.14	124.68
15	A	1140	CLA	CHB-C4A-NA	2.39	127.81	124.51
12	3	501	LUT	C22-C23-C24	-2.38	109.03	111.74
15	B	1227	CLA	C1B-CHB-C4A	-2.38	125.39	130.12
15	B	1235	CLA	C1B-CHB-C4A	-2.38	125.40	130.12
15	A	1101	CLA	O2D-CGD-CBD	2.38	115.50	111.27
16	4	610	CHL	C2C-C3C-C4C	2.38	108.19	106.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	2	608	CLA	C1B-CHB-C4A	-2.38	125.40	130.12
14	A	4004	BCR	C37-C22-C21	-2.38	119.59	122.92
13	2	502	XAT	C36-C21-C26	2.38	116.47	110.05
15	3	608	CLA	O2A-CGA-O1A	-2.38	117.59	123.59
13	1	502	XAT	C26-C27-C28	-2.38	120.97	125.99
15	A	1137	CLA	CMB-C2B-C3B	2.38	129.12	124.68
16	2	610	CHL	CMB-C2B-C1B	-2.38	124.81	128.46
15	A	1127	CLA	O2D-CGD-O1D	-2.37	119.20	123.84
14	F	4001	BCR	C24-C23-C22	-2.37	122.65	126.23
14	B	4006	BCR	C27-C26-C25	2.37	126.17	122.73
15	1	611	CLA	CHB-C4A-NA	2.37	127.79	124.51
15	1	615	CLA	C1B-CHB-C4A	-2.36	125.43	130.12
17	1	801	LHG	O8-C23-C24	2.36	119.33	111.91
15	A	1133	CLA	C1B-CHB-C4A	-2.36	125.43	130.12
16	3	604	CHL	CMB-C2B-C1B	-2.36	124.83	128.46
14	3	504	BCR	C15-C14-C13	-2.36	123.94	127.31
15	4	616	CLA	CHB-C4A-NA	2.36	127.78	124.51
15	4	605	CLA	C4-C3-C2	-2.36	117.62	123.68
15	B	1214	CLA	C1B-CHB-C4A	-2.36	125.44	130.12
14	F	4002	BCR	C8-C7-C6	-2.36	120.58	127.20
15	A	1128	CLA	CHB-C4A-NA	2.36	127.77	124.51
15	1	608	CLA	CMB-C2B-C3B	2.36	129.09	124.68
15	A	1115	CLA	CHB-C4A-NA	2.36	127.77	124.51
18	B	5003	LMG	O3-C3-C2	-2.35	104.91	110.35
15	A	1129	CLA	C1B-CHB-C4A	-2.35	125.46	130.12
14	A	4007	BCR	C38-C26-C25	-2.35	121.89	124.53
15	A	1107	CLA	C2A-C1A-CHA	2.35	127.97	123.86
13	4	502	XAT	C19-C9-C8	-2.35	114.37	118.08
15	B	1221	CLA	O2A-CGA-O1A	-2.35	117.66	123.59
14	3	504	BCR	C38-C26-C25	-2.35	121.89	124.53
15	B	1230	CLA	O2A-CGA-O1A	-2.35	117.67	123.59
15	4	604	CLA	O2A-CGA-O1A	-2.35	117.67	123.59
15	A	1123	CLA	C1B-CHB-C4A	-2.35	125.47	130.12
14	1	503	BCR	C15-C16-C17	-2.35	118.67	123.47
14	2	503	BCR	C38-C26-C25	-2.35	121.89	124.53
15	A	1113	CLA	CMB-C2B-C3B	2.34	129.06	124.68
14	A	4005	BCR	C8-C7-C6	-2.34	120.62	127.20
15	B	1023	CLA	C1B-CHB-C4A	-2.34	125.48	130.12
15	B	1204	CLA	CMB-C2B-C3B	2.34	129.06	124.68
15	A	1140	CLA	C1B-CHB-C4A	-2.34	125.48	130.12
14	A	4002	BCR	C2-C1-C6	2.34	114.08	110.48
15	A	1116	CLA	CHD-C1D-ND	-2.34	122.31	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	B	1223	CLA	CHD-C1D-ND	-2.34	122.31	124.45
16	2	613	CHL	CHD-C4C-C3C	2.34	128.27	124.84
14	J	4001	BCR	C24-C23-C22	-2.34	122.71	126.23
15	3	601	CLA	C1B-CHB-C4A	-2.33	125.49	130.12
15	A	1136	CLA	C1B-CHB-C4A	-2.33	125.50	130.12
15	A	1127	CLA	CHB-C4A-NA	2.33	127.74	124.51
15	A	1101	CLA	CMB-C2B-C1B	-2.33	124.88	128.46
15	1	603	CLA	CBA-CAA-C2A	2.33	120.75	113.86
15	A	1125	CLA	CHB-C4A-NA	2.33	127.74	124.51
15	J	1302	CLA	C1B-CHB-C4A	-2.33	125.50	130.12
16	2	609	CHL	CBA-CAA-C2A	2.33	120.74	113.86
14	4	503	BCR	C2-C1-C6	2.33	114.07	110.48
14	F	4002	BCR	C29-C30-C25	2.33	114.06	110.48
15	B	1207	CLA	C1B-CHB-C4A	-2.33	125.51	130.12
15	B	1231	CLA	CAC-C3C-C4C	2.33	127.83	124.81
15	3	601	CLA	O2A-CGA-O1A	-2.33	117.72	123.59
15	4	601	CLA	CBA-CAA-C2A	2.33	120.73	113.86
12	2	501	LUT	C22-C23-C24	-2.33	109.09	111.74
15	A	1131	CLA	CMB-C2B-C3B	2.33	129.03	124.68
15	A	1136	CLA	CHB-C4A-NA	2.32	127.72	124.51
13	2	502	XAT	C25-C24-C23	2.32	117.34	112.75
15	B	1230	CLA	C1-C2-C3	-2.32	122.03	126.04
15	4	604	CLA	CBA-CAA-C2A	2.32	120.71	113.86
15	4	603	CLA	C3A-C2A-C1A	2.32	104.81	101.34
15	A	1101	CLA	C5-C3-C2	2.32	125.81	121.12
15	4	608	CLA	C1B-CHB-C4A	-2.32	125.53	130.12
15	A	1138	CLA	O2D-CGD-CBD	2.32	115.39	111.27
15	B	1215	CLA	O2A-CGA-O1A	-2.32	117.75	123.59
16	4	611	CHL	C1-O2A-CGA	2.32	122.52	116.44
15	F	1301	CLA	CMB-C2B-C3B	2.32	129.01	124.68
15	B	1232	CLA	CMB-C2B-C1B	-2.31	124.91	128.46
14	B	4005	BCR	C38-C26-C25	-2.31	121.93	124.53
15	4	602	CLA	O2D-CGD-CBD	2.31	115.38	111.27
15	A	1139	CLA	C1B-CHB-C4A	-2.31	125.54	130.12
15	4	605	CLA	CHD-C1D-ND	-2.31	122.33	124.45
17	B	5001	LHG	C11-C10-C9	-2.31	102.70	114.42
15	A	1013	CLA	C1B-CHB-C4A	-2.31	125.54	130.12
14	A	4003	BCR	C37-C22-C21	-2.31	119.69	122.92
13	4	502	XAT	C25-C24-C23	-2.31	108.19	112.75
16	1	609	CHL	C1B-CHB-C4A	-2.31	125.55	130.12
15	B	1215	CLA	CHD-C1D-ND	-2.31	122.33	124.45
14	1	503	BCR	C37-C22-C21	-2.30	119.69	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	2	611	CHL	CHD-C4C-C3C	2.30	128.23	124.84
15	3	603	CLA	CHB-C4A-NA	2.30	127.69	124.51
15	B	1237	CLA	C1B-CHB-C4A	-2.30	125.56	130.12
14	3	504	BCR	C2-C1-C6	2.30	114.02	110.48
15	4	607	CLA	C1B-CHB-C4A	-2.30	125.56	130.12
16	3	604	CHL	C1B-CHB-C4A	-2.30	125.56	130.12
15	1	607	CLA	CHB-C4A-NA	2.30	127.69	124.51
15	B	1201	CLA	C1B-CHB-C4A	-2.30	125.56	130.12
14	B	4005	BCR	C2-C1-C6	2.30	114.02	110.48
15	B	1231	CLA	C4-C3-C2	-2.30	117.78	123.68
12	2	501	LUT	C19-C9-C8	2.30	121.70	118.08
15	B	1227	CLA	CMB-C2B-C3B	2.30	128.98	124.68
15	B	1022	CLA	C4-C3-C5	2.30	119.14	115.27
15	1	604	CLA	CAC-C3C-C4C	2.30	127.79	124.81
15	B	1206	CLA	CMB-C2B-C3B	2.30	128.97	124.68
15	4	603	CLA	C1B-CHB-C4A	-2.30	125.57	130.12
12	2	501	LUT	C20-C13-C12	2.30	121.69	118.08
15	3	612	CLA	C1B-CHB-C4A	-2.30	125.57	130.12
15	A	1136	CLA	CMB-C2B-C3B	2.29	128.97	124.68
15	A	1132	CLA	CBC-CAC-C3C	2.29	118.76	112.43
16	1	609	CHL	CMB-C2B-C1B	-2.29	124.94	128.46
15	4	609	CLA	C1B-CHB-C4A	-2.29	125.57	130.12
15	1	612	CLA	CHB-C4A-NA	2.29	127.68	124.51
19	A	1011	CL0	C9-C8-C10	2.29	119.59	111.29
14	A	4006	BCR	C8-C7-C6	-2.29	120.77	127.20
15	B	1204	CLA	O2A-CGA-O1A	-2.29	117.60	123.30
15	2	604	CLA	C1B-CHB-C4A	-2.29	125.59	130.12
14	2	503	BCR	C37-C22-C21	-2.29	119.72	122.92
15	A	1126	CLA	CHB-C4A-NA	2.29	127.67	124.51
15	B	1202	CLA	CHD-C1D-ND	-2.29	122.35	124.45
15	A	1138	CLA	O2A-CGA-O1A	-2.29	117.83	123.59
14	B	4004	BCR	C8-C7-C6	-2.28	120.79	127.20
15	B	1212	CLA	O2A-CGA-O1A	-2.28	117.83	123.59
15	1	607	CLA	C1B-CHB-C4A	-2.28	125.60	130.12
14	1	503	BCR	C27-C26-C25	2.28	126.04	122.73
15	4	606	CLA	O2A-CGA-O1A	-2.28	117.84	123.59
15	B	1212	CLA	CMB-C2B-C3B	2.28	128.94	124.68
15	B	1224	CLA	O2A-CGA-O1A	-2.28	117.84	123.59
16	1	610	CHL	CMB-C2B-C1B	-2.28	124.96	128.46
15	4	616	CLA	C1B-CHB-C4A	-2.28	125.61	130.12
15	A	1119	CLA	C1B-CHB-C4A	-2.28	125.61	130.12
15	A	1119	CLA	CHD-C1D-ND	-2.28	122.36	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	B	1210	CLA	CHB-C4A-NA	2.28	127.66	124.51
14	F	4002	BCR	C24-C23-C22	-2.27	122.80	126.23
15	B	1219	CLA	C1B-CHB-C4A	-2.27	125.61	130.12
16	2	609	CHL	CMB-C2B-C1B	-2.27	124.97	128.46
15	B	1217	CLA	C1B-CHB-C4A	-2.27	125.62	130.12
15	B	1208	CLA	CMB-C2B-C3B	2.27	128.93	124.68
15	B	1216	CLA	C2D-C1D-ND	-2.27	108.43	110.10
16	3	604	CHL	C1-O2A-CGA	2.27	122.40	116.44
15	4	606	CLA	C1B-CHB-C4A	-2.27	125.62	130.12
15	A	1109	CLA	CHD-C1D-ND	-2.27	122.37	124.45
15	1	608	CLA	C5-C3-C2	2.27	125.71	121.12
13	1	502	XAT	C20-C13-C14	-2.27	119.75	122.92
15	B	1202	CLA	CMB-C2B-C3B	2.27	128.92	124.68
15	2	601	CLA	CBA-CAA-C2A	2.27	120.55	113.86
14	3	503	BCR	C27-C26-C25	2.26	126.02	122.73
14	4	503	BCR	C15-C14-C13	-2.26	124.08	127.31
15	B	1239	CLA	CAC-C3C-C4C	2.26	127.75	124.81
14	A	4004	BCR	C33-C5-C6	-2.26	121.99	124.53
15	B	1225	CLA	CHD-C1D-ND	-2.26	122.38	124.45
16	1	610	CHL	CHD-C4C-C3C	2.26	128.16	124.84
12	3	501	LUT	C7-C6-C5	-2.26	115.98	121.46
15	B	1225	CLA	C1B-CHB-C4A	-2.26	125.64	130.12
15	B	1230	CLA	C1B-CHB-C4A	-2.26	125.64	130.12
15	A	1103	CLA	CHD-C1D-ND	-2.26	122.38	124.45
15	A	1103	CLA	C1B-CHB-C4A	-2.26	125.64	130.12
15	F	1302	CLA	CBA-CAA-C2A	2.26	120.53	113.86
15	4	605	CLA	C1B-CHB-C4A	-2.26	125.65	130.12
15	A	1012	CLA	C6-C5-C3	2.25	119.37	113.45
14	B	4001	BCR	C1-C6-C5	-2.25	119.44	122.61
13	1	502	XAT	C19-C9-C8	2.25	121.63	118.08
15	A	1105	CLA	CBC-CAC-C3C	2.25	118.64	112.43
15	B	1219	CLA	CHB-C4A-NA	2.25	127.63	124.51
15	A	1128	CLA	CMB-C2B-C3B	2.25	128.89	124.68
14	1	503	BCR	C7-C8-C9	-2.25	122.83	126.23
13	1	502	XAT	C19-C9-C10	-2.25	119.77	122.92
15	3	613	CLA	C1B-CHB-C4A	-2.25	125.67	130.12
12	1	501	LUT	C38-C25-C24	-2.25	118.75	123.56
15	2	607	CLA	C1B-CHB-C4A	-2.25	125.67	130.12
22	B	5002	DGD	CFB-CEB-CDB	-2.25	103.02	114.42
13	3	502	XAT	C19-C9-C8	-2.25	114.54	118.08
19	A	1011	CL0	C2A-C3A-C4A	2.25	105.50	101.87
15	3	612	CLA	CAC-C3C-C4C	2.25	127.72	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	5002	DGD	O6E-C5E-C4E	2.25	113.77	109.69
16	4	611	CHL	CMB-C2B-C1B	-2.24	125.01	128.46
15	A	1126	CLA	O2A-CGA-O1A	-2.24	117.93	123.59
20	B	2002	PQN	C21-C20-C18	-2.24	108.67	115.92
13	2	502	XAT	C19-C9-C10	-2.24	119.78	122.92
15	B	1212	CLA	C1B-CHB-C4A	-2.24	125.68	130.12
16	2	611	CHL	CMB-C2B-C1B	-2.24	125.02	128.46
15	4	608	CLA	CHB-C4A-NA	2.24	127.61	124.51
17	1	801	LHG	C20-C19-C18	-2.24	103.06	114.42
15	A	1121	CLA	C1B-CHB-C4A	-2.23	125.69	130.12
15	3	611	CLA	CMB-C2B-C1B	-2.23	125.03	128.46
16	1	609	CHL	CHD-C4C-C3C	2.23	128.12	124.84
14	1	503	BCR	C16-C15-C14	-2.23	118.90	123.47
14	J	4001	BCR	C33-C5-C6	-2.23	122.02	124.53
15	B	1238	CLA	C1B-CHB-C4A	-2.23	125.70	130.12
16	2	611	CHL	C3A-C2A-C1A	2.23	104.68	101.34
14	A	4005	BCR	C11-C10-C9	-2.23	124.12	127.31
16	4	610	CHL	CMB-C2B-C1B	-2.23	125.04	128.46
15	1	603	CLA	C1B-CHB-C4A	-2.23	125.70	130.12
14	A	4003	BCR	C35-C13-C14	-2.23	119.80	122.92
15	B	1240	CLA	C1B-CHB-C4A	-2.23	125.71	130.12
15	4	616	CLA	O2A-CGA-O1A	-2.23	117.97	123.59
15	3	608	CLA	CHB-C4A-NA	2.23	127.59	124.51
15	1	615	CLA	CAC-C3C-C4C	2.23	127.70	124.81
15	1	601	CLA	O2A-CGA-O1A	-2.23	117.97	123.59
15	F	1301	CLA	C1B-CHB-C4A	-2.22	125.71	130.12
15	3	607	CLA	C1B-CHB-C4A	-2.22	125.71	130.12
15	A	1110	CLA	C4-C3-C2	-2.22	117.97	123.68
15	A	1138	CLA	CMB-C2B-C3B	2.22	128.84	124.68
15	A	1129	CLA	CAC-C3C-C4C	2.22	127.69	124.81
15	B	1216	CLA	O2A-CGA-O1A	-2.22	117.98	123.59
16	2	613	CHL	CMB-C2B-C1B	-2.22	125.05	128.46
15	B	1209	CLA	CMB-C2B-C3B	2.22	128.83	124.68
15	3	608	CLA	CHD-C1D-ND	-2.22	122.41	124.45
15	B	1224	CLA	CHD-C1D-ND	-2.22	122.41	124.45
19	A	1011	CL0	C6-C5-C3	-2.22	107.64	113.45
15	2	606	CLA	C1B-CHB-C4A	-2.22	125.72	130.12
15	B	1222	CLA	O2D-CGD-O1D	-2.22	119.50	123.84
15	B	1226	CLA	CBA-CAA-C2A	2.22	120.41	113.86
15	1	608	CLA	C1B-CHB-C4A	-2.22	125.73	130.12
14	1	503	BCR	C35-C13-C14	-2.22	119.82	122.92
15	A	1105	CLA	CHD-C1D-ND	-2.22	122.42	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	A	1115	CLA	C1B-CHB-C4A	-2.22	125.73	130.12
14	3	503	BCR	C15-C16-C17	-2.21	118.94	123.47
15	2	603	CLA	CHD-C1D-ND	-2.21	122.42	124.45
15	B	1204	CLA	C1B-CHB-C4A	-2.21	125.73	130.12
15	1	611	CLA	C1B-CHB-C4A	-2.21	125.74	130.12
14	B	4005	BCR	C37-C22-C21	-2.21	119.83	122.92
14	A	4005	BCR	C16-C15-C14	-2.21	118.95	123.47
15	3	607	CLA	C5-C3-C2	2.21	125.59	121.12
15	4	608	CLA	CHD-C4C-C3C	2.21	128.09	124.84
16	4	610	CHL	CHD-C4C-NC	-2.21	120.73	124.20
19	A	1011	CL0	CMA-C3A-C4A	-2.21	105.84	111.77
22	B	5002	DGD	CDB-CCB-CBB	-2.21	103.22	114.42
13	3	502	XAT	C38-C25-C26	-2.21	118.56	122.26
15	1	604	CLA	C1B-CHB-C4A	-2.21	125.75	130.12
15	B	1238	CLA	CHD-C4C-C3C	2.20	128.08	124.84
14	A	4002	BCR	C1-C6-C5	-2.20	119.51	122.61
15	B	1222	CLA	C1-O2A-CGA	2.20	122.22	116.44
14	J	4002	BCR	C38-C26-C25	-2.20	122.06	124.53
15	F	1302	CLA	C1B-CHB-C4A	-2.20	125.76	130.12
14	4	503	BCR	C16-C15-C14	-2.20	118.96	123.47
15	B	1229	CLA	C5-C3-C2	2.20	125.57	121.12
15	A	1137	CLA	C4-C3-C2	-2.20	118.03	123.68
15	3	610	CLA	C1B-CHB-C4A	-2.20	125.76	130.12
15	A	1135	CLA	CBA-CAA-C2A	-2.20	107.38	113.86
14	B	4003	BCR	C1-C6-C5	-2.20	119.52	122.61
15	A	1138	CLA	C3A-C2A-C1A	2.20	104.63	101.34
15	A	1134	CLA	C1B-CHB-C4A	-2.20	125.77	130.12
15	A	1118	CLA	C1B-CHB-C4A	-2.20	125.77	130.12
15	A	1013	CLA	C4-C3-C2	-2.20	118.05	123.68
15	B	1216	CLA	C1-C2-C3	-2.20	122.25	126.04
15	B	1202	CLA	O2D-CGD-CBD	2.19	115.17	111.27
15	2	604	CLA	CBA-CAA-C2A	2.19	120.34	113.86
15	B	1210	CLA	C1-C2-C3	-2.19	122.25	126.04
15	B	1211	CLA	C2D-C1D-ND	-2.19	108.49	110.10
15	B	1231	CLA	O2A-CGA-O1A	-2.19	118.06	123.59
15	1	601	CLA	C1-C2-C3	-2.19	122.25	126.04
15	B	1214	CLA	O2A-CGA-O1A	-2.19	118.06	123.59
12	4	501	LUT	C8-C9-C10	2.19	122.30	118.94
16	3	604	CHL	CBA-CAA-C2A	2.19	120.33	113.86
15	B	1216	CLA	C1B-CHB-C4A	-2.19	125.78	130.12
15	B	1021	CLA	CHB-C4A-NA	2.19	127.54	124.51
14	1	503	BCR	C11-C10-C9	-2.19	124.19	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	A	1117	CLA	C11-C12-C13	-2.19	108.84	115.92
14	3	503	BCR	C2-C1-C6	2.19	113.85	110.48
15	1	603	CLA	CAC-C3C-C4C	2.19	127.65	124.81
15	4	601	CLA	O2A-CGA-O1A	-2.19	118.08	123.59
15	3	611	CLA	C1B-CHB-C4A	-2.19	125.79	130.12
14	2	503	BCR	C15-C16-C17	-2.18	119.00	123.47
15	A	1126	CLA	CBA-CAA-C2A	2.18	120.31	113.86
15	B	1230	CLA	CAC-C3C-C4C	2.18	127.64	124.81
14	3	503	BCR	C20-C21-C22	-2.18	124.19	127.31
14	B	4004	BCR	C27-C26-C25	2.18	125.90	122.73
13	4	502	XAT	C20-C13-C14	-2.18	119.87	122.92
14	B	4002	BCR	C15-C16-C17	-2.18	119.01	123.47
15	1	606	CLA	C1B-CHB-C4A	-2.18	125.80	130.12
18	2	802	LMG	O3-C3-C2	-2.18	105.31	110.35
15	A	1141	CLA	C1B-CHB-C4A	-2.18	125.80	130.12
15	A	1013	CLA	CMB-C2B-C3B	2.18	128.75	124.68
13	2	502	XAT	C39-C29-C30	-2.18	119.87	122.92
15	2	604	CLA	CAC-C3C-C4C	2.18	127.63	124.81
14	A	4003	BCR	C16-C15-C14	-2.17	119.02	123.47
15	A	1102	CLA	O2A-CGA-O1A	-2.17	118.10	123.59
16	1	609	CHL	C2C-C3C-C4C	2.17	108.04	106.49
15	A	1130	CLA	C1B-CHB-C4A	-2.17	125.81	130.12
15	B	1219	CLA	O2A-CGA-O1A	-2.17	118.11	123.59
15	3	608	CLA	CMB-C2B-C3B	2.17	128.74	124.68
15	4	607	CLA	CMB-C2B-C1B	-2.17	125.13	128.46
14	B	4003	BCR	C28-C27-C26	-2.17	110.21	114.08
15	B	1232	CLA	C1B-CHB-C4A	-2.17	125.82	130.12
15	B	1223	CLA	C1B-CHB-C4A	-2.17	125.83	130.12
15	A	1105	CLA	C1-C2-C3	-2.17	122.30	126.04
16	4	613	CHL	CMB-C2B-C1B	-2.17	125.14	128.46
13	1	502	XAT	C40-C33-C32	2.16	121.49	118.08
15	A	1120	CLA	C1B-CHB-C4A	-2.16	125.83	130.12
14	J	4001	BCR	C16-C15-C14	-2.16	119.04	123.47
15	A	1111	CLA	C1B-CHB-C4A	-2.16	125.83	130.12
14	A	4006	BCR	C38-C26-C25	-2.16	122.10	124.53
15	A	1104	CLA	C1B-CHB-C4A	-2.16	125.84	130.12
14	A	4003	BCR	C7-C8-C9	-2.16	122.97	126.23
15	1	613	CLA	C1B-CHB-C4A	-2.16	125.84	130.12
14	3	503	BCR	C7-C8-C9	-2.16	122.97	126.23
15	A	1107	CLA	C1B-CHB-C4A	-2.16	125.84	130.12
15	B	1203	CLA	C1B-CHB-C4A	-2.16	125.85	130.12
18	2	803	LMG	C1-C2-C3	-2.16	105.51	110.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	A	1125	CLA	C1B-CHB-C4A	-2.15	125.85	130.12
15	2	601	CLA	CMB-C2B-C1B	-2.15	125.16	128.46
15	B	1222	CLA	CAA-CBA-CGA	-2.15	106.96	113.25
15	A	1113	CLA	CHB-C4A-NA	2.15	127.49	124.51
17	3	801	LHG	C20-C19-C18	-2.15	103.50	114.42
15	3	606	CLA	CHD-C1D-ND	-2.15	122.48	124.45
15	B	1226	CLA	C1B-CHB-C4A	-2.15	125.86	130.12
15	A	1126	CLA	CHD-C1D-ND	-2.15	122.48	124.45
15	2	603	CLA	C1B-CHB-C4A	-2.15	125.86	130.12
16	4	611	CHL	C3A-C2A-C1A	2.15	104.56	101.34
15	B	1211	CLA	O2A-CGA-O1A	-2.15	118.17	123.59
14	A	4007	BCR	C2-C1-C6	2.15	113.79	110.48
19	A	1011	CL0	C3A-C2A-C1A	-2.15	98.13	101.34
16	4	610	CHL	C1-O2A-CGA	2.15	123.18	116.11
15	A	1117	CLA	C3A-C2A-C1A	2.15	104.55	101.34
14	J	4001	BCR	C27-C26-C25	2.14	125.84	122.73
14	B	4005	BCR	C11-C10-C9	-2.14	124.25	127.31
15	F	1302	CLA	O2A-CGA-O1A	-2.14	118.18	123.59
16	2	609	CHL	C2C-C3C-C4C	2.14	108.02	106.49
14	B	4001	BCR	C2-C3-C4	2.14	116.17	111.38
15	3	610	CLA	CHD-C1D-ND	-2.14	122.48	124.45
15	A	1124	CLA	C2A-C1A-CHA	2.14	127.60	123.86
14	B	4002	BCR	C11-C10-C9	-2.14	124.26	127.31
15	B	1202	CLA	O2A-CGA-O1A	-2.14	118.19	123.59
14	1	503	BCR	C38-C26-C25	-2.14	122.13	124.53
14	J	4002	BCR	C2-C1-C6	2.14	113.77	110.48
18	2	804	LMG	O2-C2-C1	-2.14	104.86	110.05
15	A	1137	CLA	C4-C3-C5	2.13	118.86	115.27
18	B	5003	LMG	C1-C2-C3	-2.13	105.55	110.00
15	3	607	CLA	O2A-CGA-O1A	-2.13	118.21	123.59
17	1	801	LHG	O8-C23-O10	-2.13	118.21	123.59
15	4	601	CLA	CHD-C1D-ND	-2.13	122.49	124.45
17	2	801	LHG	C5-O7-C7	-2.13	112.55	117.79
12	1	501	LUT	C19-C9-C8	2.13	121.43	118.08
15	2	616	CLA	C14-C13-C12	-2.13	103.58	111.29
14	B	4003	BCR	C24-C23-C22	-2.13	123.02	126.23
15	2	616	CLA	C16-C15-C13	2.13	122.80	115.92
15	A	1106	CLA	O2D-CGD-CBD	2.13	115.05	111.27
18	2	803	LMG	O2-C2-C1	-2.13	104.88	110.05
15	4	604	CLA	CMC-C2C-C1C	2.13	128.28	125.04
15	B	1021	CLA	O2A-CGA-O1A	-2.13	118.22	123.59
15	2	602	CLA	C2A-C1A-CHA	2.13	127.58	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	B	1206	CLA	C1B-CHB-C4A	-2.13	125.91	130.12
14	3	506	BCR	C16-C15-C14	-2.12	119.12	123.47
15	B	1209	CLA	C1B-CHB-C4A	-2.12	125.91	130.12
14	A	4005	BCR	C7-C8-C9	-2.12	123.03	126.23
15	A	1123	CLA	C2A-C1A-CHA	2.12	127.57	123.86
15	A	1116	CLA	CBA-CAA-C2A	2.12	120.13	113.86
15	A	1105	CLA	O2A-CGA-O1A	-2.12	118.23	123.59
14	B	4004	BCR	C11-C10-C9	-2.12	124.28	127.31
15	2	604	CLA	O2A-CGA-O1A	-2.12	118.24	123.59
15	A	1102	CLA	CHD-C1D-ND	-2.12	122.50	124.45
15	B	1215	CLA	CAA-C2A-C1A	-2.12	105.02	111.97
14	A	4003	BCR	C24-C23-C22	-2.12	123.03	126.23
15	A	1120	CLA	CAC-C3C-C4C	2.12	127.56	124.81
15	3	610	CLA	O2A-CGA-O1A	-2.12	118.24	123.59
18	2	802	LMG	O2-C2-C1	-2.12	104.90	110.05
22	B	5002	DGD	C3D-C4D-C5D	-2.12	106.46	110.24
16	2	613	CHL	C1B-CHB-C4A	-2.12	125.92	130.12
15	A	1130	CLA	O2D-CGD-CBD	2.12	115.03	111.27
15	B	1210	CLA	O2D-CGD-CBD	2.12	115.03	111.27
15	B	1213	CLA	O2A-CGA-O1A	-2.12	118.25	123.59
15	1	607	CLA	CAC-C3C-C4C	2.11	127.55	124.81
15	A	1134	CLA	CAA-C2A-C3A	-2.11	108.98	114.26
15	B	1236	CLA	O2A-CGA-O1A	-2.11	118.26	123.59
15	B	1225	CLA	CBA-CAA-C2A	2.11	120.10	113.86
15	A	1139	CLA	C4-C3-C2	-2.11	118.26	123.68
18	2	803	LMG	O3-C3-C2	-2.11	105.47	110.35
15	A	1117	CLA	C1B-CHB-C4A	-2.11	125.93	130.12
15	1	605	CLA	C1B-CHB-C4A	-2.11	125.93	130.12
15	A	1137	CLA	C1B-CHB-C4A	-2.11	125.93	130.12
15	A	1101	CLA	C1B-CHB-C4A	-2.11	125.94	130.12
15	B	1219	CLA	CHD-C1D-ND	-2.11	122.51	124.45
15	B	1213	CLA	C1B-CHB-C4A	-2.11	125.94	130.12
14	B	4006	BCR	C8-C7-C6	-2.11	121.28	127.20
15	3	605	CLA	CAC-C3C-C2C	-2.11	123.92	127.53
15	3	615	CLA	CMB-C2B-C1B	-2.11	125.22	128.46
15	4	604	CLA	CHD-C1D-ND	-2.11	122.52	124.45
16	4	611	CHL	CHD-C4C-C3C	2.11	127.94	124.84
15	B	1231	CLA	C1B-CHB-C4A	-2.11	125.95	130.12
15	B	1235	CLA	CHD-C1D-ND	-2.11	122.52	124.45
14	2	503	BCR	C8-C7-C6	-2.11	121.29	127.20
15	3	606	CLA	C1B-CHB-C4A	-2.10	125.95	130.12
15	A	1012	CLA	CHD-C1D-ND	-2.10	122.52	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	A	1141	CLA	CMB-C2B-C3B	2.10	128.61	124.68
17	A	5002	LHG	C11-C10-C9	-2.10	103.75	114.42
15	2	603	CLA	CMB-C2B-C3B	2.10	128.61	124.68
15	3	606	CLA	C1-O2A-CGA	2.10	121.96	116.44
15	B	1234	CLA	O2A-CGA-O1A	-2.10	118.28	123.59
14	A	4006	BCR	C37-C22-C21	-2.10	119.98	122.92
15	B	1208	CLA	C5-C3-C2	2.10	125.37	121.12
16	2	610	CHL	C1B-CHB-C4A	-2.10	125.96	130.12
14	B	4002	BCR	C34-C9-C10	-2.10	119.98	122.92
18	2	804	LMG	O3-C3-C2	-2.10	105.50	110.35
15	B	1215	CLA	O2D-CGD-CBD	2.10	114.99	111.27
15	3	609	CLA	C1B-CHB-C4A	-2.10	125.97	130.12
13	2	502	XAT	O23-C23-C22	-2.10	105.64	109.80
15	B	1201	CLA	CHD-C1D-ND	-2.09	122.53	124.45
15	B	1220	CLA	CHD-C1D-ND	-2.09	122.53	124.45
15	B	1206	CLA	CHD-C1D-ND	-2.09	122.53	124.45
15	4	603	CLA	O2A-CGA-O1A	-2.09	118.31	123.59
15	B	1239	CLA	C1B-CHB-C4A	-2.09	125.97	130.12
14	F	4001	BCR	C27-C26-C25	2.09	125.77	122.73
16	4	610	CHL	C3A-C2A-C1A	2.09	104.47	101.34
15	B	1221	CLA	C2A-C1A-CHA	2.09	127.51	123.86
15	B	1216	CLA	CHB-C4A-NA	2.09	127.40	124.51
14	A	4007	BCR	C37-C22-C21	-2.09	120.00	122.92
15	3	605	CLA	O1D-CGD-CBD	2.09	128.76	124.48
15	B	1235	CLA	CMB-C2B-C3B	2.09	128.59	124.68
12	2	501	LUT	C8-C9-C10	2.09	122.15	118.94
15	1	603	CLA	O2A-CGA-O1A	-2.09	118.32	123.59
15	A	1012	CLA	C4-C3-C5	2.09	118.78	115.27
15	2	606	CLA	CAC-C3C-C4C	2.08	127.51	124.81
15	1	604	CLA	CMC-C2C-C1C	2.08	128.21	125.04
15	3	609	CLA	CMB-C2B-C1B	-2.08	125.27	128.46
17	3	801	LHG	C11-C10-C9	-2.08	103.86	114.42
13	4	502	XAT	C24-C23-C22	-2.08	106.76	110.77
14	1	503	BCR	C2-C1-C6	2.08	113.68	110.48
20	A	2001	PQN	C2M-C2-C3	-2.08	121.01	124.40
12	4	501	LUT	C36-C21-C26	2.08	112.69	109.55
15	A	1130	CLA	CBA-CAA-C2A	2.08	120.00	113.86
14	A	4006	BCR	C2-C1-C6	2.08	113.68	110.48
15	1	613	CLA	CHD-C1D-ND	-2.08	122.55	124.45
15	A	1133	CLA	CHD-C1D-ND	-2.08	122.55	124.45
15	2	601	CLA	CHD-C1D-ND	-2.08	122.55	124.45
15	A	1139	CLA	CHD-C1D-ND	-2.08	122.55	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	A	1122	CLA	C2D-C1D-ND	-2.08	108.57	110.10
15	2	604	CLA	CHD-C1D-ND	-2.08	122.55	124.45
15	B	1220	CLA	O2D-CGD-O1D	-2.08	119.78	123.84
14	2	503	BCR	C16-C15-C14	-2.07	119.22	123.47
15	A	1105	CLA	C3A-C2A-C1A	2.07	104.44	101.34
15	3	603	CLA	O2A-CGA-O1A	-2.07	118.36	123.59
15	A	1012	CLA	C11-C12-C13	-2.07	109.22	115.92
15	3	615	CLA	C1B-CHB-C4A	-2.07	126.02	130.12
15	A	1127	CLA	CHD-C1D-ND	-2.07	122.55	124.45
15	B	1214	CLA	CHD-C1D-ND	-2.07	122.55	124.45
14	B	4001	BCR	C28-C27-C26	-2.07	110.38	114.08
14	A	4007	BCR	C27-C26-C25	2.07	125.73	122.73
15	B	1215	CLA	C1B-CHB-C4A	-2.07	126.02	130.12
15	B	1211	CLA	CHD-C1D-ND	-2.07	122.55	124.45
14	J	4001	BCR	C10-C11-C12	-2.07	116.76	123.22
14	B	4006	BCR	C35-C13-C14	-2.07	120.03	122.92
15	B	1213	CLA	CHD-C1D-ND	-2.07	122.55	124.45
15	3	614	CLA	C5-C3-C2	2.07	125.30	121.12
15	3	605	CLA	CHD-C1D-ND	-2.07	122.56	124.45
16	4	613	CHL	CHD-C4C-C3C	2.07	127.88	124.84
17	3	801	LHG	O8-C23-O10	-2.07	118.38	123.59
15	2	605	CLA	C1B-CHB-C4A	-2.07	126.03	130.12
14	A	4008	BCR	C11-C10-C9	-2.06	124.36	127.31
15	A	1125	CLA	O2A-CGA-O1A	-2.06	118.38	123.59
15	A	1110	CLA	CBA-CAA-C2A	2.06	119.95	113.86
15	3	608	CLA	C1B-CHB-C4A	-2.06	126.03	130.12
12	1	501	LUT	C20-C13-C12	2.06	121.33	118.08
15	A	1104	CLA	CHD-C1D-ND	-2.06	122.56	124.45
15	A	1114	CLA	C2A-C1A-CHA	2.06	127.46	123.86
15	B	1239	CLA	O1D-CGD-CBD	2.06	128.70	124.48
16	1	610	CHL	C4D-CHA-C1A	2.06	123.76	121.25
15	B	1237	CLA	CMB-C2B-C3B	2.06	128.53	124.68
15	B	1236	CLA	C1B-CHB-C4A	-2.06	126.04	130.12
15	4	609	CLA	O2A-CGA-O1A	-2.06	118.40	123.59
19	A	1011	CL0	CMD-C2D-C1D	2.06	128.34	124.71
14	A	4005	BCR	C27-C26-C25	2.06	125.72	122.73
15	B	1210	CLA	CAC-C3C-C4C	2.06	127.48	124.81
18	4	801	LMG	O5-C6-C5	-2.05	104.24	111.29
15	B	1023	CLA	C4-C3-C5	2.05	118.73	115.27
15	B	1222	CLA	C1B-CHB-C4A	-2.05	126.05	130.12
15	B	1234	CLA	C1B-CHB-C4A	-2.05	126.05	130.12
12	1	501	LUT	C7-C6-C5	-2.05	116.50	121.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	A	1104	CLA	C7-C6-C5	-2.05	107.79	113.36
16	2	609	CHL	CAA-C2A-C3A	2.05	118.39	112.78
16	1	610	CHL	C1-O2A-CGA	2.05	122.86	116.11
15	4	601	CLA	C4-C3-C5	2.05	118.72	115.27
16	4	613	CHL	CHA-C1A-NA	-2.05	121.71	126.40
14	3	506	BCR	C38-C26-C25	-2.05	122.23	124.53
15	A	1103	CLA	O1D-CGD-CBD	2.05	128.67	124.48
14	A	4008	BCR	C24-C23-C22	-2.05	123.14	126.23
15	B	1210	CLA	O2A-CGA-O1A	-2.05	118.42	123.59
15	B	1210	CLA	C1B-CHB-C4A	-2.05	126.06	130.12
18	2	804	LMG	O7-C10-O9	-2.05	118.76	123.70
15	A	1117	CLA	C2A-C1A-CHA	2.05	127.44	123.86
15	A	1122	CLA	C16-C15-C13	-2.04	109.31	115.92
15	A	1102	CLA	C5-C3-C2	2.04	125.25	121.12
15	4	607	CLA	C2A-C1A-CHA	2.04	127.43	123.86
14	3	506	BCR	C8-C7-C6	-2.04	121.47	127.20
14	A	4006	BCR	C7-C8-C9	-2.04	123.15	126.23
15	A	1122	CLA	C3C-C4C-NC	-2.04	108.28	110.57
15	A	1129	CLA	C2D-C1D-ND	-2.04	108.60	110.10
15	B	1214	CLA	C4-C3-C2	-2.04	118.45	123.68
15	A	1112	CLA	C1B-CHB-C4A	-2.04	126.08	130.12
14	4	503	BCR	C38-C26-C25	-2.04	122.24	124.53
15	B	1226	CLA	CHD-C1D-ND	-2.04	122.58	124.45
15	A	1107	CLA	CHA-C1A-NA	-2.04	121.74	126.40
15	A	1107	CLA	O2A-CGA-O1A	-2.04	118.45	123.59
17	3	801	LHG	C27-C26-C25	-2.04	104.09	114.42
22	B	5002	DGD	O3E-C3E-C2E	-2.04	105.64	110.35
15	A	1128	CLA	C1B-CHB-C4A	-2.03	126.09	130.12
16	2	609	CHL	CHA-C1A-NA	-2.03	121.74	126.40
15	2	605	CLA	CHD-C1D-ND	-2.03	122.58	124.45
15	A	1129	CLA	O2A-CGA-O1A	-2.03	118.46	123.59
15	B	1228	CLA	O2A-CGA-O1A	-2.03	118.46	123.59
12	3	501	LUT	C36-C21-C26	2.03	112.62	109.55
15	B	1229	CLA	C1B-CHB-C4A	-2.03	126.09	130.12
15	A	1119	CLA	O2A-CGA-O1A	-2.03	118.47	123.59
15	A	1141	CLA	CMA-C3A-C2A	-2.03	111.36	116.10
15	A	1130	CLA	CMB-C2B-C3B	2.03	128.48	124.68
22	B	5002	DGD	O6E-C1E-O5D	-2.03	105.17	109.97
15	A	1104	CLA	O2D-CGD-O1D	-2.03	119.87	123.84
15	3	610	CLA	CBA-CAA-C2A	2.03	119.86	113.86
15	A	1112	CLA	CMB-C2B-C3B	2.03	128.47	124.68
15	A	1140	CLA	CHD-C1D-ND	-2.03	122.59	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	B	1214	CLA	C2D-C1D-ND	-2.03	108.61	110.10
15	3	605	CLA	C3C-C4C-NC	-2.03	108.30	110.57
15	2	605	CLA	O2A-CGA-O1A	-2.03	118.48	123.59
15	B	1236	CLA	CMB-C2B-C1B	-2.03	125.35	128.46
15	1	608	CLA	O2A-CGA-O1A	-2.03	118.48	123.59
15	2	602	CLA	C1B-CHB-C4A	-2.03	126.11	130.12
15	3	611	CLA	CHD-C1D-ND	-2.03	122.59	124.45
14	A	4005	BCR	C37-C22-C23	2.02	121.27	118.08
14	3	504	BCR	C34-C9-C10	-2.02	120.09	122.92
14	B	4001	BCR	C35-C13-C12	2.02	121.27	118.08
18	2	804	LMG	C38-C37-C36	-2.02	104.16	114.42
15	2	603	CLA	C3A-C2A-C1A	2.02	104.37	101.34
15	1	613	CLA	O2A-CGA-O1A	-2.02	118.26	123.30
15	A	1104	CLA	O2A-CGA-O1A	-2.02	118.49	123.59
16	2	611	CHL	C1B-CHB-C4A	-2.02	126.12	130.12
15	A	1109	CLA	CMB-C2B-C3B	2.02	128.45	124.68
15	B	1230	CLA	CBA-CAA-C2A	2.02	119.81	113.86
15	1	603	CLA	CHD-C1D-ND	-2.02	122.60	124.45
15	2	612	CLA	C1-O2A-CGA	2.02	121.73	116.44
15	1	606	CLA	O2A-CGA-O1A	-2.01	118.51	123.59
18	2	804	LMG	C18-C17-C16	-2.01	104.20	114.42
14	1	503	BCR	C8-C7-C6	-2.01	121.55	127.20
15	B	1220	CLA	O2A-CGA-O1A	-2.01	118.52	123.59
14	2	503	BCR	C4-C5-C6	2.01	125.65	122.73
14	A	4003	BCR	C11-C10-C9	-2.01	124.44	127.31
15	A	1132	CLA	C1B-CHB-C4A	-2.01	126.13	130.12
15	B	1240	CLA	C1-C2-C3	2.01	129.52	126.04
15	A	1108	CLA	CHD-C1D-ND	-2.01	122.61	124.45
15	B	1220	CLA	O1D-CGD-CBD	2.01	128.60	124.48
15	A	1110	CLA	O2D-CGD-CBD	2.01	114.84	111.27
15	1	615	CLA	O2A-CGA-O1A	-2.01	118.29	123.30
15	A	1124	CLA	O2A-CGA-O1A	-2.01	118.52	123.59
15	A	1132	CLA	O2A-CGA-O1A	-2.01	118.30	123.30
17	A	5002	LHG	C18-C17-C16	-2.01	104.24	114.42
16	2	611	CHL	C4D-CHA-C1A	2.01	123.69	121.25
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
14	B	4004	BCR	C38-C26-C25	-2.00	122.28	124.53
16	3	604	CHL	CHB-C4A-NA	2.00	127.28	124.51
15	B	1211	CLA	C4-C3-C5	2.00	118.64	115.27
15	A	1131	CLA	CHD-C1D-ND	-2.00	122.61	124.45
13	2	502	XAT	C20-C13-C14	-2.00	120.12	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	B	1231	CLA	C5-C3-C2	2.00	125.17	121.12

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
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

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Mol	Chain	Res	Type	Atom
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
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

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Mol	Chain	Res	Type	Atom
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
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

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Mol	Chain	Res	Type	Atom
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	ND
15	B	1238	CLA	C8
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	ND
16	1	609	CHL	NC
16	1	609	CHL	C8
16	1	610	CHL	NA
16	1	610	CHL	ND
16	1	610	CHL	NC
16	2	609	CHL	NA
16	2	609	CHL	ND
16	2	609	CHL	NC
16	2	609	CHL	C8
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	ND
16	3	604	CHL	NC
16	3	604	CHL	C8
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

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

All (2090) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	1	501	LUT	C11-C12-C13-C14
12	1	501	LUT	C11-C12-C13-C20
12	4	501	LUT	C11-C12-C13-C14
12	4	501	LUT	C11-C12-C13-C20
12	4	501	LUT	C21-C26-C27-C28
12	4	501	LUT	C25-C26-C27-C28
12	4	501	LUT	C31-C32-C33-C34
12	4	501	LUT	C31-C32-C33-C40
13	1	502	XAT	O4-C6-C7-C8
13	2	502	XAT	C31-C32-C33-C34
13	2	502	XAT	C31-C32-C33-C40
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
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

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Mol	Chain	Res	Type	Atoms
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	2	503	BCR	C23-C24-C25-C30
14	3	503	BCR	C1-C6-C7-C8
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	C11-C12-C13-C35
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	C7-C8-C9-C34
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	C36-C18-C19-C20
14	4	503	BCR	C18-C19-C20-C21

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Mol	Chain	Res	Type	Atoms
14	4	503	BCR	C20-C21-C22-C37
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	C36-C18-C19-C20
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	C11-C12-C13-C35
14	A	4005	BCR	C36-C18-C19-C20
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

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Mol	Chain	Res	Type	Atoms
14	A	4006	BCR	C21-C22-C23-C24
14	A	4007	BCR	C7-C8-C9-C10
14	A	4007	BCR	C7-C8-C9-C34
14	A	4007	BCR	C10-C11-C12-C13
14	A	4007	BCR	C11-C12-C13-C14
14	A	4007	BCR	C11-C12-C13-C35
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	A	4008	BCR	C36-C18-C19-C20
14	B	4001	BCR	C7-C8-C9-C10
14	B	4001	BCR	C11-C12-C13-C35
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	C7-C8-C9-C34
14	B	4002	BCR	C11-C10-C9-C34
14	B	4002	BCR	C10-C11-C12-C13
14	B	4002	BCR	C11-C12-C13-C35
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

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Mol	Chain	Res	Type	Atoms
14	B	4004	BCR	C10-C11-C12-C13
14	B	4004	BCR	C11-C12-C13-C14
14	B	4004	BCR	C11-C12-C13-C35
14	B	4004	BCR	C20-C21-C22-C37
14	B	4005	BCR	C7-C8-C9-C34
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
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	C36-C18-C19-C20
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

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Mol	Chain	Res	Type	Atoms
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	CHA-CBD-CGD-O1D
15	1	601	CLA	CHA-CBD-CGD-O2D
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	607	CLA	CBD-CGD-O2D-CED
15	1	608	CLA	C2A-CAA-CBA-CGA
15	1	611	CLA	CHA-CBD-CGD-O1D
15	1	611	CLA	CHA-CBD-CGD-O2D
15	1	612	CLA	CHA-CBD-CGD-O1D
15	1	612	CLA	CHA-CBD-CGD-O2D
15	1	612	CLA	CBD-CGD-O2D-CED
15	1	613	CLA	CHA-CBD-CGD-O1D
15	1	613	CLA	CHA-CBD-CGD-O2D
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	CHA-CBD-CGD-O1D
15	2	601	CLA	CHA-CBD-CGD-O2D
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	603	CLA	CHA-CBD-CGD-O1D
15	3	603	CLA	CHA-CBD-CGD-O2D
15	3	605	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
15	3	606	CLA	CHA-CBD-CGD-O1D
15	3	606	CLA	CHA-CBD-CGD-O2D
15	3	606	CLA	CBD-CGD-O2D-CED
15	3	606	CLA	C2-C3-C5-C6
15	3	606	CLA	C4-C3-C5-C6
15	3	608	CLA	C3A-C2A-CAA-CBA
15	3	608	CLA	CBD-CGD-O2D-CED
15	3	610	CLA	CHA-CBD-CGD-O1D
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-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	606	CLA	CBD-CGD-O2D-CED
15	4	608	CLA	C2C-C3C-CAC-CBC
15	4	608	CLA	C4C-C3C-CAC-CBC
15	4	608	CLA	CHA-CBD-CGD-O1D
15	4	608	CLA	CHA-CBD-CGD-O2D
15	4	616	CLA	C1A-C2A-CAA-CBA
15	4	616	CLA	C3A-C2A-CAA-CBA
15	4	616	CLA	CHA-CBD-CGD-O1D
15	4	616	CLA	CHA-CBD-CGD-O2D
15	4	616	CLA	CBD-CGD-O2D-CED
15	A	1012	CLA	CHA-CBD-CGD-O1D
15	A	1012	CLA	CHA-CBD-CGD-O2D
15	A	1012	CLA	CAD-CBD-CGD-O1D
15	A	1012	CLA	O2A-C1-C2-C3
15	A	1012	CLA	C2-C3-C5-C6
15	A	1012	CLA	C4-C3-C5-C6
15	A	1013	CLA	C2-C3-C5-C6
15	A	1013	CLA	C4-C3-C5-C6
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	1103	CLA	CHA-CBD-CGD-O1D
15	A	1103	CLA	CHA-CBD-CGD-O2D
15	A	1105	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
15	A	1106	CLA	C1A-C2A-CAA-CBA
15	A	1106	CLA	C3A-C2A-CAA-CBA
15	A	1108	CLA	CHA-CBD-CGD-O1D
15	A	1108	CLA	CHA-CBD-CGD-O2D
15	A	1108	CLA	C2-C3-C5-C6
15	A	1108	CLA	C4-C3-C5-C6
15	A	1109	CLA	CHA-CBD-CGD-O1D
15	A	1111	CLA	C2A-CAA-CBA-CGA
15	A	1112	CLA	CBD-CGD-O2D-CED
15	A	1112	CLA	O1D-CGD-O2D-CED
15	A	1112	CLA	C4-C3-C5-C6
15	A	1114	CLA	CHA-CBD-CGD-O1D
15	A	1114	CLA	CHA-CBD-CGD-O2D
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	1119	CLA	CBD-CGD-O2D-CED
15	A	1121	CLA	CBD-CGD-O2D-CED
15	A	1121	CLA	O1D-CGD-O2D-CED
15	A	1122	CLA	C2A-CAA-CBA-CGA
15	A	1122	CLA	CHA-CBD-CGD-O1D
15	A	1122	CLA	CHA-CBD-CGD-O2D
15	A	1126	CLA	CBD-CGD-O2D-CED
15	A	1126	CLA	O2A-C1-C2-C3
15	A	1127	CLA	CHA-CBD-CGD-O1D
15	A	1127	CLA	CHA-CBD-CGD-O2D
15	A	1129	CLA	CBD-CGD-O2D-CED
15	A	1132	CLA	CBD-CGD-O2D-CED
15	A	1133	CLA	C2-C3-C5-C6
15	A	1133	CLA	C4-C3-C5-C6
15	A	1137	CLA	C2-C3-C5-C6
15	A	1137	CLA	C4-C3-C5-C6
15	A	1139	CLA	CHA-CBD-CGD-O1D
15	A	1139	CLA	CHA-CBD-CGD-O2D
15	A	1139	CLA	CBD-CGD-O2D-CED
15	A	1140	CLA	C2-C3-C5-C6
15	A	1140	CLA	C4-C3-C5-C6
15	A	1141	CLA	CHA-CBD-CGD-O1D
15	A	1141	CLA	CHA-CBD-CGD-O2D
15	A	1141	CLA	CAD-CBD-CGD-O1D
15	B	1021	CLA	CHA-CBD-CGD-O1D
15	B	1021	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
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	1201	CLA	CHA-CBD-CGD-O1D
15	B	1201	CLA	CHA-CBD-CGD-O2D
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	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	1210	CLA	CHA-CBD-CGD-O1D
15	B	1210	CLA	CHA-CBD-CGD-O2D
15	B	1217	CLA	CBA-CGA-O2A-C1
15	B	1217	CLA	O1A-CGA-O2A-C1
15	B	1217	CLA	CHA-CBD-CGD-O1D
15	B	1217	CLA	CHA-CBD-CGD-O2D
15	B	1219	CLA	CHA-CBD-CGD-O1D
15	B	1219	CLA	CHA-CBD-CGD-O2D
15	B	1220	CLA	C2A-CAA-CBA-CGA
15	B	1220	CLA	CHA-CBD-CGD-O1D
15	B	1220	CLA	CHA-CBD-CGD-O2D
15	B	1225	CLA	CHA-CBD-CGD-O1D
15	B	1225	CLA	CHA-CBD-CGD-O2D
15	B	1225	CLA	C2-C3-C5-C6
15	B	1225	CLA	C4-C3-C5-C6
15	B	1226	CLA	C11-C12-C13-C14
15	B	1227	CLA	CHA-CBD-CGD-O1D
15	B	1227	CLA	CHA-CBD-CGD-O2D
15	B	1227	CLA	CBD-CGD-O2D-CED
15	B	1228	CLA	CBD-CGD-O2D-CED
15	B	1229	CLA	C2A-CAA-CBA-CGA
15	B	1229	CLA	CHA-CBD-CGD-O1D
15	B	1229	CLA	CHA-CBD-CGD-O2D
15	B	1232	CLA	CHA-CBD-CGD-O1D
15	B	1232	CLA	CAD-CBD-CGD-O1D
15	B	1232	CLA	CAD-CBD-CGD-O2D
15	B	1235	CLA	C2-C3-C5-C6
15	B	1235	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
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	3	604	CHL	C1A-C2A-CAA-CBA
16	3	604	CHL	C3A-C2A-CAA-CBA
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	O9-C7-O7-C5
17	A	5001	LHG	O1-C1-C2-C3
17	A	5002	LHG	C1-C2-C3-O3
17	A	5002	LHG	O2-C2-C3-O3
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	C4-O6-P-O5
17	B	5001	LHG	C8-C7-O7-C5
18	2	803	LMG	C11-C10-O7-C8
18	2	804	LMG	C2-C1-O1-C7
18	2	804	LMG	O6-C1-O1-C7
18	2	804	LMG	O9-C10-O7-C8
18	2	804	LMG	C11-C10-O7-C8
19	A	1011	CL0	CAD-CBD-CGD-O1D
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	2	616	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
15	3	608	CLA	C2C-C3C-CAC-CBC
16	4	610	CHL	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	1219	CLA	CBD-CGD-O2D-CED
15	B	1225	CLA	CBD-CGD-O2D-CED
15	B	1236	CLA	CBD-CGD-O2D-CED
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
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

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Mol	Chain	Res	Type	Atoms
15	3	605	CLA	O1D-CGD-O2D-CED
15	A	1107	CLA	O1D-CGD-O2D-CED
15	B	1023	CLA	O1D-CGD-O2D-CED
15	B	1203	CLA	O1D-CGD-O2D-CED
15	B	1206	CLA	O1D-CGD-O2D-CED
15	B	1216	CLA	O1D-CGD-O2D-CED
15	B	1228	CLA	O1D-CGD-O2D-CED
15	J	1302	CLA	O1D-CGD-O2D-CED
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	1	601	CLA	O1D-CGD-O2D-CED
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	1022	CLA	O1D-CGD-O2D-CED
15	B	1227	CLA	CBA-CGA-O2A-C1
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
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	1209	CLA	CBD-CGD-O2D-CED
15	B	1221	CLA	CBD-CGD-O2D-CED
15	B	1222	CLA	CBD-CGD-O2D-CED
15	B	1224	CLA	CBD-CGD-O2D-CED
15	B	1232	CLA	CBD-CGD-O2D-CED
15	B	1237	CLA	CBD-CGD-O2D-CED
15	B	1238	CLA	CBD-CGD-O2D-CED
15	F	1302	CLA	CBD-CGD-O2D-CED
15	3	605	CLA	C2C-C3C-CAC-CBC
16	4	610	CHL	C4C-C3C-CAC-CBC
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

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Mol	Chain	Res	Type	Atoms
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
15	4	608	CLA	O1A-CGA-O2A-C1
15	F	1301	CLA	O1A-CGA-O2A-C1
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	1227	CLA	O1D-CGD-O2D-CED
15	B	1240	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	606	CLA	O1D-CGD-O2D-CED
15	3	609	CLA	CBD-CGD-O2D-CED
15	A	1113	CLA	CBD-CGD-O2D-CED
15	1	611	CLA	O1D-CGD-O2D-CED
15	4	603	CLA	O1D-CGD-O2D-CED
15	A	1133	CLA	O1D-CGD-O2D-CED
17	B	5001	LHG	O9-C7-O7-C5
18	2	803	LMG	O9-C10-O7-C8
22	B	5002	DGD	O1B-C1B-O2G-C2G
18	B	5003	LMG	C4-C5-C6-O5
15	3	601	CLA	O1A-CGA-O2A-C1
15	B	1209	CLA	CBA-CGA-O2A-C1
15	B	1209	CLA	O1A-CGA-O2A-C1
15	2	601	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
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	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
17	3	801	LHG	C8-C7-O7-C5
15	2	604	CLA	O1D-CGD-O2D-CED
15	B	1207	CLA	CBD-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	A	1105	CLA	C2A-CAA-CBA-CGA
15	A	1132	CLA	C2A-CAA-CBA-CGA
15	B	1207	CLA	C2A-CAA-CBA-CGA
15	B	1225	CLA	C2A-CAA-CBA-CGA
15	B	1228	CLA	C2A-CAA-CBA-CGA
16	1	610	CHL	C2A-CAA-CBA-CGA
16	4	610	CHL	C2A-CAA-CBA-CGA
15	A	1127	CLA	O1D-CGD-O2D-CED
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

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Mol	Chain	Res	Type	Atoms
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
15	A	1140	CLA	O1D-CGD-O2D-CED
15	3	605	CLA	C4C-C3C-CAC-CBC
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	603	CLA	O1A-CGA-O2A-C1
15	1	605	CLA	O1A-CGA-O2A-C1
15	1	606	CLA	O1A-CGA-O2A-C1
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
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	4	601	CLA	CBD-CGD-O2D-CED
15	B	1211	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
15	B	1231	CLA	CBD-CGD-O2D-CED
15	F	1301	CLA	CBD-CGD-O2D-CED
15	A	1118	CLA	O1D-CGD-O2D-CED
17	1	801	LHG	O2-C2-C3-O3
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	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	B	1207	CLA	C2C-C3C-CAC-CBC
15	B	1234	CLA	C4C-C3C-CAC-CBC
15	A	1126	CLA	O1A-CGA-O2A-C1
15	4	609	CLA	O1D-CGD-O2D-CED
15	B	1234	CLA	CBD-CGD-O2D-CED
15	B	1217	CLA	O1D-CGD-O2D-CED
15	B	1229	CLA	O1A-CGA-O2A-C1
15	A	1125	CLA	C3-C5-C6-C7
15	B	1230	CLA	C3-C5-C6-C7
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	A	1141	CLA	O1D-CGD-O2D-CED
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	1	605	CLA	C4-C3-C5-C6
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

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Mol	Chain	Res	Type	Atoms
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	A	1112	CLA	C2-C3-C5-C6
15	B	1238	CLA	C2-C3-C5-C6
15	2	602	CLA	C2A-CAA-CBA-CGA
15	A	1130	CLA	C2A-CAA-CBA-CGA
15	B	1225	CLA	O1D-CGD-O2D-CED
15	2	604	CLA	O1A-CGA-O2A-C1
15	B	1219	CLA	O1A-CGA-O2A-C1
15	B	1231	CLA	O1A-CGA-O2A-C1
15	A	1013	CLA	O1D-CGD-O2D-CED
15	A	1105	CLA	CBA-CGA-O2A-C1
15	B	1232	CLA	CBA-CGA-O2A-C1
15	1	612	CLA	C4C-C3C-CAC-CBC
15	1	602	CLA	O1D-CGD-O2D-CED
15	B	1219	CLA	O1D-CGD-O2D-CED
17	1	801	LHG	O10-C23-O8-C6
15	A	1110	CLA	O1D-CGD-O2D-CED
15	B	1224	CLA	O1D-CGD-O2D-CED
15	3	612	CLA	O1D-CGD-O2D-CED
17	1	801	LHG	O9-C7-O7-C5
15	A	1105	CLA	O1A-CGA-O2A-C1
15	1	615	CLA	C2C-C3C-CAC-CBC
15	1	608	CLA	C3-C5-C6-C7
15	3	607	CLA	C3-C5-C6-C7
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	1202	CLA	CBD-CGD-O2D-CED
14	1	503	BCR	C13-C14-C15-C16
14	4	503	BCR	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
14	F	4001	BCR	C19-C20-C21-C22
15	1	603	CLA	C8-C10-C11-C12
15	4	603	CLA	C10-C11-C12-C13
15	B	1227	CLA	C10-C11-C12-C13
17	2	801	LHG	O2-C2-C3-O3
15	1	611	CLA	O2A-C1-C2-C3
22	B	5002	DGD	O2G-C2G-C3G-O3G
15	A	1125	CLA	O1A-CGA-O2A-C1
15	1	603	CLA	C2-C3-C5-C6
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	B	1221	CLA	O1D-CGD-O2D-CED
15	F	1302	CLA	O1D-CGD-O2D-CED
12	1	501	LUT	C7-C8-C9-C19
12	1	501	LUT	C27-C28-C29-C39
12	1	501	LUT	C31-C32-C33-C40
12	2	501	LUT	C11-C12-C13-C20
12	2	501	LUT	C27-C28-C29-C39
12	3	501	LUT	C31-C32-C33-C40
13	1	502	XAT	C7-C8-C9-C19
13	2	502	XAT	C7-C8-C9-C19
13	3	502	XAT	C11-C12-C13-C20
14	1	503	BCR	C7-C8-C9-C34
14	3	503	BCR	C37-C22-C23-C24
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	4006	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	C37-C22-C23-C24
14	B	4001	BCR	C7-C8-C9-C34
14	B	4003	BCR	C7-C8-C9-C34

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Mol	Chain	Res	Type	Atoms
14	B	4003	BCR	C36-C18-C19-C20
14	F	4001	BCR	C7-C8-C9-C34
14	F	4001	BCR	C36-C18-C19-C20
14	F	4002	BCR	C7-C8-C9-C34
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
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
14	F	4001	BCR	C7-C8-C9-C10
15	2	606	CLA	C2C-C3C-CAC-CBC
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
15	1	605	CLA	C8-C10-C11-C12
15	A	1109	CLA	C15-C16-C17-C18
15	A	1138	CLA	C5-C6-C7-C8
15	B	1211	CLA	C13-C15-C16-C17
15	B	1227	CLA	C15-C16-C17-C18
15	B	1232	CLA	O1D-CGD-O2D-CED
18	2	804	LMG	O6-C5-C6-O5
15	B	1201	CLA	C2A-CAA-CBA-CGA
17	2	801	LHG	C24-C23-O8-C6
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	1123	CLA	C8-C10-C11-C12
15	A	1128	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
15	A	1138	CLA	C8-C10-C11-C12
16	4	613	CHL	C8-C10-C11-C12
18	4	801	LMG	C28-C29-C30-C31
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	3	606	CLA	C5-C6-C7-C8
15	A	1122	CLA	C5-C6-C7-C8
15	A	1123	CLA	C10-C11-C12-C13
15	B	1238	CLA	O1D-CGD-O2D-CED
17	A	5001	LHG	O1-C1-C2-O2
15	B	1225	CLA	O1A-CGA-O2A-C1
17	1	801	LHG	C23-C24-C25-C26
17	2	801	LHG	C23-C24-C25-C26
17	3	801	LHG	C23-C24-C25-C26
15	A	1102	CLA	C10-C11-C12-C13
15	A	1114	CLA	C5-C6-C7-C8
15	4	612	CLA	C3-C5-C6-C7
15	B	1240	CLA	CBA-CGA-O2A-C1
15	2	616	CLA	C2-C1-O2A-CGA
15	4	605	CLA	C13-C15-C16-C17
15	B	1022	CLA	C13-C15-C16-C17
17	A	5002	LHG	C7-C8-C9-C10
18	B	5003	LMG	C28-C29-C30-C31
16	2	610	CHL	C2A-CAA-CBA-CGA
15	A	1133	CLA	C13-C15-C16-C17
16	1	609	CHL	C13-C15-C16-C17
15	2	607	CLA	C11-C10-C8-C7
15	3	608	CLA	C12-C13-C15-C16
15	A	1139	CLA	C12-C13-C15-C16
15	B	1023	CLA	C6-C7-C8-C10
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	1207	CLA	C4C-C3C-CAC-CBC
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

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Mol	Chain	Res	Type	Atoms
14	B	4003	BCR	C15-C16-C17-C18
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	1215	CLA	C2A-CAA-CBA-CGA
15	3	609	CLA	O1D-CGD-O2D-CED
15	4	604	CLA	O1D-CGD-O2D-CED
15	A	1113	CLA	O1D-CGD-O2D-CED
15	B	1209	CLA	O1D-CGD-O2D-CED
15	B	1237	CLA	O1D-CGD-O2D-CED
15	A	1119	CLA	C5-C6-C7-C8
15	A	1139	CLA	C8-C10-C11-C12
15	B	1021	CLA	C13-C15-C16-C17
15	B	1203	CLA	C5-C6-C7-C8
15	B	1238	CLA	C5-C6-C7-C8
14	J	4001	BCR	C22-C23-C24-C25
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
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	A	4005	BCR	C18-C19-C20-C21
14	A	4006	BCR	C18-C19-C20-C21
14	B	4001	BCR	C10-C11-C12-C13
14	B	4006	BCR	C18-C19-C20-C21
15	3	603	CLA	C5-C6-C7-C8
15	4	604	CLA	C10-C11-C12-C13
15	A	1101	CLA	C13-C15-C16-C17
15	A	1123	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	1	607	CLA	C2C-C3C-CAC-CBC
15	3	615	CLA	CBD-CGD-O2D-CED
15	A	1101	CLA	CBD-CGD-O2D-CED
15	A	1128	CLA	O1A-CGA-O2A-C1
15	2	605	CLA	C10-C11-C12-C13
15	2	607	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
15	2	616	CLA	C15-C16-C17-C18
15	3	603	CLA	C13-C15-C16-C17
15	A	1117	CLA	C15-C16-C17-C18
15	A	1126	CLA	C15-C16-C17-C18
15	B	1219	CLA	C8-C10-C11-C12
15	B	1219	CLA	C13-C15-C16-C17
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
19	A	1011	CL0	C5-C6-C7-C8
17	2	801	LHG	C3-O3-P-O6
17	2	801	LHG	C4-O6-P-O3
17	3	801	LHG	C3-O3-P-O6
17	B	5001	LHG	C4-O6-P-O3
15	3	601	CLA	C3-C5-C6-C7
15	3	605	CLA	CBA-CGA-O2A-C1
15	B	1234	CLA	CBA-CGA-O2A-C1
15	4	607	CLA	C8-C10-C11-C12
15	A	1140	CLA	C10-C11-C12-C13
17	2	801	LHG	C1-C2-C3-O3
17	3	801	LHG	C1-C2-C3-O3
17	2	801	LHG	O9-C7-O7-C5
15	4	605	CLA	C10-C11-C12-C13
15	A	1109	CLA	C10-C11-C12-C13
15	A	1111	CLA	C15-C16-C17-C18
15	B	1021	CLA	C8-C10-C11-C12
15	B	1227	CLA	C13-C15-C16-C17
15	B	1207	CLA	O1D-CGD-O2D-CED
15	2	603	CLA	C2A-CAA-CBA-CGA
15	B	1023	CLA	C2A-CAA-CBA-CGA
15	A	1013	CLA	C3-C5-C6-C7
15	B	1221	CLA	C3-C5-C6-C7
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
15	B	1216	CLA	CBA-CGA-O2A-C1
15	B	1228	CLA	CBA-CGA-O2A-C1
15	A	1105	CLA	C10-C11-C12-C13
12	1	501	LUT	C29-C30-C31-C32

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Mol	Chain	Res	Type	Atoms
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	A	1108	CLA	CBD-CGD-O2D-CED
15	B	1226	CLA	CBD-CGD-O2D-CED
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
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	1105	CLA	C3-C5-C6-C7
17	A	5001	LHG	C30-C31-C32-C33
15	B	1240	CLA	O1A-CGA-O2A-C1
15	2	601	CLA	C16-C17-C18-C19
15	A	1112	CLA	C16-C17-C18-C20
15	A	1124	CLA	C11-C12-C13-C14
15	B	1211	CLA	C16-C17-C18-C19
15	4	609	CLA	CBA-CGA-O2A-C1
17	1	801	LHG	C12-C13-C14-C15
18	2	803	LMG	C11-C12-C13-C14
17	A	5001	LHG	C23-C24-C25-C26
17	3	801	LHG	C2-C3-O3-P
18	2	804	LMG	C29-C30-C31-C32
15	3	611	CLA	C8-C10-C11-C12
17	A	5002	LHG	C17-C18-C19-C20
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

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Mol	Chain	Res	Type	Atoms
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
15	A	1103	CLA	CBA-CGA-O2A-C1
15	B	1236	CLA	CBA-CGA-O2A-C1
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	O1A-CGA-O2A-C1
15	A	1109	CLA	O1A-CGA-O2A-C1
15	B	1234	CLA	O1A-CGA-O2A-C1
15	1	605	CLA	C16-C17-C18-C19
15	A	1110	CLA	C6-C7-C8-C9
15	4	601	CLA	O1D-CGD-O2D-CED
15	B	1231	CLA	O1D-CGD-O2D-CED
15	A	1138	CLA	C4-C3-C5-C6
18	2	802	LMG	C38-C39-C40-C41
15	3	608	CLA	C6-C7-C8-C9
15	A	1122	CLA	C14-C13-C15-C16
15	A	1104	CLA	CBD-CGD-O2D-CED
15	A	1131	CLA	CBD-CGD-O2D-CED
18	4	801	LMG	C33-C34-C35-C36
16	1	609	CHL	C10-C11-C12-C13
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	1214	CLA	C2A-CAA-CBA-CGA
15	3	605	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
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
17	1	801	LHG	C29-C30-C31-C32
17	1	801	LHG	O1-C1-C2-C3
17	A	5002	LHG	O1-C1-C2-C3
17	B	5001	LHG	O1-C1-C2-C3
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
17	3	801	LHG	C12-C13-C14-C15
22	B	5002	DGD	CAB-CBB-CCB-CDB
15	1	605	CLA	C16-C17-C18-C20
15	2	601	CLA	C16-C17-C18-C20
15	4	607	CLA	C11-C12-C13-C15
15	A	1128	CLA	C16-C17-C18-C20
18	2	803	LMG	O6-C1-O1-C7
15	2	603	CLA	C5-C6-C7-C8
15	A	1013	CLA	C10-C11-C12-C13
15	B	1021	CLA	C15-C16-C17-C18
17	B	5001	LHG	C27-C28-C29-C30
18	B	5003	LMG	C30-C31-C32-C33
17	1	801	LHG	C26-C27-C28-C29
17	A	5001	LHG	C32-C33-C34-C35
15	B	1022	CLA	O1A-CGA-O2A-C1
15	B	1228	CLA	O1A-CGA-O2A-C1
17	B	5001	LHG	C13-C14-C15-C16
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

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Mol	Chain	Res	Type	Atoms
15	B	1207	CLA	C3A-C2A-CAA-CBA
15	B	1210	CLA	C3A-C2A-CAA-CBA
17	B	5001	LHG	C16-C17-C18-C19
15	F	1301	CLA	O1D-CGD-O2D-CED
15	4	607	CLA	C11-C12-C13-C14
15	A	1124	CLA	C11-C12-C13-C15
15	A	1128	CLA	C16-C17-C18-C19
15	1	615	CLA	C4C-C3C-CAC-CBC
15	4	616	CLA	O2A-C1-C2-C3
15	A	1103	CLA	O2A-C1-C2-C3
15	A	1125	CLA	O2A-C1-C2-C3
14	3	506	BCR	C14-C15-C16-C17
18	2	802	LMG	C10-C11-C12-C13
15	B	1222	CLA	C8-C10-C11-C12
15	A	1103	CLA	C4-C3-C5-C6
15	A	1117	CLA	C4-C3-C5-C6
15	B	1210	CLA	C4-C3-C5-C6
15	B	1232	CLA	O1A-CGA-O2A-C1
15	A	1103	CLA	C2-C3-C5-C6
15	A	1138	CLA	C2-C3-C5-C6
15	B	1210	CLA	C2-C3-C5-C6
18	2	802	LMG	C11-C10-O7-C8
15	A	1110	CLA	C2A-CAA-CBA-CGA
17	1	801	LHG	O1-C1-C2-O2
15	1	604	CLA	C16-C17-C18-C19
15	A	1110	CLA	C6-C7-C8-C10
15	A	1112	CLA	C8-C10-C11-C12
17	A	5002	LHG	C13-C14-C15-C16
15	A	1126	CLA	C4C-C3C-CAC-CBC
15	A	1114	CLA	O1A-CGA-O2A-C1
17	A	5001	LHG	C10-C11-C12-C13
18	2	803	LMG	C29-C30-C31-C32
15	A	1012	CLA	C2-C1-O2A-CGA
15	A	1126	CLA	C2-C1-O2A-CGA
17	3	801	LHG	C5-C4-O6-P
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	1	801	LHG	C28-C29-C30-C31
15	B	1220	CLA	CBD-CGD-O2D-CED
12	1	501	LUT	C5-C6-C7-C8
12	3	501	LUT	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
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	2	503	BCR	C23-C24-C25-C26
14	3	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	C5-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	2	606	CLA	C4C-C3C-CAC-CBC
15	A	1126	CLA	C2C-C3C-CAC-CBC
17	A	5002	LHG	C28-C29-C30-C31
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	B	1212	CLA	C5-C6-C7-C8
15	B	1223	CLA	C10-C11-C12-C13
15	B	1211	CLA	O1D-CGD-O2D-CED
15	B	1236	CLA	O1A-CGA-O2A-C1
15	2	612	CLA	C5-C6-C7-C8
15	4	607	CLA	C10-C11-C12-C13
15	A	1137	CLA	C8-C10-C11-C12
15	B	1208	CLA	C8-C10-C11-C12
15	B	1221	CLA	C15-C16-C17-C18
17	A	5002	LHG	C11-C10-C9-C8
15	A	1125	CLA	C4-C3-C5-C6
15	1	603	CLA	C6-C7-C8-C10
15	3	605	CLA	C12-C13-C15-C16
15	3	612	CLA	C12-C13-C15-C16
15	A	1102	CLA	C11-C10-C8-C7
15	A	1111	CLA	C11-C12-C13-C15
15	A	1117	CLA	C2-C3-C5-C6
15	A	1122	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
15	A	1125	CLA	C2-C3-C5-C6
15	A	1127	CLA	C11-C12-C13-C15
15	B	1215	CLA	C11-C10-C8-C7
15	B	1216	CLA	O1A-CGA-O2A-C1
17	A	5001	LHG	C14-C15-C16-C17
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	1228	CLA	C10-C11-C12-C13
15	B	1240	CLA	C13-C15-C16-C17
18	2	802	LMG	O9-C10-O7-C8
15	A	1122	CLA	CBA-CGA-O2A-C1
17	2	801	LHG	C28-C29-C30-C31
18	2	803	LMG	C14-C15-C16-C17
15	A	1115	CLA	C2A-CAA-CBA-CGA
15	B	1231	CLA	C8-C10-C11-C12
15	B	1208	CLA	C2C-C3C-CAC-CBC
15	3	601	CLA	C5-C6-C7-C8
14	A	4002	BCR	C22-C23-C24-C25
14	J	4002	BCR	C22-C23-C24-C25
17	A	5001	LHG	O10-C23-O8-C6
15	B	1023	CLA	CBA-CGA-O2A-C1
15	2	604	CLA	C16-C17-C18-C20
15	A	1112	CLA	C16-C17-C18-C19
17	A	5002	LHG	C10-C11-C12-C13
17	1	801	LHG	C8-C7-O7-C5
17	2	801	LHG	C8-C7-O7-C5
15	3	611	CLA	C10-C11-C12-C13
15	B	1231	CLA	C5-C6-C7-C8
15	A	1134	CLA	CBD-CGD-O2D-CED
15	A	1114	CLA	C3-C5-C6-C7
18	B	5003	LMG	C2-C1-O1-C7
15	B	1230	CLA	C5-C6-C7-C8
17	A	5002	LHG	O7-C5-C6-O8
17	1	801	LHG	C11-C10-C9-C8
18	2	802	LMG	C15-C16-C17-C18
15	B	1202	CLA	C15-C16-C17-C18
15	B	1234	CLA	O1D-CGD-O2D-CED
15	3	608	CLA	C14-C13-C15-C16
15	3	612	CLA	C14-C13-C15-C16
15	4	603	CLA	C6-C7-C8-C9
15	A	1111	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
15	A	1122	CLA	C6-C7-C8-C9
15	A	1123	CLA	C11-C12-C13-C14
15	A	1126	CLA	C11-C12-C13-C14
15	A	1139	CLA	C14-C13-C15-C16
15	B	1203	CLA	C14-C13-C15-C16
15	B	1212	CLA	C3-C5-C6-C7
15	3	603	CLA	C2A-CAA-CBA-CGA
15	A	1104	CLA	C2A-CAA-CBA-CGA
14	F	4001	BCR	C11-C12-C13-C35
15	1	601	CLA	C10-C11-C12-C13
15	A	1137	CLA	CBD-CGD-O2D-CED
17	3	801	LHG	C14-C15-C16-C17
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	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
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	1	604	CLA	C16-C17-C18-C20
15	2	604	CLA	C16-C17-C18-C19
15	B	1211	CLA	C16-C17-C18-C20
19	A	1011	CL0	C16-C17-C18-C20
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	A	1104	CLA	C10-C11-C12-C13
15	A	1112	CLA	C5-C6-C7-C8
15	A	1133	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
17	B	5001	LHG	C3-O3-P-O6
15	1	607	CLA	C4C-C3C-CAC-CBC
15	4	605	CLA	C5-C6-C7-C8
15	B	1215	CLA	C5-C6-C7-C8
18	2	804	LMG	C31-C32-C33-C34
22	B	5002	DGD	C5A-C6A-C7A-C8A
17	3	801	LHG	C11-C12-C13-C14
15	B	1224	CLA	C4-C3-C5-C6
15	3	615	CLA	C3A-C2A-CAA-CBA
15	B	1238	CLA	C3A-C2A-CAA-CBA
15	1	605	CLA	C5-C6-C7-C8
15	2	604	CLA	C10-C11-C12-C13
18	B	5003	LMG	C11-C10-O7-C8
15	B	1023	CLA	O1A-CGA-O2A-C1
18	4	801	LMG	O10-C28-O8-C9
15	B	1023	CLA	C16-C17-C18-C19
19	A	1011	CL0	C16-C17-C18-C19
17	2	801	LHG	C4-C5-C6-O8
18	2	803	LMG	C7-C8-C9-O8
22	B	5002	DGD	O1G-C1G-C2G-C3G
15	A	1104	CLA	O1D-CGD-O2D-CED
17	3	801	LHG	C15-C16-C17-C18
17	A	5002	LHG	C25-C26-C27-C28
17	A	5002	LHG	O1-C1-C2-O2
22	B	5002	DGD	C2A-C3A-C4A-C5A
18	2	802	LMG	C32-C33-C34-C35
15	4	609	CLA	C5-C6-C7-C8
15	A	1139	CLA	C10-C11-C12-C13
14	2	503	BCR	C16-C17-C18-C36
18	2	803	LMG	O6-C5-C6-O5
15	B	1021	CLA	C4-C3-C5-C6
15	B	1225	CLA	C16-C17-C18-C20
15	B	1202	CLA	CBA-CGA-O2A-C1
16	2	609	CHL	CBA-CGA-O2A-C1
15	B	1208	CLA	CBD-CGD-O2D-CED
17	A	5001	LHG	C19-C20-C21-C22
18	4	801	LMG	C12-C13-C14-C15
15	4	605	CLA	C8-C10-C11-C12
18	2	802	LMG	C29-C30-C31-C32
18	2	802	LMG	C18-C19-C20-C21
15	A	1103	CLA	C15-C16-C17-C18
18	2	802	LMG	C34-C35-C36-C37

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Mol	Chain	Res	Type	Atoms
15	A	1133	CLA	C16-C17-C18-C20
15	B	1225	CLA	C16-C17-C18-C19
15	A	1122	CLA	O1A-CGA-O2A-C1
22	B	5002	DGD	C7B-C8B-C9B-CAB
15	B	1210	CLA	C5-C6-C7-C8
14	A	4005	BCR	C16-C17-C18-C19
15	A	1111	CLA	C2C-C3C-CAC-CBC
17	1	801	LHG	C30-C31-C32-C33
15	B	1202	CLA	O1A-CGA-O2A-C1
15	A	1131	CLA	O1D-CGD-O2D-CED
18	2	802	LMG	C41-C42-C43-C44
15	B	1211	CLA	C4-C3-C5-C6
15	B	1225	CLA	C13-C15-C16-C17
15	1	604	CLA	C11-C12-C13-C15
15	1	605	CLA	C12-C13-C15-C16
15	2	604	CLA	C11-C10-C8-C7
15	3	611	CLA	C12-C13-C15-C16
15	4	603	CLA	C6-C7-C8-C10
15	A	1116	CLA	C6-C7-C8-C10
15	A	1123	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	C2-C3-C5-C6
15	B	1021	CLA	C6-C7-C8-C10
15	B	1203	CLA	C12-C13-C15-C16
15	B	1224	CLA	C2-C3-C5-C6
15	B	1240	CLA	CAA-CBA-CGA-O2A
15	A	1124	CLA	C3-C5-C6-C7
15	B	1202	CLA	C3-C5-C6-C7
17	A	5002	LHG	C34-C35-C36-C37
15	2	601	CLA	C11-C12-C13-C14
15	2	605	CLA	C6-C7-C8-C9
15	3	611	CLA	C14-C13-C15-C16
15	A	1101	CLA	C6-C7-C8-C9
15	A	1105	CLA	C11-C10-C8-C9
15	A	1109	CLA	C6-C7-C8-C9
15	A	1116	CLA	C6-C7-C8-C9
15	A	1127	CLA	C11-C12-C13-C14
15	A	1127	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
15	A	1128	CLA	C11-C10-C8-C9
15	A	1139	CLA	C6-C7-C8-C9
15	B	1021	CLA	C6-C7-C8-C9
15	B	1023	CLA	C14-C13-C15-C16
15	B	1227	CLA	C11-C10-C8-C9
15	B	1235	CLA	C6-C7-C8-C9
19	A	1011	CL0	C6-C7-C8-C9
17	A	5001	LHG	C29-C30-C31-C32
15	A	1106	CLA	C2A-CAA-CBA-CGA
15	B	1202	CLA	O1D-CGD-O2D-CED
14	A	4002	BCR	C37-C22-C23-C24
15	A	1133	CLA	C16-C17-C18-C19
15	B	1205	CLA	C16-C17-C18-C19
15	2	607	CLA	C2C-C3C-CAC-CBC
14	F	4001	BCR	C11-C12-C13-C14
15	3	615	CLA	O1D-CGD-O2D-CED
15	1	601	CLA	C5-C6-C7-C8
18	2	804	LMG	C22-C23-C24-C25
15	4	602	CLA	CBA-CGA-O2A-C1
15	B	1235	CLA	CBA-CGA-O2A-C1
22	B	5002	DGD	C4B-C5B-C6B-C7B
15	A	1012	CLA	C8-C10-C11-C12
18	B	5003	LMG	C13-C14-C15-C16
15	B	1226	CLA	C3-C5-C6-C7
15	A	1101	CLA	O1D-CGD-O2D-CED
17	3	801	LHG	C11-C10-C9-C8
15	3	605	CLA	C10-C11-C12-C13
15	B	1211	CLA	C2-C3-C5-C6
15	A	1105	CLA	C5-C6-C7-C8
15	A	1136	CLA	C13-C15-C16-C17
15	B	1216	CLA	C8-C10-C11-C12
15	4	604	CLA	C3-C5-C6-C7
15	B	1023	CLA	C16-C17-C18-C20
15	B	1205	CLA	C16-C17-C18-C20
18	2	804	LMG	C21-C22-C23-C24
15	3	611	CLA	C2A-CAA-CBA-CGA
15	A	1124	CLA	CBA-CGA-O2A-C1
18	2	803	LMG	C15-C16-C17-C18
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

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Mol	Chain	Res	Type	Atoms
17	A	5001	LHG	C27-C28-C29-C30
15	A	1108	CLA	O1D-CGD-O2D-CED
15	A	1123	CLA	CBA-CGA-O2A-C1
15	A	1136	CLA	CBA-CGA-O2A-C1
15	B	1205	CLA	C15-C16-C17-C18
15	B	1215	CLA	C15-C16-C17-C18
17	A	5002	LHG	C4-C5-C6-O8
17	B	5001	LHG	C4-C5-C6-O8
18	2	802	LMG	O1-C7-C8-C9
22	B	5002	DGD	C1G-C2G-C3G-O3G
15	B	1221	CLA	O2A-C1-C2-C3
18	2	804	LMG	C30-C31-C32-C33
15	3	601	CLA	C4-C3-C5-C6
18	2	802	LMG	C13-C14-C15-C16
17	B	5001	LHG	C11-C12-C13-C14
18	2	803	LMG	C19-C20-C21-C22
18	B	5003	LMG	C12-C13-C14-C15
17	B	5001	LHG	O1-C1-C2-O2
15	3	607	CLA	C10-C11-C12-C13
15	1	601	CLA	CBA-CGA-O2A-C1
15	B	1220	CLA	O1D-CGD-O2D-CED
15	A	1112	CLA	C15-C16-C17-C18
15	A	1127	CLA	C15-C16-C17-C18
15	B	1235	CLA	O1A-CGA-O2A-C1
18	2	803	LMG	C17-C18-C19-C20
18	2	802	LMG	O1-C7-C8-O7
15	A	1139	CLA	C16-C17-C18-C19
16	1	609	CHL	C16-C17-C18-C19
15	A	1110	CLA	C5-C6-C7-C8
17	1	801	LHG	C1-C2-C3-O3
18	2	802	LMG	C42-C43-C44-C45
15	B	1208	CLA	C2-C1-O2A-CGA
15	B	1215	CLA	C2-C1-O2A-CGA
15	B	1214	CLA	C8-C10-C11-C12
15	1	605	CLA	C14-C13-C15-C16
15	3	605	CLA	C6-C7-C8-C9
15	A	1122	CLA	C11-C12-C13-C14
15	A	1125	CLA	C11-C12-C13-C14
15	A	1133	CLA	C11-C12-C13-C14
15	A	1136	CLA	C11-C10-C8-C9
15	B	1216	CLA	C6-C7-C8-C9
15	B	1219	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
15	B	1221	CLA	C6-C7-C8-C9
15	B	1226	CLA	O1D-CGD-O2D-CED
15	1	601	CLA	C13-C15-C16-C17
15	4	609	CLA	C2A-CAA-CBA-CGA
15	B	1204	CLA	C2A-CAA-CBA-CGA
15	A	1139	CLA	C16-C17-C18-C20
12	4	501	LUT	C5-C6-C7-C8
14	1	503	BCR	C1-C6-C7-C8
14	1	503	BCR	C5-C6-C7-C8
14	3	504	BCR	C1-C6-C7-C8
14	3	504	BCR	C5-C6-C7-C8
14	3	504	BCR	C23-C24-C25-C26
14	3	504	BCR	C23-C24-C25-C30
14	B	4005	BCR	C1-C6-C7-C8
14	B	4005	BCR	C5-C6-C7-C8
14	B	4006	BCR	C23-C24-C25-C26
14	B	4006	BCR	C23-C24-C25-C30
15	B	1223	CLA	C13-C15-C16-C17
14	B	4003	BCR	C37-C22-C23-C24
15	A	1134	CLA	O1D-CGD-O2D-CED
12	1	501	LUT	C7-C8-C9-C10
12	2	501	LUT	C27-C28-C29-C30
13	1	502	XAT	C27-C28-C29-C30
14	2	503	BCR	C7-C8-C9-C10
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	1120	CLA	C1A-C2A-CAA-CBA
15	J	1302	CLA	C1A-C2A-CAA-CBA
15	4	603	CLA	C13-C15-C16-C17
15	A	1126	CLA	C13-C15-C16-C17
14	J	4002	BCR	C14-C15-C16-C17
15	B	1219	CLA	C10-C11-C12-C13
17	3	801	LHG	C26-C27-C28-C29
18	2	804	LMG	C37-C38-C39-C40
18	2	804	LMG	C4-C5-C6-O5
15	A	1137	CLA	O1D-CGD-O2D-CED
15	B	1205	CLA	C4-C3-C5-C6
15	2	601	CLA	C11-C12-C13-C15
15	2	605	CLA	C6-C7-C8-C10
15	3	605	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
15	3	605	CLA	C11-C12-C13-C15
15	A	1013	CLA	C6-C7-C8-C10
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	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
15	B	1235	CLA	C11-C10-C8-C7
16	1	609	CHL	C6-C7-C8-C10
15	A	1129	CLA	C3-C5-C6-C7
18	2	802	LMG	C36-C37-C38-C39
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	B	1203	CLA	C13-C15-C16-C17
14	A	4008	BCR	C20-C21-C22-C37
14	B	4002	BCR	C35-C13-C14-C15
14	J	4002	BCR	C11-C10-C9-C34
15	B	1223	CLA	CBA-CGA-O2A-C1
18	B	5003	LMG	C33-C34-C35-C36
15	1	605	CLA	CAD-CBD-CGD-O2D
15	3	601	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	1012	CLA	CAD-CBD-CGD-O2D
15	A	1125	CLA	CAD-CBD-CGD-O2D
15	A	1138	CLA	CAD-CBD-CGD-O2D
15	A	1141	CLA	CAD-CBD-CGD-O2D
15	B	1023	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
15	B	1208	CLA	CAD-CBD-CGD-O2D
15	B	1216	CLA	CAD-CBD-CGD-O2D
15	B	1228	CLA	CAD-CBD-CGD-O2D
15	B	1238	CLA	CAD-CBD-CGD-O2D
18	2	802	LMG	C9-C8-O7-C10
15	3	612	CLA	C10-C11-C12-C13
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
15	4	602	CLA	O1A-CGA-O2A-C1
15	B	1226	CLA	C10-C11-C12-C13
15	B	1205	CLA	C2-C3-C5-C6
15	2	601	CLA	C5-C6-C7-C8
15	A	1101	CLA	C2A-CAA-CBA-CGA
15	B	1022	CLA	C2A-CAA-CBA-CGA
14	B	4001	BCR	C14-C15-C16-C17
15	A	1124	CLA	O1A-CGA-O2A-C1
15	B	1223	CLA	O1A-CGA-O2A-C1
15	1	615	CLA	CHA-CBD-CGD-O1D
15	1	615	CLA	CHA-CBD-CGD-O2D
15	2	603	CLA	CHA-CBD-CGD-O1D
15	2	603	CLA	CHA-CBD-CGD-O2D
15	2	616	CLA	CHA-CBD-CGD-O1D
15	2	616	CLA	CHA-CBD-CGD-O2D
15	3	610	CLA	CHA-CBD-CGD-O2D
15	3	615	CLA	CHA-CBD-CGD-O1D
15	4	604	CLA	CHA-CBD-CGD-O1D
15	4	604	CLA	CHA-CBD-CGD-O2D
15	4	606	CLA	CHA-CBD-CGD-O1D
15	4	609	CLA	CHA-CBD-CGD-O1D
15	A	1101	CLA	CHA-CBD-CGD-O1D
15	A	1106	CLA	CHA-CBD-CGD-O1D
15	A	1106	CLA	CHA-CBD-CGD-O2D
15	A	1109	CLA	CHA-CBD-CGD-O2D
15	A	1117	CLA	CHA-CBD-CGD-O1D
15	A	1117	CLA	CHA-CBD-CGD-O2D
15	A	1123	CLA	CHA-CBD-CGD-O1D
15	A	1134	CLA	CHA-CBD-CGD-O1D
15	A	1134	CLA	CHA-CBD-CGD-O2D
15	A	1137	CLA	CHA-CBD-CGD-O1D
15	A	1137	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
15	B	1022	CLA	CHA-CBD-CGD-O1D
15	B	1022	CLA	CHA-CBD-CGD-O2D
15	B	1204	CLA	CHA-CBD-CGD-O1D
15	B	1204	CLA	CHA-CBD-CGD-O2D
15	B	1211	CLA	CHA-CBD-CGD-O1D
15	B	1213	CLA	CHA-CBD-CGD-O1D
15	B	1213	CLA	CHA-CBD-CGD-O2D
15	B	1218	CLA	CHA-CBD-CGD-O1D
15	B	1218	CLA	CHA-CBD-CGD-O2D
15	B	1221	CLA	CHA-CBD-CGD-O1D
15	B	1221	CLA	CHA-CBD-CGD-O2D
15	B	1234	CLA	CHA-CBD-CGD-O1D
15	B	1234	CLA	CHA-CBD-CGD-O2D
15	F	1302	CLA	CHA-CBD-CGD-O1D
15	F	1302	CLA	CHA-CBD-CGD-O2D
15	J	1302	CLA	CHA-CBD-CGD-O1D
15	J	1302	CLA	CHA-CBD-CGD-O2D
16	1	609	CHL	CHA-CBD-CGD-O1D
16	1	609	CHL	CHA-CBD-CGD-O2D
16	2	609	CHL	CHA-CBD-CGD-O1D
15	1	601	CLA	O1A-CGA-O2A-C1
15	A	1123	CLA	O1A-CGA-O2A-C1
15	A	1136	CLA	O1A-CGA-O2A-C1
17	2	801	LHG	O10-C23-O8-C6
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
17	B	5001	LHG	O7-C5-C6-O8
16	2	609	CHL	O1A-CGA-O2A-C1
16	1	609	CHL	C16-C17-C18-C20
19	A	1011	CL0	C3-C5-C6-C7
15	2	612	CLA	C4-C3-C5-C6
15	A	1136	CLA	C8-C10-C11-C12
15	2	601	CLA	C6-C7-C8-C9
15	3	605	CLA	C11-C12-C13-C14
15	B	1202	CLA	C11-C10-C8-C9
15	B	1215	CLA	C11-C10-C8-C9
15	B	1235	CLA	C11-C10-C8-C9
15	B	1208	CLA	O1D-CGD-O2D-CED
15	A	1013	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
13	1	502	XAT	C11-C12-C13-C20
14	F	4002	BCR	C37-C22-C23-C24
17	3	801	LHG	C16-C17-C18-C19
13	1	502	XAT	C11-C12-C13-C14
14	2	503	BCR	C11-C12-C13-C14
14	2	503	BCR	C21-C22-C23-C24
14	A	4004	BCR	C21-C22-C23-C24
14	B	4006	BCR	C7-C8-C9-C10
14	B	4006	BCR	C21-C22-C23-C24
15	2	602	CLA	C1A-C2A-CAA-CBA
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	4	605	CLA	C16-C17-C18-C20
17	A	5002	LHG	C24-C23-O8-C6
14	B	4002	BCR	C19-C20-C21-C22
17	1	801	LHG	C3-O3-P-O6
17	A	5001	LHG	C4-O6-P-O3
17	A	5002	LHG	C3-O3-P-O6
18	4	801	LMG	C4-C5-C6-O5
15	A	1139	CLA	C4-C3-C5-C6
17	A	5002	LHG	C2-C3-O3-P
17	1	801	LHG	C3-O3-P-O4
17	2	801	LHG	C3-O3-P-O5
17	3	801	LHG	C3-O3-P-O5
17	A	5001	LHG	C4-O6-P-O4
17	A	5002	LHG	C3-O3-P-O4
17	B	5001	LHG	C3-O3-P-O4
17	B	5001	LHG	C4-O6-P-O4
15	B	1219	CLA	C16-C17-C18-C20
18	2	804	LMG	C33-C34-C35-C36
15	B	1021	CLA	C3-C5-C6-C7
16	2	609	CHL	C3-C5-C6-C7
15	3	614	CLA	C3-C5-C6-C7
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	4	606	CLA	CAD-CBD-CGD-O1D
15	A	1103	CLA	CAD-CBD-CGD-O1D
15	A	1135	CLA	C2-C3-C5-C6
15	B	1217	CLA	CAD-CBD-CGD-O1D
15	B	1227	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
15	B	1239	CLA	CAD-CBD-CGD-O1D
16	1	609	CHL	CAD-CBD-CGD-O1D
16	2	609	CHL	CAD-CBD-CGD-O1D
16	4	613	CHL	C11-C12-C13-C15
12	3	501	LUT	C25-C26-C27-C28
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	1102	CLA	C12-C13-C15-C16
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
15	B	1226	CLA	C11-C12-C13-C15
19	A	1011	CL0	C11-C10-C8-C7
17	B	5001	LHG	C15-C16-C17-C18
15	A	1105	CLA	O1D-CGD-O2D-CED
15	4	612	CLA	C16-C17-C18-C19
18	2	803	LMG	C2-C1-O1-C7
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	2	607	CLA	C4C-C3C-CAC-CBC
15	2	608	CLA	C2C-C3C-CAC-CBC
22	B	5002	DGD	C3B-C4B-C5B-C6B
18	2	804	LMG	C24-C25-C26-C27
15	2	616	CLA	C4-C3-C5-C6
15	A	1126	CLA	CAA-CBA-CGA-O2A
15	A	1102	CLA	C8-C10-C11-C12
15	3	607	CLA	C11-C10-C8-C9
15	A	1013	CLA	C6-C7-C8-C9
15	A	1117	CLA	C14-C13-C15-C16
15	A	1123	CLA	C6-C7-C8-C9
15	A	1136	CLA	C11-C12-C13-C14
15	B	1223	CLA	C6-C7-C8-C9
15	B	1224	CLA	C6-C7-C8-C9
16	2	609	CHL	C14-C13-C15-C16
15	B	1023	CLA	C3-C5-C6-C7
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

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Mol	Chain	Res	Type	Atoms
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
17	A	5001	LHG	C25-C26-C27-C28
14	B	4004	BCR	C36-C18-C19-C20
15	A	1124	CLA	C10-C11-C12-C13
14	A	4002	BCR	C16-C17-C18-C36
18	2	802	LMG	C39-C40-C41-C42
17	2	801	LHG	C10-C11-C12-C13
15	2	612	CLA	C2-C3-C5-C6
15	A	1013	CLA	C5-C6-C7-C8
15	A	1136	CLA	CBD-CGD-O2D-CED
15	B	1224	CLA	C8-C10-C11-C12
15	B	1236	CLA	C1-C2-C3-C4
15	B	1203	CLA	C3-C5-C6-C7
15	B	1234	CLA	C3-C5-C6-C7
15	B	1224	CLA	CAA-CBA-CGA-O2A
15	A	1136	CLA	C10-C11-C12-C13
17	1	801	LHG	C4-C5-O7-C7
18	2	804	LMG	C9-C8-O7-C10
15	A	1138	CLA	C2A-CAA-CBA-CGA
15	B	1222	CLA	C2-C1-O2A-CGA
19	A	1011	CL0	C2-C1-O2A-CGA
22	B	5002	DGD	CAA-CBA-CCA-CDA
15	F	1302	CLA	O2A-C1-C2-C3
15	3	601	CLA	C2-C3-C5-C6
17	A	5002	LHG	C31-C32-C33-C34
15	1	611	CLA	O1A-CGA-O2A-C1
15	A	1111	CLA	C4C-C3C-CAC-CBC
15	B	1219	CLA	C16-C17-C18-C19
15	B	1219	CLA	C5-C6-C7-C8
17	2	801	LHG	O7-C5-C6-O8
15	3	610	CLA	O1D-CGD-O2D-CED
17	3	801	LHG	C28-C29-C30-C31
22	B	5002	DGD	C7A-C8A-C9A-CAA
18	2	804	LMG	C36-C37-C38-C39
15	A	1012	CLA	C15-C16-C17-C18
15	B	1211	CLA	C15-C16-C17-C18
15	A	1136	CLA	C11-C12-C13-C15
15	1	604	CLA	C11-C12-C13-C14
15	2	604	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
15	4	609	CLA	C6-C7-C8-C9
15	A	1111	CLA	C11-C10-C8-C9
14	A	4006	BCR	C19-C20-C21-C22
14	F	4002	BCR	C19-C20-C21-C22
15	4	605	CLA	C16-C17-C18-C19
20	B	2002	PQN	C26-C27-C28-C29
15	A	1128	CLA	C3-C5-C6-C7
20	B	2002	PQN	C26-C27-C28-C30
17	1	801	LHG	C2-C3-O3-P
19	A	1011	CL0	CAA-CBA-CGA-O2A
15	A	1136	CLA	O1D-CGD-O2D-CED
15	1	611	CLA	CBA-CGA-O2A-C1
15	A	1116	CLA	O1D-CGD-O2D-CED
15	A	1012	CLA	C13-C15-C16-C17
15	3	610	CLA	CBD-CGD-O2D-CED
15	A	1105	CLA	CBD-CGD-O2D-CED
15	A	1133	CLA	CBA-CGA-O2A-C1
15	A	1136	CLA	C2A-CAA-CBA-CGA
15	3	601	CLA	C11-C12-C13-C15
12	1	501	LUT	C33-C34-C35-C15
12	2	501	LUT	C9-C10-C11-C12
14	3	503	BCR	C9-C10-C11-C12
22	B	5002	DGD	C9B-CAB-CBB-CCB
17	2	801	LHG	C9-C10-C11-C12
14	J	4001	BCR	C18-C19-C20-C21
15	B	1021	CLA	C5-C6-C7-C8
15	A	1133	CLA	O1A-CGA-O2A-C1
18	2	803	LMG	C30-C31-C32-C33
16	2	613	CHL	CAA-CBA-CGA-O2A
15	3	608	CLA	CAA-CBA-CGA-O2A
15	1	605	CLA	C2-C1-O2A-CGA
15	2	601	CLA	C2-C1-O2A-CGA
15	B	1221	CLA	C2-C1-O2A-CGA
15	B	1235	CLA	C2-C1-O2A-CGA
15	B	1214	CLA	C15-C16-C17-C18
15	3	614	CLA	C2A-CAA-CBA-CGA
15	4	604	CLA	C2A-CAA-CBA-CGA
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	1234	CLA	C3A-C2A-CAA-CBA
18	2	802	LMG	C30-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
15	B	1236	CLA	O2A-C1-C2-C3
15	A	1130	CLA	CAA-CBA-CGA-O1A
15	B	1022	CLA	C4-C3-C5-C6
15	A	1140	CLA	C6-C7-C8-C9
15	B	1240	CLA	C14-C13-C15-C16
16	2	613	CHL	CAA-CBA-CGA-O1A
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
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
17	A	5002	LHG	O9-C7-O7-C5
17	A	5002	LHG	C11-C12-C13-C14
15	2	605	CLA	C16-C17-C18-C19
13	1	502	XAT	C27-C28-C29-C39
14	B	4005	BCR	C37-C22-C23-C24
14	F	4001	BCR	C37-C22-C23-C24
17	A	5001	LHG	C34-C35-C36-C37
15	A	1129	CLA	C2C-C3C-CAC-CBC
15	B	1221	CLA	C4-C3-C5-C6
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

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Mol	Chain	Res	Type	Atoms
15	2	616	CLA	C11-C12-C13-C15
15	4	604	CLA	C11-C10-C8-C7
15	4	612	CLA	C11-C12-C13-C15
15	A	1122	CLA	C11-C12-C13-C15
15	A	1125	CLA	C11-C10-C8-C7
15	A	1125	CLA	C12-C13-C15-C16
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	1224	CLA	C6-C7-C8-C10
15	B	1225	CLA	C6-C7-C8-C10
15	B	1226	CLA	C11-C10-C8-C7
19	A	1011	CL0	C6-C7-C8-C10
18	2	803	LMG	C31-C32-C33-C34
19	A	1011	CL0	C2A-CAA-CBA-CGA
15	A	1111	CLA	C10-C11-C12-C13
15	3	601	CLA	C11-C12-C13-C14
15	1	606	CLA	O1D-CGD-O2D-CED
22	B	5002	DGD	O1A-C1A-O1G-C1G
15	A	1116	CLA	CBD-CGD-O2D-CED
22	B	5002	DGD	C2B-C3B-C4B-C5B
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
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
18	B	5003	LMG	C14-C15-C16-C17
15	A	1117	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
15	4	606	CLA	C2A-CAA-CBA-CGA
15	A	1130	CLA	CAA-CBA-CGA-O2A
17	1	801	LHG	C15-C16-C17-C18
15	A	1127	CLA	C4-C3-C5-C6
15	2	604	CLA	C2-C1-O2A-CGA
15	3	610	CLA	C2-C1-O2A-CGA
15	A	1105	CLA	C2-C1-O2A-CGA
16	1	609	CHL	C2-C1-O2A-CGA
15	B	1022	CLA	C2-C3-C5-C6
17	A	5002	LHG	C30-C31-C32-C33
18	4	801	LMG	C30-C31-C32-C33
15	B	1224	CLA	C10-C11-C12-C13
15	A	1135	CLA	C4-C3-C5-C6
15	A	1116	CLA	CAA-CBA-CGA-O2A
18	2	804	LMG	C19-C20-C21-C22
18	2	804	LMG	C34-C35-C36-C37
15	A	1125	CLA	C8-C10-C11-C12
15	2	605	CLA	C2A-CAA-CBA-CGA
15	B	1224	CLA	C2A-CAA-CBA-CGA
15	3	605	CLA	C16-C17-C18-C20
15	B	1240	CLA	C16-C17-C18-C19
14	4	503	BCR	C1-C6-C7-C8
14	B	4004	BCR	C1-C6-C7-C8
14	F	4001	BCR	C1-C6-C7-C8
14	F	4002	BCR	C1-C6-C7-C8
15	B	1229	CLA	C10-C11-C12-C13
15	1	607	CLA	CAA-CBA-CGA-O2A
18	2	804	LMG	C7-C8-C9-O8
15	A	1121	CLA	CAA-CBA-CGA-O2A
15	A	1131	CLA	CAA-CBA-CGA-O2A
15	2	604	CLA	C15-C16-C17-C18
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
14	J	4001	BCR	C13-C14-C15-C16
17	A	5001	LHG	C24-C23-O8-C6
15	4	607	CLA	C4-C3-C5-C6
15	A	1119	CLA	C4-C3-C5-C6
12	2	501	LUT	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
15	A	1118	CLA	C1A-C2A-CAA-CBA
15	2	616	CLA	C2-C3-C5-C6
15	1	613	CLA	CAA-CBA-CGA-O2A
15	A	1113	CLA	CAA-CBA-CGA-O2A
15	B	1240	CLA	CAA-CBA-CGA-O1A
17	A	5001	LHG	C24-C25-C26-C27
15	B	1215	CLA	C8-C10-C11-C12
15	B	1216	CLA	C10-C11-C12-C13
15	2	606	CLA	C2A-CAA-CBA-CGA
15	A	1108	CLA	C2A-CAA-CBA-CGA
15	A	1128	CLA	C2A-CAA-CBA-CGA
18	2	802	LMG	C28-C29-C30-C31
15	A	1115	CLA	CAA-CBA-CGA-O2A
15	3	607	CLA	C11-C10-C8-C7
15	B	1211	CLA	C11-C12-C13-C15
15	B	1239	CLA	O1D-CGD-O2D-CED
14	A	4008	BCR	C13-C14-C15-C16
15	A	1117	CLA	CBD-CGD-O2D-CED
15	B	1203	CLA	O1A-CGA-O2A-C1
15	B	1203	CLA	CBA-CGA-O2A-C1
15	A	1128	CLA	C13-C15-C16-C17
15	1	615	CLA	CAA-CBA-CGA-O2A
15	A	1012	CLA	CAA-CBA-CGA-O2A
16	2	609	CHL	CAA-CBA-CGA-O2A
15	B	1212	CLA	C4-C3-C5-C6
15	B	1227	CLA	C4-C3-C5-C6
15	B	1202	CLA	C13-C15-C16-C17
15	1	615	CLA	CAA-CBA-CGA-O1A
15	A	1012	CLA	C11-C12-C13-C14
15	A	1104	CLA	C6-C7-C8-C9
15	A	1133	CLA	C6-C7-C8-C9
15	A	1136	CLA	C14-C13-C15-C16
15	B	1023	CLA	C11-C10-C8-C9
15	B	1208	CLA	C6-C7-C8-C9
15	B	1223	CLA	C11-C10-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
19	A	1011	CL0	C14-C13-C15-C16
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	A	1115	CLA	CAA-CBA-CGA-O1A
15	1	602	CLA	CAD-CBD-CGD-O2D
15	1	607	CLA	CAD-CBD-CGD-O2D
15	3	612	CLA	CAD-CBD-CGD-O2D
15	4	609	CLA	CAD-CBD-CGD-O2D
15	A	1104	CLA	CAD-CBD-CGD-O2D
15	A	1133	CLA	CAD-CBD-CGD-O2D
15	B	1214	CLA	CAD-CBD-CGD-O2D
15	B	1230	CLA	CAD-CBD-CGD-O2D
15	3	612	CLA	C3-C5-C6-C7
15	4	604	CLA	C2-C1-O2A-CGA
15	A	1111	CLA	C2-C1-O2A-CGA
15	B	1208	CLA	C4C-C3C-CAC-CBC
17	B	5001	LHG	C23-C24-C25-C26
15	1	605	CLA	CAA-CBA-CGA-O2A
15	A	1129	CLA	CAA-CBA-CGA-O2A
14	A	4003	BCR	C6-C7-C8-C9
15	B	1203	CLA	C4-C3-C5-C6
15	A	1121	CLA	CAA-CBA-CGA-O1A
15	B	1237	CLA	CAA-CBA-CGA-O2A
15	A	1013	CLA	CAA-CBA-CGA-O2A
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
13	1	502	XAT	O24-C26-C27-C28
13	2	502	XAT	O4-C6-C7-C8
13	3	502	XAT	O24-C26-C27-C28
18	2	804	LMG	O1-C7-C8-C9
18	B	5003	LMG	O1-C7-C8-C9
15	A	1132	CLA	CAA-CBA-CGA-O2A
15	B	1022	CLA	CAA-CBA-CGA-O2A
15	1	613	CLA	CAA-CBA-CGA-O1A
15	A	1113	CLA	CAA-CBA-CGA-O1A
15	B	1218	CLA	CAA-CBA-CGA-O1A
15	3	608	CLA	O2A-C1-C2-C3
15	A	1114	CLA	O2A-C1-C2-C3
15	A	1123	CLA	O2A-C1-C2-C3
15	A	1128	CLA	O2A-C1-C2-C3
15	A	1129	CLA	O2A-C1-C2-C3
15	B	1023	CLA	O2A-C1-C2-C3
15	B	1203	CLA	O2A-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
15	B	1212	CLA	O2A-C1-C2-C3
16	1	609	CHL	O2A-C1-C2-C3
16	1	609	CHL	CAA-CBA-CGA-O2A
17	A	5002	LHG	O8-C23-C24-C25
15	A	1101	CLA	C3-C5-C6-C7
15	B	1240	CLA	C16-C17-C18-C20
15	1	606	CLA	CBD-CGD-O2D-CED
15	1	604	CLA	CHA-CBD-CGD-O1D
15	1	604	CLA	CHA-CBD-CGD-O2D
15	3	609	CLA	CHA-CBD-CGD-O1D
15	3	609	CLA	CHA-CBD-CGD-O2D
15	4	606	CLA	CHA-CBD-CGD-O2D
15	A	1102	CLA	CHA-CBD-CGD-O1D
15	A	1123	CLA	CHA-CBD-CGD-O2D
15	A	1128	CLA	CHA-CBD-CGD-O1D
15	A	1128	CLA	CHA-CBD-CGD-O2D
15	A	1130	CLA	CHA-CBD-CGD-O1D
15	A	1130	CLA	CHA-CBD-CGD-O2D
15	B	1202	CLA	CHA-CBD-CGD-O1D
15	B	1202	CLA	CHA-CBD-CGD-O2D
15	B	1211	CLA	CHA-CBD-CGD-O2D
15	B	1215	CLA	CHA-CBD-CGD-O1D
15	B	1215	CLA	CHA-CBD-CGD-O2D
15	B	1222	CLA	CHA-CBD-CGD-O1D
15	B	1222	CLA	CHA-CBD-CGD-O2D
15	B	1232	CLA	CHA-CBD-CGD-O2D
16	1	610	CHL	CHA-CBD-CGD-O1D
16	1	610	CHL	CHA-CBD-CGD-O2D
16	2	609	CHL	CHA-CBD-CGD-O2D
15	A	1131	CLA	CAA-CBA-CGA-O1A
15	B	1235	CLA	CAA-CBA-CGA-O2A
14	J	4001	BCR	C16-C17-C18-C19
15	A	1132	CLA	CAA-CBA-CGA-O1A
15	B	1221	CLA	C16-C17-C18-C19
15	B	1023	CLA	CAA-CBA-CGA-O2A
17	B	5001	LHG	O7-C7-C8-C9
17	1	801	LHG	C9-C10-C11-C12
15	B	1221	CLA	C5-C6-C7-C8
15	B	1218	CLA	CAA-CBA-CGA-O2A
15	2	604	CLA	CAA-CBA-CGA-O2A
15	4	602	CLA	CAA-CBA-CGA-O2A
15	F	1302	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
15	3	608	CLA	C10-C11-C12-C13
15	1	608	CLA	CAA-CBA-CGA-O2A
17	3	801	LHG	O7-C7-C8-C9
17	2	801	LHG	C11-C12-C13-C14
15	2	601	CLA	C6-C7-C8-C10
15	A	1122	CLA	C12-C13-C15-C16
15	A	1139	CLA	C2-C3-C5-C6
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	1117	CLA	C11-C12-C13-C14
15	B	1214	CLA	C14-C13-C15-C16
19	A	1011	CL0	C11-C12-C13-C14
15	B	1221	CLA	C16-C17-C18-C20
15	B	1237	CLA	CAA-CBA-CGA-O1A
15	3	605	CLA	C16-C17-C18-C19
18	2	803	LMG	O7-C10-C11-C12
15	A	1012	CLA	CAA-CBA-CGA-O1A
15	B	1022	CLA	CAA-CBA-CGA-O1A
15	4	612	CLA	C1A-C2A-CAA-CBA
15	B	1225	CLA	C1A-C2A-CAA-CBA
15	B	1236	CLA	C1A-C2A-CAA-CBA
15	F	1302	CLA	C1A-C2A-CAA-CBA
15	4	609	CLA	C11-C12-C13-C15
16	1	609	CHL	CAA-CBA-CGA-O1A
17	B	5001	LHG	O9-C7-C8-C9
18	4	801	LMG	O10-C28-C29-C30
18	2	802	LMG	C33-C34-C35-C36
15	B	1219	CLA	C2-C1-O2A-CGA
17	B	5001	LHG	O10-C23-C24-C25
18	B	5003	LMG	C7-C8-C9-O8
15	F	1301	CLA	C2C-C3C-CAC-CBC
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	A	1120	CLA	C2C-C3C-CAC-CBC
15	4	602	CLA	CAA-CBA-CGA-O1A
15	3	603	CLA	CAA-CBA-CGA-O2A
15	1	605	CLA	CAA-CBA-CGA-O1A
18	2	804	LMG	C23-C24-C25-C26
16	2	609	CHL	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
17	1	801	LHG	O9-C7-C8-C9
15	4	604	CLA	CAA-CBA-CGA-O2A
15	B	1206	CLA	CAA-CBA-CGA-O2A
15	A	1103	CLA	C5-C6-C7-C8
15	B	1204	CLA	CAA-CBA-CGA-O1A
14	B	4006	BCR	C10-C11-C12-C13
15	4	602	CLA	C2A-CAA-CBA-CGA
15	A	1103	CLA	C2A-CAA-CBA-CGA
15	A	1013	CLA	CAA-CBA-CGA-O1A
15	A	1125	CLA	C5-C6-C7-C8
15	B	1234	CLA	C4-C3-C5-C6
19	A	1011	CL0	C4-C3-C5-C6
15	2	616	CLA	C8-C10-C11-C12
15	A	1129	CLA	C4C-C3C-CAC-CBC
15	A	1105	CLA	CAD-CBD-CGD-O1D
15	A	1107	CLA	CAD-CBD-CGD-O1D
15	A	1117	CLA	CAD-CBD-CGD-O1D
15	A	1120	CLA	CAD-CBD-CGD-O1D
15	B	1215	CLA	CAD-CBD-CGD-O1D
15	B	1229	CLA	CAD-CBD-CGD-O1D
16	1	610	CHL	CAD-CBD-CGD-O1D
16	2	610	CHL	CAD-CBD-CGD-O1D
16	2	611	CHL	CAD-CBD-CGD-O1D
18	2	804	LMG	C7-C8-O7-C10
15	2	604	CLA	CAA-CBA-CGA-O1A
15	A	1129	CLA	CAA-CBA-CGA-O1A
15	B	1205	CLA	C10-C11-C12-C13
15	2	603	CLA	C11-C10-C8-C9
15	A	1119	CLA	C11-C12-C13-C14
15	A	1137	CLA	C6-C7-C8-C9
15	B	1210	CLA	C6-C7-C8-C9
15	B	1211	CLA	C6-C7-C8-C9
15	B	1215	CLA	C6-C7-C8-C9
15	F	1302	CLA	CAA-CBA-CGA-O1A
15	F	1301	CLA	CAA-CBA-CGA-O2A
16	1	610	CHL	CAA-CBA-CGA-O2A
18	2	803	LMG	C16-C17-C18-C19
15	B	1235	CLA	CAA-CBA-CGA-O1A
17	A	5002	LHG	C12-C13-C14-C15
15	3	610	CLA	CAA-CBA-CGA-O2A
15	1	608	CLA	C5-C6-C7-C8
15	A	1101	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
15	2	606	CLA	CAA-CBA-CGA-O2A
15	1	608	CLA	CAA-CBA-CGA-O1A
18	4	801	LMG	C14-C15-C16-C17
12	2	501	LUT	C25-C26-C27-C28
15	2	608	CLA	C3A-C2A-CAA-CBA
15	2	616	CLA	C11-C10-C8-C7
15	4	607	CLA	C3A-C2A-CAA-CBA
15	A	1101	CLA	C11-C10-C8-C7
15	A	1107	CLA	C3A-C2A-CAA-CBA
15	A	1117	CLA	C11-C10-C8-C7
15	A	1137	CLA	C11-C12-C13-C15
15	B	1218	CLA	C3A-C2A-CAA-CBA
15	B	1223	CLA	C6-C7-C8-C10
15	B	1224	CLA	C11-C10-C8-C7
15	B	1225	CLA	C12-C13-C15-C16
15	B	1226	CLA	C3A-C2A-CAA-CBA
19	A	1011	CL0	C11-C12-C13-C15
17	A	5002	LHG	O10-C23-C24-C25
15	A	1123	CLA	CAA-CBA-CGA-O2A
15	B	1221	CLA	CAA-CBA-CGA-O2A
17	B	5001	LHG	O8-C23-C24-C25
18	4	801	LMG	O8-C28-C29-C30
12	4	501	LUT	C7-C8-C9-C10
14	3	504	BCR	C7-C8-C9-C10
14	J	4001	BCR	C7-C8-C9-C10
15	3	610	CLA	CAA-CBA-CGA-O1A
15	4	604	CLA	CAA-CBA-CGA-O1A
15	B	1023	CLA	CAA-CBA-CGA-O1A
17	3	801	LHG	O9-C7-C8-C9
14	2	503	BCR	C19-C20-C21-C22
15	3	601	CLA	CAA-CBA-CGA-O2A
15	3	603	CLA	CAA-CBA-CGA-O1A
15	B	1221	CLA	CAA-CBA-CGA-O1A
15	F	1301	CLA	CAA-CBA-CGA-O1A
15	A	1122	CLA	C3-C5-C6-C7
15	3	603	CLA	C8-C10-C11-C12
16	2	609	CHL	C8-C10-C11-C12
15	B	1209	CLA	CAA-CBA-CGA-O2A
15	3	612	CLA	C5-C6-C7-C8
15	2	605	CLA	C16-C17-C18-C20
15	2	606	CLA	CAA-CBA-CGA-O1A
15	B	1206	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
15	B	1204	CLA	CAA-CBA-CGA-O2A

There are no ring outliers.

115 monomers are involved in 201 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	A	5001	LHG	1	0
15	1	605	CLA	4	0
15	3	614	CLA	1	0
14	3	506	BCR	2	0
15	B	1207	CLA	1	0
16	4	610	CHL	1	0
15	B	1238	CLA	1	0
15	B	1206	CLA	2	0
15	A	1122	CLA	1	0
14	3	504	BCR	3	0
15	B	1215	CLA	1	0
13	1	502	XAT	3	0
14	B	4004	BCR	2	0
15	B	1216	CLA	1	0
12	1	501	LUT	11	0
15	A	1126	CLA	6	0
15	1	615	CLA	2	0
13	2	502	XAT	2	0
14	J	4001	BCR	3	0
15	B	1226	CLA	2	0
15	A	1104	CLA	2	0
15	3	615	CLA	1	0
15	A	1129	CLA	2	0
21	C	3003	SF4	1	0
15	2	604	CLA	1	0
14	B	4002	BCR	2	0
16	3	604	CHL	1	0
15	A	1133	CLA	1	0
15	A	1119	CLA	2	0
15	B	1214	CLA	2	0
14	A	4007	BCR	4	0
15	B	1208	CLA	2	0
14	A	4006	BCR	6	0
14	A	4004	BCR	1	0
15	B	1240	CLA	2	0
15	2	602	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	A	1013	CLA	4	0
15	3	608	CLA	3	0
15	B	1225	CLA	1	0
15	3	611	CLA	1	0
15	2	616	CLA	2	0
15	A	1103	CLA	1	0
15	B	1210	CLA	2	0
15	1	611	CLA	3	0
15	B	1234	CLA	2	0
14	B	4001	BCR	1	0
15	3	612	CLA	2	0
15	A	1121	CLA	1	0
14	J	4002	BCR	2	0
15	B	1022	CLA	2	0
15	A	1114	CLA	2	0
15	1	603	CLA	6	0
15	B	1209	CLA	1	0
16	1	609	CHL	1	0
15	4	601	CLA	1	0
15	A	1125	CLA	5	0
14	B	4003	BCR	1	0
16	2	610	CHL	1	0
16	1	610	CHL	1	0
15	2	603	CLA	1	0
13	3	502	XAT	2	0
15	A	1112	CLA	3	0
14	F	4001	BCR	2	0
14	B	4006	BCR	2	0
15	B	1231	CLA	4	0
18	B	5003	LMG	2	0
15	1	601	CLA	2	0
17	1	801	LHG	1	0
15	A	1127	CLA	2	0
15	A	1123	CLA	2	0
15	A	1108	CLA	1	0
15	B	1236	CLA	2	0
15	A	1141	CLA	2	0
16	2	609	CHL	1	0
15	B	1220	CLA	2	0
14	B	4005	BCR	3	0
15	B	1230	CLA	2	0
15	3	603	CLA	2	0

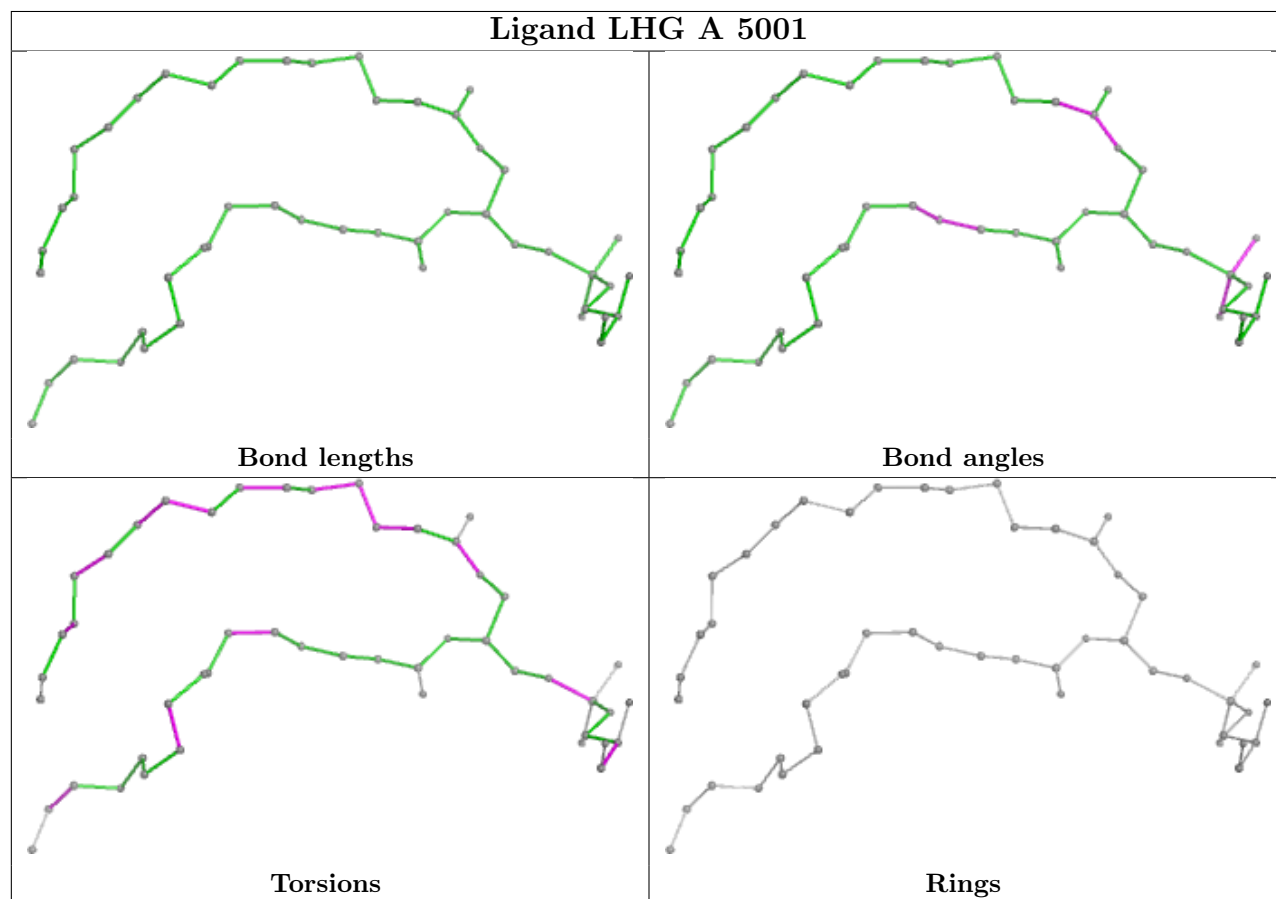
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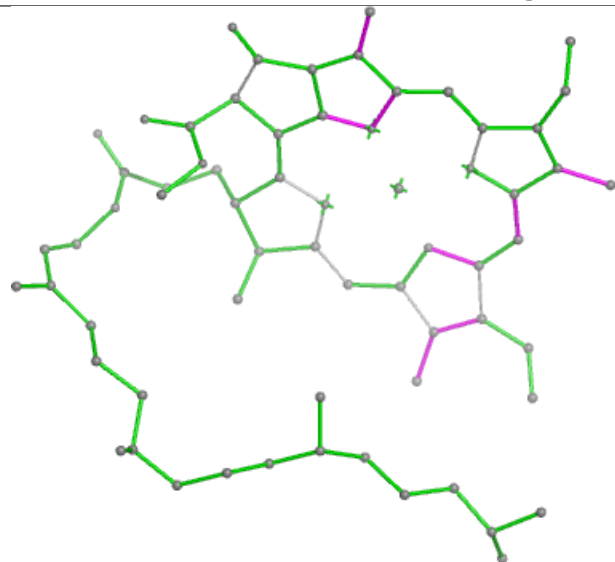
Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	B	1239	CLA	3	0
15	A	1111	CLA	3	0
15	B	1023	CLA	2	0
15	A	1012	CLA	10	0
15	1	613	CLA	1	0
15	B	1221	CLA	2	0
14	A	4008	BCR	1	0
15	B	1021	CLA	3	0
15	2	608	CLA	1	0
15	3	605	CLA	5	0
13	4	502	XAT	6	0
14	A	4002	BCR	2	0
15	4	603	CLA	1	0
15	1	607	CLA	2	0
15	2	601	CLA	2	0
22	B	5002	DGD	2	0
15	B	1224	CLA	2	0
15	4	608	CLA	2	0
15	A	1105	CLA	2	0
15	A	1132	CLA	1	0
12	3	501	LUT	8	0
15	A	1137	CLA	1	0
12	2	501	LUT	5	0
15	3	601	CLA	4	0
19	A	1011	CL0	3	0
15	4	604	CLA	2	0
15	1	612	CLA	3	0
15	2	612	CLA	2	0
15	B	1229	CLA	2	0
15	4	609	CLA	1	0
15	A	1117	CLA	3	0
12	4	501	LUT	6	0
15	A	1128	CLA	1	0
15	B	1202	CLA	2	0
15	B	1223	CLA	2	0
17	A	5002	LHG	1	0
15	2	606	CLA	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.

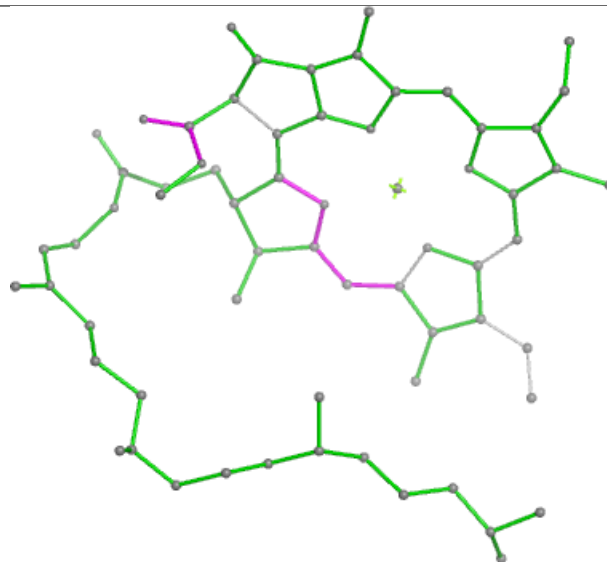
Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD 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.



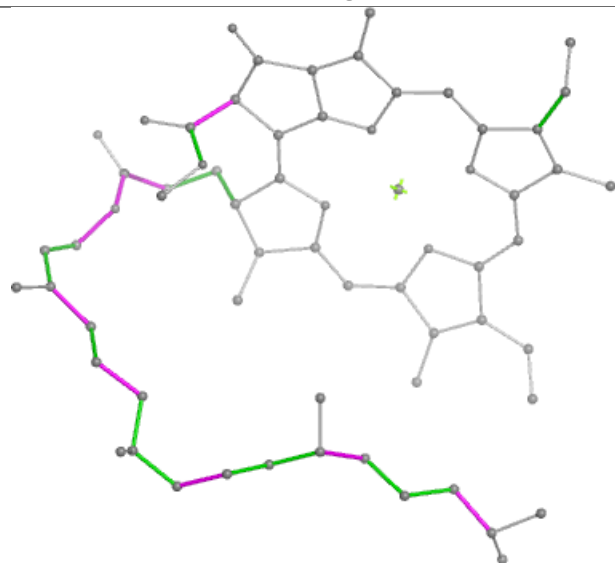
Ligand CLA 1 605



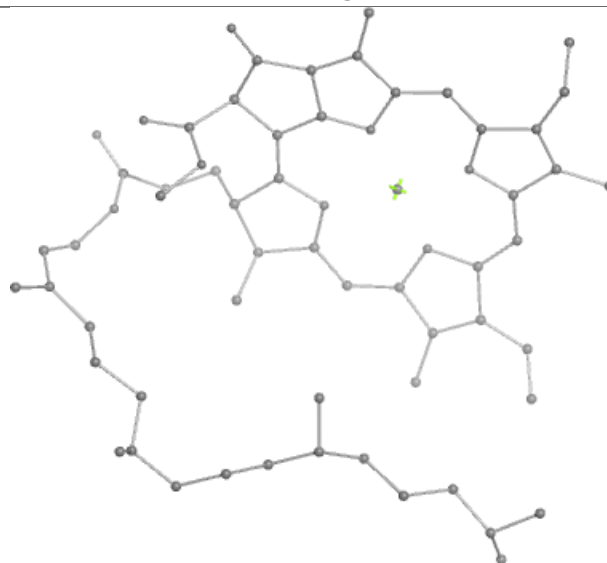
Bond lengths



Bond angles

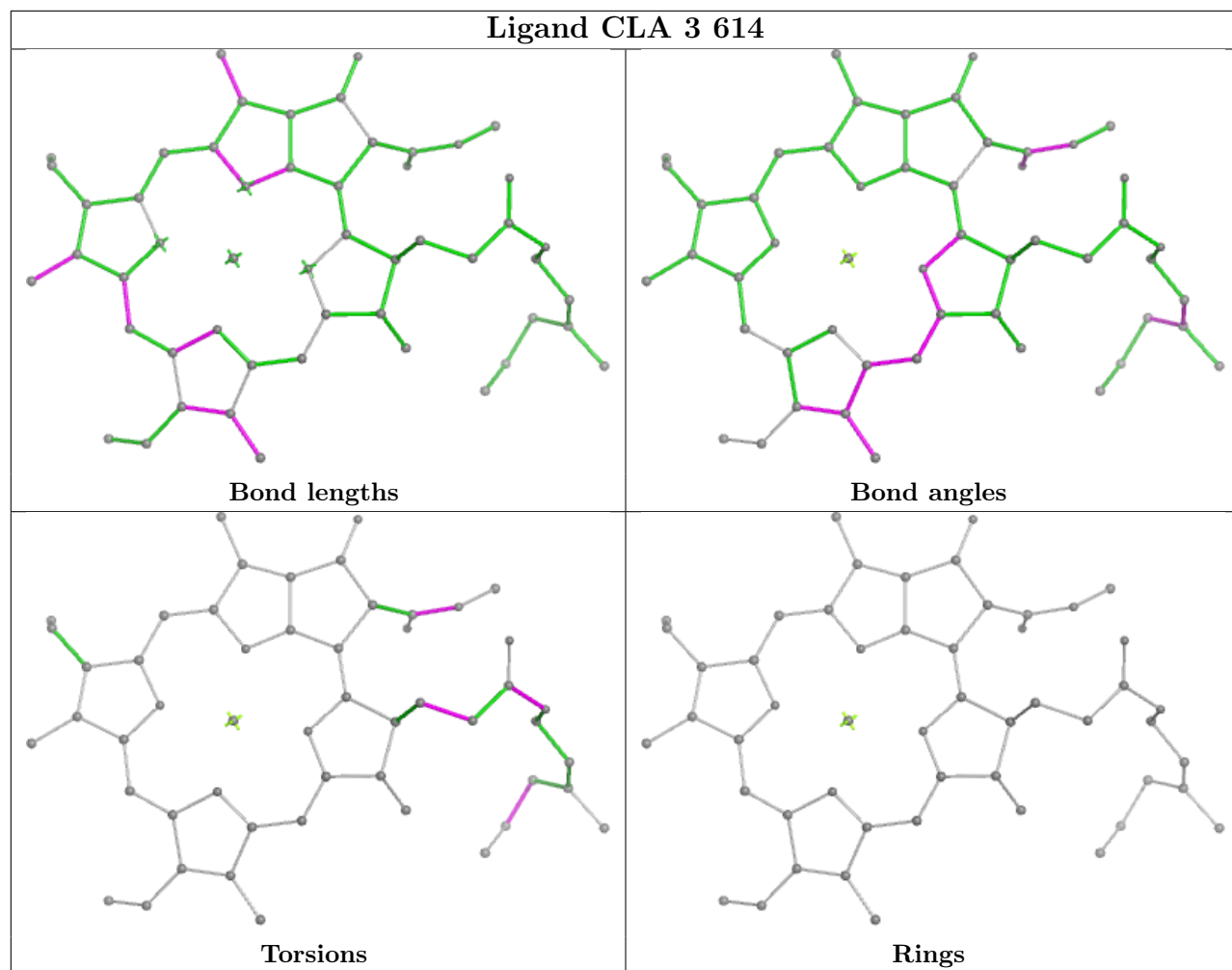


Torsions

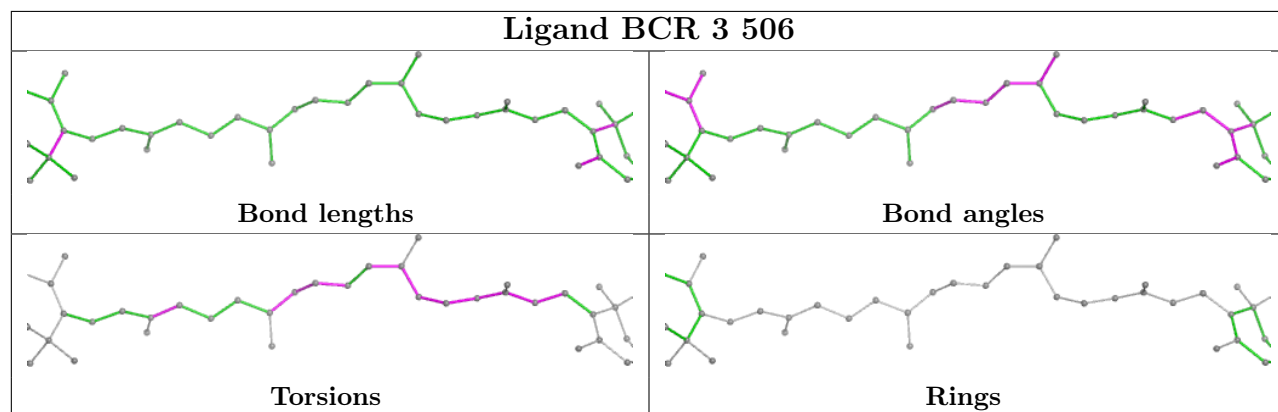


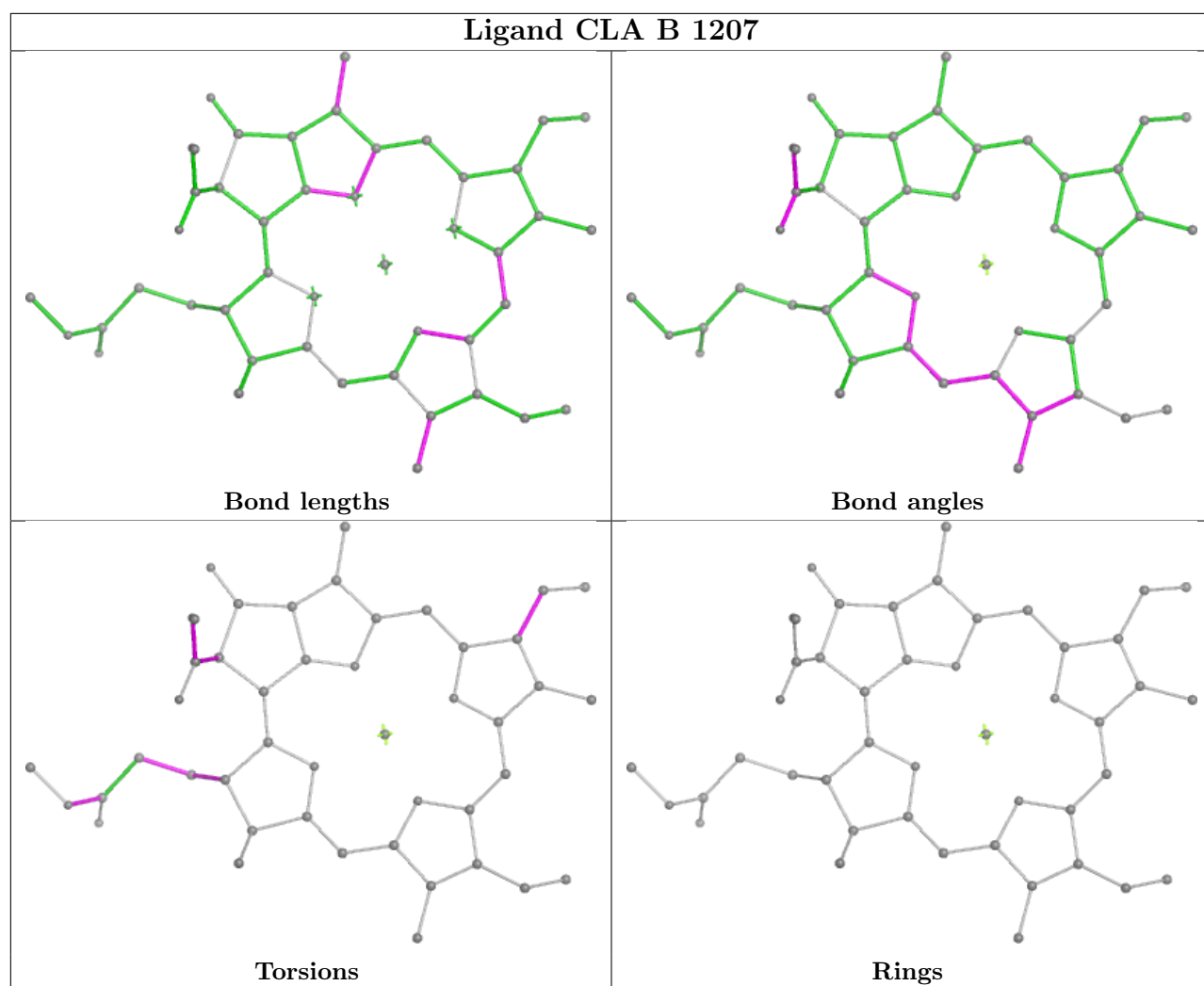
Rings

Ligand CLA 3 614

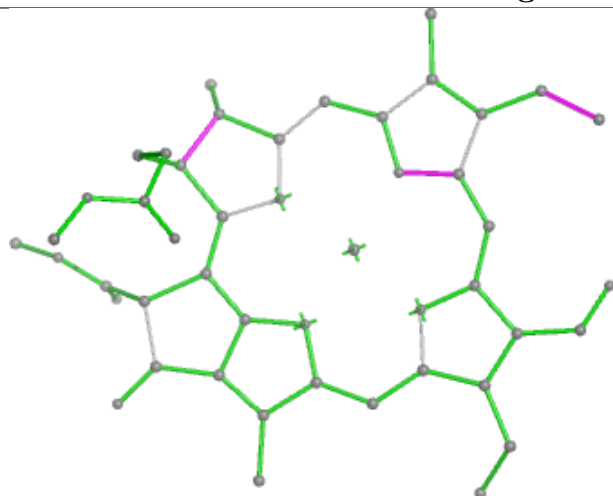


Ligand BCR 3 506

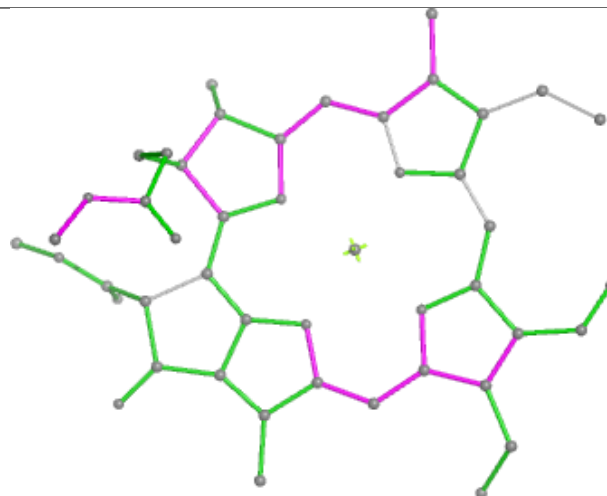




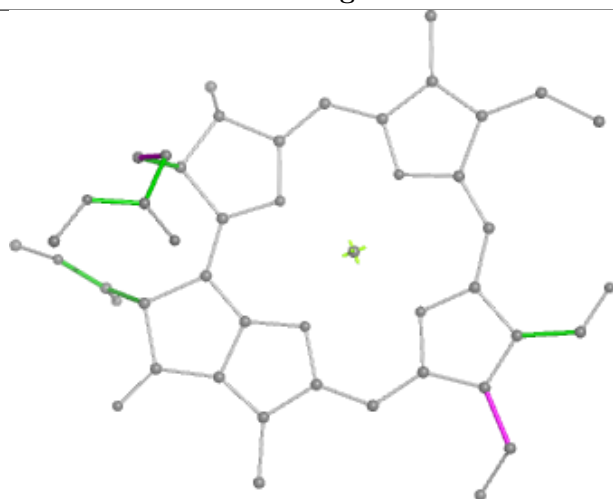
Ligand CHL 4 610



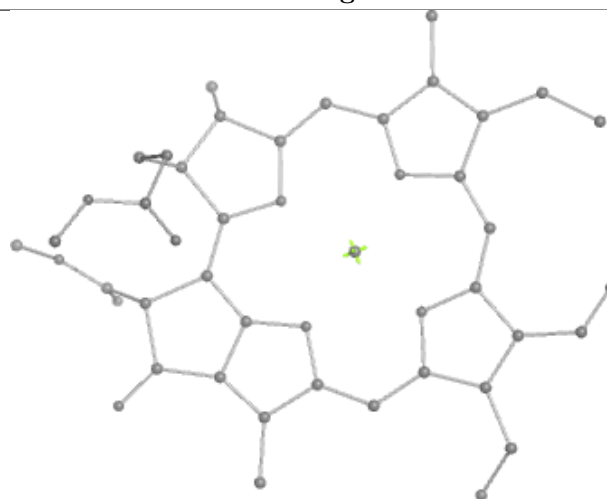
Bond lengths



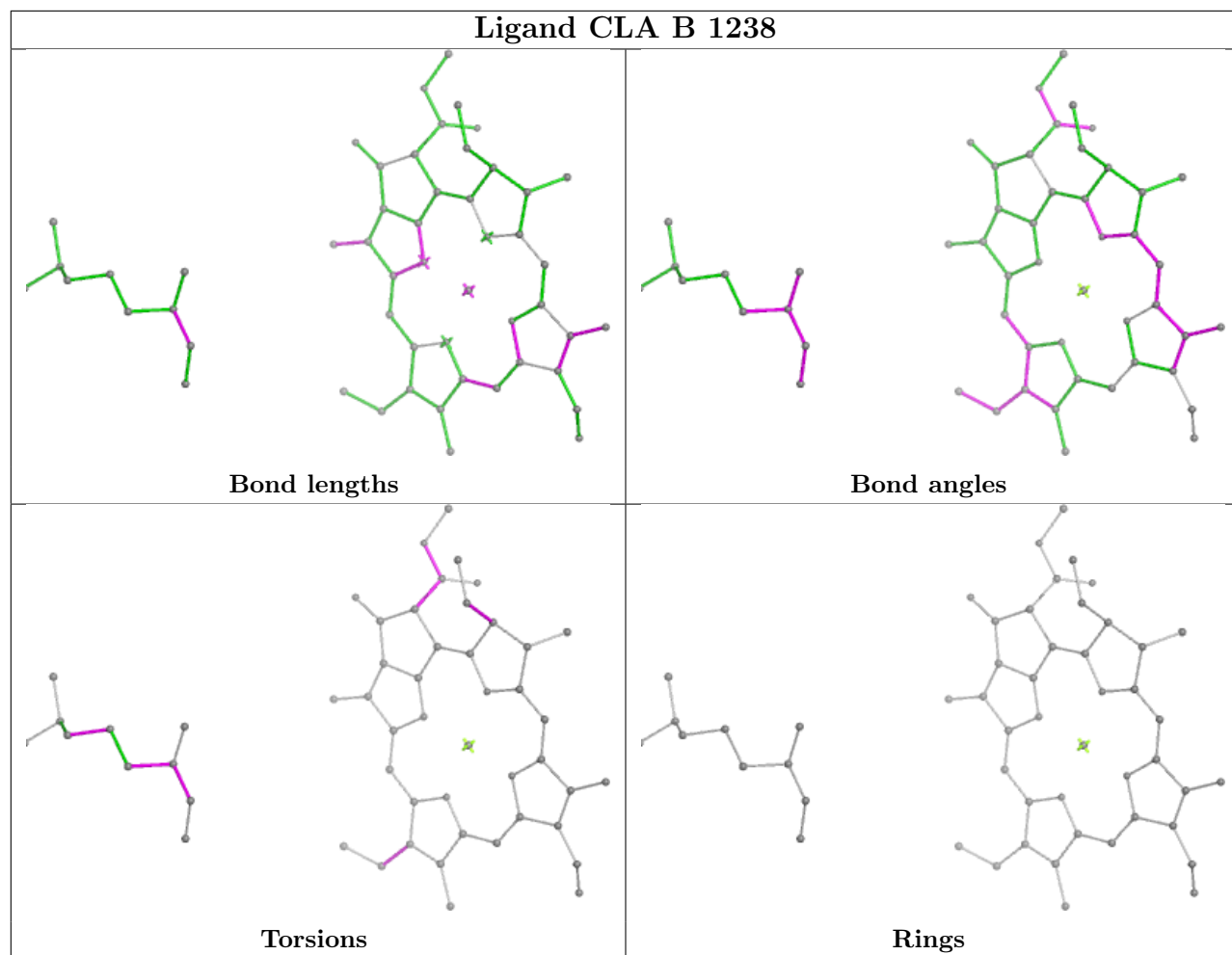
Bond angles

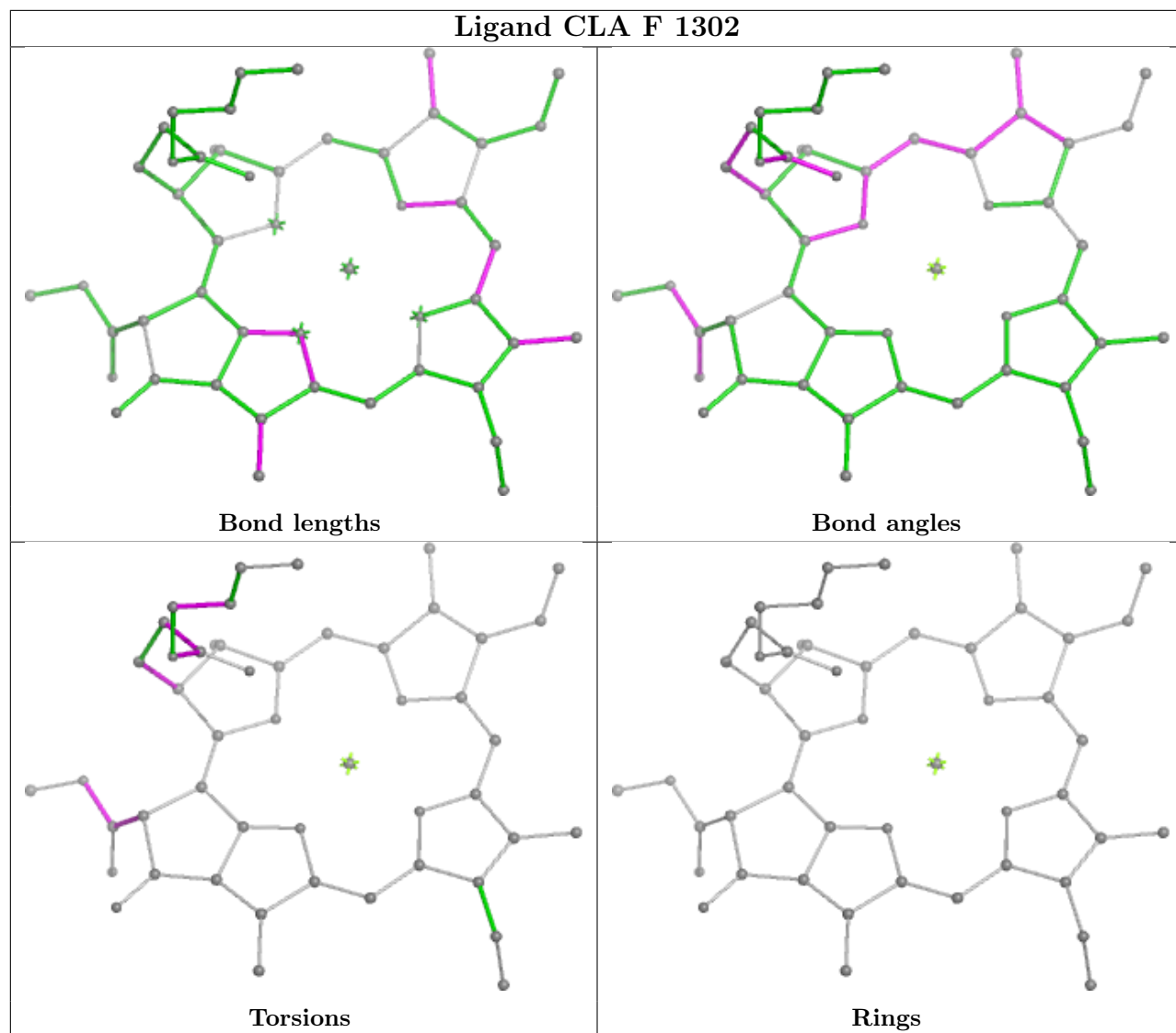


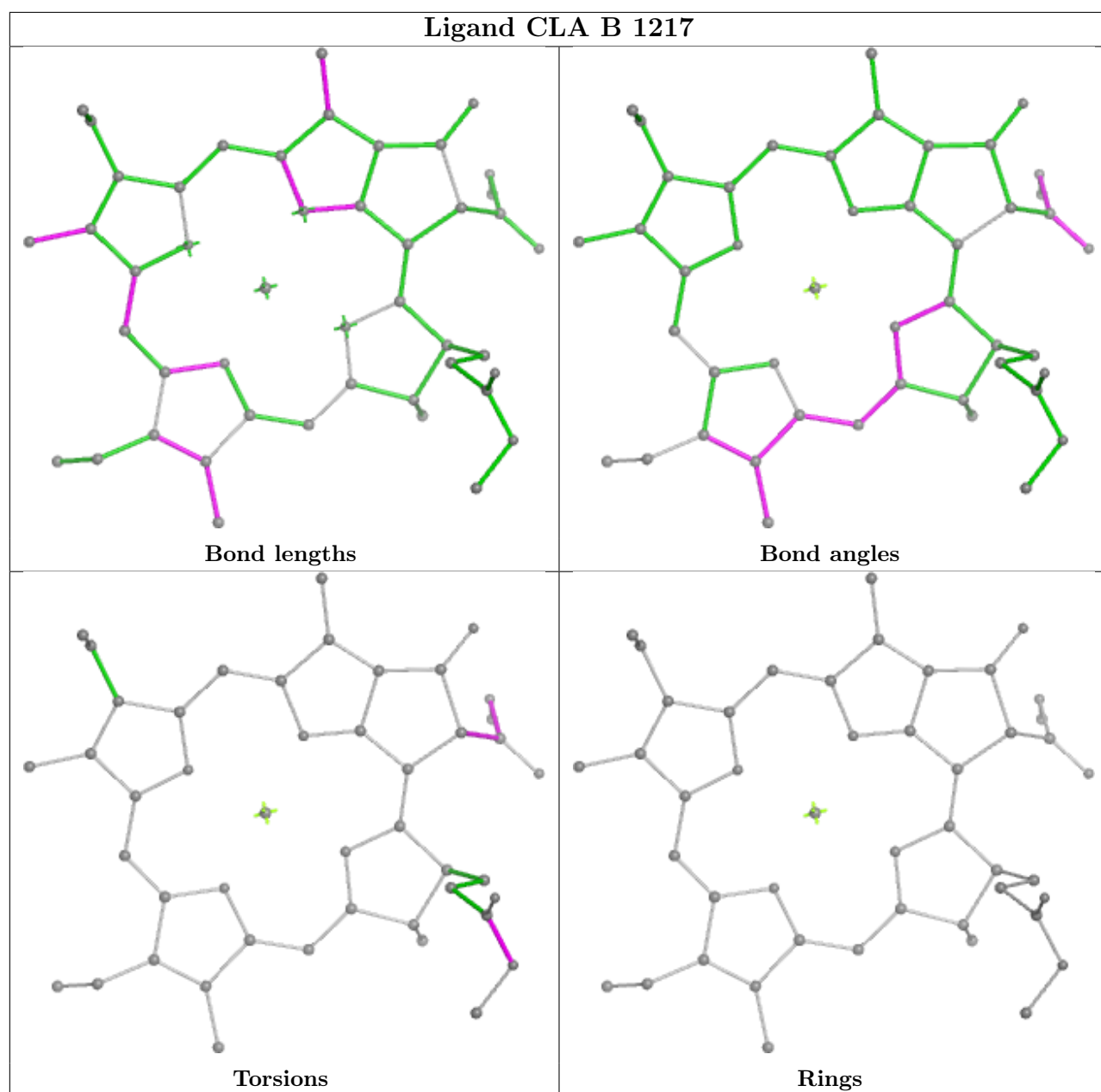
Torsions



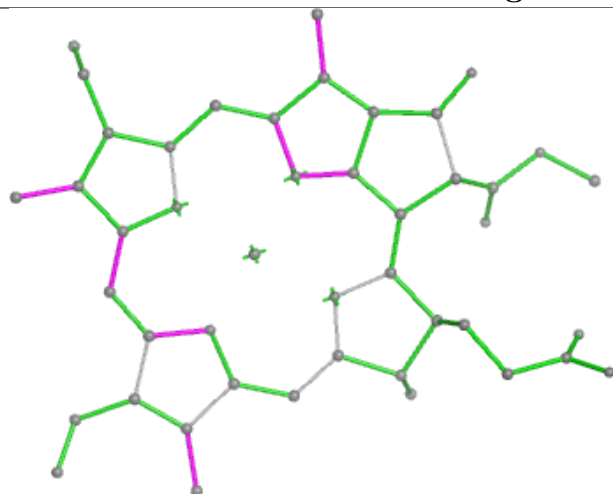
Rings



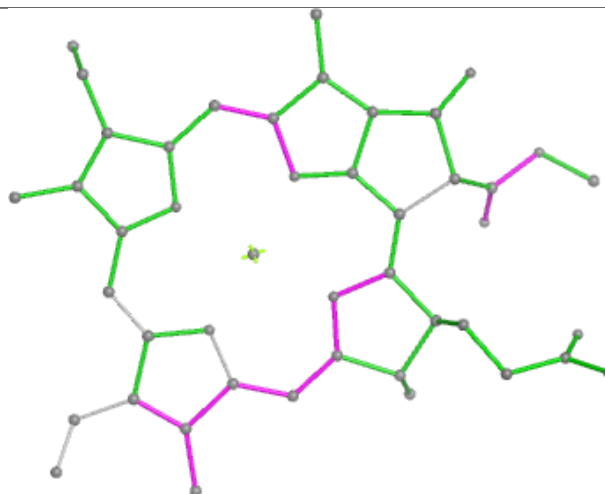




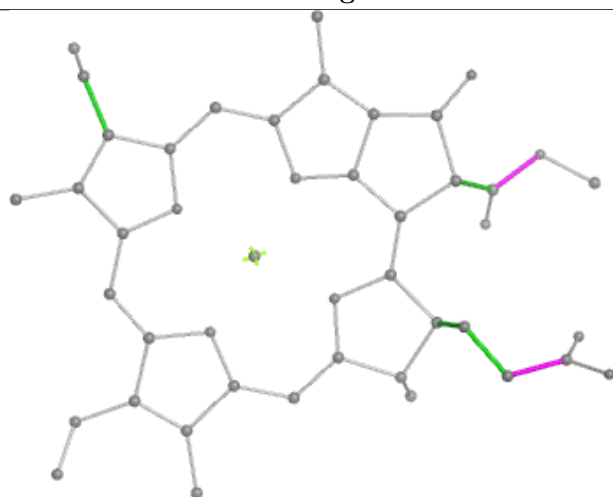
Ligand CLA B 1206



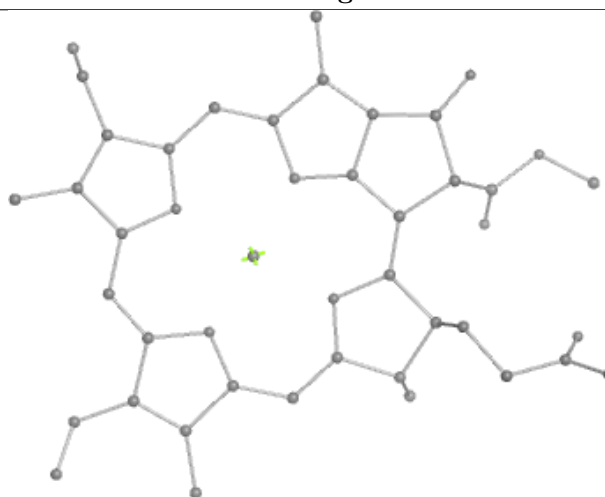
Bond lengths



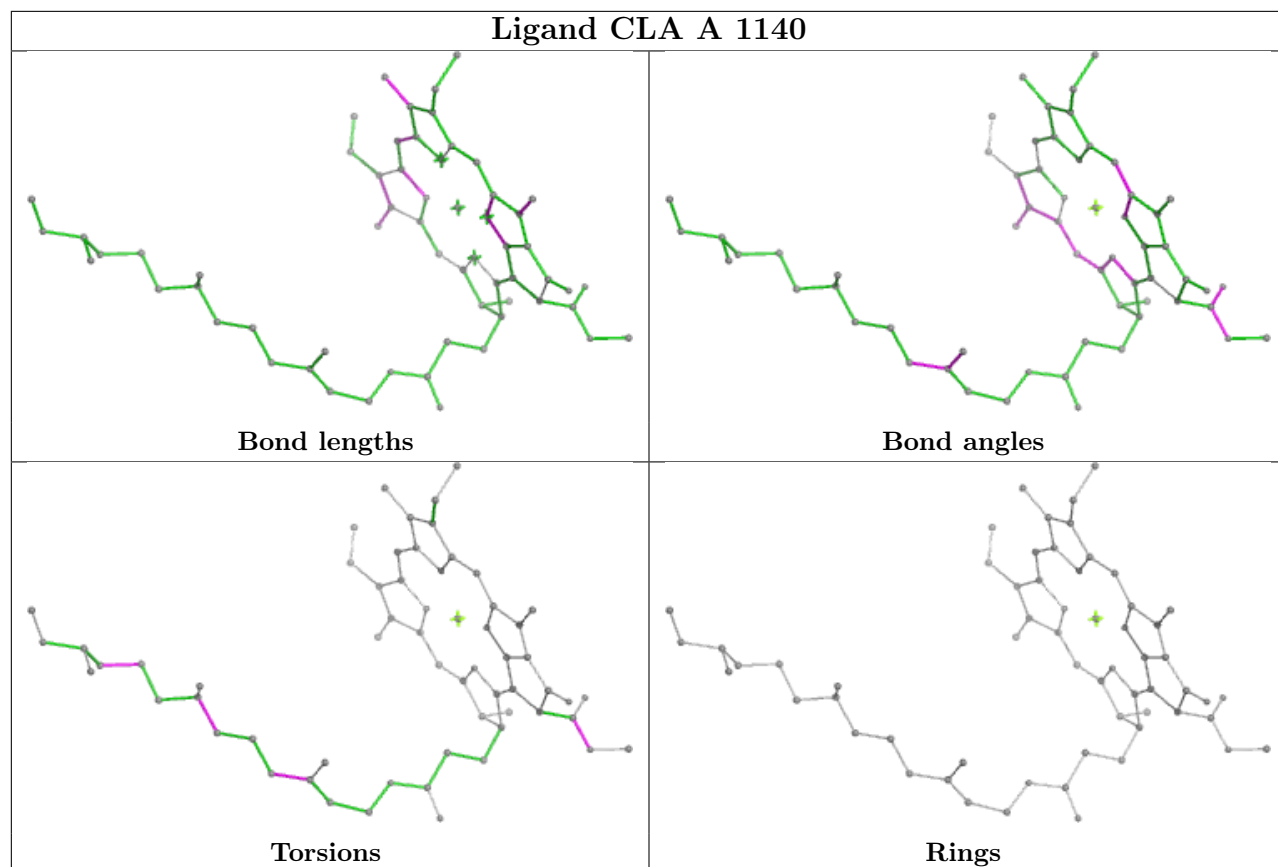
Bond angles

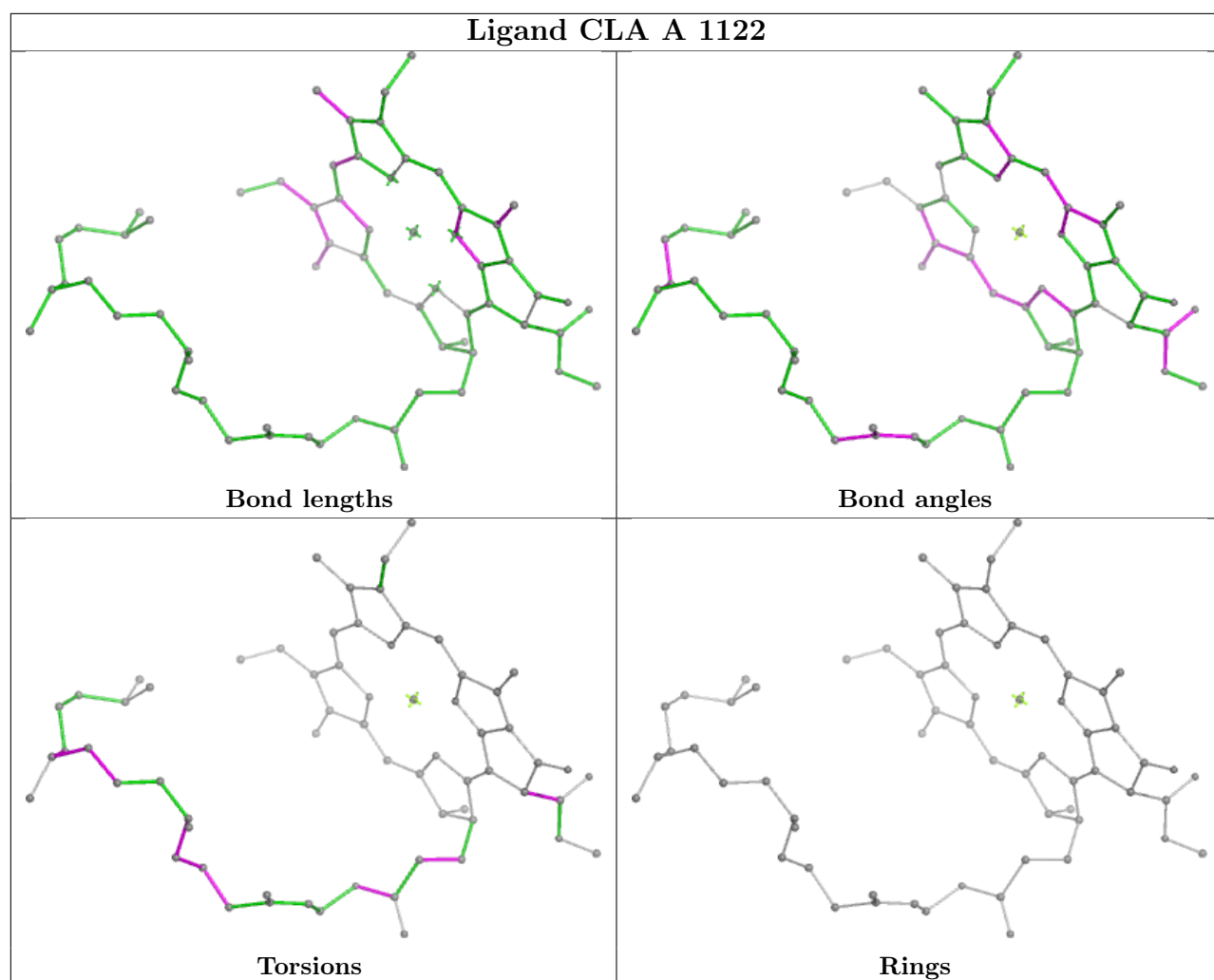


Torsions

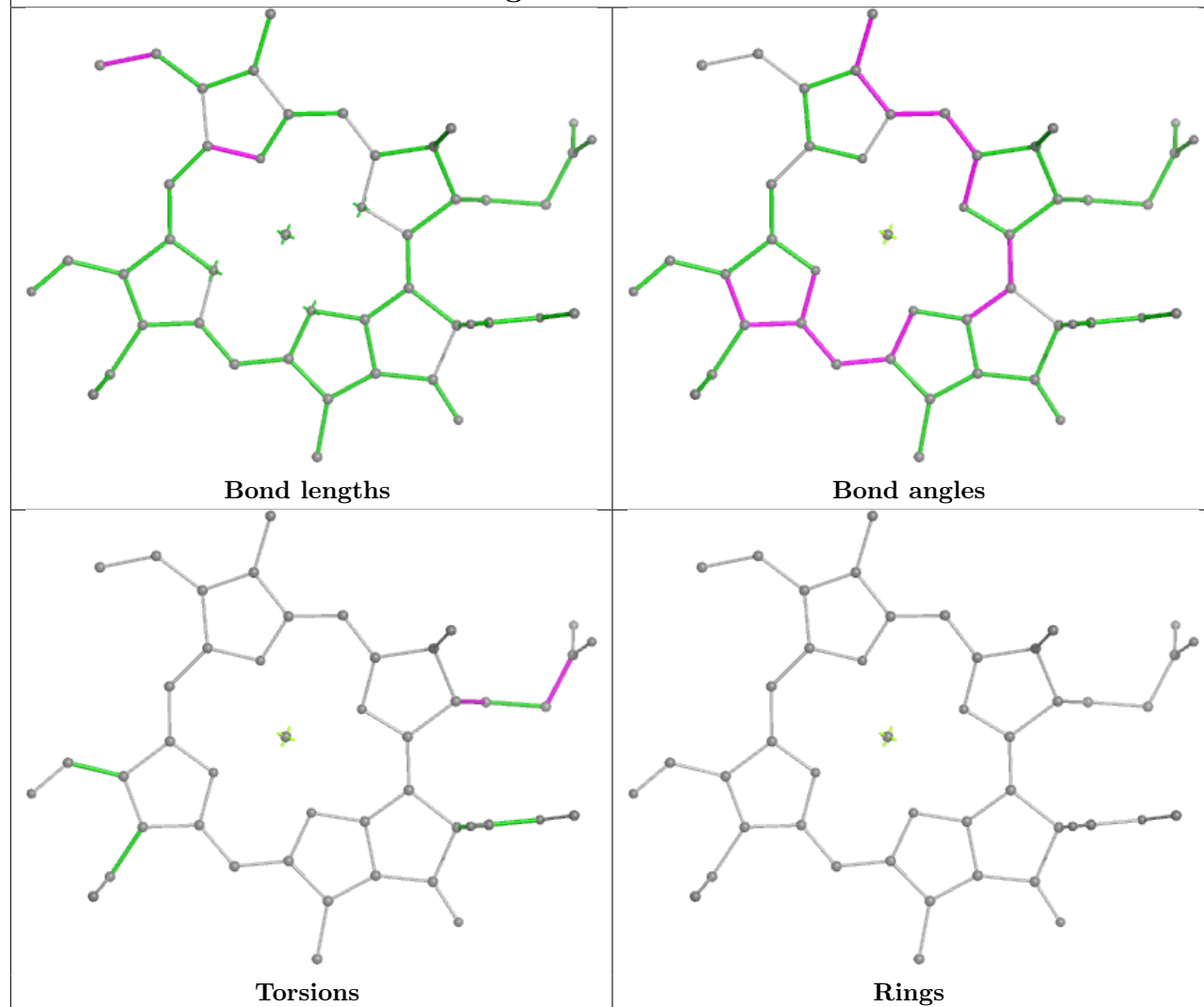


Rings

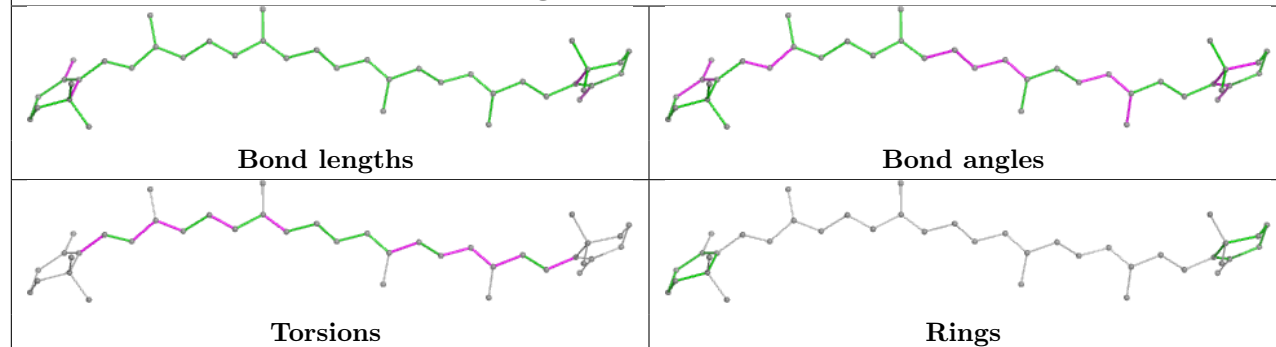




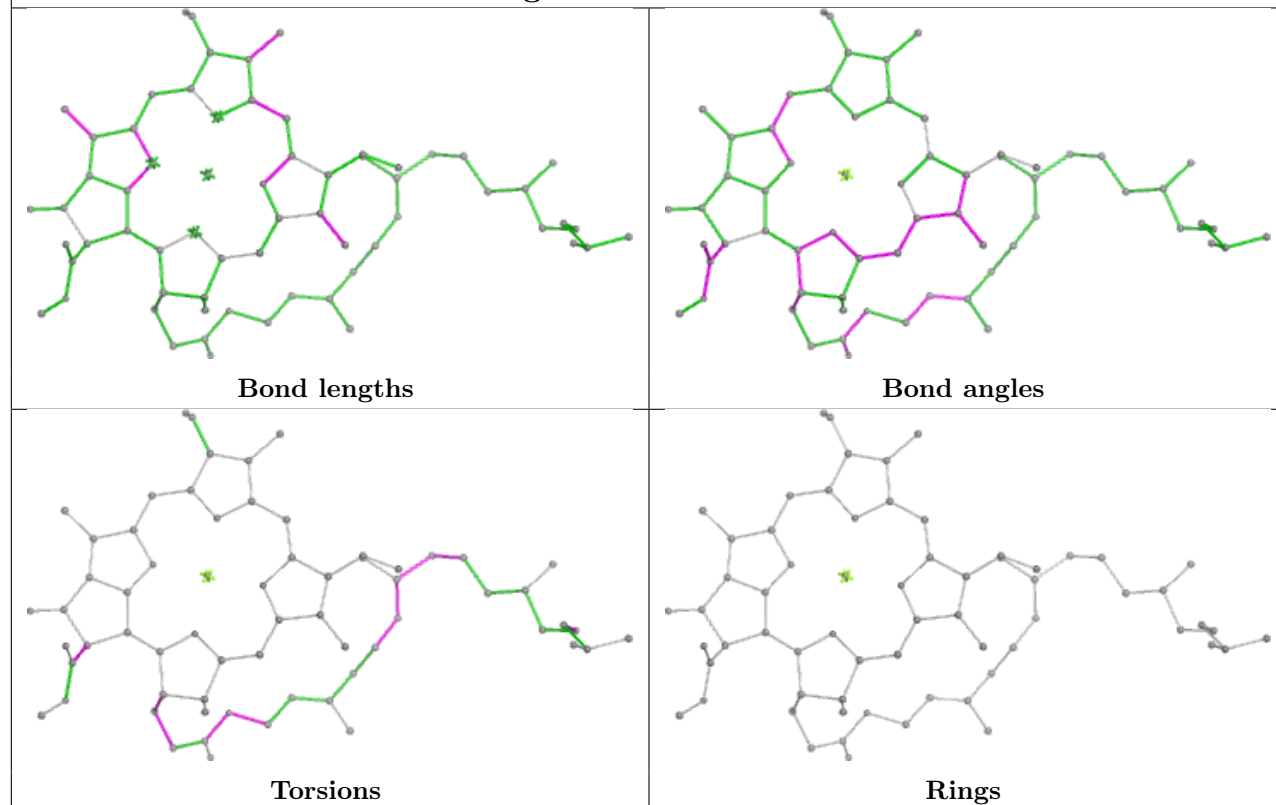
Ligand CHL 2 613



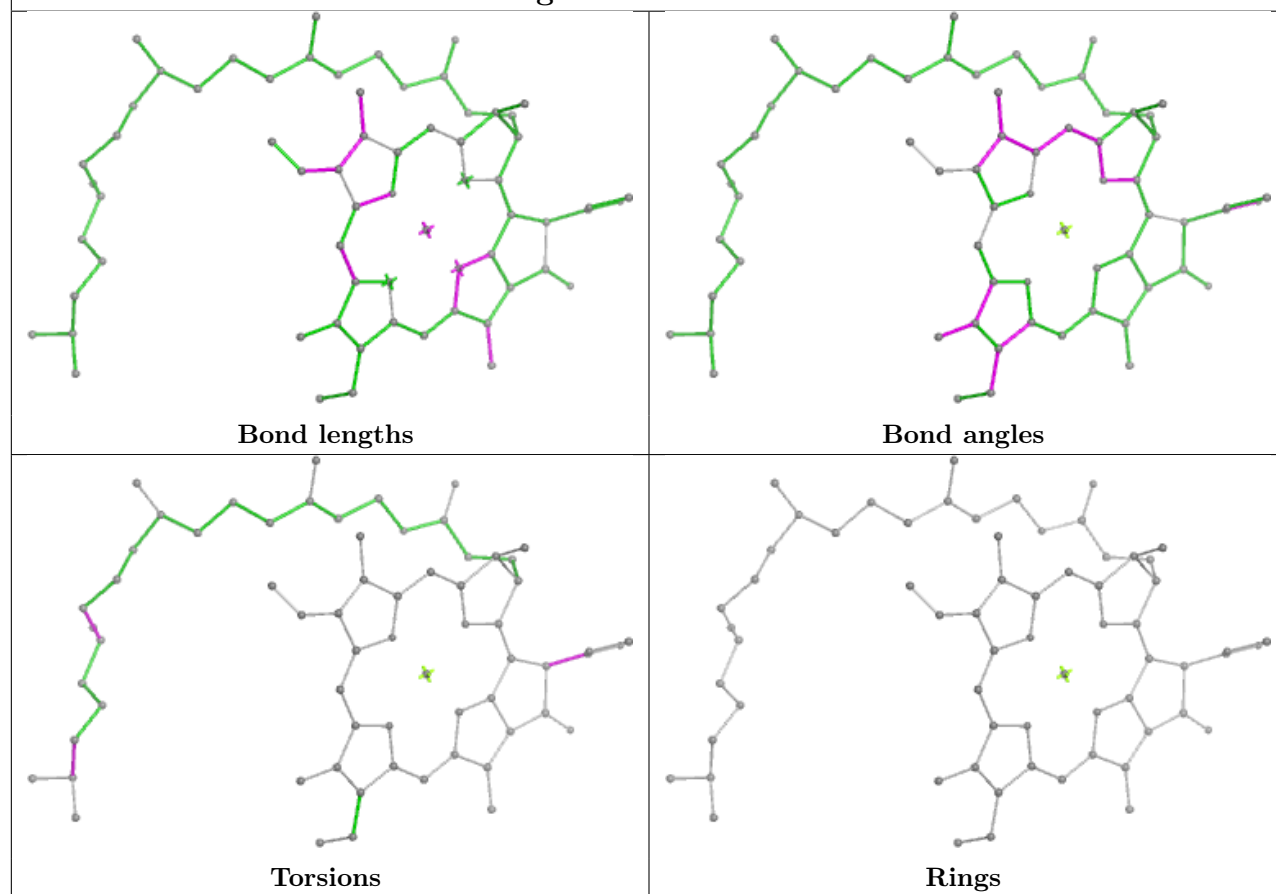
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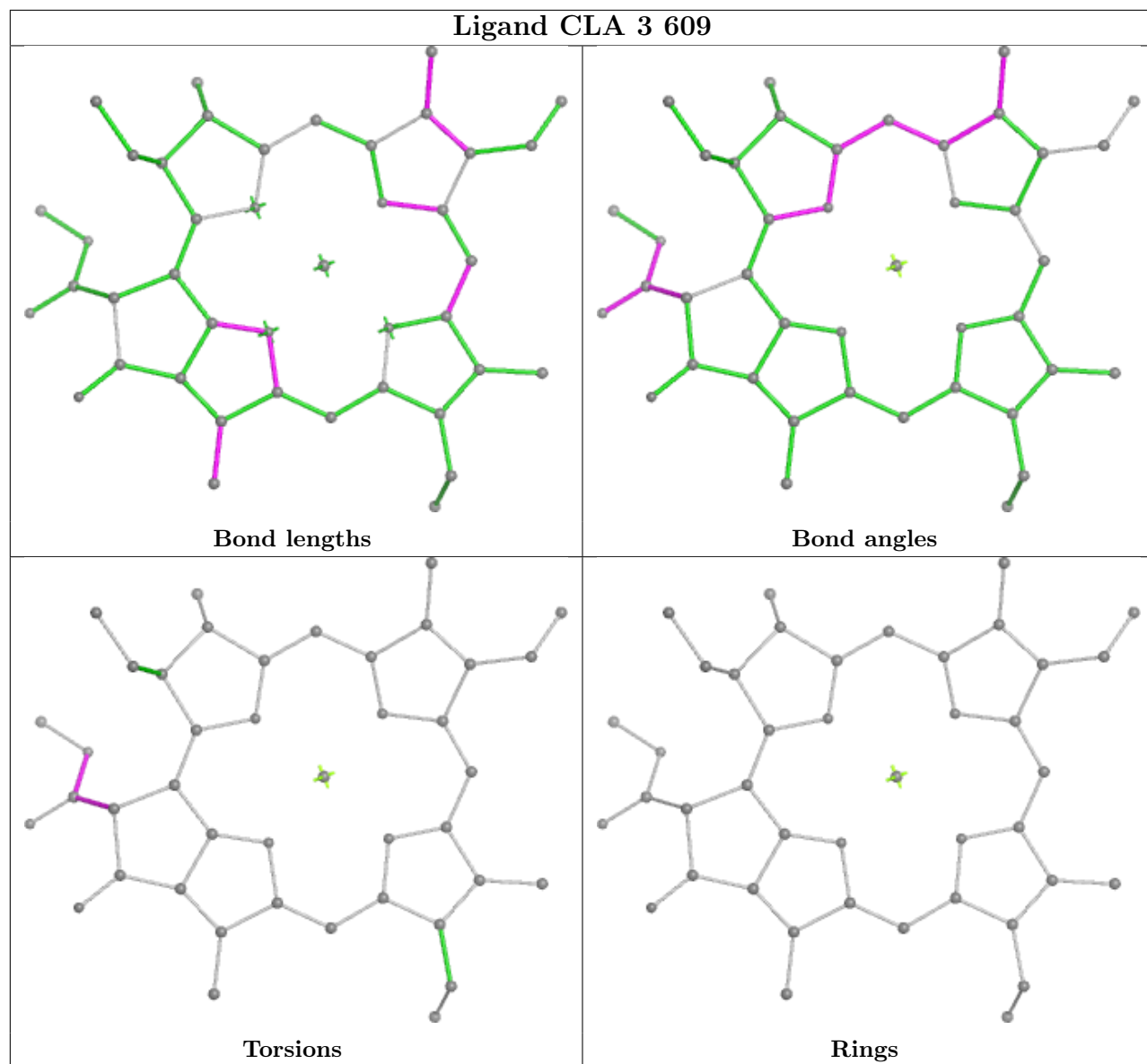


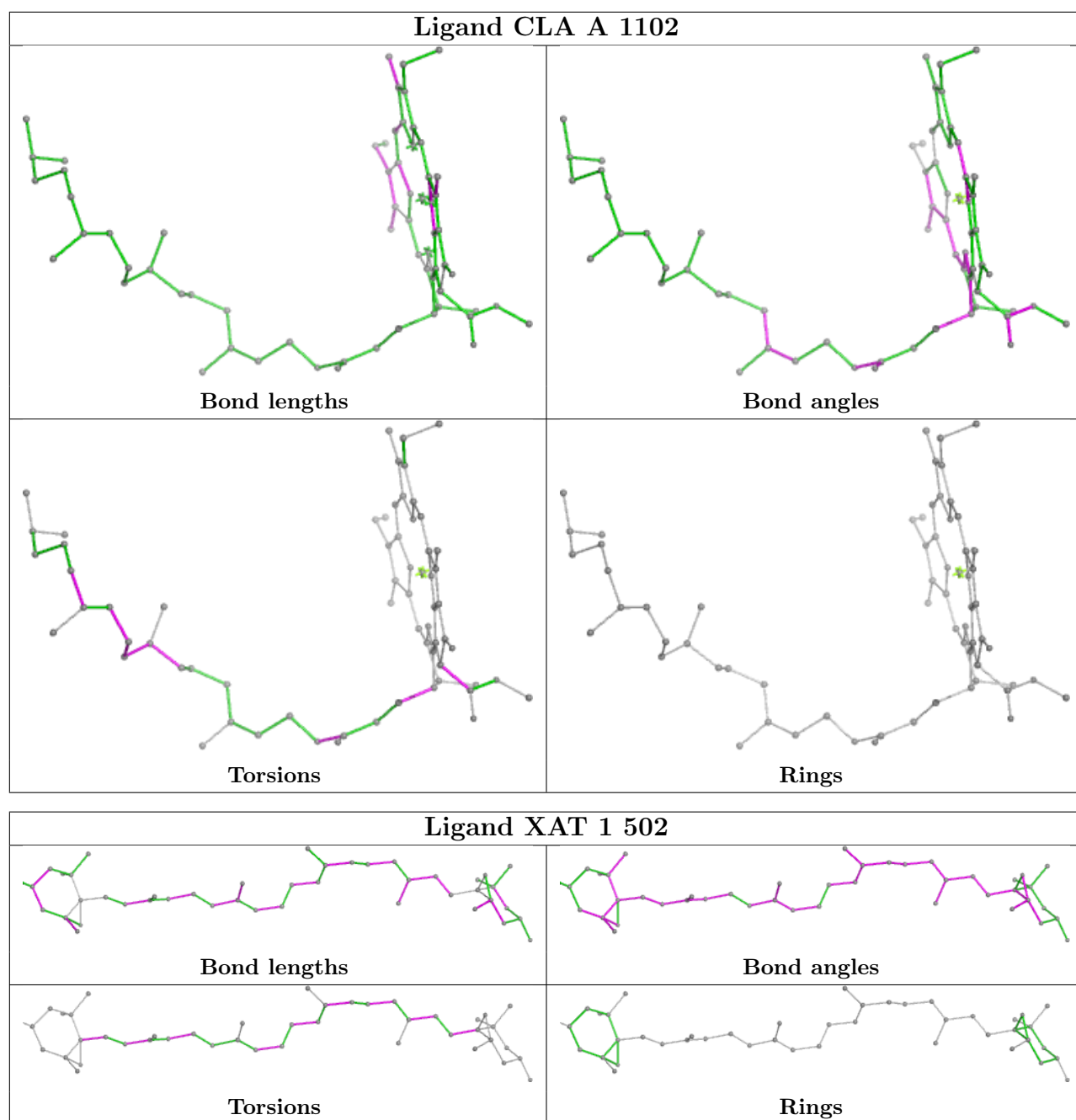
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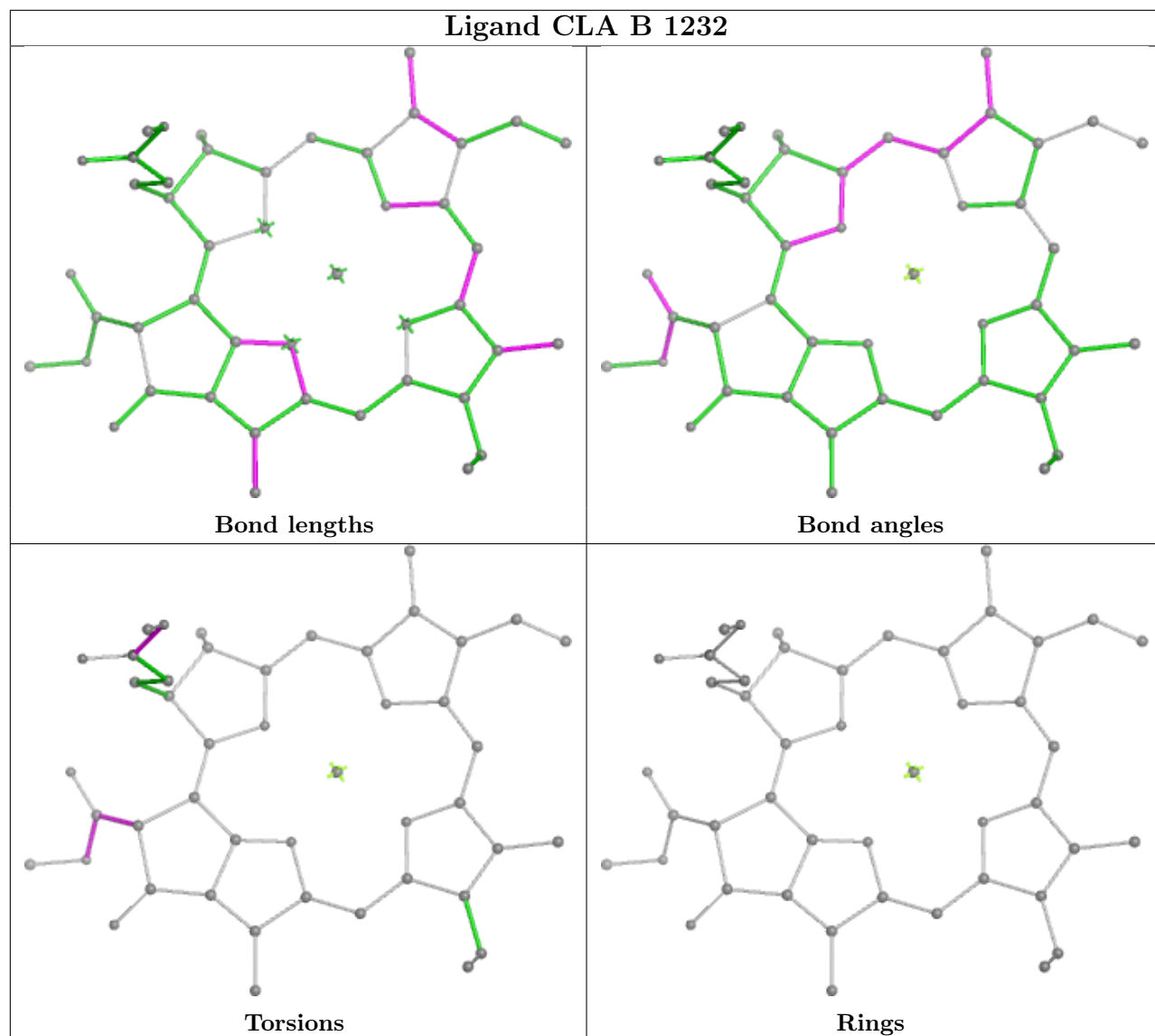


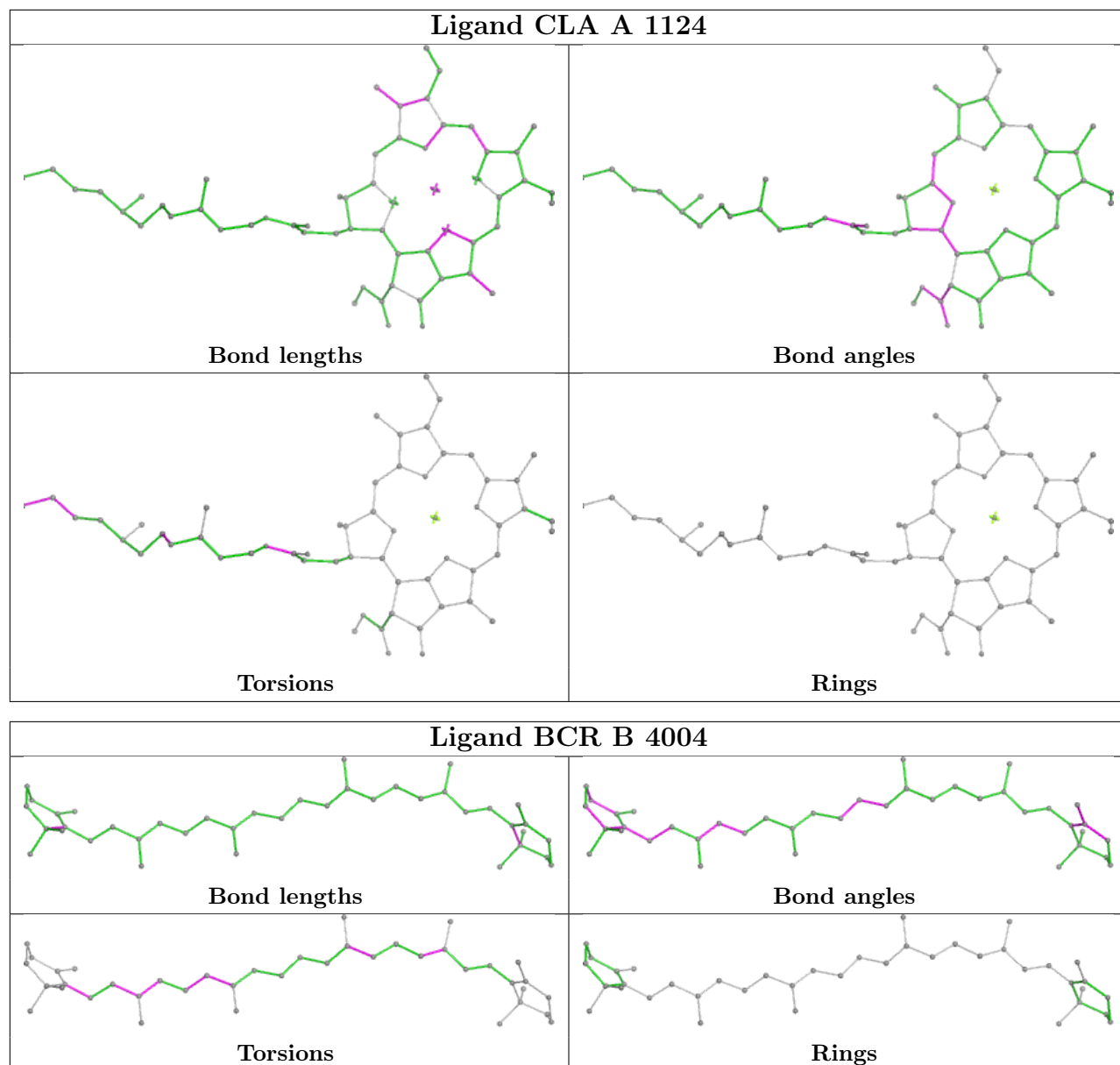
Ligand CLA 1 604

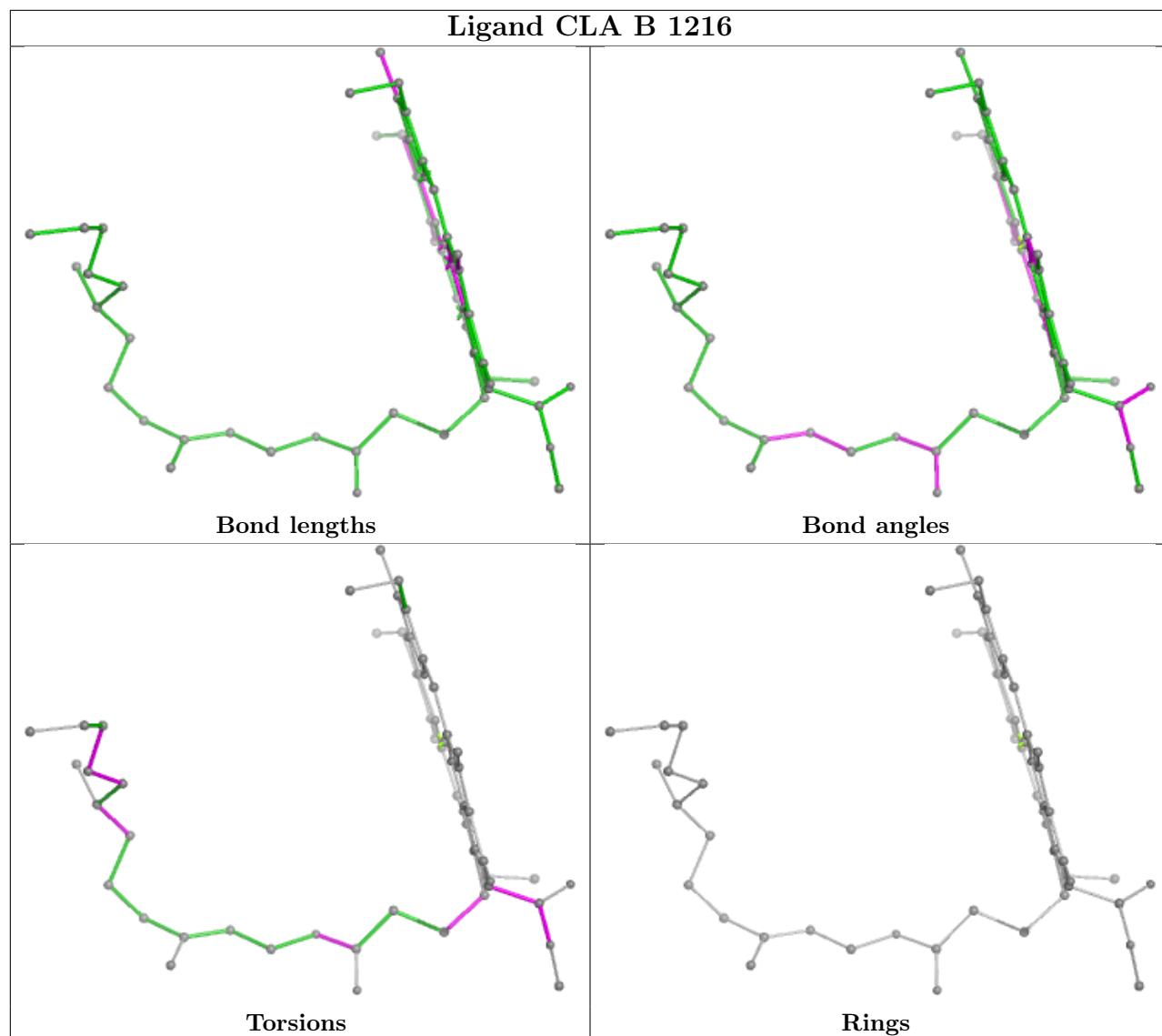




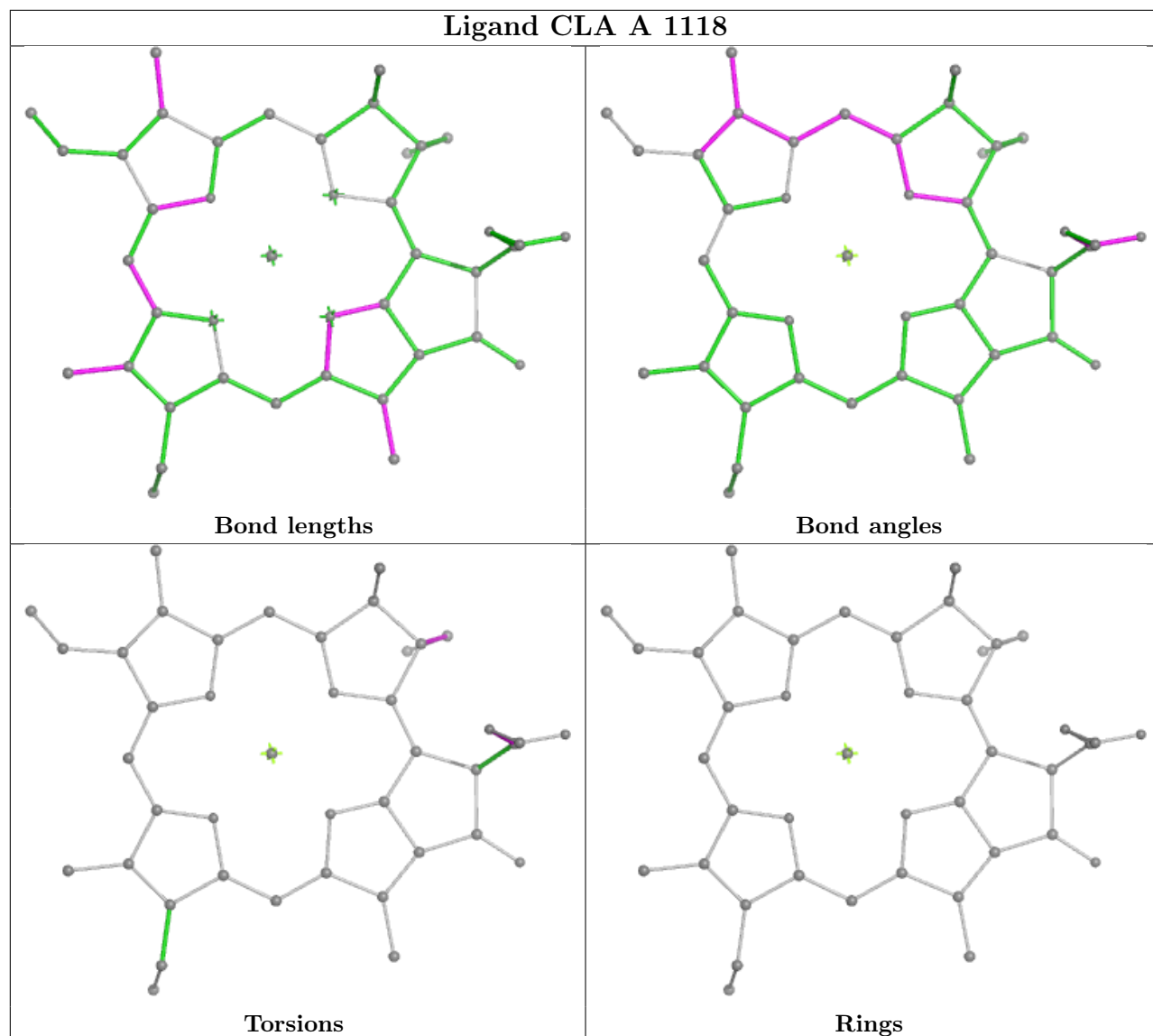




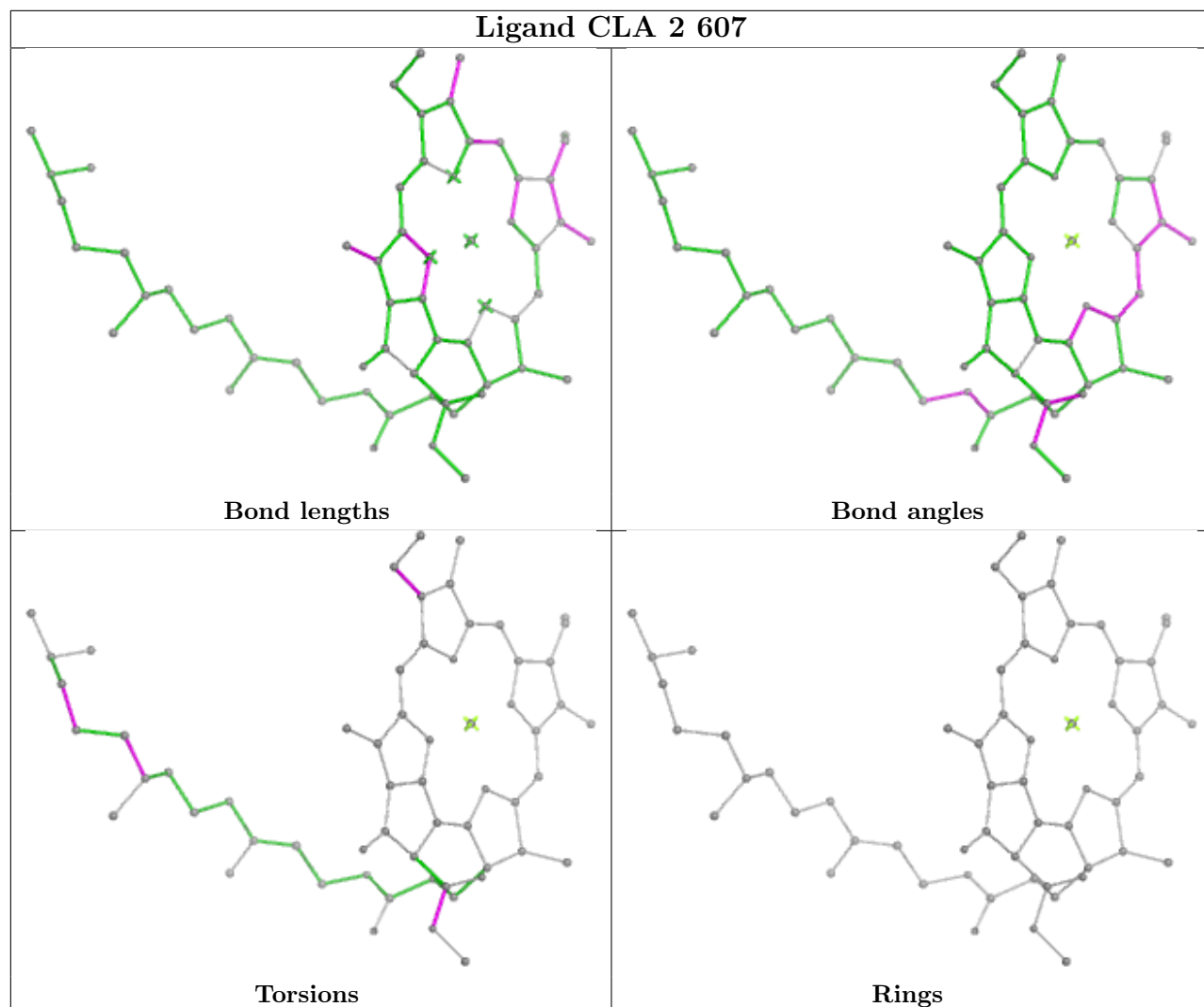




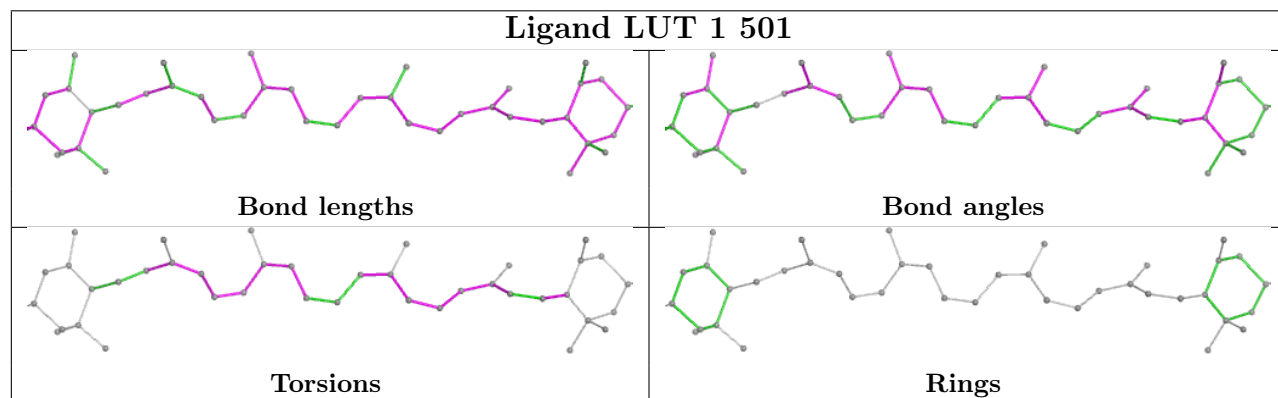
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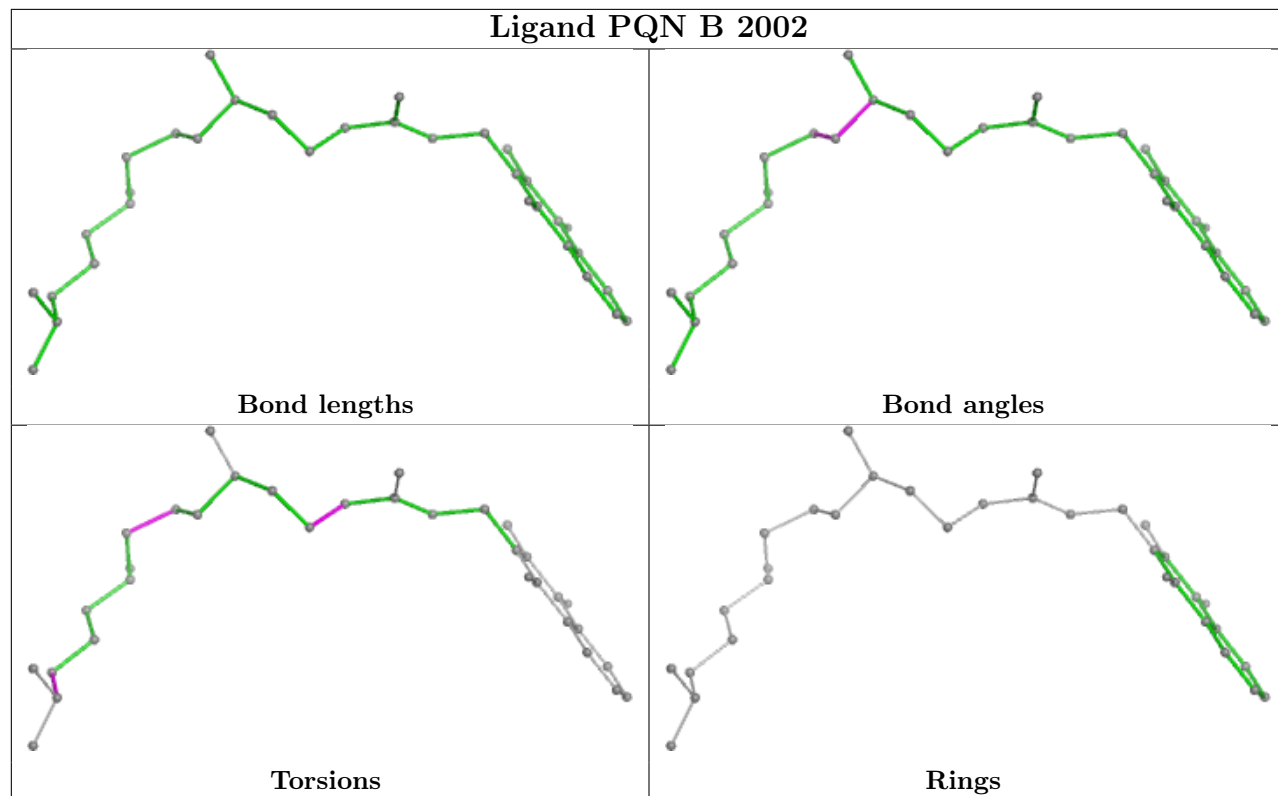
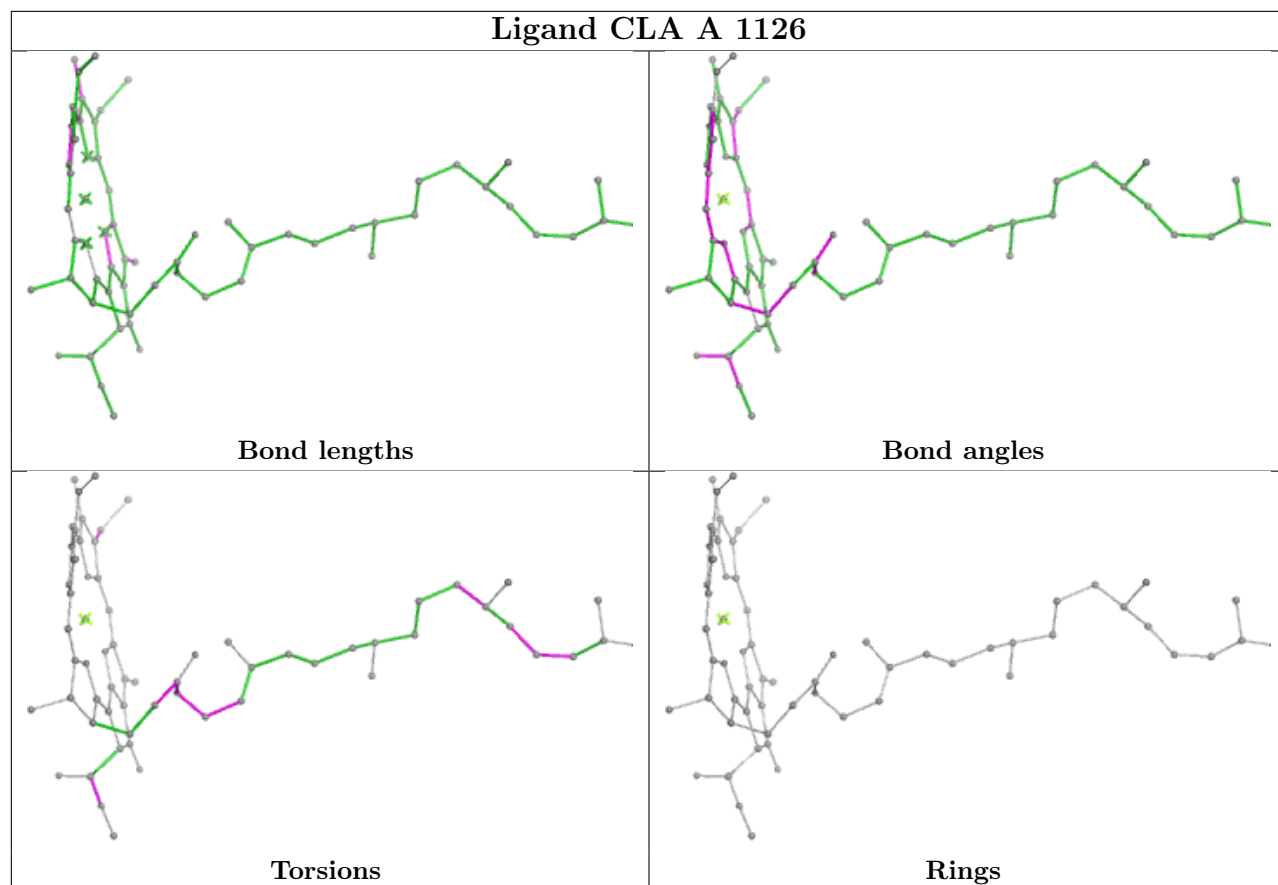


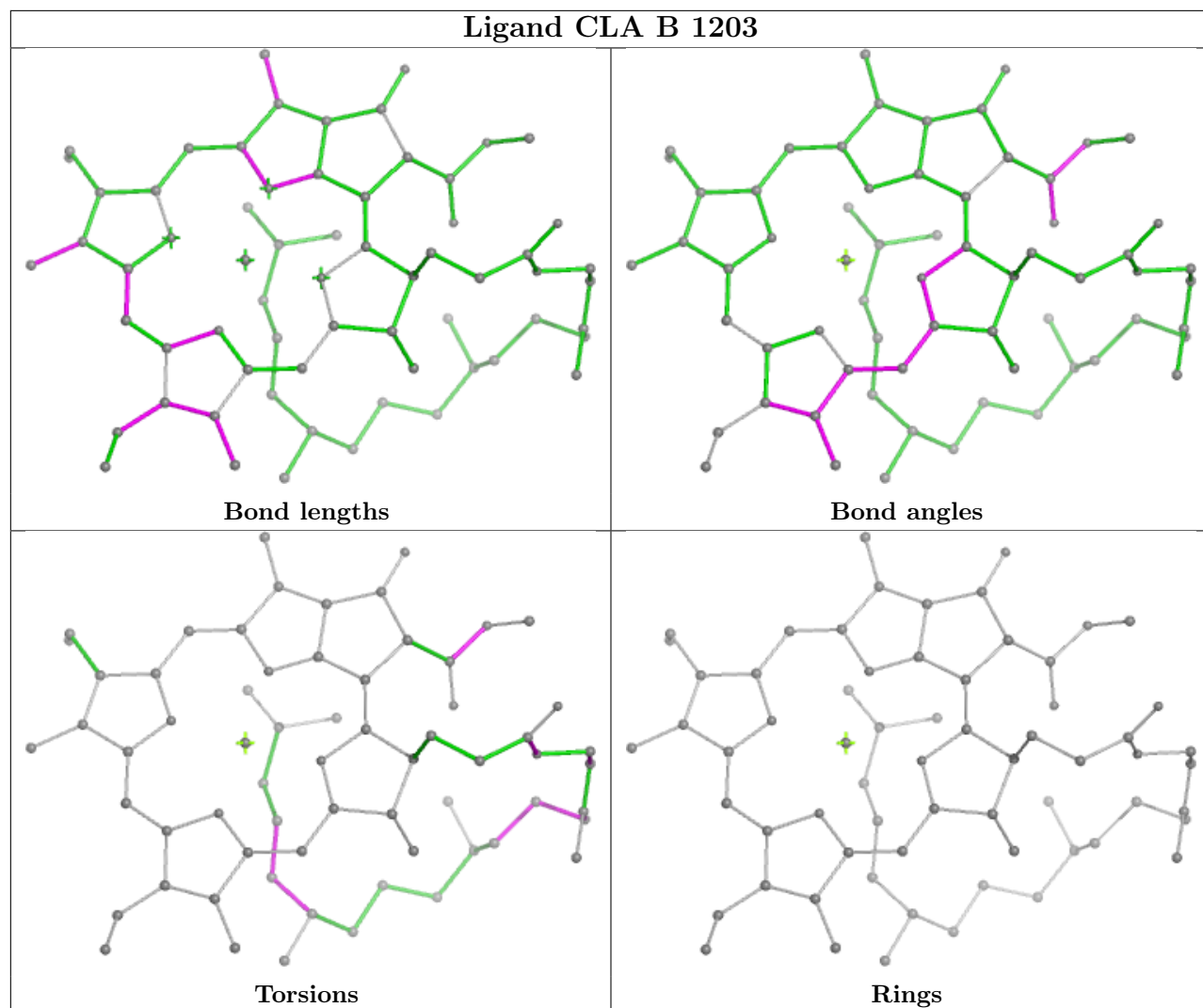
Ligand CLA 2 607



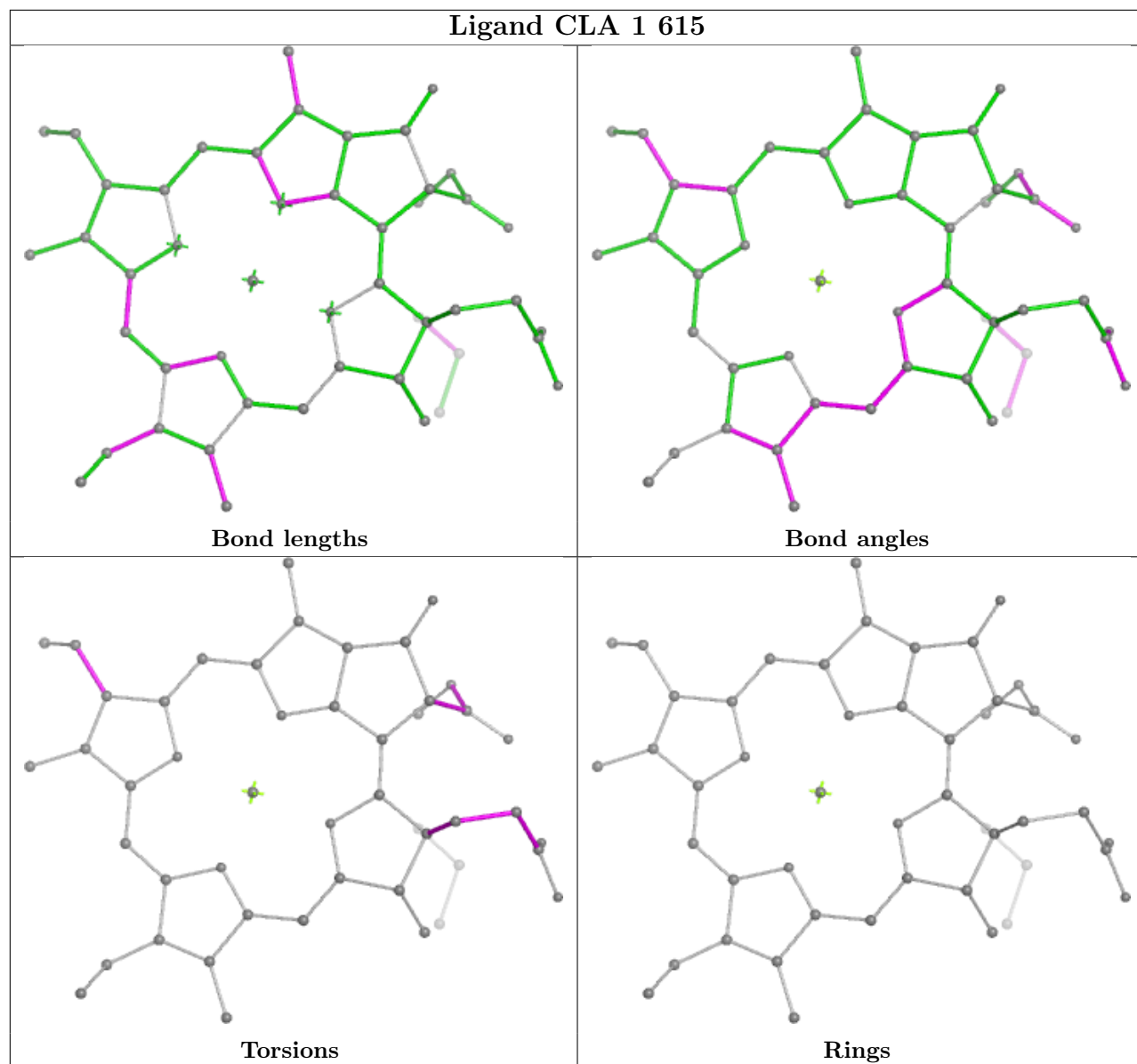
Ligand LUT 1 501



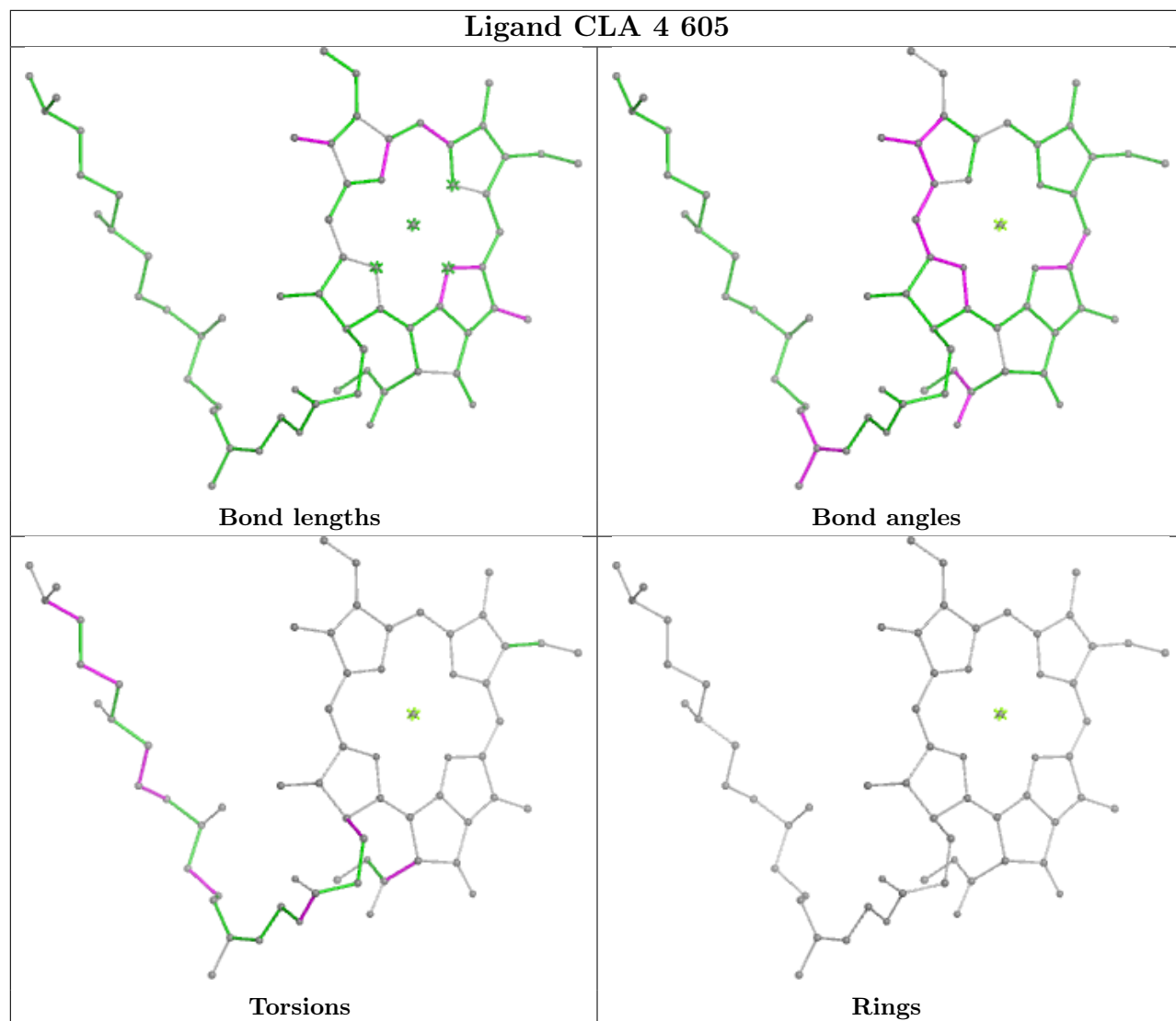




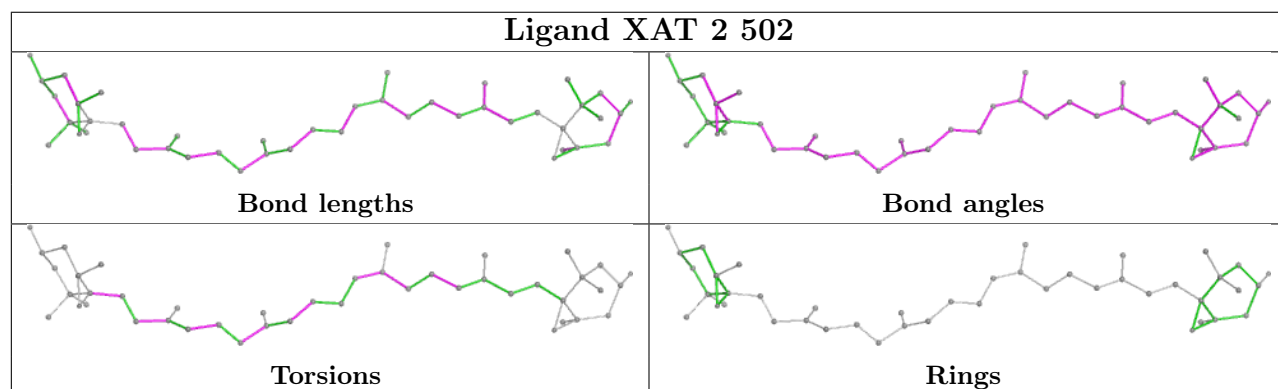
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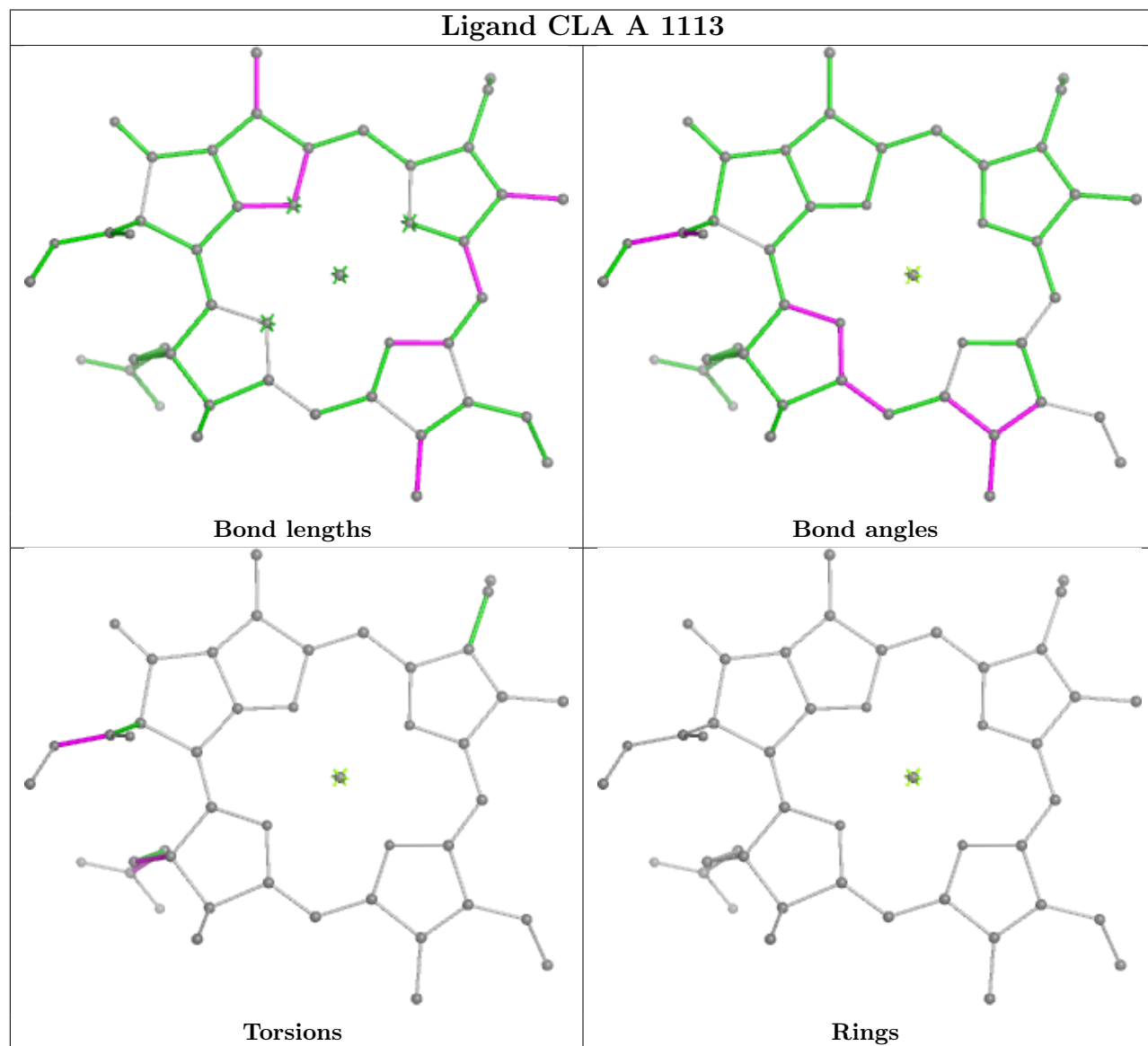
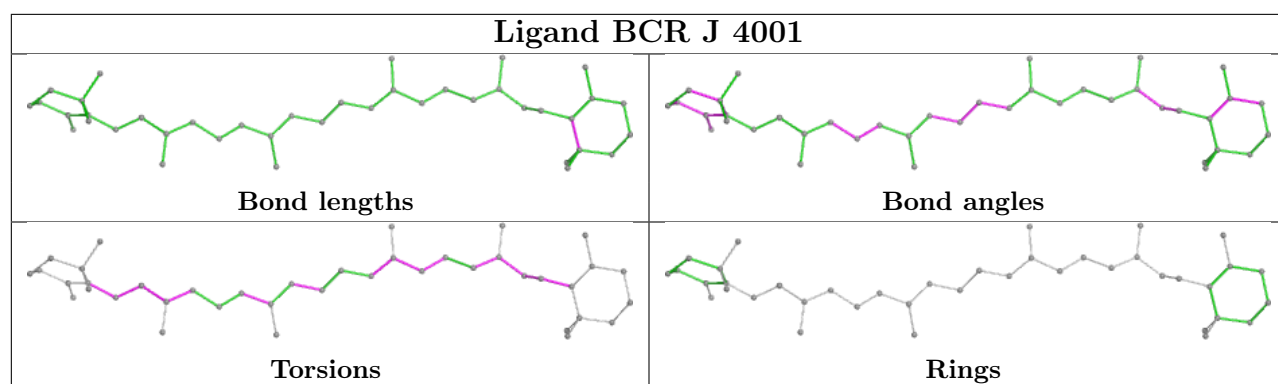


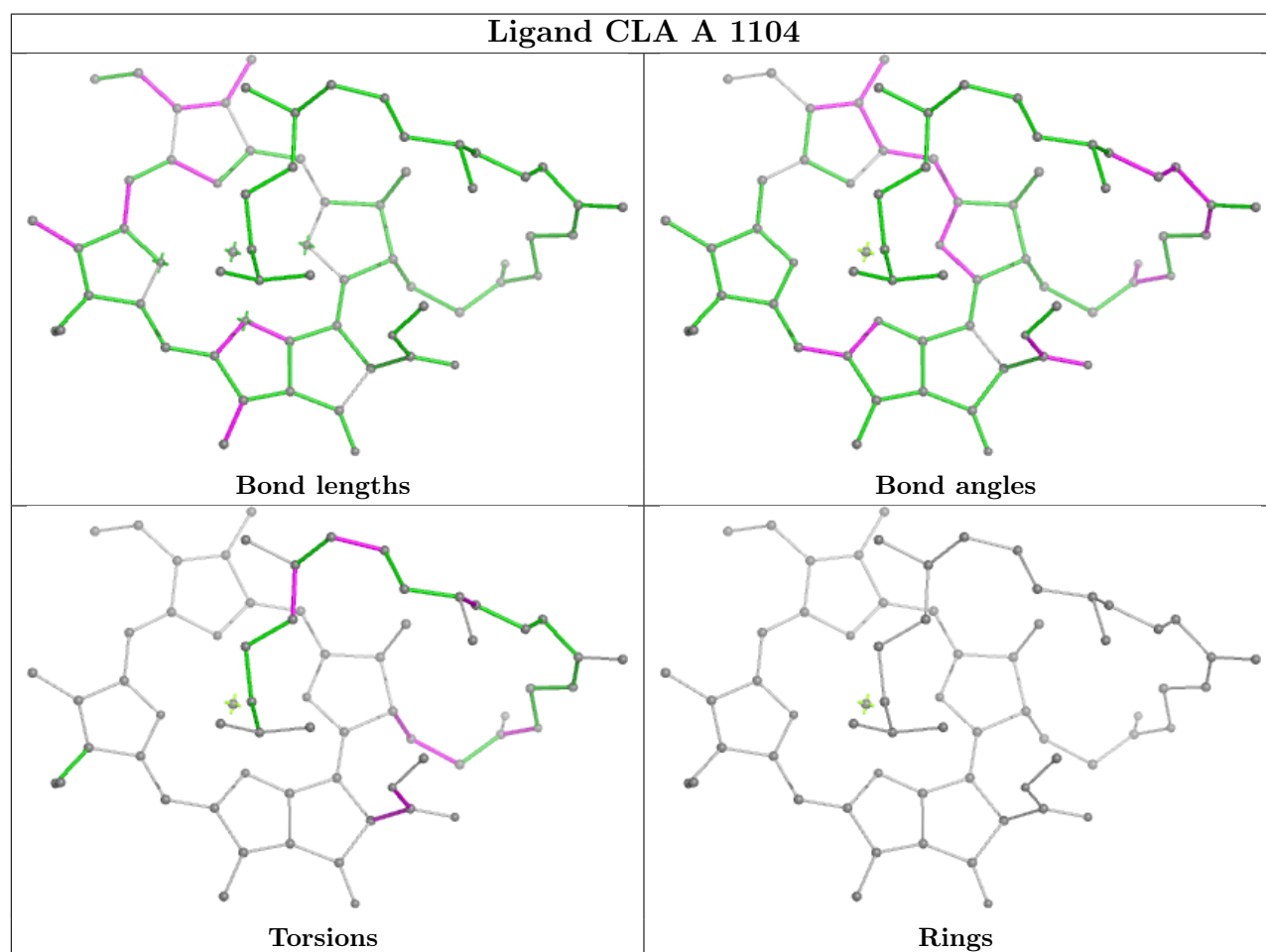
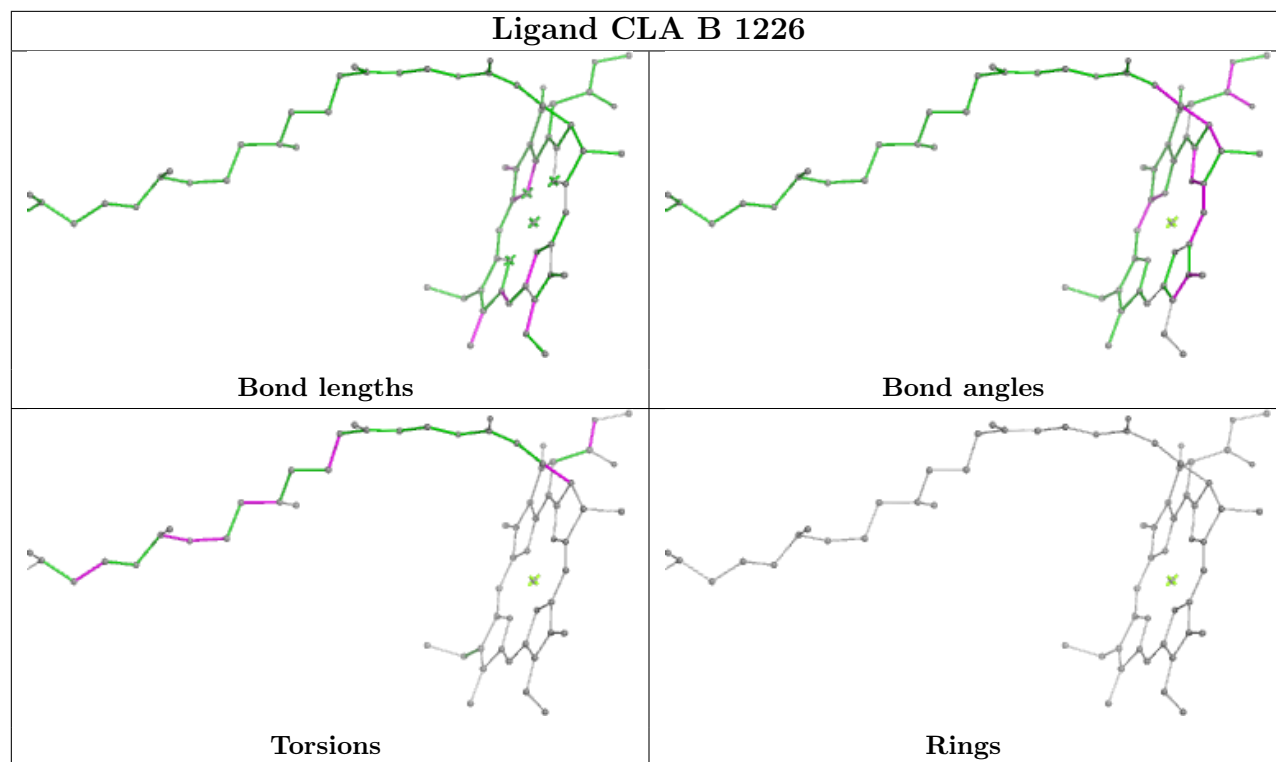
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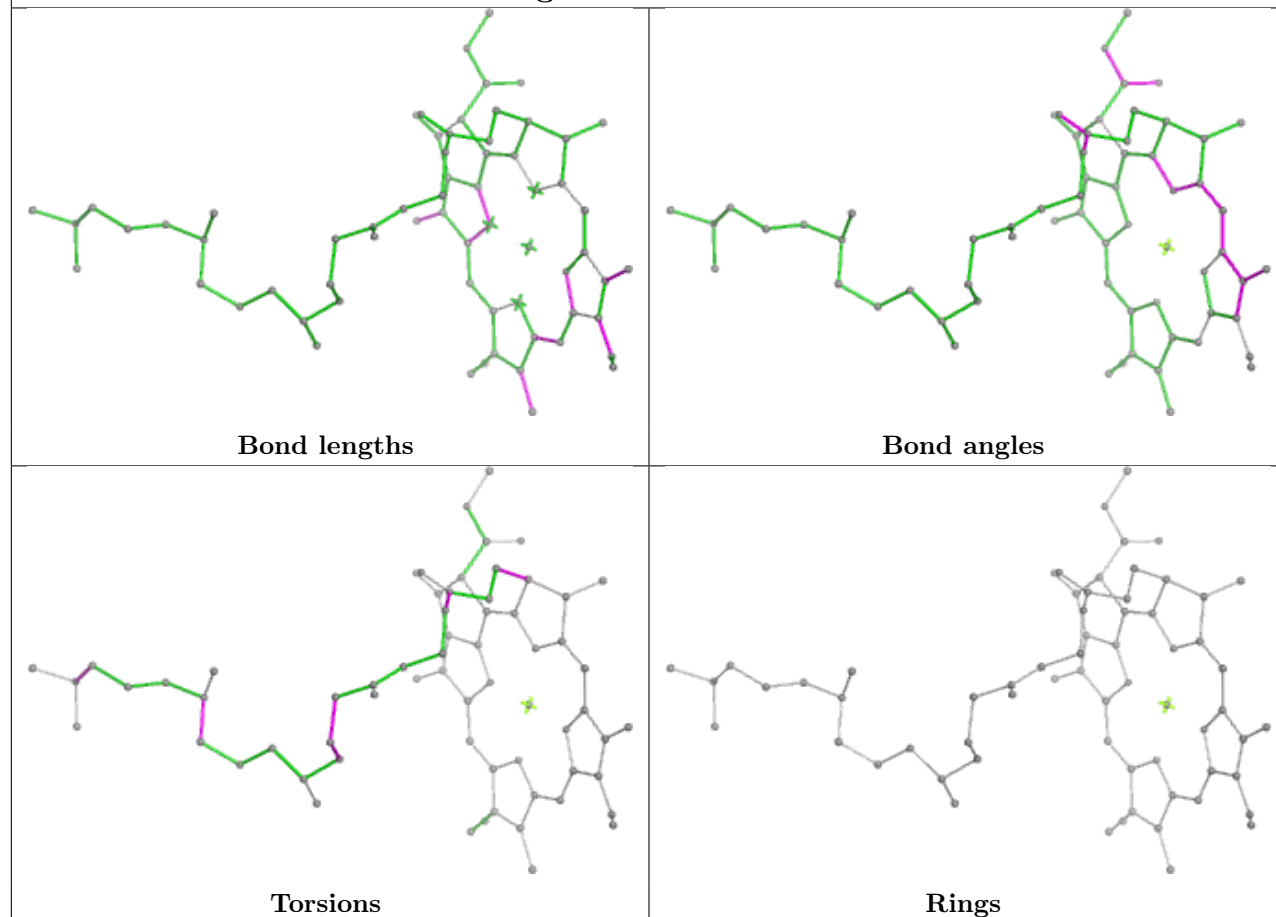
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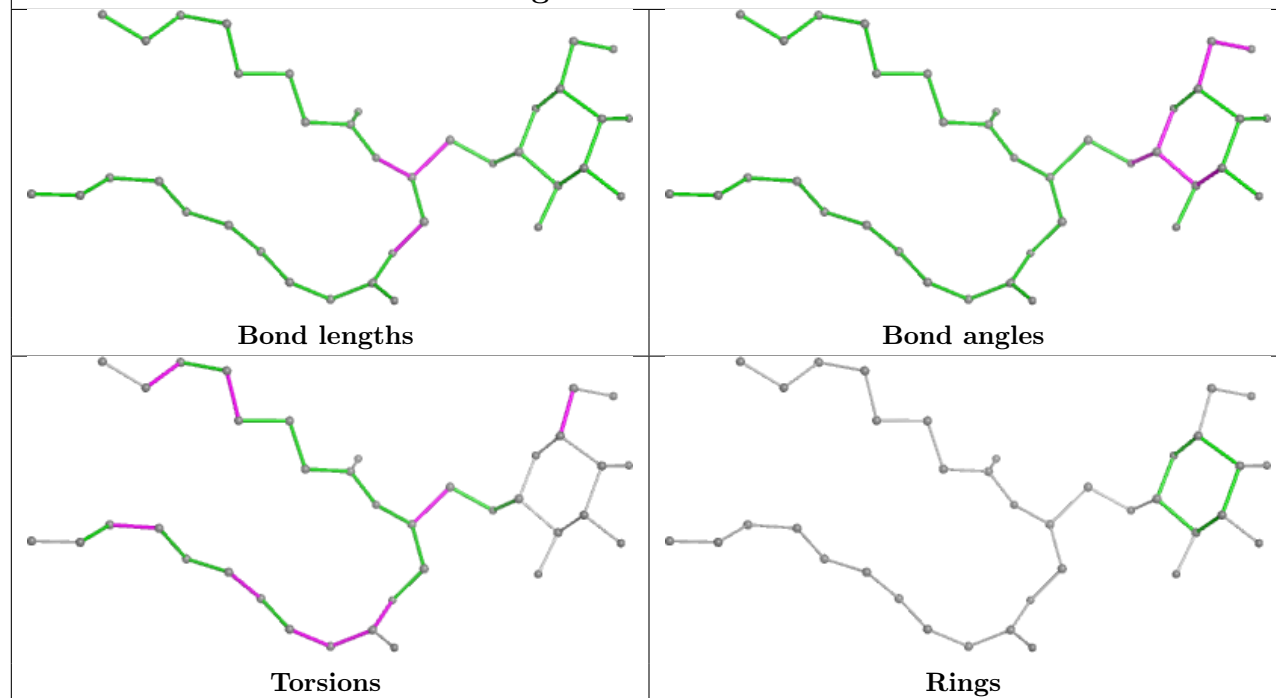




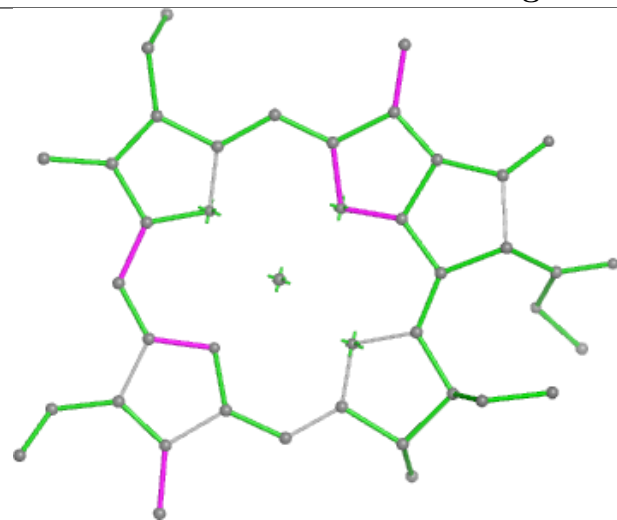
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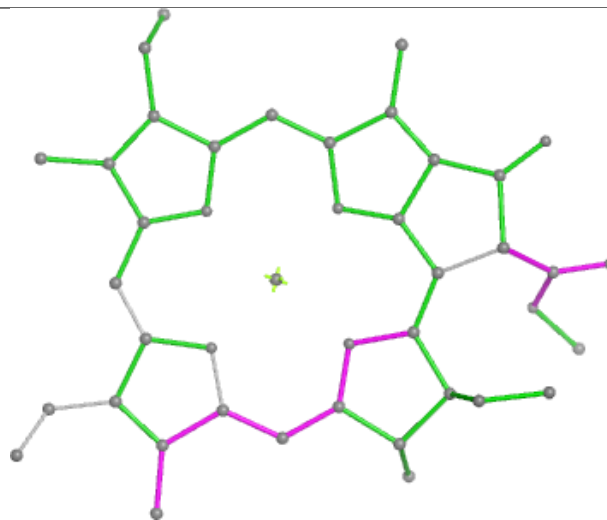
Ligand LMG 4 801



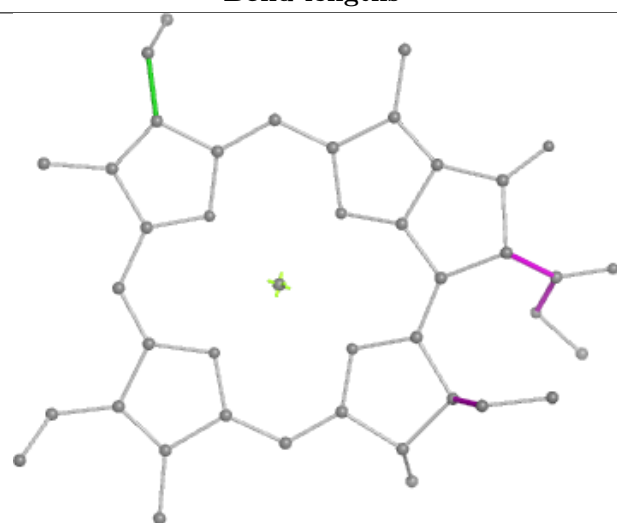
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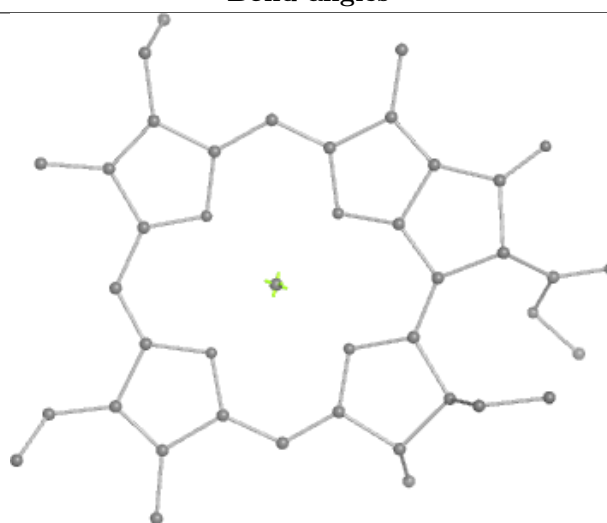
Bond lengths



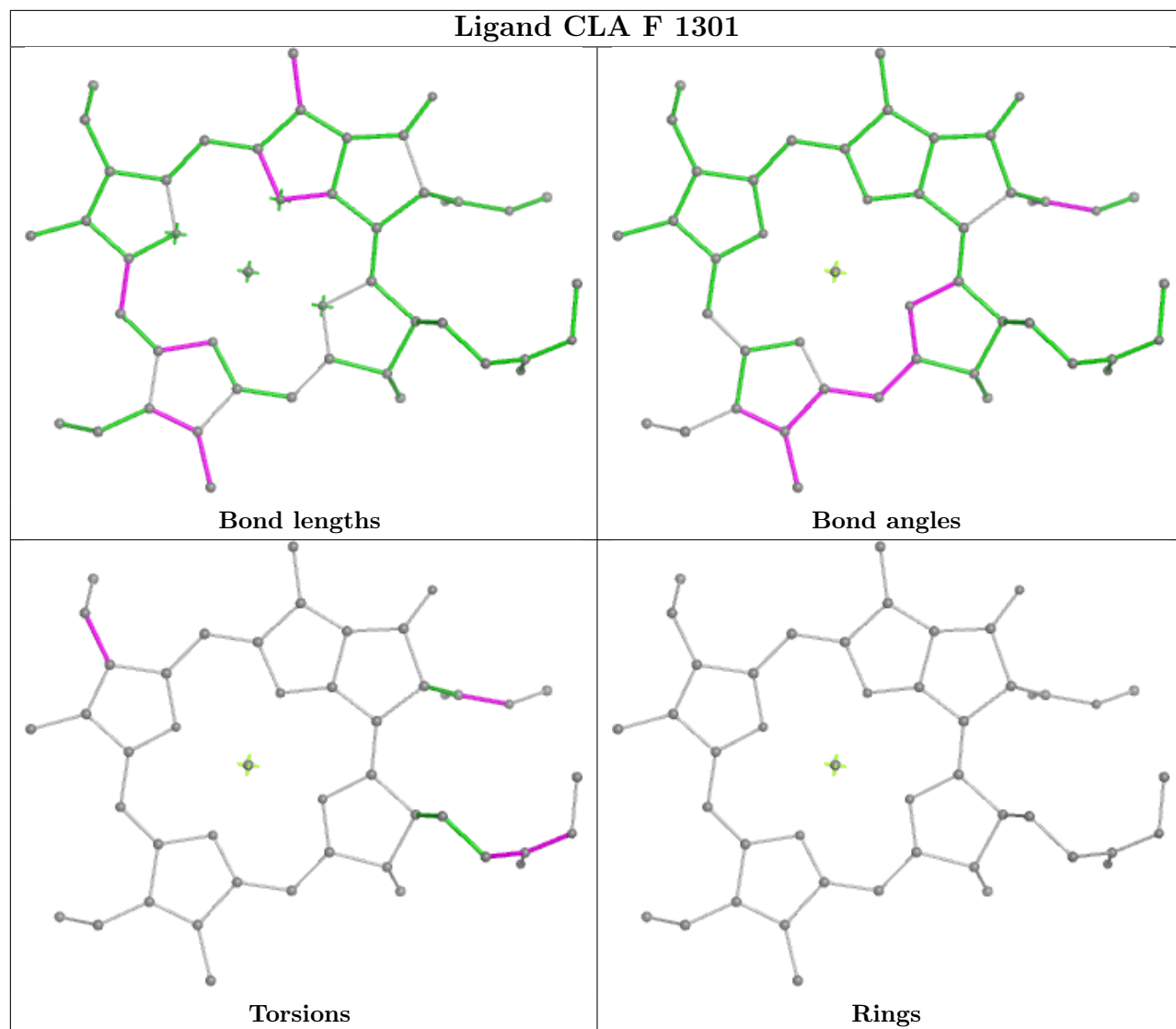
Bond angles

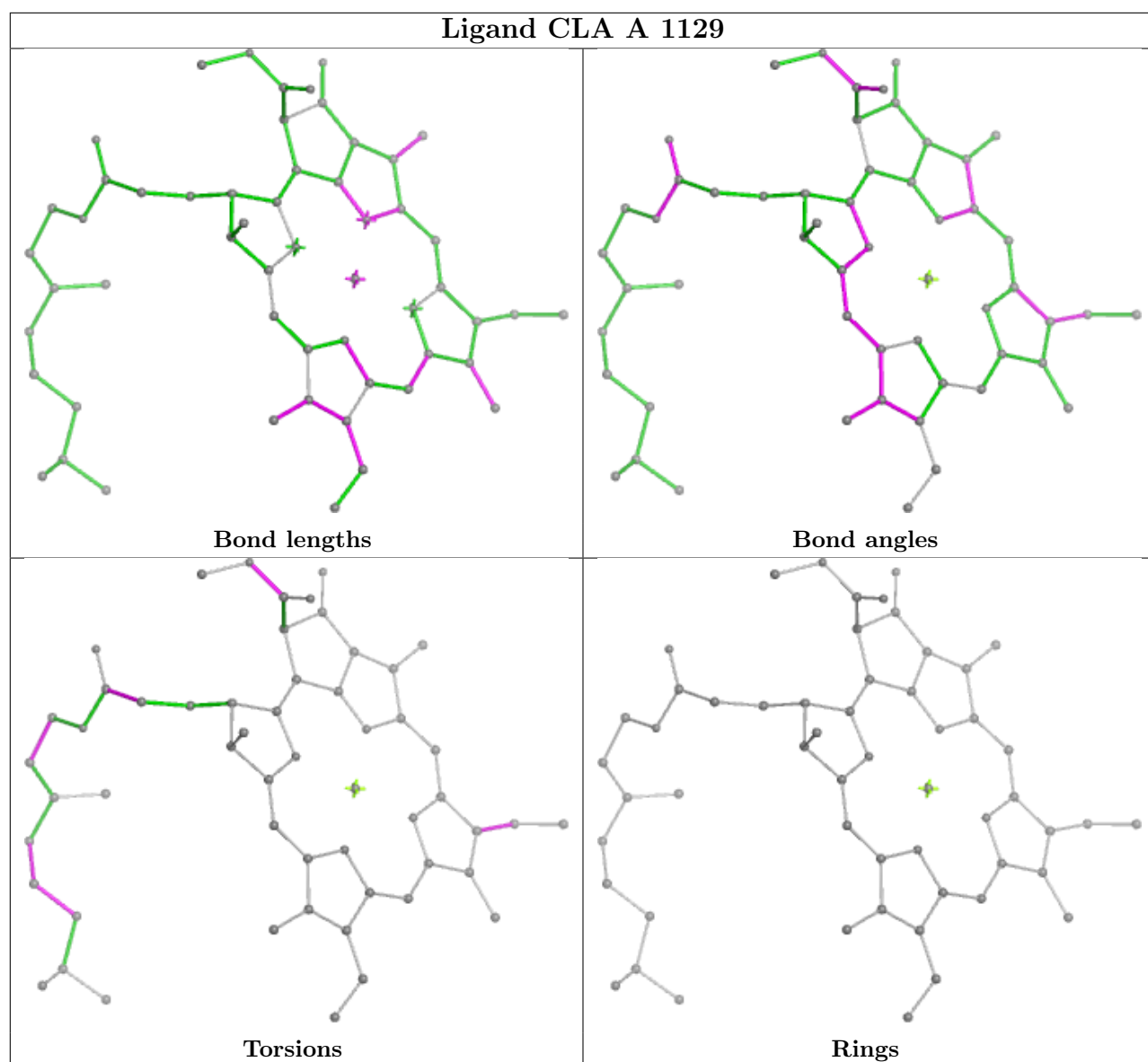


Torsions

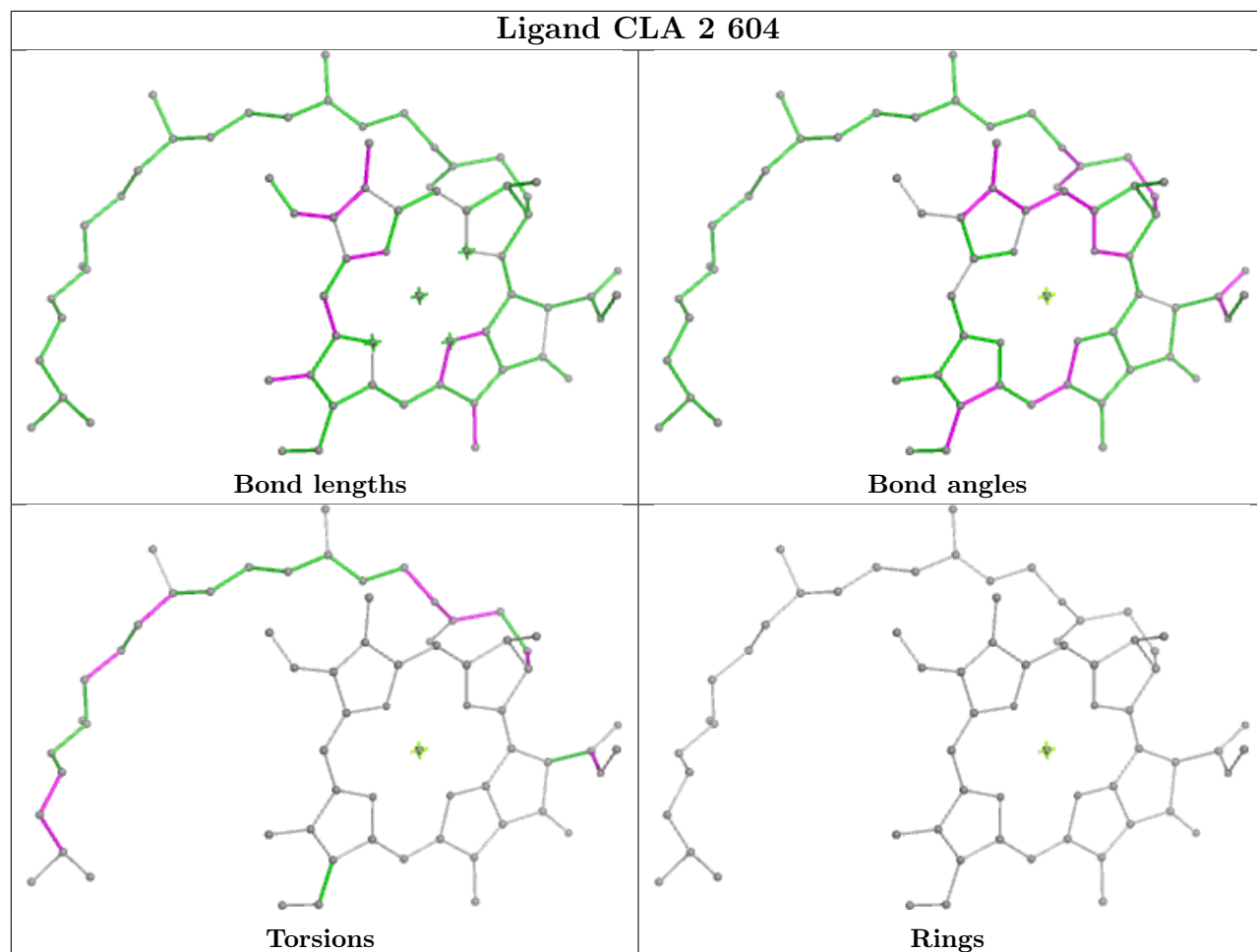


Rings

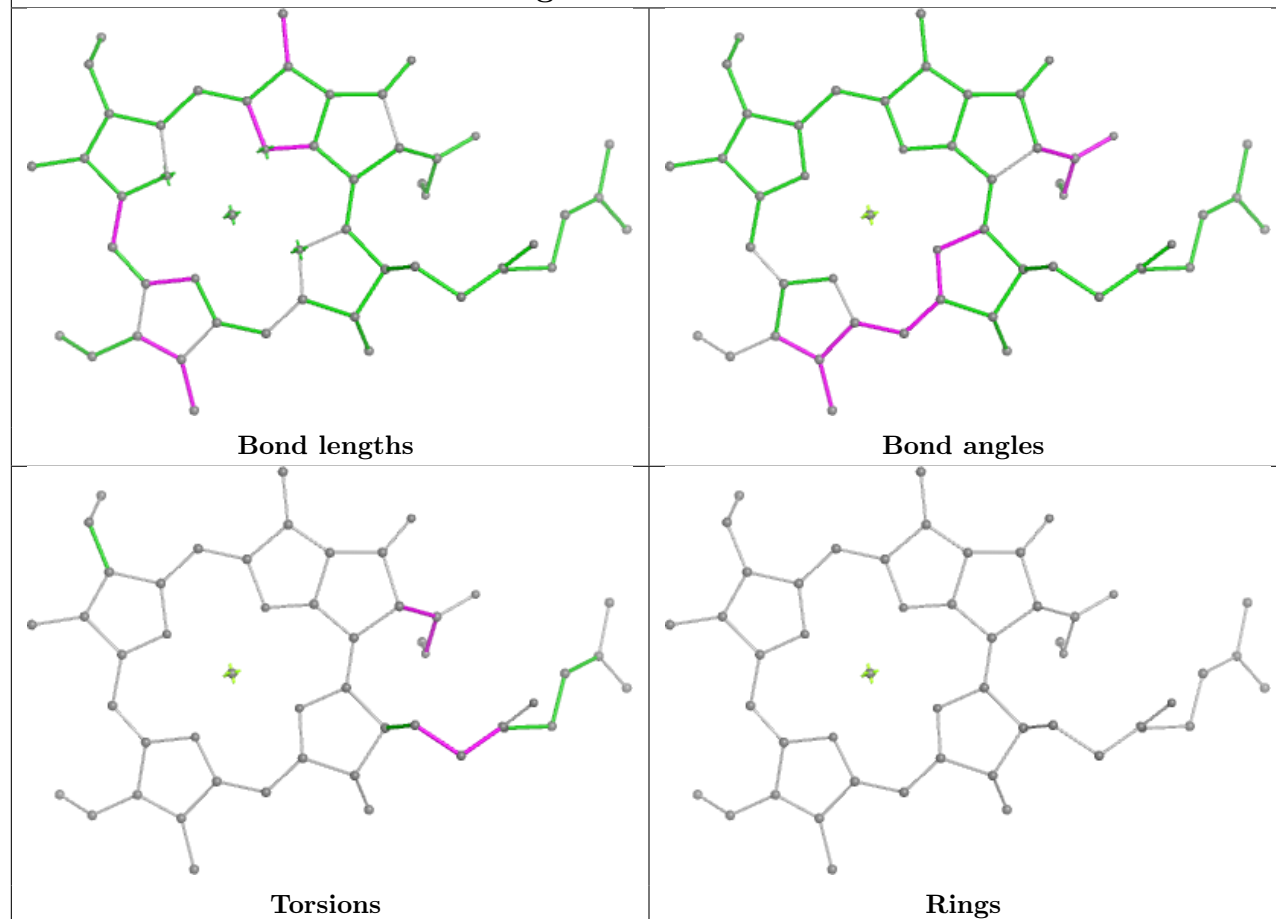




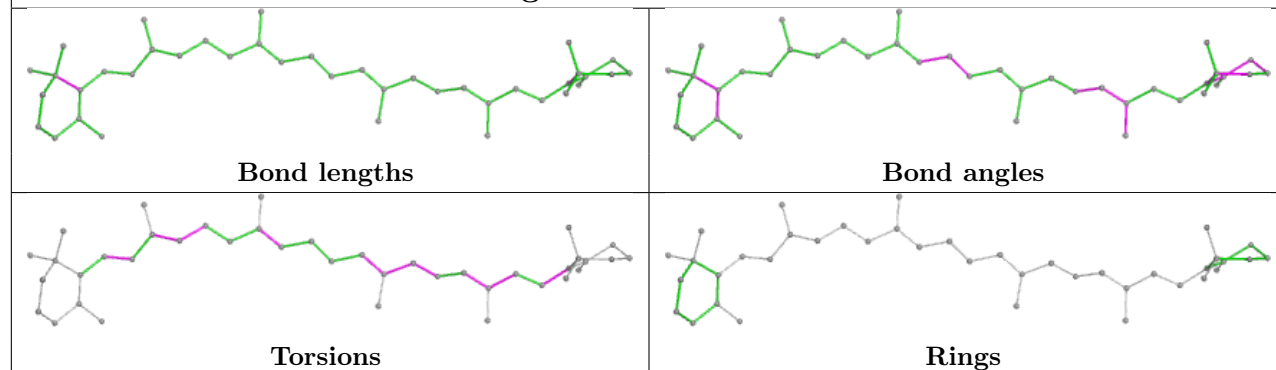
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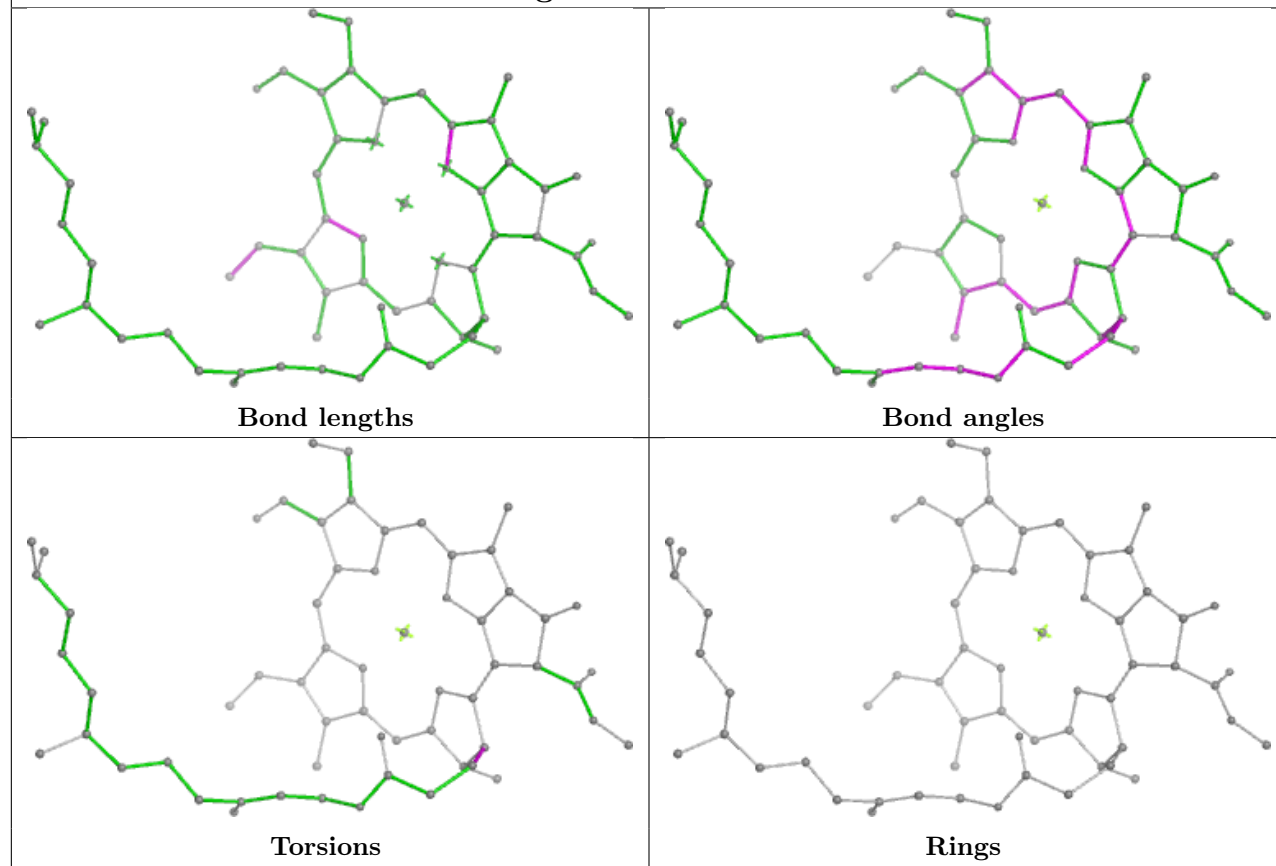
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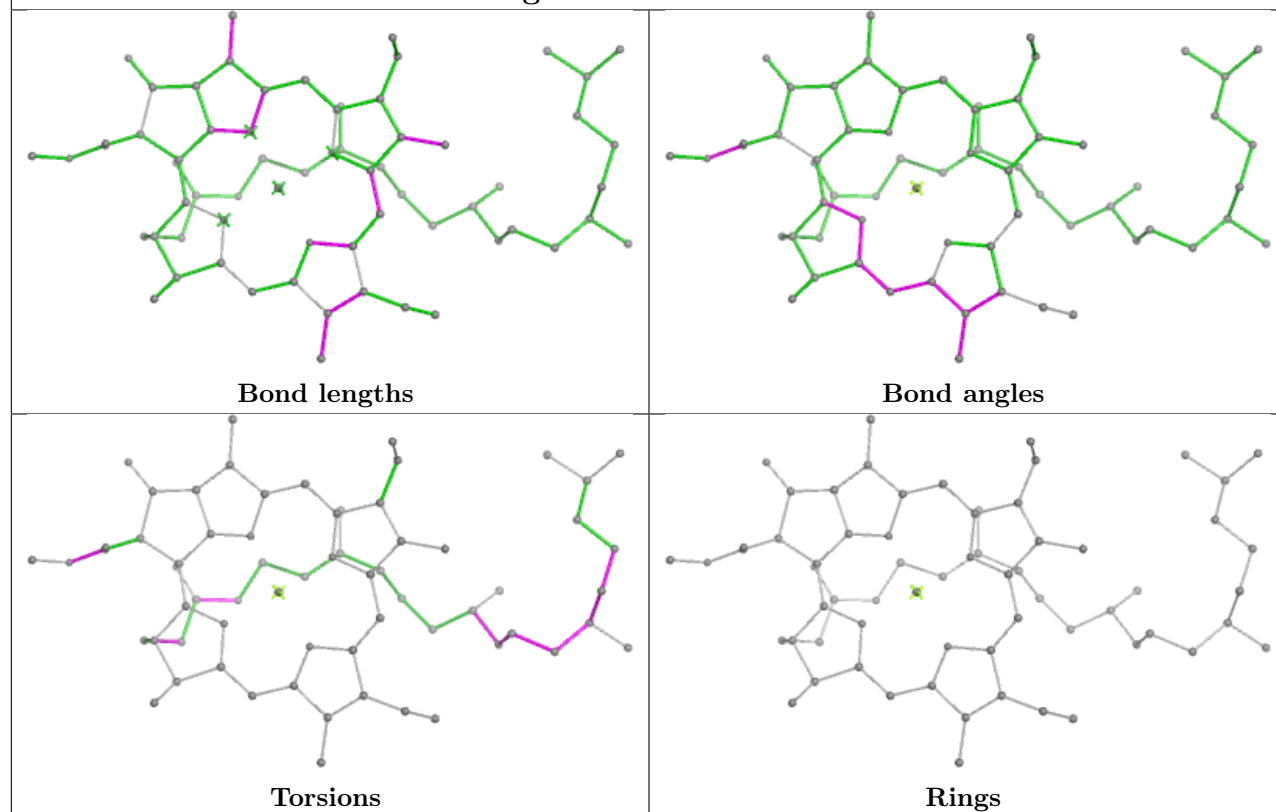
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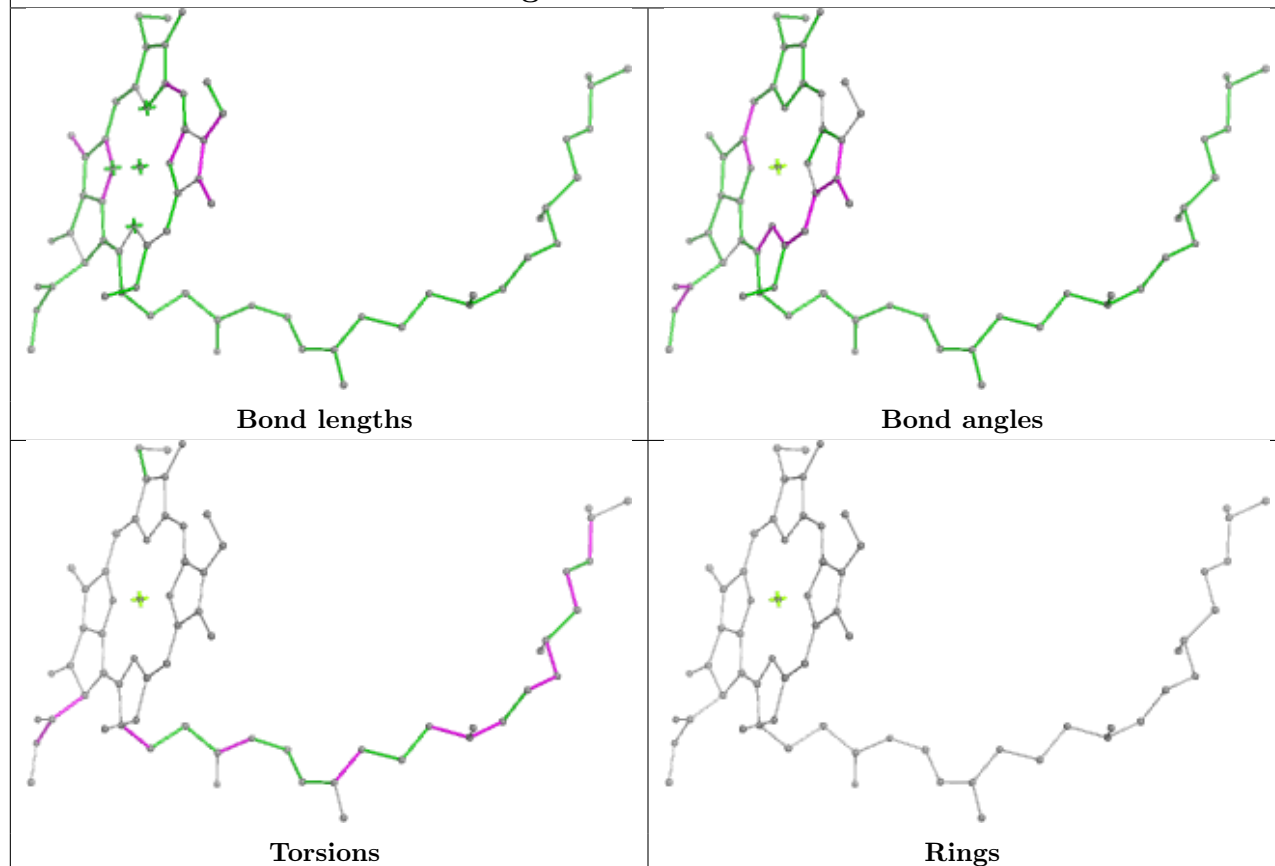
Ligand CHL 3 604



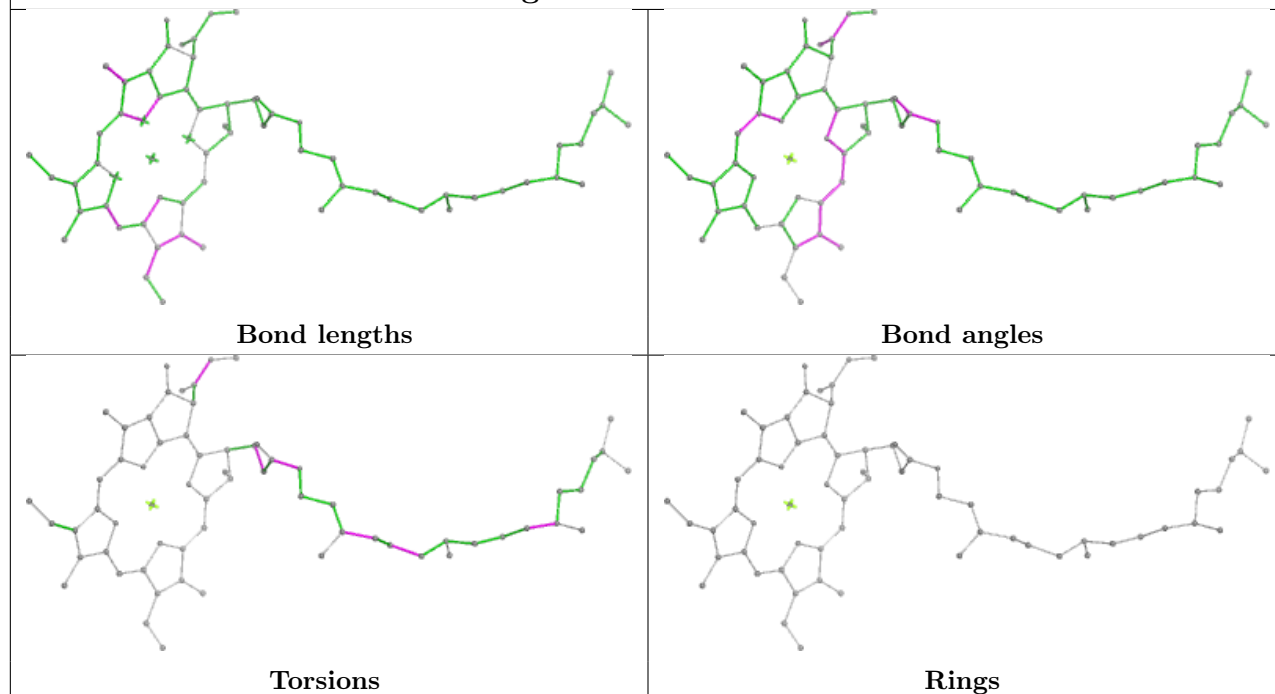
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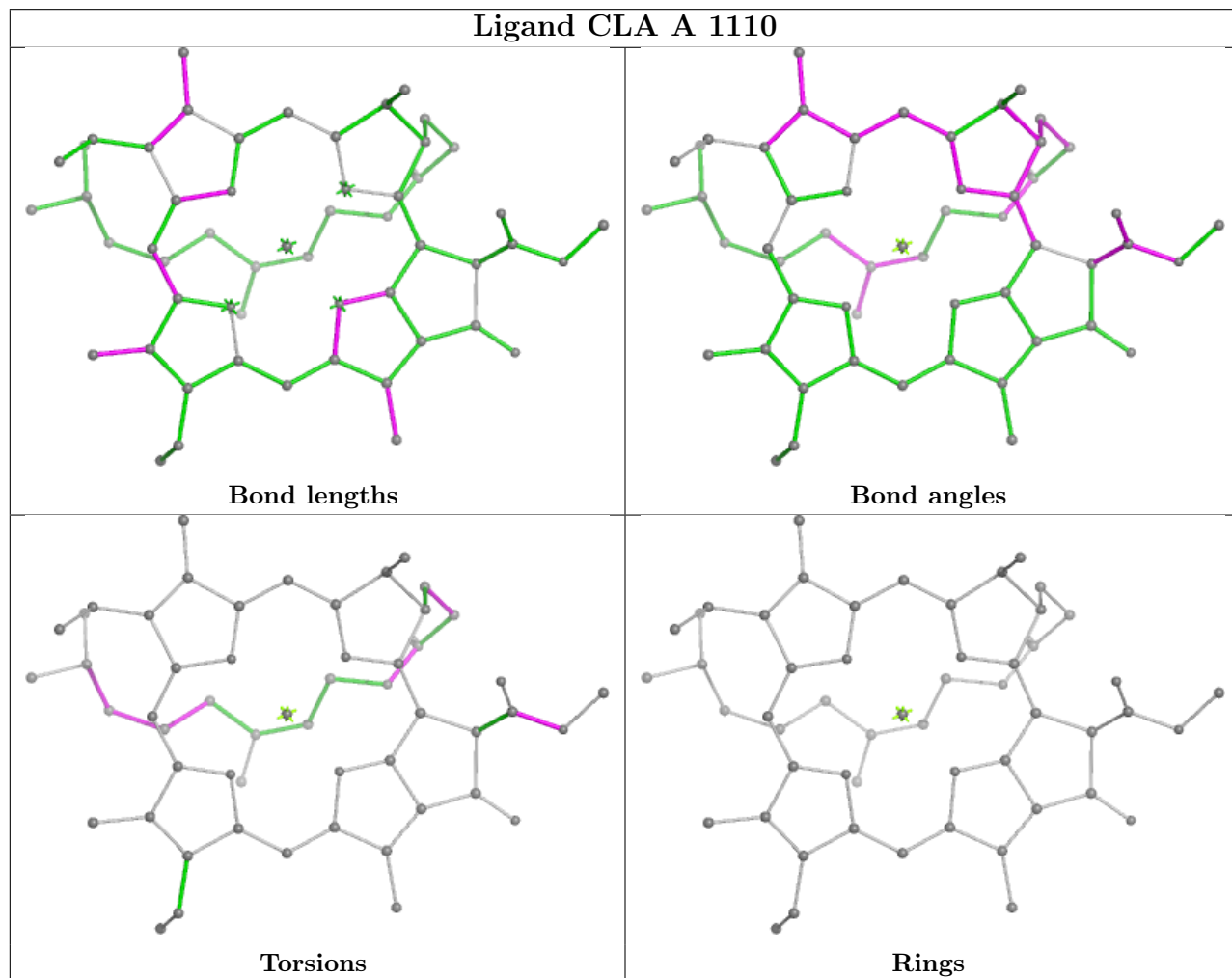
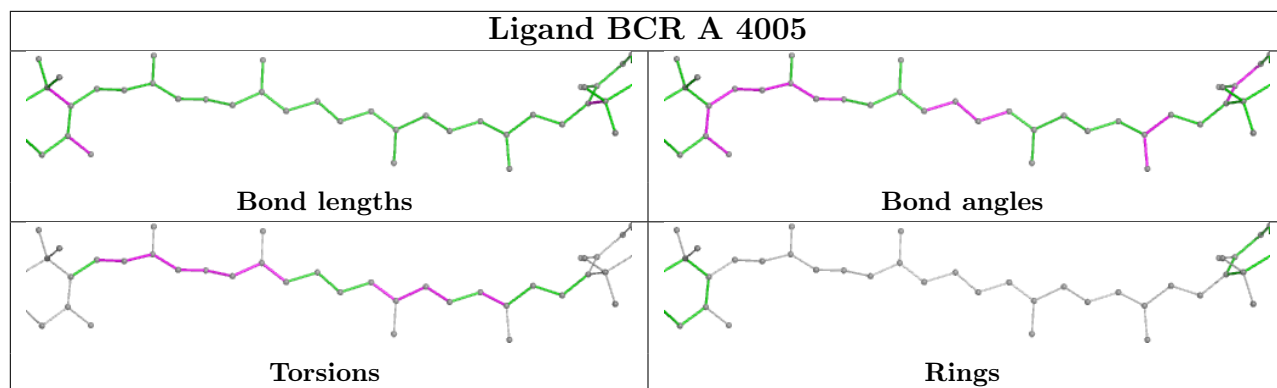


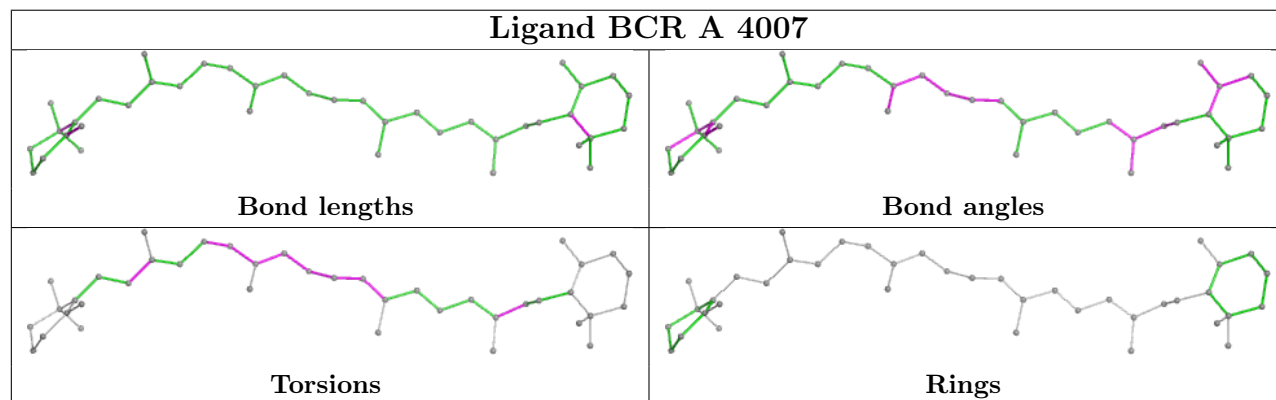
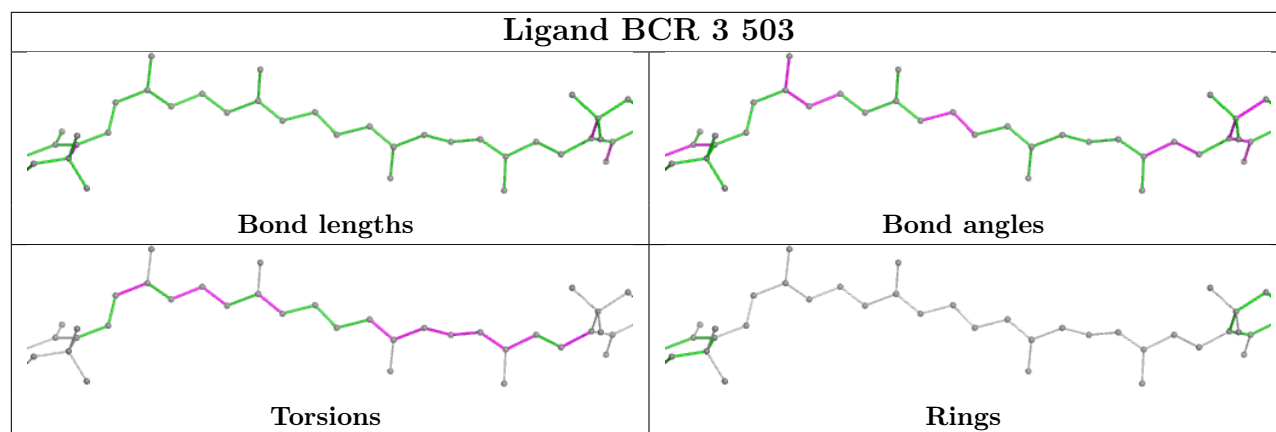
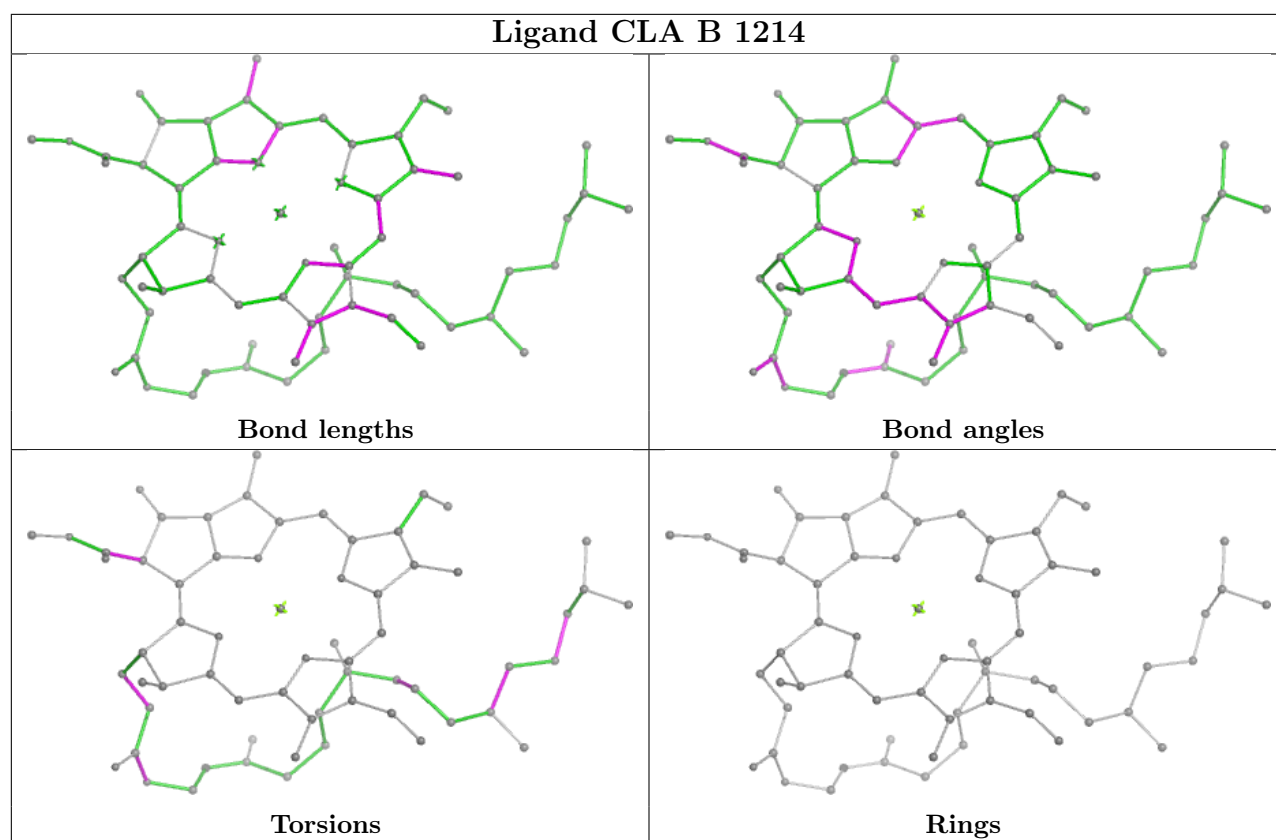
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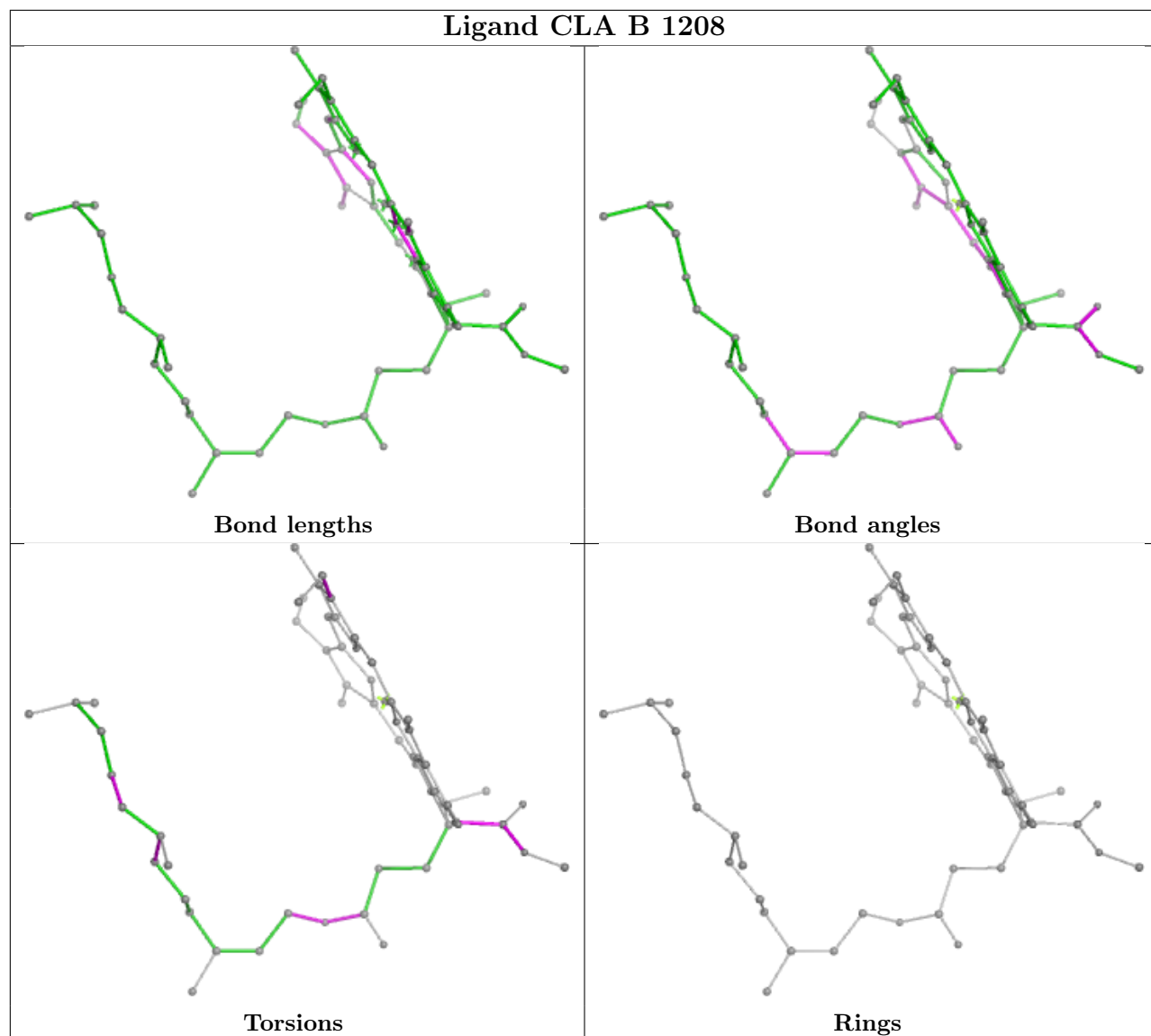


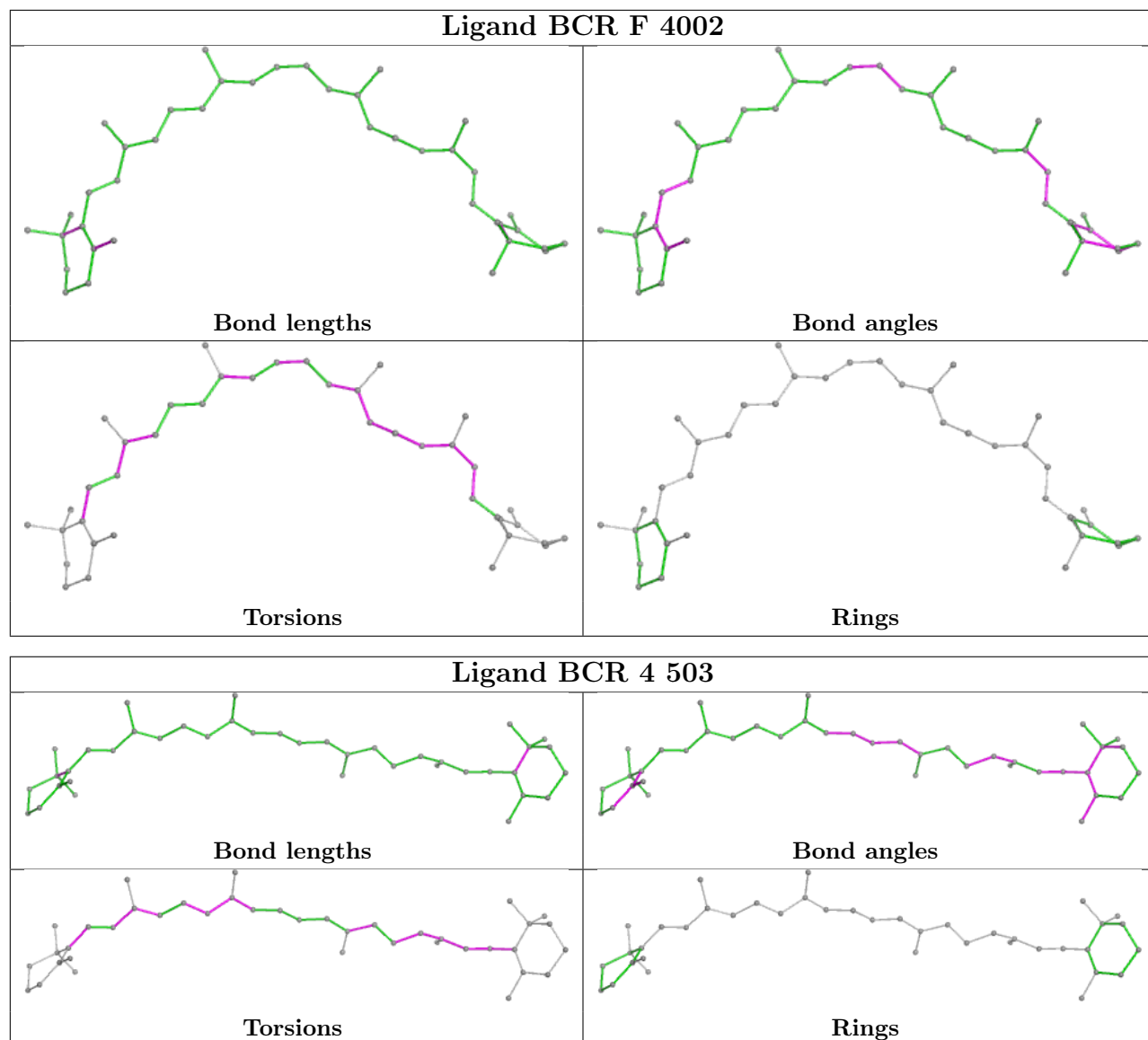
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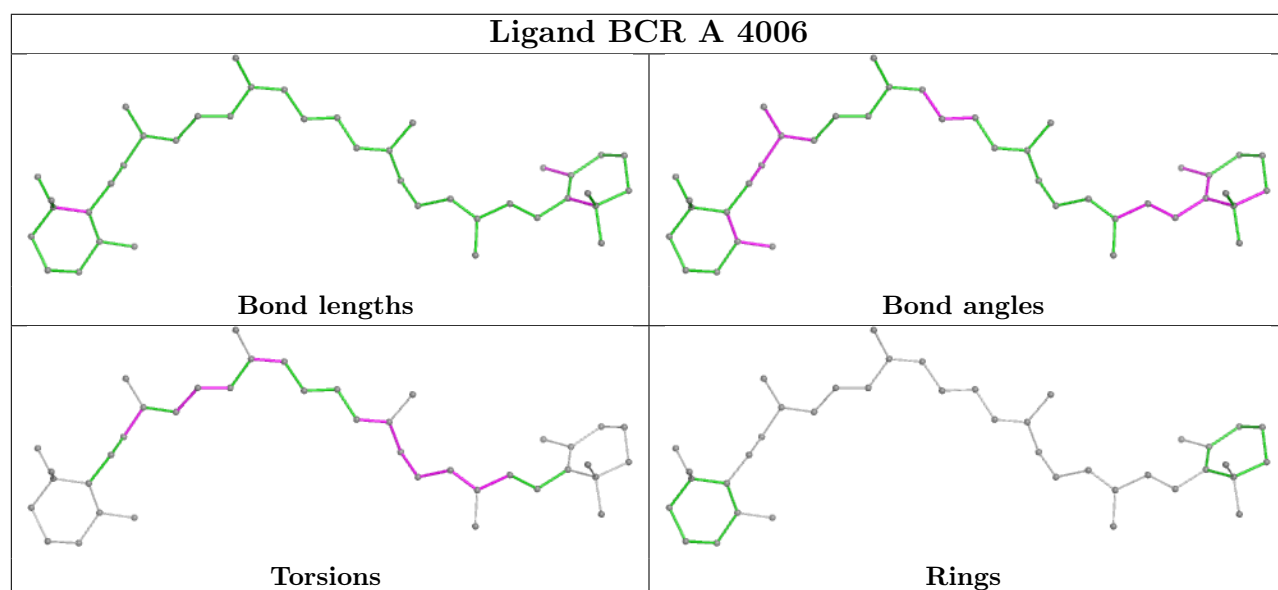
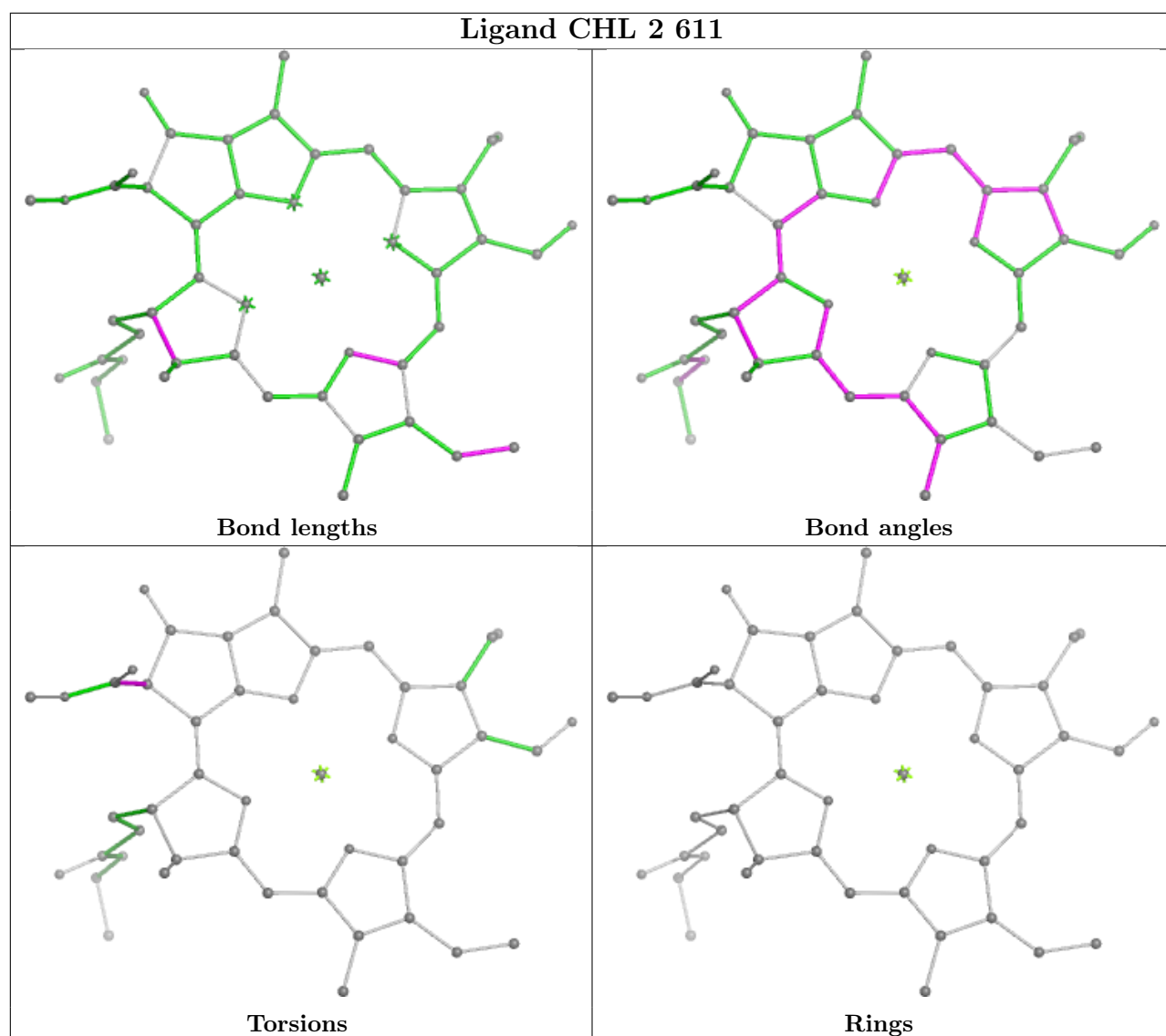


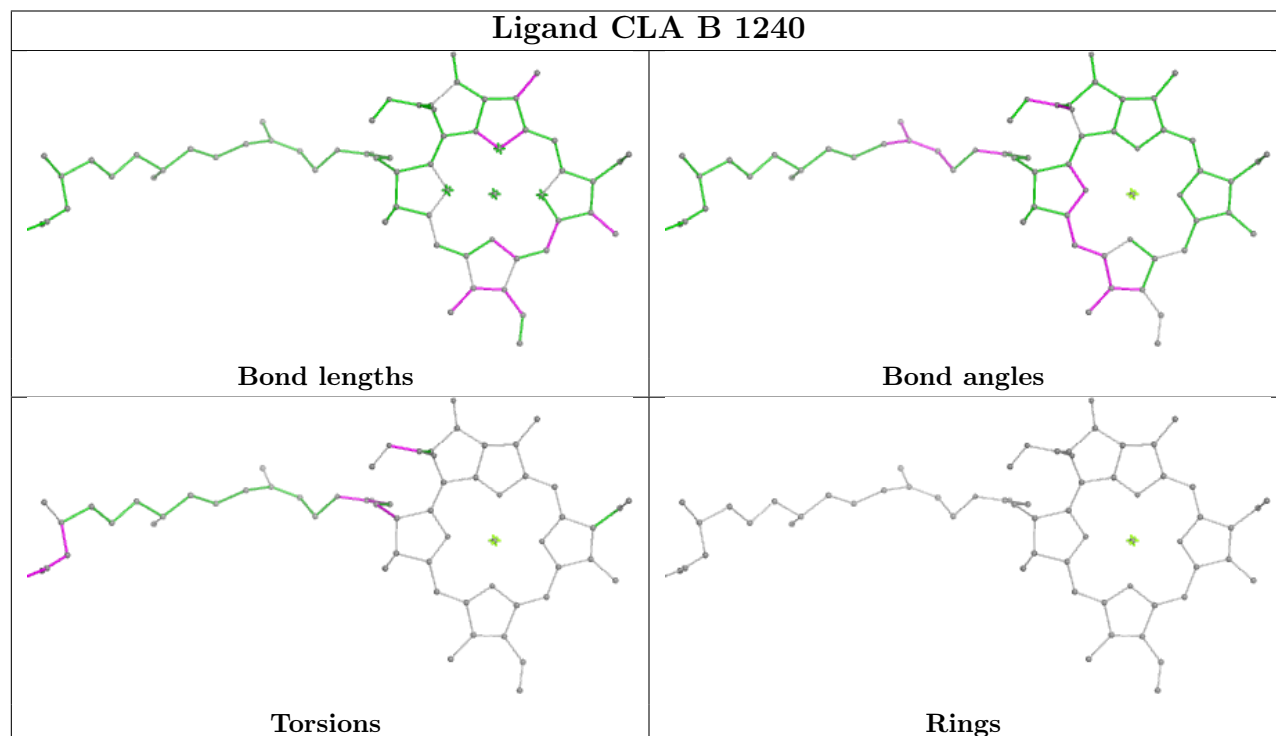
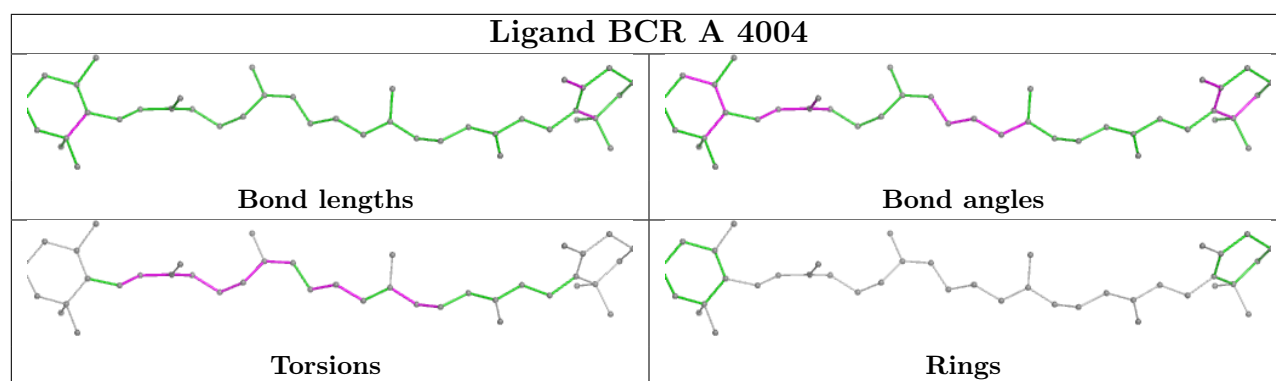




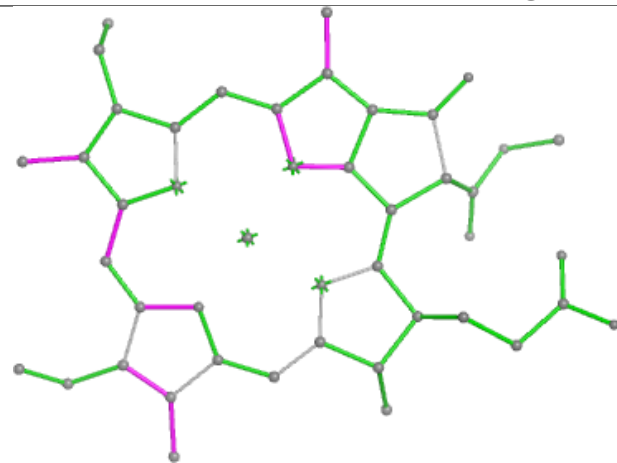




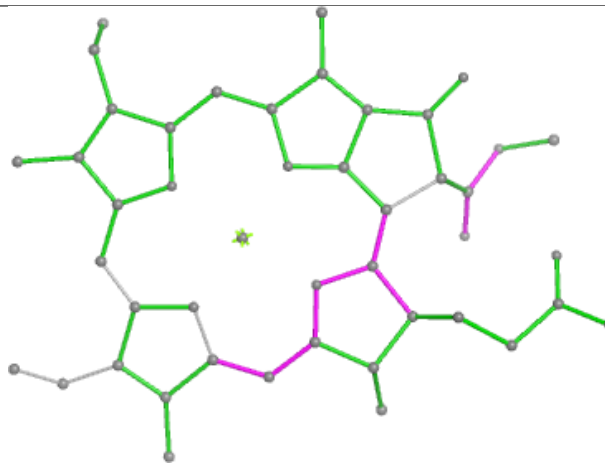




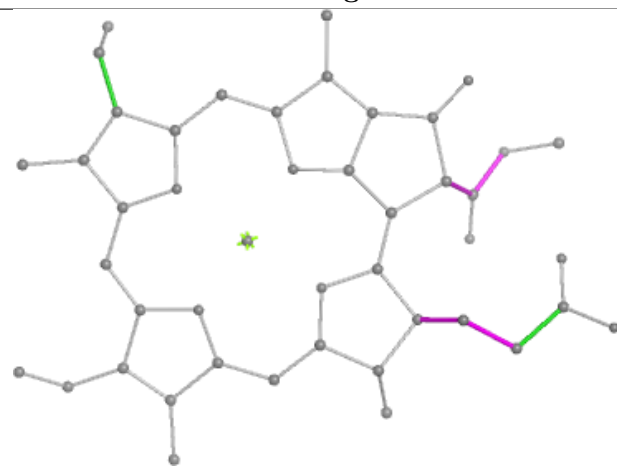
Ligand CLA 2 602



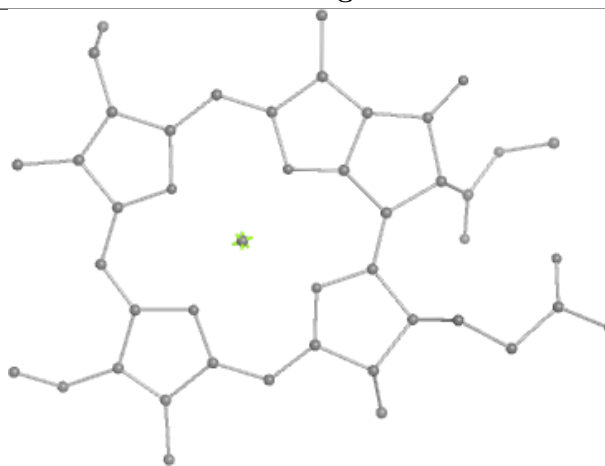
Bond lengths



Bond angles

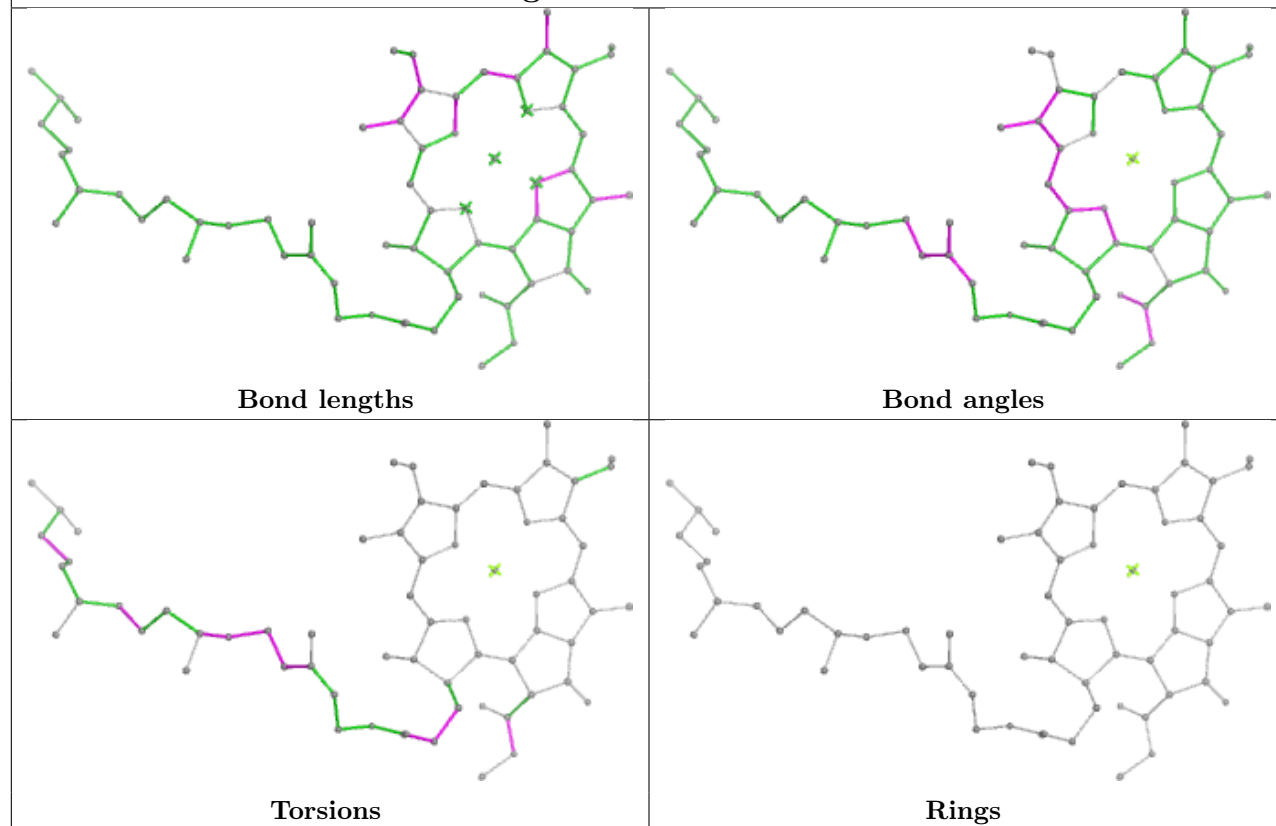


Torsions

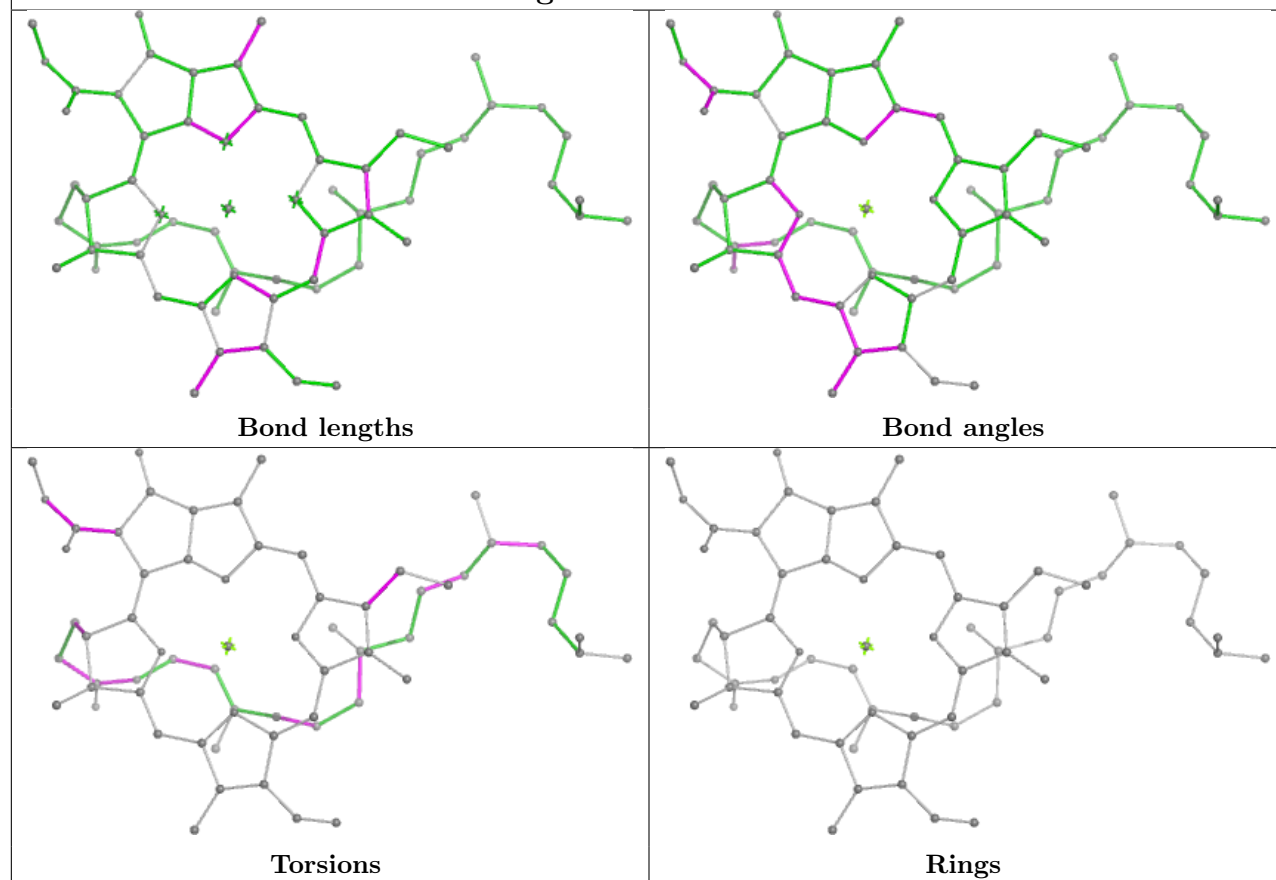


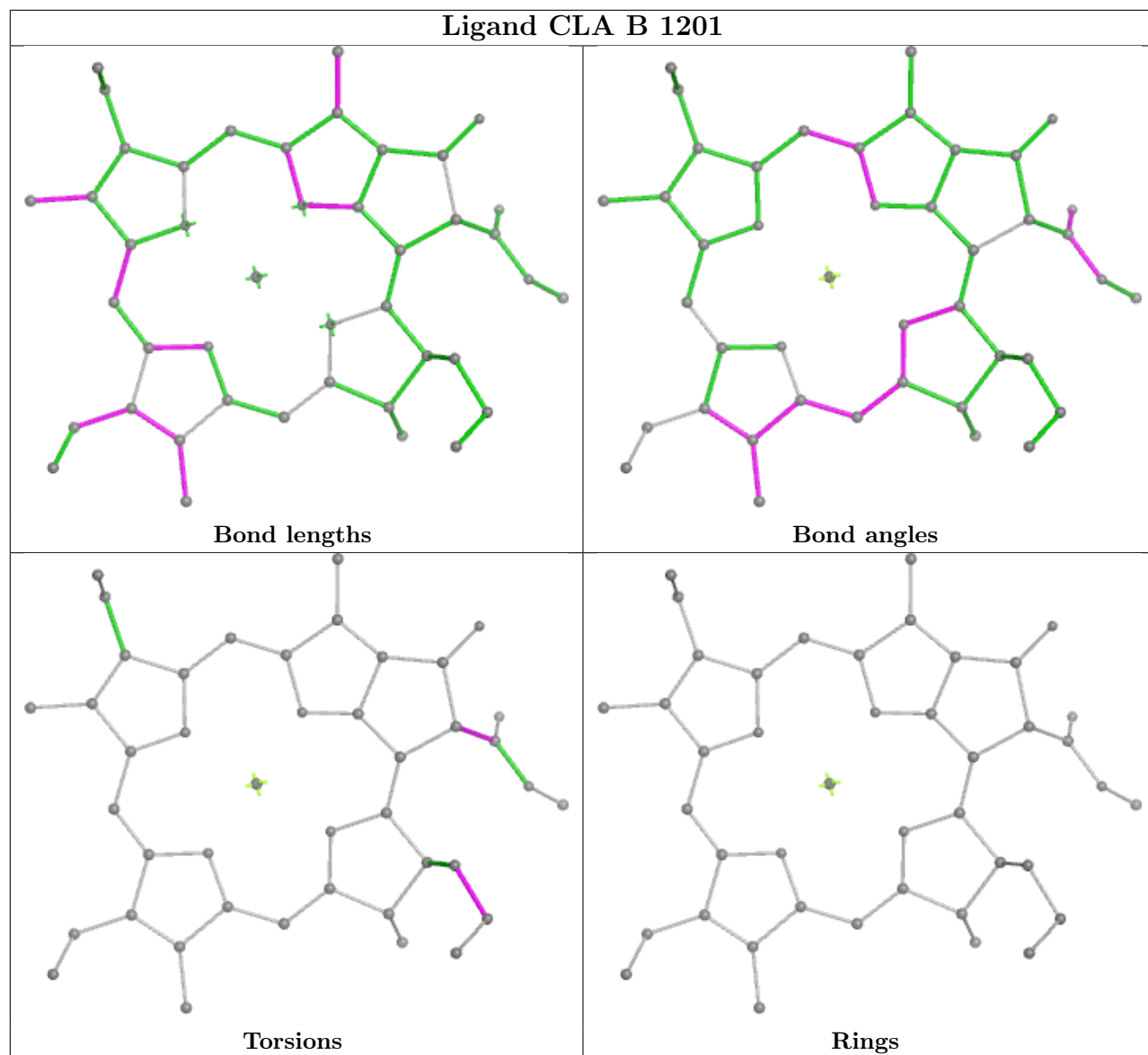
Rings

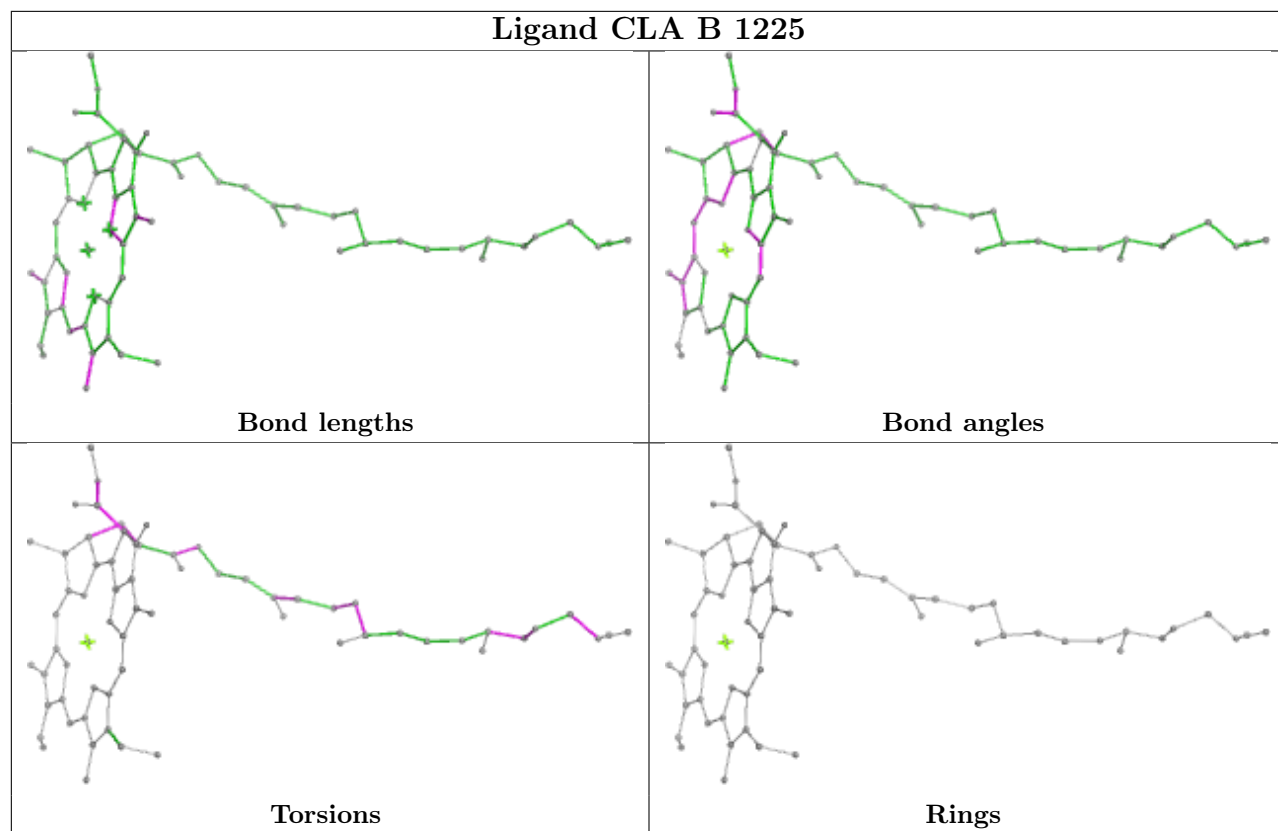
Ligand CLA A 1013



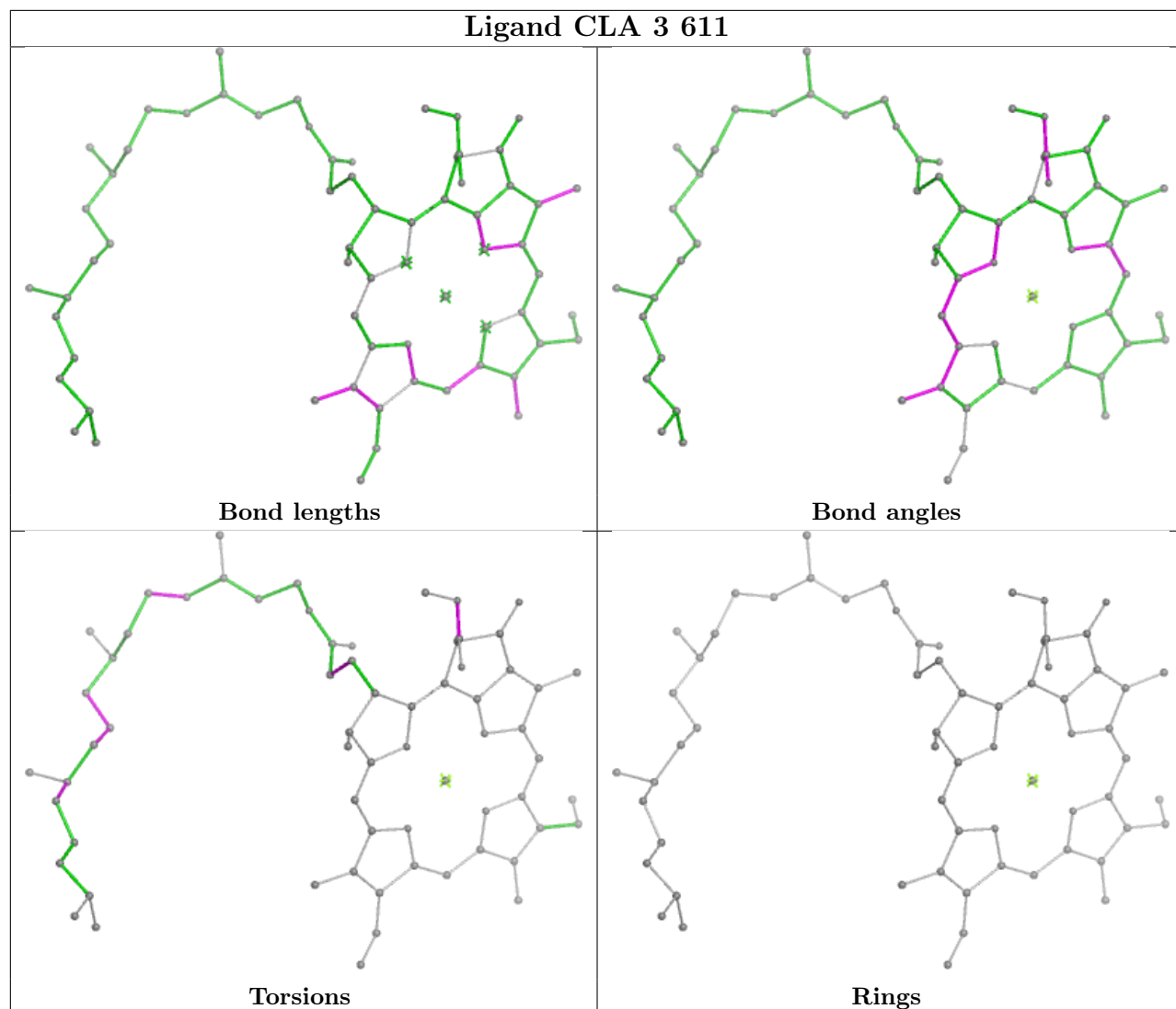
Ligand CLA 3 608



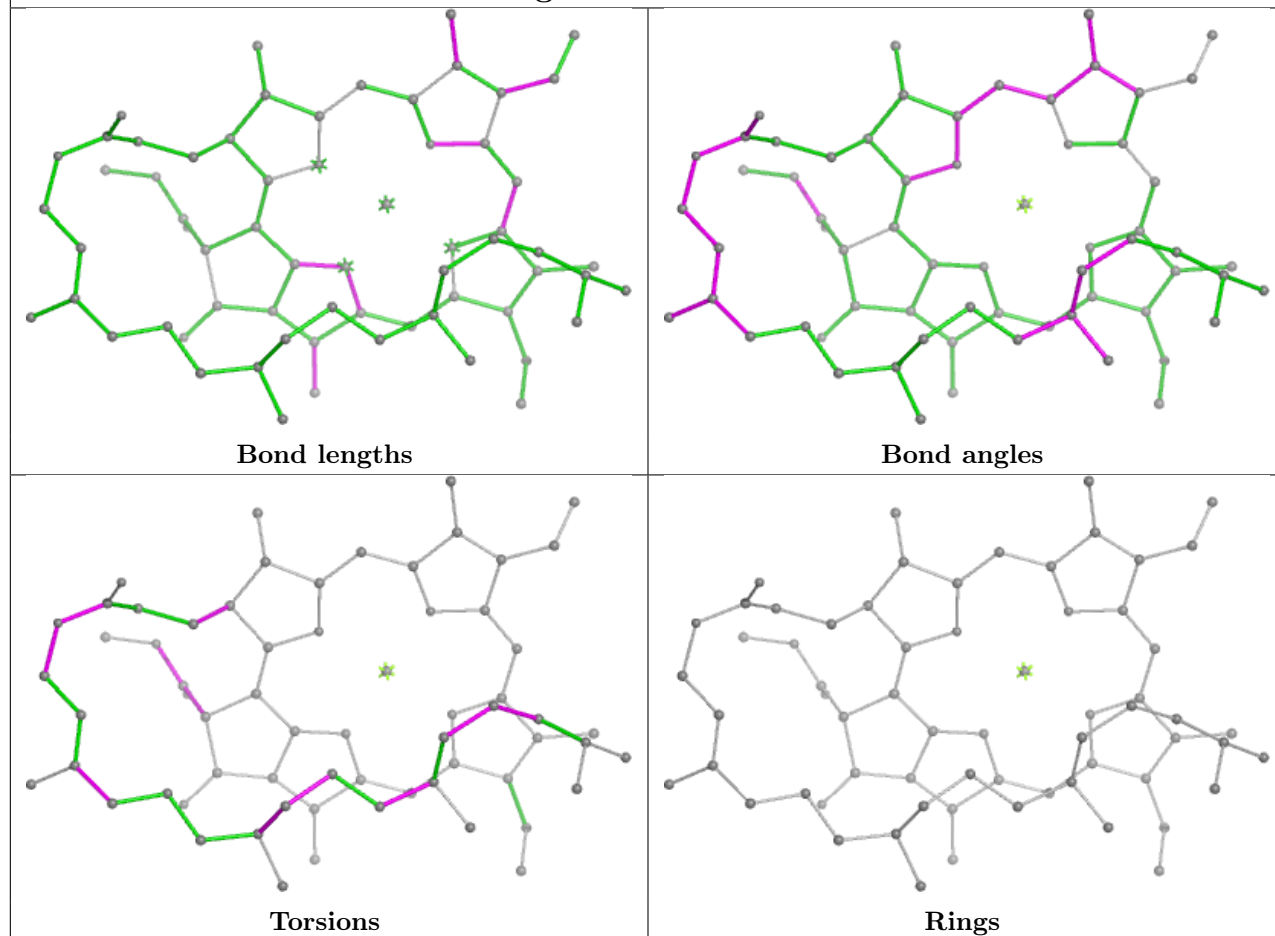




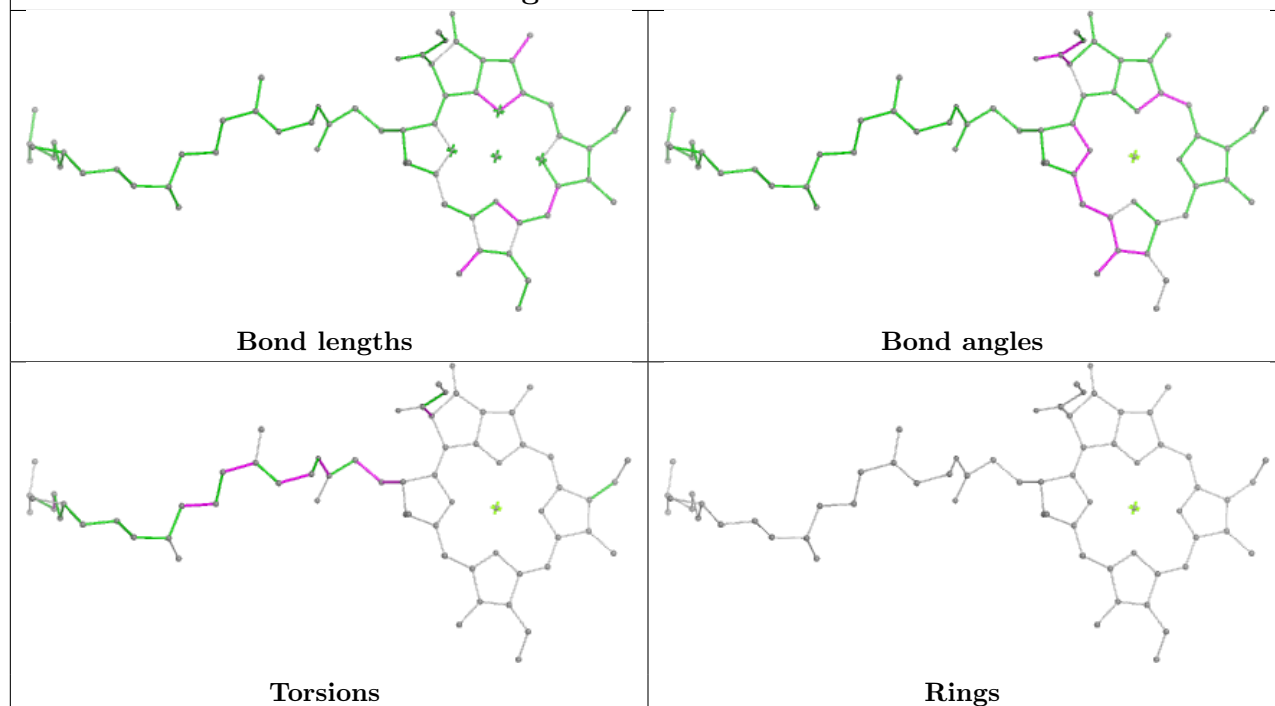
Ligand CLA 3 611

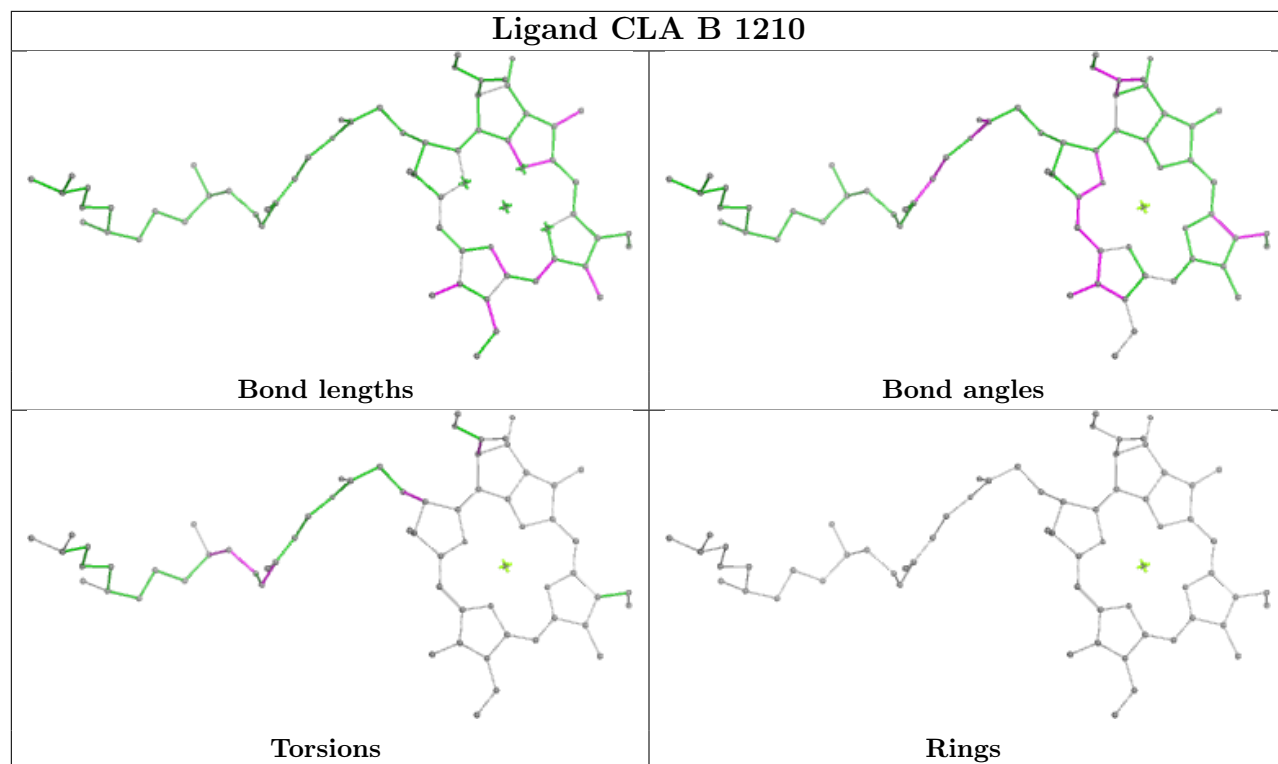


Ligand CLA 2 616

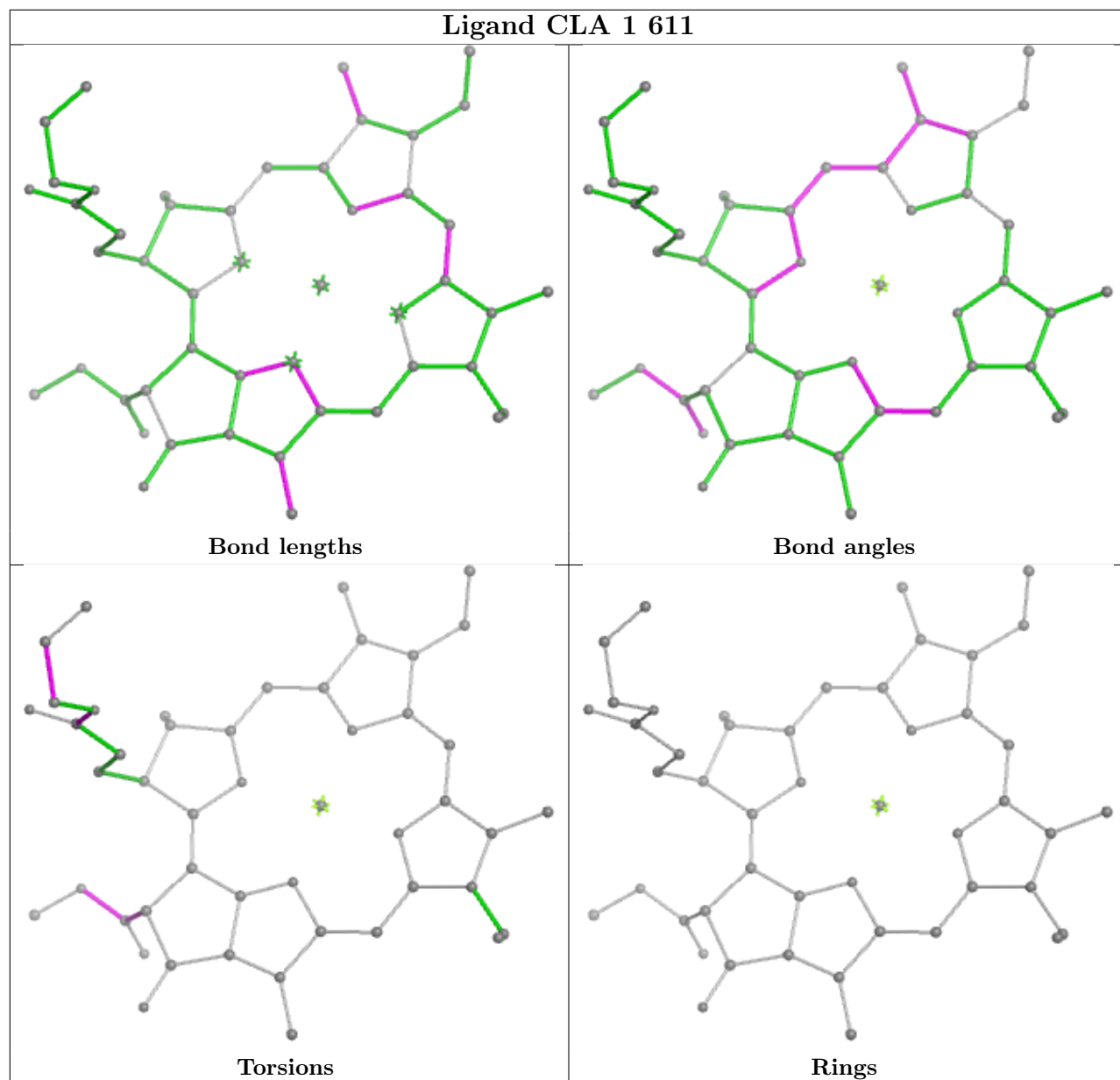


Ligand CLA A 1103

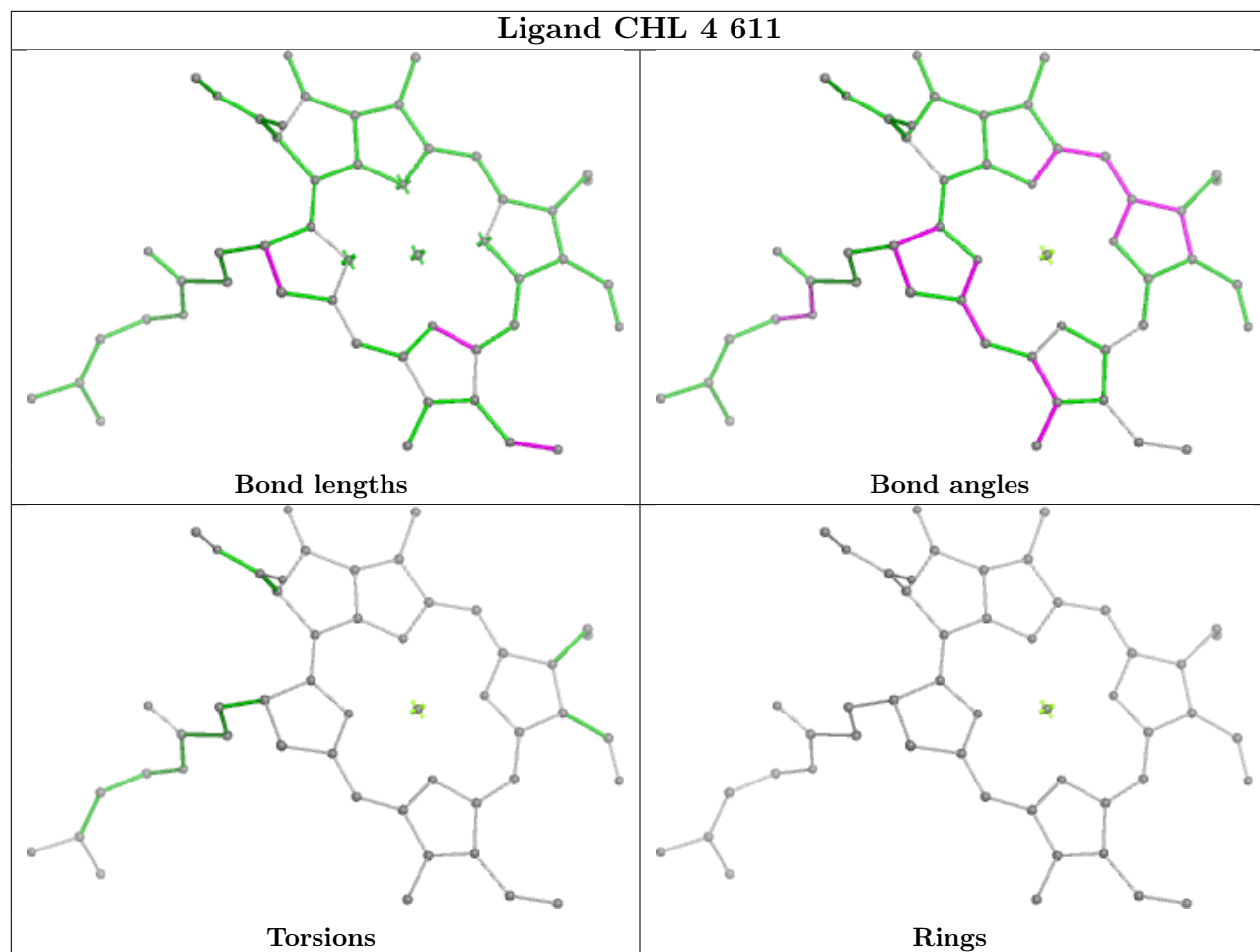




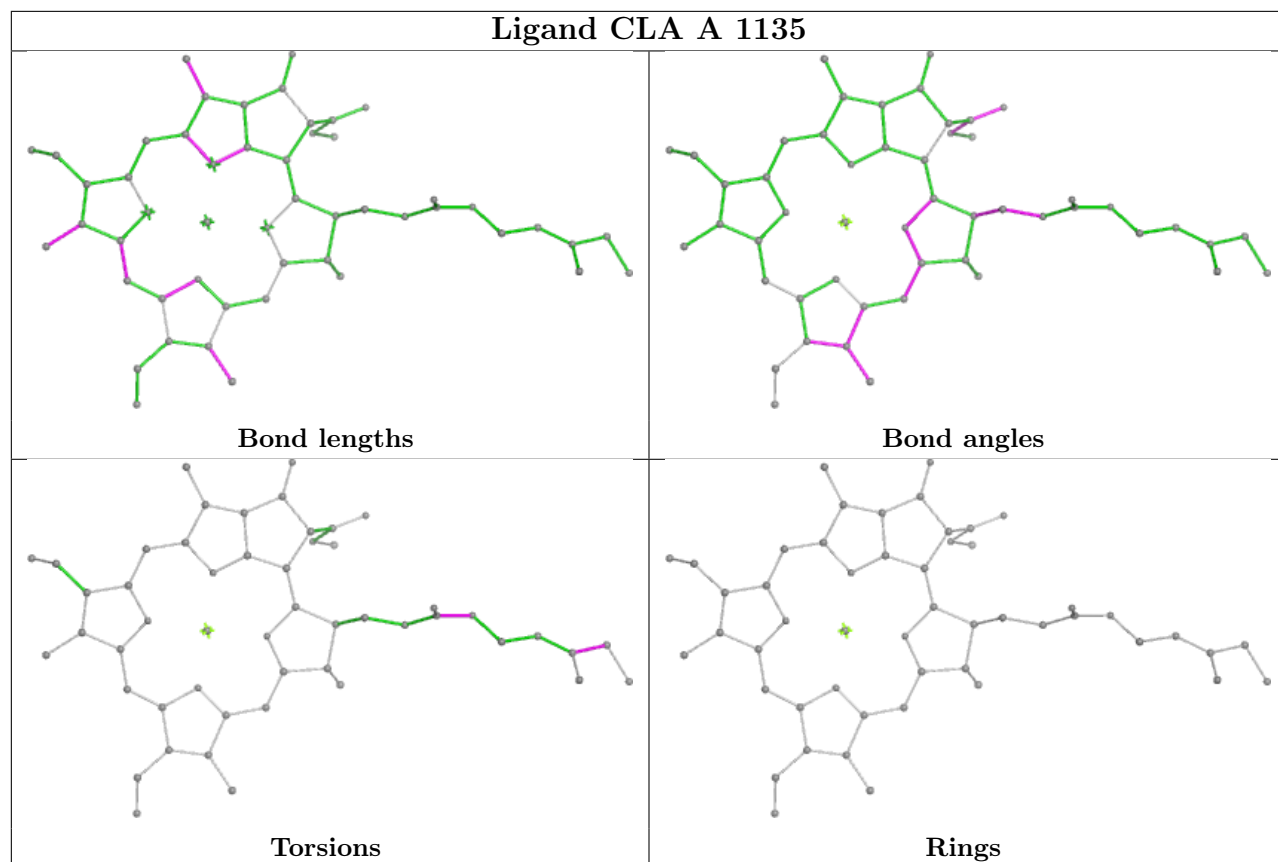
Ligand CLA 1 611



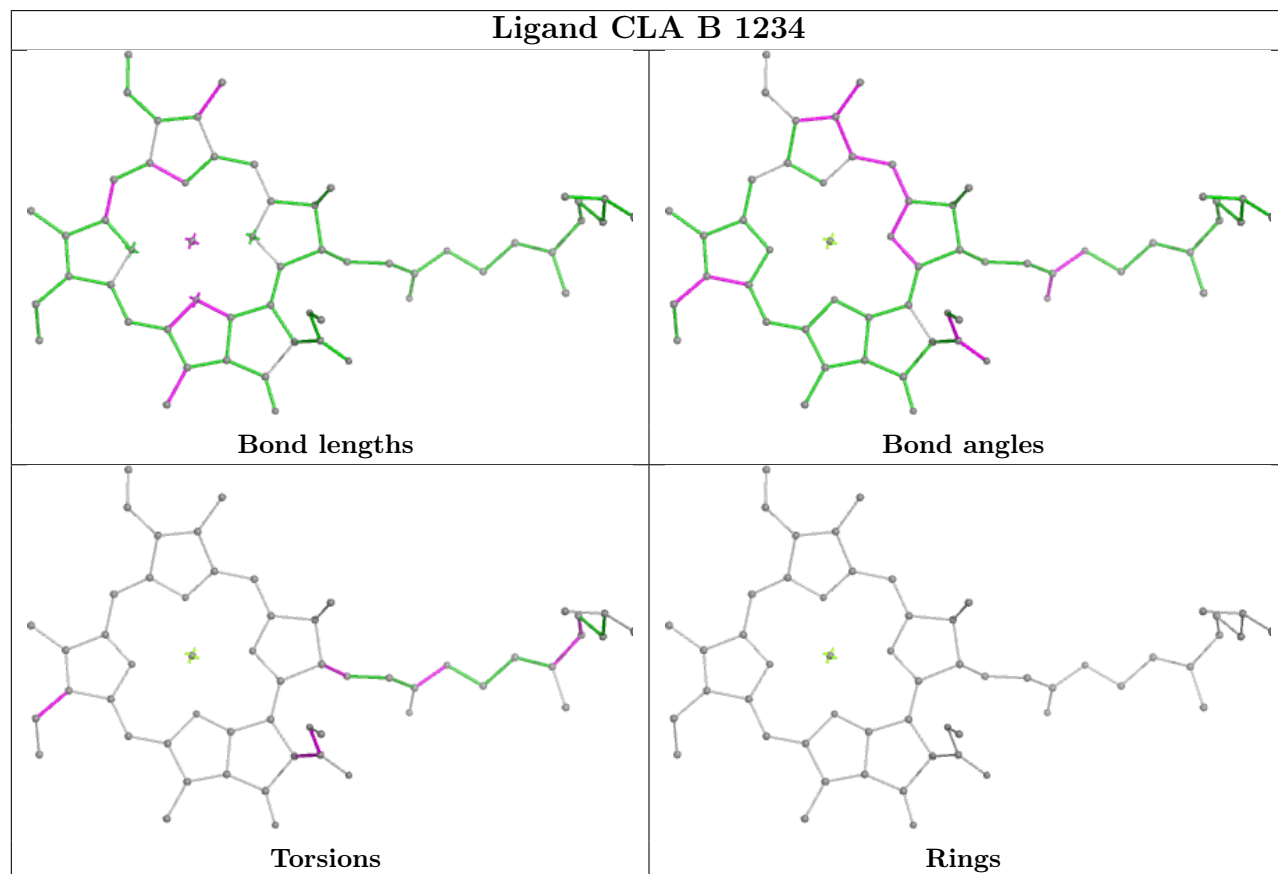
Ligand CHL 4 611

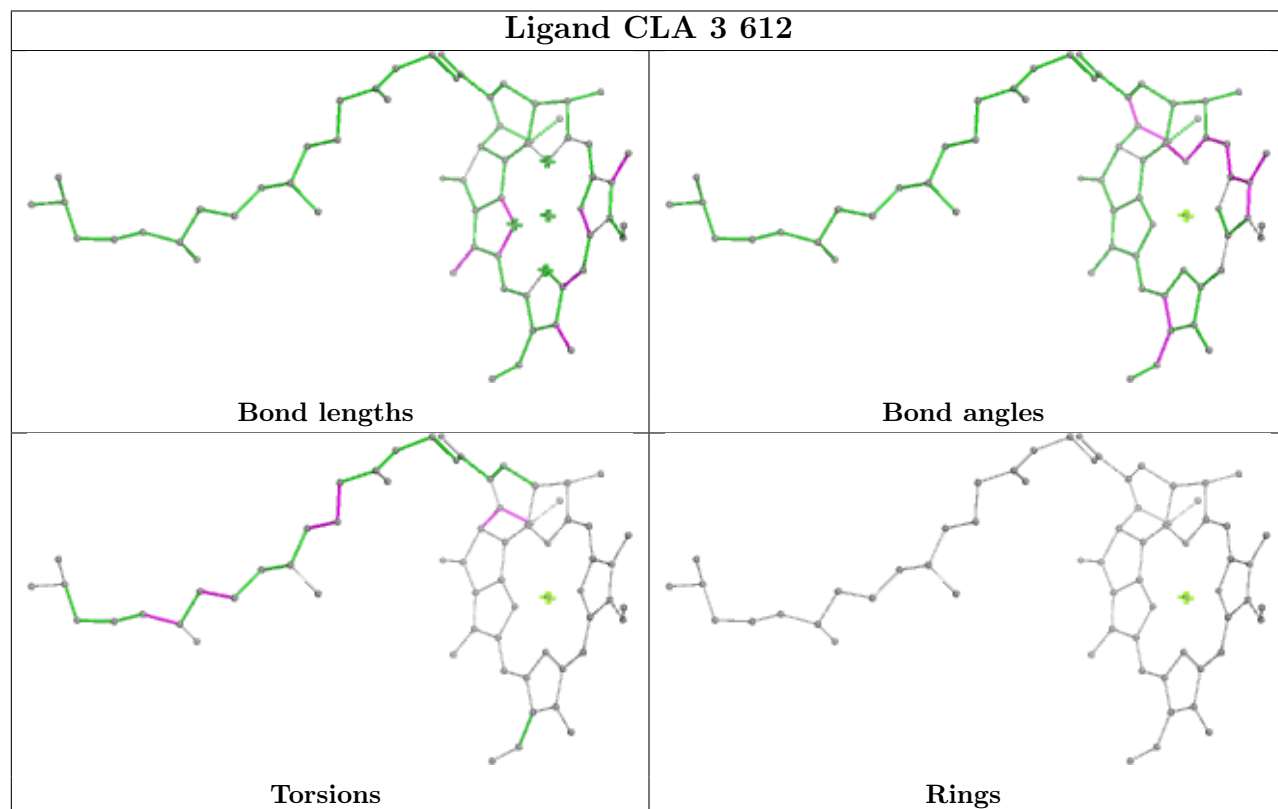
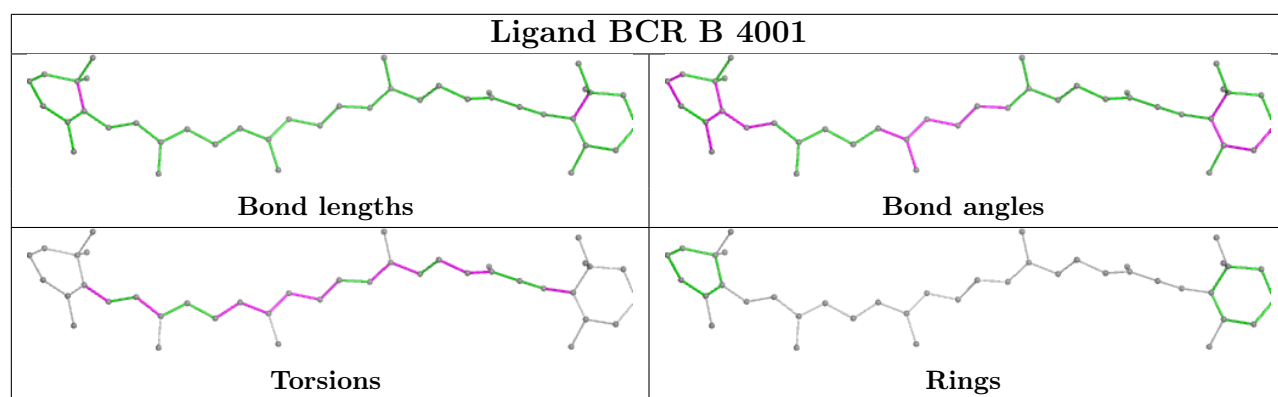


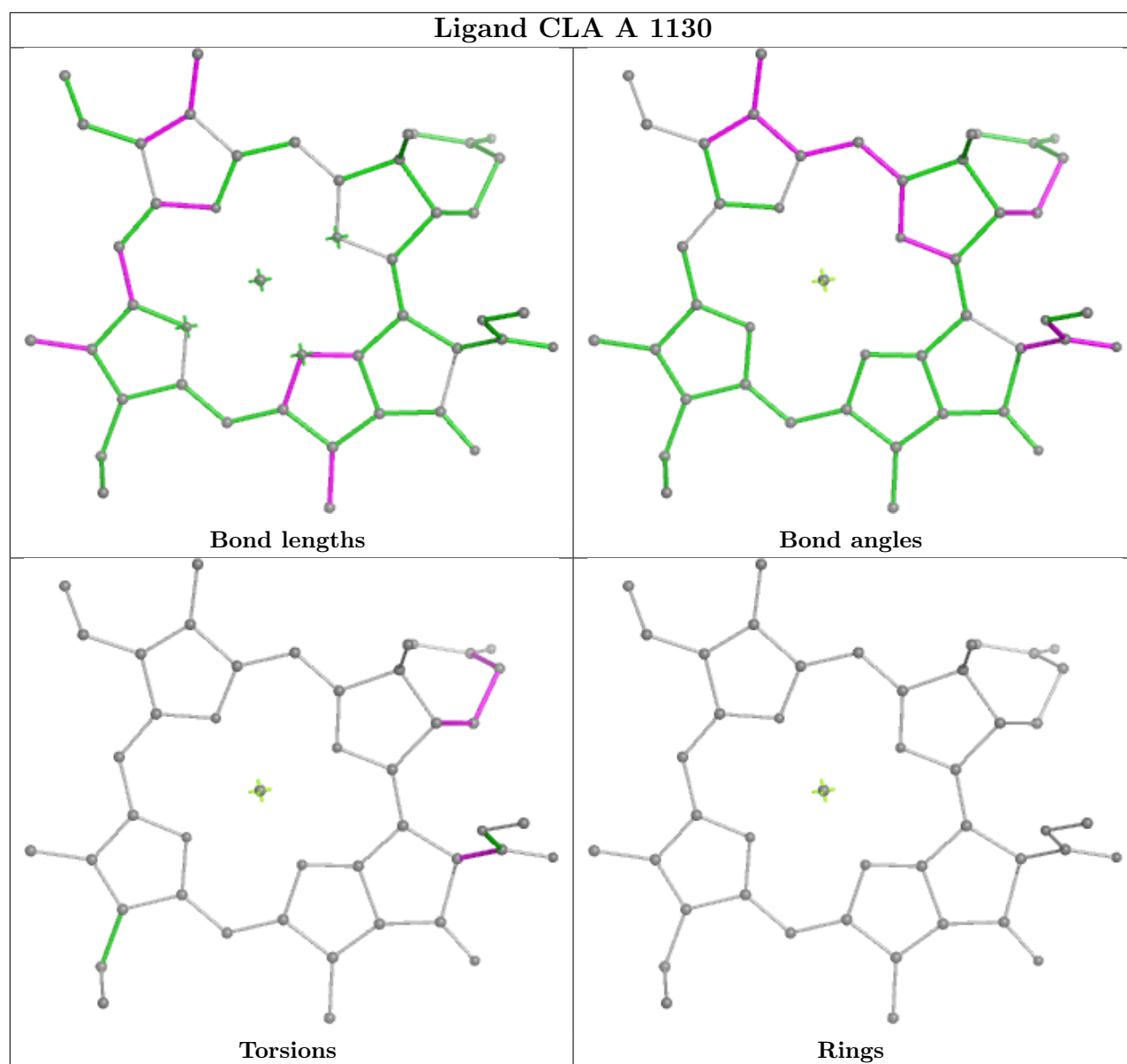
Ligand CLA A 1135



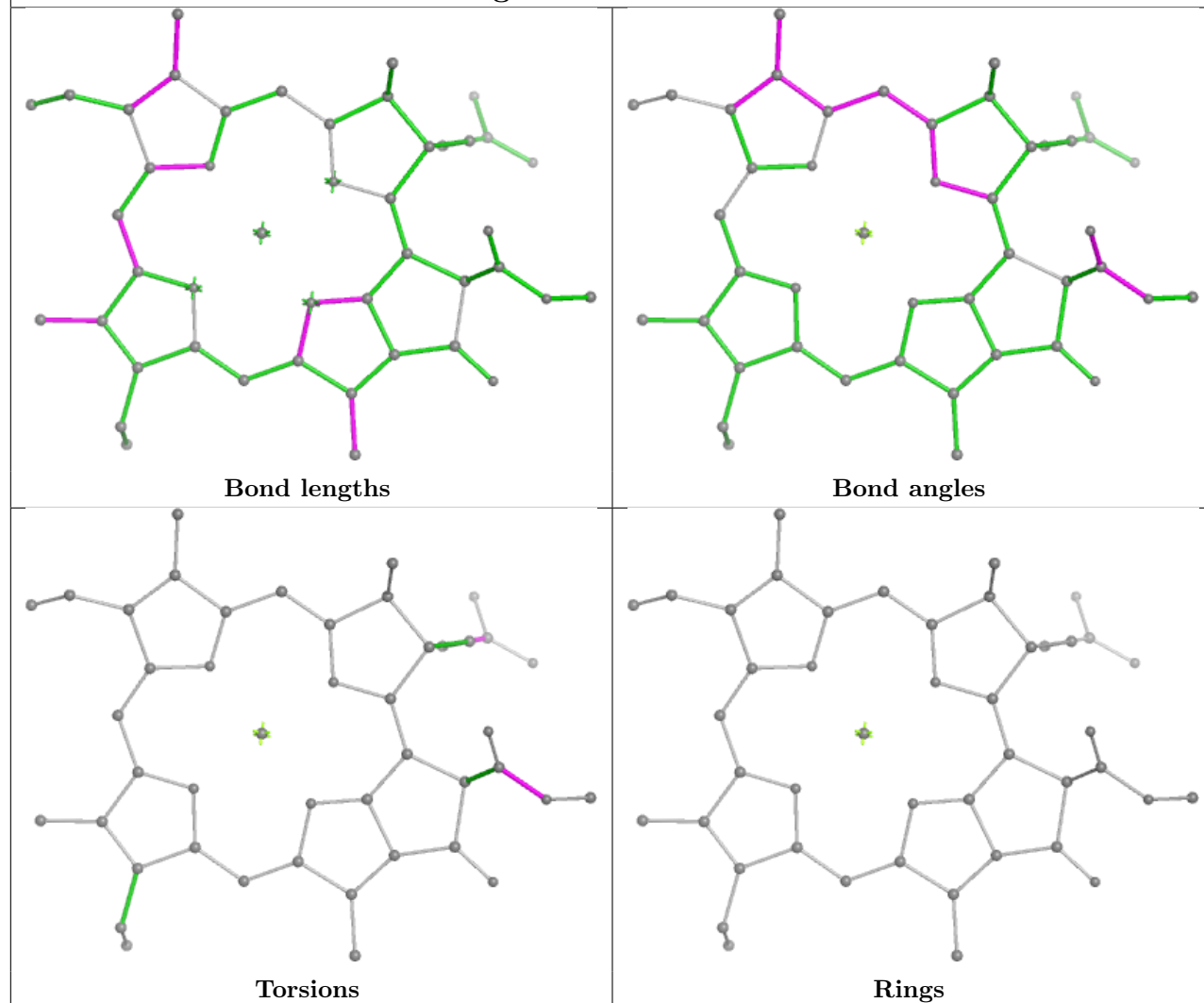
Ligand CLA B 1234



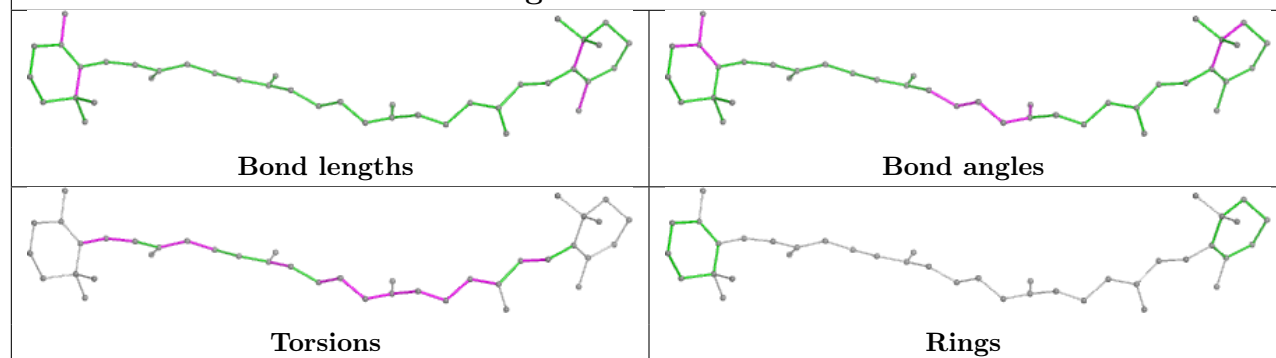


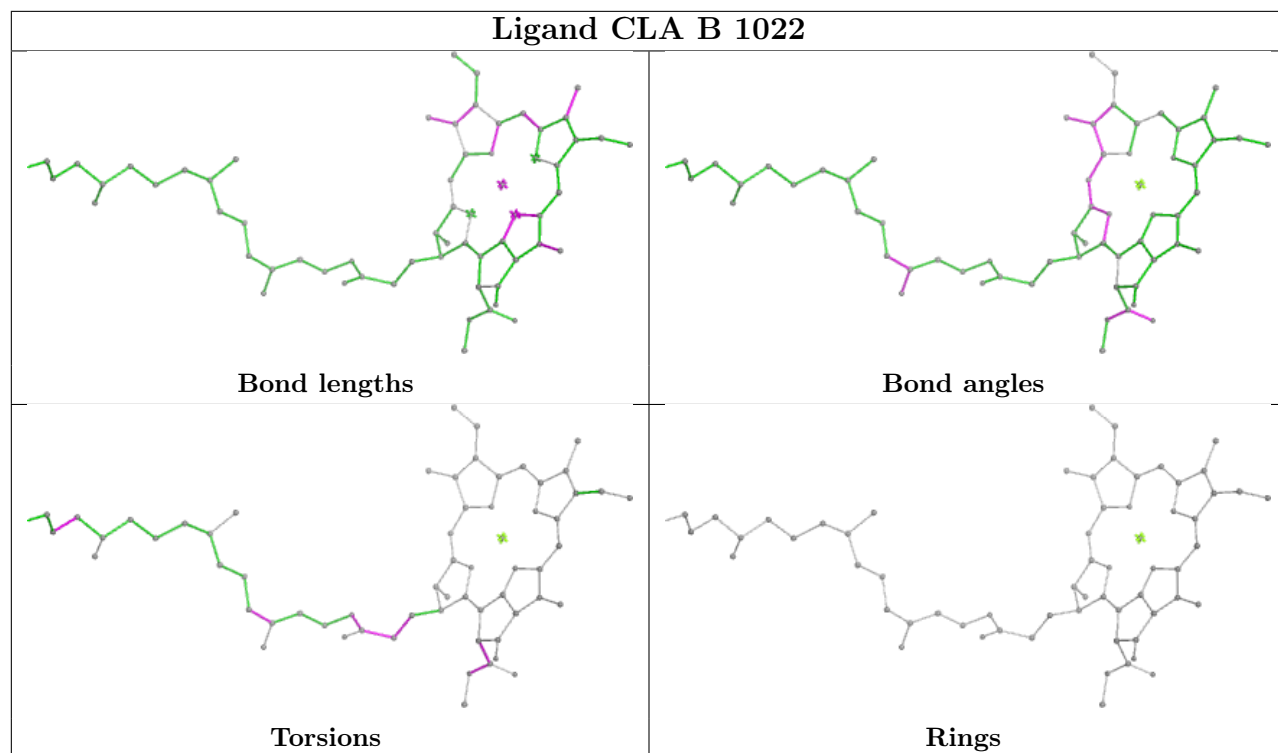


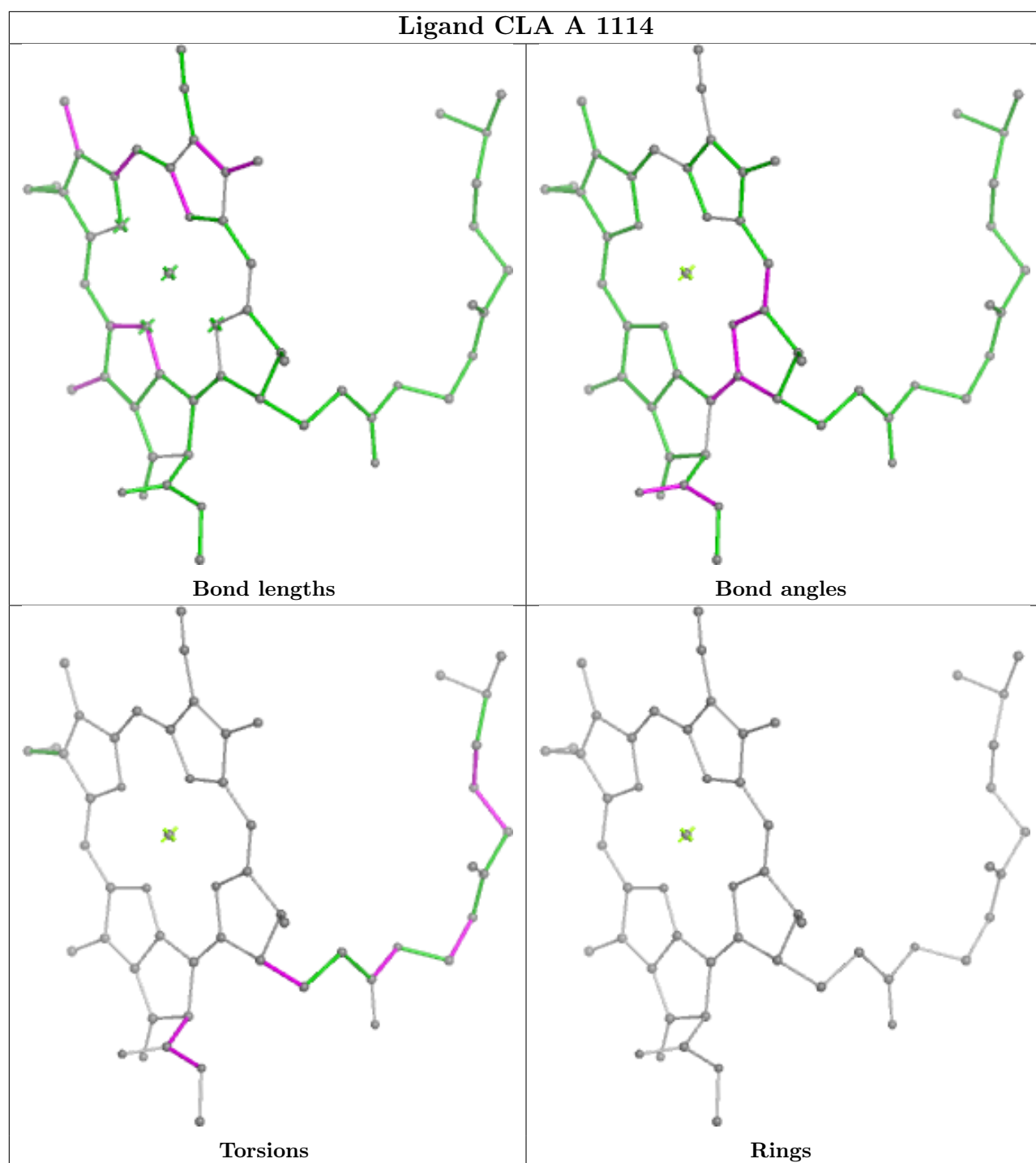
Ligand CLA A 1121



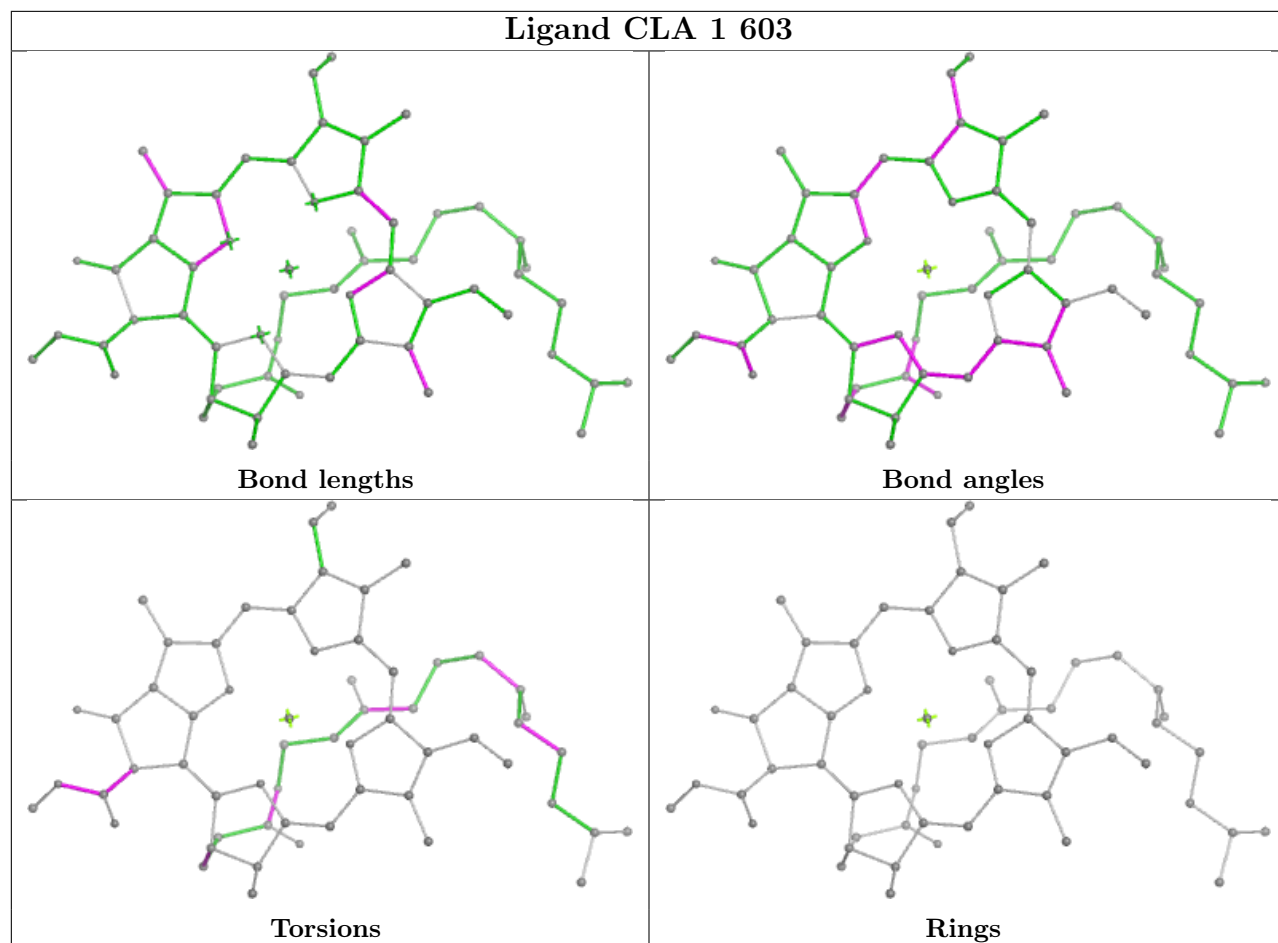
Ligand BCR J 4002

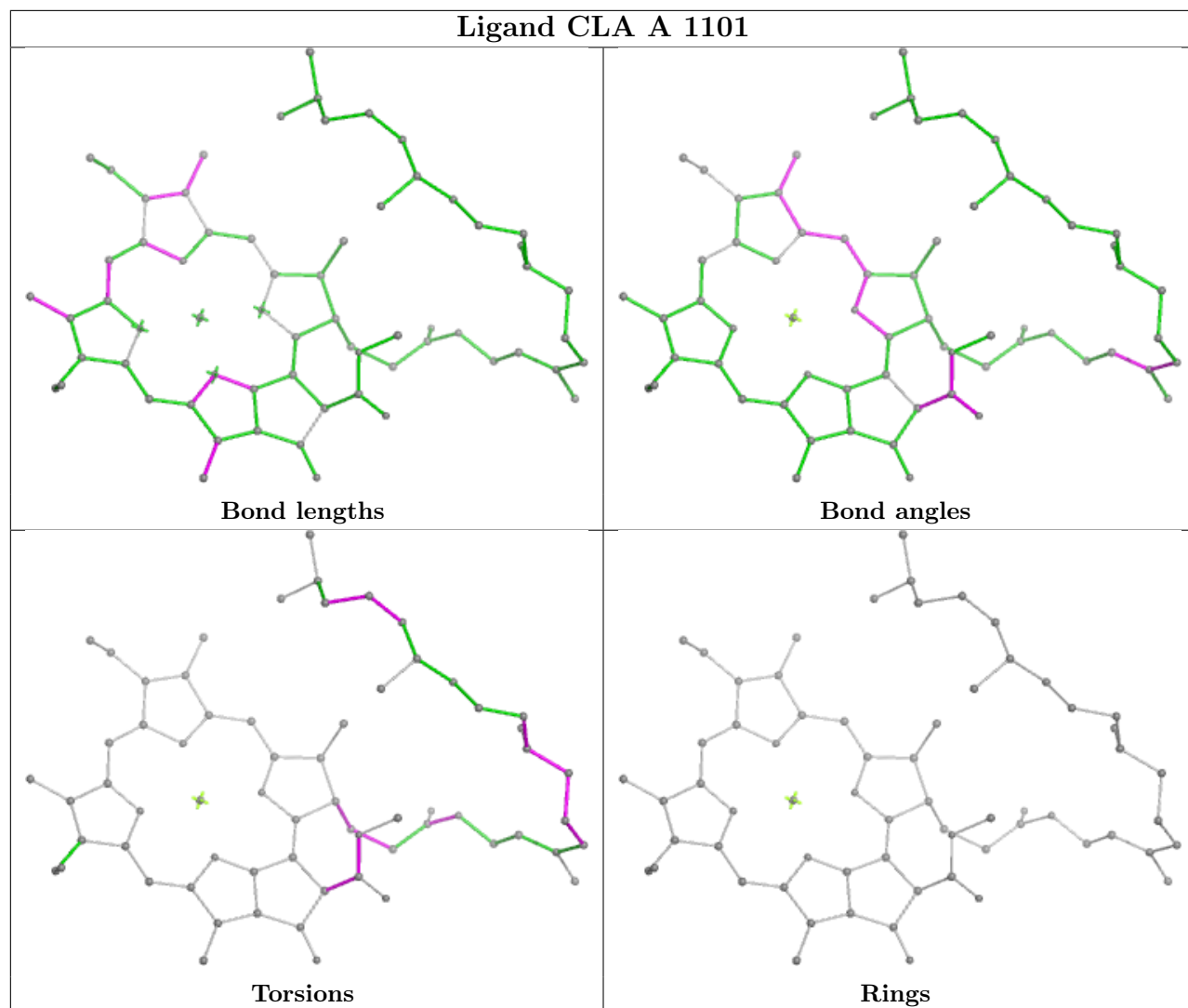


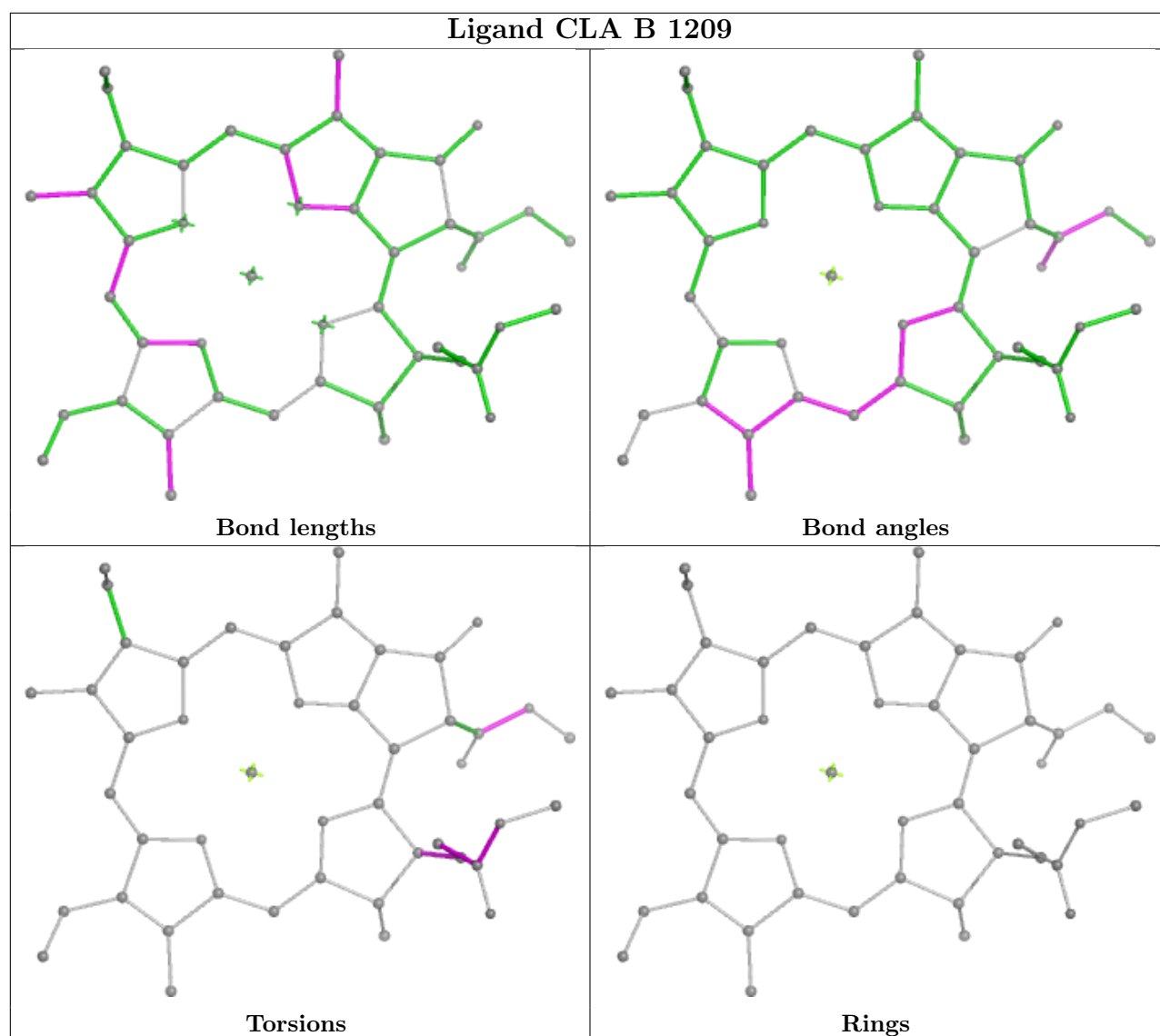




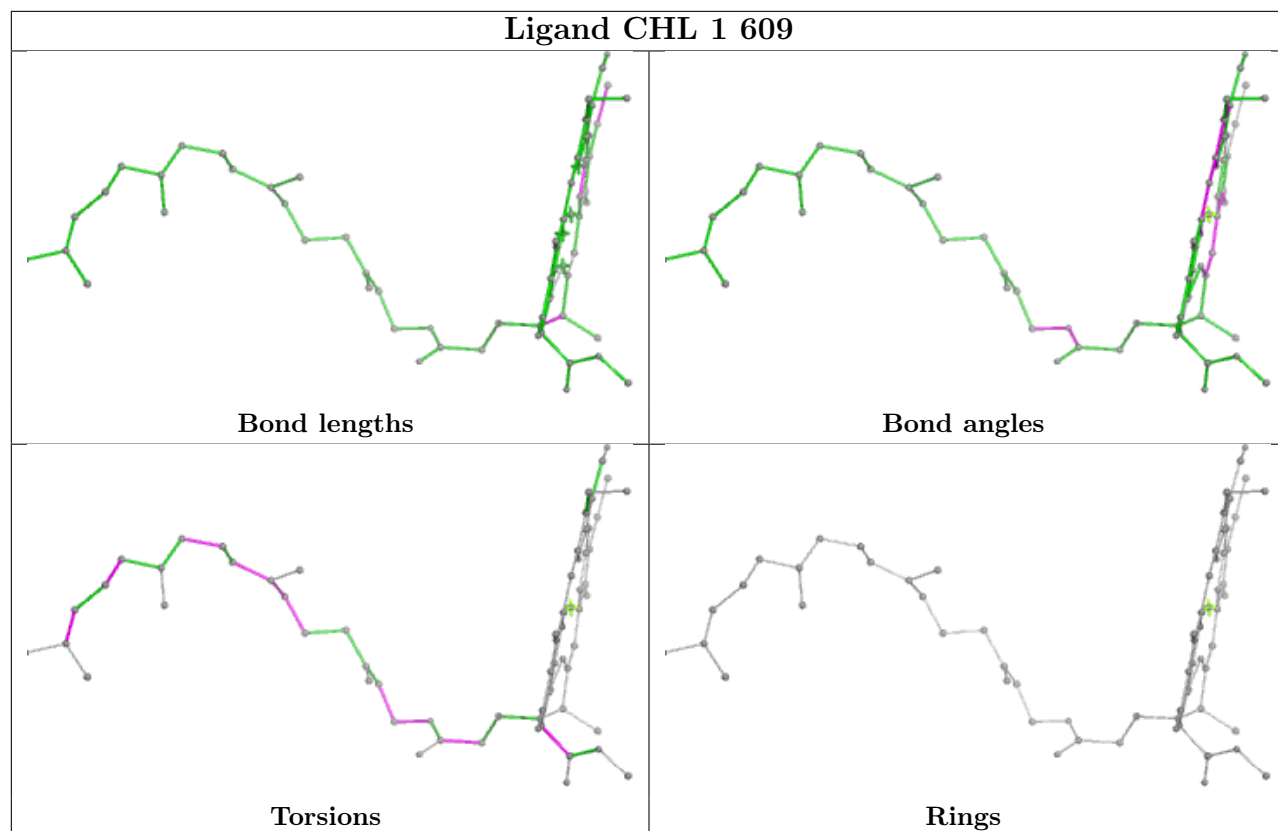
Ligand CLA 1 603



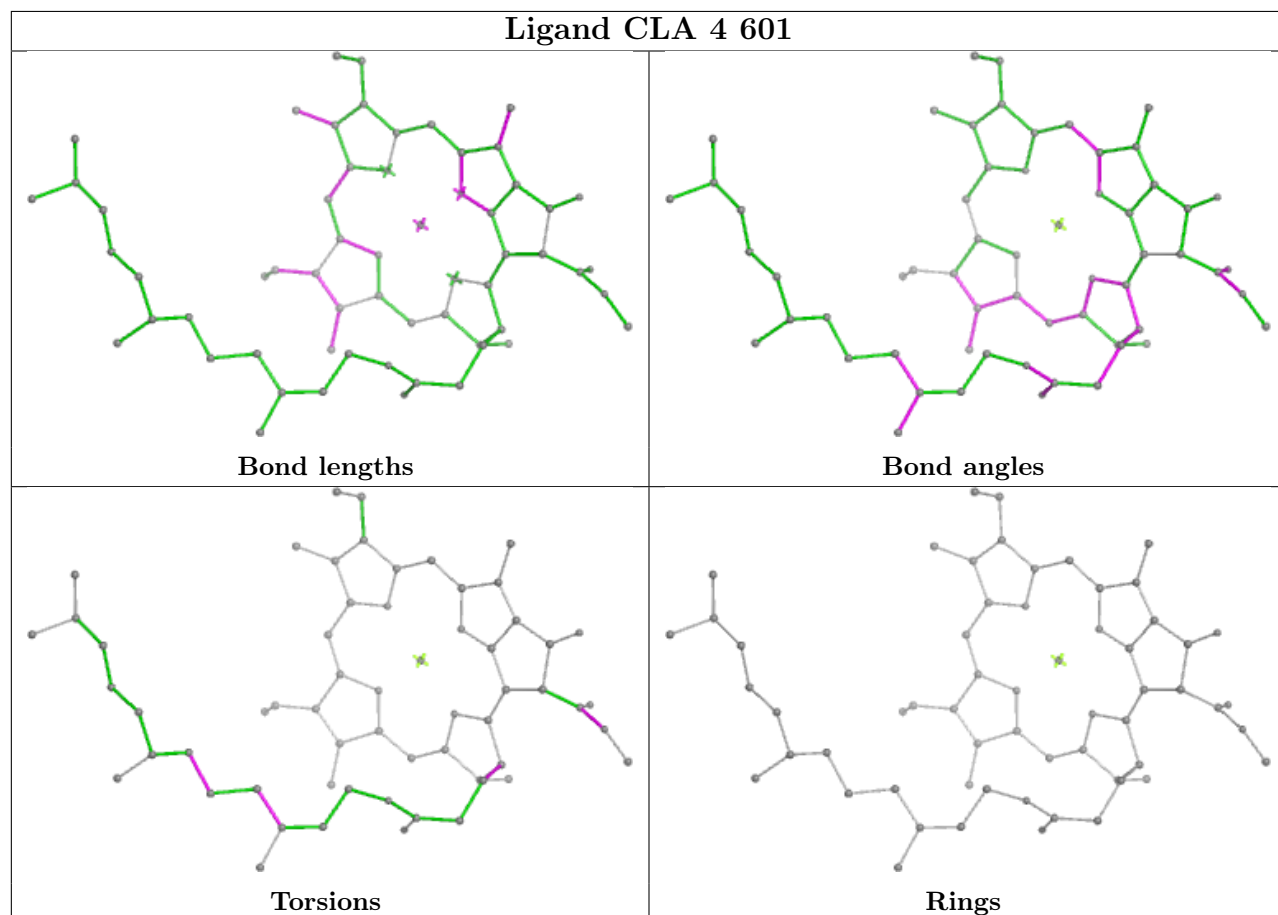


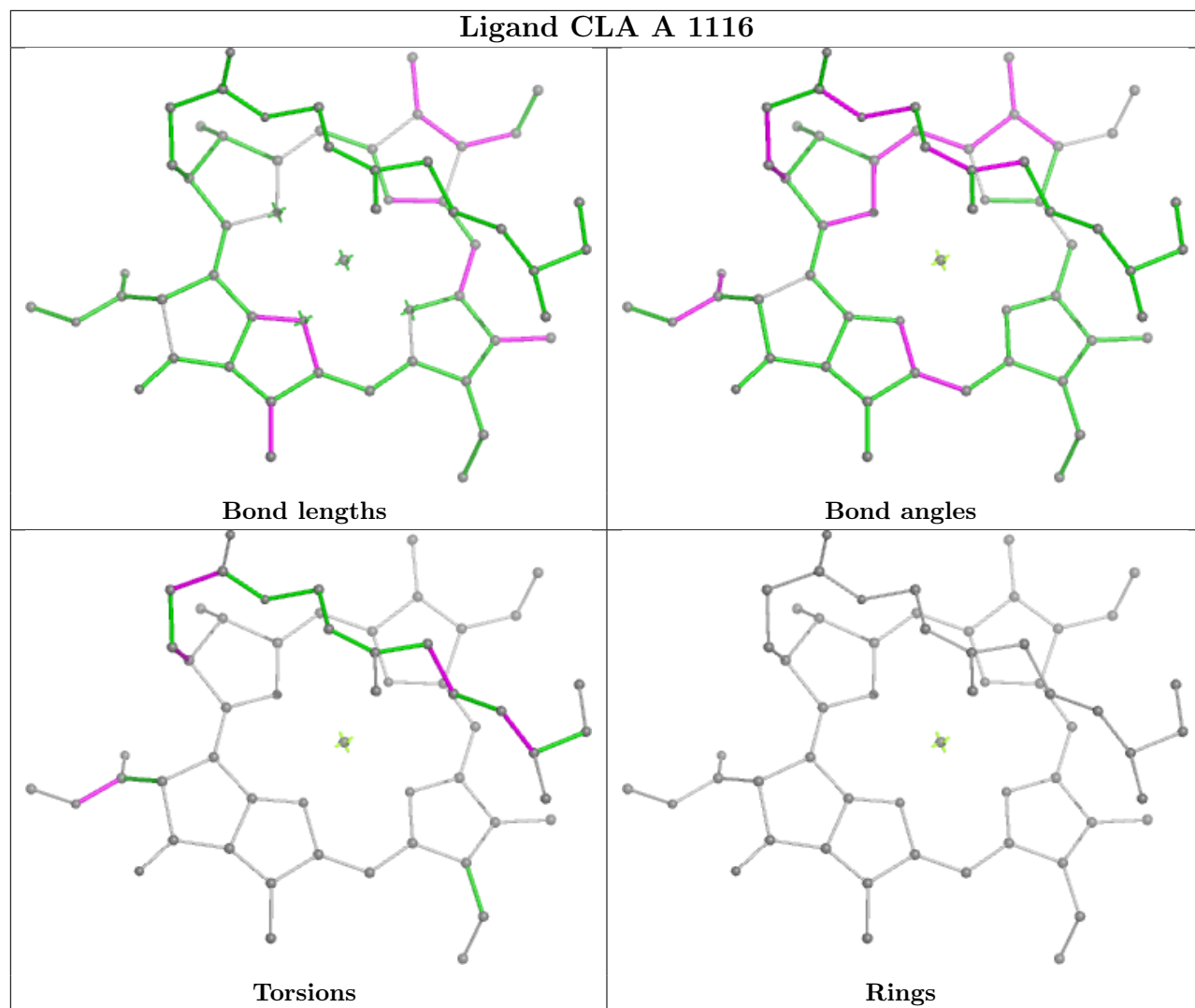


Ligand CHL 1 609

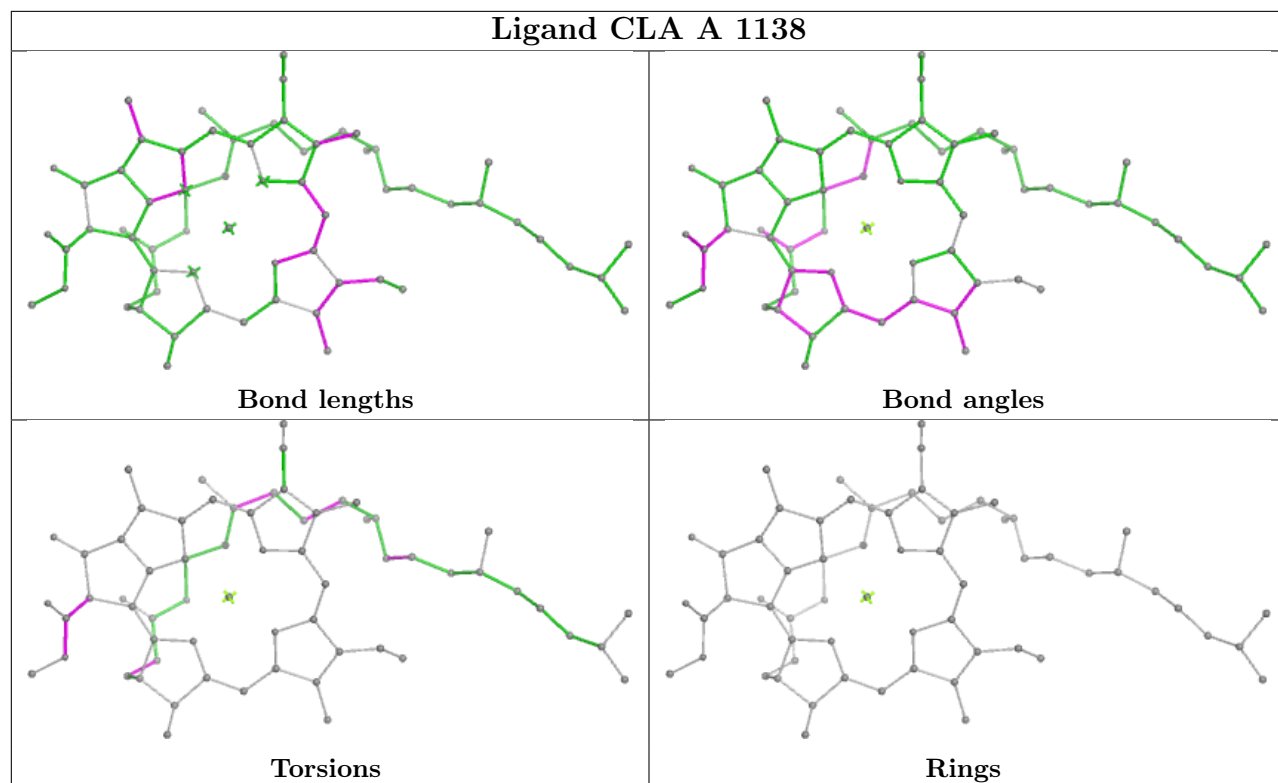


Ligand CLA 4 601

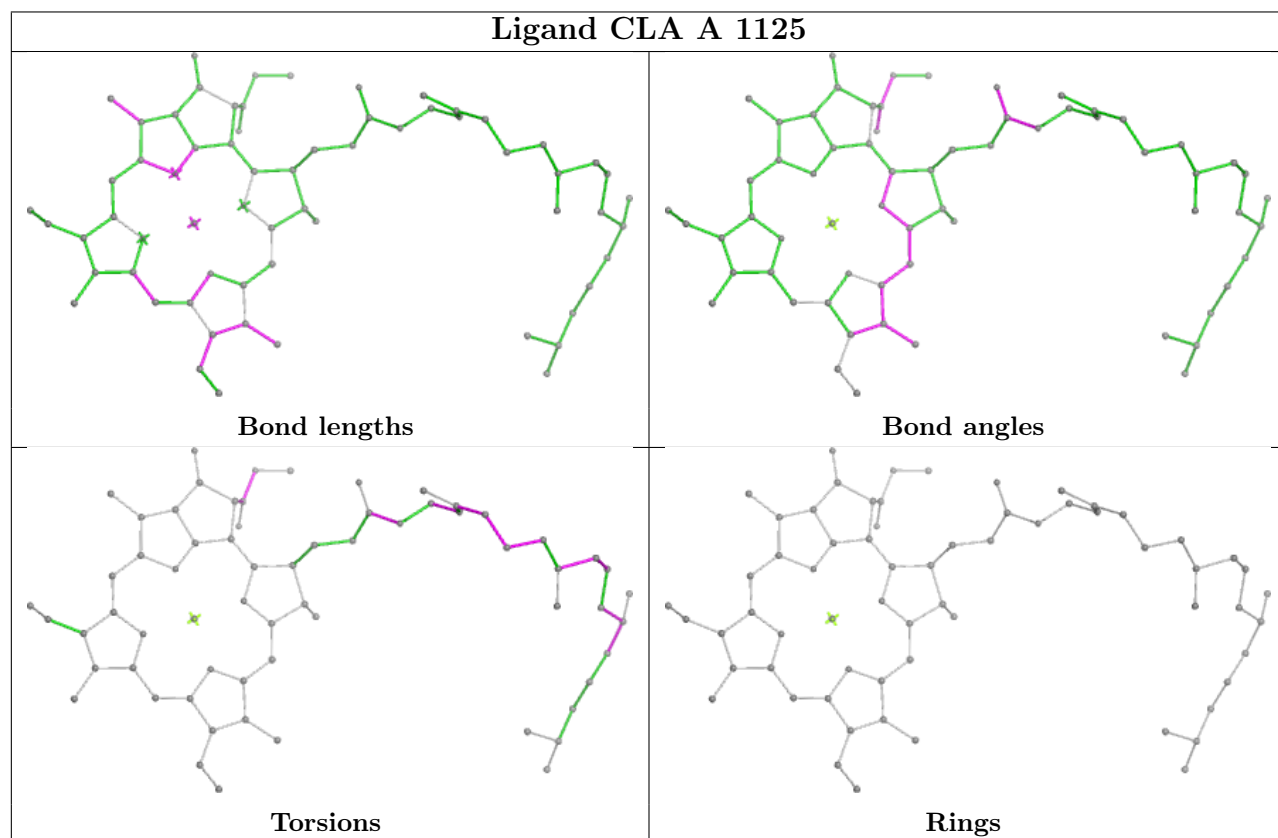


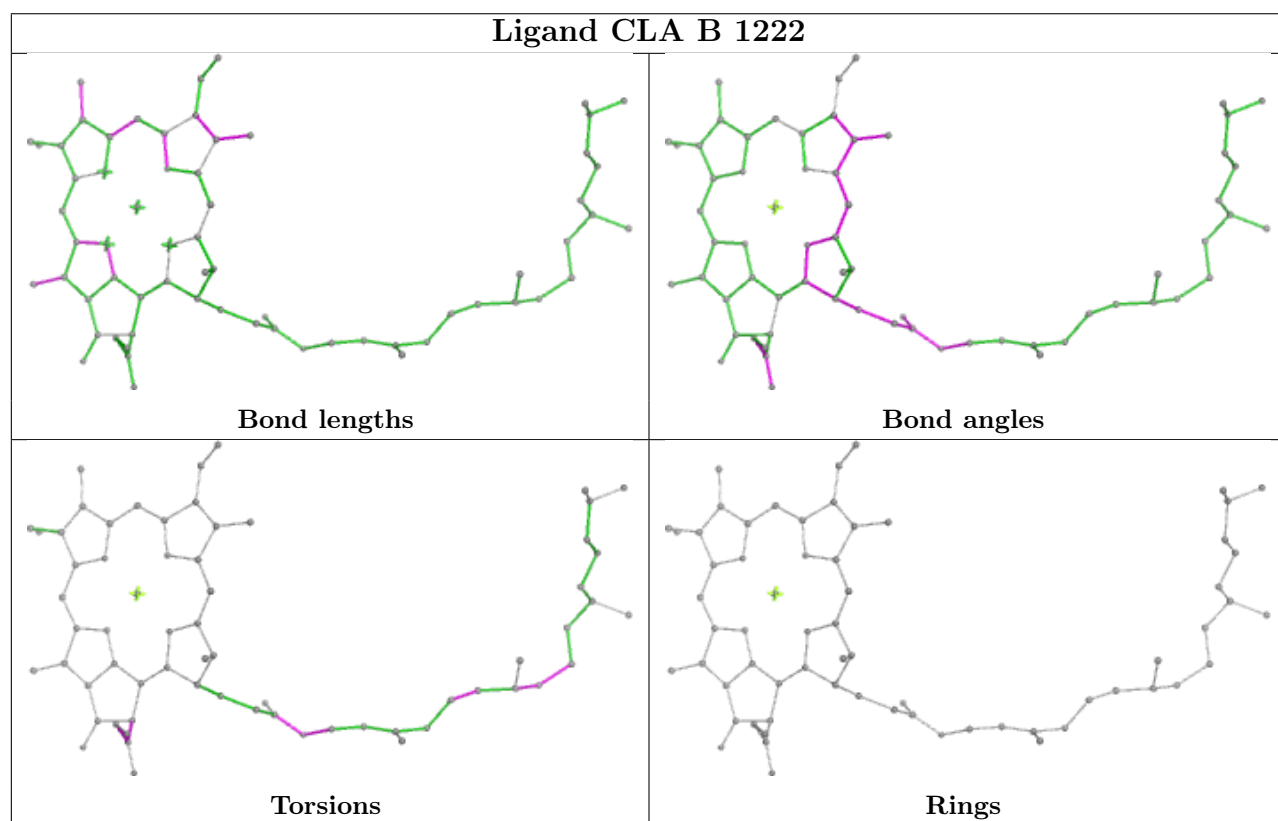
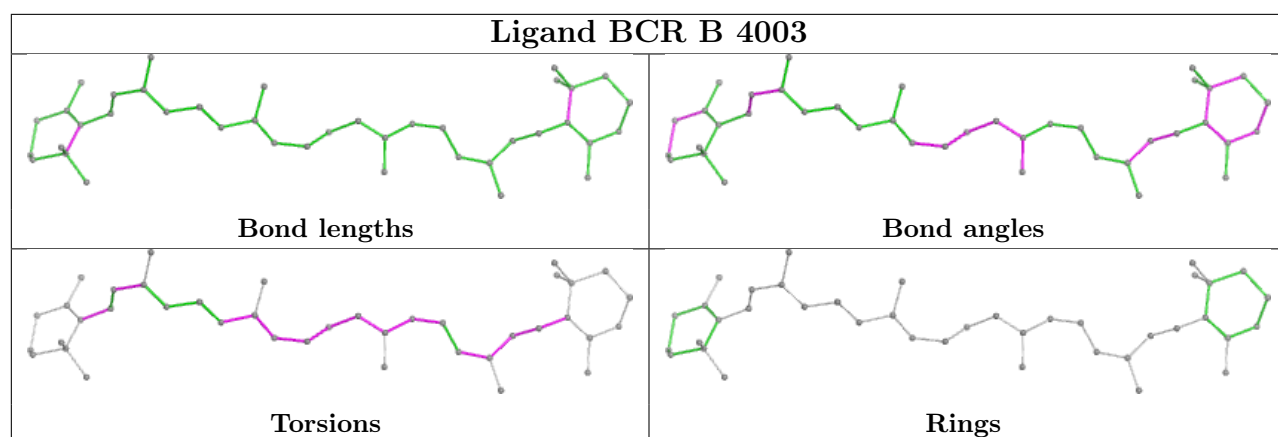


Ligand CLA A 1138

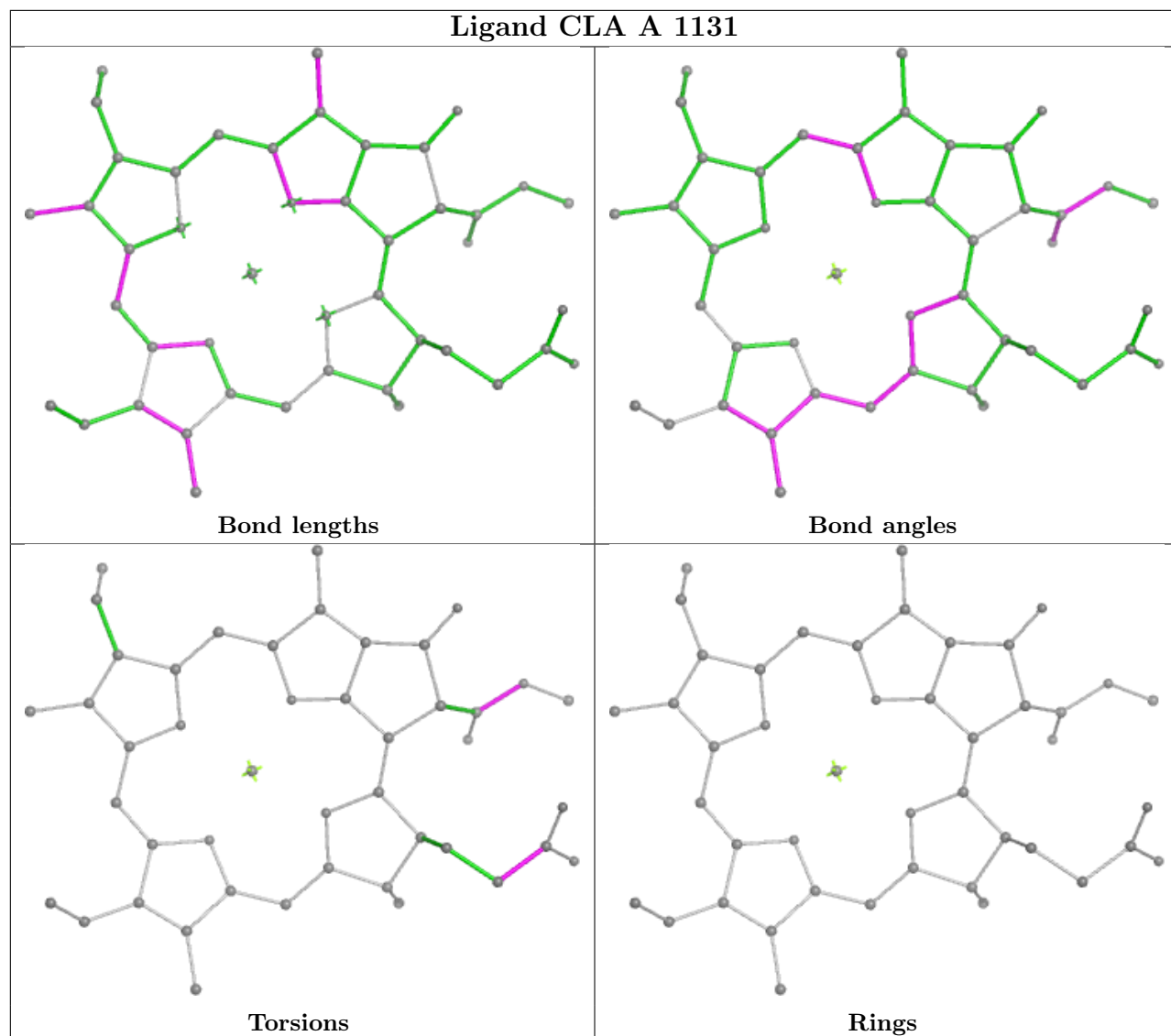


Ligand CLA A 1125

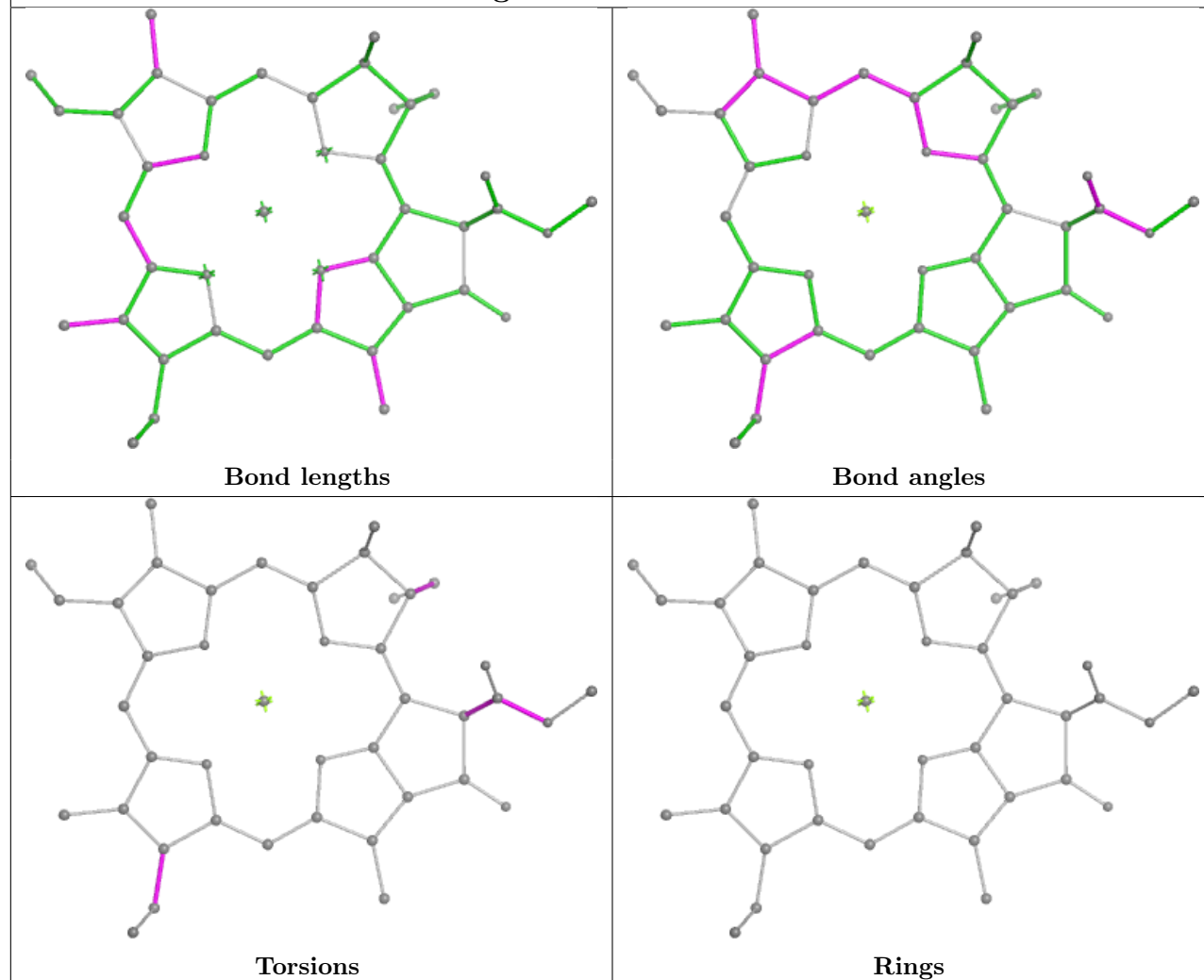




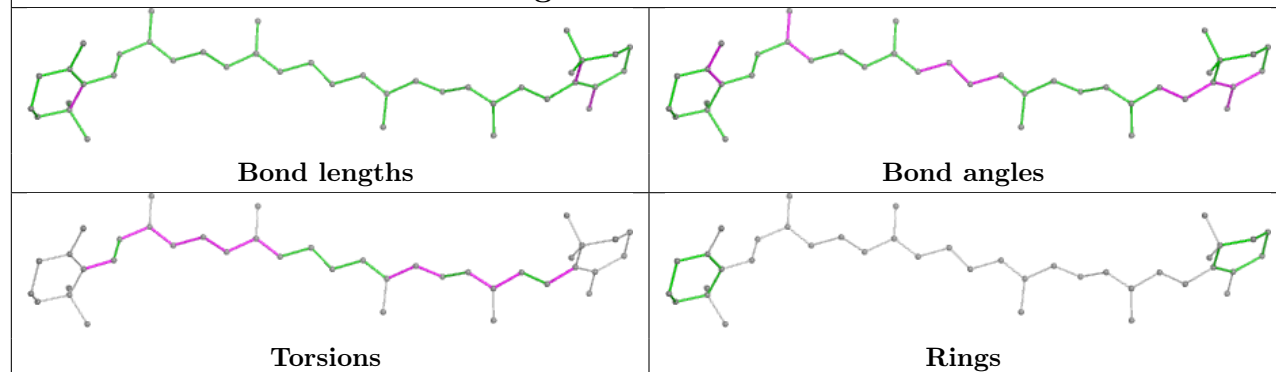
Ligand CLA A 1131



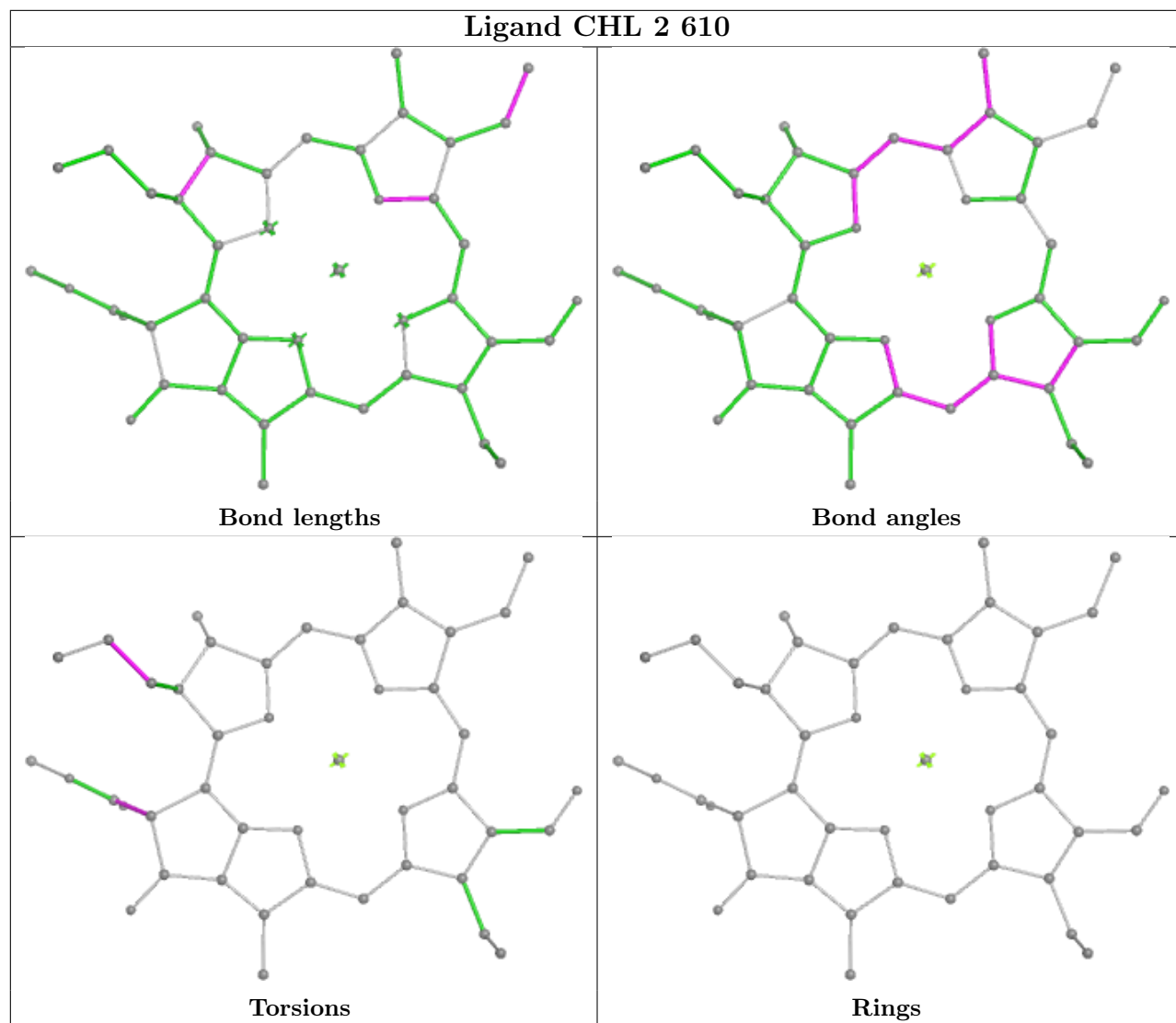
Ligand CLA A 1120



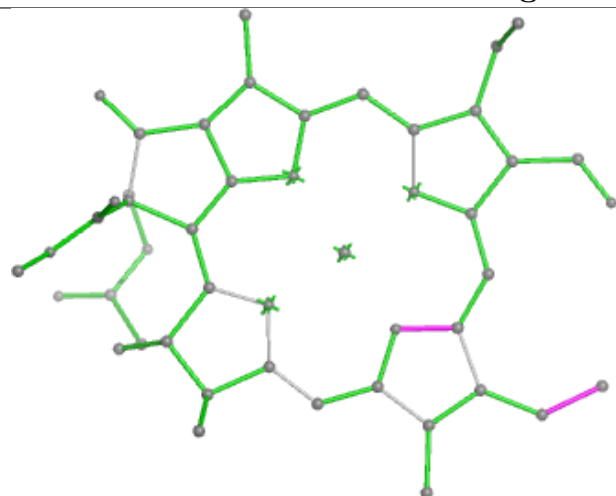
Ligand BCR 2 503



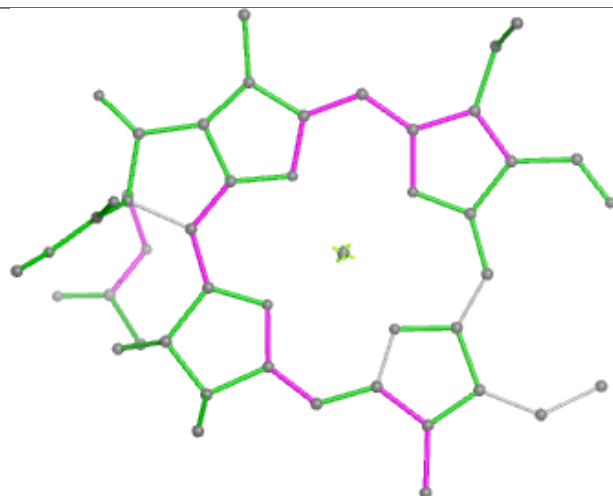
Ligand CHL 2 610



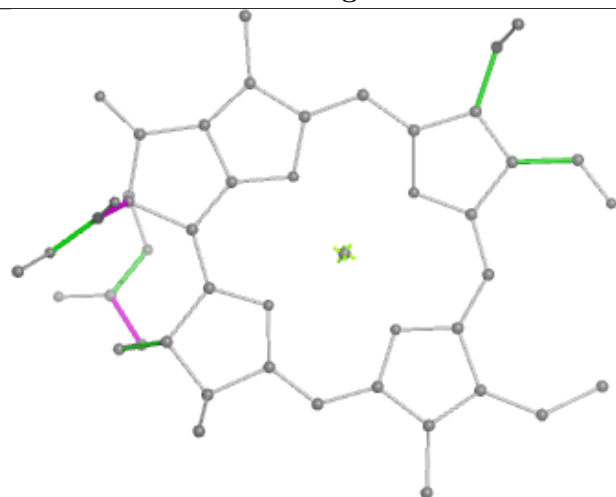
Ligand CHL 1 610



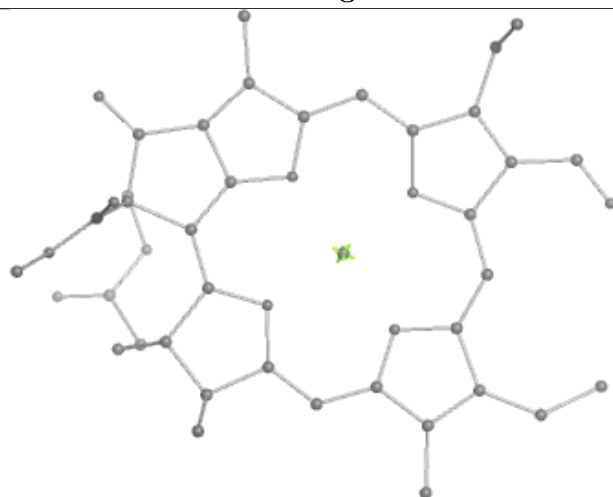
Bond lengths



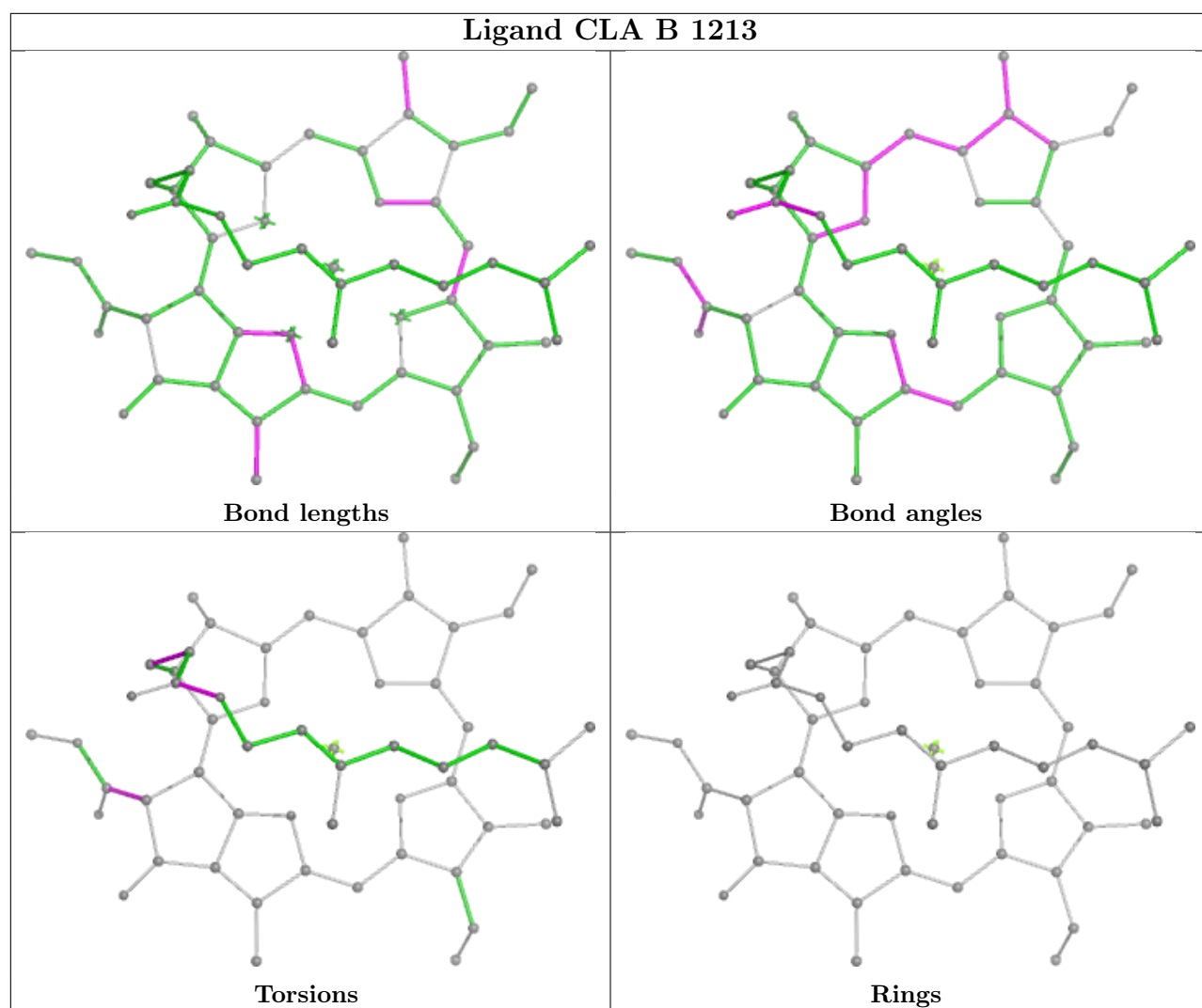
Bond angles



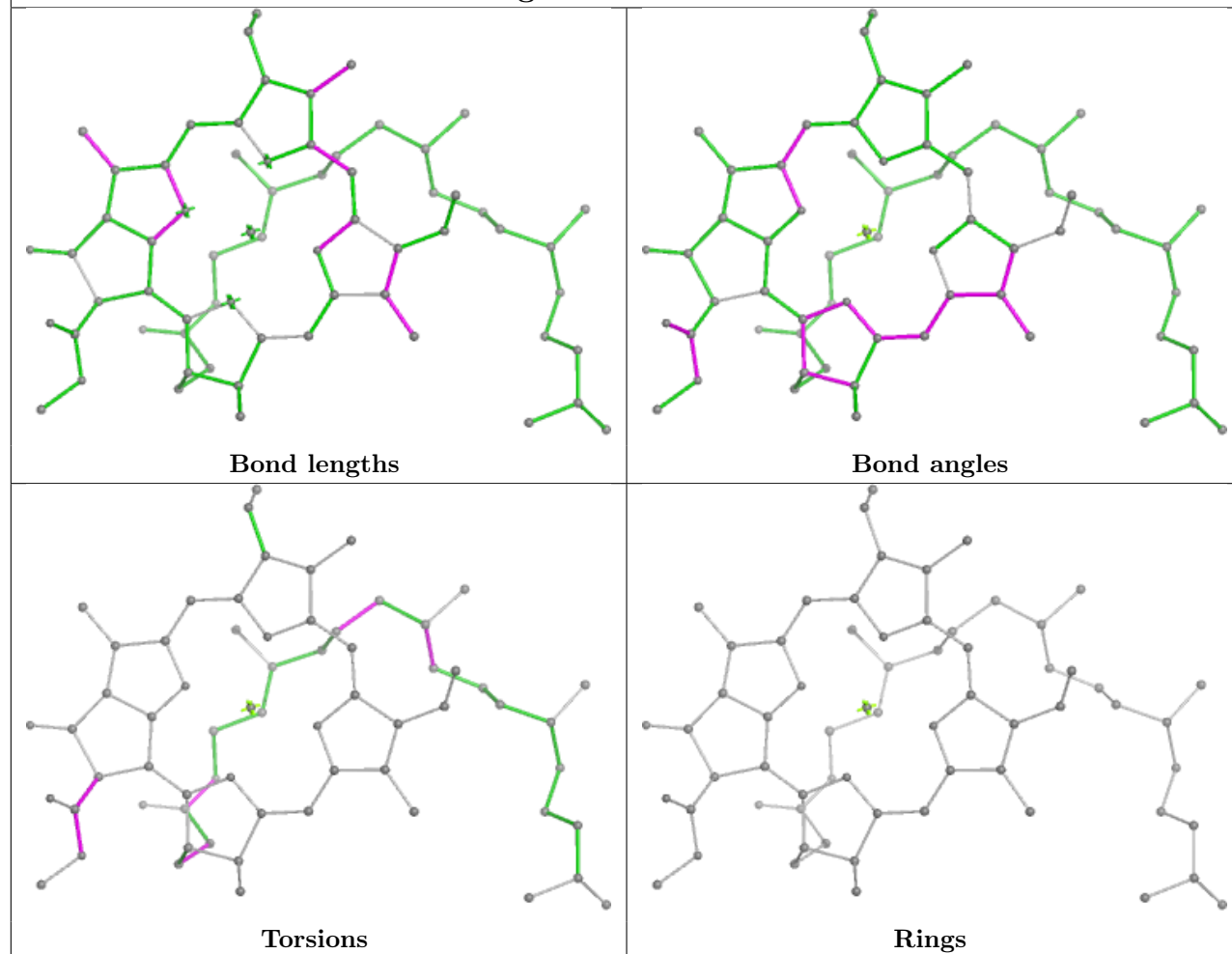
Torsions



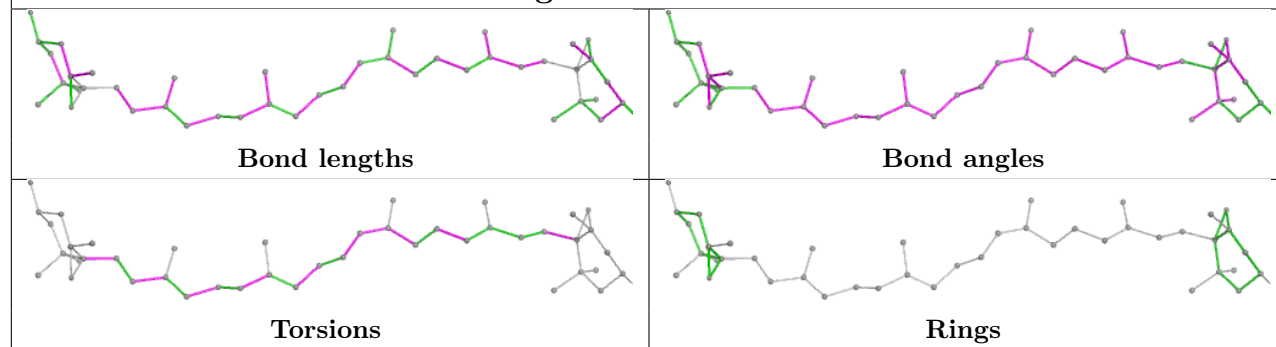
Rings

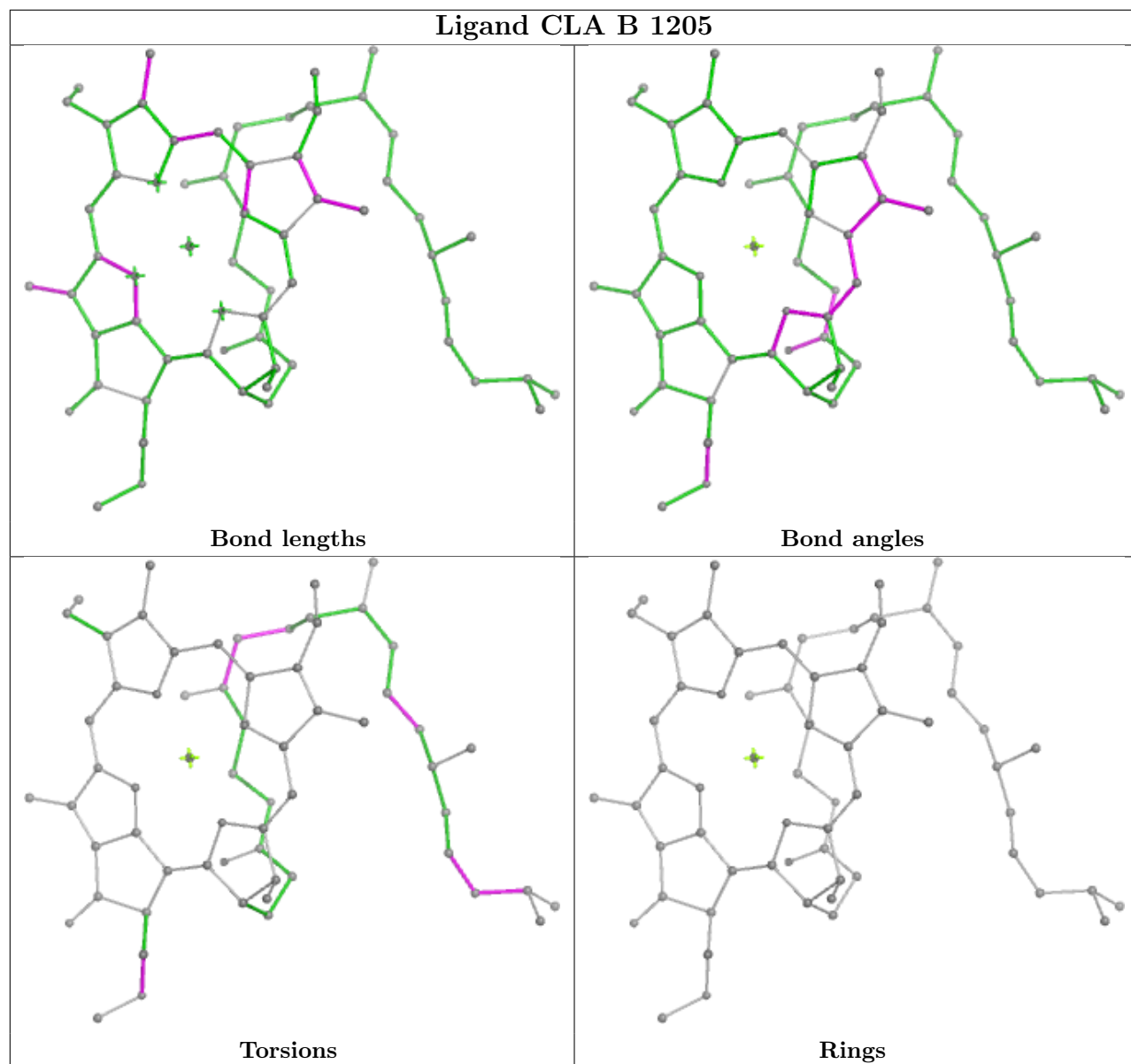


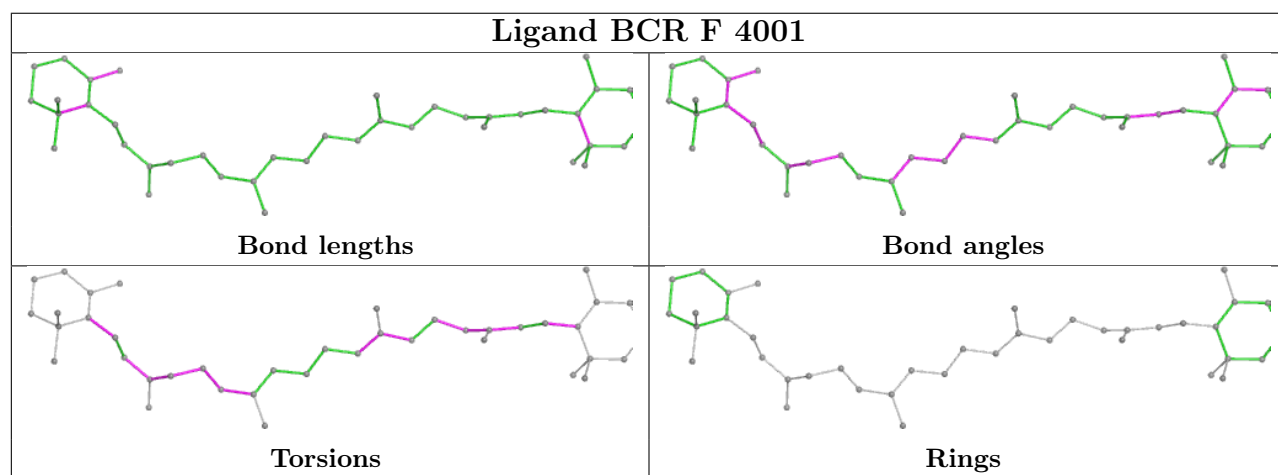
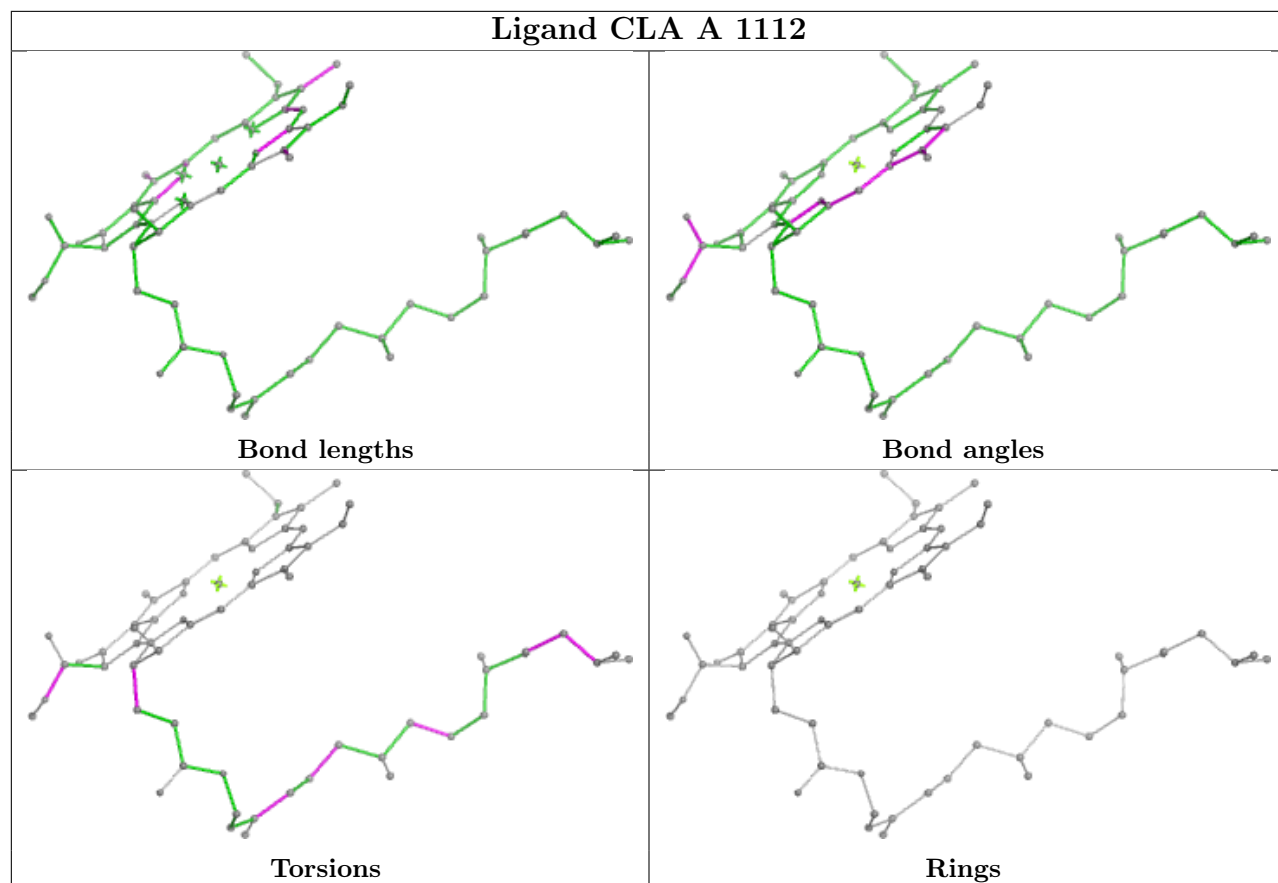
Ligand CLA 2 603

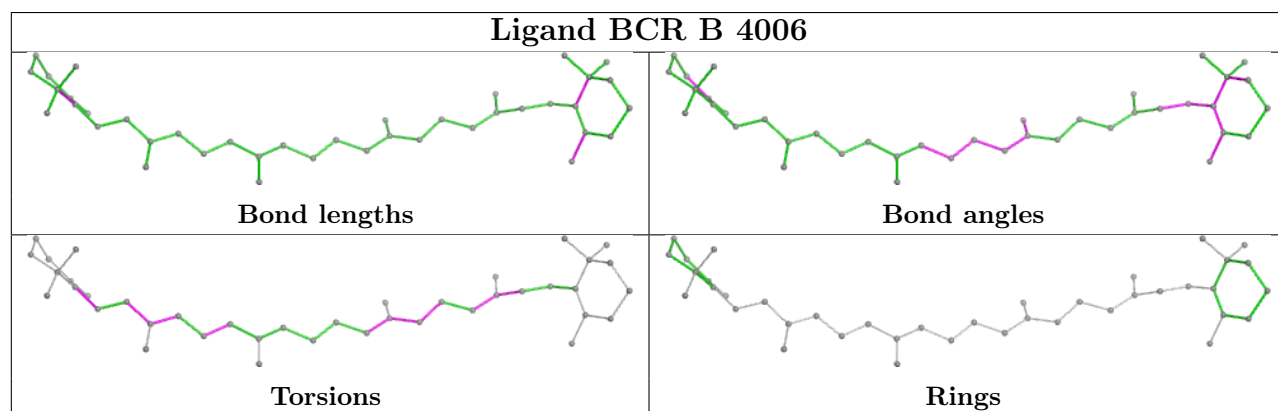
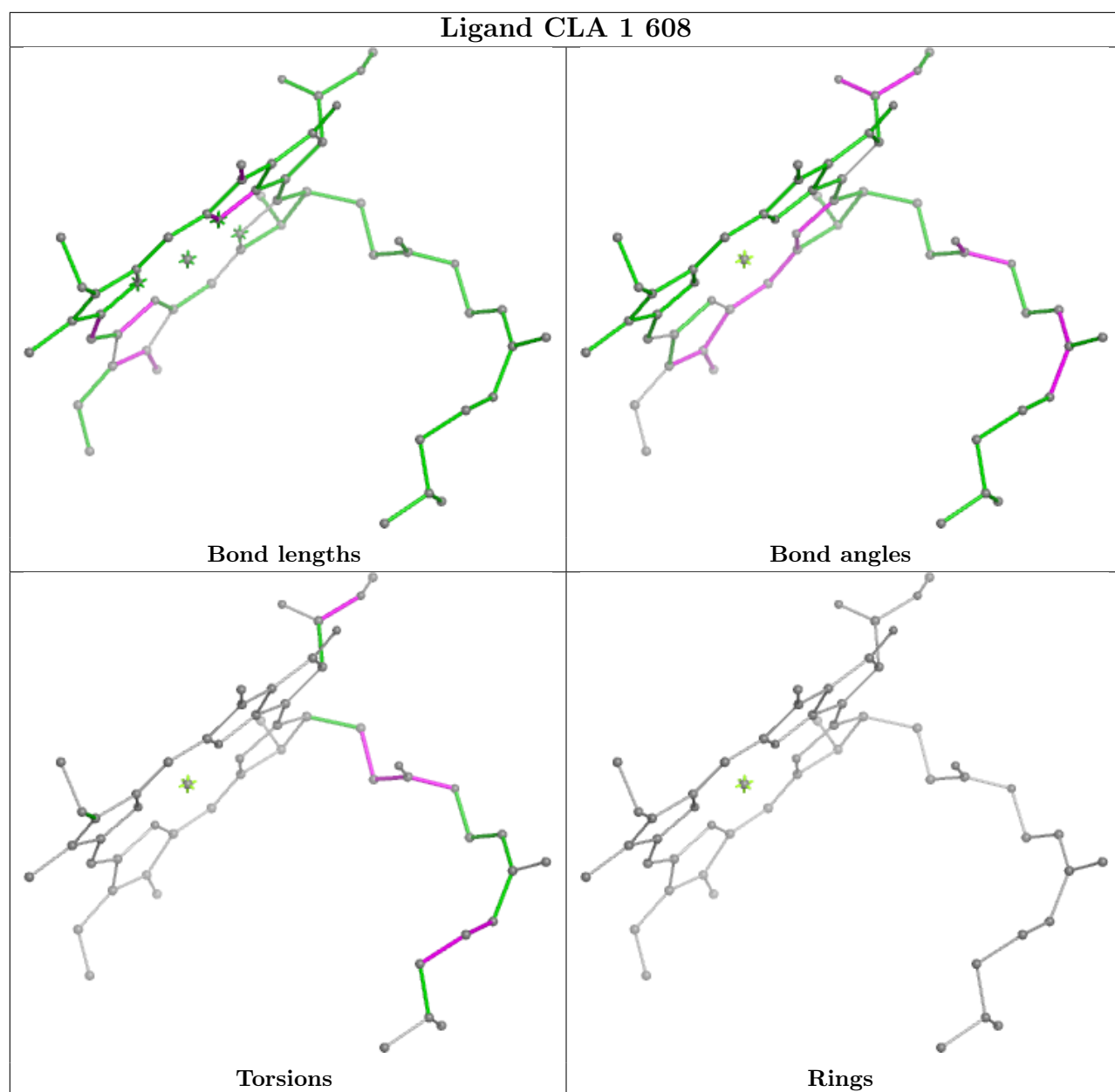


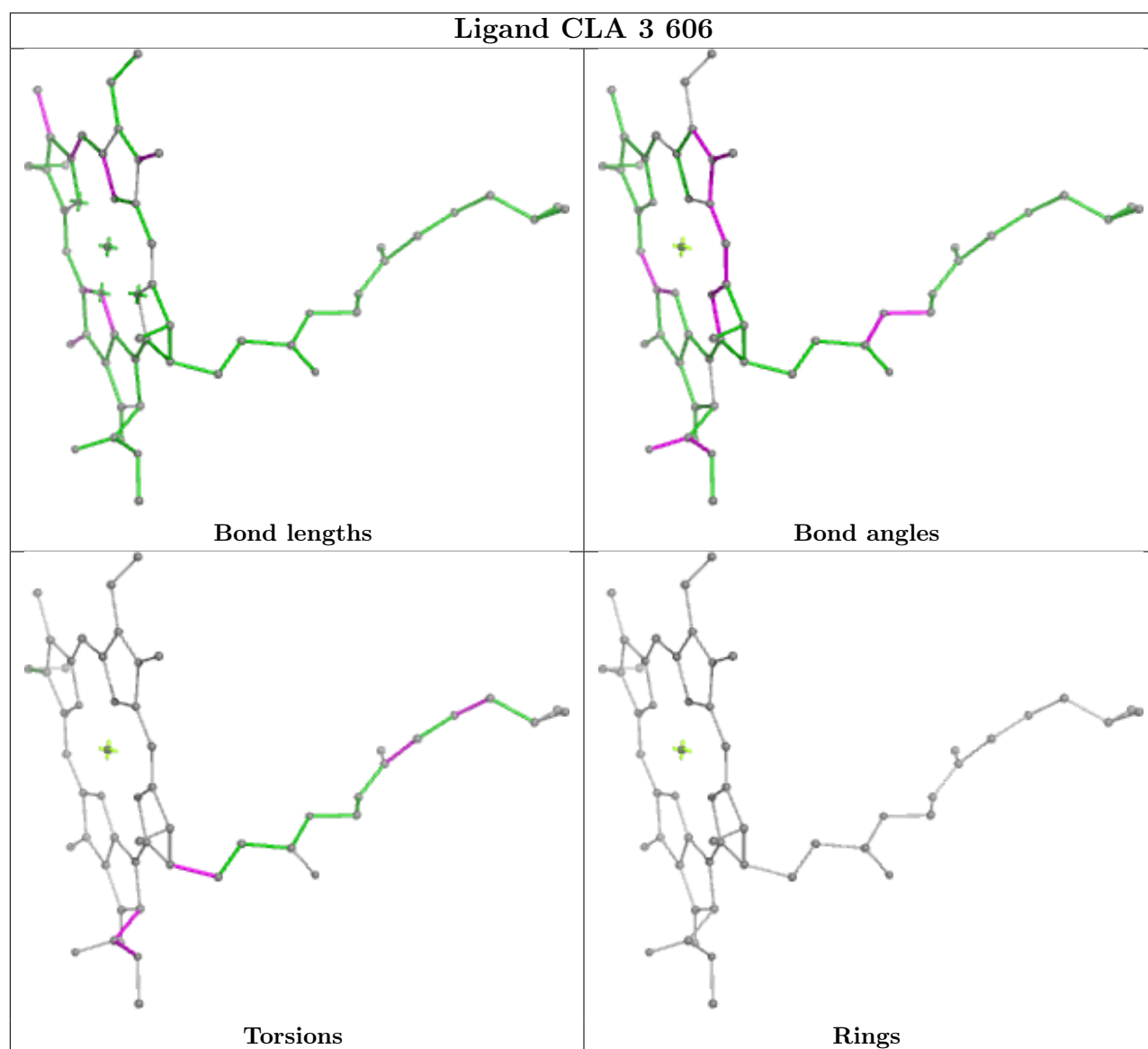
Ligand XAT 3 502



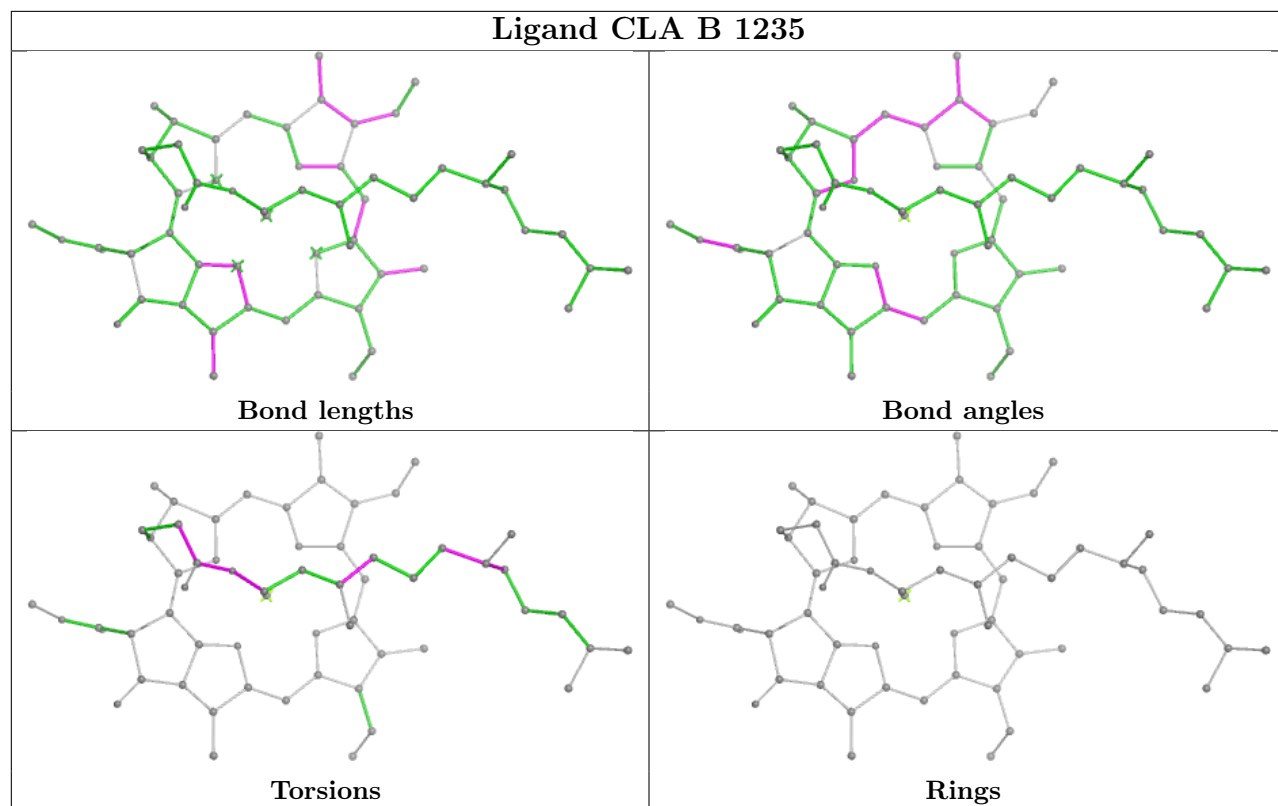




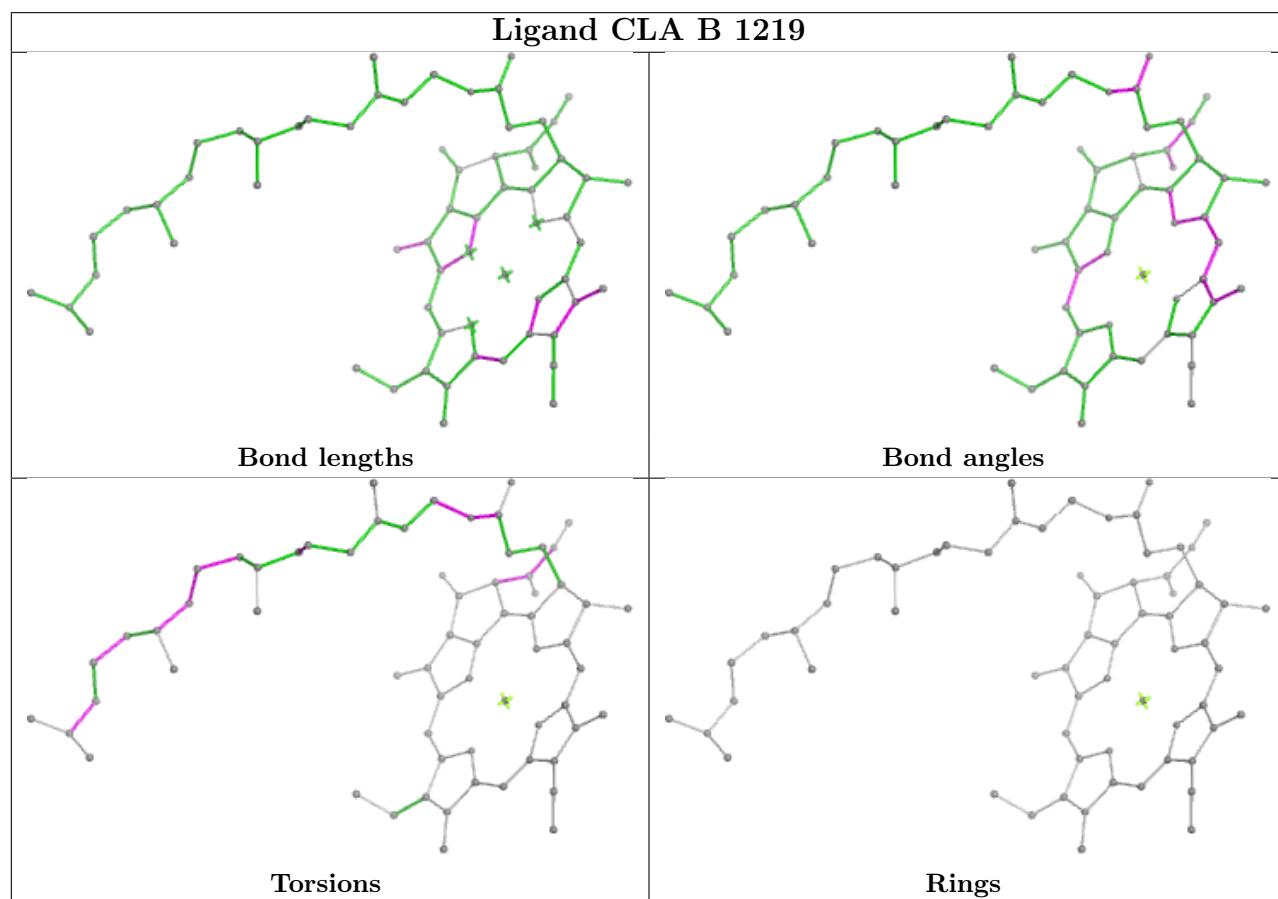


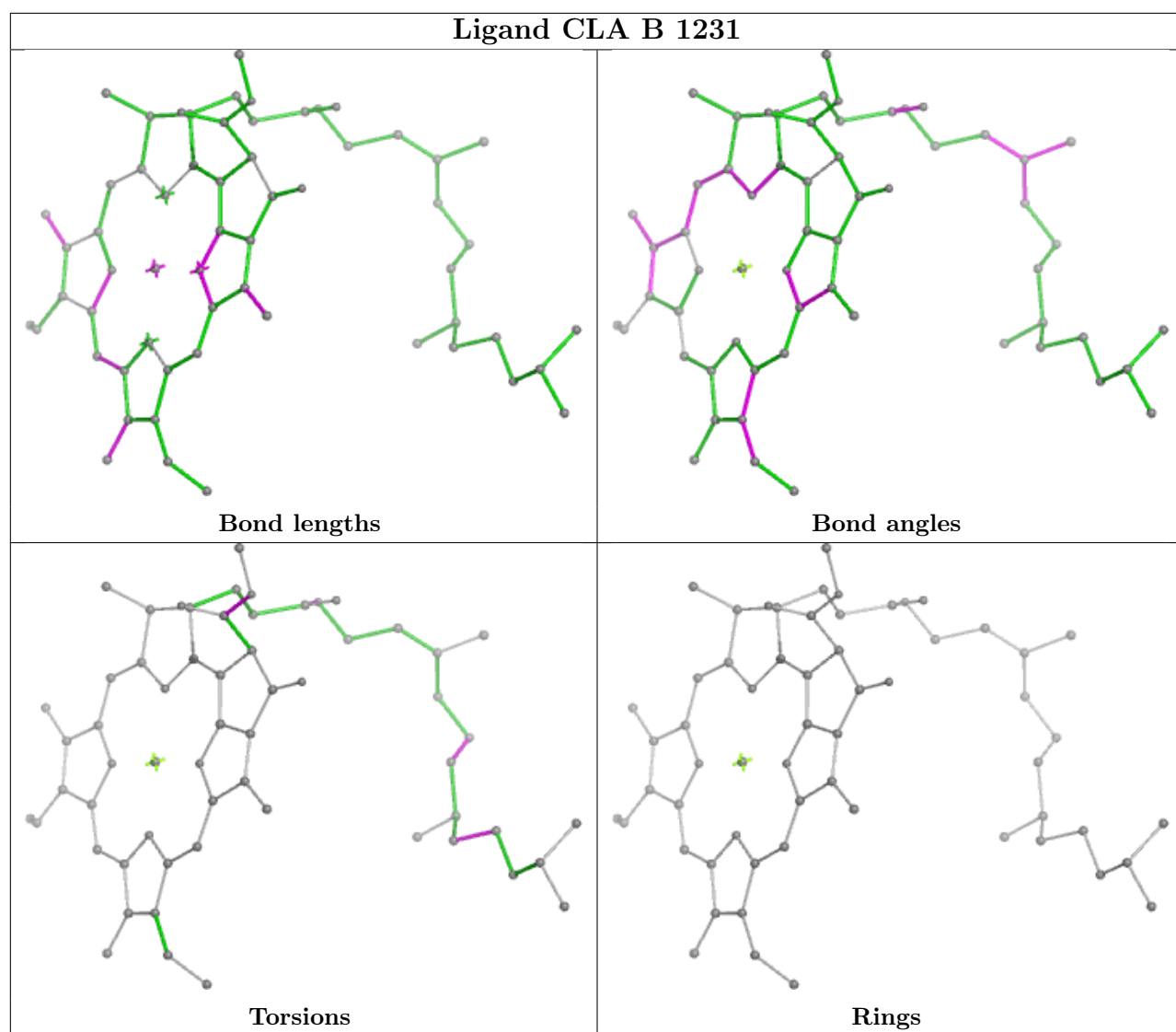


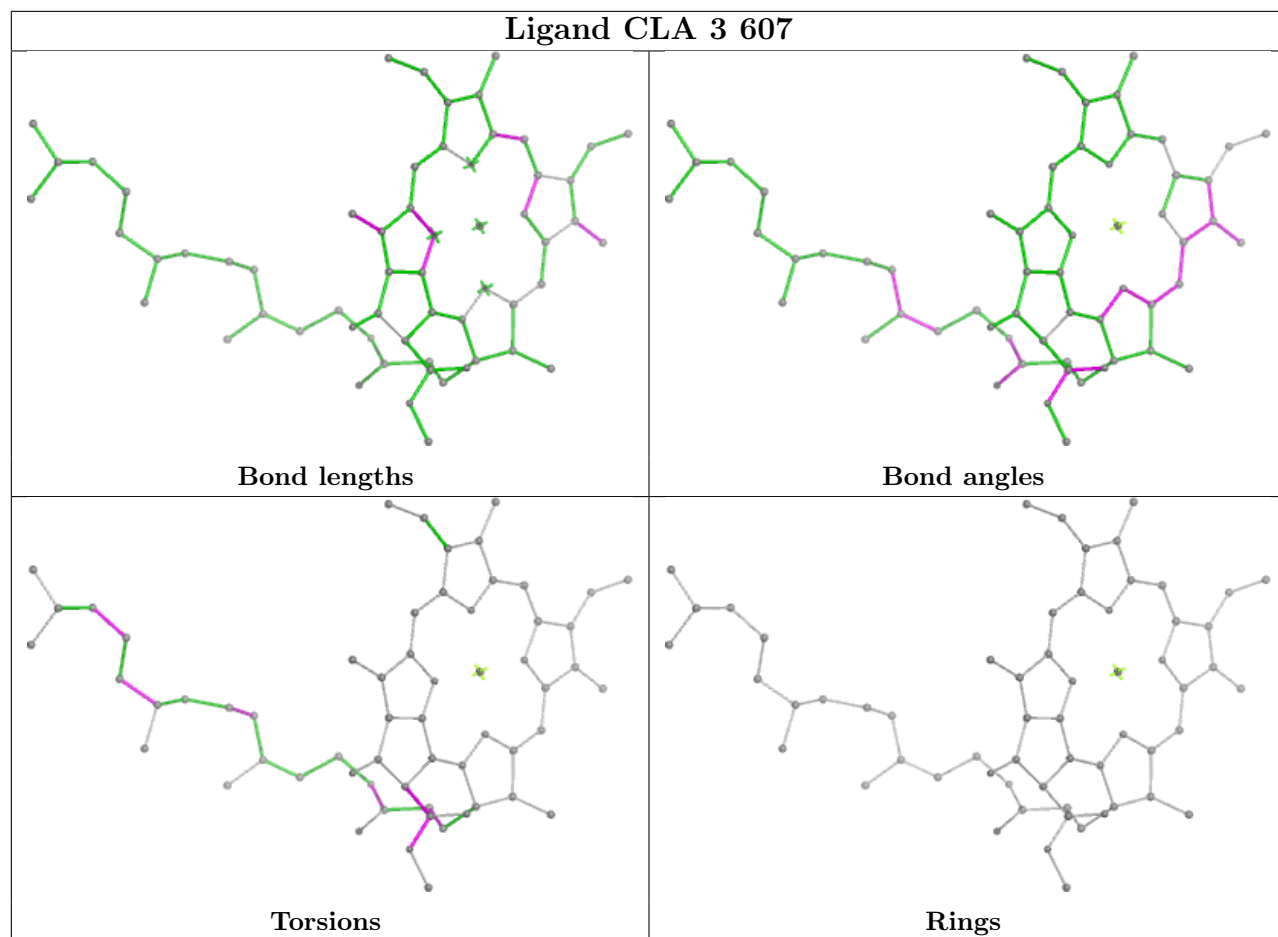
Ligand CLA B 1235

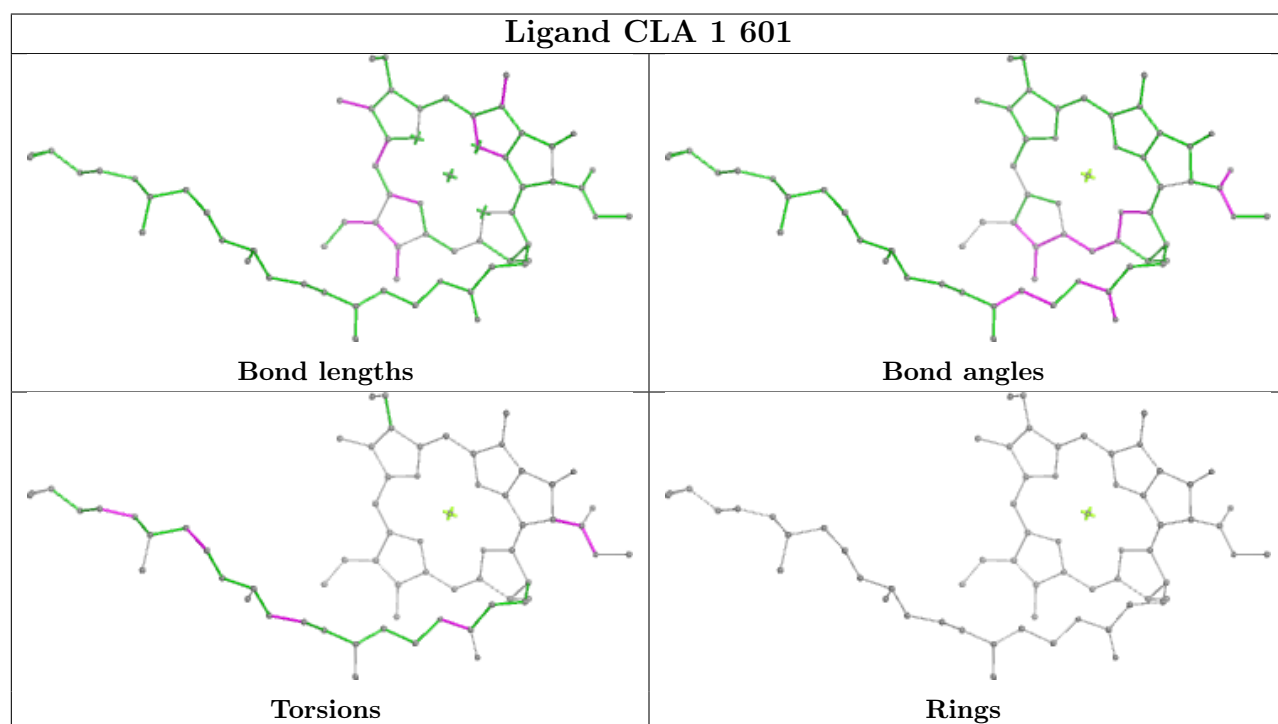
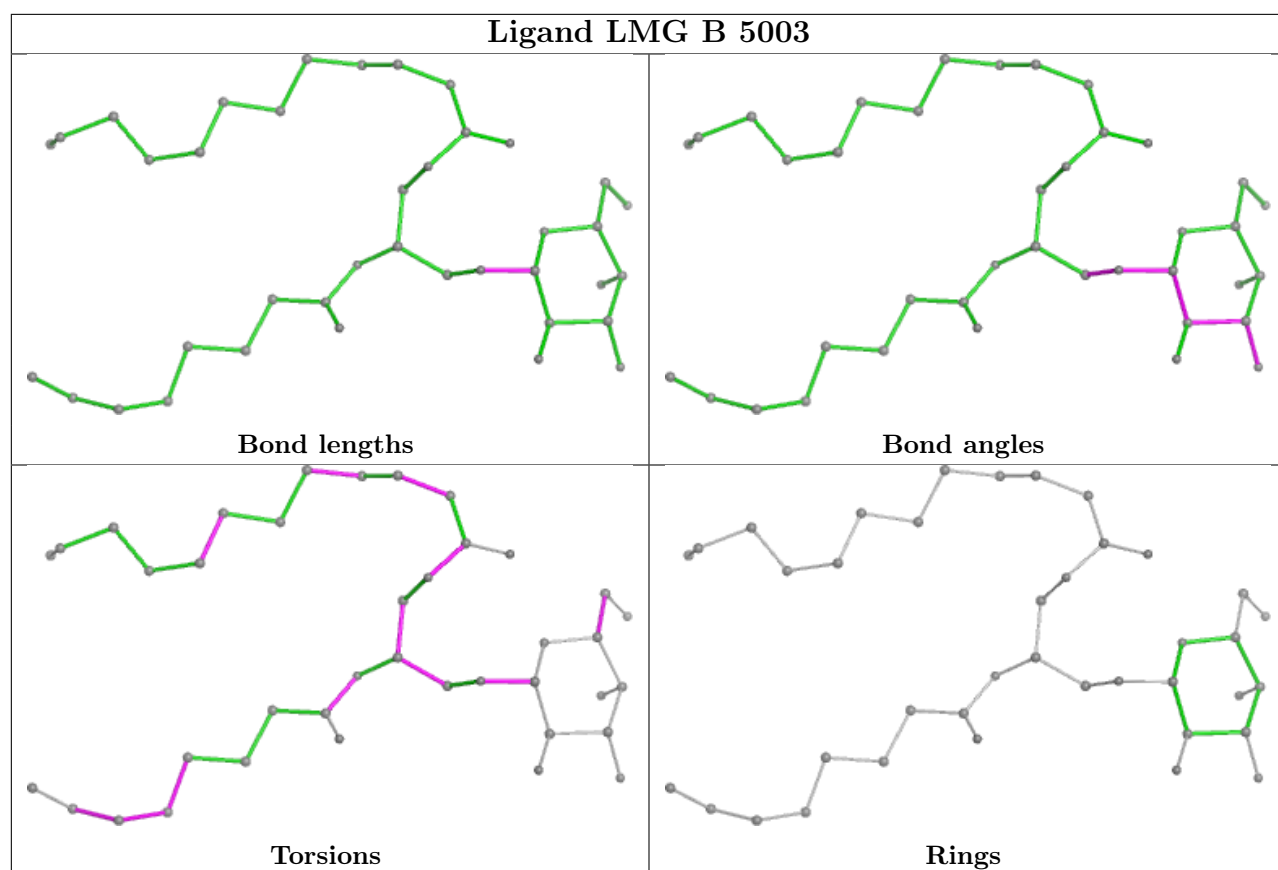


Ligand CLA B 1219

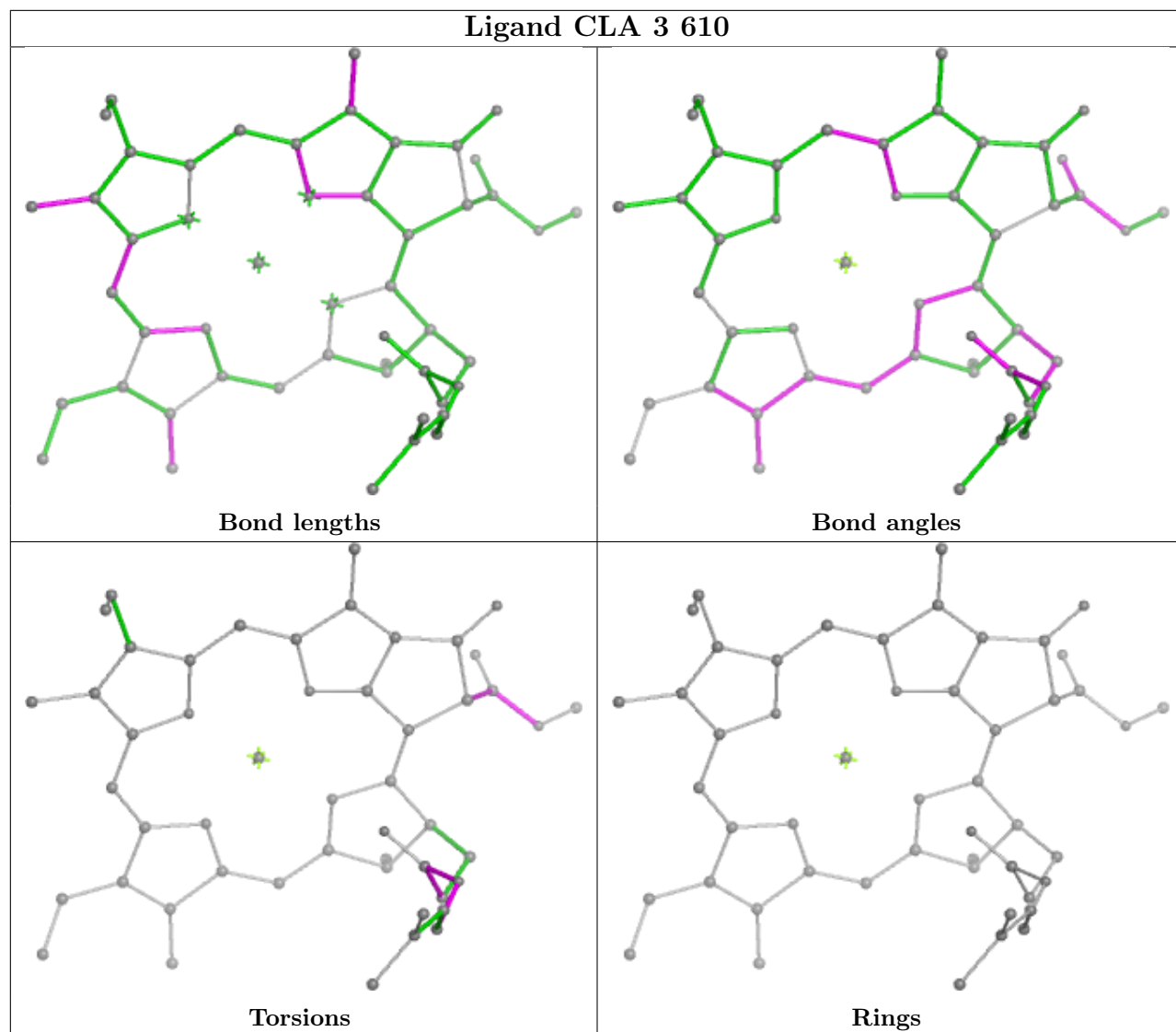


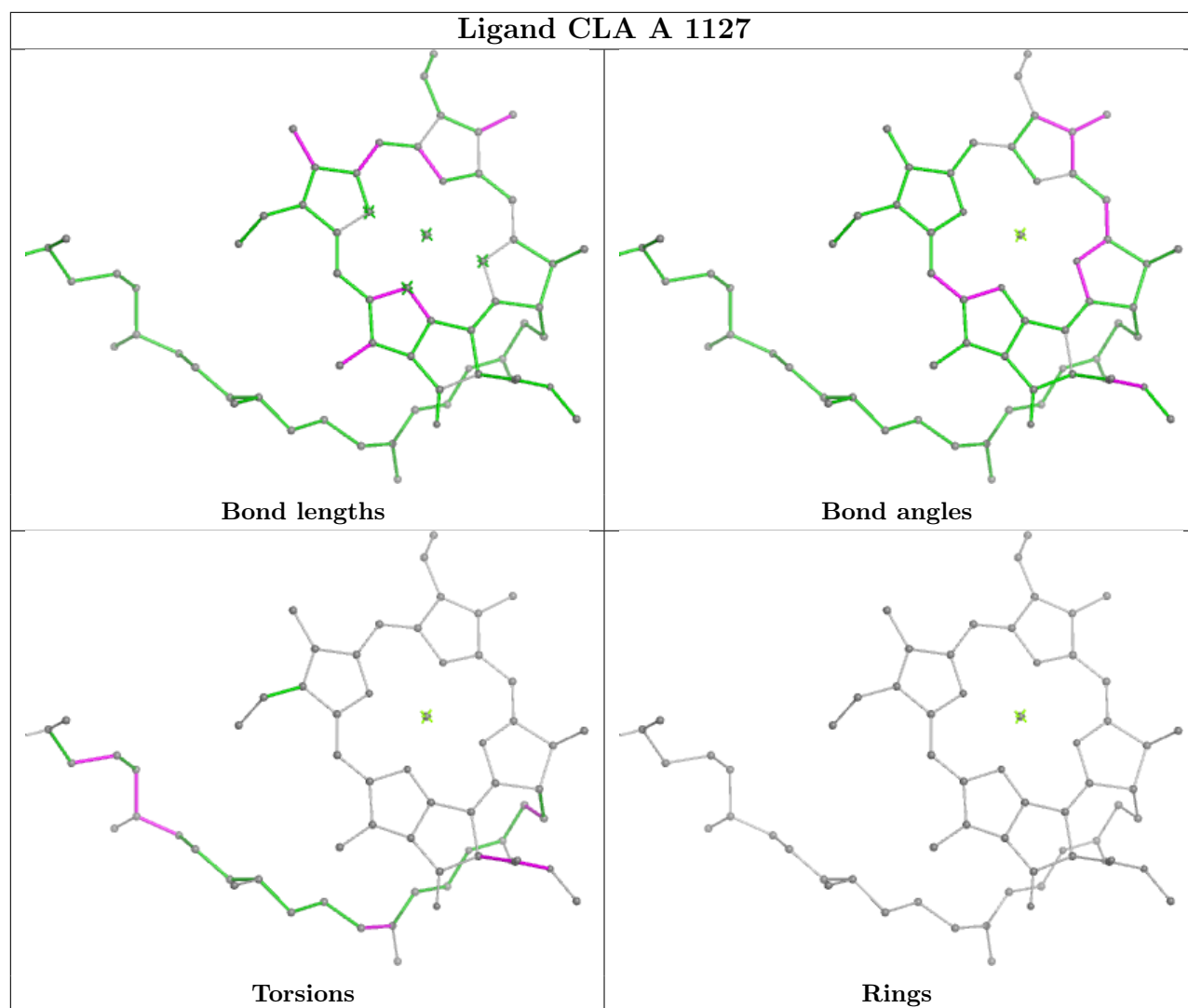
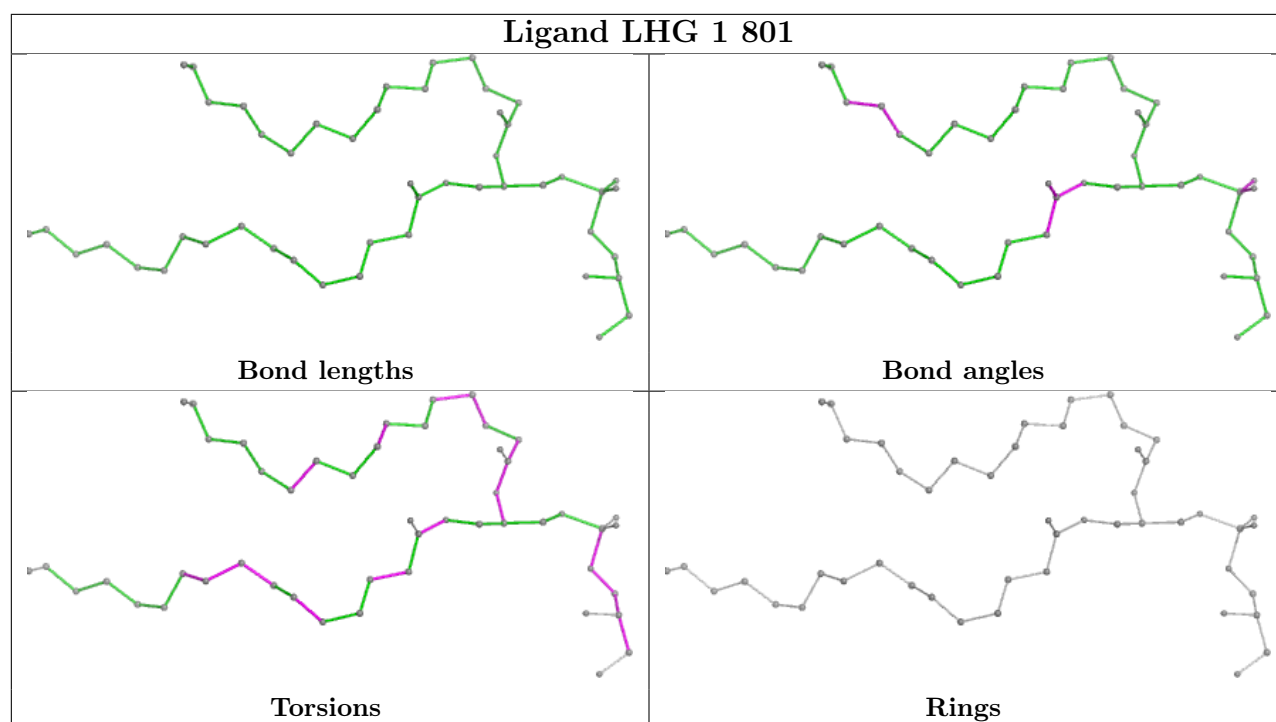




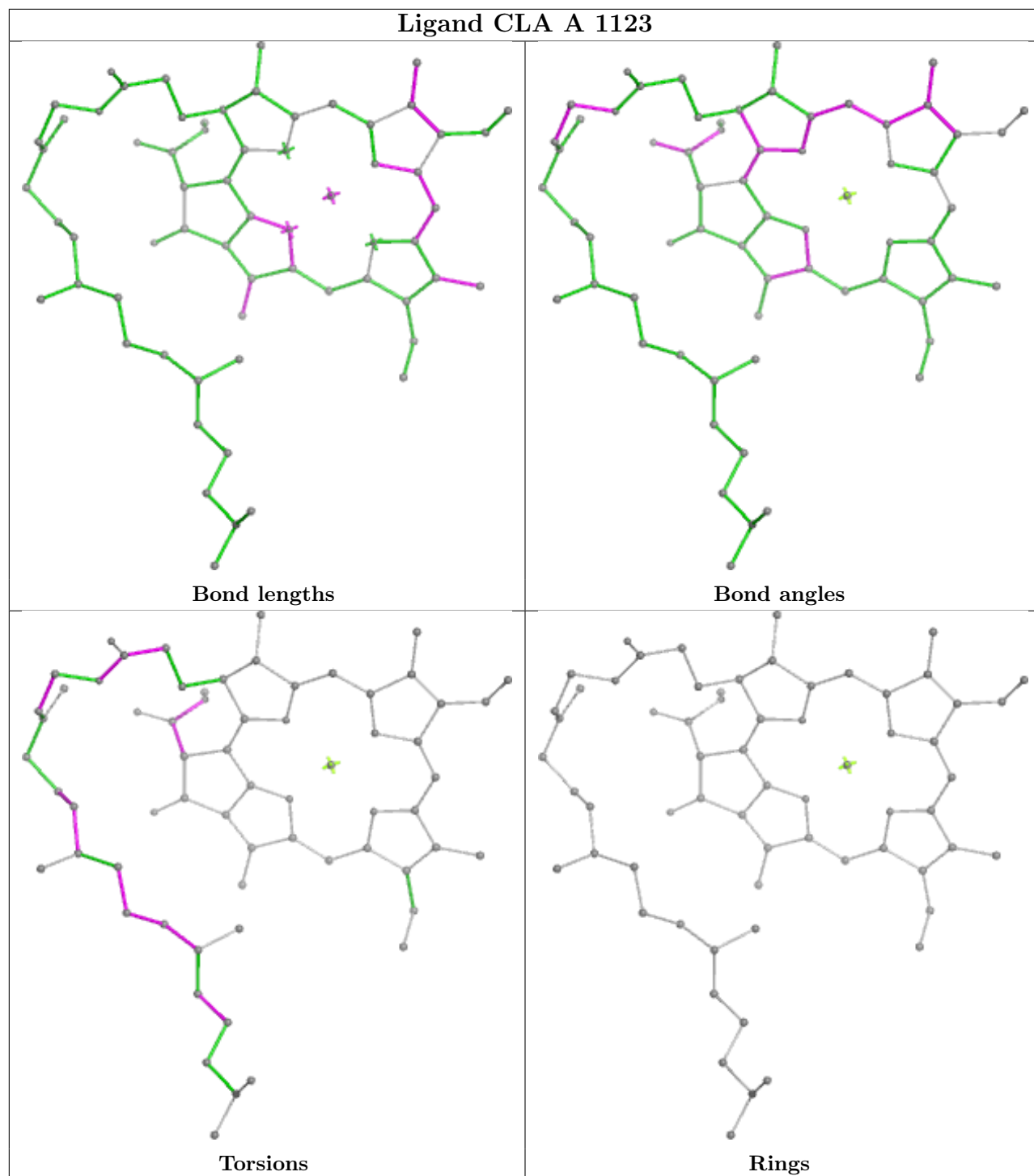


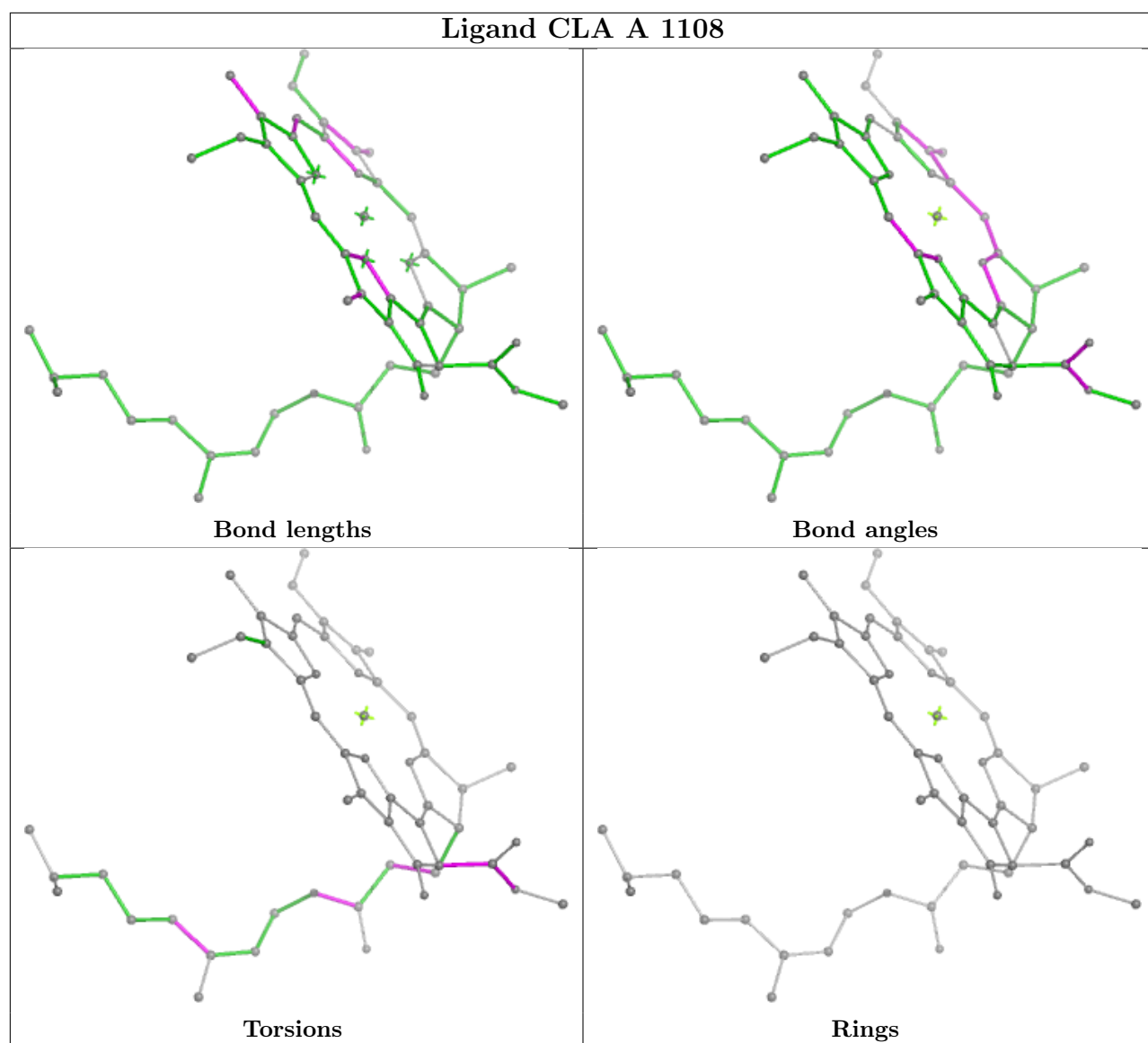
Ligand CLA 3 610

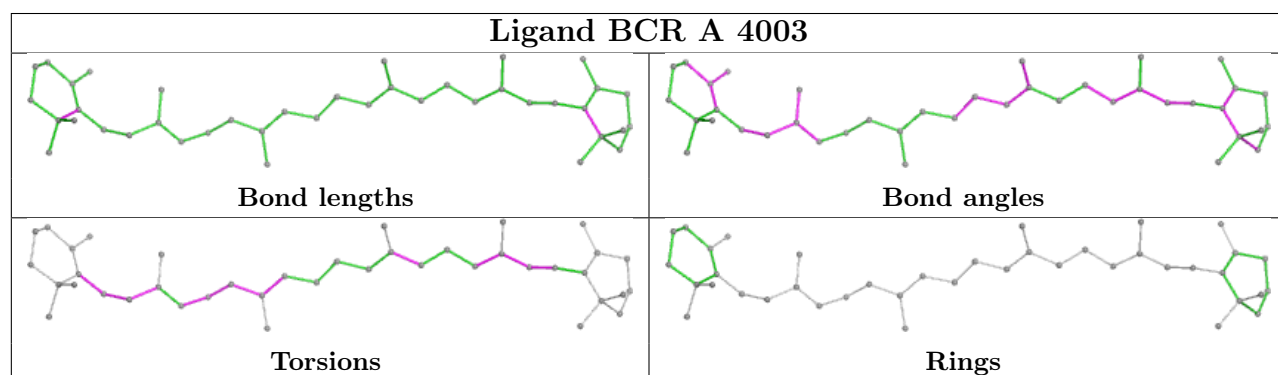
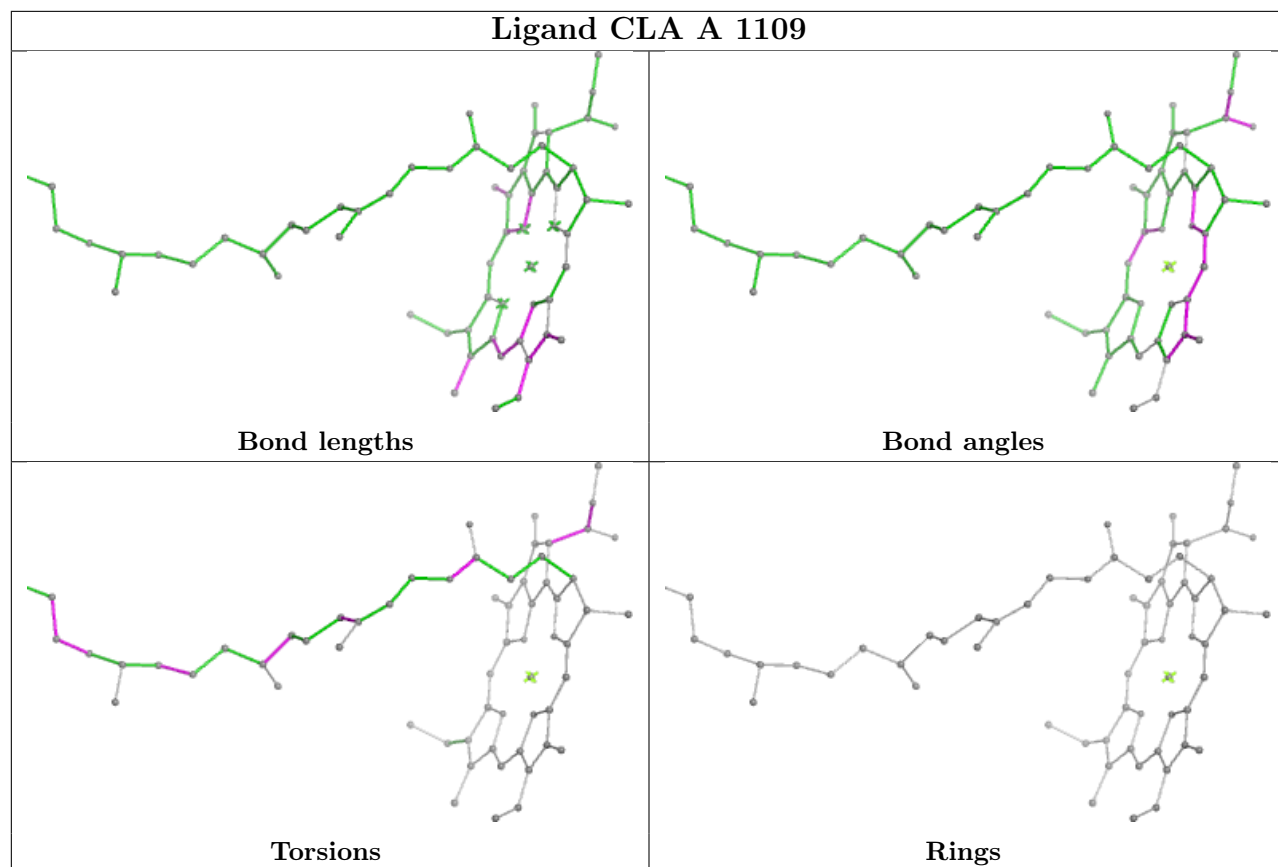




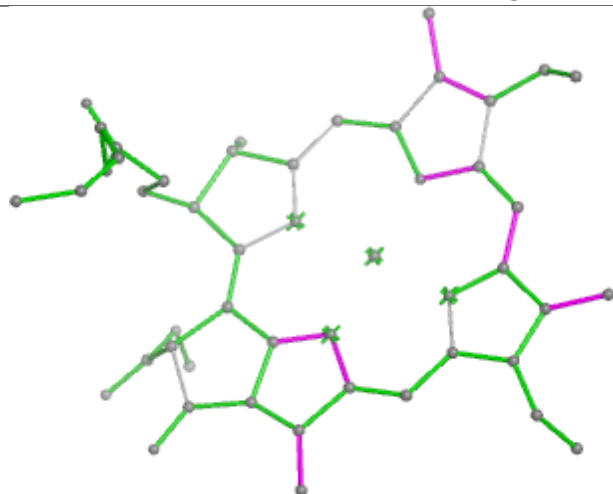
Ligand CLA A 1123



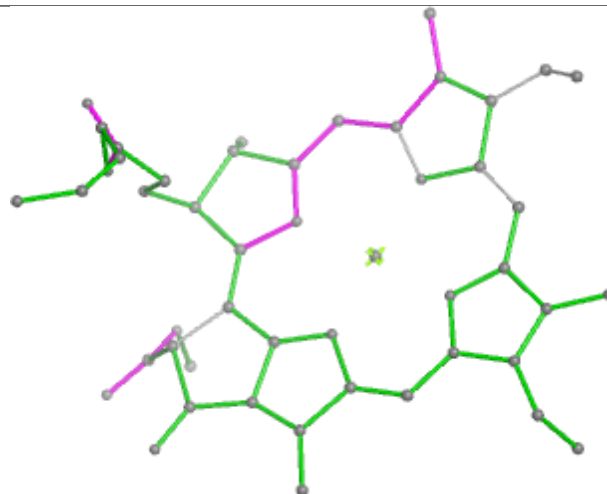




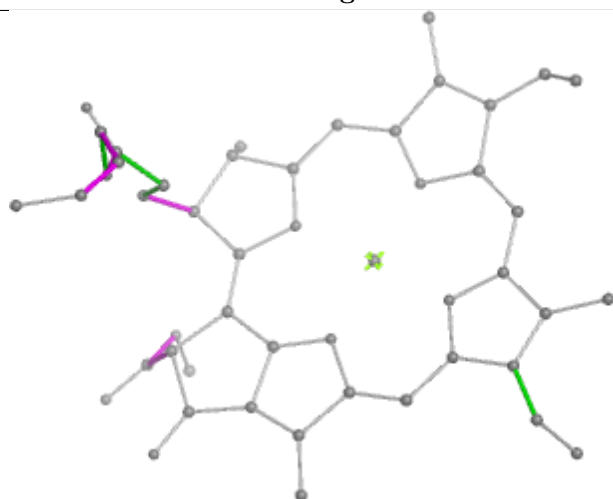
Ligand CLA B 1236



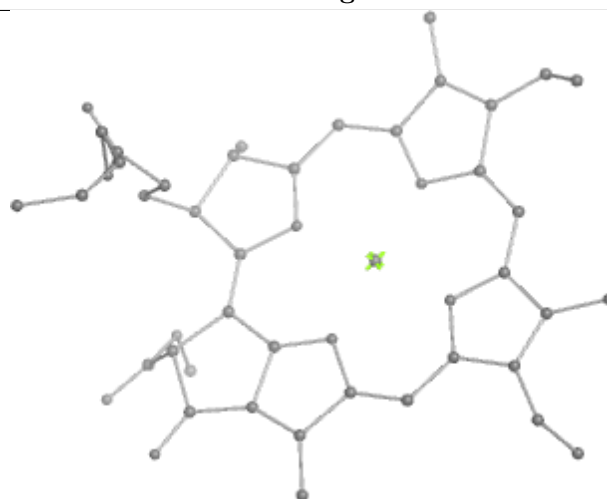
Bond lengths



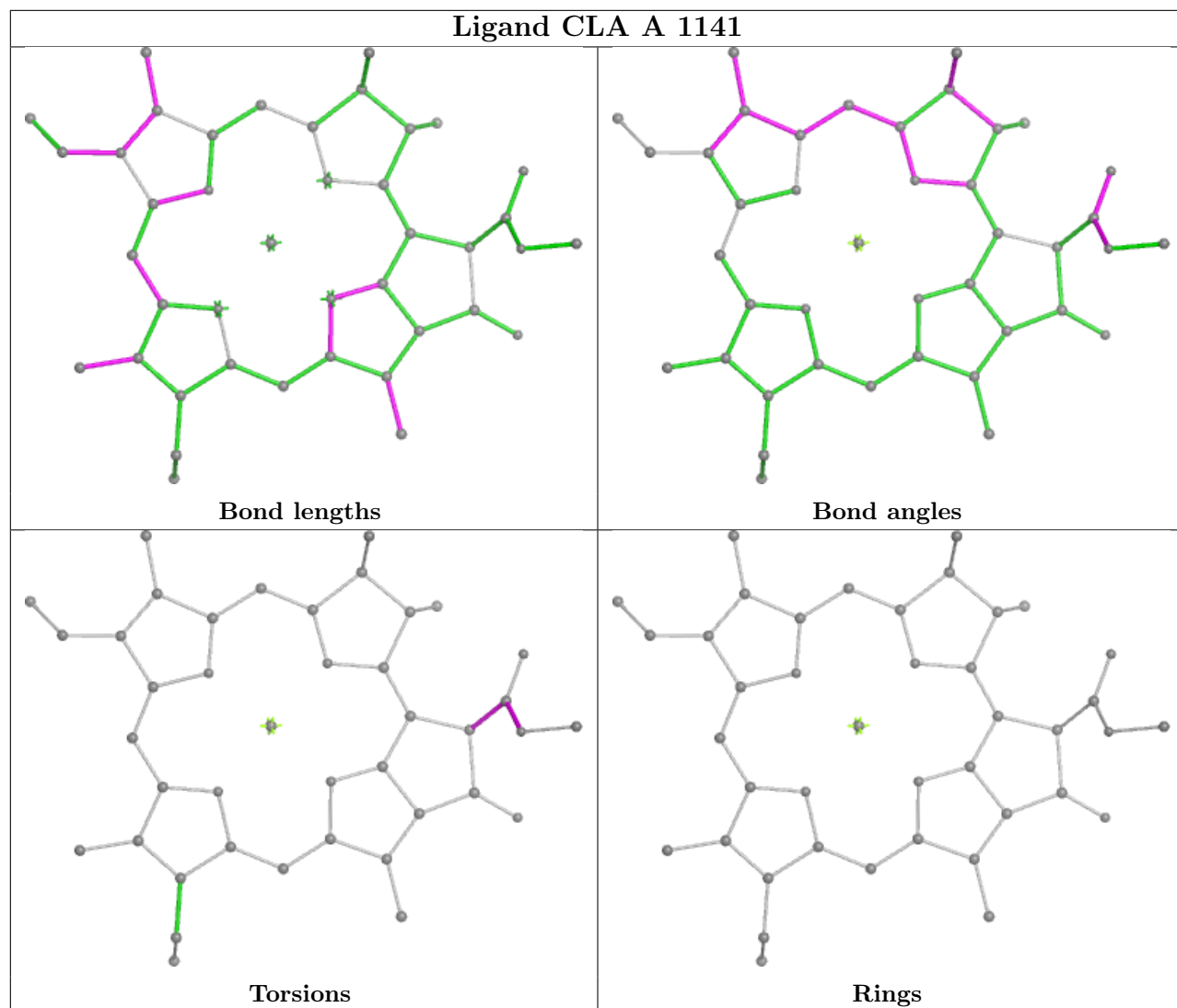
Bond angles



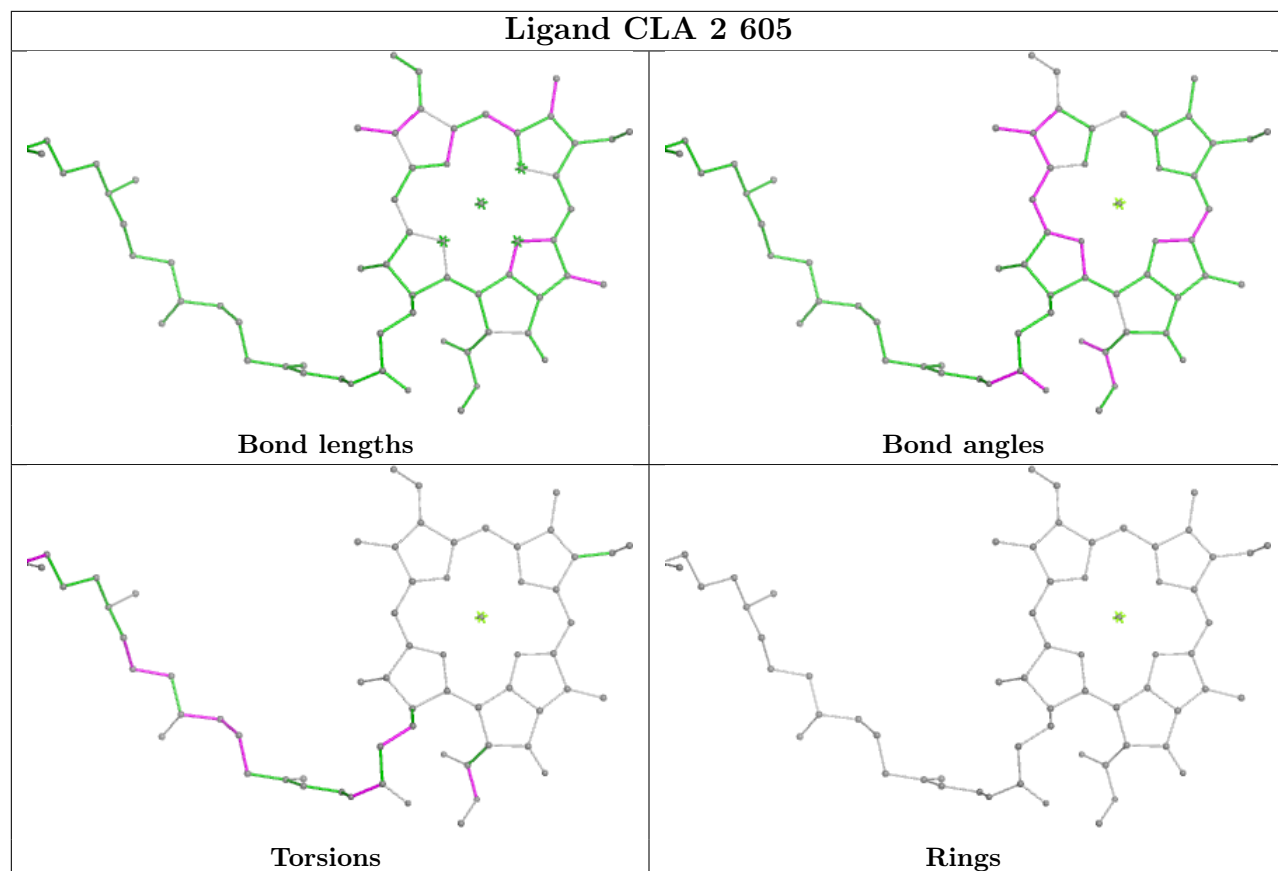
Torsions



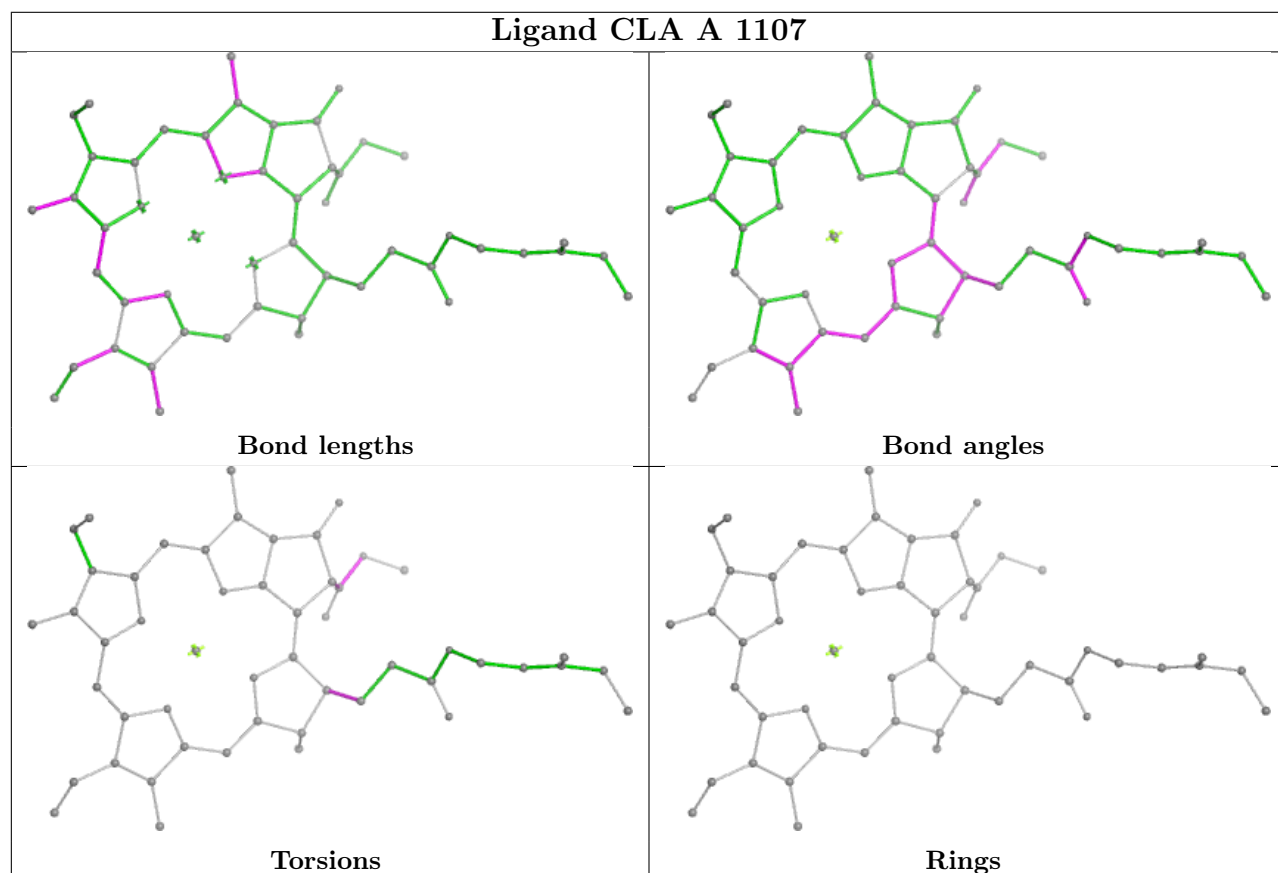
Rings



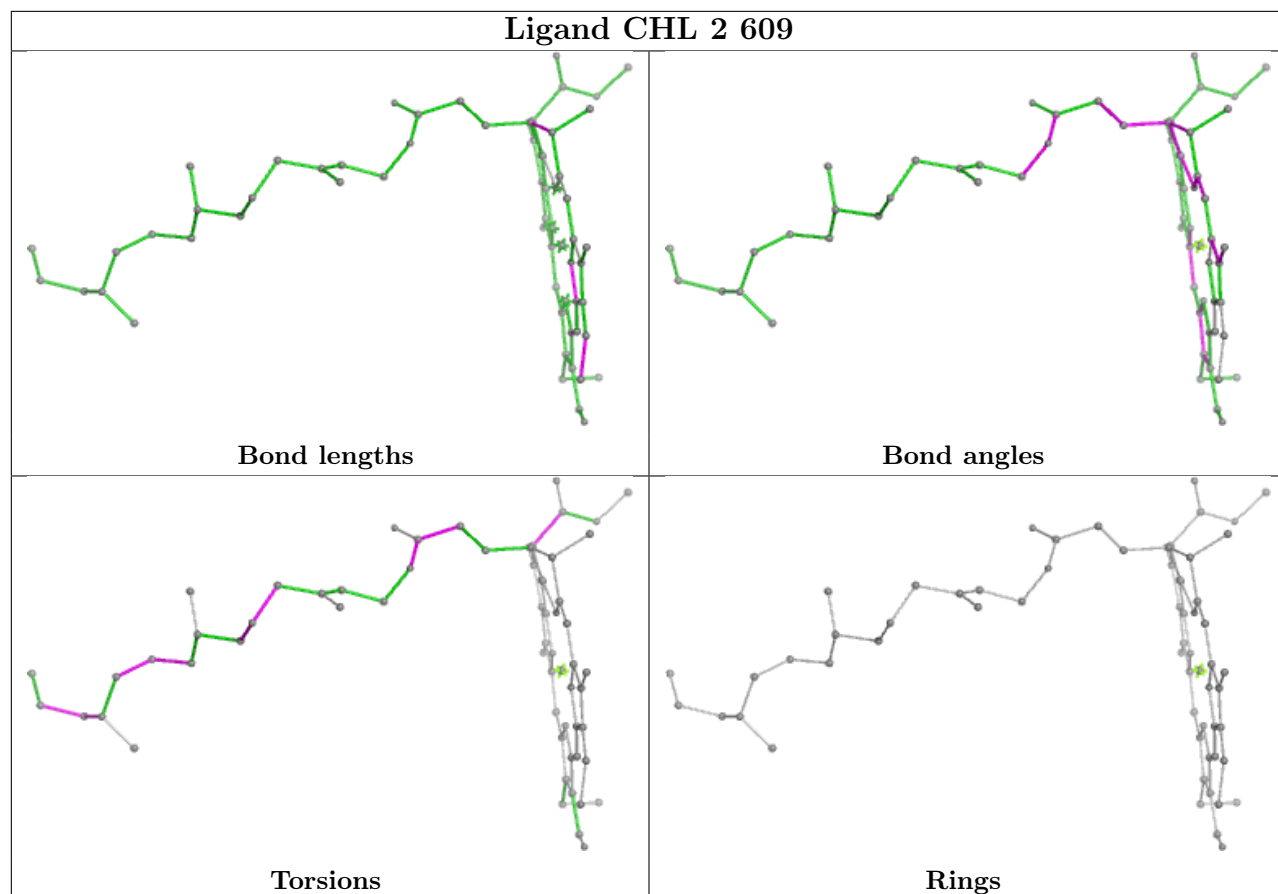
Ligand CLA 2 605



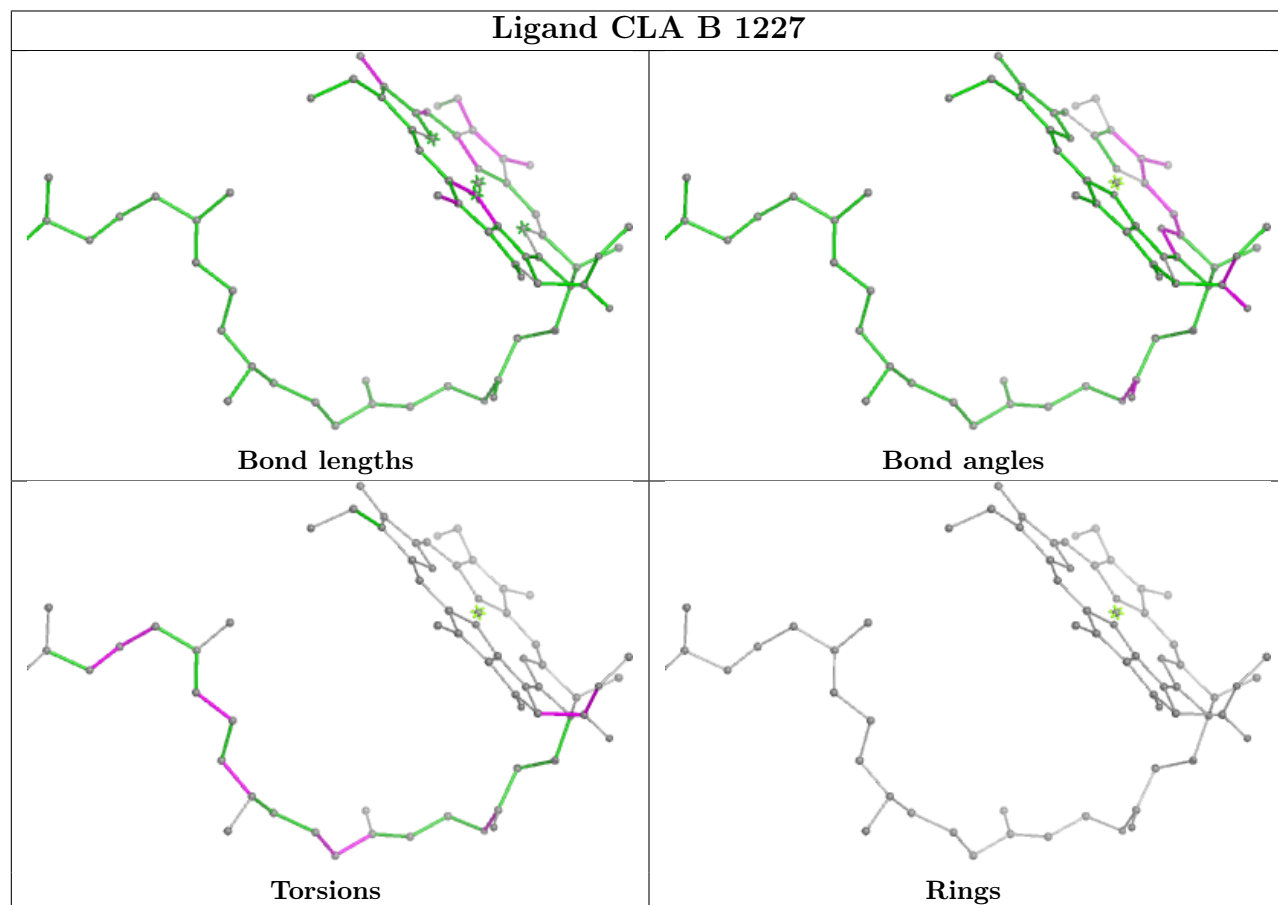
Ligand CLA A 1107

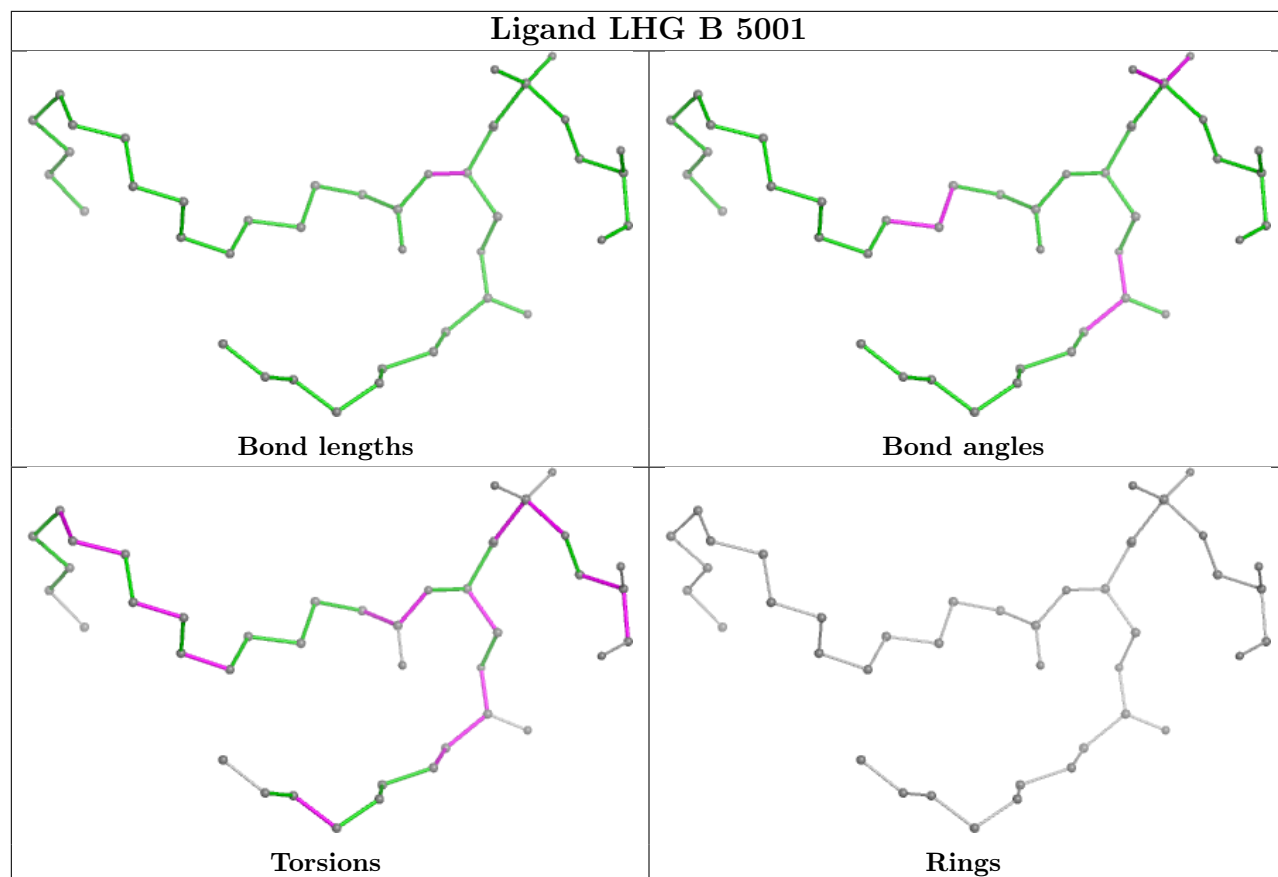


Ligand CHL 2 609

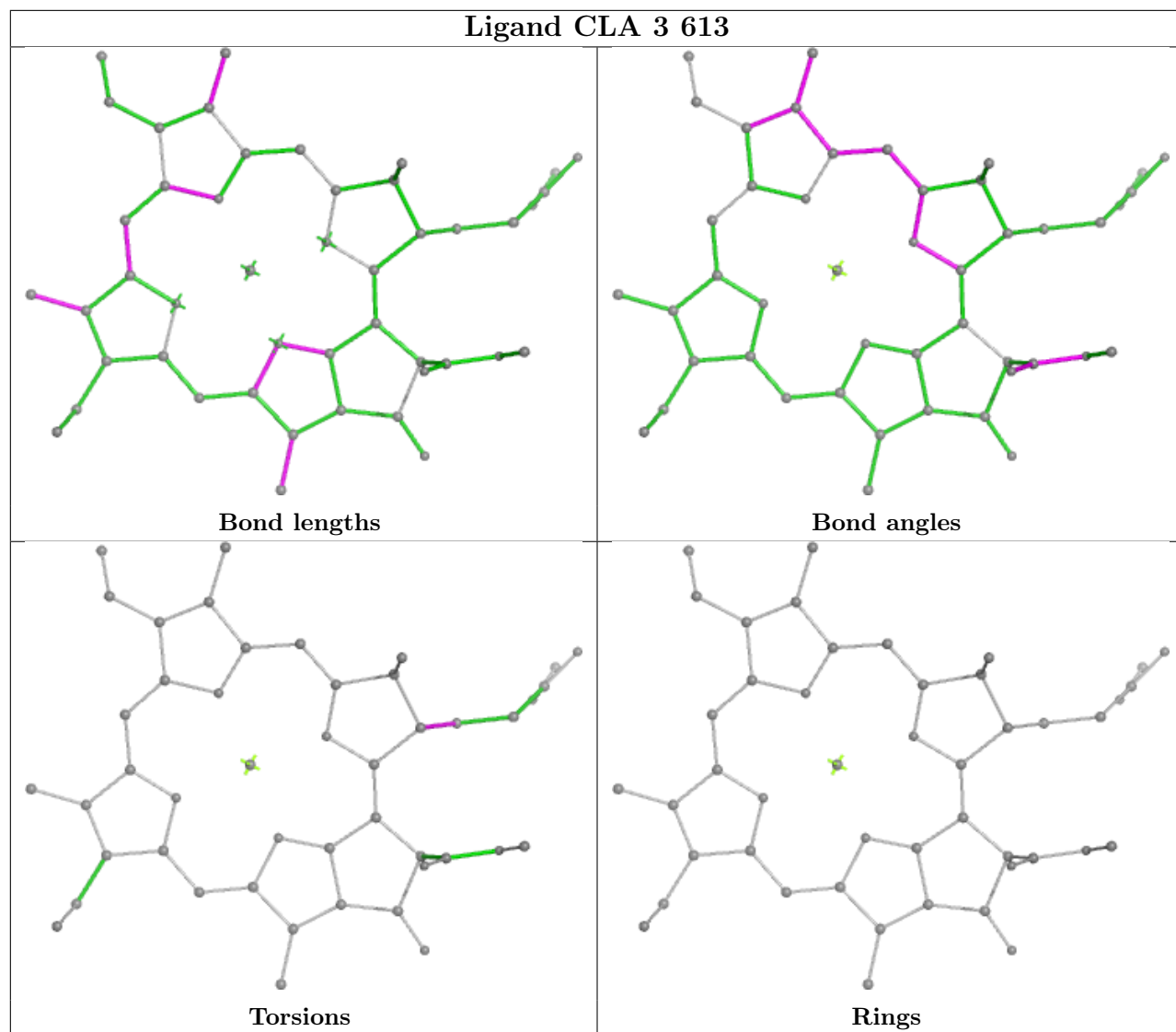


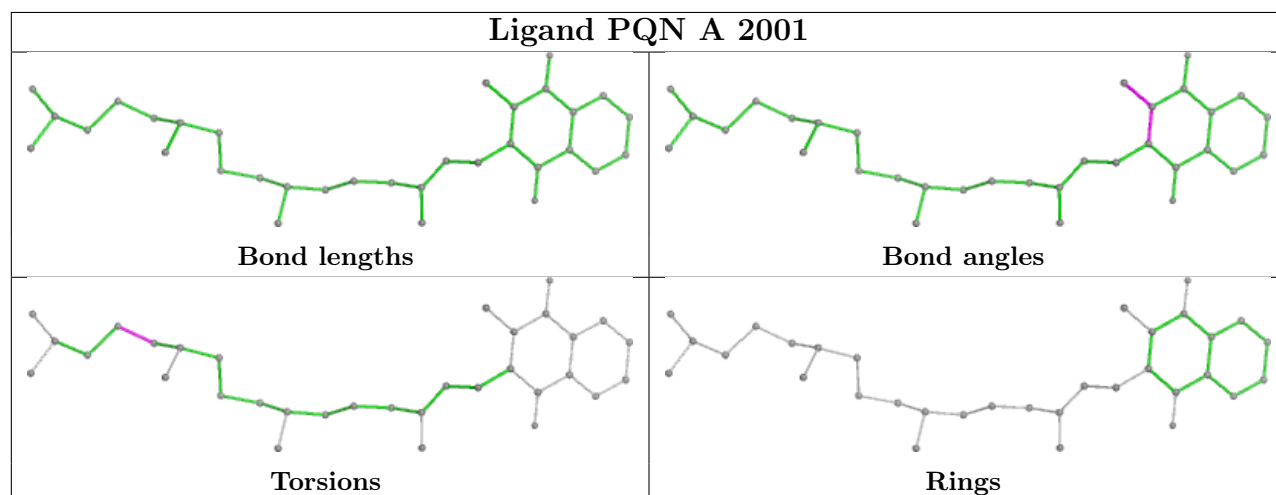
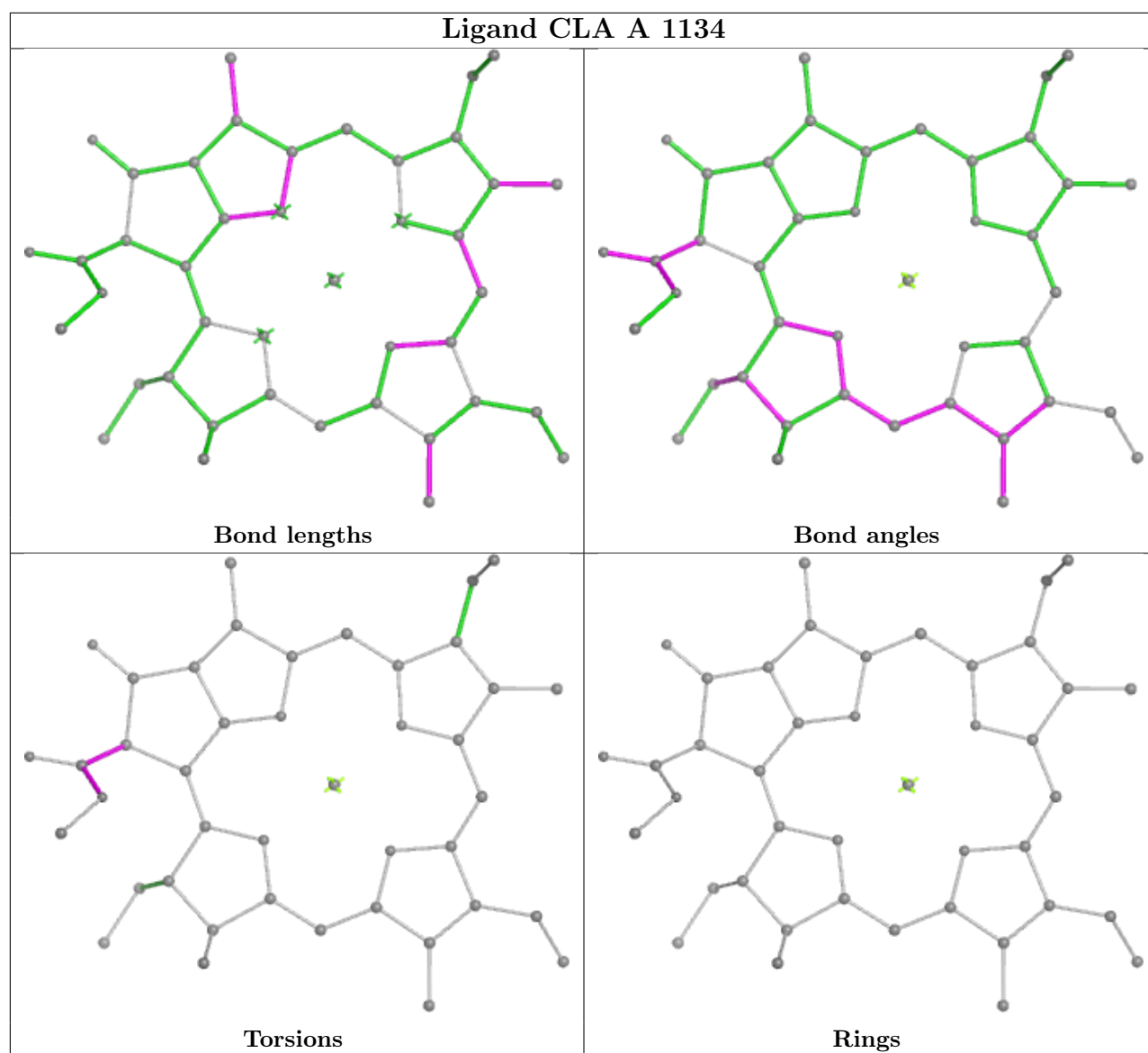
Ligand CLA B 1227



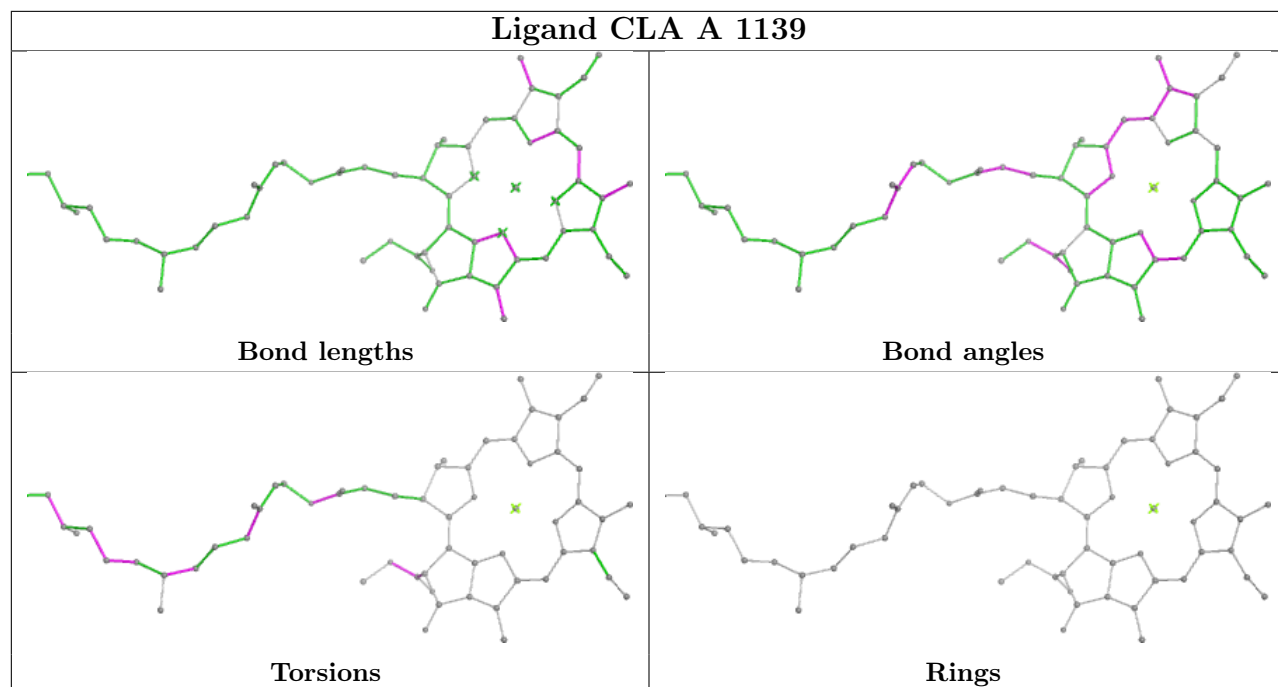


Ligand CLA 3 613

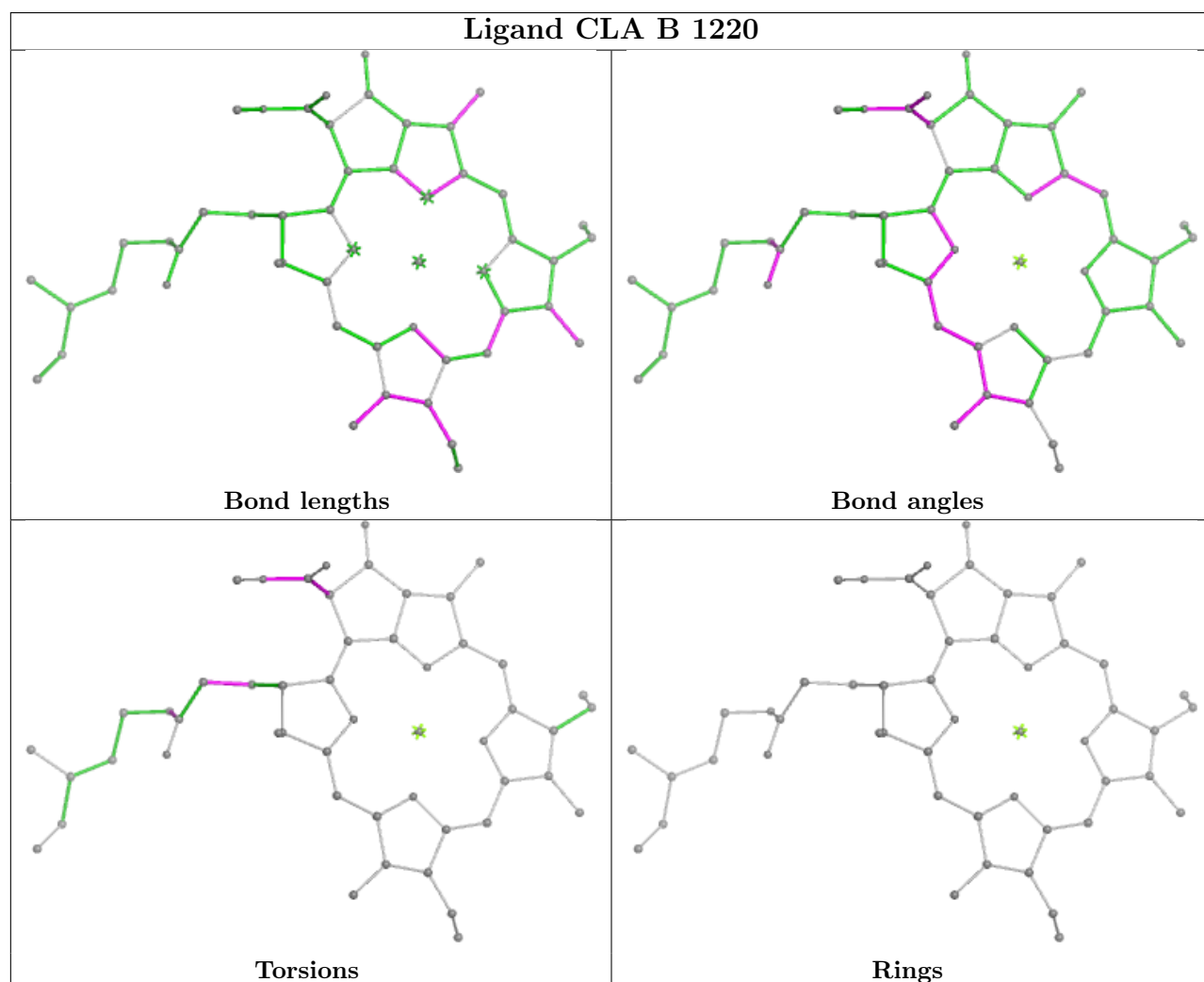


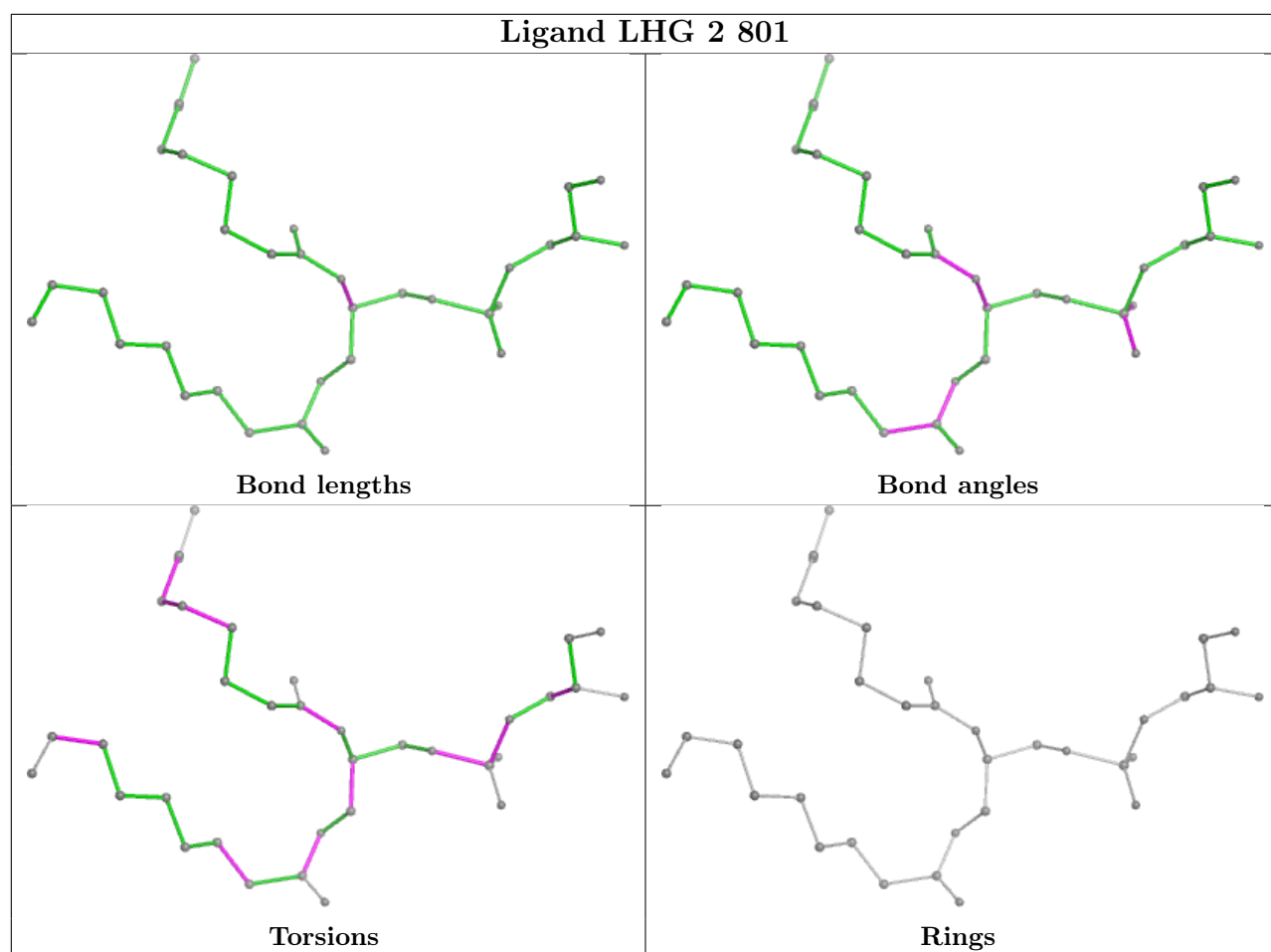


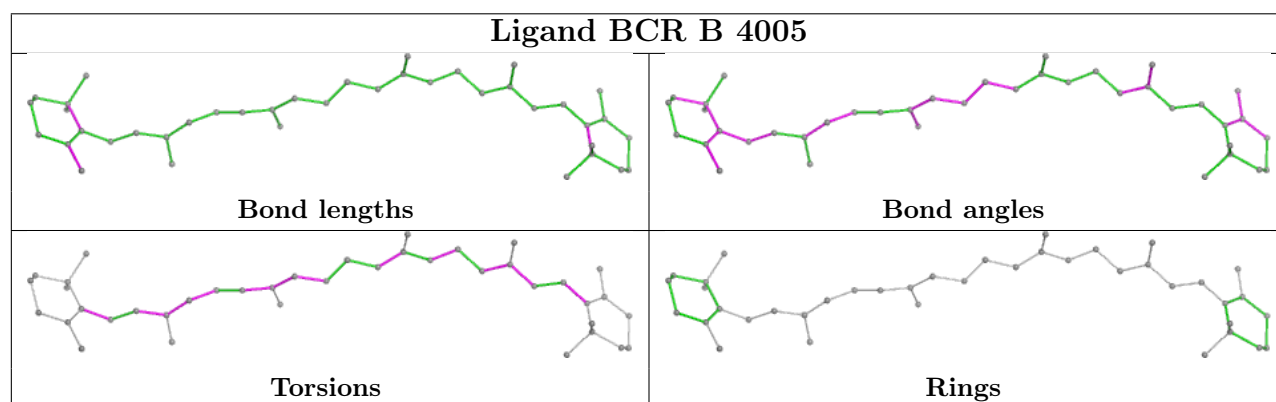
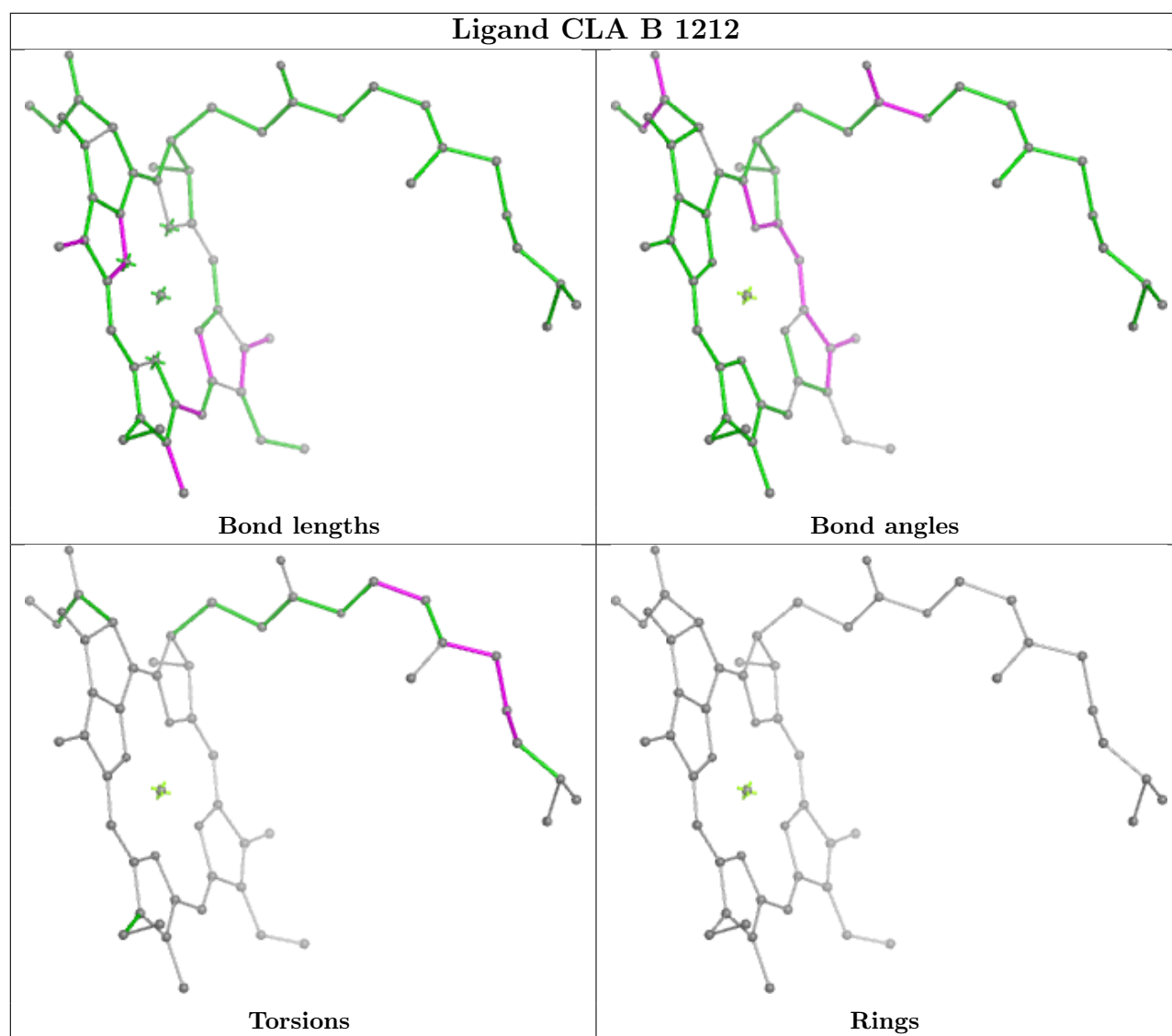
Ligand CLA A 1139

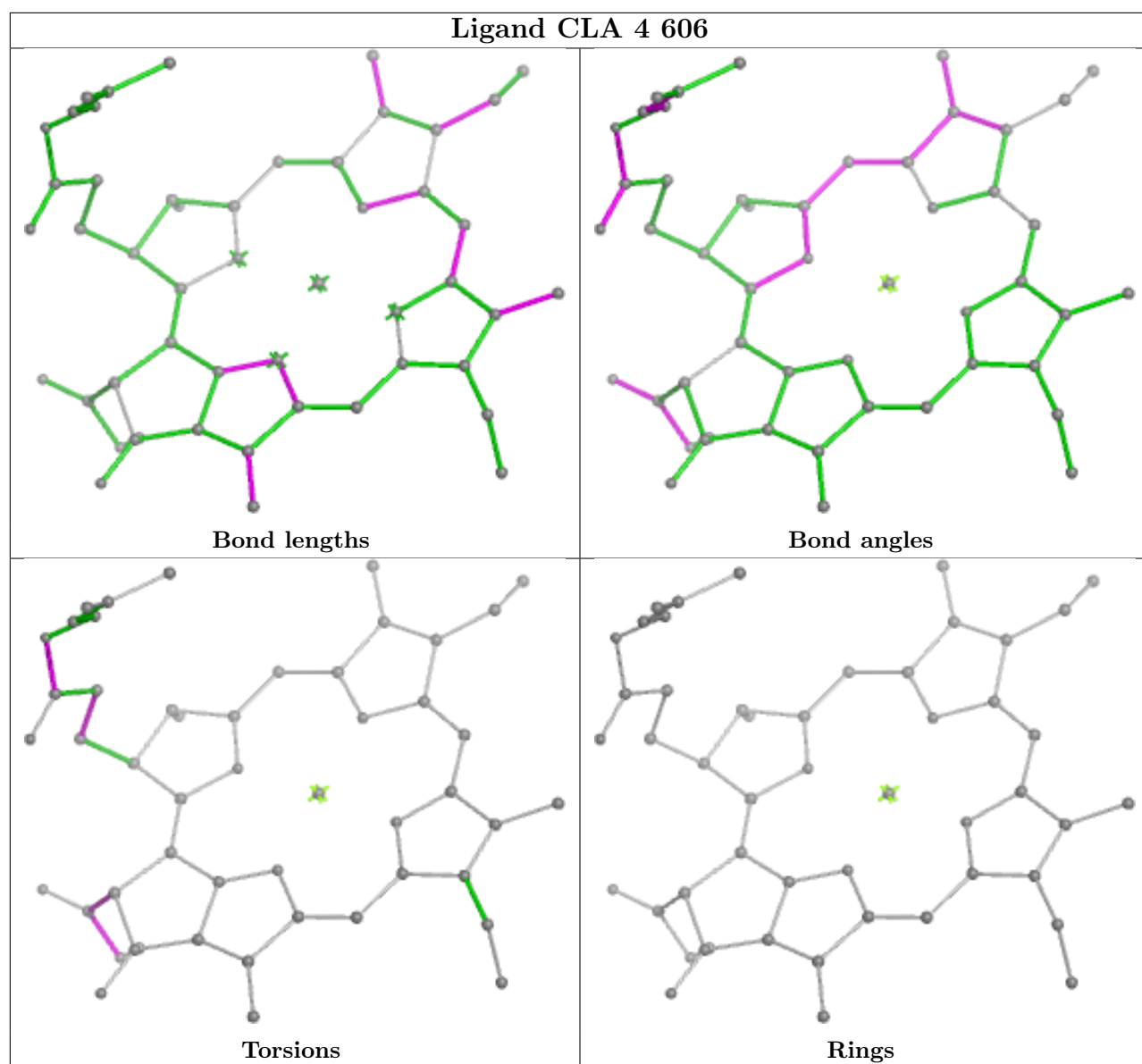


Ligand CLA B 1220

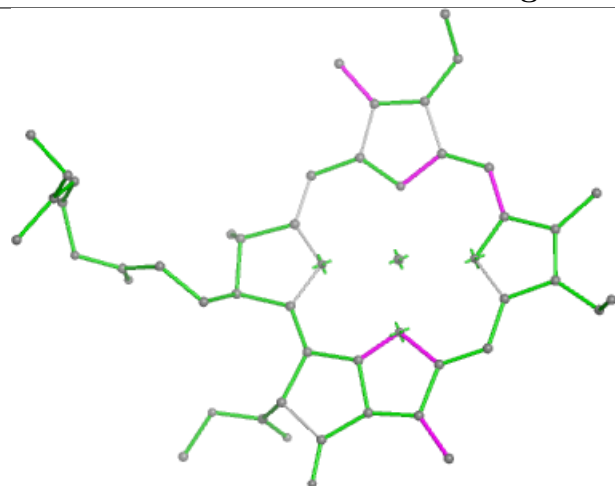




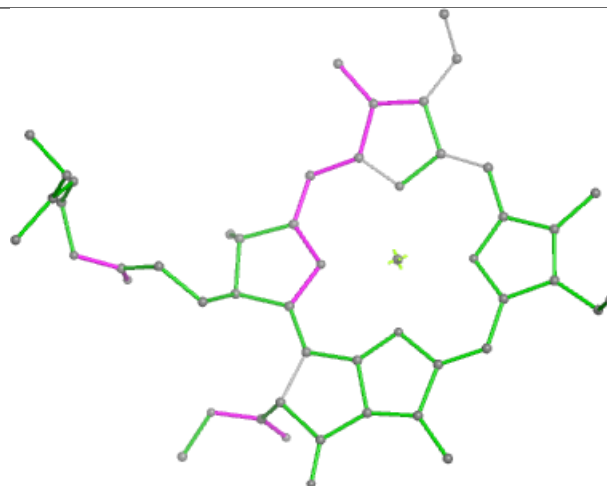




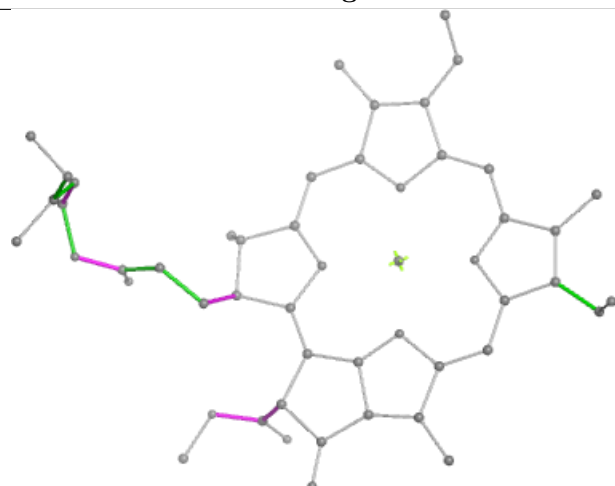
Ligand CLA 4 616



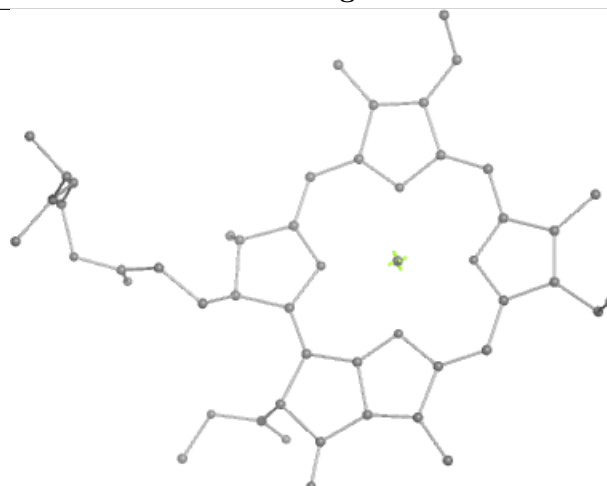
Bond lengths



Bond angles

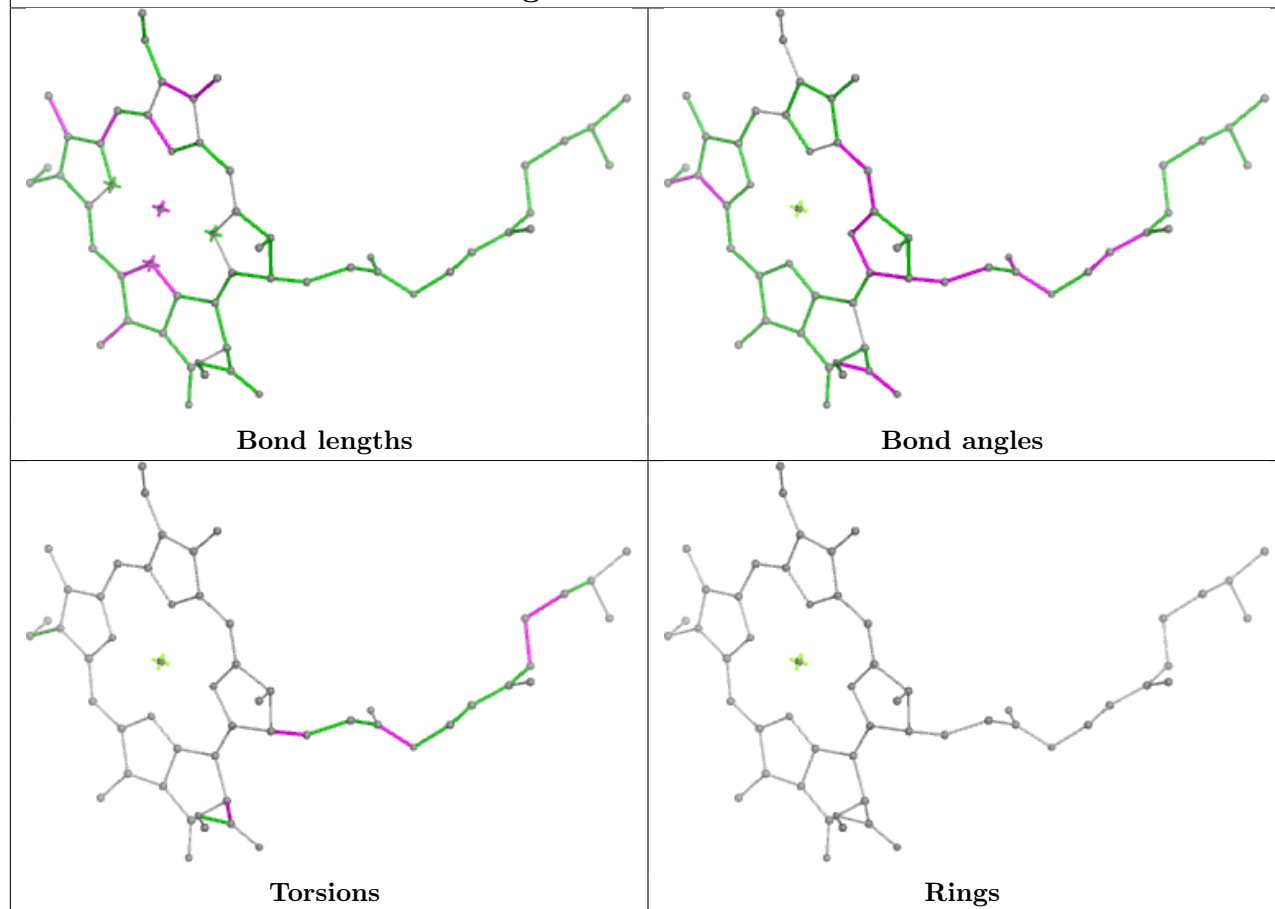


Torsions

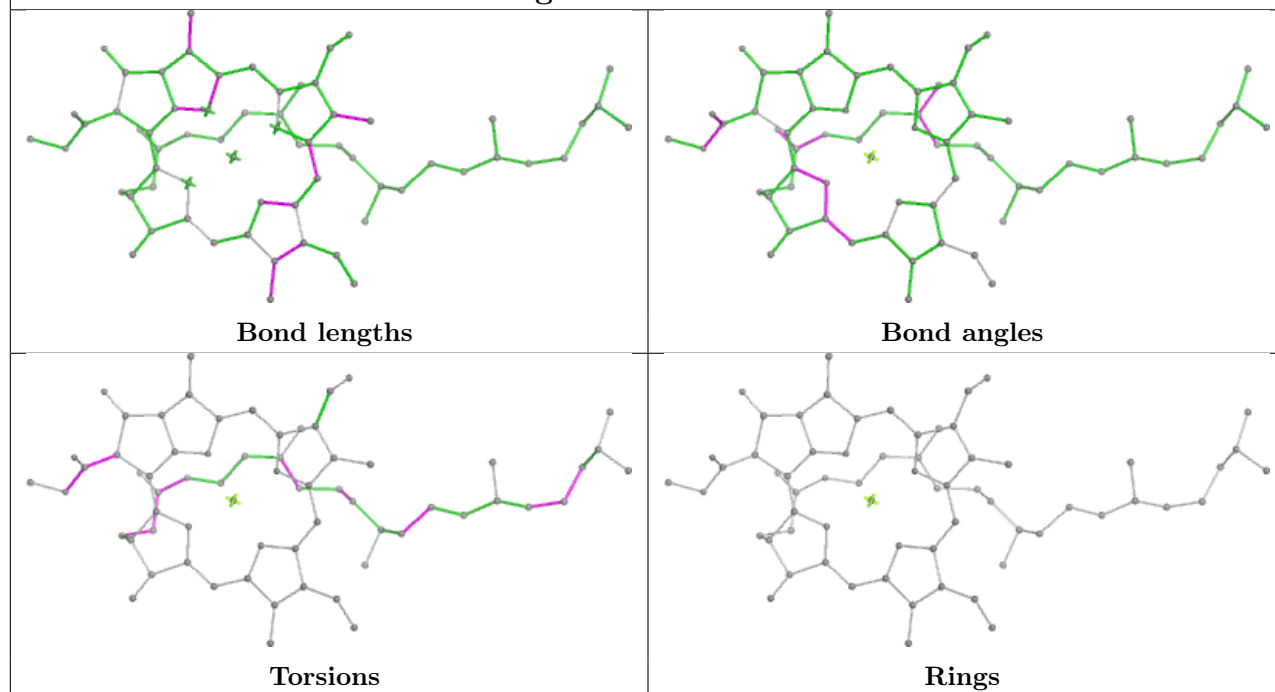


Rings

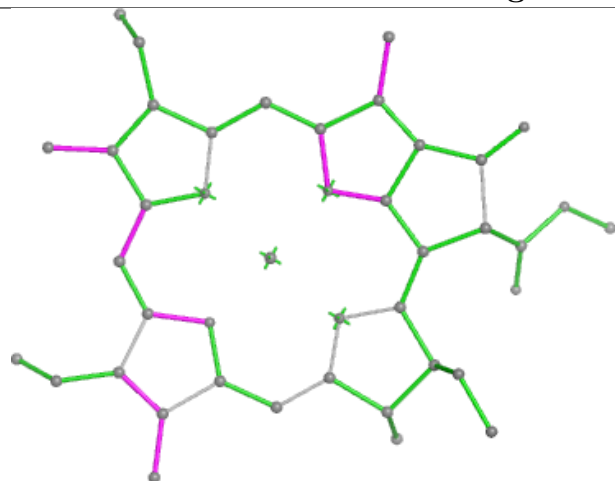
Ligand CLA B 1230



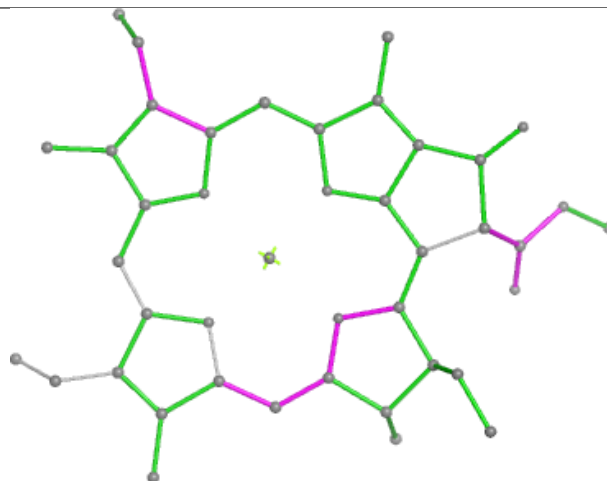
Ligand CLA 3 603



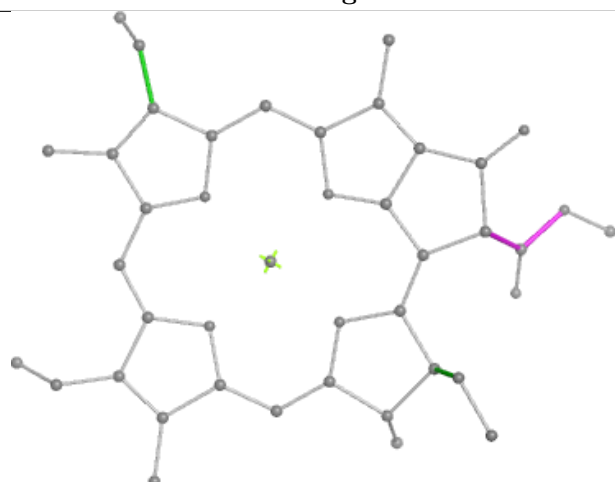
Ligand CLA B 1239



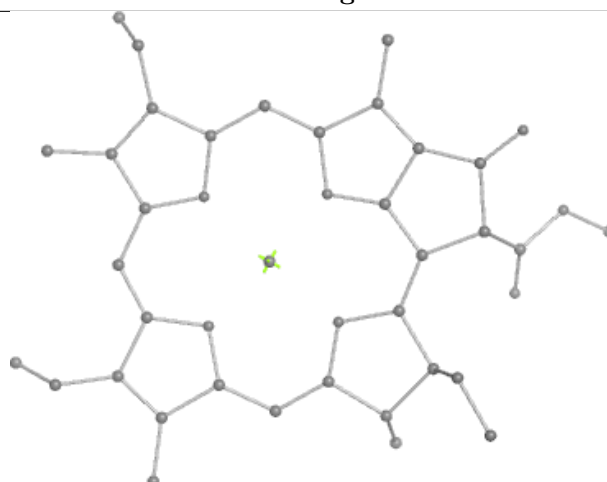
Bond lengths



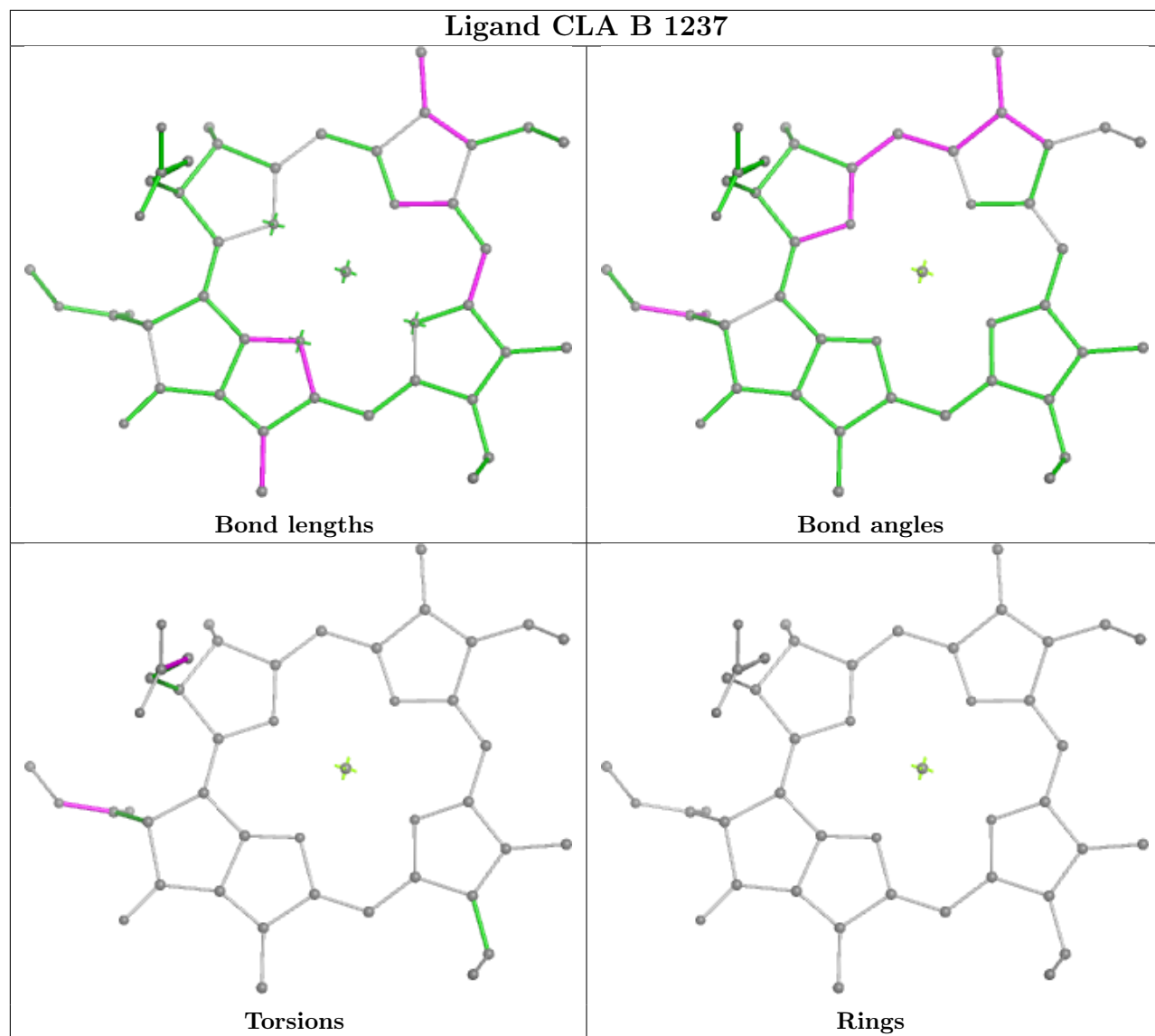
Bond angles



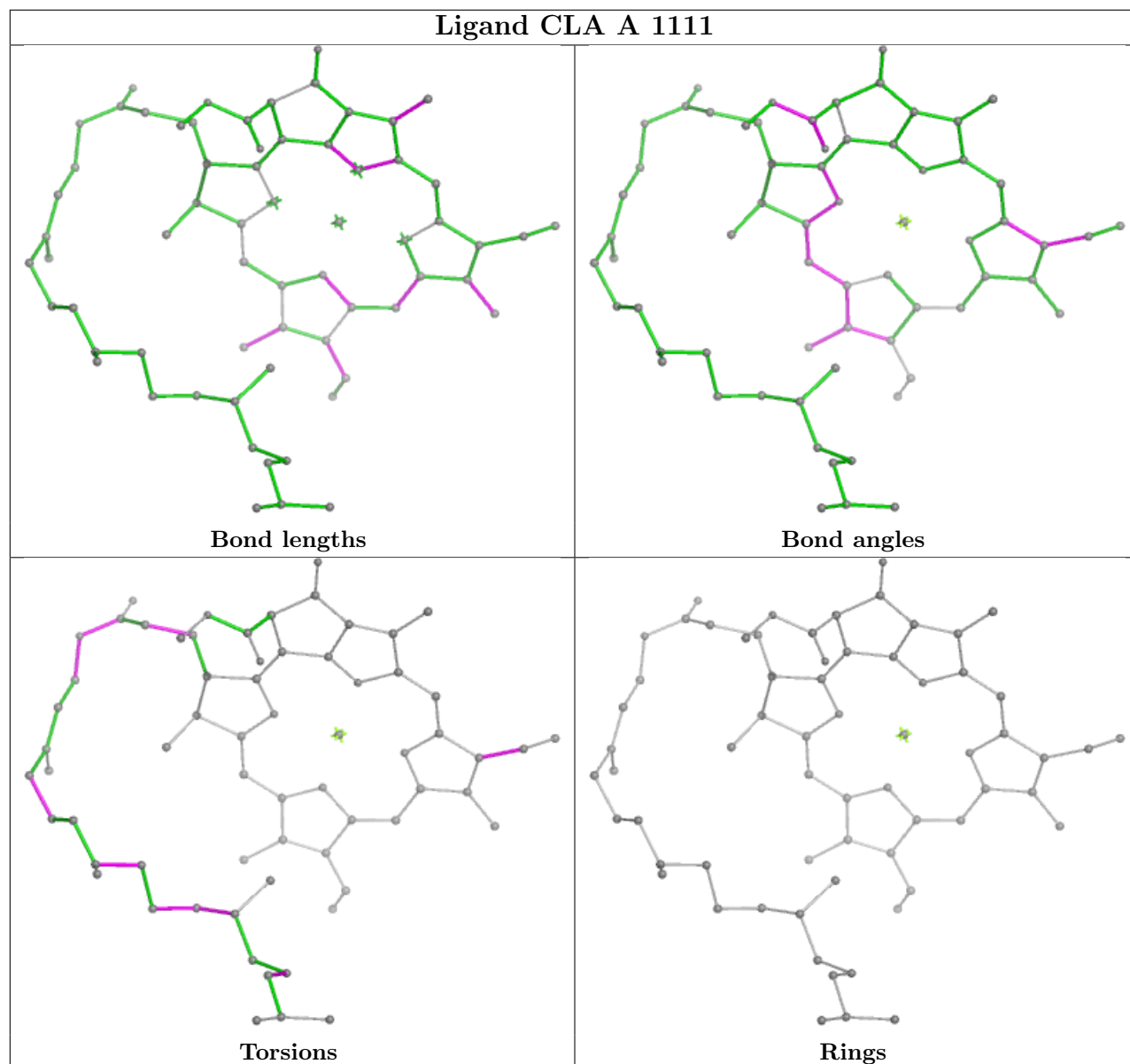
Torsions

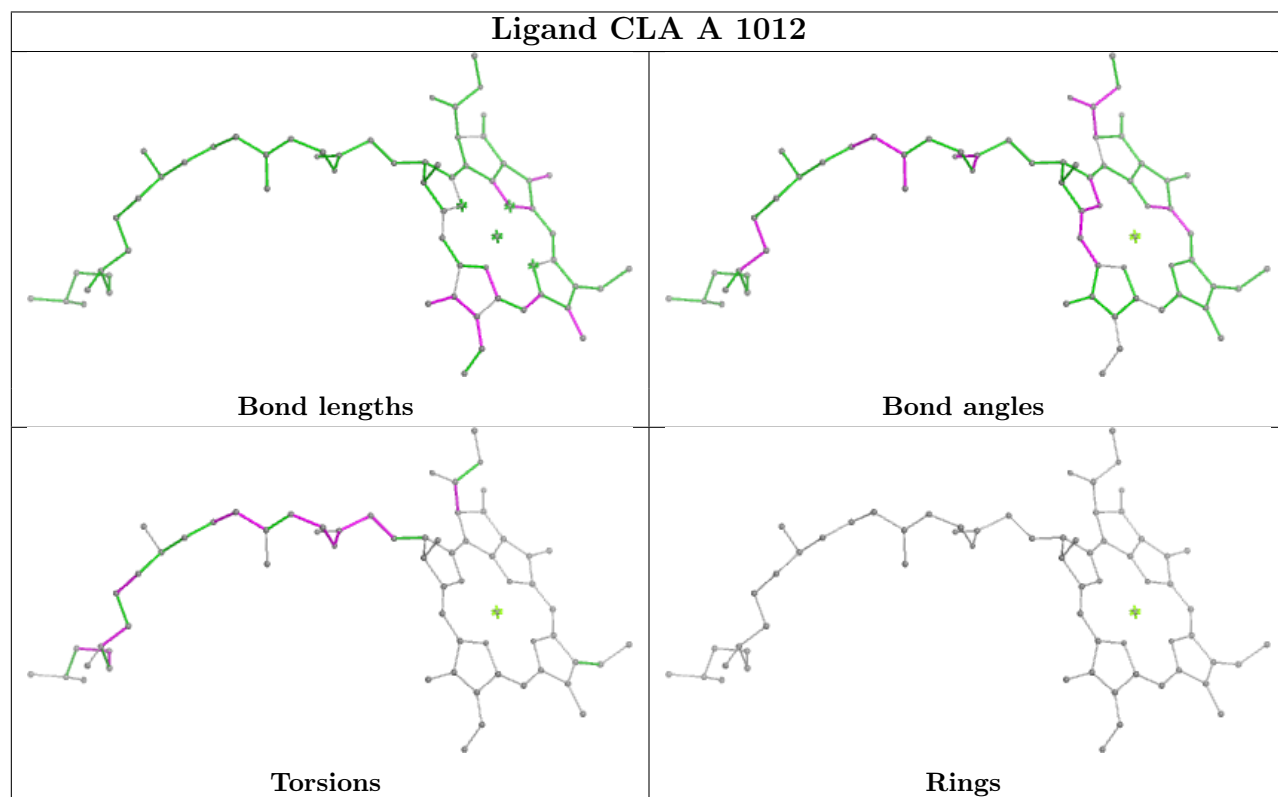
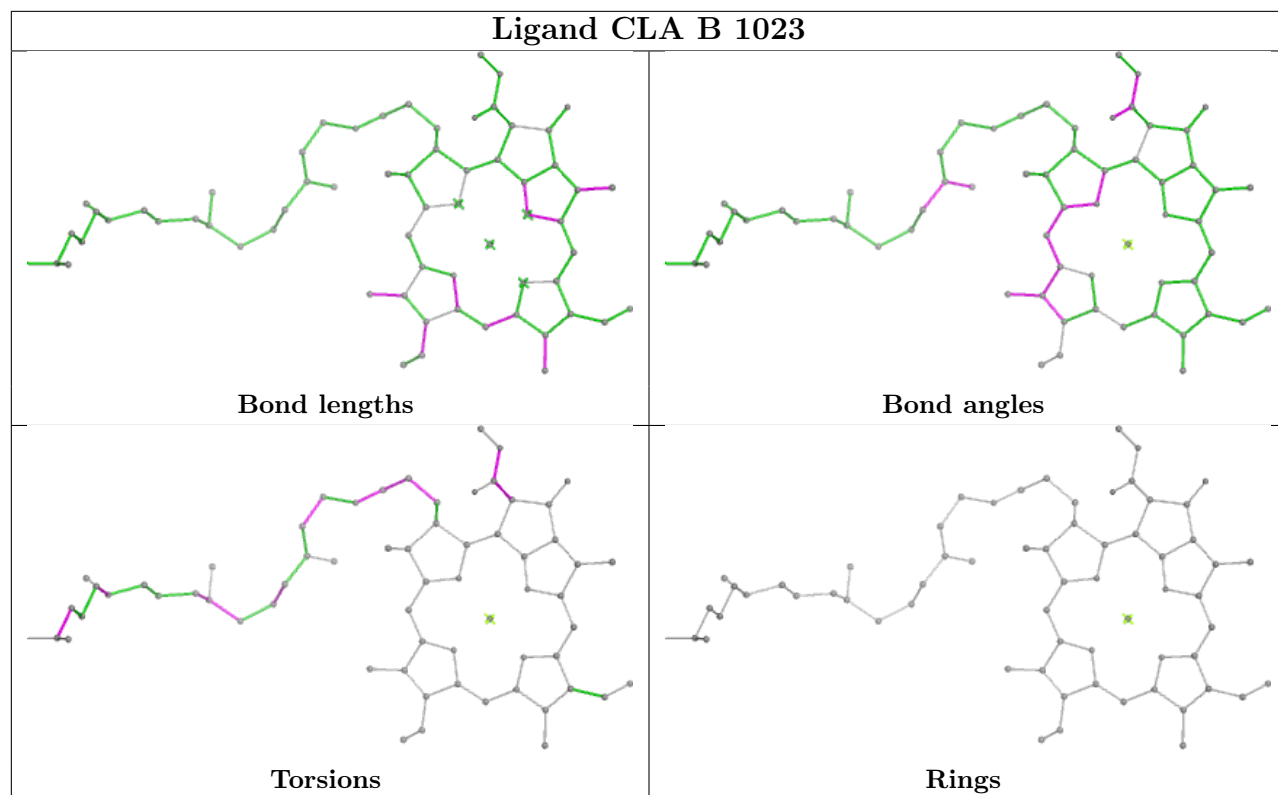


Rings

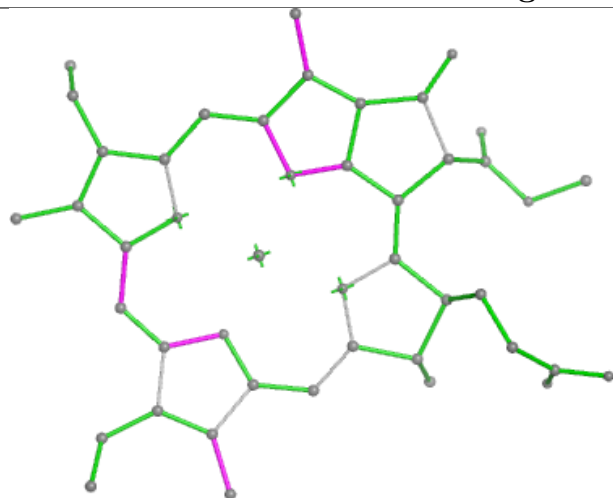


Ligand CLA A 1111

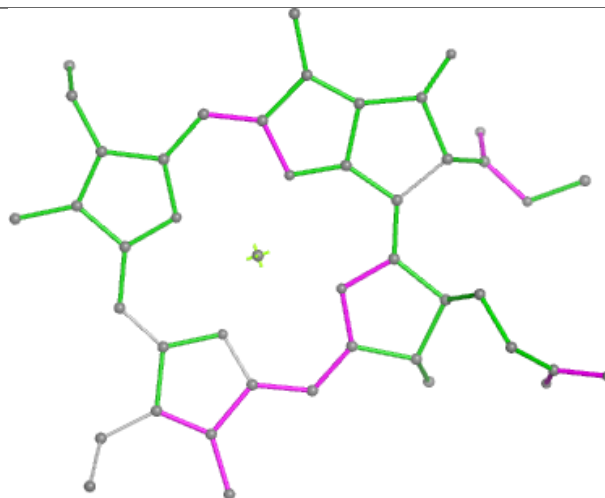




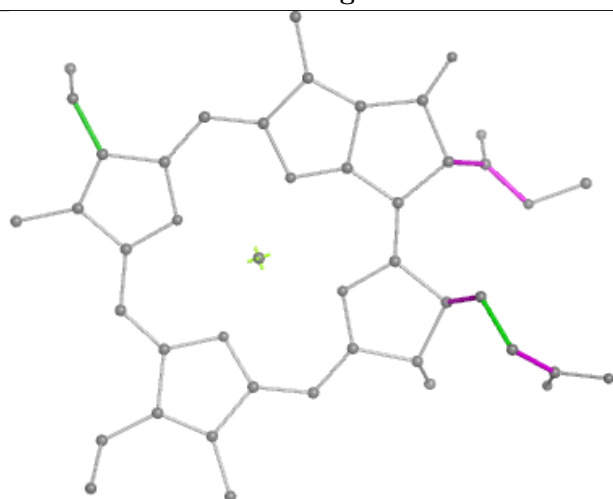
Ligand CLA 1 613



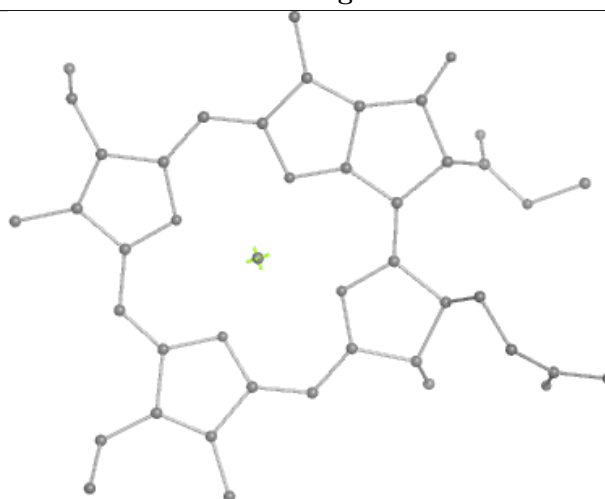
Bond lengths



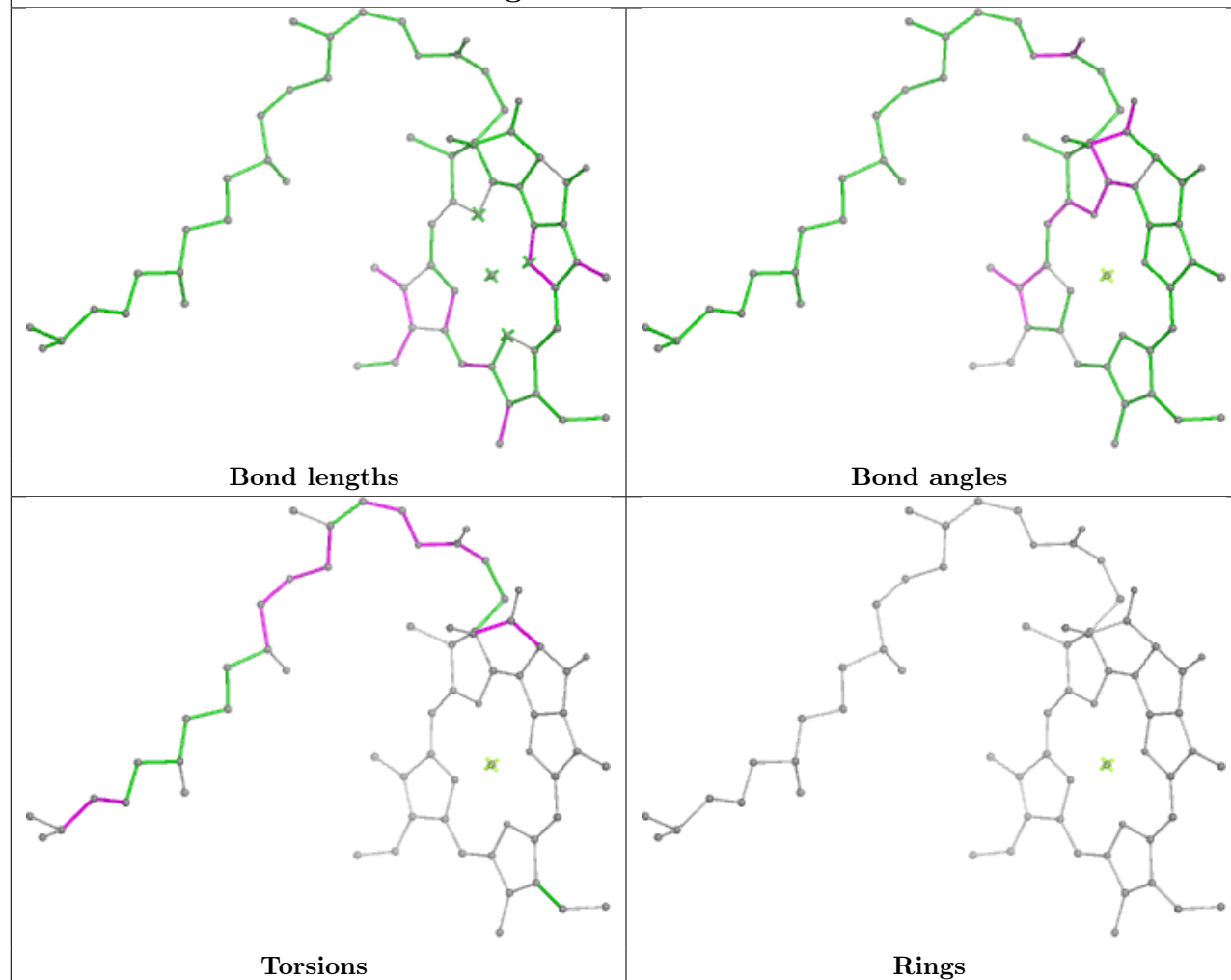
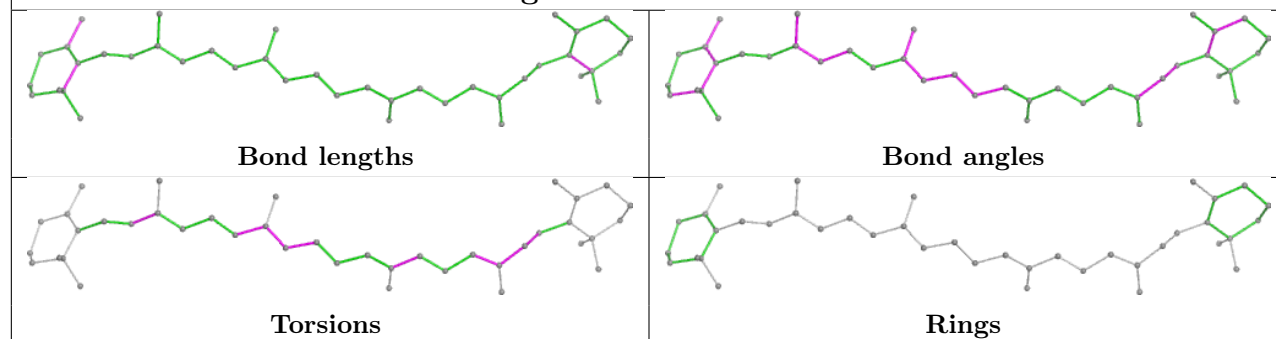
Bond angles

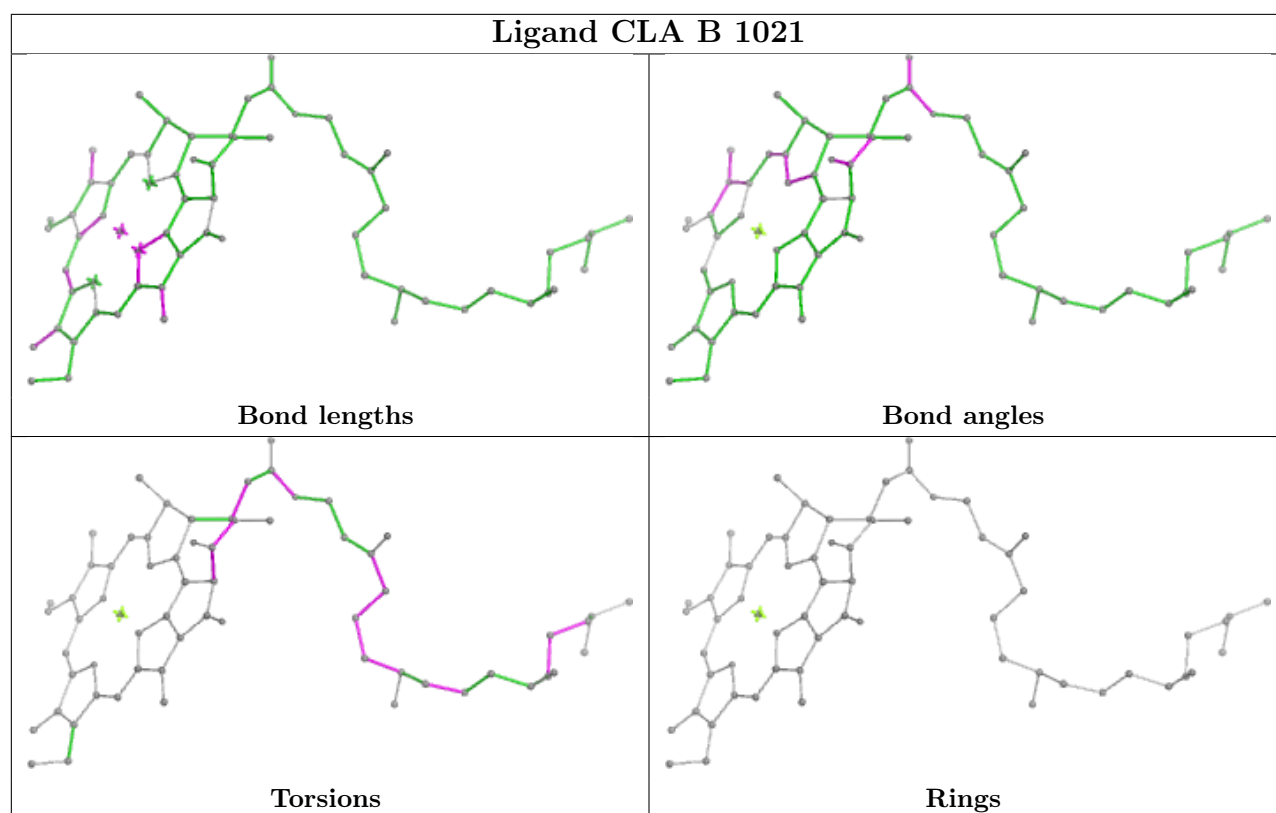


Torsions

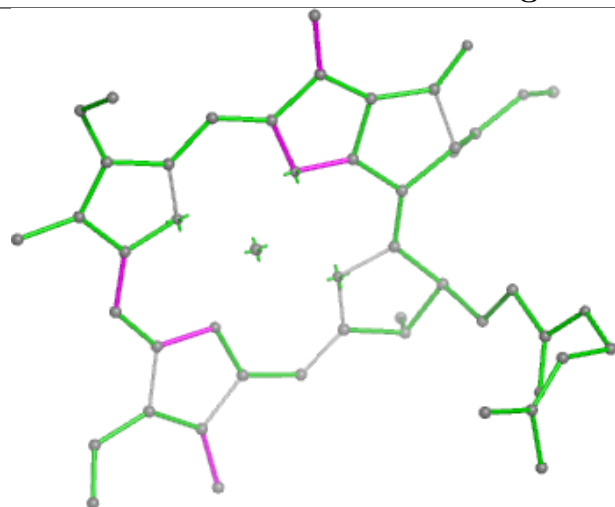


Rings

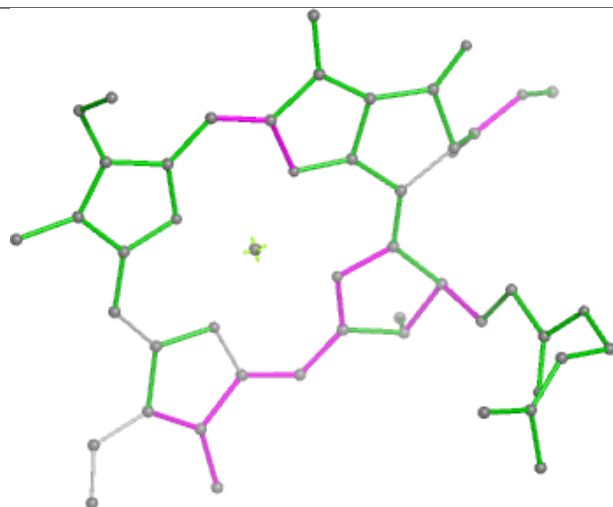
Ligand CLA B 1221**Ligand BCR A 4008**



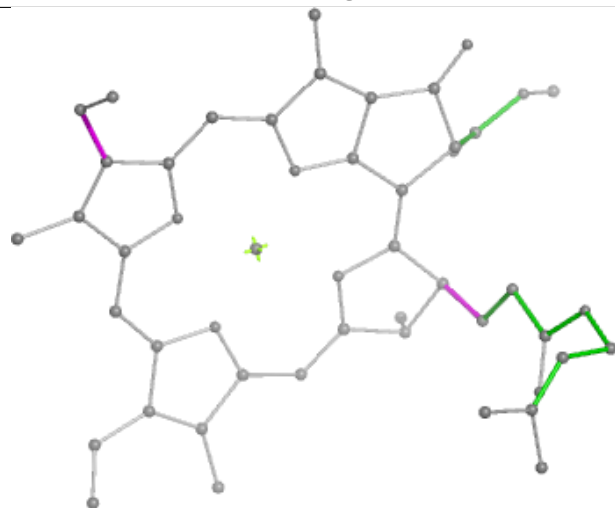
Ligand CLA 2 608



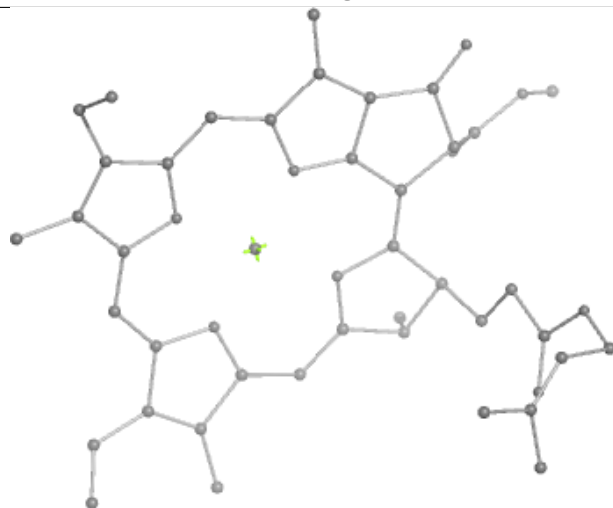
Bond lengths



Bond angles

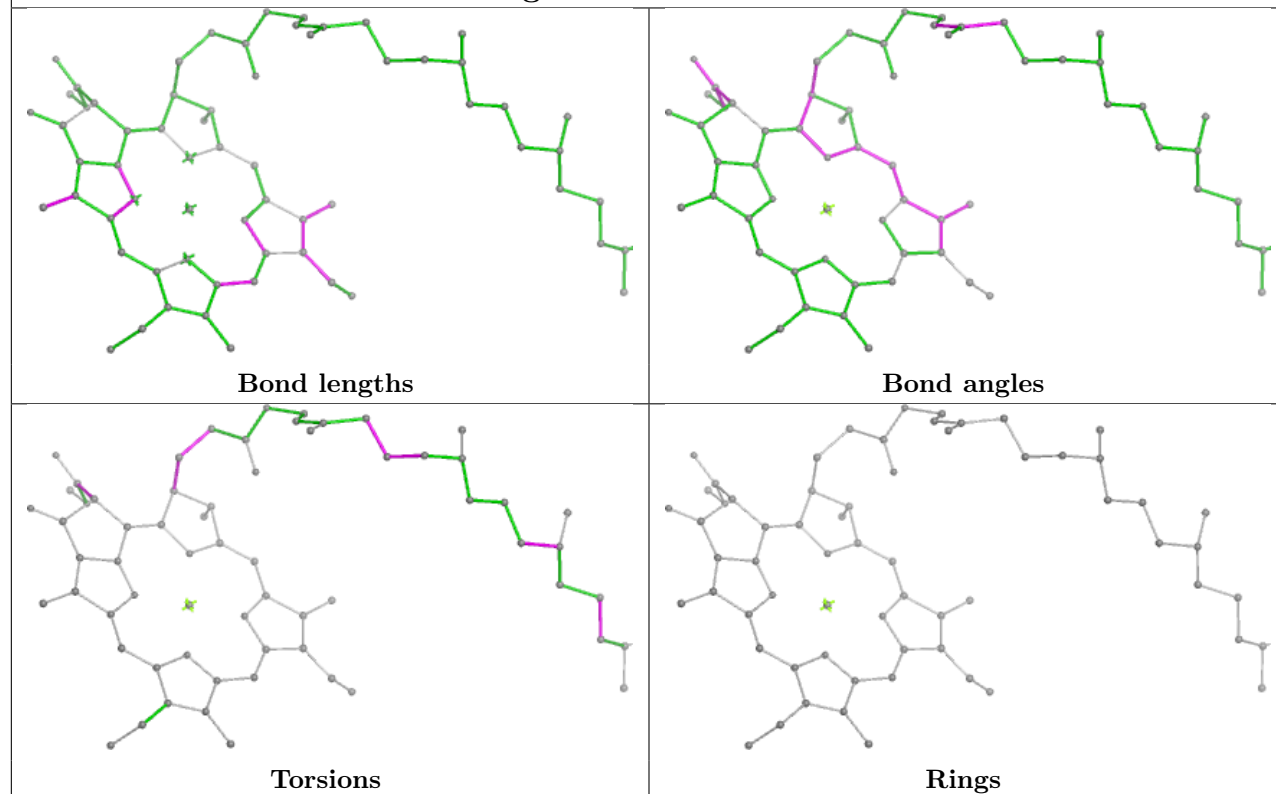


Torsions

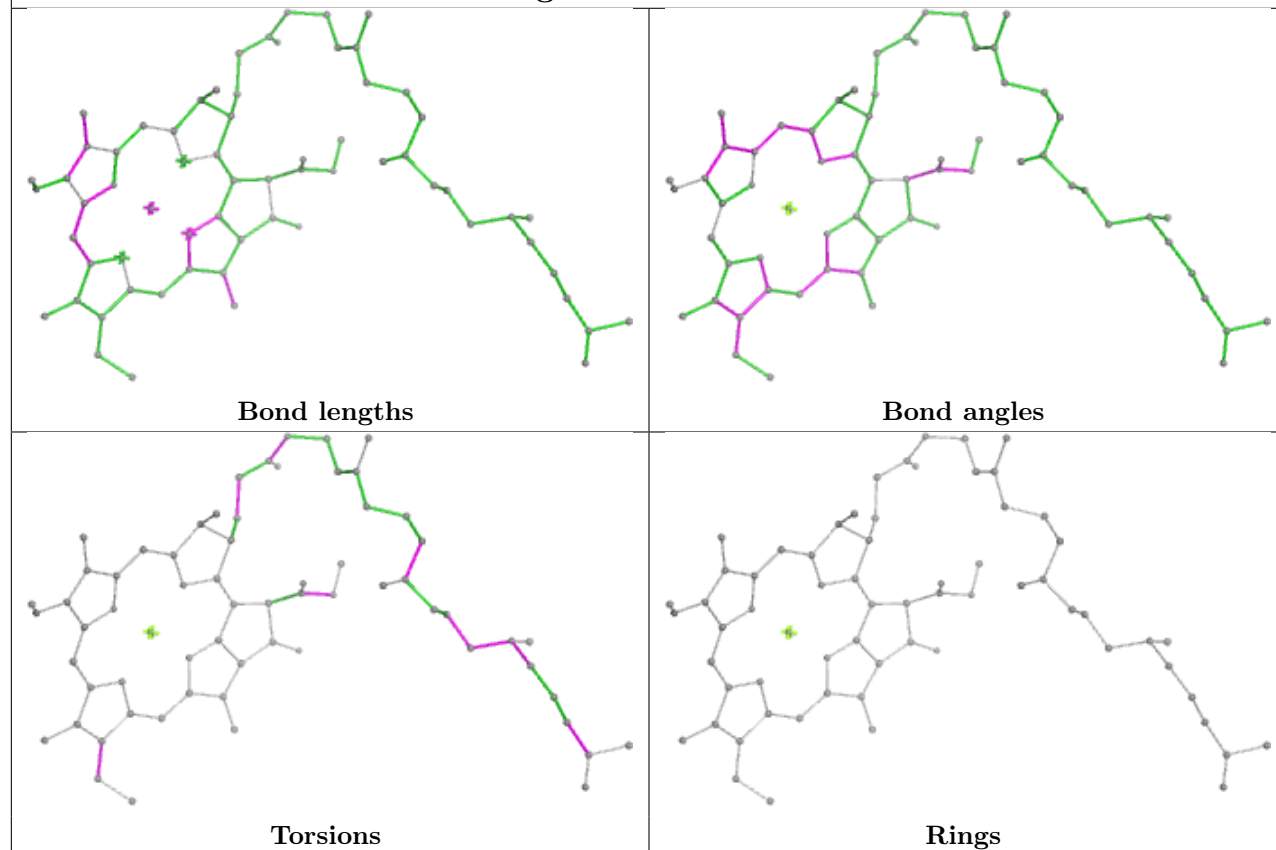


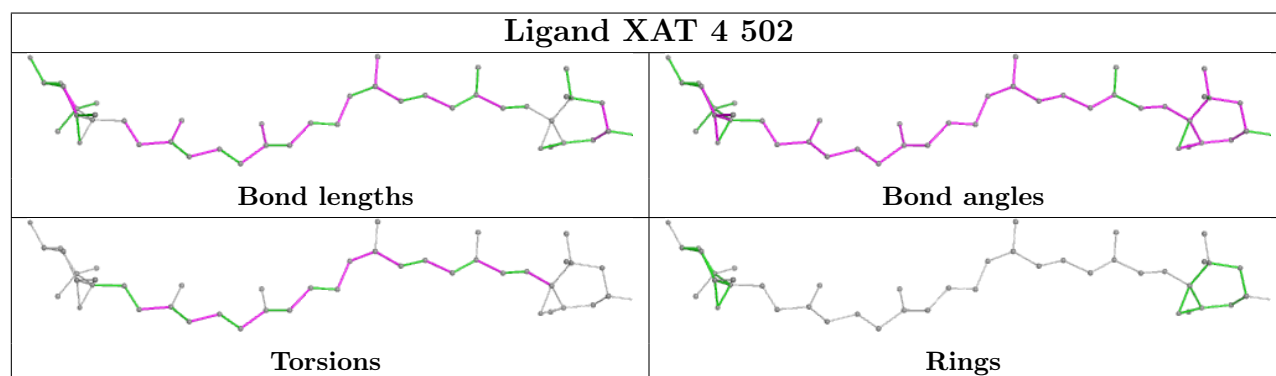
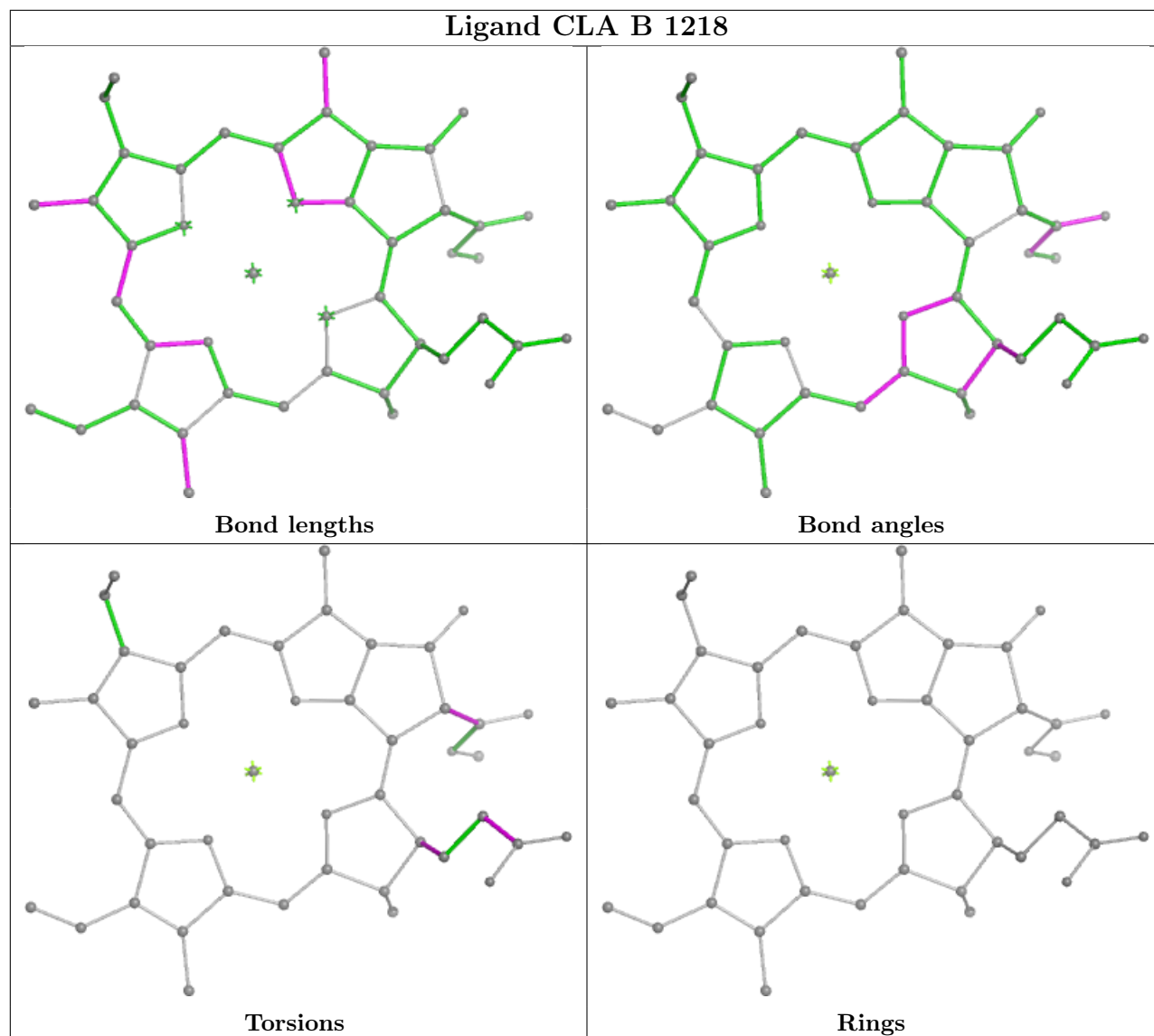
Rings

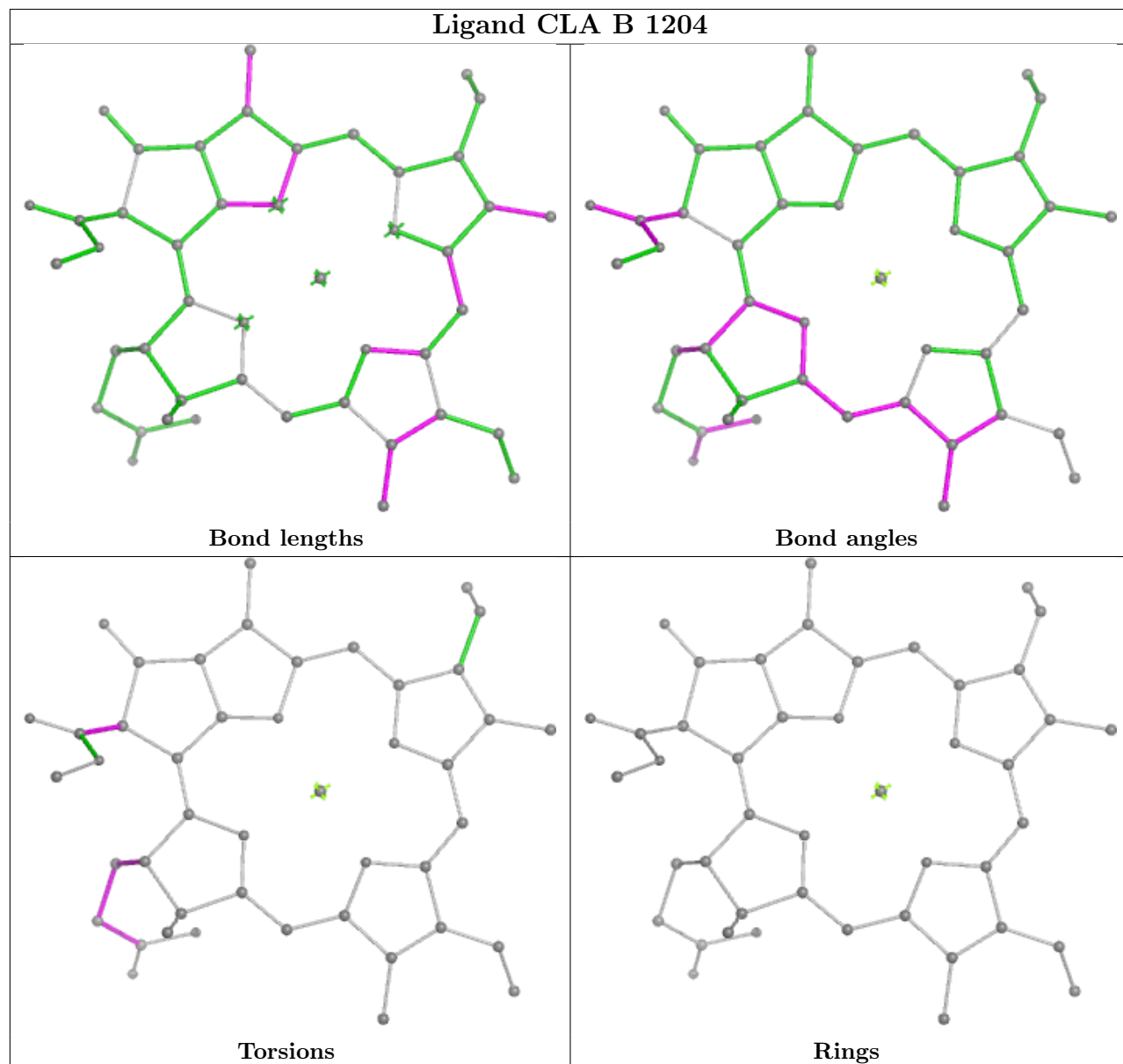
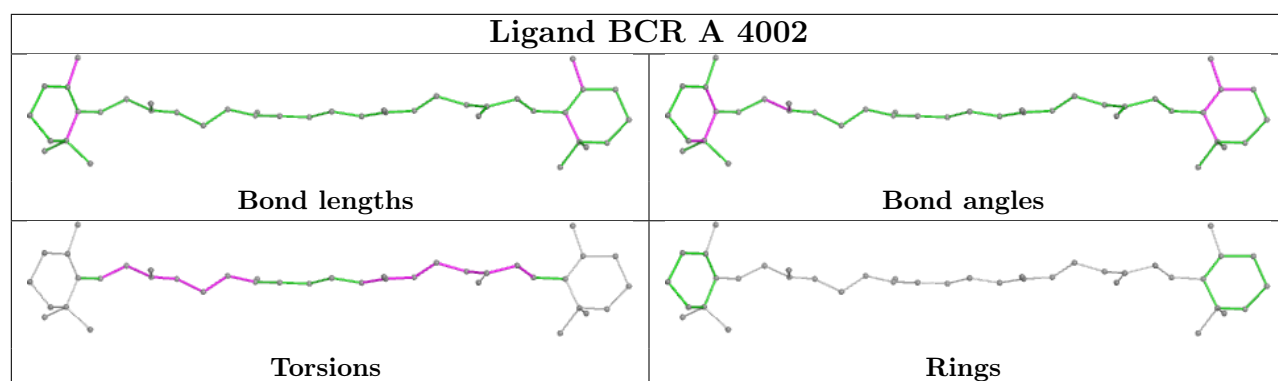
Ligand CLA A 1106

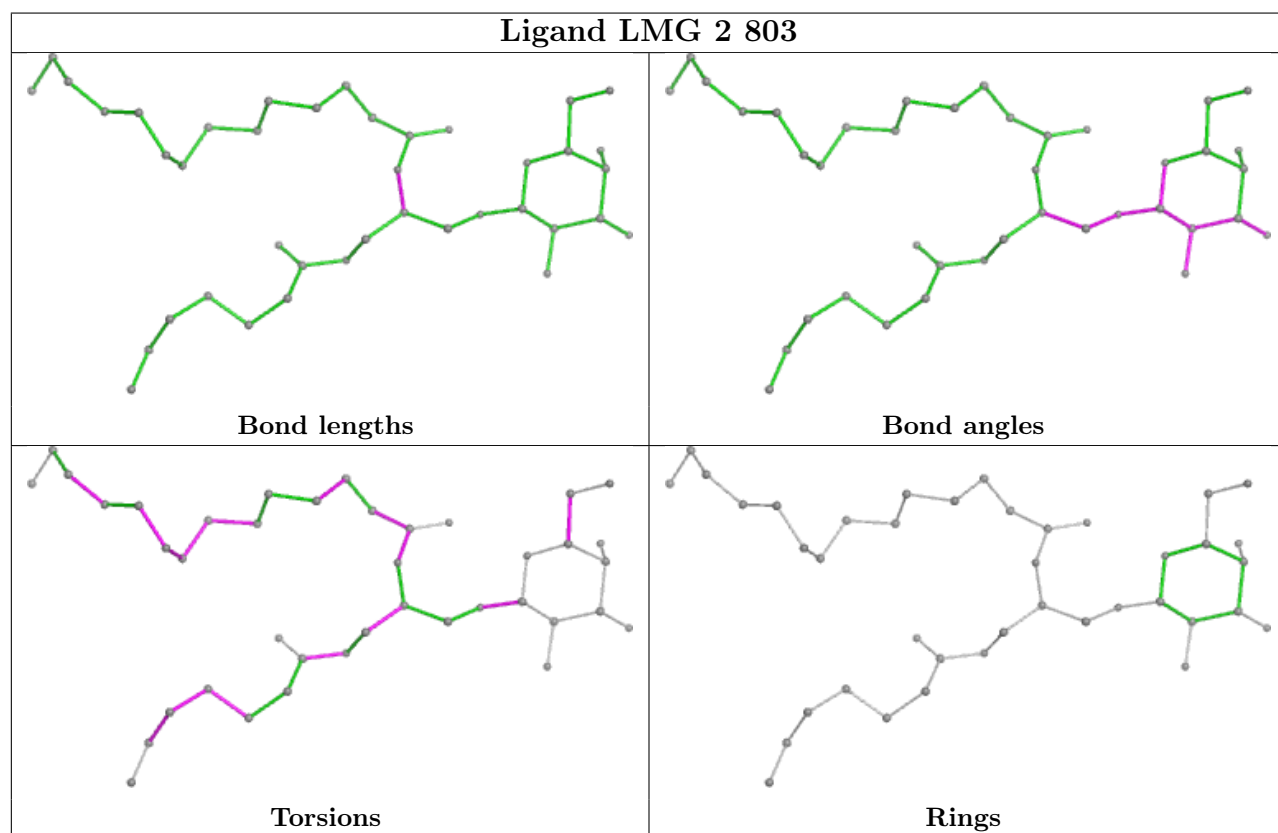
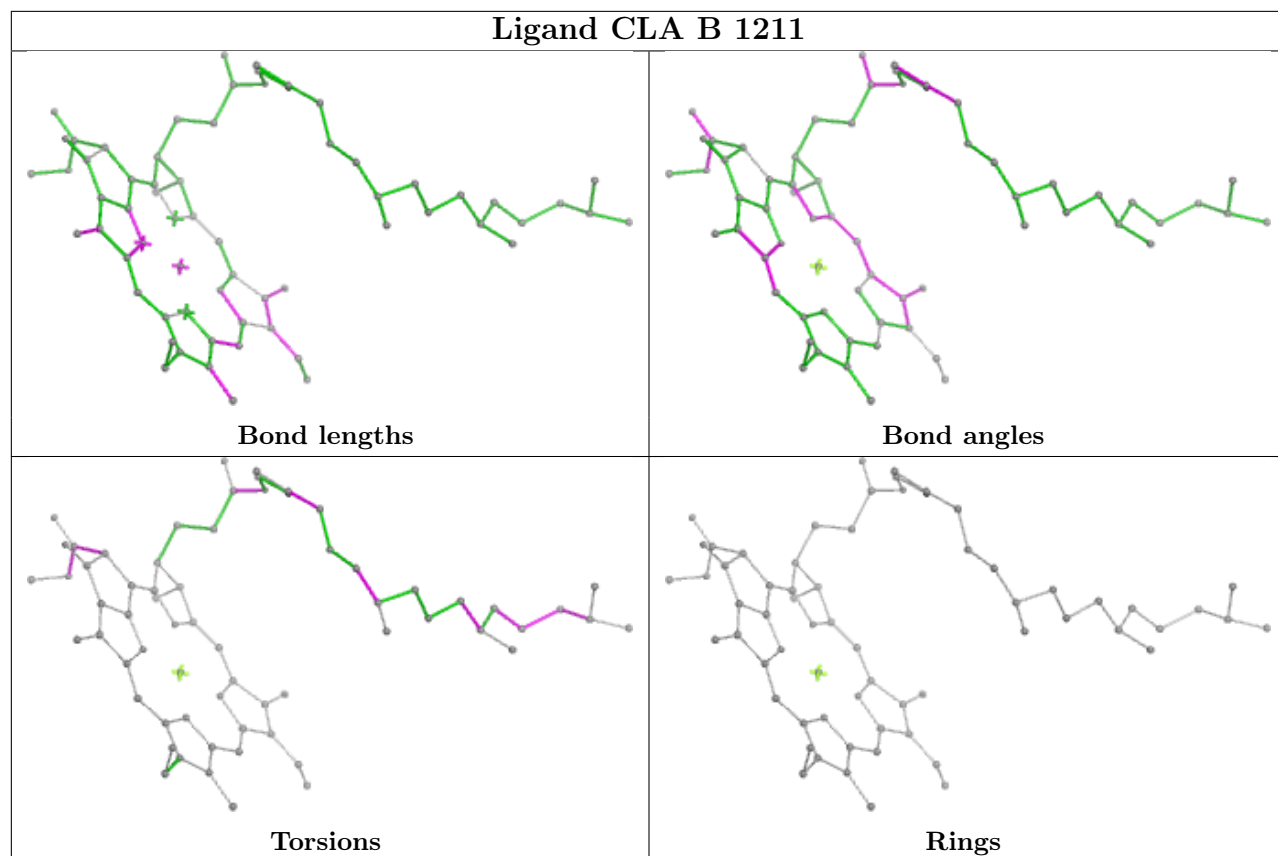


Ligand CLA 3 605

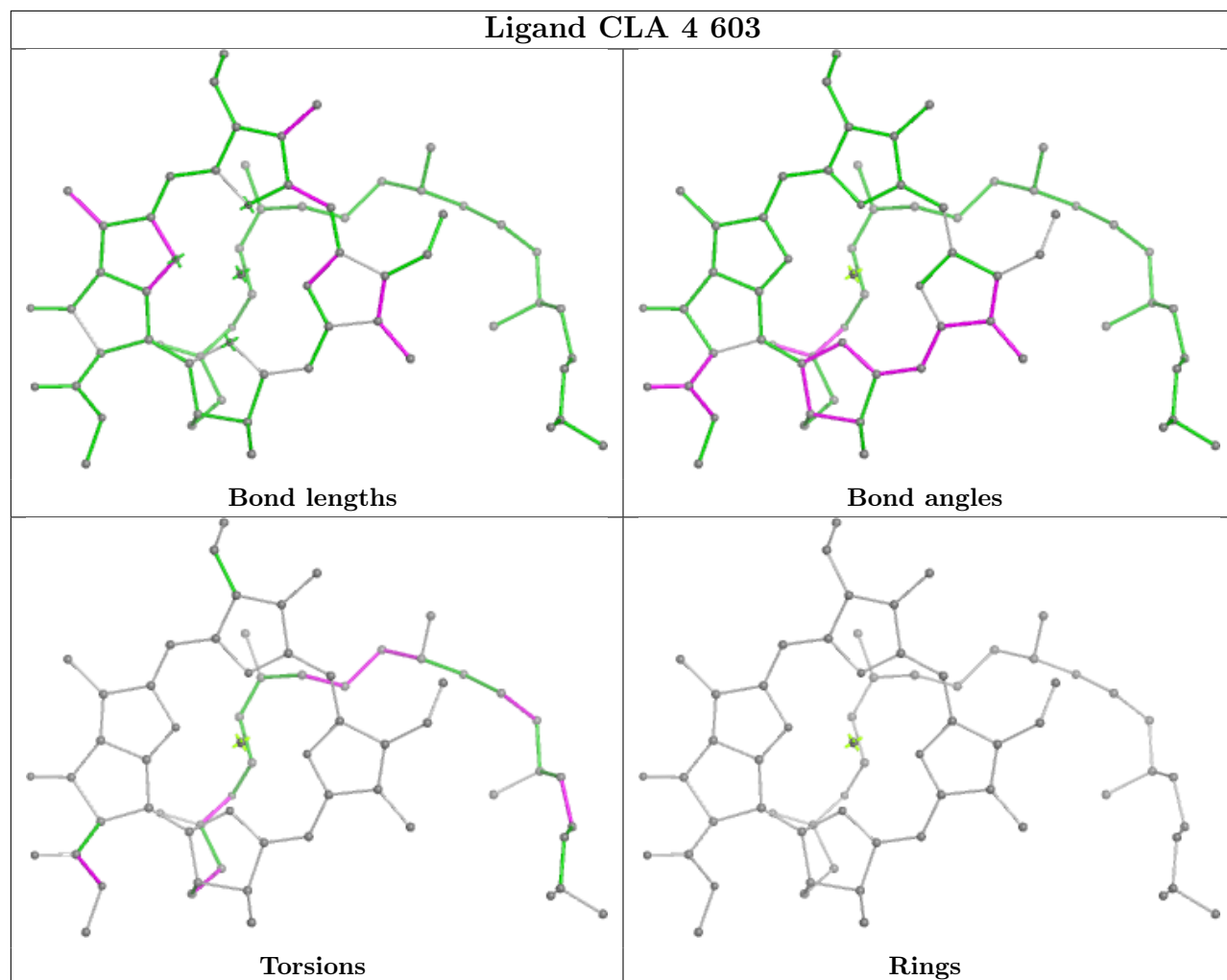




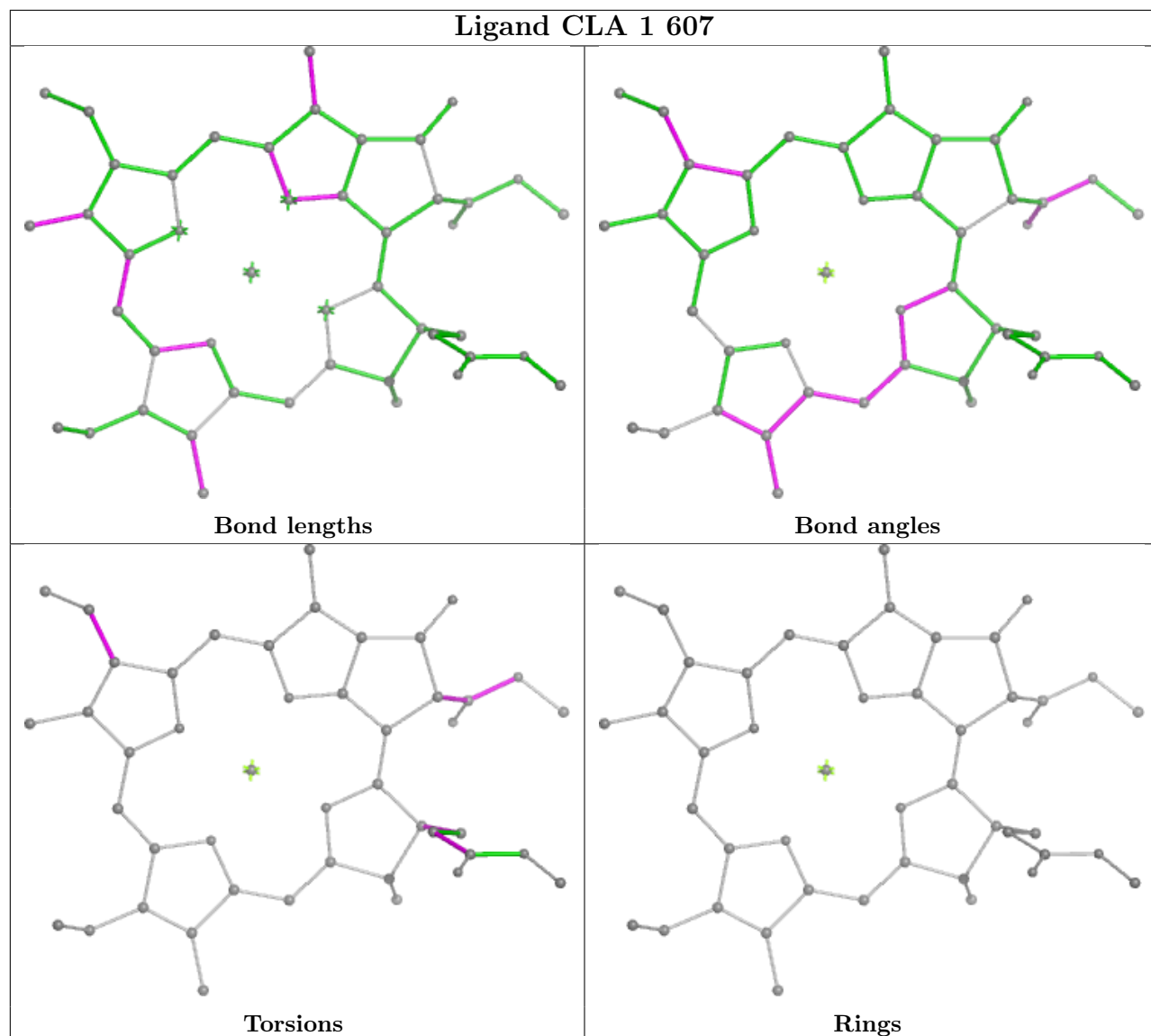




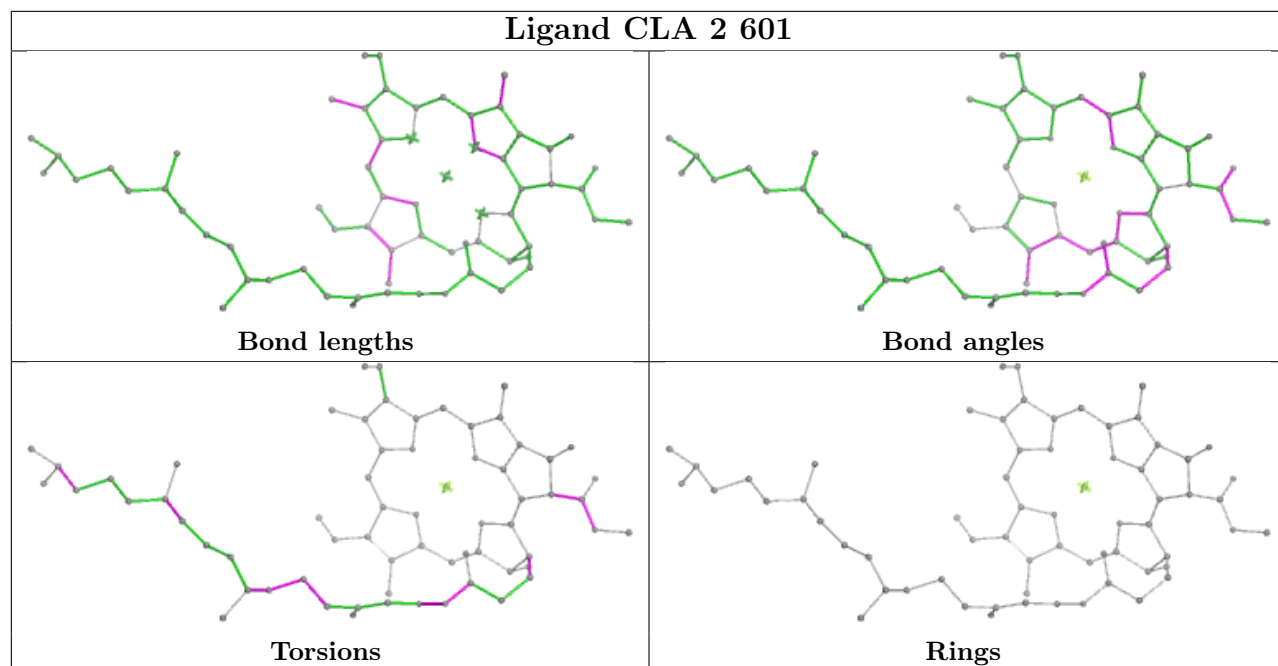
Ligand CLA 4 603



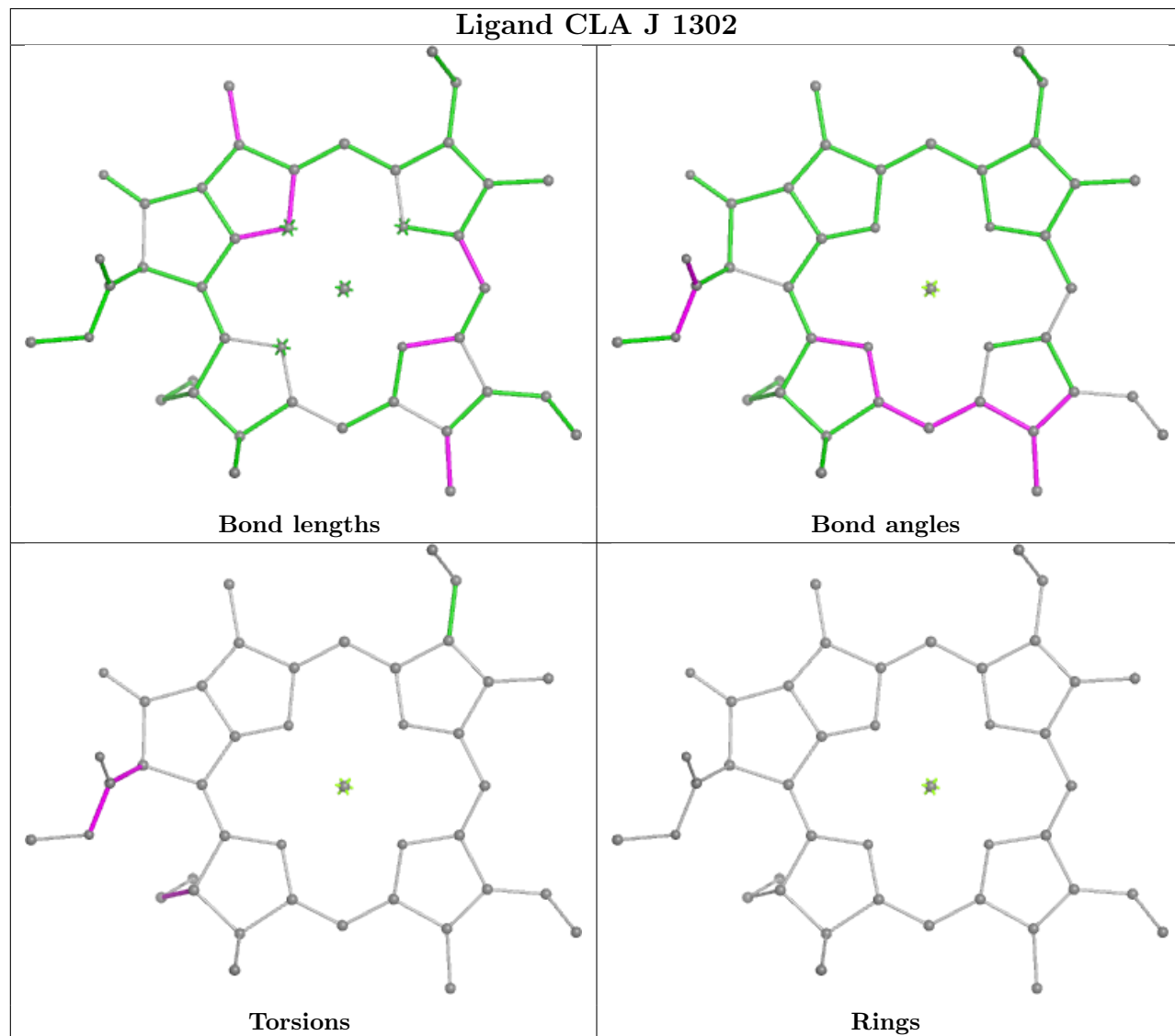
Ligand CLA 1 607

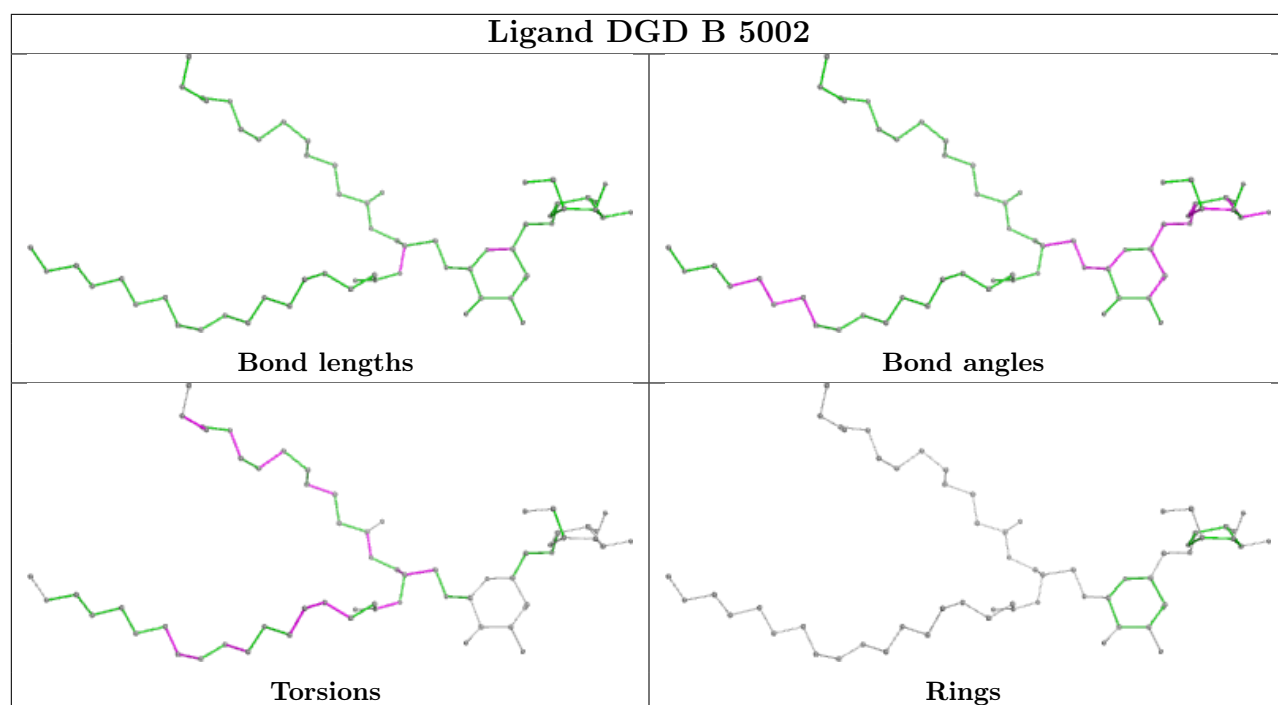


Ligand CLA 2 601

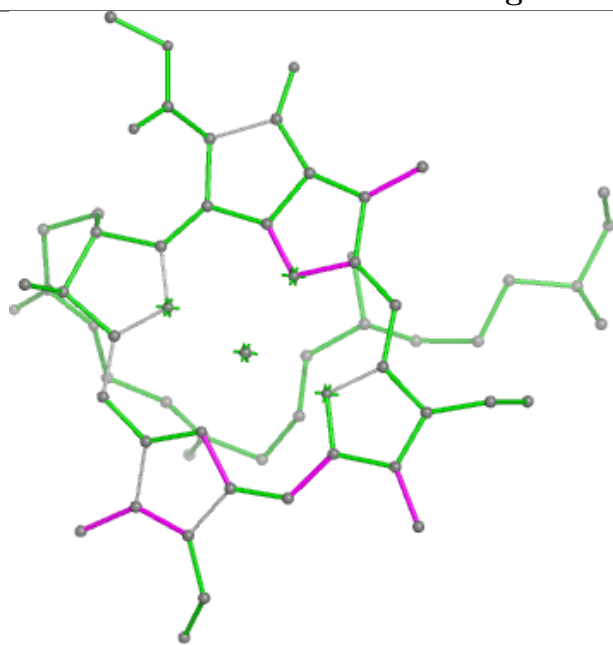


Ligand CLA J 1302

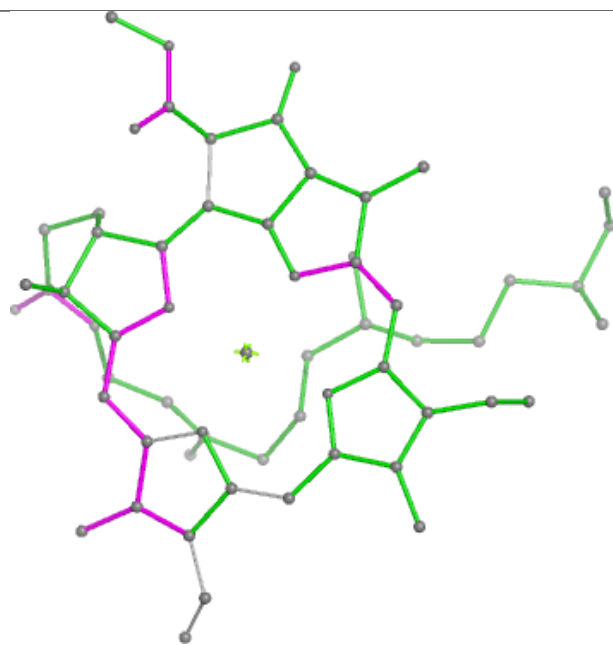




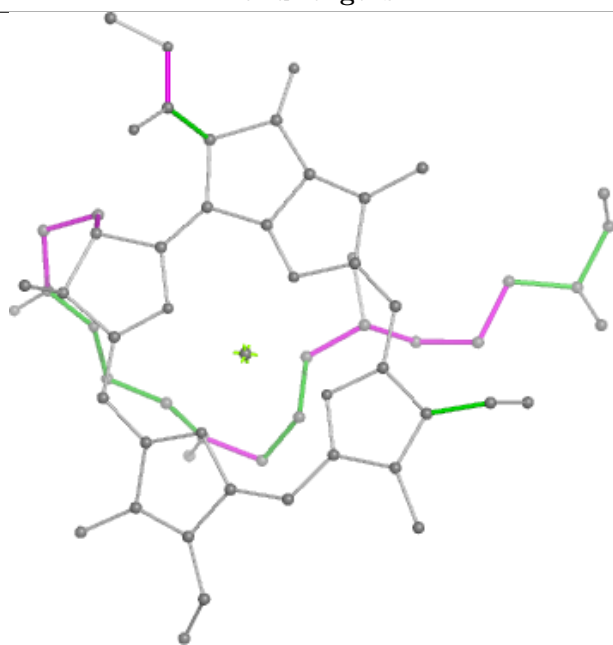
Ligand CLA B 1224



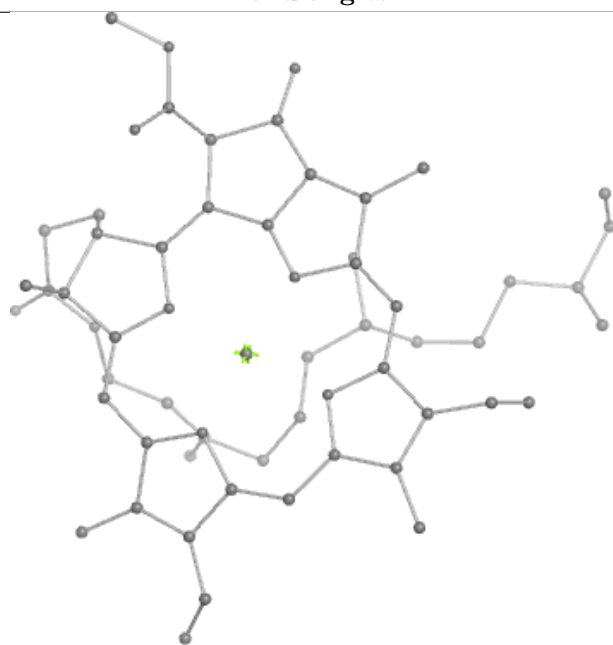
Bond lengths



Bond angles

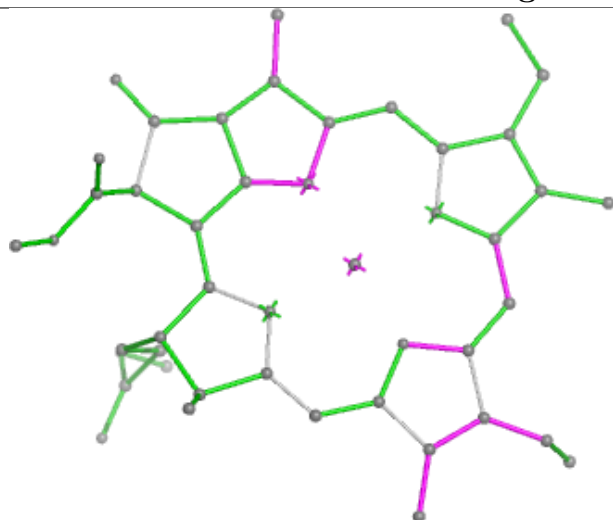


Torsions

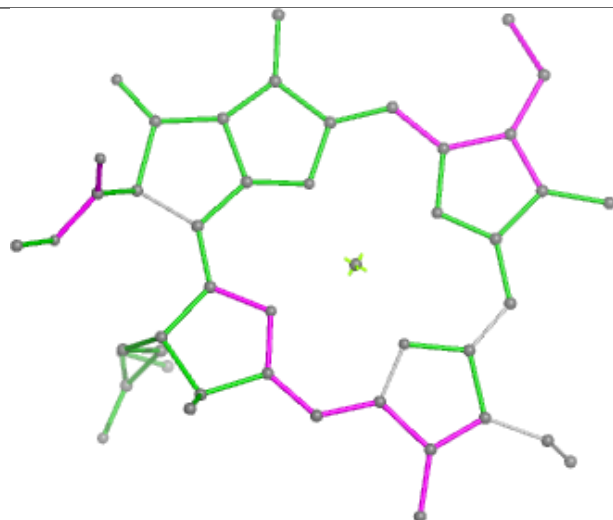


Rings

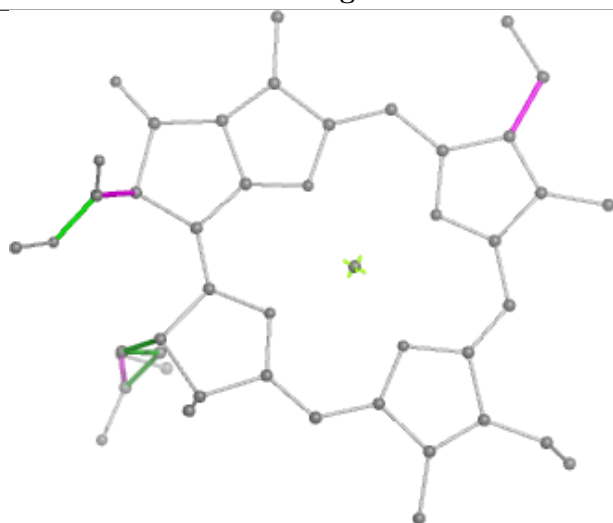
Ligand CLA 4 608



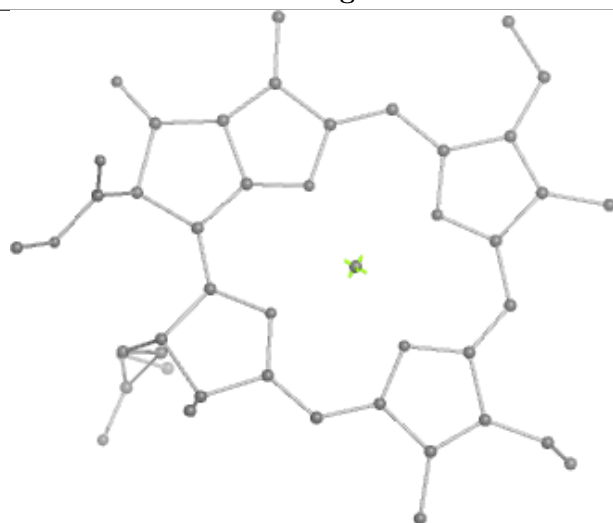
Bond lengths



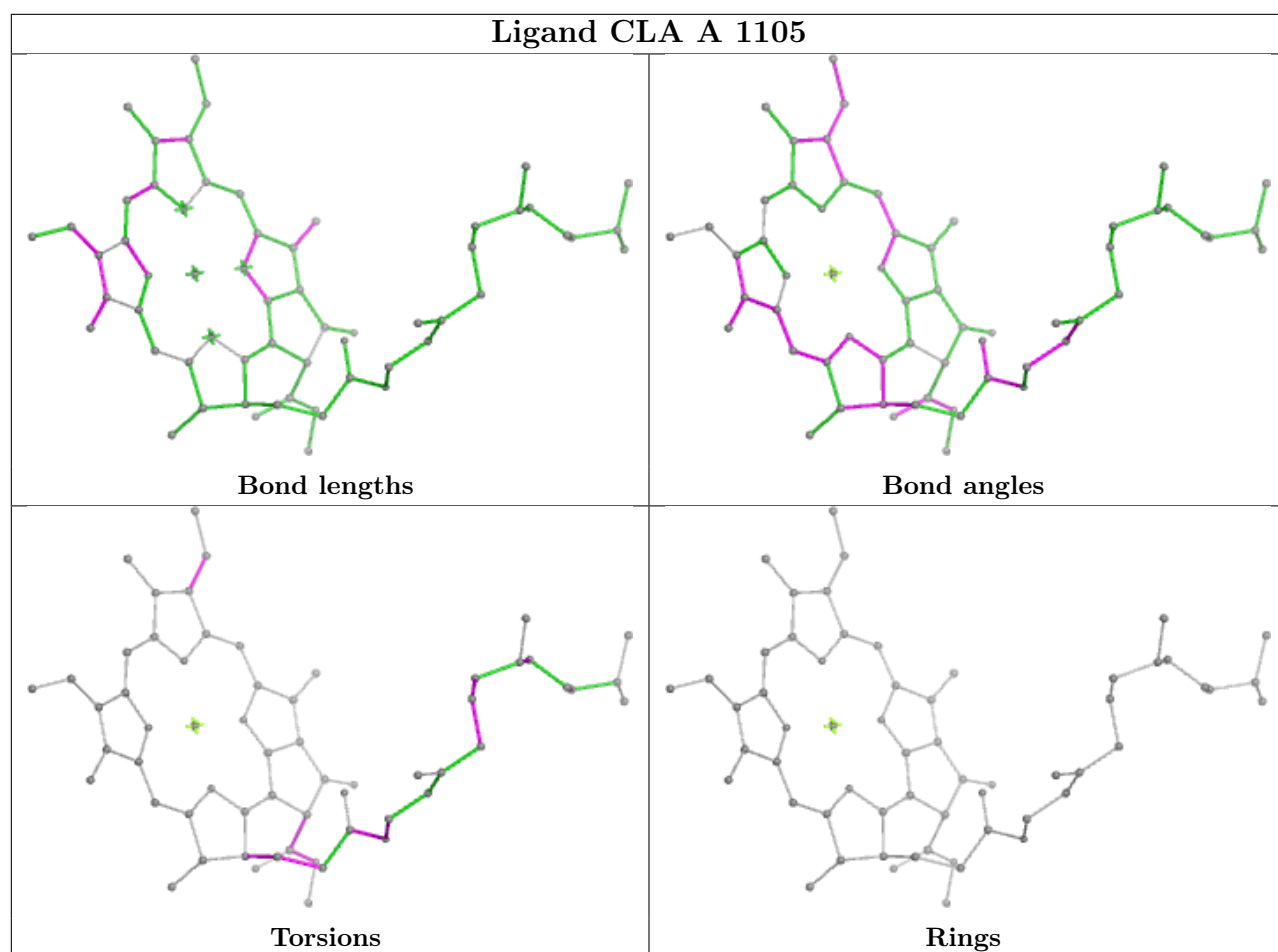
Bond angles

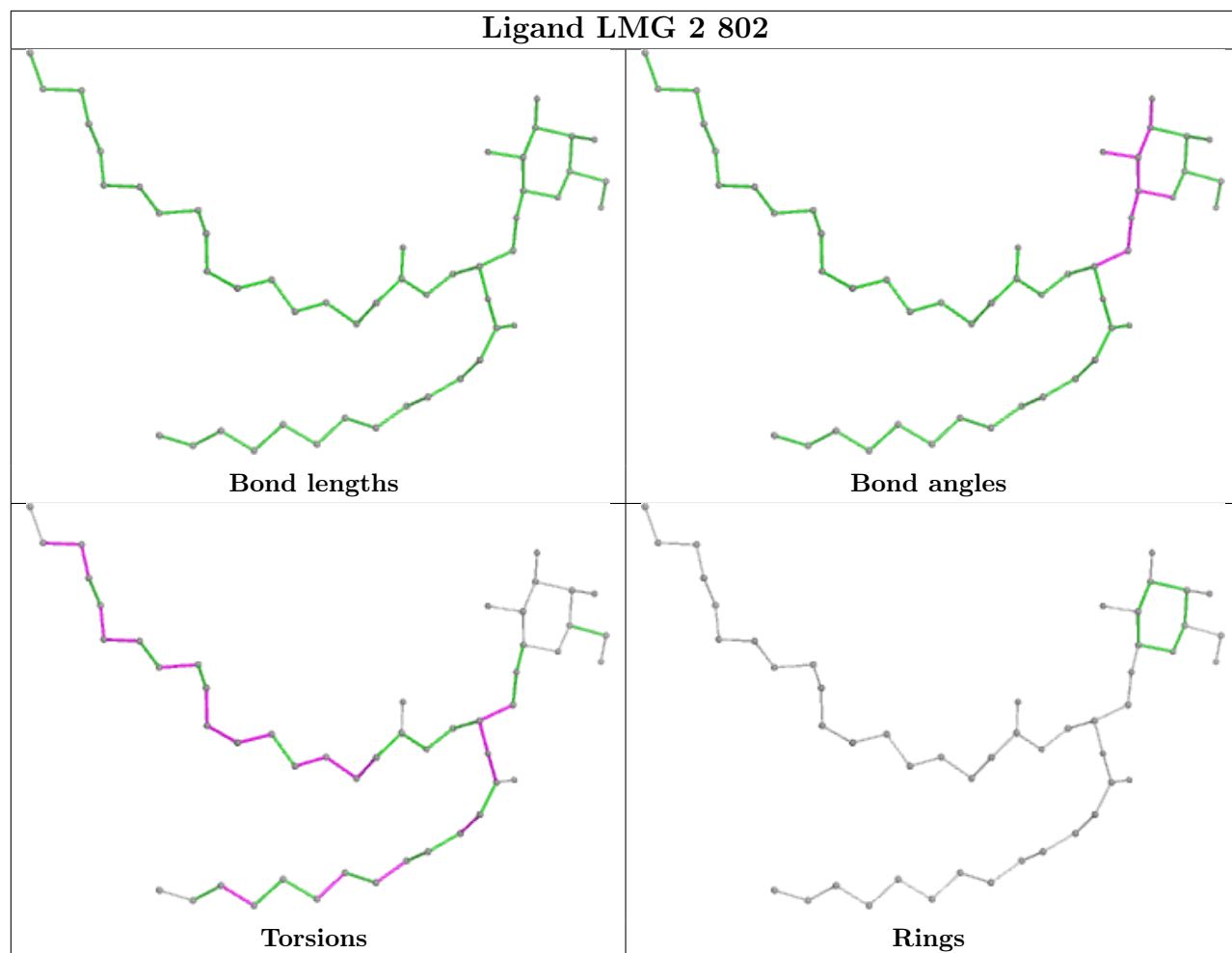


Torsions

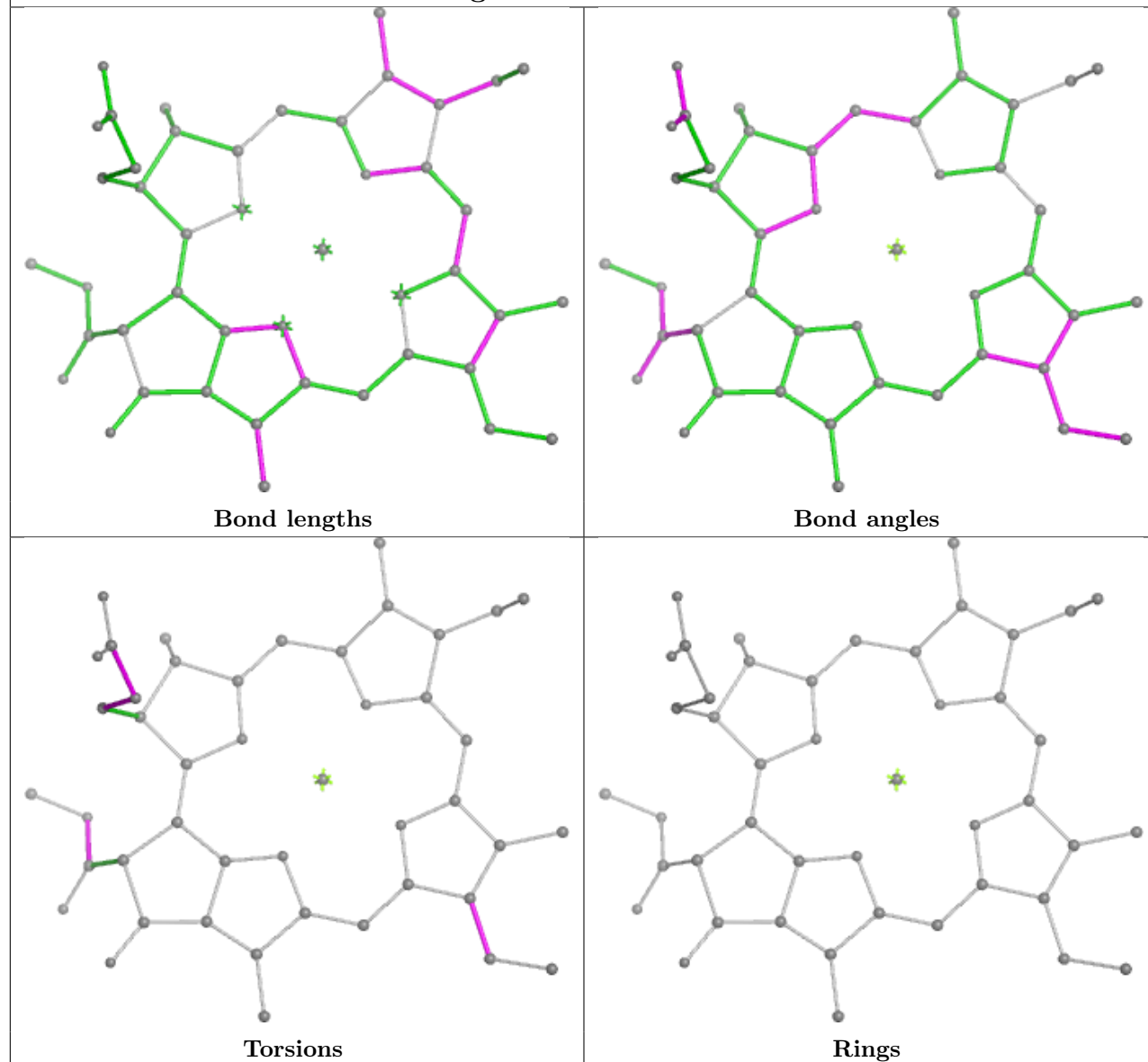


Rings

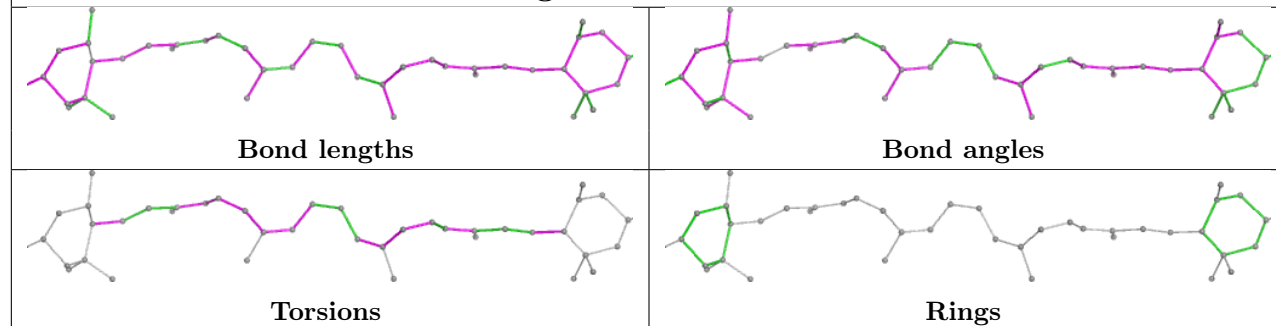


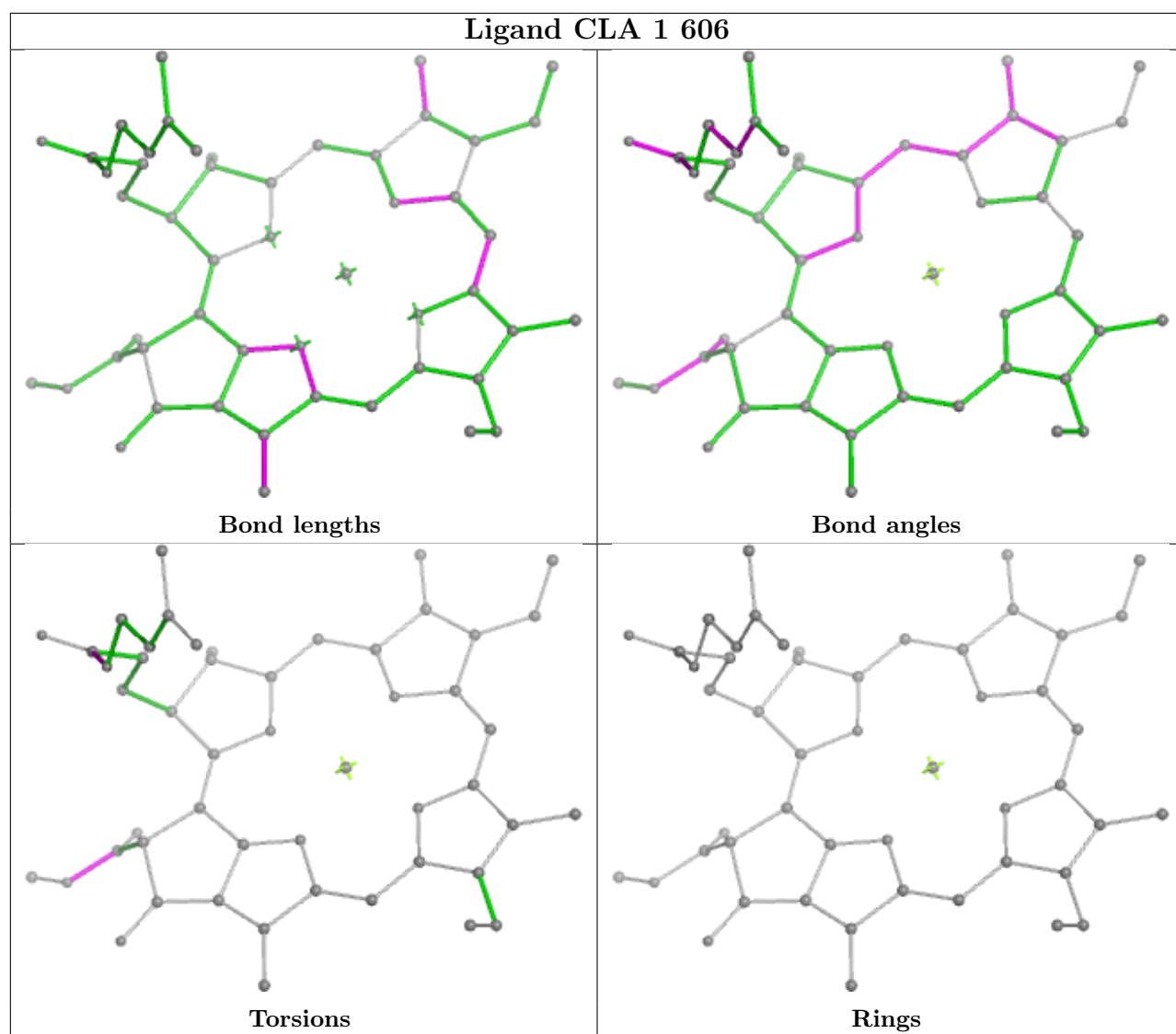


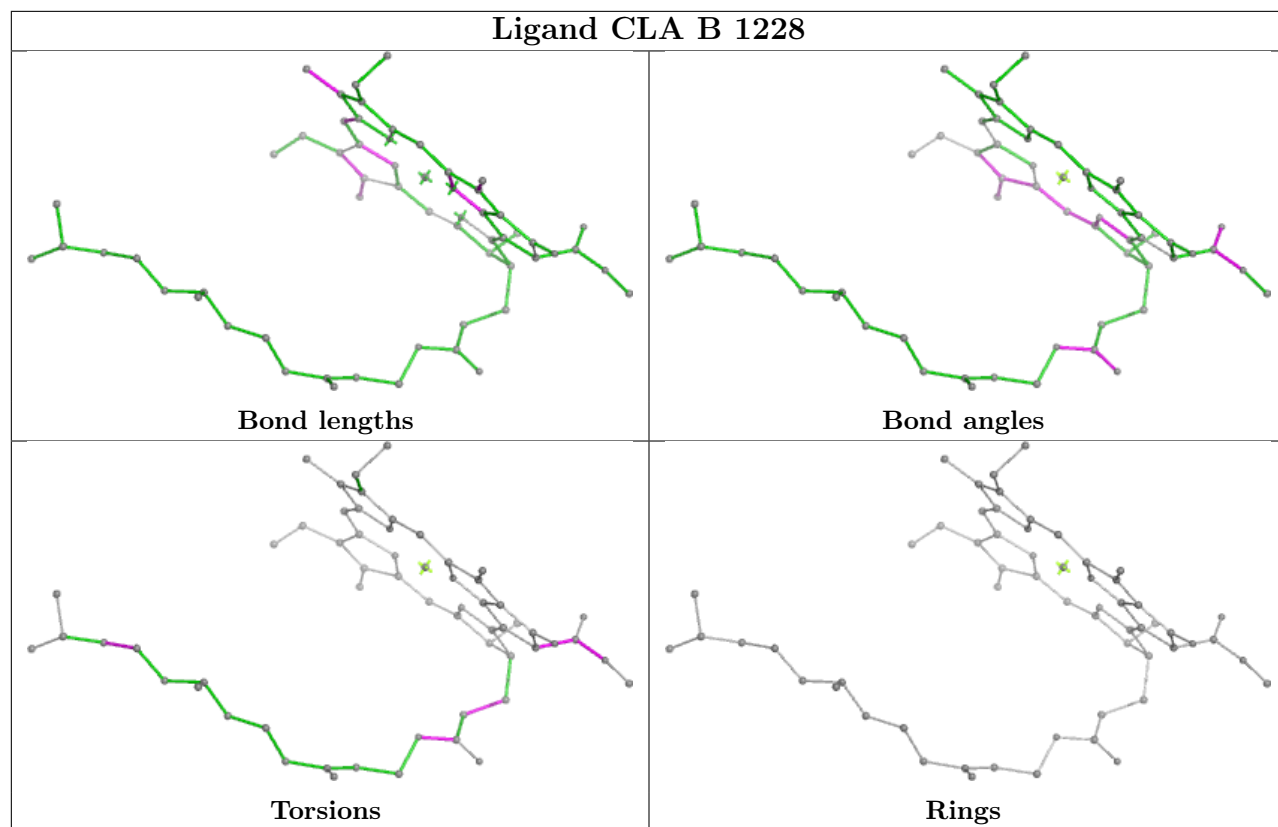
Ligand CLA A 1132

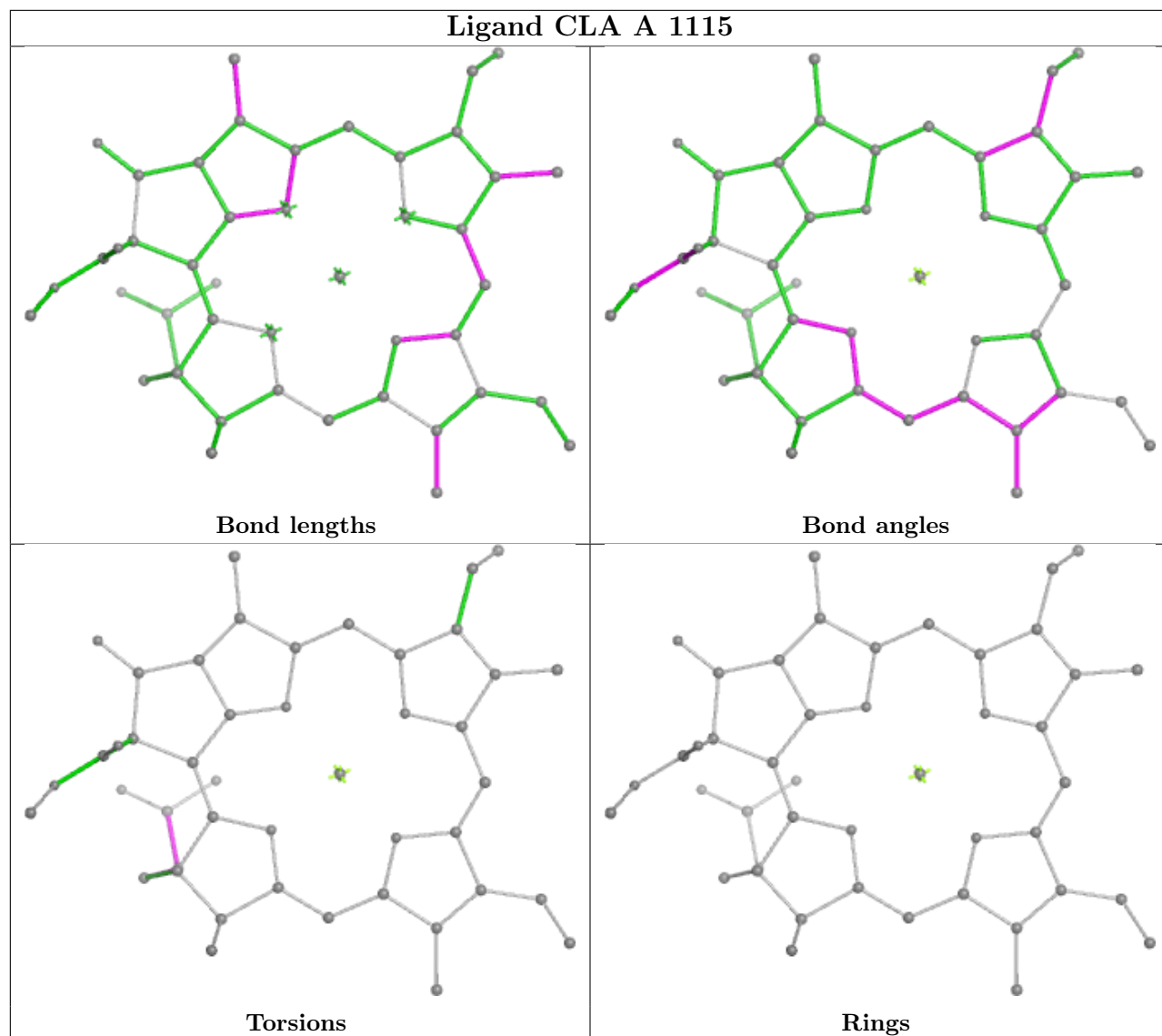


Ligand LUT 3 501

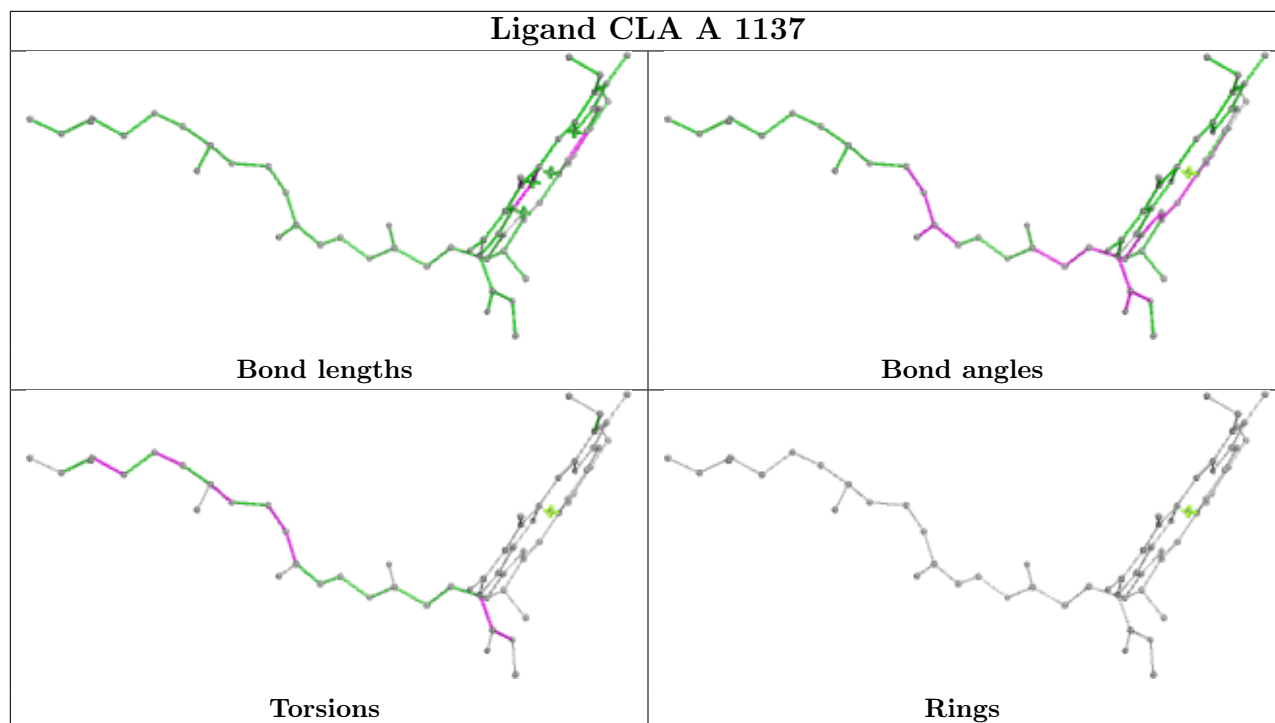




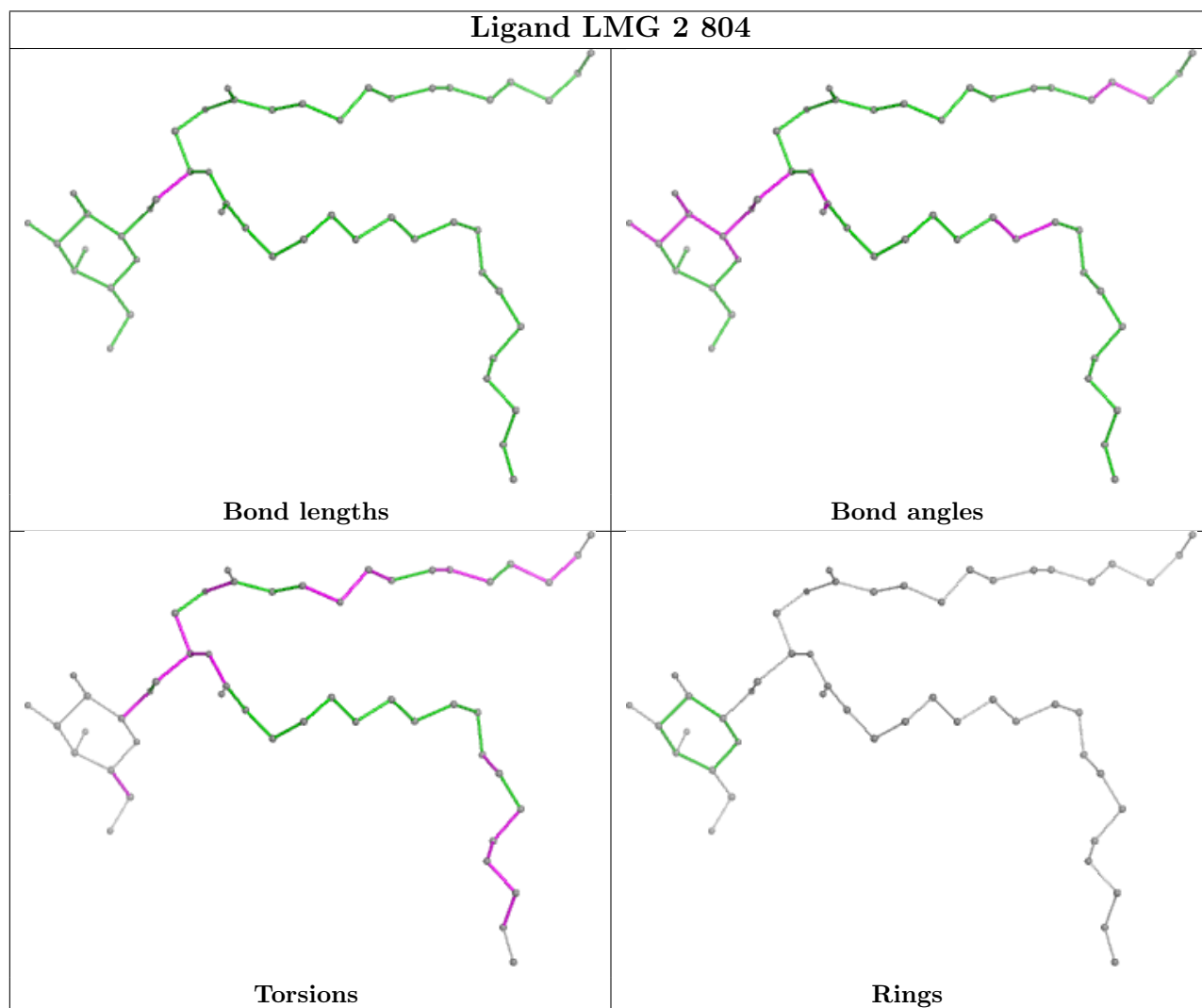


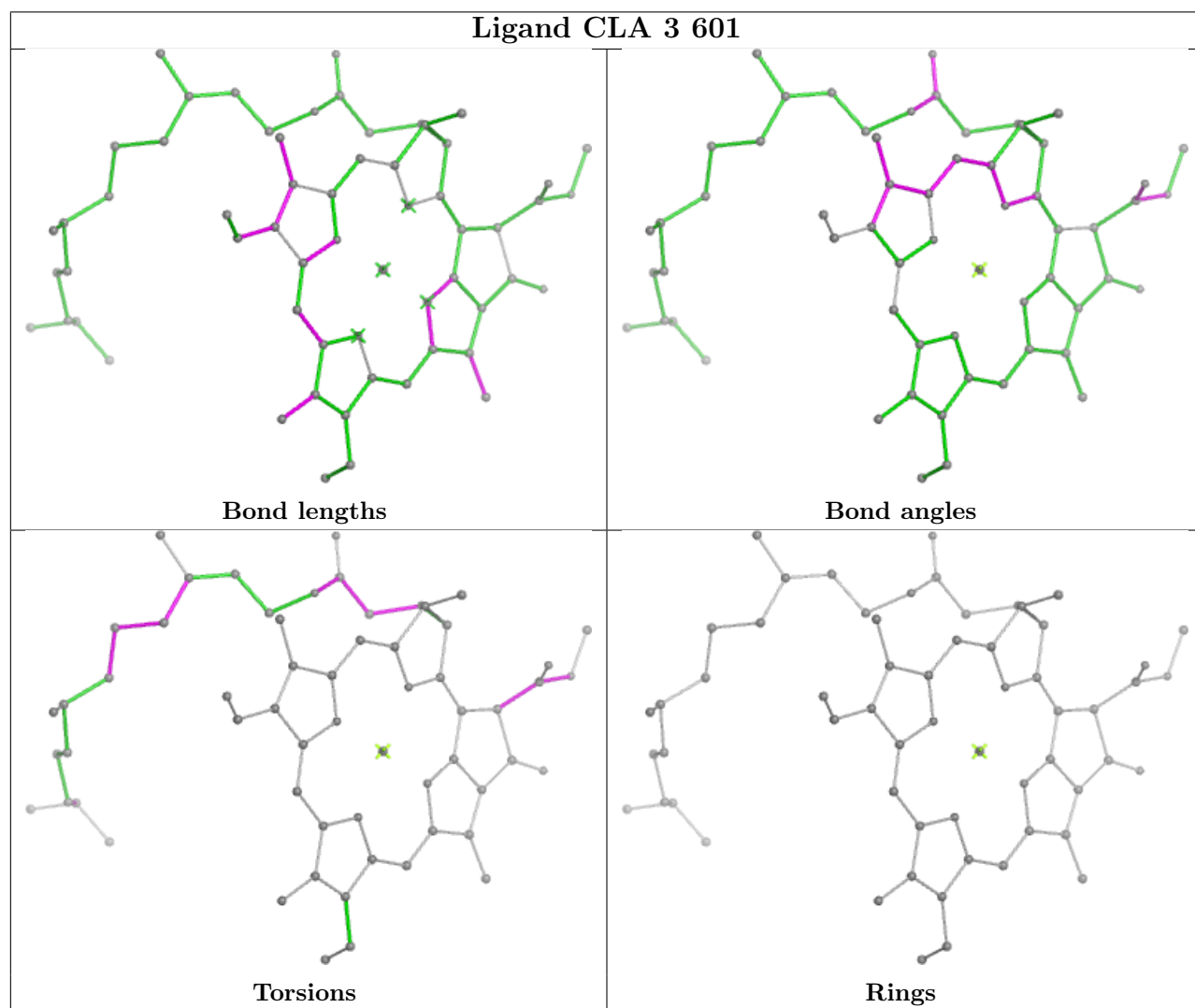
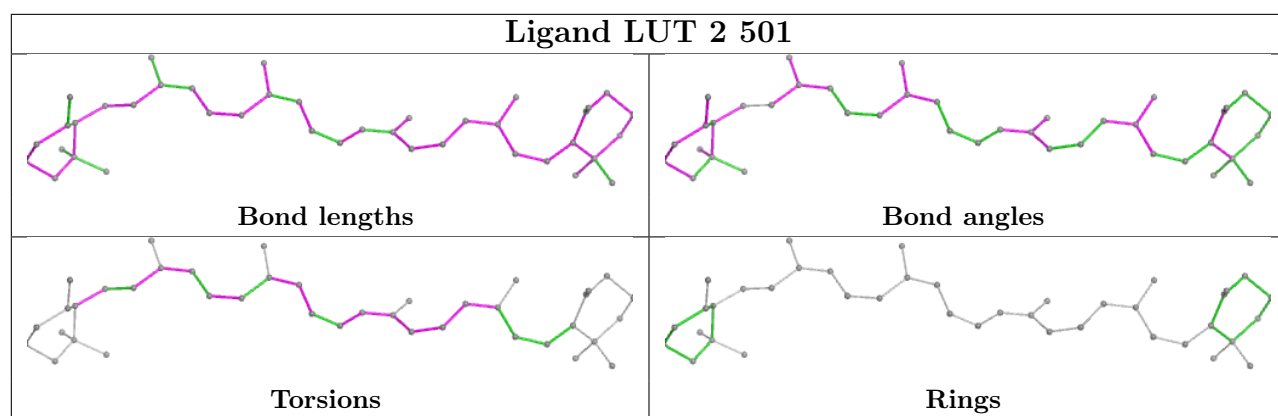


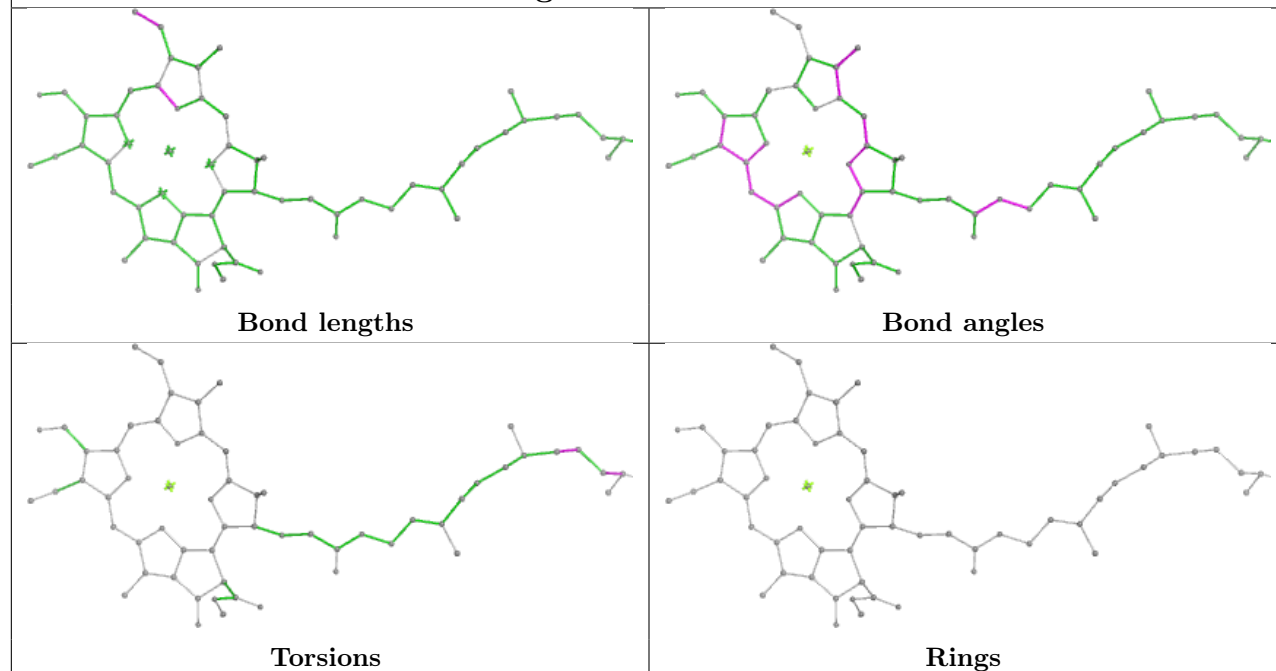
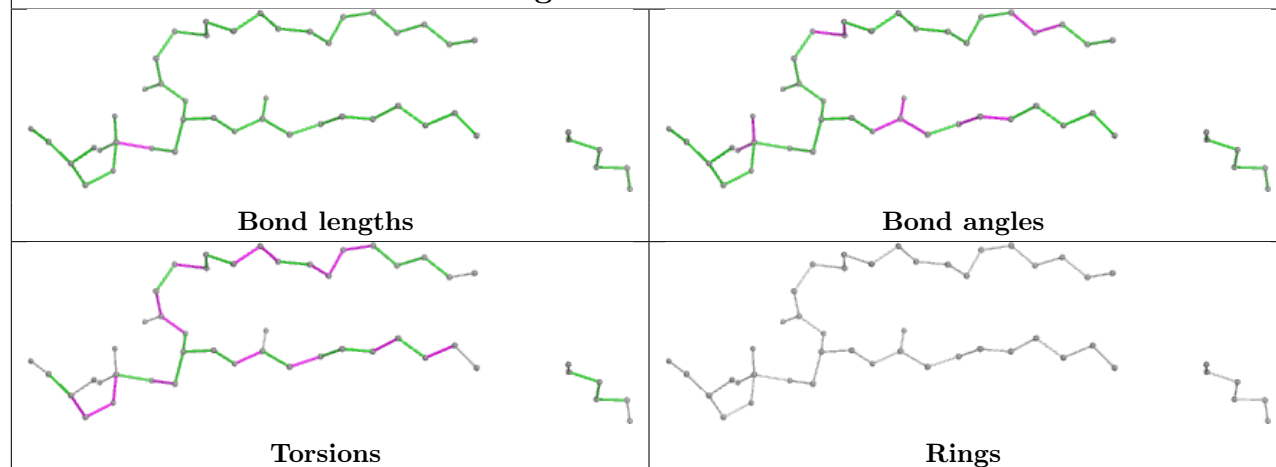
Ligand CLA A 1137

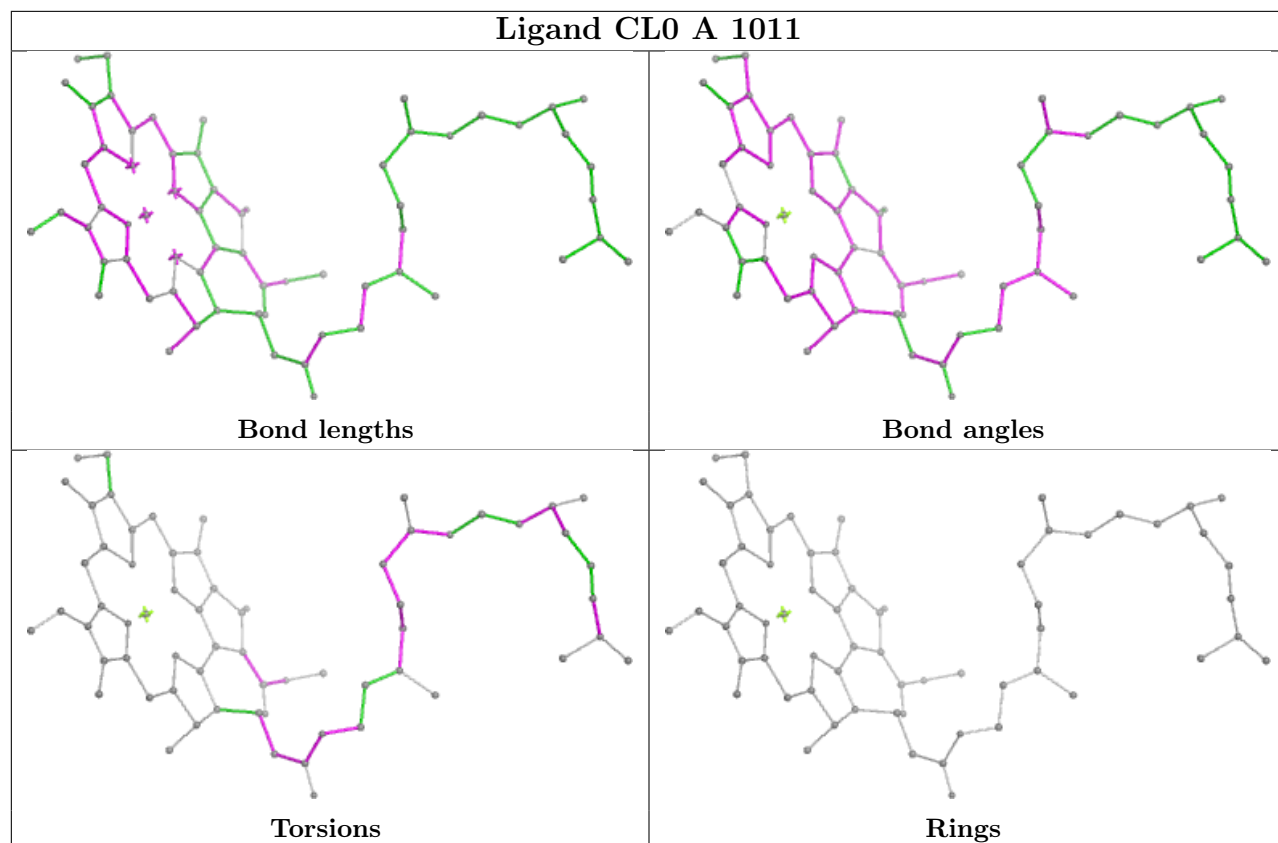


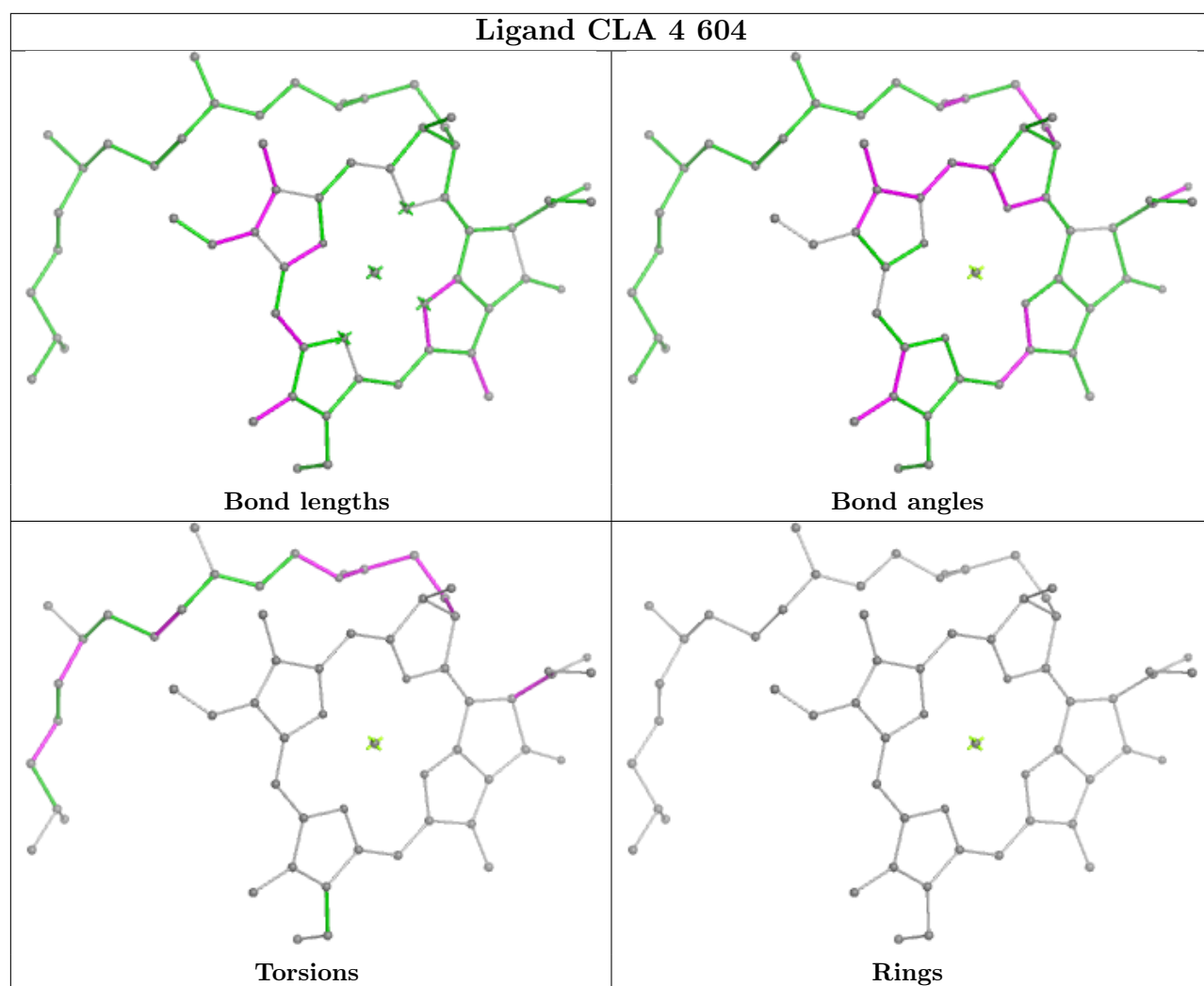
Ligand LMG 2 804



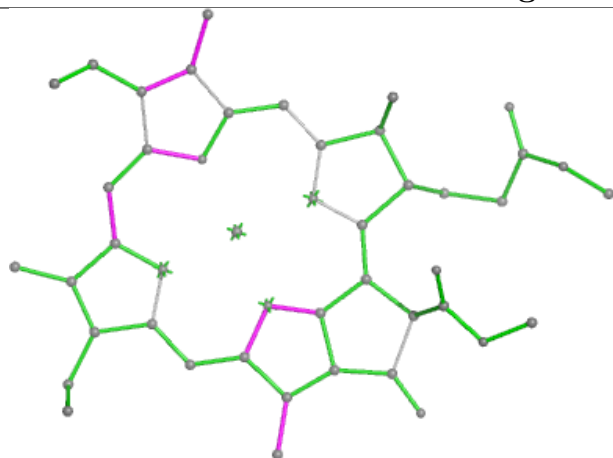


Ligand CHL 4 613**Ligand LHG 3 801**

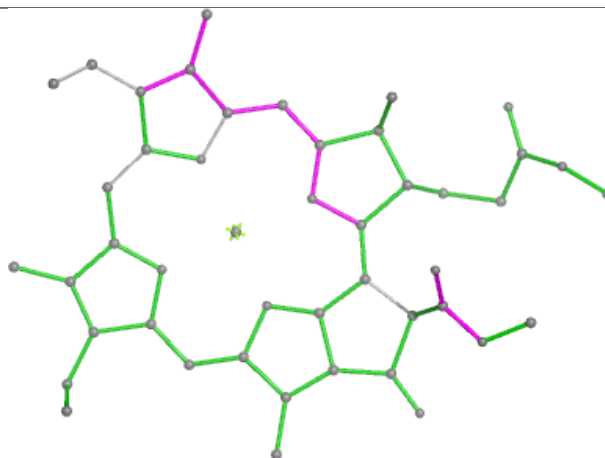




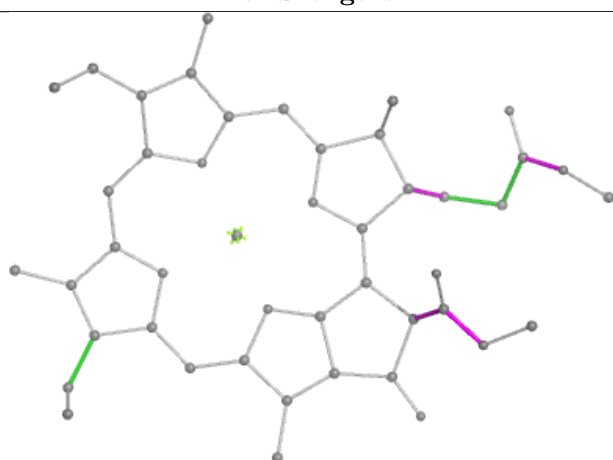
Ligand CLA 1 602



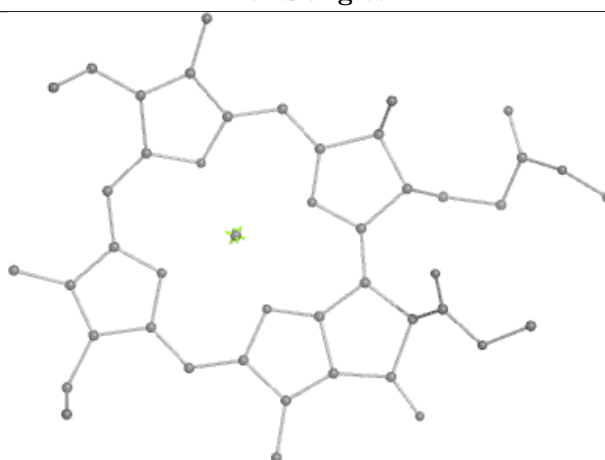
Bond lengths



Bond angles

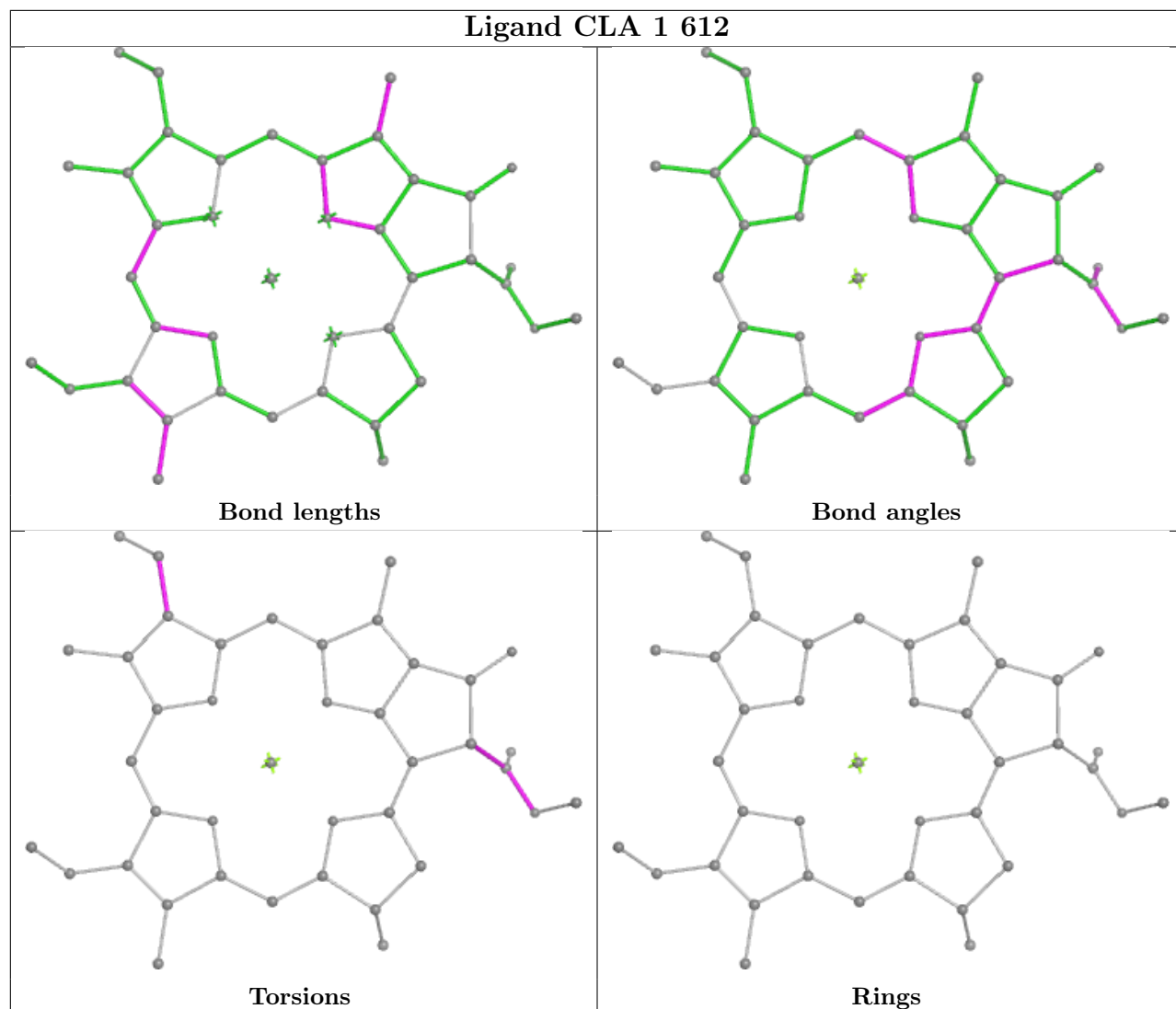


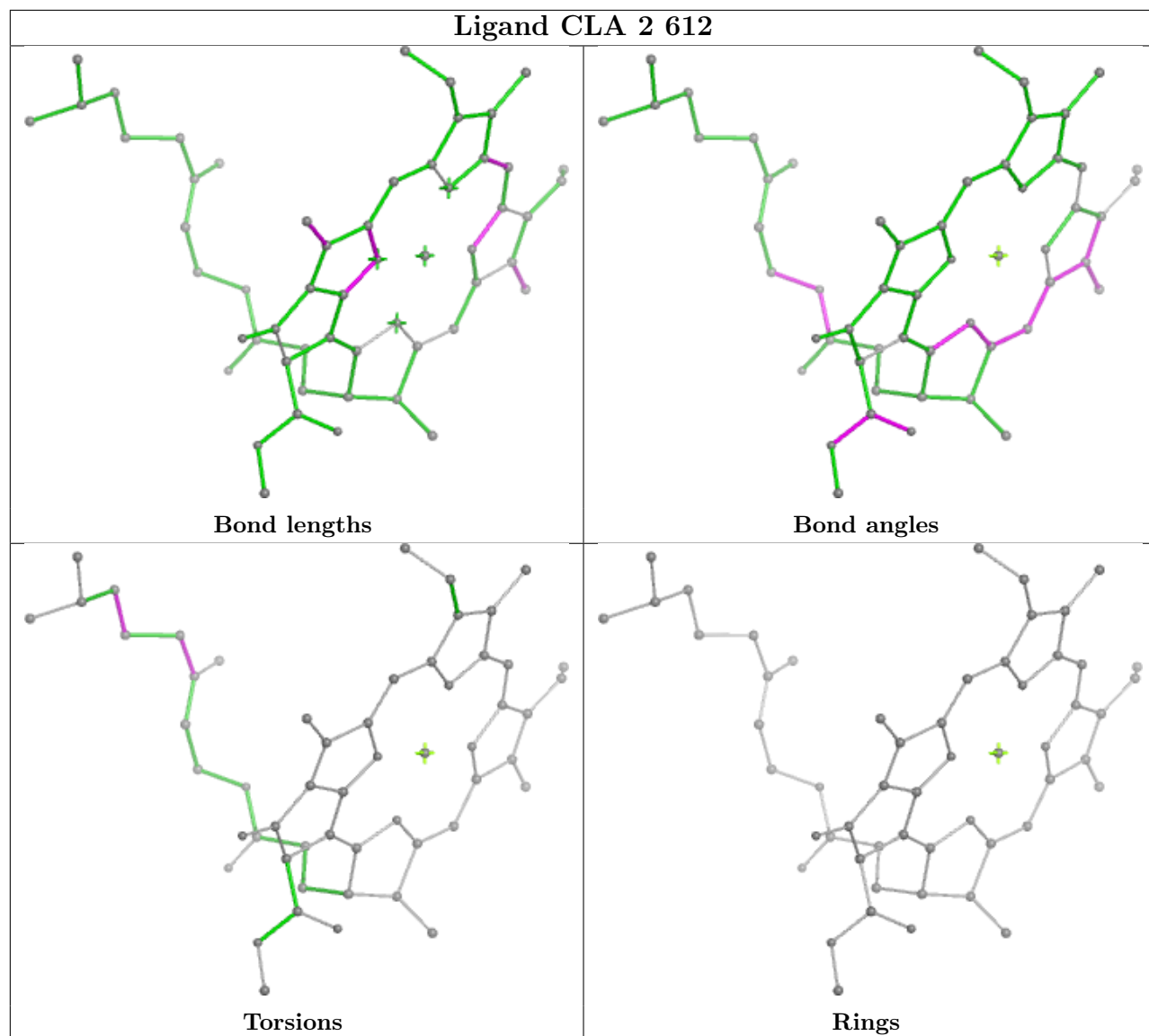
Torsions

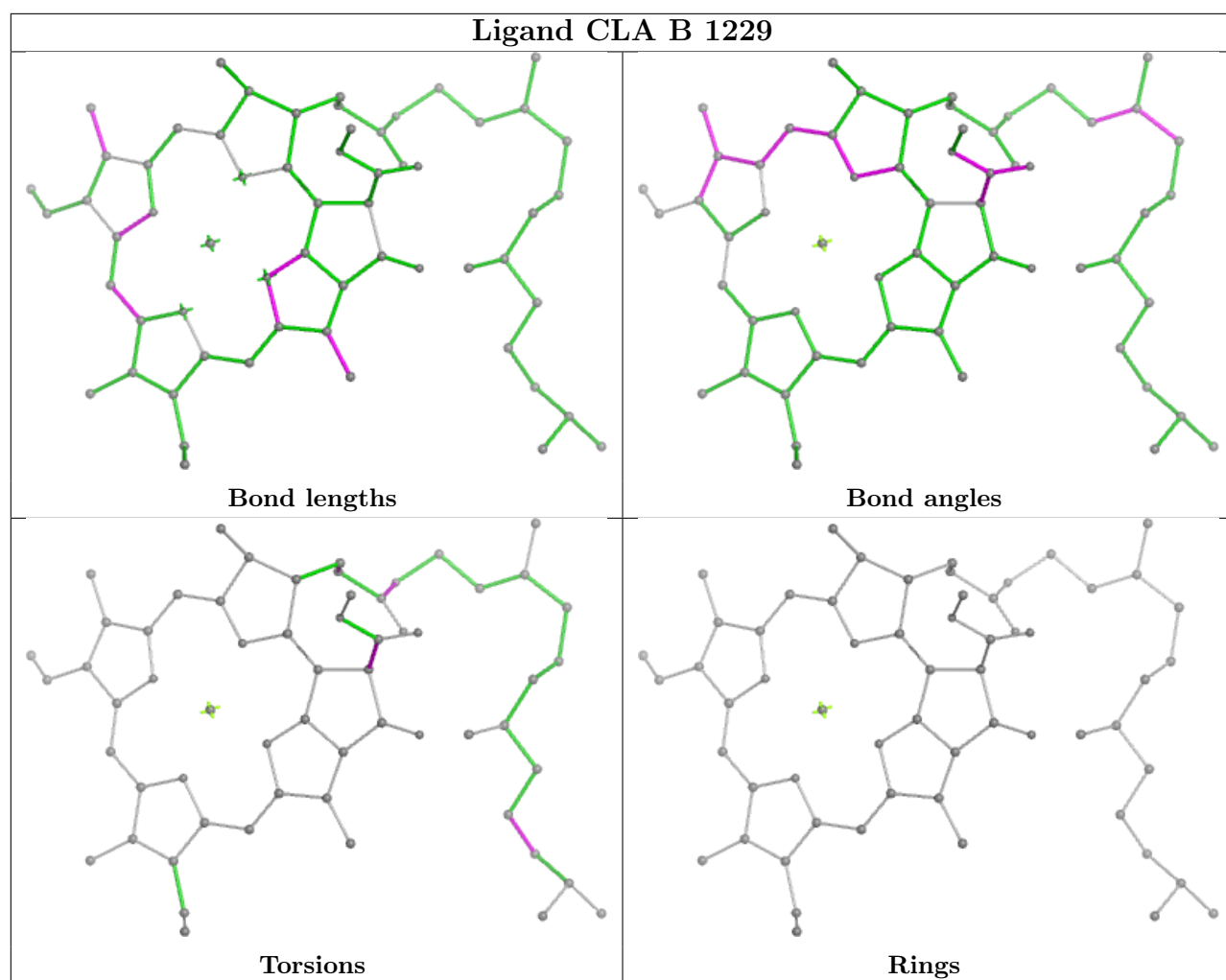


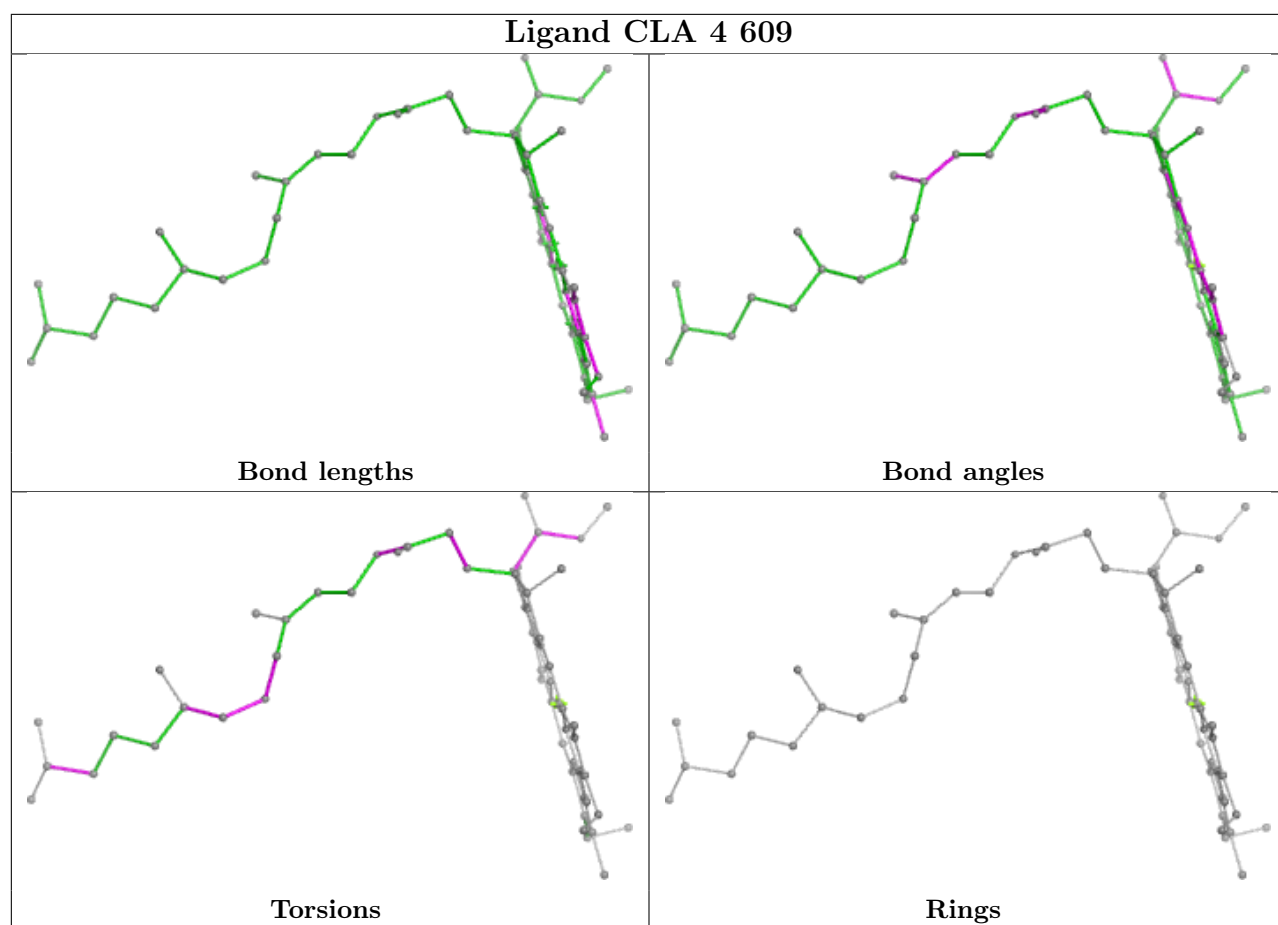
Rings

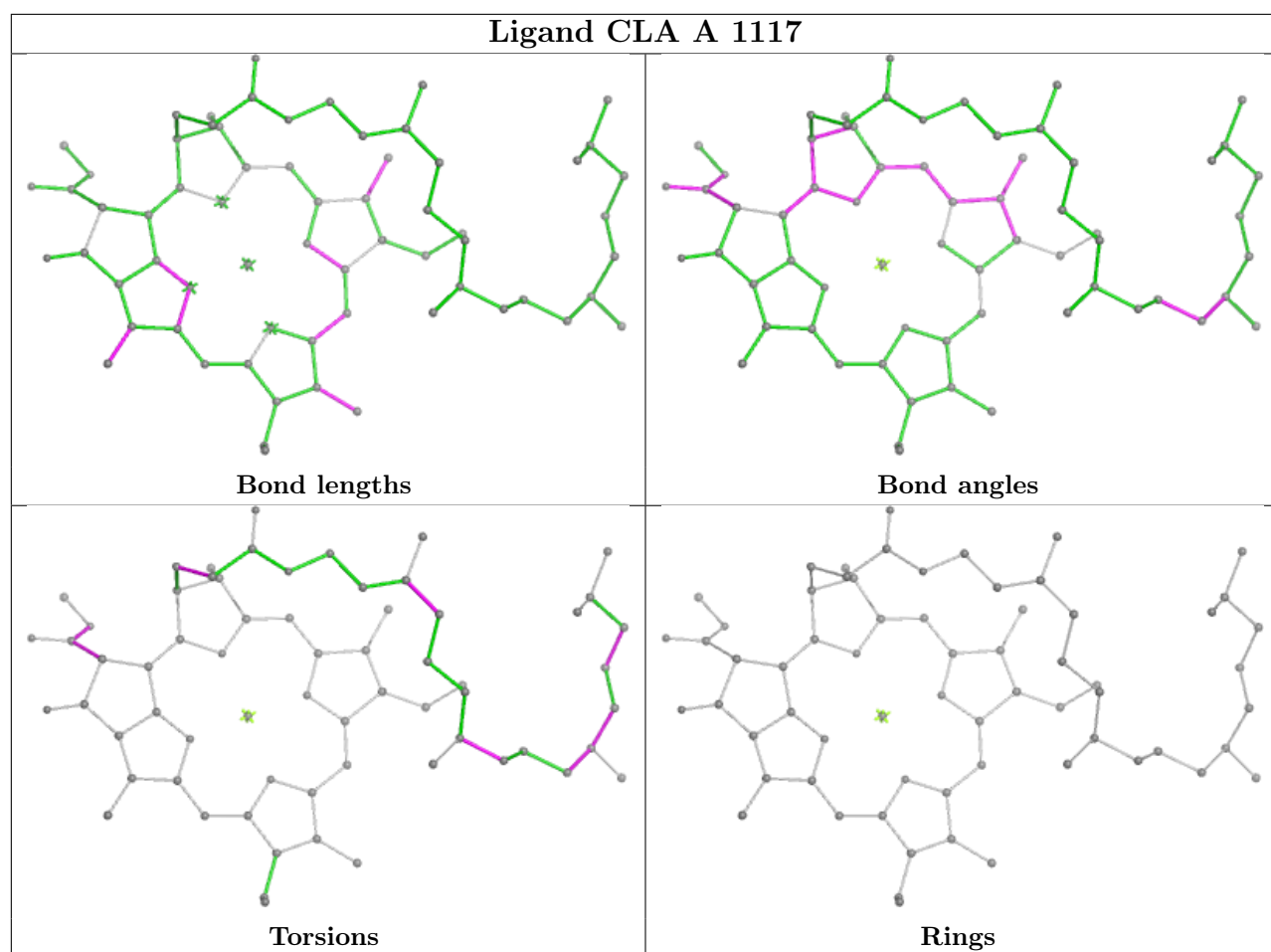
Ligand CLA 1 612

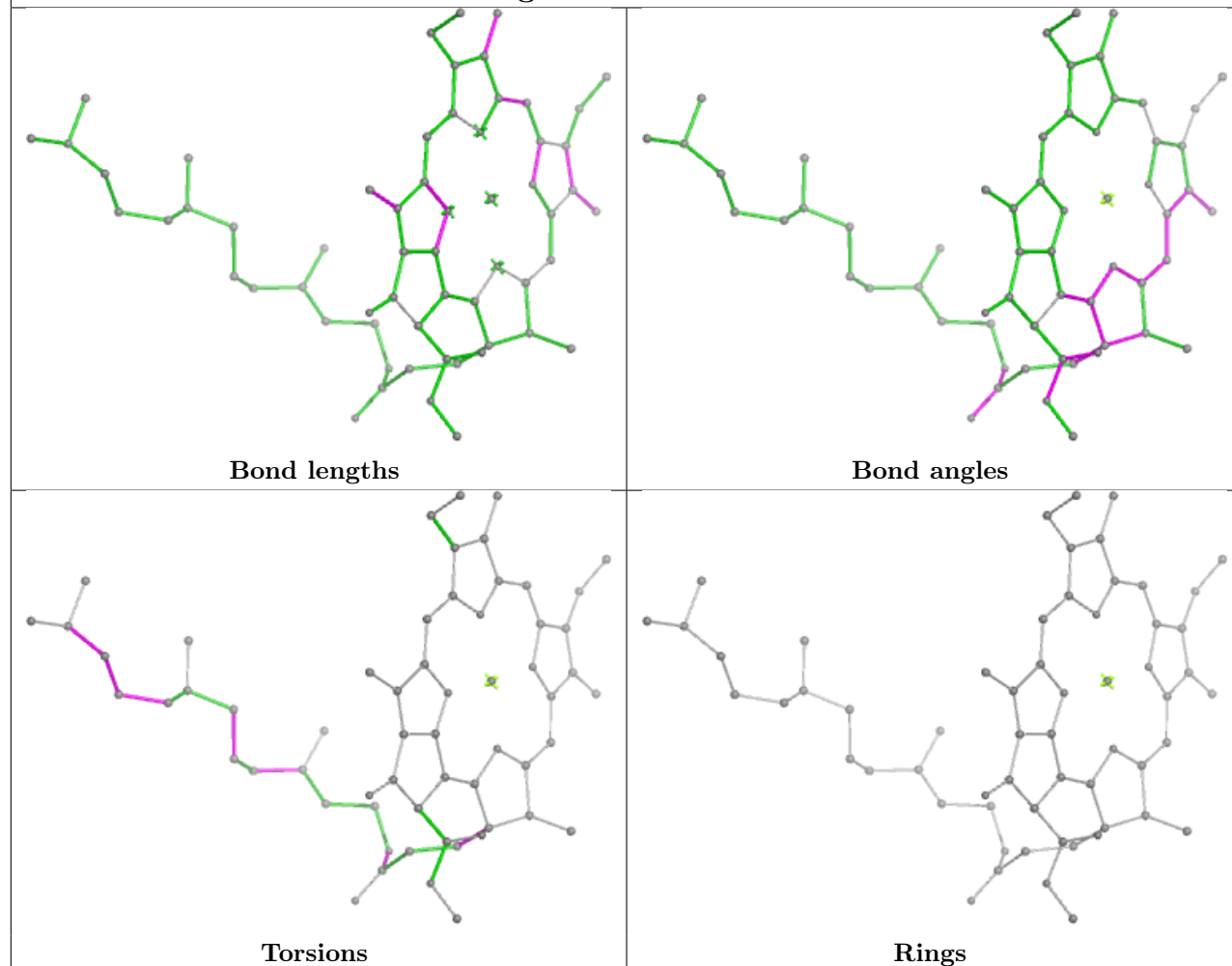
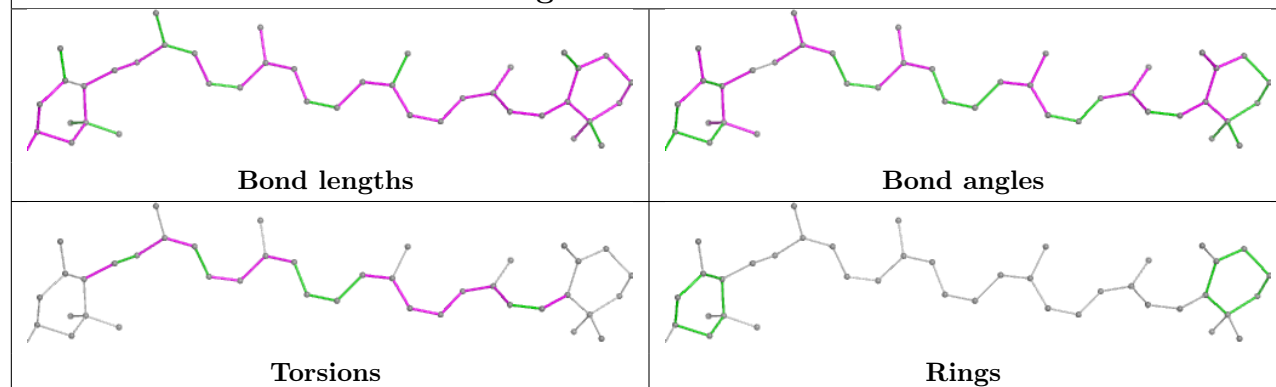


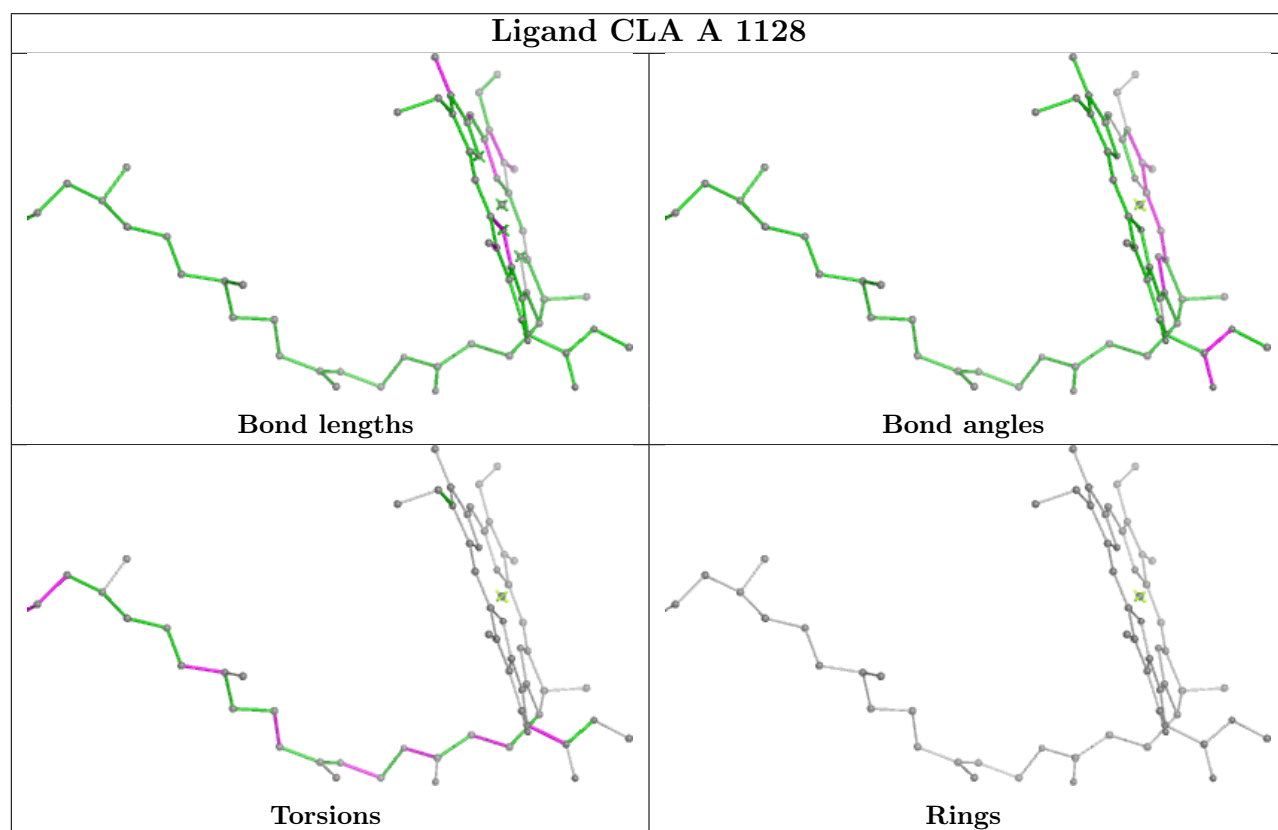
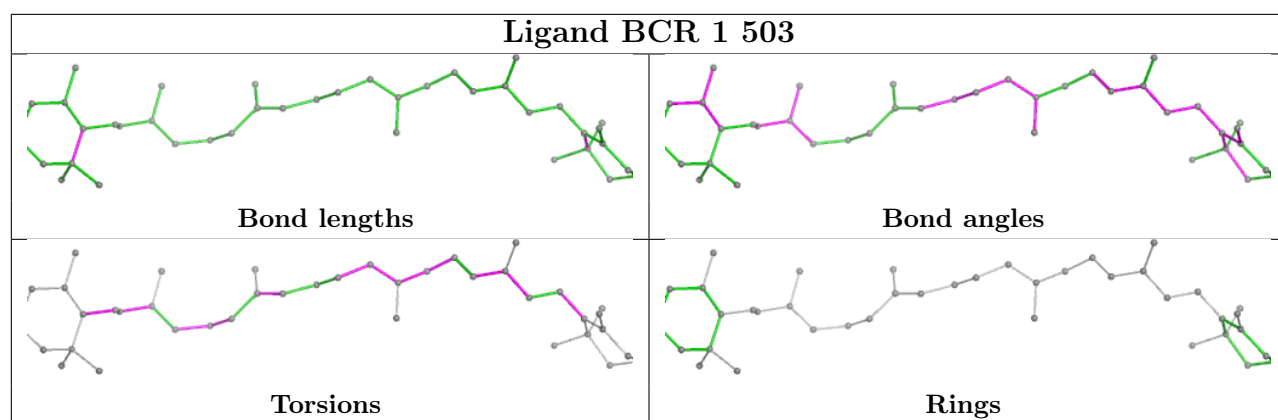


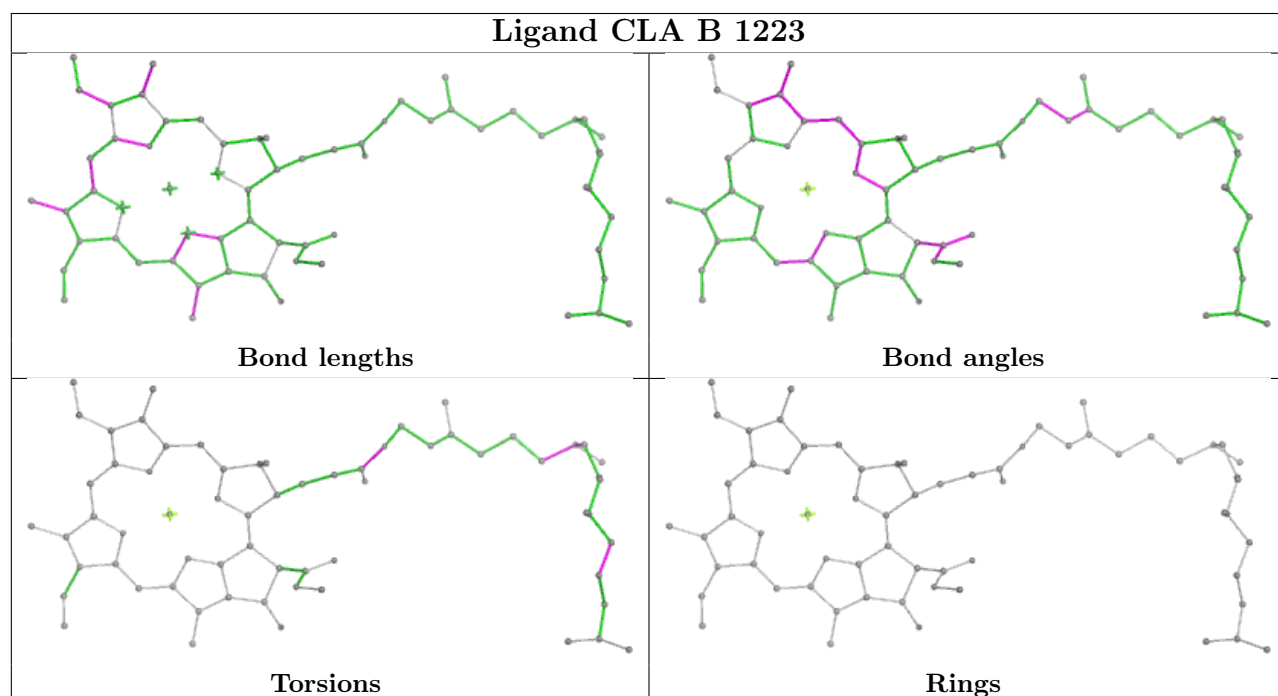
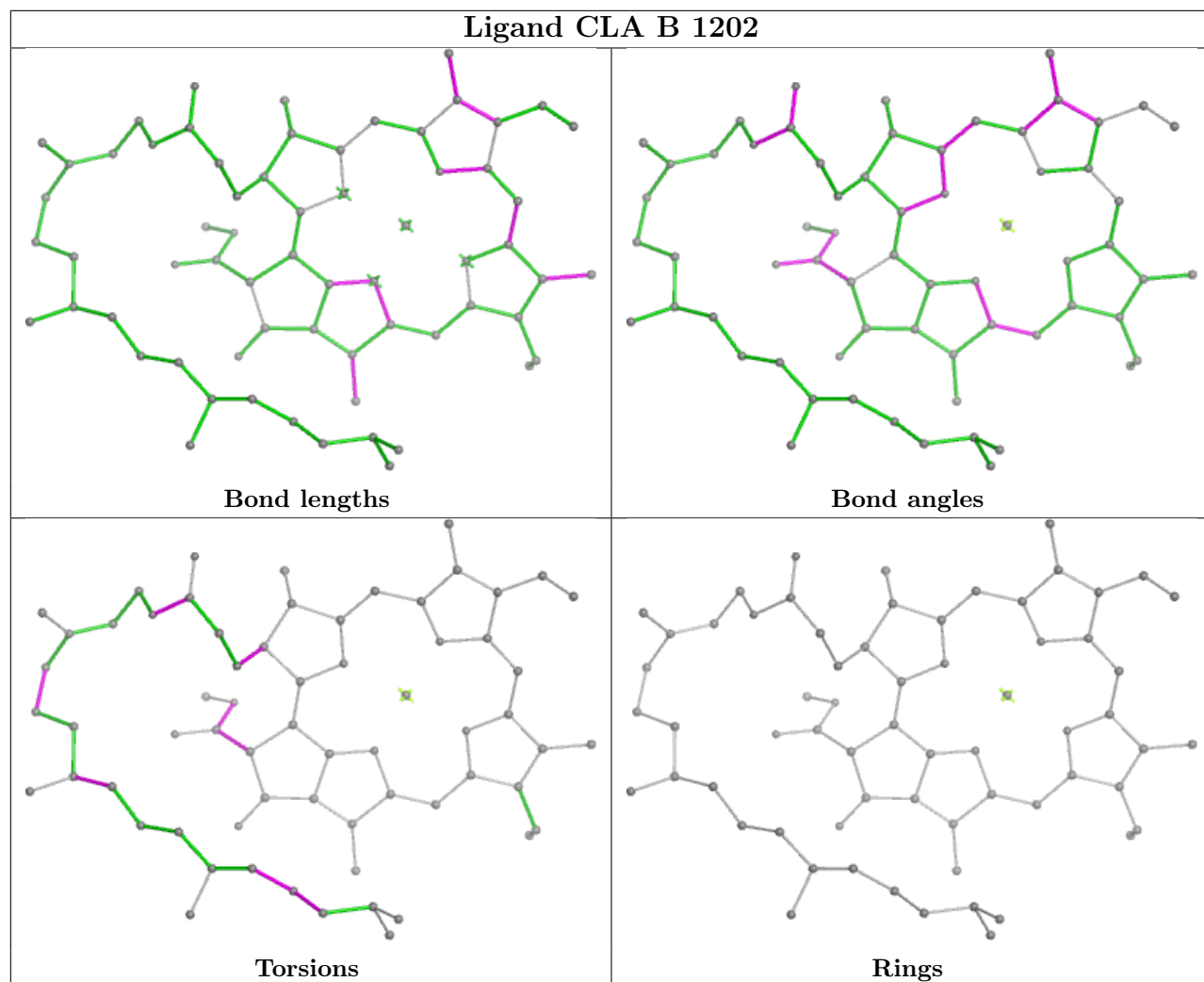


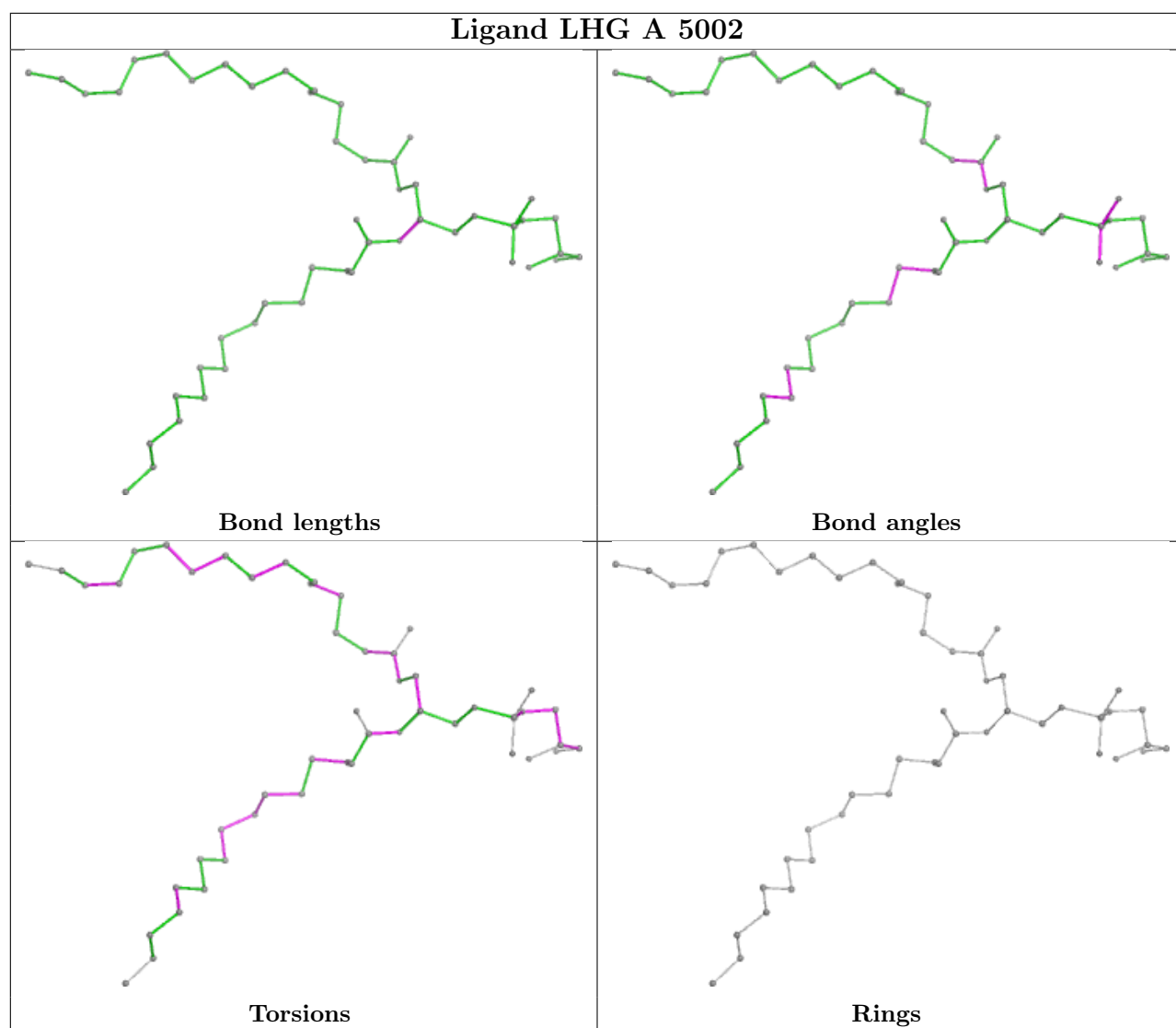


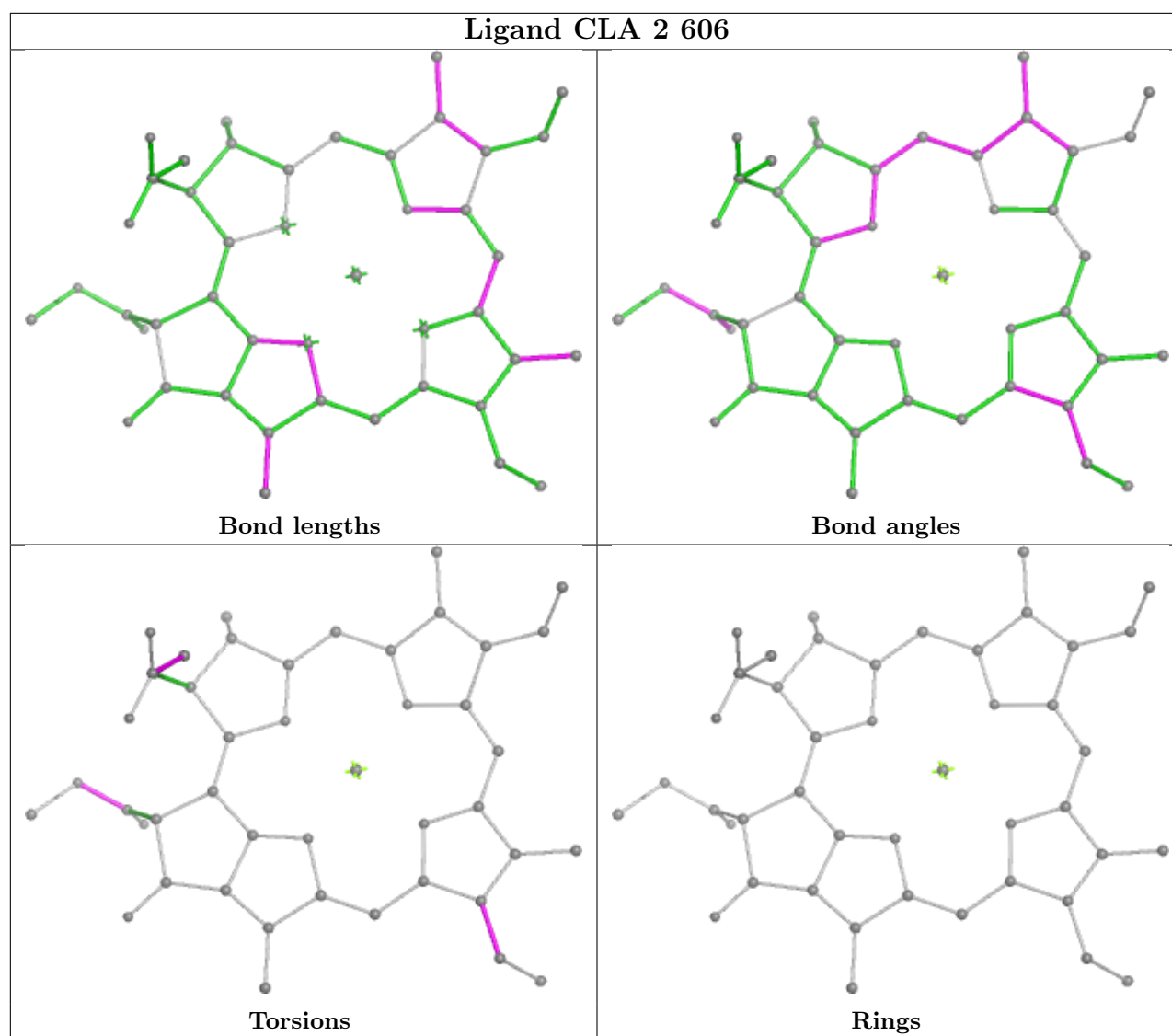


Ligand CLA 4 607**Ligand LUT 4 501**









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.

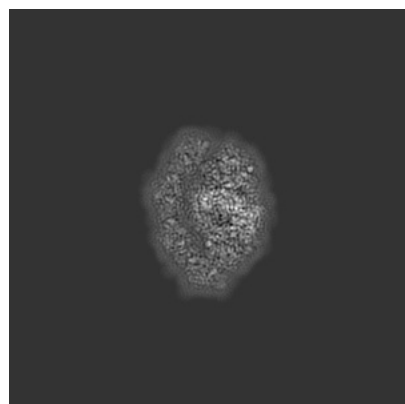
6 Map visualisation [i](#)

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.

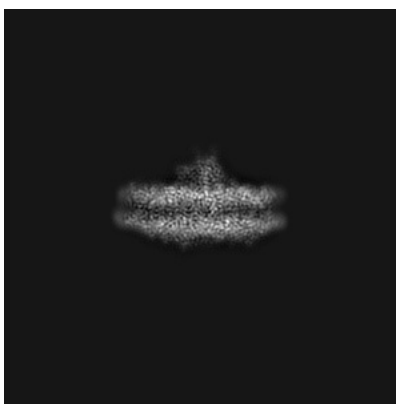
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

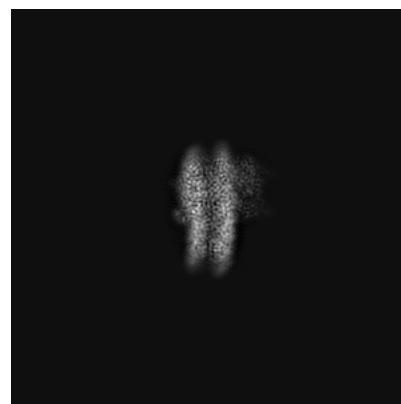
6.1.1 Primary map



X

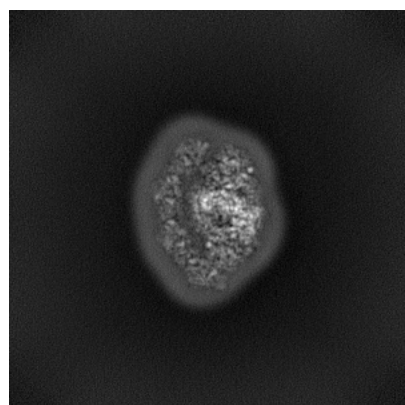


Y

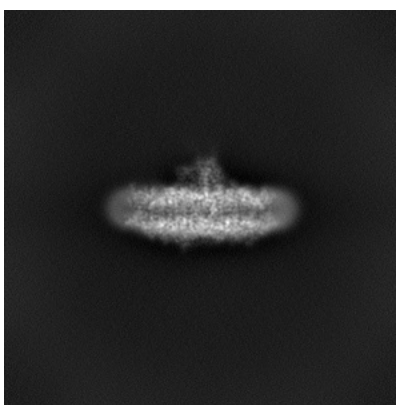


Z

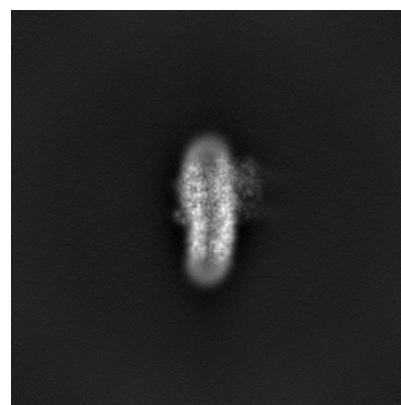
6.1.2 Raw map



X



Y

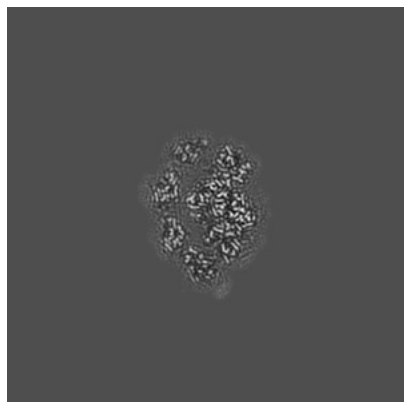


Z

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

6.2 Central slices [i](#)

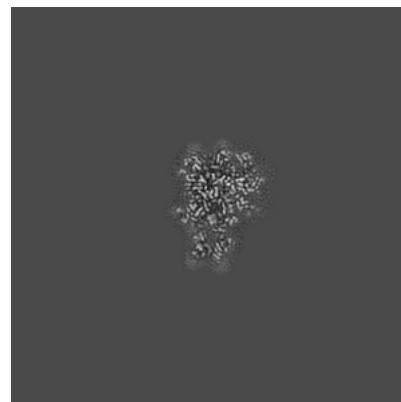
6.2.1 Primary map



X Index: 200

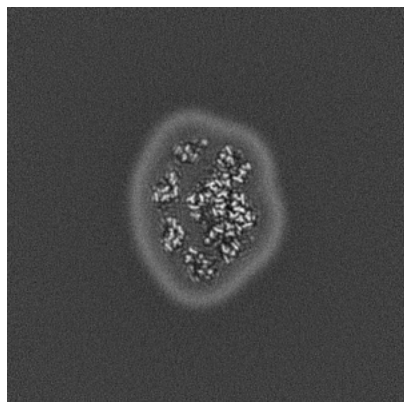


Y Index: 200

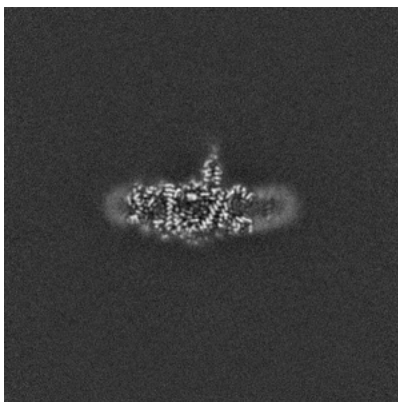


Z Index: 200

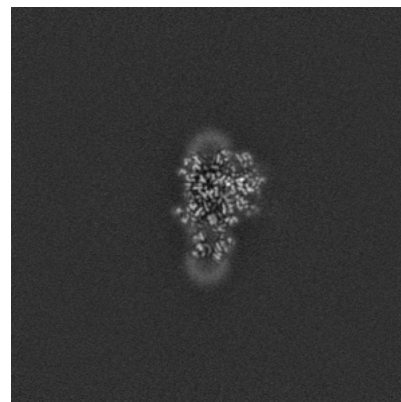
6.2.2 Raw map



X Index: 200



Y Index: 200

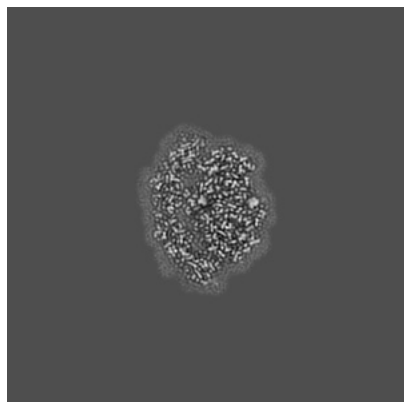


Z Index: 200

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

6.3 Largest variance slices [i](#)

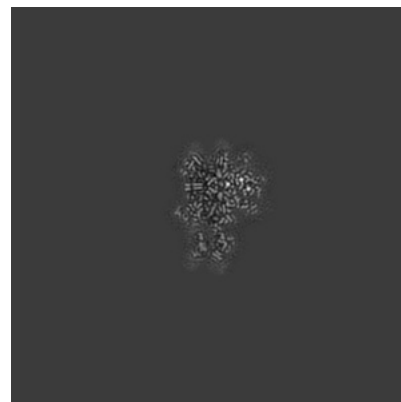
6.3.1 Primary map



X Index: 210

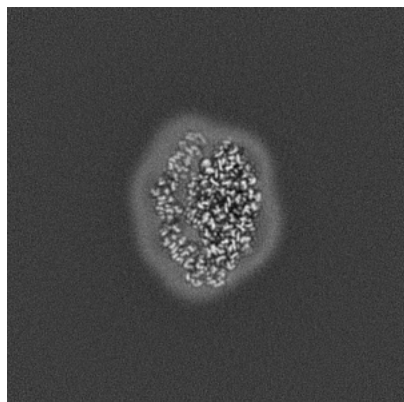


Y Index: 222

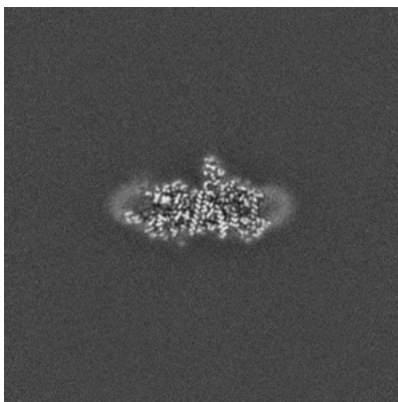


Z Index: 202

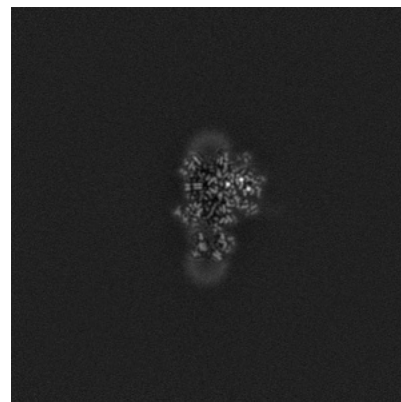
6.3.2 Raw map



X Index: 186



Y Index: 214

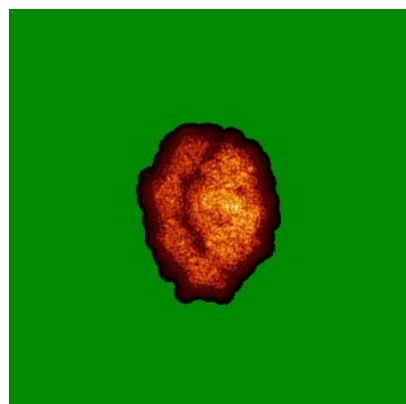


Z Index: 202

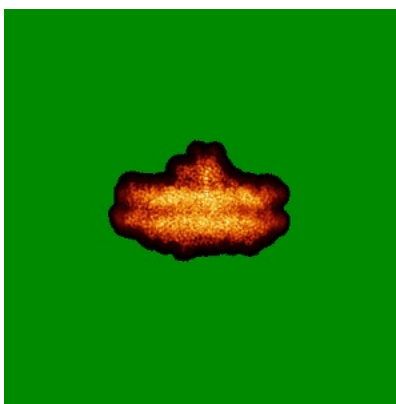
The images above show the largest variance slices of the map in three orthogonal directions.

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

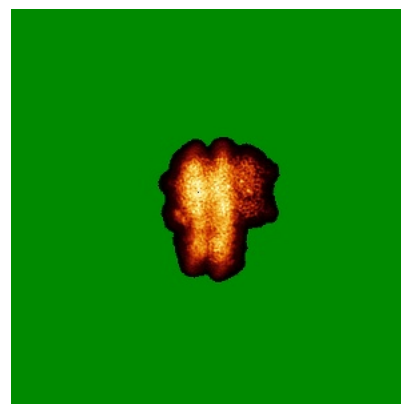
6.4.1 Primary map



X

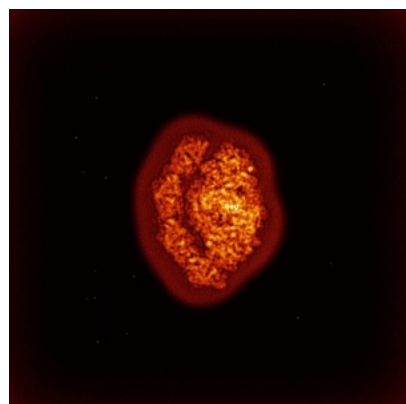


Y

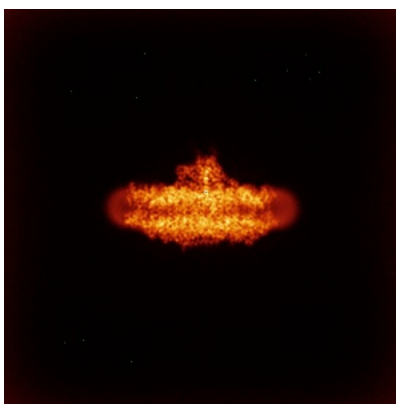


Z

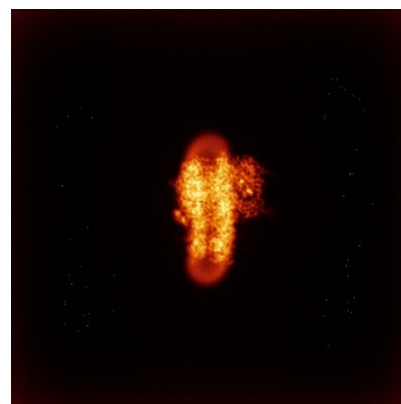
6.4.2 Raw map



X



Y

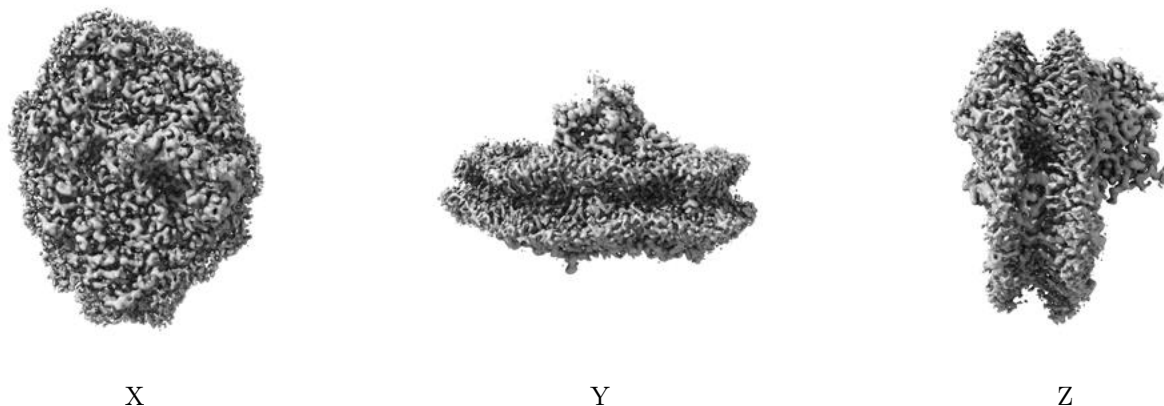


Z

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.

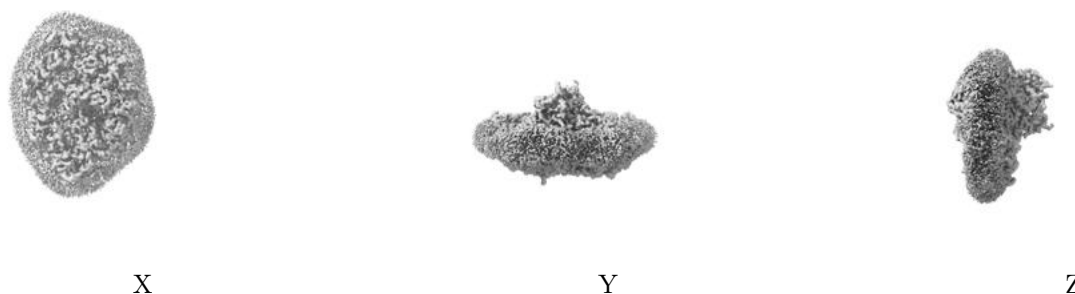
6.5 Orthogonal surface views [i](#)

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.

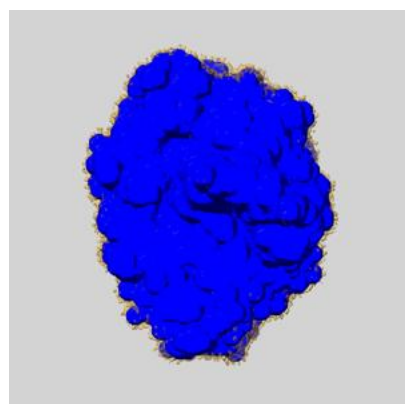
6.6 Mask visualisation [i](#)

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

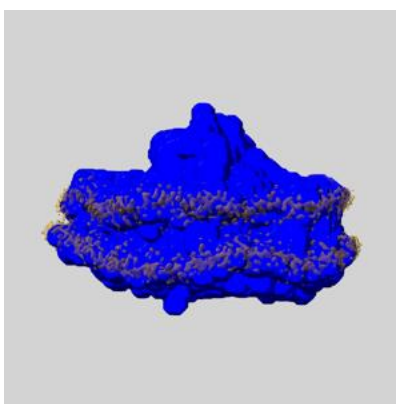
A mask typically either:

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

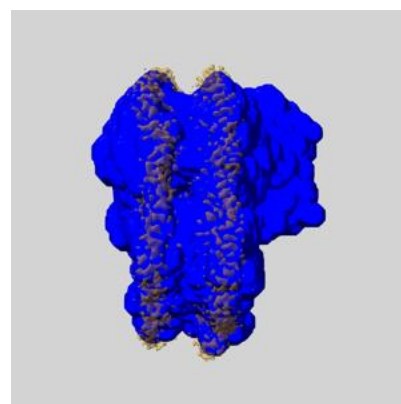
6.6.1 emd_4883_msk_1.map [i](#)



X



Y

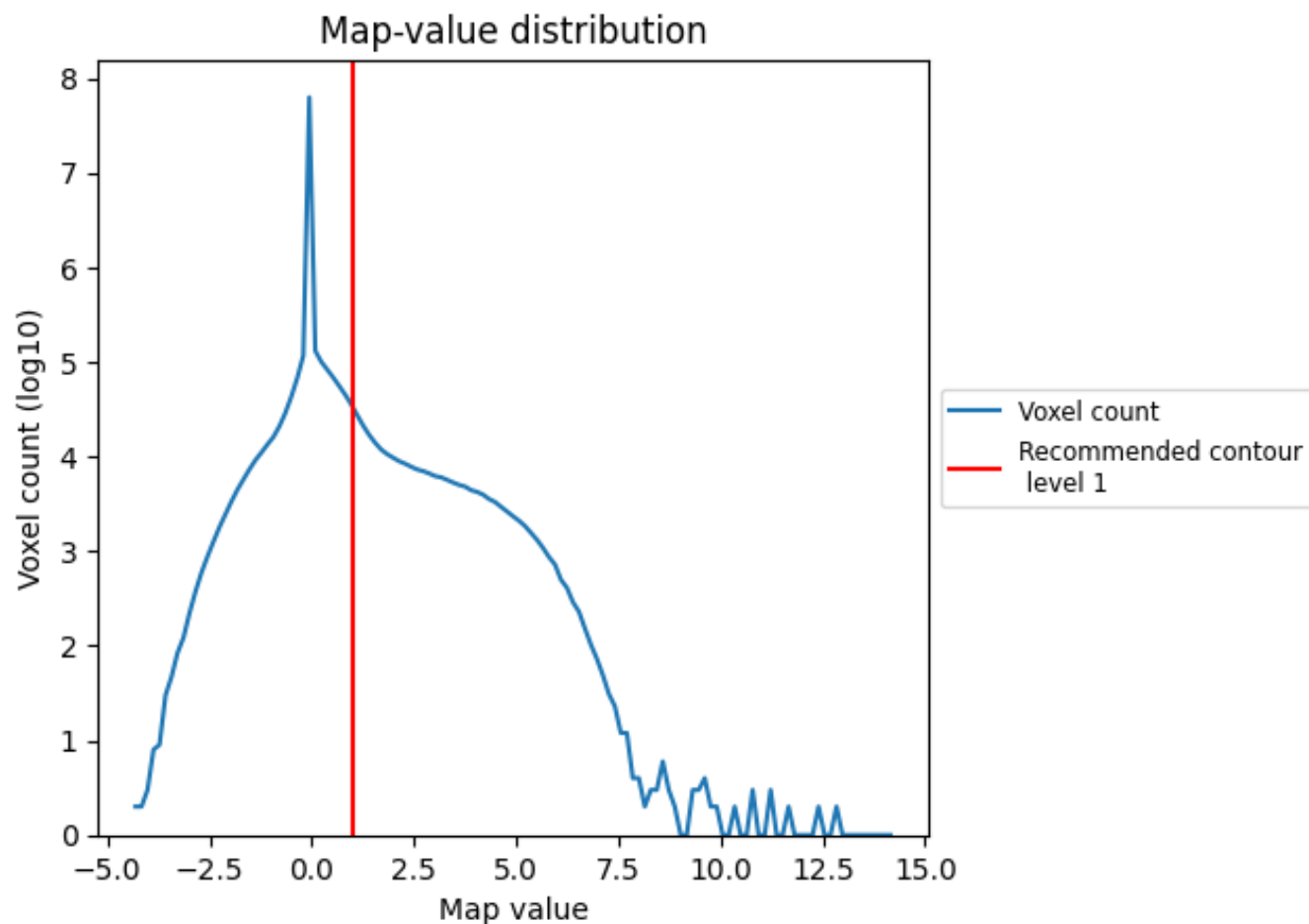


Z

7 Map analysis [i](#)

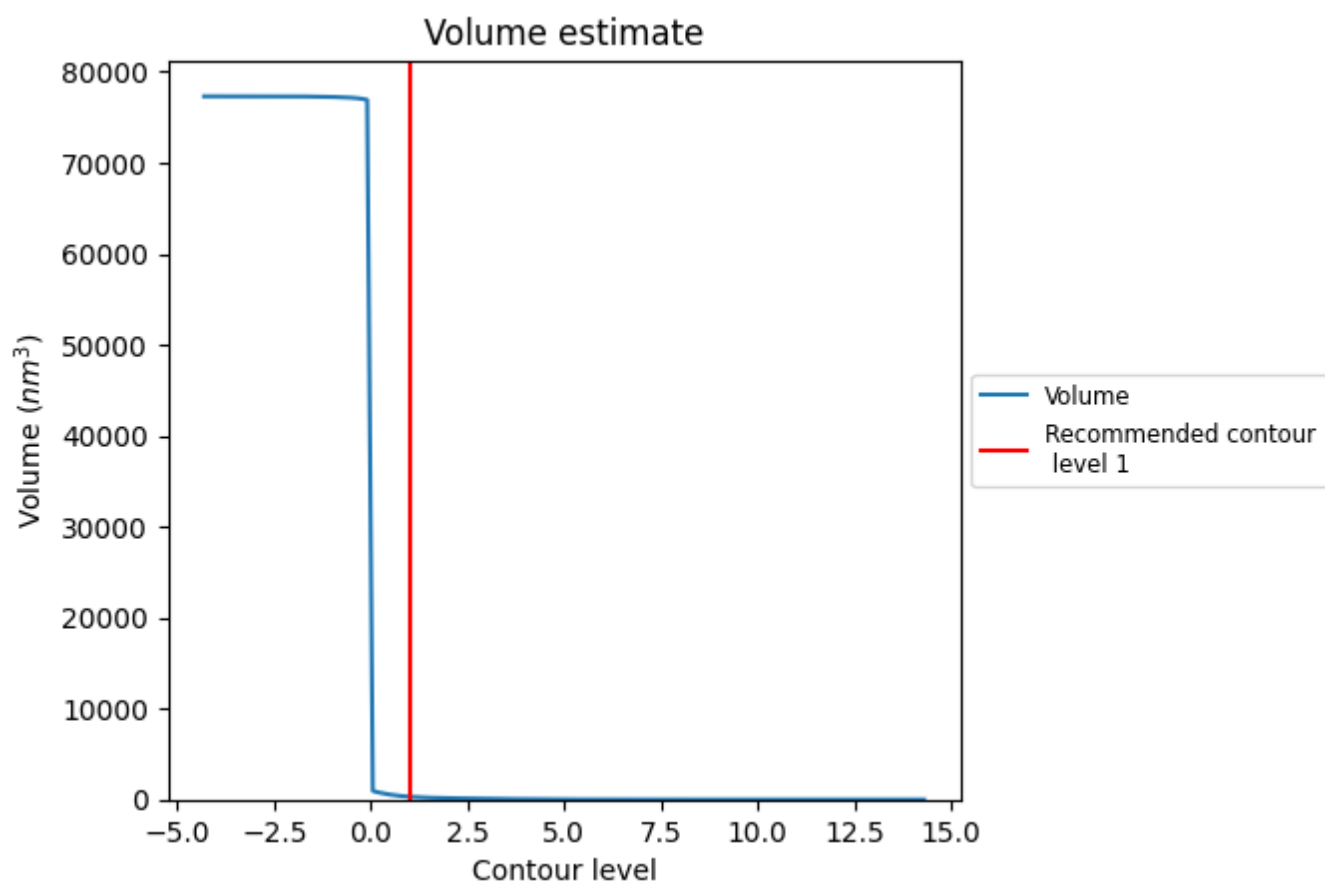
This section contains the results of statistical analysis of the map.

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.

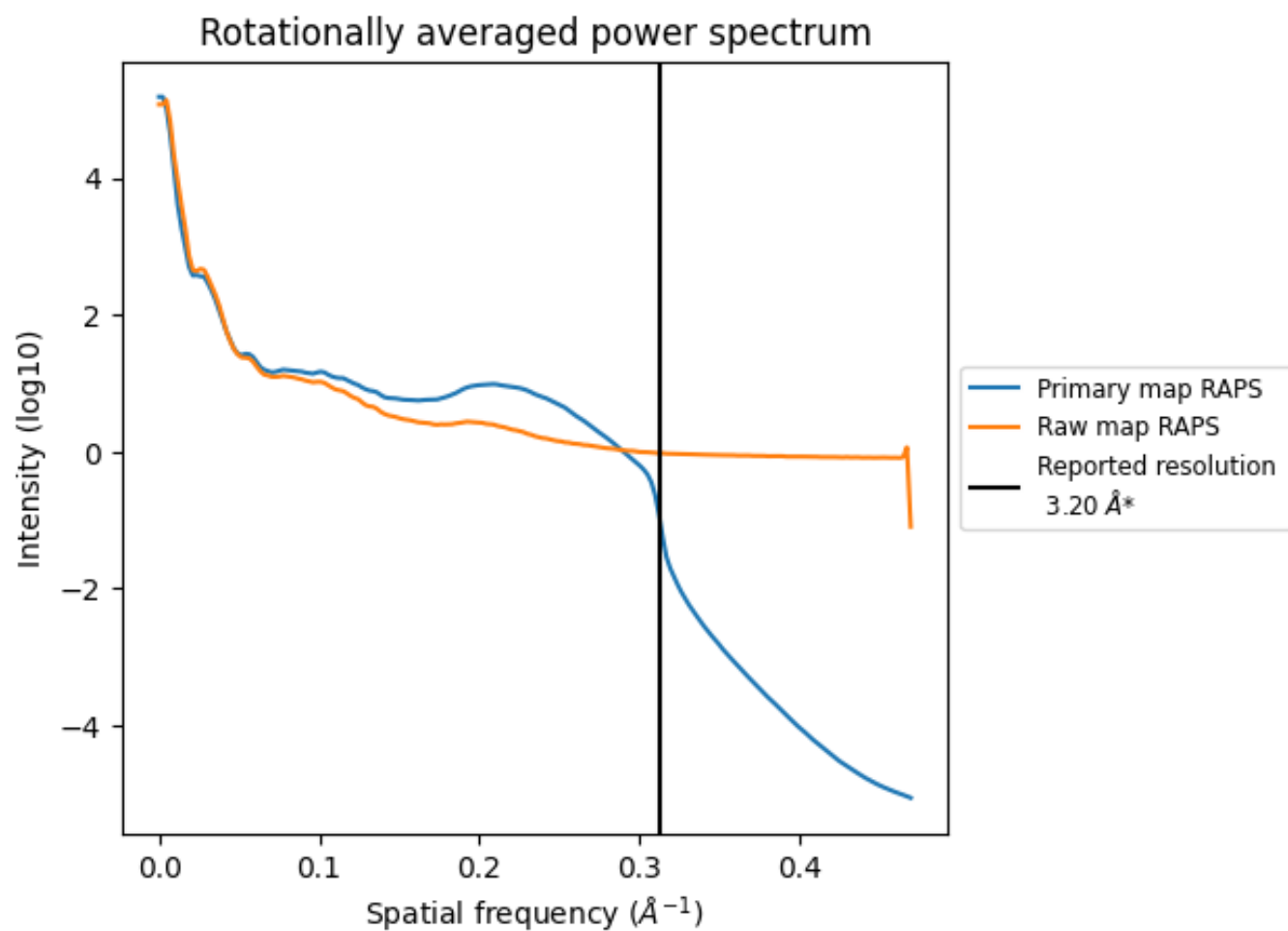
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 312 nm^3 ; 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 ⓘ

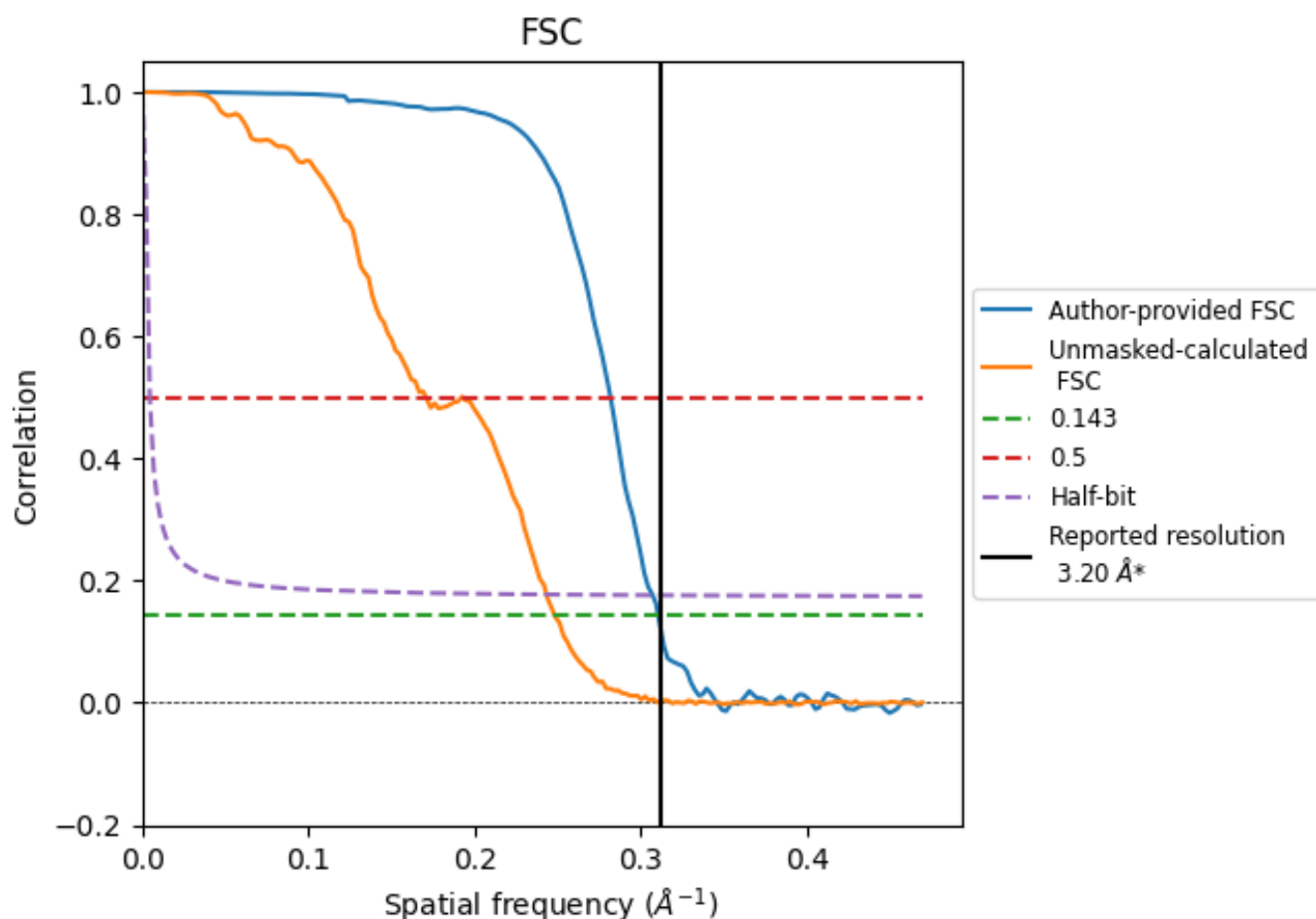


*Reported resolution corresponds to spatial frequency of 0.312 Å⁻¹

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 \AA^{-1}

8.2 Resolution estimates [i](#)

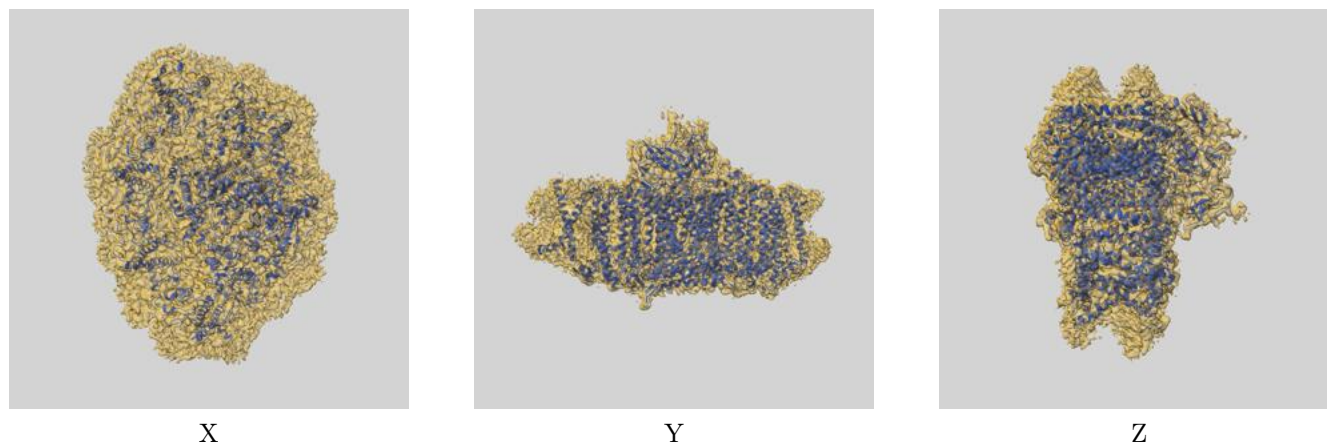
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	3.22	3.55	3.25
Unmasked-calculated*	4.03	5.85	4.11

*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](#)



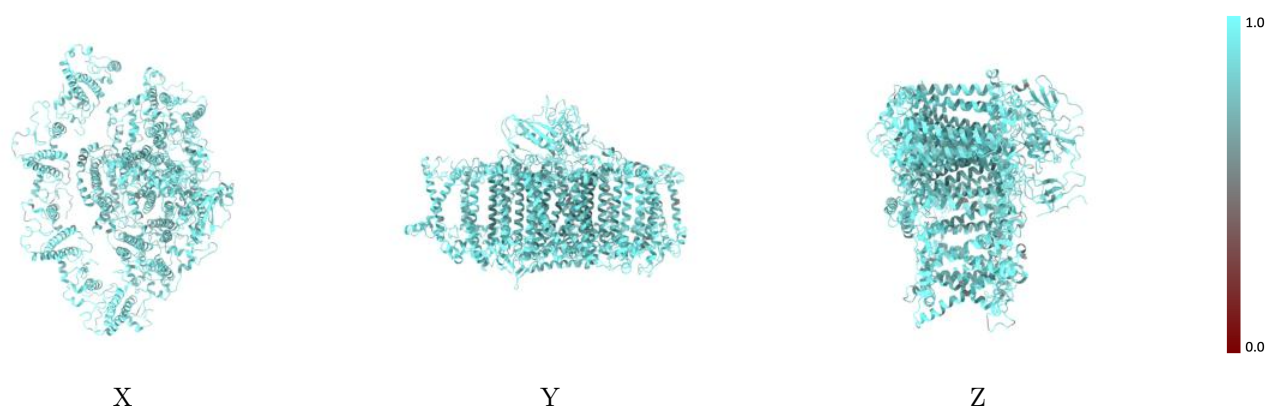
The images above show the 3D surface view of the map at the recommended contour level 1.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



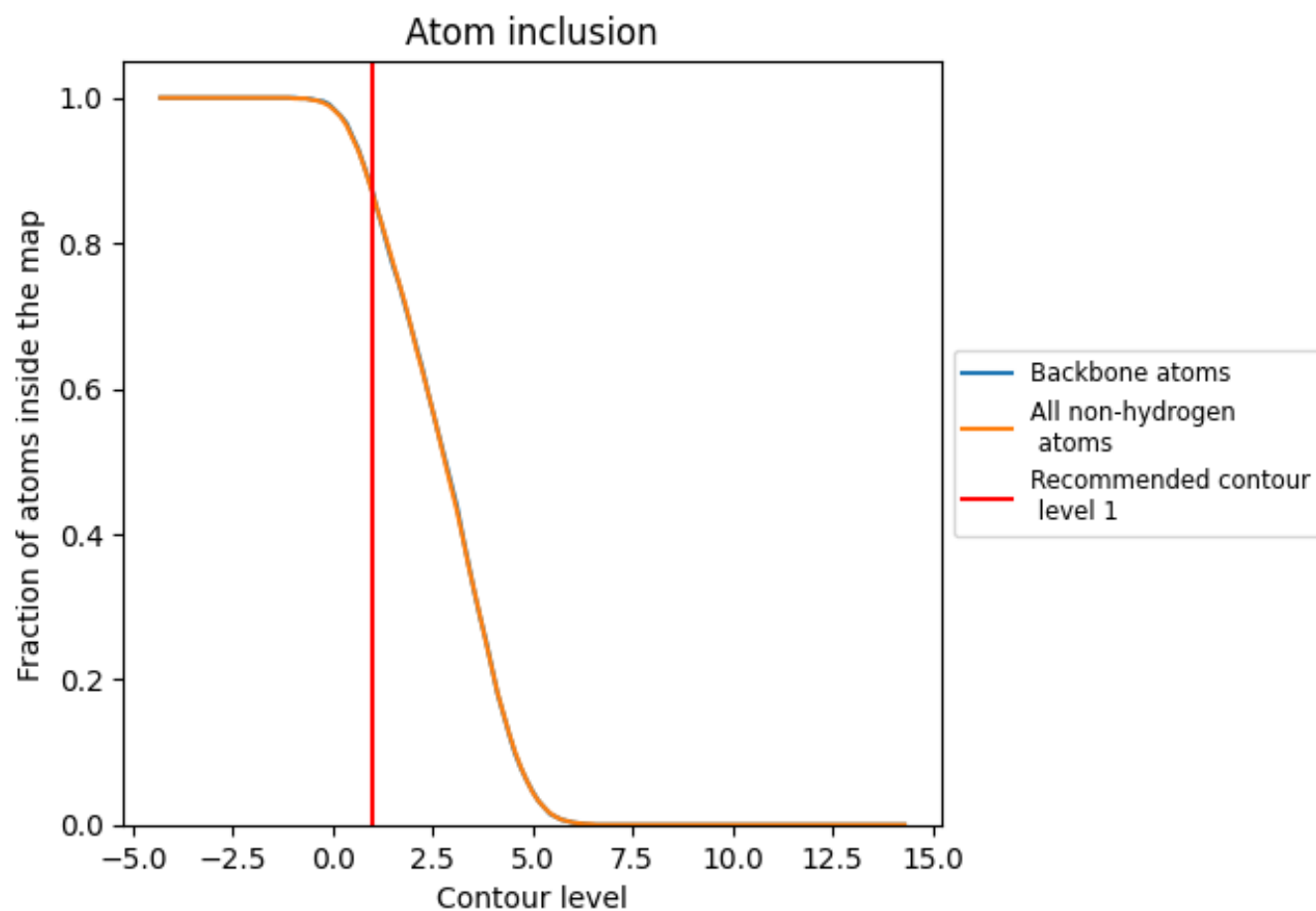
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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	<div><div></div></div> 0.8680	<div><div></div></div> 0.4670
1	<div><div></div></div> 0.8400	<div><div></div></div> 0.4240
2	<div><div></div></div> 0.8680	<div><div></div></div> 0.4760
3	<div><div></div></div> 0.8630	<div><div></div></div> 0.4740
4	<div><div></div></div> 0.8460	<div><div></div></div> 0.4470
A	<div><div></div></div> 0.8830	<div><div></div></div> 0.4870
B	<div><div></div></div> 0.8730	<div><div></div></div> 0.4650
C	<div><div></div></div> 0.8900	<div><div></div></div> 0.4440
D	<div><div></div></div> 0.8610	<div><div></div></div> 0.4330
E	<div><div></div></div> 0.8840	<div><div></div></div> 0.4690
F	<div><div></div></div> 0.8370	<div><div></div></div> 0.4540
J	<div><div></div></div> 0.8860	<div><div></div></div> 0.4880

1.0

0.0

<0.0