



Full wwPDB EM Validation Report ⓘ

Aug 5, 2026 – 07:11 AM EDT

PDB ID : 7KSQ / pdb_00007ksq
EMDB ID : EMD-23023
Title : The Structure of the moss PSI-LHCI reveals the evolution of the LHCI antenna
Authors : Riddle, R.; Gorski, C.; Toporik, H.; Dobson, Z.; Da, Z.; Williams, D.; Mazor, Y.
Deposited on : 2020-11-23
Resolution : 2.80 Å(reported)

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:

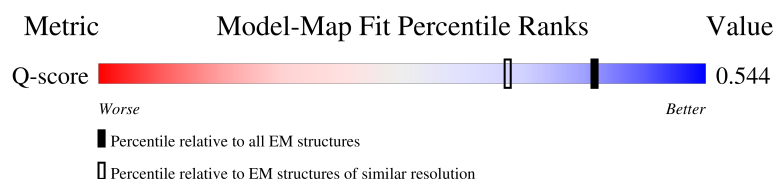
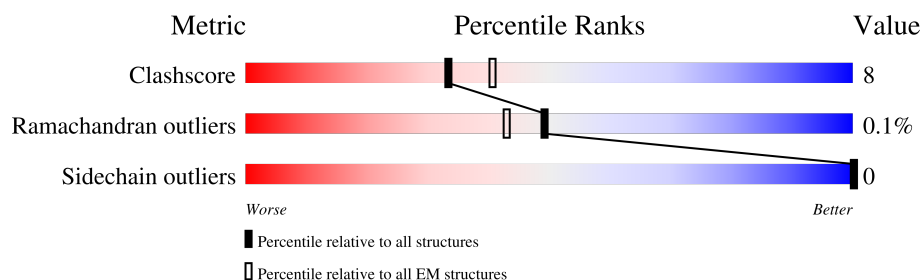
EMDB validation analysis : 0.0.1.dev133
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

1 Overall quality at a glance

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

The reported resolution of this entry is 2.80 Å.

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



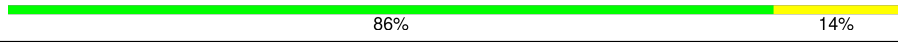
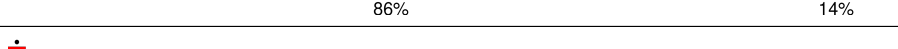
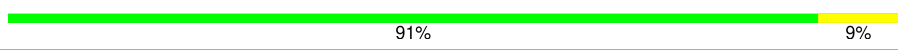
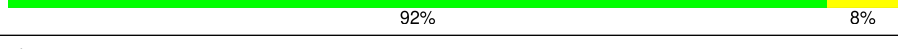
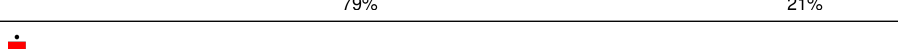
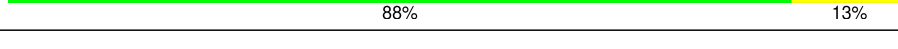
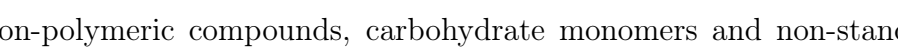
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	11806 (2.30 - 3.30)

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

Mol	Chain	Length	Quality of chain
1	A	742	
2	B	732	
3	1	192	
4	2	203	

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Mol	Chain	Length	Quality of chain
5	3	218	
6	4	203	
7	C	80	
8	D	142	
9	E	63	
10	F	160	
11	G	91	
12	H	87	
13	I	34	
14	J	41	
15	K	81	
16	L	160	
17	M	30	
18	O	88	

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
29	LUT	2	623	X	-	-	-
29	LUT	4	623	X	-	-	-

2 Entry composition

There are 30 unique types of molecules in this entry. The entry contains 36553 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	742	Total	C	N	O	S	0	0
			5837	3827	993	998	19		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	732	Total	C	N	O	S	0	0
			5845	3836	995	998	16		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	1	192	Total	C	N	O	S	0	0
			1473	961	247	264	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	2	203	Total	C	N	O	S	0	0
			1567	1021	262	280	4		

- Molecule 5 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	3	218	Total	C	N	O	S	0	0
			1678	1099	272	300	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	4	203	Total	C	N	O	S	0	0
			1574	1024	264	281	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	C	80	Total	C	N	O	S	0	0
			596	365	103	117	11		

- Molecule 8 is a protein called PsaD.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	D	142	Total	C	N	O	S	0	0
			1109	711	195	200	3		

- Molecule 9 is a protein called PsaE.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	E	63	Total	C	N	O	0	0
			500	317	89	94		

- Molecule 10 is a protein called PSI-F.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	F	160	Total	C	N	O	S	0	0
			1239	801	215	220	3		

- Molecule 11 is a protein called PSI-G.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	G	91	Total	C	N	O	0	0
			689	444	119	126		

- Molecule 12 is a protein called PsaH.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	H	87	Total	C	N	O	S	0	0
			659	418	114	126	1		

- Molecule 13 is a protein called Photosystem I reaction center subunit VIII.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	I	34	Total	C	N	O	S	0	0
			266	181	35	48	2		

- Molecule 14 is a protein called Photosystem I reaction center subunit IX.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	J	41	Total	C	N	O	S	0	0
			325	222	48	54	1		

- Molecule 15 is a protein called PsaK.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	K	81	Total	C	N	O	S	0	0
			561	352	97	108	4		

- Molecule 16 is a protein called PSI subunit V.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	L	160	Total	C	N	O	S	0	0
			1171	771	188	210	2		

- Molecule 17 is a protein called Photosystem I reaction center subunit XII.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	M	30	Total	C	N	O	S	0	0
			223	146	36	41			

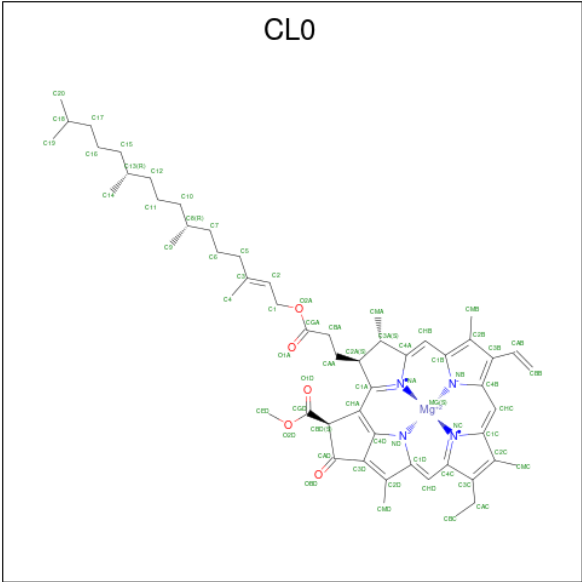
- Molecule 18 is a protein called PsaO.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	O	88	Total	C	N	O	S	0	0
			655	432	113	109	1		

There are 2 discrepancies between the modelled and reference sequences:

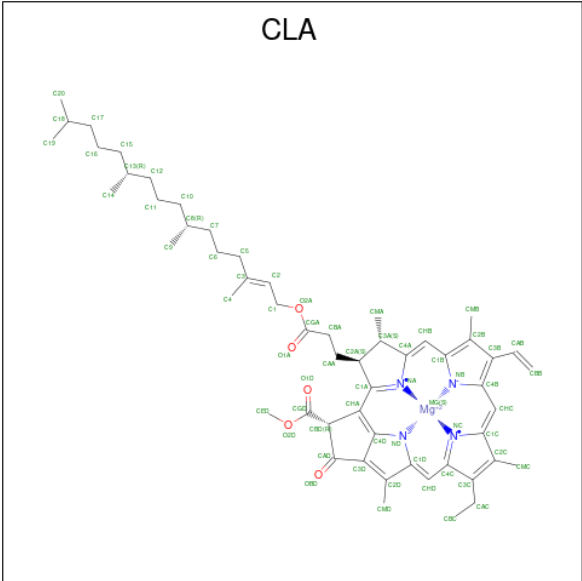
Chain	Residue	Modelled	Actual	Comment	Reference
O	62	ARG	LYS	conflict	UNP A0A2K1JDE1
O	130	PHE	LEU	conflict	UNP A0A2K1JDE1

- Molecule 19 is CHLOROPHYLL A ISOMER (CCD ID: CL0) (formula: $C_{55}H_{72}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 20 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
20	A	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
20	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			51	41	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
20	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			61	51	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
20	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			54	44	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
20	B	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	1	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
20	1	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
20	1	1	Total	C	Mg	N	O	0
			50	40	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
20	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
20	1	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
20	1	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
20	1	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
20	1	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
20	1	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
20	1	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
20	1	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
20	1	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
20	2	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
20	2	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
20	2	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
20	2	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
20	2	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
20	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	2	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
20	3	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
20	3	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
20	3	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
20	3	1	Total	C	Mg	N	O	0
			27	22	1	4		
20	3	1	Total	C	Mg	N	O	0
			46	36	1	4	5	

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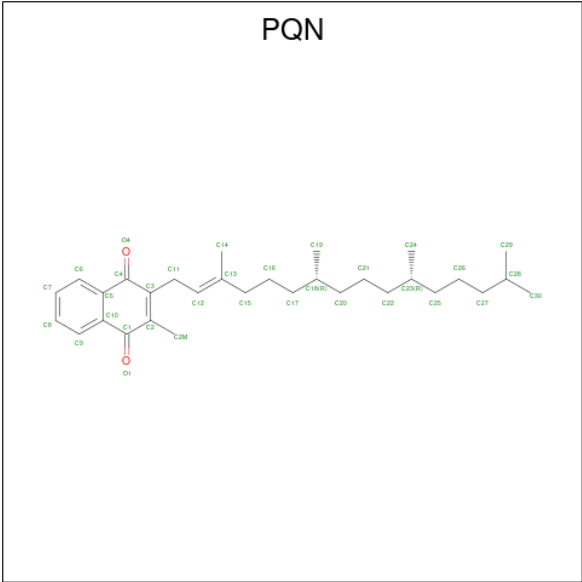
Mol	Chain	Residues	Atoms					AltConf
20	3	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
20	3	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
20	3	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
20	3	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
20	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
20	3	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
20	3	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
20	3	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
20	4	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
20	4	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
20	4	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
20	4	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
20	4	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
20	4	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
20	4	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
20	4	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
20	4	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
20	F	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
20	F	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
20	F	1	Total	C	Mg	N		0
			27	22	1	4		

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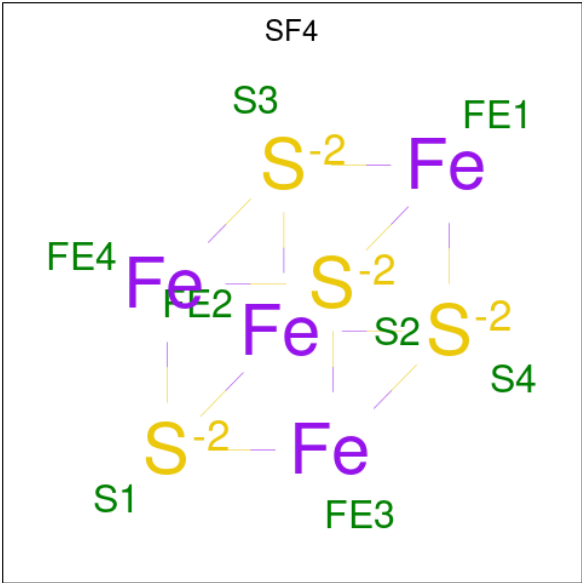
Mol	Chain	Residues	Atoms					AltConf
20	G	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
20	G	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
20	G	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
20	H	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
20	I	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	J	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
20	K	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
20	K	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
20	K	1	Total	C	Mg	N		0
			27	22	1	4		
20	K	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
20	L	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
20	L	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
20	L	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
20	O	1	Total	C	Mg	N		0
			27	22	1	4		
20	O	1	Total	C	Mg	N		0
			27	22	1	4		
20	O	1	Total	C	Mg	N		0
			27	22	1	4		

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



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

- Molecule 22 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



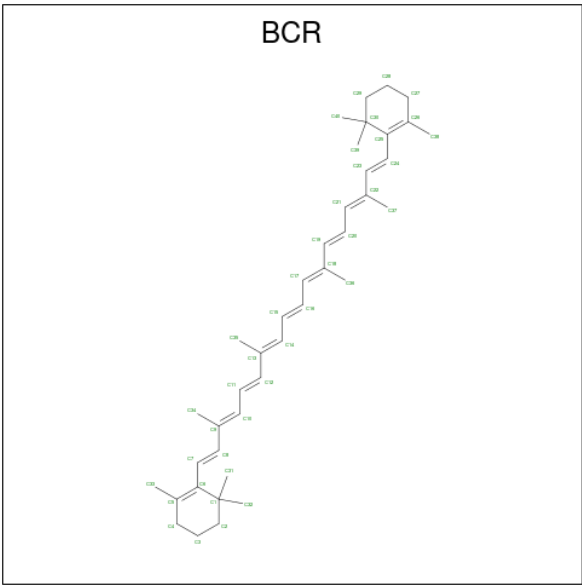
Mol	Chain	Residues	Atoms			AltConf
22	A	1	Total	Fe	S	0
			8	4	4	
22	C	1	Total	Fe	S	0
			8	4	4	

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

- Molecule 23 is BETA-CAROTENE (CCD ID: BCR) (formula: C₄₀H₅₆) (labeled as "Ligand of Interest" by depositor).



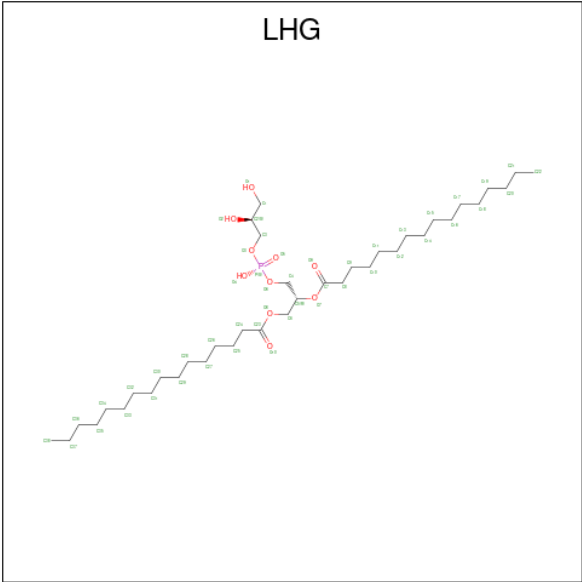
Mol	Chain	Residues	Atoms		AltConf
23	A	1	Total	C	0
			40	40	
23	A	1	Total	C	0
			40	40	
23	A	1	Total	C	0
			40	40	
23	A	1	Total	C	0
			40	40	
23	A	1	Total	C	0
			40	40	
23	A	1	Total	C	0
			40	40	
23	B	1	Total	C	0
			40	40	
23	B	1	Total	C	0
			40	40	
23	B	1	Total	C	0
			40	40	
23	B	1	Total	C	0
			40	40	

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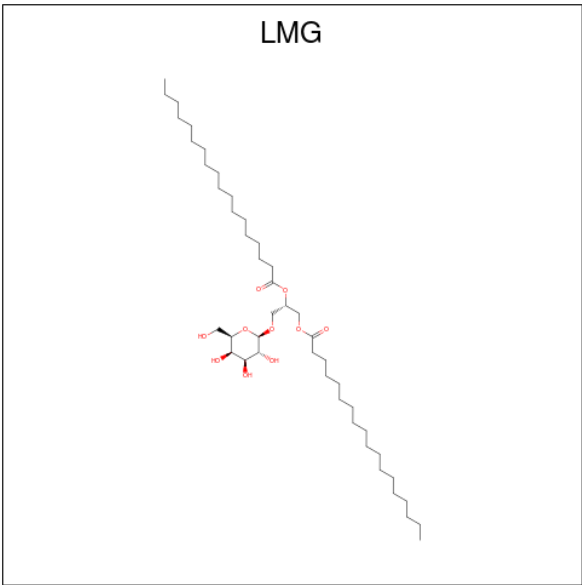
Mol	Chain	Residues	Atoms	AltConf
23	B	1	Total C 40 40	0
23	B	1	Total C 40 40	0
23	B	1	Total C 40 40	0
23	1	1	Total C 25 25	0
23	3	1	Total C 40 40	0
23	3	1	Total C 40 40	0
23	F	1	Total C 40 40	0
23	G	1	Total C 40 40	0
23	I	1	Total C 40 40	0
23	I	1	Total C 40 40	0
23	J	1	Total C 40 40	0
23	J	1	Total C 40 40	0
23	K	1	Total C 40 40	0
23	L	1	Total C 40 40	0
23	L	1	Total C 40 40	0
23	M	1	Total C 40 40	0
23	O	1	Total C 14 14	0

- Molecule 24 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P) (labeled as "Ligand of Interest" by depositor).



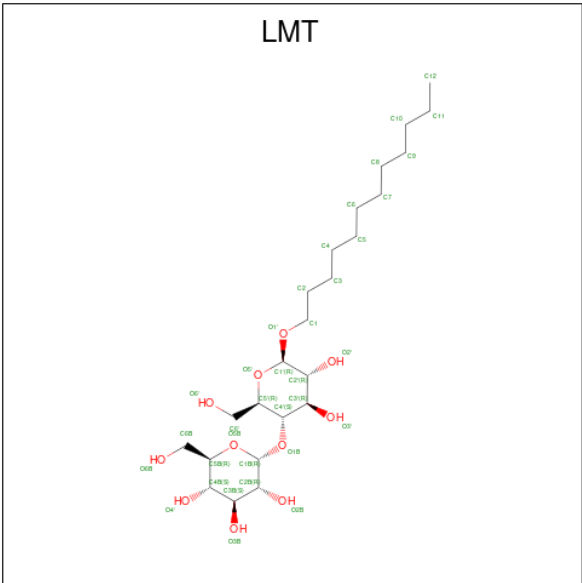
Mol	Chain	Residues	Atoms				AltConf
24	A	1	Total	C	O	P	0
			49	38	10	1	
24	A	1	Total	C	O	P	0
			31	20	10	1	
24	B	1	Total	C	O	P	0
			35	24	10	1	
24	1	1	Total	C	O	P	0
			37	26	10	1	
24	2	1	Total	C	O	P	0
			32	21	10	1	
24	3	1	Total	C	O	P	0
			34	23	10	1	
24	4	1	Total	C	O	P	0
			38	27	10	1	

- Molecule 25 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: C₄₅H₈₆O₁₀) (labeled as "Ligand of Interest" by depositor).



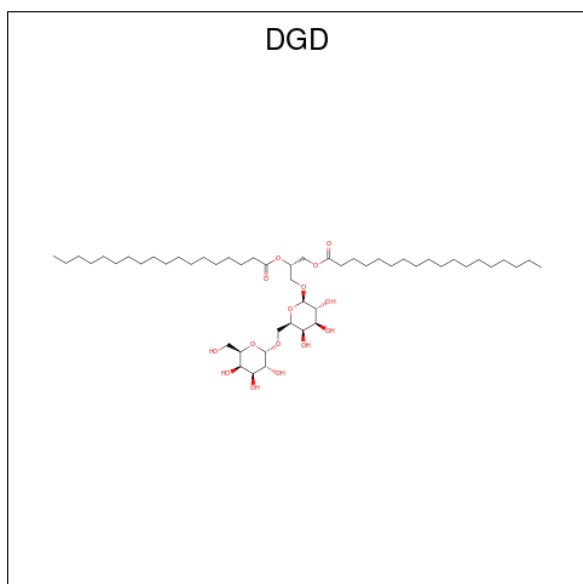
Mol	Chain	Residues	Atoms			AltConf
25	A	1	Total	C	O	0
			34	24	10	
25	2	1	Total	C	O	0
			36	26	10	
25	J	1	Total	C	O	0
			49	39	10	
25	J	1	Total	C	O	0
			26	16	10	

- Molecule 26 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: C₂₄H₄₆O₁₁) (labeled as "Ligand of Interest" by depositor).



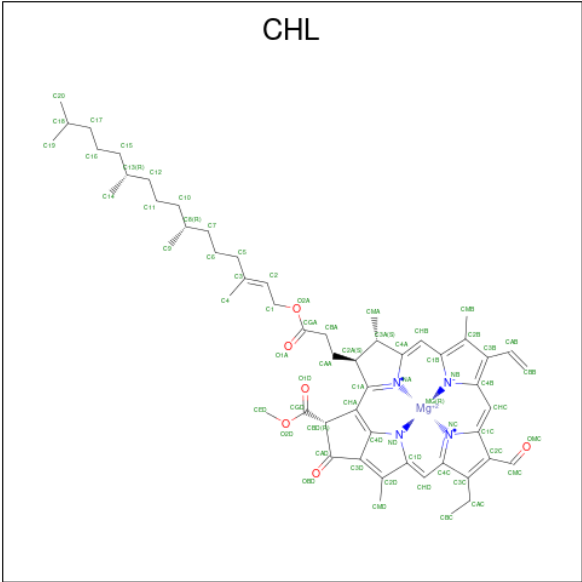
Mol	Chain	Residues	Atoms			AltConf
26	A	1	Total	C	O	0
			33	22	11	
26	B	1	Total	C	O	0
			31	20	11	
26	1	1	Total	C	O	0
			35	24	11	
26	4	1	Total	C	O	0
			35	24	11	
26	G	1	Total	C	O	0
			35	24	11	
26	G	1	Total	C	O	0
			31	20	11	

- Molecule 27 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$) (labeled as "Ligand of Interest" by depositor).



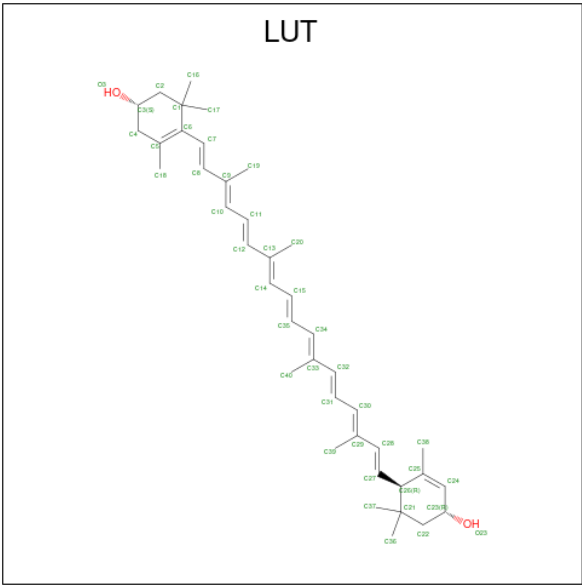
Mol	Chain	Residues	Atoms			AltConf
27	B	1	Total	C	O	0
			61	46	15	

- Molecule 28 is CHLOROPHYLL B (CCD ID: CHL) (formula: $C_{55}H_{70}MgN_4O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
28	1	1	Total 47	C 36	Mg 1	N 4	O 6	0
28	1	1	Total 56	C 45	Mg 1	N 4	O 6	0
28	2	1	Total 56	C 45	Mg 1	N 4	O 6	0
28	2	1	Total 46	C 35	Mg 1	N 4	O 6	0
28	2	1	Total 47	C 36	Mg 1	N 4	O 6	0
28	2	1	Total 48	C 37	Mg 1	N 4	O 6	0
28	2	1	Total 56	C 45	Mg 1	N 4	O 6	0
28	2	1	Total 47	C 36	Mg 1	N 4	O 6	0
28	2	1	Total 66	C 55	Mg 1	N 4	O 6	0
28	3	1	Total 47	C 36	Mg 1	N 4	O 6	0
28	4	1	Total 47	C 36	Mg 1	N 4	O 6	0
28	4	1	Total 47	C 36	Mg 1	N 4	O 6	0
28	4	1	Total 51	C 40	Mg 1	N 4	O 6	0
28	4	1	Total 43	C 34	Mg 1	N 4	O 4	0

- Molecule 29 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (CCD ID: LUT) (formula: C₄₀H₅₆O₂) (labeled as "Ligand of Interest" by depositor).



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

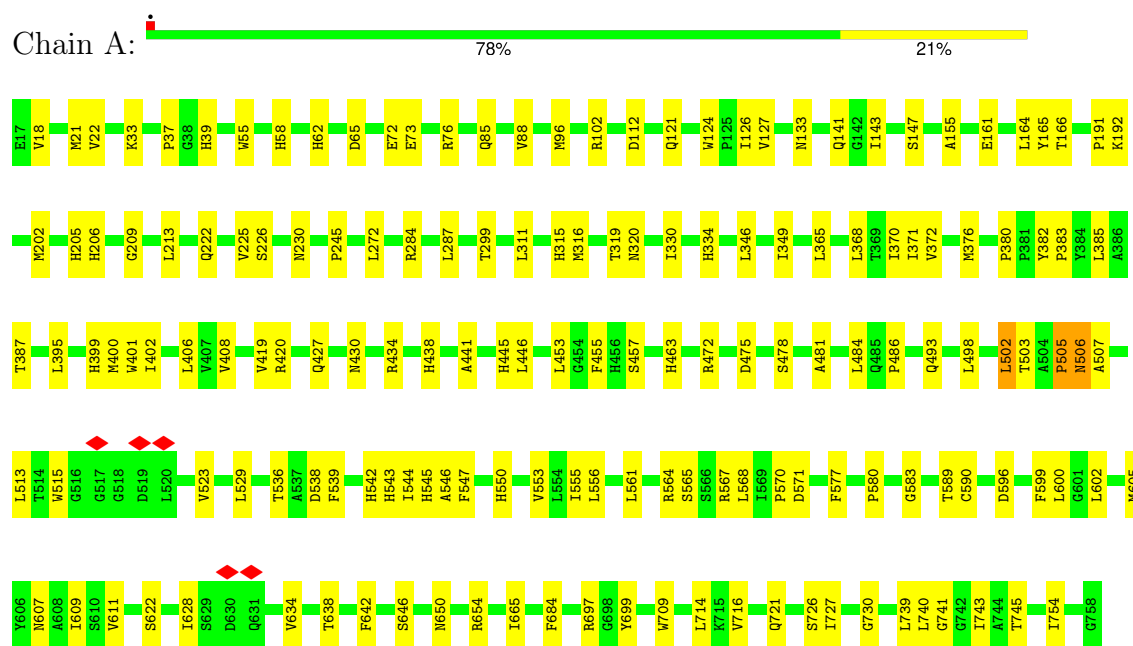
- Molecule 30 is water.

Mol	Chain	Residues	Atoms		AltConf
30	A	15	Total 15	O 15	0
30	B	23	Total 23	O 23	0
30	3	1	Total 1	O 1	0
30	4	1	Total 1	O 1	0
30	C	2	Total 2	O 2	0
30	D	1	Total 1	O 1	0
30	F	1	Total 1	O 1	0
30	G	1	Total 1	O 1	0

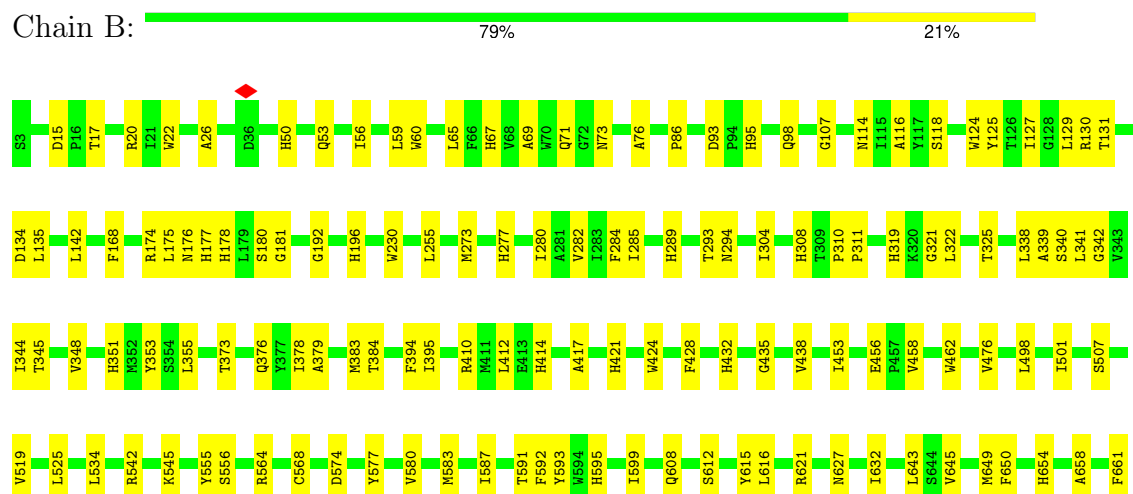
3 Residue-property plots

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

- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2





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

Chain 1: 91% 9%



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

Chain 2: 86% 14%



- Molecule 5: Chlorophyll a-b binding protein, chloroplastic

Chain 3: 84% 16%



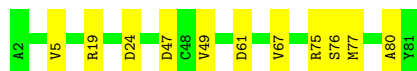
- Molecule 6: Chlorophyll a-b binding protein, chloroplastic

Chain 4: 86% 14%



- Molecule 7: Photosystem I iron-sulfur center

Chain C: 86% 14%



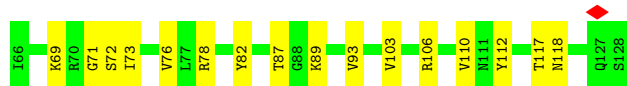
- Molecule 8: PsaD

Chain D: 88% 12%



- Molecule 9: PsaE

Chain E:  75% 25%



- Molecule 10: PSI-F

Chain F:  85% 15%

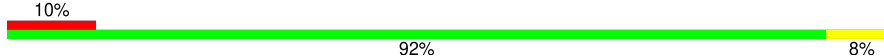


- Molecule 11: PSI-G

Chain G:  91% 9%



- Molecule 12: PsaH

Chain H:  10% 92% 8%



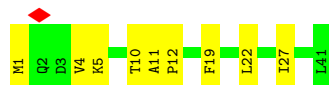
- Molecule 13: Photosystem I reaction center subunit VIII

Chain I:  79% 21%



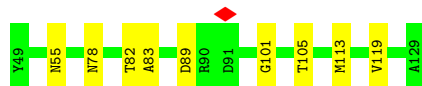
- Molecule 14: Photosystem I reaction center subunit IX

Chain J:  78% 22%



- Molecule 15: PsaK

Chain K:  89% 11%



• Molecule 16: PSI subunit V

Chain L:  89% 11%



• Molecule 17: Photosystem I reaction center subunit XII

Chain M:  87% 13%



• Molecule 18: PsaO

Chain O:  88% 13%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	114608	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.6	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	33.849	Depositor
Minimum map value	-23.604	Depositor
Average map value	0.022	Depositor
Map value standard deviation	0.825	Depositor
Recommended contour level	1.5	Depositor
Map size (Å)	291.2, 291.2, 291.2	wwPDB
Map dimensions	280, 280, 280	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0400001, 1.0400001, 1.0400001	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, CL0, CLA, PQN, LMG, SF4, LHG, LMT, LUT, DGD, 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	A	0.30	0/6032	0.61	3/8227 (0.0%)
2	B	0.30	0/6059	0.64	0/8267
3	1	0.22	0/1522	0.51	0/2081
4	2	0.18	0/1618	0.42	0/2218
5	3	0.20	0/1729	0.46	0/2349
6	4	0.24	0/1623	0.57	0/2219
7	C	0.23	0/606	0.57	0/821
8	D	0.17	0/1136	0.46	0/1538
9	E	0.15	0/511	0.37	0/694
10	F	0.30	1/1265 (0.1%)	0.54	0/1710
11	G	0.16	0/704	0.40	0/960
12	H	0.19	0/673	0.48	0/909
13	I	0.29	0/273	0.61	0/373
14	J	0.20	0/334	0.46	0/457
15	K	0.16	0/567	0.41	0/768
16	L	0.22	0/1202	0.57	0/1645
17	M	0.16	0/224	0.46	0/302
18	O	0.30	0/680	0.76	0/933
All	All	0.26	1/26758 (0.0%)	0.56	3/36471 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	F	213	TRP	C-N	6.98	1.42	1.34

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	498	LEU	CA-CB-CG	5.62	135.98	116.30
1	A	502	LEU	CA-CB-CG	5.19	134.46	116.30
1	A	506	ASN	N-CA-C	5.11	121.67	110.80

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	667	TRP	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5837	0	5725	125	0
2	B	5845	0	5618	120	0
3	1	1473	0	1448	15	0
4	2	1567	0	1527	22	0
5	3	1678	0	1638	31	0
6	4	1574	0	1549	22	0
7	C	596	0	573	9	0
8	D	1109	0	1111	14	0
9	E	500	0	494	10	0
10	F	1239	0	1288	21	0
11	G	689	0	681	6	0
12	H	659	0	636	6	0
13	I	266	0	274	7	0
14	J	325	0	341	9	0
15	K	561	0	574	7	0
16	L	1171	0	1186	15	0
17	M	223	0	244	4	0
18	O	655	0	599	6	0
19	A	65	0	72	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	1	614	0	508	9	0
20	2	378	0	334	4	0
20	3	648	0	530	14	0
20	4	527	0	448	9	0
20	A	2384	0	2226	105	0
20	B	2177	0	1998	104	0
20	F	118	0	69	4	0
20	G	151	0	121	0	0
20	H	45	0	33	2	0
20	I	65	0	72	7	0
20	J	45	0	33	0	0
20	K	173	0	118	3	0
20	L	155	0	131	9	0
20	O	81	0	9	0	0
21	A	33	0	46	2	0
21	B	33	0	46	5	0
22	A	8	0	0	0	0
22	C	16	0	0	0	0
23	1	25	0	33	0	0
23	3	80	0	112	4	0
23	A	240	0	336	8	0
23	B	280	0	392	29	0
23	F	40	0	56	2	0
23	G	40	0	56	3	0
23	I	80	0	112	5	0
23	J	80	0	112	4	0
23	K	40	0	56	1	0
23	L	80	0	112	7	0
23	M	40	0	56	5	0
23	O	14	0	20	0	0
24	1	37	0	44	1	0
24	2	32	0	34	2	0
24	3	34	0	38	1	0
24	4	38	0	46	2	0
24	A	80	0	106	4	0
24	B	35	0	40	0	0
25	2	36	0	42	0	0
25	A	34	0	38	2	0
25	J	75	0	90	4	0
26	1	35	0	46	2	0
26	4	35	0	45	3	0
26	A	33	0	39	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	B	31	0	35	0	0
26	G	66	0	80	3	0
27	B	61	0	83	5	0
28	1	103	0	78	2	0
28	2	366	0	290	11	0
28	3	47	0	31	2	0
28	4	188	0	128	1	0
29	1	84	0	112	8	0
29	2	126	0	165	9	0
29	3	84	0	110	9	0
29	4	126	0	166	7	0
30	3	1	0	0	0	0
30	4	1	0	0	0	0
30	A	15	0	0	0	0
30	B	23	0	0	0	0
30	C	2	0	0	0	0
30	D	1	0	0	0	0
30	F	1	0	0	0	0
30	G	1	0	0	0	0
All	All	36553	0	35639	601	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 8.

All (601) 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)
20:A:1134:CLA:H2A	20:A:1134:CLA:HED3	1.63	0.80
20:4:601:CLA:HBB2	20:4:602:CLA:HHH	1.64	0.79
20:3:610:CLA:HAB	29:3:620:LUT:H32	1.67	0.75
20:4:610:CLA:HAB	29:4:620:LUT:H32	1.69	0.75
1:A:209:GLY:HA3	20:A:1111:CLA:HBB1	1.71	0.72
20:1:603:CLA:H11	20:1:603:CLA:H2A	1.72	0.71
20:A:1106:CLA:HAB	20:A:1126:CLA:H102	1.72	0.69
1:A:743:ILE:HG23	20:A:1126:CLA:HAB	1.75	0.69
20:B:1208:CLA:HBB2	20:B:1210:CLA:HMA3	1.74	0.68
20:K:204:CLA:H3A	23:K:301:BCR:H363	1.74	0.67
20:A:1124:CLA:H2	20:A:1133:CLA:HBB2	1.78	0.66
20:B:1201:CLA:H3A	17:M:29:LEU:HD13	1.78	0.66
6:4:251:LEU:HB2	29:4:620:LUT:H22	1.76	0.66
4:2:158:ILE:HG23	20:2:609:CLA:HBB2	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:1:602:CLA:HHD	28:1:601:CHL:HBB2	1.78	0.65
4:2:234:VAL:HG11	29:2:621:LUT:H10	1.79	0.65
2:B:180:SER:HB3	20:B:1217:CLA:HAC2	1.78	0.64
20:H:200:CLA:HBB2	23:L:420:BCR:H311	1.78	0.64
20:A:1114:CLA:HHD	5:3:192:PRO:HG3	1.79	0.63
5:3:286:VAL:HG11	29:3:621:LUT:H12	1.81	0.63
2:B:181:GLY:HA3	20:B:1210:CLA:HBB1	1.81	0.63
1:A:85:GLN:HG2	20:A:1103:CLA:H3A	1.81	0.63
20:A:1130:CLA:H43	20:L:302:CLA:H43	1.82	0.62
1:A:133:ASN:HB3	1:A:141:GLN:HB3	1.81	0.62
5:3:219:ARG:HA	5:3:230:MET:HE3	1.81	0.62
2:B:348:VAL:HG21	20:B:1225:CLA:HHD	1.81	0.61
1:A:455:PHE:HB3	20:A:1132:CLA:HBB2	1.81	0.61
2:B:355:LEU:HD13	20:B:1214:CLA:HAA1	1.82	0.61
5:3:304:LEU:HB2	29:3:620:LUT:H22	1.83	0.61
1:A:371:ILE:HD13	20:A:1124:CLA:HED3	1.83	0.61
20:A:1131:CLA:H92	23:B:4017:BCR:H362	1.83	0.61
1:A:453:LEU:HB3	1:A:547:PHE:HB2	1.83	0.60
8:D:103:ILE:HD13	8:D:141:LEU:HD23	1.83	0.60
20:A:1105:CLA:HMB3	20:A:1106:CLA:H3A	1.83	0.60
20:A:1139:CLA:HMC2	23:B:4014:BCR:H381	1.82	0.60
14:J:12:PRO:HB2	23:J:213:BCR:H391	1.83	0.60
2:B:595:HIS:HE2	2:B:729:THR:HG1	1.47	0.60
6:4:251:LEU:HD13	29:4:620:LUT:H163	1.83	0.60
1:A:147:SER:HA	20:A:1126:CLA:HMA2	1.84	0.60
2:B:545:LYS:HD2	9:E:82:TYR:HA	1.83	0.60
20:A:1110:CLA:H11	5:3:129:LEU:HD23	1.83	0.60
20:A:1137:CLA:HMC2	20:A:5005:CLA:HBB2	1.84	0.60
20:B:1209:CLA:HHC	20:B:1217:CLA:HBC2	1.83	0.59
2:B:342:GLY:HA3	2:B:383:MET:HG2	1.84	0.59
2:B:15:ASP:HB3	2:B:20:ARG:HB2	1.84	0.59
2:B:192:GLY:O	2:B:196:HIS:HB2	2.02	0.59
20:A:1104:CLA:H151	20:A:1127:CLA:HBB2	1.84	0.59
20:3:604:CLA:HMC1	23:3:624:BCR:H21C	1.83	0.59
2:B:687:LEU:HB2	23:I:120:BCR:H282	1.84	0.58
9:E:71:GLY:HA2	9:E:89:LYS:HE2	1.84	0.58
20:B:1239:CLA:HAA1	27:B:5002:DGD:HAW2	1.85	0.58
3:1:142:PRO:HG3	11:G:147:ILE:HD11	1.85	0.58
20:3:610:CLA:H61	29:3:620:LUT:H30	1.84	0.58
20:A:1118:CLA:HAA2	15:K:105:THR:HG23	1.85	0.58
2:B:353:TYR:O	2:B:507:SER:OG	2.22	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:376:GLN:HG3	2:B:587:ILE:HD12	1.86	0.58
20:B:1204:CLA:HMB3	20:B:1205:CLA:HMB	1.86	0.58
6:4:197:PRO:HB3	28:4:608:CHL:HBC2	1.86	0.58
20:4:603:CLA:H93	26:4:631:LMT:H91	1.85	0.57
1:A:126:ILE:HG23	1:A:127:VAL:HG22	1.86	0.57
2:B:168:PHE:O	2:B:174:ARG:NH1	2.37	0.57
7:C:24:ASP:HB2	8:D:139:LEU:HD21	1.87	0.57
2:B:689:ASN:O	2:B:692:ARG:NH1	2.38	0.57
12:H:114:LEU:HA	12:H:117:THR:HG22	1.87	0.56
1:A:402:ILE:HD12	20:A:1104:CLA:H143	1.85	0.56
1:A:739:LEU:O	1:A:743:ILE:HB	2.04	0.56
20:B:1210:CLA:H151	20:B:1225:CLA:HMD2	1.87	0.56
2:B:56:ILE:HD11	23:M:4021:BCR:HC7	1.87	0.56
2:B:595:HIS:O	2:B:599:ILE:HB	2.05	0.56
20:B:1237:CLA:H162	16:L:151:LEU:HD11	1.86	0.56
6:4:91:LEU:HA	10:F:209:LYS:HG2	1.87	0.56
1:A:546:ALA:HB2	20:A:1136:CLA:HMA1	1.87	0.56
1:A:441:ALA:O	1:A:445:HIS:ND1	2.35	0.56
2:B:178:HIS:HB3	20:B:1221:CLA:HED3	1.87	0.56
20:B:1220:CLA:HAB	20:B:1227:CLA:HHD	1.87	0.56
2:B:273:MET:O	2:B:277:HIS:ND1	2.39	0.56
20:B:1208:CLA:HBA2	26:G:401:LMT:H42	1.88	0.56
23:A:4011:BCR:H362	20:B:1012:CLA:H51	1.88	0.55
20:A:1108:CLA:H2A	20:A:1108:CLA:HED3	1.89	0.55
20:A:1117:CLA:H193	20:A:1125:CLA:HAA1	1.87	0.55
1:A:272:LEU:HD11	15:K:119:VAL:HG22	1.88	0.55
2:B:394:PHE:O	2:B:542:ARG:NH1	2.39	0.55
20:F:301:CLA:HBB1	14:J:22:LEU:HD21	1.88	0.55
5:3:304:LEU:HD22	29:3:620:LUT:H172	1.88	0.55
1:A:446:LEU:HD21	1:A:553:VAL:HG12	1.88	0.55
1:A:502:LEU:HD12	1:A:503:THR:HG23	1.88	0.55
2:B:50:HIS:HE1	20:B:1202:CLA:H171	1.71	0.55
3:1:160:ASN:ND2	26:1:631:LMT:O2'	2.39	0.55
8:D:135:LYS:HE3	8:D:167:LEU:HD13	1.88	0.54
7:C:61:ASP:O	9:E:118:ASN:ND2	2.40	0.54
1:A:401:TRP:HB3	20:A:1126:CLA:HMC3	1.89	0.54
4:2:112:ARG:NH2	28:2:608:CHL:OBD	2.40	0.54
5:3:189:VAL:HG21	29:3:621:LUT:H22	1.88	0.54
1:A:287:LEU:HD21	1:A:380:PRO:HD2	1.90	0.54
1:A:427:GLN:OE1	1:A:430:ASN:ND2	2.41	0.54
1:A:607:ASN:HD21	19:A:1011:CL0:H65	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:A:1022:CLA:HBD	2:B:654:HIS:HB3	1.89	0.54
2:B:627:ASN:HB3	2:B:728:SER:HB2	1.89	0.54
20:A:1122:CLA:H122	20:A:1137:CLA:HAA2	1.90	0.54
1:A:226:SER:O	1:A:230:ASN:HB2	2.08	0.54
1:A:371:ILE:HG21	20:A:1117:CLA:H201	1.90	0.54
20:A:1022:CLA:H122	23:B:4017:BCR:H12C	1.90	0.54
3:1:160:ASN:HB3	26:1:631:LMT:H1'	1.90	0.54
6:4:158:LEU:HA	6:4:161:MET:HB2	1.89	0.54
2:B:417:ALA:O	2:B:421:HIS:ND1	2.40	0.54
1:A:743:ILE:HG21	20:A:1126:CLA:HMC2	1.90	0.53
5:3:170:LEU:HD23	5:3:173:ILE:HD11	1.89	0.53
1:A:121:GLN:NE2	20:A:1107:CLA:OBD	2.39	0.53
5:3:142:ASP:OD1	5:3:142:ASP:N	2.42	0.53
1:A:478:SER:HB2	1:A:481:ALA:H	1.74	0.53
20:B:1238:CLA:H191	13:I:20:ALA:HB2	1.90	0.53
1:A:346:LEU:HD21	20:A:1122:CLA:HBC3	1.90	0.53
1:A:472:ARG:NH2	20:A:1132:CLA:O1D	2.42	0.53
1:A:486:PRO:HG3	1:A:539:PHE:HB2	1.91	0.53
1:A:85:GLN:HB2	20:A:1103:CLA:HMB2	1.89	0.53
20:A:1116:CLA:HED2	20:A:1117:CLA:H3A	1.90	0.53
2:B:114:ASN:ND2	20:B:1206:CLA:OBD	2.42	0.53
2:B:525:LEU:HD21	20:B:1012:CLA:HBB1	1.90	0.53
6:4:110:HIS:HB3	6:4:230:MET:HE3	1.90	0.53
10:F:99:ILE:HD12	10:F:123:ILE:HG23	1.91	0.53
23:A:4001:BCR:H23C	15:K:113:MET:HG2	1.90	0.53
2:B:73:ASN:HB2	2:B:76:ALA:HB3	1.91	0.53
2:B:658:ALA:O	2:B:661:PHE:HB2	2.09	0.53
1:A:408:VAL:HG22	1:A:556:LEU:HD11	1.91	0.53
20:A:1102:CLA:HAA1	20:A:1109:CLA:H2	1.89	0.53
1:A:33:LYS:HD2	20:A:1109:CLA:H2A	1.91	0.53
1:A:58:HIS:HB2	24:A:5001:LHG:H102	1.91	0.52
1:A:370:ILE:HG23	1:A:400:MET:HE1	1.91	0.52
2:B:384:THR:HG22	2:B:534:LEU:HD11	1.90	0.52
4:2:65:ARG:NH2	4:2:85:ASP:OD1	2.43	0.52
20:2:610:CLA:HAB	29:2:620:LUT:H10	1.90	0.52
2:B:435:GLY:HA3	20:B:1230:CLA:HAB	1.91	0.52
5:3:304:LEU:HD13	29:3:620:LUT:H163	1.92	0.52
18:O:61:ARG:NH2	18:O:132:GLN:OE1	2.42	0.52
15:K:55:ASN:ND2	20:K:204:CLA:OBD	2.42	0.52
1:A:628:ILE:HG12	1:A:634:VAL:HG22	1.91	0.52
25:A:5002:LMG:H111	4:2:92:GLY:HA3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:B:1237:CLA:H152	23:I:120:BCR:H16C	1.91	0.52
8:D:134:ARG:HB2	8:D:137:GLN:HG3	1.91	0.52
3:1:108:GLU:HB3	3:1:220:LEU:HD12	1.92	0.52
5:3:153:ASN:ND2	20:3:609:CLA:OBD	2.43	0.52
1:A:206:HIS:ND1	20:A:8895:CLA:OBD	2.42	0.52
2:B:395:ILE:HD13	2:B:555:TYR:HA	1.92	0.52
20:B:1220:CLA:H3A	20:B:1240:CLA:HED3	1.92	0.52
4:2:193:ASP:OD2	4:2:220:ARG:NH1	2.42	0.52
1:A:18:VAL:O	1:A:320:ASN:ND2	2.43	0.52
1:A:567:ARG:NH2	8:D:88:THR:O	2.42	0.52
20:A:1128:CLA:HMD2	24:A:5001:LHG:H281	1.90	0.52
3:1:79:VAL:HB	3:1:82:ASN:HB2	1.91	0.52
20:3:613:CLA:HHB	29:3:620:LUT:H162	1.92	0.52
16:L:213:LEU:HD22	16:L:219:LEU:HD11	1.92	0.52
3:1:101:VAL:HG11	29:1:620:LUT:H12	1.90	0.52
1:A:513:LEU:HD12	1:A:529:LEU:HB2	1.92	0.52
2:B:694:LYS:NZ	13:I:31:GLU:O	2.42	0.52
20:B:1237:CLA:HBA1	23:I:120:BCR:H23C	1.91	0.52
4:2:197:PRO:HB3	28:2:608:CHL:HBC2	1.92	0.51
20:A:1132:CLA:H162	20:L:302:CLA:HMB2	1.91	0.51
2:B:340:SER:HB3	20:B:1221:CLA:H42	1.91	0.51
23:B:4014:BCR:H332	23:J:212:BCR:HC32	1.93	0.51
16:L:126:LEU:HD12	20:L:303:CLA:HMB3	1.92	0.51
1:A:602:LEU:HB3	1:A:739:LEU:HD11	1.91	0.51
20:B:1225:CLA:H51	23:B:4005:BCR:H23C	1.91	0.51
2:B:282:VAL:HG21	20:B:1213:CLA:HAB	1.93	0.51
6:4:91:LEU:HD22	10:F:209:LYS:HA	1.92	0.51
10:F:158:GLY:HA2	10:F:162:TYR:HB2	1.91	0.51
19:A:1011:CL0:H46	20:A:1022:CLA:HED2	1.92	0.51
6:4:208:GLY:HA3	20:4:610:CLA:HED3	1.93	0.51
1:A:406:LEU:HD21	20:A:1104:CLA:H142	1.93	0.51
20:A:1127:CLA:H12	23:A:4003:BCR:H392	1.92	0.51
1:A:316:MET:HA	20:A:1120:CLA:HHD	1.92	0.51
6:4:163:TRP:CG	29:4:623:LUT:H32	2.46	0.51
20:A:1022:CLA:HBA2	20:A:1022:CLA:HED3	1.92	0.51
24:2:630:LHG:H271	28:2:601:CHL:HBB1	1.93	0.51
2:B:456:GLU:OE1	10:F:147:HIS:ND1	2.44	0.51
2:B:643:LEU:HD11	2:B:731:GLY:HA3	1.93	0.51
5:3:201:ASP:OD1	5:3:201:ASP:N	2.44	0.50
1:A:568:LEU:O	8:D:134:ARG:NH1	2.43	0.50
10:F:170:ILE:HG23	20:F:301:CLA:HAA1	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:A:1138:CLA:H51	23:B:4014:BCR:H19C	1.93	0.50
2:B:60:TRP:NE1	20:B:1224:CLA:OBD	2.43	0.50
1:A:740:LEU:HD22	20:A:1140:CLA:HMA1	1.92	0.50
6:4:165:GLU:OE1	6:4:168:ARG:NH2	2.39	0.50
1:A:699:TYR:OH	20:A:1013:CLA:OBD	2.27	0.50
1:A:387:THR:HG21	1:A:523:VAL:HB	1.93	0.50
2:B:556:SER:HB3	27:B:5002:DGD:HD2	1.94	0.50
2:B:17:THR:HG21	7:C:77:MET:HG2	1.94	0.50
21:B:2002:PQN:H142	23:B:4017:BCR:H271	1.93	0.50
5:3:285:ALA:O	5:3:289:TYR:N	2.44	0.50
13:I:24:ALA:HB1	16:L:157:ILE:HG21	1.92	0.50
1:A:372:VAL:HG12	1:A:376:MET:HE2	1.94	0.50
1:A:726:SER:O	1:A:730:GLY:N	2.39	0.50
20:A:1022:CLA:H101	20:B:1023:CLA:H122	1.94	0.50
2:B:98:GLN:NE2	12:H:128:GLY:O	2.45	0.50
28:2:601:CHL:H11	5:3:211:ALA:HA	1.94	0.50
20:A:1122:CLA:HHB	20:A:1801:CLA:HAB	1.94	0.49
2:B:341:LEU:O	2:B:345:THR:OG1	2.28	0.49
20:B:1023:CLA:H121	23:B:4017:BCR:H363	1.94	0.49
1:A:382:TYR:HB2	1:A:385:LEU:HD13	1.95	0.49
1:A:400:MET:HB3	1:A:609:ILE:HG23	1.94	0.49
20:A:1128:CLA:H172	20:A:1140:CLA:H3A	1.93	0.49
2:B:417:ALA:HB1	20:B:1227:CLA:HMB3	1.94	0.49
2:B:615:TYR:OH	2:B:621:ARG:NH2	2.45	0.49
1:A:697:ARG:H	2:B:568:CYS:HB2	1.77	0.49
1:A:419:VAL:HG21	1:A:577:PHE:HB2	1.93	0.49
2:B:284:PHE:HE1	20:B:1216:CLA:HHC	1.76	0.49
2:B:670:TYR:OH	20:B:1023:CLA:OBD	2.25	0.49
3:1:121:TRP:HB2	3:1:127:GLY:HA3	1.93	0.49
8:D:175:PRO:HA	8:D:182:ARG:HH12	1.76	0.49
1:A:73:GLU:OE2	1:A:76:ARG:NH1	2.45	0.49
20:B:1225:CLA:H8	23:B:4005:BCR:H21C	1.94	0.49
15:K:89:ASP:OD1	15:K:89:ASP:N	2.46	0.49
20:A:1108:CLA:HAA1	5:3:141:ILE:HG13	1.94	0.49
2:B:694:LYS:HD2	16:L:162:SER:HA	1.94	0.49
4:2:148:THR:HG23	6:4:259:TYR:HB3	1.93	0.49
20:2:610:CLA:H13	29:2:620:LUT:H203	1.94	0.49
1:A:564:ARG:HH21	8:D:114:GLU:HG3	1.78	0.49
20:A:1140:CLA:HMC1	23:B:4014:BCR:H373	1.94	0.49
20:B:1216:CLA:HBB1	20:B:1221:CLA:H52	1.95	0.49
2:B:53:GLN:HB2	20:B:1202:CLA:HMB2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:410:ARG:O	2:B:414:HIS:ND1	2.41	0.48
20:B:1221:CLA:HBB1	20:B:1223:CLA:H102	1.95	0.48
15:K:78:ASN:ND2	15:K:101:GLY:O	2.46	0.48
20:2:613:CLA:HMC2	20:2:613:CLA:H92	1.95	0.48
5:3:124:TYR:HB2	20:3:602:CLA:HMD1	1.95	0.48
2:B:118:SER:HA	20:B:1224:CLA:HMA2	1.95	0.48
2:B:308:HIS:HA	20:B:1240:CLA:HMD1	1.94	0.48
20:B:1203:CLA:HMD3	20:B:1205:CLA:H201	1.94	0.48
20:B:1228:CLA:H11	23:F:416:BCR:H353	1.95	0.48
23:I:118:BCR:H402	23:I:120:BCR:H353	1.95	0.48
1:A:721:GLN:NE2	9:E:110:VAL:O	2.37	0.48
3:1:65:ALA:HB3	3:1:68:ASP:HB2	1.94	0.48
3:1:101:VAL:HG11	29:1:620:LUT:H10	1.95	0.48
4:2:67:LEU:O	5:3:233:GLN:NE2	2.39	0.48
5:3:202:PRO:HA	5:3:205:LEU:HB2	1.94	0.48
14:J:1:MET:HB3	14:J:5:LYS:HE2	1.96	0.48
1:A:124:TRP:HE1	26:A:5004:LMT:H6D	1.79	0.48
20:A:1108:CLA:HBB2	20:A:1111:CLA:HMA3	1.95	0.48
2:B:124:TRP:HA	2:B:127:ILE:HG12	1.94	0.48
1:A:484:LEU:HB2	1:A:536:THR:HG23	1.95	0.48
1:A:546:ALA:O	1:A:550:HIS:ND1	2.46	0.48
2:B:519:VAL:HG21	2:B:593:TYR:HB2	1.95	0.48
2:B:680:TRP:NE1	16:L:77:GLY:O	2.42	0.48
5:3:259:LEU:HD13	29:3:620:LUT:H222	1.95	0.48
4:2:212:ASP:OD1	4:2:212:ASP:N	2.44	0.48
1:A:330:ILE:O	1:A:334:HIS:ND1	2.42	0.48
4:2:231:MET:HB2	28:2:602:CHL:HMC	1.95	0.48
1:A:463:HIS:NE2	1:A:475:ASP:O	2.47	0.48
2:B:69:ALA:HB2	2:B:135:LEU:HB2	1.96	0.48
3:1:159:ARG:HH12	20:1:609:CLA:HED1	1.79	0.48
8:D:114:GLU:O	8:D:144:ARG:NH1	2.46	0.47
17:M:12:LEU:HB3	23:M:4021:BCR:H21C	1.96	0.47
1:A:55:TRP:HE3	24:A:5001:LHG:H101	1.80	0.47
28:1:607:CHL:HHC	28:1:607:CHL:HBB1	1.97	0.47
13:I:30:ILE:HG13	13:I:31:GLU:HG2	1.95	0.47
20:A:1110:CLA:HAC2	20:A:1111:CLA:H151	1.96	0.47
20:A:1113:CLA:HAA2	5:3:294:ILE:HG22	1.97	0.47
20:B:1239:CLA:HAC1	21:B:2002:PQN:H202	1.97	0.47
1:A:538:ASP:O	1:A:542:HIS:ND1	2.36	0.47
23:B:4014:BCR:H321	10:F:167:PHE:HB2	1.96	0.47
1:A:222:GLN:HA	1:A:226:SER:HB2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:299:THR:HG23	20:A:1117:CLA:HMA3	1.97	0.47
4:2:127:LEU:HB3	4:2:132:ILE:HB	1.97	0.47
20:A:1138:CLA:HBB1	20:A:1139:CLA:HMD1	1.96	0.47
2:B:592:PHE:HE2	20:B:1021:CLA:H62	1.78	0.47
1:A:39:HIS:NE2	20:A:1102:CLA:O1D	2.45	0.47
1:A:166:THR:HG21	20:A:1114:CLA:H3A	1.96	0.47
1:A:213:LEU:HD21	20:A:1118:CLA:HMC1	1.96	0.47
2:B:65:LEU:HD11	23:B:4006:BCR:H271	1.97	0.47
2:B:645:VAL:HG21	20:B:1206:CLA:HMD2	1.96	0.47
2:B:684:ARG:NE	16:L:77:GLY:O	2.47	0.47
2:B:724:PHE:O	2:B:728:SER:OG	2.31	0.47
3:1:225:THR:O	3:1:233:ASN:ND2	2.42	0.47
4:2:167:ARG:NH1	4:2:178:VAL:O	2.47	0.47
20:A:1101:CLA:HAB	23:J:213:BCR:H281	1.96	0.47
29:2:620:LUT:H15	29:2:620:LUT:H201	1.73	0.47
20:B:1208:CLA:HBD	26:G:401:LMT:H1'	1.97	0.47
24:2:630:LHG:HC81	23:3:623:BCR:H313	1.97	0.47
9:E:76:VAL:HG12	9:E:78:ARG:H	1.80	0.47
1:A:741:GLY:O	1:A:745:THR:OG1	2.29	0.47
1:A:21:MET:HB3	1:A:192:LYS:HE3	1.96	0.46
2:B:50:HIS:ND1	20:B:1210:CLA:OBD	2.41	0.46
9:E:106:ARG:NH1	9:E:117:THR:OG1	2.48	0.46
20:L:302:CLA:HMB3	20:L:303:CLA:HBC2	1.97	0.46
18:O:88:LEU:HB3	18:O:93:LEU:HD21	1.96	0.46
1:A:133:ASN:O	10:F:105:ARG:NH2	2.48	0.46
1:A:493:GLN:HG3	1:A:515:TRP:HE3	1.80	0.46
2:B:339:ALA:HB2	23:B:4010:BCR:H372	1.98	0.46
20:A:1130:CLA:H91	20:A:1136:CLA:H201	1.97	0.46
2:B:321:GLY:O	2:B:325:THR:OG1	2.34	0.46
20:B:1213:CLA:HBB2	23:G:311:BCR:H282	1.98	0.46
2:B:662:MET:O	2:B:666:SER:OG	2.30	0.46
16:L:95:ASN:O	16:L:100:ARG:NH1	2.48	0.46
20:A:1111:CLA:H121	20:A:1111:CLA:H161	1.77	0.46
2:B:373:THR:HG23	2:B:591:THR:HG21	1.97	0.46
20:B:1202:CLA:H93	20:B:1210:CLA:H2	1.97	0.46
20:L:302:CLA:H3A	20:L:302:CLA:HBA2	1.67	0.46
20:B:1223:CLA:H152	23:B:4010:BCR:H17C	1.96	0.46
23:B:4014:BCR:H11C	10:F:167:PHE:HE1	1.80	0.46
1:A:126:ILE:HG12	14:J:27:ILE:HG23	1.97	0.46
20:B:1238:CLA:HMC2	23:B:4017:BCR:H381	1.98	0.46
20:3:609:CLA:HBA2	20:3:609:CLA:H3A	1.78	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:D:105:TRP:HE1	8:D:123:MET:HE3	1.80	0.46
20:L:303:CLA:HAC1	23:L:420:BCR:H373	1.98	0.46
1:A:434:ARG:O	1:A:438:HIS:ND1	2.42	0.46
2:B:73:ASN:ND2	2:B:107:GLY:O	2.49	0.46
3:1:90:GLU:HG2	3:1:194:ILE:HD11	1.98	0.46
1:A:127:VAL:HB	20:B:1230:CLA:HMD1	1.98	0.46
2:B:545:LYS:HE3	10:F:234:THR:HG22	1.98	0.46
20:B:1202:CLA:HBA1	20:B:1202:CLA:H3A	1.76	0.46
23:L:419:BCR:H20C	23:L:419:BCR:H361	1.79	0.46
1:A:709:TRP:HH2	20:B:1228:CLA:HED3	1.81	0.45
1:A:65:ASP:HB2	1:A:420:ARG:HH21	1.82	0.45
1:A:155:ALA:HB2	1:A:383:PRO:HD2	1.99	0.45
2:B:304:ILE:O	2:B:308:HIS:ND1	2.47	0.45
2:B:338:LEU:HG	20:B:1202:CLA:HED1	1.98	0.45
4:2:69:PHE:HD2	4:2:72:SER:HB3	1.82	0.45
28:2:602:CHL:HH2	28:2:601:CHL:HBB2	1.98	0.45
20:I:121:CLA:H93	16:L:142:LEU:HB3	1.97	0.45
1:A:650:ASN:O	1:A:654:ARG:HB3	2.16	0.45
25:A:5002:LMG:H151	14:J:4:VAL:HG21	1.97	0.45
2:B:412:LEU:HB3	10:F:238:ARG:HD2	1.99	0.45
2:B:424:TRP:CE2	20:B:1228:CLA:HAB	2.51	0.45
20:B:1232:CLA:HBA1	20:B:1232:CLA:H3A	1.73	0.45
20:B:1237:CLA:HMC2	20:B:1238:CLA:H11	1.97	0.45
11:G:69:THR:HA	11:G:136:GLY:HA3	1.98	0.45
20:A:1115:CLA:HBC2	20:A:1116:CLA:HMC2	1.99	0.45
20:B:1204:CLA:HHB	20:B:1205:CLA:HHB	1.99	0.45
20:B:1224:CLA:H3A	20:B:1224:CLA:HBA2	1.73	0.45
20:B:1225:CLA:H61	23:B:4006:BCR:H392	1.98	0.45
20:1:603:CLA:H41	20:1:603:CLA:H62	1.63	0.45
6:4:190:THR:N	6:4:198:GLY:O	2.49	0.45
2:B:177:HIS:CG	20:B:1210:CLA:HMC2	2.52	0.45
2:B:255:LEU:HD11	20:B:1212:CLA:HBC1	1.98	0.45
4:2:93:LEU:HA	14:J:1:MET:HE3	1.98	0.45
5:3:120:LEU:HB2	5:3:123:ASP:HB2	1.99	0.45
20:L:302:CLA:HMD3	23:L:419:BCR:H271	1.97	0.45
2:B:691:VAL:HG11	20:B:1237:CLA:HAB	1.99	0.45
20:B:1226:CLA:H2	27:B:5002:DGD:HB41	1.98	0.45
4:2:234:VAL:HG11	29:2:621:LUT:H12	1.99	0.45
20:F:301:CLA:HBA1	20:F:301:CLA:H3A	1.67	0.45
1:A:565:SER:HB2	1:A:570:PRO:HA	1.99	0.45
20:A:1131:CLA:HMC2	20:L:303:CLA:HBB2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:A:2001:PQN:H162	23:B:4014:BCR:H382	1.99	0.45
2:B:344:ILE:HD13	20:B:1221:CLA:H43	1.99	0.45
2:B:649:MET:HE1	20:B:1205:CLA:H41	1.98	0.45
2:B:733:PHE:HB3	12:H:138:ARG:HE	1.82	0.45
28:2:601:CHL:HED2	5:3:218:HIS:HB3	1.99	0.45
5:3:120:LEU:HD13	20:3:602:CLA:HED2	1.98	0.45
10:F:150:VAL:HG12	10:F:160:PHE:HB2	1.99	0.45
2:B:59:LEU:HD21	17:M:18:THR:HG21	1.98	0.45
23:B:4005:BCR:H15C	23:B:4005:BCR:H351	1.87	0.45
21:A:2001:PQN:H201	20:A:1138:CLA:HBC1	1.98	0.45
20:B:1235:CLA:HBB1	20:B:1236:CLA:HHD	1.99	0.45
20:4:602:CLA:HBC1	24:4:630:LHG:H112	1.99	0.45
1:A:222:GLN:NE2	20:A:1117:CLA:O1D	2.50	0.45
20:A:1119:CLA:H12	20:A:8895:CLA:HBB1	1.98	0.45
2:B:498:LEU:HA	2:B:501:ILE:HG22	1.98	0.45
2:B:616:LEU:HD21	20:B:1021:CLA:H162	1.99	0.45
1:A:37:PRO:HB3	20:A:1101:CLA:HAC1	2.00	0.44
2:B:438:VAL:HG13	20:B:1012:CLA:H62	1.99	0.44
20:B:1237:CLA:H41	20:B:1237:CLA:H61	1.80	0.44
1:A:112:ASP:OD1	1:A:112:ASP:N	2.49	0.44
2:B:695:ASP:OD1	2:B:695:ASP:N	2.49	0.44
20:B:1223:CLA:H141	20:B:1223:CLA:H161	1.83	0.44
23:B:4009:BCR:H371	23:B:4009:BCR:H24C	1.76	0.44
20:F:301:CLA:HMA2	25:J:301:LMG:H381	1.98	0.44
20:A:1116:CLA:H93	20:K:201:CLA:H91	2.00	0.44
20:A:1118:CLA:H71	24:3:630:LHG:H282	1.99	0.44
20:3:607:CLA:H141	20:3:617:CLA:HBB1	2.00	0.44
6:4:114:ALA:O	6:4:118:ALA:N	2.45	0.44
23:M:4021:BCR:H20C	23:M:4021:BCR:H361	1.86	0.44
19:A:1011:CL0:H53	19:A:1011:CL0:H61	1.75	0.44
2:B:608:GLN:O	2:B:612:SER:HB2	2.17	0.44
5:3:155:ARG:NH1	28:3:608:CHL:OBD	2.46	0.44
7:C:75:ARG:NH1	8:D:99:GLU:OE2	2.50	0.44
1:A:225:VAL:HG13	1:A:245:PRO:HB3	2.00	0.44
1:A:571:ASP:OD1	1:A:571:ASP:N	2.45	0.44
23:A:4007:BCR:H371	23:A:4007:BCR:H383	1.99	0.44
20:4:603:CLA:HED1	26:4:631:LMT:H92	1.99	0.44
20:4:603:CLA:H8	10:F:214:PRO:HB2	2.00	0.44
1:A:372:VAL:HG21	20:A:1127:CLA:HHD	2.00	0.44
20:A:1128:CLA:H202	20:A:1140:CLA:HBA1	1.99	0.44
23:3:624:BCR:H24C	23:3:624:BCR:H371	1.78	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:1:85:ARG:NH2	20:1:603:CLA:O1D	2.50	0.44
4:2:204:PRO:HD2	29:2:620:LUT:H3	2.00	0.44
23:I:120:BCR:H20C	23:I:120:BCR:H361	1.83	0.44
1:A:319:THR:OG1	1:A:320:ASN:N	2.51	0.44
2:B:428:PHE:O	2:B:432:HIS:ND1	2.50	0.44
20:B:1223:CLA:C4B	20:B:1231:CLA:H3A	2.48	0.44
20:B:1238:CLA:H2A	13:I:27:PHE:CE1	2.53	0.44
4:2:252:LEU:HD22	29:2:620:LUT:H222	2.00	0.44
10:F:218:ILE:HA	10:F:221:LEU:HB3	2.00	0.44
2:B:131:THR:OG1	2:B:134:ASP:OD2	2.36	0.44
2:B:230:TRP:HB3	20:B:1213:CLA:H3A	1.99	0.44
21:B:2002:PQN:H141	21:B:2002:PQN:H161	1.80	0.44
5:3:219:ARG:HG3	28:3:608:CHL:HBB1	2.00	0.44
23:L:420:BCR:H15C	23:L:420:BCR:H351	1.87	0.44
5:3:112:SER:OG	5:3:127:ASP:O	2.33	0.43
1:A:88:VAL:HG21	20:A:1102:CLA:HBB1	2.01	0.43
1:A:622:SER:HG	1:A:638:THR:HG1	1.64	0.43
20:A:1102:CLA:HAB	20:A:1104:CLA:HBD	2.00	0.43
2:B:462:TRP:HE1	2:B:476:VAL:HG21	1.83	0.43
20:B:1209:CLA:HMD2	26:G:401:LMT:H82	2.00	0.43
13:I:19:PRO:HB2	13:I:23:MET:HE2	2.00	0.43
1:A:654:ARG:HA	2:B:632:ILE:HD12	2.01	0.43
20:A:1103:CLA:H2	20:A:1103:CLA:H62	1.67	0.43
20:A:1119:CLA:H101	23:A:4008:BCR:H10C	1.99	0.43
20:B:1204:CLA:H2A	20:B:1206:CLA:HED1	2.01	0.43
1:A:544:ILE:HG21	19:A:1011:CL0:H60	2.00	0.43
20:A:1022:CLA:H171	20:I:121:CLA:HMC2	2.00	0.43
20:B:1235:CLA:HBC2	25:J:301:LMG:H242	2.00	0.43
1:A:596:ASP:HA	1:A:599:PHE:HB3	2.00	0.43
2:B:293:THR:OG1	2:B:294:ASN:N	2.51	0.43
1:A:72:GLU:OE1	1:A:76:ARG:NH2	2.52	0.43
1:A:567:ARG:HD3	7:C:80:ALA:HB3	2.00	0.43
23:A:4008:BCR:H15C	23:A:4008:BCR:H351	1.79	0.43
2:B:458:VAL:HG11	10:F:149:ILE:HG23	2.01	0.43
20:B:1215:CLA:H41	20:B:1215:CLA:H62	1.79	0.43
2:B:545:LYS:HD3	2:B:545:LYS:HA	1.79	0.43
23:B:4010:BCR:H361	23:B:4010:BCR:H20C	1.68	0.43
2:B:142:LEU:HD11	23:B:4006:BCR:H24C	1.99	0.43
20:B:1023:CLA:H13	20:I:121:CLA:HBC1	1.99	0.43
21:B:2002:PQN:H222	23:B:4017:BCR:H17C	2.01	0.43
6:4:117:GLY:HA2	29:4:621:LUT:H181	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:4:224:LYS:HZ1	24:4:630:LHG:P	2.42	0.43
23:G:311:BCR:H20C	23:G:311:BCR:H361	1.86	0.43
1:A:22:VAL:HA	1:A:191:PRO:HA	1.99	0.43
1:A:102:ARG:HH12	1:A:165:TYR:HB2	1.84	0.43
20:A:1127:CLA:H121	23:A:4003:BCR:H21C	2.01	0.43
2:B:564:ARG:HB3	9:E:112:TYR:HB2	2.00	0.43
2:B:580:VAL:HA	2:B:583:MET:HG3	2.01	0.43
24:1:630:LHG:H162	24:1:630:LHG:H132	1.87	0.43
29:2:620:LUT:H11	29:2:620:LUT:H191	1.85	0.43
28:2:601:CHL:H203	28:2:601:CHL:H162	1.84	0.43
20:A:1137:CLA:HBB1	20:A:5005:CLA:HAB	2.01	0.43
2:B:277:HIS:HA	2:B:280:ILE:HG12	2.01	0.43
15:K:82:THR:OG1	15:K:83:ALA:N	2.52	0.43
18:O:136:LYS:NZ	18:O:140:ASP:OD2	2.50	0.43
1:A:395:LEU:O	1:A:399:HIS:ND1	2.52	0.42
1:A:642:PHE:O	1:A:646:SER:OG	2.32	0.42
1:A:665:ILE:O	2:B:621:ARG:NH1	2.49	0.42
20:A:1022:CLA:HBB2	20:B:1023:CLA:HAA1	2.01	0.42
20:A:1116:CLA:HBA2	20:A:1116:CLA:H3A	1.83	0.42
20:A:8895:CLA:H2	20:A:8895:CLA:H62	1.74	0.42
20:B:1203:CLA:H201	20:B:1224:CLA:HMD3	2.00	0.42
20:B:1219:CLA:O2D	11:G:91:GLN:NE2	2.47	0.42
23:B:4010:BCR:H15C	23:B:4010:BCR:H351	1.77	0.42
4:2:77:TRP:NE1	4:2:89:ASP:OD2	2.50	0.42
18:O:91:LEU:O	18:O:95:SER:N	2.52	0.42
20:A:1118:CLA:H41	20:A:1118:CLA:H62	1.85	0.42
20:A:1132:CLA:H151	20:A:1136:CLA:H202	2.01	0.42
20:B:1238:CLA:H142	20:B:1238:CLA:H112	1.88	0.42
4:2:149:ASP:HB3	4:2:152:THR:HG22	2.01	0.42
6:4:218:ILE:HG13	20:4:610:CLA:H3A	2.01	0.42
23:M:4021:BCR:H24C	23:M:4021:BCR:H371	1.84	0.42
20:1:602:CLA:H52	29:1:621:LUT:H8	2.01	0.42
28:2:601:CHL:H92	28:2:601:CHL:H61	1.93	0.42
5:3:200:ALA:HB3	5:3:205:LEU:HG	2.01	0.42
10:F:89:LYS:HA	10:F:89:LYS:HD3	1.88	0.42
20:H:200:CLA:HAB	23:L:420:BCR:H321	2.02	0.42
14:J:19:PHE:HA	14:J:22:LEU:HB3	2.00	0.42
1:A:583:GLY:O	1:A:589:THR:OG1	2.37	0.42
19:A:1011:CL0:H62	20:A:1022:CLA:HMA1	2.01	0.42
2:B:53:GLN:HG2	20:B:1202:CLA:H3A	2.01	0.42
20:I:121:CLA:H141	20:I:121:CLA:H162	1.73	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:A:1138:CLA:HED2	2:B:424:TRP:HB2	2.01	0.42
2:B:86:PRO:O	2:B:116:ALA:N	2.37	0.42
2:B:176:ASN:O	2:B:180:SER:HB2	2.19	0.42
20:B:1229:CLA:HBB2	20:B:1230:CLA:HBB	2.01	0.42
5:3:271:LEU:HD21	20:3:610:CLA:HBA2	2.01	0.42
1:A:457:SER:HB3	1:A:543:HIS:HB3	2.00	0.42
2:B:453:ILE:HG21	25:J:301:LMG:H191	2.02	0.42
20:B:1214:CLA:HBA2	20:B:1223:CLA:HBB2	2.01	0.42
29:1:621:LUT:H27	29:1:621:LUT:H30	1.83	0.42
5:3:283:MET:SD	20:3:602:CLA:HAB	2.59	0.42
20:3:613:CLA:H2	20:3:613:CLA:H61	1.75	0.42
6:4:157:GLU:O	6:4:161:MET:N	2.44	0.42
6:4:165:GLU:O	6:4:169:TRP:N	2.53	0.42
1:A:205:HIS:CG	20:A:1111:CLA:HMC2	2.55	0.42
2:B:26:ALA:HA	20:B:1226:CLA:H11	2.01	0.42
2:B:129:LEU:HD13	2:B:135:LEU:HD23	2.02	0.42
2:B:319:HIS:HB3	2:B:322:LEU:HD12	2.01	0.42
29:4:621:LUT:H401	29:4:621:LUT:H35	1.76	0.42
10:F:197:ILE:HG12	14:J:10:THR:HG22	2.00	0.42
24:A:5003:LHG:HC92	20:A:5005:CLA:HBA1	2.02	0.42
20:B:1201:CLA:H11	17:M:26:GLY:HA3	2.01	0.42
20:B:1237:CLA:H142	20:B:1238:CLA:H101	2.02	0.42
12:H:101:LYS:HA	12:H:101:LYS:HD3	1.78	0.42
1:A:365:LEU:HG	20:A:1127:CLA:HMC1	2.01	0.42
2:B:175:LEU:HD23	2:B:175:LEU:HA	1.93	0.42
2:B:649:MET:HE2	23:B:4017:BCR:H333	2.02	0.42
20:3:610:CLA:HBA2	20:3:610:CLA:H3A	1.81	0.42
7:C:47:ASP:OD2	8:D:135:LYS:NZ	2.52	0.42
9:E:69:LYS:HB3	9:E:72:SER:HB3	2.01	0.42
9:E:73:ILE:HG23	9:E:87:THR:HG23	2.02	0.42
16:L:82:PRO:O	16:L:86:SER:OG	2.33	0.42
1:A:580:PRO:HB3	1:A:727:ILE:HB	2.02	0.42
20:A:1124:CLA:HAA2	20:A:1135:CLA:HMB3	2.02	0.42
2:B:67:HIS:ND1	2:B:71:GLN:OE1	2.45	0.42
2:B:93:ASP:OD2	2:B:95:HIS:ND1	2.39	0.42
2:B:285:ILE:O	2:B:289:HIS:ND1	2.48	0.42
20:B:1237:CLA:H122	20:B:1237:CLA:H8	1.87	0.42
28:2:601:CHL:H91	28:2:601:CHL:H112	1.83	0.42
7:C:5:VAL:HG22	7:C:67:VAL:HG13	2.01	0.42
8:D:116:PRO:HD3	8:D:141:LEU:HD13	2.02	0.42
16:L:96:LEU:HD23	20:L:301:CLA:HHC	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:A:1130:CLA:OBD	20:A:5005:CLA:H3A	2.20	0.41
20:A:1138:CLA:H52	20:A:1138:CLA:H11	1.85	0.41
1:A:561:LEU:HD23	1:A:561:LEU:HA	1.89	0.41
11:G:125:THR:OG1	11:G:126:ILE:N	2.53	0.41
1:A:754:ILE:HD12	1:A:754:ILE:HA	1.95	0.41
20:A:1127:CLA:H172	20:A:1127:CLA:H13	1.72	0.41
2:B:574:ASP:HA	2:B:577:TYR:HB3	2.01	0.41
20:I:121:CLA:H122	16:L:146:GLY:HA2	2.02	0.41
20:A:1117:CLA:H122	20:A:1125:CLA:H92	2.02	0.41
20:A:1133:CLA:HHC	20:A:1133:CLA:HBB1	2.02	0.41
2:B:22:TRP:CG	2:B:704:GLN:HE22	2.38	0.41
20:B:1217:CLA:HMB2	11:G:130:LEU:HD22	2.01	0.41
6:4:133:LEU:HB3	6:4:135:THR:HG23	2.02	0.41
1:A:590:CYS:HB2	2:B:668:ARG:H	1.86	0.41
20:A:1104:CLA:H112	20:A:1104:CLA:H72	1.90	0.41
23:B:4006:BCR:H20C	23:B:4006:BCR:H361	1.91	0.41
27:B:5002:DGD:HA42	27:B:5002:DGD:HA71	1.89	0.41
20:1:609:CLA:H61	20:1:609:CLA:H2	1.85	0.41
5:3:145:TRP:O	5:3:149:ALA:N	2.50	0.41
10:F:201:PRO:HD3	25:J:302:LMG:HC91	2.01	0.41
16:L:175:THR:OG1	16:L:176:LEU:N	2.52	0.41
1:A:62:HIS:HB2	20:A:1128:CLA:HAA2	2.02	0.41
1:A:368:LEU:HD11	20:A:1117:CLA:H71	2.03	0.41
2:B:378:ILE:HG23	20:B:1203:CLA:H143	2.02	0.41
20:B:1206:CLA:H3A	20:I:121:CLA:CBB	2.51	0.41
20:1:603:CLA:HBC1	20:1:609:CLA:HAC1	2.02	0.41
6:4:126:LEU:HA	6:4:248:ILE:HG21	2.03	0.41
20:4:603:CLA:H61	10:F:215:VAL:HG22	2.02	0.41
23:G:311:BCR:H24C	23:G:311:BCR:H371	1.84	0.41
1:A:622:SER:OG	1:A:638:THR:OG1	2.38	0.41
20:A:1103:CLA:H192	20:A:1111:CLA:H8	2.02	0.41
7:C:49:VAL:HA	7:C:76:SER:HA	2.03	0.41
1:A:96:MET:HE1	20:A:1106:CLA:HMA2	2.02	0.41
1:A:684:PHE:HB2	20:B:1012:CLA:HBA1	2.02	0.41
1:A:716:VAL:HG23	10:F:179:ARG:HA	2.02	0.41
20:B:1012:CLA:H61	20:B:1012:CLA:H41	1.73	0.41
20:3:612:CLA:HBB2	23:3:624:BCR:H382	2.03	0.41
1:A:124:TRP:HB3	23:J:213:BCR:H323	2.03	0.41
1:A:161:GLU:HA	1:A:164:LEU:HD12	2.03	0.41
1:A:311:LEU:O	1:A:315:HIS:ND1	2.49	0.41
1:A:346:LEU:HA	1:A:349:ILE:HD12	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:545:HIS:HE1	1:A:611:VAL:HG12	1.86	0.41
1:A:555:ILE:HG21	1:A:600:LEU:HB2	2.02	0.41
1:A:714:LEU:HD13	23:F:416:BCR:H321	2.03	0.41
20:A:1128:CLA:H71	20:A:1128:CLA:H112	1.89	0.41
20:A:1134:CLA:HMD2	18:O:84:ASN:HB3	2.02	0.41
2:B:71:GLN:NE2	20:B:1204:CLA:O1D	2.45	0.41
2:B:310:PRO:HA	2:B:311:PRO:HD3	1.85	0.41
2:B:693:TRP:HE3	20:B:1238:CLA:HMD3	1.86	0.41
21:B:2002:PQN:H251	21:B:2002:PQN:H212	1.91	0.41
20:1:606:CLA:HBA1	20:1:606:CLA:H3A	1.86	0.41
29:2:623:LUT:H31	29:2:623:LUT:H391	1.97	0.41
29:4:620:LUT:H27	29:4:620:LUT:H30	1.88	0.41
9:E:93:VAL:HG22	9:E:103:VAL:HG13	2.03	0.41
10:F:196:ILE:O	14:J:11:ALA:N	2.54	0.41
13:I:27:PHE:HA	13:I:30:ILE:HG12	2.02	0.41
18:O:101:ALA:HB1	18:O:108:ALA:HB2	2.02	0.41
1:A:121:GLN:HB3	1:A:143:ILE:HB	2.03	0.41
1:A:126:ILE:HG13	1:A:127:VAL:HG13	2.03	0.41
1:A:202:MET:HE1	20:A:8895:CLA:H142	2.03	0.41
2:B:345:THR:HB	2:B:379:ALA:HB2	2.02	0.41
2:B:650:PHE:O	2:B:654:HIS:ND1	2.50	0.41
20:B:1208:CLA:HAA2	11:G:108:ARG:HD3	2.02	0.41
20:B:1217:CLA:HBA2	20:B:1217:CLA:H3A	1.62	0.41
3:1:204:PHE:CD2	29:1:621:LUT:H32	2.56	0.41
29:1:620:LUT:H35	29:1:620:LUT:H401	1.88	0.41
4:2:163:TRP:CD1	28:2:608:CHL:HAB	2.56	0.41
7:C:19:ARG:HG2	8:D:176:GLU:HG2	2.03	0.41
20:I:121:CLA:H12	16:L:129:PRO:HG2	2.03	0.41
1:A:365:LEU:HD12	1:A:365:LEU:HA	1.93	0.40
20:A:1013:CLA:HAA1	20:B:1012:CLA:HBB2	2.03	0.40
2:B:580:VAL:HB	2:B:710:LEU:HD11	2.03	0.40
20:B:1203:CLA:H112	20:B:1203:CLA:H152	1.77	0.40
23:B:4004:BCR:H20C	23:B:4004:BCR:H361	1.84	0.40
12:H:121:ASP:N	12:H:121:ASP:OD1	2.48	0.40
2:B:125:TYR:O	2:B:130:ARG:NH1	2.40	0.40
2:B:351:HIS:HD1	20:B:1214:CLA:CAD	2.32	0.40
23:B:4009:BCR:H15C	23:B:4009:BCR:H351	1.90	0.40
29:1:621:LUT:H35	29:1:621:LUT:H401	1.91	0.40
6:4:102:TRP:HB2	26:4:631:LMT:H3B	2.02	0.40
12:H:96:ARG:NH1	16:L:159:GLY:O	2.54	0.40
1:A:505:PRO:O	1:A:507:ALA:N	2.53	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:515:TRP:HH2	20:A:1135:CLA:HED3	1.87	0.40
23:A:4007:BCR:H15C	23:A:4007:BCR:H351	1.87	0.40
4:2:228:ARG:HG2	4:2:231:MET:HE2	2.03	0.40
1:A:605:MET:HE3	1:A:605:MET:HB3	1.97	0.40
23:M:4021:BCR:H15C	23:M:4021:BCR:H351	1.92	0.40
20:B:1204:CLA:H3A	20:B:1205:CLA:HMB3	2.02	0.40
20:B:1223:CLA:H13	23:B:4010:BCR:H15C	2.03	0.40
20:B:1226:CLA:H41	27:B:5002:DGD:HA92	2.04	0.40
3:1:194:ILE:HD12	3:1:194:ILE:HA	1.96	0.40
29:1:621:LUT:H31	29:1:621:LUT:H391	1.93	0.40
5:3:151:ILE:HG21	5:3:249:ALA:HB1	2.02	0.40
6:4:111:CYS:HB3	6:4:226:GLY:HA3	2.04	0.40
23:L:419:BCR:H11C	23:L:419:BCR:H341	1.95	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	740/742 (100%)	699 (94%)	38 (5%)	3 (0%)	30	60
2	B	730/732 (100%)	708 (97%)	22 (3%)	0	100	100
3	1	190/192 (99%)	182 (96%)	8 (4%)	0	100	100
4	2	201/203 (99%)	198 (98%)	3 (2%)	0	100	100
5	3	216/218 (99%)	206 (95%)	10 (5%)	0	100	100
6	4	201/203 (99%)	197 (98%)	4 (2%)	0	100	100
7	C	78/80 (98%)	74 (95%)	4 (5%)	0	100	100
8	D	140/142 (99%)	136 (97%)	4 (3%)	0	100	100
9	E	61/63 (97%)	56 (92%)	5 (8%)	0	100	100
10	F	158/160 (99%)	153 (97%)	5 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	G	89/91 (98%)	88 (99%)	1 (1%)	0	100	100
12	H	85/87 (98%)	82 (96%)	3 (4%)	0	100	100
13	I	32/34 (94%)	31 (97%)	1 (3%)	0	100	100
14	J	39/41 (95%)	39 (100%)	0	0	100	100
15	K	79/81 (98%)	78 (99%)	1 (1%)	0	100	100
16	L	158/160 (99%)	149 (94%)	9 (6%)	0	100	100
17	M	28/30 (93%)	28 (100%)	0	0	100	100
18	O	86/88 (98%)	75 (87%)	11 (13%)	0	100	100
All	All	3311/3347 (99%)	3179 (96%)	129 (4%)	3 (0%)	49	77

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	506	ASN
1	A	505	PRO
1	A	284	ARG

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	603/603 (100%)	603 (100%)	0	100	100
2	B	595/595 (100%)	595 (100%)	0	100	100
3	1	148/148 (100%)	148 (100%)	0	100	100
4	2	160/160 (100%)	160 (100%)	0	100	100
5	3	169/171 (99%)	169 (100%)	0	100	100
6	4	161/162 (99%)	161 (100%)	0	100	100
7	C	67/67 (100%)	67 (100%)	0	100	100
8	D	114/115 (99%)	114 (100%)	0	100	100
9	E	55/55 (100%)	55 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	F	130/131 (99%)	130 (100%)	0	100	100
11	G	72/72 (100%)	72 (100%)	0	100	100
12	H	66/68 (97%)	66 (100%)	0	100	100
13	I	30/30 (100%)	30 (100%)	0	100	100
14	J	35/35 (100%)	35 (100%)	0	100	100
15	K	57/58 (98%)	57 (100%)	0	100	100
16	L	116/118 (98%)	116 (100%)	0	100	100
17	M	25/25 (100%)	25 (100%)	0	100	100
18	O	60/72 (83%)	60 (100%)	0	100	100
All	All	2663/2685 (99%)	2663 (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 (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	115	HIS
1	A	224	HIS
1	A	251	ASN
1	A	621	GLN
2	B	158	GLN
2	B	266	GLN
2	B	275	HIS
2	B	636	ASN
3	1	55	ASN
3	1	237	HIS
4	2	262	ASN
5	3	303	ASN
6	4	179	ASN
9	E	127	GLN
10	F	97	GLN
12	H	82	GLN
17	M	7	GLN
18	O	56	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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](#)

219 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	$\# Z > 2$
20	CLA	B	1224	-	65,69,73	1.22	10 (15%)	77,108,113	1.46	10 (12%)
20	CLA	B	1226	-	59,63,73	1.31	9 (15%)	70,101,113	1.71	11 (15%)
20	CLA	4	611	-	59,63,73	1.26	9 (15%)	70,101,113	1.47	7 (10%)
20	CLA	3	610	-	59,63,73	1.25	8 (13%)	70,101,113	1.24	7 (10%)
28	CHL	4	607	-	51,55,74	2.17	18 (35%)	56,91,114	2.90	22 (39%)
20	CLA	A	1102	-	49,53,73	1.36	9 (18%)	58,89,113	1.35	7 (12%)
23	BCR	B	4017	-	41,41,41	1.11	3 (7%)	56,56,56	1.26	5 (8%)
23	BCR	F	416	-	41,41,41	1.02	2 (4%)	56,56,56	1.36	10 (17%)
25	LMG	2	631	-	36,36,55	0.94	0	44,44,63	1.21	5 (11%)
20	CLA	A	1107	-	49,53,73	1.39	8 (16%)	58,89,113	1.60	7 (12%)
23	BCR	B	4006	-	41,41,41	1.06	2 (4%)	56,56,56	1.22	5 (8%)
20	CLA	A	1105	-	54,58,73	1.31	8 (14%)	64,95,113	1.63	7 (10%)
20	CLA	B	1209	-	49,53,73	1.41	7 (14%)	58,89,113	1.54	6 (10%)
23	BCR	3	624	-	41,41,41	0.99	2 (4%)	56,56,56	1.36	9 (16%)
20	CLA	B	1220	-	49,53,73	1.38	8 (16%)	58,89,113	1.39	6 (10%)
20	CLA	2	610	-	64,68,73	1.21	7 (10%)	76,107,113	1.16	5 (6%)
20	CLA	4	614	-	50,54,73	1.37	8 (16%)	59,90,113	1.38	5 (8%)
29	LUT	4	623	-	42,43,43	2.42	1 (2%)	51,60,60	1.79	8 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	BCR	B	4010	-	41,41,41	1.08	1 (2%)	56,56,56	1.70	13 (23%)
20	CLA	F	302	-	50,54,73	1.36	8 (16%)	59,90,113	1.38	5 (8%)
24	LHG	A	5001	-	48,48,48	0.68	1 (2%)	51,54,54	1.29	6 (11%)
20	CLA	A	1022	-	69,73,73	1.19	7 (10%)	82,113,113	1.27	6 (7%)
20	CLA	A	1130	-	64,68,73	1.21	8 (12%)	76,107,113	1.29	9 (11%)
20	CLA	B	1212	-	49,53,73	1.37	9 (18%)	58,89,113	1.54	7 (12%)
20	CLA	B	1237	-	69,73,73	1.21	8 (11%)	82,113,113	1.32	7 (8%)
20	CLA	3	611	-	45,49,73	1.43	8 (17%)	54,84,113	1.37	3 (5%)
20	CLA	A	1136	-	69,73,73	1.18	8 (11%)	82,113,113	1.40	9 (10%)
20	CLA	A	1116	-	58,62,73	1.27	10 (17%)	68,99,113	1.33	7 (10%)
23	BCR	A	4008	-	41,41,41	1.01	1 (2%)	56,56,56	1.86	15 (26%)
20	CLA	B	1227	-	49,53,73	1.40	10 (20%)	58,89,113	1.71	10 (17%)
20	CLA	1	611	-	50,54,73	1.36	7 (14%)	59,90,113	1.28	4 (6%)
29	LUT	4	621	-	42,43,43	2.53	4 (9%)	51,60,60	3.06	14 (27%)
20	CLA	B	1228	-	53,57,73	1.31	9 (16%)	61,93,113	1.42	7 (11%)
20	CLA	2	604	-	54,58,73	1.32	8 (14%)	64,95,113	1.36	6 (9%)
20	CLA	B	1205	-	69,73,73	1.18	9 (13%)	82,113,113	1.47	10 (12%)
20	CLA	B	1211	-	60,64,73	1.25	7 (11%)	71,102,113	1.45	7 (9%)
29	LUT	3	621	-	42,43,43	2.44	1 (2%)	51,60,60	1.85	10 (19%)
20	CLA	A	1121	-	55,59,73	1.32	8 (14%)	64,96,113	1.54	8 (12%)
26	LMT	4	631	-	36,36,36	1.18	5 (13%)	47,47,47	0.95	1 (2%)
20	CLA	B	1234	-	55,59,73	1.30	9 (16%)	64,96,113	1.49	8 (12%)
26	LMT	1	631	-	36,36,36	1.15	4 (11%)	47,47,47	0.97	2 (4%)
28	CHL	2	615	-	51,55,74	2.17	17 (33%)	56,91,114	2.92	23 (41%)
23	BCR	A	4002	-	41,41,41	1.06	2 (4%)	56,56,56	1.21	5 (8%)
29	LUT	1	620	-	42,43,43	2.72	2 (4%)	51,60,60	2.30	14 (27%)
20	CLA	A	5005	-	54,58,73	1.31	8 (14%)	64,95,113	1.39	8 (12%)
20	CLA	3	607	-	64,68,73	1.21	8 (12%)	76,107,113	1.26	4 (5%)
20	CLA	3	612	-	49,53,73	1.39	7 (14%)	58,89,113	1.34	5 (8%)
23	BCR	B	4005	-	41,41,41	1.04	2 (4%)	56,56,56	1.20	5 (8%)
23	BCR	1	623	-	25,25,41	1.04	2 (8%)	33,33,56	1.29	5 (15%)
20	CLA	B	1012	-	59,63,73	1.30	8 (13%)	70,101,113	1.45	10 (14%)
20	CLA	B	1230	-	49,53,73	1.39	8 (16%)	58,89,113	1.36	5 (8%)
20	CLA	3	606	-	50,54,73	1.38	9 (18%)	59,90,113	1.30	3 (5%)
20	CLA	A	1108	-	49,53,73	1.36	8 (16%)	58,89,113	1.66	6 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	BCR	A	4007	-	41,41,41	1.11	3 (7%)	56,56,56	1.88	18 (32%)
20	CLA	A	1119	-	69,73,73	1.16	9 (13%)	82,113,113	1.49	8 (9%)
28	CHL	2	608	-	52,56,74	2.09	15 (28%)	57,92,114	2.96	22 (38%)
20	CLA	A	1135	-	55,59,73	1.33	8 (14%)	64,96,113	1.44	7 (10%)
20	CLA	1	602	-	64,68,73	1.22	8 (12%)	76,107,113	1.45	7 (9%)
28	CHL	2	607	-	51,55,74	2.17	16 (31%)	56,91,114	2.95	25 (44%)
20	CLA	B	1240	-	69,73,73	1.19	9 (13%)	82,113,113	1.37	9 (10%)
20	CLA	B	1202	-	69,73,73	1.15	8 (11%)	82,113,113	1.43	7 (8%)
20	CLA	1	603	-	59,63,73	1.26	8 (13%)	70,101,113	1.38	8 (11%)
25	LMG	J	302	-	26,26,55	1.12	2 (7%)	34,34,63	1.16	4 (11%)
20	CLA	B	1023	-	65,69,73	1.20	9 (13%)	77,108,113	1.52	12 (15%)
28	CHL	4	608	-	55,59,74	2.08	19 (34%)	61,96,114	2.80	23 (37%)
20	CLA	A	1101	-	54,58,73	1.32	9 (16%)	64,95,113	1.42	7 (10%)
20	CLA	A	1132	-	69,73,73	1.14	8 (11%)	82,113,113	1.63	14 (17%)
20	CLA	A	1134	-	49,53,73	1.38	8 (16%)	58,89,113	1.62	6 (10%)
20	CLA	A	1140	-	55,59,73	1.31	8 (14%)	64,96,113	1.39	9 (14%)
28	CHL	1	607	-	51,55,74	2.20	18 (35%)	56,91,114	3.00	27 (48%)
23	BCR	A	4001	-	41,41,41	1.04	2 (4%)	56,56,56	1.37	7 (12%)
23	BCR	I	120	-	41,41,41	1.06	3 (7%)	56,56,56	1.77	15 (26%)
24	LHG	A	5003	-	30,30,48	0.78	1 (3%)	33,36,54	1.28	3 (9%)
23	BCR	L	420	-	41,41,41	0.99	1 (2%)	56,56,56	1.50	10 (17%)
20	CLA	B	1213	-	59,63,73	1.22	8 (13%)	70,101,113	1.48	9 (12%)
23	BCR	G	311	-	41,41,41	0.99	2 (4%)	56,56,56	1.36	9 (16%)
29	LUT	2	621	-	42,43,43	2.38	1 (2%)	51,60,60	1.58	6 (11%)
20	CLA	I	121	-	69,73,73	1.17	8 (11%)	82,113,113	1.28	6 (7%)
28	CHL	2	601	-	70,74,74	1.84	16 (22%)	79,114,114	2.62	30 (37%)
23	BCR	L	419	-	41,41,41	0.97	1 (2%)	56,56,56	1.59	12 (21%)
20	CLA	B	1222	-	50,54,73	1.34	8 (16%)	59,90,113	1.57	9 (15%)
23	BCR	B	4009	-	41,41,41	0.99	1 (2%)	56,56,56	1.56	11 (19%)
20	CLA	A	1128	-	69,73,73	1.21	9 (13%)	82,113,113	1.41	14 (17%)
20	CLA	3	613	-	59,63,73	1.29	8 (13%)	70,101,113	1.32	3 (4%)
20	CLA	K	202	-	50,54,73	1.37	8 (16%)	59,90,113	1.36	6 (10%)
20	CLA	K	203	-	27,35,73	1.85	6 (22%)	32,60,113	1.60	5 (15%)
20	CLA	O	203	-	27,35,73	1.86	7 (25%)	32,60,113	1.65	5 (15%)
28	CHL	2	606	-	50,54,74	2.19	17 (34%)	55,90,114	2.95	21 (38%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	CLA	A	1013	-	60,64,73	1.23	10 (16%)	71,102,113	1.82	14 (19%)
29	LUT	2	623	-	42,43,43	2.55	1 (2%)	51,60,60	1.76	9 (17%)
20	CLA	G	218	-	59,63,73	1.27	7 (11%)	70,101,113	1.28	4 (5%)
20	CLA	A	1118	-	59,63,73	1.28	6 (10%)	70,101,113	1.25	6 (8%)
20	CLA	A	1110	-	59,63,73	1.28	9 (15%)	70,101,113	1.45	6 (8%)
20	CLA	B	1232	-	49,53,73	1.44	8 (16%)	58,89,113	1.78	7 (12%)
23	BCR	J	213	-	41,41,41	1.03	2 (4%)	56,56,56	1.37	7 (12%)
29	LUT	1	621	-	42,43,43	2.66	2 (4%)	51,60,60	2.23	9 (17%)
20	CLA	3	614	-	52,56,73	1.35	7 (13%)	61,92,113	1.53	6 (9%)
20	CLA	K	204	-	49,53,73	1.40	9 (18%)	58,89,113	1.49	9 (15%)
20	CLA	A	1127	-	69,73,73	1.18	11 (15%)	82,113,113	1.56	11 (13%)
23	BCR	K	301	-	41,41,41	1.04	2 (4%)	56,56,56	1.31	6 (10%)
20	CLA	A	1114	-	49,53,73	1.39	6 (12%)	58,89,113	1.70	9 (15%)
20	CLA	4	613	-	59,63,73	1.27	9 (15%)	70,101,113	1.35	5 (7%)
23	BCR	A	4011	-	41,41,41	1.03	2 (4%)	56,56,56	1.23	6 (10%)
20	CLA	A	1109	-	69,73,73	1.18	10 (14%)	82,113,113	1.31	7 (8%)
23	BCR	J	212	-	41,41,41	1.09	2 (4%)	56,56,56	1.29	7 (12%)
24	LHG	3	630	-	33,33,48	0.75	1 (3%)	36,39,54	1.30	4 (11%)
20	CLA	1	604	-	54,58,73	1.30	8 (14%)	64,95,113	1.49	7 (10%)
20	CLA	A	1112	-	49,53,73	1.38	9 (18%)	58,89,113	1.31	8 (13%)
20	CLA	2	603	-	50,54,73	1.34	8 (16%)	59,90,113	1.38	4 (6%)
23	BCR	B	4004	-	41,41,41	1.05	2 (4%)	56,56,56	1.29	5 (8%)
20	CLA	1	606	-	49,53,73	1.39	9 (18%)	58,89,113	1.53	8 (13%)
20	CLA	O	202	-	27,35,73	1.85	7 (25%)	32,60,113	1.62	5 (15%)
20	CLA	A	1138	-	64,68,73	1.20	8 (12%)	76,107,113	1.42	7 (9%)
25	LMG	A	5002	-	34,34,55	0.95	0	42,42,63	1.23	3 (7%)
20	CLA	A	1137	-	49,53,73	1.40	7 (14%)	58,89,113	1.41	5 (8%)
20	CLA	1	613	-	59,63,73	1.27	9 (15%)	70,101,113	1.31	6 (8%)
21	PQN	A	2001	-	34,34,34	0.41	0	43,45,45	1.04	1 (2%)
21	PQN	B	2002	-	34,34,34	0.42	0	43,45,45	1.07	1 (2%)
29	LUT	2	620	-	42,43,43	2.47	1 (2%)	51,60,60	2.11	19 (37%)
20	CLA	1	610	-	59,63,73	1.24	7 (11%)	70,101,113	1.65	9 (12%)
20	CLA	1	615	-	50,54,73	1.38	8 (16%)	59,90,113	1.45	5 (8%)
22	SF4	C	1003	7	0,12,12	-	-	-	-	-
24	LHG	B	5101	-	34,34,48	0.75	1 (2%)	37,40,54	1.29	4 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	CLA	A	1111	-	69,73,73	1.19	9 (13%)	82,113,113	1.34	6 (7%)
20	CLA	4	612	-	50,54,73	1.37	7 (14%)	59,90,113	1.28	4 (6%)
20	CLA	B	1223	-	69,73,73	1.15	7 (10%)	82,113,113	1.33	10 (12%)
23	BCR	O	301	-	14,14,41	1.09	1 (7%)	20,20,56	1.06	1 (5%)
20	CLA	B	1236	-	51,55,73	1.33	8 (15%)	60,91,113	1.41	5 (8%)
20	CLA	1	609	-	64,68,73	1.24	8 (12%)	76,107,113	1.59	3 (3%)
20	CLA	3	617	-	50,54,73	1.36	8 (16%)	59,90,113	1.33	5 (8%)
20	CLA	3	609	-	64,68,73	1.21	8 (12%)	76,107,113	1.31	8 (10%)
22	SF4	C	1002	7	0,12,12	-	-	-	-	-
27	DGD	B	5002	-	62,62,67	0.97	4 (6%)	76,76,81	1.26	8 (10%)
20	CLA	L	302	-	64,68,73	1.21	7 (10%)	76,107,113	1.21	7 (9%)
24	LHG	2	630	-	31,31,48	0.79	2 (6%)	34,37,54	1.24	3 (8%)
20	CLA	B	1225	-	69,73,73	1.17	9 (13%)	82,113,113	1.36	8 (9%)
20	CLA	B	1221	-	58,62,73	1.30	10 (17%)	68,99,113	1.64	9 (13%)
28	CHL	4	606	-	51,55,74	2.16	17 (33%)	56,91,114	2.92	23 (41%)
24	LHG	4	630	-	37,37,48	0.83	2 (5%)	40,43,54	1.26	3 (7%)
20	CLA	A	1126	-	64,68,73	1.19	9 (14%)	76,107,113	1.81	16 (21%)
20	CLA	B	1201	-	54,58,73	1.30	8 (14%)	64,95,113	1.40	10 (15%)
20	CLA	O	201	-	27,35,73	1.84	7 (25%)	32,60,113	1.62	5 (15%)
24	LHG	1	630	-	36,36,48	0.68	1 (2%)	39,42,54	1.26	4 (10%)
20	CLA	A	1131	-	69,73,73	1.18	8 (11%)	82,113,113	1.30	6 (7%)
20	CLA	A	8895	-	69,73,73	1.19	9 (13%)	82,113,113	1.46	5 (6%)
28	CHL	2	611	-	60,64,74	1.99	18 (30%)	67,102,114	2.72	26 (38%)
28	CHL	3	608	-	51,55,74	2.12	16 (31%)	56,91,114	2.91	24 (42%)
25	LMG	J	301	-	49,49,55	0.81	1 (2%)	57,57,63	1.27	5 (8%)
20	CLA	A	1125	-	64,68,73	1.22	9 (14%)	76,107,113	1.69	14 (18%)
20	CLA	4	610	-	59,63,73	1.26	10 (16%)	70,101,113	1.55	8 (11%)
20	CLA	G	201	-	54,58,73	1.33	8 (14%)	64,95,113	1.36	5 (7%)
20	CLA	2	613	-	69,73,73	1.18	9 (13%)	82,113,113	1.27	6 (7%)
26	LMT	A	5004	-	34,34,36	1.20	4 (11%)	45,45,47	1.05	1 (2%)
23	BCR	I	118	-	41,41,41	1.03	2 (4%)	56,56,56	1.30	8 (14%)
20	CLA	H	200	-	49,53,73	1.39	6 (12%)	58,89,113	1.33	6 (10%)
20	CLA	1	612	-	50,54,73	1.37	8 (16%)	59,90,113	1.30	7 (11%)
20	CLA	B	1203	-	69,73,73	1.17	8 (11%)	82,113,113	1.30	9 (10%)
28	CHL	1	601	-	60,64,74	1.96	17 (28%)	67,102,114	2.86	28 (41%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	CLA	A	1139	-	54,58,73	1.31	9 (16%)	64,95,113	1.45	6 (9%)
20	CLA	B	1208	-	49,53,73	1.38	8 (16%)	58,89,113	1.56	7 (12%)
20	CLA	B	1217	-	49,53,73	1.38	7 (14%)	58,89,113	1.37	6 (10%)
20	CLA	3	603	-	59,63,73	1.28	9 (15%)	70,101,113	1.39	5 (7%)
20	CLA	F	301	-	49,53,73	1.38	8 (16%)	58,89,113	1.47	4 (6%)
23	BCR	M	4021	-	41,41,41	0.99	2 (4%)	56,56,56	1.31	9 (16%)
26	LMT	G	401	-	36,36,36	1.15	5 (13%)	47,47,47	1.04	1 (2%)
20	CLA	F	303	-	27,35,73	1.85	6 (22%)	32,60,113	1.62	5 (15%)
20	CLA	A	1115	-	58,62,73	1.26	8 (13%)	68,99,113	1.41	10 (14%)
20	CLA	G	202	-	50,54,73	1.36	7 (14%)	59,90,113	1.34	4 (6%)
20	CLA	3	605	-	27,35,73	1.85	7 (25%)	32,60,113	1.64	6 (18%)
20	CLA	B	1231	-	49,53,73	1.40	7 (14%)	58,89,113	1.46	6 (10%)
20	CLA	L	303	-	49,53,73	1.37	8 (16%)	58,89,113	1.61	8 (13%)
20	CLA	A	1801	-	54,58,73	1.32	9 (16%)	64,95,113	1.46	5 (7%)
20	CLA	J	102	-	49,53,73	1.39	8 (16%)	58,89,113	1.51	4 (6%)
20	CLA	B	1239	-	49,53,73	1.38	7 (14%)	58,89,113	1.58	9 (15%)
20	CLA	4	602	-	64,68,73	1.19	7 (10%)	76,107,113	1.37	8 (10%)
20	CLA	B	1206	-	51,55,73	1.34	9 (17%)	60,91,113	1.49	6 (10%)
20	CLA	3	602	-	64,68,73	1.22	8 (12%)	76,107,113	1.53	9 (11%)
20	CLA	A	1133	-	49,53,73	1.41	6 (12%)	58,89,113	1.18	4 (6%)
20	CLA	4	601	-	54,58,73	1.32	7 (12%)	64,95,113	1.43	5 (7%)
20	CLA	B	1238	-	69,73,73	1.17	8 (11%)	82,113,113	1.32	7 (8%)
20	CLA	K	201	-	59,63,73	1.27	8 (13%)	70,101,113	1.35	6 (8%)
20	CLA	3	604	-	54,58,73	1.33	8 (14%)	64,95,113	1.45	8 (12%)
28	CHL	2	602	-	60,64,74	2.03	21 (35%)	67,102,114	2.77	26 (38%)
20	CLA	B	1210	-	69,73,73	1.18	8 (11%)	82,113,113	1.50	9 (10%)
29	LUT	3	620	-	42,43,43	2.39	1 (2%)	51,60,60	1.58	5 (9%)
20	CLA	A	1103	-	69,73,73	1.19	9 (13%)	82,113,113	1.22	6 (7%)
20	CLA	A	1124	-	61,65,73	1.23	7 (11%)	72,103,113	1.27	5 (6%)
20	CLA	B	1219	-	49,53,73	1.40	9 (18%)	58,89,113	1.62	9 (15%)
23	BCR	B	4014	-	41,41,41	1.03	2 (4%)	56,56,56	1.41	9 (16%)
20	CLA	A	1104	-	69,73,73	1.18	9 (13%)	82,113,113	1.27	9 (10%)
20	CLA	4	609	-	59,63,73	1.26	8 (13%)	70,101,113	1.69	9 (12%)
20	CLA	4	603	-	59,63,73	1.25	8 (13%)	70,101,113	1.32	7 (10%)
20	CLA	B	1235	-	59,63,73	1.26	9 (15%)	70,101,113	1.32	5 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	CLA	A	1117	-	69,73,73	1.17	9 (13%)	82,113,113	1.48	13 (15%)
20	CLA	B	1204	-	65,69,73	1.19	8 (12%)	77,108,113	1.13	6 (7%)
20	CLA	A	1122	-	64,68,73	1.22	9 (14%)	76,107,113	1.42	5 (6%)
20	CLA	B	1229	-	59,63,73	1.28	8 (13%)	70,101,113	1.31	7 (10%)
20	CLA	2	609	-	59,63,73	1.26	7 (11%)	70,101,113	1.63	6 (8%)
22	SF4	A	3001	2,1	0,12,12	-	-	-	-	-
23	BCR	3	623	-	41,41,41	1.05	2 (4%)	56,56,56	1.25	7 (12%)
20	CLA	A	1113	-	49,53,73	1.38	8 (16%)	58,89,113	1.57	10 (17%)
20	CLA	A	1120	-	49,53,73	1.37	8 (16%)	58,89,113	1.45	4 (6%)
20	CLA	B	1021	-	69,73,73	1.16	10 (14%)	82,113,113	1.27	9 (10%)
26	LMT	B	5001	-	32,32,36	1.24	6 (18%)	43,43,47	0.96	0
26	LMT	G	402	-	32,32,36	1.23	5 (15%)	43,43,47	0.91	0
20	CLA	4	604	-	54,58,73	1.31	8 (14%)	64,95,113	1.39	7 (10%)
20	CLA	1	614	-	50,54,73	1.37	8 (16%)	59,90,113	1.50	7 (11%)
20	CLA	1	608	-	54,58,73	1.31	7 (12%)	64,95,113	1.44	7 (10%)
28	CHL	4	615	-	47,51,74	2.18	16 (34%)	50,86,114	3.03	22 (44%)
20	CLA	2	612	-	56,60,73	1.31	7 (12%)	65,97,113	1.42	6 (9%)
20	CLA	L	301	-	54,58,73	1.35	8 (14%)	64,95,113	1.63	9 (14%)
20	CLA	B	1215	-	64,68,73	1.22	9 (14%)	76,107,113	1.70	11 (14%)
23	BCR	A	4003	-	41,41,41	1.01	2 (4%)	56,56,56	1.35	8 (14%)
19	CL0	A	1011	-	69,73,73	1.18	10 (14%)	82,113,113	1.28	7 (8%)
20	CLA	A	1106	-	59,63,73	1.25	9 (15%)	70,101,113	1.60	6 (8%)
20	CLA	B	1216	-	59,63,73	1.27	10 (16%)	70,101,113	1.72	11 (15%)
20	CLA	2	614	-	54,58,73	1.31	8 (14%)	64,95,113	1.51	7 (10%)
20	CLA	B	1214	-	63,67,73	1.24	10 (15%)	74,105,113	1.51	11 (14%)
29	LUT	4	620	-	42,43,43	2.51	2 (4%)	51,60,60	2.04	12 (23%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	B	1224	-	-	11/35/111/115	-
20	CLA	B	1226	-	-	6/27/103/115	-
20	CLA	4	611	-	-	6/27/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	3	610	-	-	9/27/103/115	-
28	CHL	4	607	-	-	9/19/95/117	-
20	CLA	A	1102	-	-	8/15/91/115	-
23	BCR	B	4017	-	-	17/29/63/63	0/2/2/2
23	BCR	F	416	-	-	17/29/63/63	0/2/2/2
25	LMG	2	631	-	-	6/31/51/70	0/1/1/1
20	CLA	A	1107	-	-	9/15/91/115	-
23	BCR	B	4006	-	-	11/29/63/63	0/2/2/2
20	CLA	A	1105	-	-	0/21/97/115	-
20	CLA	B	1209	-	-	2/15/91/115	-
23	BCR	3	624	-	-	16/29/63/63	0/2/2/2
20	CLA	B	1220	-	-	4/15/91/115	-
29	LUT	4	623	-	1/1/12/27	12/29/67/67	0/2/2/2
20	CLA	2	610	-	-	10/33/109/115	-
20	CLA	4	614	-	-	7/17/93/115	-
23	BCR	B	4010	-	-	6/29/63/63	0/2/2/2
20	CLA	F	302	-	-	7/17/93/115	-
24	LHG	A	5001	-	-	20/53/53/53	-
20	CLA	A	1022	-	-	9/39/115/115	-
20	CLA	A	1130	-	-	6/33/109/115	-
20	CLA	B	1212	-	-	3/15/91/115	-
20	CLA	B	1237	-	-	11/39/115/115	-
20	CLA	3	611	-	-	4/10/86/115	-
20	CLA	A	1136	-	-	10/39/115/115	-
20	CLA	A	1116	-	-	8/26/102/115	-
23	BCR	A	4008	-	-	11/29/63/63	0/2/2/2
20	CLA	B	1227	-	-	1/15/91/115	-
20	CLA	1	611	-	-	4/17/93/115	-
29	LUT	4	621	-	-	4/29/67/67	0/2/2/2
20	CLA	B	1228	-	-	9/20/96/115	-
20	CLA	2	604	-	-	5/21/97/115	-
20	CLA	B	1205	-	-	9/39/115/115	-
20	CLA	B	1211	-	-	9/29/105/115	-
29	LUT	3	621	-	-	8/29/67/67	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	A	1121	-	-	9/23/99/115	-
26	LMT	4	631	-	-	4/21/61/61	0/2/2/2
20	CLA	B	1234	-	-	6/23/99/115	-
26	LMT	1	631	-	-	6/21/61/61	0/2/2/2
28	CHL	2	615	-	-	13/19/95/117	-
23	BCR	A	4002	-	-	9/29/63/63	0/2/2/2
29	LUT	1	620	-	-	5/29/67/67	0/2/2/2
20	CLA	A	5005	-	-	6/21/97/115	-
20	CLA	3	607	-	-	18/33/109/115	-
20	CLA	3	612	-	-	5/15/91/115	-
23	BCR	B	4005	-	-	8/29/63/63	0/2/2/2
23	BCR	1	623	-	-	5/18/35/63	0/1/1/2
20	CLA	B	1012	-	-	14/27/103/115	-
20	CLA	B	1230	-	-	8/15/91/115	-
20	CLA	3	606	-	-	11/17/93/115	-
20	CLA	A	1108	-	-	5/15/91/115	-
23	BCR	A	4007	-	-	7/29/63/63	0/2/2/2
20	CLA	A	1119	-	-	10/39/115/115	-
28	CHL	2	608	-	-	11/20/96/117	-
20	CLA	A	1135	-	-	8/23/99/115	-
20	CLA	1	602	-	-	2/33/109/115	-
28	CHL	2	607	-	-	10/19/95/117	-
20	CLA	B	1240	-	-	13/39/115/115	-
20	CLA	B	1202	-	-	10/39/115/115	-
20	CLA	1	603	-	-	14/27/103/115	-
25	LMG	J	302	-	-	6/21/41/70	0/1/1/1
20	CLA	B	1023	-	-	8/35/111/115	-
28	CHL	4	608	-	-	10/23/99/117	-
20	CLA	A	1101	-	-	10/21/97/115	-
20	CLA	A	1132	-	-	8/39/115/115	-
20	CLA	A	1134	-	-	6/15/91/115	-
20	CLA	A	1140	-	-	8/23/99/115	-
28	CHL	1	607	-	-	8/19/95/117	-
23	BCR	A	4001	-	-	15/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	BCR	I	120	-	-	14/29/63/63	0/2/2/2
24	LHG	A	5003	-	-	11/35/35/53	-
23	BCR	L	420	-	-	7/29/63/63	0/2/2/2
20	CLA	B	1213	-	-	6/27/103/115	-
23	BCR	G	311	-	-	7/29/63/63	0/2/2/2
29	LUT	2	621	-	-	2/29/67/67	0/2/2/2
20	CLA	I	121	-	-	12/39/115/115	-
28	CHL	2	601	-	-	22/41/117/117	-
23	BCR	L	419	-	-	4/29/63/63	0/2/2/2
20	CLA	B	1222	-	-	6/17/93/115	-
23	BCR	B	4009	-	-	3/29/63/63	0/2/2/2
20	CLA	A	1128	-	-	12/39/115/115	-
20	CLA	3	613	-	-	10/27/103/115	-
20	CLA	K	202	-	-	8/17/93/115	-
28	CHL	2	606	-	-	9/17/93/117	-
20	CLA	A	1013	-	-	3/29/105/115	-
29	LUT	2	623	-	1/1/12/27	9/29/67/67	0/2/2/2
20	CLA	G	218	-	-	10/27/103/115	-
20	CLA	A	1118	-	-	13/27/103/115	-
20	CLA	A	1110	-	-	7/27/103/115	-
20	CLA	B	1232	-	-	6/15/91/115	-
23	BCR	J	213	-	-	8/29/63/63	0/2/2/2
29	LUT	1	621	-	-	5/29/67/67	0/2/2/2
20	CLA	3	614	-	-	9/19/95/115	-
20	CLA	K	204	-	-	8/15/91/115	-
20	CLA	A	1127	-	-	18/39/115/115	-
23	BCR	K	301	-	-	14/29/63/63	0/2/2/2
20	CLA	A	1114	-	-	6/15/91/115	-
20	CLA	4	613	-	-	8/27/103/115	-
23	BCR	A	4011	-	-	18/29/63/63	0/2/2/2
20	CLA	A	1109	-	-	10/39/115/115	-
23	BCR	J	212	-	-	14/29/63/63	0/2/2/2
24	LHG	3	630	-	-	12/38/38/53	-
20	CLA	1	604	-	-	4/21/97/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	A	1112	-	-	6/15/91/115	-
20	CLA	2	603	-	-	7/17/93/115	-
23	BCR	B	4004	-	-	14/29/63/63	0/2/2/2
20	CLA	1	606	-	-	6/15/91/115	-
25	LMG	A	5002	-	-	13/29/49/70	0/1/1/1
20	CLA	A	1138	-	-	9/33/109/115	-
20	CLA	A	1137	-	-	5/15/91/115	-
20	CLA	1	613	-	-	9/27/103/115	-
21	PQN	A	2001	-	-	6/23/43/43	0/2/2/2
21	PQN	B	2002	-	-	8/23/43/43	0/2/2/2
29	LUT	2	620	-	-	6/29/67/67	0/2/2/2
20	CLA	1	610	-	-	6/27/103/115	-
20	CLA	1	615	-	-	8/17/93/115	-
24	LHG	B	5101	-	-	9/39/39/53	-
22	SF4	C	1003	7	-	-	0/6/5/5
20	CLA	A	1111	-	-	15/39/115/115	-
20	CLA	4	612	-	-	10/17/93/115	-
20	CLA	B	1223	-	-	6/39/115/115	-
23	BCR	O	301	-	-	3/5/22/63	0/1/1/2
20	CLA	B	1236	-	-	6/18/94/115	-
20	CLA	1	609	-	-	6/33/109/115	-
20	CLA	3	617	-	-	6/17/93/115	-
20	CLA	3	609	-	-	10/33/109/115	-
22	SF4	C	1002	7	-	-	0/6/5/5
27	DGD	B	5002	-	-	18/50/90/95	0/2/2/2
20	CLA	L	302	-	-	12/33/109/115	-
24	LHG	2	630	-	-	10/36/36/53	-
20	CLA	B	1225	-	-	15/39/115/115	-
20	CLA	B	1221	-	-	1/26/102/115	-
28	CHL	4	606	-	-	11/19/95/117	-
24	LHG	4	630	-	-	15/42/42/53	-
20	CLA	A	1126	-	-	11/33/109/115	-
20	CLA	B	1201	-	-	10/21/97/115	-
24	LHG	1	630	-	-	14/41/41/53	-
20	CLA	A	1131	-	-	6/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	A	8895	-	-	9/39/115/115	-
28	CHL	2	611	-	-	8/29/105/117	-
28	CHL	3	608	-	-	5/19/95/117	-
25	LMG	J	301	-	-	15/44/64/70	0/1/1/1
20	CLA	A	1125	-	-	13/33/109/115	-
20	CLA	4	610	-	-	7/27/103/115	-
20	CLA	G	201	-	-	6/21/97/115	-
20	CLA	2	613	-	-	13/39/115/115	-
26	LMT	A	5004	-	-	7/19/59/61	0/2/2/2
23	BCR	I	118	-	-	11/29/63/63	0/2/2/2
20	CLA	H	200	-	-	5/15/91/115	-
20	CLA	1	612	-	-	8/17/93/115	-
20	CLA	B	1203	-	-	13/39/115/115	-
28	CHL	1	601	-	-	10/29/105/117	-
20	CLA	A	1139	-	-	6/21/97/115	-
20	CLA	B	1208	-	-	3/15/91/115	-
20	CLA	B	1217	-	-	5/15/91/115	-
20	CLA	3	603	-	-	12/27/103/115	-
20	CLA	F	301	-	-	3/15/91/115	-
23	BCR	M	4021	-	-	5/29/63/63	0/2/2/2
26	LMT	G	401	-	-	5/21/61/61	0/2/2/2
20	CLA	A	1115	-	-	6/26/102/115	-
20	CLA	G	202	-	-	8/17/93/115	-
20	CLA	B	1231	-	-	7/15/91/115	-
20	CLA	L	303	-	-	7/15/91/115	-
20	CLA	A	1801	-	-	7/21/97/115	-
20	CLA	J	102	-	-	9/15/91/115	-
20	CLA	B	1239	-	-	6/15/91/115	-
20	CLA	4	602	-	-	3/33/109/115	-
20	CLA	B	1206	-	-	7/18/94/115	-
20	CLA	3	602	-	-	8/33/109/115	-
20	CLA	A	1133	-	-	7/15/91/115	-
20	CLA	4	601	-	-	9/21/97/115	-
20	CLA	B	1238	-	-	16/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	K	201	-	-	7/27/103/115	-
20	CLA	3	604	-	-	6/21/97/115	-
28	CHL	2	602	-	-	15/29/105/117	-
20	CLA	B	1210	-	-	22/39/115/115	-
29	LUT	3	620	-	-	2/29/67/67	0/2/2/2
20	CLA	A	1103	-	-	17/39/115/115	-
20	CLA	A	1124	-	-	11/30/106/115	-
20	CLA	B	1219	-	-	3/15/91/115	-
23	BCR	B	4014	-	-	19/29/63/63	0/2/2/2
20	CLA	A	1104	-	-	19/39/115/115	-
20	CLA	4	609	-	-	10/27/103/115	-
20	CLA	4	603	-	-	12/27/103/115	-
20	CLA	B	1235	-	-	9/27/103/115	-
20	CLA	A	1117	-	-	10/39/115/115	-
20	CLA	B	1204	-	-	8/35/111/115	-
20	CLA	A	1122	-	-	14/33/109/115	-
20	CLA	B	1229	-	-	9/27/103/115	-
20	CLA	2	609	-	-	3/27/103/115	-
23	BCR	3	623	-	-	14/29/63/63	0/2/2/2
22	SF4	A	3001	2,1	-	-	0/6/5/5
20	CLA	A	1113	-	-	4/15/91/115	-
20	CLA	A	1120	-	-	3/15/91/115	-
20	CLA	B	1021	-	-	16/39/115/115	-
26	LMT	B	5001	-	-	4/17/57/61	0/2/2/2
26	LMT	G	402	-	-	6/17/57/61	0/2/2/2
20	CLA	4	604	-	-	6/21/97/115	-
20	CLA	1	614	-	-	8/17/93/115	-
20	CLA	1	608	-	-	3/21/97/115	-
28	CHL	4	615	-	-	4/14/90/117	-
20	CLA	2	612	-	-	7/24/100/115	-
20	CLA	L	301	-	-	7/21/97/115	-
20	CLA	B	1215	-	-	11/33/109/115	-
23	BCR	A	4003	-	-	12/29/63/63	0/2/2/2
19	CL0	A	1011	-	-	7/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	A	1106	-	-	8/27/103/115	-
20	CLA	B	1216	-	-	9/27/103/115	-
20	CLA	2	614	-	-	5/21/97/115	-
20	CLA	B	1214	-	-	8/32/108/115	-
29	LUT	4	620	-	-	9/29/67/67	0/2/2/2

All (1536) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	1	620	LUT	C24-C25	16.76	1.53	1.33
29	1	621	LUT	C24-C25	16.27	1.52	1.33
29	2	623	LUT	C24-C25	15.79	1.51	1.33
29	4	620	LUT	C24-C25	15.47	1.51	1.33
29	2	620	LUT	C24-C25	15.22	1.51	1.33
29	3	621	LUT	C24-C25	15.10	1.51	1.33
29	4	621	LUT	C24-C25	14.92	1.50	1.33
29	4	623	LUT	C24-C25	14.84	1.50	1.33
29	3	620	LUT	C24-C25	14.81	1.50	1.33
29	2	621	LUT	C24-C25	14.74	1.50	1.33
28	4	615	CHL	O2D-CGD	5.15	1.45	1.33
28	4	606	CHL	O2D-CGD	5.14	1.45	1.33
28	2	606	CHL	O2D-CGD	5.13	1.45	1.33
28	2	607	CHL	O2D-CGD	5.12	1.45	1.33
28	2	615	CHL	O2D-CGD	5.11	1.45	1.33
28	4	607	CHL	O2D-CGD	5.10	1.45	1.33
28	1	607	CHL	O2D-CGD	5.09	1.45	1.33
28	3	608	CHL	O2D-CGD	5.07	1.45	1.33
28	2	602	CHL	O2D-CGD	5.06	1.45	1.33
28	2	611	CHL	O2D-CGD	5.04	1.45	1.33
28	2	608	CHL	O2D-CGD	5.03	1.45	1.33
28	4	608	CHL	O2D-CGD	5.02	1.45	1.33
28	2	601	CHL	O2D-CGD	4.98	1.45	1.33
28	1	601	CHL	O2D-CGD	4.86	1.45	1.33
28	2	608	CHL	C3D-C4D	-4.73	1.33	1.44
28	3	608	CHL	C3D-C4D	-4.63	1.33	1.44
28	2	608	CHL	CHC-C1C	4.58	1.47	1.38
28	4	608	CHL	C3D-C4D	-4.56	1.33	1.44
28	1	607	CHL	C3D-C4D	-4.55	1.33	1.44
28	2	606	CHL	O2A-CGA	4.55	1.45	1.30
28	4	608	CHL	CHC-C1C	4.54	1.47	1.38
28	2	611	CHL	C3D-C4D	-4.52	1.34	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	2	615	CHL	C3D-C4D	-4.51	1.34	1.44
28	4	607	CHL	C3D-C4D	-4.50	1.34	1.44
28	2	602	CHL	O2A-CGA	4.49	1.46	1.33
28	1	601	CHL	C3D-C4D	-4.48	1.34	1.44
28	2	602	CHL	CHC-C1C	4.48	1.47	1.38
28	2	607	CHL	C3D-C4D	-4.47	1.34	1.44
28	2	606	CHL	CHC-C1C	4.47	1.47	1.38
28	4	606	CHL	CHC-C1C	4.45	1.47	1.38
28	2	601	CHL	C3D-C4D	-4.45	1.34	1.44
28	4	615	CHL	C3D-C4D	-4.45	1.34	1.44
20	O	202	CLA	C2B-C1B	4.44	1.49	1.40
28	4	606	CHL	C3D-C4D	-4.44	1.34	1.44
28	2	606	CHL	C3D-C4D	-4.44	1.34	1.44
20	O	203	CLA	C2B-C1B	4.42	1.49	1.40
20	K	203	CLA	C2B-C1B	4.40	1.49	1.40
20	3	605	CLA	C2B-C1B	4.40	1.49	1.40
28	2	611	CHL	O2A-CGA	4.39	1.46	1.33
20	F	303	CLA	C2B-C1B	4.39	1.49	1.40
20	O	201	CLA	C2B-C1B	4.39	1.49	1.40
20	K	203	CLA	C3B-C4B	4.37	1.49	1.40
28	2	602	CHL	C3D-C4D	-4.37	1.34	1.44
20	3	605	CLA	C3B-C4B	4.36	1.49	1.40
20	F	303	CLA	C3B-C4B	4.36	1.49	1.40
20	O	202	CLA	C3B-C4B	4.36	1.49	1.40
20	O	203	CLA	C3B-C4B	4.34	1.49	1.40
28	4	615	CHL	CHC-C1C	4.33	1.47	1.38
20	O	201	CLA	C3B-C4B	4.33	1.49	1.40
28	4	607	CHL	CHC-C1C	4.32	1.47	1.38
28	2	607	CHL	CHC-C1C	4.31	1.47	1.38
28	2	611	CHL	CHC-C1C	4.30	1.47	1.38
28	2	608	CHL	O2A-CGA	4.30	1.45	1.33
28	1	607	CHL	CHC-C1C	4.29	1.47	1.38
28	2	601	CHL	CHC-C1C	4.27	1.47	1.38
28	2	601	CHL	O2A-CGA	4.26	1.45	1.33
28	4	608	CHL	O2A-CGA	4.26	1.45	1.33
28	2	615	CHL	CHC-C1C	4.24	1.47	1.38
28	2	607	CHL	CHD-C1D	4.23	1.46	1.38
28	1	601	CHL	O2A-CGA	4.23	1.45	1.33
28	4	607	CHL	CHD-C1D	4.22	1.46	1.38
28	2	615	CHL	O2A-CGA	4.16	1.45	1.33
28	4	607	CHL	O2A-CGA	4.15	1.45	1.33
28	1	607	CHL	CHD-C1D	4.15	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	1	607	CHL	C2C-C3C	4.14	1.46	1.37
28	4	606	CHL	O2A-CGA	4.14	1.45	1.33
28	2	607	CHL	O2A-CGA	4.13	1.45	1.33
28	1	607	CHL	O2A-CGA	4.13	1.45	1.33
28	4	608	CHL	CHD-C1D	4.12	1.46	1.38
28	3	608	CHL	CHC-C1C	4.12	1.46	1.38
28	3	608	CHL	O2A-CGA	4.12	1.45	1.33
28	4	606	CHL	CHD-C1D	4.11	1.46	1.38
28	4	615	CHL	CHD-C1D	4.10	1.46	1.38
28	1	601	CHL	CHC-C1C	4.09	1.46	1.38
28	2	602	CHL	CHD-C1D	4.08	1.46	1.38
28	2	615	CHL	CHD-C1D	4.07	1.46	1.38
28	2	606	CHL	CHD-C1D	4.05	1.46	1.38
28	4	607	CHL	C2C-C3C	4.00	1.46	1.37
28	2	601	CHL	C2C-C3C	4.00	1.46	1.37
28	2	611	CHL	C2C-C3C	3.99	1.46	1.37
28	2	615	CHL	C2C-C3C	3.98	1.46	1.37
28	2	611	CHL	CHD-C1D	3.97	1.46	1.38
28	2	602	CHL	C2C-C3C	3.95	1.46	1.37
28	4	615	CHL	C2C-C3C	3.94	1.46	1.37
28	2	607	CHL	C2C-C3C	3.92	1.46	1.37
28	2	601	CHL	CHD-C1D	3.91	1.46	1.38
28	3	608	CHL	CHD-C1D	3.89	1.46	1.38
28	4	608	CHL	C2C-C3C	3.88	1.46	1.37
28	2	607	CHL	CHD-C4C	3.85	1.48	1.39
28	1	607	CHL	CHD-C4C	3.83	1.47	1.39
28	4	607	CHL	CHD-C4C	3.83	1.47	1.39
28	3	608	CHL	C2C-C3C	3.80	1.45	1.37
28	2	615	CHL	CHD-C4C	3.79	1.47	1.39
28	2	606	CHL	CHD-C4C	3.78	1.47	1.39
28	2	607	CHL	OBD-CAD	3.78	1.29	1.22
28	2	608	CHL	C2C-C3C	3.78	1.45	1.37
28	2	615	CHL	OBD-CAD	3.77	1.29	1.22
28	1	607	CHL	OBD-CAD	3.76	1.29	1.22
20	G	218	CLA	C1D-ND	3.75	1.42	1.37
28	4	615	CHL	CHD-C4C	3.75	1.47	1.39
28	4	606	CHL	CHD-C4C	3.74	1.47	1.39
28	4	606	CHL	C2C-C3C	3.74	1.45	1.37
28	2	602	CHL	CHD-C4C	3.74	1.47	1.39
28	4	607	CHL	OBD-CAD	3.74	1.28	1.22
28	2	606	CHL	C2C-C3C	3.72	1.45	1.37
28	2	601	CHL	CHD-C4C	3.72	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	4	608	CHL	CHD-C4C	3.71	1.47	1.39
28	2	606	CHL	OBD-CAD	3.70	1.28	1.22
20	2	613	CLA	C1D-ND	3.69	1.42	1.37
28	4	615	CHL	OBD-CAD	3.69	1.28	1.22
20	A	1130	CLA	C1D-ND	3.68	1.42	1.37
28	2	608	CHL	CHD-C1D	3.67	1.45	1.38
28	1	601	CHL	C2C-C3C	3.66	1.45	1.37
28	3	608	CHL	CHD-C4C	3.65	1.47	1.39
28	2	601	CHL	OBD-CAD	3.65	1.28	1.22
20	B	1217	CLA	C1D-ND	3.63	1.42	1.37
28	1	601	CHL	CHD-C1D	3.63	1.45	1.38
28	2	611	CHL	CHD-C4C	3.62	1.47	1.39
20	B	1240	CLA	C1D-ND	3.61	1.42	1.37
28	4	606	CHL	OBD-CAD	3.61	1.28	1.22
28	4	608	CHL	OBD-CAD	3.60	1.28	1.22
20	A	1133	CLA	C1D-ND	3.60	1.42	1.37
20	A	1107	CLA	C1D-ND	3.59	1.42	1.37
20	A	1118	CLA	C4B-NB	3.59	1.42	1.37
20	L	301	CLA	C1D-ND	3.58	1.42	1.37
20	F	303	CLA	C2D-C1D	3.56	1.48	1.42
20	1	606	CLA	C1D-ND	3.56	1.42	1.37
28	2	611	CHL	OBD-CAD	3.56	1.28	1.22
20	A	1101	CLA	C1D-ND	3.55	1.42	1.37
20	3	611	CLA	C1D-ND	3.54	1.42	1.37
29	4	621	LUT	C22-C21	3.54	1.59	1.54
20	B	1237	CLA	C1D-ND	3.54	1.42	1.37
20	4	601	CLA	C1D-ND	3.53	1.42	1.37
20	4	612	CLA	C1D-ND	3.53	1.42	1.37
28	2	602	CHL	OBD-CAD	3.53	1.28	1.22
20	B	1232	CLA	C1D-ND	3.52	1.42	1.37
20	3	614	CLA	C1D-ND	3.52	1.42	1.37
28	1	601	CHL	OBD-CAD	3.51	1.28	1.22
20	A	1113	CLA	C1D-ND	3.51	1.42	1.37
28	4	606	CHL	CHC-C4B	3.50	1.47	1.39
20	1	608	CLA	C1D-ND	3.50	1.42	1.37
20	3	605	CLA	C2D-C1D	3.50	1.48	1.42
20	1	610	CLA	C1D-ND	3.50	1.42	1.37
20	K	203	CLA	C2D-C1D	3.50	1.48	1.42
20	G	202	CLA	C1D-ND	3.50	1.42	1.37
28	1	601	CHL	CHD-C4C	3.49	1.47	1.39
28	2	608	CHL	CHC-C4B	3.49	1.47	1.39
20	O	202	CLA	C2D-C1D	3.49	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	A	1111	CLA	C1D-ND	3.48	1.42	1.37
20	O	203	CLA	C2D-C1D	3.48	1.48	1.42
20	H	200	CLA	C1D-ND	3.47	1.42	1.37
20	3	607	CLA	C1D-ND	3.47	1.42	1.37
20	3	612	CLA	C1D-ND	3.47	1.42	1.37
20	O	201	CLA	C2D-C1D	3.46	1.48	1.42
20	B	1209	CLA	C1D-ND	3.46	1.42	1.37
20	4	613	CLA	C1D-ND	3.46	1.42	1.37
20	L	302	CLA	C1D-ND	3.46	1.42	1.37
20	1	609	CLA	C1D-ND	3.46	1.42	1.37
20	L	303	CLA	C1D-ND	3.46	1.42	1.37
20	3	609	CLA	C1D-ND	3.46	1.42	1.37
20	3	617	CLA	C1D-ND	3.46	1.42	1.37
20	J	102	CLA	C1D-ND	3.45	1.42	1.37
20	B	1012	CLA	C1D-ND	3.45	1.42	1.37
28	2	606	CHL	CHC-C4B	3.45	1.47	1.39
20	3	603	CLA	C1D-ND	3.44	1.42	1.37
20	4	614	CLA	C1D-ND	3.44	1.42	1.37
28	2	608	CHL	CHD-C4C	3.43	1.47	1.39
28	1	607	CHL	CHC-C4B	3.43	1.47	1.39
20	A	1128	CLA	C4B-NB	3.42	1.42	1.37
20	B	1237	CLA	C4B-NB	3.42	1.42	1.37
20	1	615	CLA	C1D-ND	3.42	1.42	1.37
20	1	604	CLA	C1D-ND	3.42	1.42	1.37
20	1	611	CLA	C1D-ND	3.42	1.42	1.37
28	2	601	CHL	CHC-C4B	3.41	1.47	1.39
20	3	613	CLA	C1D-ND	3.41	1.42	1.37
20	A	1104	CLA	C1D-ND	3.41	1.42	1.37
28	1	601	CHL	CHC-C4B	3.41	1.47	1.39
20	K	201	CLA	C1D-ND	3.41	1.42	1.37
28	3	608	CHL	CHC-C4B	3.41	1.47	1.39
20	B	1239	CLA	C1D-ND	3.40	1.42	1.37
20	1	614	CLA	C1D-ND	3.39	1.42	1.37
20	2	610	CLA	C1D-ND	3.39	1.42	1.37
28	2	611	CHL	CHC-C4B	3.39	1.47	1.39
20	B	1205	CLA	C1D-ND	3.39	1.42	1.37
20	3	606	CLA	C1D-ND	3.39	1.42	1.37
20	A	1122	CLA	C1D-ND	3.39	1.42	1.37
20	A	1133	CLA	C4B-NB	3.39	1.42	1.37
20	B	1231	CLA	C1D-ND	3.38	1.42	1.37
20	B	1202	CLA	C1D-ND	3.38	1.42	1.37
20	A	1103	CLA	C1D-ND	3.38	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B	1208	CLA	C1D-ND	3.37	1.42	1.37
20	B	1212	CLA	C1D-ND	3.37	1.42	1.37
20	4	604	CLA	C1D-ND	3.36	1.42	1.37
20	B	1214	CLA	C1D-ND	3.36	1.42	1.37
20	A	1134	CLA	C1D-ND	3.36	1.42	1.37
20	G	201	CLA	C1D-ND	3.35	1.42	1.37
20	2	612	CLA	C1D-ND	3.35	1.42	1.37
20	A	1137	CLA	C4B-NB	3.35	1.42	1.37
20	A	1120	CLA	C1D-ND	3.35	1.42	1.37
28	4	608	CHL	CHC-C4B	3.35	1.46	1.39
20	3	610	CLA	C1D-ND	3.34	1.42	1.37
20	2	609	CLA	C1D-ND	3.33	1.42	1.37
23	B	4017	BCR	C30-C25	-3.33	1.49	1.53
28	2	607	CHL	CHC-C4B	3.33	1.46	1.39
20	B	1219	CLA	C1D-ND	3.33	1.42	1.37
20	K	204	CLA	C1D-ND	3.33	1.42	1.37
20	B	1209	CLA	C4B-NB	3.33	1.42	1.37
20	K	202	CLA	C1D-ND	3.33	1.42	1.37
20	A	1131	CLA	C1D-ND	3.32	1.42	1.37
20	A	1106	CLA	C1D-ND	3.32	1.42	1.37
20	1	603	CLA	C1D-ND	3.32	1.42	1.37
20	2	603	CLA	C1D-ND	3.32	1.42	1.37
28	4	615	CHL	CHC-C4B	3.31	1.46	1.39
20	B	1234	CLA	C1D-ND	3.31	1.42	1.37
28	2	615	CHL	CHC-C4B	3.31	1.46	1.39
20	2	604	CLA	C1D-ND	3.30	1.42	1.37
28	4	607	CHL	CHC-C4B	3.30	1.46	1.39
20	B	1220	CLA	C1D-ND	3.29	1.42	1.37
20	F	301	CLA	C1D-ND	3.29	1.42	1.37
20	B	1229	CLA	C4B-NB	3.29	1.42	1.37
20	B	1211	CLA	C1D-ND	3.29	1.42	1.37
20	A	1110	CLA	C1D-ND	3.29	1.42	1.37
20	3	604	CLA	C1D-ND	3.29	1.42	1.37
20	B	1206	CLA	C1D-ND	3.28	1.42	1.37
28	2	602	CHL	CHC-C4B	3.28	1.46	1.39
20	A	1118	CLA	C1D-ND	3.28	1.42	1.37
20	A	5005	CLA	C1D-ND	3.27	1.42	1.37
20	A	1140	CLA	C4B-NB	3.27	1.42	1.37
20	I	121	CLA	C1D-ND	3.27	1.42	1.37
20	A	1114	CLA	C1D-ND	3.27	1.42	1.37
20	A	1137	CLA	C1D-ND	3.27	1.42	1.37
20	A	1135	CLA	C1D-ND	3.26	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B	1229	CLA	C1D-ND	3.26	1.42	1.37
20	2	614	CLA	C1D-ND	3.26	1.42	1.37
20	A	1115	CLA	C1D-ND	3.25	1.42	1.37
20	A	1121	CLA	C1D-ND	3.24	1.42	1.37
20	F	302	CLA	C1D-ND	3.24	1.42	1.37
20	B	1201	CLA	C1D-ND	3.23	1.42	1.37
20	1	612	CLA	C1D-ND	3.23	1.42	1.37
20	A	1117	CLA	C1D-ND	3.23	1.42	1.37
20	B	1228	CLA	C1D-ND	3.23	1.42	1.37
20	B	1238	CLA	C1D-ND	3.22	1.42	1.37
20	1	615	CLA	C4B-NB	3.22	1.42	1.37
20	B	1236	CLA	C1D-ND	3.21	1.42	1.37
20	B	1203	CLA	C1D-ND	3.21	1.42	1.37
20	B	1204	CLA	C1D-ND	3.20	1.42	1.37
20	1	613	CLA	C1D-ND	3.20	1.42	1.37
20	A	1124	CLA	C1D-ND	3.20	1.42	1.37
20	A	1112	CLA	C1D-ND	3.20	1.42	1.37
20	4	603	CLA	C1D-ND	3.20	1.42	1.37
20	A	1801	CLA	C1D-ND	3.20	1.42	1.37
28	3	608	CHL	OBD-CAD	3.19	1.28	1.22
20	A	1108	CLA	C1D-ND	3.18	1.42	1.37
20	A	1102	CLA	C1D-ND	3.18	1.42	1.37
20	4	612	CLA	C4B-NB	3.17	1.42	1.37
20	3	611	CLA	C4B-NB	3.17	1.42	1.37
20	B	1216	CLA	C1D-ND	3.17	1.42	1.37
20	A	1119	CLA	C1D-ND	3.17	1.42	1.37
20	B	1222	CLA	C1D-ND	3.17	1.42	1.37
20	3	603	CLA	C4B-NB	3.16	1.42	1.37
20	3	602	CLA	C1D-ND	3.16	1.42	1.37
20	4	611	CLA	C1D-ND	3.16	1.42	1.37
20	B	1232	CLA	C4B-NB	3.16	1.42	1.37
20	B	1235	CLA	C1D-ND	3.16	1.42	1.37
20	A	8895	CLA	C1D-ND	3.15	1.42	1.37
20	A	1136	CLA	C1D-ND	3.15	1.42	1.37
20	A	1128	CLA	C1D-ND	3.15	1.42	1.37
29	1	621	LUT	C23-C24	3.13	1.54	1.50
20	A	1140	CLA	C1D-ND	3.13	1.42	1.37
23	I	120	BCR	C1-C6	-3.13	1.49	1.53
20	4	610	CLA	C1D-ND	3.13	1.42	1.37
20	A	1128	CLA	CMB-C2B	-3.12	1.44	1.50
20	B	1230	CLA	C1D-ND	3.12	1.42	1.37
20	1	602	CLA	C1D-ND	3.12	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	A	1022	CLA	C1D-ND	3.12	1.42	1.37
23	A	4007	BCR	C1-C6	-3.12	1.49	1.53
20	B	1215	CLA	C1D-ND	3.12	1.42	1.37
20	B	1023	CLA	CMC-C2C	-3.11	1.44	1.50
23	J	212	BCR	C1-C6	-3.11	1.49	1.53
20	A	1103	CLA	C4B-NB	3.11	1.41	1.37
29	1	620	LUT	C23-C24	3.11	1.54	1.50
20	1	611	CLA	C4B-NB	3.10	1.41	1.37
20	G	201	CLA	C4B-NB	3.10	1.41	1.37
20	A	1138	CLA	C1D-ND	3.10	1.41	1.37
20	4	609	CLA	C1D-ND	3.10	1.41	1.37
20	A	1105	CLA	C1D-ND	3.10	1.41	1.37
28	2	611	CHL	CHB-C1B	3.09	1.46	1.39
20	B	1213	CLA	C1D-ND	3.09	1.41	1.37
20	A	1116	CLA	C1D-ND	3.09	1.41	1.37
20	B	1210	CLA	C1D-ND	3.08	1.41	1.37
20	B	1224	CLA	C1D-ND	3.07	1.41	1.37
20	4	602	CLA	C1D-ND	3.07	1.41	1.37
20	K	204	CLA	C4B-NB	3.07	1.41	1.37
28	1	607	CHL	CHB-C1B	3.07	1.46	1.39
20	3	613	CLA	C4B-NB	3.06	1.41	1.37
28	2	608	CHL	OBD-CAD	3.06	1.27	1.22
20	B	1225	CLA	C1D-ND	3.06	1.41	1.37
20	3	612	CLA	C4B-NB	3.05	1.41	1.37
28	2	602	CHL	C3D-C2D	3.05	1.47	1.39
20	A	1135	CLA	C4B-NB	3.05	1.41	1.37
28	3	608	CHL	CHB-C1B	3.04	1.46	1.39
23	J	212	BCR	C30-C25	-3.04	1.49	1.53
28	4	615	CHL	CHB-C1B	3.03	1.46	1.39
23	3	623	BCR	C1-C6	-3.02	1.49	1.53
28	2	607	CHL	CHB-C1B	3.02	1.46	1.39
20	A	1139	CLA	C1D-ND	3.02	1.41	1.37
20	B	1214	CLA	C4B-NB	3.02	1.41	1.37
20	B	1223	CLA	C4B-NB	3.02	1.41	1.37
20	1	609	CLA	C4B-NB	3.01	1.41	1.37
20	A	1107	CLA	C4B-NB	3.01	1.41	1.37
20	B	1231	CLA	C4B-NB	3.01	1.41	1.37
20	3	604	CLA	C4B-NB	3.01	1.41	1.37
20	1	612	CLA	C4B-NB	3.01	1.41	1.37
20	L	302	CLA	C4B-NB	3.01	1.41	1.37
20	B	1217	CLA	C4B-NB	3.00	1.41	1.37
20	J	102	CLA	C4B-NB	3.00	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	2	615	CHL	CHB-C1B	3.00	1.46	1.39
29	4	621	LUT	C22-C23	3.00	1.56	1.52
28	2	608	CHL	CHB-C1B	3.00	1.46	1.39
20	3	614	CLA	C4B-NB	3.00	1.41	1.37
20	A	1139	CLA	C4B-NB	3.00	1.41	1.37
20	B	1226	CLA	CMB-C2B	-3.00	1.44	1.50
20	3	606	CLA	C4B-NB	3.00	1.41	1.37
20	A	1126	CLA	C1D-ND	2.99	1.41	1.37
20	4	614	CLA	C4B-NB	2.99	1.41	1.37
20	2	612	CLA	C4B-NB	2.99	1.41	1.37
20	F	302	CLA	C4B-NB	2.99	1.41	1.37
20	A	1109	CLA	C1D-ND	2.98	1.41	1.37
20	4	601	CLA	C4B-NB	2.98	1.41	1.37
20	G	218	CLA	C4B-NB	2.98	1.41	1.37
28	4	606	CHL	CHB-C1B	2.98	1.46	1.39
20	A	1136	CLA	C4B-NB	2.97	1.41	1.37
23	K	301	BCR	C1-C6	-2.97	1.50	1.53
20	3	610	CLA	C4B-NB	2.96	1.41	1.37
28	2	601	CHL	CHB-C1B	2.96	1.46	1.39
20	2	613	CLA	C4B-NB	2.96	1.41	1.37
20	2	604	CLA	C4B-NB	2.96	1.41	1.37
20	4	613	CLA	C4B-NB	2.96	1.41	1.37
28	2	606	CHL	CHB-C1B	2.96	1.46	1.39
20	K	202	CLA	C4B-NB	2.96	1.41	1.37
20	A	1102	CLA	C4B-NB	2.95	1.41	1.37
20	1	613	CLA	C4B-NB	2.95	1.41	1.37
20	4	611	CLA	C4B-NB	2.95	1.41	1.37
20	A	1127	CLA	C1D-ND	2.95	1.41	1.37
20	3	607	CLA	C4B-NB	2.95	1.41	1.37
20	L	301	CLA	C4B-NB	2.94	1.41	1.37
20	A	1022	CLA	C4B-NB	2.94	1.41	1.37
20	B	1226	CLA	CMD-C2D	-2.94	1.44	1.50
20	1	610	CLA	C4B-NB	2.93	1.41	1.37
20	A	1132	CLA	C1D-ND	2.93	1.41	1.37
20	H	200	CLA	C4B-NB	2.93	1.41	1.37
20	A	1137	CLA	C3B-C4B	2.92	1.51	1.42
20	1	614	CLA	C4B-NB	2.92	1.41	1.37
28	1	601	CHL	CHB-C1B	2.91	1.46	1.39
20	A	1116	CLA	C4B-NB	2.91	1.41	1.37
20	B	1221	CLA	C1D-ND	2.91	1.41	1.37
23	B	4005	BCR	C1-C6	-2.91	1.50	1.53
23	F	416	BCR	C1-C6	-2.91	1.50	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B	1228	CLA	C4B-NB	2.91	1.41	1.37
28	2	615	CHL	C3D-C2D	2.90	1.46	1.39
20	B	1240	CLA	C4B-NB	2.90	1.41	1.37
20	L	303	CLA	C1B-C2B	2.90	1.49	1.43
20	A	1801	CLA	C4B-NB	2.89	1.41	1.37
20	B	1236	CLA	C4B-NB	2.89	1.41	1.37
23	B	4006	BCR	C1-C6	-2.89	1.50	1.53
20	B	1223	CLA	C1D-ND	2.89	1.41	1.37
28	4	607	CHL	C3D-C2D	2.89	1.46	1.39
20	A	1125	CLA	C1D-ND	2.89	1.41	1.37
20	A	1118	CLA	C3B-C4B	2.89	1.51	1.42
20	B	1227	CLA	C1D-ND	2.89	1.41	1.37
20	3	617	CLA	C4B-NB	2.89	1.41	1.37
20	A	8895	CLA	C4B-NB	2.88	1.41	1.37
23	B	4004	BCR	C1-C6	-2.88	1.50	1.53
23	O	301	BCR	C30-C25	-2.88	1.50	1.53
28	4	615	CHL	C3D-C2D	2.88	1.46	1.39
20	B	1206	CLA	C4B-NB	2.88	1.41	1.37
20	2	614	CLA	C4B-NB	2.87	1.41	1.37
23	A	4002	BCR	C30-C25	-2.87	1.50	1.53
28	4	607	CHL	CHB-C1B	2.87	1.45	1.39
20	B	1230	CLA	C1B-C2B	2.87	1.49	1.43
20	1	606	CLA	C1B-C2B	2.87	1.49	1.43
23	A	4001	BCR	C1-C6	-2.87	1.50	1.53
20	2	609	CLA	C4B-NB	2.86	1.41	1.37
23	1	623	BCR	C30-C25	-2.86	1.50	1.53
20	A	1112	CLA	C4B-NB	2.85	1.41	1.37
20	A	1110	CLA	C4B-NB	2.85	1.41	1.37
20	B	1201	CLA	C4B-NB	2.85	1.41	1.37
20	A	1113	CLA	C4B-NB	2.85	1.41	1.37
20	B	1226	CLA	C1D-ND	2.85	1.41	1.37
20	B	1012	CLA	C4B-NB	2.84	1.41	1.37
20	G	202	CLA	C4B-NB	2.84	1.41	1.37
23	A	4003	BCR	C1-C6	-2.84	1.50	1.53
20	A	1125	CLA	C4B-NB	2.84	1.41	1.37
20	B	1221	CLA	C4B-NB	2.84	1.41	1.37
20	A	1101	CLA	C4B-NB	2.84	1.41	1.37
23	B	4006	BCR	C30-C25	-2.83	1.50	1.53
20	B	1021	CLA	C1D-ND	2.83	1.41	1.37
20	1	604	CLA	C4B-NB	2.83	1.41	1.37
28	2	606	CHL	C3D-C2D	2.83	1.46	1.39
20	A	1122	CLA	C4B-NB	2.82	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	4	630	LHG	O7-C7	2.82	1.42	1.34
20	B	1222	CLA	C1B-C2B	2.82	1.49	1.43
20	1	602	CLA	C1B-C2B	2.82	1.49	1.43
20	2	612	CLA	C1B-C2B	2.82	1.49	1.43
28	1	607	CHL	C1D-C2D	2.81	1.50	1.45
23	3	623	BCR	C30-C25	-2.81	1.50	1.53
28	4	606	CHL	C3D-C2D	2.81	1.46	1.39
20	A	1130	CLA	C4B-NB	2.81	1.41	1.37
23	I	118	BCR	C30-C25	-2.81	1.50	1.53
20	1	610	CLA	C1B-C2B	2.81	1.49	1.43
28	2	611	CHL	C3D-C2D	2.81	1.46	1.39
20	4	611	CLA	C1B-C2B	2.80	1.49	1.43
20	B	1230	CLA	C4B-NB	2.80	1.41	1.37
20	B	1217	CLA	C1B-C2B	2.80	1.49	1.43
20	B	1227	CLA	C4B-NB	2.80	1.41	1.37
20	A	1107	CLA	C1B-C2B	2.80	1.49	1.43
20	4	613	CLA	C1B-C2B	2.80	1.49	1.43
20	2	613	CLA	C1B-C2B	2.79	1.49	1.43
23	A	4011	BCR	C30-C25	-2.79	1.50	1.53
28	4	608	CHL	CHB-C1B	2.79	1.45	1.39
20	G	202	CLA	C1B-C2B	2.79	1.49	1.43
20	A	1122	CLA	C1B-C2B	2.79	1.49	1.43
20	L	302	CLA	C1B-C2B	2.79	1.49	1.43
20	1	608	CLA	C1B-C2B	2.79	1.49	1.43
20	1	608	CLA	C4B-NB	2.78	1.41	1.37
20	4	609	CLA	C1B-C2B	2.78	1.49	1.43
28	1	607	CHL	C3D-C2D	2.78	1.46	1.39
19	A	1011	CL0	C4B-NB	2.78	1.41	1.37
20	K	201	CLA	C4B-NB	2.77	1.41	1.37
20	A	1109	CLA	C4B-NB	2.77	1.41	1.37
20	2	609	CLA	C1B-C2B	2.77	1.49	1.43
20	1	615	CLA	C1B-C2B	2.77	1.49	1.43
19	A	1011	CL0	C1D-ND	2.77	1.41	1.37
20	1	603	CLA	C4B-NB	2.77	1.41	1.37
28	2	606	CHL	C1D-C2D	2.77	1.50	1.45
20	A	1104	CLA	C4B-NB	2.77	1.41	1.37
20	K	204	CLA	C1B-C2B	2.77	1.49	1.43
20	4	614	CLA	C1B-C2B	2.77	1.49	1.43
20	3	612	CLA	C1B-C2B	2.77	1.49	1.43
20	A	1114	CLA	C1B-C2B	2.76	1.49	1.43
20	3	611	CLA	C1B-C2B	2.76	1.49	1.43
20	B	1225	CLA	CMD-C2D	-2.76	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	A	5005	CLA	C4B-NB	2.76	1.41	1.37
28	4	607	CHL	C1D-C2D	2.76	1.50	1.45
20	A	1126	CLA	CHC-C1C	2.76	1.44	1.38
20	A	1013	CLA	MG-NB	-2.76	2.00	2.05
23	A	4002	BCR	C1-C6	-2.76	1.50	1.53
20	B	1239	CLA	C4B-NB	2.76	1.41	1.37
20	3	617	CLA	C1B-C2B	2.75	1.49	1.43
20	2	610	CLA	C4B-NB	2.75	1.41	1.37
20	B	1205	CLA	C4B-NB	2.75	1.41	1.37
20	1	611	CLA	C1B-C2B	2.75	1.49	1.43
20	1	614	CLA	C1B-C2B	2.75	1.49	1.43
20	K	201	CLA	C1B-C2B	2.75	1.49	1.43
20	A	1120	CLA	C4B-NB	2.75	1.41	1.37
28	2	607	CHL	C3D-C2D	2.75	1.46	1.39
20	A	1133	CLA	C3B-C4B	2.75	1.50	1.42
20	2	603	CLA	C4B-NB	2.75	1.41	1.37
20	4	603	CLA	C4B-NB	2.74	1.41	1.37
20	4	604	CLA	C4B-NB	2.74	1.41	1.37
20	1	604	CLA	C1B-C2B	2.74	1.49	1.43
23	B	4017	BCR	C1-C6	-2.74	1.50	1.53
20	A	1121	CLA	C4B-NB	2.74	1.41	1.37
20	1	609	CLA	C1B-C2B	2.74	1.49	1.43
20	1	613	CLA	C1B-C2B	2.74	1.49	1.43
20	J	102	CLA	C1B-C2B	2.73	1.49	1.43
20	B	1203	CLA	C1B-C2B	2.73	1.49	1.43
20	K	202	CLA	C1B-C2B	2.73	1.49	1.43
20	B	1201	CLA	C1B-C2B	2.73	1.49	1.43
20	4	602	CLA	C4B-NB	2.73	1.41	1.37
20	B	1209	CLA	C3B-C4B	2.73	1.50	1.42
20	3	602	CLA	C4B-NB	2.73	1.41	1.37
28	1	601	CHL	C3D-C2D	2.73	1.46	1.39
20	B	1222	CLA	C4B-NB	2.73	1.41	1.37
20	B	1012	CLA	CHC-C1C	2.72	1.43	1.38
20	A	1111	CLA	C4B-NB	2.72	1.41	1.37
20	F	301	CLA	C4B-NB	2.72	1.41	1.37
20	A	1131	CLA	C1B-C2B	2.72	1.49	1.43
28	2	601	CHL	C3D-C2D	2.72	1.46	1.39
20	2	610	CLA	C1B-C2B	2.72	1.49	1.43
20	3	614	CLA	C1B-C2B	2.72	1.49	1.43
20	B	1212	CLA	C1B-C2B	2.72	1.49	1.43
20	B	1221	CLA	CMD-C2D	-2.72	1.45	1.50
28	2	607	CHL	C1D-C2D	2.71	1.50	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	A	1125	CLA	C1B-C2B	2.71	1.49	1.43
20	3	607	CLA	C1B-C2B	2.71	1.49	1.43
20	3	613	CLA	C1B-C2B	2.71	1.49	1.43
20	A	1115	CLA	C4B-NB	2.71	1.41	1.37
20	A	1134	CLA	C1B-C2B	2.71	1.49	1.43
20	B	1211	CLA	C1B-C2B	2.71	1.49	1.43
20	F	302	CLA	C1B-C2B	2.71	1.49	1.43
20	4	603	CLA	C1B-C2B	2.70	1.49	1.43
20	B	1221	CLA	C1B-C2B	2.70	1.49	1.43
20	B	1204	CLA	C1B-C2B	2.70	1.49	1.43
20	B	1021	CLA	C1B-C2B	2.70	1.49	1.43
23	L	420	BCR	C1-C6	-2.70	1.50	1.53
20	A	1121	CLA	C1B-C2B	2.70	1.49	1.43
20	1	606	CLA	C4B-NB	2.70	1.41	1.37
20	3	609	CLA	C4B-NB	2.70	1.41	1.37
20	A	8895	CLA	C1B-C2B	2.70	1.49	1.43
20	A	1101	CLA	C1B-C2B	2.70	1.49	1.43
20	A	1120	CLA	C1B-C2B	2.70	1.49	1.43
20	I	121	CLA	C1B-C2B	2.70	1.49	1.43
23	J	213	BCR	C1-C6	-2.69	1.50	1.53
20	4	612	CLA	C1B-C2B	2.69	1.49	1.43
20	3	602	CLA	CHC-C1C	2.69	1.43	1.38
28	4	606	CHL	C1D-C2D	2.69	1.50	1.45
20	B	1211	CLA	C4B-NB	2.69	1.41	1.37
20	B	1202	CLA	C4B-NB	2.69	1.41	1.37
20	B	1235	CLA	C4B-NB	2.68	1.41	1.37
20	B	1236	CLA	C1B-C2B	2.68	1.49	1.43
20	2	604	CLA	C1B-C2B	2.68	1.49	1.43
28	2	615	CHL	C1D-C2D	2.68	1.50	1.45
20	B	1226	CLA	MG-NB	-2.68	2.00	2.05
20	A	1115	CLA	C1B-C2B	2.68	1.49	1.43
20	B	1226	CLA	C4B-NB	2.68	1.41	1.37
28	2	602	CHL	CHB-C1B	2.67	1.45	1.39
20	G	201	CLA	C1B-C2B	2.67	1.49	1.43
20	B	1216	CLA	MG-NB	-2.67	2.00	2.05
20	2	614	CLA	C1B-C2B	2.67	1.49	1.43
20	O	203	CLA	CAD-C3D	-2.67	1.45	1.50
20	3	606	CLA	C1B-C2B	2.67	1.49	1.43
20	B	1238	CLA	C4B-NB	2.67	1.41	1.37
20	4	602	CLA	C1B-C2B	2.67	1.49	1.43
28	4	608	CHL	C3D-C2D	2.67	1.46	1.39
20	B	1216	CLA	CHC-C1C	2.67	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B	1023	CLA	C1B-C2B	2.67	1.49	1.43
20	B	1210	CLA	C1B-C2B	2.67	1.49	1.43
20	A	1106	CLA	C4B-NB	2.67	1.41	1.37
20	2	603	CLA	C1B-C2B	2.66	1.49	1.43
20	A	1138	CLA	C4B-NB	2.66	1.41	1.37
20	B	1225	CLA	C4B-NB	2.66	1.41	1.37
20	H	200	CLA	C1B-C2B	2.66	1.49	1.43
20	1	612	CLA	C1B-C2B	2.66	1.49	1.43
28	4	615	CHL	C1D-C2D	2.66	1.50	1.45
20	A	1124	CLA	C1B-C2B	2.66	1.49	1.43
20	4	610	CLA	C4B-NB	2.66	1.41	1.37
20	A	1110	CLA	C1B-C2B	2.66	1.49	1.43
20	3	603	CLA	C1B-C2B	2.65	1.49	1.43
19	A	1011	CL0	C1B-C2B	2.65	1.49	1.43
20	B	1224	CLA	C4B-NB	2.65	1.41	1.37
20	B	1237	CLA	C1B-C2B	2.65	1.49	1.43
20	A	1108	CLA	C1B-C2B	2.64	1.49	1.43
20	A	1134	CLA	C4B-NB	2.64	1.41	1.37
20	1	603	CLA	C1B-C2B	2.64	1.49	1.43
20	L	303	CLA	C4B-NB	2.64	1.41	1.37
20	A	1140	CLA	C1B-C2B	2.64	1.49	1.43
20	G	218	CLA	C1B-C2B	2.64	1.49	1.43
20	B	1237	CLA	C3B-C4B	2.64	1.50	1.42
20	B	1208	CLA	C4B-NB	2.63	1.41	1.37
20	B	1227	CLA	MG-NB	-2.63	2.00	2.05
20	B	1205	CLA	CMC-C2C	-2.63	1.45	1.50
20	1	602	CLA	C4B-NB	2.63	1.41	1.37
20	A	1109	CLA	C1B-C2B	2.63	1.49	1.43
20	B	1240	CLA	C1B-C2B	2.63	1.49	1.43
20	F	301	CLA	C1B-C2B	2.63	1.49	1.43
23	A	4008	BCR	C1-C6	-2.63	1.50	1.53
20	A	1111	CLA	C1B-C2B	2.63	1.49	1.43
20	O	201	CLA	CAD-C3D	-2.63	1.45	1.50
28	3	608	CHL	C3D-C2D	2.63	1.46	1.39
20	B	1229	CLA	C3B-C4B	2.63	1.50	1.42
20	B	1219	CLA	C1B-C2B	2.63	1.49	1.43
20	A	1104	CLA	C1B-C2B	2.62	1.49	1.43
20	3	609	CLA	C1B-C2B	2.62	1.49	1.43
20	B	1208	CLA	C1B-C2B	2.62	1.49	1.43
20	B	1204	CLA	C4B-NB	2.61	1.41	1.37
20	B	1205	CLA	C1B-C2B	2.61	1.49	1.43
20	B	1219	CLA	C4B-NB	2.61	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	3	605	CLA	CAD-C3D	-2.61	1.45	1.50
20	B	1210	CLA	C4B-NB	2.61	1.41	1.37
20	4	604	CLA	C1B-C2B	2.60	1.49	1.43
20	B	1231	CLA	C1B-C2B	2.60	1.49	1.43
20	4	610	CLA	C1B-C2B	2.60	1.49	1.43
20	3	602	CLA	C1B-C2B	2.60	1.49	1.43
20	B	1220	CLA	C1B-C2B	2.59	1.49	1.43
20	B	1215	CLA	C4B-NB	2.59	1.41	1.37
20	I	121	CLA	C4B-NB	2.59	1.41	1.37
20	A	1022	CLA	C1B-C2B	2.59	1.49	1.43
20	4	609	CLA	C4B-NB	2.59	1.41	1.37
28	2	601	CHL	C1D-C2D	2.59	1.50	1.45
20	B	1202	CLA	C1B-C2B	2.59	1.49	1.43
20	A	1103	CLA	CMC-C2C	-2.58	1.45	1.50
20	A	1103	CLA	C1B-C2B	2.58	1.49	1.43
20	B	1021	CLA	C4B-NB	2.58	1.41	1.37
20	B	1012	CLA	C3B-C4B	2.58	1.50	1.42
19	A	1011	CL0	CMD-C2D	-2.58	1.45	1.50
20	A	1127	CLA	MG-NB	-2.58	2.00	2.05
20	L	301	CLA	C1B-C2B	2.58	1.49	1.43
20	A	1136	CLA	C3B-C4B	2.57	1.50	1.42
26	G	402	LMT	O3'-C3'	-2.57	1.36	1.43
20	3	602	CLA	C3B-C4B	2.57	1.50	1.42
20	4	601	CLA	C3B-C4B	2.57	1.50	1.42
20	O	202	CLA	CAD-C3D	-2.57	1.45	1.50
20	A	1105	CLA	C4B-NB	2.57	1.41	1.37
28	1	607	CHL	C3B-C4B	2.57	1.50	1.42
28	2	607	CHL	C1B-C2B	2.56	1.49	1.43
20	K	203	CLA	CAD-C3D	-2.56	1.45	1.50
20	B	1205	CLA	C3B-C4B	2.56	1.50	1.42
20	B	1234	CLA	C4B-NB	2.56	1.41	1.37
20	B	1224	CLA	CHC-C1C	2.56	1.43	1.38
20	A	1106	CLA	C1B-C2B	2.55	1.49	1.43
20	A	1117	CLA	C1B-C2B	2.55	1.49	1.43
28	3	608	CHL	C1D-C2D	2.55	1.50	1.45
20	B	1023	CLA	CHC-C1C	2.55	1.43	1.38
28	4	615	CHL	C1B-C2B	2.55	1.49	1.43
20	A	1130	CLA	C1B-C2B	2.55	1.49	1.43
20	B	1228	CLA	C1B-C2B	2.55	1.49	1.43
20	B	1225	CLA	C1B-C2B	2.55	1.49	1.43
26	4	631	LMT	O3'-C3'	-2.55	1.36	1.43
23	3	624	BCR	C1-C6	-2.55	1.50	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	3	604	CLA	C1B-C2B	2.55	1.49	1.43
20	B	1239	CLA	CMB-C2B	-2.54	1.45	1.50
20	B	1209	CLA	C1B-C2B	2.54	1.49	1.43
23	L	419	BCR	C1-C6	-2.54	1.50	1.53
20	A	5005	CLA	C1B-C2B	2.54	1.49	1.43
28	2	602	CHL	C1D-C2D	2.54	1.50	1.45
20	F	303	CLA	CAD-C3D	-2.54	1.45	1.50
20	A	1112	CLA	C1B-C2B	2.53	1.49	1.43
23	B	4014	BCR	C30-C25	-2.53	1.50	1.53
20	3	610	CLA	C1B-C2B	2.53	1.49	1.43
20	A	1102	CLA	C3B-C4B	2.53	1.50	1.42
28	2	608	CHL	C3D-C2D	2.53	1.45	1.39
20	B	1206	CLA	C1B-C2B	2.52	1.49	1.43
20	B	1232	CLA	MG-NB	-2.52	2.00	2.05
20	B	1232	CLA	CHC-C1C	2.52	1.43	1.38
20	A	1135	CLA	C3B-C4B	2.52	1.50	1.42
28	2	615	CHL	C1B-C2B	2.52	1.49	1.43
20	B	1213	CLA	C1B-C2B	2.52	1.49	1.43
20	B	1210	CLA	CHC-C1C	2.52	1.43	1.38
20	A	1126	CLA	C3B-C4B	2.52	1.50	1.42
20	B	1229	CLA	C1B-C2B	2.52	1.49	1.43
20	A	1801	CLA	C1B-C2B	2.52	1.49	1.43
24	A	5001	LHG	O7-C5	-2.51	1.40	1.46
28	4	608	CHL	C1D-C2D	2.51	1.50	1.45
20	A	1131	CLA	C4B-NB	2.51	1.41	1.37
20	A	1105	CLA	C1B-C2B	2.51	1.49	1.43
20	B	1220	CLA	C4B-NB	2.51	1.41	1.37
20	A	1139	CLA	C1B-C2B	2.51	1.49	1.43
20	A	1022	CLA	CMB-C2B	-2.51	1.45	1.50
28	2	611	CHL	C1B-C2B	2.50	1.49	1.43
20	B	1223	CLA	C1B-C2B	2.50	1.49	1.43
20	A	1113	CLA	C1B-C2B	2.50	1.49	1.43
20	A	1124	CLA	C3B-C4B	2.50	1.50	1.42
20	A	1127	CLA	C4B-NB	2.49	1.41	1.37
20	4	601	CLA	C1B-C2B	2.49	1.49	1.43
20	A	1109	CLA	MG-NB	-2.49	2.00	2.05
20	B	1212	CLA	CMC-C2C	-2.49	1.45	1.50
20	A	1116	CLA	C3B-C4B	2.48	1.50	1.42
20	A	1106	CLA	CHC-C1C	2.48	1.43	1.38
20	A	1131	CLA	C3B-C4B	2.48	1.50	1.42
20	B	1214	CLA	C3B-C4B	2.48	1.50	1.42
20	4	609	CLA	MG-NB	-2.48	2.00	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	A	1126	CLA	C1B-C2B	2.48	1.48	1.43
20	A	1127	CLA	CHC-C1C	2.48	1.43	1.38
20	B	1216	CLA	C3B-C4B	2.48	1.49	1.42
20	B	1023	CLA	C1D-ND	2.48	1.41	1.37
20	B	1238	CLA	CMD-C2D	-2.48	1.45	1.50
20	B	1232	CLA	CMB-C2B	-2.48	1.45	1.50
20	A	1109	CLA	CMD-C2D	-2.47	1.45	1.50
20	B	1220	CLA	CHC-C1C	2.47	1.43	1.38
20	B	1021	CLA	CMD-C2D	-2.47	1.45	1.50
20	B	1214	CLA	CMB-C2B	-2.47	1.45	1.50
20	A	1136	CLA	C1B-C2B	2.47	1.48	1.43
20	3	613	CLA	C3B-C4B	2.47	1.49	1.42
20	A	1132	CLA	C3B-C4B	2.47	1.49	1.42
20	1	612	CLA	C3B-C4B	2.47	1.49	1.42
20	1	603	CLA	C3B-C4B	2.46	1.49	1.42
28	2	601	CHL	C1B-C2B	2.46	1.48	1.43
20	4	612	CLA	C3B-C4B	2.46	1.49	1.42
20	B	1235	CLA	C1B-C2B	2.46	1.48	1.43
20	B	1236	CLA	C3B-C4B	2.46	1.49	1.42
23	M	4021	BCR	C1-C6	-2.46	1.50	1.53
20	A	1013	CLA	CMD-C2D	-2.46	1.45	1.50
28	2	606	CHL	C1B-C2B	2.46	1.48	1.43
20	B	1215	CLA	C1B-C2B	2.46	1.48	1.43
26	B	5001	LMT	O3'-C3'	-2.46	1.36	1.43
20	A	1139	CLA	CHC-C1C	2.46	1.43	1.38
20	A	1132	CLA	C1B-C2B	2.45	1.48	1.43
20	B	1213	CLA	CHC-C1C	2.45	1.43	1.38
20	A	1119	CLA	C3B-C4B	2.45	1.49	1.42
28	4	607	CHL	C4C-C3C	2.45	1.49	1.45
20	B	1215	CLA	MG-NB	-2.45	2.00	2.05
20	B	1231	CLA	C3B-C4B	2.45	1.49	1.42
20	A	1105	CLA	CHC-C1C	2.45	1.43	1.38
20	A	1124	CLA	C4B-NB	2.45	1.41	1.37
20	B	1215	CLA	CMB-C2B	-2.45	1.45	1.50
20	B	1227	CLA	C1B-C2B	2.45	1.48	1.43
20	B	1210	CLA	C3B-C4B	2.45	1.49	1.42
26	A	5004	LMT	O3'-C3'	-2.44	1.36	1.43
26	1	631	LMT	O3'-C3'	-2.44	1.36	1.43
20	A	1118	CLA	C1B-C2B	2.44	1.48	1.43
20	A	1133	CLA	C1B-C2B	2.44	1.48	1.43
20	I	121	CLA	CMD-C2D	-2.44	1.45	1.50
20	1	614	CLA	CHC-C1C	2.44	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	A	1108	CLA	MG-NB	-2.44	2.01	2.05
20	A	1140	CLA	CMD-C2D	-2.44	1.45	1.50
28	4	607	CHL	C1B-NB	-2.44	1.34	1.37
20	A	1125	CLA	MG-NB	-2.44	2.01	2.05
20	A	1126	CLA	MG-NB	-2.44	2.01	2.05
20	B	1212	CLA	C4B-NB	2.44	1.41	1.37
20	4	609	CLA	CHC-C1C	2.43	1.43	1.38
20	A	1134	CLA	C3B-C4B	2.43	1.49	1.42
20	A	1013	CLA	C3B-C4B	2.43	1.49	1.42
26	G	401	LMT	O3'-C3'	-2.43	1.36	1.43
20	B	1239	CLA	C1B-C2B	2.43	1.48	1.43
20	A	1132	CLA	CHC-C1C	2.43	1.43	1.38
20	A	1127	CLA	C1B-C2B	2.43	1.48	1.43
20	A	1102	CLA	C1B-C2B	2.43	1.48	1.43
20	B	1021	CLA	CMC-C2C	-2.43	1.45	1.50
19	A	1011	CL0	MG-NB	-2.42	2.01	2.05
20	A	1126	CLA	CMC-C2C	-2.42	1.45	1.50
20	B	1235	CLA	CMB-C2B	-2.42	1.45	1.50
20	3	611	CLA	C3B-C4B	2.42	1.49	1.42
28	1	601	CHL	C4C-C3C	2.42	1.49	1.45
20	A	1114	CLA	CMB-C2B	-2.42	1.45	1.50
20	A	1114	CLA	C4B-NB	2.42	1.41	1.37
20	A	1113	CLA	C3B-C4B	2.42	1.49	1.42
20	A	1109	CLA	CHC-C1C	2.42	1.43	1.38
20	B	1227	CLA	CMB-C2B	-2.42	1.45	1.50
20	A	1110	CLA	C3B-C4B	2.42	1.49	1.42
20	A	1102	CLA	CHC-C1C	2.42	1.43	1.38
20	A	1124	CLA	CHC-C1C	2.42	1.43	1.38
20	3	604	CLA	CMB-C2B	-2.42	1.45	1.50
20	4	602	CLA	C3B-C4B	2.42	1.49	1.42
20	G	218	CLA	C3B-C4B	2.41	1.49	1.42
20	B	1224	CLA	C1B-C2B	2.41	1.48	1.43
20	4	614	CLA	CHC-C1C	2.41	1.43	1.38
28	3	608	CHL	C1B-C2B	2.41	1.48	1.43
20	A	1119	CLA	C1B-C2B	2.41	1.48	1.43
20	A	1139	CLA	C3B-C4B	2.41	1.49	1.42
28	2	607	CHL	C4C-C3C	2.41	1.49	1.45
20	A	1108	CLA	C4B-NB	2.41	1.41	1.37
20	3	606	CLA	C3B-C4B	2.41	1.49	1.42
20	L	301	CLA	CMB-C2B	-2.41	1.45	1.50
20	K	204	CLA	C3B-C4B	2.41	1.49	1.42
20	B	1221	CLA	MG-NB	-2.41	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	A	1105	CLA	MG-NB	-2.40	2.01	2.05
20	A	1108	CLA	CHC-C1C	2.40	1.43	1.38
23	B	4004	BCR	C30-C25	-2.40	1.50	1.53
20	B	1203	CLA	C4B-NB	2.40	1.41	1.37
28	1	601	CHL	C1B-C2B	2.40	1.48	1.43
20	A	1113	CLA	CHC-C1C	2.40	1.43	1.38
20	B	1219	CLA	CMD-C2D	-2.40	1.45	1.50
20	A	1022	CLA	MG-NB	-2.40	2.01	2.05
20	1	602	CLA	CMD-C2D	-2.40	1.45	1.50
20	B	1232	CLA	C3B-C4B	2.40	1.49	1.42
20	A	1119	CLA	CHC-C1C	2.40	1.43	1.38
20	B	1023	CLA	C4B-NB	2.40	1.41	1.37
20	G	201	CLA	C3B-C4B	2.40	1.49	1.42
20	4	604	CLA	C3B-C4B	2.40	1.49	1.42
20	A	1109	CLA	C3B-C4B	2.40	1.49	1.42
20	A	1013	CLA	CHC-C1C	2.39	1.43	1.38
20	B	1219	CLA	MG-NB	-2.39	2.01	2.05
20	A	1117	CLA	C4B-NB	2.39	1.41	1.37
28	2	608	CHL	C1B-C2B	2.39	1.48	1.43
28	4	606	CHL	C1B-C2B	2.39	1.48	1.43
28	1	607	CHL	C1B-C2B	2.39	1.48	1.43
20	B	1222	CLA	CMD-C2D	-2.39	1.45	1.50
20	1	614	CLA	C3B-C4B	2.39	1.49	1.42
20	B	1210	CLA	CMC-C2C	-2.39	1.45	1.50
20	4	611	CLA	CHC-C1C	2.39	1.43	1.38
20	3	610	CLA	C3B-C4B	2.39	1.49	1.42
20	A	1130	CLA	CHC-C1C	2.39	1.43	1.38
20	2	609	CLA	CHC-C1C	2.39	1.43	1.38
20	B	1221	CLA	CHC-C1C	2.39	1.43	1.38
23	J	213	BCR	C30-C25	-2.38	1.50	1.53
20	F	302	CLA	C3B-C4B	2.38	1.49	1.42
20	A	8895	CLA	MG-NB	-2.38	2.01	2.05
20	A	1138	CLA	MG-NB	-2.38	2.01	2.05
20	A	1022	CLA	CMD-C2D	-2.38	1.45	1.50
20	1	613	CLA	CHC-C1C	2.38	1.43	1.38
20	B	1211	CLA	CHC-C1C	2.38	1.43	1.38
20	A	1127	CLA	CMD-C2D	-2.38	1.45	1.50
20	B	1227	CLA	CHC-C1C	2.38	1.43	1.38
20	L	301	CLA	CHC-C1C	2.38	1.43	1.38
20	A	1135	CLA	C1B-C2B	2.38	1.48	1.43
20	B	1222	CLA	CHC-C1C	2.38	1.43	1.38
20	4	602	CLA	CHC-C1C	2.38	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	F	301	CLA	C3B-C4B	2.38	1.49	1.42
20	3	603	CLA	C3B-C4B	2.38	1.49	1.42
20	B	1206	CLA	MG-NB	-2.38	2.01	2.05
20	A	1138	CLA	C3B-C4B	2.38	1.49	1.42
20	A	1140	CLA	C3B-C4B	2.38	1.49	1.42
20	A	1111	CLA	MG-NB	-2.37	2.01	2.05
20	B	1021	CLA	MG-NB	-2.37	2.01	2.05
20	A	8895	CLA	CMD-C2D	-2.37	1.45	1.50
20	K	203	CLA	CHC-C1C	2.37	1.43	1.38
20	1	615	CLA	CHC-C1C	2.37	1.43	1.38
20	A	1121	CLA	C3B-C4B	2.37	1.49	1.42
20	B	1224	CLA	C3B-C4B	2.37	1.49	1.42
20	A	1132	CLA	C4B-NB	2.37	1.41	1.37
20	A	1125	CLA	CHC-C1C	2.37	1.43	1.38
20	B	1231	CLA	CMD-C2D	-2.37	1.45	1.50
20	F	303	CLA	CHC-C1C	2.37	1.43	1.38
20	B	1216	CLA	C1B-C2B	2.37	1.48	1.43
20	B	1213	CLA	C3B-C4B	2.37	1.49	1.42
20	2	603	CLA	C3B-C4B	2.37	1.49	1.42
20	1	613	CLA	MG-NB	-2.37	2.01	2.05
20	3	614	CLA	CHC-C1C	2.37	1.43	1.38
20	1	612	CLA	CHC-C1C	2.37	1.43	1.38
20	A	1106	CLA	C3B-C4B	2.37	1.49	1.42
20	A	1118	CLA	CMD-C2D	-2.37	1.45	1.50
20	A	1106	CLA	MG-NB	-2.37	2.01	2.05
20	A	1119	CLA	MG-NB	-2.36	2.01	2.05
28	2	602	CHL	C1B-C2B	2.36	1.48	1.43
20	3	609	CLA	CHC-C1C	2.36	1.43	1.38
20	2	614	CLA	C3B-C4B	2.36	1.49	1.42
20	A	1126	CLA	C4B-NB	2.36	1.41	1.37
20	B	1234	CLA	C1B-C2B	2.36	1.48	1.43
20	F	302	CLA	CHC-C1C	2.36	1.43	1.38
23	B	4005	BCR	C30-C25	-2.36	1.50	1.53
20	B	1220	CLA	CMD-C2D	-2.36	1.45	1.50
20	A	1133	CLA	CMB-C2B	-2.36	1.45	1.50
23	A	4001	BCR	C30-C25	-2.36	1.50	1.53
20	B	1228	CLA	CHC-C1C	2.36	1.43	1.38
20	B	1225	CLA	MG-NB	-2.36	2.01	2.05
20	A	1137	CLA	C1B-C2B	2.36	1.48	1.43
20	A	1135	CLA	MG-NB	-2.36	2.01	2.05
20	A	1103	CLA	C3B-C4B	2.36	1.49	1.42
20	B	1210	CLA	CMD-C2D	-2.36	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	4	604	CLA	CHC-C1C	2.36	1.43	1.38
20	A	1127	CLA	C3B-C4B	2.36	1.49	1.42
20	B	1213	CLA	C4B-NB	2.36	1.41	1.37
20	B	1238	CLA	C1B-C2B	2.36	1.48	1.43
20	B	1230	CLA	CHC-C1C	2.36	1.43	1.38
20	B	1023	CLA	MG-NB	-2.35	2.01	2.05
20	B	1215	CLA	C3B-C4B	2.35	1.49	1.42
20	B	1239	CLA	C3B-C4B	2.35	1.49	1.42
20	G	201	CLA	CHC-C1C	2.35	1.43	1.38
20	L	301	CLA	MG-NB	-2.35	2.01	2.05
20	B	1235	CLA	C3B-C4B	2.35	1.49	1.42
20	B	1224	CLA	CMC-C2C	-2.35	1.46	1.50
20	K	201	CLA	CHC-C1C	2.35	1.43	1.38
20	B	1205	CLA	MG-NB	-2.35	2.01	2.05
20	4	610	CLA	MG-NB	-2.35	2.01	2.05
20	B	1220	CLA	C3B-C4B	2.35	1.49	1.42
20	B	1236	CLA	CHC-C1C	2.35	1.43	1.38
20	O	202	CLA	CHC-C1C	2.35	1.43	1.38
20	B	1228	CLA	C3B-C4B	2.35	1.49	1.42
20	B	1240	CLA	C3B-C4B	2.35	1.49	1.42
20	A	1104	CLA	CHC-C1C	2.35	1.43	1.38
20	3	607	CLA	C3B-C4B	2.35	1.49	1.42
20	A	1112	CLA	C3B-C4B	2.35	1.49	1.42
20	B	1238	CLA	C3B-C4B	2.35	1.49	1.42
20	K	202	CLA	C3B-C4B	2.35	1.49	1.42
29	4	620	LUT	C23-C24	2.34	1.53	1.50
20	4	603	CLA	C3B-C4B	2.34	1.49	1.42
20	2	612	CLA	CHC-C1C	2.34	1.43	1.38
26	A	5004	LMT	O2B-C2B	-2.34	1.37	1.43
20	J	102	CLA	C3B-C4B	2.34	1.49	1.42
20	A	1013	CLA	CMC-C2C	-2.34	1.46	1.50
20	1	609	CLA	C3B-C4B	2.34	1.49	1.42
20	A	1104	CLA	CMD-C2D	-2.34	1.46	1.50
20	H	200	CLA	CHC-C1C	2.34	1.43	1.38
20	B	1226	CLA	MG-ND	-2.34	2.01	2.05
20	O	203	CLA	CHC-C1C	2.33	1.43	1.38
20	3	614	CLA	C3B-C4B	2.33	1.49	1.42
20	B	1238	CLA	CHC-C1C	2.33	1.43	1.38
20	B	1230	CLA	C3B-C4B	2.33	1.49	1.42
20	3	602	CLA	MG-NB	-2.33	2.01	2.05
20	2	604	CLA	C3B-C4B	2.33	1.49	1.42
26	4	631	LMT	O2B-C2B	-2.33	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	A	1121	CLA	CHC-C1C	2.33	1.43	1.38
20	1	610	CLA	CHC-C1C	2.33	1.43	1.38
20	A	1128	CLA	MG-NB	-2.33	2.01	2.05
20	B	1211	CLA	C3B-C4B	2.33	1.49	1.42
23	B	4009	BCR	C30-C25	-2.33	1.50	1.53
20	A	1130	CLA	C3B-C4B	2.33	1.49	1.42
20	4	614	CLA	C3B-C4B	2.33	1.49	1.42
20	A	1013	CLA	CMB-C2B	-2.32	1.46	1.50
20	A	1121	CLA	CMD-C2D	-2.32	1.46	1.50
20	A	1119	CLA	C4B-NB	2.32	1.40	1.37
20	A	1138	CLA	CHC-C1C	2.32	1.43	1.38
20	4	610	CLA	C3B-C4B	2.32	1.49	1.42
20	A	1111	CLA	CHC-C1C	2.32	1.43	1.38
20	B	1012	CLA	MG-NB	-2.32	2.01	2.05
20	G	202	CLA	CHC-C1C	2.32	1.43	1.38
20	4	610	CLA	CHC-C1C	2.32	1.43	1.38
20	A	1801	CLA	CMB-C2B	-2.32	1.46	1.50
28	1	607	CHL	C4C-C3C	2.32	1.49	1.45
20	3	604	CLA	C3B-C4B	2.32	1.49	1.42
20	B	1235	CLA	MG-NB	-2.32	2.01	2.05
20	A	1117	CLA	C3B-C4B	2.32	1.49	1.42
20	4	613	CLA	C3B-C4B	2.32	1.49	1.42
20	3	613	CLA	CHC-C1C	2.32	1.43	1.38
20	A	1013	CLA	MG-ND	-2.32	2.01	2.05
20	3	605	CLA	CHC-C1C	2.32	1.43	1.38
20	B	1202	CLA	C3B-C4B	2.32	1.49	1.42
20	A	5005	CLA	CMD-C2D	-2.32	1.46	1.50
20	A	1115	CLA	C3B-C4B	2.31	1.49	1.42
20	A	1121	CLA	MG-NB	-2.31	2.01	2.05
28	2	608	CHL	C1D-C2D	2.31	1.49	1.45
20	A	1105	CLA	C3B-C4B	2.31	1.49	1.42
20	1	602	CLA	CMC-C2C	-2.31	1.46	1.50
20	B	1224	CLA	MG-NB	-2.31	2.01	2.05
28	1	601	CHL	C3B-C4B	2.31	1.49	1.42
20	A	1139	CLA	MG-NB	-2.31	2.01	2.05
20	A	1101	CLA	CMC-C2C	-2.31	1.46	1.50
20	A	1128	CLA	CMD-C2D	-2.31	1.46	1.50
20	B	1212	CLA	CHC-C1C	2.31	1.43	1.38
20	B	1023	CLA	C3B-C4B	2.31	1.49	1.42
20	1	602	CLA	CHC-C1C	2.31	1.43	1.38
20	1	603	CLA	CMB-C2B	-2.31	1.46	1.50
20	B	1234	CLA	C3B-C4B	2.31	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	A	1137	CLA	CHC-C1C	2.31	1.43	1.38
20	A	1114	CLA	MG-NB	-2.31	2.01	2.05
20	A	1136	CLA	CMB-C2B	-2.31	1.46	1.50
20	B	1012	CLA	CMC-C2C	-2.31	1.46	1.50
20	A	1124	CLA	MG-NB	-2.31	2.01	2.05
20	A	1104	CLA	C3B-C4B	2.30	1.49	1.42
20	2	610	CLA	C3B-C4B	2.30	1.49	1.42
20	1	602	CLA	C3B-C4B	2.30	1.49	1.42
20	A	1131	CLA	MG-NB	-2.30	2.01	2.05
20	B	1212	CLA	C3B-C4B	2.30	1.49	1.42
20	B	1202	CLA	CHC-C1C	2.30	1.43	1.38
20	4	611	CLA	C3B-C4B	2.30	1.49	1.42
20	A	1115	CLA	CHC-C1C	2.30	1.43	1.38
20	K	204	CLA	CHC-C1C	2.30	1.43	1.38
20	1	615	CLA	C3B-C4B	2.30	1.49	1.42
20	K	201	CLA	C3B-C4B	2.30	1.49	1.42
20	B	1219	CLA	CMB-C2B	-2.30	1.46	1.50
20	3	612	CLA	C3B-C4B	2.30	1.49	1.42
20	B	1234	CLA	MG-NB	-2.30	2.01	2.05
20	A	1127	CLA	MG-ND	-2.30	2.01	2.05
20	A	1116	CLA	CMB-C2B	-2.30	1.46	1.50
20	2	614	CLA	CHC-C1C	2.30	1.43	1.38
20	A	1132	CLA	MG-NB	-2.30	2.01	2.05
20	A	1103	CLA	CHC-C1C	2.30	1.43	1.38
20	B	1219	CLA	C3B-C4B	2.29	1.49	1.42
20	3	610	CLA	CHC-C1C	2.29	1.43	1.38
20	A	1110	CLA	CHC-C1C	2.29	1.43	1.38
20	2	603	CLA	CHC-C1C	2.29	1.43	1.38
20	B	1210	CLA	MG-NB	-2.29	2.01	2.05
20	A	1120	CLA	C3B-C4B	2.29	1.49	1.42
20	3	609	CLA	C3B-C4B	2.29	1.49	1.42
20	B	1209	CLA	CHC-C1C	2.29	1.43	1.38
20	B	1208	CLA	C3B-C4B	2.29	1.49	1.42
20	3	617	CLA	CHC-C1C	2.29	1.43	1.38
20	A	1104	CLA	MG-NB	-2.29	2.01	2.05
20	A	1101	CLA	C3B-C4B	2.29	1.49	1.42
20	3	607	CLA	CHC-C1C	2.29	1.43	1.38
20	B	1234	CLA	CHC-C1C	2.29	1.43	1.38
20	B	1240	CLA	CHC-C1C	2.29	1.43	1.38
20	3	617	CLA	C3B-C4B	2.29	1.49	1.42
20	A	1101	CLA	CHC-C1C	2.29	1.43	1.38
23	B	4014	BCR	C1-C6	-2.29	1.50	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	4010	BCR	C30-C25	-2.29	1.50	1.53
20	A	1116	CLA	CMD-C2D	-2.29	1.46	1.50
20	A	1013	CLA	C1B-NB	-2.29	1.34	1.37
26	4	631	LMT	O2'-C2'	-2.29	1.37	1.43
20	A	5005	CLA	C3B-C4B	2.29	1.49	1.42
20	1	611	CLA	C3B-C4B	2.29	1.49	1.42
20	B	1235	CLA	CHC-C1C	2.28	1.43	1.38
20	A	1138	CLA	CMB-C2B	-2.28	1.46	1.50
20	B	1217	CLA	CMD-C2D	-2.28	1.46	1.50
20	A	1125	CLA	MG-ND	-2.28	2.01	2.05
20	B	1023	CLA	MG-ND	-2.28	2.01	2.05
20	A	1108	CLA	C3B-C4B	2.28	1.49	1.42
20	A	8895	CLA	C3B-C4B	2.28	1.49	1.42
20	1	613	CLA	C3B-C4B	2.28	1.49	1.42
20	2	609	CLA	C3B-C4B	2.28	1.49	1.42
20	A	1125	CLA	C3B-C4B	2.28	1.49	1.42
20	A	1116	CLA	MG-NB	-2.28	2.01	2.05
20	A	1125	CLA	CMD-C2D	-2.28	1.46	1.50
20	B	1208	CLA	CHC-C1C	2.28	1.43	1.38
20	K	202	CLA	CHC-C1C	2.28	1.43	1.38
20	A	1138	CLA	C1B-C2B	2.28	1.48	1.43
20	A	1136	CLA	CHC-C1C	2.28	1.43	1.38
20	A	8895	CLA	CHC-C1C	2.28	1.43	1.38
20	B	1222	CLA	MG-NB	-2.28	2.01	2.05
20	B	1238	CLA	MG-NB	-2.28	2.01	2.05
20	3	603	CLA	CMC-C2C	-2.27	1.46	1.50
19	A	1011	CL0	CMB-C2B	-2.27	1.46	1.50
20	4	609	CLA	C3B-C4B	2.27	1.49	1.42
20	B	1222	CLA	C3B-C4B	2.27	1.49	1.42
23	G	311	BCR	C30-C25	-2.27	1.50	1.53
20	2	613	CLA	C3B-C4B	2.27	1.49	1.42
20	1	604	CLA	C3B-C4B	2.27	1.49	1.42
20	B	1221	CLA	C3B-C4B	2.27	1.49	1.42
20	1	610	CLA	C3B-C4B	2.27	1.49	1.42
20	2	612	CLA	C3B-C4B	2.27	1.49	1.42
20	F	301	CLA	CHC-C1C	2.27	1.43	1.38
26	1	631	LMT	O2'-C2'	-2.27	1.37	1.43
20	3	604	CLA	MG-NB	-2.27	2.01	2.05
28	4	608	CHL	C1B-NB	-2.27	1.34	1.37
20	A	1801	CLA	CHC-C1C	2.27	1.43	1.38
20	G	202	CLA	C3B-C4B	2.27	1.49	1.42
20	A	1116	CLA	C1B-C2B	2.26	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	A	1801	CLA	MG-NB	-2.26	2.01	2.05
20	B	1204	CLA	C3B-C4B	2.26	1.49	1.42
20	B	1021	CLA	CHC-C1C	2.26	1.43	1.38
20	4	613	CLA	CHC-C1C	2.26	1.43	1.38
20	B	1223	CLA	CMC-C2C	-2.26	1.46	1.50
20	B	1237	CLA	CMB-C2B	-2.26	1.46	1.50
20	G	218	CLA	CHC-C1C	2.26	1.43	1.38
20	B	1202	CLA	CMD-C2D	-2.26	1.46	1.50
28	1	601	CHL	C1D-C2D	2.26	1.49	1.45
28	3	608	CHL	C1B-NB	-2.26	1.34	1.37
28	3	608	CHL	C3B-C4B	2.26	1.49	1.42
20	B	1232	CLA	C1B-C2B	2.26	1.48	1.43
19	A	1011	CL0	CHC-C1C	2.26	1.43	1.38
20	B	1206	CLA	CHC-C1C	2.26	1.43	1.38
20	L	301	CLA	C3B-C4B	2.26	1.49	1.42
23	I	118	BCR	C1-C6	-2.26	1.50	1.53
20	B	1201	CLA	CMD-C2D	-2.26	1.46	1.50
20	B	1227	CLA	CMD-C2D	-2.26	1.46	1.50
20	B	1219	CLA	CHC-C1C	2.26	1.43	1.38
28	4	606	CHL	C3B-C4B	2.26	1.49	1.42
26	B	5001	LMT	O2B-C2B	-2.26	1.37	1.43
26	1	631	LMT	O2B-C2B	-2.26	1.37	1.43
20	A	1119	CLA	CMB-C2B	-2.26	1.46	1.50
20	B	1229	CLA	CHC-C1C	2.26	1.43	1.38
28	1	601	CHL	C1B-NB	-2.26	1.34	1.37
20	A	1117	CLA	MG-NB	-2.25	2.01	2.05
20	B	1216	CLA	CMB-C2B	-2.25	1.46	1.50
20	B	1023	CLA	CMD-C2D	-2.25	1.46	1.50
20	1	606	CLA	MG-NB	-2.25	2.01	2.05
20	2	604	CLA	CHC-C1C	2.25	1.43	1.38
20	3	604	CLA	CHC-C1C	2.25	1.43	1.38
20	A	1111	CLA	CMC-C2C	-2.25	1.46	1.50
24	B	5101	LHG	O7-C5	-2.25	1.41	1.46
20	A	5005	CLA	CHC-C1C	2.25	1.43	1.38
20	3	611	CLA	CHC-C1C	2.25	1.43	1.38
20	3	609	CLA	MG-NB	-2.25	2.01	2.05
20	H	200	CLA	C3B-C4B	2.25	1.49	1.42
19	A	1011	CL0	C3B-C4B	2.25	1.49	1.42
28	4	615	CHL	C4C-C3C	2.25	1.48	1.45
20	B	1213	CLA	MG-NB	-2.25	2.01	2.05
20	A	1139	CLA	CMD-C2D	-2.25	1.46	1.50
20	B	1216	CLA	CMD-C2D	-2.25	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	A	1117	CLA	CMB-C2B	-2.25	1.46	1.50
20	B	1203	CLA	MG-NB	-2.25	2.01	2.05
20	B	1223	CLA	C3B-C4B	2.25	1.49	1.42
20	A	1103	CLA	MG-NB	-2.24	2.01	2.05
20	A	1133	CLA	CMD-C2D	-2.24	1.46	1.50
20	A	1111	CLA	CMB-C2B	-2.24	1.46	1.50
20	L	303	CLA	C3B-C4B	2.24	1.49	1.42
28	4	608	CHL	C1B-C2B	2.24	1.48	1.43
20	B	1215	CLA	CHC-C1C	2.24	1.43	1.38
20	B	1217	CLA	C3B-C4B	2.24	1.49	1.42
26	G	401	LMT	O2'-C2'	-2.24	1.37	1.43
28	4	615	CHL	C2C-C1C	2.24	1.49	1.44
20	A	1013	CLA	C4B-NB	2.24	1.40	1.37
20	1	609	CLA	MG-NB	-2.24	2.01	2.05
20	B	1225	CLA	CMC-C2C	-2.24	1.46	1.50
20	A	1120	CLA	CHC-C1C	2.24	1.43	1.38
20	A	1101	CLA	MG-NB	-2.24	2.01	2.05
20	4	602	CLA	MG-NB	-2.24	2.01	2.05
20	A	1126	CLA	CMD-C2D	-2.24	1.46	1.50
20	A	5005	CLA	CMB-C2B	-2.24	1.46	1.50
20	3	612	CLA	CHC-C1C	2.24	1.43	1.38
23	A	4011	BCR	C1-C6	-2.24	1.50	1.53
20	A	1122	CLA	MG-NB	-2.24	2.01	2.05
28	4	608	CHL	C2C-C1C	2.24	1.49	1.44
20	B	1208	CLA	MG-NB	-2.24	2.01	2.05
20	B	1238	CLA	CMB-C2B	-2.23	1.46	1.50
28	2	606	CHL	C2C-C1C	2.23	1.49	1.44
20	A	1136	CLA	MG-NB	-2.23	2.01	2.05
20	B	1206	CLA	C3B-C4B	2.23	1.49	1.42
20	A	5005	CLA	MG-NB	-2.23	2.01	2.05
20	B	1012	CLA	CMD-C2D	-2.23	1.46	1.50
20	4	603	CLA	CHC-C1C	2.23	1.43	1.38
28	4	606	CHL	C1B-NB	-2.23	1.34	1.37
20	A	1103	CLA	CMB-C2B	-2.23	1.46	1.50
26	G	402	LMT	O2B-C2B	-2.23	1.37	1.43
20	A	1122	CLA	C3B-C4B	2.23	1.49	1.42
28	4	607	CHL	C1B-C2B	2.23	1.48	1.43
20	A	1122	CLA	CMB-C2B	-2.23	1.46	1.50
20	B	1234	CLA	CMB-C2B	-2.23	1.46	1.50
20	F	301	CLA	MG-NB	-2.23	2.01	2.05
20	G	218	CLA	CMD-C2D	-2.23	1.46	1.50
28	4	606	CHL	C4C-C3C	2.23	1.48	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	1	609	CLA	CHC-C1C	2.23	1.43	1.38
20	A	1128	CLA	C3B-C4B	2.23	1.49	1.42
20	A	1135	CLA	CHC-C1C	2.23	1.43	1.38
20	4	612	CLA	CHC-C1C	2.23	1.43	1.38
20	1	614	CLA	MG-NB	-2.23	2.01	2.05
28	2	601	CHL	C1B-NB	-2.23	1.34	1.37
20	O	201	CLA	CHC-C1C	2.23	1.42	1.38
20	L	302	CLA	C3B-C4B	2.23	1.49	1.42
26	A	5004	LMT	O2'-C2'	-2.22	1.37	1.43
20	B	1206	CLA	CMB-C2B	-2.22	1.46	1.50
20	I	121	CLA	MG-NB	-2.22	2.01	2.05
20	A	1116	CLA	CHC-C1C	2.22	1.42	1.38
28	2	601	CHL	C3B-C4B	2.22	1.49	1.42
20	B	1212	CLA	MG-NB	-2.22	2.01	2.05
20	F	301	CLA	CMB-C2B	-2.22	1.46	1.50
26	B	5001	LMT	O2'-C2'	-2.22	1.37	1.43
28	2	611	CHL	C1B-NB	-2.22	1.34	1.37
20	4	611	CLA	CMD-C2D	-2.22	1.46	1.50
20	B	1205	CLA	CHC-C1C	2.22	1.42	1.38
20	A	1801	CLA	C3B-C4B	2.22	1.49	1.42
20	2	609	CLA	MG-NB	-2.22	2.01	2.05
20	A	1104	CLA	CMC-C2C	-2.22	1.46	1.50
26	G	401	LMT	O2B-C2B	-2.22	1.37	1.43
26	G	402	LMT	O2'-C2'	-2.22	1.37	1.43
20	B	1234	CLA	CMC-C2C	-2.22	1.46	1.50
20	A	1112	CLA	CHC-C1C	2.22	1.42	1.38
28	2	611	CHL	C1D-C2D	2.22	1.49	1.45
20	B	1230	CLA	CMC-C2C	-2.22	1.46	1.50
20	B	1227	CLA	C3B-C4B	2.21	1.49	1.42
20	A	1131	CLA	CHC-C1C	2.21	1.42	1.38
20	1	604	CLA	CHC-C1C	2.21	1.42	1.38
20	B	1231	CLA	CHC-C1C	2.21	1.42	1.38
20	4	610	CLA	CMD-C2D	-2.21	1.46	1.50
20	B	1240	CLA	CMD-C2D	-2.21	1.46	1.50
20	B	1211	CLA	MG-NB	-2.21	2.01	2.05
20	B	1220	CLA	CMC-C2C	-2.21	1.46	1.50
20	B	1220	CLA	MG-NB	-2.21	2.01	2.05
26	4	631	LMT	O3B-C3B	-2.21	1.37	1.43
20	A	1106	CLA	CMD-C2D	-2.21	1.46	1.50
28	2	611	CHL	C4C-C3C	2.21	1.48	1.45
20	1	608	CLA	C3B-C4B	2.20	1.49	1.42
20	A	1134	CLA	CMD-C2D	-2.20	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	A	1139	CLA	CMB-C2B	-2.20	1.46	1.50
23	M	4021	BCR	C30-C25	-2.20	1.51	1.53
20	I	121	CLA	C3B-C4B	2.20	1.49	1.42
20	B	1227	CLA	MG-ND	-2.20	2.01	2.05
20	2	610	CLA	MG-NB	-2.20	2.01	2.05
20	B	1229	CLA	CMB-C2B	-2.20	1.46	1.50
20	2	610	CLA	CHC-C1C	2.20	1.42	1.38
20	A	1107	CLA	MG-NB	-2.20	2.01	2.05
20	B	1224	CLA	CMB-C2B	-2.20	1.46	1.50
29	4	621	LUT	C26-C27	-2.20	1.47	1.50
20	B	1231	CLA	CMB-C2B	-2.20	1.46	1.50
28	4	608	CHL	C4C-C3C	2.20	1.48	1.45
20	J	102	CLA	CHC-C1C	2.20	1.42	1.38
20	B	1211	CLA	CMD-C2D	-2.20	1.46	1.50
20	1	602	CLA	MG-NB	-2.20	2.01	2.05
19	A	1011	CL0	CMC-C2C	-2.19	1.46	1.50
20	B	1206	CLA	CMD-C2D	-2.19	1.46	1.50
28	2	615	CHL	C1B-NB	-2.19	1.35	1.37
20	A	1120	CLA	CMD-C2D	-2.19	1.46	1.50
20	A	1140	CLA	CHC-C1C	2.19	1.42	1.38
20	A	1134	CLA	MG-NB	-2.19	2.01	2.05
26	G	402	LMT	O3B-C3B	-2.19	1.37	1.43
20	A	1111	CLA	C3B-C4B	2.19	1.49	1.42
26	A	5004	LMT	O3B-C3B	-2.19	1.37	1.43
20	A	1124	CLA	CMD-C2D	-2.19	1.46	1.50
20	B	1223	CLA	CHC-C1C	2.19	1.42	1.38
20	3	606	CLA	CHC-C1C	2.19	1.42	1.38
20	1	611	CLA	CHC-C1C	2.19	1.42	1.38
20	B	1228	CLA	MG-NB	-2.18	2.01	2.05
28	2	602	CHL	C1B-NB	-2.18	1.35	1.37
23	3	624	BCR	C30-C25	-2.18	1.51	1.53
26	B	5001	LMT	O3B-C3B	-2.18	1.37	1.43
28	2	602	CHL	CHB-C4A	-2.18	1.32	1.37
20	3	603	CLA	CHC-C1C	2.18	1.42	1.38
20	A	1120	CLA	MG-NB	-2.18	2.01	2.05
20	B	1205	CLA	CMD-C2D	-2.18	1.46	1.50
20	B	1235	CLA	CMD-C2D	-2.18	1.46	1.50
26	1	631	LMT	O3B-C3B	-2.18	1.37	1.43
20	A	1131	CLA	CMD-C2D	-2.18	1.46	1.50
27	B	5002	DGD	C3G-C2G	2.17	1.57	1.50
20	2	613	CLA	CHC-C1C	2.17	1.42	1.38
20	B	1216	CLA	MG-ND	-2.17	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B	1204	CLA	MG-NB	-2.17	2.01	2.05
20	K	202	CLA	MG-NB	-2.17	2.01	2.05
20	B	1225	CLA	C3B-C4B	2.17	1.49	1.42
20	A	1114	CLA	CMD-C2D	-2.17	1.46	1.50
20	3	606	CLA	CMC-C2C	-2.17	1.46	1.50
20	A	1801	CLA	CMD-C2D	-2.17	1.46	1.50
20	B	1224	CLA	CMD-C2D	-2.17	1.46	1.50
20	2	604	CLA	CMB-C2B	-2.16	1.46	1.50
28	4	615	CHL	C1B-NB	-2.16	1.35	1.37
20	A	1140	CLA	CMB-C2B	-2.16	1.46	1.50
20	B	1204	CLA	CHC-C1C	2.16	1.42	1.38
20	J	102	CLA	MG-NB	-2.16	2.01	2.05
20	K	204	CLA	MG-NB	-2.16	2.01	2.05
28	3	608	CHL	C2C-C1C	2.16	1.49	1.44
28	2	608	CHL	C1B-NB	-2.16	1.35	1.37
20	B	1214	CLA	CHC-C1C	2.16	1.42	1.38
20	B	1204	CLA	CMB-C2B	-2.16	1.46	1.50
20	A	1112	CLA	CMD-C2D	-2.16	1.46	1.50
20	A	1134	CLA	CMB-C2B	-2.16	1.46	1.50
20	I	121	CLA	CHC-C1C	2.16	1.42	1.38
20	B	1226	CLA	C1B-C2B	2.16	1.48	1.43
20	A	1113	CLA	MG-NB	-2.16	2.01	2.05
20	2	612	CLA	MG-NB	-2.16	2.01	2.05
20	B	1205	CLA	CMB-C2B	-2.16	1.46	1.50
20	2	613	CLA	CMD-C2D	-2.16	1.46	1.50
20	B	1021	CLA	C3B-C4B	2.16	1.49	1.42
20	B	1215	CLA	CMC-C2C	-2.16	1.46	1.50
20	B	1214	CLA	C1B-C2B	2.16	1.48	1.43
28	2	608	CHL	C2C-C1C	2.16	1.49	1.44
20	B	1239	CLA	CMD-C2D	-2.16	1.46	1.50
20	B	1201	CLA	CHC-C1C	2.16	1.42	1.38
26	G	401	LMT	O3B-C3B	-2.16	1.37	1.43
20	A	1122	CLA	CMC-C2C	-2.16	1.46	1.50
20	4	614	CLA	MG-NB	-2.16	2.01	2.05
20	1	603	CLA	CMD-C2D	-2.16	1.46	1.50
20	B	1202	CLA	CMC-C2C	-2.16	1.46	1.50
20	G	201	CLA	CMD-C2D	-2.15	1.46	1.50
23	G	311	BCR	C1-C6	-2.15	1.51	1.53
20	B	1203	CLA	C3B-C4B	2.15	1.49	1.42
20	A	1135	CLA	CMB-C2B	-2.15	1.46	1.50
20	3	613	CLA	MG-NB	-2.15	2.01	2.05
20	A	1108	CLA	CMC-C2C	-2.15	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	4	613	CLA	CMD-C2D	-2.15	1.46	1.50
20	B	1202	CLA	MG-NB	-2.15	2.01	2.05
23	K	301	BCR	C30-C25	-2.15	1.51	1.53
20	A	1101	CLA	CMD-C2D	-2.15	1.46	1.50
20	F	302	CLA	MG-NB	-2.15	2.01	2.05
20	4	609	CLA	CMD-C2D	-2.15	1.46	1.50
20	B	1203	CLA	CMD-C2D	-2.14	1.46	1.50
20	A	1136	CLA	CMD-C2D	-2.14	1.46	1.50
28	2	606	CHL	C1B-NB	-2.14	1.35	1.37
20	B	1230	CLA	CMD-C2D	-2.14	1.46	1.50
24	A	5003	LHG	O7-C5	-2.14	1.41	1.46
20	1	611	CLA	CMD-C2D	-2.14	1.46	1.50
20	B	1212	CLA	CMD-C2D	-2.14	1.46	1.50
20	B	1227	CLA	CMC-C2C	-2.14	1.46	1.50
20	4	611	CLA	MG-NB	-2.14	2.01	2.05
20	4	613	CLA	MG-NB	-2.14	2.01	2.05
20	1	603	CLA	MG-NB	-2.14	2.01	2.05
20	B	1201	CLA	C3B-C4B	2.14	1.49	1.42
20	A	8895	CLA	CMB-C2B	-2.14	1.46	1.50
20	A	1115	CLA	MG-NB	-2.14	2.01	2.05
20	A	1121	CLA	CMB-C2B	-2.14	1.46	1.50
23	I	120	BCR	C33-C5	-2.14	1.47	1.50
20	3	613	CLA	CMD-C2D	-2.14	1.46	1.50
20	A	1111	CLA	CMD-C2D	-2.13	1.46	1.50
20	1	603	CLA	CHC-C1C	2.13	1.42	1.38
20	H	200	CLA	MG-NB	-2.13	2.01	2.05
20	L	303	CLA	CHC-C1C	2.13	1.42	1.38
20	B	1237	CLA	CMD-C2D	-2.13	1.46	1.50
20	A	1139	CLA	CMC-C2C	-2.13	1.46	1.50
20	4	604	CLA	MG-NB	-2.13	2.01	2.05
20	A	1105	CLA	CMB-C2B	-2.13	1.46	1.50
20	3	602	CLA	CMD-C2D	-2.13	1.46	1.50
20	3	617	CLA	MG-NB	-2.13	2.01	2.05
20	K	201	CLA	MG-NB	-2.13	2.01	2.05
20	1	606	CLA	C3B-C4B	2.13	1.48	1.42
24	4	630	LHG	P-O6	2.13	1.67	1.59
26	B	5001	LMT	O4'-C4B	-2.13	1.37	1.43
20	B	1217	CLA	CHC-C1C	2.13	1.42	1.38
20	B	1234	CLA	CMD-C2D	-2.13	1.46	1.50
20	A	1130	CLA	MG-NB	-2.13	2.01	2.05
20	3	606	CLA	CMD-C2D	-2.13	1.46	1.50
20	3	609	CLA	CMB-C2B	-2.13	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B	1224	CLA	MG-ND	-2.12	2.01	2.05
28	2	602	CHL	C4C-C3C	2.12	1.48	1.45
20	B	1203	CLA	CMC-C2C	-2.12	1.46	1.50
20	2	614	CLA	MG-NB	-2.12	2.01	2.05
20	A	1115	CLA	CMD-C2D	-2.12	1.46	1.50
20	B	1240	CLA	MG-NB	-2.12	2.01	2.05
20	1	608	CLA	CHC-C1C	2.12	1.42	1.38
28	2	601	CHL	C4C-C3C	2.12	1.48	1.45
20	1	610	CLA	CMC-C2C	-2.12	1.46	1.50
23	F	416	BCR	C30-C25	-2.12	1.51	1.53
20	B	1230	CLA	MG-NB	-2.12	2.01	2.05
20	A	1103	CLA	CMD-C2D	-2.12	1.46	1.50
20	A	1105	CLA	CMD-C2D	-2.12	1.46	1.50
20	A	1106	CLA	CMC-C2C	-2.12	1.46	1.50
28	2	606	CHL	C4C-C3C	2.12	1.48	1.45
20	2	603	CLA	MG-NB	-2.12	2.01	2.05
26	B	5001	LMT	O1'-C1'	-2.12	1.36	1.40
20	A	1110	CLA	CMD-C2D	-2.12	1.46	1.50
20	F	301	CLA	CMD-C2D	-2.12	1.46	1.50
28	4	608	CHL	CHB-C4A	-2.12	1.32	1.37
20	1	606	CLA	CMD-C2D	-2.12	1.46	1.50
28	2	602	CHL	C4B-NB	-2.12	1.35	1.37
20	3	604	CLA	CMD-C2D	-2.12	1.46	1.50
20	B	1223	CLA	CMD-C2D	-2.12	1.46	1.50
28	1	607	CHL	C1B-NB	-2.12	1.35	1.37
28	4	607	CHL	C3B-C4B	2.12	1.48	1.42
20	K	204	CLA	CMC-C2C	-2.11	1.46	1.50
20	B	1012	CLA	C1B-C2B	2.11	1.48	1.43
20	3	611	CLA	CMD-C2D	-2.11	1.46	1.50
28	2	606	CHL	C3B-C4B	2.11	1.48	1.42
20	G	201	CLA	MG-NB	-2.11	2.01	2.05
20	A	1107	CLA	CMD-C2D	-2.11	1.46	1.50
23	A	4003	BCR	C30-C25	-2.11	1.51	1.53
20	A	1109	CLA	CMB-C2B	-2.11	1.46	1.50
20	B	1215	CLA	CMD-C2D	-2.11	1.46	1.50
20	4	610	CLA	CMB-C2B	-2.11	1.46	1.50
20	A	1107	CLA	CMB-C2B	-2.11	1.46	1.50
20	1	612	CLA	MG-NB	-2.11	2.01	2.05
20	K	203	CLA	C3C-C2C	2.11	1.40	1.35
20	B	1225	CLA	CHC-C1C	2.11	1.42	1.38
20	A	1120	CLA	CMB-C2B	-2.11	1.46	1.50
20	A	1118	CLA	CMB-C2B	-2.11	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B	1214	CLA	CMC-C2C	-2.11	1.46	1.50
20	3	603	CLA	CMB-C2B	-2.11	1.46	1.50
20	A	1112	CLA	CMB-C2B	-2.11	1.46	1.50
23	1	623	BCR	C12-C13	-2.11	1.44	1.50
20	3	606	CLA	CMB-C2B	-2.11	1.46	1.50
20	B	1021	CLA	MG-ND	-2.11	2.01	2.05
20	A	1112	CLA	MG-NB	-2.11	2.01	2.05
20	B	1221	CLA	C4-C3	-2.11	1.45	1.50
20	B	1237	CLA	CMC-C2C	-2.10	1.46	1.50
20	3	610	CLA	MG-NB	-2.10	2.01	2.05
20	B	1213	CLA	CMD-C2D	-2.10	1.46	1.50
20	B	1240	CLA	CMC-C2C	-2.10	1.46	1.50
20	A	1138	CLA	CMD-C2D	-2.10	1.46	1.50
20	I	121	CLA	CMC-C2C	-2.10	1.46	1.50
20	A	1137	CLA	CMD-C2D	-2.10	1.46	1.50
20	3	614	CLA	MG-NB	-2.10	2.01	2.05
20	1	608	CLA	CMD-C2D	-2.10	1.46	1.50
26	4	631	LMT	O4'-C4B	-2.10	1.37	1.43
28	4	607	CHL	CHB-C4A	-2.10	1.32	1.37
20	A	1102	CLA	CMC-C2C	-2.10	1.46	1.50
20	B	1214	CLA	MG-NB	-2.10	2.01	2.05
20	A	1134	CLA	CHC-C1C	2.10	1.42	1.38
20	F	302	CLA	CMB-C2B	-2.10	1.46	1.50
20	A	1101	CLA	CMB-C2B	-2.10	1.46	1.50
20	B	1226	CLA	C3B-C4B	2.10	1.48	1.42
20	2	609	CLA	CMD-C2D	-2.10	1.46	1.50
20	3	611	CLA	MG-NB	-2.10	2.01	2.05
20	1	612	CLA	CMB-C2B	-2.09	1.46	1.50
20	2	603	CLA	CMD-C2D	-2.09	1.46	1.50
28	2	607	CHL	C1B-NB	-2.09	1.35	1.37
28	1	601	CHL	CHB-C4A	-2.09	1.32	1.37
20	2	604	CLA	MG-NB	-2.09	2.01	2.05
20	A	1119	CLA	CMC-C2C	-2.09	1.46	1.50
20	L	303	CLA	MG-NB	-2.09	2.01	2.05
20	4	601	CLA	CMD-C2D	-2.09	1.46	1.50
20	F	303	CLA	C3C-C2C	2.09	1.40	1.35
28	2	602	CHL	C3B-C4B	2.09	1.48	1.42
20	B	1236	CLA	CMD-C2D	-2.09	1.46	1.50
20	B	1209	CLA	CMD-C2D	-2.09	1.46	1.50
20	4	603	CLA	CMD-C2D	-2.09	1.46	1.50
28	1	607	CHL	C2C-C1C	2.09	1.49	1.44
20	2	610	CLA	CMD-C2D	-2.09	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B	1239	CLA	MG-NB	-2.09	2.01	2.05
20	J	102	CLA	CMD-C2D	-2.09	1.46	1.50
20	K	204	CLA	CMD-C2D	-2.09	1.46	1.50
20	O	203	CLA	MG-NB	-2.08	2.01	2.05
20	B	1213	CLA	CMC-C2C	-2.08	1.46	1.50
20	2	604	CLA	CMD-C2D	-2.08	1.46	1.50
20	3	605	CLA	C3C-C2C	2.08	1.40	1.35
20	3	617	CLA	CMD-C2D	-2.08	1.46	1.50
20	F	302	CLA	CMD-C2D	-2.08	1.46	1.50
20	B	1201	CLA	MG-NB	-2.08	2.01	2.05
20	3	609	CLA	CMD-C2D	-2.08	1.46	1.50
20	4	614	CLA	CMD-C2D	-2.08	1.46	1.50
20	G	202	CLA	MG-NB	-2.08	2.01	2.05
20	A	1119	CLA	CMD-C2D	-2.08	1.46	1.50
20	A	1137	CLA	CMB-C2B	-2.08	1.46	1.50
20	A	1132	CLA	CMD-C2D	-2.08	1.46	1.50
20	A	1128	CLA	MG-ND	-2.08	2.01	2.05
20	1	609	CLA	CMB-C2B	-2.08	1.46	1.50
20	A	1126	CLA	MG-ND	-2.08	2.01	2.05
25	J	302	LMG	C4-C5	2.08	1.57	1.53
20	1	614	CLA	CMD-C2D	-2.08	1.46	1.50
28	4	606	CHL	C2C-C1C	2.08	1.49	1.44
20	A	1022	CLA	CHC-C1C	2.08	1.42	1.38
20	A	1107	CLA	CHC-C1C	2.08	1.42	1.38
20	B	1208	CLA	CMD-C2D	-2.08	1.46	1.50
24	2	630	LHG	O7-C5	-2.08	1.41	1.46
20	A	1130	CLA	CMD-C2D	-2.07	1.46	1.50
20	B	1232	CLA	CMD-C2D	-2.07	1.46	1.50
20	B	1237	CLA	CHC-C1C	2.07	1.42	1.38
20	B	1228	CLA	CMC-C2C	-2.07	1.46	1.50
27	B	5002	DGD	C3D-C2D	2.07	1.57	1.52
28	4	615	CHL	C3B-C4B	2.07	1.48	1.42
20	3	605	CLA	MG-NB	-2.07	2.01	2.05
20	A	1135	CLA	CMD-C2D	-2.07	1.46	1.50
20	B	1209	CLA	CMB-C2B	-2.07	1.46	1.50
20	A	1117	CLA	CMD-C2D	-2.07	1.46	1.50
20	3	610	CLA	CMD-C2D	-2.07	1.46	1.50
20	K	202	CLA	CMB-C2B	-2.07	1.46	1.50
20	L	303	CLA	CMC-C2C	-2.07	1.46	1.50
27	B	5002	DGD	O5D-C6D	-2.07	1.40	1.43
20	B	1203	CLA	CHC-C1C	2.07	1.42	1.38
20	J	102	CLA	CMB-C2B	-2.07	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	L	301	CLA	CMD-C2D	-2.07	1.46	1.50
20	1	614	CLA	CMB-C2B	-2.07	1.46	1.50
20	K	202	CLA	CMD-C2D	-2.07	1.46	1.50
23	A	4007	BCR	C4-C5	-2.07	1.47	1.51
20	3	613	CLA	CMB-C2B	-2.06	1.46	1.50
20	A	1108	CLA	CMD-C2D	-2.06	1.46	1.50
20	2	612	CLA	CMD-C2D	-2.06	1.46	1.50
20	3	606	CLA	MG-NB	-2.06	2.01	2.05
20	B	1229	CLA	CMD-C2D	-2.06	1.46	1.50
20	2	614	CLA	CMD-C2D	-2.06	1.46	1.50
20	L	302	CLA	CMD-C2D	-2.06	1.46	1.50
20	A	1132	CLA	CMC-C2C	-2.06	1.46	1.50
20	1	604	CLA	CMD-C2D	-2.06	1.46	1.50
20	L	303	CLA	CMD-C2D	-2.06	1.46	1.50
20	A	1122	CLA	CMD-C2D	-2.06	1.46	1.50
20	1	615	CLA	CMD-C2D	-2.06	1.46	1.50
20	4	602	CLA	CMD-C2D	-2.06	1.46	1.50
20	A	1110	CLA	MG-NB	-2.06	2.01	2.05
20	3	603	CLA	MG-NB	-2.06	2.01	2.05
20	A	1122	CLA	CHC-C1C	2.06	1.42	1.38
20	A	1104	CLA	CMB-C2B	-2.06	1.46	1.50
20	A	1801	CLA	CMC-C2C	-2.06	1.46	1.50
20	3	603	CLA	CMD-C2D	-2.06	1.46	1.50
20	K	201	CLA	CMC-C2C	-2.06	1.46	1.50
28	2	607	CHL	C3B-C4B	2.06	1.48	1.42
24	3	630	LHG	O7-C5	-2.06	1.41	1.46
20	O	201	CLA	C3C-C2C	2.06	1.40	1.35
20	A	1140	CLA	CMC-C2C	-2.06	1.46	1.50
20	A	1112	CLA	CMC-C2C	-2.06	1.46	1.50
20	4	611	CLA	CMB-C2B	-2.06	1.46	1.50
20	4	612	CLA	CMB-C2B	-2.06	1.46	1.50
20	A	1013	CLA	C1D-ND	2.06	1.40	1.37
20	B	1214	CLA	CMD-C2D	-2.05	1.46	1.50
20	A	1106	CLA	CMB-C2B	-2.05	1.46	1.50
20	B	1221	CLA	CMC-C2C	-2.05	1.46	1.50
20	1	609	CLA	CMD-C2D	-2.05	1.46	1.50
20	B	1206	CLA	CMC-C2C	-2.05	1.46	1.50
20	4	601	CLA	CMB-C2B	-2.05	1.46	1.50
20	A	1107	CLA	C3B-C4B	2.05	1.48	1.42
20	A	1109	CLA	CMC-C2C	-2.05	1.46	1.50
20	A	1127	CLA	CMC-C2C	-2.05	1.46	1.50
20	O	202	CLA	MG-NB	-2.05	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	A	1113	CLA	CMC-C2C	-2.05	1.46	1.50
20	G	218	CLA	CMB-C2B	-2.05	1.46	1.50
20	B	1236	CLA	MG-NB	-2.05	2.01	2.05
20	O	203	CLA	C3C-C2C	2.05	1.40	1.35
20	K	204	CLA	CMB-C2B	-2.05	1.46	1.50
20	3	607	CLA	MG-NB	-2.05	2.01	2.05
20	4	601	CLA	MG-NB	-2.05	2.01	2.05
20	B	1228	CLA	CMD-C2D	-2.05	1.46	1.50
20	B	1225	CLA	CMB-C2B	-2.05	1.46	1.50
20	A	1115	CLA	CMC-C2C	-2.05	1.46	1.50
20	B	1212	CLA	CMB-C2B	-2.05	1.46	1.50
20	1	612	CLA	CMD-C2D	-2.05	1.46	1.50
20	2	613	CLA	CMB-C2B	-2.05	1.46	1.50
20	A	1109	CLA	MG-ND	-2.05	2.01	2.05
20	O	201	CLA	MG-NB	-2.05	2.01	2.05
28	2	602	CHL	C2C-C1C	2.05	1.48	1.44
20	K	201	CLA	CMD-C2D	-2.04	1.46	1.50
28	4	607	CHL	C4D-CHA	2.04	1.45	1.38
20	A	1117	CLA	CHC-C1C	2.04	1.42	1.38
28	2	615	CHL	C4C-C3C	2.04	1.48	1.45
20	A	1113	CLA	CMD-C2D	-2.04	1.46	1.50
20	L	302	CLA	CMB-C2B	-2.04	1.46	1.50
20	A	1110	CLA	CMB-C2B	-2.04	1.46	1.50
20	2	613	CLA	MG-NB	-2.04	2.01	2.05
28	2	602	CHL	C3A-C2A	-2.04	1.48	1.54
20	B	1216	CLA	CMC-C2C	-2.04	1.46	1.50
20	1	606	CLA	CMC-C2C	-2.04	1.46	1.50
28	2	602	CHL	C4D-CHA	2.04	1.45	1.38
20	A	1131	CLA	CMB-C2B	-2.04	1.46	1.50
28	2	615	CHL	C3B-C4B	2.04	1.48	1.42
20	1	611	CLA	CMB-C2B	-2.04	1.46	1.50
20	4	604	CLA	CMB-C2B	-2.04	1.46	1.50
28	4	608	CHL	C4D-CHA	2.04	1.45	1.38
20	3	611	CLA	CMB-C2B	-2.04	1.46	1.50
20	4	614	CLA	CMB-C2B	-2.04	1.46	1.50
20	B	1214	CLA	MG-ND	-2.04	2.01	2.05
20	3	612	CLA	CMD-C2D	-2.04	1.46	1.50
20	4	612	CLA	CMD-C2D	-2.04	1.46	1.50
20	G	202	CLA	CMD-C2D	-2.04	1.46	1.50
20	B	1216	CLA	C4B-NB	2.04	1.40	1.37
20	B	1222	CLA	CMC-C2C	-2.04	1.46	1.50
20	1	604	CLA	MG-NB	-2.04	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	J	302	LMG	O7-C8	-2.03	1.41	1.46
20	B	1219	CLA	MG-ND	-2.03	2.01	2.05
20	B	1221	CLA	MG-ND	-2.03	2.01	2.05
20	A	1102	CLA	CMB-C2B	-2.03	1.46	1.50
20	A	1127	CLA	CMB-C2B	-2.03	1.46	1.50
20	2	603	CLA	CMB-C2B	-2.03	1.46	1.50
28	2	611	CHL	C1D-ND	-2.03	1.35	1.37
19	A	1011	CL0	MG-ND	-2.03	2.01	2.05
20	B	1208	CLA	CMB-C2B	-2.03	1.46	1.50
20	A	1116	CLA	MG-ND	-2.03	2.01	2.05
20	A	1128	CLA	CMC-C2C	-2.03	1.46	1.50
20	B	1226	CLA	CHC-C1C	2.03	1.42	1.38
26	G	402	LMT	O4'-C4B	-2.03	1.37	1.43
20	A	8895	CLA	MG-ND	-2.03	2.01	2.05
24	1	630	LHG	P-O6	2.03	1.67	1.59
20	4	603	CLA	CMB-C2B	-2.03	1.46	1.50
20	3	607	CLA	CMD-C2D	-2.03	1.46	1.50
20	4	611	CLA	CMC-C2C	-2.03	1.46	1.50
20	B	1201	CLA	CMB-C2B	-2.03	1.46	1.50
20	1	610	CLA	CMD-C2D	-2.02	1.46	1.50
20	3	610	CLA	CMB-C2B	-2.02	1.46	1.50
20	4	610	CLA	CMC-C2C	-2.02	1.46	1.50
20	O	202	CLA	C3C-C2C	2.02	1.39	1.35
20	3	614	CLA	CMD-C2D	-2.02	1.46	1.50
20	A	1127	CLA	C1B-NB	-2.02	1.35	1.37
20	1	613	CLA	CMB-C2B	-2.02	1.46	1.50
20	B	1204	CLA	CMD-C2D	-2.02	1.46	1.50
28	2	611	CHL	C2C-C1C	2.02	1.48	1.44
20	A	1128	CLA	C1B-C2B	2.02	1.47	1.43
20	A	1102	CLA	CMD-C2D	-2.02	1.46	1.50
20	A	1110	CLA	CMC-C2C	-2.02	1.46	1.50
28	2	615	CHL	C2C-C1C	2.02	1.48	1.44
20	3	602	CLA	CMC-C2C	-2.02	1.46	1.50
20	1	615	CLA	MG-NB	-2.02	2.01	2.05
26	G	401	LMT	O1'-C1'	-2.02	1.36	1.40
20	A	1116	CLA	CMC-C2C	-2.02	1.46	1.50
20	1	613	CLA	CMC-C2C	-2.02	1.46	1.50
20	1	613	CLA	CMD-C2D	-2.02	1.46	1.50
20	2	614	CLA	CMB-C2B	-2.02	1.46	1.50
28	4	608	CHL	C3B-C4B	2.02	1.48	1.42
20	4	609	CLA	CMB-C2B	-2.02	1.46	1.50
24	2	630	LHG	P-O6	2.02	1.67	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	3	617	CLA	CMC-C2C	-2.01	1.46	1.50
20	B	1228	CLA	CMB-C2B	-2.01	1.46	1.50
20	2	613	CLA	CMC-C2C	-2.01	1.46	1.50
28	1	607	CHL	CHB-C4A	-2.01	1.32	1.37
20	A	1125	CLA	CMC-C2C	-2.01	1.46	1.50
20	4	603	CLA	CMC-C2C	-2.01	1.46	1.50
20	1	606	CLA	CHC-C1C	2.01	1.42	1.38
25	J	301	LMG	O7-C8	-2.01	1.41	1.46
28	2	611	CHL	C3B-C4B	2.01	1.48	1.42
20	B	1217	CLA	CMB-C2B	-2.01	1.46	1.50
20	B	1240	CLA	CMB-C2B	-2.01	1.46	1.50
20	3	612	CLA	CMB-C2B	-2.01	1.46	1.50
20	B	1235	CLA	CMC-C2C	-2.01	1.46	1.50
20	1	604	CLA	CMB-C2B	-2.01	1.46	1.50
20	1	608	CLA	MG-NB	-2.01	2.01	2.05
20	4	613	CLA	CMC-C2C	-2.01	1.46	1.50
23	I	120	BCR	C29-C28	-2.01	1.47	1.52
20	B	1229	CLA	MG-NB	-2.01	2.01	2.05
27	B	5002	DGD	C4E-C3E	2.01	1.57	1.52
20	A	1102	CLA	MG-NB	-2.01	2.01	2.05
20	B	1236	CLA	CMB-C2B	-2.01	1.46	1.50
20	A	1130	CLA	CMC-C2C	-2.01	1.46	1.50
23	B	4017	BCR	C38-C26	-2.01	1.47	1.50
20	3	607	CLA	CMB-C2B	-2.01	1.46	1.50
20	4	610	CLA	MG-ND	-2.01	2.01	2.05
20	4	604	CLA	CMD-C2D	-2.01	1.46	1.50
20	A	1117	CLA	CMC-C2C	-2.01	1.46	1.50
23	A	4007	BCR	C38-C26	-2.00	1.47	1.50
20	B	1021	CLA	CMB-C2B	-2.00	1.46	1.50
20	1	606	CLA	CMB-C2B	-2.00	1.46	1.50
20	1	615	CLA	CMC-C2C	-2.00	1.46	1.50
20	L	302	CLA	CHC-C1C	2.00	1.42	1.38
20	4	613	CLA	CMB-C2B	-2.00	1.46	1.50
20	G	201	CLA	CMB-C2B	-2.00	1.46	1.50

All (1773) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	4	621	LUT	O23-C23-C22	-11.92	88.94	110.06
20	2	609	CLA	C4A-NA-C1A	10.10	111.29	106.68
20	4	609	CLA	C4A-NA-C1A	9.85	111.17	106.68
20	1	609	CLA	C4A-NA-C1A	9.25	110.90	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	1106	CLA	C4A-NA-C1A	9.16	110.86	106.68
20	1	610	CLA	C4A-NA-C1A	9.13	110.84	106.68
29	4	621	LUT	C37-C21-C22	9.08	126.32	109.41
28	3	608	CHL	CMD-C2D-C1D	8.73	140.09	124.73
20	3	602	CLA	C4A-NA-C1A	8.70	110.65	106.68
28	2	607	CHL	CMD-C2D-C1D	8.64	139.94	124.73
28	1	607	CHL	CMD-C2D-C1D	8.62	139.92	124.73
20	4	610	CLA	C4A-NA-C1A	8.61	110.61	106.68
20	A	1127	CLA	C4A-NA-C1A	8.57	110.59	106.68
28	2	601	CHL	CMD-C2D-C1D	8.53	139.75	124.73
28	4	608	CHL	CMD-C2D-C1D	8.47	139.65	124.73
28	2	608	CHL	CMD-C2D-C1D	8.43	139.58	124.73
20	B	1232	CLA	C4A-NA-C1A	8.39	110.51	106.68
28	2	606	CHL	CMD-C2D-C1D	8.36	139.46	124.73
20	B	1215	CLA	C4A-NA-C1A	8.35	110.49	106.68
28	4	606	CHL	CMD-C2D-C1D	8.26	139.28	124.73
28	4	607	CHL	CMD-C2D-C1D	8.25	139.26	124.73
28	4	615	CHL	CMD-C2D-C1D	8.24	139.24	124.73
28	2	615	CHL	CMD-C2D-C1D	8.22	139.21	124.73
28	1	601	CHL	C2C-C3C-C4C	-8.12	100.56	106.43
20	A	1125	CLA	C4A-NA-C1A	8.06	110.36	106.68
28	2	608	CHL	C2C-C3C-C4C	-8.06	100.60	106.43
28	1	601	CHL	CMD-C2D-C1D	8.05	138.90	124.73
20	B	1221	CLA	C4A-NA-C1A	7.94	110.30	106.68
20	A	1105	CLA	C4A-NA-C1A	7.88	110.27	106.68
20	3	614	CLA	C4A-NA-C1A	7.85	110.26	106.68
20	1	602	CLA	C4A-NA-C1A	7.79	110.23	106.68
20	B	1205	CLA	C4A-NA-C1A	7.64	110.16	106.68
20	A	1114	CLA	C4A-NA-C1A	7.60	110.15	106.68
20	1	614	CLA	C4A-NA-C1A	7.60	110.15	106.68
20	A	1108	CLA	C4A-NA-C1A	7.60	110.14	106.68
28	2	611	CHL	C2C-C3C-C4C	-7.59	100.94	106.43
20	A	1121	CLA	C4A-NA-C1A	7.58	110.14	106.68
28	2	602	CHL	C2C-C3C-C4C	-7.57	100.95	106.43
28	4	607	CHL	C2C-C3C-C4C	-7.56	100.96	106.43
29	1	621	LUT	O23-C23-C22	7.56	123.44	110.06
20	L	303	CLA	C4A-NA-C1A	7.50	110.10	106.68
28	2	601	CHL	C2C-C3C-C4C	-7.50	101.00	106.43
20	B	1211	CLA	C4A-NA-C1A	7.43	110.07	106.68
28	2	611	CHL	CMD-C2D-C1D	7.41	137.78	124.73
20	L	301	CLA	C4A-NA-C1A	7.41	110.06	106.68
28	2	602	CHL	C2B-C1B-NB	7.40	118.00	110.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	1240	CLA	C4A-NA-C1A	7.39	110.05	106.68
28	2	602	CHL	CMD-C2D-C1D	7.38	137.73	124.73
20	B	1202	CLA	C4A-NA-C1A	7.35	110.03	106.68
28	2	607	CHL	C2C-C3C-C4C	-7.31	101.14	106.43
20	A	1134	CLA	C4A-NA-C1A	7.31	110.01	106.68
29	1	620	LUT	O23-C23-C22	7.31	123.01	110.06
20	A	1132	CLA	C4A-NA-C1A	7.29	110.00	106.68
28	1	607	CHL	C2C-C3C-C4C	-7.27	101.17	106.43
28	4	608	CHL	C2C-C3C-C4C	-7.26	101.18	106.43
28	4	606	CHL	C2C-C3C-C4C	-7.24	101.19	106.43
20	A	1113	CLA	C4A-NA-C1A	7.24	109.98	106.68
20	A	1107	CLA	C4A-NA-C1A	7.21	109.97	106.68
20	A	1110	CLA	C4A-NA-C1A	7.17	109.95	106.68
29	4	621	LUT	C36-C21-C22	-7.14	96.10	109.41
20	2	614	CLA	C4A-NA-C1A	7.13	109.93	106.68
20	A	1122	CLA	C4A-NA-C1A	7.12	109.93	106.68
20	B	1212	CLA	C4A-NA-C1A	7.05	109.90	106.68
28	4	615	CHL	C2C-C3C-C4C	-7.03	101.34	106.43
20	J	102	CLA	C4A-NA-C1A	7.03	109.89	106.68
20	B	1210	CLA	C4A-NA-C1A	7.00	109.87	106.68
20	A	8895	CLA	C4A-NA-C1A	6.96	109.85	106.68
28	1	601	CHL	C2B-C1B-NB	6.95	117.53	110.33
20	B	1209	CLA	C4A-NA-C1A	6.95	109.85	106.68
28	4	608	CHL	C2B-C1B-NB	6.94	117.52	110.33
20	A	1126	CLA	C4A-NA-C1A	6.92	109.83	106.68
20	1	604	CLA	C4A-NA-C1A	6.90	109.83	106.68
20	4	601	CLA	C4A-NA-C1A	6.89	109.82	106.68
20	1	606	CLA	C4A-NA-C1A	6.87	109.81	106.68
20	A	1111	CLA	C4A-NA-C1A	6.85	109.81	106.68
28	4	606	CHL	C2B-C1B-NB	6.83	117.40	110.33
28	1	607	CHL	C2B-C1B-NB	6.82	117.39	110.33
20	1	608	CLA	C4A-NA-C1A	6.81	109.79	106.68
28	4	607	CHL	C2B-C1B-NB	6.81	117.39	110.33
20	3	603	CLA	C4A-NA-C1A	6.81	109.78	106.68
20	4	602	CLA	C4A-NA-C1A	6.81	109.78	106.68
28	4	615	CHL	C2B-C1B-NB	6.80	117.38	110.33
29	4	623	LUT	C21-C26-C27	6.79	120.63	112.83
20	A	1139	CLA	C4A-NA-C1A	6.79	109.78	106.68
28	2	607	CHL	C2B-C1B-NB	6.78	117.36	110.33
28	2	601	CHL	C2B-C1B-NB	6.78	117.36	110.33
28	2	615	CHL	C2B-C1B-NB	6.78	117.35	110.33
28	2	606	CHL	C2B-C1B-NB	6.74	117.31	110.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	1222	CLA	C4A-NA-C1A	6.72	109.74	106.68
28	2	606	CHL	C2C-C3C-C4C	-6.69	101.59	106.43
20	3	607	CLA	C4A-NA-C1A	6.67	109.72	106.68
20	3	604	CLA	C4A-NA-C1A	6.65	109.71	106.68
20	B	1226	CLA	CMB-C2B-C1B	-6.64	115.30	125.42
29	3	620	LUT	C21-C26-C27	6.64	120.46	112.83
20	4	611	CLA	C4A-NA-C1A	6.63	109.70	106.68
20	A	1801	CLA	C4A-NA-C1A	6.60	109.69	106.68
20	B	1216	CLA	CMB-C2B-C1B	-6.59	115.38	125.42
20	A	1138	CLA	C4A-NA-C1A	6.58	109.68	106.68
28	3	608	CHL	C2B-C1B-NB	6.57	117.14	110.33
20	1	615	CLA	C4A-NA-C1A	6.54	109.66	106.68
20	4	613	CLA	C4A-NA-C1A	6.54	109.66	106.68
20	B	1208	CLA	C4A-NA-C1A	6.53	109.66	106.68
28	2	611	CHL	C2B-C1B-NB	6.53	117.10	110.33
28	2	608	CHL	C2B-C1B-NB	6.53	117.09	110.33
20	B	1229	CLA	C4A-NA-C1A	6.52	109.65	106.68
28	3	608	CHL	C2C-C3C-C4C	-6.49	101.73	106.43
20	3	613	CLA	C4A-NA-C1A	6.46	109.63	106.68
29	4	621	LUT	C38-C25-C24	-6.44	108.12	123.36
20	F	301	CLA	C4A-NA-C1A	6.44	109.62	106.68
28	2	615	CHL	C2C-C3C-C4C	-6.43	101.78	106.43
20	G	218	CLA	C4A-NA-C1A	6.41	109.60	106.68
28	2	611	CHL	O2D-CGD-CBD	6.40	122.43	111.23
29	3	621	LUT	C21-C26-C27	6.40	120.18	112.83
20	G	201	CLA	C4A-NA-C1A	6.37	109.58	106.68
29	1	621	LUT	C26-C27-C28	6.34	134.44	124.58
29	2	621	LUT	C21-C26-C27	6.32	120.09	112.83
20	2	613	CLA	C4A-NA-C1A	6.31	109.56	106.68
28	2	601	CHL	O2D-CGD-CBD	6.25	122.15	111.23
29	4	621	LUT	C37-C21-C36	-6.23	98.80	107.87
20	2	604	CLA	C4A-NA-C1A	6.21	109.51	106.68
19	A	1011	CL0	C4A-NA-C1A	6.20	109.51	106.68
20	B	1227	CLA	C4A-NA-C1A	6.18	109.50	106.68
20	B	1214	CLA	C4A-NA-C1A	6.18	109.50	106.68
28	2	602	CHL	C3B-C2B-C1B	-6.17	99.90	107.17
20	O	201	CLA	C4A-NA-C1A	6.16	109.49	106.68
20	O	203	CLA	C4A-NA-C1A	6.14	109.48	106.68
20	3	605	CLA	C4A-NA-C1A	6.14	109.48	106.68
20	B	1228	CLA	C4A-NA-C1A	6.09	109.46	106.68
20	A	1103	CLA	C4A-NA-C1A	6.06	109.44	106.68
20	A	1101	CLA	C4A-NA-C1A	6.06	109.44	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	1013	CLA	C3B-C4B-NB	-6.05	105.13	110.53
20	F	303	CLA	C4A-NA-C1A	6.04	109.44	106.68
20	O	202	CLA	C4A-NA-C1A	6.03	109.43	106.68
20	B	1216	CLA	C3B-C4B-NB	-6.02	105.16	110.53
28	1	601	CHL	CAC-C3C-C4C	6.02	132.62	124.79
20	2	612	CLA	C4A-NA-C1A	5.99	109.41	106.68
20	B	1231	CLA	C4A-NA-C1A	5.99	109.41	106.68
29	1	620	LUT	C26-C27-C28	5.98	133.89	124.58
20	K	203	CLA	C4A-NA-C1A	5.98	109.41	106.68
20	A	1120	CLA	C4A-NA-C1A	5.87	109.36	106.68
20	B	1237	CLA	C4A-NA-C1A	5.84	109.34	106.68
20	A	1135	CLA	C4A-NA-C1A	5.84	109.34	106.68
23	A	4008	BCR	C40-C30-C25	5.83	119.38	110.24
20	3	609	CLA	C4A-NA-C1A	5.82	109.33	106.68
20	B	1206	CLA	C4A-NA-C1A	5.82	109.33	106.68
20	A	1117	CLA	C4A-NA-C1A	5.81	109.33	106.68
29	2	620	LUT	C21-C26-C27	5.79	119.48	112.83
28	4	608	CHL	C3B-C2B-C1B	-5.78	100.35	107.17
20	F	302	CLA	C4A-NA-C1A	5.78	109.32	106.68
20	B	1227	CLA	C3B-C4B-NB	-5.77	105.38	110.53
23	I	120	BCR	C40-C30-C25	5.77	119.28	110.24
28	2	608	CHL	C3B-C2B-C1B	-5.74	100.41	107.17
20	4	614	CLA	C4A-NA-C1A	5.73	109.29	106.68
20	B	1225	CLA	C4A-NA-C1A	5.72	109.29	106.68
28	4	615	CHL	C3B-C2B-C1B	-5.72	100.43	107.17
28	2	607	CHL	C3B-C2B-C1B	-5.70	100.44	107.17
29	2	623	LUT	C21-C26-C27	5.70	119.37	112.83
23	A	4007	BCR	C40-C30-C25	5.68	119.16	110.24
20	3	611	CLA	C4A-NA-C1A	5.67	109.27	106.68
20	G	202	CLA	C4A-NA-C1A	5.65	109.26	106.68
28	2	615	CHL	C3B-C2B-C1B	-5.65	100.51	107.17
28	2	608	CHL	CHD-C4C-C3C	-5.63	116.56	124.77
28	2	611	CHL	C3B-C2B-C1B	-5.61	100.55	107.17
20	A	1109	CLA	C4A-NA-C1A	5.61	109.24	106.68
28	1	601	CHL	C3B-C2B-C1B	-5.56	100.61	107.17
20	A	1104	CLA	C4A-NA-C1A	5.56	109.22	106.68
28	2	606	CHL	C3B-C2B-C1B	-5.56	100.61	107.17
20	4	604	CLA	C4A-NA-C1A	5.55	109.21	106.68
20	B	1023	CLA	C4A-NA-C1A	5.55	109.21	106.68
29	4	620	LUT	C22-C23-C24	-5.51	103.00	111.18
20	3	606	CLA	C4A-NA-C1A	5.51	109.19	106.68
29	2	620	LUT	C40-C33-C32	5.50	126.48	118.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	K	204	CLA	C4A-NA-C1A	5.49	109.18	106.68
28	2	601	CHL	C3B-C2B-C1B	-5.47	100.72	107.17
28	1	601	CHL	O2D-CGD-CBD	5.45	120.75	111.23
28	2	608	CHL	C3C-C4C-NC	5.43	117.39	110.43
20	A	1124	CLA	C4A-NA-C1A	5.43	109.16	106.68
28	4	606	CHL	C3B-C2B-C1B	-5.42	100.78	107.17
20	4	612	CLA	C4A-NA-C1A	5.40	109.14	106.68
20	B	1219	CLA	C4A-NA-C1A	5.39	109.14	106.68
29	1	620	LUT	C38-C25-C24	-5.37	110.65	123.36
20	3	612	CLA	C4A-NA-C1A	5.35	109.12	106.68
20	2	603	CLA	C4A-NA-C1A	5.33	109.11	106.68
28	1	607	CHL	O2D-CGD-CBD	5.33	120.55	111.23
20	A	1131	CLA	C4A-NA-C1A	5.33	109.11	106.68
29	4	620	LUT	C26-C27-C28	5.32	132.85	124.58
20	B	1230	CLA	C4A-NA-C1A	5.31	109.10	106.68
20	B	1213	CLA	C3B-C4B-NB	-5.30	105.80	110.53
28	4	607	CHL	C3B-C2B-C1B	-5.29	100.93	107.17
20	A	1137	CLA	C4A-NA-C1A	5.26	109.08	106.68
28	2	611	CHL	C3C-C4C-NC	5.25	117.15	110.43
28	3	608	CHL	C3B-C2B-C1B	-5.25	100.98	107.17
20	B	1021	CLA	C4A-NA-C1A	5.24	109.07	106.68
20	B	1226	CLA	C2D-C1D-ND	-5.23	104.94	110.13
28	2	608	CHL	C3D-C2D-C1D	-5.22	98.71	105.83
28	2	615	CHL	O2D-CGD-CBD	5.20	120.33	111.23
28	2	606	CHL	O2D-CGD-CBD	5.19	120.30	111.23
20	B	1203	CLA	C4A-NA-C1A	5.19	109.05	106.68
28	1	601	CHL	C3D-C2D-C1D	-5.18	98.76	105.83
28	4	606	CHL	O2D-CGD-CBD	5.14	120.22	111.23
20	B	1219	CLA	CMB-C2B-C1B	-5.14	117.59	125.42
28	1	607	CHL	C3B-C2B-C1B	-5.12	101.14	107.17
28	3	608	CHL	C3D-C2D-C1D	-5.11	98.85	105.83
20	A	1119	CLA	CMB-C2B-C1B	-5.10	117.65	125.42
29	1	621	LUT	C38-C25-C24	-5.08	111.33	123.36
20	B	1236	CLA	C4A-NA-C1A	5.08	109.00	106.68
20	K	201	CLA	C4A-NA-C1A	5.08	109.00	106.68
20	B	1214	CLA	C3B-C4B-NB	-5.08	106.00	110.53
28	4	607	CHL	O2D-CGD-CBD	5.08	120.11	111.23
28	1	601	CHL	C3C-C4C-NC	5.06	116.92	110.43
20	4	611	CLA	C3B-C4B-NB	-5.05	106.02	110.53
28	2	602	CHL	O2D-CGD-CBD	5.05	120.06	111.23
29	1	621	LUT	C21-C26-C27	5.04	118.62	112.83
28	4	608	CHL	C3C-C4C-NC	5.02	116.86	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	4	615	CHL	O2D-CGD-CBD	5.01	119.98	111.23
20	A	1134	CLA	C3B-C4B-NB	-5.00	106.06	110.53
20	1	609	CLA	C3B-C4B-NB	-5.00	106.07	110.53
20	A	1126	CLA	C3B-C4B-NB	-4.99	106.08	110.53
20	A	1119	CLA	C3B-C4B-NB	-4.98	106.08	110.53
20	1	603	CLA	C3B-C4B-NB	-4.96	106.11	110.53
20	A	1128	CLA	CMB-C2B-C1B	-4.95	117.88	125.42
20	I	121	CLA	C4A-NA-C1A	4.95	108.94	106.68
20	B	1224	CLA	C4A-NA-C1A	4.94	108.94	106.68
28	2	601	CHL	C3D-C2D-C1D	-4.94	99.09	105.83
28	4	615	CHL	C3C-C4C-NC	4.92	116.73	110.43
20	3	617	CLA	C4A-NA-C1A	4.92	108.92	106.68
28	2	602	CHL	C3C-C4C-NC	4.91	116.72	110.43
28	2	601	CHL	C3C-C4C-NC	4.91	116.72	110.43
20	A	1136	CLA	C3B-C4B-NB	-4.91	106.15	110.53
20	A	1013	CLA	CMB-C2B-C1B	-4.90	117.95	125.42
28	3	608	CHL	C3C-C4C-NC	4.90	116.70	110.43
28	2	602	CHL	C3D-C2D-C1D	-4.90	99.15	105.83
28	3	608	CHL	CHD-C4C-C3C	-4.89	117.65	124.77
20	A	1126	CLA	CMB-C2B-C1B	-4.88	117.98	125.42
20	B	1220	CLA	C4A-NA-C1A	4.87	108.90	106.68
28	4	606	CHL	C3C-C4C-NC	4.86	116.66	110.43
20	A	1119	CLA	C4A-NA-C1A	4.86	108.90	106.68
29	3	621	LUT	C40-C33-C32	4.86	125.51	118.09
28	1	607	CHL	C3C-C4C-NC	4.86	116.65	110.43
28	4	615	CHL	C3D-C2D-C1D	-4.85	99.21	105.83
28	2	615	CHL	C3D-C2D-C1D	-4.85	99.21	105.83
20	B	1238	CLA	C3B-C4B-NB	-4.84	106.21	110.53
20	A	1131	CLA	C3B-C4B-NB	-4.82	106.22	110.53
28	2	606	CHL	C3D-C2D-C1D	-4.82	99.25	105.83
20	A	1102	CLA	C4A-NA-C1A	4.81	108.87	106.68
20	B	1023	CLA	C3B-C4B-NB	-4.80	106.24	110.53
20	A	1022	CLA	C3B-C4B-NB	-4.80	106.25	110.53
28	4	606	CHL	C3D-C2D-C1D	-4.80	99.29	105.83
20	1	613	CLA	C4A-NA-C1A	4.80	108.87	106.68
28	4	607	CHL	C3D-C2D-C1D	-4.80	99.29	105.83
20	K	202	CLA	C4A-NA-C1A	4.79	108.86	106.68
20	B	1208	CLA	C3B-C4B-NB	-4.77	106.27	110.53
20	B	1238	CLA	C4A-NA-C1A	4.77	108.85	106.68
28	4	607	CHL	C3C-C4C-NC	4.76	116.53	110.43
29	4	623	LUT	C7-C8-C9	-4.74	119.23	126.23
23	B	4010	BCR	C15-C16-C17	-4.73	113.83	123.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	3	608	CHL	O2D-CGD-CBD	4.73	119.50	111.23
28	2	611	CHL	CHD-C4C-C3C	-4.73	117.88	124.77
28	2	607	CHL	C3C-C4C-NC	4.72	116.48	110.43
20	B	1216	CLA	C2B-C1B-NB	-4.72	105.43	110.33
28	2	606	CHL	C3C-C4C-NC	4.72	116.47	110.43
20	H	200	CLA	C4A-NA-C1A	4.71	108.83	106.68
20	A	5005	CLA	C3B-C4B-NB	-4.71	106.32	110.53
20	B	1217	CLA	C4A-NA-C1A	4.71	108.83	106.68
28	2	615	CHL	C3C-C4C-NC	4.71	116.46	110.43
20	B	1202	CLA	CMB-C2B-C1B	-4.70	118.26	125.42
20	A	1116	CLA	C3B-C4B-NB	-4.69	106.34	110.53
28	2	607	CHL	C3D-C2D-C1D	-4.68	99.44	105.83
20	A	1115	CLA	C3B-C4B-NB	-4.68	106.36	110.53
20	B	1224	CLA	C3B-C4B-NB	-4.67	106.36	110.53
20	L	302	CLA	C4A-NA-C1A	4.66	108.81	106.68
28	2	607	CHL	O2D-CGD-CBD	4.66	119.38	111.23
28	4	608	CHL	CHD-C4C-C3C	-4.66	117.98	124.77
29	4	620	LUT	C38-C25-C24	-4.66	112.33	123.36
28	4	608	CHL	C3D-C2D-C1D	-4.65	99.48	105.83
20	A	1107	CLA	C3B-C4B-NB	-4.65	106.38	110.53
28	2	606	CHL	CHD-C4C-C3C	-4.64	118.01	124.77
20	B	1012	CLA	C4A-NA-C1A	4.63	108.79	106.68
20	B	1206	CLA	CMB-C2B-C1B	-4.61	118.40	125.42
28	2	602	CHL	CHD-C4C-C3C	-4.61	118.06	124.77
29	4	621	LUT	C26-C27-C28	-4.60	117.42	124.58
28	2	615	CHL	CHD-C4C-C3C	-4.60	118.07	124.77
20	A	1126	CLA	C4-C3-C5	4.59	123.20	115.23
20	B	1215	CLA	C3B-C4B-NB	-4.59	106.43	110.53
28	2	601	CHL	CHD-C4C-C3C	-4.59	118.08	124.77
28	1	607	CHL	C3D-C2D-C1D	-4.58	99.57	105.83
28	4	615	CHL	CHD-C4C-C3C	-4.58	118.09	124.77
28	4	606	CHL	CHD-C4C-C3C	-4.57	118.11	124.77
23	L	419	BCR	C40-C30-C25	4.57	117.41	110.24
23	L	420	BCR	C40-C30-C25	4.56	117.39	110.24
29	4	620	LUT	C21-C26-C27	4.55	118.05	112.83
20	B	1234	CLA	C3B-C4B-NB	-4.50	106.51	110.53
24	1	630	LHG	O4-P-O5	4.50	133.37	112.44
20	B	1213	CLA	CMB-C2B-C1B	-4.49	118.58	125.42
20	B	1232	CLA	C3B-C4B-NB	-4.47	106.54	110.53
24	A	5001	LHG	O4-P-O5	4.46	133.19	112.44
20	B	1239	CLA	CMB-C2B-C1B	-4.46	118.63	125.42
23	B	4009	BCR	C31-C1-C6	4.45	117.23	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	L	301	CLA	C3B-C4B-NB	-4.44	106.56	110.53
20	4	603	CLA	C4A-NA-C1A	4.44	108.70	106.68
24	A	5003	LHG	O4-P-O5	4.43	133.07	112.44
20	B	1215	CLA	CMB-C2B-C1B	-4.43	118.67	125.42
28	2	611	CHL	C3D-C2D-C1D	-4.41	99.82	105.83
20	A	1109	CLA	C3B-C4B-NB	-4.40	106.60	110.53
20	A	1013	CLA	C2B-C1B-NB	-4.40	105.76	110.33
28	1	607	CHL	CHD-C4C-C3C	-4.40	118.36	124.77
24	3	630	LHG	O4-P-O5	4.40	132.90	112.44
28	2	615	CHL	C3B-C4B-NB	4.39	114.45	110.53
24	B	5101	LHG	O4-P-O5	4.39	132.88	112.44
29	2	620	LUT	C7-C8-C9	-4.39	119.74	126.23
28	2	607	CHL	CHD-C4C-C3C	-4.39	118.37	124.77
28	2	608	CHL	O2D-CGD-CBD	4.38	118.89	111.23
28	4	615	CHL	C3B-C4B-NB	4.38	114.44	110.53
20	A	1114	CLA	CMB-C2B-C1B	-4.38	118.75	125.42
20	A	1122	CLA	C3B-C4B-NB	-4.37	106.63	110.53
28	1	607	CHL	CAA-C2A-C3A	-4.36	101.22	113.00
20	K	201	CLA	C3B-C4B-NB	-4.36	106.64	110.53
28	4	607	CHL	C3B-C4B-NB	4.35	114.41	110.53
20	B	1234	CLA	CMB-C2B-C1B	-4.34	118.81	125.42
28	2	607	CHL	C3B-C4B-NB	4.33	114.40	110.53
20	A	1136	CLA	C4A-NA-C1A	4.32	108.65	106.68
20	1	603	CLA	C4A-NA-C1A	4.32	108.65	106.68
20	A	1135	CLA	C3B-C4B-NB	-4.32	106.68	110.53
23	I	120	BCR	C7-C8-C9	-4.30	119.87	126.23
24	2	630	LHG	O4-P-O5	4.30	132.46	112.44
20	A	1013	CLA	O2D-CGD-O1D	-4.28	115.51	123.85
28	4	608	CHL	O2D-CGD-CBD	4.27	118.70	111.23
20	B	1209	CLA	C3B-C4B-NB	-4.27	106.72	110.53
24	4	630	LHG	O4-P-O5	4.26	132.28	112.44
29	1	620	LUT	C21-C26-C27	4.26	117.72	112.83
28	2	602	CHL	CHB-C4A-NA	4.25	130.54	124.40
20	1	611	CLA	C3B-C4B-NB	-4.25	106.73	110.53
20	B	1012	CLA	C3B-C4B-NB	-4.25	106.74	110.53
23	B	4010	BCR	C15-C14-C13	-4.24	121.33	127.28
23	A	4007	BCR	C2-C1-C6	4.24	116.60	110.44
29	1	621	LUT	C36-C21-C26	4.24	115.97	109.55
28	4	607	CHL	CHD-C4C-C3C	-4.24	118.60	124.77
20	B	1210	CLA	CMB-C2B-C1B	-4.23	118.97	125.42
28	1	601	CHL	C3B-C4B-NB	4.22	114.30	110.53
20	1	610	CLA	CMB-C2B-C1B	-4.19	119.04	125.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	1224	CLA	CMB-C2B-C1B	-4.17	119.06	125.42
20	A	8895	CLA	CAC-C3C-C4C	-4.17	119.36	124.79
28	1	607	CHL	C3B-C4B-NB	4.17	114.25	110.53
28	4	606	CHL	CAC-C3C-C4C	4.16	130.20	124.79
28	2	606	CHL	CAC-C3C-C4C	4.15	130.19	124.79
28	2	602	CHL	C3B-C4B-NB	4.15	114.23	110.53
20	A	1116	CLA	C4A-NA-C1A	4.15	108.57	106.68
28	2	601	CHL	C1D-ND-C4D	-4.14	103.41	106.31
28	2	601	CHL	C3B-C4B-NB	4.14	114.22	110.53
29	1	620	LUT	C36-C21-C26	4.14	115.81	109.55
28	3	608	CHL	C3B-C4B-NB	4.14	114.22	110.53
20	3	610	CLA	C4A-NA-C1A	4.12	108.56	106.68
23	J	213	BCR	C2-C1-C6	4.12	116.43	110.44
20	B	1012	CLA	CMB-C2B-C1B	-4.11	119.16	125.42
28	1	601	CHL	CHD-C4C-C3C	-4.10	118.79	124.77
29	4	623	LUT	C40-C33-C32	4.10	124.35	118.09
28	1	607	CHL	CHD-C1D-ND	-4.09	119.04	124.80
28	4	606	CHL	C3B-C4B-NB	4.09	114.18	110.53
20	A	1128	CLA	C4A-NA-C1A	4.08	108.54	106.68
28	2	606	CHL	CHD-C1D-ND	-4.07	119.07	124.80
20	2	612	CLA	C3B-C4B-NB	-4.07	106.89	110.53
28	2	615	CHL	CHD-C1D-ND	-4.07	119.08	124.80
20	A	1119	CLA	C2B-C1B-NB	-4.07	106.11	110.33
20	B	1201	CLA	C4A-NA-C1A	4.06	108.53	106.68
20	B	1239	CLA	C2B-C1B-NB	-4.05	106.12	110.33
28	2	601	CHL	CHD-C1D-ND	-4.05	119.10	124.80
20	B	1234	CLA	C4A-NA-C1A	4.04	108.52	106.68
20	2	603	CLA	C3B-C4B-NB	-4.04	106.92	110.53
20	1	612	CLA	C4A-NA-C1A	4.04	108.52	106.68
29	2	623	LUT	C11-C12-C13	-4.03	115.31	126.36
28	2	611	CHL	C3B-C4B-NB	4.03	114.12	110.53
20	A	1113	CLA	C3B-C4B-NB	-4.01	106.95	110.53
28	2	607	CHL	CHD-C1D-ND	-4.01	119.17	124.80
28	2	606	CHL	C3B-C4B-NB	3.99	114.10	110.53
20	A	1132	CLA	C3B-C4B-NB	-3.99	106.97	110.53
20	B	1235	CLA	C4A-NA-C1A	3.98	108.50	106.68
28	4	606	CHL	CHD-C1D-ND	-3.98	119.20	124.80
20	A	1130	CLA	C4A-NA-C1A	3.98	108.49	106.68
20	B	1223	CLA	C4A-NA-C1A	3.97	108.49	106.68
20	A	1118	CLA	C4A-NA-C1A	3.97	108.49	106.68
20	B	1204	CLA	C4A-NA-C1A	3.97	108.49	106.68
20	4	603	CLA	C3B-C4B-NB	-3.96	106.99	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	1	621	LUT	C37-C21-C26	-3.96	103.55	109.55
20	A	1105	CLA	C3B-C4B-NB	-3.95	107.00	110.53
28	1	607	CHL	C1D-ND-C4D	-3.95	103.54	106.31
29	4	620	LUT	C36-C21-C26	3.94	115.51	109.55
20	B	1238	CLA	CMB-C2B-C1B	-3.94	119.42	125.42
20	A	1137	CLA	C3B-C4B-NB	-3.93	107.02	110.53
20	A	1013	CLA	C4A-NA-C1A	3.93	108.47	106.68
28	2	606	CHL	CAA-C2A-C3A	-3.93	102.38	113.00
28	1	601	CHL	C1D-ND-C4D	-3.93	103.56	106.31
20	B	1227	CLA	CMB-C2B-C1B	-3.92	119.45	125.42
20	B	1226	CLA	C3B-C4B-NB	-3.91	107.04	110.53
20	A	1130	CLA	CMB-C2B-C1B	-3.91	119.46	125.42
28	1	601	CHL	C2D-C1D-ND	3.91	114.00	110.13
28	2	607	CHL	CAC-C3C-C4C	3.90	129.87	124.79
28	2	615	CHL	CAA-C2A-C3A	-3.90	102.45	113.00
28	4	615	CHL	CHD-C1D-ND	-3.90	119.31	124.80
20	B	1232	CLA	CMB-C2B-C1B	-3.89	119.49	125.42
20	B	1221	CLA	C3B-C4B-NB	-3.89	107.06	110.53
20	A	1105	CLA	CMB-C2B-C1B	-3.89	119.50	125.42
28	4	607	CHL	CHD-C1D-ND	-3.88	119.35	124.80
20	A	1140	CLA	C4A-NA-C1A	3.87	108.45	106.68
20	B	1226	CLA	C4A-NA-C1A	3.87	108.45	106.68
20	A	1127	CLA	C3B-C4B-NB	-3.87	107.08	110.53
20	B	1223	CLA	CMB-C2B-C1B	-3.86	119.54	125.42
28	1	601	CHL	CHB-C4A-NA	3.86	129.97	124.40
29	3	621	LUT	C7-C8-C9	-3.86	120.53	126.23
20	A	1013	CLA	CAA-CBA-CGA	-3.85	102.27	113.21
28	3	608	CHL	CHD-C1D-ND	-3.85	119.38	124.80
23	B	4010	BCR	C38-C26-C27	-3.85	105.39	113.60
20	A	8895	CLA	C3B-C4B-NB	-3.85	107.10	110.53
20	B	1212	CLA	CMB-C2B-C1B	-3.85	119.56	125.42
28	4	608	CHL	CHD-C1D-ND	-3.84	119.40	124.80
20	A	1121	CLA	C3B-C4B-NB	-3.83	107.11	110.53
20	A	1136	CLA	CMB-C2B-C1B	-3.82	119.60	125.42
20	A	1120	CLA	C3B-C4B-NB	-3.81	107.13	110.53
20	L	303	CLA	CMB-C2B-C1B	-3.81	119.62	125.42
20	B	1236	CLA	C3B-C4B-NB	-3.80	107.13	110.53
20	A	1101	CLA	C3B-C4B-NB	-3.80	107.14	110.53
20	B	1237	CLA	C3B-C4B-NB	-3.79	107.15	110.53
20	1	604	CLA	CMB-C2B-C1B	-3.78	119.66	125.42
20	B	1205	CLA	C3B-C4B-NB	-3.78	107.16	110.53
20	4	604	CLA	CMB-C2B-C1B	-3.77	119.67	125.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	4	608	CHL	CAC-C3C-C4C	3.77	129.69	124.79
21	B	2002	PQN	C14-C13-C15	3.76	121.75	115.23
29	1	620	LUT	O23-C23-C24	3.76	118.06	110.39
20	A	1801	CLA	CMB-C2B-C1B	-3.76	119.70	125.42
28	2	602	CHL	CHD-C1D-ND	-3.75	119.52	124.80
20	A	1117	CLA	CMB-C2B-C1B	-3.75	119.70	125.42
20	2	613	CLA	C3B-C4B-NB	-3.74	107.19	110.53
20	A	1022	CLA	C4A-NA-C1A	3.73	108.38	106.68
28	2	607	CHL	C1D-ND-C4D	-3.73	103.69	106.31
28	4	608	CHL	C3B-C4B-NB	3.73	113.86	110.53
20	B	1213	CLA	C4A-NA-C1A	3.72	108.38	106.68
28	3	608	CHL	C1D-ND-C4D	-3.72	103.70	106.31
28	2	615	CHL	C1D-ND-C4D	-3.72	103.70	106.31
28	4	606	CHL	C1D-ND-C4D	-3.72	103.70	106.31
28	2	606	CHL	C1D-ND-C4D	-3.72	103.70	106.31
20	I	121	CLA	CMB-C2B-C1B	-3.71	119.77	125.42
29	2	620	LUT	C40-C33-C34	-3.71	116.81	122.82
23	A	4008	BCR	C15-C16-C17	-3.70	115.94	123.52
20	A	1124	CLA	CMB-C2B-C1B	-3.70	119.78	125.42
29	3	620	LUT	C7-C8-C9	-3.69	120.77	126.23
20	1	602	CLA	CMB-C2B-C1B	-3.69	119.80	125.42
28	2	608	CHL	C1D-ND-C4D	-3.69	103.72	106.31
28	4	607	CHL	CAC-C3C-C4C	3.69	129.59	124.79
20	1	615	CLA	C3B-C4B-NB	-3.68	107.24	110.53
20	L	301	CLA	CMB-C2B-C1B	-3.68	119.82	125.42
28	4	615	CHL	C1D-ND-C4D	-3.67	103.74	106.31
23	B	4010	BCR	C38-C26-C25	3.67	128.49	124.48
20	A	1108	CLA	CMB-C2B-C1B	-3.67	119.84	125.42
28	2	608	CHL	CHD-C1D-ND	-3.66	119.65	124.80
20	2	610	CLA	C3B-C4B-NB	-3.66	107.27	110.53
20	3	602	CLA	C3B-C4B-NB	-3.66	107.27	110.53
23	3	624	BCR	C2-C1-C6	3.65	115.75	110.44
20	B	1225	CLA	CMB-C2B-C1B	-3.65	119.86	125.42
28	2	601	CHL	C2D-C1D-ND	3.65	113.74	110.13
20	F	301	CLA	C3B-C4B-NB	-3.65	107.28	110.53
28	2	601	CHL	CHB-C4A-NA	3.64	129.66	124.40
20	B	1224	CLA	C2D-C1D-ND	-3.64	106.53	110.13
20	B	1239	CLA	C4A-NA-C1A	3.63	108.34	106.68
28	4	608	CHL	CHB-C4A-NA	3.63	129.63	124.40
20	A	1132	CLA	CMB-C2B-C1B	-3.63	119.90	125.42
20	A	1106	CLA	C3B-C4B-NB	-3.62	107.30	110.53
20	A	1125	CLA	CMB-C2B-C1B	-3.62	119.90	125.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	1139	CLA	C3B-C4B-NB	-3.62	107.30	110.53
20	K	202	CLA	C3B-C4B-NB	-3.62	107.30	110.53
20	B	1220	CLA	C3B-C4B-NB	-3.62	107.30	110.53
23	A	4008	BCR	C15-C14-C13	-3.61	122.21	127.28
20	A	1116	CLA	CMB-C2B-C1B	-3.61	119.92	125.42
28	1	601	CHL	CHD-C1D-ND	-3.60	119.74	124.80
20	J	102	CLA	C3B-C4B-NB	-3.60	107.32	110.53
28	4	607	CHL	CHB-C4A-NA	3.59	129.59	124.40
28	2	607	CHL	CHB-C4A-NA	3.59	129.58	124.40
28	2	615	CHL	CHB-C4A-NA	3.59	129.58	124.40
20	I	121	CLA	CAC-C3C-C2C	-3.59	120.97	127.56
28	2	602	CHL	C1D-ND-C4D	-3.58	103.80	106.31
28	2	608	CHL	C2D-C1D-ND	3.57	113.66	110.13
20	B	1239	CLA	C3B-C4B-NB	-3.57	107.34	110.53
20	B	1021	CLA	C3B-C4B-NB	-3.56	107.35	110.53
20	3	609	CLA	C3B-C4B-NB	-3.56	107.35	110.53
20	B	1235	CLA	C3B-C4B-NB	-3.55	107.36	110.53
20	A	1130	CLA	C3B-C4B-NB	-3.55	107.36	110.53
20	1	613	CLA	C3B-C4B-NB	-3.55	107.36	110.53
28	2	602	CHL	C2D-C1D-ND	3.55	113.64	110.13
23	B	4014	BCR	C2-C1-C6	3.55	115.59	110.44
28	2	602	CHL	CAC-C3C-C4C	3.54	129.40	124.79
20	3	614	CLA	C3B-C4B-NB	-3.54	107.37	110.53
23	A	4008	BCR	C23-C24-C25	3.54	136.45	127.00
28	2	611	CHL	CHB-C4A-NA	3.53	129.50	124.40
20	B	1216	CLA	CHA-C1A-NA	-3.53	118.40	126.39
28	4	615	CHL	CAC-C3C-C4C	3.51	129.36	124.79
20	A	1104	CLA	C3B-C4B-NB	-3.51	107.40	110.53
28	2	608	CHL	C3B-C4B-NB	3.51	113.66	110.53
28	3	608	CHL	CHB-C4A-NA	3.51	129.46	124.40
20	B	1225	CLA	C3B-C4B-NB	-3.50	107.41	110.53
28	2	608	CHL	CHB-C4A-NA	3.49	129.44	124.40
20	B	1219	CLA	C3B-C4B-NB	-3.49	107.42	110.53
28	3	608	CHL	C2D-C1D-ND	3.49	113.58	110.13
20	A	1115	CLA	C4A-NA-C1A	3.49	108.27	106.68
28	4	615	CHL	CHB-C4A-NA	3.48	129.43	124.40
23	A	4007	BCR	C27-C26-C25	3.48	127.41	122.70
28	1	607	CHL	C3D-C4D-ND	3.48	115.65	109.99
20	2	609	CLA	C3B-C4B-NB	-3.48	107.42	110.53
20	B	1215	CLA	C4-C3-C5	3.48	121.26	115.23
20	4	614	CLA	C3B-C4B-NB	-3.47	107.44	110.53
20	A	1102	CLA	C3B-C4B-NB	-3.46	107.44	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	4	601	CLA	C3B-C4B-NB	-3.46	107.44	110.53
20	A	5005	CLA	CMB-C2B-C1B	-3.46	120.14	125.42
20	1	614	CLA	C3B-C4B-NB	-3.46	107.44	110.53
20	3	617	CLA	C3B-C4B-NB	-3.46	107.44	110.53
20	A	1124	CLA	C3B-C4B-NB	-3.46	107.44	110.53
20	B	1217	CLA	C3B-C4B-NB	-3.46	107.44	110.53
20	A	1013	CLA	O2D-CGD-CBD	3.46	117.28	111.23
20	B	1211	CLA	C3B-C4B-NB	-3.45	107.45	110.53
20	3	613	CLA	C3B-C4B-NB	-3.45	107.45	110.53
20	A	1140	CLA	C3B-C4B-NB	-3.43	107.46	110.53
20	A	1112	CLA	C4A-NA-C1A	3.43	108.24	106.68
28	2	606	CHL	CHB-C4A-NA	3.42	129.34	124.40
29	2	620	LUT	C38-C25-C24	-3.42	115.26	123.36
20	B	1206	CLA	C3B-C4B-NB	-3.42	107.48	110.53
20	A	1013	CLA	CHD-C1D-ND	-3.42	119.99	124.80
20	A	1103	CLA	C3B-C4B-NB	-3.42	107.48	110.53
29	1	620	LUT	C11-C10-C9	3.41	132.06	127.28
20	B	1228	CLA	C3B-C4B-NB	-3.40	107.49	110.53
20	B	1222	CLA	C3B-C4B-NB	-3.40	107.50	110.53
28	4	607	CHL	C1D-ND-C4D	-3.40	103.93	106.31
20	A	1110	CLA	C3B-C4B-NB	-3.40	107.50	110.53
28	2	611	CHL	O2D-CGD-O1D	-3.39	117.24	123.85
20	A	1101	CLA	O2D-CGD-O1D	-3.39	117.26	123.85
20	4	602	CLA	CMB-C2B-C1B	-3.39	120.26	125.42
20	A	1138	CLA	CMB-C2B-C1B	-3.38	120.27	125.42
28	2	611	CHL	C1D-ND-C4D	-3.38	103.94	106.31
20	4	604	CLA	C3B-C4B-NB	-3.38	107.52	110.53
20	1	606	CLA	CMB-C2B-C1B	-3.38	120.28	125.42
20	4	609	CLA	C3B-C4B-NB	-3.38	107.52	110.53
20	B	1203	CLA	CMB-C2B-C1B	-3.37	120.28	125.42
20	A	1140	CLA	C2D-C1D-ND	-3.37	106.80	110.13
20	1	612	CLA	C3B-C4B-NB	-3.36	107.53	110.53
20	B	1213	CLA	O2D-CGD-O1D	-3.36	117.30	123.85
29	2	620	LUT	C31-C32-C33	3.36	135.58	126.36
28	4	615	CHL	C2D-C1D-ND	3.36	113.45	110.13
28	4	606	CHL	CHB-C4A-NA	3.35	129.23	124.40
20	4	610	CLA	C3B-C4B-NB	-3.34	107.54	110.53
20	A	1111	CLA	C3B-C4B-NB	-3.34	107.55	110.53
20	A	1801	CLA	C3B-C4B-NB	-3.34	107.55	110.53
20	B	1222	CLA	CHD-C1D-ND	-3.34	120.10	124.80
29	2	623	LUT	C38-C25-C24	-3.34	115.45	123.36
20	A	1138	CLA	C3B-C4B-NB	-3.34	107.55	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	4	602	CLA	C3B-C4B-NB	-3.34	107.55	110.53
28	2	615	CHL	C2D-C1D-ND	3.32	113.42	110.13
29	4	621	LUT	O23-C23-C24	-3.31	103.63	110.39
20	A	1132	CLA	CMB-C2B-C3B	3.31	134.34	126.55
28	1	601	CHL	C1-O2A-CGA	3.31	124.67	116.65
20	4	613	CLA	C3B-C4B-NB	-3.31	107.57	110.53
20	A	1117	CLA	C7-C6-C5	-3.31	104.45	113.26
23	A	4007	BCR	C23-C24-C25	3.30	135.82	127.00
28	4	606	CHL	C2D-C1D-ND	3.30	113.39	110.13
20	B	1227	CLA	CHD-C1D-ND	-3.30	120.16	124.80
20	2	614	CLA	C3B-C4B-NB	-3.30	107.59	110.53
28	2	606	CHL	C2D-C1D-ND	3.29	113.39	110.13
20	B	1021	CLA	O2D-CGD-O1D	-3.29	117.44	123.85
20	B	1223	CLA	C1D-ND-C4D	-3.29	104.01	106.31
20	B	1210	CLA	C3B-C4B-NB	-3.28	107.60	110.53
20	3	603	CLA	C3B-C4B-NB	-3.28	107.60	110.53
23	I	118	BCR	C2-C1-C6	3.28	115.20	110.44
19	A	1011	CL0	CMB-C2B-C1B	-3.27	120.44	125.42
20	B	1201	CLA	C3B-C4B-NB	-3.27	107.61	110.53
28	4	608	CHL	C1D-ND-C4D	-3.26	104.02	106.31
29	2	623	LUT	C22-C23-C24	-3.26	106.35	111.18
23	B	4014	BCR	C11-C10-C9	-3.25	122.72	127.28
29	2	623	LUT	C8-C7-C6	3.25	135.68	127.00
20	K	204	CLA	C3B-C4B-NB	-3.25	107.63	110.53
28	2	611	CHL	CHD-C1D-ND	-3.24	120.24	124.80
20	A	1140	CLA	C1D-ND-C4D	-3.24	104.04	106.31
23	J	213	BCR	C15-C16-C17	-3.24	116.88	123.52
29	2	621	LUT	C7-C8-C9	-3.24	121.44	126.23
20	A	1108	CLA	C3B-C4B-NB	-3.24	107.64	110.53
20	A	1132	CLA	C3C-C4C-NC	-3.23	106.29	110.43
20	A	1133	CLA	CMB-C2B-C1B	-3.23	120.51	125.42
28	2	615	CHL	C1C-C2C-C3C	-3.22	104.32	107.28
20	A	5005	CLA	C4A-NA-C1A	3.22	108.15	106.68
20	3	612	CLA	C3B-C4B-NB	-3.21	107.66	110.53
29	1	621	LUT	O23-C23-C24	3.21	116.95	110.39
23	B	4014	BCR	C3-C4-C5	-3.21	108.33	114.06
28	3	608	CHL	C1C-C2C-C3C	-3.20	104.34	107.28
20	A	1131	CLA	O2D-CGD-O1D	-3.20	117.62	123.85
20	B	1219	CLA	C2D-C1D-ND	-3.20	106.96	110.13
20	A	1126	CLA	C6-C5-C3	3.20	121.25	113.47
29	3	621	LUT	C38-C25-C24	-3.20	115.80	123.36
20	B	1230	CLA	C3B-C4B-NB	-3.19	107.68	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	2	620	LUT	C11-C12-C13	-3.19	117.61	126.36
20	1	610	CLA	O2D-CGD-O1D	-3.19	117.64	123.85
20	F	302	CLA	C3B-C4B-NB	-3.19	107.68	110.53
20	B	1211	CLA	CMB-C2B-C1B	-3.18	120.57	125.42
20	A	5005	CLA	O2D-CGD-O1D	-3.18	117.65	123.85
20	H	200	CLA	C3B-C4B-NB	-3.18	107.69	110.53
20	A	1127	CLA	CMB-C2B-C1B	-3.17	120.59	125.42
28	2	615	CHL	C3D-C4D-ND	3.17	115.14	109.99
23	A	4008	BCR	C27-C26-C25	3.17	126.99	122.70
20	G	218	CLA	C3B-C4B-NB	-3.17	107.70	110.53
20	B	1012	CLA	O2D-CGD-O1D	-3.17	117.68	123.85
20	A	1138	CLA	O2D-CGD-O1D	-3.17	117.68	123.85
29	3	621	LUT	C40-C33-C34	-3.17	117.69	122.82
20	A	1139	CLA	O2D-CGD-O1D	-3.16	117.69	123.85
20	A	1112	CLA	C3B-C4B-NB	-3.16	107.71	110.53
28	2	606	CHL	C3D-C4D-ND	3.16	115.12	109.99
28	2	601	CHL	C3D-C4D-ND	3.16	115.12	109.99
28	2	601	CHL	CAC-C3C-C4C	3.16	128.90	124.79
20	B	1231	CLA	C3B-C4B-NB	-3.15	107.71	110.53
28	3	608	CHL	CAC-C3C-C4C	3.15	128.89	124.79
28	2	608	CHL	CAA-C2A-C3A	-3.15	104.48	113.00
20	G	202	CLA	C3B-C4B-NB	-3.15	107.72	110.53
20	B	1235	CLA	CMB-C2B-C1B	-3.15	120.62	125.42
28	2	606	CHL	CMB-C2B-C1B	3.15	130.22	125.42
28	2	607	CHL	C3D-C4D-ND	3.15	115.11	109.99
20	1	603	CLA	O2D-CGD-O1D	-3.15	117.72	123.85
20	B	1023	CLA	O2D-CGD-O1D	-3.15	117.72	123.85
23	F	416	BCR	C11-C10-C9	-3.14	122.87	127.28
20	A	1127	CLA	C2D-C1D-ND	-3.14	107.02	110.13
23	L	419	BCR	C27-C26-C25	3.14	126.95	122.70
28	2	607	CHL	C2D-C1D-ND	3.14	113.23	110.13
20	B	1240	CLA	C3B-C4B-NB	-3.14	107.73	110.53
28	2	611	CHL	CAC-C3C-C4C	3.14	128.87	124.79
20	B	1236	CLA	O2D-CGD-O1D	-3.14	117.74	123.85
20	A	1117	CLA	O2D-CGD-O1D	-3.13	117.75	123.85
20	B	1224	CLA	O2D-CGD-CBD	3.13	116.71	111.23
28	1	607	CHL	CMD-C2D-C3D	-3.13	120.50	127.69
28	2	608	CHL	CAC-C3C-C4C	3.13	128.87	124.79
20	A	1136	CLA	O2A-CGA-O1A	-3.13	115.80	123.63
29	4	621	LUT	C32-C33-C34	3.13	123.93	119.01
20	A	1125	CLA	C6-C5-C3	3.13	121.09	113.47
20	3	610	CLA	O2D-CGD-O1D	-3.13	117.76	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	4	606	CHL	C3D-C4D-ND	3.13	115.07	109.99
20	3	611	CLA	C3B-C4B-NB	-3.12	107.74	110.53
28	1	607	CHL	CHB-C4A-NA	3.12	128.90	124.40
28	2	607	CHL	CAA-C2A-C3A	-3.12	104.57	113.00
28	4	607	CHL	C2D-C1D-ND	3.12	113.21	110.13
28	2	611	CHL	C2D-C1D-ND	3.11	113.21	110.13
20	3	609	CLA	O2D-CGD-O1D	-3.11	117.80	123.85
20	B	1023	CLA	CHD-C1D-ND	-3.11	120.43	124.80
28	4	615	CHL	C3D-C4D-ND	3.10	115.03	109.99
19	A	1011	CL0	C3B-C4B-NB	-3.10	107.76	110.53
20	B	1221	CLA	CMB-C2B-C1B	-3.10	120.70	125.42
20	1	608	CLA	C3B-C4B-NB	-3.10	107.77	110.53
29	2	620	LUT	C22-C23-C24	-3.10	106.59	111.18
23	I	120	BCR	C24-C25-C26	-3.10	114.42	121.56
23	A	4008	BCR	C24-C23-C22	-3.10	121.66	126.23
28	2	608	CHL	CMB-C2B-C1B	3.09	130.13	125.42
20	B	1237	CLA	C1-O2A-CGA	3.09	124.14	116.65
29	1	620	LUT	C15-C14-C13	3.09	131.62	127.28
20	B	1221	CLA	O2D-CGD-O1D	-3.08	117.85	123.85
28	2	607	CHL	CMD-C2D-C3D	-3.08	120.62	127.69
20	B	1226	CLA	C2A-C1A-CHA	3.08	129.21	123.87
28	2	602	CHL	C3D-C4D-ND	3.08	114.99	109.99
20	A	1111	CLA	CMB-C2B-C1B	-3.07	120.74	125.42
20	A	1108	CLA	C3C-C4C-NC	-3.07	106.49	110.43
20	A	1022	CLA	O2D-CGD-O1D	-3.07	117.87	123.85
20	B	1217	CLA	CMB-C2B-C1B	-3.07	120.75	125.42
23	A	4003	BCR	C40-C30-C25	3.06	115.05	110.24
23	L	419	BCR	C15-C14-C13	-3.06	122.98	127.28
28	4	607	CHL	C3D-C4D-ND	3.06	114.95	109.99
28	1	607	CHL	C2D-C1D-ND	3.05	113.15	110.13
20	A	1125	CLA	C2D-C1D-ND	-3.05	107.11	110.13
20	O	201	CLA	C3A-C4A-CHB	-3.05	120.18	123.91
20	B	1206	CLA	O2D-CGD-O1D	-3.04	117.92	123.85
20	A	1122	CLA	O2D-CGD-O1D	-3.04	117.92	123.85
20	A	1128	CLA	C3B-C4B-NB	-3.04	107.81	110.53
20	F	301	CLA	O2D-CGD-O1D	-3.04	117.94	123.85
20	B	1215	CLA	O2D-CGD-O1D	-3.03	117.94	123.85
20	A	1109	CLA	O2D-CGD-O1D	-3.03	117.95	123.85
28	1	607	CHL	CAC-C3C-C4C	3.03	128.73	124.79
28	4	608	CHL	CMB-C2B-C1B	3.02	130.03	125.42
28	2	611	CHL	C3D-C4D-ND	3.02	114.90	109.99
23	A	4003	BCR	C27-C26-C25	3.02	126.78	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	1112	CLA	O2D-CGD-O1D	-3.02	117.97	123.85
20	1	611	CLA	O2D-CGD-O1D	-3.02	117.97	123.85
23	A	4007	BCR	C33-C5-C6	3.01	127.77	124.48
23	A	4008	BCR	C30-C25-C24	3.01	123.82	115.65
23	I	120	BCR	C27-C26-C25	3.01	126.78	122.70
20	3	606	CLA	O2D-CGD-O1D	-3.01	117.98	123.85
28	1	601	CHL	C4-C3-C5	3.01	120.46	115.23
20	A	1134	CLA	O2D-CGD-O1D	-3.01	117.99	123.85
23	B	4004	BCR	C15-C16-C17	-3.01	117.36	123.52
20	A	1132	CLA	O2D-CGD-O1D	-3.01	117.99	123.85
23	L	420	BCR	C27-C26-C25	3.01	126.77	122.70
20	4	611	CLA	O2D-CGD-O1D	-3.00	118.00	123.85
20	O	202	CLA	C3A-C4A-CHB	-3.00	120.23	123.91
20	B	1222	CLA	O2D-CGD-O1D	-3.00	118.01	123.85
23	A	4007	BCR	C1-C6-C5	-3.00	118.54	122.64
20	A	1119	CLA	O2D-CGD-O1D	-3.00	118.01	123.85
20	3	610	CLA	C3B-C4B-NB	-3.00	107.86	110.53
20	O	203	CLA	C1B-NB-C4B	2.99	108.41	106.31
23	A	4001	BCR	C24-C23-C22	-2.99	121.81	126.23
20	I	121	CLA	O2D-CGD-O1D	-2.99	118.03	123.85
20	B	1236	CLA	CHD-C1D-ND	-2.99	120.59	124.80
20	3	607	CLA	C3B-C4B-NB	-2.99	107.86	110.53
20	A	1118	CLA	C1D-ND-C4D	-2.98	104.22	106.31
20	B	1204	CLA	O2D-CGD-O1D	-2.98	118.05	123.85
20	3	617	CLA	CMB-C2B-C1B	-2.98	120.88	125.42
20	K	202	CLA	CMB-C2B-C1B	-2.98	120.89	125.42
29	1	620	LUT	C31-C32-C33	-2.98	118.20	126.36
20	A	1108	CLA	O2D-CGD-O1D	-2.98	118.06	123.85
28	4	608	CHL	C2D-C1D-ND	2.97	113.07	110.13
20	2	614	CLA	O2D-CGD-O1D	-2.97	118.06	123.85
20	J	102	CLA	O2D-CGD-O1D	-2.97	118.06	123.85
28	4	608	CHL	CMD-C2D-C3D	-2.97	120.87	127.69
28	2	602	CHL	CAA-C2A-C3A	-2.97	104.97	113.00
20	1	613	CLA	O2D-CGD-O1D	-2.97	118.07	123.85
20	B	1208	CLA	O2D-CGD-O1D	-2.97	118.07	123.85
20	B	1223	CLA	C2D-C1D-ND	-2.97	107.19	110.13
20	B	1210	CLA	CAC-C3C-C2C	-2.97	122.11	127.56
20	3	602	CLA	CHA-C1A-NA	-2.97	119.68	126.39
23	J	212	BCR	C11-C10-C9	-2.96	123.12	127.28
28	3	608	CHL	CAA-C2A-C3A	-2.96	105.00	113.00
20	B	1230	CLA	O2D-CGD-O1D	-2.96	118.09	123.85
20	G	201	CLA	C3B-C4B-NB	-2.96	107.89	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	M	4021	BCR	C31-C1-C6	2.95	114.88	110.24
20	B	1023	CLA	CMB-C2B-C1B	-2.95	120.92	125.42
20	G	218	CLA	O2D-CGD-O1D	-2.95	118.10	123.85
23	A	4001	BCR	C15-C16-C17	-2.95	117.48	123.52
20	B	1211	CLA	O2D-CGD-O1D	-2.95	118.11	123.85
23	B	4009	BCR	C38-C26-C27	-2.95	107.31	113.60
20	2	604	CLA	O2D-CGD-O1D	-2.95	118.11	123.85
20	K	201	CLA	O2D-CGD-O1D	-2.95	118.11	123.85
20	A	1106	CLA	CMB-C2B-C1B	-2.95	120.93	125.42
20	3	609	CLA	CMB-C2B-C1B	-2.94	120.94	125.42
23	I	120	BCR	C23-C24-C25	2.94	134.86	127.00
20	A	1104	CLA	O2D-CGD-O1D	-2.94	118.12	123.85
23	K	301	BCR	C24-C23-C22	-2.94	121.89	126.23
20	1	608	CLA	O2D-CGD-O1D	-2.94	118.13	123.85
23	L	420	BCR	C2-C1-C6	2.94	114.70	110.44
20	4	609	CLA	O2D-CGD-O1D	-2.94	118.14	123.85
23	B	4010	BCR	C11-C10-C9	-2.93	123.16	127.28
20	1	606	CLA	C3B-C4B-NB	-2.93	107.91	110.53
20	B	1240	CLA	O2D-CGD-O1D	-2.93	118.14	123.85
20	B	1232	CLA	O2D-CGD-O1D	-2.93	118.14	123.85
20	F	302	CLA	O2D-CGD-O1D	-2.93	118.14	123.85
20	A	1125	CLA	C3C-C4C-NC	-2.93	106.68	110.43
20	A	8895	CLA	CMB-C2B-C1B	-2.93	120.96	125.42
27	B	5002	DGD	O5D-C6D-C5D	-2.93	102.82	109.42
20	B	1221	CLA	C5-C3-C2	2.93	127.73	121.17
23	J	212	BCR	C27-C26-C25	2.93	126.66	122.70
20	O	203	CLA	C3A-C4A-CHB	-2.93	120.33	123.91
20	3	611	CLA	O2D-CGD-O1D	-2.92	118.16	123.85
20	A	1120	CLA	CMB-C2B-C1B	-2.92	120.97	125.42
20	B	1229	CLA	C3B-C4B-NB	-2.92	107.92	110.53
20	A	1111	CLA	CHD-C1D-ND	-2.92	120.69	124.80
20	L	303	CLA	O2D-CGD-O1D	-2.92	118.16	123.85
23	A	4008	BCR	C24-C25-C26	-2.92	114.83	121.56
28	4	606	CHL	CAA-C2A-C3A	-2.92	105.11	113.00
29	4	621	LUT	C40-C33-C34	-2.92	118.09	122.82
20	4	614	CLA	O2D-CGD-O1D	-2.91	118.17	123.85
20	B	1239	CLA	O2D-CGD-O1D	-2.91	118.18	123.85
20	2	604	CLA	C3B-C4B-NB	-2.91	107.93	110.53
20	B	1208	CLA	CMB-C2B-C1B	-2.91	120.99	125.42
23	I	120	BCR	C30-C25-C24	2.91	123.54	115.65
20	2	610	CLA	O2D-CGD-O1D	-2.91	118.19	123.85
20	3	604	CLA	O2D-CGD-O1D	-2.91	118.19	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	2	602	CHL	CMB-C2B-C1B	2.91	129.85	125.42
20	B	1223	CLA	CMB-C2B-C3B	2.91	133.39	126.55
20	A	1125	CLA	O2D-CGD-O1D	-2.91	118.19	123.85
20	O	202	CLA	C1B-NB-C4B	2.90	108.35	106.31
29	2	621	LUT	C11-C10-C9	2.90	131.35	127.28
23	B	4017	BCR	C15-C16-C17	-2.90	117.58	123.52
20	B	1216	CLA	O2D-CGD-O1D	-2.90	118.20	123.85
20	3	614	CLA	O2D-CGD-O1D	-2.90	118.20	123.85
20	A	1013	CLA	CMD-C2D-C1D	-2.90	119.62	124.73
20	B	1214	CLA	C2D-C1D-ND	-2.90	107.26	110.13
20	K	201	CLA	CMB-C2B-C1B	-2.90	121.00	125.42
20	B	1203	CLA	O2D-CGD-O1D	-2.90	118.21	123.85
23	B	4009	BCR	C15-C16-C17	-2.90	117.59	123.52
20	4	604	CLA	O2D-CGD-O1D	-2.90	118.21	123.85
28	3	608	CHL	CMD-C2D-C3D	-2.89	121.06	127.69
20	A	1103	CLA	O2D-CGD-O1D	-2.89	118.22	123.85
28	2	615	CHL	CMB-C2B-C1B	2.89	129.82	125.42
20	A	1130	CLA	O2D-CGD-O1D	-2.89	118.22	123.85
20	B	1202	CLA	O2D-CGD-O1D	-2.89	118.22	123.85
20	A	1135	CLA	O2D-CGD-O1D	-2.89	118.22	123.85
20	H	200	CLA	O2D-CGD-O1D	-2.89	118.22	123.85
28	4	608	CHL	C3D-C4D-ND	2.89	114.68	109.99
20	A	1126	CLA	O2A-CGA-O1A	-2.89	116.40	123.63
20	3	604	CLA	CMB-C2B-C1B	-2.89	121.02	125.42
20	3	617	CLA	O2D-CGD-O1D	-2.89	118.23	123.85
20	A	1126	CLA	O2D-CGD-O1D	-2.89	118.23	123.85
29	4	623	LUT	C40-C33-C34	-2.88	118.14	122.82
25	A	5002	LMG	O6-C1-O1	-2.88	103.23	110.04
28	3	608	CHL	C3D-C4D-ND	2.88	114.67	109.99
20	F	303	CLA	C1B-NB-C4B	2.88	108.33	106.31
20	B	1226	CLA	O2D-CGD-O1D	-2.88	118.24	123.85
20	2	603	CLA	O2D-CGD-O1D	-2.88	118.25	123.85
20	3	606	CLA	C3B-C4B-NB	-2.88	107.96	110.53
20	B	1220	CLA	O2D-CGD-O1D	-2.88	118.25	123.85
20	A	1113	CLA	O2D-CGD-O1D	-2.87	118.26	123.85
20	A	1801	CLA	O2D-CGD-O1D	-2.87	118.26	123.85
28	2	601	CHL	CMB-C2B-C1B	2.87	129.79	125.42
28	2	601	CHL	O2A-CGA-CBA	2.87	120.58	111.83
20	1	606	CLA	O2D-CGD-O1D	-2.87	118.27	123.85
23	A	4003	BCR	C30-C25-C26	-2.87	118.72	122.64
20	4	610	CLA	O2D-CGD-O1D	-2.87	118.27	123.85
20	4	602	CLA	O2D-CGD-O1D	-2.86	118.27	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	3	603	CLA	O2D-CGD-O1D	-2.86	118.27	123.85
23	G	311	BCR	C31-C1-C6	2.86	114.73	110.24
28	1	601	CHL	C3D-C4D-ND	2.86	114.64	109.99
20	3	612	CLA	O2D-CGD-O1D	-2.86	118.29	123.85
20	B	1205	CLA	O2D-CGD-O1D	-2.86	118.29	123.85
20	K	202	CLA	O2D-CGD-O1D	-2.86	118.29	123.85
20	4	613	CLA	O2D-CGD-O1D	-2.86	118.29	123.85
28	2	607	CHL	CMB-C2B-C1B	2.85	129.76	125.42
20	A	1013	CLA	CMB-C2B-C3B	2.85	133.25	126.55
28	2	601	CHL	CMD-C2D-C3D	-2.85	121.16	127.69
20	1	615	CLA	O2D-CGD-O1D	-2.84	118.31	123.85
23	L	420	BCR	C1-C6-C5	-2.84	118.75	122.64
20	G	201	CLA	O2D-CGD-O1D	-2.84	118.31	123.85
20	K	204	CLA	O2D-CGD-O1D	-2.84	118.31	123.85
20	A	1110	CLA	O2D-CGD-O1D	-2.84	118.32	123.85
28	2	615	CHL	CAC-C3C-C4C	2.84	128.49	124.79
23	G	311	BCR	C15-C16-C17	-2.84	117.72	123.52
28	4	607	CHL	CAA-C2A-C3A	-2.84	105.34	113.00
21	A	2001	PQN	C14-C13-C15	2.83	120.14	115.23
28	2	608	CHL	O2A-CGA-CBA	2.83	120.47	111.83
23	I	120	BCR	C33-C5-C6	-2.83	121.39	124.48
24	3	630	LHG	O8-C23-C24	2.83	120.46	111.83
29	4	621	LUT	C31-C32-C33	-2.83	118.61	126.36
20	A	1107	CLA	O2D-CGD-O1D	-2.82	118.35	123.85
23	I	120	BCR	C40-C30-C29	-2.82	98.11	108.95
20	A	1121	CLA	O2D-CGD-O1D	-2.82	118.35	123.85
29	4	620	LUT	C31-C32-C33	-2.82	118.62	126.36
20	A	1105	CLA	O2D-CGD-O1D	-2.82	118.36	123.85
20	B	1229	CLA	CHA-C1A-NA	-2.82	120.01	126.39
20	A	1133	CLA	C3B-C4B-NB	-2.82	108.02	110.53
23	L	419	BCR	C30-C25-C24	2.81	123.28	115.65
20	A	1114	CLA	O2D-CGD-O1D	-2.81	118.37	123.85
20	2	612	CLA	O2D-CGD-O1D	-2.81	118.37	123.85
29	3	621	LUT	C31-C32-C33	2.81	134.07	126.36
20	B	1219	CLA	O2D-CGD-O1D	-2.81	118.38	123.85
20	2	609	CLA	O2D-CGD-O1D	-2.81	118.38	123.85
28	2	602	CHL	O2A-CGA-CBA	2.81	120.41	111.83
20	G	202	CLA	O2D-CGD-O1D	-2.81	118.38	123.85
20	B	1201	CLA	C2A-C1A-CHA	2.81	128.75	123.87
20	B	1023	CLA	C2D-C1D-ND	-2.81	107.35	110.13
23	A	4007	BCR	C15-C16-C17	-2.81	117.77	123.52
20	4	603	CLA	C1-C2-C3	-2.81	121.60	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	1234	CLA	O2D-CGD-O1D	-2.81	118.39	123.85
20	2	613	CLA	O2D-CGD-O1D	-2.81	118.39	123.85
20	K	203	CLA	C1B-NB-C4B	2.80	108.28	106.31
20	3	604	CLA	C3B-C4B-NB	-2.80	108.03	110.53
20	A	1128	CLA	O2D-CGD-O1D	-2.80	118.40	123.85
23	A	4001	BCR	C15-C14-C13	-2.80	123.36	127.28
25	A	5002	LMG	O1-C7-C8	-2.80	104.02	110.82
20	A	1111	CLA	O2D-CGD-O1D	-2.79	118.41	123.85
28	2	601	CHL	O2D-CGD-O1D	-2.79	118.41	123.85
20	A	1115	CLA	O2D-CGD-O1D	-2.79	118.41	123.85
24	4	630	LHG	O8-C23-C24	2.79	120.35	111.83
28	2	606	CHL	CMD-C2D-C3D	-2.79	121.29	127.69
19	A	1011	CL0	O2D-CGD-O1D	-2.79	118.42	123.85
20	B	1222	CLA	CMB-C2B-C1B	-2.79	121.17	125.42
20	1	604	CLA	O2D-CGD-O1D	-2.79	118.42	123.85
20	B	1235	CLA	O2D-CGD-O1D	-2.79	118.42	123.85
20	B	1240	CLA	C1-O2A-CGA	2.79	123.39	116.65
20	4	603	CLA	O2D-CGD-O1D	-2.78	118.43	123.85
20	4	612	CLA	O2D-CGD-O1D	-2.78	118.43	123.85
23	3	624	BCR	C15-C14-C13	-2.78	123.38	127.28
20	3	610	CLA	CMB-C2B-C1B	-2.77	121.19	125.42
20	A	1140	CLA	O2D-CGD-O1D	-2.77	118.45	123.85
20	B	1222	CLA	CMD-C2D-C1D	-2.77	119.84	124.73
20	1	602	CLA	O2D-CGD-O1D	-2.77	118.45	123.85
24	1	630	LHG	C11-C10-C9	-2.77	100.36	114.37
20	B	1204	CLA	CMB-C2B-C1B	-2.77	121.20	125.42
23	K	301	BCR	C15-C16-C17	-2.77	117.86	123.52
20	B	1228	CLA	O2D-CGD-O1D	-2.77	118.46	123.85
20	L	302	CLA	C3B-C4B-NB	-2.77	108.06	110.53
20	3	605	CLA	C1B-NB-C4B	2.76	108.25	106.31
28	2	608	CHL	C3D-C4D-ND	2.76	114.48	109.99
28	1	607	CHL	C1C-C2C-C3C	-2.76	104.74	107.28
20	A	1121	CLA	C2D-C1D-ND	-2.76	107.40	110.13
20	1	612	CLA	O2D-CGD-O1D	-2.76	118.48	123.85
20	3	607	CLA	O2D-CGD-O1D	-2.76	118.48	123.85
20	A	1106	CLA	O2D-CGD-O1D	-2.76	118.48	123.85
23	B	4010	BCR	C32-C1-C6	2.75	114.56	110.24
20	A	1118	CLA	O2D-CGD-O1D	-2.75	118.49	123.85
29	2	621	LUT	C38-C25-C24	-2.75	116.85	123.36
20	A	1120	CLA	O2D-CGD-O1D	-2.75	118.49	123.85
23	B	4010	BCR	C24-C23-C22	-2.75	122.17	126.23
20	A	1128	CLA	C2D-C1D-ND	-2.75	107.41	110.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	G	311	BCR	C28-C27-C26	-2.75	109.16	114.06
20	B	1214	CLA	CMB-C2B-C1B	-2.75	121.24	125.42
20	1	602	CLA	C3B-C4B-NB	-2.75	108.08	110.53
20	1	610	CLA	CHB-C1B-C2B	-2.75	119.46	127.43
28	3	608	CHL	CMB-C2B-C1B	2.74	129.60	125.42
20	B	1210	CLA	O2D-CGD-O1D	-2.74	118.51	123.85
20	A	1126	CLA	C2D-C1D-ND	-2.74	107.41	110.13
20	3	602	CLA	O2D-CGD-O1D	-2.74	118.51	123.85
20	B	1205	CLA	C6-C5-C3	2.74	120.15	113.47
20	B	1023	CLA	C1D-ND-C4D	-2.74	104.39	106.31
23	A	4007	BCR	C15-C14-C13	-2.74	123.43	127.28
23	B	4009	BCR	C27-C26-C25	2.74	126.41	122.70
20	B	1214	CLA	C4B-C3B-C2B	-2.74	103.89	107.30
20	A	1115	CLA	CMB-C2B-C1B	-2.74	121.24	125.42
23	3	623	BCR	C27-C26-C25	2.74	126.40	122.70
20	A	1125	CLA	CHD-C1D-ND	-2.74	120.95	124.80
25	2	631	LMG	O6-C1-O1	-2.74	103.58	110.04
28	2	611	CHL	CMB-C2B-C1B	2.74	129.59	125.42
20	1	610	CLA	C6-C5-C3	2.73	120.13	113.47
28	1	607	CHL	CBA-CAA-C2A	2.73	121.93	113.79
20	B	1201	CLA	O2D-CGD-O1D	-2.73	118.53	123.85
20	A	1109	CLA	C2B-C1B-NB	-2.73	107.49	110.33
29	1	620	LUT	C37-C21-C36	-2.73	103.90	107.87
20	B	1231	CLA	O2D-CGD-O1D	-2.73	118.53	123.85
20	K	203	CLA	C3A-C4A-CHB	-2.73	120.57	123.91
28	4	615	CHL	CMB-C2B-C1B	2.73	129.57	125.42
29	4	620	LUT	C36-C21-C22	-2.73	104.32	109.41
28	4	606	CHL	CMD-C2D-C3D	-2.73	121.43	127.69
20	B	1234	CLA	CHA-C1A-NA	-2.72	120.22	126.39
28	1	607	CHL	CMB-C2B-C1B	2.72	129.57	125.42
20	1	608	CLA	CMB-C2B-C1B	-2.72	121.28	125.42
28	4	607	CHL	CMD-C2D-C3D	-2.72	121.45	127.69
23	L	419	BCR	C2-C1-C6	2.72	114.39	110.44
20	L	303	CLA	C3B-C4B-NB	-2.72	108.10	110.53
23	B	4017	BCR	C24-C23-C22	-2.72	122.21	126.23
20	A	1133	CLA	O2D-CGD-O1D	-2.72	118.56	123.85
23	J	213	BCR	C29-C30-C25	2.72	114.38	110.44
20	3	613	CLA	O2D-CGD-O1D	-2.72	118.56	123.85
28	1	601	CHL	O2A-CGA-CBA	2.71	120.11	111.83
20	A	1105	CLA	CHD-C1D-ND	-2.71	120.98	124.80
29	2	620	LUT	C35-C15-C14	2.71	129.07	123.52
20	A	1102	CLA	O2D-CGD-O1D	-2.71	118.57	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	1137	CLA	O2D-CGD-O1D	-2.71	118.57	123.85
23	3	624	BCR	C28-C27-C26	-2.71	109.23	114.06
20	1	611	CLA	C4A-NA-C1A	2.71	107.91	106.68
26	1	631	LMT	C3'-C4'-C5'	-2.70	104.93	110.93
23	1	623	BCR	C27-C26-C25	2.70	126.35	122.70
20	B	1217	CLA	O2D-CGD-O1D	-2.70	118.59	123.85
23	B	4004	BCR	C15-C14-C13	-2.70	123.50	127.28
28	4	615	CHL	C1C-C2C-C3C	-2.70	104.80	107.28
29	4	620	LUT	C15-C14-C13	2.70	131.06	127.28
29	1	620	LUT	C37-C21-C26	-2.69	105.47	109.55
20	B	1239	CLA	C3C-C4C-NC	-2.69	106.99	110.43
20	A	1127	CLA	CHA-C1A-NA	-2.69	120.31	126.39
20	A	1125	CLA	C3B-C4B-NB	-2.69	108.13	110.53
20	A	1115	CLA	CMB-C2B-C3B	2.68	132.87	126.55
20	B	1209	CLA	O2D-CGD-O1D	-2.68	118.62	123.85
20	1	609	CLA	O2D-CGD-O1D	-2.68	118.62	123.85
20	1	614	CLA	O2D-CGD-O1D	-2.68	118.63	123.85
20	L	301	CLA	O2D-CGD-O1D	-2.68	118.63	123.85
20	I	121	CLA	C3B-C4B-NB	-2.68	108.14	110.53
28	4	615	CHL	CMD-C2D-C3D	-2.68	121.55	127.69
29	3	621	LUT	C22-C23-C24	-2.67	107.22	111.18
20	B	1229	CLA	O2D-CGD-O1D	-2.67	118.65	123.85
20	B	1220	CLA	CMB-C2B-C1B	-2.67	121.35	125.42
20	3	602	CLA	CMB-C2B-C1B	-2.67	121.35	125.42
24	A	5003	LHG	O8-C23-C24	2.67	119.97	111.83
20	B	1222	CLA	C2D-C1D-ND	-2.67	107.49	110.13
23	I	118	BCR	C27-C26-C25	2.66	126.31	122.70
20	B	1224	CLA	O2D-CGD-O1D	-2.66	118.67	123.85
28	2	615	CHL	CMD-C2D-C3D	-2.66	121.58	127.69
20	L	301	CLA	C3C-C4C-NC	-2.66	107.02	110.43
20	L	302	CLA	O2D-CGD-O1D	-2.66	118.67	123.85
23	I	120	BCR	C11-C10-C9	-2.66	123.55	127.28
20	A	1134	CLA	CMB-C2B-C1B	-2.66	121.37	125.42
28	1	601	CHL	O2D-CGD-O1D	-2.66	118.68	123.85
20	F	303	CLA	C3A-C4A-CHB	-2.65	120.66	123.91
20	B	1223	CLA	CHD-C1D-ND	-2.65	121.08	124.80
20	A	1117	CLA	CMB-C2B-C3B	2.65	132.78	126.55
28	2	611	CHL	O2A-CGA-CBA	2.65	119.90	111.83
20	K	204	CLA	CMC-C2C-C1C	-2.64	120.90	125.03
20	L	302	CLA	CHD-C1D-ND	-2.64	121.08	124.80
28	1	601	CHL	CMB-C2B-C1B	2.64	129.44	125.42
20	1	613	CLA	CHD-C1D-ND	-2.64	121.09	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	3	612	CLA	CMB-C2B-C1B	-2.64	121.40	125.42
20	B	1225	CLA	CMB-C2B-C3B	2.64	132.76	126.55
28	4	606	CHL	CMB-C2B-C1B	2.64	129.43	125.42
20	B	1232	CLA	CHA-C1A-NA	-2.64	120.42	126.39
20	A	1136	CLA	O2D-CGD-O1D	-2.64	118.72	123.85
20	K	204	CLA	C1C-C2C-C3C	-2.64	104.21	106.98
23	O	301	BCR	C27-C26-C25	2.64	126.27	122.70
20	B	1227	CLA	O2D-CGD-O1D	-2.63	118.72	123.85
20	B	1212	CLA	O2D-CGD-O1D	-2.63	118.72	123.85
20	A	1102	CLA	CMB-C2B-C1B	-2.63	121.42	125.42
20	3	605	CLA	C1C-NC-C4C	2.63	107.88	106.68
20	B	1216	CLA	CHB-C1B-C2B	-2.63	119.80	127.43
29	4	620	LUT	C37-C21-C26	-2.63	105.57	109.55
23	A	4011	BCR	C1-C6-C5	-2.62	119.05	122.64
23	B	4004	BCR	C39-C30-C25	2.62	114.35	110.24
23	A	4008	BCR	C31-C1-C6	2.62	114.34	110.24
23	B	4006	BCR	C27-C26-C25	2.62	126.24	122.70
29	2	620	LUT	C20-C13-C14	-2.61	118.58	122.82
23	A	4002	BCR	C27-C26-C25	2.61	126.23	122.70
29	2	620	LUT	C15-C14-C13	-2.61	123.62	127.28
20	B	1222	CLA	C2A-C1A-CHA	2.61	128.39	123.87
28	2	608	CHL	CMD-C2D-C3D	-2.61	121.71	127.69
20	A	1101	CLA	CHD-C1D-ND	-2.61	121.13	124.80
20	A	1125	CLA	CAA-CBA-CGA	-2.61	105.81	113.21
28	2	611	CHL	C4D-CHA-C1A	-2.60	118.14	121.24
23	B	4010	BCR	C7-C8-C9	-2.60	122.39	126.23
20	B	1209	CLA	CMB-C2B-C1B	-2.60	121.46	125.42
24	1	630	LHG	O8-C23-C24	2.60	119.75	111.83
26	G	401	LMT	C3'-C4'-C5'	-2.59	105.18	110.93
20	O	201	CLA	C1B-NB-C4B	2.59	108.13	106.31
24	A	5001	LHG	O8-C23-C24	2.59	119.74	111.83
20	G	202	CLA	CMB-C2B-C1B	-2.59	121.47	125.42
20	B	1205	CLA	C1-C2-C3	-2.59	121.95	126.20
20	B	1230	CLA	C4D-C3D-CAD	-2.59	105.29	108.11
20	B	1203	CLA	C3C-C4C-NC	-2.59	107.11	110.43
20	A	1135	CLA	CAC-C3C-C2C	-2.59	122.80	127.56
20	A	1128	CLA	CHB-C1B-NB	2.59	127.94	124.05
23	1	623	BCR	C15-C16-C17	-2.59	118.22	123.52
23	G	311	BCR	C2-C1-C6	2.59	114.20	110.44
20	A	1125	CLA	CMB-C2B-C3B	2.59	132.64	126.55
20	B	1223	CLA	O2D-CGD-O1D	-2.59	118.81	123.85
20	B	1237	CLA	O2D-CGD-O1D	-2.58	118.82	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	1204	CLA	C3B-C4B-NB	-2.58	108.22	110.53
23	B	4017	BCR	C27-C26-C25	2.58	126.19	122.70
23	L	420	BCR	C15-C14-C13	-2.58	123.66	127.28
23	K	301	BCR	C15-C14-C13	-2.58	123.66	127.28
20	B	1216	CLA	CAC-C3C-C2C	-2.58	122.82	127.56
20	1	603	CLA	CMB-C2B-C1B	-2.58	121.49	125.42
27	B	5002	DGD	CDB-CCB-CBB	-2.58	101.34	114.37
20	B	1021	CLA	CMB-C2B-C1B	-2.58	121.50	125.42
28	2	601	CHL	O1D-CGD-CBD	-2.58	119.44	124.52
29	4	623	LUT	C15-C35-C34	-2.57	118.25	123.52
23	A	4008	BCR	C40-C30-C29	-2.57	99.07	108.95
20	B	1232	CLA	C2A-C1A-CHA	2.57	128.33	123.87
23	A	4007	BCR	C11-C10-C9	-2.57	123.67	127.28
20	B	1213	CLA	CHD-C1D-ND	-2.57	121.19	124.80
20	A	1132	CLA	CHD-C1D-C2D	2.57	130.83	125.49
23	L	419	BCR	C15-C16-C17	-2.57	118.27	123.52
20	4	610	CLA	CMB-C2B-C1B	-2.57	121.51	125.42
28	2	611	CHL	C1C-C2C-C3C	-2.57	104.92	107.28
24	2	630	LHG	O8-C23-C24	2.56	119.65	111.83
20	2	604	CLA	CMB-C2B-C1B	-2.56	121.52	125.42
20	A	1126	CLA	C4B-C3B-C2B	-2.56	104.12	107.30
20	A	1114	CLA	C3B-C4B-NB	-2.56	108.25	110.53
20	4	601	CLA	O2D-CGD-O1D	-2.56	118.87	123.85
20	B	1231	CLA	C3C-C4C-NC	-2.55	107.16	110.43
20	4	611	CLA	C2D-C1D-ND	-2.55	107.60	110.13
29	4	623	LUT	C38-C25-C24	-2.55	117.33	123.36
23	A	4007	BCR	C30-C25-C24	2.54	122.54	115.65
20	A	1126	CLA	C3B-C2B-C1B	-2.53	104.18	107.17
20	K	204	CLA	C2C-C1C-NC	-2.53	107.32	109.98
20	A	1109	CLA	C2D-C1D-ND	-2.53	107.62	110.13
28	1	607	CHL	C4B-C3B-C2B	-2.53	104.16	107.30
23	L	420	BCR	C33-C5-C4	-2.52	108.22	113.60
28	4	608	CHL	O2A-CGA-CBA	2.52	119.53	111.83
23	A	4011	BCR	C27-C26-C25	2.52	126.11	122.70
20	1	603	CLA	O2A-CGA-O1A	-2.52	117.32	123.63
23	G	311	BCR	C24-C23-C22	-2.52	122.51	126.23
23	L	419	BCR	C24-C25-C26	-2.52	115.75	121.56
23	B	4010	BCR	C27-C26-C25	2.52	126.11	122.70
29	3	621	LUT	C15-C14-C13	2.52	130.81	127.28
20	4	612	CLA	C3B-C4B-NB	-2.52	108.28	110.53
20	A	8895	CLA	O2D-CGD-O1D	-2.52	118.95	123.85
29	1	621	LUT	C7-C8-C9	-2.52	122.51	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	4009	BCR	C24-C23-C22	-2.51	122.52	126.23
20	B	1212	CLA	C3B-C4B-NB	-2.51	108.29	110.53
20	B	1214	CLA	CHA-C1A-NA	-2.51	120.71	126.39
20	B	1012	CLA	CMB-C2B-C3B	2.51	132.45	126.55
20	B	1216	CLA	C4A-NA-C1A	2.51	107.82	106.68
20	A	1124	CLA	O2D-CGD-O1D	-2.51	118.97	123.85
23	K	301	BCR	C7-C8-C9	-2.50	122.53	126.23
29	1	621	LUT	C39-C29-C30	-2.50	118.76	122.82
20	B	1214	CLA	O2D-CGD-O1D	-2.50	118.98	123.85
20	3	603	CLA	CHB-C4A-NA	2.50	128.01	124.40
23	A	4008	BCR	C33-C5-C6	-2.50	121.76	124.48
23	B	4006	BCR	C15-C16-C17	-2.50	118.41	123.52
28	2	615	CHL	O2D-CGD-O1D	-2.50	118.99	123.85
23	B	4005	BCR	C27-C26-C25	2.50	126.08	122.70
20	2	609	CLA	CHA-C1A-NA	-2.49	120.74	126.39
20	A	1132	CLA	C2D-C1D-ND	-2.49	107.66	110.13
29	3	621	LUT	C30-C31-C32	2.49	130.42	123.20
23	A	4007	BCR	C7-C6-C5	2.49	127.29	121.56
20	4	603	CLA	CHB-C4A-NA	2.49	127.99	124.40
29	2	620	LUT	C30-C31-C32	2.49	130.41	123.20
20	1	610	CLA	C4-C3-C5	2.49	119.55	115.23
24	A	5003	LHG	C11-C10-C9	-2.49	101.80	114.37
20	A	1013	CLA	C2D-C1D-ND	-2.48	107.67	110.13
20	B	1023	CLA	CMD-C2D-C1D	-2.48	120.36	124.73
23	J	212	BCR	C16-C15-C14	-2.48	118.45	123.52
20	B	1226	CLA	C2B-C1B-NB	-2.48	107.76	110.33
20	B	1238	CLA	CHA-C1A-NA	-2.48	120.78	126.39
20	A	1132	CLA	C2B-C1B-NB	-2.48	107.76	110.33
23	B	4010	BCR	C1-C6-C5	-2.47	119.25	122.64
23	A	4007	BCR	C38-C26-C27	-2.47	108.32	113.60
20	A	1109	CLA	C3C-C4C-NC	-2.47	107.26	110.43
20	1	604	CLA	C3B-C4B-NB	-2.47	108.32	110.53
20	4	602	CLA	CHA-C1A-NA	-2.47	120.80	126.39
20	B	1210	CLA	CAA-CBA-CGA	-2.47	106.20	113.21
23	G	311	BCR	C29-C30-C25	2.47	114.02	110.44
20	3	605	CLA	C3A-C4A-CHB	-2.47	120.89	123.91
20	B	1203	CLA	O2A-CGA-O1A	-2.47	117.46	123.63
23	B	4010	BCR	C20-C19-C18	-2.47	119.60	126.36
20	B	1203	CLA	CHB-C4A-NA	2.46	127.96	124.40
20	L	303	CLA	CHB-C4A-NA	2.46	127.96	124.40
20	A	1115	CLA	CHD-C1D-ND	-2.46	121.33	124.80
26	A	5004	LMT	O1B-C4'-C3'	2.46	113.49	107.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	2	610	CLA	C4A-NA-C1A	2.46	107.80	106.68
20	B	1238	CLA	O2D-CGD-O1D	-2.46	119.06	123.85
20	B	1219	CLA	C3C-C4C-NC	-2.46	107.28	110.43
20	K	202	CLA	CAC-C3C-C2C	-2.46	123.04	127.56
20	A	1132	CLA	CHD-C1D-ND	-2.46	121.34	124.80
28	2	611	CHL	CAA-C2A-C3A	-2.46	106.36	113.00
23	B	4004	BCR	C27-C26-C25	2.46	126.02	122.70
23	1	623	BCR	C35-C13-C12	2.45	120.23	114.59
20	2	614	CLA	C2D-C1D-ND	-2.45	107.70	110.13
20	1	612	CLA	CHB-C4A-NA	2.45	127.94	124.40
20	F	303	CLA	C1C-NC-C4C	2.45	107.80	106.68
20	A	1104	CLA	C11-C12-C13	-2.45	107.83	115.97
23	L	420	BCR	C7-C6-C5	2.45	127.19	121.56
20	4	603	CLA	CMB-C2B-C1B	-2.45	121.69	125.42
28	2	601	CHL	C4-C3-C5	2.44	119.47	115.23
20	B	1219	CLA	CHD-C1D-ND	-2.44	121.37	124.80
20	A	5005	CLA	CHA-C1A-NA	-2.44	120.87	126.39
20	A	1127	CLA	C1-C2-C3	-2.44	122.20	126.20
23	B	4014	BCR	C15-C16-C17	-2.44	118.53	123.52
20	B	1238	CLA	CHB-C1B-C2B	-2.44	120.36	127.43
23	3	624	BCR	C29-C30-C25	2.44	113.98	110.44
20	A	1128	CLA	CHD-C1D-ND	-2.44	121.38	124.80
28	2	606	CHL	C1C-C2C-C3C	-2.43	105.04	107.28
20	1	612	CLA	C2D-C1D-ND	-2.43	107.72	110.13
20	1	610	CLA	O2A-CGA-O1A	-2.43	117.54	123.63
28	2	606	CHL	O2D-CGD-O1D	-2.43	119.11	123.85
24	A	5001	LHG	C20-C19-C18	-2.43	102.08	114.37
20	4	613	CLA	CMB-C2B-C1B	-2.43	121.72	125.42
24	B	5101	LHG	C11-C10-C9	-2.43	102.08	114.37
20	A	1126	CLA	CMB-C2B-C3B	2.43	132.26	126.55
20	L	302	CLA	CMB-C2B-C1B	-2.43	121.72	125.42
20	B	1220	CLA	C2D-C1D-ND	-2.43	107.72	110.13
20	A	1131	CLA	C1-C2-C3	-2.43	122.22	126.20
20	A	1112	CLA	C3C-C4C-NC	-2.43	107.32	110.43
23	3	623	BCR	C11-C10-C9	-2.43	123.88	127.28
20	A	5005	CLA	O2D-CGD-CBD	2.42	115.47	111.23
20	A	1116	CLA	O2D-CGD-O1D	-2.42	119.13	123.85
20	A	1101	CLA	CMB-C2B-C1B	-2.42	121.73	125.42
20	1	613	CLA	C2D-C1D-ND	-2.42	107.73	110.13
23	M	4021	BCR	C15-C16-C17	-2.42	118.57	123.52
20	4	609	CLA	CHA-C1A-NA	-2.42	120.91	126.39
28	2	601	CHL	CAA-C2A-C3A	-2.42	106.46	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	2	620	LUT	C1-C6-C5	-2.42	119.33	122.64
23	A	4003	BCR	C38-C26-C27	-2.42	108.44	113.60
28	2	602	CHL	C1-C2-C3	-2.42	122.24	126.20
20	A	1139	CLA	CMB-C2B-C1B	-2.42	121.74	125.42
23	A	4011	BCR	C32-C1-C6	2.42	114.03	110.24
28	4	606	CHL	O2D-CGD-O1D	-2.42	119.14	123.85
20	A	1126	CLA	C3C-C4C-NC	-2.42	107.33	110.43
23	B	4009	BCR	C10-C11-C12	-2.41	116.21	123.20
20	4	610	CLA	CHA-C1A-NA	-2.41	120.93	126.39
20	L	301	CLA	C2C-C1C-NC	-2.41	107.45	109.98
20	A	1127	CLA	CHD-C1D-ND	-2.41	121.41	124.80
20	1	610	CLA	CHA-C1A-NA	-2.41	120.94	126.39
23	J	213	BCR	C28-C27-C26	-2.41	109.76	114.06
28	1	601	CHL	CAA-C2A-C3A	-2.41	106.50	113.00
20	A	1104	CLA	CMB-C2B-C1B	-2.41	121.76	125.42
20	3	609	CLA	CHD-C1D-ND	-2.40	121.42	124.80
20	A	1137	CLA	CMB-C2B-C1B	-2.40	121.76	125.42
20	B	1210	CLA	C1-C2-C3	-2.40	122.26	126.20
20	1	603	CLA	CHA-C1A-NA	-2.40	120.96	126.39
20	B	1213	CLA	CMB-C2B-C3B	2.40	132.19	126.55
20	2	609	CLA	CMB-C2B-C1B	-2.40	121.77	125.42
28	4	607	CHL	C4B-C3B-C2B	-2.39	104.33	107.30
20	L	303	CLA	CHD-C1D-ND	-2.39	121.43	124.80
20	A	5005	CLA	O2A-CGA-O1A	-2.39	117.64	123.63
20	B	1202	CLA	CMB-C2B-C3B	2.39	132.17	126.55
29	4	621	LUT	C35-C15-C14	2.39	128.41	123.52
23	J	213	BCR	C24-C23-C22	-2.39	122.70	126.23
29	2	620	LUT	C12-C13-C14	2.39	122.76	119.01
20	B	1235	CLA	CHD-C1D-ND	-2.39	121.44	124.80
23	J	212	BCR	C15-C16-C17	-2.38	118.64	123.52
20	A	1127	CLA	O2D-CGD-O1D	-2.38	119.21	123.85
28	2	601	CHL	C1C-C2C-C3C	-2.38	105.09	107.28
24	3	630	LHG	C11-C10-C9	-2.38	102.33	114.37
23	3	624	BCR	C24-C23-C22	-2.38	122.71	126.23
20	B	1202	CLA	CHA-C1A-NA	-2.38	121.00	126.39
28	2	611	CHL	C4-C3-C5	2.38	119.36	115.23
20	A	1013	CLA	CHB-C1B-C2B	-2.38	120.52	127.43
23	B	4005	BCR	C24-C23-C22	-2.38	122.72	126.23
23	B	4010	BCR	C20-C21-C22	-2.38	123.94	127.28
20	B	1234	CLA	CMB-C2B-C3B	2.38	132.14	126.55
20	4	604	CLA	CHA-C1A-NA	-2.38	121.01	126.39
20	A	5005	CLA	CHD-C1D-ND	-2.38	121.46	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	4	610	CLA	C2D-C1D-ND	-2.37	107.78	110.13
23	M	4021	BCR	C29-C30-C25	2.37	113.89	110.44
23	L	419	BCR	C23-C24-C25	2.37	133.33	127.00
20	A	1121	CLA	CHD-C1D-ND	-2.37	121.47	124.80
28	4	607	CHL	O2D-CGD-O1D	-2.37	119.23	123.85
20	B	1012	CLA	CAA-C2A-C3A	-2.37	106.60	113.00
23	3	624	BCR	C11-C10-C9	-2.37	123.96	127.28
20	B	1202	CLA	C3B-C4B-NB	-2.37	108.42	110.53
20	B	1231	CLA	CHB-C4A-NA	2.37	127.81	124.40
23	3	624	BCR	C3-C4-C5	-2.36	109.84	114.06
23	A	4011	BCR	C2-C1-C6	2.36	113.87	110.44
20	K	204	CLA	CHD-C1D-ND	-2.36	121.48	124.80
20	B	1215	CLA	CHD-C1D-ND	-2.36	121.48	124.80
23	B	4006	BCR	C29-C30-C25	2.36	113.87	110.44
20	B	1224	CLA	C3C-C4C-NC	-2.36	107.41	110.43
20	A	1126	CLA	CHD-C1D-ND	-2.36	121.49	124.80
20	4	611	CLA	CHD-C1D-ND	-2.35	121.49	124.80
20	4	613	CLA	O2A-CGA-O1A	-2.35	117.74	123.63
20	B	1216	CLA	C1-C2-C3	-2.35	122.34	126.20
20	A	1117	CLA	C16-C17-C18	-2.35	105.44	115.94
27	B	5002	DGD	C3D-C4D-C5D	-2.35	105.97	110.23
20	A	1107	CLA	CHB-C4A-NA	2.35	127.79	124.40
29	2	620	LUT	C1-C6-C7	2.35	122.03	115.65
23	B	4014	BCR	C29-C30-C25	2.35	113.85	110.44
23	B	4009	BCR	C15-C14-C13	-2.35	123.99	127.28
29	4	620	LUT	C11-C10-C9	2.35	130.57	127.28
20	B	1227	CLA	CHA-C1A-NA	-2.34	121.08	126.39
23	J	213	BCR	C15-C14-C13	-2.34	123.99	127.28
23	F	416	BCR	C15-C16-C17	-2.34	118.73	123.52
23	L	419	BCR	C31-C1-C6	2.34	113.92	110.24
28	1	601	CHL	CMD-C2D-C3D	-2.34	122.32	127.69
20	B	1203	CLA	C3B-C4B-NB	-2.34	108.44	110.53
20	B	1229	CLA	CHD-C1D-ND	-2.34	121.51	124.80
27	B	5002	DGD	O3G-C3G-C2G	-2.34	105.13	110.82
23	I	118	BCR	C3-C4-C5	-2.34	109.89	114.06
23	A	4007	BCR	C40-C30-C29	-2.34	99.98	108.95
20	B	1226	CLA	C3C-C4C-NC	-2.33	107.44	110.43
20	B	1230	CLA	CHD-C1D-ND	-2.33	121.52	124.80
28	4	608	CHL	C1C-C2C-C3C	-2.33	105.14	107.28
28	3	608	CHL	C4B-C3B-C2B	-2.33	104.41	107.30
20	A	1126	CLA	CHA-C1A-NA	-2.33	121.12	126.39
20	2	612	CLA	O2A-CGA-O1A	-2.33	117.81	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	4	615	CHL	CHB-C1B-NB	-2.33	120.56	124.05
20	1	613	CLA	C2A-C1A-CHA	2.33	127.90	123.87
20	A	1107	CLA	C3B-C2B-C1B	-2.33	104.43	107.17
20	A	1113	CLA	C3C-C4C-NC	-2.33	107.45	110.43
28	4	615	CHL	O2D-CGD-O1D	-2.32	119.32	123.85
20	4	611	CLA	CMB-C2B-C1B	-2.32	121.88	125.42
20	B	1219	CLA	C4D-C3D-CAD	-2.32	105.58	108.11
28	1	607	CHL	O2A-CGA-CBA	2.32	120.92	112.14
24	4	630	LHG	C11-C10-C9	-2.32	102.62	114.37
20	B	1023	CLA	CMD-C2D-C3D	2.32	133.02	127.69
28	2	615	CHL	CHB-C1B-NB	-2.32	120.57	124.05
20	B	1212	CLA	CHD-C1D-ND	-2.32	121.54	124.80
23	I	120	BCR	C28-C27-C26	-2.32	109.92	114.06
20	A	1114	CLA	CHA-C1A-NA	-2.32	121.14	126.39
20	B	1203	CLA	CHD-C1D-ND	-2.32	121.54	124.80
25	J	301	LMG	O6-C1-O1	-2.32	104.57	110.04
24	B	5101	LHG	O8-C23-C24	2.32	118.90	111.83
25	J	301	LMG	O3-C3-C2	-2.32	104.92	110.38
20	A	1128	CLA	C1-C2-C3	-2.32	122.40	126.20
23	L	419	BCR	C40-C30-C29	-2.31	100.06	108.95
20	L	302	CLA	C1-O2A-CGA	2.31	122.25	116.65
23	3	624	BCR	C7-C8-C9	-2.31	122.81	126.23
28	2	607	CHL	CHB-C1B-NB	-2.31	120.58	124.05
28	2	602	CHL	CHB-C1B-NB	-2.31	120.58	124.05
20	1	608	CLA	C1-C2-C3	-2.31	123.02	126.76
20	B	1214	CLA	C3C-C4C-NC	-2.31	107.47	110.43
20	B	1206	CLA	CHD-C1D-ND	-2.31	121.55	124.80
20	A	1127	CLA	O2A-CGA-O1A	-2.31	117.85	123.63
20	A	1117	CLA	CHD-C1D-ND	-2.31	121.56	124.80
20	B	1202	CLA	O2A-CGA-O1A	-2.31	117.86	123.63
23	M	4021	BCR	C24-C23-C22	-2.31	122.82	126.23
28	2	611	CHL	CMD-C2D-C3D	-2.31	122.40	127.69
23	A	4001	BCR	C28-C27-C26	-2.31	109.94	114.06
20	B	1023	CLA	C1-C2-C3	-2.31	122.42	126.20
29	2	621	LUT	C20-C13-C12	2.30	121.61	118.09
20	A	1116	CLA	O2A-CGA-O1A	-2.30	117.86	123.63
20	H	200	CLA	CMB-C2B-C1B	-2.30	121.91	125.42
29	4	621	LUT	C35-C34-C33	-2.30	124.05	127.28
20	A	1136	CLA	CHD-C1D-ND	-2.30	121.56	124.80
20	A	1105	CLA	CHA-C1A-NA	-2.30	121.18	126.39
25	J	301	LMG	C38-C37-C36	-2.30	102.73	114.37
20	B	1209	CLA	C3C-C4C-NC	-2.30	107.48	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	1221	CLA	C4-C3-C5	-2.30	111.23	115.23
20	A	1116	CLA	C2D-C1D-ND	-2.30	107.85	110.13
20	B	1221	CLA	C2D-C1D-ND	-2.30	107.85	110.13
20	B	1201	CLA	CHB-C4A-NA	2.30	127.72	124.40
20	A	1115	CLA	CAC-C3C-C2C	-2.30	123.33	127.56
23	I	118	BCR	C15-C16-C17	-2.30	118.81	123.52
28	2	607	CHL	C1C-C2C-C3C	-2.30	105.17	107.28
20	A	1128	CLA	C4B-C3B-C2B	-2.30	104.44	107.30
20	A	1112	CLA	C2D-C1D-ND	-2.29	107.86	110.13
20	A	1107	CLA	CHA-C1A-NA	-2.29	121.20	126.39
20	B	1210	CLA	CHD-C1D-ND	-2.29	121.57	124.80
20	A	1126	CLA	C2A-C1A-CHA	2.29	127.85	123.87
23	B	4009	BCR	C40-C30-C25	2.29	113.84	110.24
23	L	420	BCR	C24-C23-C22	-2.29	122.84	126.23
23	A	4003	BCR	C15-C16-C17	-2.29	118.83	123.52
20	K	201	CLA	CHD-C1D-ND	-2.29	121.58	124.80
20	F	301	CLA	CMB-C2B-C1B	-2.29	121.94	125.42
20	A	1130	CLA	CHA-C1A-NA	-2.29	121.21	126.39
20	O	202	CLA	CHB-C4A-NA	2.29	127.68	124.43
20	2	613	CLA	CMB-C2B-C1B	-2.28	121.94	125.42
20	A	1113	CLA	O2A-CGA-O1A	-2.28	117.46	123.33
23	B	4005	BCR	C15-C16-C17	-2.28	118.85	123.52
23	B	4006	BCR	C24-C23-C22	-2.28	122.86	126.23
23	M	4021	BCR	C28-C27-C26	-2.28	109.98	114.06
28	1	607	CHL	O1D-CGD-CBD	-2.28	120.02	124.52
23	L	420	BCR	C15-C16-C17	-2.28	118.85	123.52
20	A	1132	CLA	CAC-C3C-C4C	-2.28	121.82	124.79
20	B	1211	CLA	CMB-C2B-C3B	2.28	131.92	126.55
20	B	1205	CLA	O2A-CGA-O1A	-2.28	117.92	123.63
29	2	623	LUT	C7-C8-C9	2.28	129.61	126.23
20	2	604	CLA	CHB-C4A-NA	2.28	127.69	124.40
23	A	4011	BCR	C24-C23-C22	-2.28	122.86	126.23
20	3	617	CLA	CHB-C4A-NA	2.28	127.69	124.40
23	I	118	BCR	C16-C15-C14	-2.28	118.86	123.52
20	3	604	CLA	CHA-C1A-NA	-2.27	121.24	126.39
20	O	201	CLA	CHB-C4A-NA	2.27	127.66	124.43
23	F	416	BCR	C7-C8-C9	-2.27	122.88	126.23
20	A	1127	CLA	CMB-C2B-C3B	2.27	131.89	126.55
20	B	1231	CLA	C2D-C1D-ND	-2.27	107.88	110.13
23	I	118	BCR	C31-C1-C6	2.27	113.80	110.24
20	F	302	CLA	CHD-C1D-ND	-2.27	121.61	124.80
20	4	609	CLA	C3C-C4C-NC	-2.27	107.52	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	1119	CLA	C4D-C3D-CAD	-2.27	105.64	108.11
28	1	607	CHL	O2D-CGD-O1D	-2.27	119.44	123.85
28	3	608	CHL	O2D-CGD-O1D	-2.27	119.44	123.85
20	1	611	CLA	C2D-C1D-ND	-2.27	107.88	110.13
23	A	4007	BCR	C30-C25-C26	-2.27	119.54	122.64
23	B	4005	BCR	C15-C14-C13	-2.27	124.10	127.28
26	1	631	LMT	O5B-C5B-C4B	2.26	113.78	109.70
23	A	4007	BCR	C37-C22-C23	2.26	121.55	118.09
20	A	1136	CLA	C7-C6-C5	-2.26	107.23	113.26
24	A	5001	LHG	C27-C26-C25	-2.26	102.93	114.37
20	4	601	CLA	CHA-C1A-NA	-2.26	121.27	126.39
20	A	1118	CLA	CMB-C2B-C1B	-2.26	121.97	125.42
20	4	601	CLA	CMB-C2B-C1B	-2.26	121.97	125.42
23	J	212	BCR	C24-C23-C22	-2.26	122.89	126.23
24	2	630	LHG	C27-C26-C25	-2.26	102.94	114.37
20	B	1239	CLA	C4B-C3B-C2B	-2.26	104.49	107.30
20	4	603	CLA	CHD-C1D-ND	-2.26	121.62	124.80
28	2	602	CHL	O2D-CGD-O1D	-2.26	119.45	123.85
20	B	1201	CLA	C1C-C2C-C3C	-2.26	104.61	106.98
23	A	4001	BCR	C29-C30-C25	2.26	113.72	110.44
20	B	1229	CLA	O2A-CGA-O1A	-2.26	117.98	123.63
28	1	601	CHL	C4D-CHA-C1A	-2.26	118.55	121.24
20	3	614	CLA	CMB-C2B-C1B	-2.26	121.98	125.42
20	B	1208	CLA	CHB-C4A-NA	2.25	127.65	124.40
20	4	609	CLA	CMB-C2B-C1B	-2.25	121.99	125.42
23	M	4021	BCR	C10-C11-C12	-2.25	116.67	123.20
28	2	601	CHL	CHB-C1B-NB	-2.25	120.67	124.05
25	2	631	LMG	O1-C7-C8	-2.25	105.34	110.82
20	B	1206	CLA	CHB-C4A-NA	2.25	127.65	124.40
29	4	621	LUT	C17-C1-C6	2.25	113.77	110.24
24	B	5101	LHG	C27-C26-C25	-2.25	103.00	114.37
20	B	1216	CLA	C4D-C3D-CAD	-2.25	105.66	108.11
20	A	1131	CLA	C2B-C1B-NB	-2.25	108.00	110.33
24	A	5001	LHG	C18-C17-C16	-2.25	103.01	114.37
20	3	602	CLA	CMB-C2B-C3B	2.25	131.84	126.55
20	A	1117	CLA	CHD-C1D-C2D	2.25	130.16	125.49
23	B	4017	BCR	C10-C11-C12	-2.25	116.69	123.20
20	A	1119	CLA	CHA-C1A-NA	-2.25	121.31	126.39
20	B	1239	CLA	C1C-C2C-C3C	-2.24	104.62	106.98
20	A	1117	CLA	C1-C2-C3	-2.24	122.52	126.20
20	B	1214	CLA	C4D-C3D-CAD	-2.24	105.67	108.11
20	B	1240	CLA	CMB-C2B-C1B	-2.24	122.01	125.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	1210	CLA	C16-C17-C18	-2.24	105.94	115.94
20	B	1205	CLA	CMD-C2D-C1D	-2.24	120.78	124.73
20	A	1115	CLA	C2A-C1A-CHA	2.24	127.75	123.87
20	4	610	CLA	CMB-C2B-C3B	2.24	131.81	126.55
20	3	605	CLA	CHB-C4A-NA	2.24	127.61	124.43
28	2	606	CHL	CHB-C1B-NB	-2.24	120.69	124.05
20	K	204	CLA	CHB-C4A-NA	2.24	127.63	124.40
23	A	4003	BCR	C15-C14-C13	-2.24	124.14	127.28
23	1	623	BCR	C24-C23-C22	-2.24	122.93	126.23
28	4	608	CHL	C4D-C3D-CAD	2.24	110.53	108.11
29	3	620	LUT	C38-C25-C24	-2.24	118.07	123.36
20	A	1128	CLA	CMD-C2D-C1D	-2.24	120.79	124.73
20	B	1217	CLA	O1A-CGA-CBA	2.23	130.18	123.09
23	M	4021	BCR	C1-C6-C5	-2.23	119.58	122.64
23	F	416	BCR	C16-C15-C14	-2.23	118.95	123.52
28	1	601	CHL	C4B-C3B-C2B	-2.23	104.52	107.30
27	B	5002	DGD	O6D-C1D-O3G	-2.23	104.77	110.04
20	4	612	CLA	CHB-C4A-NA	2.23	127.62	124.40
28	1	607	CHL	CHC-C4B-NB	-2.23	120.70	124.05
23	3	623	BCR	C7-C8-C9	-2.23	122.93	126.23
20	A	1128	CLA	C3C-C4C-NC	-2.23	107.57	110.43
20	B	1240	CLA	CHD-C1D-ND	-2.23	121.66	124.80
23	3	623	BCR	C33-C5-C6	-2.23	122.05	124.48
23	B	4009	BCR	C30-C25-C26	-2.23	119.59	122.64
20	B	1023	CLA	C4D-C3D-CAD	-2.23	105.68	108.11
20	B	1223	CLA	CHA-C1A-NA	-2.23	121.34	126.39
28	2	611	CHL	CHB-C1B-NB	-2.23	120.70	124.05
23	I	118	BCR	C30-C25-C26	-2.23	119.59	122.64
20	3	614	CLA	CHA-C1A-NA	-2.23	121.34	126.39
20	A	1111	CLA	C4D-C3D-CAD	-2.23	105.69	108.11
20	A	1113	CLA	CHA-C1A-NA	-2.23	121.35	126.39
23	A	4002	BCR	C24-C23-C22	-2.23	122.94	126.23
20	1	615	CLA	CMB-C2B-C1B	-2.22	122.03	125.42
27	B	5002	DGD	O6E-C1E-O5D	-2.22	104.79	110.04
20	2	614	CLA	O2D-CGD-CBD	2.22	115.12	111.23
20	B	1215	CLA	C3C-C4C-NC	-2.22	107.58	110.43
20	O	203	CLA	C1C-NC-C4C	2.22	107.69	106.68
20	3	604	CLA	C2D-C1D-ND	-2.22	107.93	110.13
20	A	1130	CLA	C2A-C1A-CHA	2.22	127.72	123.87
28	2	602	CHL	CBA-CAA-C2A	2.22	120.40	113.79
20	O	203	CLA	CHB-C4A-NA	2.22	127.59	124.43
20	1	603	CLA	C4-C3-C5	2.22	119.08	115.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	4	606	CHL	C1C-C2C-C3C	-2.22	105.24	107.28
20	L	303	CLA	CHA-C1A-NA	-2.22	121.37	126.39
20	B	1226	CLA	CHD-C1D-ND	-2.22	121.68	124.80
28	2	608	CHL	C4D-CHA-C1A	-2.22	118.60	121.24
20	A	1106	CLA	CHD-C1D-ND	-2.22	121.68	124.80
20	A	1119	CLA	O2A-CGA-O1A	-2.22	118.08	123.63
23	I	120	BCR	C38-C26-C27	-2.22	108.87	113.60
20	1	615	CLA	CHB-C4A-NA	2.21	127.59	124.40
23	G	311	BCR	C15-C14-C13	-2.21	124.17	127.28
20	B	1021	CLA	CMD-C2D-C1D	-2.21	120.83	124.73
27	B	5002	DGD	CFB-CEB-CDB	-2.21	103.19	114.37
20	A	1105	CLA	C2D-C1D-ND	-2.21	107.94	110.13
20	1	606	CLA	CHB-C4A-NA	2.21	127.59	124.40
28	1	601	CHL	CHB-C1B-NB	-2.21	120.73	124.05
20	B	1201	CLA	CMB-C2B-C1B	-2.21	122.05	125.42
20	A	1140	CLA	C3C-C4C-NC	-2.21	107.60	110.43
23	I	120	BCR	C16-C17-C18	-2.21	124.18	127.28
20	B	1228	CLA	CHB-C4A-NA	2.21	127.59	124.40
29	2	620	LUT	C39-C29-C30	-2.21	119.24	122.82
20	B	1239	CLA	CHB-C4A-NA	2.21	127.58	124.40
23	A	4002	BCR	C15-C16-C17	-2.21	119.00	123.52
20	A	1101	CLA	O2D-CGD-CBD	2.21	115.09	111.23
20	B	1240	CLA	C2D-C1D-ND	-2.21	107.94	110.13
20	4	611	CLA	CHA-C1A-NA	-2.21	121.40	126.39
20	B	1217	CLA	O2A-CGA-O1A	-2.21	117.66	123.33
20	B	1227	CLA	C2D-C1D-ND	-2.20	107.94	110.13
20	B	1226	CLA	CHA-C1A-NA	-2.20	121.40	126.39
20	B	1227	CLA	C4D-C3D-CAD	-2.20	105.71	108.11
20	1	604	CLA	O2A-CGA-O1A	-2.20	118.12	123.63
20	2	610	CLA	C2D-C1D-ND	-2.20	107.95	110.13
20	1	610	CLA	O2D-CGD-CBD	2.20	115.08	111.23
23	L	419	BCR	C1-C6-C5	-2.20	119.63	122.64
28	4	606	CHL	C4B-C3B-C2B	-2.20	104.57	107.30
20	B	1213	CLA	C4D-C3D-CAD	-2.20	105.72	108.11
23	B	4009	BCR	C7-C8-C9	-2.20	122.98	126.23
23	F	416	BCR	C24-C23-C22	-2.20	122.98	126.23
20	K	202	CLA	CHD-C1D-ND	-2.20	121.71	124.80
20	1	612	CLA	C2B-C1B-NB	-2.20	108.05	110.33
20	4	609	CLA	O2D-CGD-CBD	2.20	115.07	111.23
20	F	303	CLA	CHB-C4A-NA	2.20	127.55	124.43
20	A	1132	CLA	CAA-CBA-CGA	-2.19	106.98	113.21
24	3	630	LHG	C27-C26-C25	-2.19	103.29	114.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	4014	BCR	C15-C14-C13	-2.19	124.21	127.28
20	3	610	CLA	CHB-C4A-NA	2.19	127.56	124.40
23	J	213	BCR	C3-C4-C5	-2.19	110.16	114.06
23	F	416	BCR	C27-C26-C25	2.19	125.66	122.70
20	B	1227	CLA	CHD-C1D-C2D	2.19	130.03	125.49
20	B	1221	CLA	CHB-C4A-NA	2.19	127.55	124.40
28	2	602	CHL	C1C-C2C-C3C	-2.19	105.27	107.28
29	4	620	LUT	C40-C33-C34	-2.18	119.28	122.82
20	A	1122	CLA	O2A-CGA-O1A	-2.18	118.17	123.63
28	2	602	CHL	C4-C3-C5	2.18	119.02	115.23
23	K	301	BCR	C29-C30-C25	2.18	113.61	110.44
20	F	302	CLA	CHB-C4A-NA	2.18	127.55	124.40
23	B	4004	BCR	C24-C23-C22	-2.18	123.01	126.23
23	J	212	BCR	C7-C8-C9	-2.18	123.01	126.23
20	A	1131	CLA	O1D-CGD-CBD	2.18	128.82	124.52
29	2	623	LUT	C19-C9-C10	-2.18	119.28	122.82
20	3	609	CLA	CHA-C1A-NA	-2.18	121.45	126.39
20	A	1114	CLA	CHB-C4A-NA	2.18	127.55	124.40
23	A	4008	BCR	C28-C27-C26	-2.18	110.17	114.06
20	A	1113	CLA	CMB-C2B-C1B	-2.18	122.10	125.42
20	B	1021	CLA	O2A-CGA-O1A	-2.18	118.18	123.63
20	K	204	CLA	C3C-C4C-NC	-2.18	107.64	110.43
20	B	1201	CLA	O2A-CGA-O1A	-2.18	118.18	123.63
20	2	613	CLA	CHB-C4A-NA	2.18	127.54	124.40
20	A	1138	CLA	C2A-C1A-CHA	2.18	127.64	123.87
20	A	1114	CLA	CHD-C1D-ND	-2.18	121.74	124.80
20	B	1214	CLA	CHB-C1B-C2B	-2.18	121.11	127.43
20	2	604	CLA	CHA-C1A-NA	-2.17	121.47	126.39
24	A	5001	LHG	C11-C10-C9	-2.17	103.38	114.37
28	4	607	CHL	C1C-C2C-C3C	-2.17	105.28	107.28
20	A	1140	CLA	CMB-C2B-C1B	-2.17	122.11	125.42
23	F	416	BCR	C40-C30-C25	2.17	113.65	110.24
20	A	1125	CLA	C2A-C1A-CHA	2.17	127.63	123.87
20	A	1126	CLA	C11-C10-C8	-2.17	108.76	115.97
20	B	1225	CLA	C1-O2A-CGA	2.17	121.90	116.65
20	A	1121	CLA	C2B-C1B-NB	-2.17	108.08	110.33
20	B	1234	CLA	C2B-C1B-NB	-2.17	108.08	110.33
20	B	1236	CLA	CHB-C4A-NA	2.17	127.53	124.40
20	2	614	CLA	CMB-C2B-C1B	-2.17	122.12	125.42
23	M	4021	BCR	C2-C1-C6	2.17	113.59	110.44
29	2	621	LUT	C19-C9-C8	2.17	121.40	118.09
20	B	1224	CLA	O2A-CGA-O1A	-2.17	118.21	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	4002	BCR	C15-C14-C13	-2.17	124.24	127.28
28	3	608	CHL	C4D-CHA-C1A	-2.16	118.66	121.24
29	2	620	LUT	C18-C5-C4	2.16	118.40	114.42
20	4	602	CLA	CHD-C1D-ND	-2.16	121.76	124.80
20	A	1114	CLA	CHD-C1D-C2D	2.16	129.99	125.49
25	J	301	LMG	O2-C2-C1	-2.16	104.92	110.08
23	A	4007	BCR	C33-C5-C4	-2.16	108.99	113.60
29	1	620	LUT	C20-C13-C12	2.16	121.39	118.09
23	A	4008	BCR	C38-C26-C27	-2.16	108.99	113.60
28	2	601	CHL	C4B-C3B-C2B	-2.16	104.62	107.30
25	A	5002	LMG	O3-C3-C2	-2.16	105.29	110.38
20	B	1237	CLA	CHB-C4A-NA	2.16	127.52	124.40
23	3	623	BCR	C15-C14-C13	-2.16	124.25	127.28
20	A	1128	CLA	O2A-CGA-O1A	-2.16	118.23	123.63
20	B	1222	CLA	CHA-C1A-NA	-2.16	121.51	126.39
20	A	1104	CLA	CHB-C4A-NA	2.16	127.51	124.40
20	B	1223	CLA	C3B-C4B-NB	-2.16	108.61	110.53
20	B	1215	CLA	CHD-C1D-C2D	2.16	129.97	125.49
23	B	4014	BCR	C16-C15-C14	-2.16	119.11	123.52
20	B	1211	CLA	CHB-C4A-NA	2.16	127.51	124.40
28	4	608	CHL	O2D-CGD-O1D	-2.15	119.65	123.85
28	4	606	CHL	O2A-CGA-CBA	2.15	120.27	112.14
20	A	1102	CLA	CHB-C4A-NA	2.15	127.50	124.40
20	A	1134	CLA	CHA-C1A-NA	-2.15	121.52	126.39
20	A	1138	CLA	C3C-C4C-NC	-2.15	107.67	110.43
20	2	614	CLA	CHB-C4A-NA	2.15	127.50	124.40
20	A	1102	CLA	CMB-C2B-C3B	2.15	131.61	126.55
20	A	1136	CLA	C1-O2A-CGA	-2.15	111.45	116.65
20	A	1128	CLA	CMB-C2B-C3B	2.15	131.60	126.55
20	L	302	CLA	CAA-CBA-CGA	-2.15	107.11	113.21
25	J	302	LMG	C1-C2-C3	-2.15	105.50	110.01
20	B	1224	CLA	CHD-C1D-ND	-2.15	121.78	124.80
20	B	1228	CLA	CMB-C2B-C1B	-2.15	122.15	125.42
20	K	203	CLA	C1C-NC-C4C	2.14	107.66	106.68
20	H	200	CLA	CHB-C4A-NA	2.14	127.49	124.40
25	2	631	LMG	O3-C3-C2	-2.14	105.33	110.38
20	B	1234	CLA	O2A-CGA-O1A	-2.14	118.27	123.63
23	B	4014	BCR	C30-C25-C26	-2.14	119.71	122.64
28	1	601	CHL	C4D-C3D-CAD	2.14	110.43	108.11
20	B	1216	CLA	O2A-CGA-O1A	-2.14	118.28	123.63
20	A	1115	CLA	CHB-C4A-NA	2.14	127.48	124.40
20	A	1130	CLA	CHD-C1D-ND	-2.14	121.80	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	1	607	CHL	C4D-C3D-CAD	2.14	110.42	108.11
20	B	1213	CLA	O2D-CGD-CBD	2.13	114.96	111.23
20	1	606	CLA	C2D-C1D-ND	-2.13	108.02	110.13
20	B	1201	CLA	C1-C2-C3	-2.13	123.31	126.76
20	L	301	CLA	CHA-C1A-NA	-2.13	121.56	126.39
23	B	4017	BCR	C16-C15-C14	-2.13	119.16	123.52
20	B	1208	CLA	O2A-CGA-O1A	-2.13	117.85	123.33
20	B	1225	CLA	C2D-C1D-ND	-2.13	108.02	110.13
20	A	1117	CLA	C3C-C4C-NC	-2.13	107.70	110.43
20	2	612	CLA	C3C-C4C-NC	-2.13	107.70	110.43
28	2	611	CHL	O1D-CGD-CBD	-2.13	120.31	124.52
20	3	607	CLA	O2A-CGA-O1A	-2.13	118.30	123.63
20	3	609	CLA	O2A-CGA-O1A	-2.13	118.30	123.63
20	A	1110	CLA	CHD-C1D-ND	-2.13	121.81	124.80
20	4	609	CLA	C2D-C1D-ND	-2.13	108.02	110.13
20	B	1203	CLA	CAA-C2A-C3A	-2.13	107.25	113.00
20	B	1220	CLA	CHD-C1D-ND	-2.13	121.81	124.80
20	G	218	CLA	CHA-C1A-NA	-2.13	121.57	126.39
20	1	614	CLA	CHD-C1D-ND	-2.13	121.81	124.80
20	1	602	CLA	CHA-C1A-NA	-2.13	121.58	126.39
20	A	1117	CLA	C3B-C4B-NB	-2.13	108.63	110.53
20	B	1212	CLA	CMC-C2C-C1C	-2.13	121.71	125.03
20	A	1130	CLA	C1D-ND-C4D	-2.13	104.82	106.31
20	A	1104	CLA	O2A-CGA-O1A	-2.12	118.31	123.63
20	3	604	CLA	O2A-CGA-O1A	-2.12	118.31	123.63
20	A	1135	CLA	CHA-C1A-NA	-2.12	121.58	126.39
20	A	1140	CLA	O2D-CGD-CBD	2.12	114.94	111.23
23	A	4003	BCR	C11-C10-C9	-2.12	124.30	127.28
20	3	610	CLA	CMB-C2B-C3B	2.12	131.54	126.55
28	2	615	CHL	O2A-CGA-CBA	2.12	120.16	112.14
23	B	4005	BCR	C38-C26-C27	-2.12	109.07	113.60
28	2	608	CHL	O2D-CGD-O1D	-2.12	119.72	123.85
20	A	1103	CLA	CHB-C4A-NA	2.12	127.46	124.40
28	2	608	CHL	CHB-C1B-NB	-2.12	120.87	124.05
20	B	1224	CLA	CHA-C1A-NA	-2.12	121.59	126.39
20	G	201	CLA	CHB-C4A-NA	2.12	127.46	124.40
29	2	623	LUT	C28-C29-C30	2.12	122.34	119.01
20	1	606	CLA	O1A-CGA-CBA	2.12	129.81	123.09
20	1	604	CLA	C1-C2-C3	-2.12	123.34	126.76
29	3	620	LUT	C20-C13-C12	2.12	121.32	118.09
19	A	1011	CL0	O2A-CGA-O1A	-2.12	118.34	123.63
20	A	1135	CLA	O2A-CGA-O1A	-2.12	118.34	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	1237	CLA	CBA-CAA-C2A	2.12	120.09	113.79
20	A	1022	CLA	CMD-C2D-C1D	-2.12	121.00	124.73
23	3	623	BCR	C24-C23-C22	-2.11	123.11	126.23
28	3	608	CHL	O2A-CGA-CBA	2.11	120.12	112.14
29	4	623	LUT	C31-C32-C33	2.11	132.15	126.36
20	L	303	CLA	O2A-CGA-O1A	-2.11	117.90	123.33
20	B	1205	CLA	C11-C10-C8	-2.11	108.95	115.97
20	A	1013	CLA	C1-C2-C3	-2.11	122.74	126.20
20	3	603	CLA	O2A-CGA-O1A	-2.11	118.35	123.63
20	L	301	CLA	CHB-C4A-NA	2.11	127.44	124.40
20	I	121	CLA	C2D-C1D-ND	-2.11	108.04	110.13
20	3	604	CLA	CHB-C4A-NA	2.11	127.44	124.40
25	2	631	LMG	O2-C2-C1	-2.11	105.05	110.08
20	A	1134	CLA	O2A-CGA-O1A	-2.11	117.91	123.33
20	3	609	CLA	C2B-C1B-NB	-2.11	108.14	110.33
20	A	1112	CLA	O2A-CGA-O1A	-2.11	117.91	123.33
23	A	4007	BCR	C20-C21-C22	-2.10	124.33	127.28
20	A	1132	CLA	CHB-C4A-NA	2.10	127.44	124.40
20	B	1225	CLA	O2D-CGD-CBD	2.10	114.91	111.23
28	2	601	CHL	C6-C5-C3	-2.10	108.34	113.47
20	B	1208	CLA	CHA-C1A-NA	-2.10	121.63	126.39
20	A	1118	CLA	C3B-C4B-NB	-2.10	108.65	110.53
23	1	623	BCR	C15-C14-C13	-2.10	124.27	127.48
20	A	1117	CLA	O2D-CGD-CBD	2.10	114.91	111.23
28	4	607	CHL	CHB-C1B-C2B	-2.10	121.32	127.43
23	F	416	BCR	C15-C14-C13	-2.10	124.33	127.28
20	O	201	CLA	C1C-NC-C4C	2.10	107.64	106.68
28	2	607	CHL	O2A-CGA-CBA	2.10	120.08	112.14
20	A	1101	CLA	CHB-C4A-NA	2.10	127.43	124.40
20	B	1240	CLA	CHA-C1A-NA	-2.10	121.63	126.39
20	A	1121	CLA	O2A-CGA-O1A	-2.10	118.37	123.63
20	A	1112	CLA	C2A-C1A-CHA	2.10	127.51	123.87
29	4	621	LUT	C11-C10-C9	2.10	130.22	127.28
25	J	302	LMG	O6-C1-O1	-2.10	105.08	110.04
23	A	4001	BCR	C11-C10-C9	-2.10	124.33	127.28
28	2	607	CHL	C4D-C3D-CAD	2.10	110.39	108.11
20	1	606	CLA	O2A-CGA-O1A	-2.10	117.94	123.33
23	B	4014	BCR	C27-C26-C25	2.10	125.54	122.70
20	B	1012	CLA	CHB-C1B-C2B	-2.10	121.34	127.43
20	A	1022	CLA	CMB-C2B-C1B	-2.10	122.23	125.42
25	J	302	LMG	O3-C3-C2	-2.10	105.44	110.38
20	A	1125	CLA	CHB-C4A-NA	2.09	127.42	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	G	311	BCR	C1-C6-C5	-2.09	119.77	122.64
20	B	1012	CLA	C3C-C4C-NC	-2.09	107.75	110.43
20	B	1209	CLA	O2A-CGA-O1A	-2.09	117.95	123.33
20	A	1136	CLA	C1-C2-C3	-2.09	122.77	126.20
20	A	1127	CLA	C3C-C4C-NC	-2.09	107.75	110.43
28	2	601	CHL	C4D-C3D-CAD	2.09	110.38	108.11
20	3	602	CLA	C2D-C1D-ND	-2.09	108.06	110.13
28	2	615	CHL	C4B-C3B-C2B	-2.09	104.70	107.30
20	3	612	CLA	CHB-C4A-NA	2.09	127.42	124.40
20	4	614	CLA	C2D-C1D-ND	-2.09	108.06	110.13
20	B	1215	CLA	O2D-CGD-CBD	2.09	114.88	111.23
20	B	1213	CLA	CHB-C1B-C2B	-2.09	121.37	127.43
20	A	1110	CLA	O2A-CGA-O1A	-2.09	118.41	123.63
20	B	1211	CLA	CHA-C1A-NA	-2.09	121.67	126.39
20	A	1121	CLA	CMB-C2B-C1B	-2.08	122.25	125.42
28	3	608	CHL	CHB-C1B-NB	-2.08	120.92	124.05
28	2	611	CHL	C1-C2-C3	-2.08	122.78	126.20
20	A	1102	CLA	O2A-CGA-O1A	-2.08	117.97	123.33
20	B	1225	CLA	O2D-CGD-O1D	-2.08	119.79	123.85
20	A	1801	CLA	O2A-CGA-O1A	-2.08	118.42	123.63
20	2	609	CLA	O2A-CGA-O1A	-2.08	118.42	123.63
20	B	1238	CLA	O2A-CGA-O1A	-2.08	118.42	123.63
20	B	1232	CLA	CHD-C1D-ND	-2.08	121.88	124.80
25	J	302	LMG	O2-C2-C1	-2.08	105.12	110.08
28	1	607	CHL	CHB-C1B-C2B	-2.08	121.39	127.43
23	A	4002	BCR	C16-C15-C14	-2.08	119.27	123.52
29	1	620	LUT	C19-C9-C8	2.08	121.26	118.09
23	L	420	BCR	C38-C26-C27	-2.08	109.17	113.60
20	A	1116	CLA	CHB-C1B-NB	2.08	127.16	124.05
20	4	610	CLA	O2A-CGA-O1A	-2.07	118.44	123.63
26	4	631	LMT	O1'-C1'-C2'	2.07	111.42	108.27
20	A	1138	CLA	O2D-CGD-CBD	2.07	114.86	111.23
20	A	1118	CLA	CAA-CBA-CGA	-2.07	107.32	113.21
28	4	608	CHL	CHB-C1B-C2B	-2.07	121.41	127.43
23	A	4007	BCR	C24-C25-C26	-2.07	116.78	121.56
20	A	1130	CLA	C4D-CHA-C1A	-2.07	118.77	121.24
28	4	607	CHL	O2A-CGA-CBA	2.07	119.97	112.14
20	1	603	CLA	O2D-CGD-CBD	2.07	114.85	111.23
20	B	1228	CLA	CHD-C1D-ND	-2.07	121.89	124.80
20	A	1113	CLA	CMB-C2B-C3B	2.07	131.42	126.55
28	2	602	CHL	CHB-C1B-C2B	-2.07	121.42	127.43
20	A	1125	CLA	C7-C6-C5	2.07	118.78	113.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	1021	CLA	CHB-C4A-NA	2.07	127.39	124.40
20	A	1139	CLA	CHD-C1D-ND	-2.07	121.89	124.80
20	A	1137	CLA	C2B-C1B-NB	-2.07	108.18	110.33
20	A	1109	CLA	O2A-CGA-O1A	-2.07	118.45	123.63
20	A	1110	CLA	C3C-C4C-NC	-2.07	107.78	110.43
20	A	1122	CLA	C3C-C4C-NC	-2.07	107.78	110.43
28	4	606	CHL	CHB-C1B-NB	-2.07	120.95	124.05
23	K	301	BCR	C27-C26-C25	2.07	125.50	122.70
20	1	602	CLA	CHB-C4A-NA	2.07	127.38	124.40
20	4	604	CLA	O2A-CGA-O1A	-2.07	118.46	123.63
20	3	614	CLA	O2A-CGA-O1A	-2.07	118.46	123.63
29	2	620	LUT	C19-C9-C10	-2.07	119.47	122.82
23	A	4008	BCR	C11-C10-C9	-2.07	124.38	127.28
23	B	4009	BCR	C1-C6-C5	-2.07	119.81	122.64
23	I	120	BCR	C21-C20-C19	-2.07	117.21	123.20
20	K	201	CLA	C4D-C3D-CAD	-2.07	105.86	108.11
20	1	614	CLA	CHA-C1A-NA	-2.07	121.71	126.39
23	3	624	BCR	C15-C16-C17	-2.06	119.29	123.52
28	4	608	CHL	C4D-CHA-C1A	-2.06	118.78	121.24
20	A	1022	CLA	O2A-CGA-O1A	-2.06	118.47	123.63
20	A	1013	CLA	CAA-C2A-C1A	-2.06	105.22	111.97
28	4	615	CHL	C4B-C3B-C2B	-2.06	104.74	107.30
20	B	1226	CLA	CHB-C1B-C2B	-2.06	121.44	127.43
28	2	607	CHL	C4D-CHA-C1A	-2.06	118.79	121.24
23	L	419	BCR	C24-C23-C22	-2.06	123.19	126.23
20	3	610	CLA	C2D-C1D-ND	-2.06	108.09	110.13
28	2	602	CHL	O1D-CGD-CBD	-2.06	120.46	124.52
20	O	202	CLA	C1C-NC-C4C	2.06	107.62	106.68
20	K	203	CLA	C2A-C1A-CHA	2.06	125.90	122.71
20	B	1237	CLA	CHA-C1A-NA	-2.06	121.73	126.39
23	B	4010	BCR	C24-C25-C26	2.06	126.29	121.56
20	1	604	CLA	CHA-C1A-NA	-2.06	121.73	126.39
29	3	621	LUT	C20-C13-C12	2.05	121.23	118.09
29	3	620	LUT	C31-C32-C33	-2.05	120.74	126.36
20	B	1223	CLA	CHB-C1B-NB	2.05	127.13	124.05
20	H	200	CLA	C2D-C1D-ND	-2.05	108.10	110.13
23	3	623	BCR	C15-C16-C17	-2.05	119.32	123.52
20	L	301	CLA	O2A-CGA-O1A	-2.05	118.50	123.63
23	I	120	BCR	C1-C6-C5	-2.05	119.83	122.64
20	2	610	CLA	CMB-C2B-C1B	-2.05	122.30	125.42
28	2	607	CHL	CED-O2D-CGD	2.05	120.56	115.92
20	A	1125	CLA	CAC-C3C-C4C	-2.05	122.12	124.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	1204	CLA	CHB-C4A-NA	2.05	127.36	124.40
23	F	416	BCR	C29-C30-C25	2.05	113.41	110.44
20	1	608	CLA	CHA-C1A-NA	-2.05	121.75	126.39
20	A	1133	CLA	CHB-C4A-NA	2.05	127.35	124.40
28	2	601	CHL	C1-C2-C3	-2.05	122.84	126.20
20	2	612	CLA	CMB-C2B-C1B	-2.05	122.31	125.42
20	B	1219	CLA	CHA-C1A-NA	-2.05	121.76	126.39
20	B	1021	CLA	O1D-CGD-CBD	2.04	128.55	124.52
23	B	4006	BCR	C33-C5-C6	-2.04	122.25	124.48
20	B	1023	CLA	C2A-C1A-CHA	2.04	127.41	123.87
20	A	1104	CLA	CMB-C2B-C3B	2.04	131.35	126.55
29	1	620	LUT	C40-C33-C34	-2.04	119.51	122.82
23	I	118	BCR	C38-C26-C27	-2.04	109.25	113.60
20	B	1012	CLA	C2A-C1A-CHA	2.04	127.41	123.87
24	1	630	LHG	O8-C23-O10	-2.04	118.53	123.63
23	A	4003	BCR	C16-C15-C14	-2.04	119.35	123.52
20	G	201	CLA	O2A-CGA-O1A	-2.04	118.53	123.63
29	4	623	LUT	C20-C13-C14	-2.04	119.51	122.82
20	A	1103	CLA	CHD-C1D-ND	-2.04	121.94	124.80
20	A	1128	CLA	CHA-C1A-NA	-2.04	121.78	126.39
19	A	1011	CL0	C1-C2-C3	-2.04	122.86	126.20
20	2	603	CLA	C2D-C1D-ND	-2.03	108.11	110.13
23	A	4001	BCR	C20-C21-C22	-2.03	124.42	127.28
20	1	614	CLA	C2D-C1D-ND	-2.03	108.11	110.13
20	1	614	CLA	C3C-C4C-NC	-2.03	107.83	110.43
23	F	416	BCR	C28-C27-C26	-2.03	110.43	114.06
20	A	1108	CLA	CHB-C4A-NA	2.03	127.33	124.40
23	J	212	BCR	C2-C1-C6	2.03	113.39	110.44
23	A	4008	BCR	C10-C11-C12	-2.03	117.31	123.20
20	A	1114	CLA	C2D-C1D-ND	-2.03	108.12	110.13
20	B	1012	CLA	C2C-C1C-NC	-2.03	107.85	109.98
20	2	613	CLA	C2A-C1A-CHA	2.03	127.39	123.87
20	A	1107	CLA	CMB-C2B-C1B	-2.03	122.33	125.42
20	1	608	CLA	CHD-C1D-ND	-2.03	121.95	124.80
20	B	1212	CLA	CHB-C4A-NA	2.03	127.33	124.40
20	A	1115	CLA	C2C-C1C-NC	-2.03	107.85	109.98
20	B	1205	CLA	C2C-C1C-NC	-2.03	107.85	109.98
20	B	1215	CLA	O2A-CGA-O1A	-2.03	118.55	123.63
19	A	1011	CL0	CMD-C2D-C1D	-2.03	121.16	124.73
20	A	1106	CLA	CHA-C1A-NA	-2.03	121.80	126.39
28	2	607	CHL	O2D-CGD-O1D	-2.03	119.90	123.85
20	A	1140	CLA	CHB-C1B-NB	2.03	127.09	124.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	M	4021	BCR	C16-C15-C14	-2.03	119.37	123.52
20	B	1240	CLA	CHB-C4A-NA	2.03	127.32	124.40
28	4	615	CHL	C4D-CHA-C1A	-2.03	118.83	121.24
20	A	1135	CLA	C2B-C1B-NB	-2.03	108.23	110.33
20	B	1021	CLA	CHD-C1D-ND	-2.02	121.95	124.80
20	3	602	CLA	CHD-C1D-ND	-2.02	121.95	124.80
25	J	301	LMG	O1-C1-C2	-2.02	105.20	108.27
28	2	601	CHL	OMC-CMC-C2C	-2.02	121.05	125.62
20	B	1214	CLA	CMB-C2B-C3B	2.02	131.31	126.55
20	A	1132	CLA	CMC-C2C-C1C	-2.02	121.87	125.03
23	I	120	BCR	C4-C5-C6	2.02	125.44	122.70
20	J	102	CLA	CHB-C4A-NA	2.02	127.32	124.40
20	A	1139	CLA	CHB-C4A-NA	2.02	127.32	124.40
28	2	601	CHL	C4D-CHA-C1A	-2.02	118.83	121.24
20	A	1124	CLA	O2A-CGA-O1A	-2.02	118.58	123.63
20	A	1113	CLA	O1A-CGA-CBA	2.02	129.50	123.09
20	A	1103	CLA	O2A-CGA-O1A	-2.02	118.58	123.63
20	3	605	CLA	C2A-C1A-CHA	2.02	125.84	122.71
20	A	1117	CLA	C2D-C1D-ND	-2.02	108.13	110.13
20	4	604	CLA	C1-C2-C3	-2.02	123.50	126.76
20	B	1205	CLA	C4B-C3B-C2B	-2.02	104.79	107.30
20	4	602	CLA	C1-C2-C3	-2.02	122.89	126.20
23	A	4011	BCR	C11-C10-C9	-2.02	124.45	127.28
20	A	1113	CLA	CHB-C4A-NA	2.02	127.31	124.40
20	A	1112	CLA	CMB-C2B-C1B	-2.02	122.35	125.42
20	B	1201	CLA	CMB-C2B-C3B	2.02	131.29	126.55
23	G	311	BCR	C11-C10-C9	-2.01	124.45	127.28
20	3	602	CLA	CHD-C1D-C2D	2.01	129.68	125.49
29	2	623	LUT	C39-C29-C30	-2.01	119.55	122.82
20	B	1227	CLA	O2A-CGA-O1A	-2.01	118.16	123.33
20	B	1229	CLA	O1D-CGD-CBD	2.01	128.49	124.52
29	4	620	LUT	C35-C15-C14	-2.01	119.41	123.52
20	B	1204	CLA	O2A-CGA-O1A	-2.01	118.60	123.63
28	1	601	CHL	O1D-CGD-CBD	-2.01	120.56	124.52
20	1	602	CLA	C1-C2-C3	-2.01	122.91	126.20
29	2	620	LUT	C28-C29-C30	2.01	122.17	119.01
28	1	601	CHL	C4A-NA-C1A	2.01	107.59	106.68
20	4	609	CLA	C2B-C1B-NB	-2.01	108.25	110.33
20	4	602	CLA	CMB-C2B-C3B	2.01	131.27	126.55
25	2	631	LMG	O1-C1-C2	-2.01	105.23	108.27
20	B	1228	CLA	CHA-C1A-NA	-2.00	121.85	126.39
20	A	1104	CLA	C1-C2-C3	-2.00	122.92	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	1221	CLA	CHA-C1A-NA	-2.00	121.86	126.39
27	B	5002	DGD	C9B-C8B-C7B	-2.00	104.25	114.37
20	B	1215	CLA	C2B-C1B-NB	-2.00	108.25	110.33
20	1	612	CLA	CHA-C1A-NA	-2.00	121.86	126.39
20	4	614	CLA	CMB-C2B-C1B	-2.00	122.37	125.42

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
29	2	623	LUT	C26
29	4	623	LUT	C26

All (1828) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
20	A	1013	CLA	CBD-CGD-O2D-CED
20	A	1022	CLA	C1A-C2A-CAA-CBA
20	A	1022	CLA	C3A-C2A-CAA-CBA
20	A	1101	CLA	CHA-CBD-CGD-O1D
20	A	1101	CLA	CHA-CBD-CGD-O2D
20	A	1102	CLA	C1A-C2A-CAA-CBA
20	A	1102	CLA	C3A-C2A-CAA-CBA
20	A	1102	CLA	CHA-CBD-CGD-O2D
20	A	1103	CLA	C3A-C2A-CAA-CBA
20	A	1103	CLA	C4B-C3B-CAB-CBB
20	A	1104	CLA	CHA-CBD-CGD-O1D
20	A	1104	CLA	CHA-CBD-CGD-O2D
20	A	1106	CLA	CHA-CBD-CGD-O1D
20	A	1106	CLA	CHA-CBD-CGD-O2D
20	A	1107	CLA	C1A-C2A-CAA-CBA
20	A	1109	CLA	C1A-C2A-CAA-CBA
20	A	1109	CLA	C3A-C2A-CAA-CBA
20	A	1109	CLA	C4B-C3B-CAB-CBB
20	A	1110	CLA	CBA-CGA-O2A-C1
20	A	1110	CLA	C4B-C3B-CAB-CBB
20	A	1112	CLA	C1A-C2A-CAA-CBA
20	A	1112	CLA	C3A-C2A-CAA-CBA
20	A	1112	CLA	C4B-C3B-CAB-CBB
20	A	1116	CLA	C3A-C2A-CAA-CBA
20	A	1117	CLA	CBD-CGD-O2D-CED
20	A	1119	CLA	C6-C7-C8-C9
20	A	1121	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
20	A	1122	CLA	C4B-C3B-CAB-CBB
20	A	1122	CLA	CAD-CBD-CGD-O2D
20	A	1125	CLA	C1A-C2A-CAA-CBA
20	A	1126	CLA	C1A-C2A-CAA-CBA
20	A	1126	CLA	CBD-CGD-O2D-CED
20	A	1128	CLA	C1A-C2A-CAA-CBA
20	A	1128	CLA	CHA-CBD-CGD-O1D
20	A	1128	CLA	CHA-CBD-CGD-O2D
20	A	1130	CLA	C1A-C2A-CAA-CBA
20	A	1131	CLA	CAD-CBD-CGD-O2D
20	A	1132	CLA	CBD-CGD-O2D-CED
20	A	1135	CLA	C1A-C2A-CAA-CBA
20	A	1136	CLA	C11-C10-C8-C7
20	A	1137	CLA	C1A-C2A-CAA-CBA
20	A	1140	CLA	C4B-C3B-CAB-CBB
20	A	1140	CLA	C2-C3-C5-C6
20	A	1140	CLA	C4-C3-C5-C6
20	A	1138	CLA	C4B-C3B-CAB-CBB
20	A	1138	CLA	CBD-CGD-O2D-CED
20	A	1139	CLA	C4B-C3B-CAB-CBB
20	A	1801	CLA	CBD-CGD-O2D-CED
20	B	1023	CLA	CBD-CGD-O2D-CED
20	B	1012	CLA	C1A-C2A-CAA-CBA
20	B	1012	CLA	CAD-CBD-CGD-O1D
20	B	1012	CLA	CAD-CBD-CGD-O2D
20	B	1021	CLA	CBD-CGD-O2D-CED
20	B	1201	CLA	C1A-C2A-CAA-CBA
20	B	1202	CLA	C1A-C2A-CAA-CBA
20	B	1202	CLA	C3A-C2A-CAA-CBA
20	B	1203	CLA	C1A-C2A-CAA-CBA
20	B	1205	CLA	CHA-CBD-CGD-O1D
20	B	1205	CLA	CHA-CBD-CGD-O2D
20	B	1211	CLA	CBD-CGD-O2D-CED
20	B	1216	CLA	C1A-C2A-CAA-CBA
20	B	1216	CLA	C2B-C3B-CAB-CBB
20	B	1217	CLA	C1A-C2A-CAA-CBA
20	B	1217	CLA	C3A-C2A-CAA-CBA
20	B	1219	CLA	CBD-CGD-O2D-CED
20	B	1220	CLA	C1A-C2A-CAA-CBA
20	B	1220	CLA	C3A-C2A-CAA-CBA
20	B	1222	CLA	CHA-CBD-CGD-O1D
20	B	1222	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
20	B	1222	CLA	CBD-CGD-O2D-CED
20	B	1223	CLA	C1A-C2A-CAA-CBA
20	B	1223	CLA	C3A-C2A-CAA-CBA
20	B	1224	CLA	C1A-C2A-CAA-CBA
20	B	1225	CLA	C1A-C2A-CAA-CBA
20	B	1225	CLA	C3A-C2A-CAA-CBA
20	B	1226	CLA	C1A-C2A-CAA-CBA
20	B	1229	CLA	CBD-CGD-O2D-CED
20	B	1230	CLA	C1A-C2A-CAA-CBA
20	B	1230	CLA	C3A-C2A-CAA-CBA
20	B	1231	CLA	C4B-C3B-CAB-CBB
20	B	1232	CLA	C4B-C3B-CAB-CBB
20	B	1232	CLA	CBD-CGD-O2D-CED
20	B	1234	CLA	C2-C3-C5-C6
20	B	1236	CLA	C4B-C3B-CAB-CBB
20	B	1237	CLA	C1A-C2A-CAA-CBA
20	B	1238	CLA	C4B-C3B-CAB-CBB
20	B	1239	CLA	C1A-C2A-CAA-CBA
20	B	1240	CLA	CAD-CBD-CGD-O2D
20	1	603	CLA	C1A-C2A-CAA-CBA
20	1	603	CLA	CHA-CBD-CGD-O1D
20	1	603	CLA	CHA-CBD-CGD-O2D
20	1	603	CLA	CBD-CGD-O2D-CED
20	1	604	CLA	CBD-CGD-O2D-CED
20	1	606	CLA	CBD-CGD-O2D-CED
20	1	610	CLA	CHA-CBD-CGD-O1D
20	1	610	CLA	CHA-CBD-CGD-O2D
20	1	612	CLA	C4B-C3B-CAB-CBB
20	1	613	CLA	C1A-C2A-CAA-CBA
20	1	613	CLA	CAD-CBD-CGD-O1D
20	1	613	CLA	CAD-CBD-CGD-O2D
20	1	614	CLA	C4B-C3B-CAB-CBB
20	1	615	CLA	C1A-C2A-CAA-CBA
20	1	615	CLA	C3A-C2A-CAA-CBA
20	1	615	CLA	CHA-CBD-CGD-O1D
20	1	615	CLA	CHA-CBD-CGD-O2D
20	2	603	CLA	CBD-CGD-O2D-CED
20	2	604	CLA	CBD-CGD-O2D-CED
20	2	610	CLA	C6-C7-C8-C9
20	3	603	CLA	CBD-CGD-O2D-CED
20	3	604	CLA	CBD-CGD-O2D-CED
20	3	606	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
20	3	606	CLA	C3A-C2A-CAA-CBA
20	3	606	CLA	C4B-C3B-CAB-CBB
20	3	607	CLA	C1A-C2A-CAA-CBA
20	3	609	CLA	CBD-CGD-O2D-CED
20	3	610	CLA	C3A-C2A-CAA-CBA
20	3	611	CLA	C4B-C3B-CAB-CBB
20	3	612	CLA	CBD-CGD-O2D-CED
20	3	613	CLA	C4B-C3B-CAB-CBB
20	3	614	CLA	C1A-C2A-CAA-CBA
20	3	614	CLA	CBD-CGD-O2D-CED
20	4	614	CLA	CAD-CBD-CGD-O1D
20	4	614	CLA	CAD-CBD-CGD-O2D
20	4	603	CLA	CBD-CGD-O2D-CED
20	4	604	CLA	CBD-CGD-O2D-CED
20	4	612	CLA	C4B-C3B-CAB-CBB
20	4	612	CLA	CHA-CBD-CGD-O2D
20	F	301	CLA	C4B-C3B-CAB-CBB
20	F	301	CLA	CBD-CGD-O2D-CED
20	F	302	CLA	C4B-C3B-CAB-CBB
20	F	302	CLA	CHA-CBD-CGD-O2D
20	G	218	CLA	C4B-C3B-CAB-CBB
20	G	218	CLA	CHA-CBD-CGD-O2D
20	G	201	CLA	C4B-C3B-CAB-CBB
20	G	201	CLA	CBD-CGD-O2D-CED
20	G	202	CLA	C1A-C2A-CAA-CBA
20	H	200	CLA	CBD-CGD-O2D-CED
20	J	102	CLA	CAD-CBD-CGD-O1D
20	J	102	CLA	CAD-CBD-CGD-O2D
20	K	201	CLA	C1A-C2A-CAA-CBA
20	K	201	CLA	CHA-CBD-CGD-O1D
20	K	201	CLA	CHA-CBD-CGD-O2D
20	K	202	CLA	C1A-C2A-CAA-CBA
20	K	202	CLA	CBA-CGA-O2A-C1
20	K	204	CLA	C1A-C2A-CAA-CBA
20	K	204	CLA	C4B-C3B-CAB-CBB
20	L	302	CLA	C1A-C2A-CAA-CBA
20	L	302	CLA	C3A-C2A-CAA-CBA
20	L	303	CLA	C1A-C2A-CAA-CBA
20	L	303	CLA	CBD-CGD-O2D-CED
23	A	4001	BCR	C7-C8-C9-C10
23	A	4001	BCR	C21-C22-C23-C24
23	A	4003	BCR	C7-C8-C9-C34

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Mol	Chain	Res	Type	Atoms
23	A	4003	BCR	C21-C22-C23-C24
23	A	4007	BCR	C22-C23-C24-C25
23	A	4007	BCR	C23-C24-C25-C26
23	A	4007	BCR	C23-C24-C25-C30
23	A	4008	BCR	C7-C8-C9-C10
23	A	4008	BCR	C22-C23-C24-C25
23	A	4011	BCR	C7-C8-C9-C34
23	A	4011	BCR	C18-C19-C20-C21
23	A	4011	BCR	C20-C21-C22-C23
23	A	4011	BCR	C20-C21-C22-C37
23	A	4011	BCR	C22-C23-C24-C25
23	B	4004	BCR	C11-C12-C13-C14
23	B	4004	BCR	C37-C22-C23-C24
23	B	4004	BCR	C22-C23-C24-C25
23	B	4006	BCR	C6-C7-C8-C9
23	B	4010	BCR	C6-C7-C8-C9
23	B	4010	BCR	C7-C8-C9-C10
23	B	4010	BCR	C21-C22-C23-C24
23	B	4017	BCR	C10-C11-C12-C13
23	B	4017	BCR	C18-C19-C20-C21
23	B	4017	BCR	C20-C21-C22-C23
23	B	4017	BCR	C20-C21-C22-C37
23	B	4017	BCR	C21-C22-C23-C24
23	B	4017	BCR	C22-C23-C24-C25
23	B	4014	BCR	C6-C7-C8-C9
23	B	4014	BCR	C9-C10-C11-C12
23	B	4014	BCR	C10-C11-C12-C13
23	B	4014	BCR	C11-C12-C13-C14
23	B	4014	BCR	C11-C12-C13-C35
23	B	4014	BCR	C14-C15-C16-C17
23	B	4014	BCR	C21-C22-C23-C24
23	3	623	BCR	C11-C10-C9-C8
23	3	623	BCR	C11-C12-C13-C14
23	3	623	BCR	C14-C15-C16-C17
23	3	623	BCR	C15-C16-C17-C18
23	3	623	BCR	C16-C17-C18-C36
23	3	624	BCR	C6-C7-C8-C9
23	F	416	BCR	C7-C8-C9-C10
23	F	416	BCR	C18-C19-C20-C21
23	F	416	BCR	C21-C22-C23-C24
23	F	416	BCR	C37-C22-C23-C24
23	F	416	BCR	C22-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
23	I	118	BCR	C6-C7-C8-C9
23	I	118	BCR	C7-C8-C9-C10
23	I	118	BCR	C7-C8-C9-C34
23	I	118	BCR	C21-C22-C23-C24
23	I	120	BCR	C6-C7-C8-C9
23	I	120	BCR	C21-C22-C23-C24
23	I	120	BCR	C37-C22-C23-C24
23	J	212	BCR	C6-C7-C8-C9
23	J	212	BCR	C7-C8-C9-C10
23	J	212	BCR	C7-C8-C9-C34
23	J	212	BCR	C21-C22-C23-C24
23	J	212	BCR	C37-C22-C23-C24
23	J	213	BCR	C6-C7-C8-C9
23	J	213	BCR	C22-C23-C24-C25
23	K	301	BCR	C6-C7-C8-C9
23	K	301	BCR	C7-C8-C9-C34
23	K	301	BCR	C21-C22-C23-C24
23	L	419	BCR	C7-C8-C9-C10
23	L	419	BCR	C22-C23-C24-C25
23	L	420	BCR	C18-C19-C20-C21
23	L	420	BCR	C22-C23-C24-C25
23	M	4021	BCR	C6-C7-C8-C9
24	A	5001	LHG	C3-O3-P-O5
24	A	5003	LHG	O7-C5-C6-O8
24	B	5101	LHG	C3-O3-P-O5
24	1	630	LHG	O1-C1-C2-O2
24	1	630	LHG	O1-C1-C2-C3
24	1	630	LHG	C3-O3-P-O5
24	1	630	LHG	C3-O3-P-O6
24	1	630	LHG	C4-O6-P-O5
24	2	630	LHG	C3-O3-P-O6
24	3	630	LHG	O6-C4-C5-O7
24	4	630	LHG	C4-O6-P-O5
25	A	5002	LMG	O9-C10-O7-C8
25	A	5002	LMG	C11-C10-O7-C8
26	B	5001	LMT	C2-C1-O1'-C1'
27	B	5002	DGD	C2B-C1B-O2G-C2G
27	B	5002	DGD	O1B-C1B-O2G-C2G
28	1	607	CHL	C1A-C2A-CAA-CBA
28	1	607	CHL	C3C-C2C-CMC-OMC
28	2	602	CHL	C1A-C2A-CAA-CBA
28	2	602	CHL	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
28	2	602	CHL	C1C-C2C-CMC-OMC
28	2	602	CHL	C3C-C2C-CMC-OMC
28	2	602	CHL	CHA-CBD-CGD-O1D
28	2	602	CHL	CHA-CBD-CGD-O2D
28	2	606	CHL	C3A-C2A-CAA-CBA
28	2	607	CHL	C1C-C2C-CMC-OMC
28	2	607	CHL	C3C-C2C-CMC-OMC
28	2	608	CHL	C2B-C3B-CAB-CBB
28	2	608	CHL	C4B-C3B-CAB-CBB
28	2	608	CHL	C3C-C2C-CMC-OMC
28	2	611	CHL	C1C-C2C-CMC-OMC
28	2	611	CHL	C3C-C2C-CMC-OMC
28	2	615	CHL	CHA-CBD-CGD-O1D
28	2	615	CHL	CHA-CBD-CGD-O2D
28	2	601	CHL	C1C-C2C-CMC-OMC
28	2	601	CHL	C3C-C2C-CMC-OMC
28	2	601	CHL	CHA-CBD-CGD-O1D
28	2	601	CHL	CHA-CBD-CGD-O2D
28	3	608	CHL	CBD-CGD-O2D-CED
28	4	606	CHL	C3C-C2C-CMC-OMC
28	4	607	CHL	C1C-C2C-CMC-OMC
28	4	607	CHL	C3C-C2C-CMC-OMC
28	4	608	CHL	C1A-C2A-CAA-CBA
28	4	608	CHL	C4B-C3B-CAB-CBB
28	4	608	CHL	CBD-CGD-O2D-CED
29	1	620	LUT	C21-C26-C27-C28
29	1	620	LUT	C25-C26-C27-C28
29	1	621	LUT	C21-C26-C27-C28
29	1	621	LUT	C25-C26-C27-C28
29	2	620	LUT	C21-C26-C27-C28
29	2	621	LUT	C21-C26-C27-C28
29	2	621	LUT	C29-C30-C31-C32
29	2	623	LUT	C7-C8-C9-C10
29	2	623	LUT	C7-C8-C9-C19
29	2	623	LUT	C11-C12-C13-C14
29	2	623	LUT	C11-C12-C13-C20
29	2	623	LUT	C25-C26-C27-C28
29	3	620	LUT	C21-C26-C27-C28
29	3	621	LUT	C21-C26-C27-C28
29	3	621	LUT	C27-C28-C29-C30
29	3	621	LUT	C27-C28-C29-C39
29	3	621	LUT	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
29	3	621	LUT	C31-C32-C33-C40
29	4	620	LUT	C21-C26-C27-C28
29	4	620	LUT	C25-C26-C27-C28
29	4	621	LUT	C1-C6-C7-C8
29	4	621	LUT	C5-C6-C7-C8
29	4	623	LUT	C25-C26-C27-C28
29	4	623	LUT	C27-C28-C29-C30
29	4	623	LUT	C27-C28-C29-C39
20	A	1022	CLA	O1D-CGD-O2D-CED
20	A	1104	CLA	O1D-CGD-O2D-CED
20	A	1108	CLA	O1D-CGD-O2D-CED
20	A	1121	CLA	O1D-CGD-O2D-CED
20	A	1126	CLA	O1D-CGD-O2D-CED
20	A	1134	CLA	O1D-CGD-O2D-CED
20	A	1139	CLA	O1D-CGD-O2D-CED
20	B	1023	CLA	O1D-CGD-O2D-CED
20	B	1219	CLA	O1D-CGD-O2D-CED
20	B	1229	CLA	O1D-CGD-O2D-CED
20	B	1232	CLA	O1D-CGD-O2D-CED
20	1	604	CLA	O1D-CGD-O2D-CED
20	3	612	CLA	O1D-CGD-O2D-CED
20	H	200	CLA	O1D-CGD-O2D-CED
20	L	303	CLA	O1D-CGD-O2D-CED
28	4	608	CHL	O1D-CGD-O2D-CED
20	A	1122	CLA	O1D-CGD-O2D-CED
20	1	606	CLA	O1D-CGD-O2D-CED
20	1	608	CLA	O1D-CGD-O2D-CED
20	1	613	CLA	O1D-CGD-O2D-CED
20	2	603	CLA	O1D-CGD-O2D-CED
20	3	614	CLA	O1D-CGD-O2D-CED
20	4	604	CLA	O1D-CGD-O2D-CED
20	K	204	CLA	O1D-CGD-O2D-CED
20	A	1022	CLA	CBD-CGD-O2D-CED
20	A	1103	CLA	CBD-CGD-O2D-CED
20	A	1104	CLA	CBD-CGD-O2D-CED
20	A	1108	CLA	CBD-CGD-O2D-CED
20	A	1109	CLA	CBD-CGD-O2D-CED
20	A	1112	CLA	CBD-CGD-O2D-CED
20	A	1121	CLA	CBD-CGD-O2D-CED
20	A	1122	CLA	CBD-CGD-O2D-CED
20	A	1131	CLA	CBD-CGD-O2D-CED
20	A	1134	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
20	A	1139	CLA	CBD-CGD-O2D-CED
20	B	1206	CLA	CBD-CGD-O2D-CED
20	B	1235	CLA	CBD-CGD-O2D-CED
20	B	1239	CLA	CBD-CGD-O2D-CED
20	1	608	CLA	CBD-CGD-O2D-CED
20	1	610	CLA	CBD-CGD-O2D-CED
20	1	611	CLA	CBD-CGD-O2D-CED
20	1	613	CLA	CBD-CGD-O2D-CED
20	3	606	CLA	CBD-CGD-O2D-CED
20	4	614	CLA	CBD-CGD-O2D-CED
20	4	613	CLA	CBD-CGD-O2D-CED
20	F	302	CLA	CBD-CGD-O2D-CED
20	K	204	CLA	CBD-CGD-O2D-CED
28	2	608	CHL	CBD-CGD-O2D-CED
20	A	1110	CLA	O1A-CGA-O2A-C1
20	A	1138	CLA	O1D-CGD-O2D-CED
20	2	604	CLA	O1D-CGD-O2D-CED
28	2	608	CHL	O1D-CGD-O2D-CED
20	1	614	CLA	CBA-CGA-O2A-C1
26	A	5004	LMT	C3'-C4'-O1B-C1B
20	A	1131	CLA	O1D-CGD-O2D-CED
20	3	606	CLA	O1D-CGD-O2D-CED
20	4	614	CLA	O1D-CGD-O2D-CED
20	L	301	CLA	CBA-CGA-O2A-C1
24	3	630	LHG	C24-C23-O8-C6
20	A	1118	CLA	O1A-CGA-O2A-C1
20	A	1121	CLA	O1A-CGA-O2A-C1
20	A	1138	CLA	O1A-CGA-O2A-C1
20	B	1012	CLA	O1A-CGA-O2A-C1
20	1	603	CLA	O1A-CGA-O2A-C1
20	2	609	CLA	O1A-CGA-O2A-C1
20	3	603	CLA	O1A-CGA-O2A-C1
20	4	603	CLA	O1A-CGA-O2A-C1
20	4	613	CLA	O1A-CGA-O2A-C1
20	L	301	CLA	O1A-CGA-O2A-C1
24	3	630	LHG	O10-C23-O8-C6
20	1	614	CLA	O1A-CGA-O2A-C1
20	K	202	CLA	O1A-CGA-O2A-C1
20	A	1109	CLA	O1D-CGD-O2D-CED
20	B	1021	CLA	O1D-CGD-O2D-CED
20	B	1239	CLA	O1D-CGD-O2D-CED
20	4	603	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
20	A	1013	CLA	O1D-CGD-O2D-CED
20	A	1132	CLA	O1D-CGD-O2D-CED
20	B	1211	CLA	O1D-CGD-O2D-CED
20	1	603	CLA	O1D-CGD-O2D-CED
20	3	604	CLA	O1D-CGD-O2D-CED
20	F	301	CLA	O1D-CGD-O2D-CED
20	G	201	CLA	O1D-CGD-O2D-CED
20	A	1801	CLA	O1D-CGD-O2D-CED
20	4	612	CLA	O1A-CGA-O2A-C1
20	F	302	CLA	O1A-CGA-O2A-C1
20	A	1103	CLA	C3-C5-C6-C7
20	A	1124	CLA	C3-C5-C6-C7
20	A	1128	CLA	C3-C5-C6-C7
20	A	1138	CLA	C3-C5-C6-C7
20	B	1214	CLA	C3-C5-C6-C7
20	3	602	CLA	C3-C5-C6-C7
20	G	218	CLA	C3-C5-C6-C7
20	A	1117	CLA	O1D-CGD-O2D-CED
20	3	603	CLA	O1D-CGD-O2D-CED
28	3	608	CHL	O1D-CGD-O2D-CED
20	A	1121	CLA	CBA-CGA-O2A-C1
20	1	603	CLA	CBA-CGA-O2A-C1
20	2	609	CLA	CBA-CGA-O2A-C1
20	3	603	CLA	CBA-CGA-O2A-C1
20	3	614	CLA	CBA-CGA-O2A-C1
20	4	603	CLA	CBA-CGA-O2A-C1
20	4	613	CLA	CBA-CGA-O2A-C1
20	G	201	CLA	CBA-CGA-O2A-C1
20	A	1101	CLA	CBD-CGD-O2D-CED
20	A	1107	CLA	CBD-CGD-O2D-CED
20	A	1111	CLA	CBD-CGD-O2D-CED
20	A	1113	CLA	CBD-CGD-O2D-CED
20	B	1204	CLA	CBD-CGD-O2D-CED
20	B	1208	CLA	CBD-CGD-O2D-CED
20	B	1213	CLA	CBD-CGD-O2D-CED
20	B	1226	CLA	CBD-CGD-O2D-CED
20	B	1230	CLA	CBD-CGD-O2D-CED
20	3	610	CLA	CBD-CGD-O2D-CED
20	4	611	CLA	CBD-CGD-O2D-CED
20	G	218	CLA	CBD-CGD-O2D-CED
20	G	202	CLA	CBD-CGD-O2D-CED
20	J	102	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
20	K	201	CLA	CBD-CGD-O2D-CED
20	K	202	CLA	CBD-CGD-O2D-CED
28	4	607	CHL	CBD-CGD-O2D-CED
20	A	1103	CLA	O1D-CGD-O2D-CED
20	B	1222	CLA	O1D-CGD-O2D-CED
20	3	609	CLA	O1D-CGD-O2D-CED
20	A	1122	CLA	O1A-CGA-O2A-C1
20	B	1222	CLA	O1A-CGA-O2A-C1
20	1	611	CLA	O1A-CGA-O2A-C1
20	B	1012	CLA	C4-C3-C5-C6
20	1	603	CLA	C4-C3-C5-C6
20	B	1012	CLA	C2-C3-C5-C6
20	1	603	CLA	C2-C3-C5-C6
20	B	1222	CLA	CBA-CGA-O2A-C1
20	1	611	CLA	CBA-CGA-O2A-C1
20	3	617	CLA	CBA-CGA-O2A-C1
20	F	302	CLA	CBA-CGA-O2A-C1
20	G	202	CLA	CBA-CGA-O2A-C1
20	A	1114	CLA	CBD-CGD-O2D-CED
20	B	1203	CLA	CBD-CGD-O2D-CED
20	B	1225	CLA	CBD-CGD-O2D-CED
20	3	617	CLA	CBD-CGD-O2D-CED
20	A	1112	CLA	O1D-CGD-O2D-CED
20	B	1201	CLA	C2A-CAA-CBA-CGA
28	2	607	CHL	C2A-CAA-CBA-CGA
20	B	1229	CLA	C3-C5-C6-C7
20	2	610	CLA	C3-C5-C6-C7
20	3	607	CLA	C3-C5-C6-C7
20	A	1118	CLA	CBA-CGA-O2A-C1
20	A	1128	CLA	CBA-CGA-O2A-C1
20	A	1135	CLA	CBA-CGA-O2A-C1
20	A	1138	CLA	CBA-CGA-O2A-C1
20	B	1012	CLA	CBA-CGA-O2A-C1
20	B	1203	CLA	CBA-CGA-O2A-C1
20	B	1228	CLA	CBA-CGA-O2A-C1
20	3	604	CLA	CBA-CGA-O2A-C1
20	4	604	CLA	CBA-CGA-O2A-C1
20	3	617	CLA	O1A-CGA-O2A-C1
20	G	202	CLA	O1A-CGA-O2A-C1
20	B	1228	CLA	O1A-CGA-O2A-C1
20	3	604	CLA	O1A-CGA-O2A-C1
25	A	5002	LMG	O10-C28-O8-C9

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Mol	Chain	Res	Type	Atoms
20	4	612	CLA	CBA-CGA-O2A-C1
20	1	610	CLA	O1D-CGD-O2D-CED
19	A	1011	CL0	C3-C5-C6-C7
20	3	610	CLA	C3-C5-C6-C7
20	A	1130	CLA	CBD-CGD-O2D-CED
20	B	1231	CLA	CBD-CGD-O2D-CED
20	2	610	CLA	CBD-CGD-O2D-CED
24	4	630	LHG	O2-C2-C3-O3
20	1	611	CLA	O1D-CGD-O2D-CED
20	4	613	CLA	O1D-CGD-O2D-CED
20	A	1122	CLA	CBA-CGA-O2A-C1
20	B	1229	CLA	CBA-CGA-O2A-C1
20	3	614	CLA	O1A-CGA-O2A-C1
20	G	201	CLA	O1A-CGA-O2A-C1
20	B	1210	CLA	C2C-C3C-CAC-CBC
20	B	1216	CLA	C2C-C3C-CAC-CBC
20	1	615	CLA	CBD-CGD-O2D-CED
20	3	611	CLA	CBD-CGD-O2D-CED
24	4	630	LHG	C8-C7-O7-C5
20	F	302	CLA	O1D-CGD-O2D-CED
20	2	613	CLA	C3-C5-C6-C7
20	B	1216	CLA	CBD-CGD-O2D-CED
20	2	613	CLA	CBD-CGD-O2D-CED
20	4	601	CLA	CBD-CGD-O2D-CED
26	G	402	LMT	O5'-C5'-C6'-O6'
20	B	1235	CLA	O1D-CGD-O2D-CED
20	B	1215	CLA	C4-C3-C5-C6
20	B	1215	CLA	C2-C3-C5-C6
20	A	1128	CLA	O1A-CGA-O2A-C1
20	A	1135	CLA	O1A-CGA-O2A-C1
24	4	630	LHG	O9-C7-O7-C5
20	B	1206	CLA	O1D-CGD-O2D-CED
20	A	1133	CLA	CBD-CGD-O2D-CED
20	2	612	CLA	CBD-CGD-O2D-CED
25	J	301	LMG	O6-C5-C6-O5
20	L	303	CLA	C2A-CAA-CBA-CGA
20	B	1229	CLA	O1A-CGA-O2A-C1
20	4	604	CLA	O1A-CGA-O2A-C1
25	A	5002	LMG	O6-C1-O1-C7
27	B	5002	DGD	O6D-C1D-O3G-C3G
20	A	1127	CLA	CBA-CGA-O2A-C1
20	B	1021	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
25	A	5002	LMG	C29-C28-O8-C9
20	A	1124	CLA	CBD-CGD-O2D-CED
20	B	1236	CLA	CBD-CGD-O2D-CED
20	1	612	CLA	CBD-CGD-O2D-CED
20	3	613	CLA	CBD-CGD-O2D-CED
20	4	612	CLA	CBD-CGD-O2D-CED
28	2	615	CHL	CBD-CGD-O2D-CED
28	4	615	CHL	CBD-CGD-O2D-CED
26	G	401	LMT	O5'-C5'-C6'-O6'
20	K	202	CLA	C2C-C3C-CAC-CBC
20	A	1116	CLA	CBD-CGD-O2D-CED
20	4	610	CLA	CBD-CGD-O2D-CED
28	2	607	CHL	CBD-CGD-O2D-CED
23	L	420	BCR	C19-C20-C21-C22
20	A	1127	CLA	O1A-CGA-O2A-C1
20	B	1021	CLA	O1A-CGA-O2A-C1
20	B	1203	CLA	O1A-CGA-O2A-C1
20	G	218	CLA	O1A-CGA-O2A-C1
19	A	1011	CL0	CBA-CGA-O2A-C1
20	A	1104	CLA	CBA-CGA-O2A-C1
20	A	1125	CLA	CBA-CGA-O2A-C1
20	A	1136	CLA	CBA-CGA-O2A-C1
20	B	1201	CLA	CBA-CGA-O2A-C1
20	B	1240	CLA	CBA-CGA-O2A-C1
20	1	604	CLA	CBA-CGA-O2A-C1
20	3	607	CLA	CBA-CGA-O2A-C1
20	G	218	CLA	CBA-CGA-O2A-C1
24	B	5101	LHG	C24-C23-O8-C6
24	1	630	LHG	C24-C23-O8-C6
20	A	1119	CLA	CBD-CGD-O2D-CED
28	4	606	CHL	CBD-CGD-O2D-CED
25	J	301	LMG	C4-C5-C6-O5
20	A	1115	CLA	C2C-C3C-CAC-CBC
20	B	1230	CLA	O1D-CGD-O2D-CED
20	G	202	CLA	O1D-CGD-O2D-CED
20	L	302	CLA	C4C-C3C-CAC-CBC
20	A	1106	CLA	C3-C5-C6-C7
20	3	609	CLA	C3-C5-C6-C7
20	B	1210	CLA	C11-C12-C13-C14
20	B	1214	CLA	C6-C7-C8-C9
20	B	1215	CLA	C6-C7-C8-C9
20	B	1223	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
20	B	1224	CLA	C6-C7-C8-C9
28	2	601	CHL	C6-C7-C8-C9
28	2	601	CHL	C11-C12-C13-C14
20	A	1107	CLA	O1D-CGD-O2D-CED
20	A	1113	CLA	O1D-CGD-O2D-CED
20	G	218	CLA	O1D-CGD-O2D-CED
28	4	607	CHL	O1D-CGD-O2D-CED
25	A	5002	LMG	C2-C1-O1-C7
27	B	5002	DGD	C2D-C1D-O3G-C3G
20	B	1226	CLA	O1D-CGD-O2D-CED
19	A	1011	CL0	O1A-CGA-O2A-C1
20	A	1104	CLA	O1A-CGA-O2A-C1
20	A	1125	CLA	O1A-CGA-O2A-C1
20	B	1201	CLA	O1A-CGA-O2A-C1
20	A	1101	CLA	O1D-CGD-O2D-CED
23	A	4001	BCR	C37-C22-C23-C24
23	A	4003	BCR	C37-C22-C23-C24
23	A	4008	BCR	C7-C8-C9-C34
23	A	4011	BCR	C37-C22-C23-C24
23	B	4005	BCR	C37-C22-C23-C24
23	B	4006	BCR	C7-C8-C9-C34
23	B	4010	BCR	C7-C8-C9-C34
23	B	4010	BCR	C37-C22-C23-C24
23	B	4017	BCR	C36-C18-C19-C20
23	B	4014	BCR	C37-C22-C23-C24
23	1	623	BCR	C37-C22-C23-C24
23	3	623	BCR	C11-C12-C13-C35
23	3	624	BCR	C7-C8-C9-C34
23	F	416	BCR	C7-C8-C9-C34
23	I	118	BCR	C37-C22-C23-C24
23	L	419	BCR	C7-C8-C9-C34
29	1	621	LUT	C27-C28-C29-C39
29	4	623	LUT	C7-C8-C9-C19
29	4	623	LUT	C31-C32-C33-C40
23	A	4011	BCR	C21-C22-C23-C24
23	B	4004	BCR	C7-C8-C9-C10
23	B	4005	BCR	C21-C22-C23-C24
23	B	4006	BCR	C7-C8-C9-C10
23	B	4014	BCR	C7-C8-C9-C10
23	3	623	BCR	C21-C22-C23-C24
29	1	621	LUT	C27-C28-C29-C30
29	4	620	LUT	C27-C28-C29-C30

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Mol	Chain	Res	Type	Atoms
29	4	623	LUT	C7-C8-C9-C10
29	4	623	LUT	C31-C32-C33-C34
20	A	1125	CLA	C2A-CAA-CBA-CGA
20	A	1140	CLA	C2A-CAA-CBA-CGA
20	B	1240	CLA	O1A-CGA-O2A-C1
20	1	604	CLA	O1A-CGA-O2A-C1
20	4	609	CLA	C3-C5-C6-C7
26	G	402	LMT	C4'-C5'-C6'-O6'
20	B	1228	CLA	CBD-CGD-O2D-CED
20	1	615	CLA	CBA-CGA-O2A-C1
20	4	614	CLA	CBA-CGA-O2A-C1
20	A	1801	CLA	CBA-CGA-O2A-C1
20	B	1214	CLA	CBA-CGA-O2A-C1
20	A	1118	CLA	C2-C1-O2A-CGA
20	A	1111	CLA	O1D-CGD-O2D-CED
20	B	1204	CLA	O1D-CGD-O2D-CED
20	K	202	CLA	O1D-CGD-O2D-CED
23	3	624	BCR	C14-C15-C16-C17
20	A	1111	CLA	C8-C10-C11-C12
20	B	1210	CLA	C10-C11-C12-C13
20	B	1213	CLA	O1D-CGD-O2D-CED
24	B	5101	LHG	C23-C24-C25-C26
20	4	611	CLA	O1D-CGD-O2D-CED
20	A	1127	CLA	CBD-CGD-O2D-CED
20	B	1021	CLA	C6-C7-C8-C10
20	J	102	CLA	O1D-CGD-O2D-CED
20	A	1106	CLA	CBA-CGA-O2A-C1
20	2	610	CLA	C4-C3-C5-C6
20	B	1208	CLA	O1D-CGD-O2D-CED
26	1	631	LMT	C4'-C5'-C6'-O6'
26	4	631	LMT	C4B-C5B-C6B-O6B
20	3	607	CLA	O1A-CGA-O2A-C1
20	K	201	CLA	O1D-CGD-O2D-CED
20	B	1237	CLA	C5-C6-C7-C8
21	A	2001	PQN	C23-C25-C26-C27
20	B	1214	CLA	C2A-CAA-CBA-CGA
20	B	1224	CLA	C2A-CAA-CBA-CGA
20	B	1237	CLA	C2A-CAA-CBA-CGA
20	B	1238	CLA	C2A-CAA-CBA-CGA
20	K	202	CLA	C2A-CAA-CBA-CGA
28	1	607	CHL	C2A-CAA-CBA-CGA
28	1	601	CHL	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
28	2	608	CHL	C2A-CAA-CBA-CGA
28	3	608	CHL	C2A-CAA-CBA-CGA
28	4	607	CHL	C2A-CAA-CBA-CGA
28	4	608	CHL	C2A-CAA-CBA-CGA
20	B	1225	CLA	O1D-CGD-O2D-CED
23	A	4001	BCR	C10-C11-C12-C13
23	A	4001	BCR	C18-C19-C20-C21
23	B	4004	BCR	C10-C11-C12-C13
23	B	4014	BCR	C18-C19-C20-C21
20	A	1127	CLA	C8-C10-C11-C12
20	B	1238	CLA	C5-C6-C7-C8
20	2	610	CLA	C5-C6-C7-C8
21	B	2002	PQN	C15-C16-C17-C18
28	2	601	CHL	C13-C15-C16-C17
20	A	8895	CLA	C3-C5-C6-C7
27	B	5002	DGD	O6E-C1E-O5D-C6D
20	3	610	CLA	O1D-CGD-O2D-CED
26	A	5004	LMT	C4'-C5'-C6'-O6'
20	A	1119	CLA	C15-C16-C17-C18
20	B	1023	CLA	C10-C11-C12-C13
20	B	1238	CLA	C10-C11-C12-C13
20	2	613	CLA	C5-C6-C7-C8
21	B	2002	PQN	C20-C21-C22-C23
28	2	601	CHL	C5-C6-C7-C8
28	2	601	CHL	C15-C16-C17-C18
28	2	601	CHL	C8-C10-C11-C12
20	2	610	CLA	O1D-CGD-O2D-CED
20	A	1114	CLA	O1D-CGD-O2D-CED
20	3	617	CLA	O1D-CGD-O2D-CED
20	B	1215	CLA	CBD-CGD-O2D-CED
20	A	1801	CLA	O1A-CGA-O2A-C1
20	B	1203	CLA	O1D-CGD-O2D-CED
20	A	1103	CLA	CBA-CGA-O2A-C1
20	A	1124	CLA	CBA-CGA-O2A-C1
20	A	1126	CLA	CBA-CGA-O2A-C1
20	B	1237	CLA	CBA-CGA-O2A-C1
20	3	613	CLA	CBA-CGA-O2A-C1
26	1	631	LMT	C4B-C5B-C6B-O6B
20	3	614	CLA	O2A-C1-C2-C3
20	A	1135	CLA	C2C-C3C-CAC-CBC
20	A	1106	CLA	O1A-CGA-O2A-C1
20	A	1136	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
20	1	612	CLA	CBA-CGA-O2A-C1
20	2	603	CLA	CBA-CGA-O2A-C1
24	A	5003	LHG	C23-C24-C25-C26
20	B	1210	CLA	C15-C16-C17-C18
20	A	1130	CLA	O1D-CGD-O2D-CED
20	B	1021	CLA	C5-C6-C7-C8
24	4	630	LHG	C1-C2-C3-O3
20	A	1110	CLA	C2A-CAA-CBA-CGA
20	A	1121	CLA	C2A-CAA-CBA-CGA
28	2	602	CHL	C2A-CAA-CBA-CGA
20	B	1231	CLA	O1D-CGD-O2D-CED
20	B	1225	CLA	C15-C16-C17-C18
20	3	609	CLA	C8-C10-C11-C12
20	1	615	CLA	O1D-CGD-O2D-CED
20	3	611	CLA	O1D-CGD-O2D-CED
20	4	601	CLA	O1D-CGD-O2D-CED
20	A	1127	CLA	C15-C16-C17-C18
20	B	1215	CLA	C5-C6-C7-C8
20	4	611	CLA	C5-C6-C7-C8
20	3	609	CLA	C10-C11-C12-C13
27	B	5002	DGD	C2A-C1A-O1G-C1G
21	B	2002	PQN	C14-C13-C15-C16
20	A	1111	CLA	C10-C11-C12-C13
20	A	1138	CLA	C5-C6-C7-C8
20	B	1203	CLA	C3-C5-C6-C7
20	B	1226	CLA	C3-C5-C6-C7
24	A	5001	LHG	C8-C7-O7-C5
26	B	5001	LMT	C4'-C5'-C6'-O6'
26	A	5004	LMT	C2'-C1'-O1'-C1
27	B	5002	DGD	C2E-C1E-O5D-C6D
23	A	4002	BCR	C16-C17-C18-C36
23	A	4002	BCR	C20-C21-C22-C37
23	A	4003	BCR	C16-C17-C18-C36
23	A	4008	BCR	C20-C21-C22-C37
23	B	4017	BCR	C16-C17-C18-C36
23	B	4014	BCR	C35-C13-C14-C15
23	3	623	BCR	C11-C10-C9-C34
23	F	416	BCR	C20-C21-C22-C37
23	G	311	BCR	C20-C21-C22-C37
23	I	120	BCR	C11-C10-C9-C34
23	I	120	BCR	C35-C13-C14-C15
23	J	212	BCR	C16-C17-C18-C36

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Mol	Chain	Res	Type	Atoms
23	J	213	BCR	C20-C21-C22-C37
23	K	301	BCR	C11-C10-C9-C34
28	2	606	CHL	CBD-CGD-O2D-CED
23	A	4001	BCR	C7-C8-C9-C34
23	B	4004	BCR	C7-C8-C9-C34
23	B	4014	BCR	C7-C8-C9-C34
23	I	120	BCR	C7-C8-C9-C34
29	1	620	LUT	C27-C28-C29-C39
29	4	620	LUT	C11-C12-C13-C20
29	4	620	LUT	C27-C28-C29-C39
23	I	120	BCR	C7-C8-C9-C10
29	1	620	LUT	C27-C28-C29-C30
20	B	1214	CLA	O1A-CGA-O2A-C1
20	A	1106	CLA	C2A-CAA-CBA-CGA
20	A	1114	CLA	C2A-CAA-CBA-CGA
20	A	1127	CLA	C2A-CAA-CBA-CGA
20	L	302	CLA	C2A-CAA-CBA-CGA
28	2	615	CHL	C2A-CAA-CBA-CGA
20	K	201	CLA	C2C-C3C-CAC-CBC
20	B	1229	CLA	C5-C6-C7-C8
24	A	5003	LHG	O1-C1-C2-C3
24	2	630	LHG	O1-C1-C2-C3
20	1	603	CLA	C6-C7-C8-C9
20	3	603	CLA	C6-C7-C8-C9
20	2	613	CLA	O1D-CGD-O2D-CED
20	A	1126	CLA	O1A-CGA-O2A-C1
23	A	4003	BCR	C11-C10-C9-C8
23	A	4003	BCR	C16-C17-C18-C19
23	A	4008	BCR	C20-C21-C22-C23
23	A	4011	BCR	C12-C13-C14-C15
23	B	4014	BCR	C11-C10-C9-C8
23	B	4014	BCR	C20-C21-C22-C23
23	3	623	BCR	C16-C17-C18-C19
23	3	624	BCR	C16-C17-C18-C19
23	I	118	BCR	C11-C10-C9-C8
23	I	118	BCR	C20-C21-C22-C23
23	I	120	BCR	C11-C10-C9-C8
23	I	120	BCR	C12-C13-C14-C15
23	J	212	BCR	C12-C13-C14-C15
23	J	212	BCR	C16-C17-C18-C19
23	J	213	BCR	C11-C10-C9-C8
23	K	301	BCR	C20-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
21	B	2002	PQN	C12-C13-C15-C16
20	A	1133	CLA	O1D-CGD-O2D-CED
20	B	1216	CLA	O1D-CGD-O2D-CED
20	2	612	CLA	O1D-CGD-O2D-CED
20	3	609	CLA	CBA-CGA-O2A-C1
20	A	1118	CLA	C5-C6-C7-C8
20	B	1201	CLA	CBD-CGD-O2D-CED
26	G	401	LMT	C4'-C5'-C6'-O6'
20	L	301	CLA	C2-C1-O2A-CGA
20	B	1012	CLA	C6-C7-C8-C10
20	B	1213	CLA	C6-C7-C8-C10
20	3	603	CLA	C6-C7-C8-C10
23	A	4011	BCR	C14-C15-C16-C17
23	F	416	BCR	C14-C15-C16-C17
20	B	1224	CLA	C2C-C3C-CAC-CBC
24	2	630	LHG	C26-C27-C28-C29
26	G	401	LMT	C2-C1-O1'-C1'
20	4	612	CLA	O1D-CGD-O2D-CED
20	B	1021	CLA	C8-C10-C11-C12
20	A	1104	CLA	C4B-C3B-CAB-CBB
20	B	1228	CLA	C4B-C3B-CAB-CBB
20	B	1239	CLA	C4B-C3B-CAB-CBB
20	2	603	CLA	C4B-C3B-CAB-CBB
20	2	612	CLA	C4B-C3B-CAB-CBB
20	3	607	CLA	C4B-C3B-CAB-CBB
20	J	102	CLA	C4B-C3B-CAB-CBB
28	2	606	CHL	C4B-C3B-CAB-CBB
28	2	607	CHL	CBA-CGA-O2A-C1
20	A	1111	CLA	C16-C17-C18-C19
20	B	1012	CLA	C6-C7-C8-C9
20	B	1213	CLA	C6-C7-C8-C9
20	1	603	CLA	C6-C7-C8-C10
20	3	602	CLA	C11-C12-C13-C14
20	L	302	CLA	C11-C12-C13-C15
28	1	601	CHL	C6-C7-C8-C9
20	3	613	CLA	O1A-CGA-O2A-C1
20	A	1103	CLA	C6-C7-C8-C10
20	B	1210	CLA	C11-C12-C13-C15
20	B	1214	CLA	C6-C7-C8-C10
20	B	1225	CLA	C11-C10-C8-C7
25	J	301	LMG	C18-C19-C20-C21
20	B	1238	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
20	A	1103	CLA	O1A-CGA-O2A-C1
20	B	1215	CLA	C3-C5-C6-C7
20	A	1101	CLA	C3A-C2A-CAA-CBA
20	A	1107	CLA	C3A-C2A-CAA-CBA
20	A	1111	CLA	C3A-C2A-CAA-CBA
20	A	1125	CLA	C3A-C2A-CAA-CBA
20	A	1128	CLA	C3A-C2A-CAA-CBA
20	A	1130	CLA	C3A-C2A-CAA-CBA
20	A	1135	CLA	C3A-C2A-CAA-CBA
20	A	5005	CLA	C3A-C2A-CAA-CBA
20	B	1012	CLA	C3A-C2A-CAA-CBA
20	B	1203	CLA	C3A-C2A-CAA-CBA
20	B	1210	CLA	C3A-C2A-CAA-CBA
20	B	1216	CLA	C3A-C2A-CAA-CBA
20	B	1234	CLA	C3A-C2A-CAA-CBA
20	B	1239	CLA	C3A-C2A-CAA-CBA
20	1	603	CLA	C3A-C2A-CAA-CBA
20	3	603	CLA	C3A-C2A-CAA-CBA
20	3	607	CLA	C3A-C2A-CAA-CBA
20	3	617	CLA	C3A-C2A-CAA-CBA
20	4	603	CLA	C3A-C2A-CAA-CBA
20	G	202	CLA	C3A-C2A-CAA-CBA
20	J	102	CLA	C3A-C2A-CAA-CBA
20	K	201	CLA	C3A-C2A-CAA-CBA
20	K	204	CLA	C3A-C2A-CAA-CBA
20	L	303	CLA	C3A-C2A-CAA-CBA
28	1	607	CHL	C3A-C2A-CAA-CBA
28	2	615	CHL	C3A-C2A-CAA-CBA
20	3	613	CLA	O1D-CGD-O2D-CED
28	4	615	CHL	O1D-CGD-O2D-CED
23	A	4003	BCR	C19-C20-C21-C22
20	A	1111	CLA	C16-C17-C18-C20
20	3	602	CLA	C11-C12-C13-C15
20	L	302	CLA	C11-C12-C13-C14
24	A	5003	LHG	C24-C25-C26-C27
20	A	1140	CLA	CBA-CGA-O2A-C1
20	1	610	CLA	CBA-CGA-O2A-C1
24	A	5003	LHG	C24-C23-O8-C6
24	1	630	LHG	C12-C13-C14-C15
20	A	1124	CLA	O1A-CGA-O2A-C1
20	3	609	CLA	O1A-CGA-O2A-C1
27	B	5002	DGD	CAA-CBA-CCA-CDA

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Mol	Chain	Res	Type	Atoms
24	2	630	LHG	C27-C28-C29-C30
20	A	1022	CLA	C4C-C3C-CAC-CBC
20	A	8895	CLA	C4C-C3C-CAC-CBC
20	1	612	CLA	O1D-CGD-O2D-CED
20	B	1236	CLA	O1D-CGD-O2D-CED
20	A	1103	CLA	C2B-C3B-CAB-CBB
23	A	4008	BCR	C1-C6-C7-C8
23	A	4008	BCR	C5-C6-C7-C8
23	A	4008	BCR	C23-C24-C25-C26
23	B	4006	BCR	C1-C6-C7-C8
23	B	4006	BCR	C5-C6-C7-C8
23	B	4017	BCR	C23-C24-C25-C26
23	B	4017	BCR	C23-C24-C25-C30
23	1	623	BCR	C23-C24-C25-C30
23	3	623	BCR	C1-C6-C7-C8
23	3	623	BCR	C5-C6-C7-C8
23	3	623	BCR	C23-C24-C25-C26
23	3	623	BCR	C23-C24-C25-C30
23	I	120	BCR	C1-C6-C7-C8
23	I	120	BCR	C5-C6-C7-C8
23	J	212	BCR	C23-C24-C25-C30
23	L	420	BCR	C23-C24-C25-C30
28	2	602	CHL	C2B-C3B-CAB-CBB
28	2	606	CHL	C2B-C3B-CAB-CBB
28	2	611	CHL	C2B-C3B-CAB-CBB
28	4	608	CHL	C2B-C3B-CAB-CBB
29	2	623	LUT	C1-C6-C7-C8
29	2	623	LUT	C5-C6-C7-C8
28	2	602	CHL	C5-C6-C7-C8
24	3	630	LHG	C24-C25-C26-C27
20	A	1124	CLA	O1D-CGD-O2D-CED
28	2	615	CHL	O1D-CGD-O2D-CED
20	B	1225	CLA	C2A-CAA-CBA-CGA
20	2	610	CLA	C2A-CAA-CBA-CGA
20	3	607	CLA	C2A-CAA-CBA-CGA
20	3	613	CLA	C2A-CAA-CBA-CGA
27	B	5002	DGD	C1B-C2B-C3B-C4B
24	A	5001	LHG	C27-C28-C29-C30
20	3	607	CLA	C4-C3-C5-C6
28	2	607	CHL	O1D-CGD-O2D-CED
23	A	4003	BCR	C18-C19-C20-C21
23	3	624	BCR	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
23	J	212	BCR	C18-C19-C20-C21
23	K	301	BCR	C18-C19-C20-C21
20	2	610	CLA	C2-C3-C5-C6
26	4	631	LMT	O5B-C5B-C6B-O6B
20	3	607	CLA	C11-C12-C13-C14
24	1	630	LHG	C23-C24-C25-C26
25	2	631	LMG	C28-C29-C30-C31
20	B	1216	CLA	CBA-CGA-O2A-C1
20	B	1223	CLA	C13-C15-C16-C17
20	1	615	CLA	O1A-CGA-O2A-C1
20	A	1116	CLA	O1D-CGD-O2D-CED
26	G	402	LMT	C2'-C1'-O1'-C1
20	B	1237	CLA	O1A-CGA-O2A-C1
24	A	5001	LHG	C24-C25-C26-C27
25	J	301	LMG	C16-C17-C18-C19
20	4	610	CLA	O1D-CGD-O2D-CED
23	B	4004	BCR	C13-C14-C15-C16
20	B	1235	CLA	C6-C7-C8-C10
24	A	5003	LHG	C8-C7-O7-C5
25	J	302	LMG	C11-C10-O7-C8
20	B	1214	CLA	C5-C6-C7-C8
20	4	614	CLA	O1A-CGA-O2A-C1
20	B	1210	CLA	CBD-CGD-O2D-CED
23	A	4008	BCR	C11-C12-C13-C35
23	K	301	BCR	C37-C22-C23-C24
23	A	4011	BCR	C7-C8-C9-C10
23	B	4004	BCR	C21-C22-C23-C24
20	1	613	CLA	C2A-CAA-CBA-CGA
20	4	604	CLA	C2A-CAA-CBA-CGA
20	4	613	CLA	C2A-CAA-CBA-CGA
20	A	1127	CLA	C16-C17-C18-C19
20	B	1202	CLA	C16-C17-C18-C20
20	B	1235	CLA	C6-C7-C8-C9
20	B	1240	CLA	C16-C17-C18-C20
20	3	607	CLA	C11-C12-C13-C15
20	I	121	CLA	C16-C17-C18-C19
20	I	121	CLA	CBD-CGD-O2D-CED
20	4	609	CLA	C4-C3-C5-C6
25	J	301	LMG	C34-C35-C36-C37
20	B	1238	CLA	O1A-CGA-O2A-C1
20	1	603	CLA	C3-C5-C6-C7
20	4	613	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
20	3	609	CLA	C11-C12-C13-C15
28	1	601	CHL	C6-C7-C8-C10
20	A	1140	CLA	O1A-CGA-O2A-C1
24	A	5001	LHG	O7-C5-C6-O8
25	2	631	LMG	C29-C28-O8-C9
28	3	608	CHL	CBA-CGA-O2A-C1
20	A	1140	CLA	C2-C1-O2A-CGA
28	4	606	CHL	O1D-CGD-O2D-CED
20	B	1210	CLA	C13-C15-C16-C17
20	3	613	CLA	C3-C5-C6-C7
20	3	607	CLA	C2-C3-C5-C6
20	4	609	CLA	C2-C3-C5-C6
24	A	5001	LHG	O9-C7-O7-C5
20	A	1106	CLA	C5-C6-C7-C8
20	A	1126	CLA	C2A-CAA-CBA-CGA
20	B	1211	CLA	C2A-CAA-CBA-CGA
28	2	606	CHL	C2A-CAA-CBA-CGA
20	3	607	CLA	CBD-CGD-O2D-CED
20	B	1201	CLA	C4C-C3C-CAC-CBC
20	A	1119	CLA	O1D-CGD-O2D-CED
20	1	610	CLA	O1A-CGA-O2A-C1
20	L	302	CLA	C3-C5-C6-C7
20	B	1225	CLA	C2C-C3C-CAC-CBC
25	J	301	LMG	C32-C33-C34-C35
20	A	1101	CLA	C1A-C2A-CAA-CBA
20	A	1103	CLA	C1A-C2A-CAA-CBA
20	A	1111	CLA	C1A-C2A-CAA-CBA
20	A	1116	CLA	C1A-C2A-CAA-CBA
20	A	1119	CLA	C1A-C2A-CAA-CBA
20	A	1132	CLA	C1A-C2A-CAA-CBA
20	A	1133	CLA	C1A-C2A-CAA-CBA
20	A	1134	CLA	C1A-C2A-CAA-CBA
20	A	5005	CLA	C1A-C2A-CAA-CBA
20	B	1209	CLA	C1A-C2A-CAA-CBA
20	B	1210	CLA	C1A-C2A-CAA-CBA
20	B	1212	CLA	C1A-C2A-CAA-CBA
20	B	1215	CLA	C1A-C2A-CAA-CBA
20	B	1219	CLA	C1A-C2A-CAA-CBA
20	B	1228	CLA	C1A-C2A-CAA-CBA
20	B	1229	CLA	C1A-C2A-CAA-CBA
20	B	1231	CLA	C1A-C2A-CAA-CBA
20	B	1234	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
20	B	1236	CLA	C1A-C2A-CAA-CBA
20	2	604	CLA	C1A-C2A-CAA-CBA
20	3	603	CLA	C1A-C2A-CAA-CBA
20	3	604	CLA	C1A-C2A-CAA-CBA
20	3	610	CLA	C1A-C2A-CAA-CBA
20	3	617	CLA	C1A-C2A-CAA-CBA
20	4	601	CLA	C1A-C2A-CAA-CBA
20	4	603	CLA	C1A-C2A-CAA-CBA
20	4	604	CLA	C1A-C2A-CAA-CBA
20	4	609	CLA	C1A-C2A-CAA-CBA
20	4	611	CLA	C1A-C2A-CAA-CBA
20	J	102	CLA	C1A-C2A-CAA-CBA
20	L	301	CLA	C1A-C2A-CAA-CBA
28	2	606	CHL	C1A-C2A-CAA-CBA
28	2	607	CHL	C1A-C2A-CAA-CBA
28	2	608	CHL	C1A-C2A-CAA-CBA
28	2	615	CHL	C1A-C2A-CAA-CBA
20	B	1228	CLA	O1D-CGD-O2D-CED
24	B	5101	LHG	O6-C4-C5-C6
20	A	1127	CLA	C2C-C3C-CAC-CBC
20	A	1104	CLA	C6-C7-C8-C10
20	A	1104	CLA	C12-C13-C15-C16
20	A	1122	CLA	C11-C10-C8-C7
20	A	1124	CLA	C11-C10-C8-C7
20	A	1127	CLA	C11-C12-C13-C15
20	A	1132	CLA	C12-C13-C15-C16
20	B	1215	CLA	C6-C7-C8-C10
21	B	2002	PQN	C21-C22-C23-C25
28	2	601	CHL	C11-C12-C13-C15
20	A	1127	CLA	C16-C17-C18-C20
20	B	1202	CLA	C15-C16-C17-C18
20	B	1210	CLA	CBA-CGA-O2A-C1
28	4	606	CHL	CBA-CGA-O2A-C1
25	A	5002	LMG	C10-C11-C12-C13
20	B	1238	CLA	C4-C3-C5-C6
20	B	1235	CLA	C2-C3-C5-C6
24	B	5101	LHG	O10-C23-O8-C6
23	O	301	BCR	C37-C22-C23-C24
26	A	5004	LMT	O5'-C5'-C6'-O6'
24	A	5001	LHG	C31-C32-C33-C34
20	4	613	CLA	C3-C5-C6-C7
24	2	630	LHG	C8-C7-O7-C5

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Mol	Chain	Res	Type	Atoms
20	4	603	CLA	C2A-CAA-CBA-CGA
20	A	1104	CLA	C14-C13-C15-C16
20	A	1122	CLA	C11-C10-C8-C9
20	A	1124	CLA	C11-C10-C8-C9
20	A	1127	CLA	C11-C12-C13-C14
20	A	1132	CLA	C14-C13-C15-C16
20	A	1136	CLA	C6-C7-C8-C9
20	A	8895	CLA	C14-C13-C15-C16
20	B	1021	CLA	C6-C7-C8-C9
20	B	1021	CLA	C11-C10-C8-C9
26	1	631	LMT	O5B-C5B-C6B-O6B
20	A	1139	CLA	CBA-CGA-O2A-C1
24	3	630	LHG	O9-C7-O7-C5
24	A	5003	LHG	C4-C5-C6-O8
27	B	5002	DGD	O1A-C1A-O1G-C1G
26	1	631	LMT	O5'-C5'-C6'-O6'
20	3	609	CLA	C11-C12-C13-C14
20	1	612	CLA	O1A-CGA-O2A-C1
20	2	603	CLA	O1A-CGA-O2A-C1
20	B	1235	CLA	C4-C3-C5-C6
20	B	1238	CLA	C2-C3-C5-C6
20	L	302	CLA	C5-C6-C7-C8
23	1	623	BCR	C21-C22-C23-C24
23	K	301	BCR	C7-C8-C9-C10
29	4	620	LUT	C11-C12-C13-C14
24	4	630	LHG	C11-C10-C9-C8
28	2	615	CHL	CBA-CGA-O2A-C1
25	J	302	LMG	O6-C5-C6-O5
20	A	1127	CLA	O1D-CGD-O2D-CED
20	4	601	CLA	O2A-C1-C2-C3
24	A	5001	LHG	C25-C26-C27-C28
23	A	4008	BCR	C10-C11-C12-C13
23	B	4017	BCR	C9-C10-C11-C12
28	2	615	CHL	C3C-C2C-CMC-OMC
24	1	630	LHG	C7-C8-C9-C10
28	1	607	CHL	CBA-CGA-O2A-C1
23	A	4003	BCR	C20-C21-C22-C23
23	B	4017	BCR	C6-C7-C8-C9
20	B	1206	CLA	CBA-CGA-O2A-C1
20	B	1240	CLA	C16-C17-C18-C19
20	2	614	CLA	CBA-CGA-O2A-C1
24	A	5001	LHG	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
20	B	1216	CLA	O1A-CGA-O2A-C1
20	B	1210	CLA	C8-C10-C11-C12
20	A	1101	CLA	CBA-CGA-O2A-C1
28	2	608	CHL	CBA-CGA-O2A-C1
20	A	1126	CLA	C2C-C3C-CAC-CBC
20	B	1223	CLA	C2C-C3C-CAC-CBC
25	J	301	LMG	C20-C21-C22-C23
20	B	1238	CLA	C13-C15-C16-C17
20	A	1104	CLA	C3-C5-C6-C7
25	2	631	LMG	C30-C31-C32-C33
20	B	1202	CLA	CBA-CGA-O2A-C1
25	A	5002	LMG	C12-C13-C14-C15
24	A	5003	LHG	O9-C7-O7-C5
24	A	5003	LHG	O1-C1-C2-O2
24	4	630	LHG	O1-C1-C2-O2
20	A	1103	CLA	C6-C7-C8-C9
20	B	1215	CLA	O1D-CGD-O2D-CED
20	2	613	CLA	C4B-C3B-CAB-CBB
20	3	603	CLA	C4B-C3B-CAB-CBB
20	4	609	CLA	C4B-C3B-CAB-CBB
20	4	613	CLA	C4B-C3B-CAB-CBB
20	G	202	CLA	C4B-C3B-CAB-CBB
20	H	200	CLA	C4B-C3B-CAB-CBB
28	2	607	CHL	C4B-C3B-CAB-CBB
28	2	611	CHL	C4B-C3B-CAB-CBB
28	4	607	CHL	C4B-C3B-CAB-CBB
24	A	5001	LHG	C35-C36-C37-C38
20	A	1111	CLA	C2A-CAA-CBA-CGA
20	B	1215	CLA	C2A-CAA-CBA-CGA
28	2	611	CHL	C2A-CAA-CBA-CGA
24	3	630	LHG	O6-C4-C5-C6
20	A	1119	CLA	C6-C7-C8-C10
20	A	1136	CLA	C6-C7-C8-C10
20	A	8895	CLA	C12-C13-C15-C16
20	B	1021	CLA	C11-C10-C8-C7
20	B	1203	CLA	C12-C13-C15-C16
20	B	1210	CLA	C12-C13-C15-C16
20	B	1224	CLA	C11-C12-C13-C15
20	2	610	CLA	C6-C7-C8-C10
21	A	2001	PQN	C21-C22-C23-C25
20	B	1021	CLA	C15-C16-C17-C18
20	A	1115	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
24	1	630	LHG	O10-C23-O8-C6
25	2	631	LMG	C17-C18-C19-C20
20	A	1127	CLA	C4-C3-C5-C6
20	A	1133	CLA	C3A-C2A-CAA-CBA
20	A	1137	CLA	C3A-C2A-CAA-CBA
20	B	1224	CLA	C3A-C2A-CAA-CBA
28	2	602	CHL	C3A-C2A-CAA-CBA
28	4	608	CHL	C3A-C2A-CAA-CBA
25	J	301	LMG	C33-C34-C35-C36
26	A	5004	LMT	O5'-C1'-O1'-C1
20	A	1139	CLA	O1A-CGA-O2A-C1
28	2	606	CHL	O1D-CGD-O2D-CED
20	B	1225	CLA	CBA-CGA-O2A-C1
23	3	623	BCR	C37-C22-C23-C24
20	B	1234	CLA	C4-C3-C5-C6
23	B	4017	BCR	C11-C12-C13-C14
25	A	5002	LMG	C7-C8-C9-O8
24	2	630	LHG	C23-C24-C25-C26
24	A	5001	LHG	C26-C27-C28-C29
20	3	613	CLA	C4-C3-C5-C6
20	A	5005	CLA	CBA-CGA-O2A-C1
20	3	613	CLA	C2-C3-C5-C6
20	B	1201	CLA	O1D-CGD-O2D-CED
20	3	606	CLA	CBA-CGA-O2A-C1
20	3	606	CLA	C2B-C3B-CAB-CBB
23	A	4001	BCR	C1-C6-C7-C8
23	A	4002	BCR	C1-C6-C7-C8
23	A	4002	BCR	C23-C24-C25-C30
23	A	4003	BCR	C1-C6-C7-C8
23	A	4003	BCR	C5-C6-C7-C8
23	A	4011	BCR	C23-C24-C25-C30
23	B	4004	BCR	C1-C6-C7-C8
23	B	4005	BCR	C1-C6-C7-C8
23	B	4009	BCR	C1-C6-C7-C8
23	B	4017	BCR	C1-C6-C7-C8
23	1	623	BCR	C23-C24-C25-C26
23	3	624	BCR	C1-C6-C7-C8
23	3	624	BCR	C23-C24-C25-C30
23	F	416	BCR	C1-C6-C7-C8
23	G	311	BCR	C23-C24-C25-C30
23	J	212	BCR	C1-C6-C7-C8
23	J	212	BCR	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
23	J	213	BCR	C1-C6-C7-C8
23	J	213	BCR	C23-C24-C25-C30
23	K	301	BCR	C1-C6-C7-C8
23	M	4021	BCR	C23-C24-C25-C30
23	O	301	BCR	C23-C24-C25-C30
28	2	607	CHL	C2B-C3B-CAB-CBB
28	4	607	CHL	C2B-C3B-CAB-CBB
29	4	620	LUT	C1-C6-C7-C8
23	B	4004	BCR	C19-C20-C21-C22
25	J	301	LMG	O7-C8-C9-O8
20	B	1210	CLA	O1A-CGA-O2A-C1
23	I	120	BCR	C18-C19-C20-C21
20	A	1127	CLA	C2-C3-C5-C6
20	B	1202	CLA	C16-C17-C18-C19
20	A	1122	CLA	C6-C7-C8-C9
20	A	1130	CLA	C6-C7-C8-C9
21	A	2001	PQN	C21-C22-C23-C24
20	L	302	CLA	C2C-C3C-CAC-CBC
23	G	311	BCR	C22-C23-C24-C25
23	J	212	BCR	C14-C15-C16-C17
20	A	1136	CLA	C3-C5-C6-C7
20	B	1012	CLA	CBD-CGD-O2D-CED
20	1	609	CLA	C5-C6-C7-C8
20	A	1120	CLA	CBD-CGD-O2D-CED
24	2	630	LHG	O1-C1-C2-O2
20	I	121	CLA	CBA-CGA-O2A-C1
28	1	601	CHL	CBA-CGA-O2A-C1
20	2	613	CLA	C16-C17-C18-C20
19	A	1011	CL0	C8-C10-C11-C12
20	1	609	CLA	C8-C10-C11-C12
28	2	607	CHL	O1A-CGA-O2A-C1
23	A	4001	BCR	C20-C21-C22-C37
23	A	4002	BCR	C35-C13-C14-C15
23	B	4004	BCR	C11-C10-C9-C34
23	1	623	BCR	C20-C21-C22-C37
23	3	624	BCR	C11-C10-C9-C34
23	3	624	BCR	C16-C17-C18-C36
23	G	311	BCR	C35-C13-C14-C15
23	K	301	BCR	C20-C21-C22-C37
24	A	5001	LHG	O6-C4-C5-C6
20	I	121	CLA	O1D-CGD-O2D-CED
20	I	121	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
26	B	5001	LMT	O5'-C5'-C6'-O6'
26	G	402	LMT	O5B-C5B-C6B-O6B
19	A	1011	CL0	C12-C13-C15-C16
20	A	1122	CLA	C6-C7-C8-C10
20	A	1125	CLA	C11-C10-C8-C7
20	A	1128	CLA	C12-C13-C15-C16
20	A	1136	CLA	C11-C12-C13-C15
20	B	1023	CLA	C11-C10-C8-C7
28	2	601	CHL	C12-C13-C15-C16
20	4	602	CLA	C10-C11-C12-C13
23	3	624	BCR	C7-C8-C9-C10
23	3	624	BCR	C11-C12-C13-C14
20	2	614	CLA	O1A-CGA-O2A-C1
20	B	1210	CLA	O1D-CGD-O2D-CED
20	B	1205	CLA	C4-C3-C5-C6
20	B	1224	CLA	CAA-CBA-CGA-O2A
20	A	5005	CLA	O1A-CGA-O2A-C1
20	B	1206	CLA	O1A-CGA-O2A-C1
28	2	608	CHL	O1A-CGA-O2A-C1
24	4	630	LHG	O1-C1-C2-C3
28	2	602	CHL	C3-C5-C6-C7
27	B	5002	DGD	C3G-C2G-O2G-C1B
28	1	601	CHL	O2A-C1-C2-C3
20	B	1202	CLA	O1A-CGA-O2A-C1
20	B	1225	CLA	O1A-CGA-O2A-C1
23	A	4007	BCR	C19-C20-C21-C22
20	A	1118	CLA	C6-C7-C8-C9
20	A	1101	CLA	O1A-CGA-O2A-C1
20	A	1117	CLA	C15-C16-C17-C18
20	G	218	CLA	C5-C6-C7-C8
23	F	416	BCR	C12-C13-C14-C15
23	F	416	BCR	C20-C21-C22-C23
24	A	5001	LHG	O6-C4-C5-O7
24	B	5101	LHG	O6-C4-C5-O7
25	J	301	LMG	C7-C8-C9-O8
24	4	630	LHG	C7-C8-C9-C10
20	3	607	CLA	O1D-CGD-O2D-CED
20	B	1211	CLA	C3-C5-C6-C7
20	B	1238	CLA	C3-C5-C6-C7
25	A	5002	LMG	O7-C8-C9-O8
20	A	1119	CLA	C14-C13-C15-C16
20	A	1125	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
20	B	1205	CLA	C14-C13-C15-C16
20	B	1211	CLA	C6-C7-C8-C9
21	A	2001	PQN	C19-C18-C20-C21
20	B	1239	CLA	C4C-C3C-CAC-CBC
28	1	601	CHL	O1A-CGA-O2A-C1
20	A	8895	CLA	C8-C10-C11-C12
25	2	631	LMG	O6-C5-C6-O5
20	3	603	CLA	C5-C6-C7-C8
20	1	603	CLA	C5-C6-C7-C8
20	B	1023	CLA	C2A-CAA-CBA-CGA
27	B	5002	DGD	O6E-C5E-C6E-O5E
20	I	121	CLA	O1A-CGA-O2A-C1
28	2	601	CHL	C3-C5-C6-C7
20	4	609	CLA	C6-C7-C8-C9
20	A	1127	CLA	C3-C5-C6-C7
20	B	1205	CLA	C3-C5-C6-C7
20	B	1203	CLA	C15-C16-C17-C18
20	B	1226	CLA	C5-C6-C7-C8
20	A	1108	CLA	C1A-C2A-CAA-CBA
20	A	1110	CLA	C1A-C2A-CAA-CBA
20	A	1116	CLA	C4B-C3B-CAB-CBB
20	A	1131	CLA	C4B-C3B-CAB-CBB
20	B	1205	CLA	C4B-C3B-CAB-CBB
20	B	1216	CLA	C4B-C3B-CAB-CBB
20	B	1229	CLA	C4B-C3B-CAB-CBB
20	1	608	CLA	C1A-C2A-CAA-CBA
20	2	614	CLA	C1A-C2A-CAA-CBA
20	4	610	CLA	C1A-C2A-CAA-CBA
28	2	615	CHL	C4B-C3B-CAB-CBB
28	4	606	CHL	C4B-C3B-CAB-CBB
28	4	615	CHL	C4B-C3B-CAB-CBB
20	L	302	CLA	C4-C3-C5-C6
20	A	1104	CLA	C5-C6-C7-C8
23	K	301	BCR	C22-C23-C24-C25
20	B	1240	CLA	CAA-CBA-CGA-O2A
20	A	1118	CLA	C6-C7-C8-C10
20	A	1113	CLA	C2A-CAA-CBA-CGA
24	A	5001	LHG	C29-C30-C31-C32
20	A	1126	CLA	C3-C5-C6-C7
26	G	402	LMT	C4B-C5B-C6B-O6B
20	A	1022	CLA	C12-C13-C15-C16
20	A	1109	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
20	A	1119	CLA	C12-C13-C15-C16
20	B	1021	CLA	C11-C12-C13-C15
20	B	1225	CLA	C6-C7-C8-C10
20	B	1240	CLA	C11-C12-C13-C15
28	2	601	CHL	C6-C7-C8-C10
20	A	1104	CLA	C16-C17-C18-C19
20	2	613	CLA	C16-C17-C18-C19
20	1	609	CLA	CBA-CGA-O2A-C1
20	2	612	CLA	CBA-CGA-O2A-C1
20	A	1118	CLA	C4-C3-C5-C6
20	K	202	CLA	C3A-C2A-CAA-CBA
20	4	603	CLA	C6-C7-C8-C10
25	J	302	LMG	O9-C10-O7-C8
20	A	1104	CLA	C6-C7-C8-C9
20	A	1136	CLA	C11-C12-C13-C14
20	B	1023	CLA	C11-C10-C8-C9
20	B	1203	CLA	C14-C13-C15-C16
20	B	1225	CLA	C6-C7-C8-C9
20	I	121	CLA	C11-C10-C8-C9
28	3	608	CHL	O1A-CGA-O2A-C1
23	A	4011	BCR	C13-C14-C15-C16
23	B	4009	BCR	C9-C10-C11-C12
23	B	4017	BCR	C19-C20-C21-C22
20	A	1120	CLA	O1D-CGD-O2D-CED
20	B	1228	CLA	C1-C2-C3-C4
28	1	607	CHL	C1C-C2C-CMC-OMC
28	2	608	CHL	C1C-C2C-CMC-OMC
28	2	615	CHL	C1C-C2C-CMC-OMC
28	4	606	CHL	C1C-C2C-CMC-OMC
25	J	301	LMG	C30-C31-C32-C33
20	B	1204	CLA	C2C-C3C-CAC-CBC
21	B	2002	PQN	C25-C26-C27-C28
24	A	5001	LHG	C4-C5-C6-O8
24	3	630	LHG	C23-C24-C25-C26
20	A	1103	CLA	CAD-CBD-CGD-O2D
20	A	1111	CLA	CAD-CBD-CGD-O2D
20	A	1118	CLA	CAD-CBD-CGD-O2D
20	A	1125	CLA	CAD-CBD-CGD-O2D
20	A	1801	CLA	CAD-CBD-CGD-O2D
20	B	1210	CLA	CAD-CBD-CGD-O2D
20	2	614	CLA	CAD-CBD-CGD-O2D
20	3	606	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
20	3	614	CLA	CAD-CBD-CGD-O2D
20	4	603	CLA	CAD-CBD-CGD-O2D
20	L	301	CLA	CAD-CBD-CGD-O2D
28	1	601	CHL	CAD-CBD-CGD-O2D
26	G	402	LMT	O5'-C1'-O1'-C1
20	A	1118	CLA	C2C-C3C-CAC-CBC
20	I	121	CLA	C2C-C3C-CAC-CBC
20	2	613	CLA	C2A-CAA-CBA-CGA
20	3	607	CLA	C5-C6-C7-C8
20	1	609	CLA	O1A-CGA-O2A-C1
28	4	606	CHL	O1A-CGA-O2A-C1
24	4	630	LHG	C28-C29-C30-C31
20	A	1102	CLA	CHA-CBD-CGD-O1D
20	A	1103	CLA	CAD-CBD-CGD-O1D
20	A	1107	CLA	CHA-CBD-CGD-O1D
20	A	1111	CLA	CAD-CBD-CGD-O1D
20	A	1115	CLA	CHA-CBD-CGD-O1D
20	A	1115	CLA	CHA-CBD-CGD-O2D
20	A	1118	CLA	CAD-CBD-CGD-O1D
20	A	1122	CLA	CAD-CBD-CGD-O1D
20	A	1125	CLA	CAD-CBD-CGD-O1D
20	A	1131	CLA	CAD-CBD-CGD-O1D
20	A	1135	CLA	CHA-CBD-CGD-O1D
20	A	1135	CLA	CHA-CBD-CGD-O2D
20	A	5005	CLA	CHA-CBD-CGD-O1D
20	A	5005	CLA	CHA-CBD-CGD-O2D
20	A	8895	CLA	CAD-CBD-CGD-O1D
20	A	1801	CLA	CAD-CBD-CGD-O1D
20	B	1201	CLA	CHA-CBD-CGD-O1D
20	B	1201	CLA	CHA-CBD-CGD-O2D
20	B	1208	CLA	CHA-CBD-CGD-O1D
20	B	1210	CLA	CAD-CBD-CGD-O1D
20	B	1212	CLA	CHA-CBD-CGD-O1D
20	B	1212	CLA	CHA-CBD-CGD-O2D
20	B	1234	CLA	CHA-CBD-CGD-O1D
20	B	1234	CLA	CHA-CBD-CGD-O2D
20	B	1240	CLA	CAD-CBD-CGD-O1D
20	1	602	CLA	CHA-CBD-CGD-O2D
20	2	614	CLA	CAD-CBD-CGD-O1D
20	3	602	CLA	CHA-CBD-CGD-O1D
20	3	602	CLA	CHA-CBD-CGD-O2D
20	3	606	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
20	3	610	CLA	CHA-CBD-CGD-O1D
20	3	614	CLA	CAD-CBD-CGD-O1D
20	4	601	CLA	CAD-CBD-CGD-O1D
20	4	602	CLA	CHA-CBD-CGD-O1D
20	4	602	CLA	CHA-CBD-CGD-O2D
20	4	603	CLA	CAD-CBD-CGD-O1D
20	4	612	CLA	CHA-CBD-CGD-O1D
20	F	302	CLA	CHA-CBD-CGD-O1D
20	G	218	CLA	CHA-CBD-CGD-O1D
20	L	301	CLA	CAD-CBD-CGD-O1D
23	A	4001	BCR	C9-C10-C11-C12
23	A	4001	BCR	C15-C16-C17-C18
23	B	4006	BCR	C11-C10-C9-C34
23	B	4014	BCR	C19-C20-C21-C22
23	3	624	BCR	C15-C16-C17-C18
23	F	416	BCR	C13-C14-C15-C16
23	L	419	BCR	C15-C16-C17-C18
24	A	5003	LHG	C3-O3-P-O5
24	1	630	LHG	C3-O3-P-O4
24	2	630	LHG	C3-O3-P-O5
24	3	630	LHG	C4-O6-P-O5
24	4	630	LHG	C3-O3-P-O5
28	1	601	CHL	CAD-CBD-CGD-O1D
29	3	620	LUT	C29-C30-C31-C32
20	A	1137	CLA	C2C-C3C-CAC-CBC
23	A	4003	BCR	C14-C15-C16-C17
20	B	1224	CLA	C4-C3-C5-C6
20	A	1107	CLA	C2B-C3B-CAB-CBB
20	A	1122	CLA	C2B-C3B-CAB-CBB
20	A	1138	CLA	C2B-C3B-CAB-CBB
20	A	1139	CLA	C2B-C3B-CAB-CBB
20	B	1231	CLA	C2B-C3B-CAB-CBB
20	B	1232	CLA	C2B-C3B-CAB-CBB
20	B	1238	CLA	C2B-C3B-CAB-CBB
20	1	612	CLA	C2B-C3B-CAB-CBB
20	1	613	CLA	C2B-C3B-CAB-CBB
20	2	610	CLA	C2B-C3B-CAB-CBB
20	3	613	CLA	C2B-C3B-CAB-CBB
28	4	615	CHL	C2B-C3B-CAB-CBB
20	A	1022	CLA	C8-C10-C11-C12
23	A	4007	BCR	C36-C18-C19-C20
23	L	420	BCR	C7-C8-C9-C34

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Mol	Chain	Res	Type	Atoms
20	A	1116	CLA	CAA-CBA-CGA-O2A
21	B	2002	PQN	C13-C15-C16-C17
24	A	5001	LHG	C18-C19-C20-C21
24	A	5001	LHG	C34-C35-C36-C37
20	A	1132	CLA	C4C-C3C-CAC-CBC
29	2	620	LUT	C30-C31-C32-C33
29	3	621	LUT	C30-C31-C32-C33
29	4	623	LUT	C30-C31-C32-C33
20	B	1205	CLA	C2-C3-C5-C6
20	3	607	CLA	C10-C11-C12-C13
20	A	1124	CLA	C6-C7-C8-C9
20	A	1128	CLA	C14-C13-C15-C16
20	B	1210	CLA	C14-C13-C15-C16
20	B	1224	CLA	C11-C12-C13-C14
20	B	1237	CLA	C6-C7-C8-C9
20	A	1124	CLA	C6-C7-C8-C10
20	B	1237	CLA	C6-C7-C8-C10
20	B	1229	CLA	C2C-C3C-CAC-CBC
23	A	4002	BCR	C12-C13-C14-C15
28	2	615	CHL	O1A-CGA-O2A-C1
23	A	4002	BCR	C6-C7-C8-C9
25	J	301	LMG	O6-C1-O1-C7
20	4	601	CLA	C2A-CAA-CBA-CGA
20	B	1021	CLA	C16-C17-C18-C20
20	4	609	CLA	C6-C7-C8-C10
20	B	1023	CLA	C8-C10-C11-C12
20	4	609	CLA	C4C-C3C-CAC-CBC
20	2	613	CLA	C4-C3-C5-C6
20	A	1801	CLA	C2C-C3C-CAC-CBC
28	4	606	CHL	CAA-CBA-CGA-O2A
20	A	1124	CLA	C5-C6-C7-C8
29	1	621	LUT	C9-C10-C11-C12
29	4	623	LUT	C13-C14-C15-C35
24	2	630	LHG	C9-C10-C11-C12
20	2	612	CLA	C2C-C3C-CAC-CBC
24	3	630	LHG	C8-C7-O7-C5
20	A	1103	CLA	CAA-CBA-CGA-O2A
24	4	630	LHG	C11-C12-C13-C14
24	3	630	LHG	C9-C10-C11-C12
20	B	1214	CLA	C2-C1-O2A-CGA
20	A	1111	CLA	CAA-CBA-CGA-O2A
24	B	5101	LHG	C24-C25-C26-C27

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Mol	Chain	Res	Type	Atoms
20	A	1119	CLA	O1A-CGA-O2A-C1
20	B	1217	CLA	C2C-C3C-CAC-CBC
20	B	1202	CLA	CAA-CBA-CGA-O2A
25	J	301	LMG	C38-C39-C40-C41
28	1	607	CHL	CAA-CBA-CGA-O2A
25	A	5002	LMG	C8-C7-O1-C1
27	B	5002	DGD	C5D-C6D-O5D-C1E
20	A	1138	CLA	C2A-CAA-CBA-CGA
20	4	609	CLA	C2A-CAA-CBA-CGA
20	B	1012	CLA	O1D-CGD-O2D-CED
29	2	623	LUT	C29-C30-C31-C32
29	4	620	LUT	C29-C30-C31-C32
20	A	1110	CLA	C6-C7-C8-C10
20	4	610	CLA	C6-C7-C8-C10
20	B	1012	CLA	C2C-C3C-CAC-CBC
20	B	1224	CLA	C2-C3-C5-C6
28	2	601	CHL	C10-C11-C12-C13
28	1	607	CHL	O1A-CGA-O2A-C1
20	3	603	CLA	C4C-C3C-CAC-CBC
27	B	5002	DGD	C2A-C3A-C4A-C5A
20	B	1021	CLA	C16-C17-C18-C19
20	A	1117	CLA	C14-C13-C15-C16
20	B	1240	CLA	C11-C10-C8-C9
28	4	608	CHL	CBA-CGA-O2A-C1
20	A	1135	CLA	C4B-C3B-CAB-CBB
20	B	1203	CLA	C4B-C3B-CAB-CBB
20	B	1204	CLA	C4B-C3B-CAB-CBB
20	1	613	CLA	C4B-C3B-CAB-CBB
20	3	604	CLA	C4B-C3B-CAB-CBB
26	1	631	LMT	C2-C3-C4-C5
20	A	1104	CLA	C15-C16-C17-C18
20	A	1127	CLA	C13-C15-C16-C17
20	A	1130	CLA	C8-C10-C11-C12
20	A	1119	CLA	CBA-CGA-O2A-C1
20	B	1228	CLA	O2A-C1-C2-C3
29	2	623	LUT	C9-C10-C11-C12
28	2	601	CHL	C16-C17-C18-C19
20	A	1117	CLA	C12-C13-C15-C16
20	A	1132	CLA	C8-C10-C11-C12
20	A	1107	CLA	CAA-CBA-CGA-O2A
20	A	1128	CLA	O1D-CGD-O2D-CED
20	4	603	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
20	A	1122	CLA	C3A-C2A-CAA-CBA
20	B	1206	CLA	C3A-C2A-CAA-CBA
20	B	1232	CLA	C3A-C2A-CAA-CBA
20	B	1237	CLA	C3A-C2A-CAA-CBA
20	1	614	CLA	C3A-C2A-CAA-CBA
20	4	609	CLA	C3A-C2A-CAA-CBA
20	A	1115	CLA	O1D-CGD-O2D-CED
23	A	4011	BCR	C11-C10-C9-C34
23	A	4011	BCR	C16-C17-C18-C36
23	B	4005	BCR	C11-C10-C9-C34
23	F	416	BCR	C35-C13-C14-C15
23	I	120	BCR	C20-C21-C22-C37
29	2	620	LUT	C39-C29-C30-C31
29	2	620	LUT	C40-C33-C34-C35
29	3	621	LUT	C39-C29-C30-C31
29	4	621	LUT	C20-C13-C14-C15
29	4	623	LUT	C39-C29-C30-C31
20	3	606	CLA	O1A-CGA-O2A-C1
28	4	607	CHL	CBA-CGA-O2A-C1
20	A	1126	CLA	C2-C1-O2A-CGA
20	A	1117	CLA	C16-C17-C18-C19
25	J	301	LMG	C31-C32-C33-C34
20	B	1203	CLA	C13-C15-C16-C17
20	B	1225	CLA	C13-C15-C16-C17
20	B	1237	CLA	C8-C10-C11-C12
20	B	1211	CLA	C2C-C3C-CAC-CBC
27	B	5002	DGD	O6D-C5D-C6D-O5D
28	2	601	CHL	C4-C3-C5-C6
20	L	302	CLA	C2-C3-C5-C6
20	A	1013	CLA	C2A-CAA-CBA-CGA
20	A	1133	CLA	C2A-CAA-CBA-CGA
20	A	1103	CLA	C11-C12-C13-C14
20	A	1131	CLA	C6-C7-C8-C9
20	A	8895	CLA	C6-C7-C8-C9
20	B	1205	CLA	C6-C7-C8-C9
20	2	613	CLA	C11-C10-C8-C9
20	L	302	CLA	C11-C10-C8-C9
28	2	601	CHL	C16-C17-C18-C20
20	B	1220	CLA	CAA-CBA-CGA-O2A
20	H	200	CLA	CAA-CBA-CGA-O1A
26	G	401	LMT	C3-C4-C5-C6
26	B	5001	LMT	O1'-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
24	A	5003	LHG	O10-C23-O8-C6
20	A	1107	CLA	CAA-CBA-CGA-O1A
20	A	1104	CLA	C2A-CAA-CBA-CGA
20	3	610	CLA	C2A-CAA-CBA-CGA
20	A	1122	CLA	C1A-C2A-CAA-CBA
20	B	1238	CLA	C1A-C2A-CAA-CBA
20	1	602	CLA	C1A-C2A-CAA-CBA
20	1	614	CLA	C1A-C2A-CAA-CBA
23	B	4005	BCR	C11-C10-C9-C8
23	B	4006	BCR	C11-C10-C9-C8
23	B	4006	BCR	C20-C21-C22-C23
23	3	624	BCR	C12-C13-C14-C15
23	I	120	BCR	C20-C21-C22-C23
29	2	620	LUT	C28-C29-C30-C31
29	2	620	LUT	C32-C33-C34-C35
29	3	621	LUT	C28-C29-C30-C31
29	4	621	LUT	C12-C13-C14-C15
29	4	623	LUT	C28-C29-C30-C31
20	A	1103	CLA	C4C-C3C-CAC-CBC
28	2	606	CHL	CAA-CBA-CGA-O1A
20	A	1101	CLA	C2B-C3B-CAB-CBB
20	A	1111	CLA	C2B-C3B-CAB-CBB
20	A	1112	CLA	C2B-C3B-CAB-CBB
20	A	1121	CLA	C2B-C3B-CAB-CBB
20	A	1140	CLA	C2B-C3B-CAB-CBB
20	B	1236	CLA	C2B-C3B-CAB-CBB
20	1	614	CLA	C2B-C3B-CAB-CBB
20	3	611	CLA	C2B-C3B-CAB-CBB
20	4	612	CLA	C2B-C3B-CAB-CBB
20	G	218	CLA	C2B-C3B-CAB-CBB
20	G	201	CLA	C2B-C3B-CAB-CBB
20	K	204	CLA	C2B-C3B-CAB-CBB
23	A	4001	BCR	C5-C6-C7-C8
23	A	4001	BCR	C23-C24-C25-C26
23	A	4001	BCR	C23-C24-C25-C30
23	A	4002	BCR	C5-C6-C7-C8
23	A	4002	BCR	C23-C24-C25-C26
23	A	4011	BCR	C23-C24-C25-C26
23	B	4004	BCR	C5-C6-C7-C8
23	B	4004	BCR	C23-C24-C25-C30
23	B	4005	BCR	C5-C6-C7-C8
23	B	4009	BCR	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
23	B	4010	BCR	C1-C6-C7-C8
23	B	4017	BCR	C5-C6-C7-C8
23	B	4014	BCR	C1-C6-C7-C8
23	B	4014	BCR	C5-C6-C7-C8
23	3	624	BCR	C5-C6-C7-C8
23	3	624	BCR	C23-C24-C25-C26
23	F	416	BCR	C5-C6-C7-C8
23	F	416	BCR	C23-C24-C25-C26
23	F	416	BCR	C23-C24-C25-C30
23	G	311	BCR	C23-C24-C25-C26
23	I	118	BCR	C23-C24-C25-C30
23	J	212	BCR	C5-C6-C7-C8
23	J	213	BCR	C5-C6-C7-C8
23	J	213	BCR	C23-C24-C25-C26
23	K	301	BCR	C5-C6-C7-C8
23	K	301	BCR	C23-C24-C25-C26
23	K	301	BCR	C23-C24-C25-C30
23	L	420	BCR	C23-C24-C25-C26
23	M	4021	BCR	C23-C24-C25-C26
23	O	301	BCR	C23-C24-C25-C26
28	2	615	CHL	C2B-C3B-CAB-CBB
28	4	606	CHL	C2B-C3B-CAB-CBB
29	4	620	LUT	C5-C6-C7-C8
20	4	611	CLA	CBA-CGA-O2A-C1
24	4	630	LHG	C10-C11-C12-C13
20	B	1235	CLA	C3-C5-C6-C7
20	B	1220	CLA	CAA-CBA-CGA-O1A
28	4	608	CHL	O1A-CGA-O2A-C1
28	2	601	CHL	C2-C3-C5-C6
27	B	5002	DGD	C4D-C5D-C6D-O5D
20	B	1210	CLA	C6-C7-C8-C10
20	B	1224	CLA	C6-C7-C8-C10
20	2	613	CLA	C11-C10-C8-C7
20	3	607	CLA	C6-C7-C8-C10
21	A	2001	PQN	C17-C18-C20-C21
20	A	1115	CLA	CBD-CGD-O2D-CED
20	B	1206	CLA	C2-C1-O2A-CGA
20	A	1022	CLA	C2A-CAA-CBA-CGA
20	A	1117	CLA	C2A-CAA-CBA-CGA
20	B	1205	CLA	C2A-CAA-CBA-CGA
28	2	606	CHL	CAA-CBA-CGA-O2A
20	A	1128	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
20	A	1110	CLA	C6-C7-C8-C9
20	4	610	CLA	C6-C7-C8-C9
23	A	4007	BCR	C7-C8-C9-C34
20	1	606	CLA	C4C-C3C-CAC-CBC
20	A	1104	CLA	C4-C3-C5-C6
20	A	1128	CLA	C4-C3-C5-C6
28	2	611	CHL	C4-C3-C5-C6
20	2	613	CLA	C2-C3-C5-C6
20	A	8895	CLA	C2-C1-O2A-CGA
20	H	200	CLA	CAA-CBA-CGA-O2A
26	G	401	LMT	O5B-C1B-O1B-C4'
25	J	302	LMG	C10-C11-C12-C13
20	I	121	CLA	C3-C5-C6-C7
20	A	1127	CLA	C6-C7-C8-C9
20	4	611	CLA	O1A-CGA-O2A-C1
20	L	301	CLA	C4C-C3C-CAC-CBC
29	4	623	LUT	C29-C30-C31-C32
27	B	5002	DGD	C8A-C9A-CAA-CBA
24	A	5001	LHG	C13-C14-C15-C16
23	B	4006	BCR	C22-C23-C24-C25
20	A	1118	CLA	C2-C3-C5-C6
20	A	1133	CLA	CAA-CBA-CGA-O2A
20	1	613	CLA	CAA-CBA-CGA-O2A
20	B	1217	CLA	CAA-CBA-CGA-O2A
20	3	612	CLA	CAA-CBA-CGA-O2A
20	A	1101	CLA	C2A-CAA-CBA-CGA
20	B	1204	CLA	C2A-CAA-CBA-CGA
20	3	609	CLA	CAA-CBA-CGA-O2A
20	K	204	CLA	CAA-CBA-CGA-O2A
28	2	602	CHL	C4-C3-C5-C6
20	A	1114	CLA	C4C-C3C-CAC-CBC
20	B	1021	CLA	CAA-CBA-CGA-O2A
20	3	606	CLA	CAA-CBA-CGA-O2A
28	2	608	CHL	CAA-CBA-CGA-O2A
20	A	1136	CLA	C15-C16-C17-C18
20	A	1102	CLA	C4B-C3B-CAB-CBB
20	A	1125	CLA	C4C-C3C-CAC-CBC
20	B	1230	CLA	C4B-C3B-CAB-CBB
20	B	1240	CLA	C4B-C3B-CAB-CBB
20	4	601	CLA	C4B-C3B-CAB-CBB
20	4	603	CLA	C4B-C3B-CAB-CBB
20	4	601	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
20	A	1134	CLA	CAA-CBA-CGA-O2A
20	2	612	CLA	O1A-CGA-O2A-C1
25	2	631	LMG	O10-C28-O8-C9
28	2	602	CHL	C6-C7-C8-C9
23	B	4006	BCR	C20-C21-C22-C37
23	B	4017	BCR	C11-C10-C9-C34
23	3	624	BCR	C35-C13-C14-C15
23	F	416	BCR	C11-C10-C9-C34
20	A	1134	CLA	CAA-CBA-CGA-O1A
20	B	1225	CLA	C4-C3-C5-C6
19	A	1011	CL0	CAA-CBA-CGA-O2A
28	2	611	CHL	C2-C3-C5-C6
26	A	5004	LMT	C5'-C4'-O1B-C1B
21	A	2001	PQN	C25-C26-C27-C28
20	A	1137	CLA	CAA-CBA-CGA-O2A
25	A	5002	LMG	C31-C32-C33-C34
23	A	4001	BCR	C13-C14-C15-C16
20	A	1022	CLA	C14-C13-C15-C16
20	A	1136	CLA	C11-C10-C8-C9
20	B	1204	CLA	C6-C7-C8-C9
20	B	1238	CLA	C11-C10-C8-C9
20	B	1231	CLA	CAA-CBA-CGA-O2A
20	B	1201	CLA	C2-C1-O2A-CGA
24	A	5001	LHG	C11-C12-C13-C14
24	A	5001	LHG	C30-C31-C32-C33
20	A	1118	CLA	C3A-C2A-CAA-CBA
20	A	1126	CLA	C3A-C2A-CAA-CBA
20	3	614	CLA	C3A-C2A-CAA-CBA
20	3	612	CLA	CAA-CBA-CGA-O1A
25	J	301	LMG	O10-C28-O8-C9
24	1	630	LHG	C13-C14-C15-C16
26	4	631	LMT	O5'-C5'-C6'-O6'
20	J	102	CLA	CAA-CBA-CGA-O2A
20	B	1221	CLA	C2A-CAA-CBA-CGA
20	B	1217	CLA	CAA-CBA-CGA-O1A
20	J	102	CLA	CAA-CBA-CGA-O1A
20	K	204	CLA	CAA-CBA-CGA-O1A
23	A	4011	BCR	C11-C10-C9-C8
23	A	4011	BCR	C16-C17-C18-C19
26	A	5004	LMT	O1'-C1-C2-C3
20	A	1133	CLA	CAA-CBA-CGA-O1A
20	B	1231	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
24	2	630	LHG	O9-C7-O7-C5
23	A	4001	BCR	C6-C7-C8-C9
23	M	4021	BCR	C22-C23-C24-C25
20	B	1023	CLA	C5-C6-C7-C8
24	4	630	LHG	C25-C26-C27-C28
20	B	1213	CLA	C5-C6-C7-C8
20	A	1111	CLA	C3-C5-C6-C7
20	B	1211	CLA	O1A-CGA-O2A-C1
20	A	1125	CLA	C5-C6-C7-C8
20	B	1210	CLA	C3-C5-C6-C7
20	A	1109	CLA	C6-C7-C8-C9
20	B	1021	CLA	C11-C12-C13-C14
20	B	1202	CLA	C11-C10-C8-C9
20	B	1240	CLA	C11-C12-C13-C14
28	2	601	CHL	C14-C13-C15-C16
20	A	1117	CLA	C16-C17-C18-C20
23	A	4008	BCR	C11-C12-C13-C14
23	I	118	BCR	C17-C18-C19-C20
24	1	630	LHG	C27-C28-C29-C30
20	A	1137	CLA	CAA-CBA-CGA-O1A
20	A	1103	CLA	C11-C12-C13-C15
20	A	1117	CLA	C11-C10-C8-C7
20	A	1126	CLA	C6-C7-C8-C10
20	A	1127	CLA	C6-C7-C8-C10
20	B	1202	CLA	C11-C10-C8-C7
20	B	1203	CLA	C11-C12-C13-C15
20	B	1223	CLA	C12-C13-C15-C16
20	B	1238	CLA	C11-C10-C8-C7
20	1	609	CLA	C6-C7-C8-C10
20	A	1102	CLA	C2B-C3B-CAB-CBB
20	A	1104	CLA	C2B-C3B-CAB-CBB
20	A	1106	CLA	C2B-C3B-CAB-CBB
20	A	1109	CLA	C2B-C3B-CAB-CBB
20	A	1113	CLA	C2B-C3B-CAB-CBB
20	B	1012	CLA	C2B-C3B-CAB-CBB
20	B	1230	CLA	C2B-C3B-CAB-CBB
20	B	1235	CLA	C2B-C3B-CAB-CBB
20	2	612	CLA	C2B-C3B-CAB-CBB
20	2	613	CLA	C2B-C3B-CAB-CBB
20	3	602	CLA	C2B-C3B-CAB-CBB
20	3	610	CLA	C2B-C3B-CAB-CBB
20	3	612	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
20	4	610	CLA	C2B-C3B-CAB-CBB
23	A	4011	BCR	C5-C6-C7-C8
23	B	4004	BCR	C23-C24-C25-C26
23	B	4005	BCR	C23-C24-C25-C26
23	B	4005	BCR	C23-C24-C25-C30
23	B	4006	BCR	C23-C24-C25-C26
23	B	4014	BCR	C23-C24-C25-C26
23	B	4014	BCR	C23-C24-C25-C30
23	G	311	BCR	C1-C6-C7-C8
23	G	311	BCR	C5-C6-C7-C8
23	I	118	BCR	C5-C6-C7-C8
23	I	118	BCR	C23-C24-C25-C26
25	J	302	LMG	O8-C28-C29-C30
20	3	603	CLA	C2-C1-O2A-CGA
20	I	121	CLA	CAA-CBA-CGA-O2A
24	3	630	LHG	O7-C7-C8-C9
20	B	1209	CLA	C2A-CAA-CBA-CGA
27	B	5002	DGD	C6A-C7A-C8A-C9A
20	4	612	CLA	CAA-CBA-CGA-O2A
20	1	609	CLA	C3-C5-C6-C7
20	B	1204	CLA	C12-C13-C15-C16
20	B	1210	CLA	CAA-CBA-CGA-O2A
28	1	601	CHL	C3-C5-C6-C7
20	A	1109	CLA	CAA-CBA-CGA-O2A
20	1	614	CLA	CAA-CBA-CGA-O2A
20	B	1238	CLA	C11-C12-C13-C14
29	1	620	LUT	C31-C32-C33-C40
20	A	1121	CLA	CAA-CBA-CGA-O2A
19	A	1011	CL0	C4B-C3B-CAB-CBB
20	B	1206	CLA	C1A-C2A-CAA-CBA
20	B	1232	CLA	C1A-C2A-CAA-CBA
20	B	1240	CLA	C1A-C2A-CAA-CBA
20	2	604	CLA	C4B-C3B-CAB-CBB
20	2	609	CLA	C4B-C3B-CAB-CBB
20	4	614	CLA	C1A-C2A-CAA-CBA
28	4	606	CHL	C1A-C2A-CAA-CBA
20	A	1114	CLA	CAA-CBA-CGA-O2A
26	1	631	LMT	O5'-C1'-O1'-C1
20	1	612	CLA	CAA-CBA-CGA-O2A
20	2	603	CLA	CAA-CBA-CGA-O2A
28	2	601	CHL	CAA-CBA-CGA-O2A
20	L	303	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
23	A	4007	BCR	C17-C18-C19-C20
23	L	420	BCR	C7-C8-C9-C10
23	M	4021	BCR	C19-C20-C21-C22
20	B	1237	CLA	C16-C17-C18-C20
24	4	630	LHG	C27-C28-C29-C30
20	A	8895	CLA	C15-C16-C17-C18
20	A	1116	CLA	CAA-CBA-CGA-O1A
20	B	1237	CLA	C2C-C3C-CAC-CBC
20	A	1125	CLA	C2-C1-O2A-CGA
20	B	1210	CLA	C2-C1-O2A-CGA
28	1	601	CHL	C2-C1-O2A-CGA
28	2	602	CHL	C2-C1-O2A-CGA
28	2	611	CHL	C2-C1-O2A-CGA
26	4	631	LMT	C6-C7-C8-C9
20	I	121	CLA	O2A-C1-C2-C3
20	A	1108	CLA	CAA-CBA-CGA-O2A
20	B	1213	CLA	C2A-CAA-CBA-CGA
20	B	1235	CLA	C2A-CAA-CBA-CGA
24	3	630	LHG	O9-C7-C8-C9
20	B	1227	CLA	CAA-CBA-CGA-O2A
20	A	1134	CLA	C3A-C2A-CAA-CBA
20	B	1228	CLA	C3A-C2A-CAA-CBA
20	B	1236	CLA	C3A-C2A-CAA-CBA
28	4	606	CHL	C3A-C2A-CAA-CBA
20	B	1238	CLA	C16-C17-C18-C20
20	1	606	CLA	CAA-CBA-CGA-O2A
20	3	602	CLA	C10-C11-C12-C13
20	B	1240	CLA	CAA-CBA-CGA-O1A
20	B	1211	CLA	CBA-CGA-O2A-C1
28	2	602	CHL	CAA-CBA-CGA-O2A
20	I	121	CLA	CAA-CBA-CGA-O1A
20	3	602	CLA	C2A-CAA-CBA-CGA
20	4	610	CLA	CBA-CGA-O2A-C1
20	3	607	CLA	C6-C7-C8-C9
21	B	2002	PQN	C21-C22-C23-C24
20	2	603	CLA	CAA-CBA-CGA-O1A
20	A	1102	CLA	CAA-CBA-CGA-O2A
20	B	1211	CLA	C4-C3-C5-C6
25	A	5002	LMG	O10-C28-C29-C30
20	G	202	CLA	CAA-CBA-CGA-O2A
20	A	1111	CLA	O1A-CGA-O2A-C1
20	1	614	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
25	J	302	LMG	C8-C7-O1-C1
20	3	610	CLA	O1A-CGA-O2A-C1
20	A	1121	CLA	CAA-CBA-CGA-O1A
28	2	601	CHL	CAA-CBA-CGA-O1A
20	A	1107	CLA	C4C-C3C-CAC-CBC
20	B	1230	CLA	CAA-CBA-CGA-O2A
20	A	1104	CLA	C2-C3-C5-C6
20	B	1225	CLA	C2-C3-C5-C6
20	A	1108	CLA	CAA-CBA-CGA-O1A
20	A	1114	CLA	CAA-CBA-CGA-O1A
28	4	607	CHL	O1A-CGA-O2A-C1
20	4	612	CLA	CAA-CBA-CGA-O1A
24	B	5101	LHG	O9-C7-C8-C9
20	2	604	CLA	C4C-C3C-CAC-CBC
20	A	1116	CLA	CAD-CBD-CGD-O2D
20	A	1124	CLA	CAD-CBD-CGD-O2D
20	B	1215	CLA	CAD-CBD-CGD-O2D
20	1	606	CLA	CAD-CBD-CGD-O2D
20	4	601	CLA	CAD-CBD-CGD-O2D
20	A	1117	CLA	C10-C11-C12-C13
28	4	608	CHL	C2-C1-O2A-CGA
20	L	303	CLA	CAA-CBA-CGA-O2A
20	A	1109	CLA	CAA-CBA-CGA-O1A
20	3	607	CLA	CAA-CBA-CGA-O2A
20	A	1102	CLA	CAA-CBA-CGA-O1A
20	A	1120	CLA	CAA-CBA-CGA-O2A
20	1	606	CLA	CAA-CBA-CGA-O1A
20	B	1204	CLA	C6-C7-C8-C10
20	A	1118	CLA	CAA-CBA-CGA-O2A
20	A	1125	CLA	CAA-CBA-CGA-O2A
20	A	1132	CLA	CAA-CBA-CGA-O2A
20	B	1226	CLA	CAA-CBA-CGA-O2A
24	B	5101	LHG	O7-C7-C8-C9
20	B	1230	CLA	CAA-CBA-CGA-O1A
20	B	1210	CLA	CAA-CBA-CGA-O1A
20	1	612	CLA	CAA-CBA-CGA-O1A
24	1	630	LHG	O10-C23-C24-C25

There are no ring outliers.

163 monomers are involved in 359 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	B	1224	CLA	4	0
20	B	1226	CLA	3	0
20	3	610	CLA	4	0
20	A	1102	CLA	4	0
23	B	4017	BCR	7	0
23	F	416	BCR	2	0
20	A	1107	CLA	1	0
23	B	4006	BCR	4	0
20	A	1105	CLA	1	0
20	B	1209	CLA	2	0
23	3	624	BCR	3	0
20	B	1220	CLA	2	0
20	2	610	CLA	2	0
29	4	623	LUT	1	0
23	B	4010	BCR	5	0
24	A	5001	LHG	3	0
20	A	1022	CLA	8	0
20	A	1130	CLA	3	0
20	B	1212	CLA	1	0
20	B	1237	CLA	8	0
20	A	1136	CLA	3	0
20	A	1116	CLA	4	0
23	A	4008	BCR	2	0
20	B	1227	CLA	2	0
29	4	621	LUT	2	0
20	B	1228	CLA	3	0
20	B	1205	CLA	5	0
29	3	621	LUT	2	0
26	4	631	LMT	3	0
26	1	631	LMT	2	0
29	1	620	LUT	3	0
20	A	5005	CLA	4	0
20	3	607	CLA	1	0
20	3	612	CLA	1	0
23	B	4005	BCR	3	0
20	B	1012	CLA	6	0
20	B	1230	CLA	3	0
20	A	1108	CLA	3	0
23	A	4007	BCR	2	0
20	A	1119	CLA	2	0
28	2	608	CHL	3	0
20	A	1135	CLA	2	0
20	1	602	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	B	1240	CLA	2	0
20	B	1202	CLA	6	0
20	1	603	CLA	4	0
25	J	302	LMG	1	0
20	B	1023	CLA	5	0
28	4	608	CHL	1	0
20	A	1101	CLA	2	0
20	A	1132	CLA	4	0
20	A	1134	CLA	2	0
20	A	1140	CLA	4	0
28	1	607	CHL	1	0
23	A	4001	BCR	1	0
23	I	120	BCR	5	0
24	A	5003	LHG	1	0
23	L	420	BCR	4	0
20	B	1213	CLA	3	0
23	G	311	BCR	3	0
29	2	621	LUT	2	0
20	I	121	CLA	7	0
28	2	601	CHL	7	0
23	L	419	BCR	3	0
23	B	4009	BCR	2	0
20	A	1128	CLA	5	0
20	3	613	CLA	2	0
20	A	1013	CLA	2	0
29	2	623	LUT	1	0
20	A	1118	CLA	4	0
20	A	1110	CLA	2	0
20	B	1232	CLA	1	0
23	J	213	BCR	3	0
29	1	621	LUT	5	0
20	K	204	CLA	2	0
20	A	1127	CLA	6	0
23	K	301	BCR	1	0
20	A	1114	CLA	2	0
23	A	4011	BCR	1	0
20	A	1109	CLA	2	0
23	J	212	BCR	1	0
24	3	630	LHG	1	0
23	B	4004	BCR	1	0
20	1	606	CLA	1	0
20	A	1138	CLA	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	A	5002	LMG	2	0
20	A	1137	CLA	3	0
21	A	2001	PQN	2	0
21	B	2002	PQN	5	0
29	2	620	LUT	6	0
20	A	1111	CLA	6	0
20	B	1223	CLA	6	0
20	B	1236	CLA	1	0
20	1	609	CLA	3	0
20	3	617	CLA	1	0
20	3	609	CLA	2	0
27	B	5002	DGD	5	0
20	L	302	CLA	5	0
24	2	630	LHG	2	0
20	B	1225	CLA	5	0
20	B	1221	CLA	5	0
24	4	630	LHG	2	0
20	A	1126	CLA	5	0
20	B	1201	CLA	2	0
24	1	630	LHG	1	0
20	A	1131	CLA	2	0
20	A	8895	CLA	4	0
28	3	608	CHL	2	0
25	J	301	LMG	3	0
20	A	1125	CLA	2	0
20	4	610	CLA	3	0
20	2	613	CLA	1	0
26	A	5004	LMT	1	0
23	I	118	BCR	1	0
20	H	200	CLA	2	0
20	B	1203	CLA	4	0
28	1	601	CHL	1	0
20	A	1139	CLA	2	0
20	B	1208	CLA	4	0
20	B	1217	CLA	4	0
20	F	301	CLA	4	0
23	M	4021	BCR	5	0
26	G	401	LMT	3	0
20	A	1115	CLA	1	0
20	B	1231	CLA	1	0
20	L	303	CLA	4	0
20	A	1801	CLA	1	0

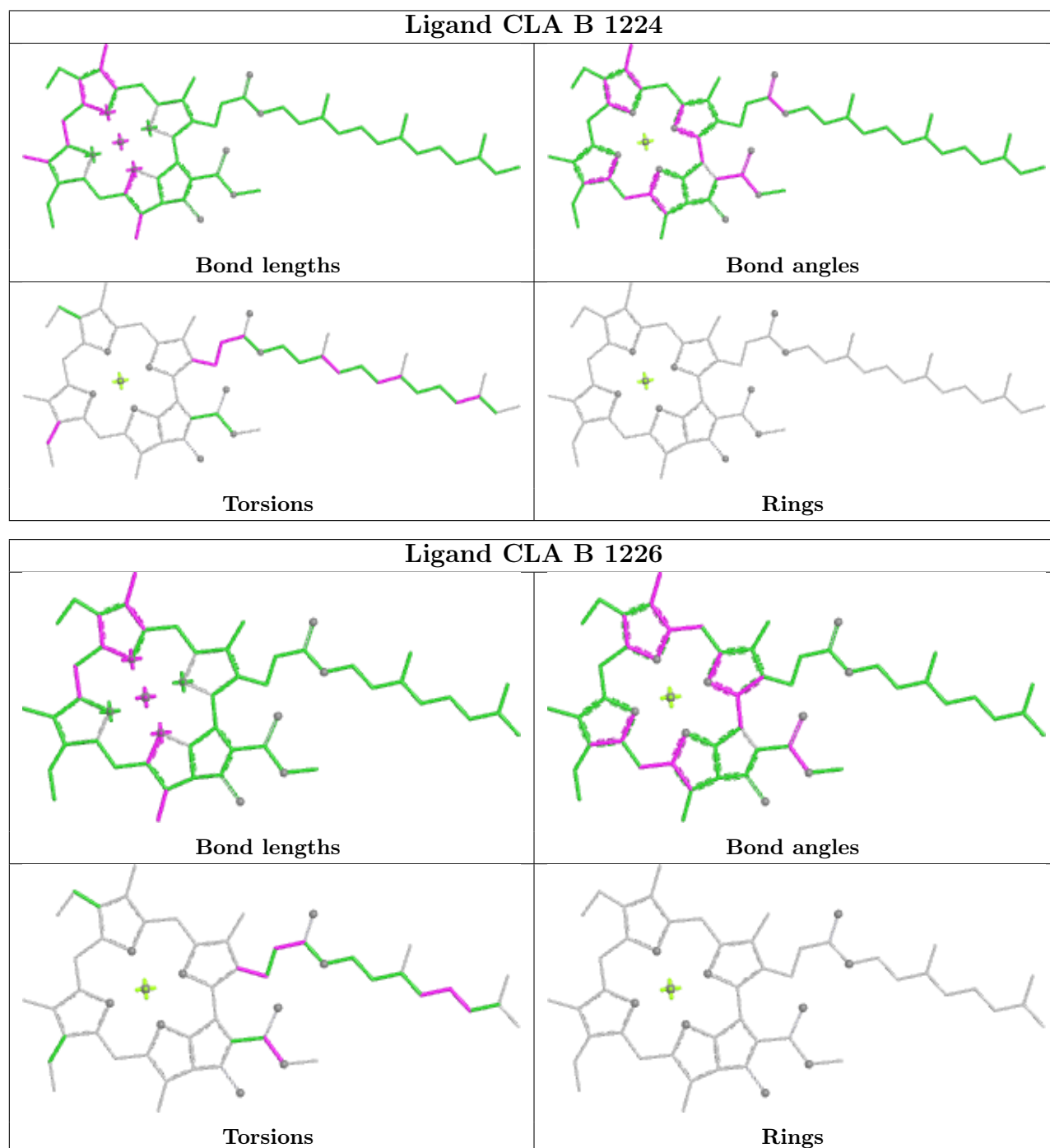
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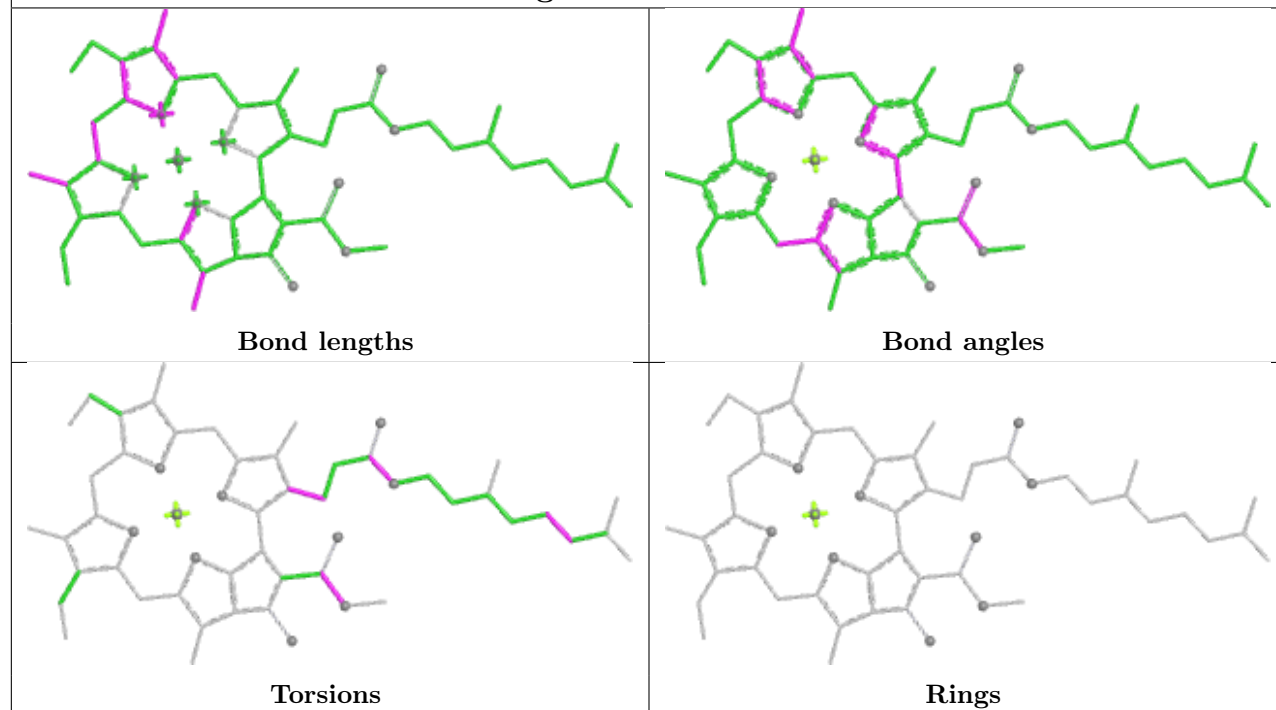
Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	B	1239	CLA	2	0
20	4	602	CLA	2	0
20	B	1206	CLA	4	0
20	3	602	CLA	3	0
20	A	1133	CLA	2	0
20	4	601	CLA	1	0
20	B	1238	CLA	7	0
20	K	201	CLA	1	0
20	3	604	CLA	1	0
28	2	602	CHL	2	0
20	B	1210	CLA	6	0
29	3	620	LUT	7	0
20	A	1103	CLA	4	0
20	A	1124	CLA	3	0
20	B	1219	CLA	1	0
23	B	4014	BCR	7	0
20	A	1104	CLA	5	0
20	4	603	CLA	4	0
20	B	1235	CLA	2	0
20	A	1117	CLA	7	0
20	B	1204	CLA	5	0
20	A	1122	CLA	3	0
20	B	1229	CLA	1	0
20	2	609	CLA	1	0
23	3	623	BCR	1	0
20	A	1113	CLA	1	0
20	A	1120	CLA	1	0
20	B	1021	CLA	2	0
20	L	301	CLA	1	0
20	B	1215	CLA	1	0
23	A	4003	BCR	2	0
19	A	1011	CL0	5	0
20	A	1106	CLA	3	0
20	B	1216	CLA	2	0
20	B	1214	CLA	3	0
29	4	620	LUT	4	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

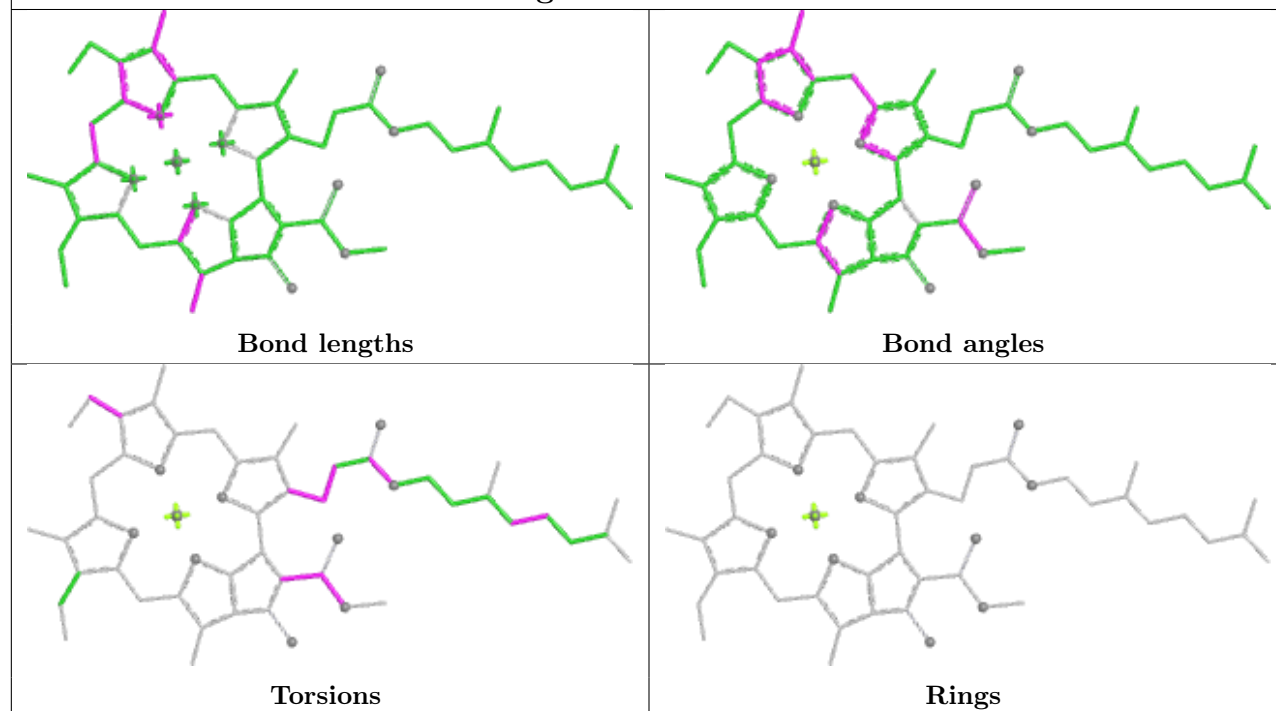
highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified 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.

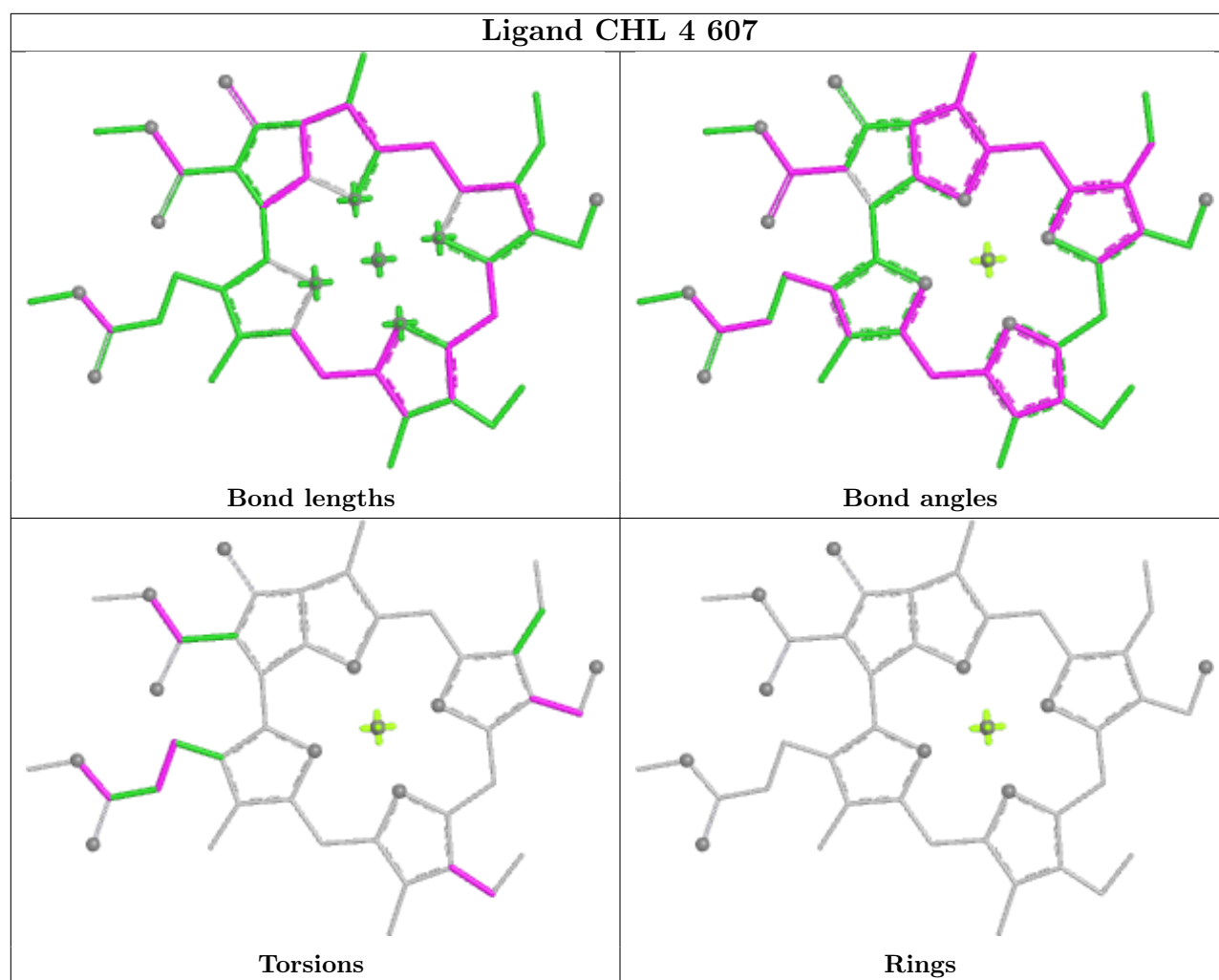


Ligand CLA 4 611

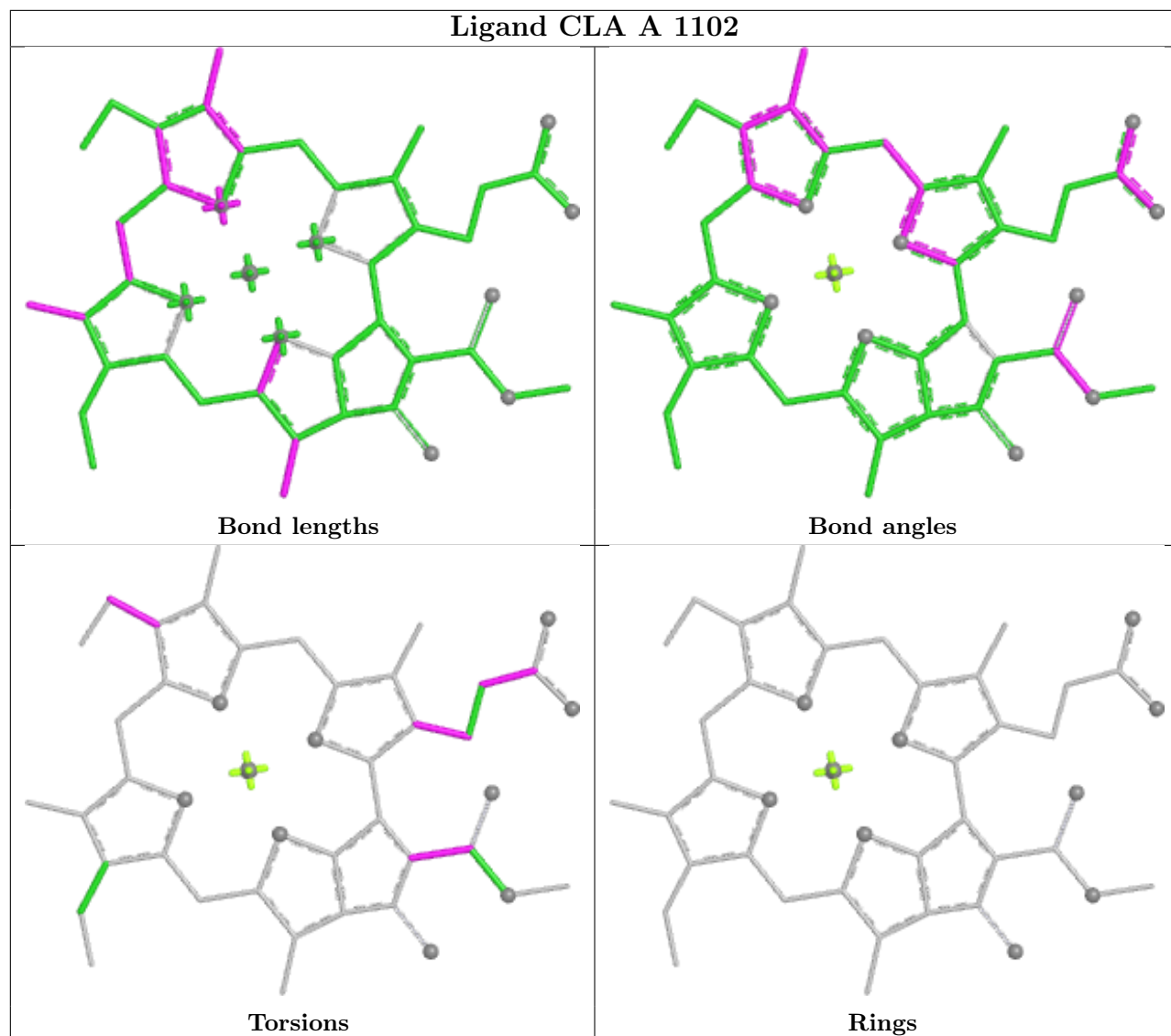


Ligand CLA 3 610

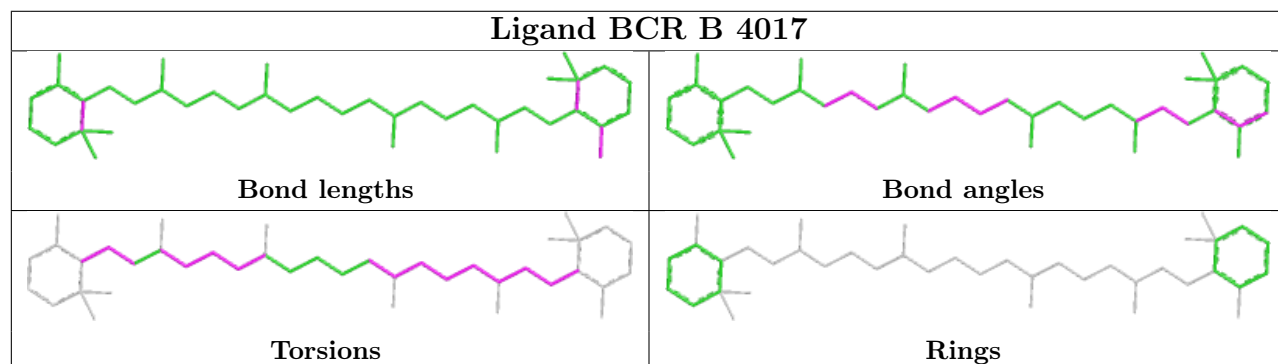


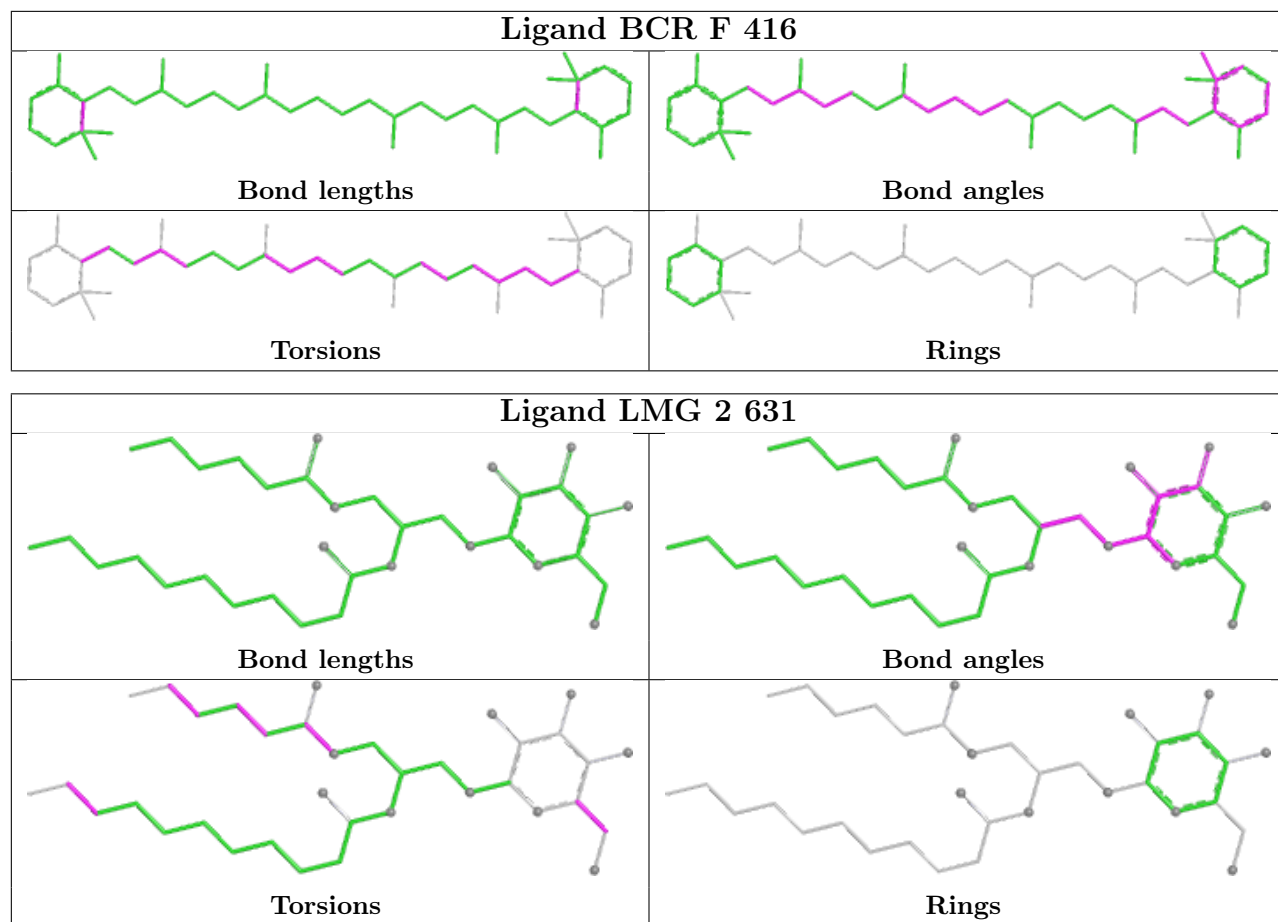


Ligand CLA A 1102

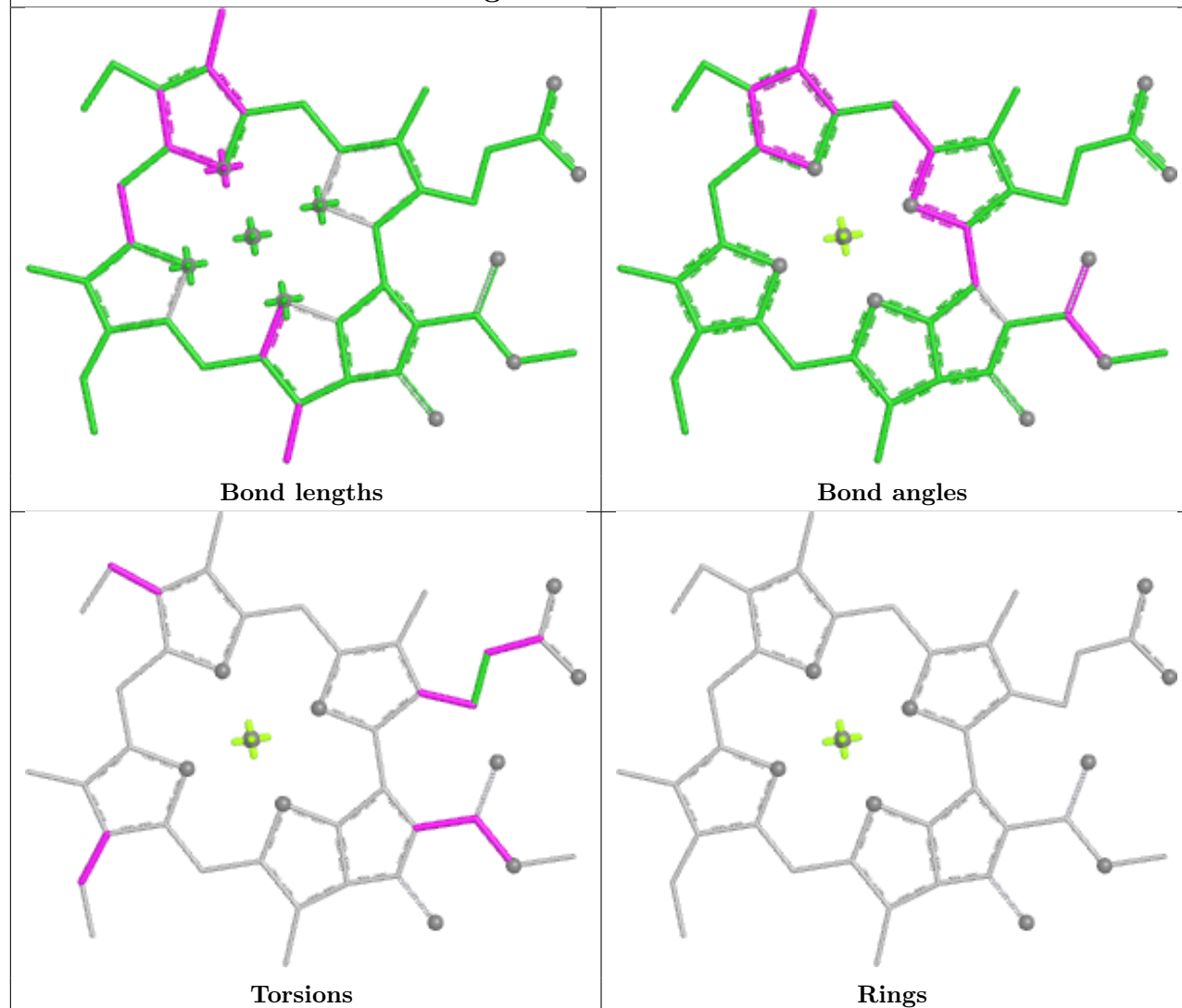


Ligand BCR B 4017

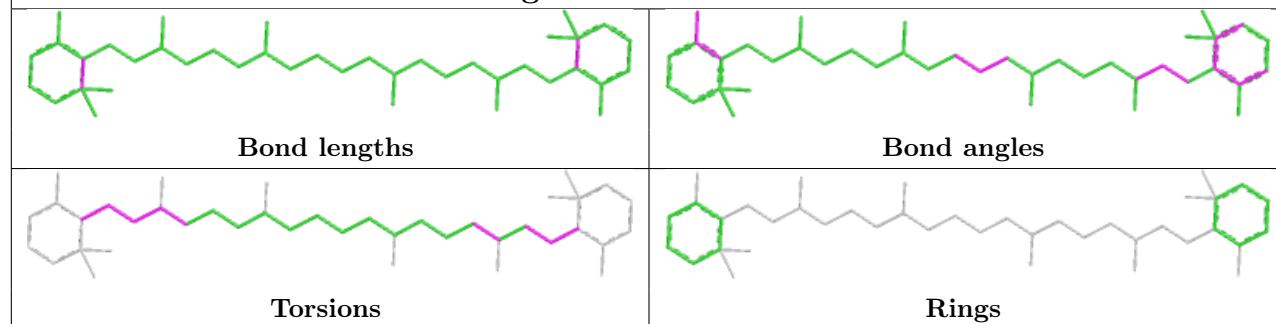


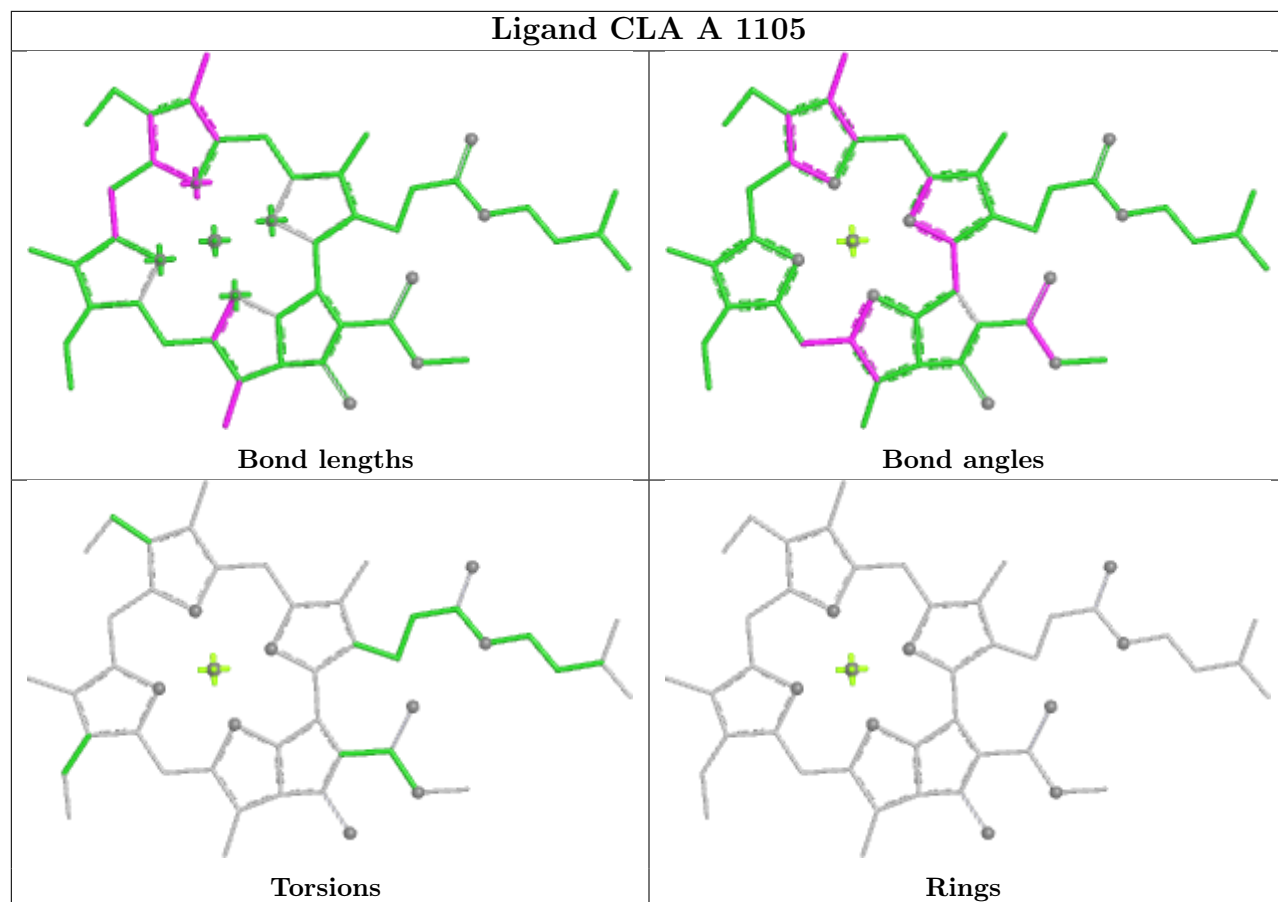


Ligand CLA A 1107

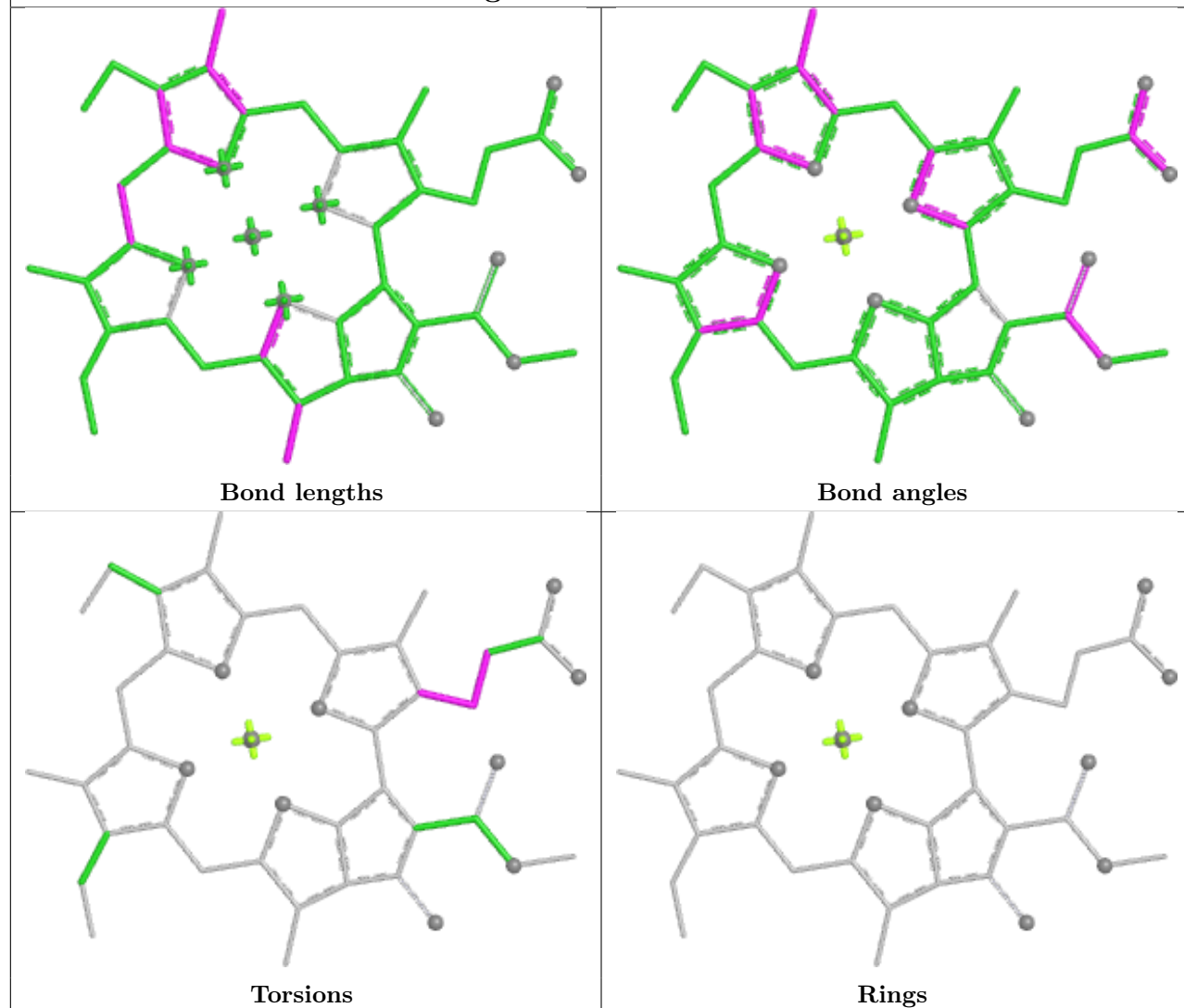


Ligand BCR B 4006

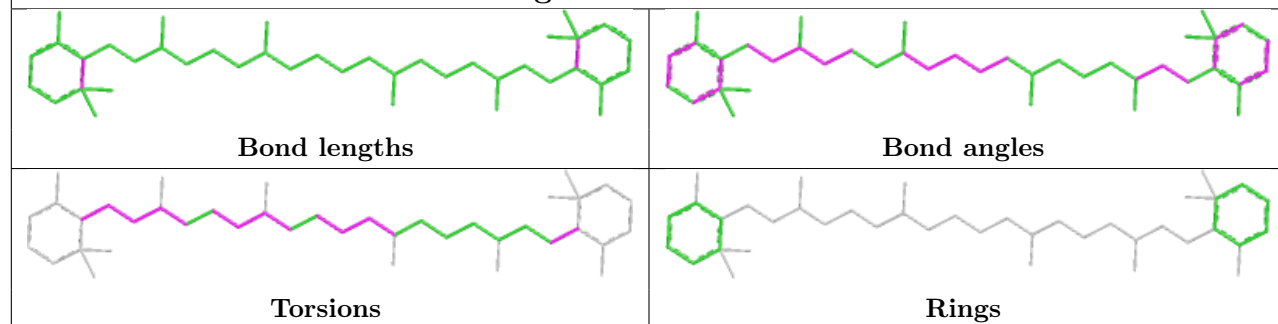




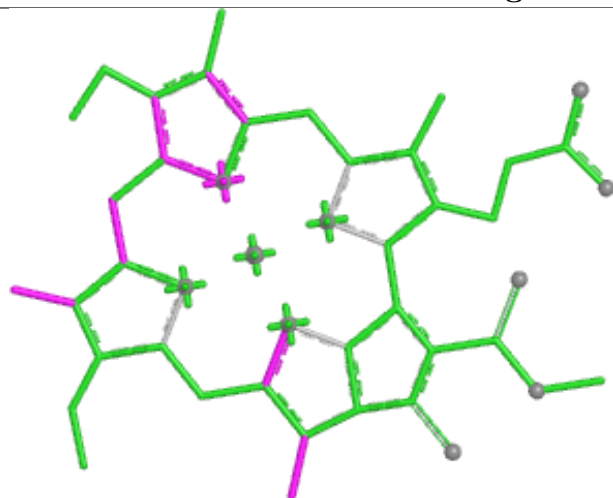
Ligand CLA B 1209



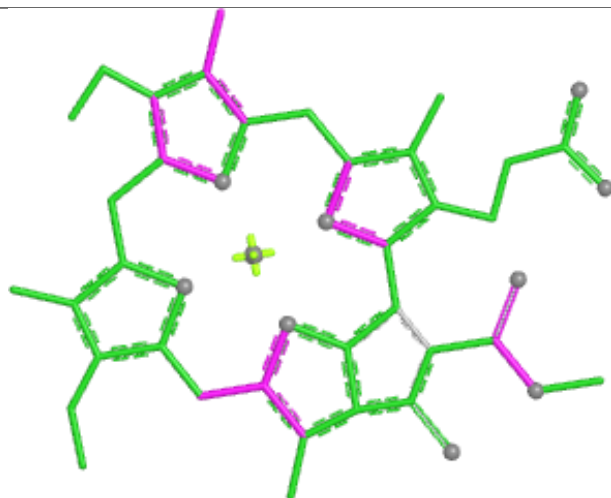
Ligand BCR 3 624



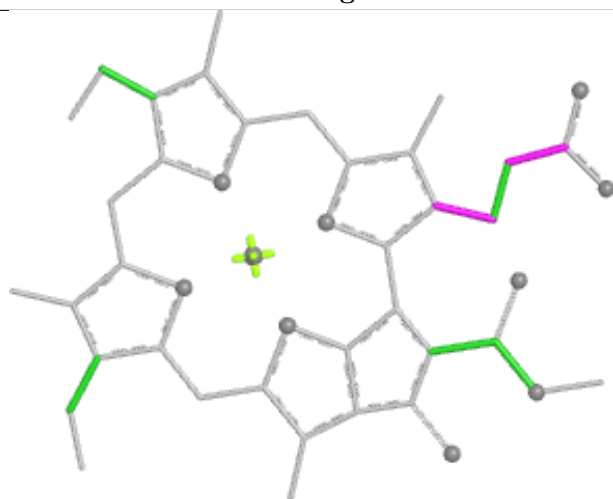
Ligand CLA B 1220



Bond lengths



Bond angles

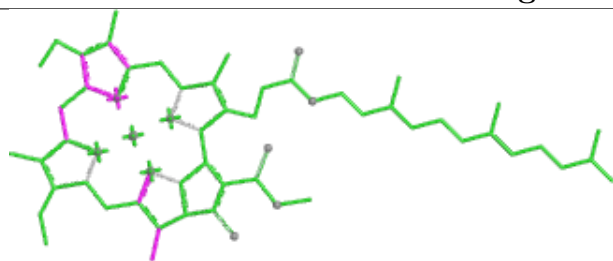


Torsions

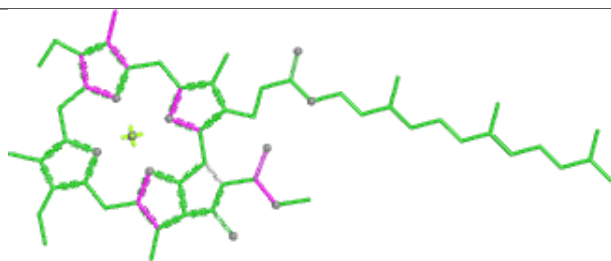


Rings

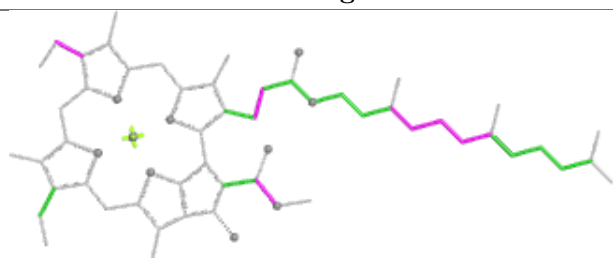
Ligand CLA 2 610



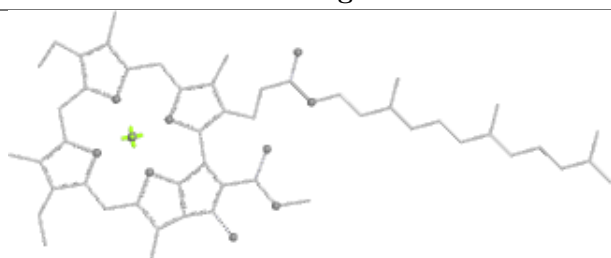
Bond lengths



Bond angles

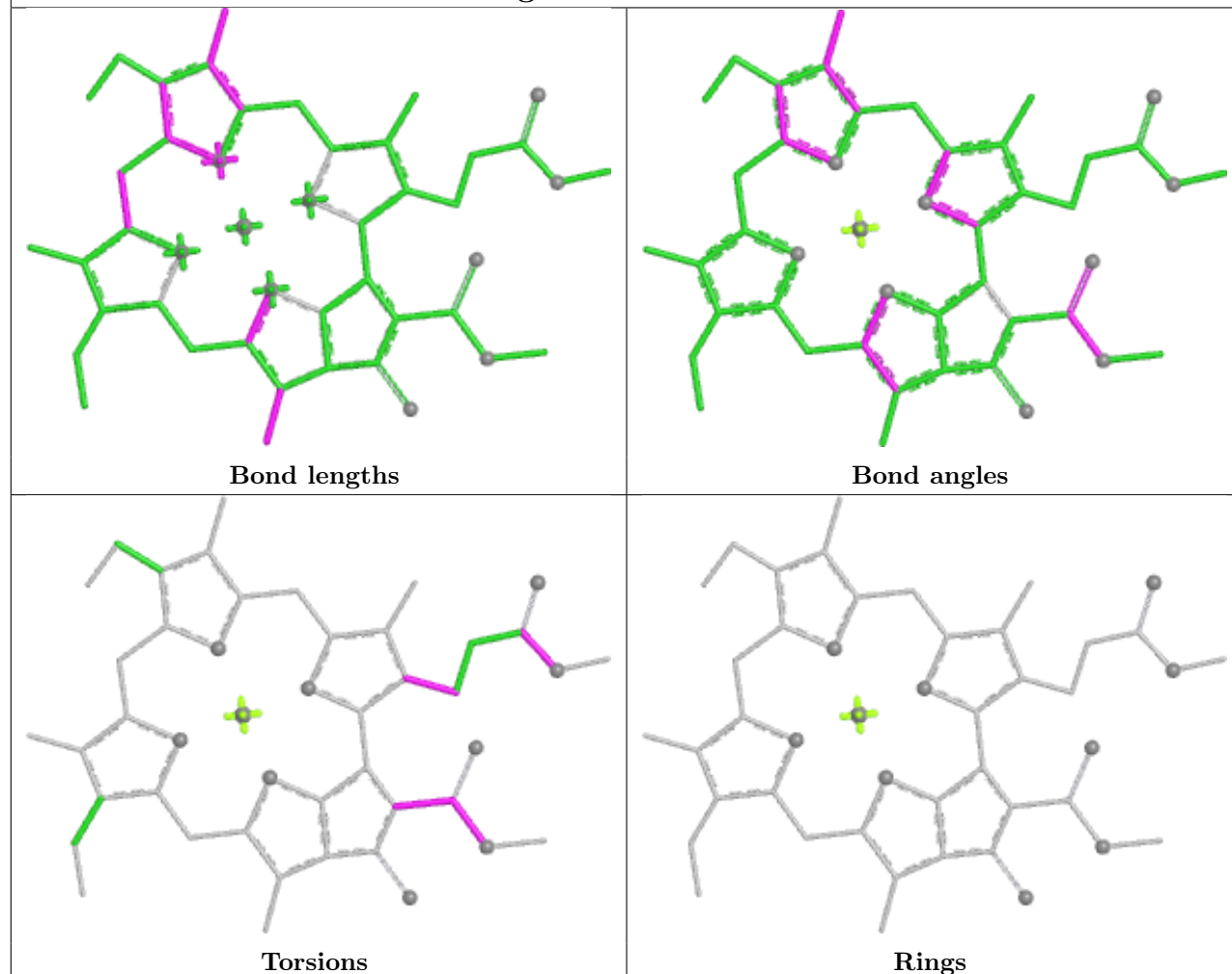


Torsions

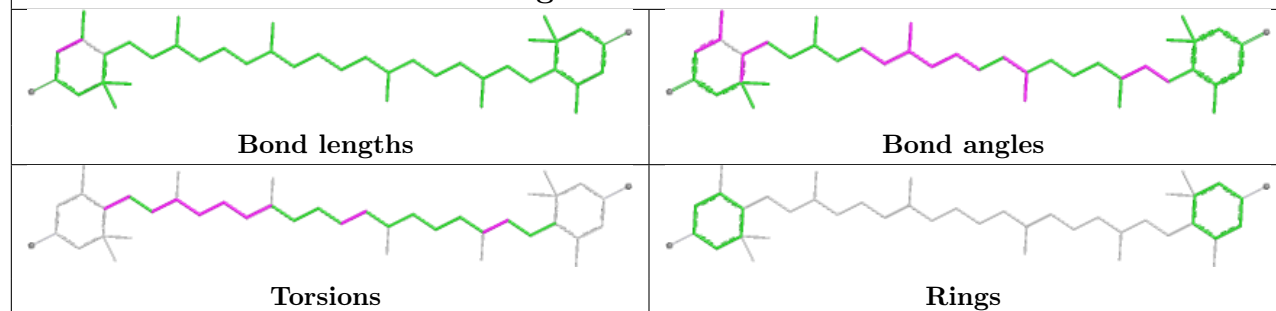


Rings

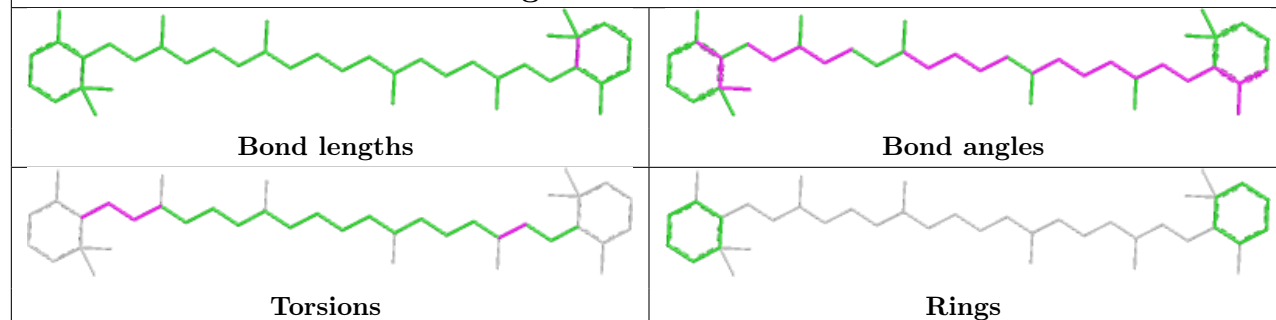
Ligand CLA 4 614



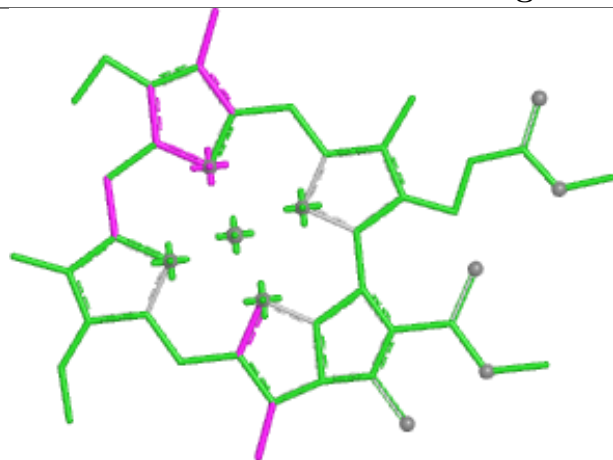
Ligand LUT 4 623



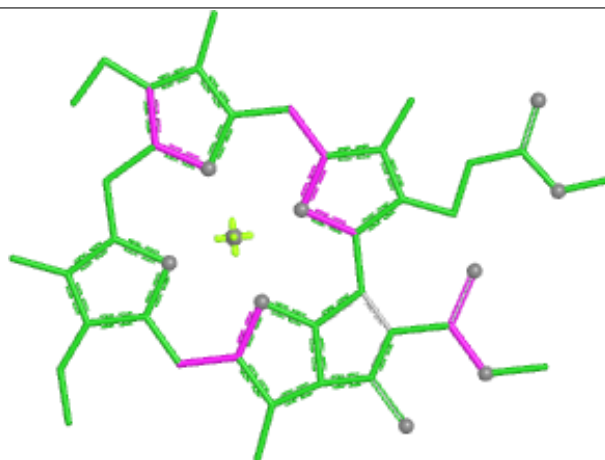
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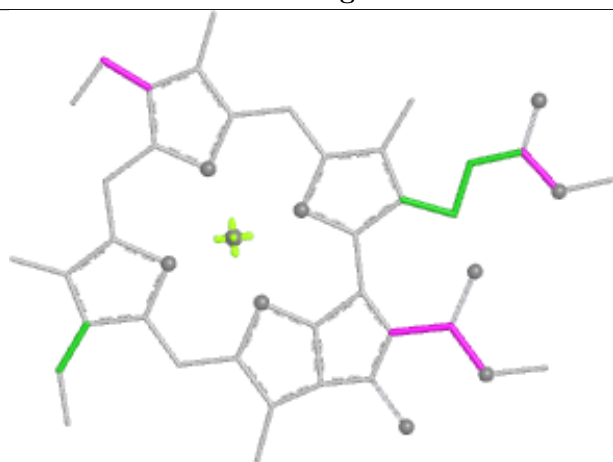
Ligand CLA F 302



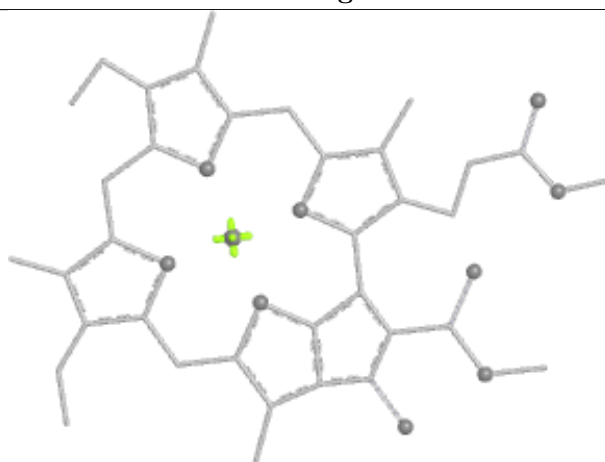
Bond lengths



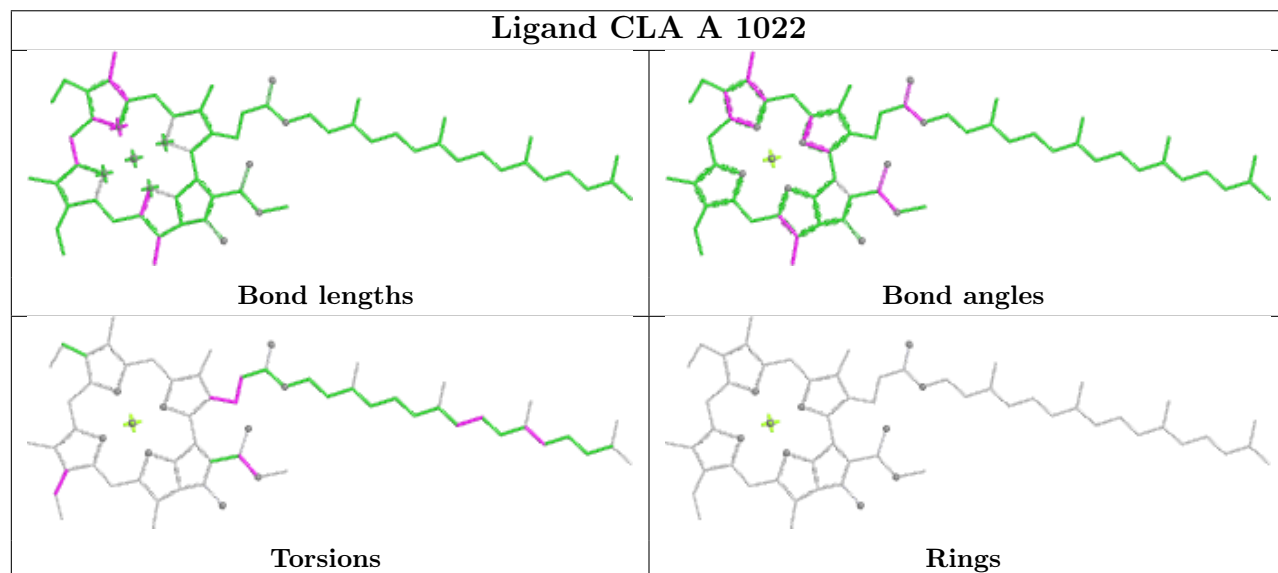
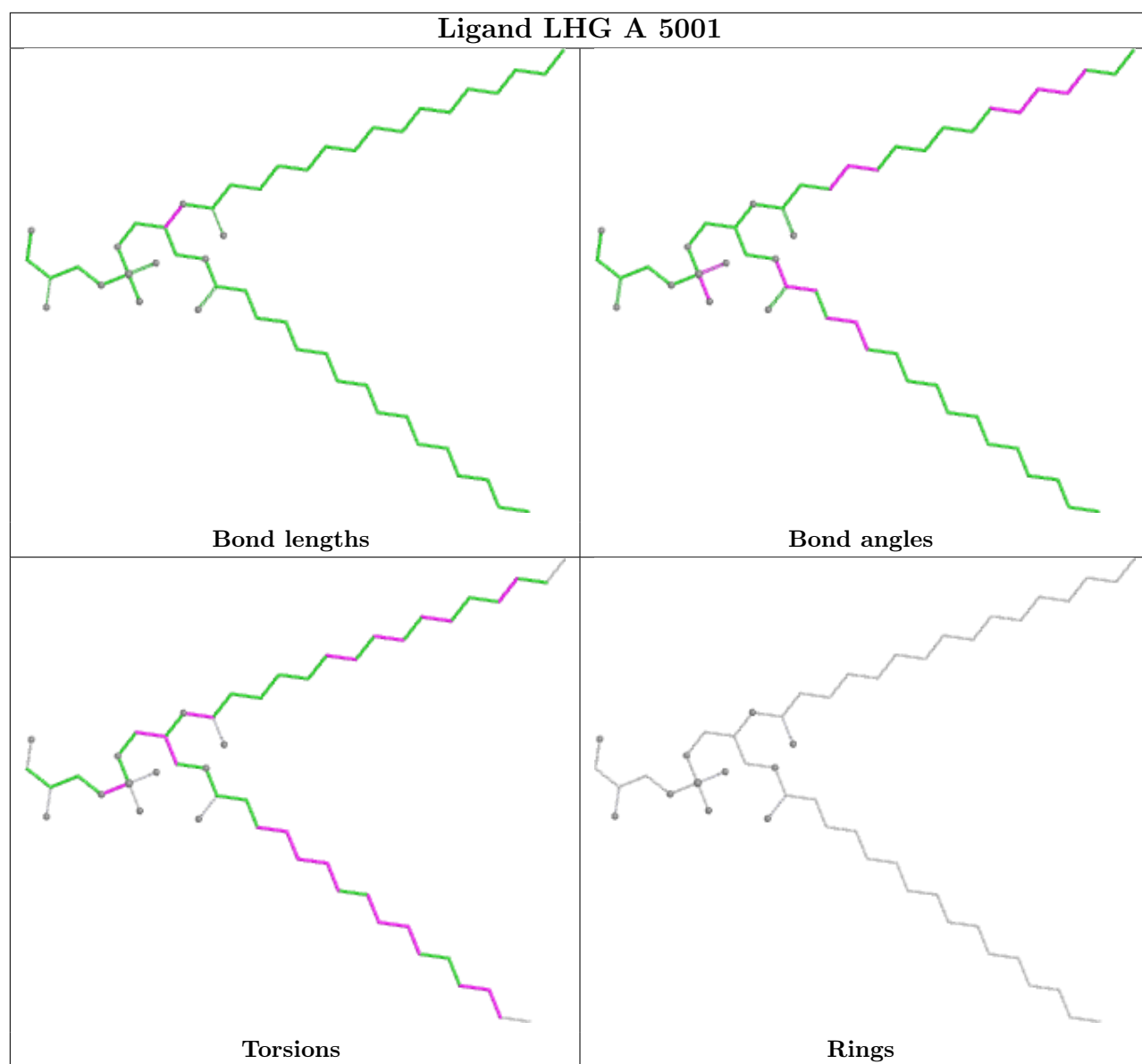
Bond angles



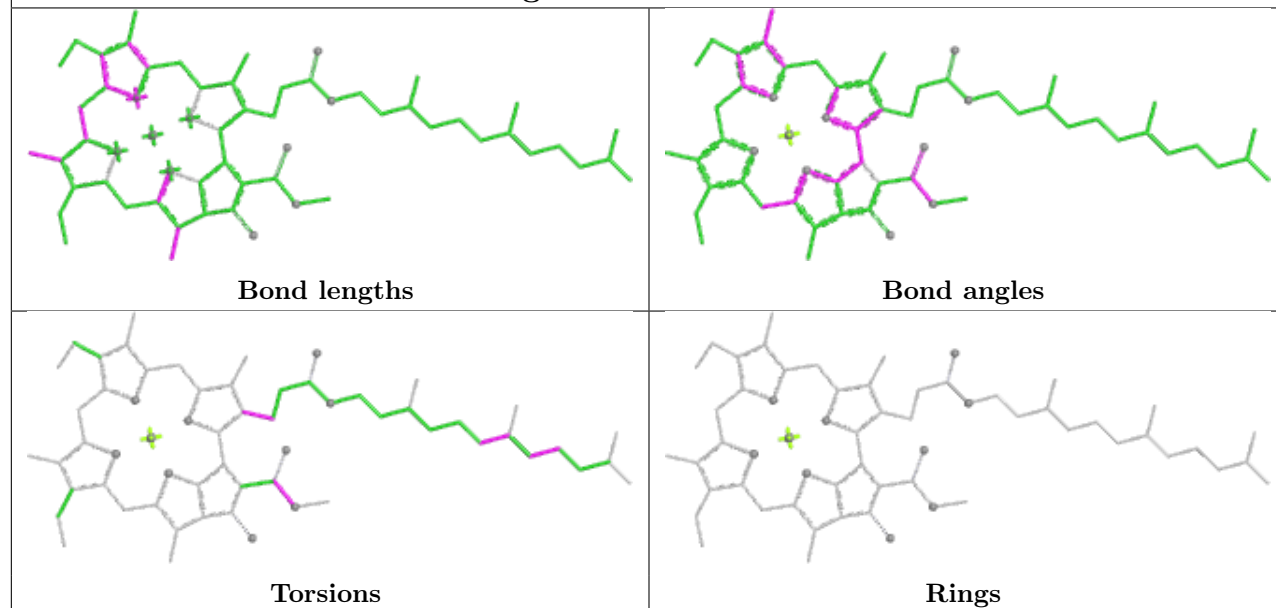
Torsions



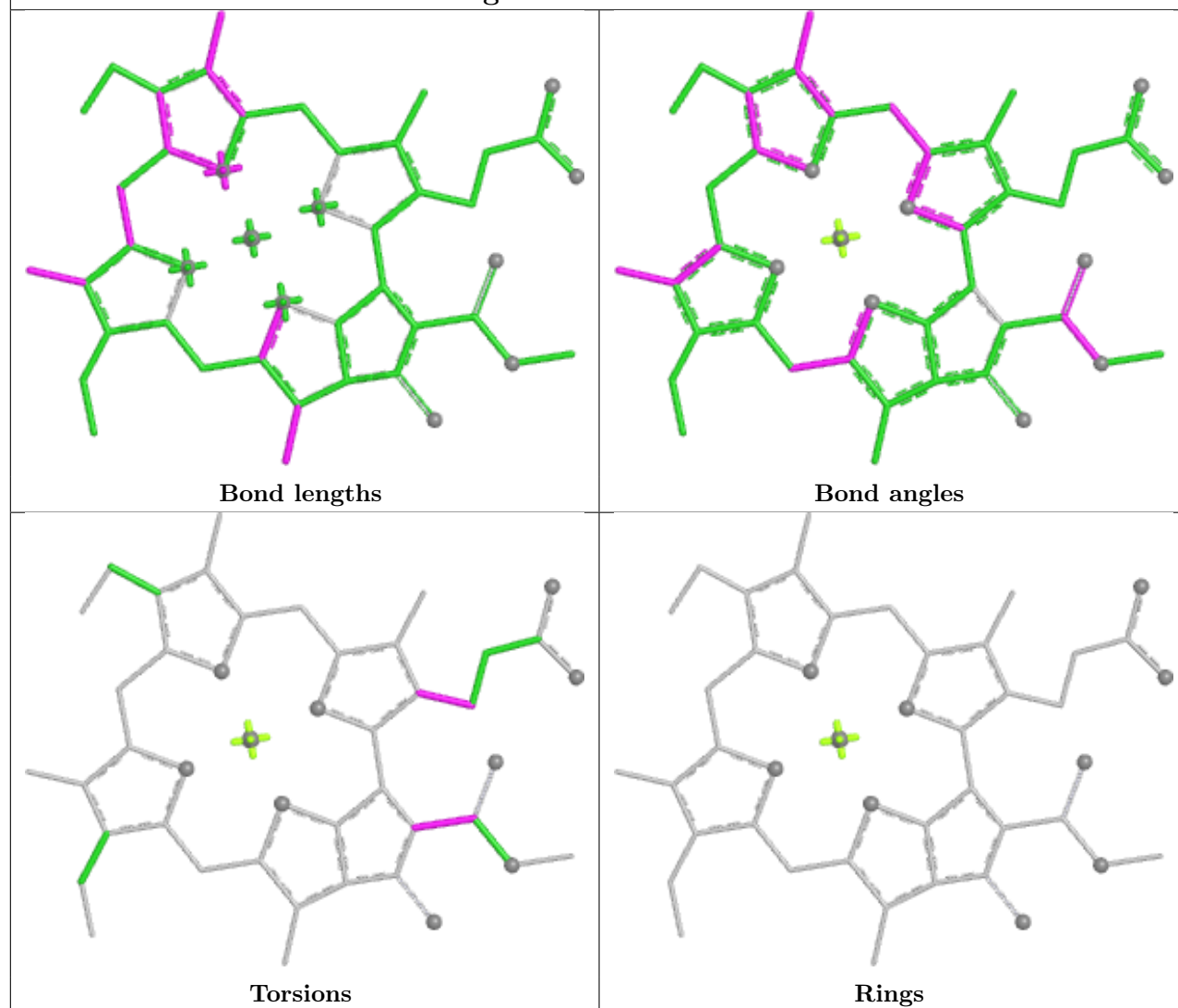
Rings

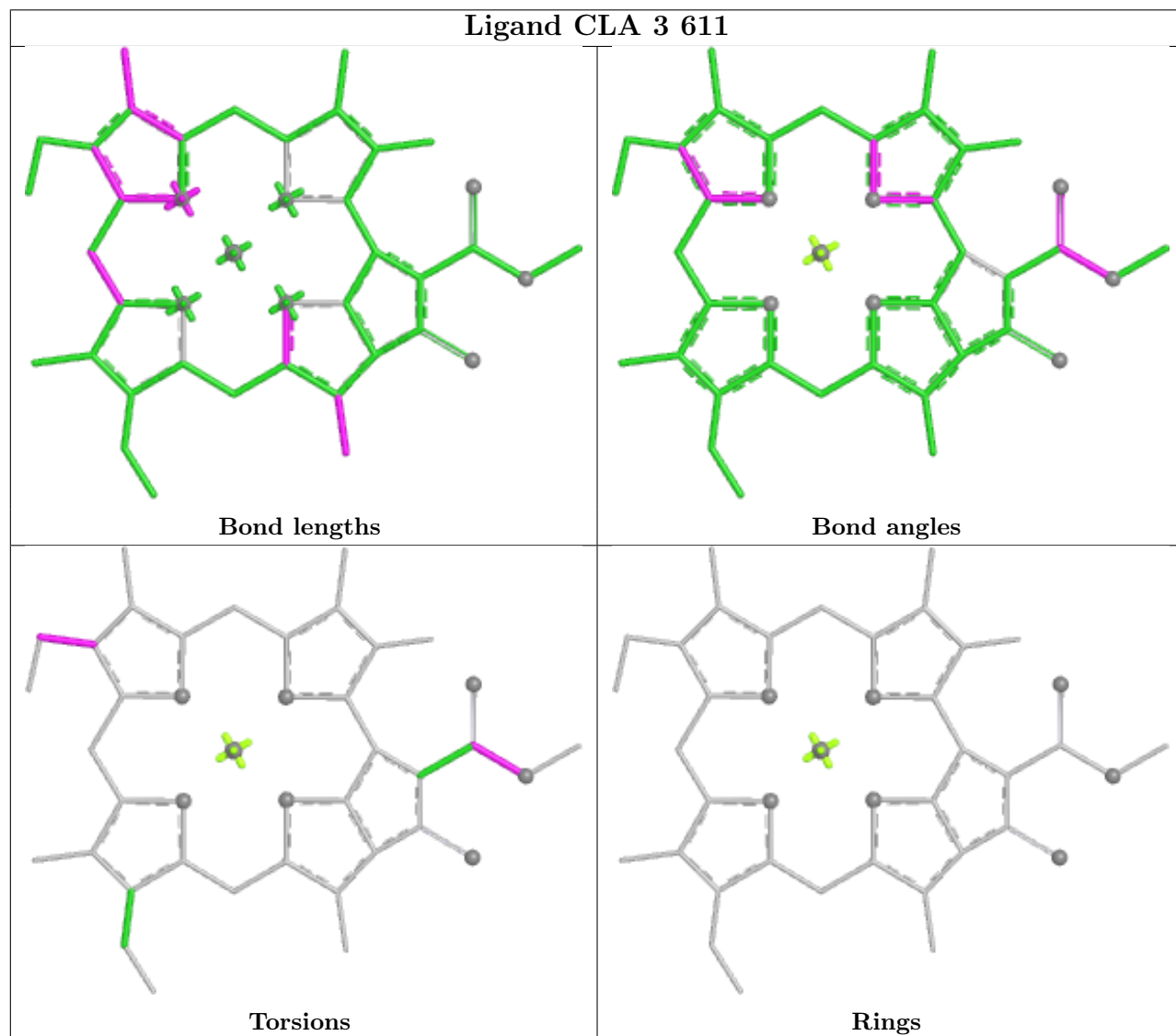
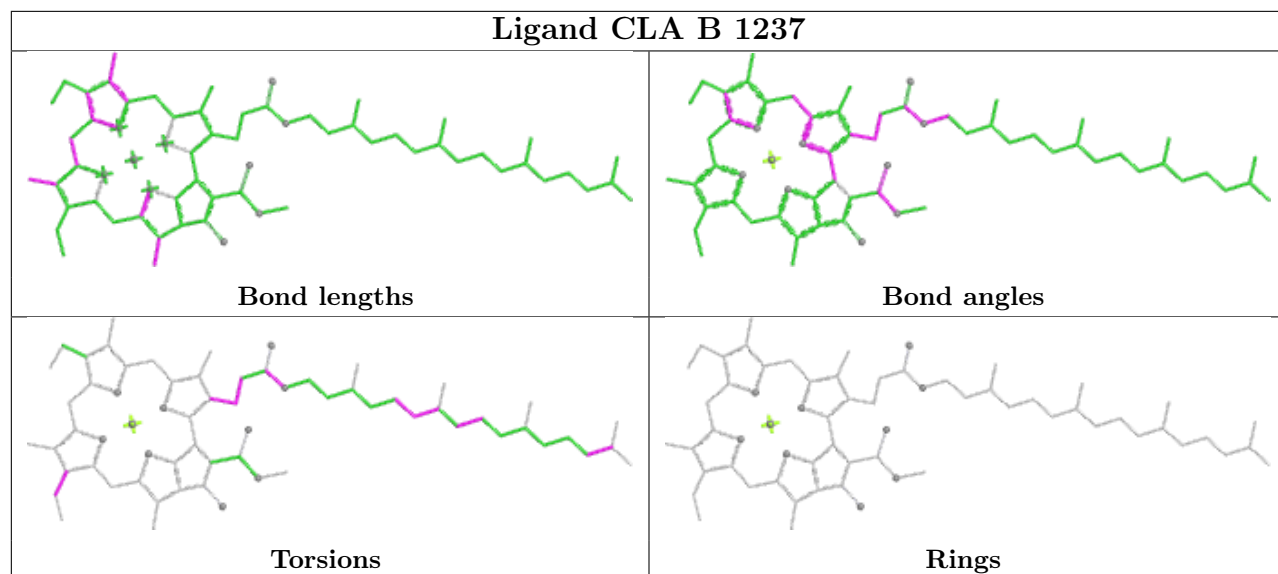


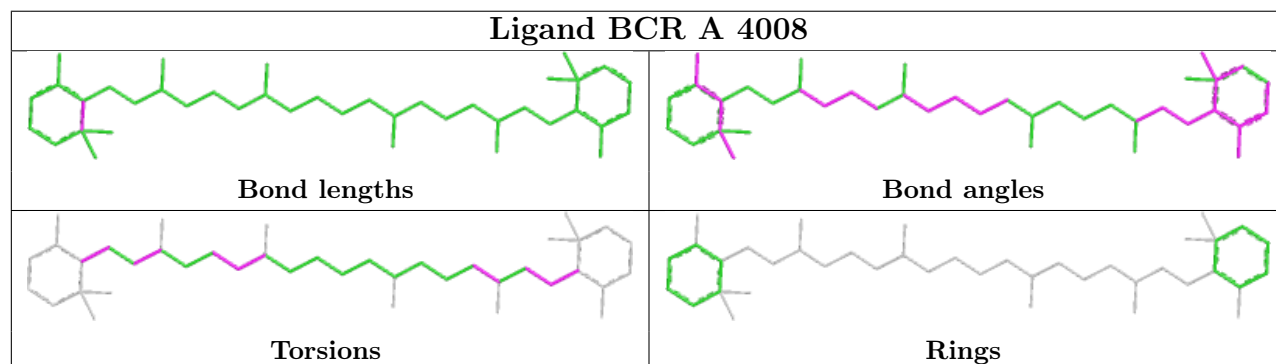
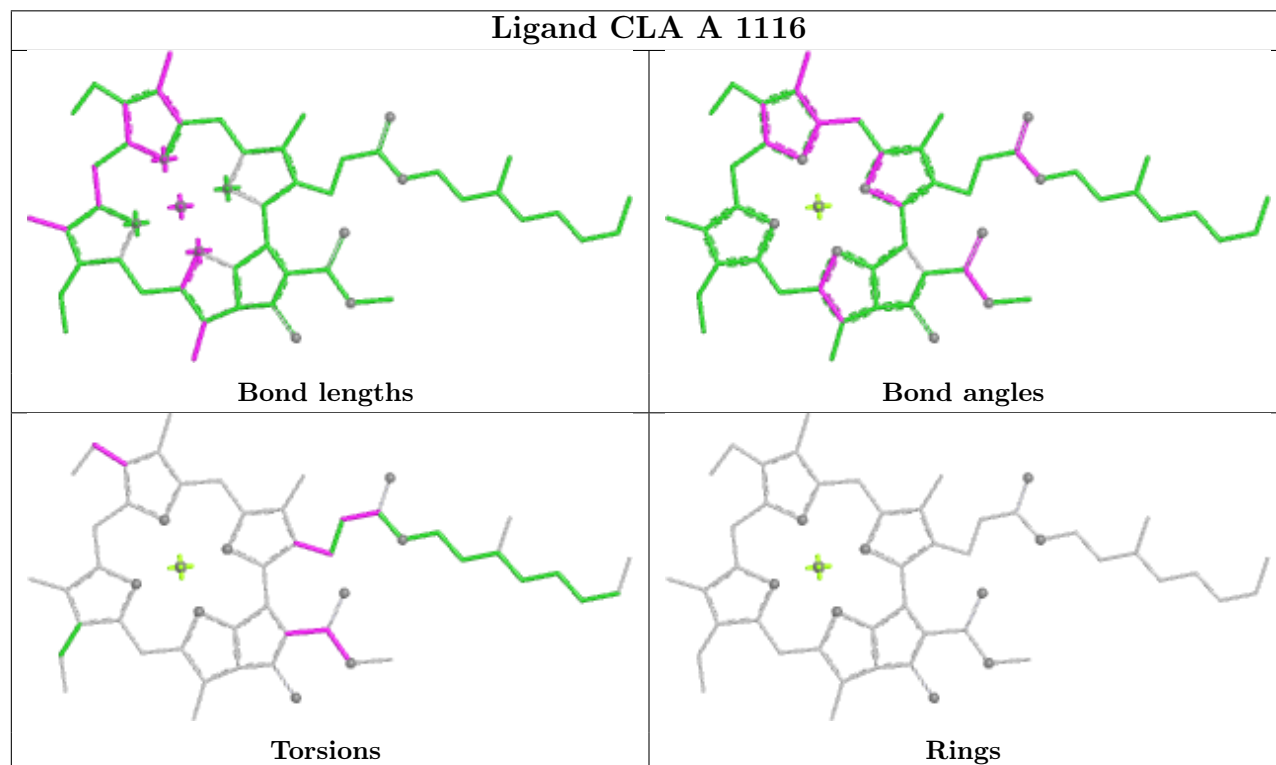
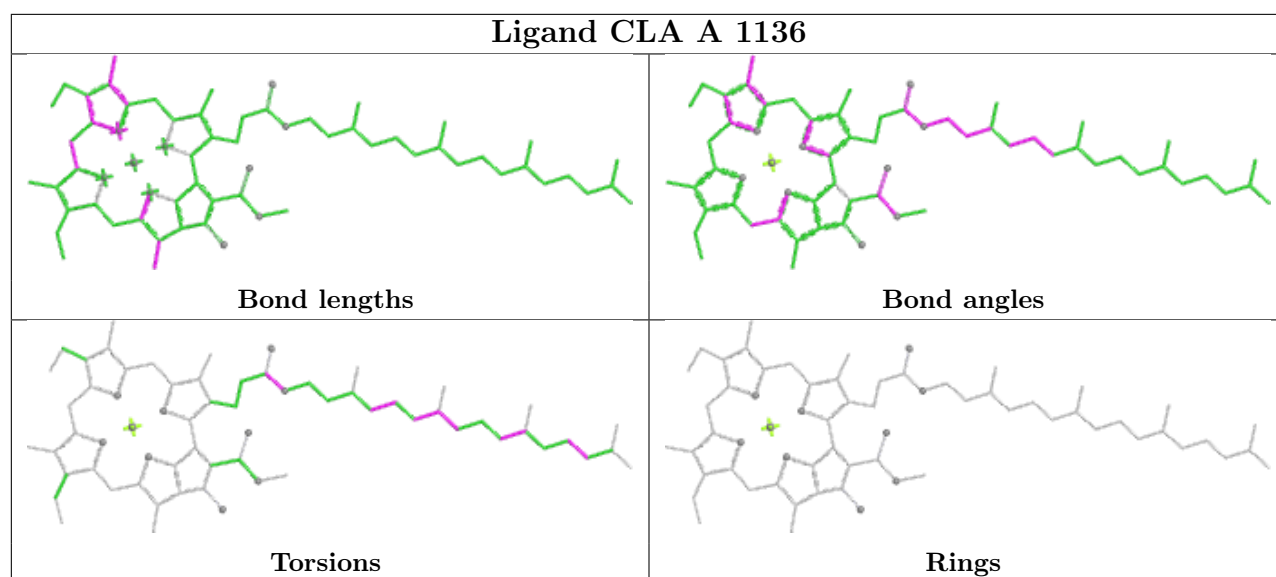
Ligand CLA A 1130

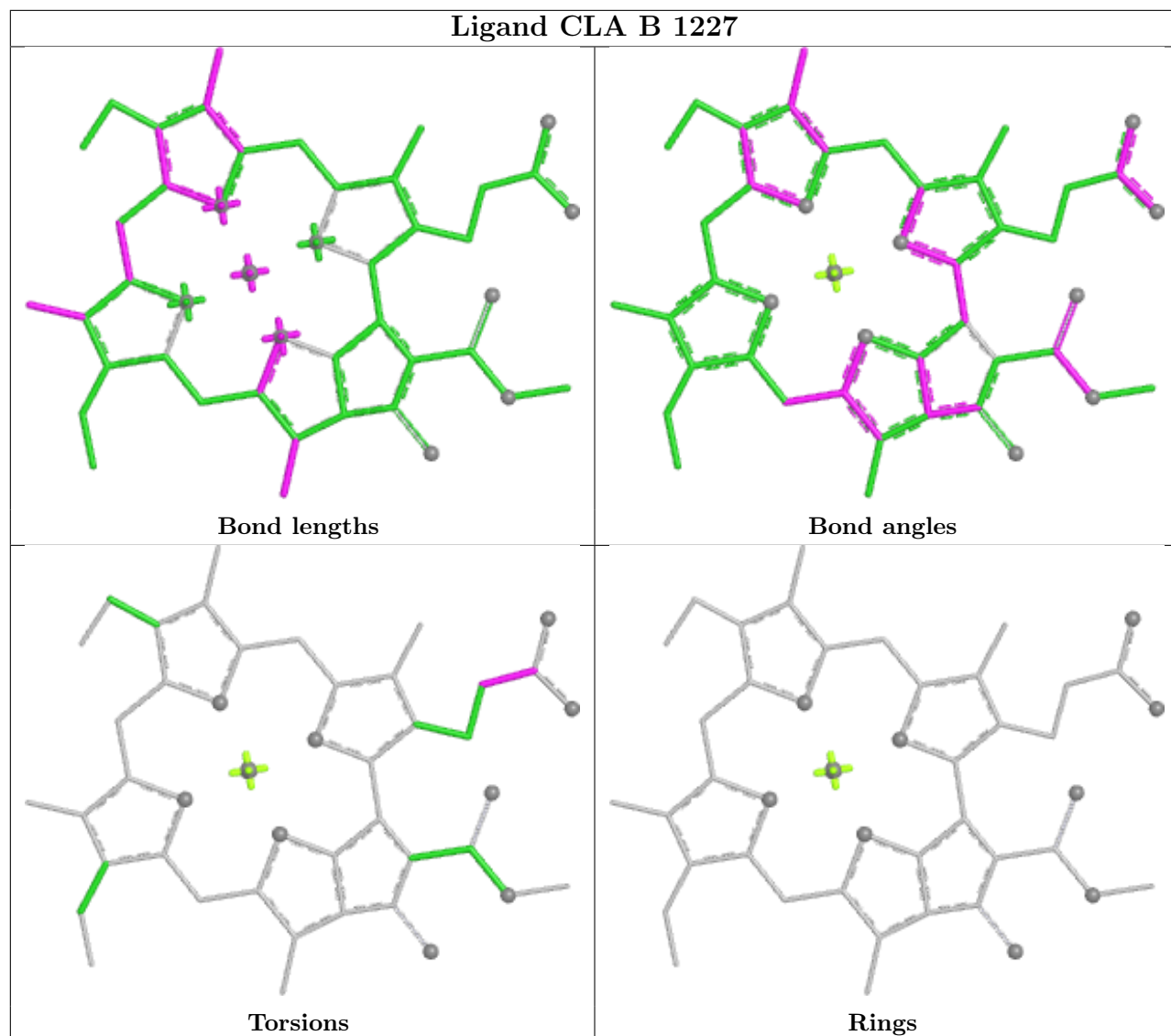


Ligand CLA B 1212

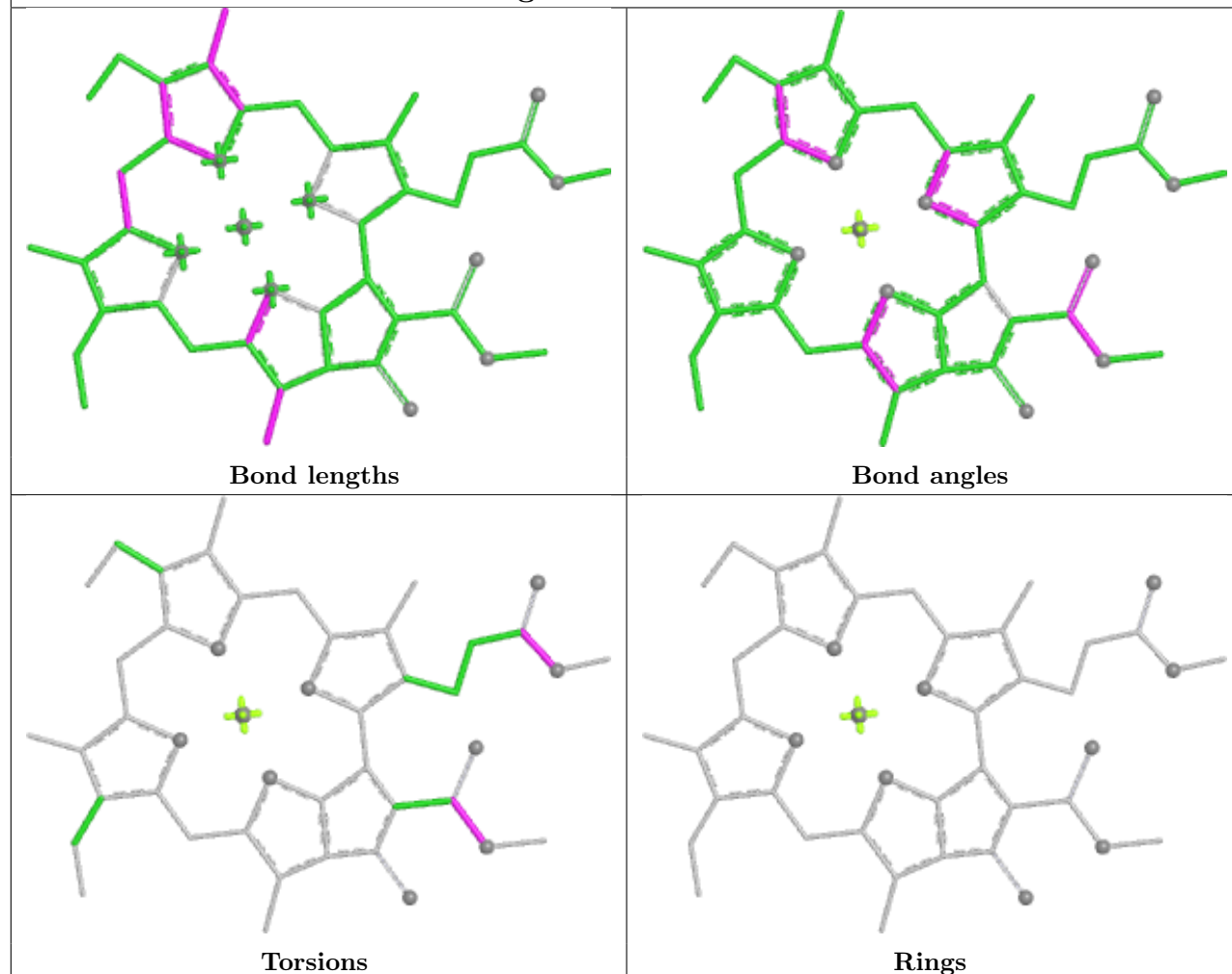




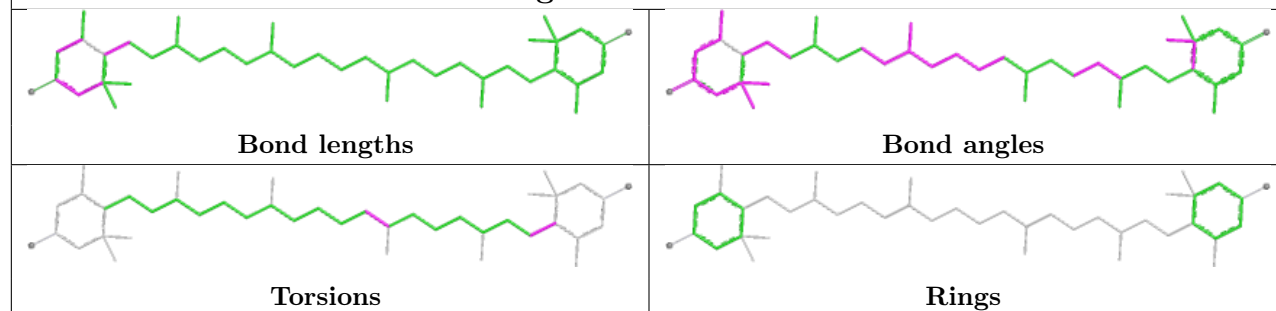


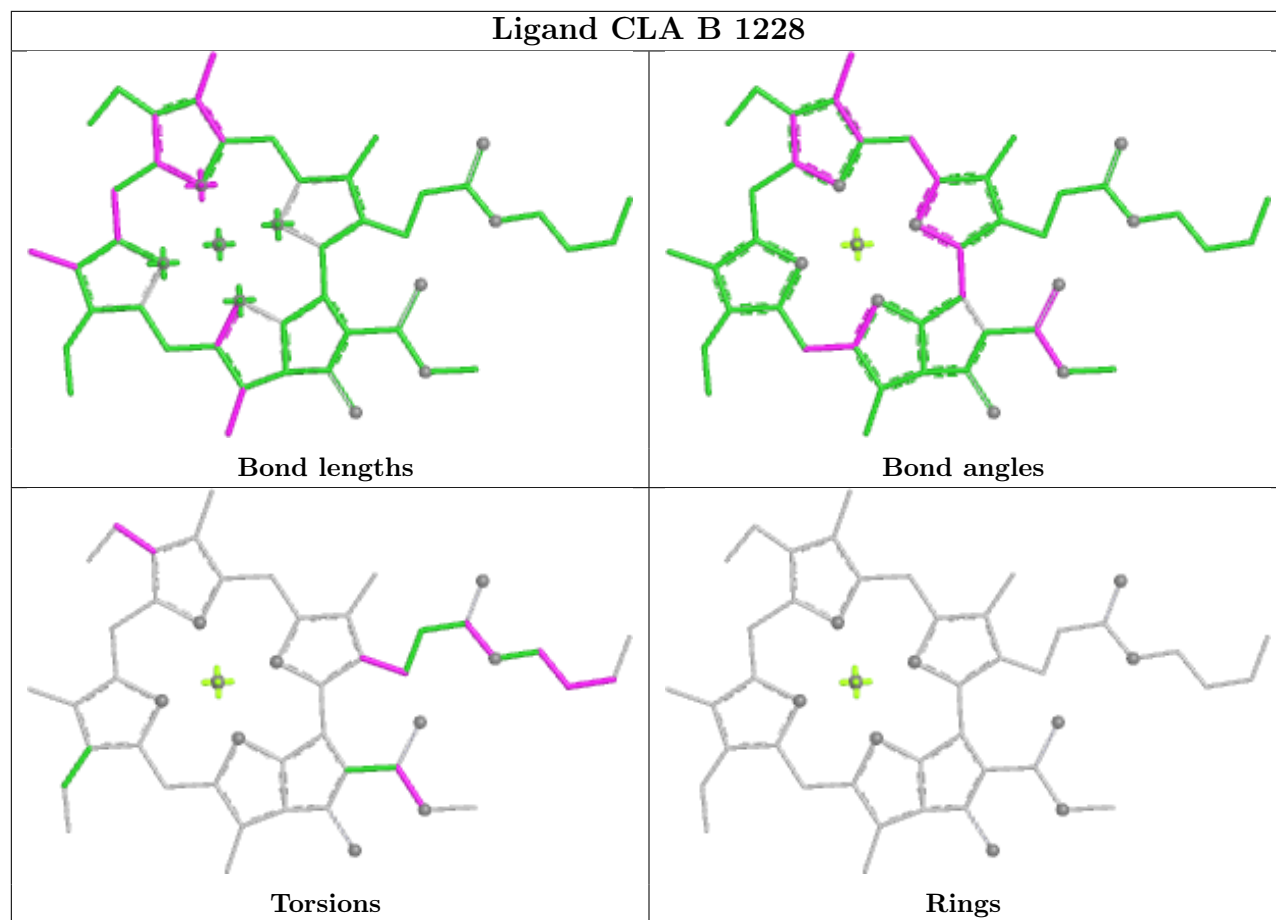


Ligand CLA 1 611

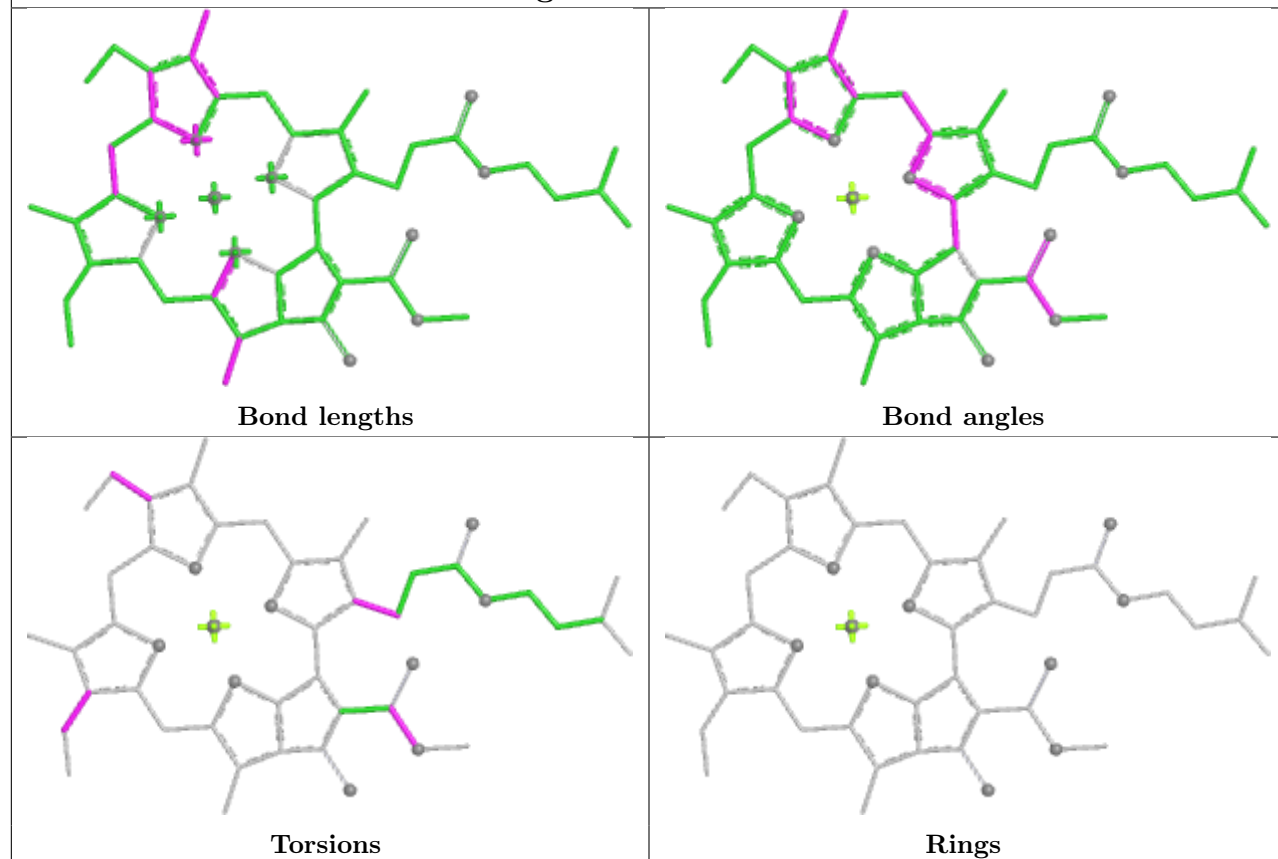


Ligand LUT 4 621

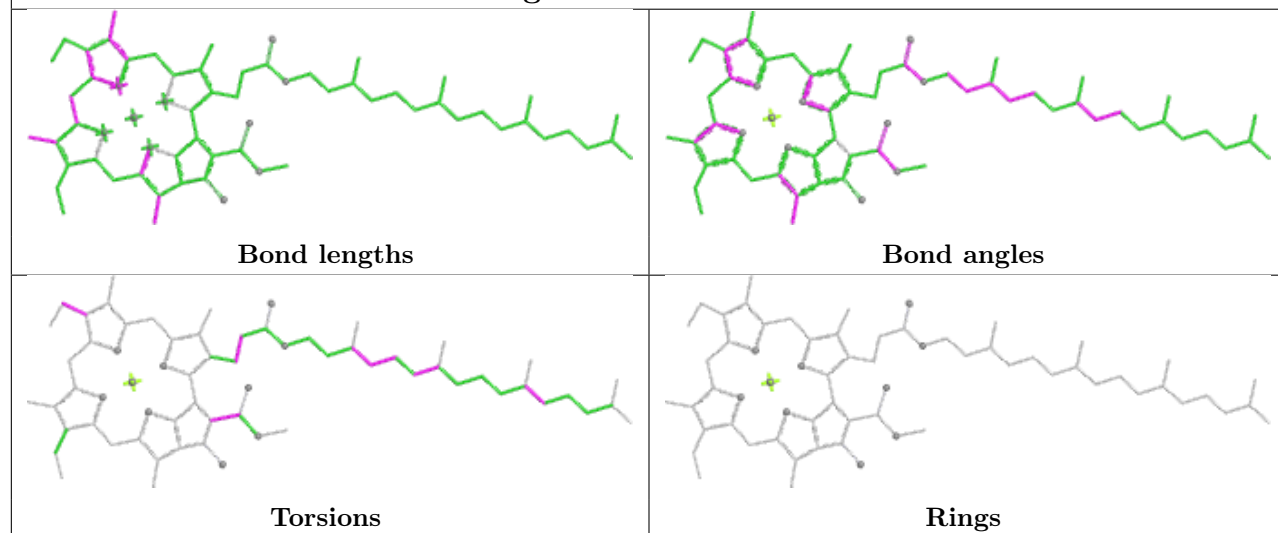


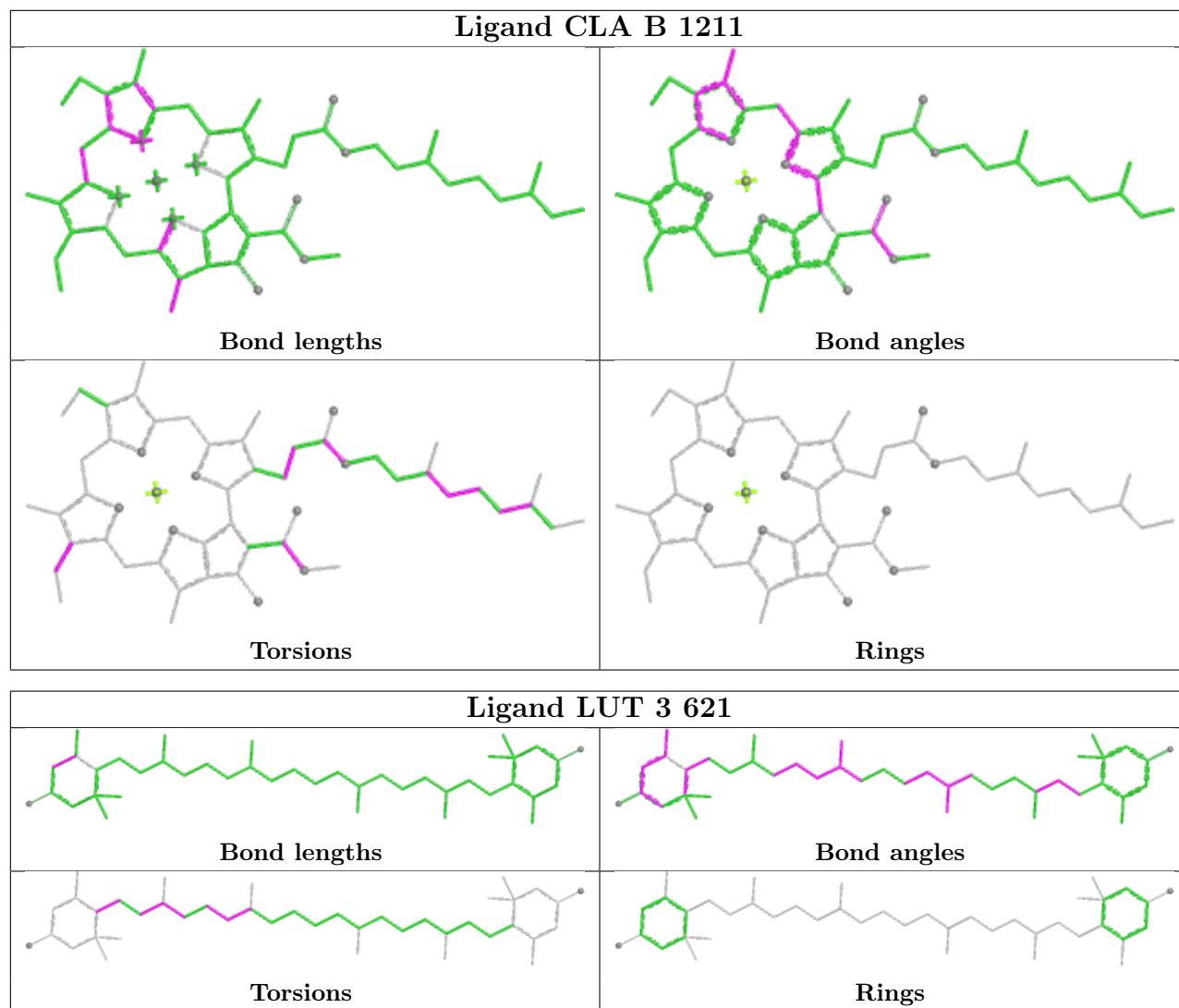


Ligand CLA 2 604

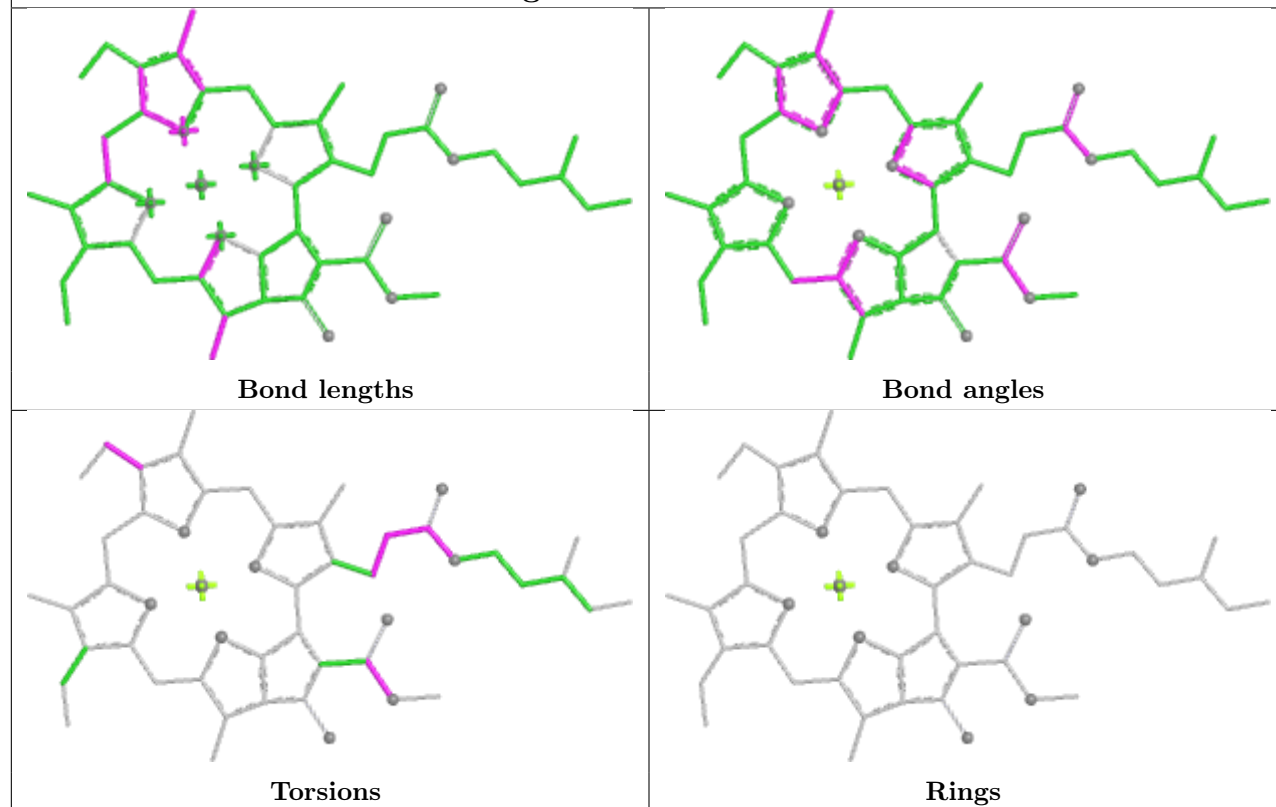


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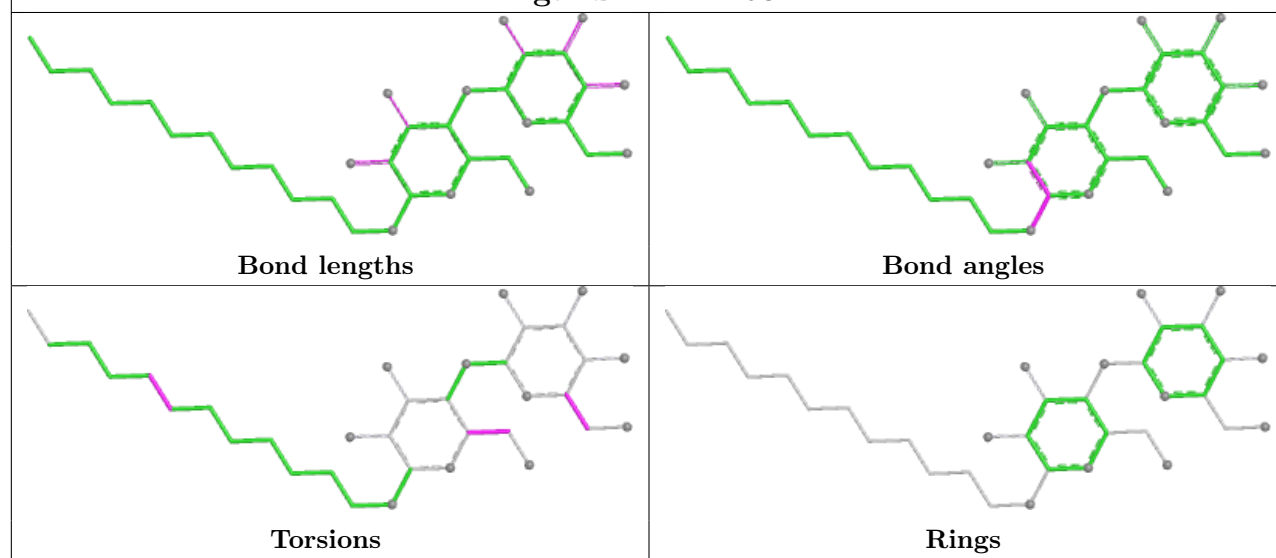


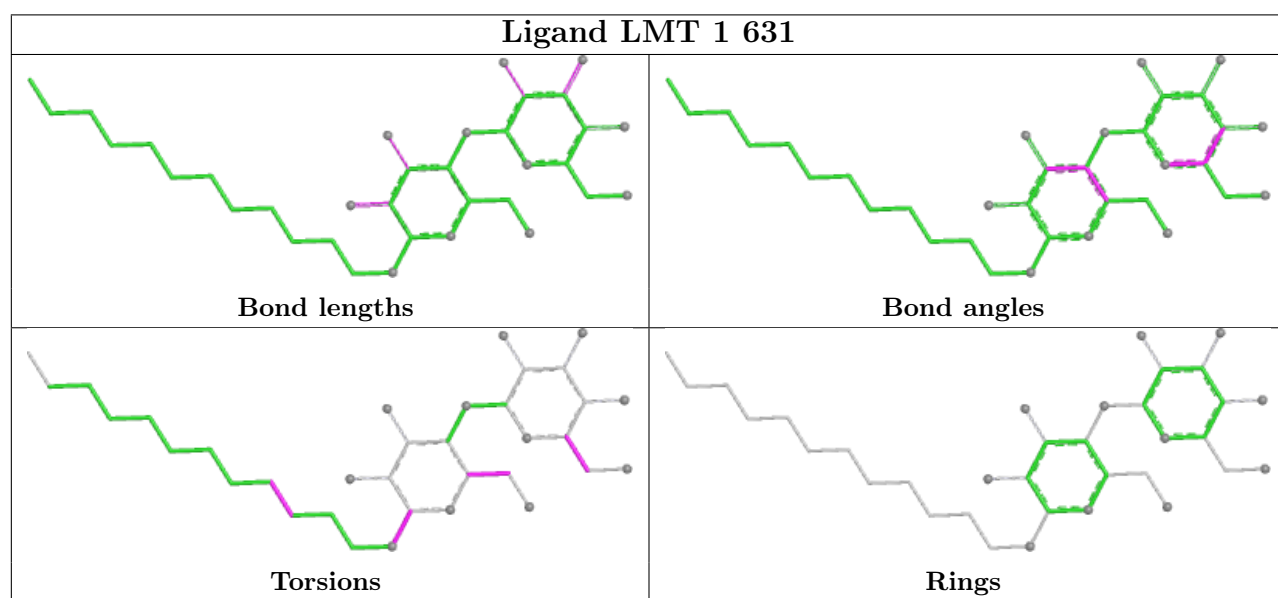
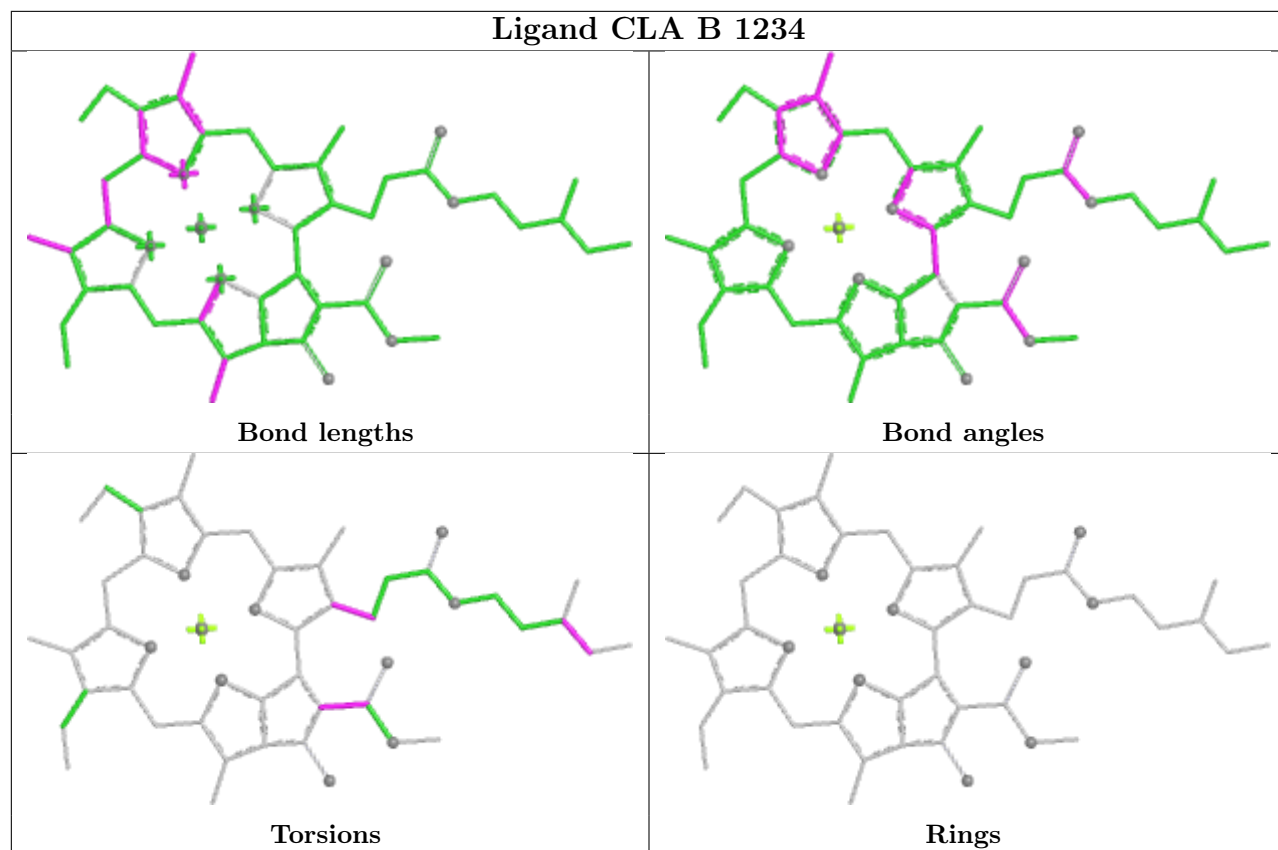


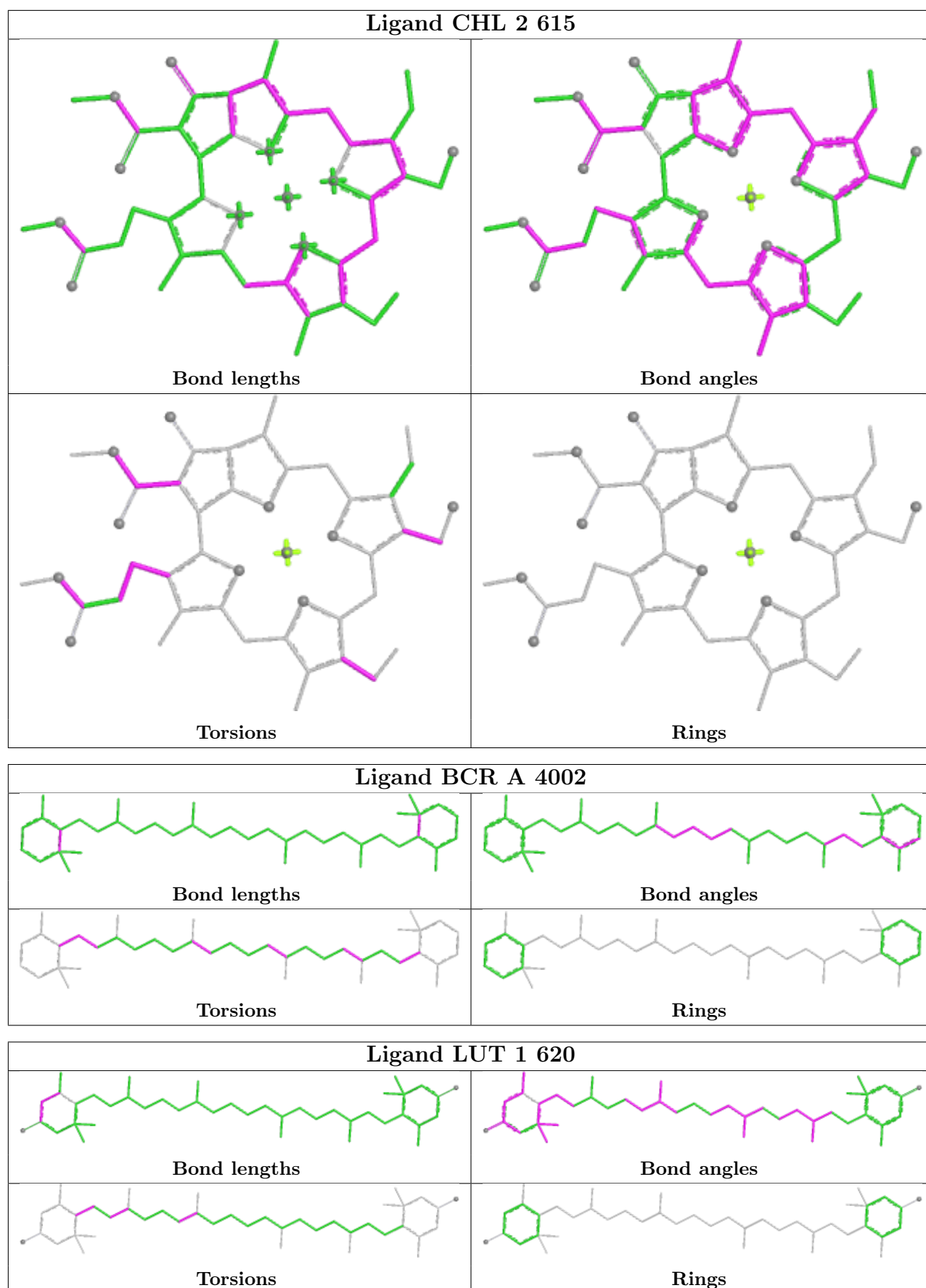
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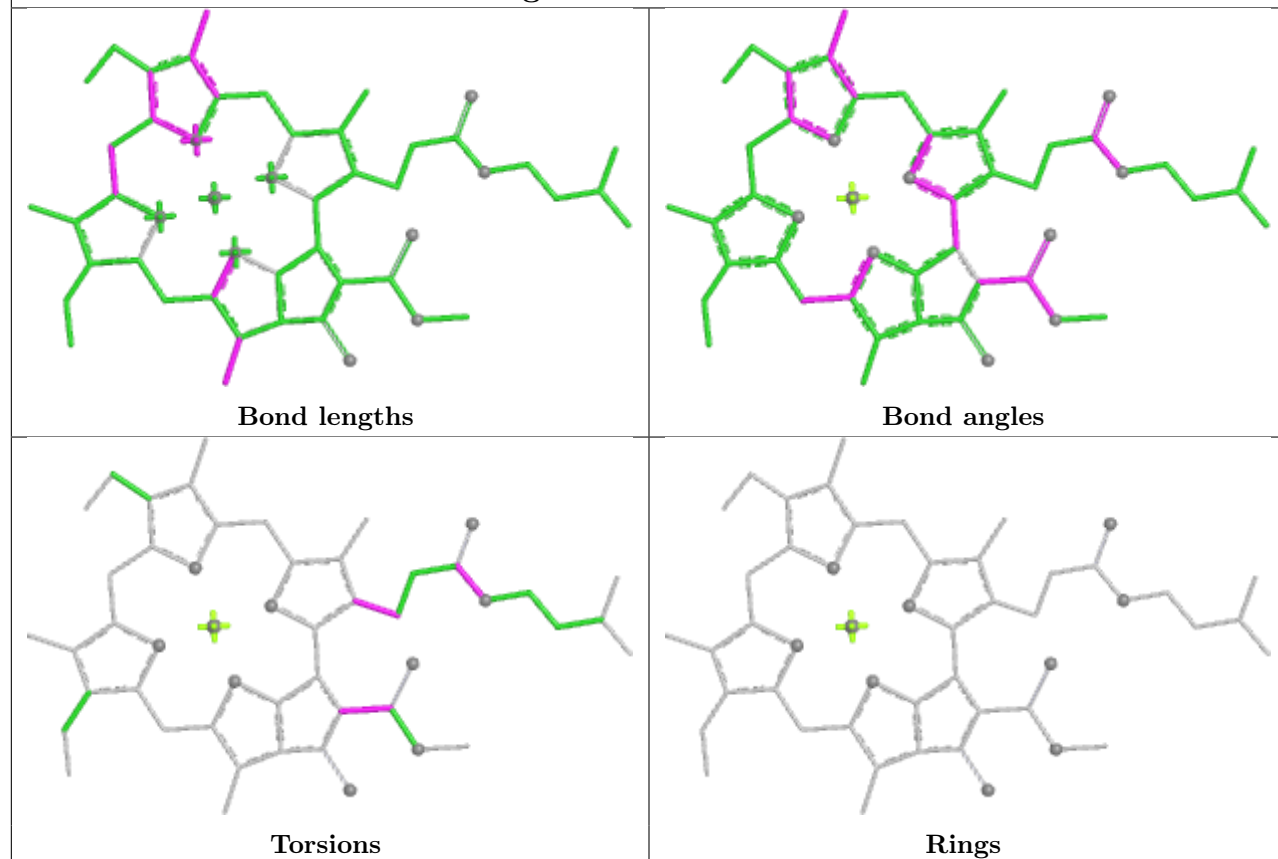
Ligand LMT 4 631



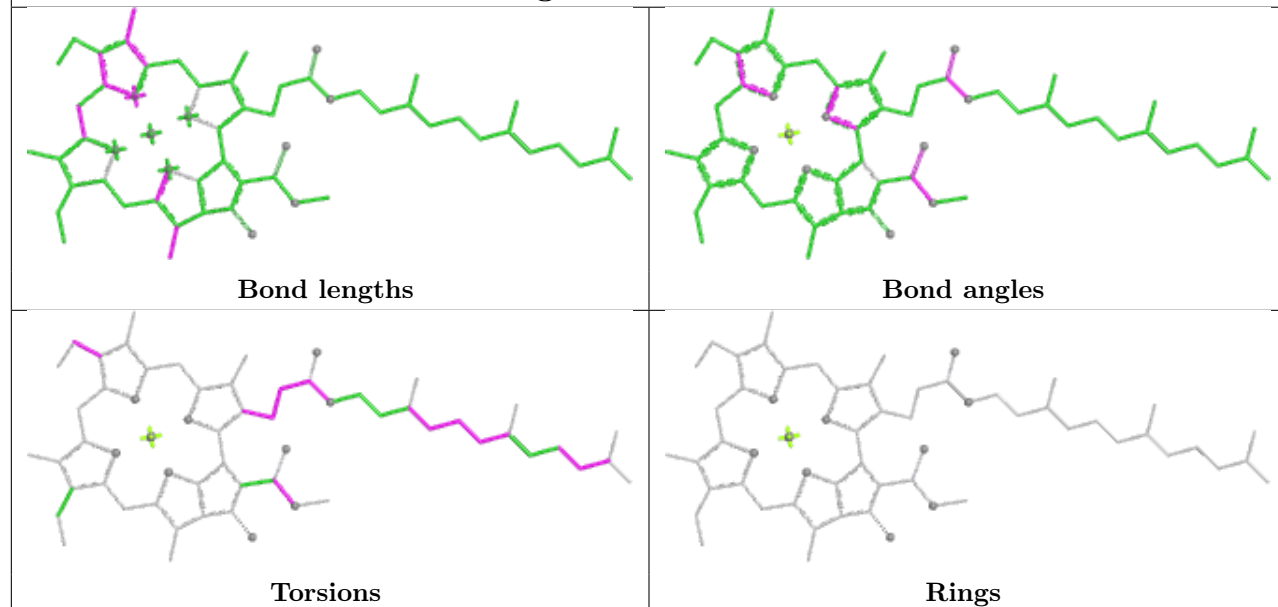




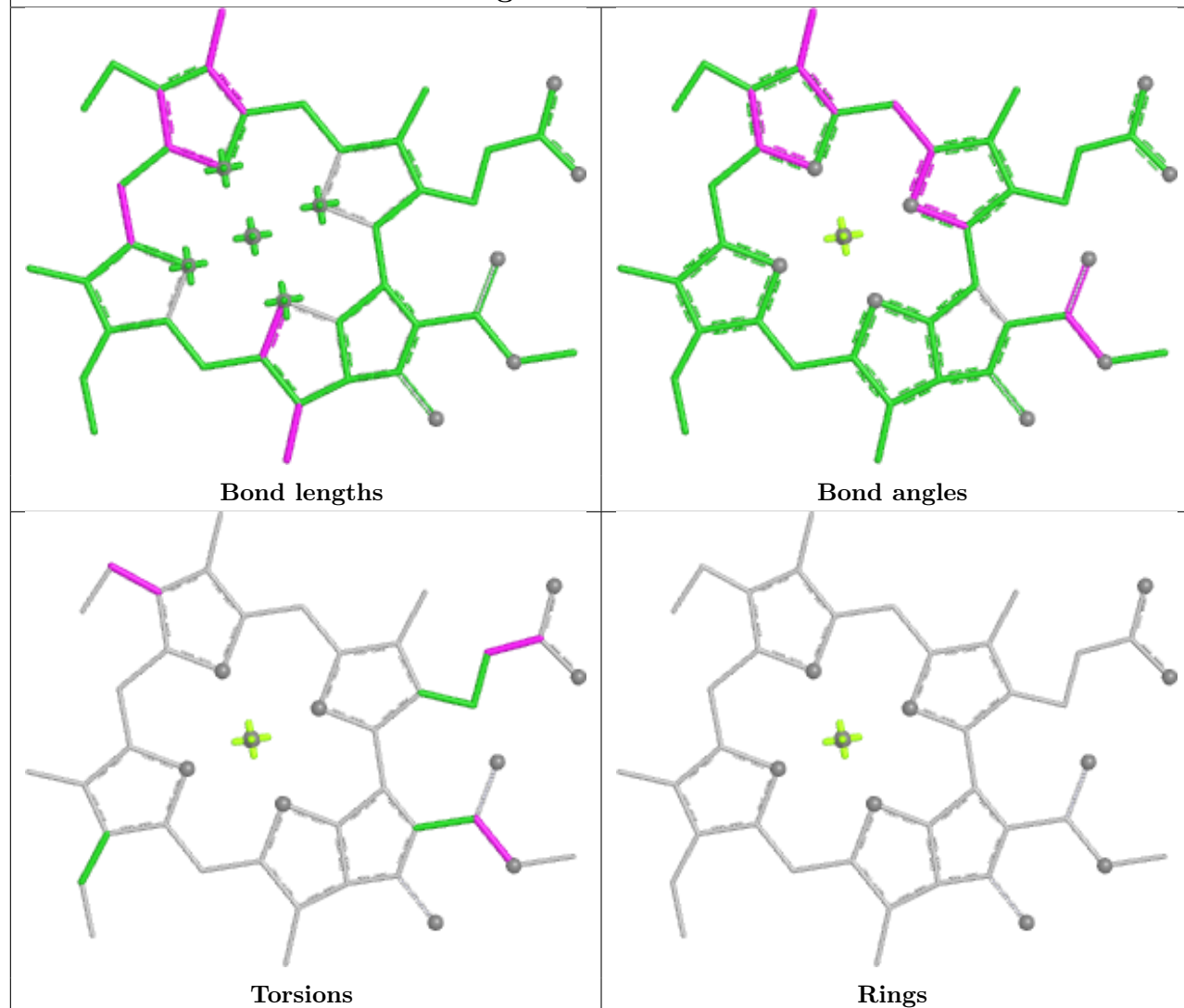
Ligand CLA A 5005



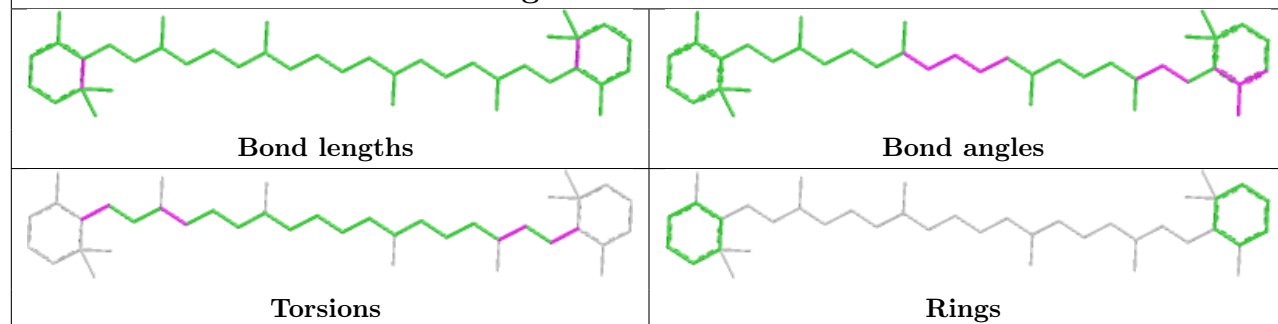
Ligand CLA 3 607

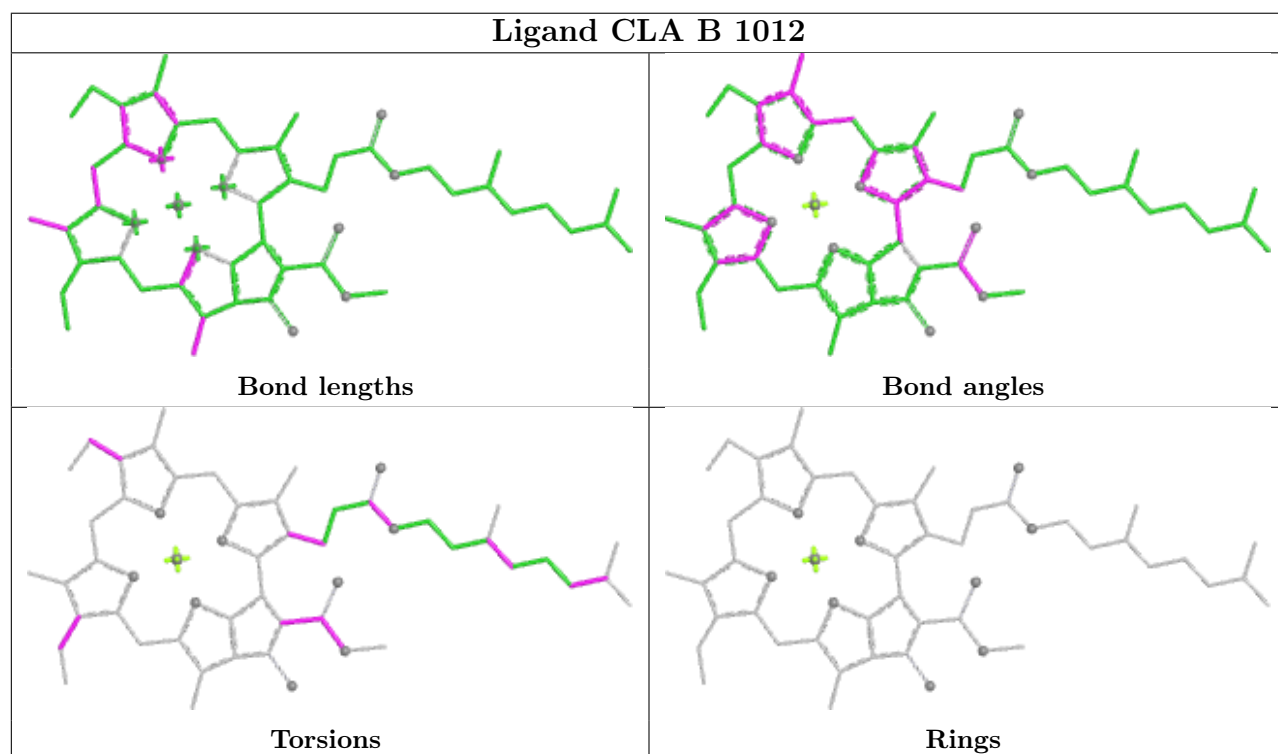
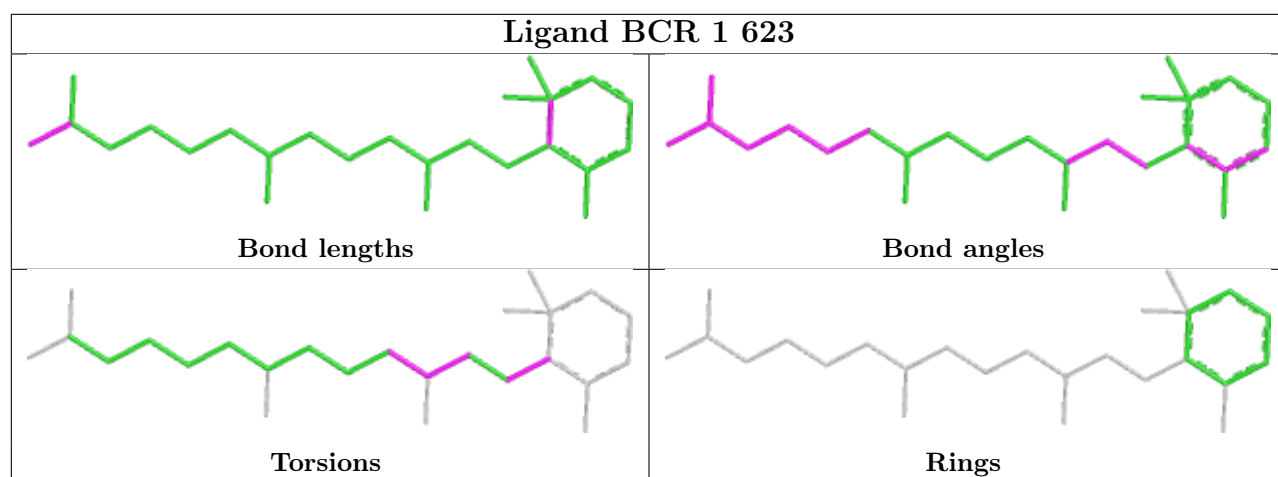


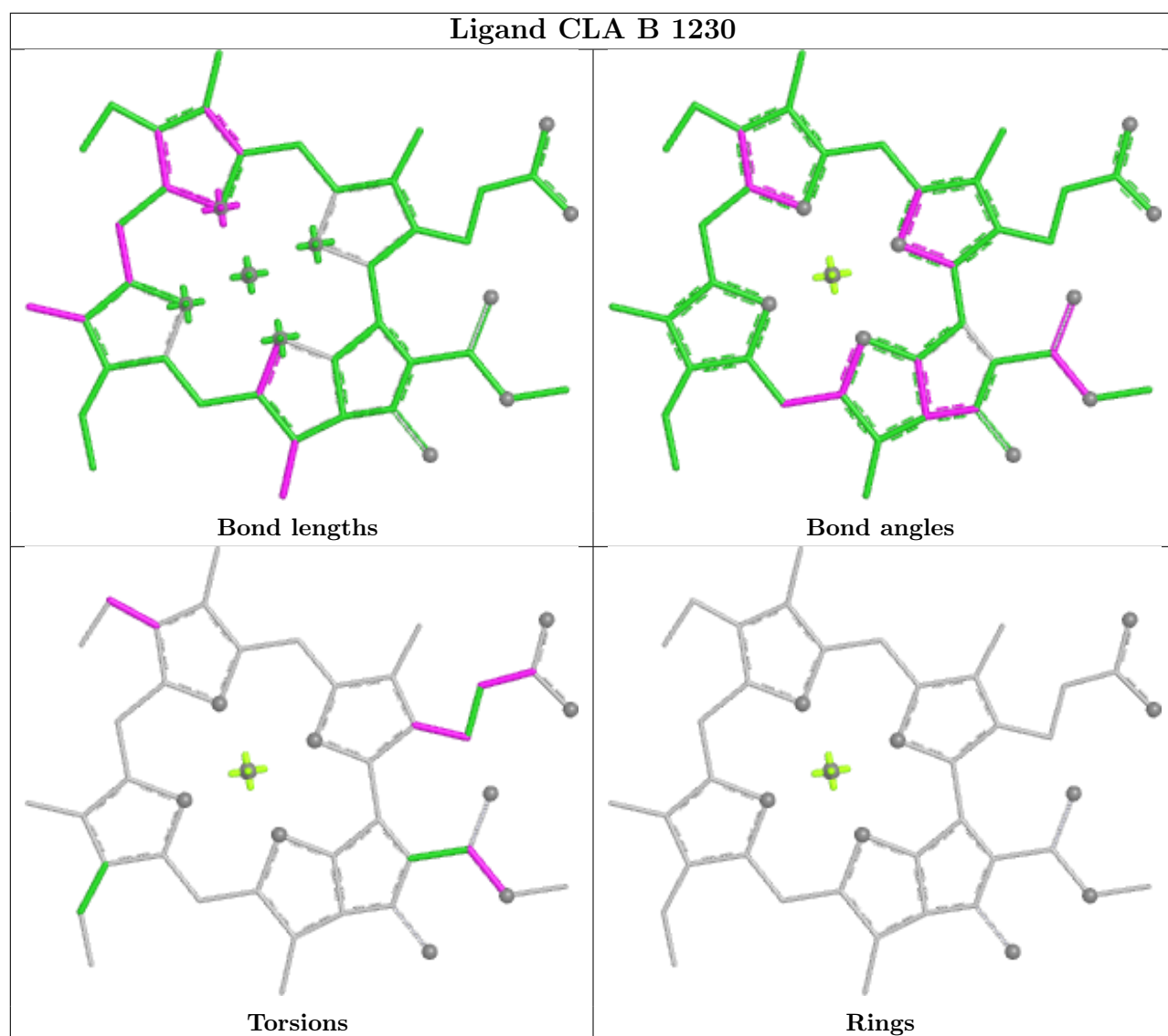
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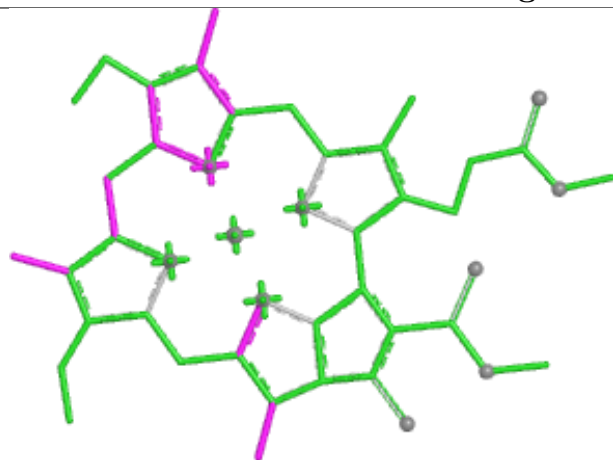
Ligand BCR B 4005



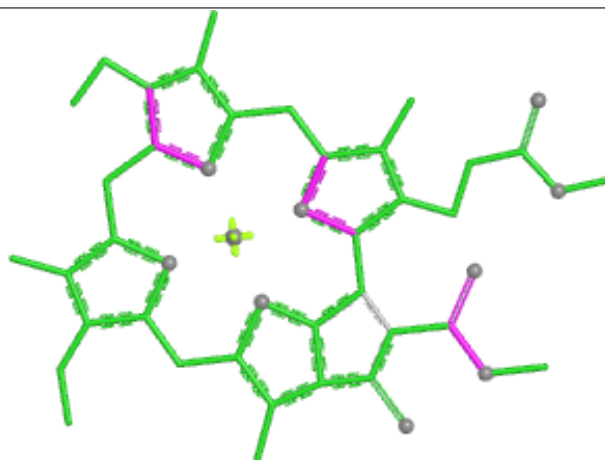




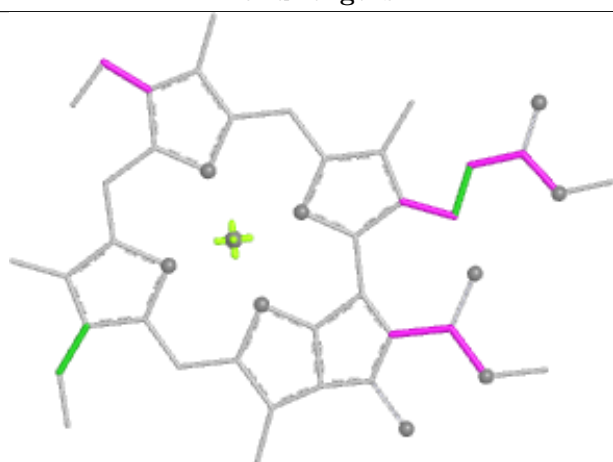
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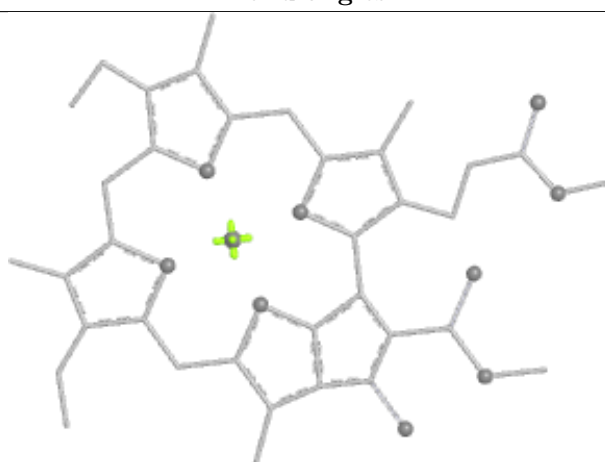
Bond lengths



Bond angles

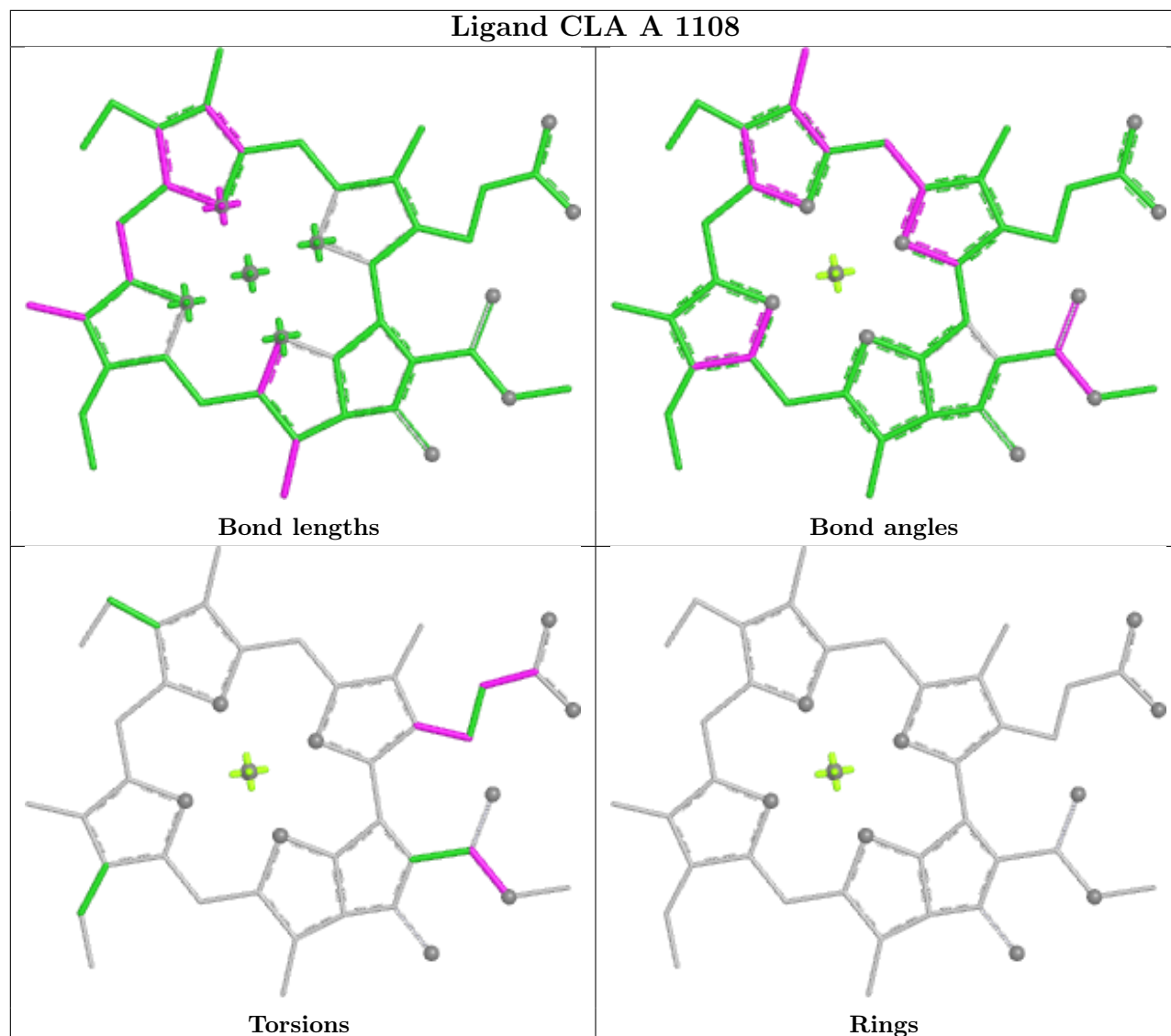


Torsions

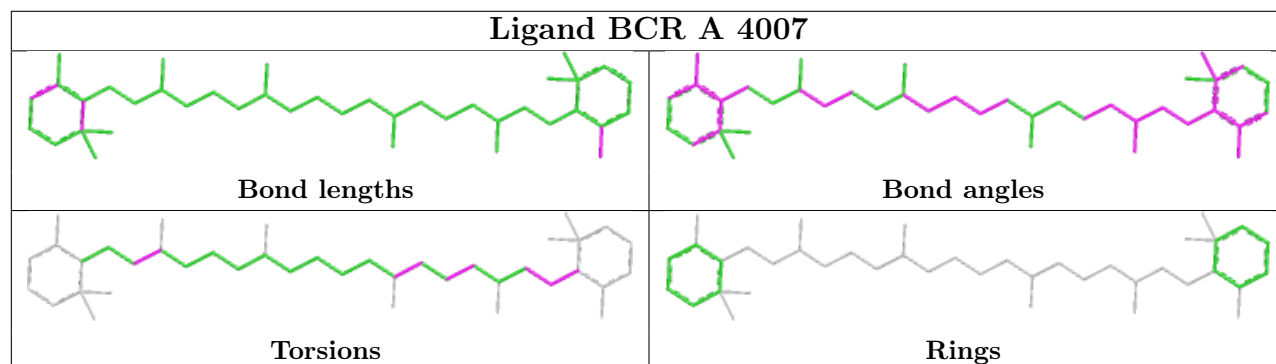


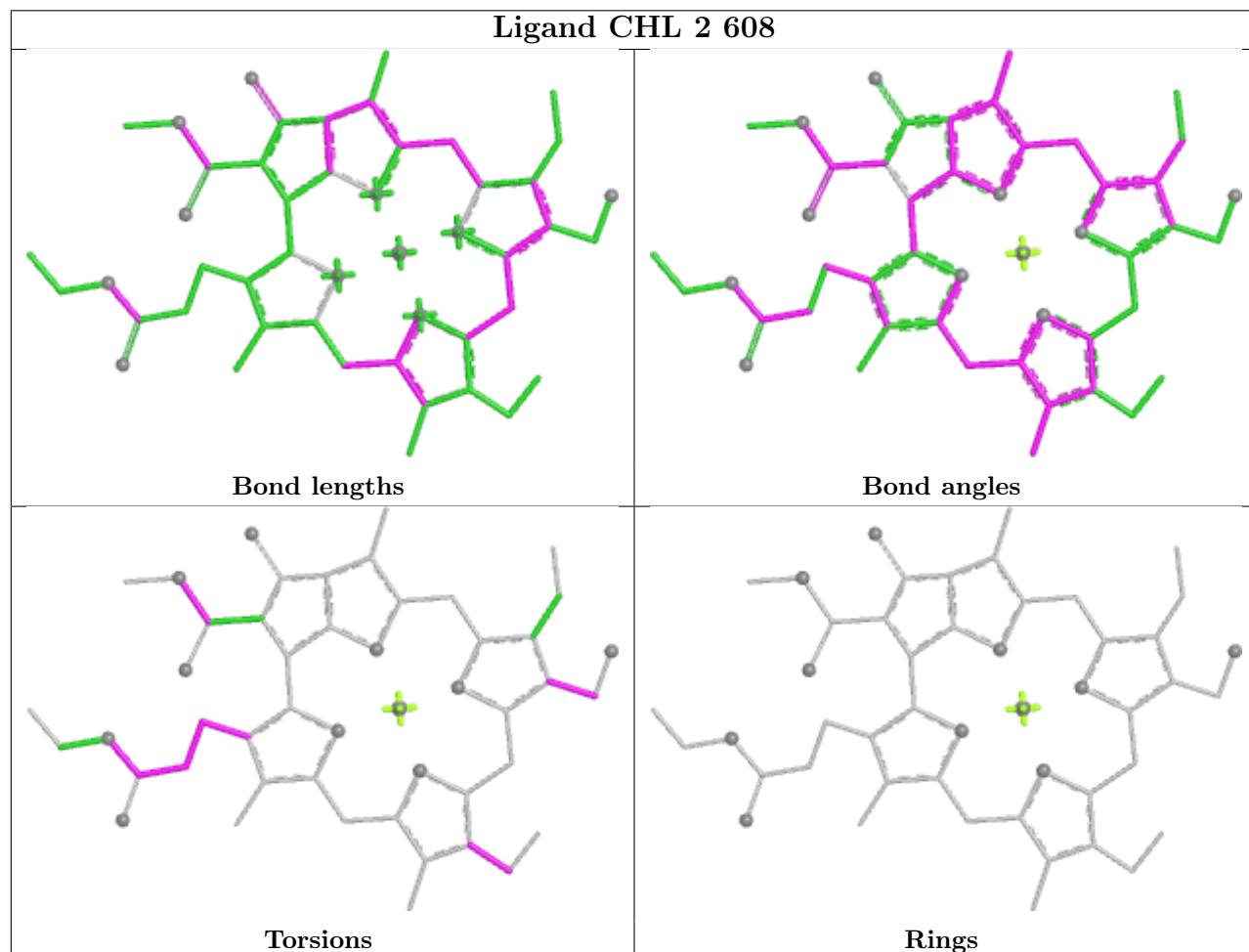
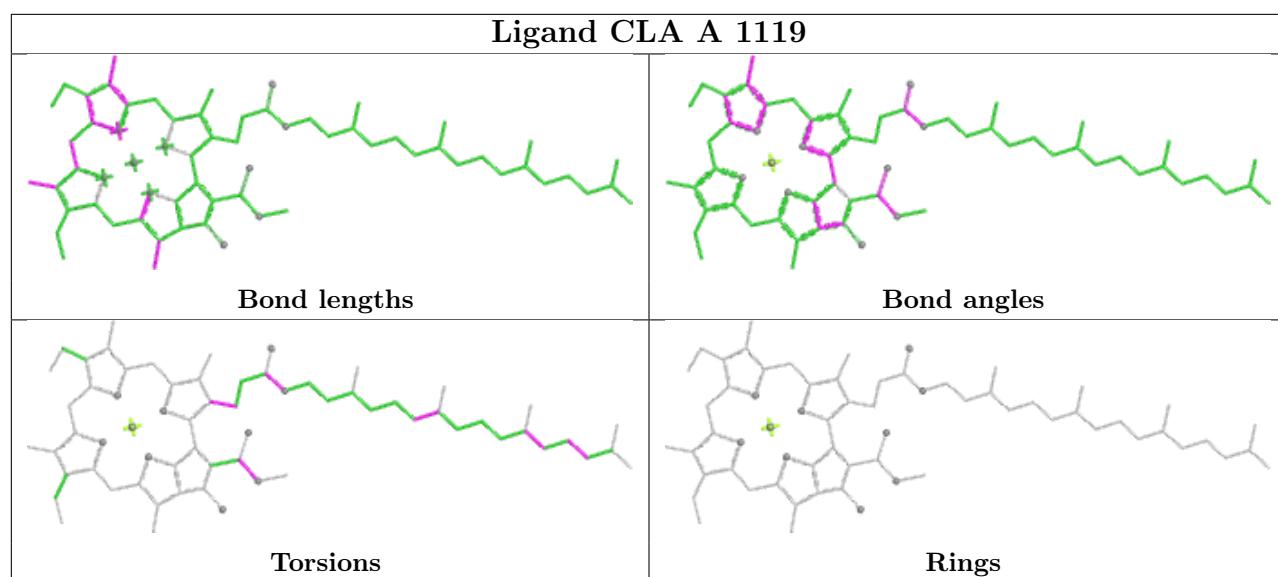
Rings

Ligand CLA A 1108

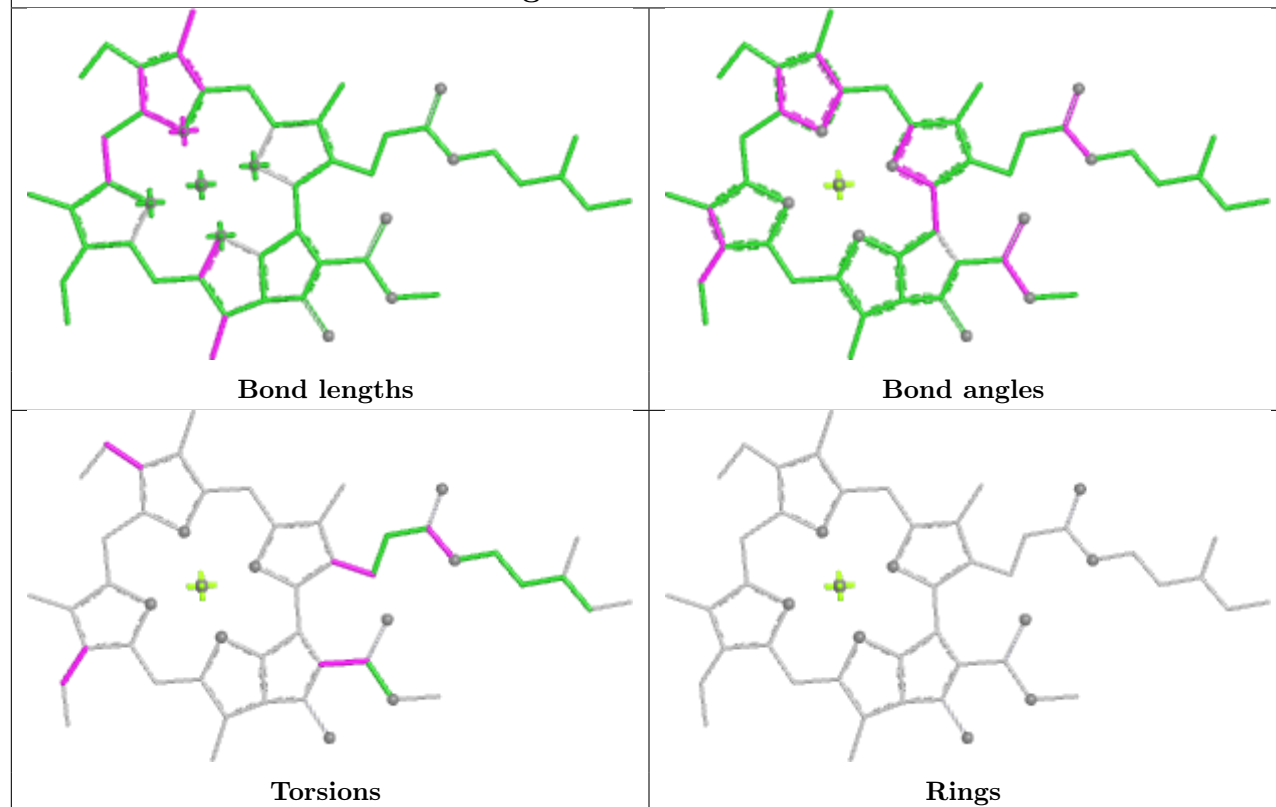


Ligand BCR A 4007

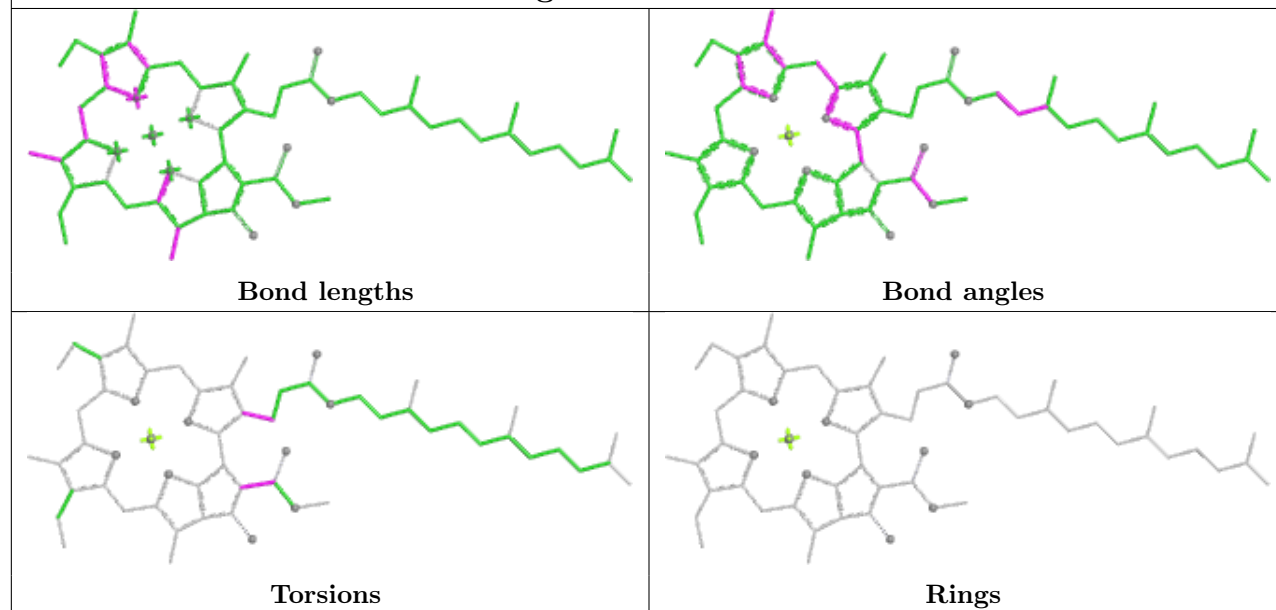




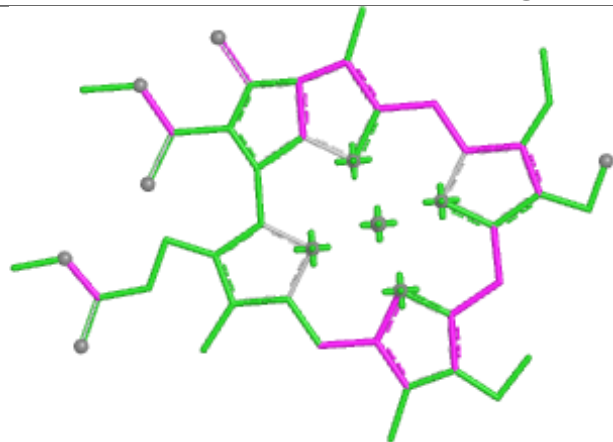
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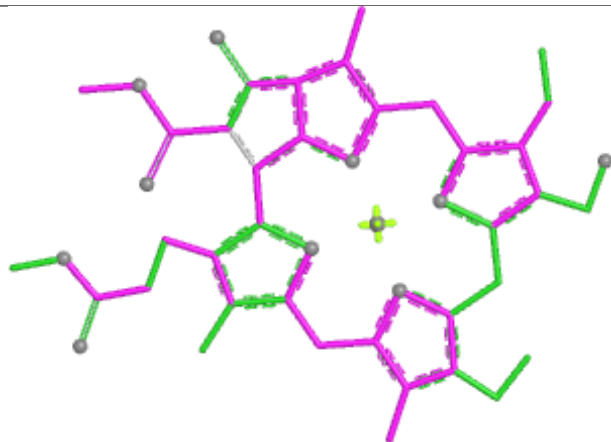
Ligand CLA 1 602



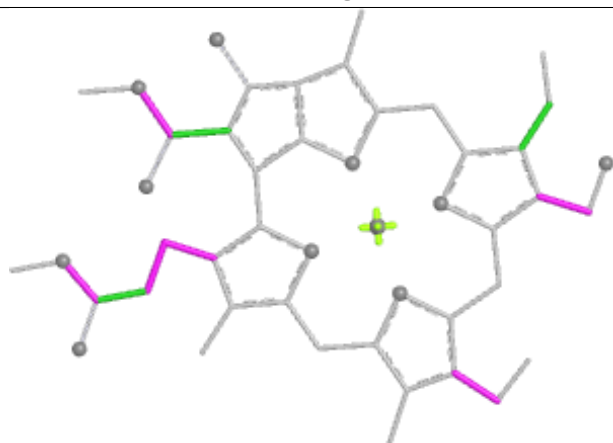
Ligand CHL 2 607



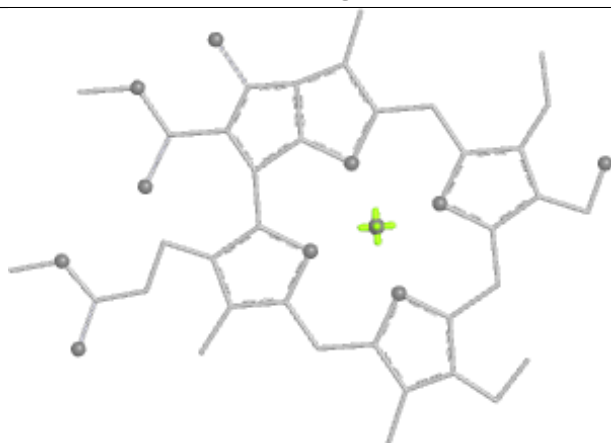
Bond lengths



Bond angles

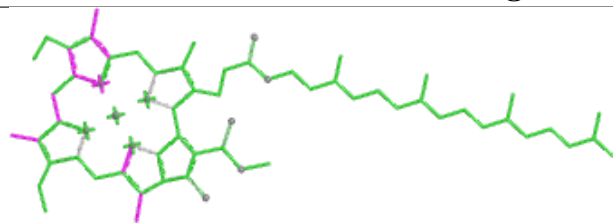


Torsions

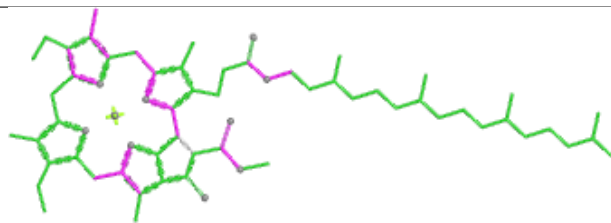


Rings

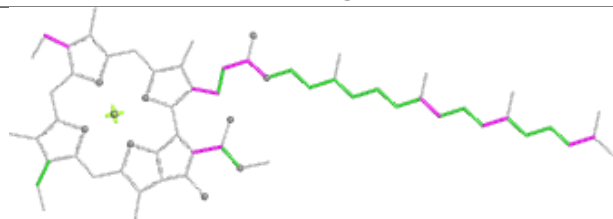
Ligand CLA B 1240



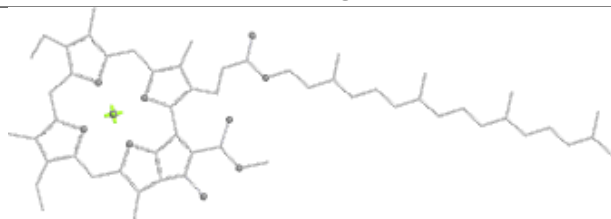
Bond lengths



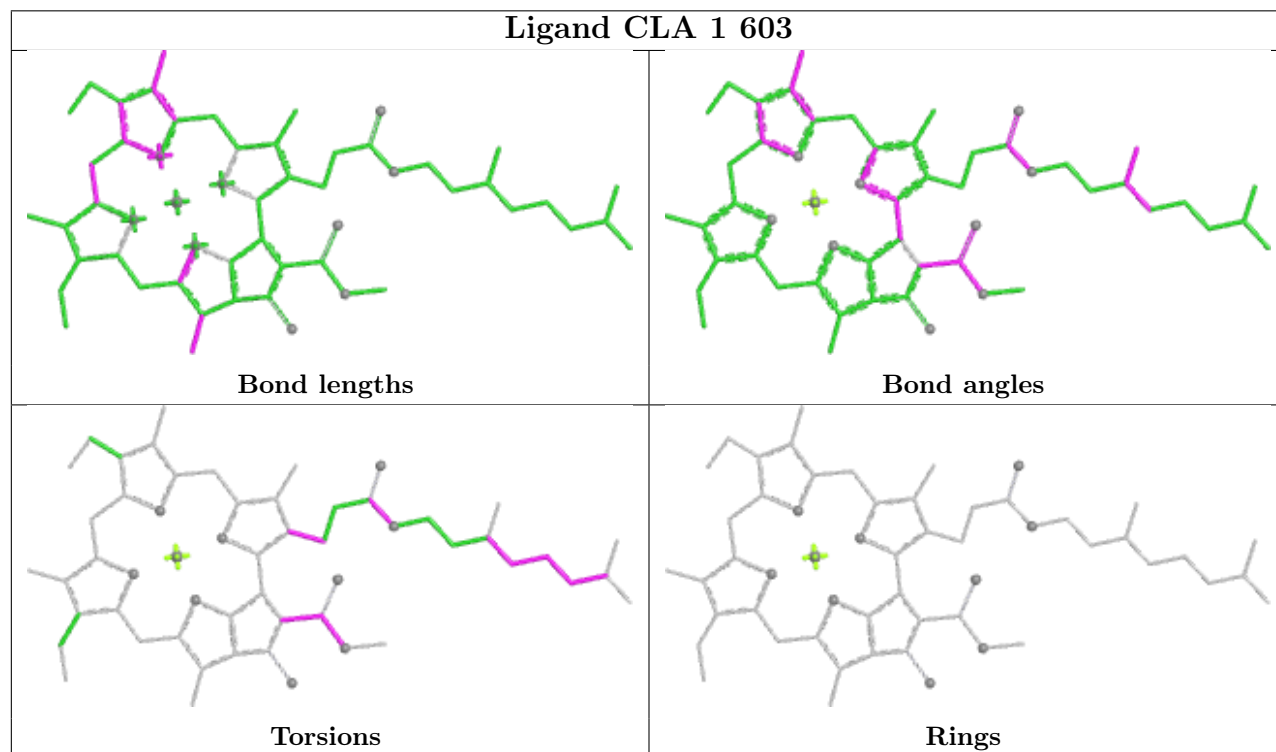
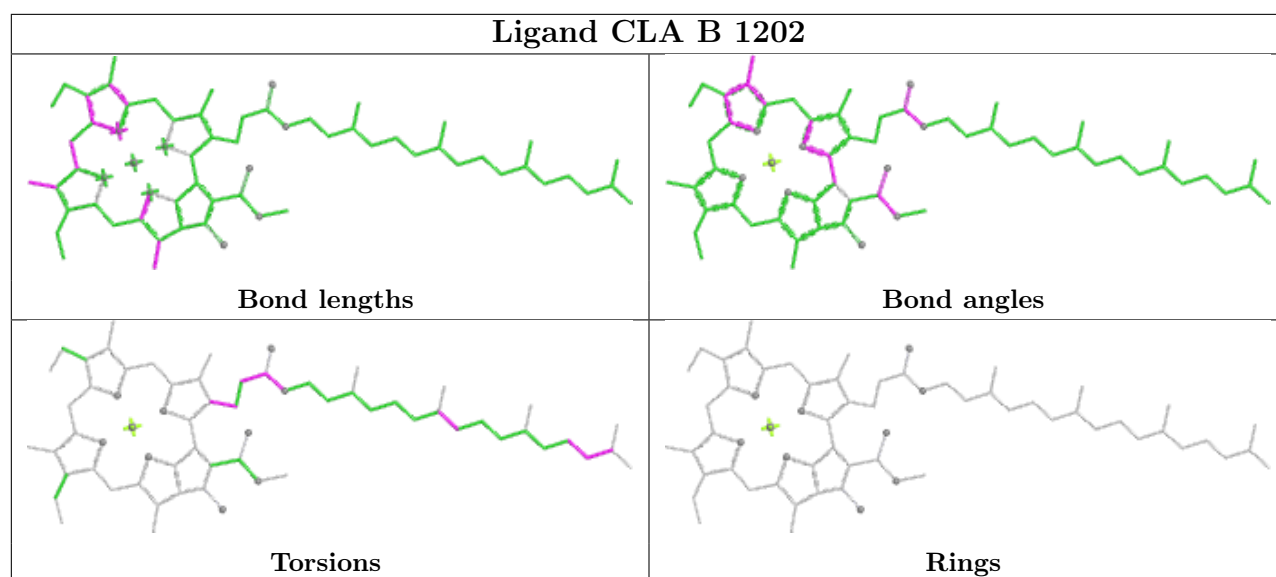
Bond angles

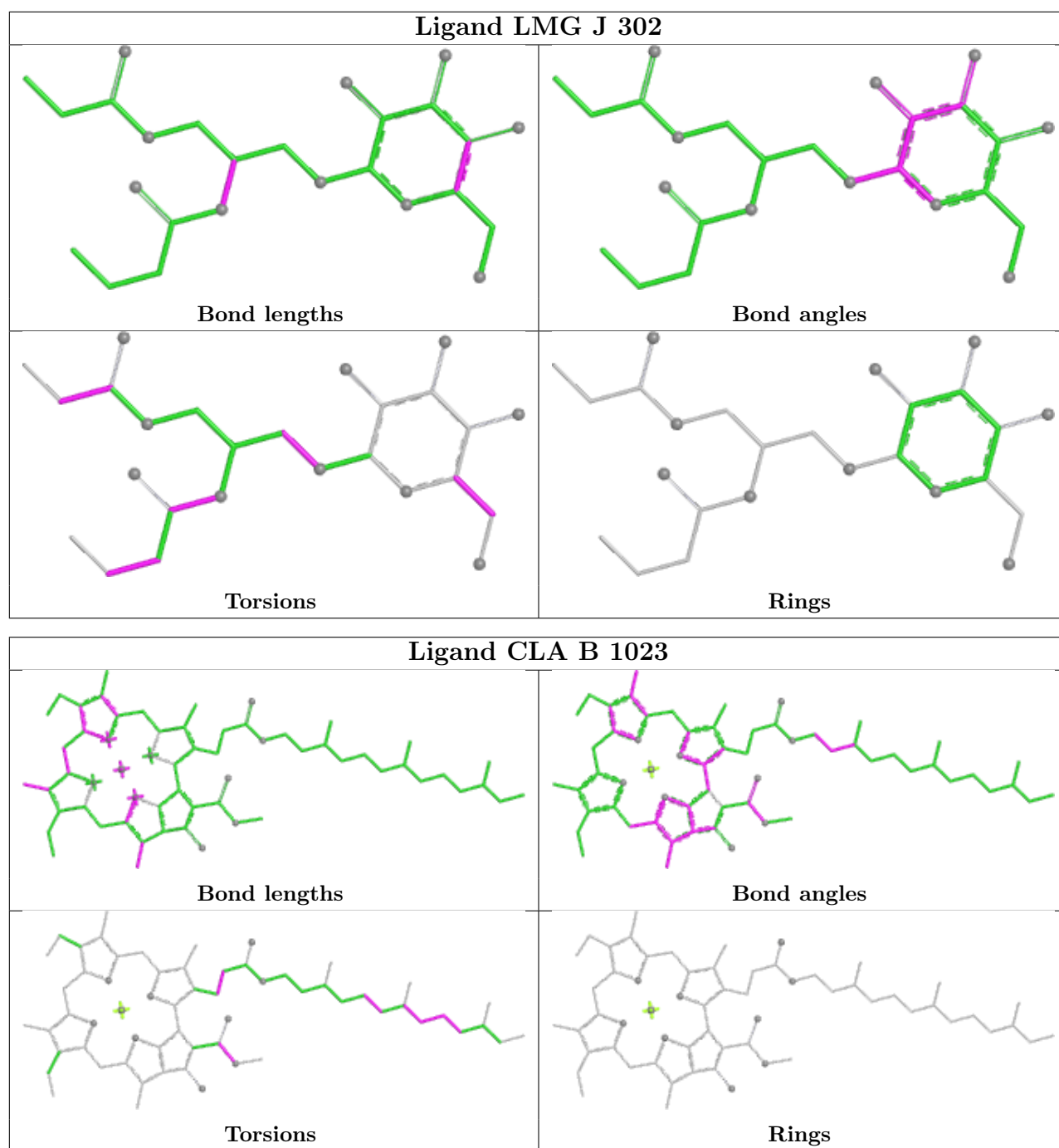


Torsions

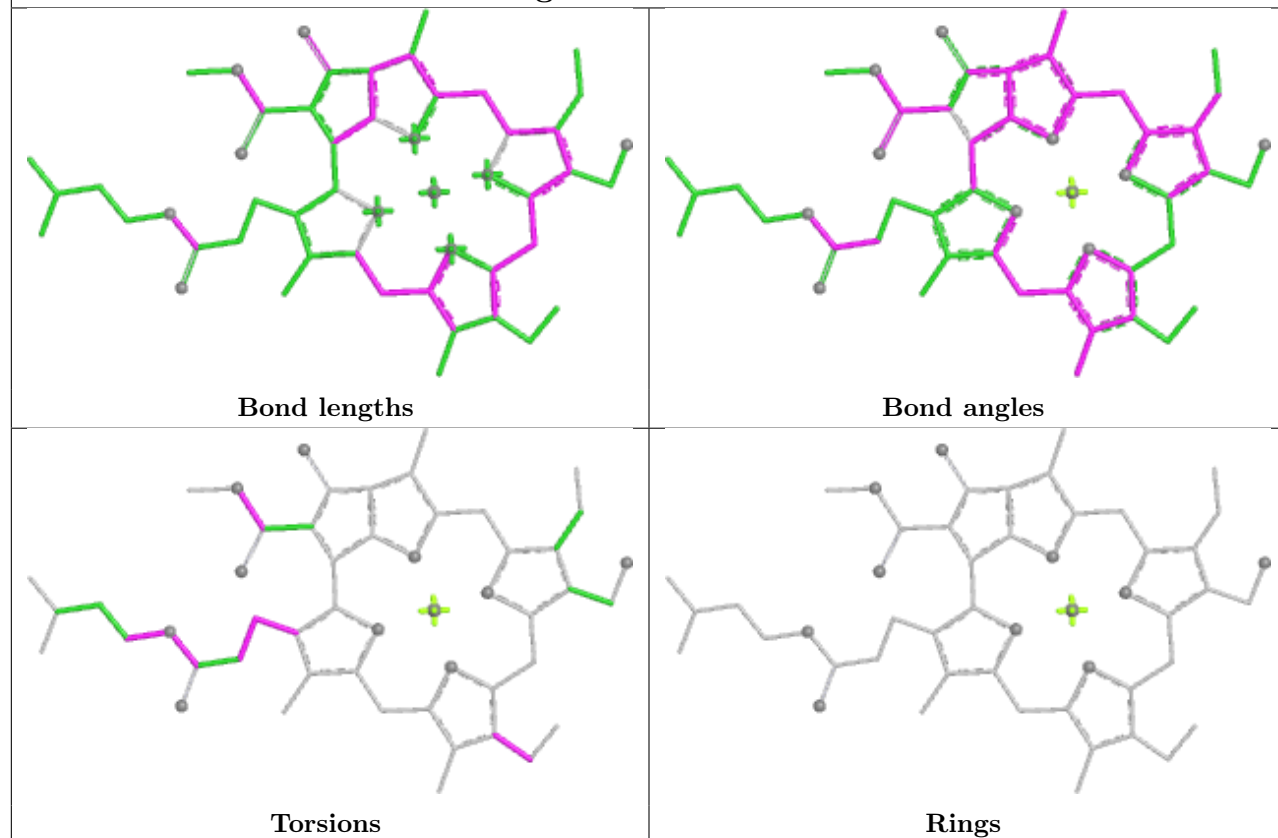


Rings

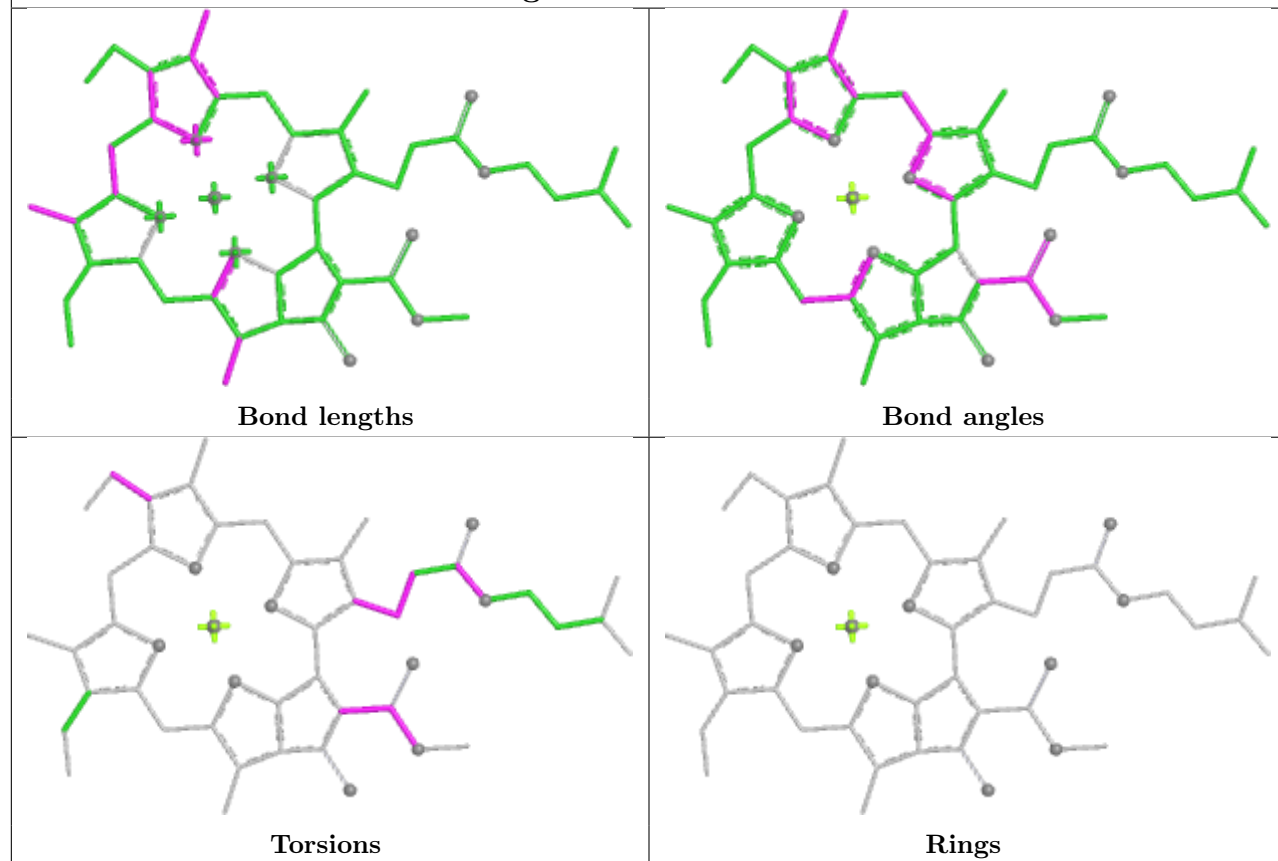


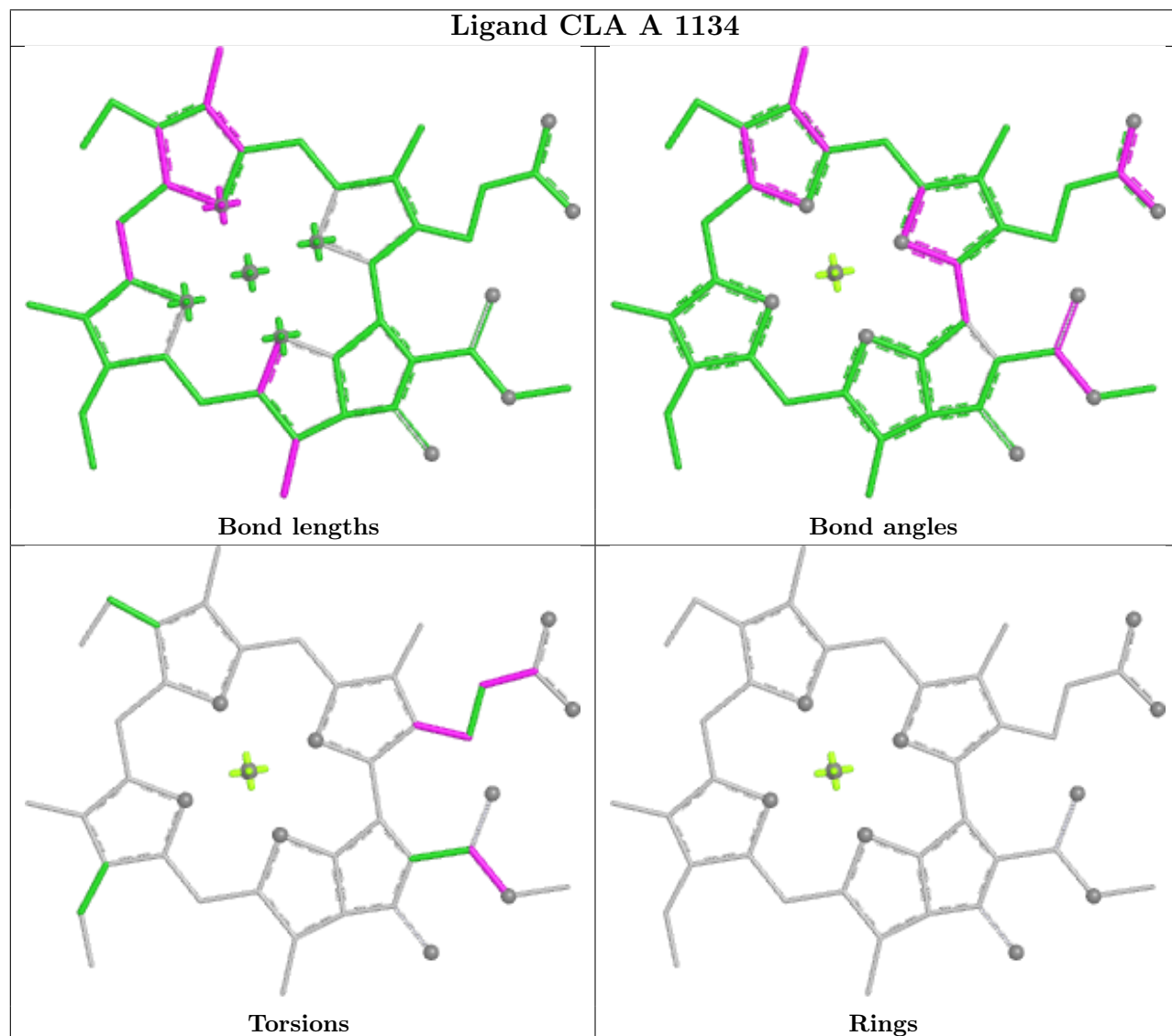
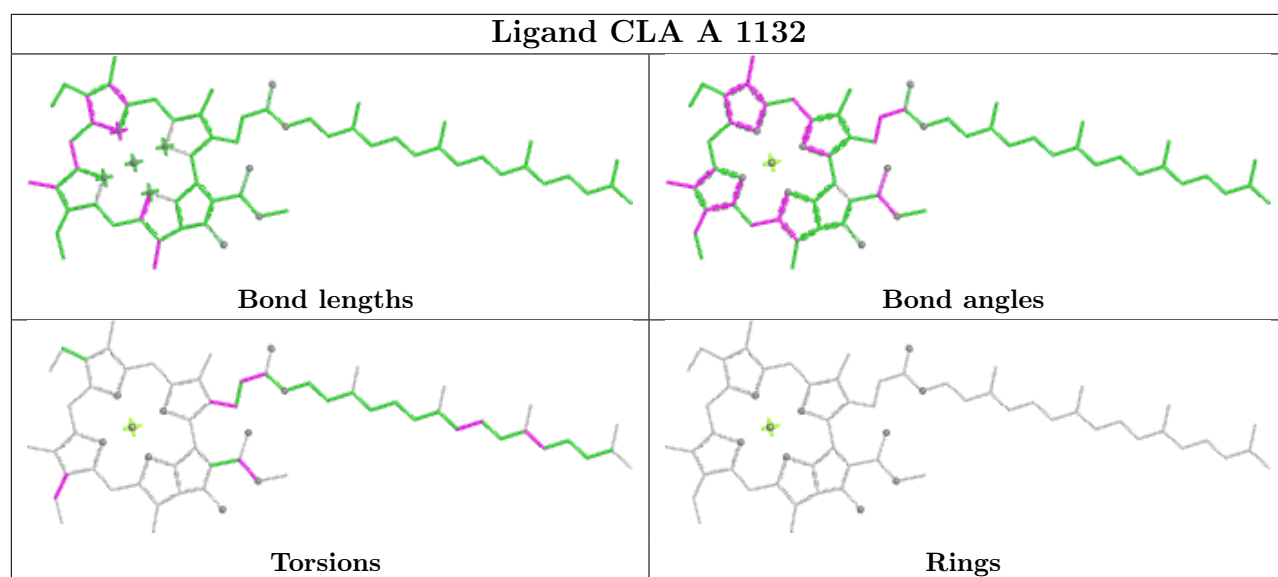


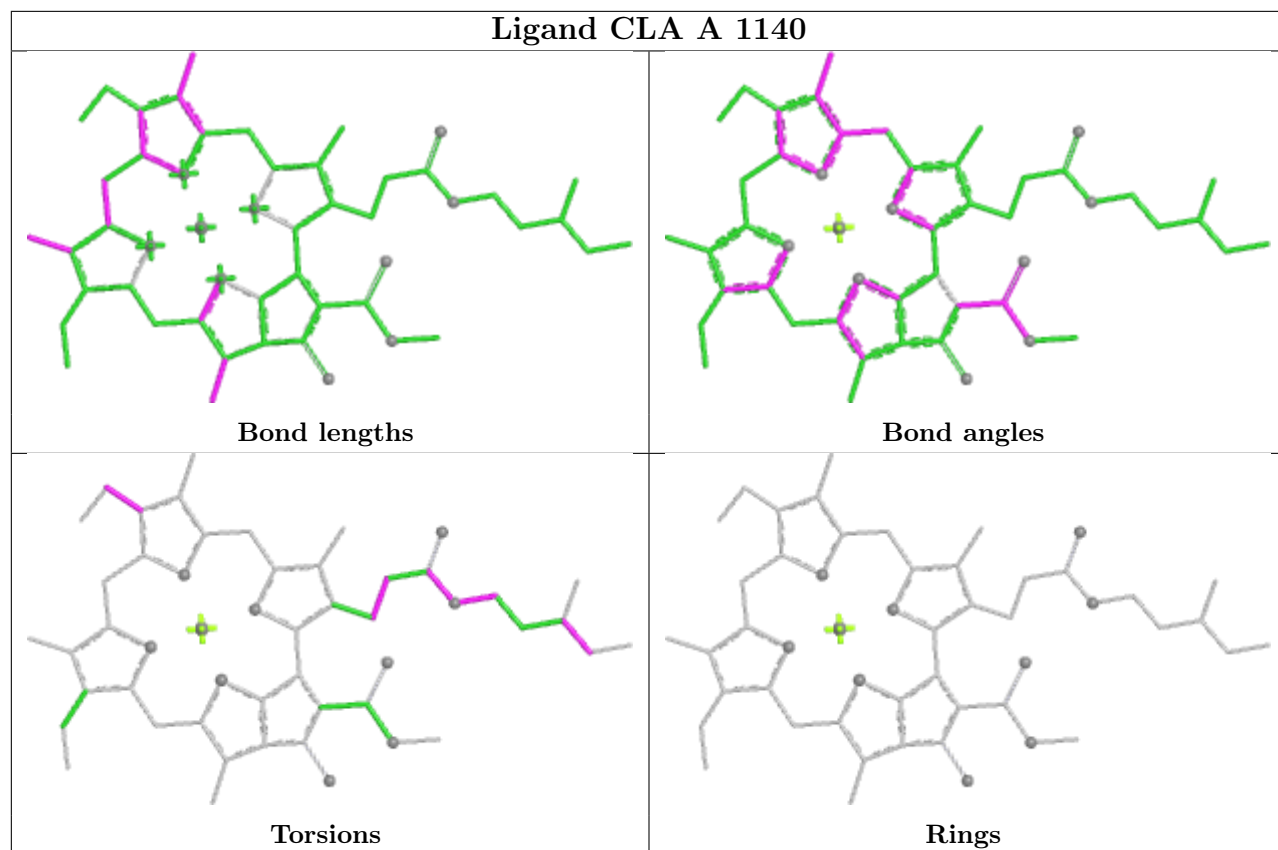
Ligand CHL 4 608

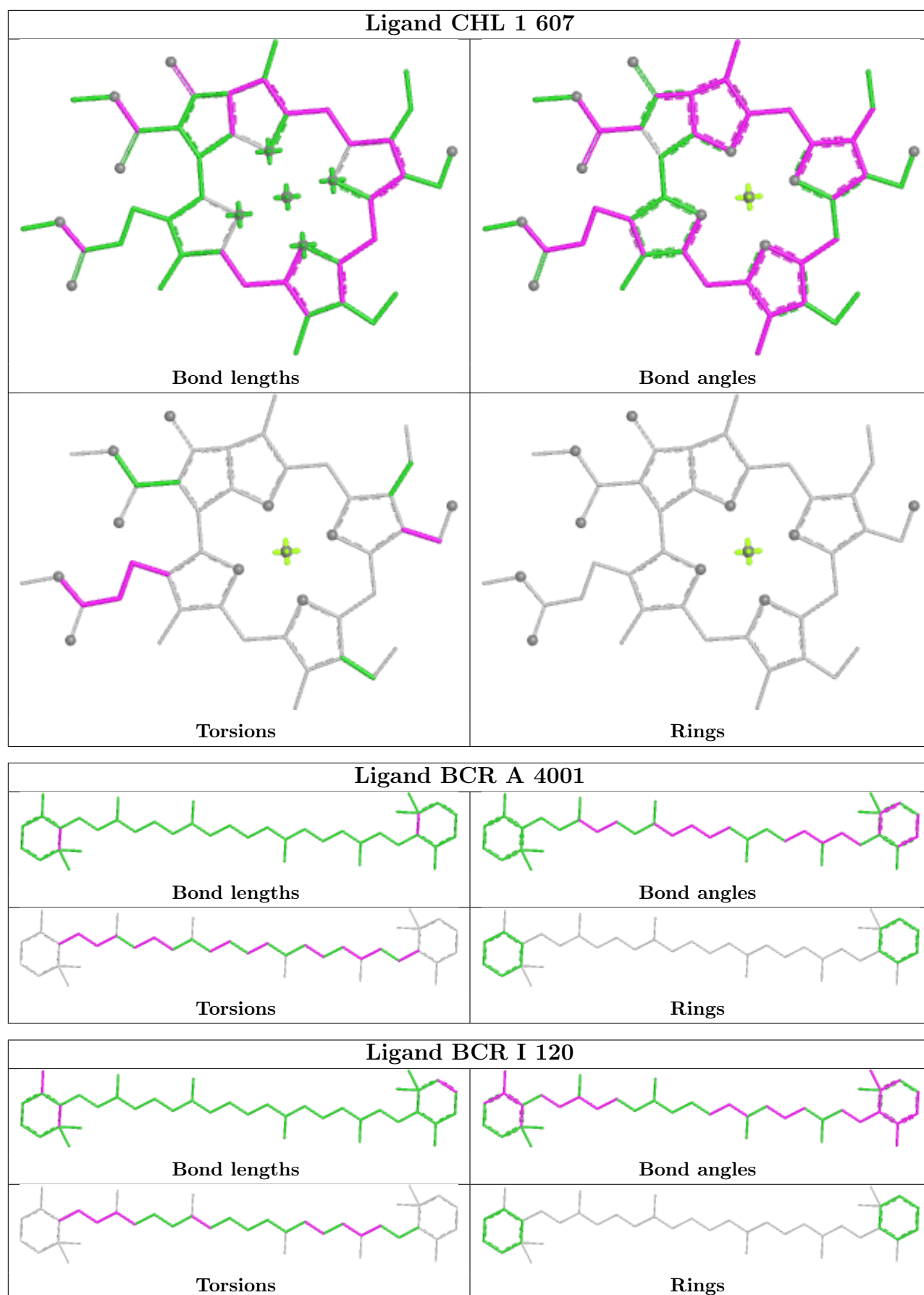


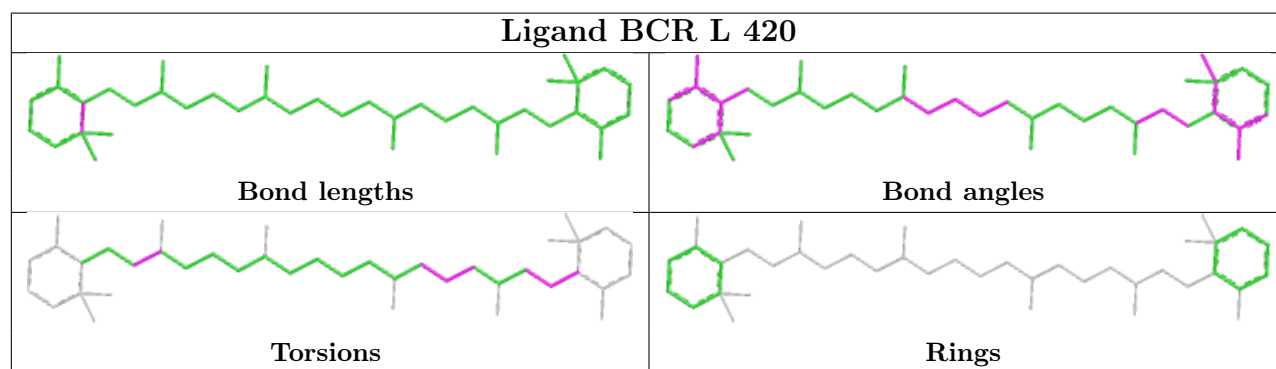
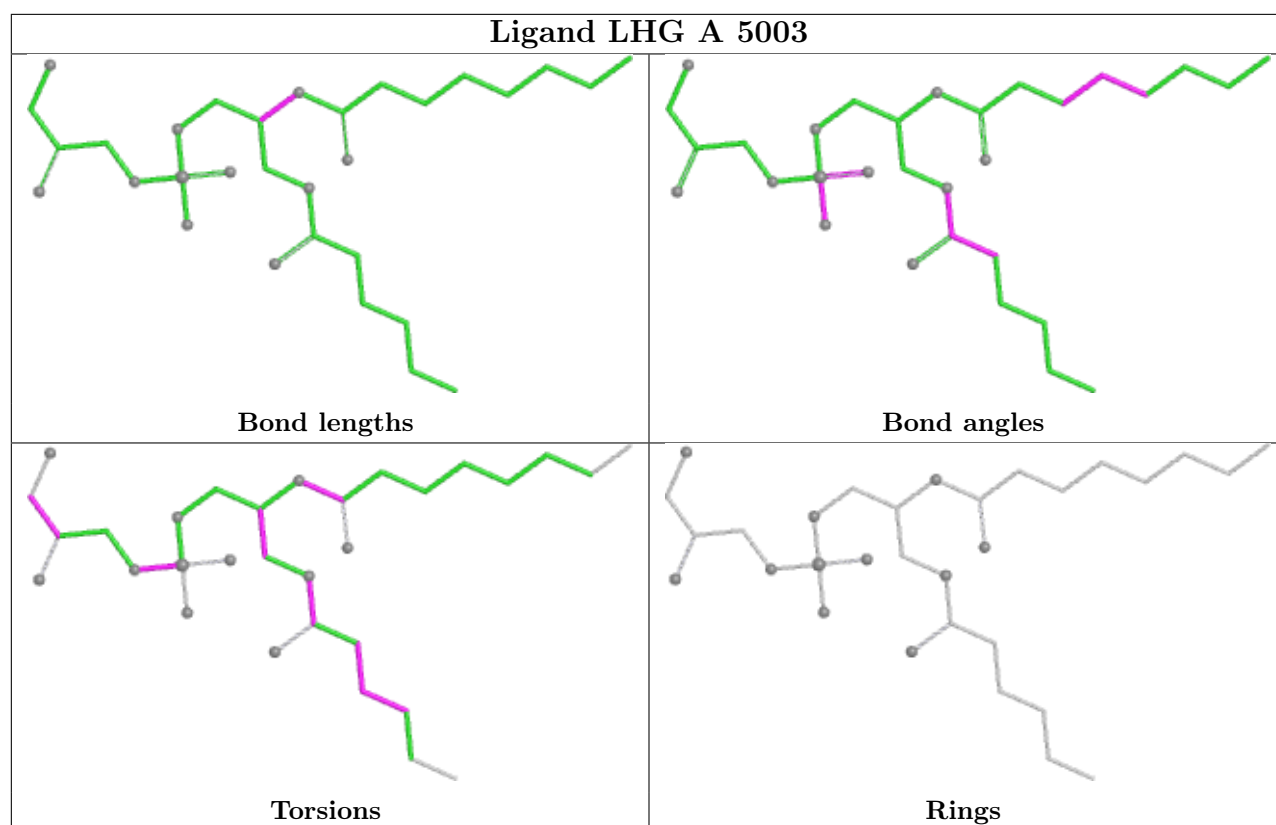
Ligand CLA A 1101

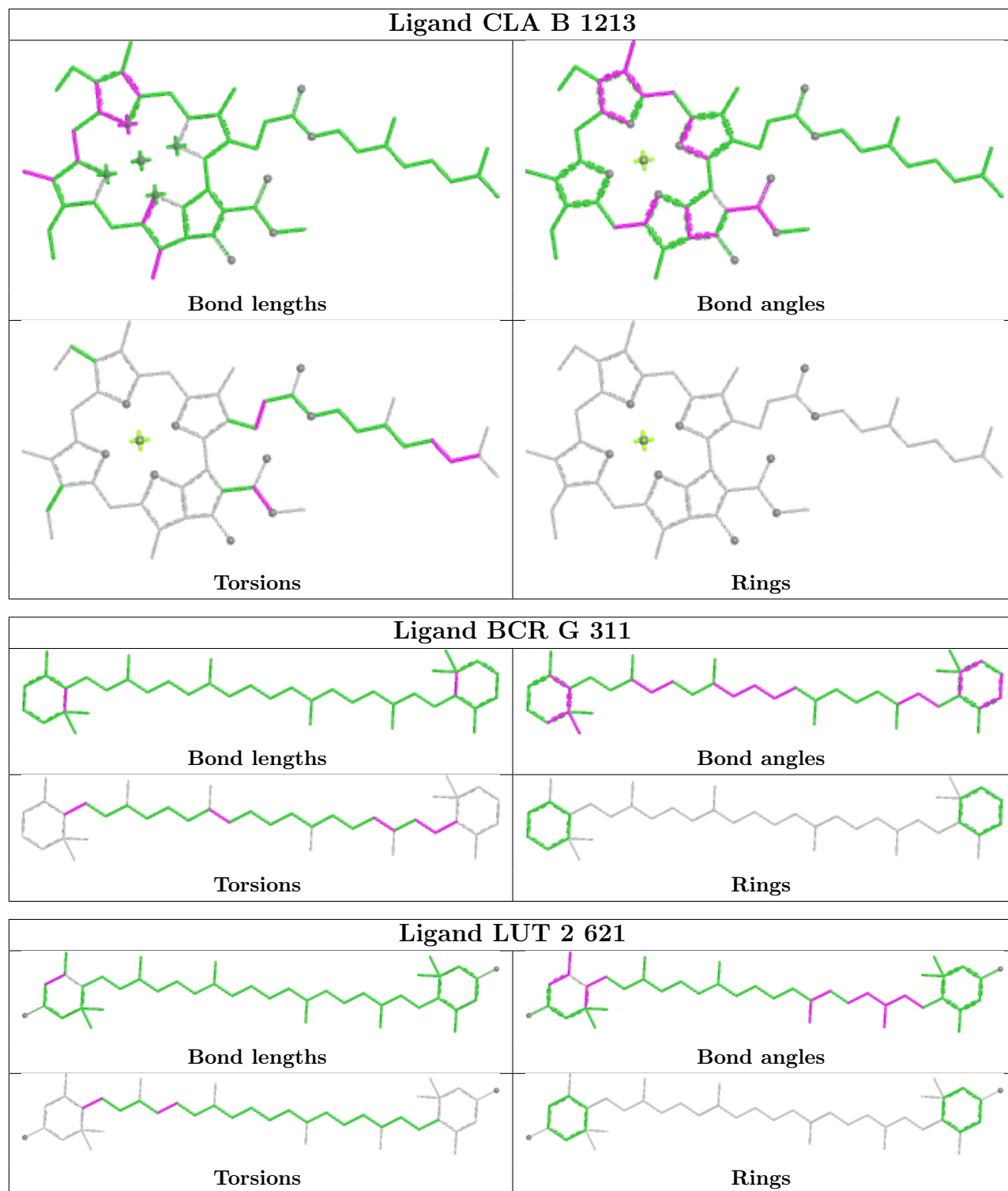


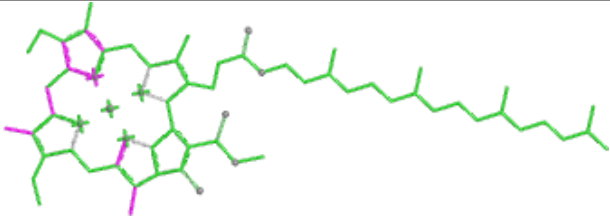
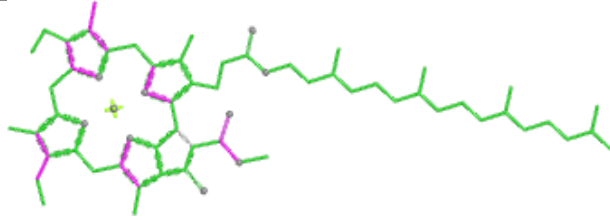
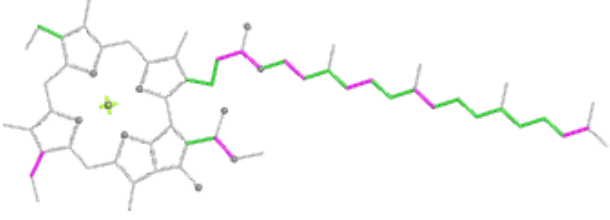
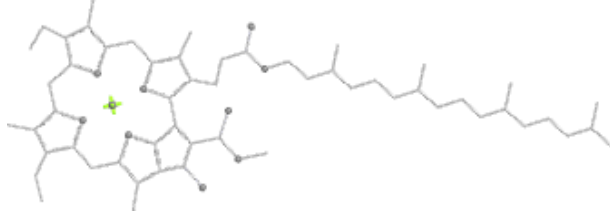
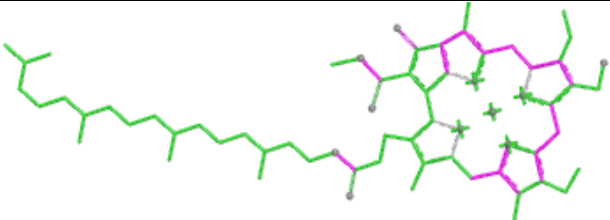
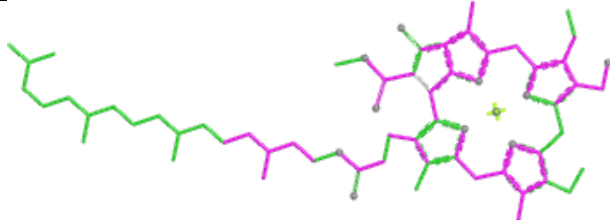
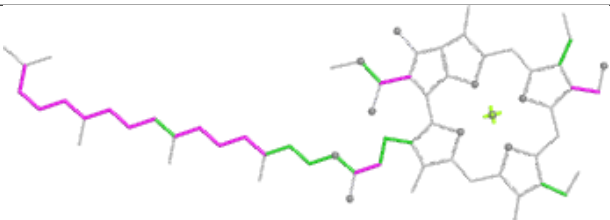
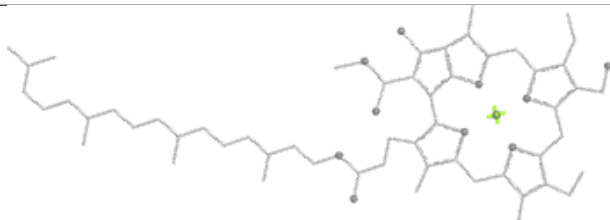
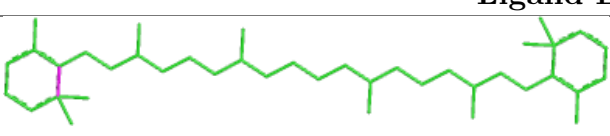
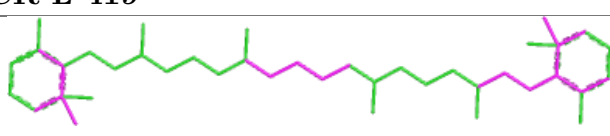
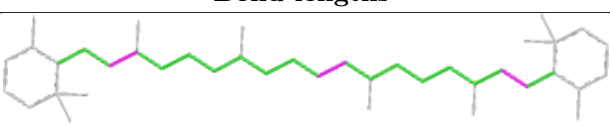
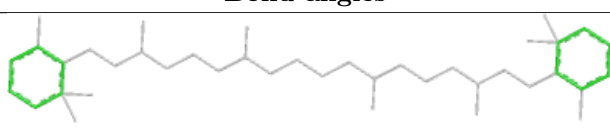


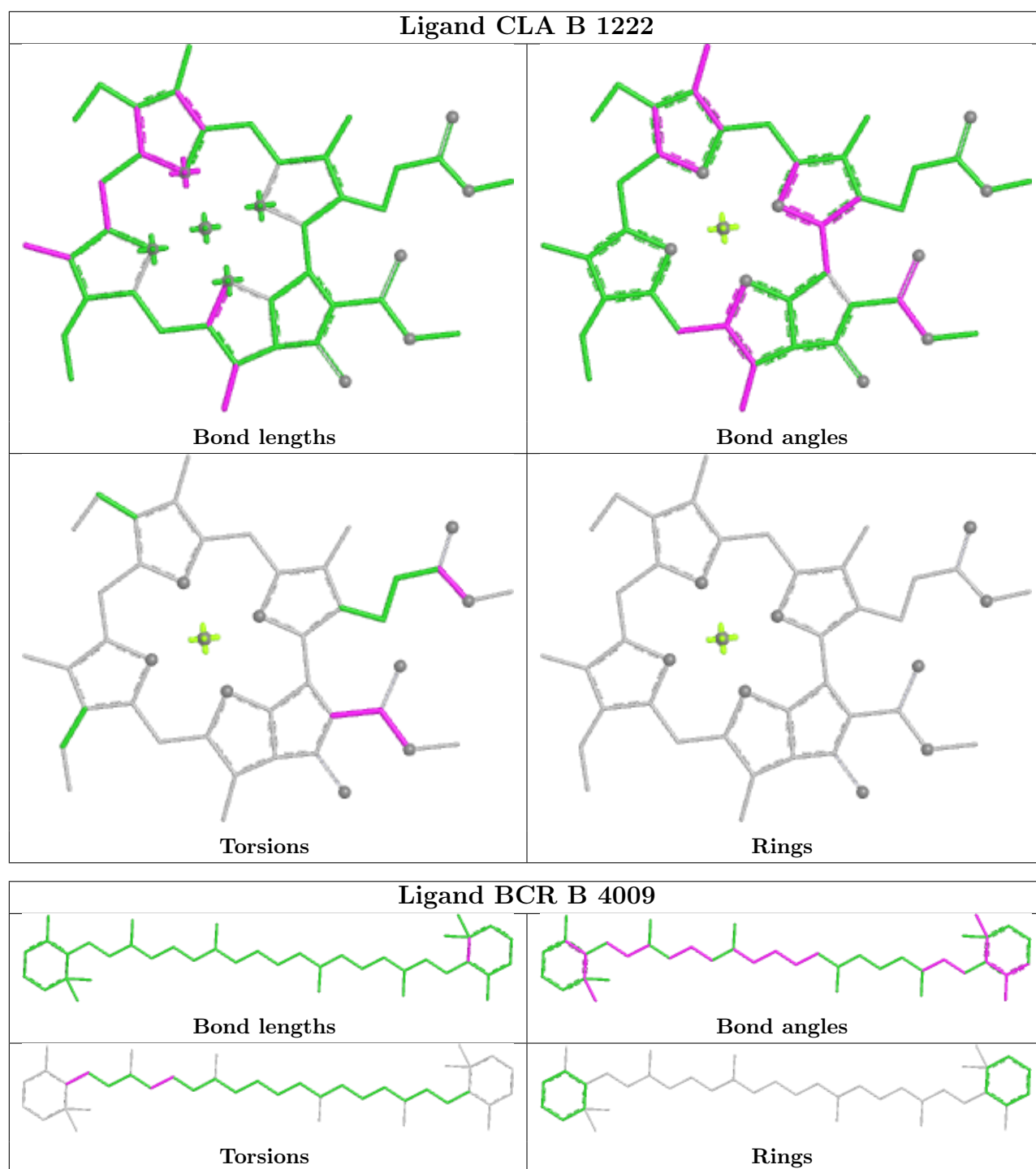


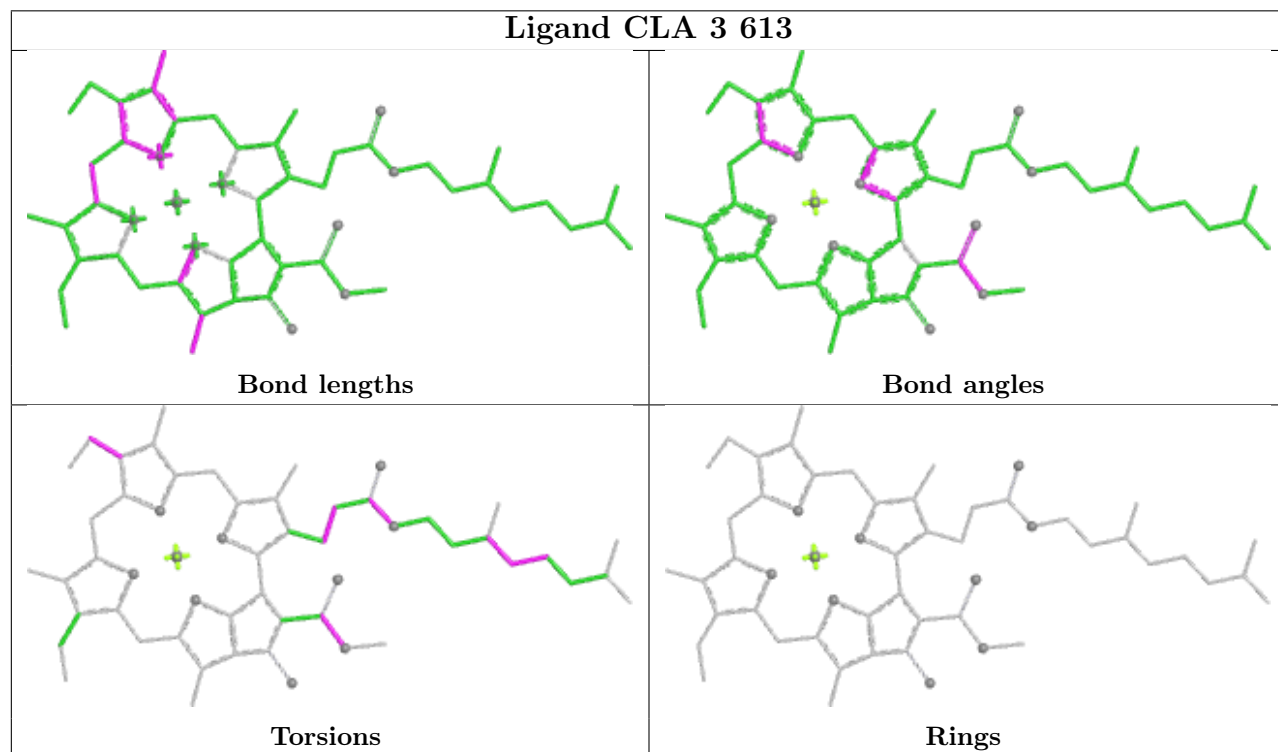
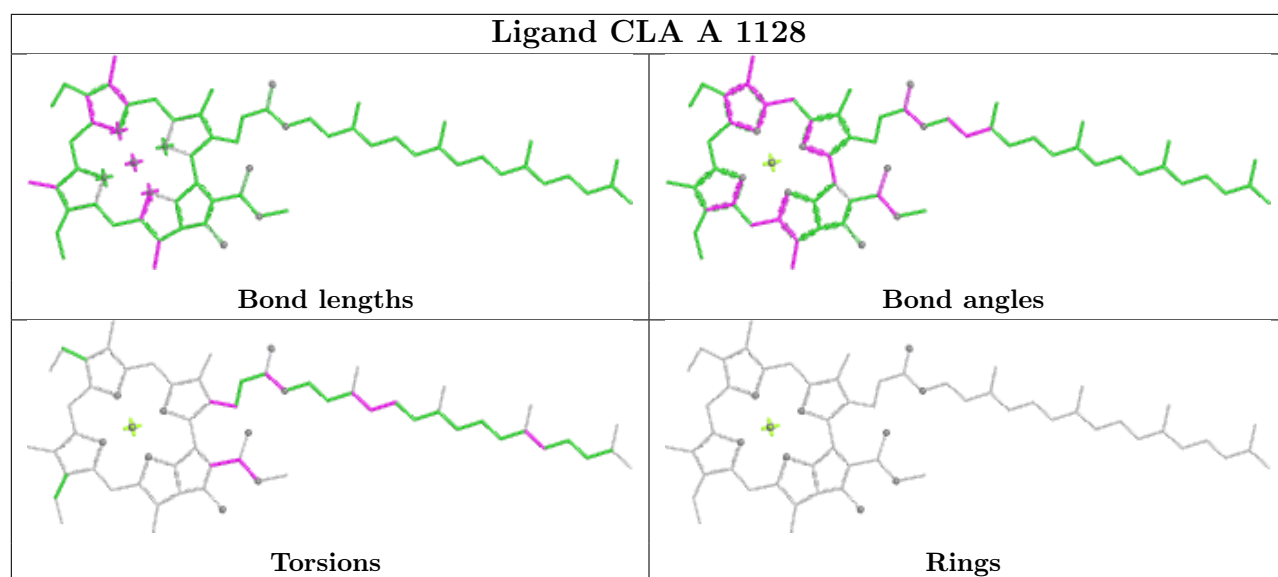


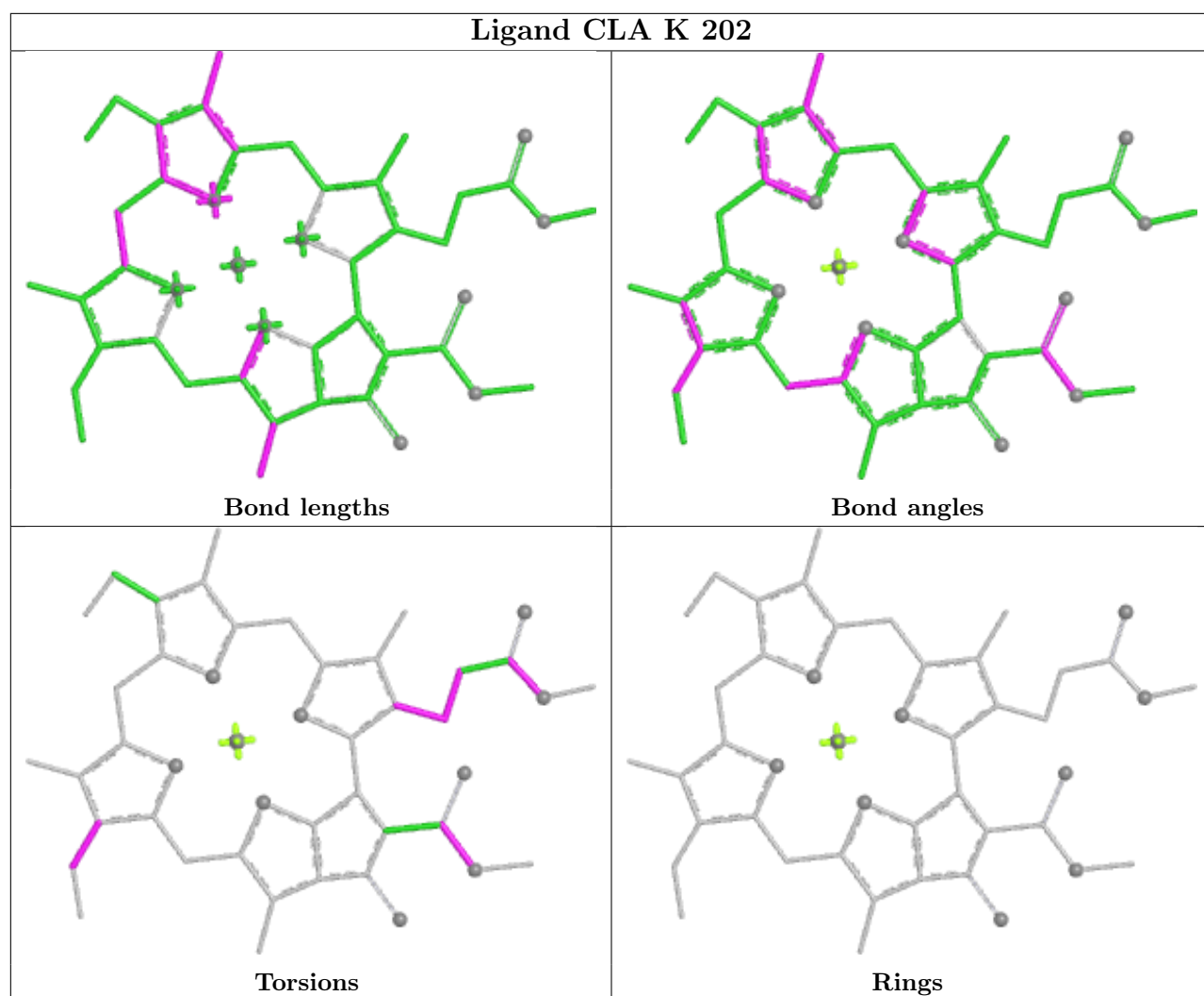




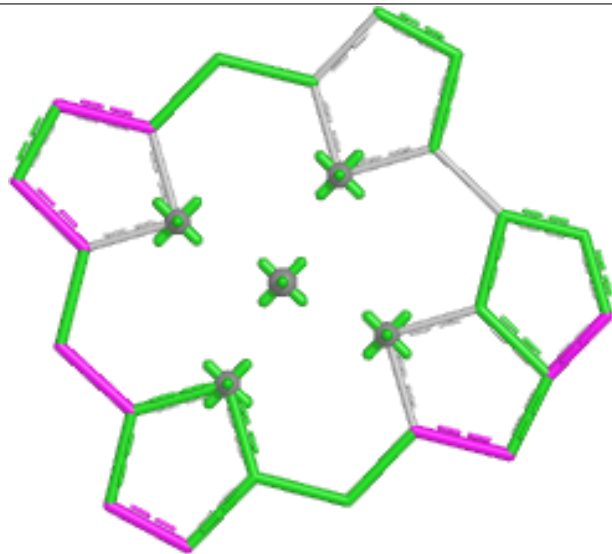
Ligand CLA I 121	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand CHL 2 601	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR L 419	
 Bond lengths	 Bond angles
 Torsions	 Rings



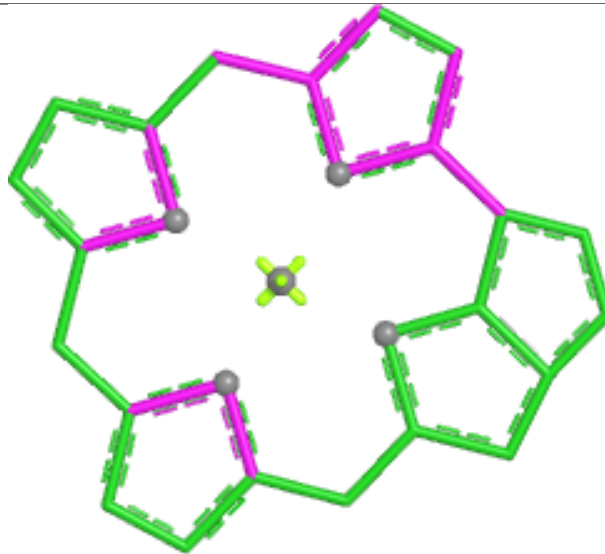




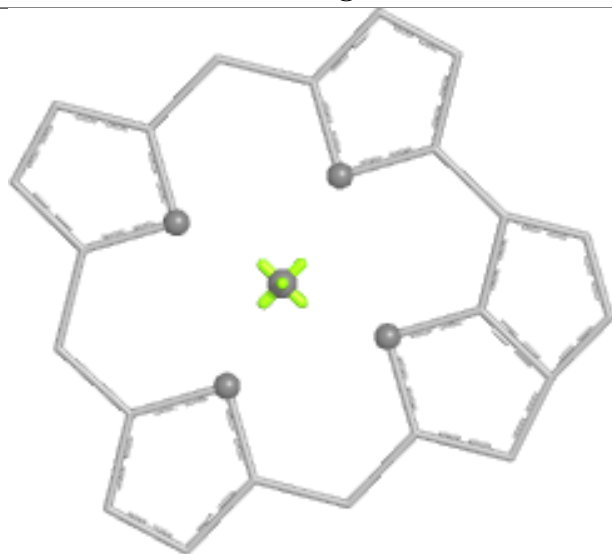
Ligand CLA K 203



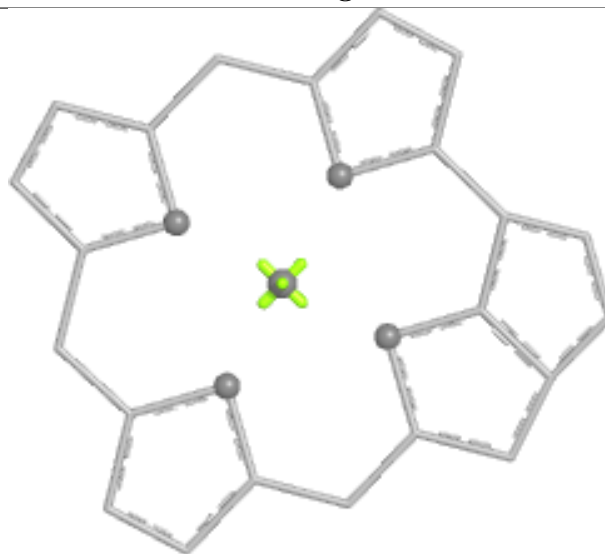
Bond lengths



Bond angles

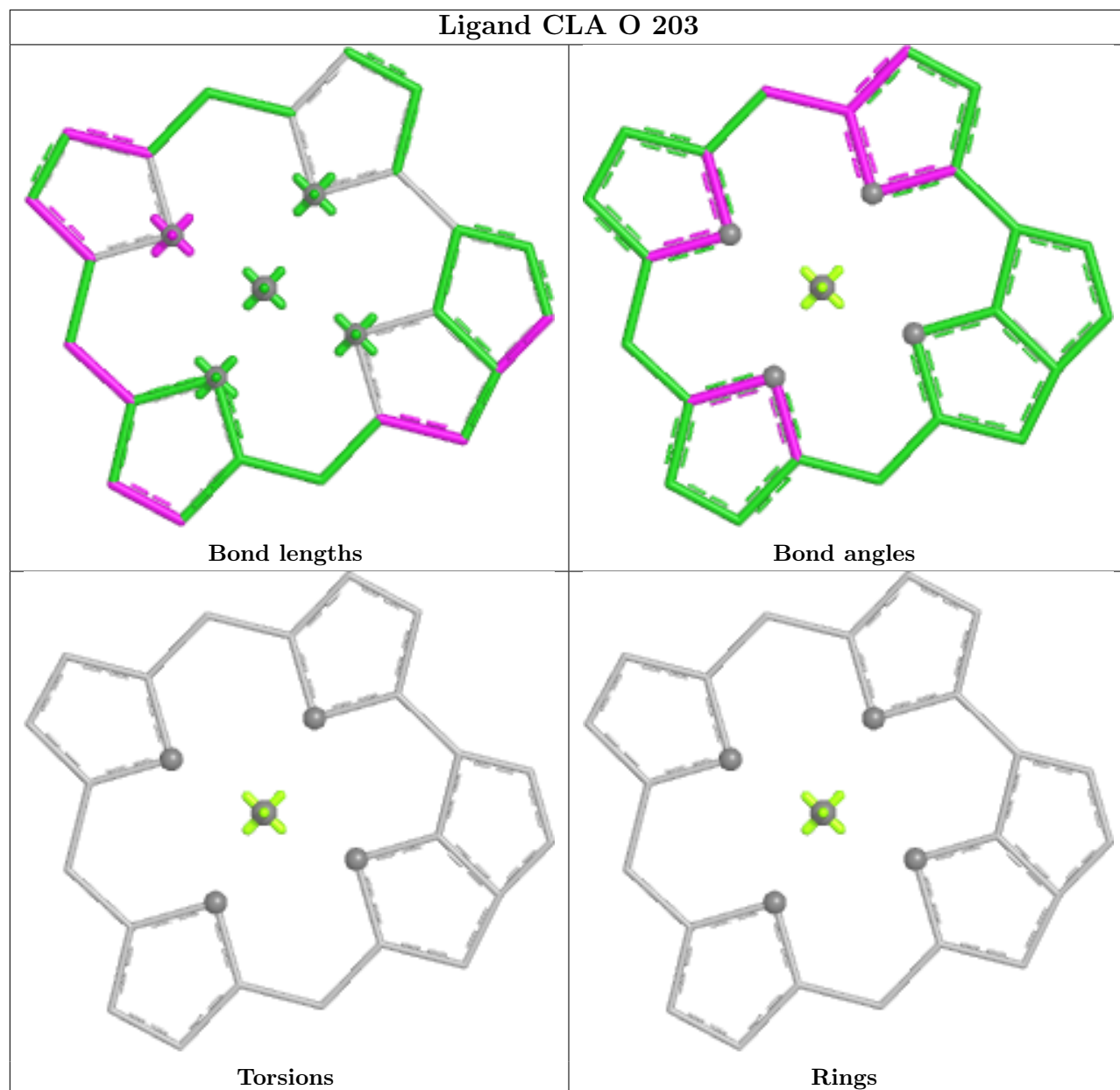


Torsions

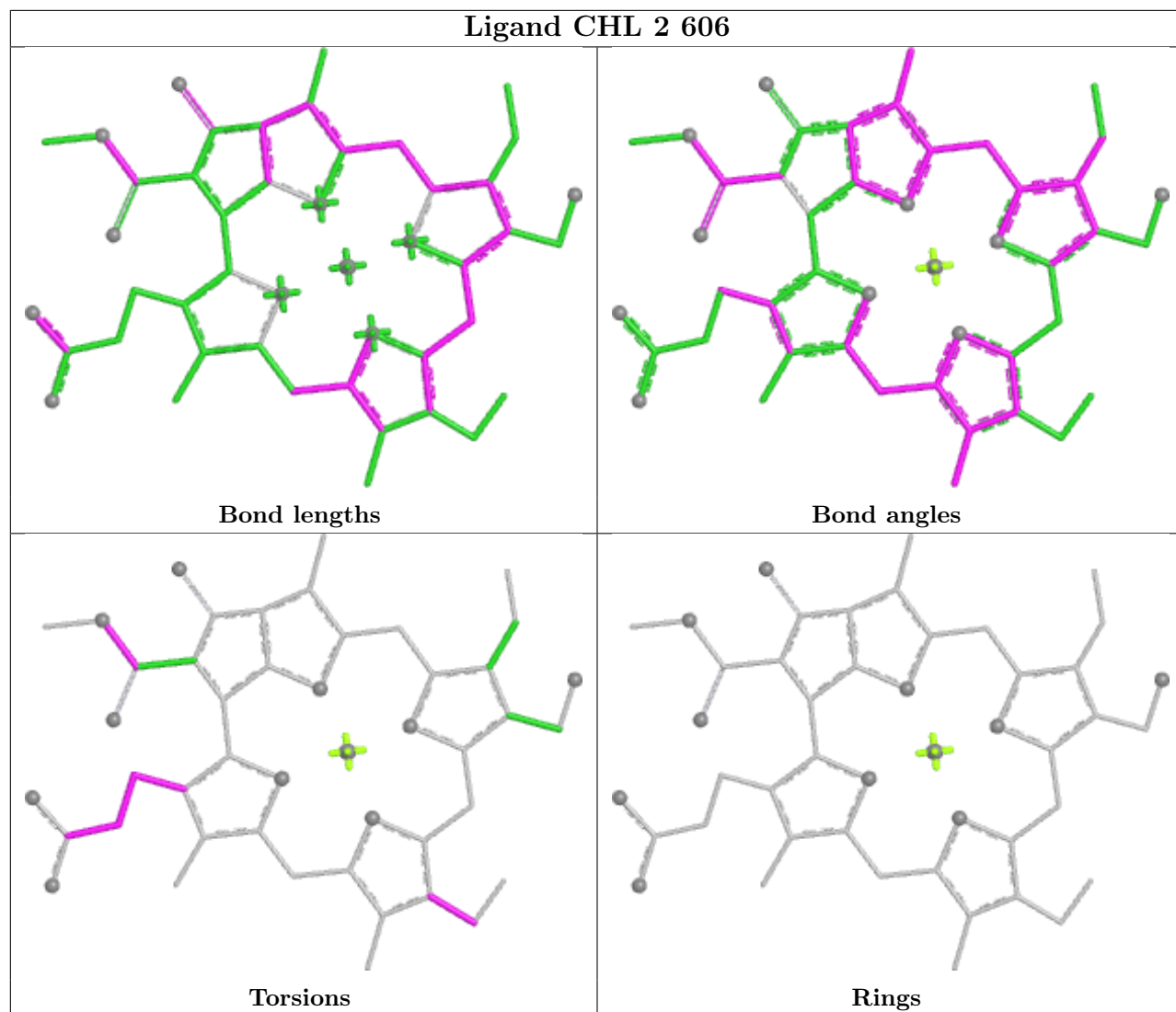


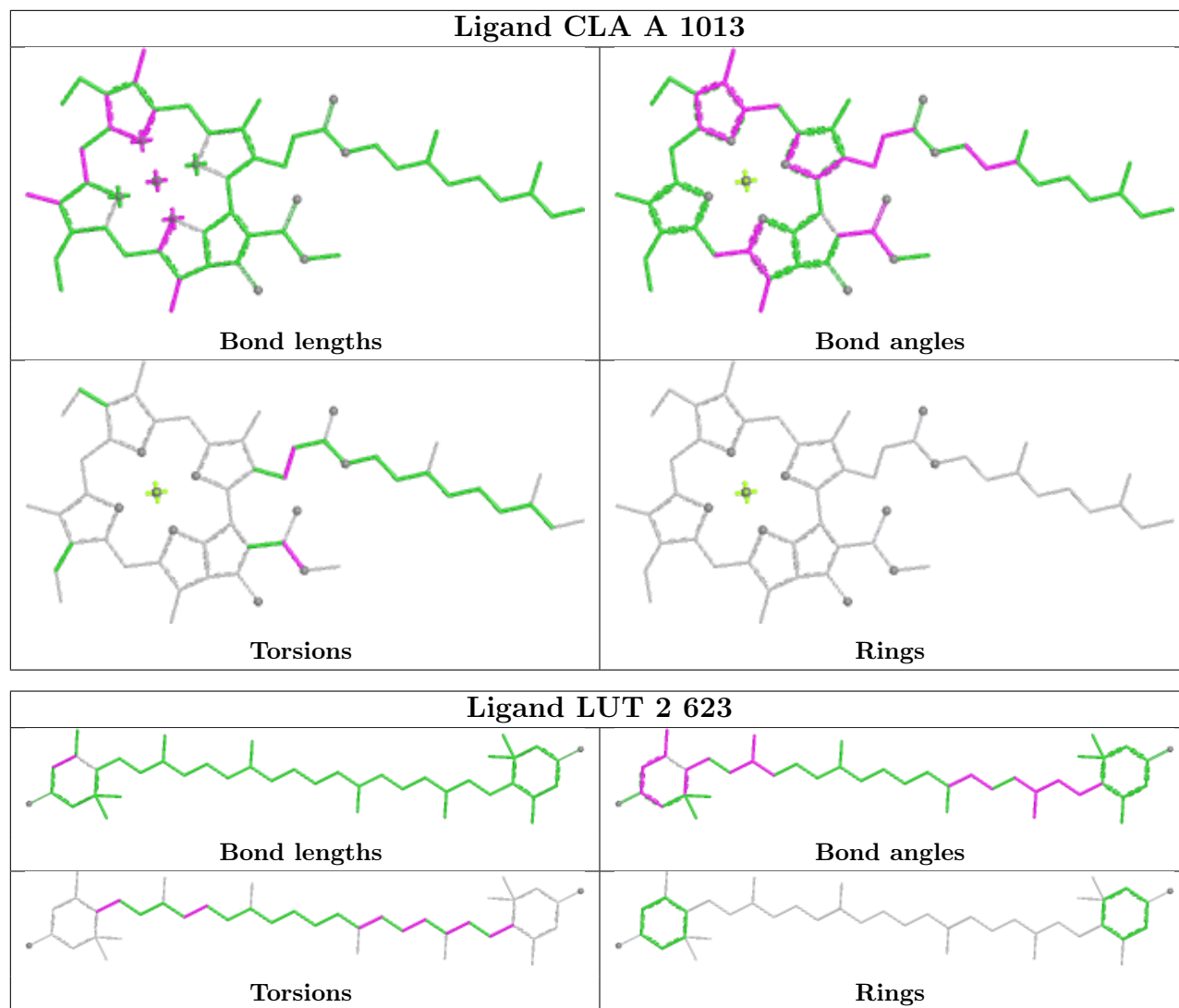
Rings

Ligand CLA O 203

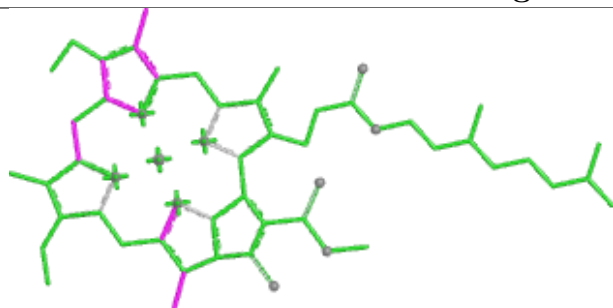


Ligand CHL 2 606

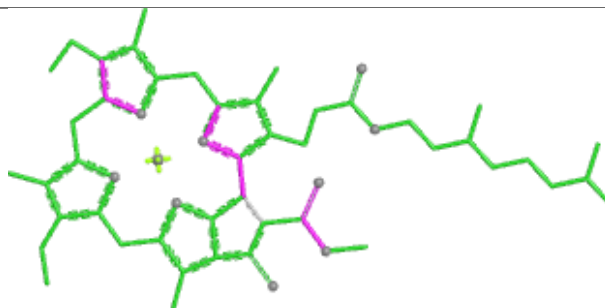




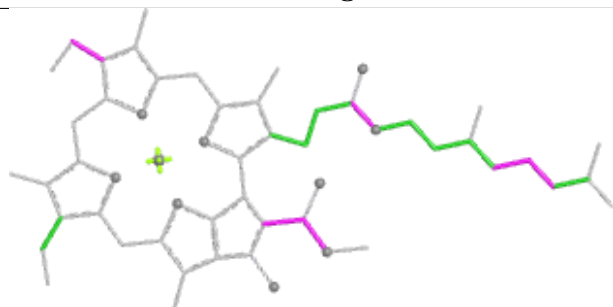
Ligand CLA G 218



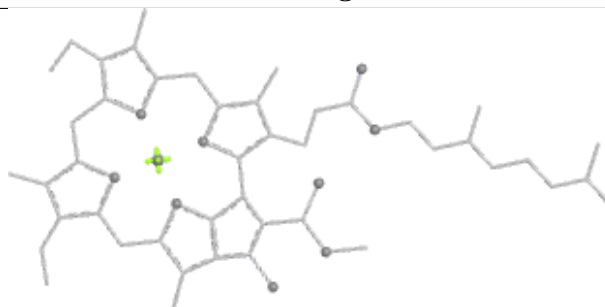
Bond lengths



Bond angles

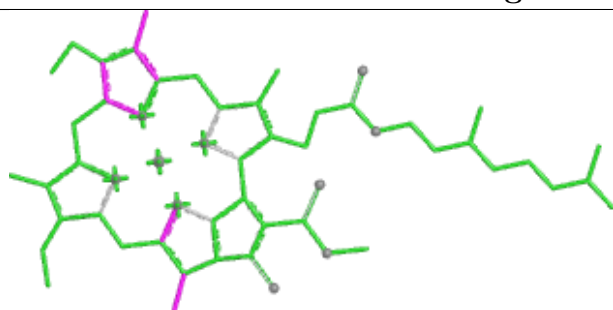


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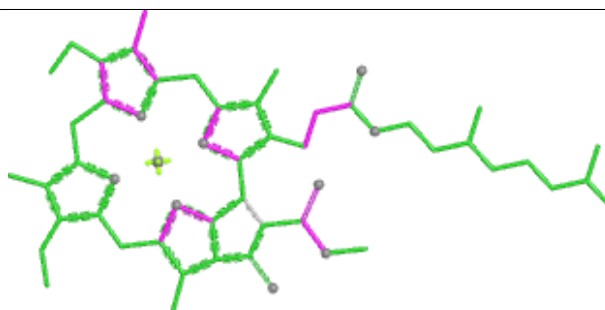


Rings

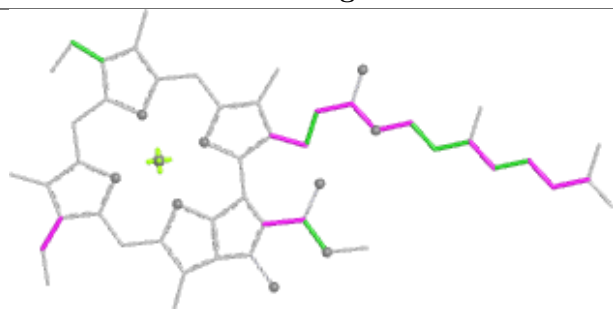
Ligand CLA A 1118



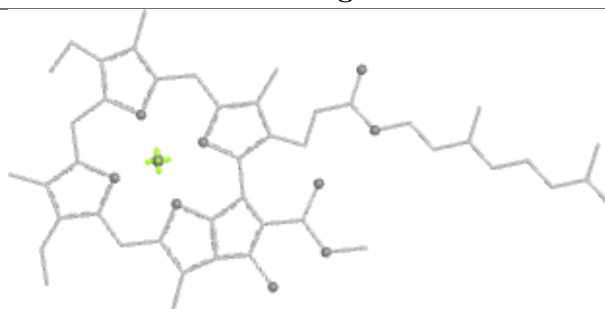
Bond lengths



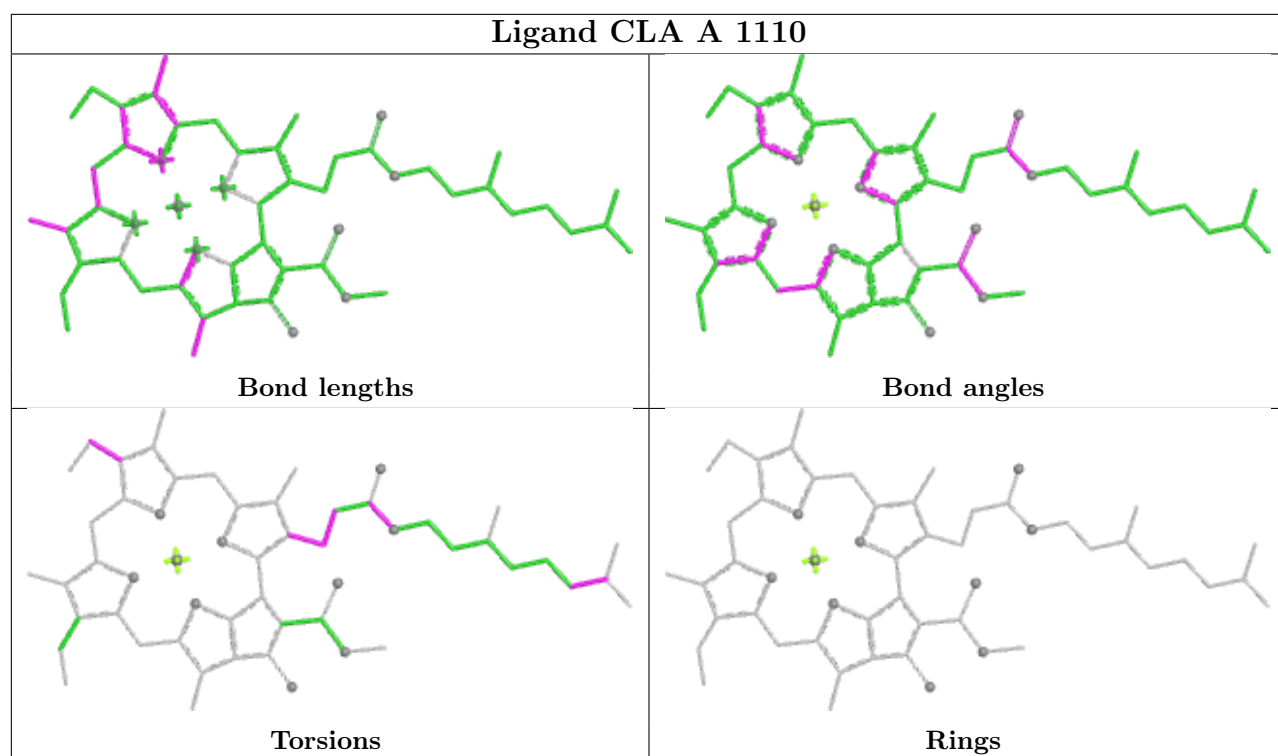
Bond angles

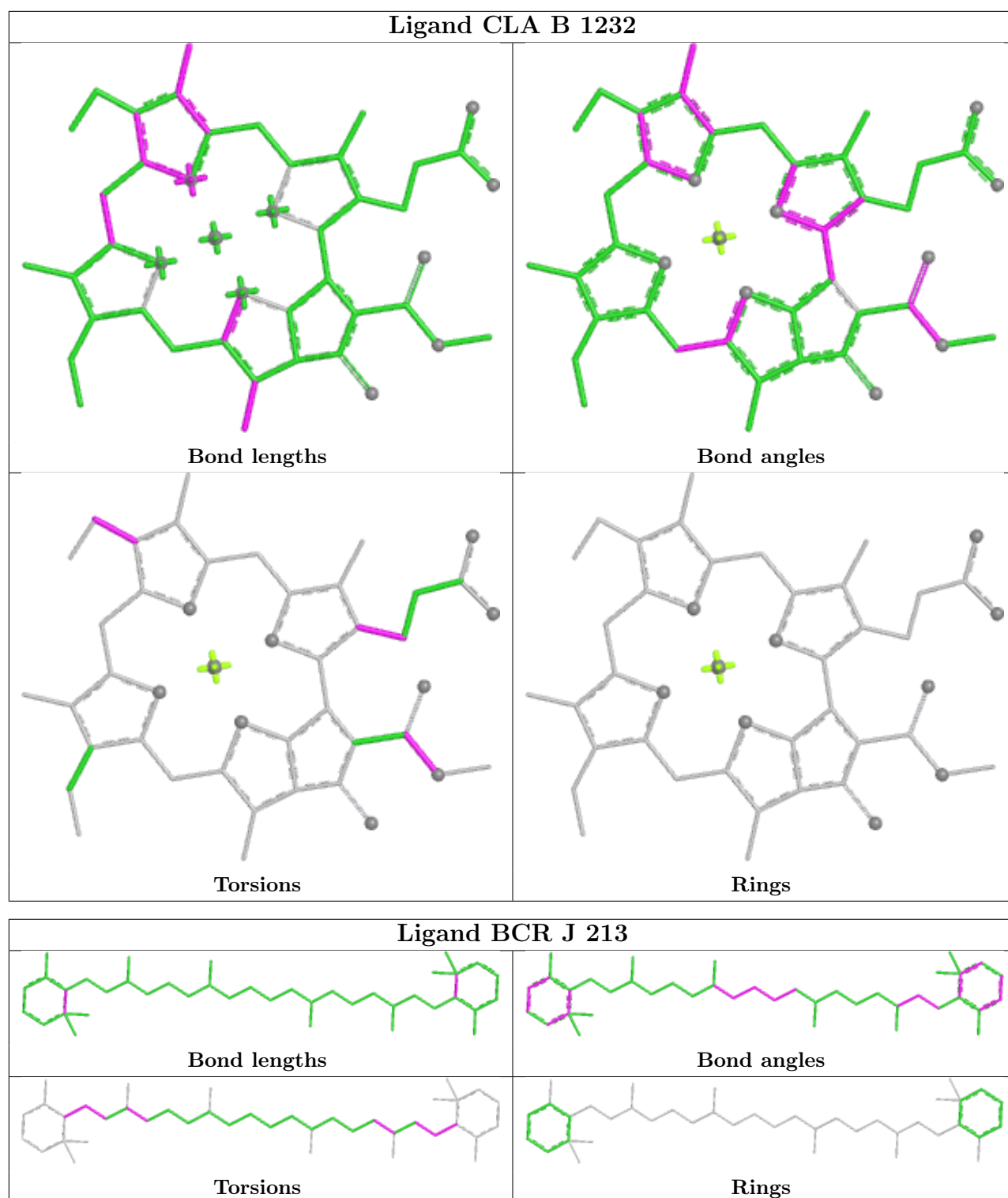


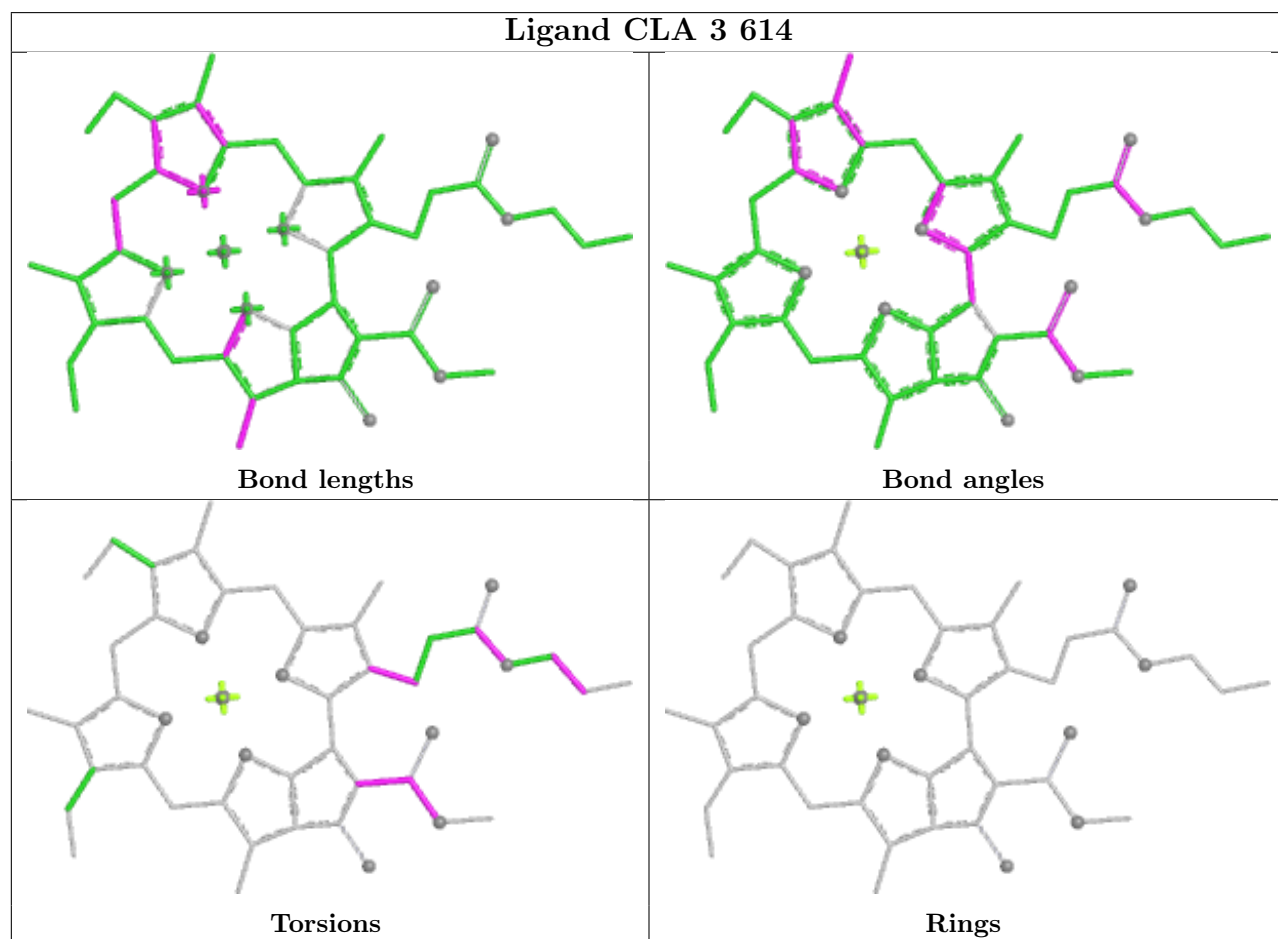
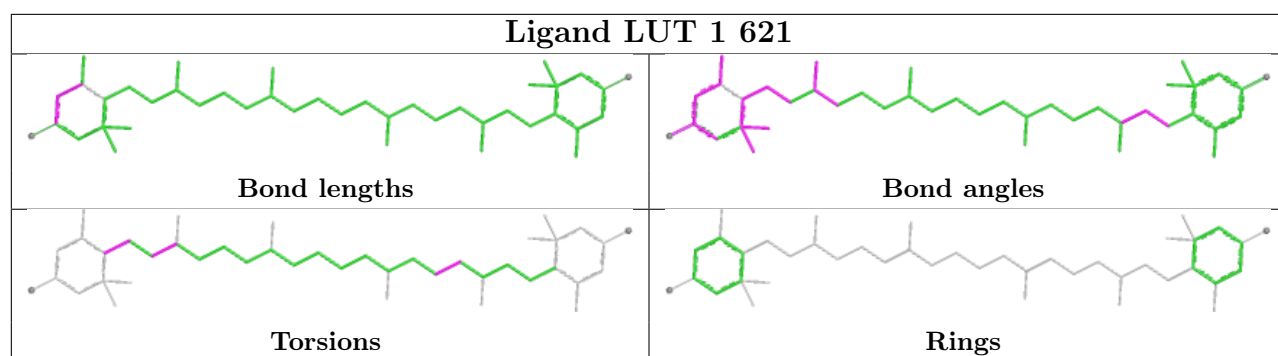
Torsions

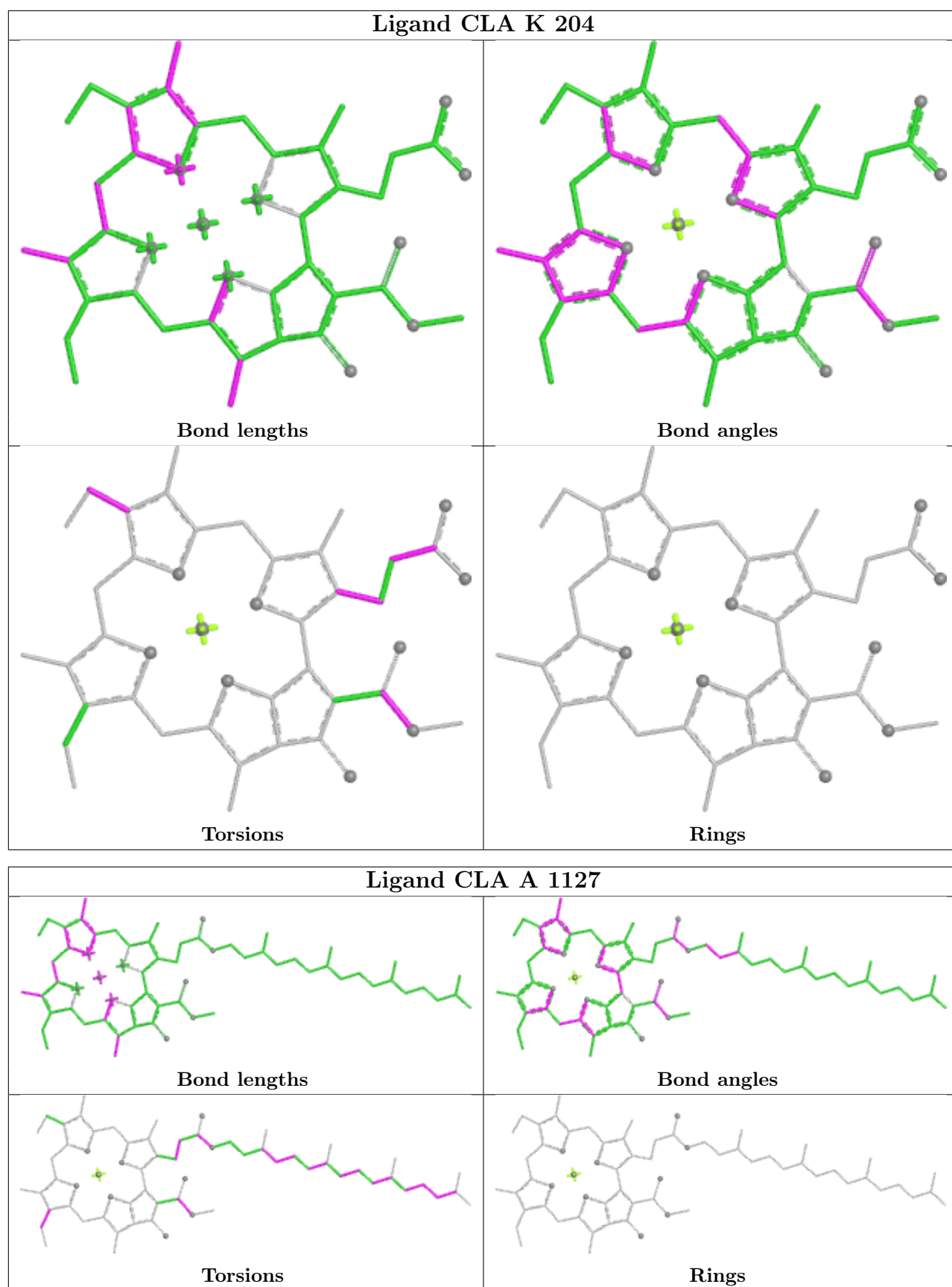


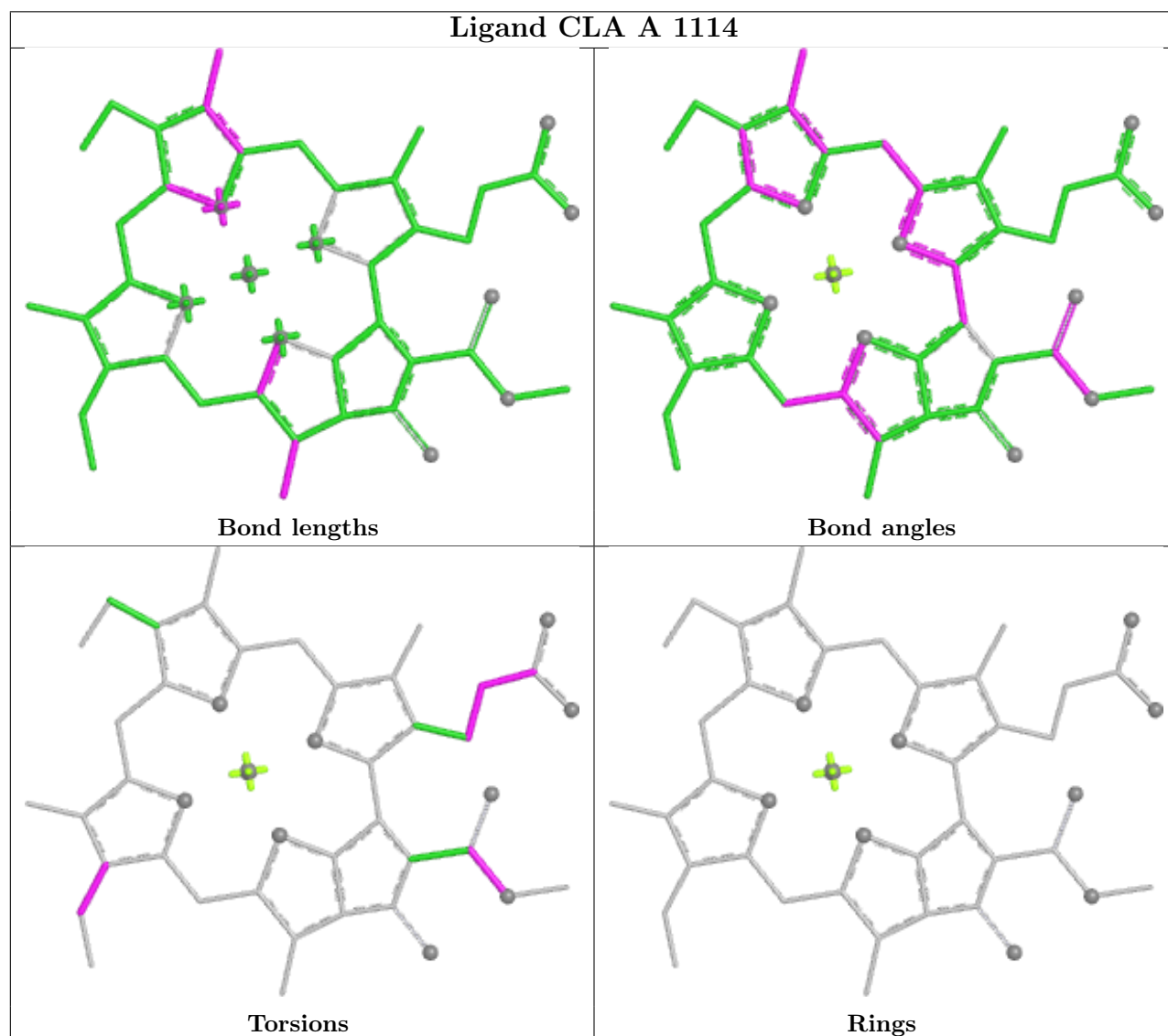
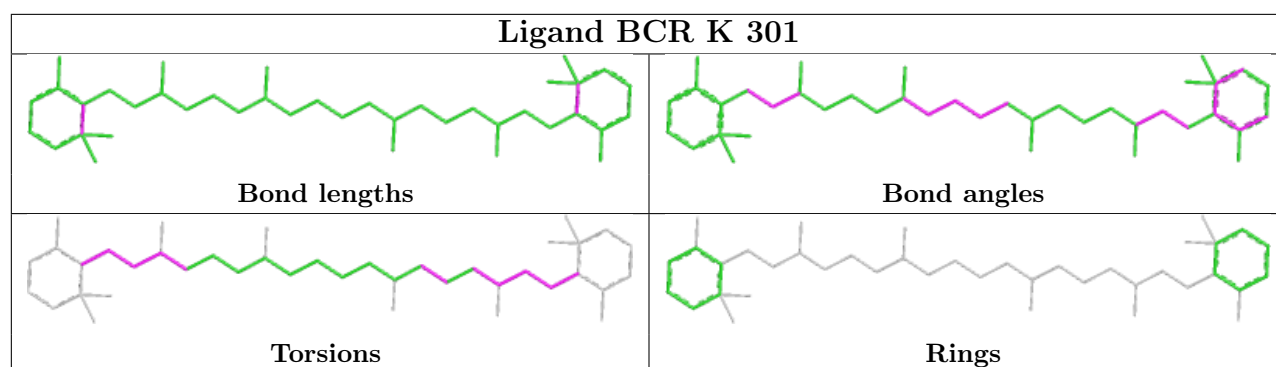
Rings



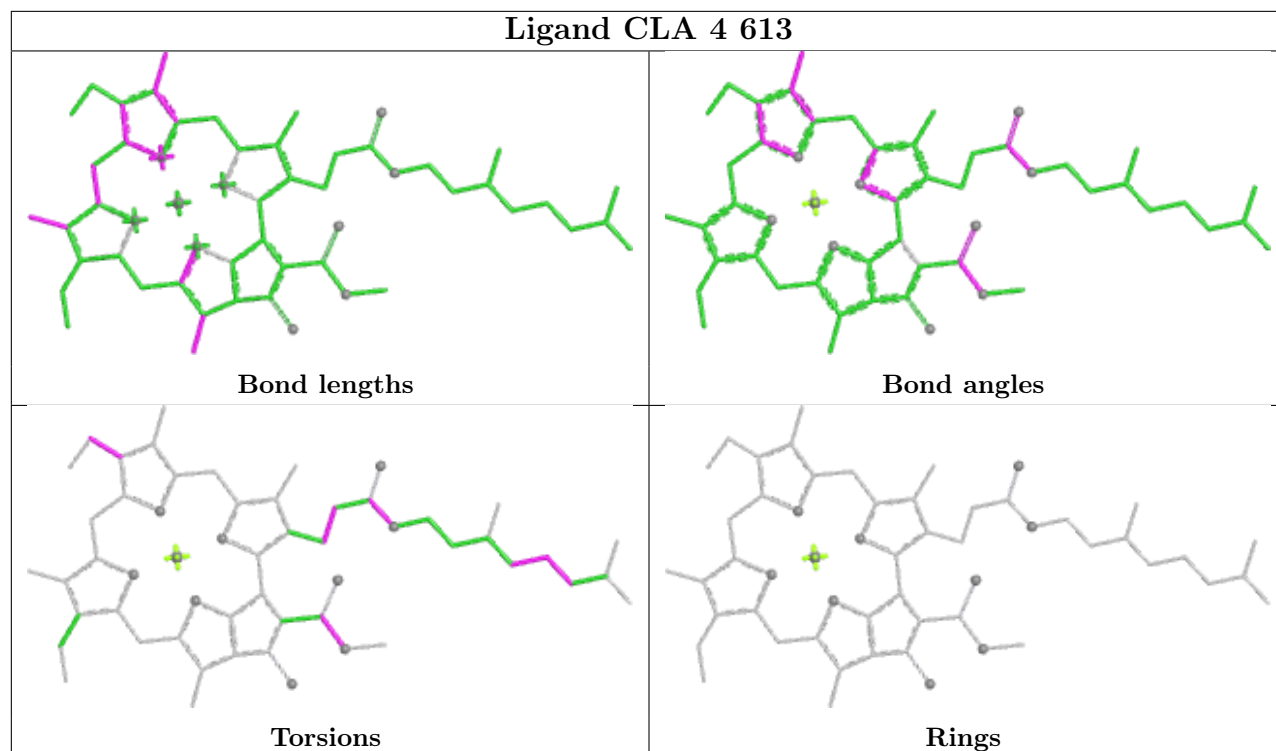




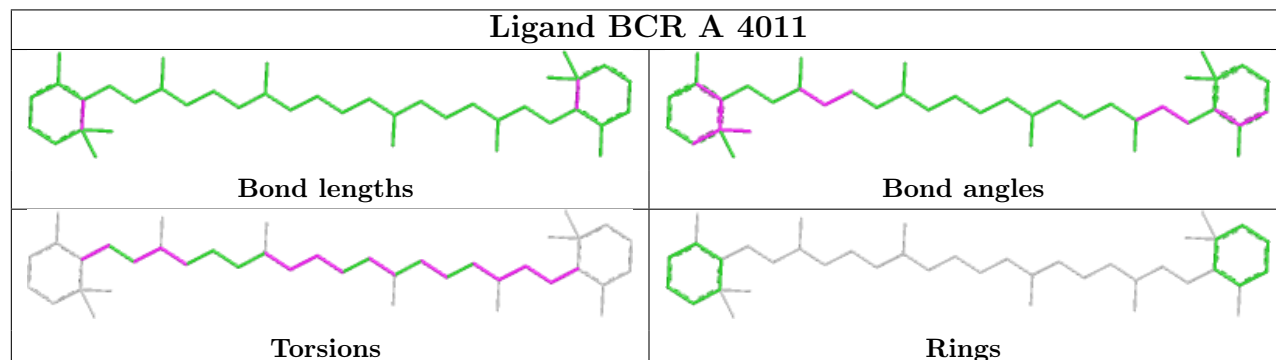




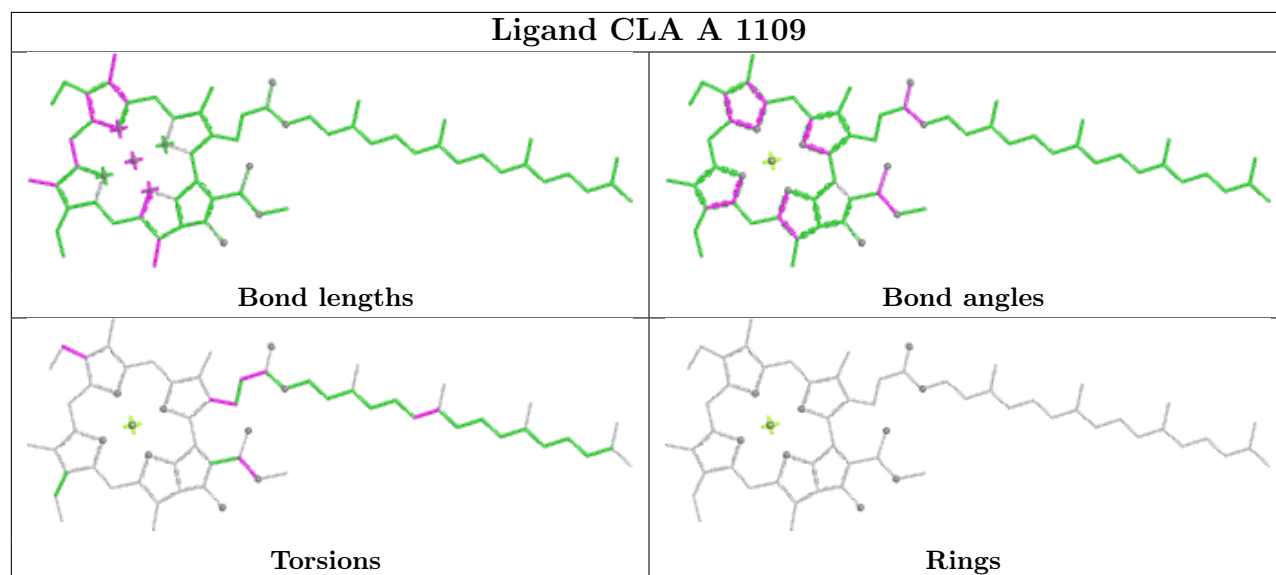
Ligand CLA 4 613

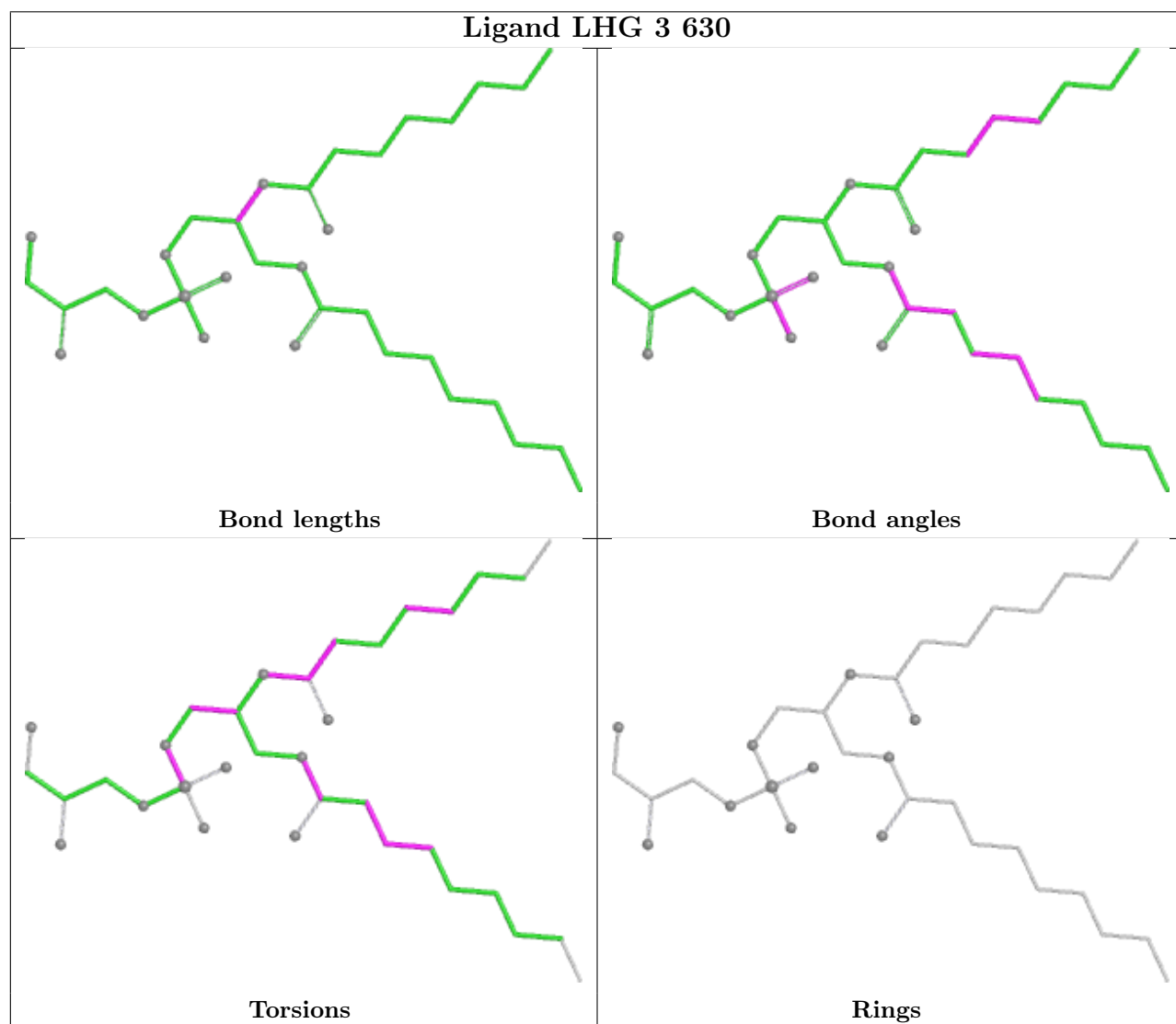
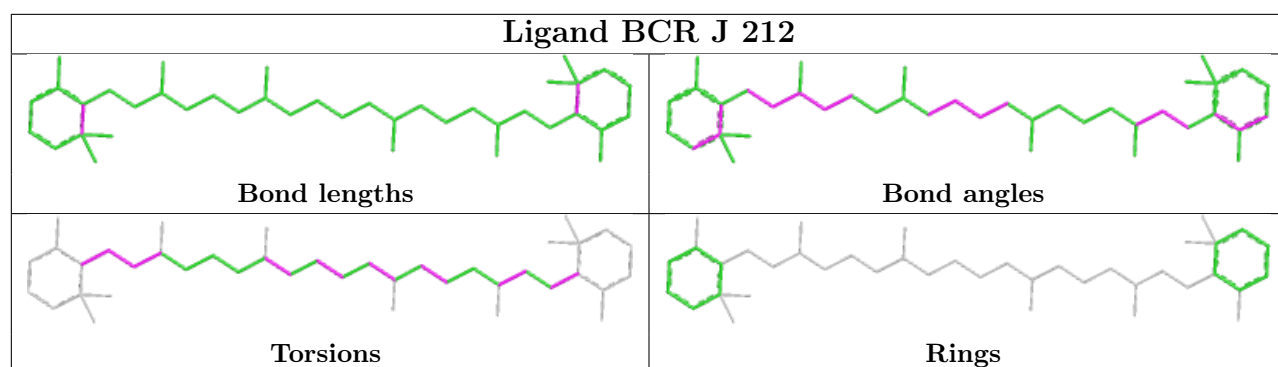


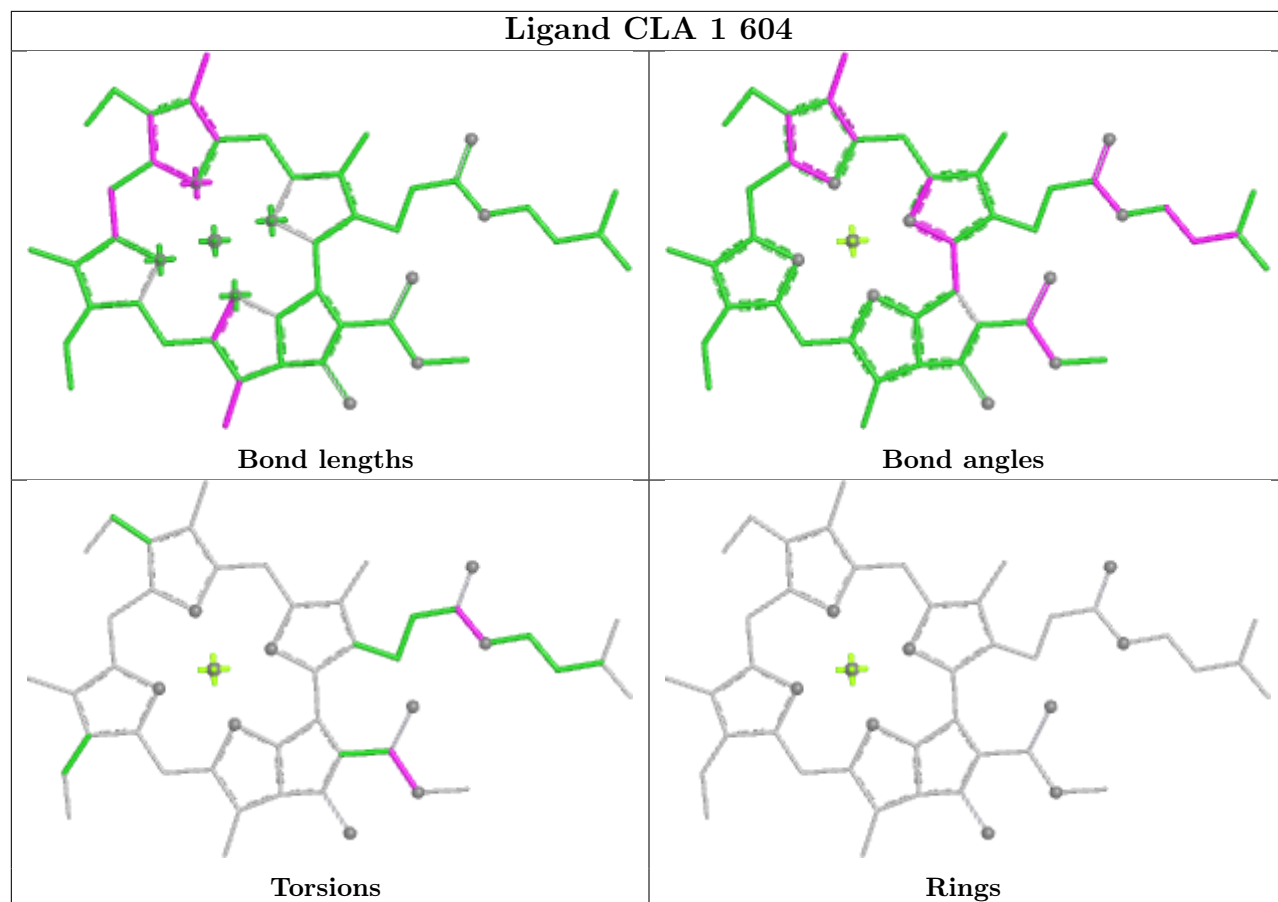
Ligand BCR A 4011

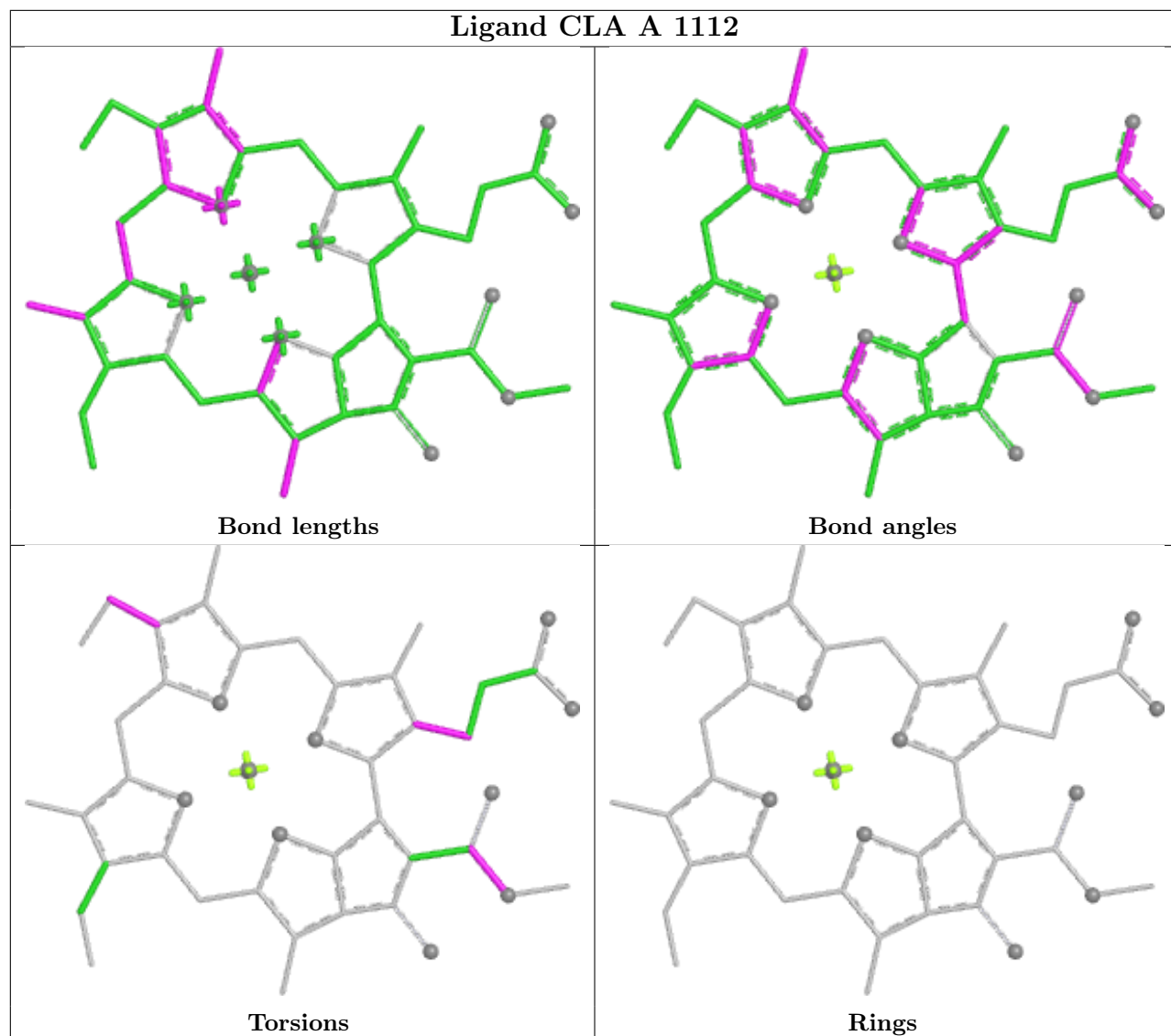


Ligand CLA A 1109

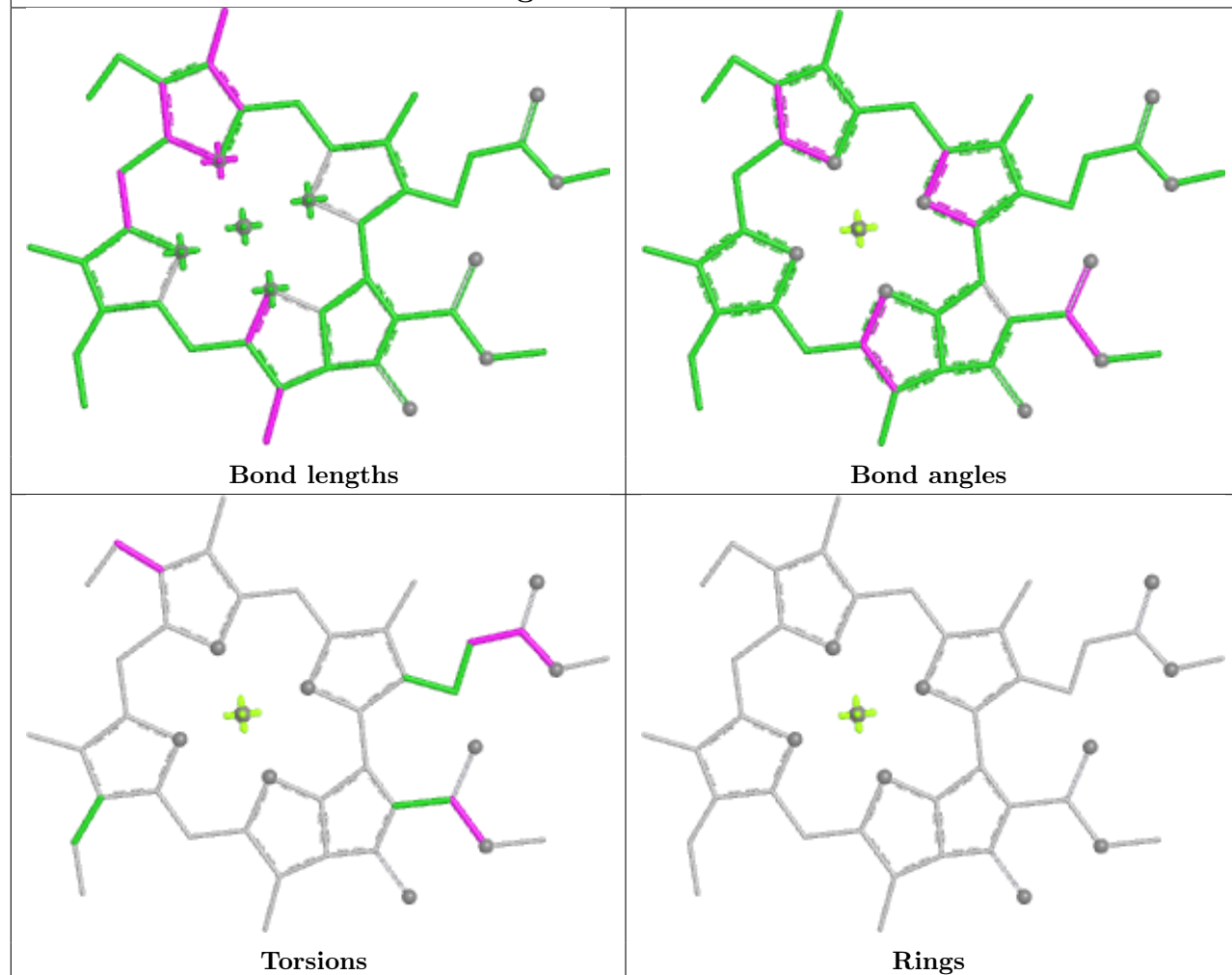




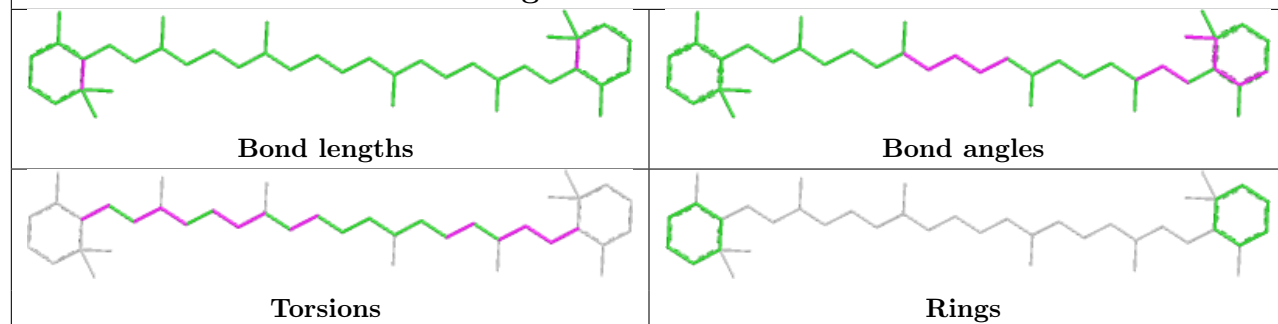




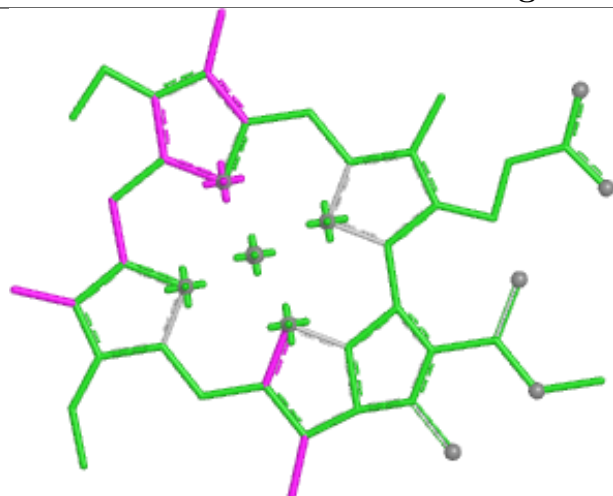
Ligand CLA 2 603



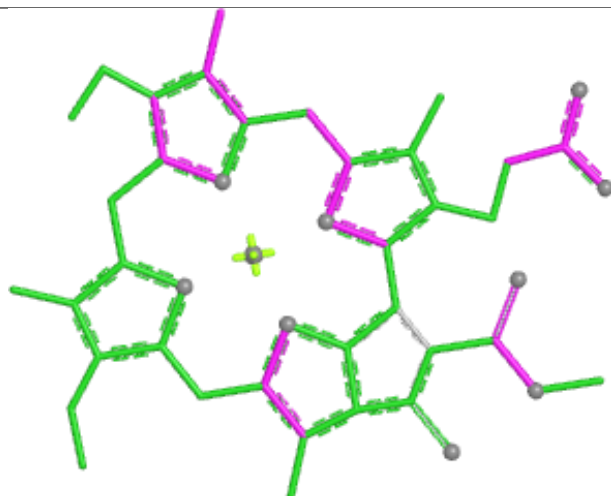
Ligand BCR B 4004



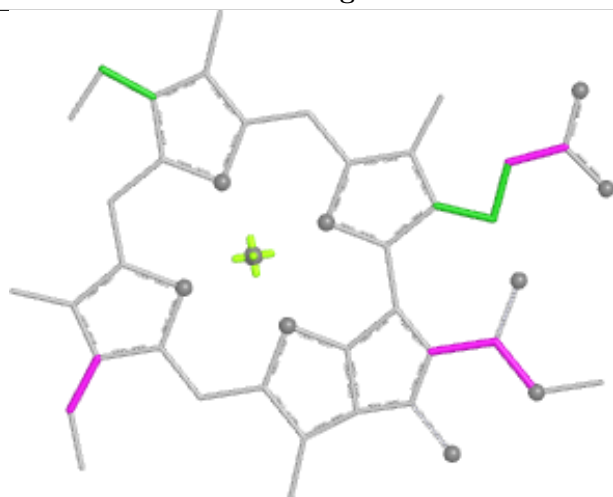
Ligand CLA 1 606



Bond lengths



Bond angles

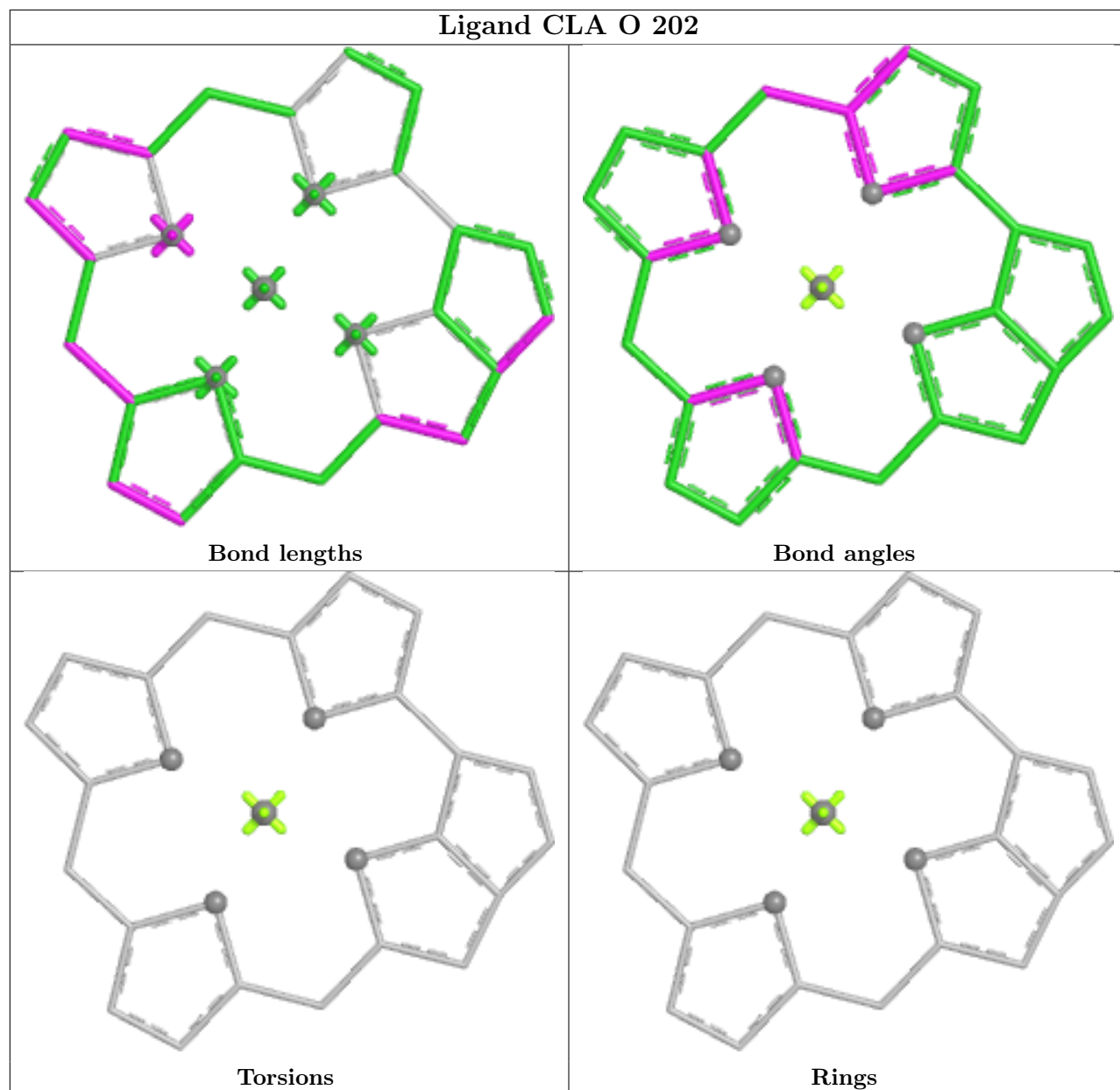


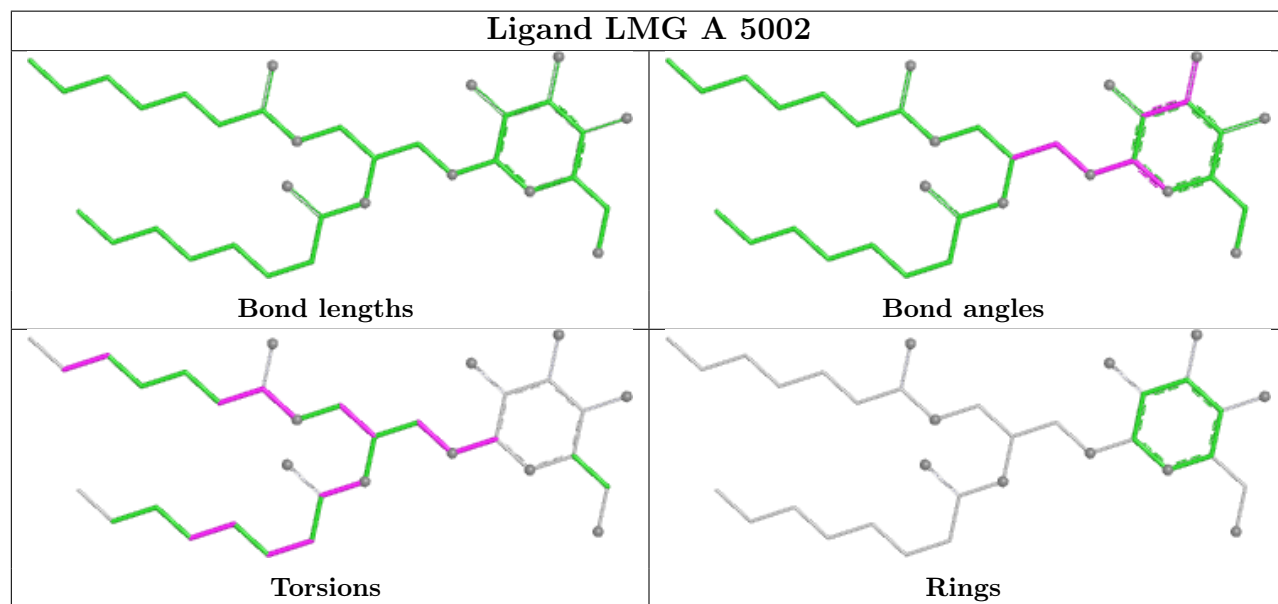
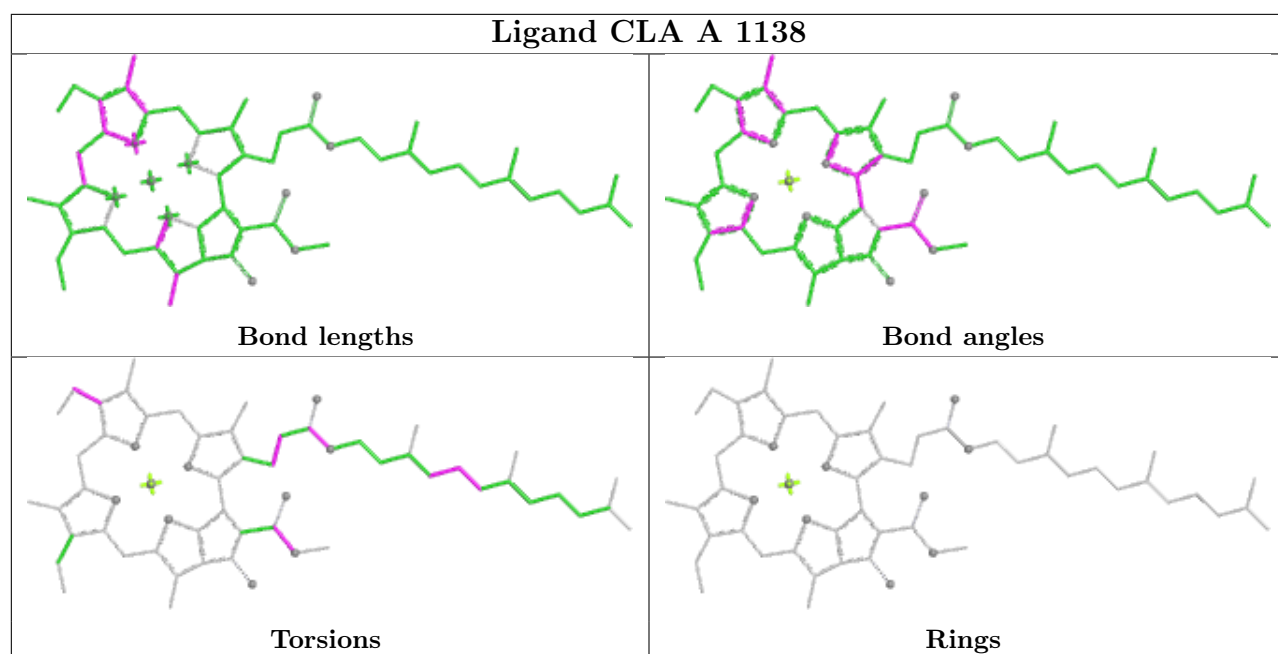
Torsions

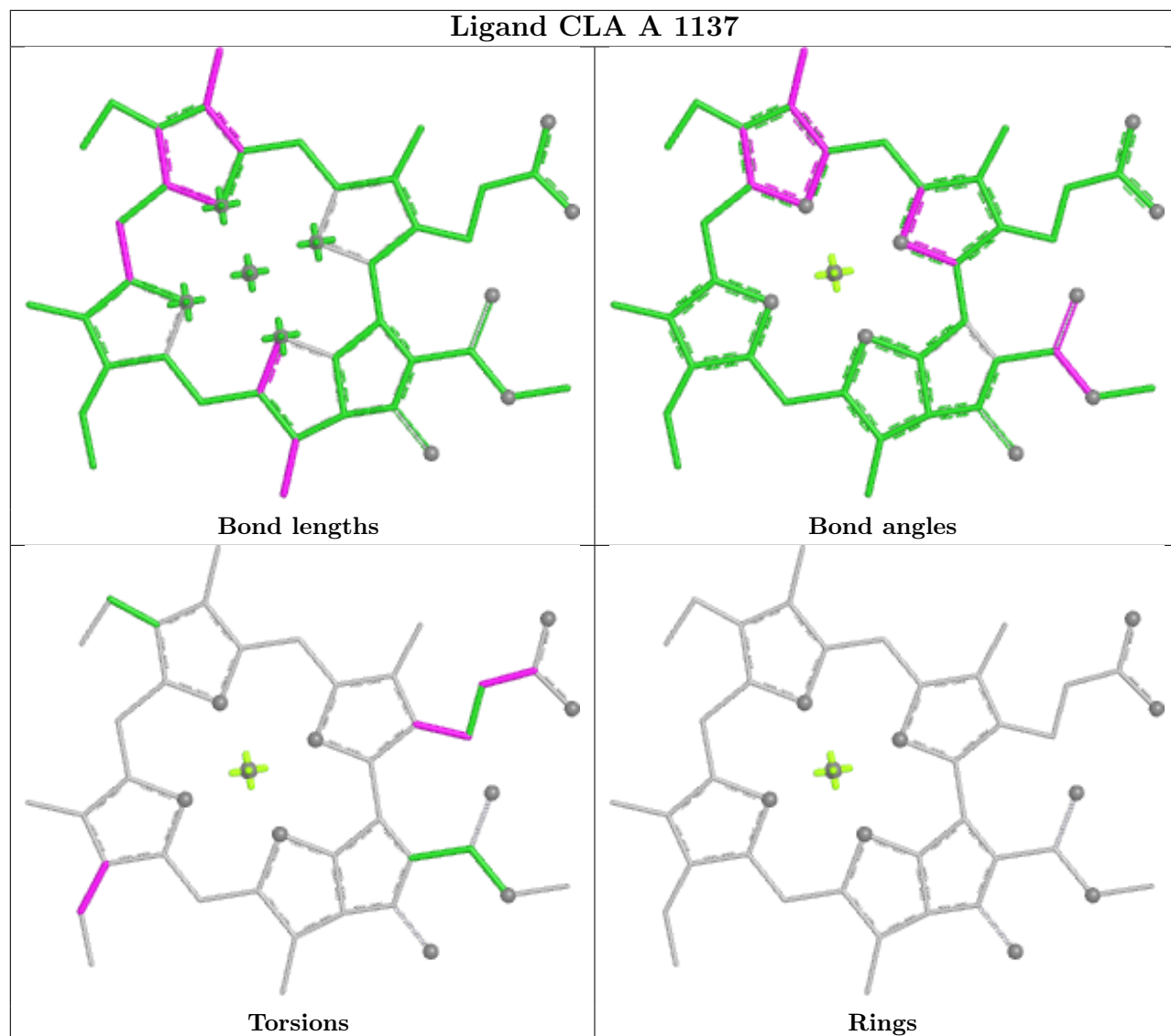


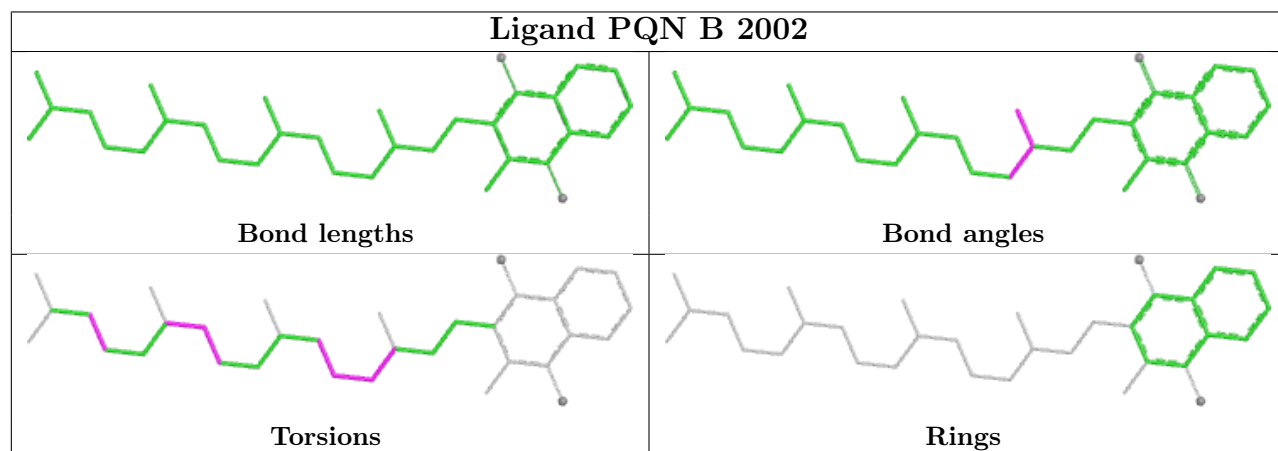
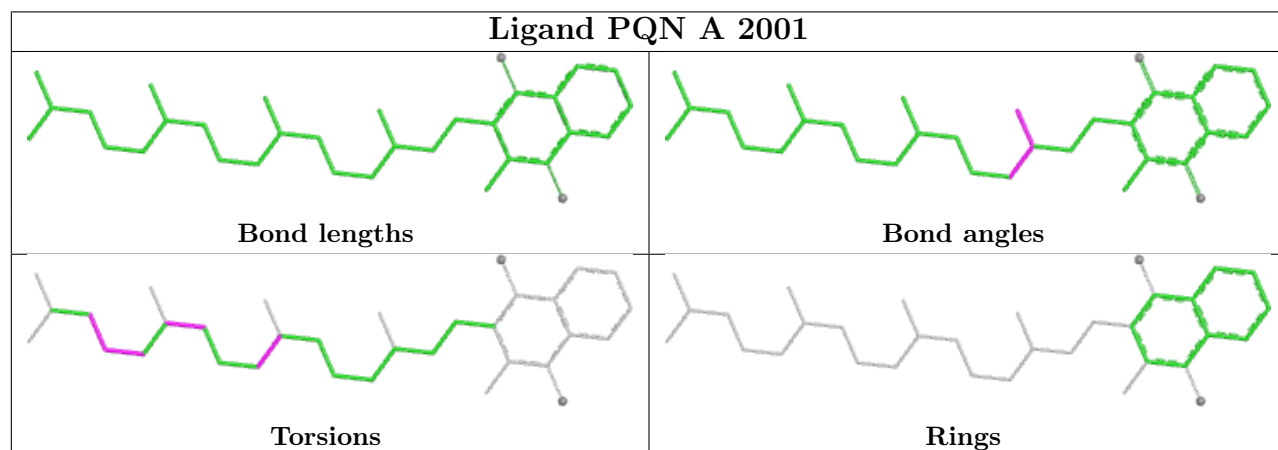
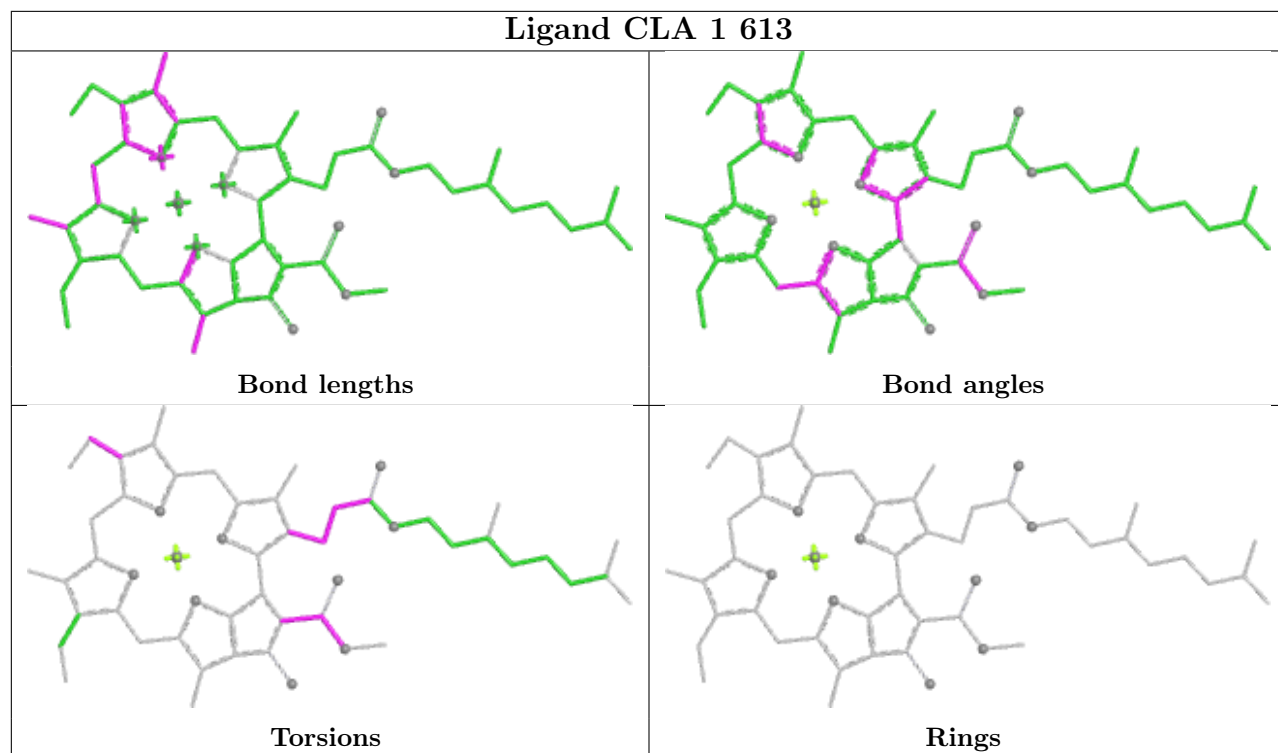
Rings

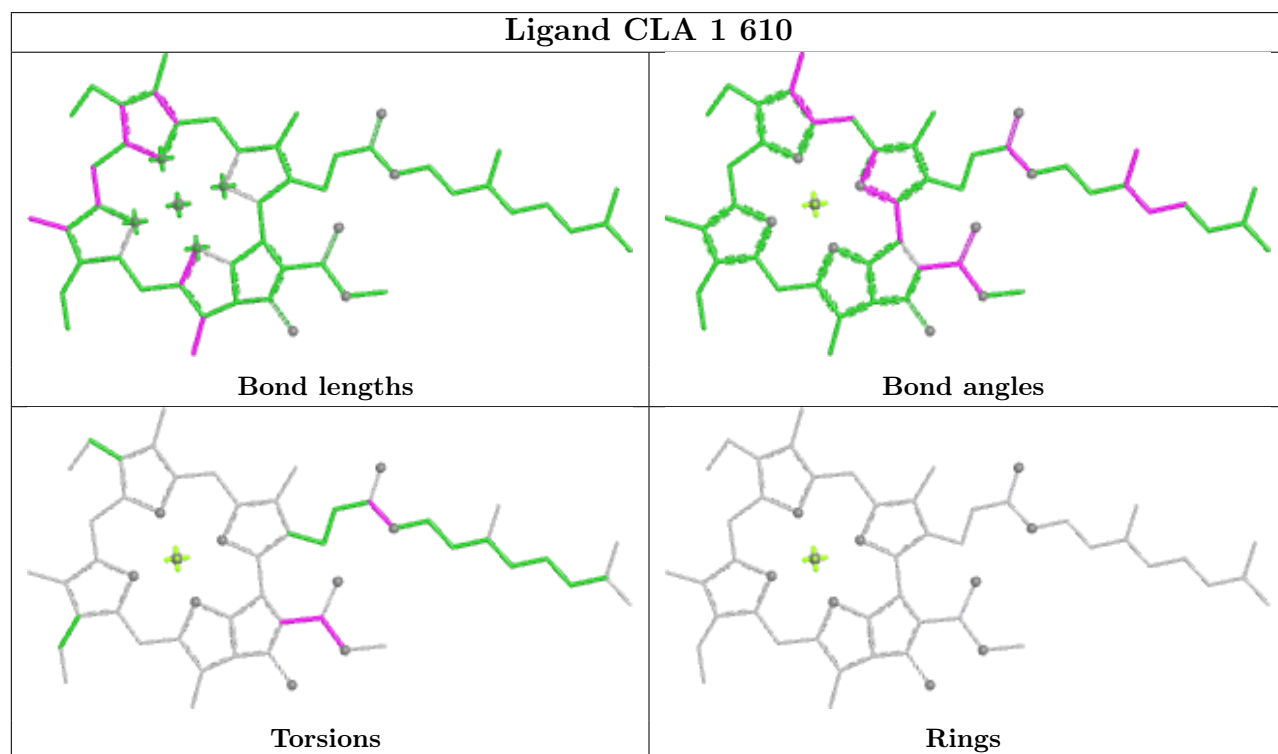
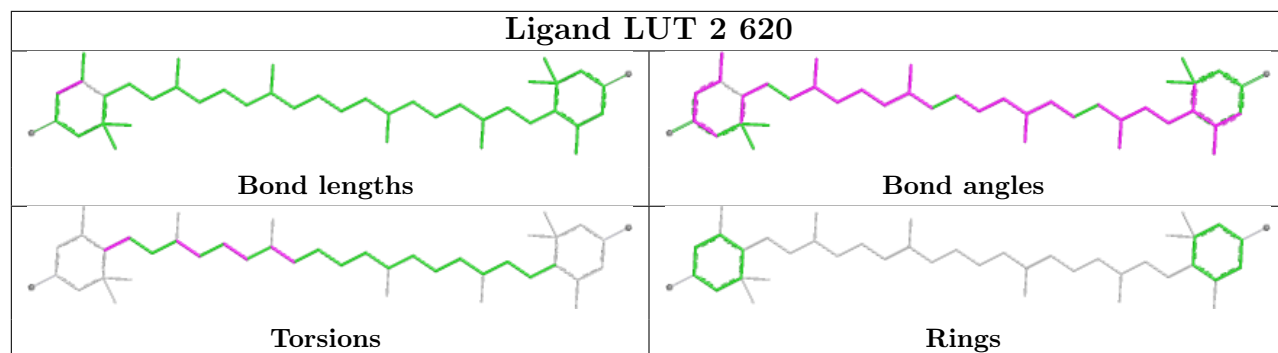
Ligand CLA O 202



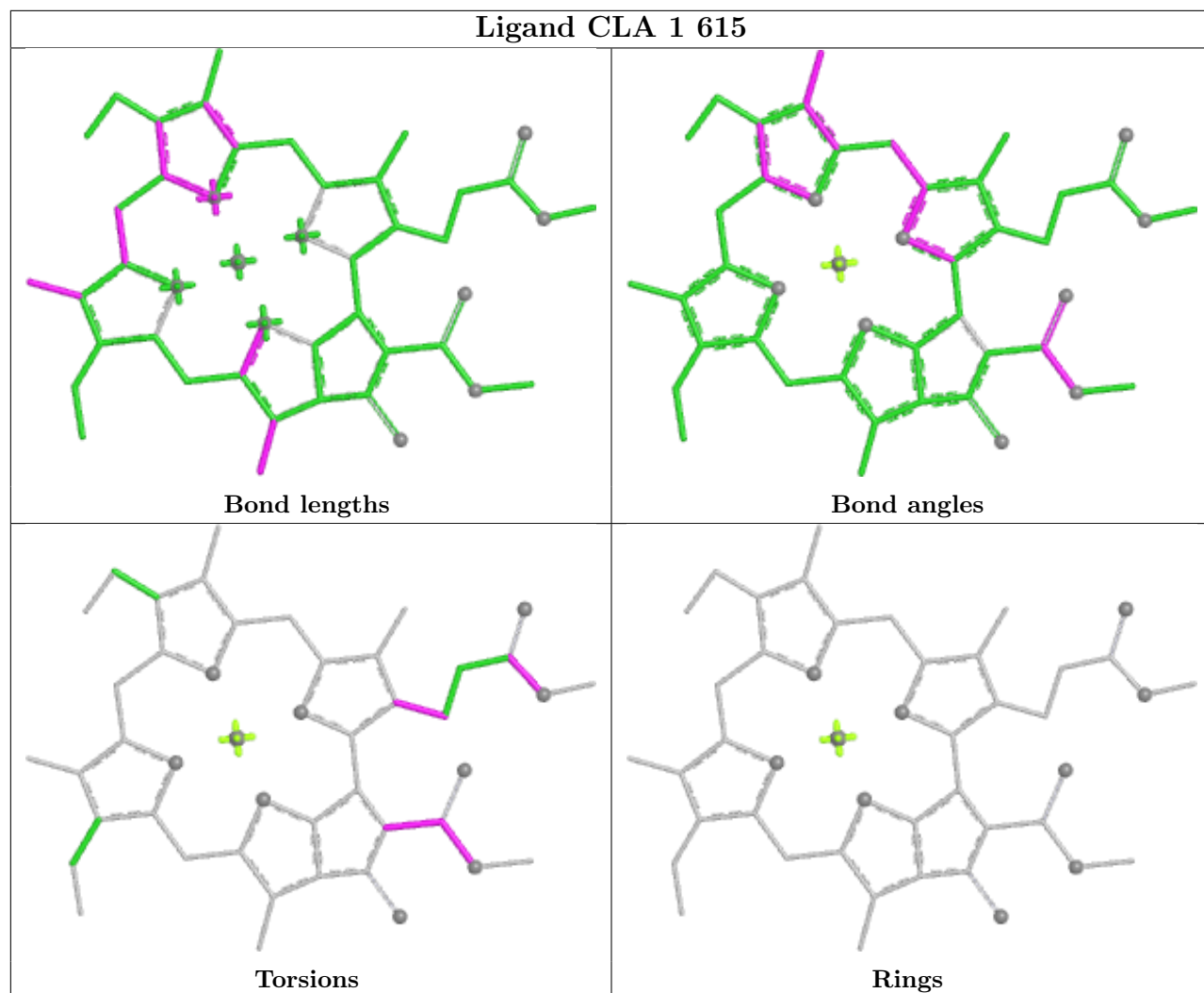


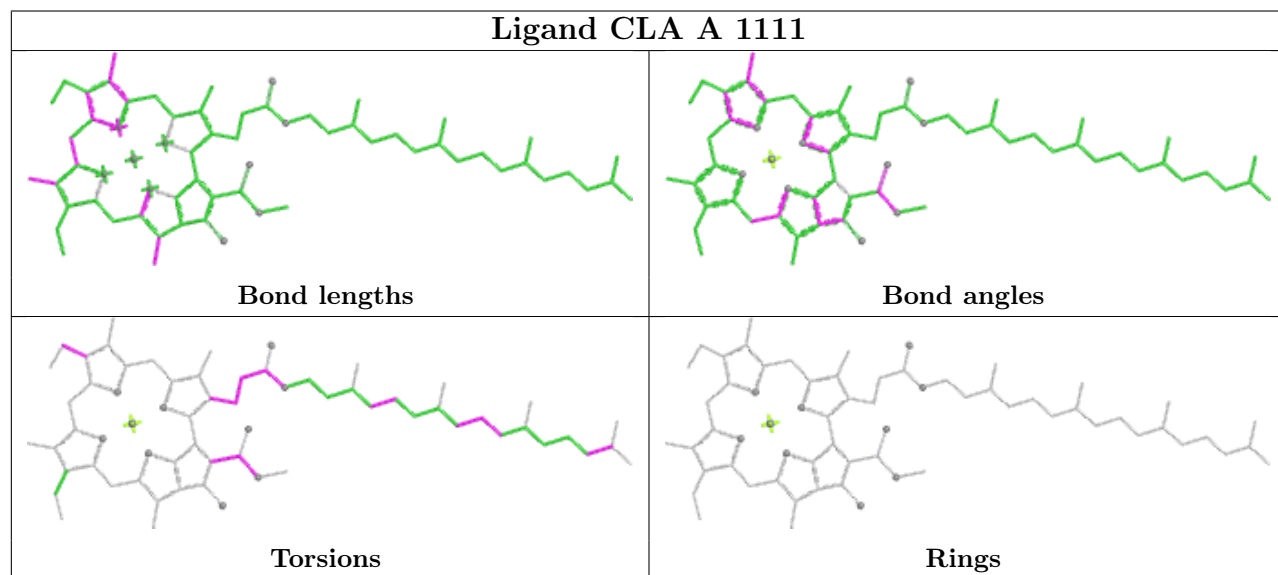
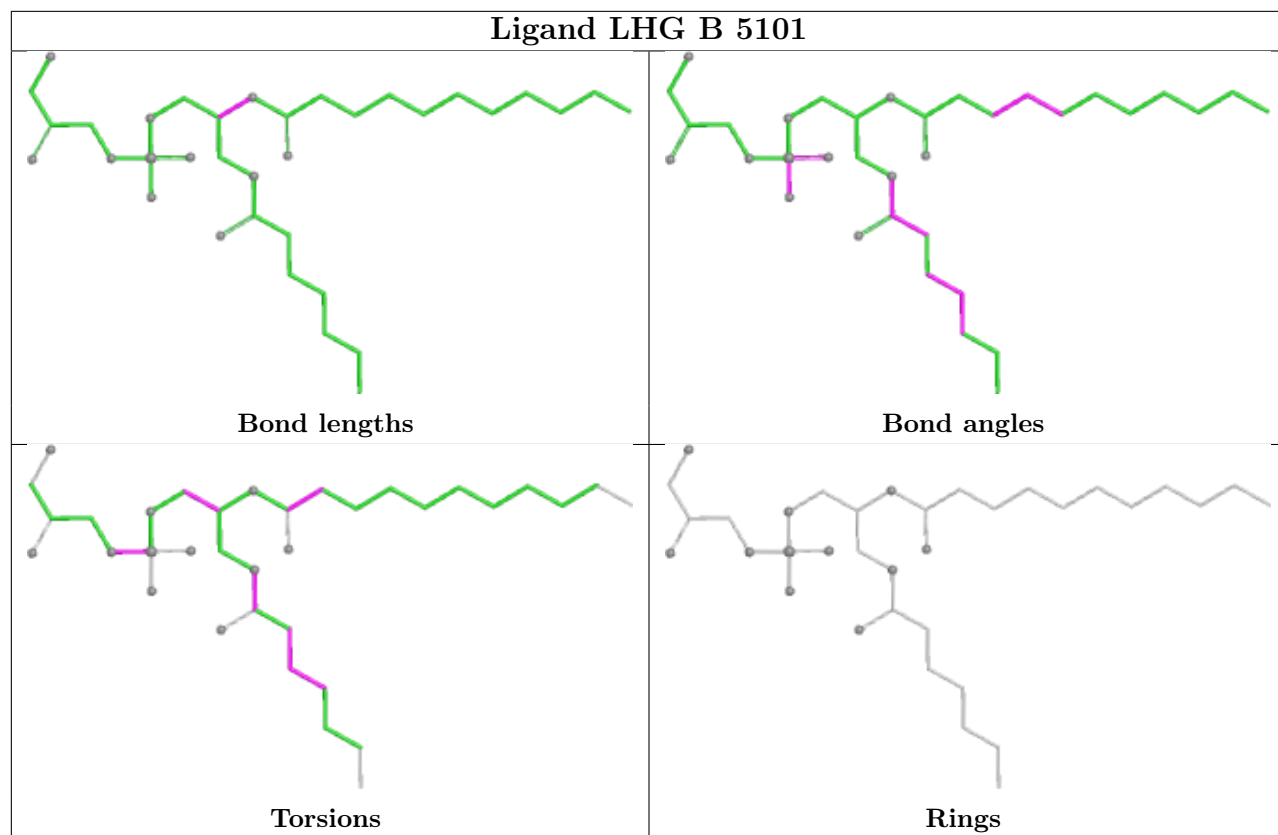




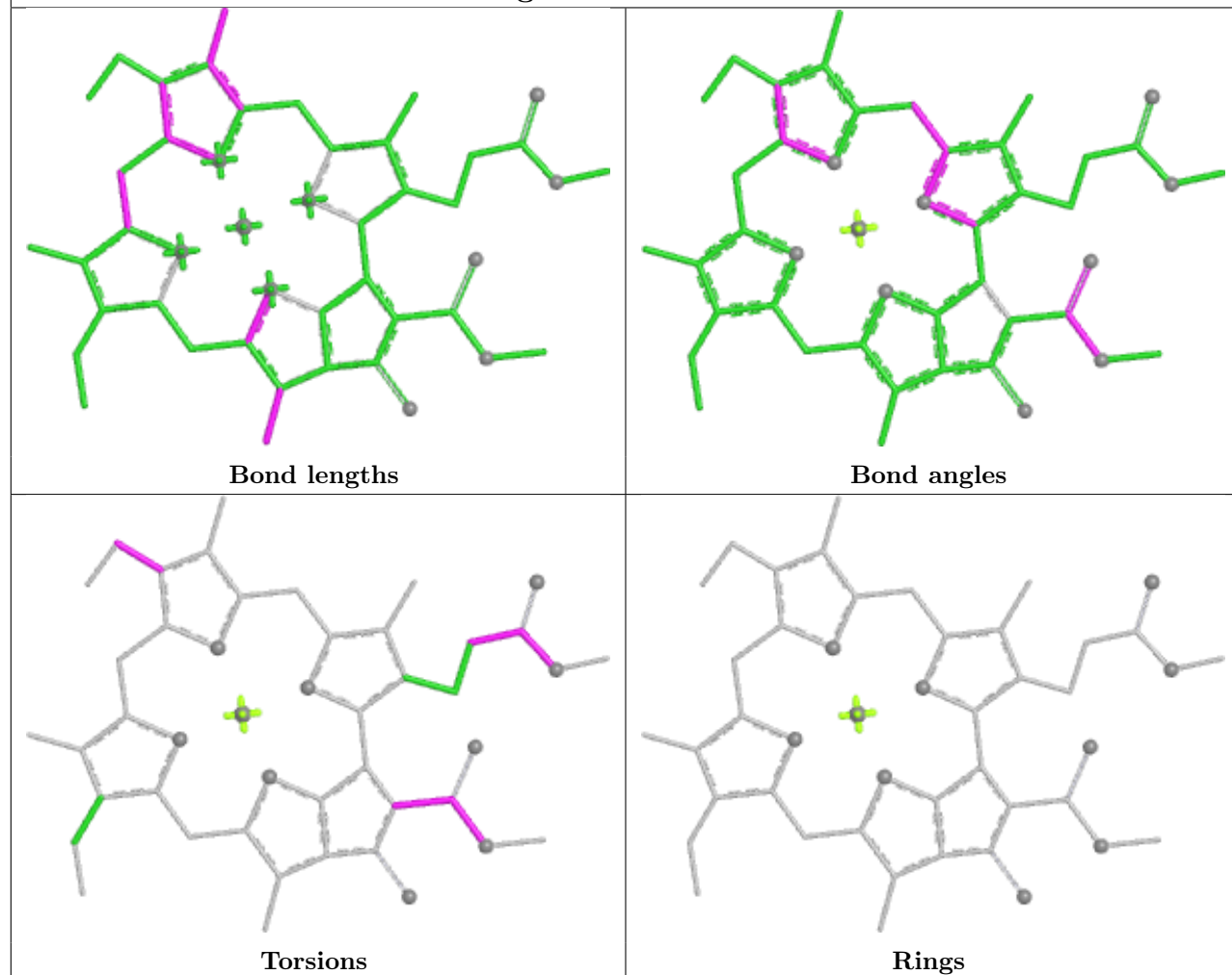


Ligand CLA 1 615

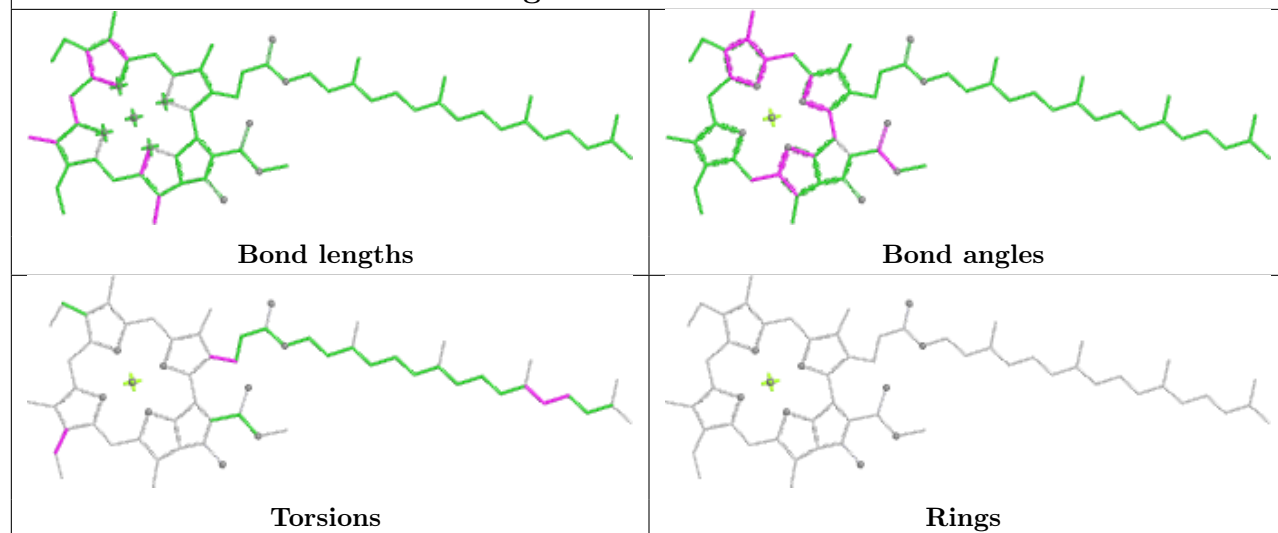


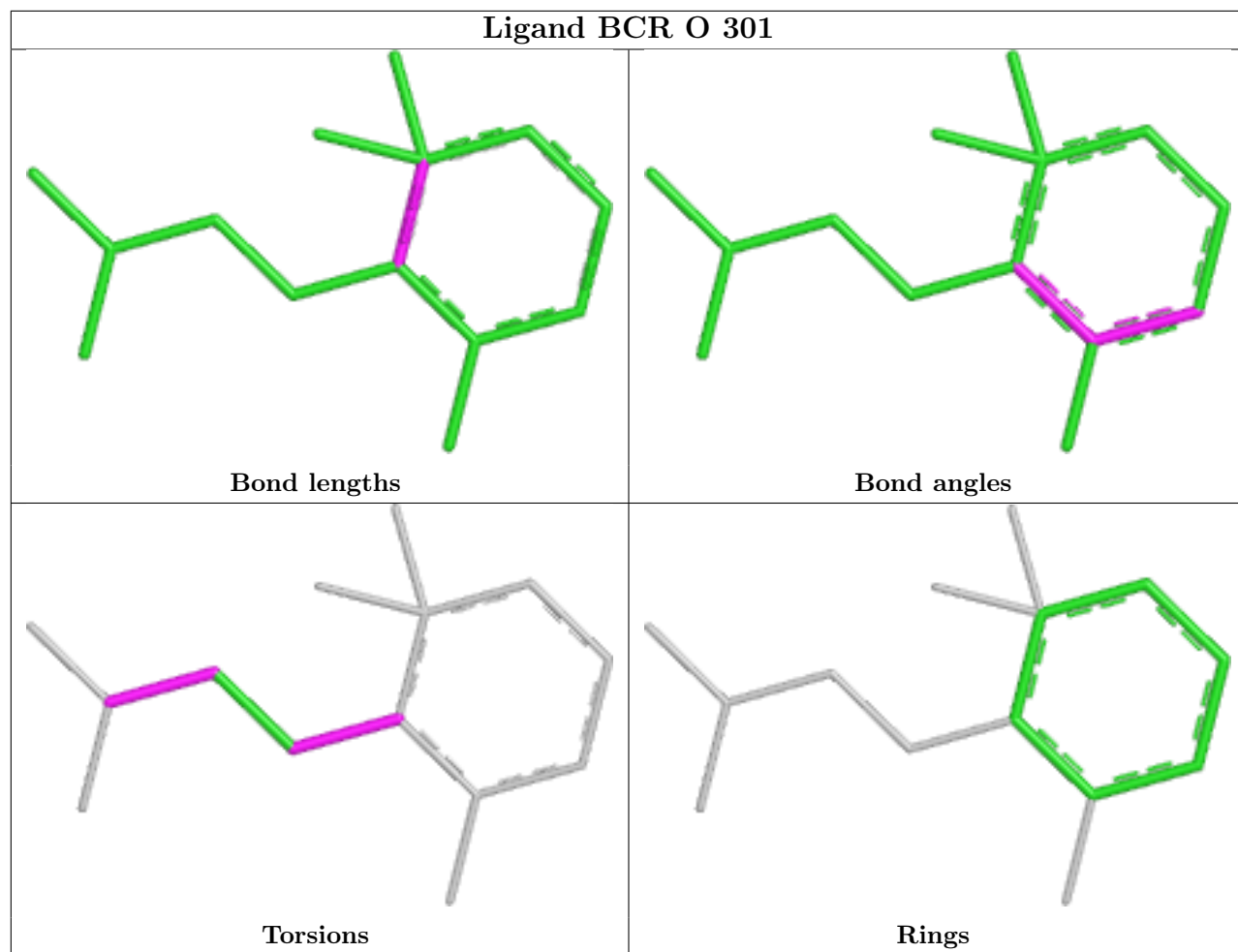


Ligand CLA 4 612

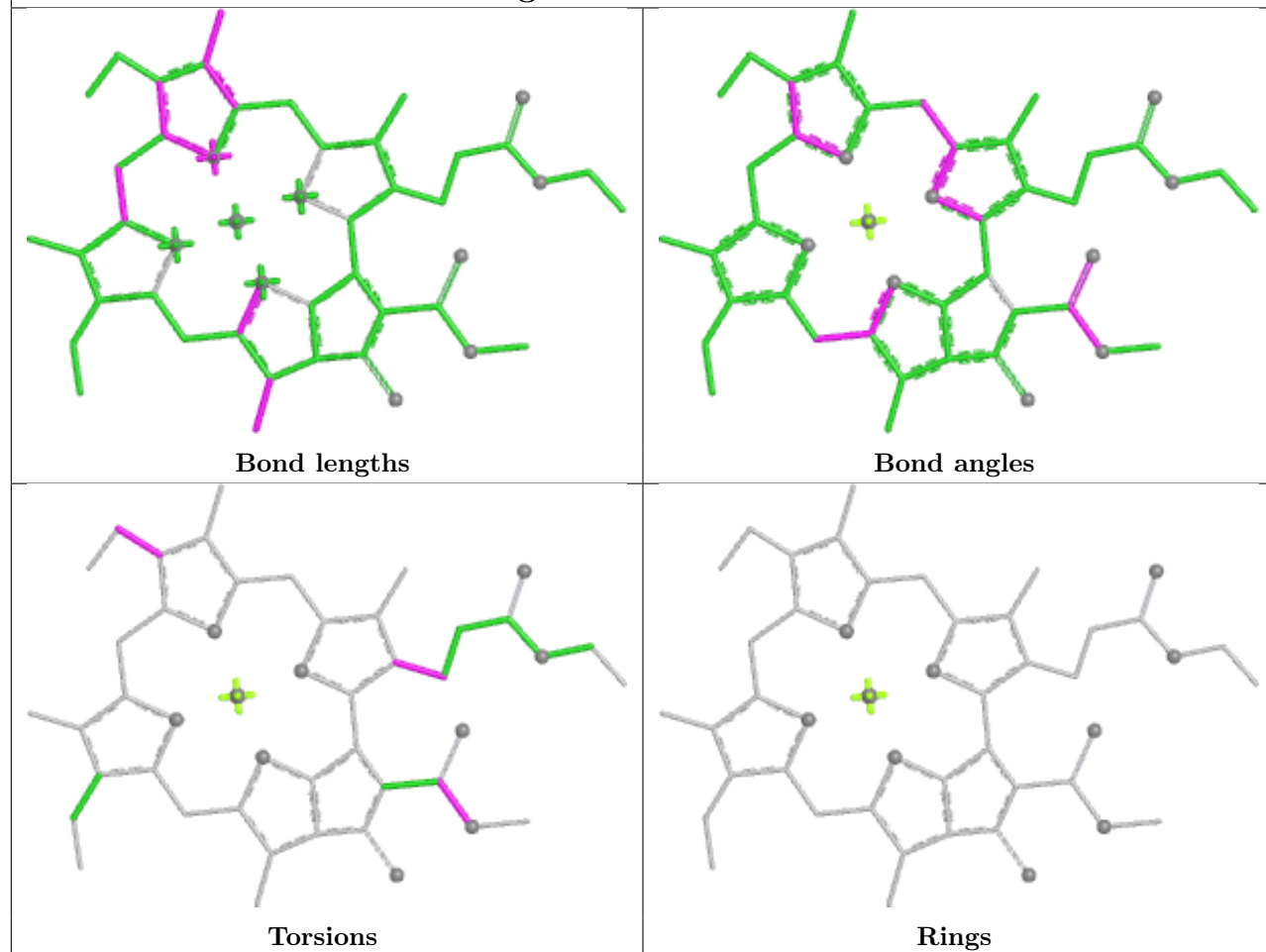


Ligand CLA B 1223

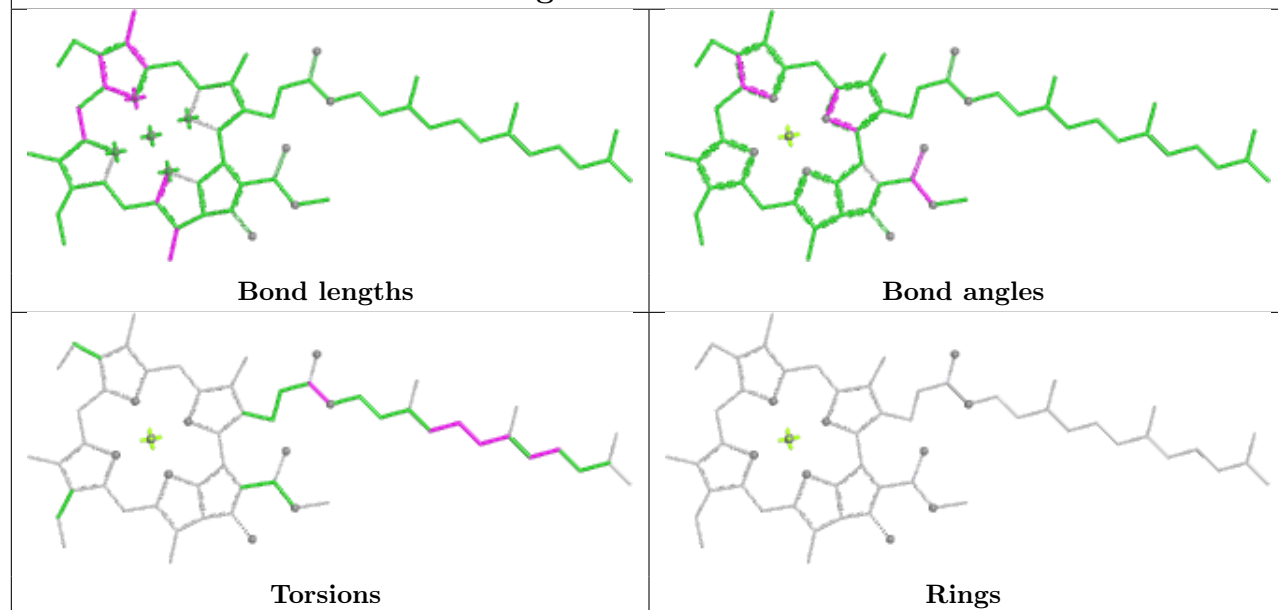




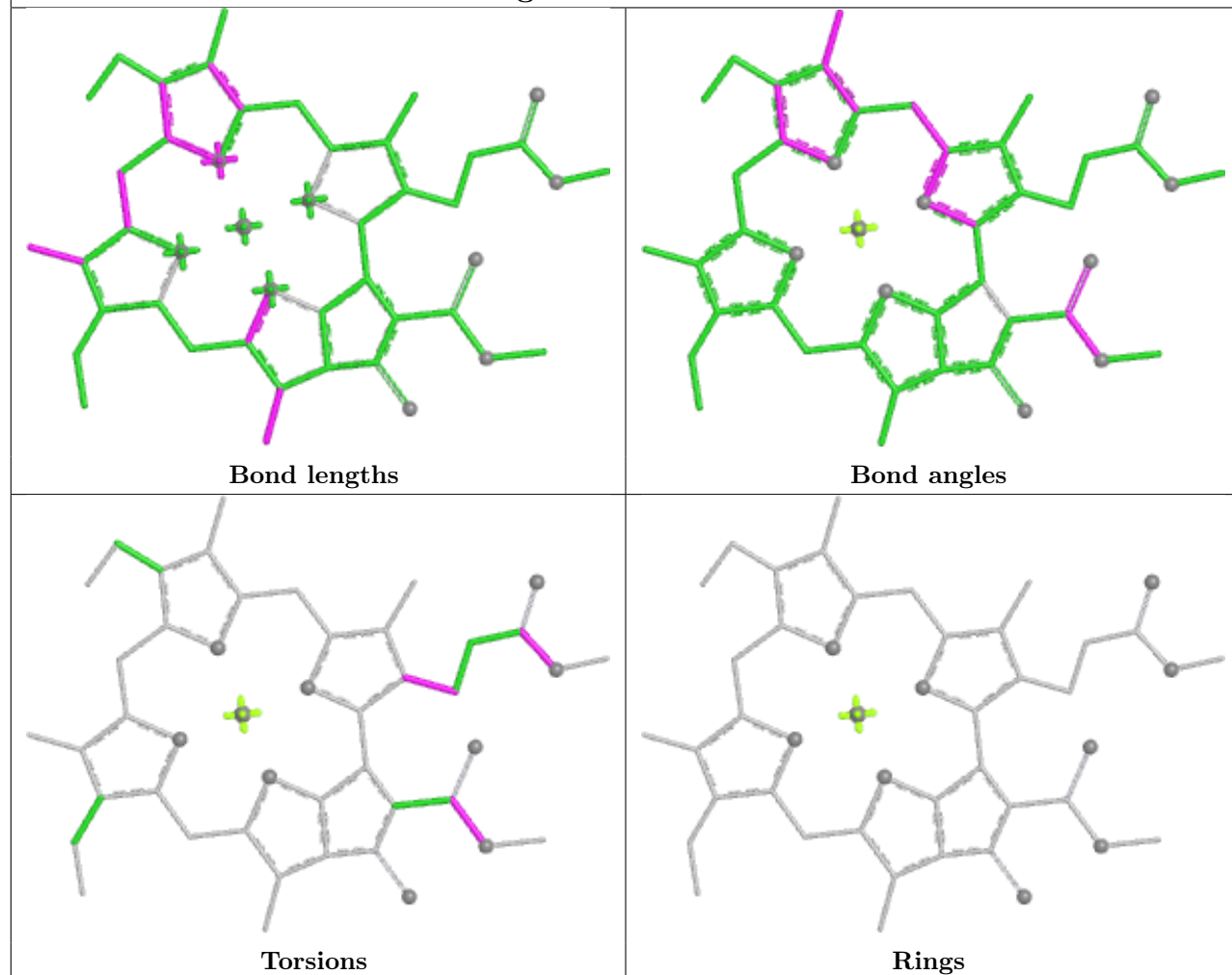
Ligand CLA B 1236



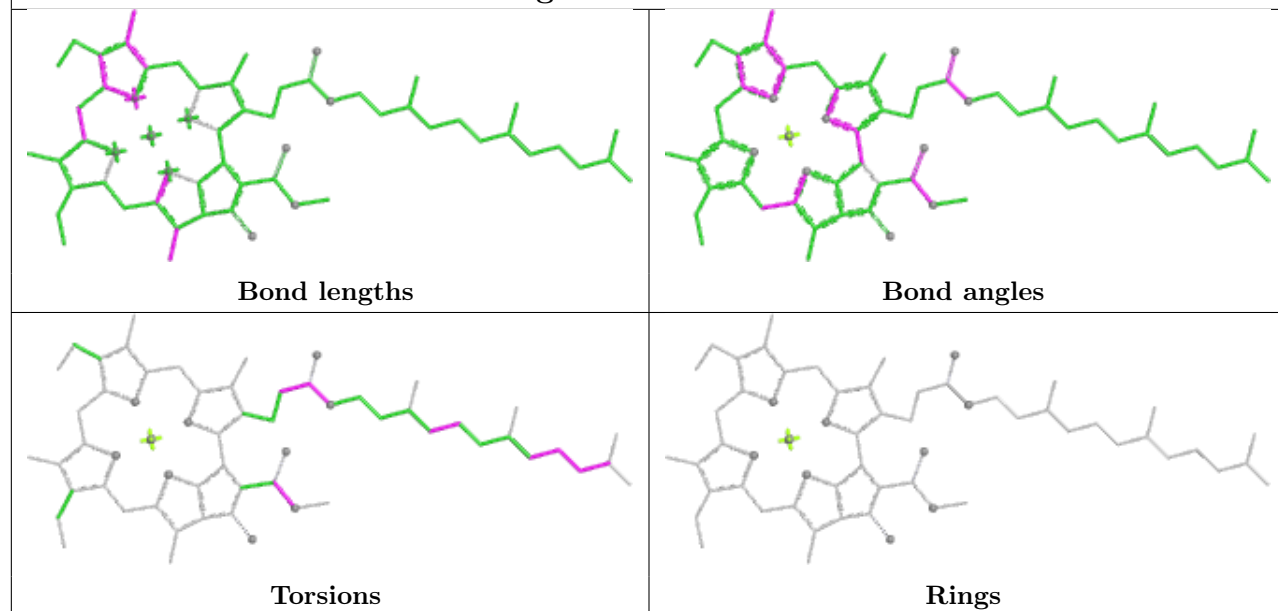
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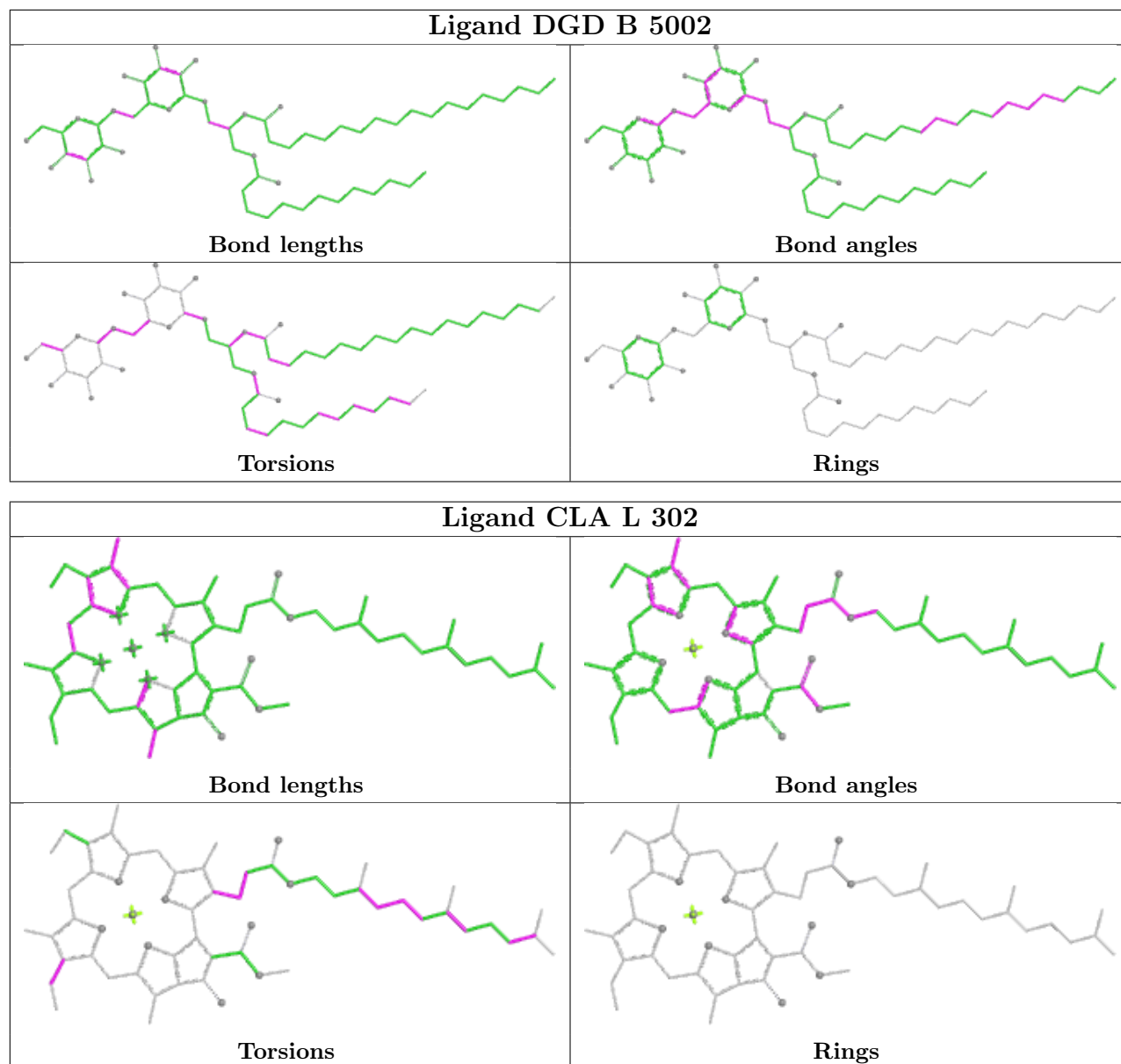


Ligand CLA 3 617

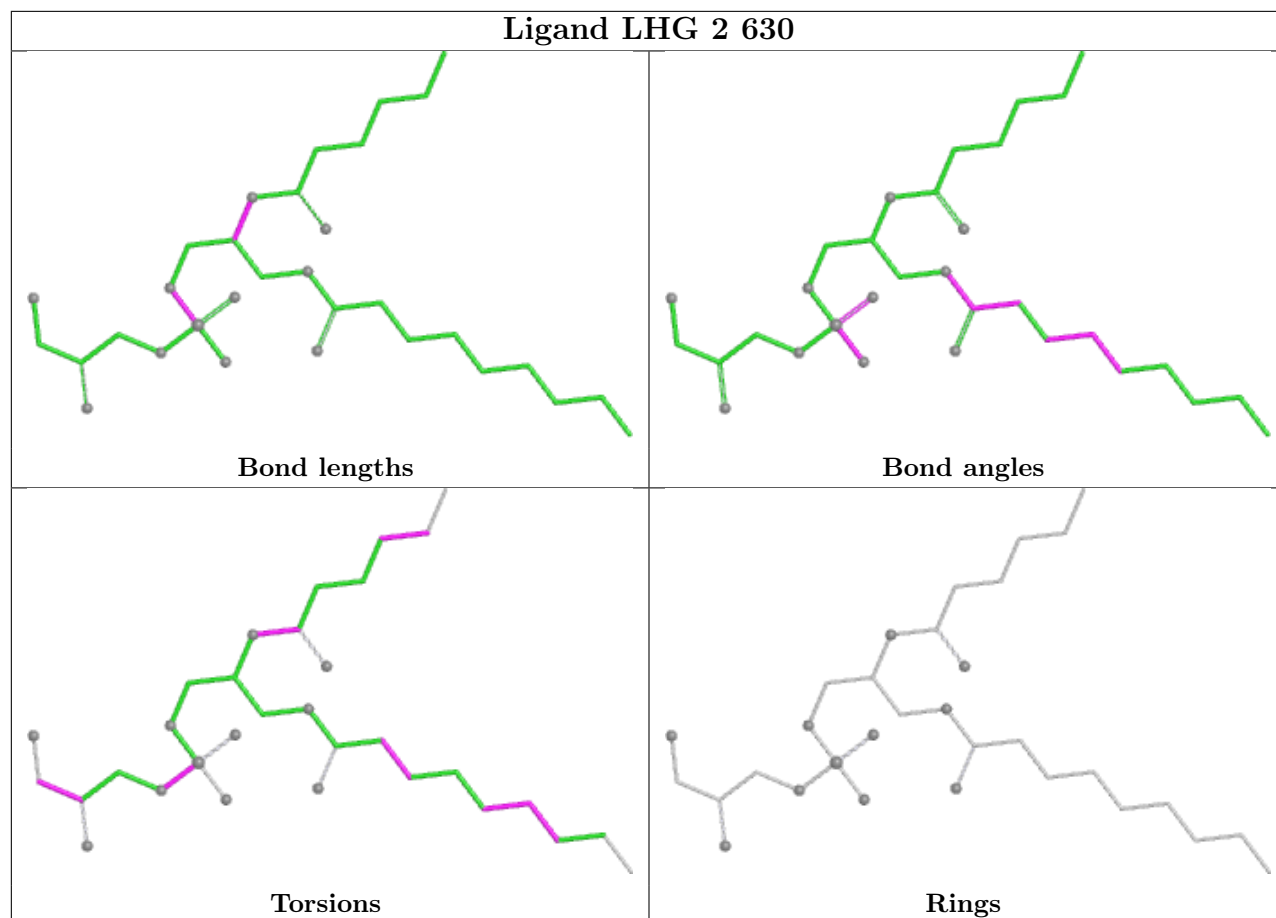


Ligand CLA 3 609

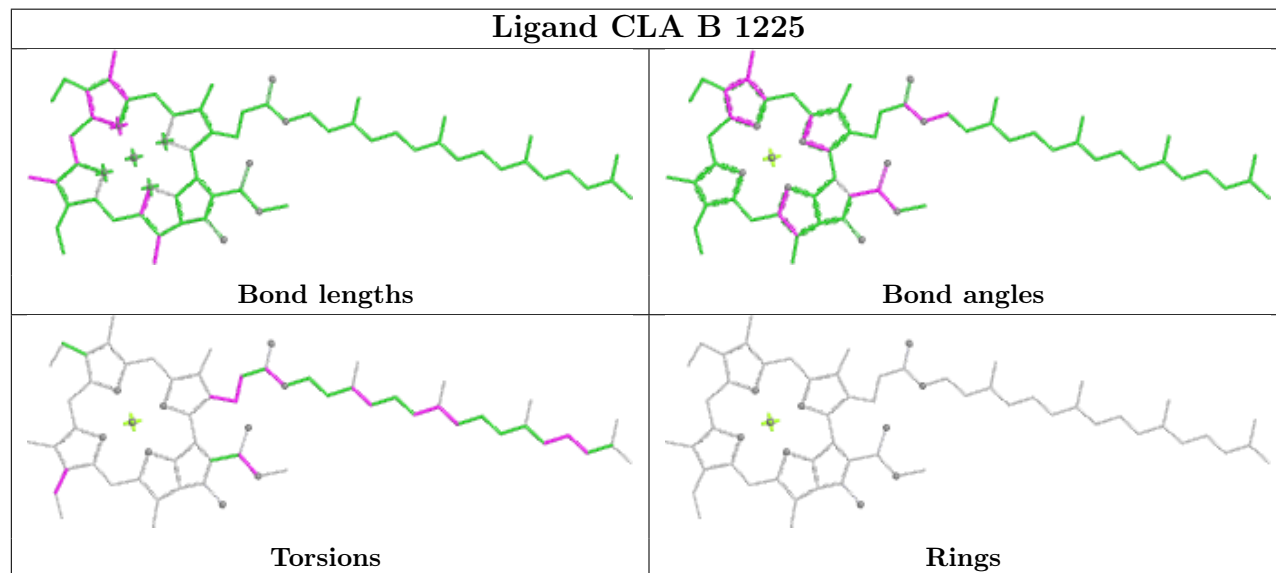


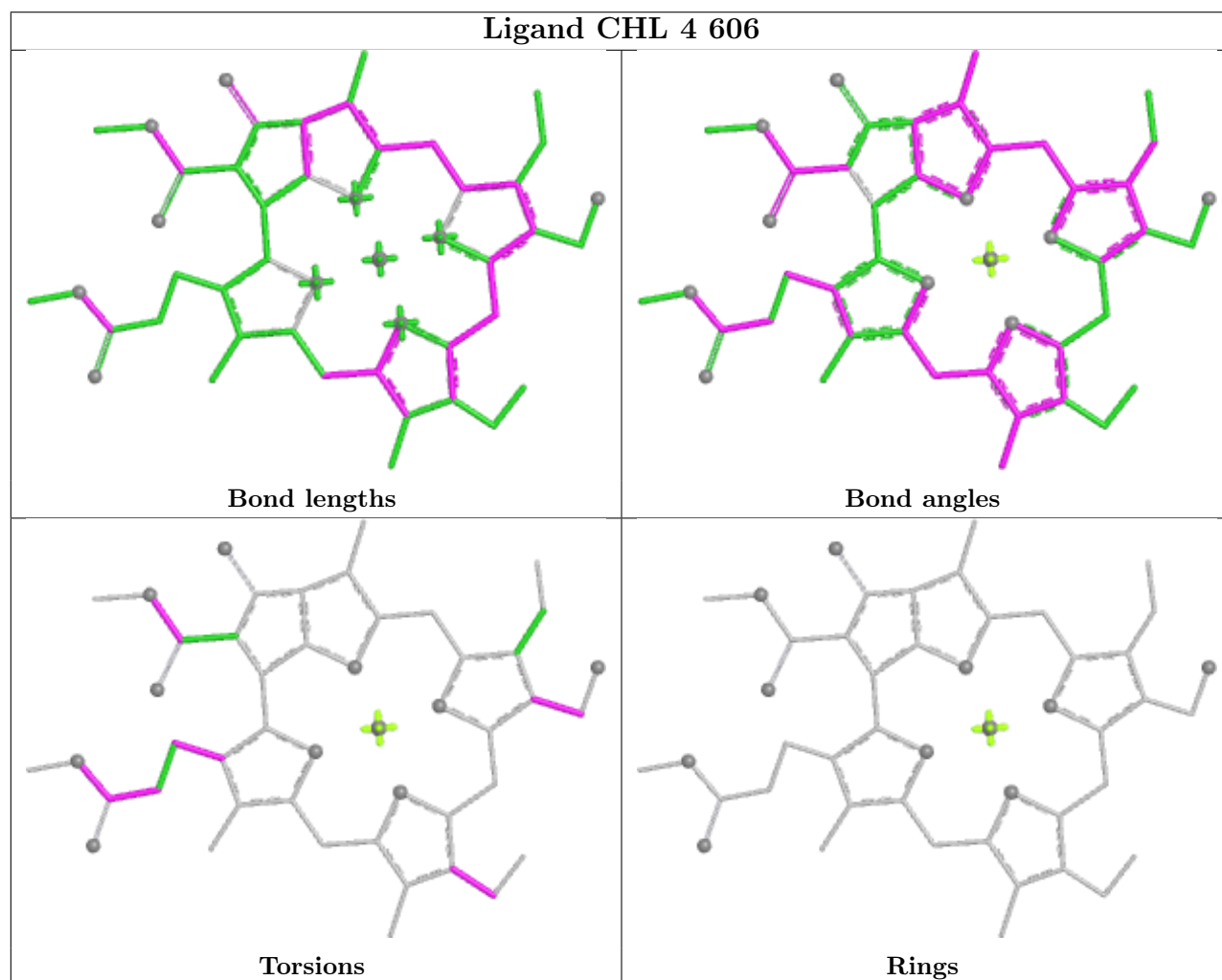
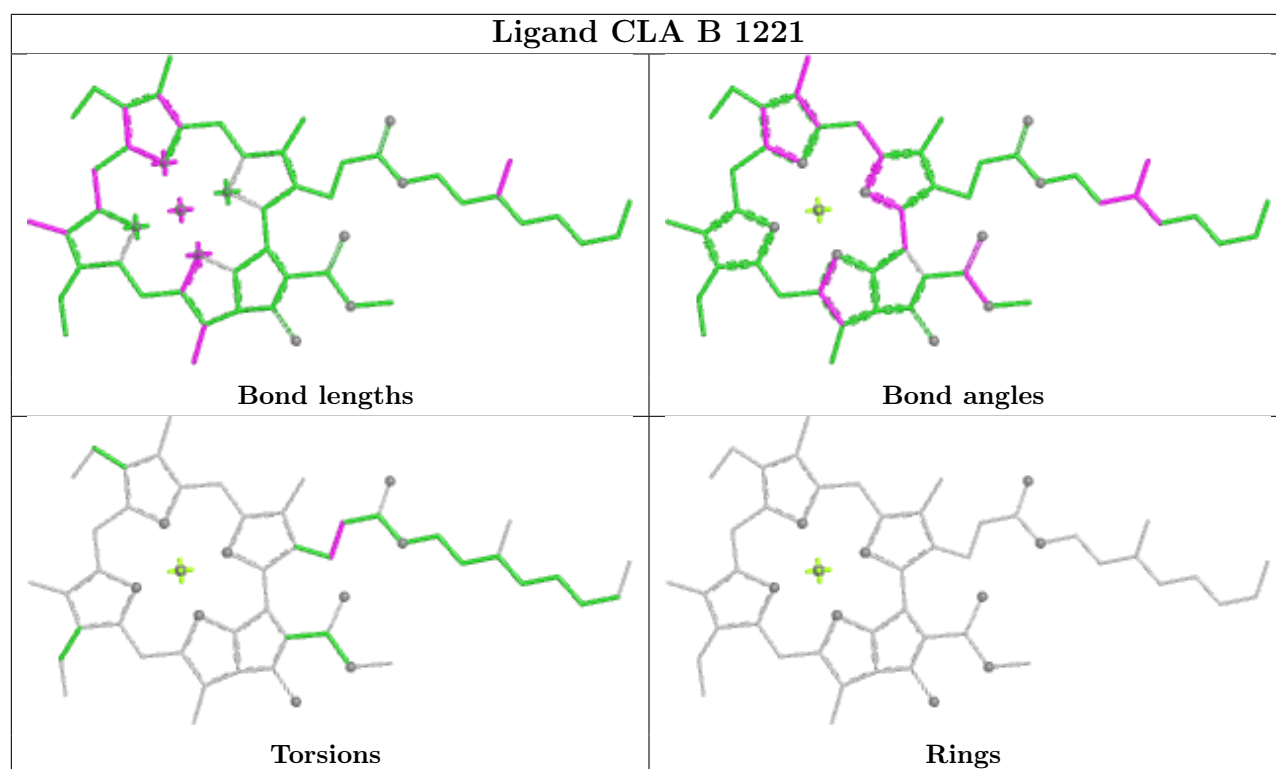


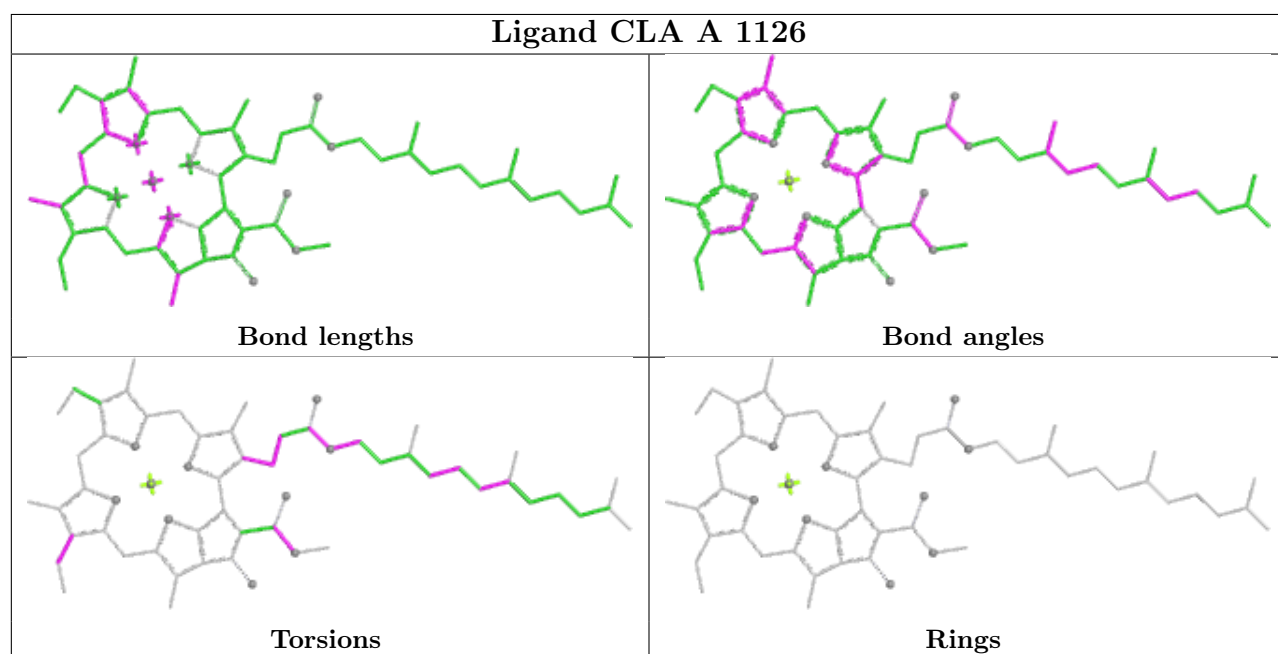
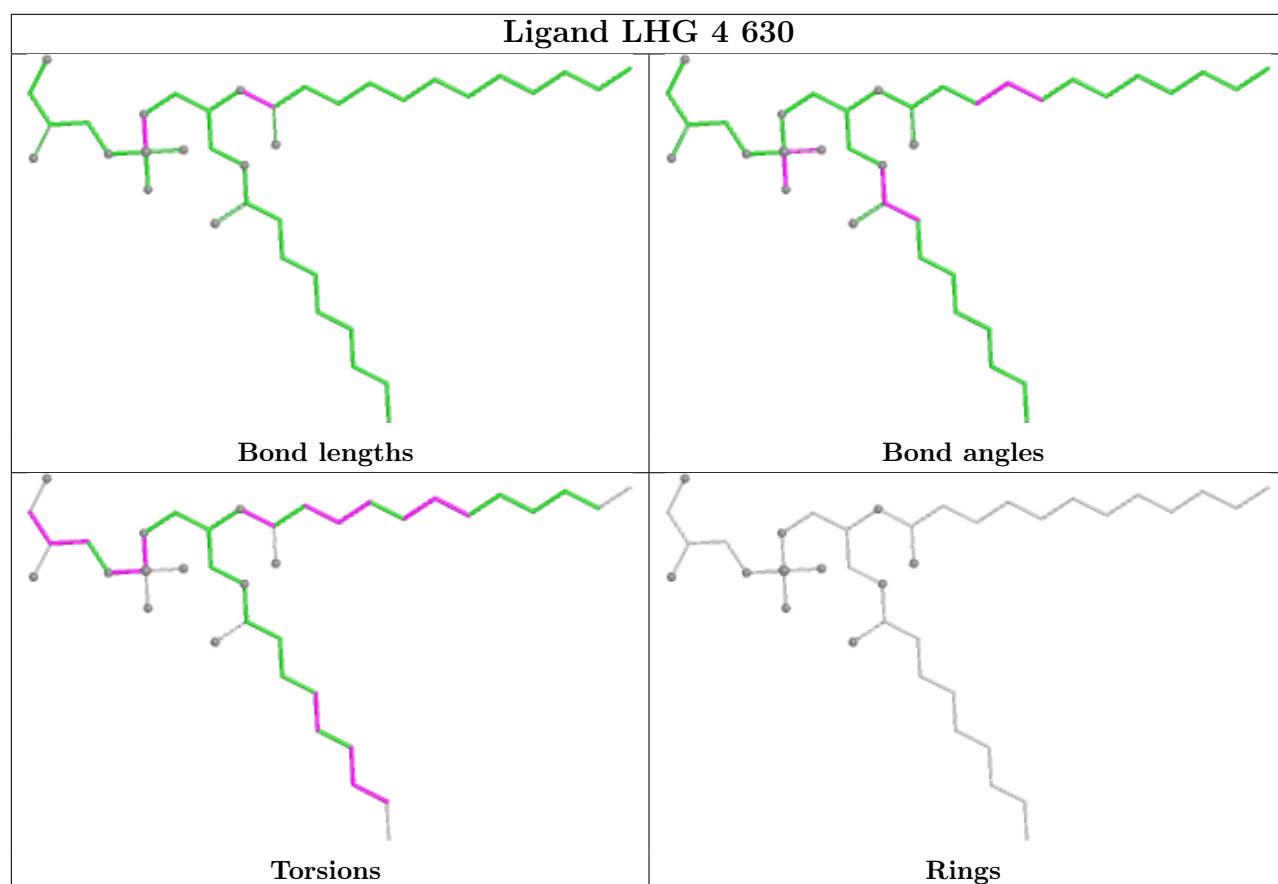
Ligand LHG 2 630

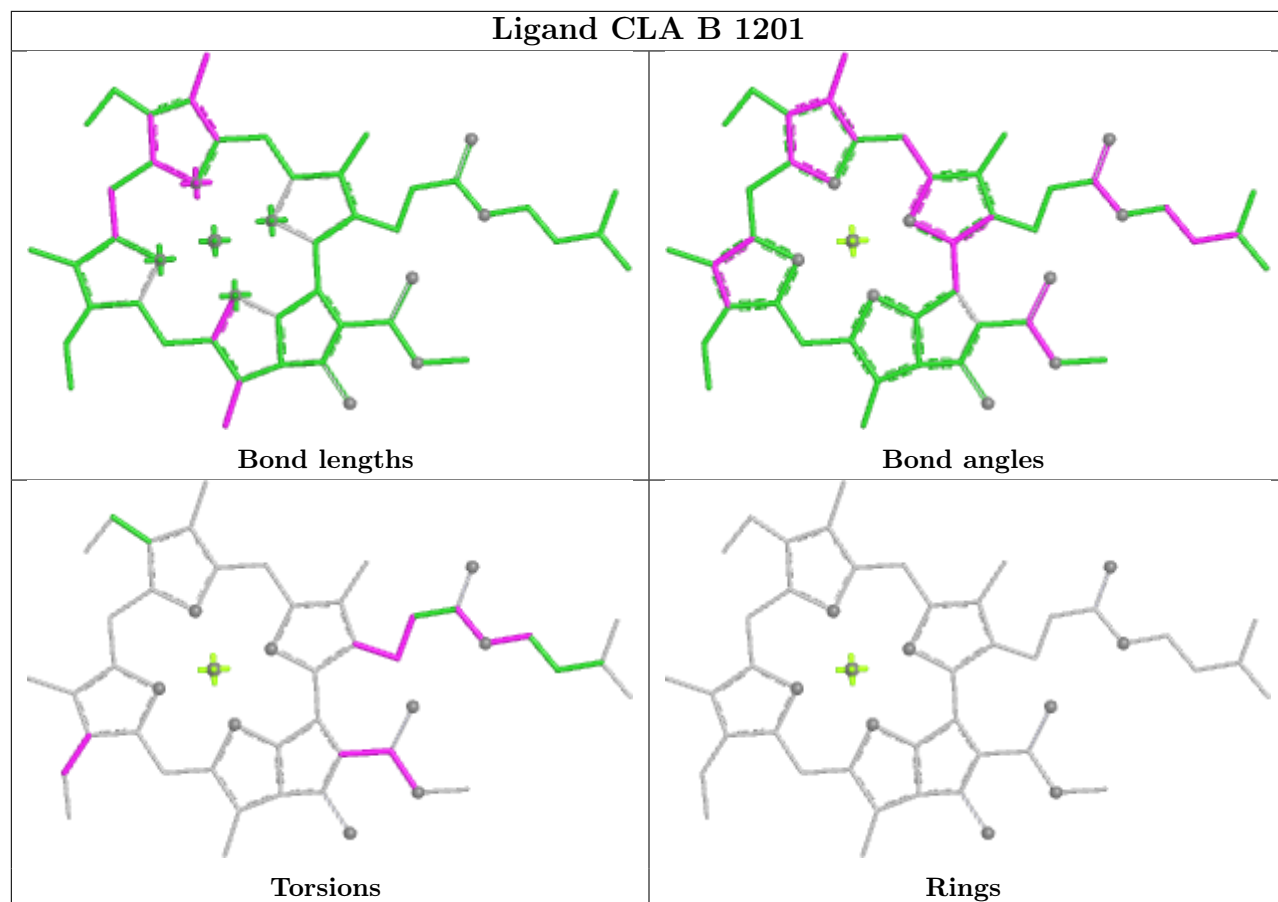


Ligand CLA B 1225

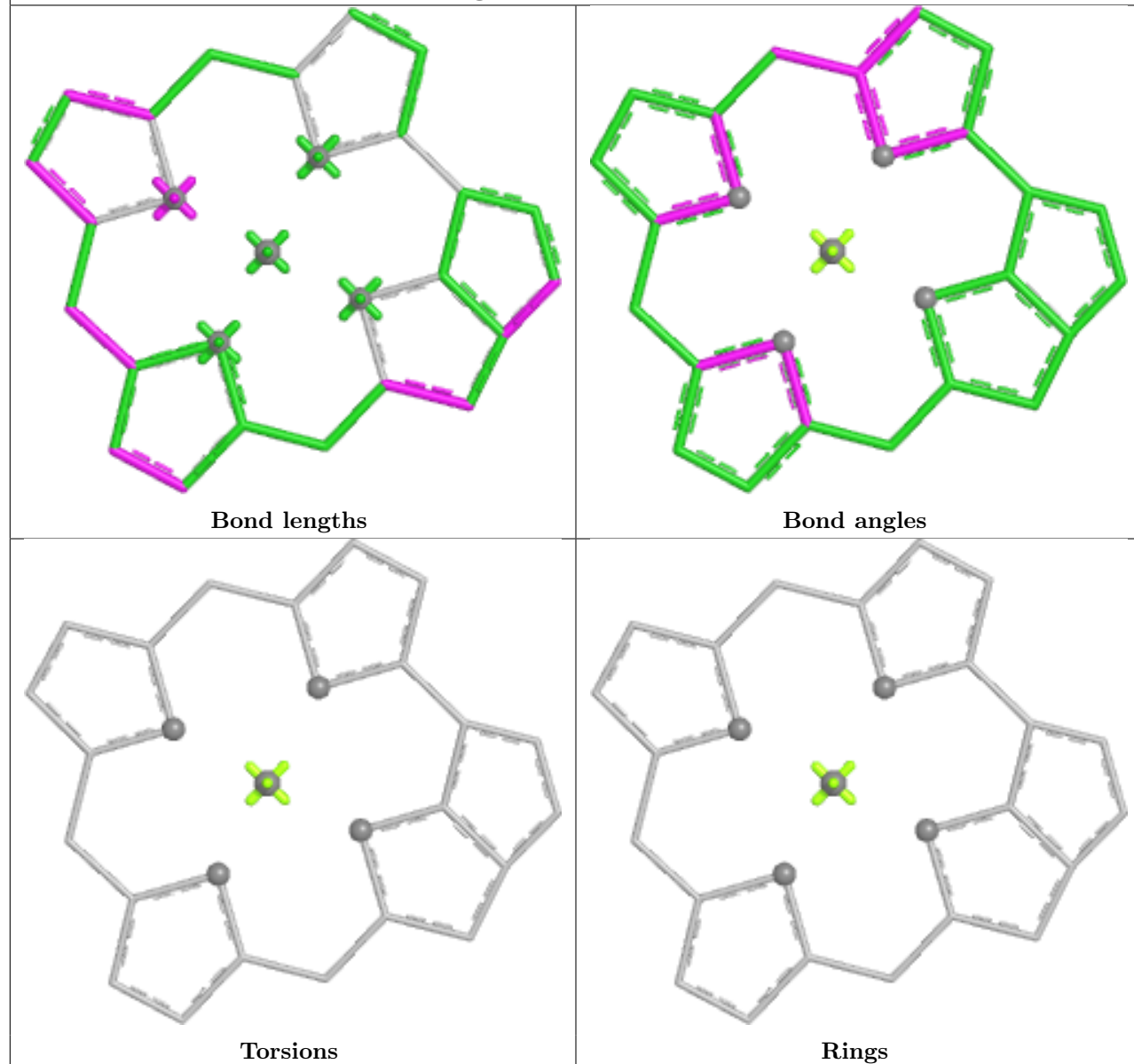


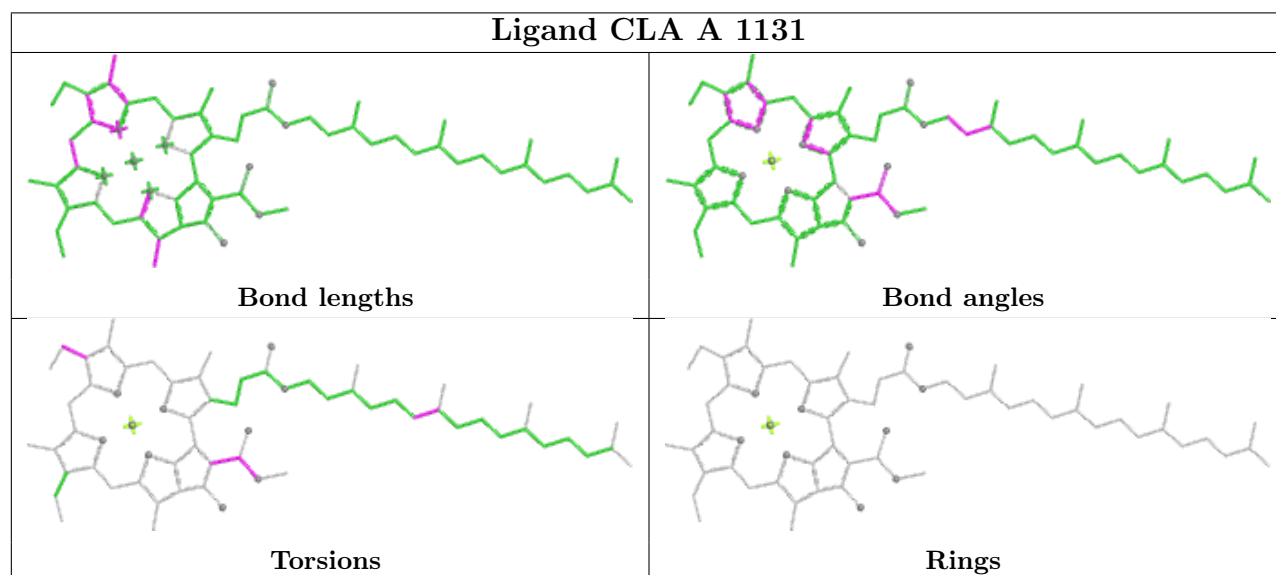
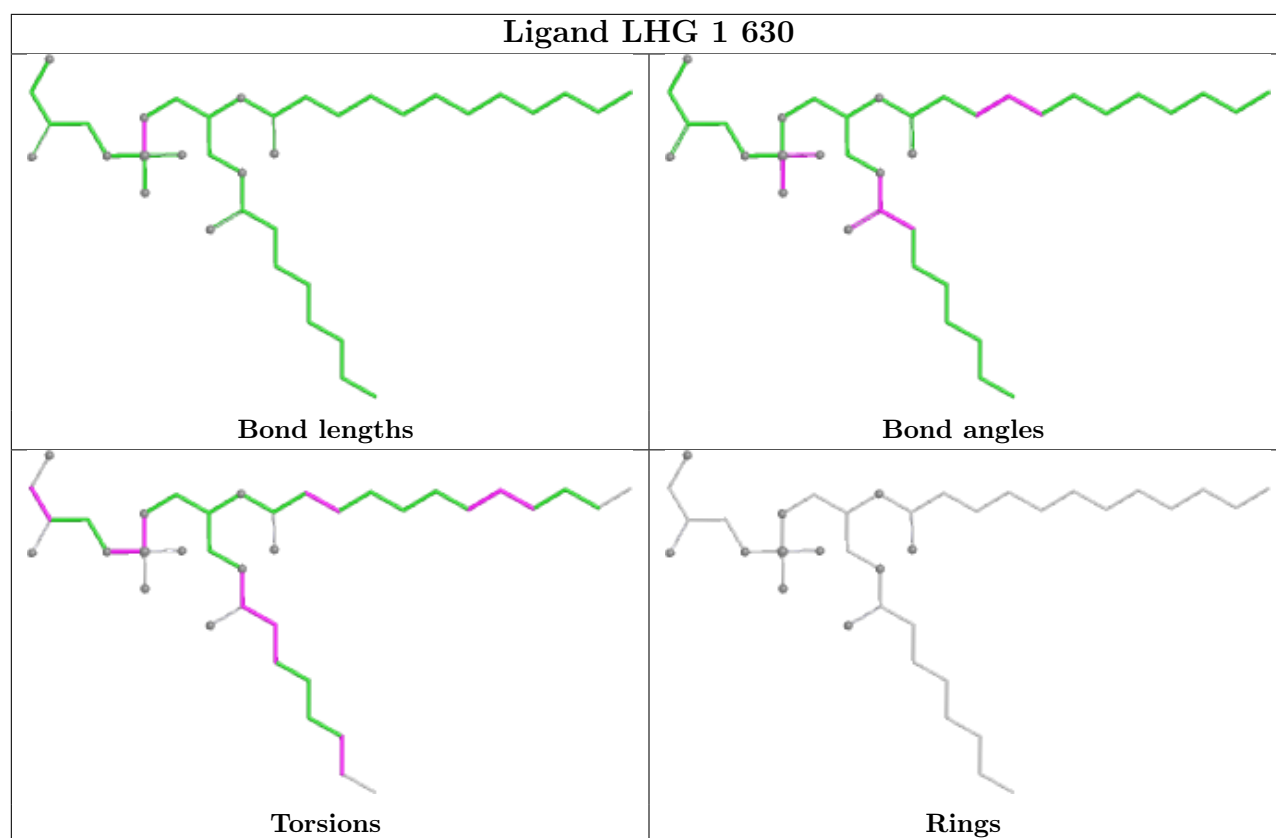


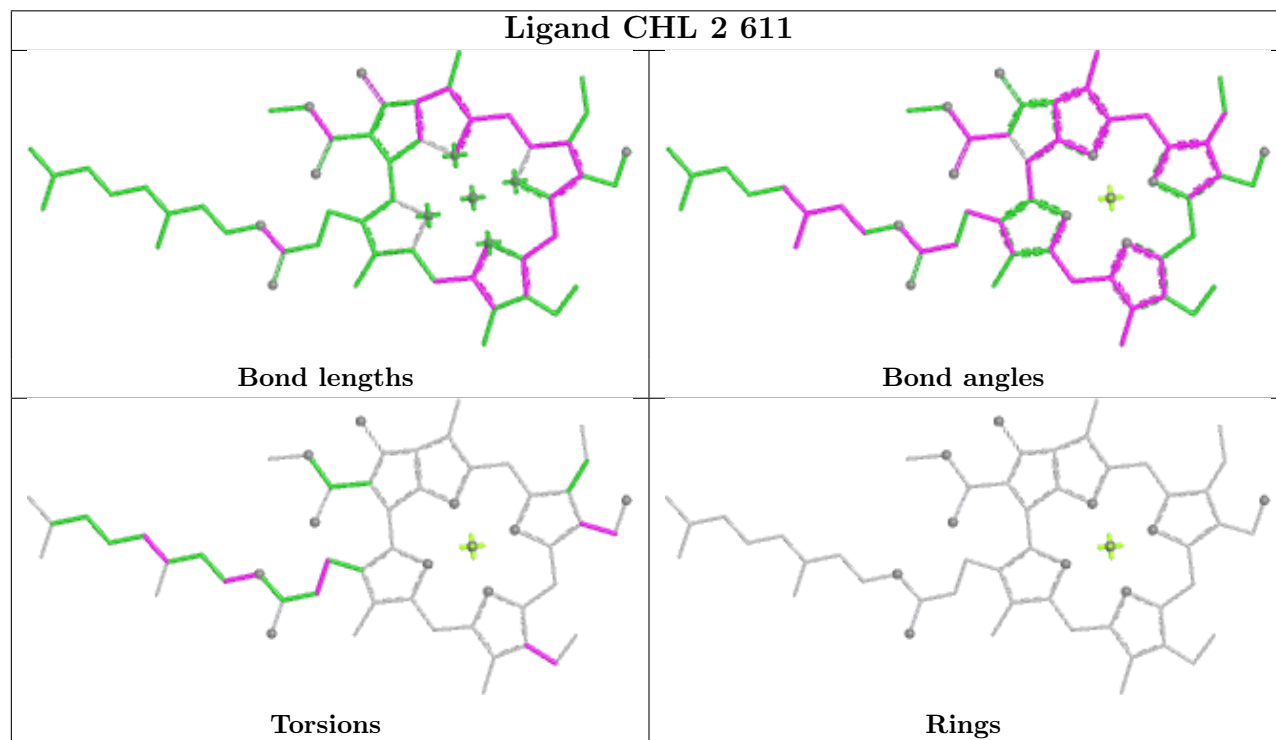
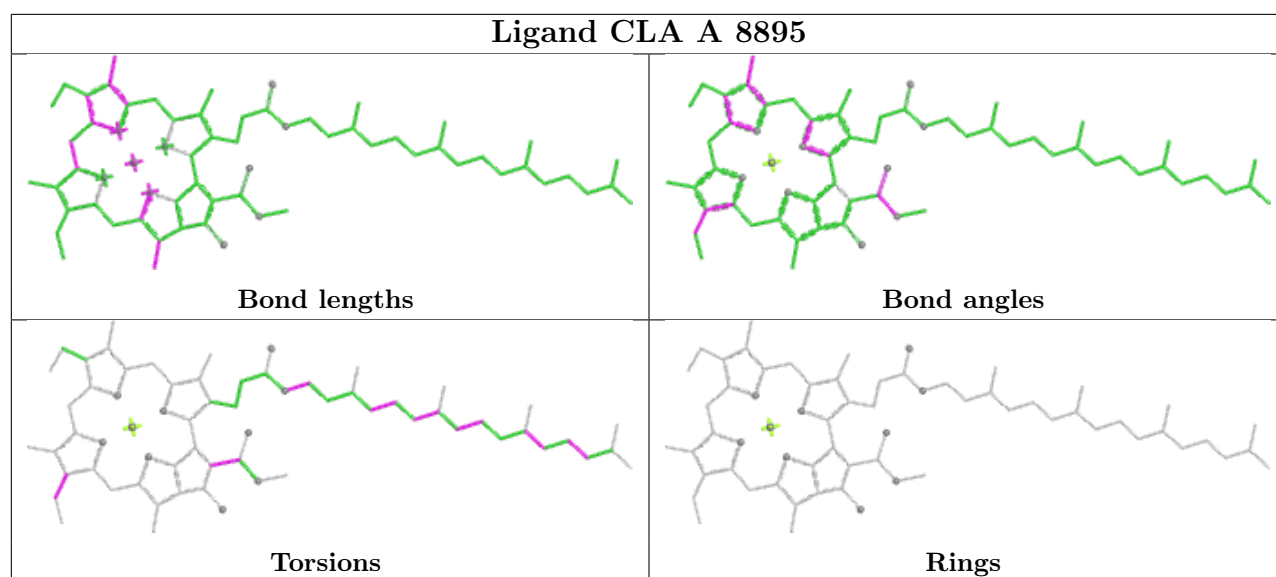




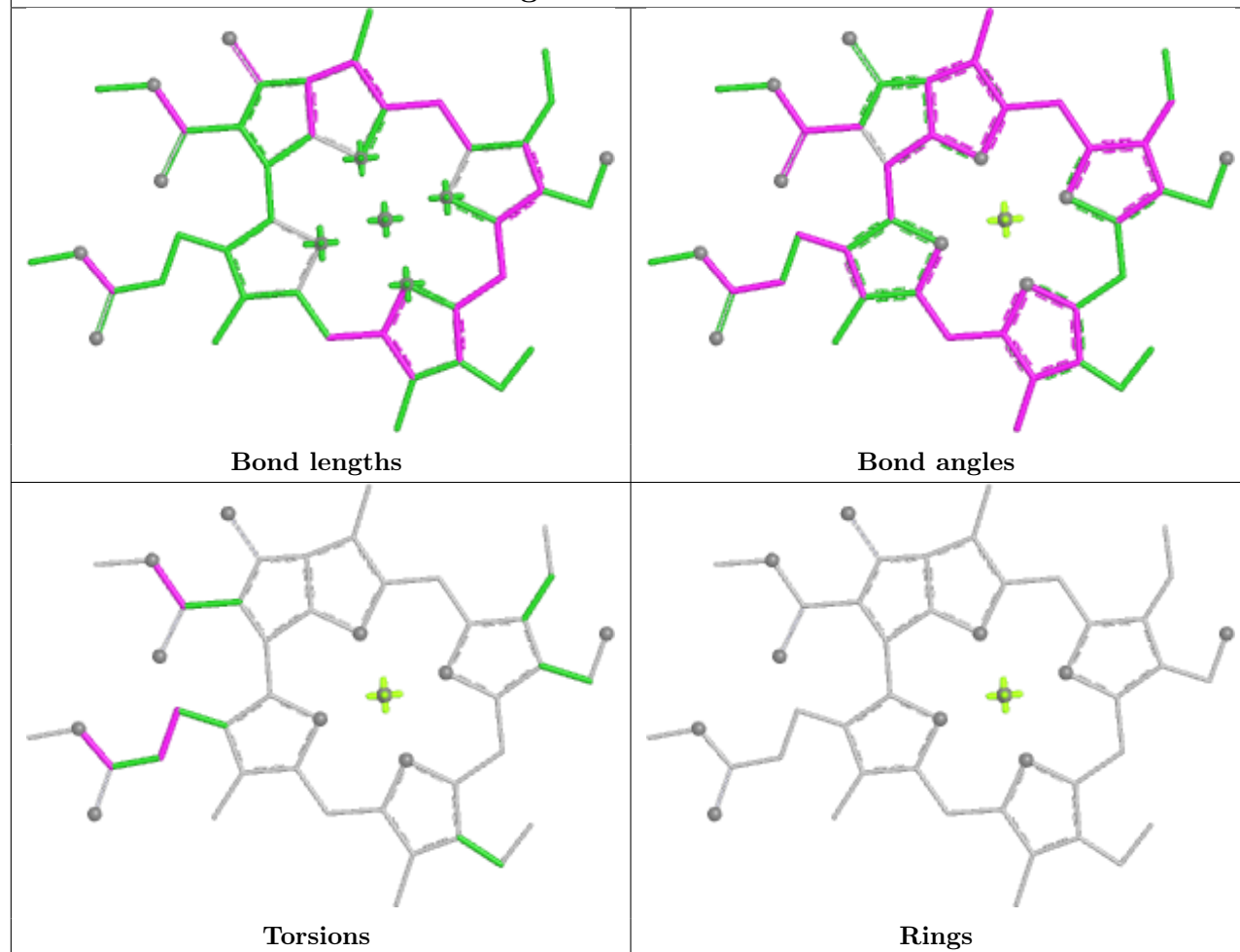
Ligand CLA O 201



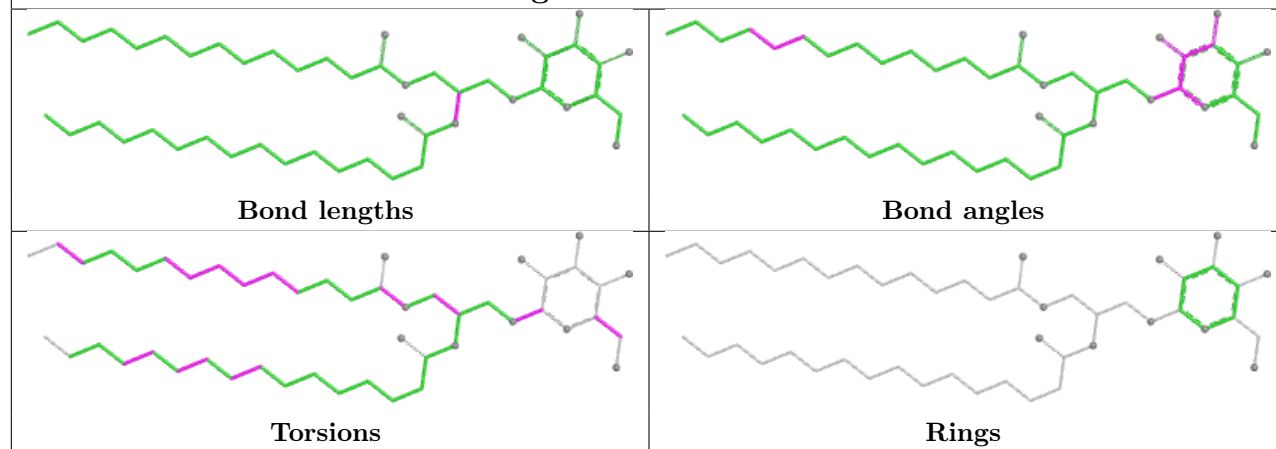




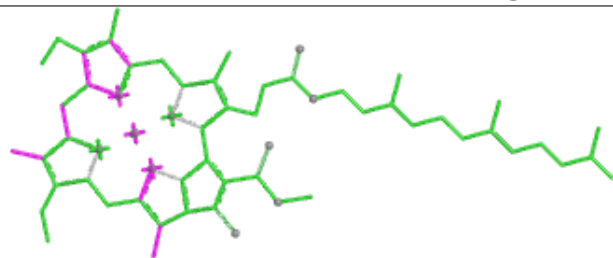
Ligand CHL 3 608



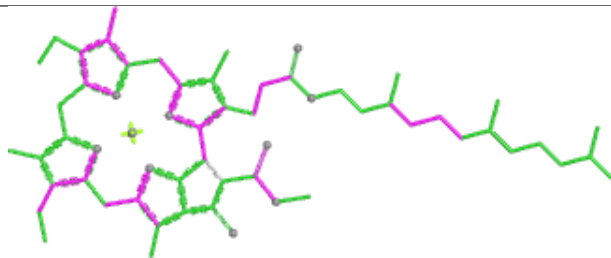
Ligand LMG J 301



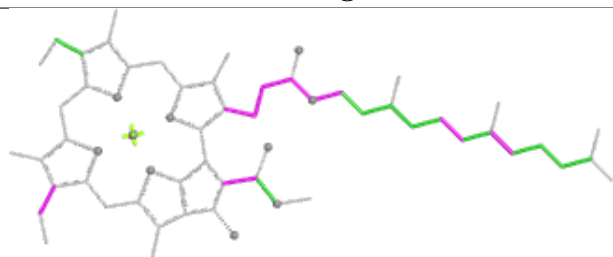
Ligand CLA A 1125



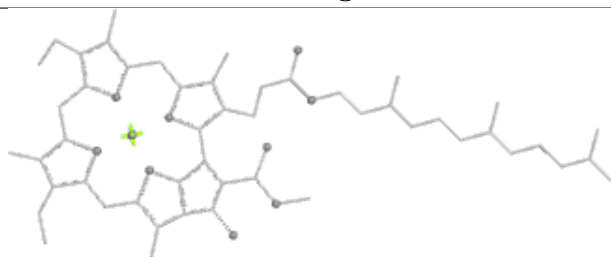
Bond lengths



Bond angles

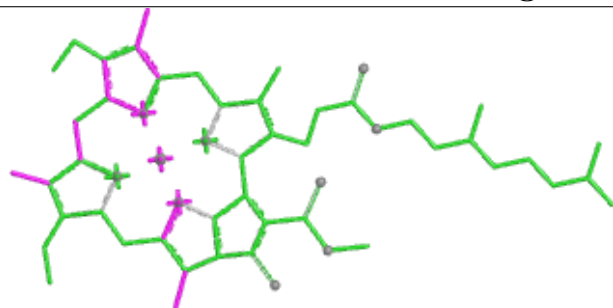


Torsions

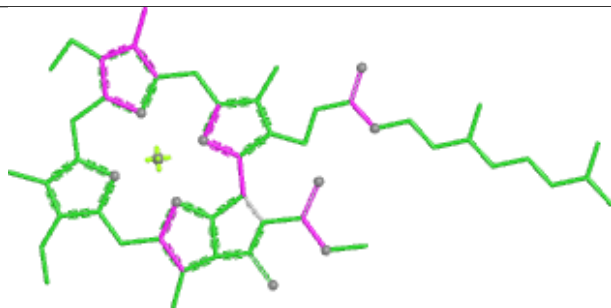


Rings

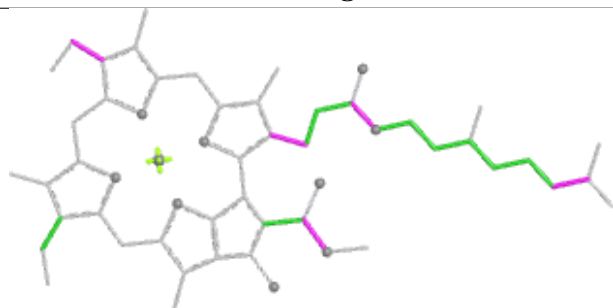
Ligand CLA 4 610



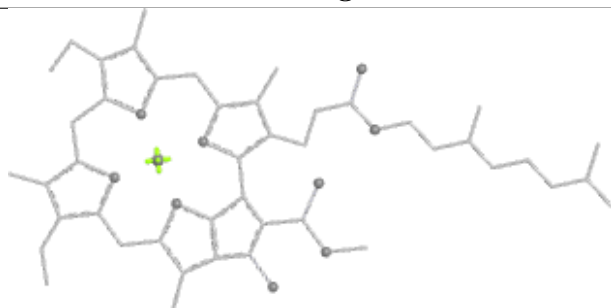
Bond lengths



Bond angles

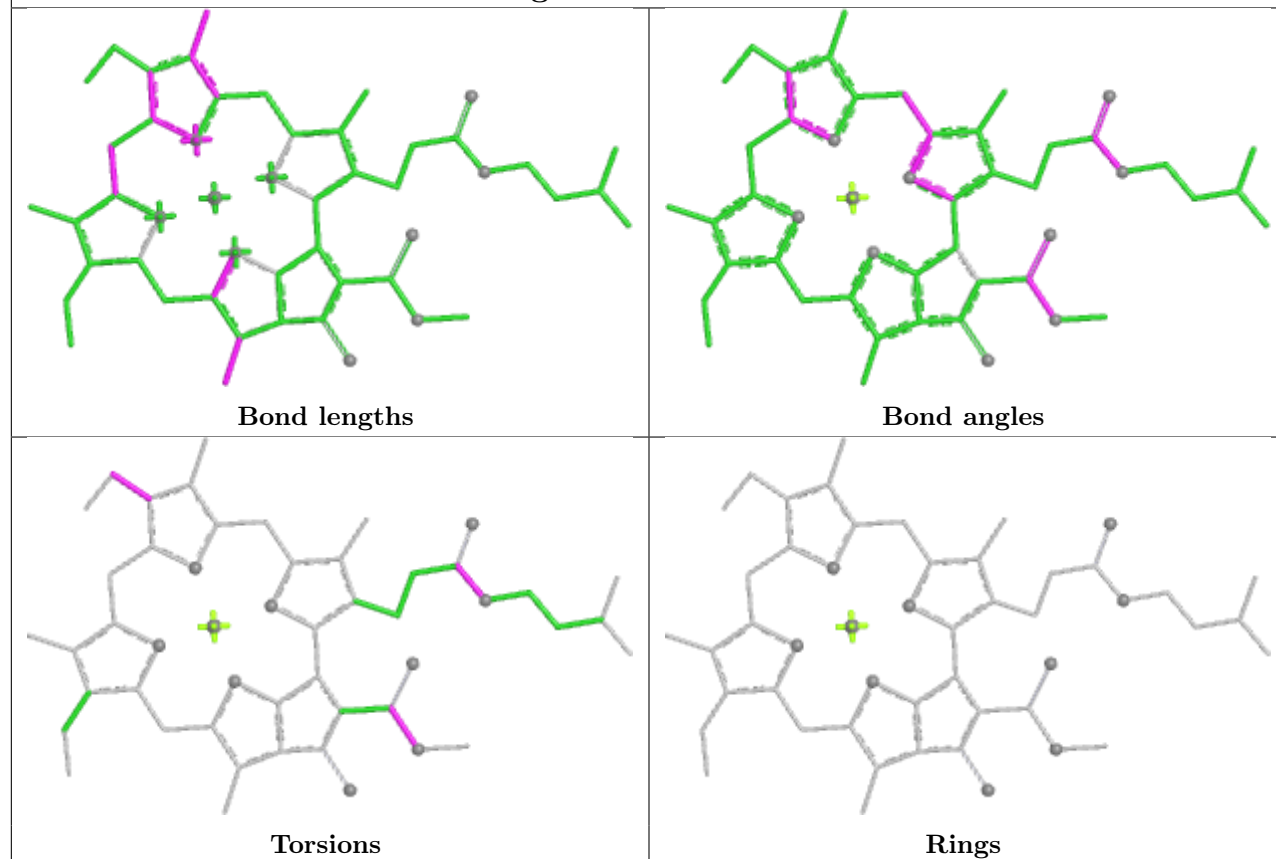


Torsions

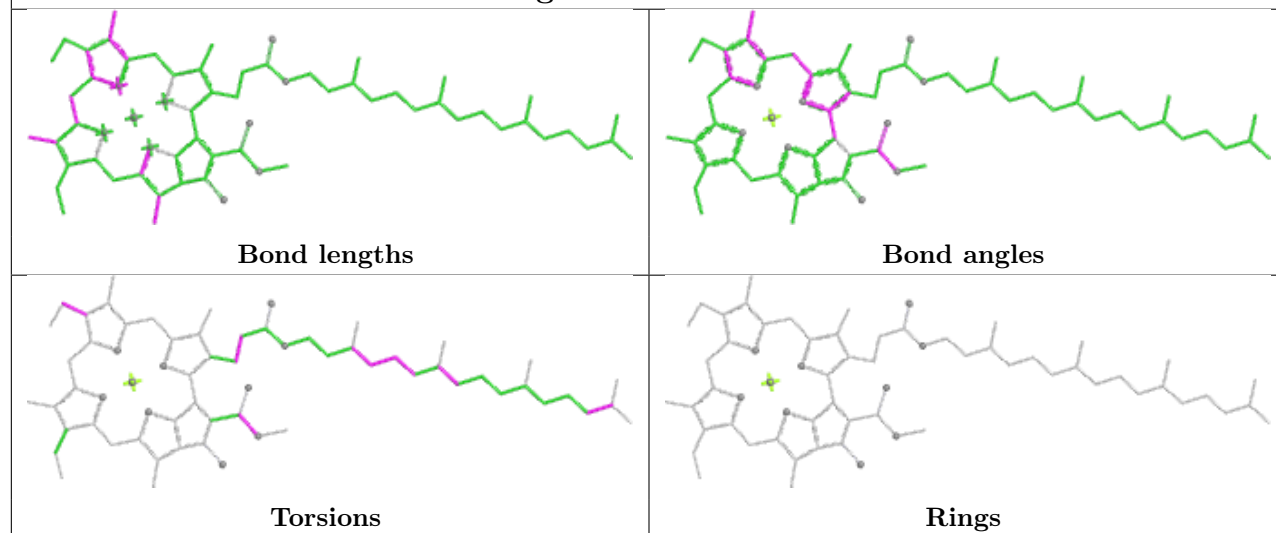


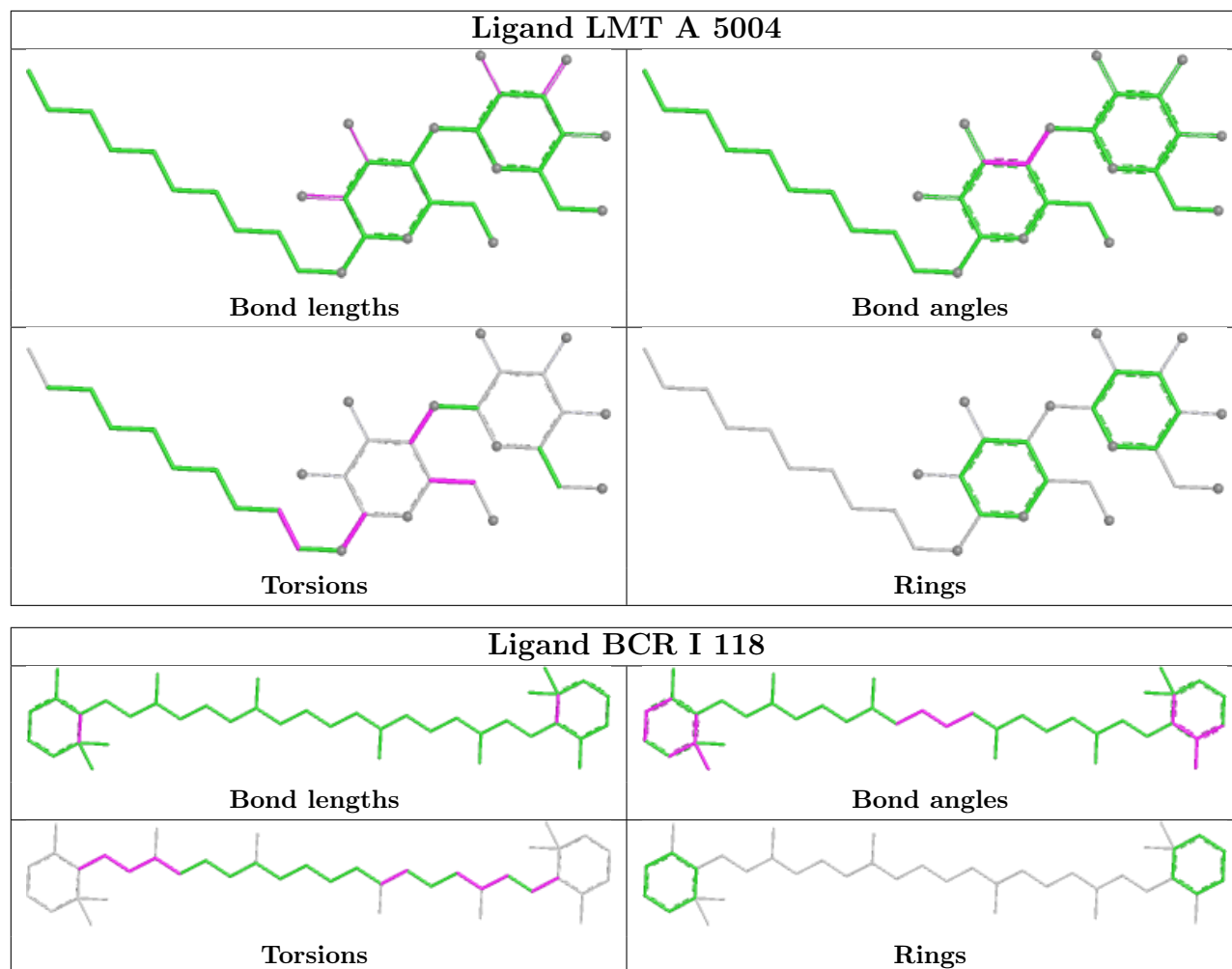
Rings

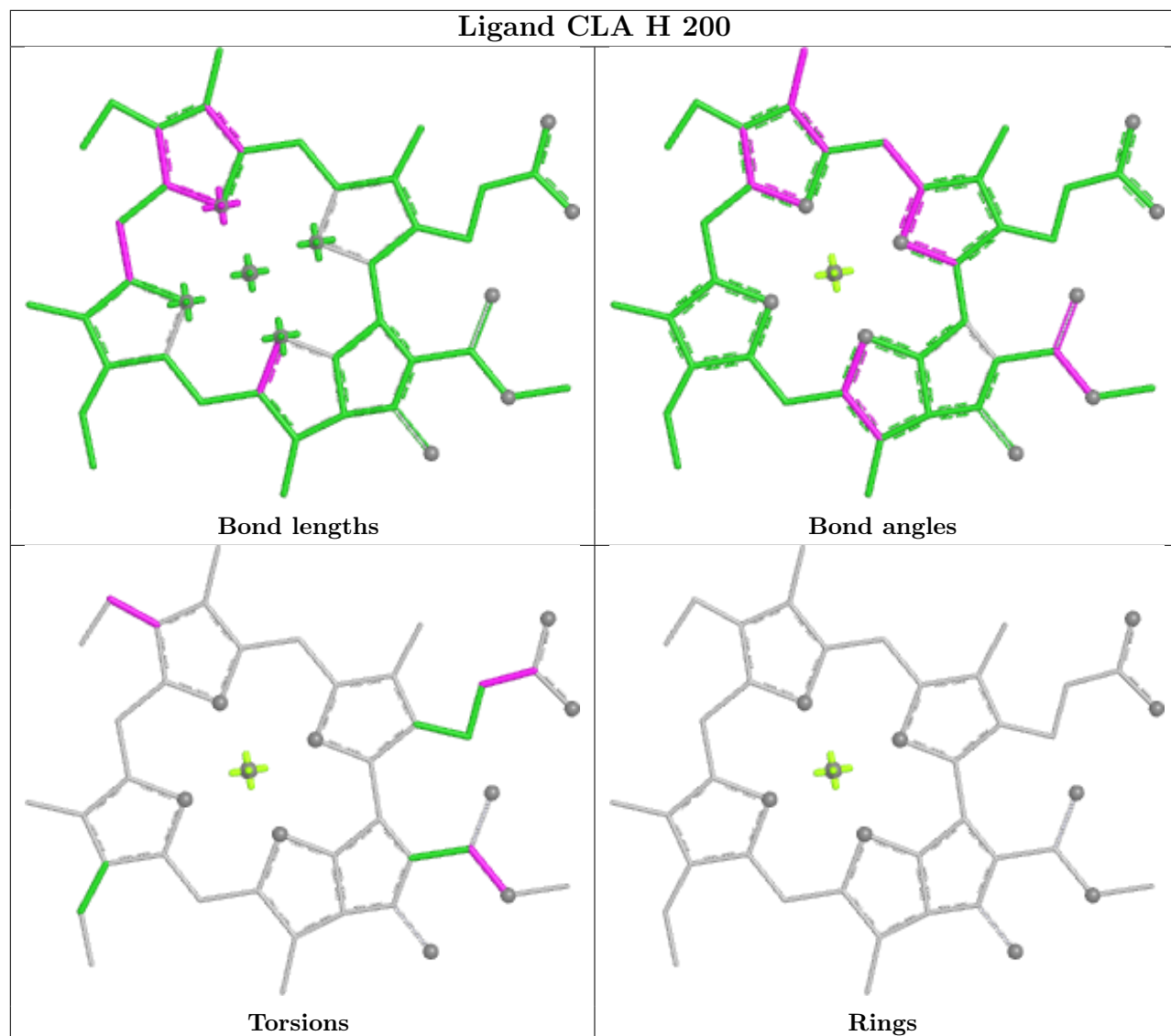
Ligand CLA G 201



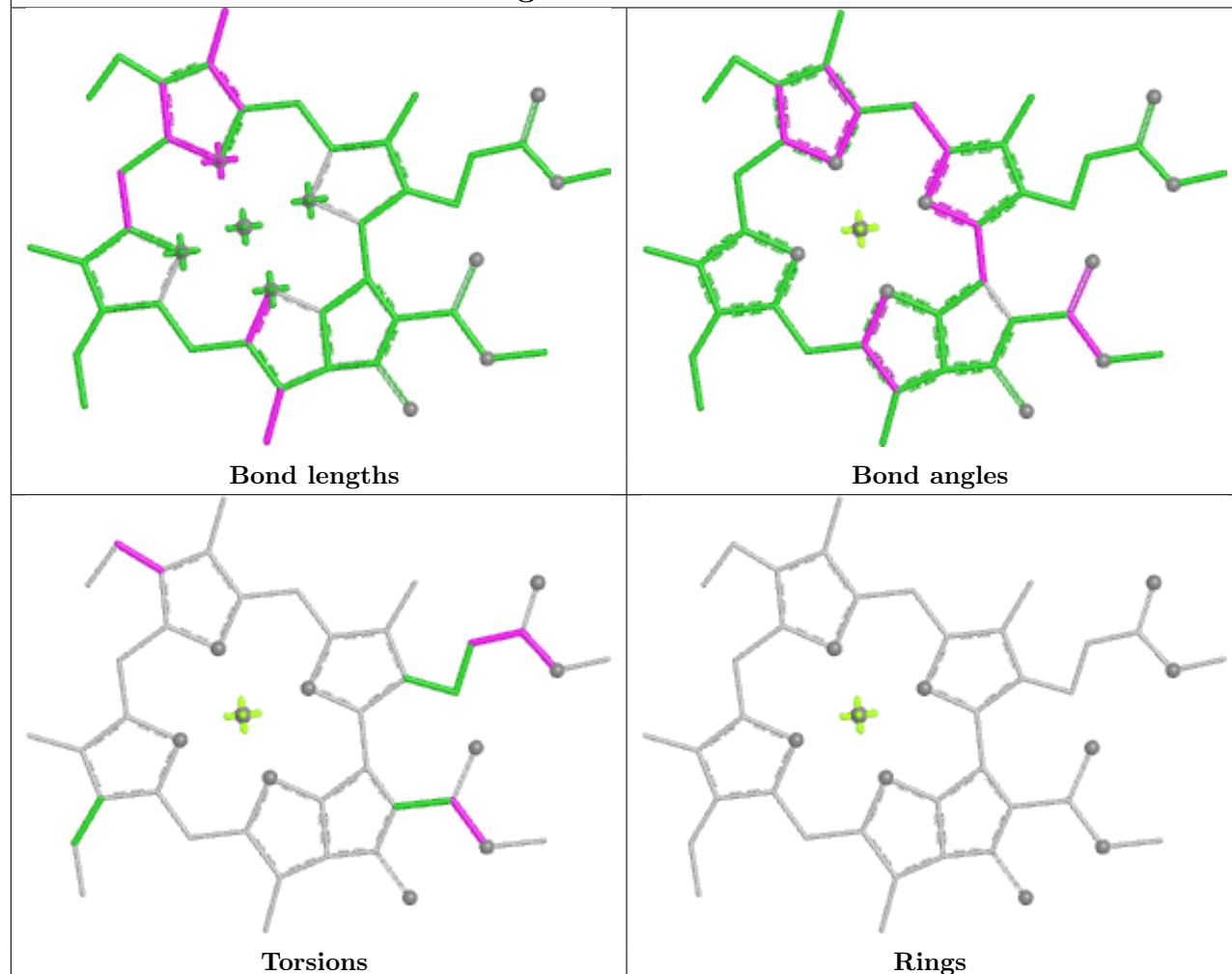
Ligand CLA 2 613



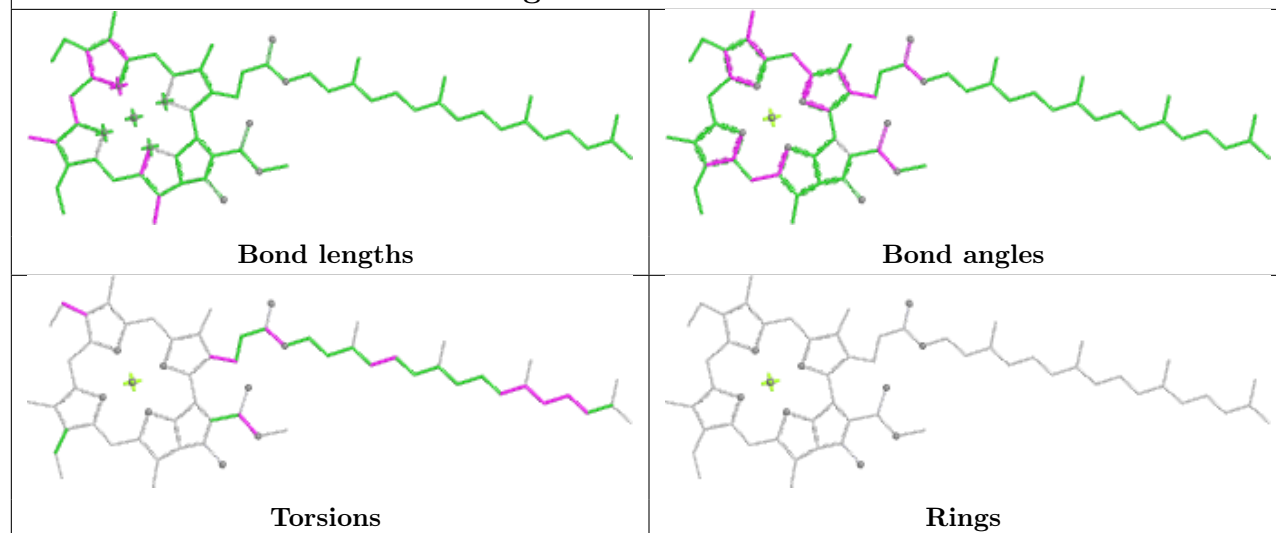




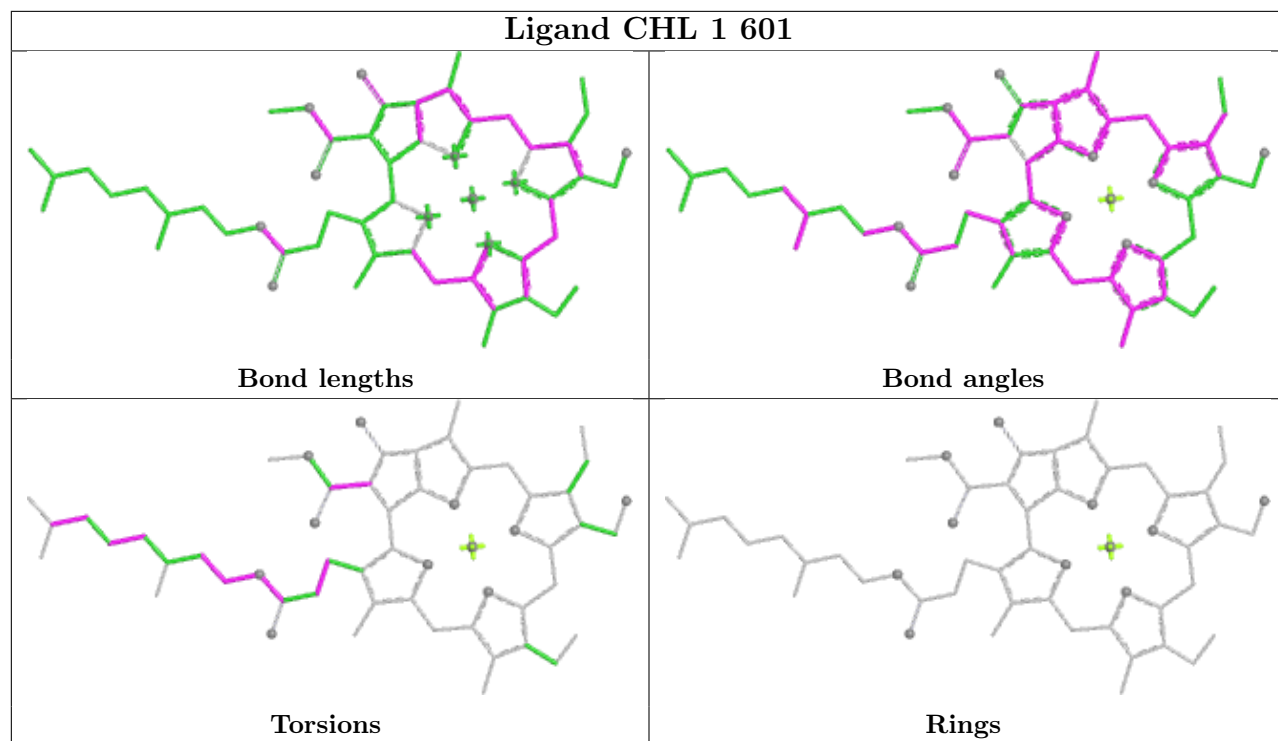
Ligand CLA 1 612



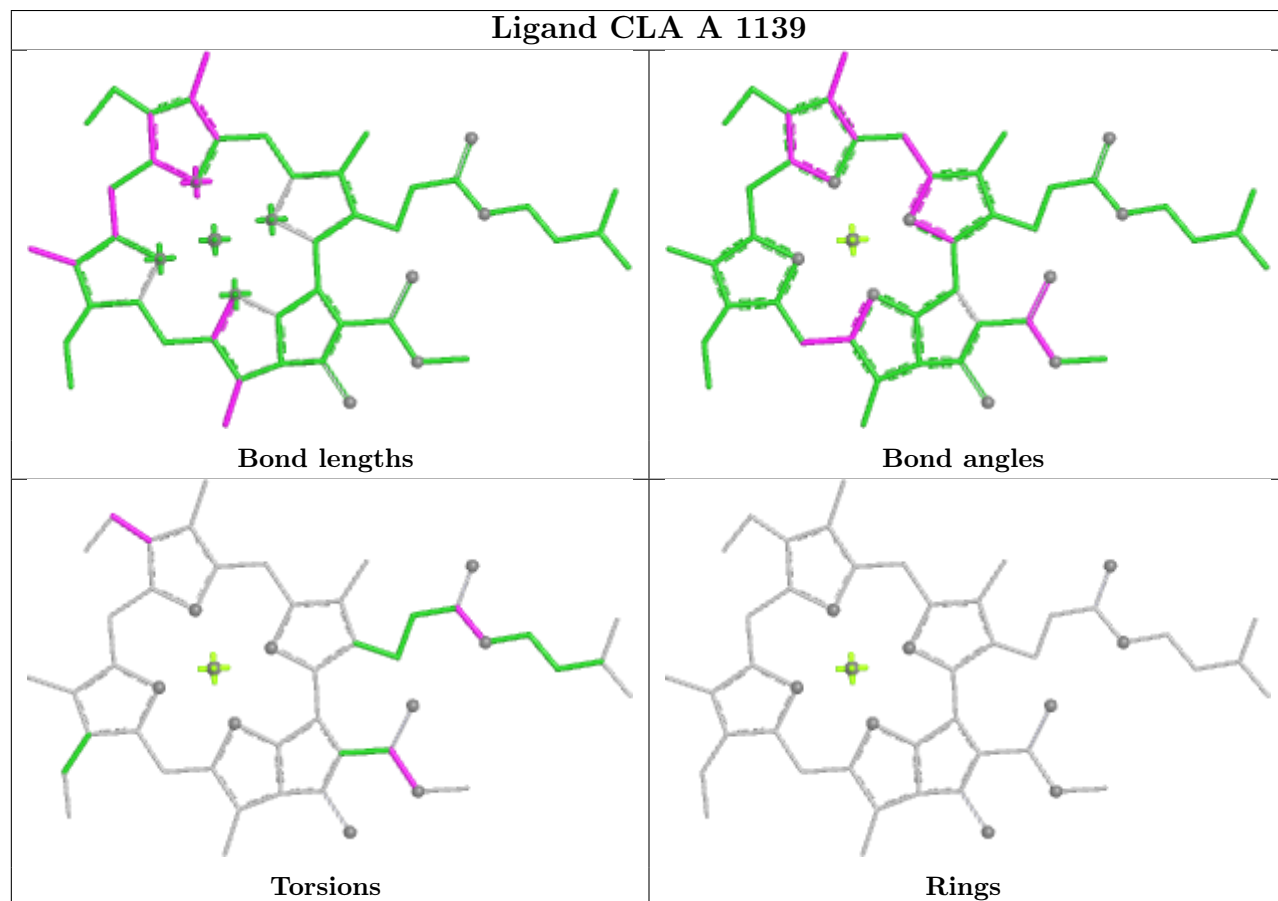
Ligand CLA B 1203

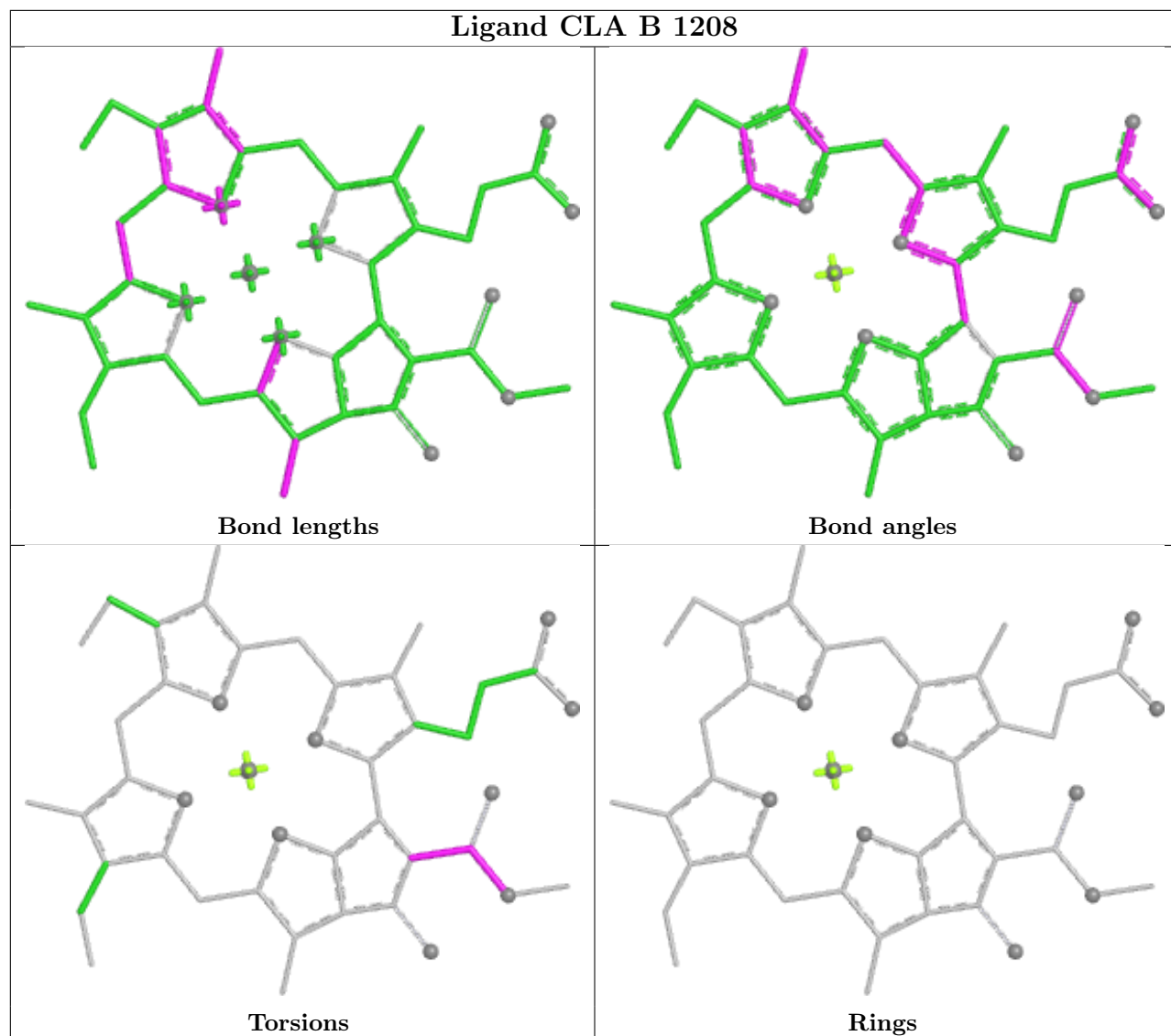


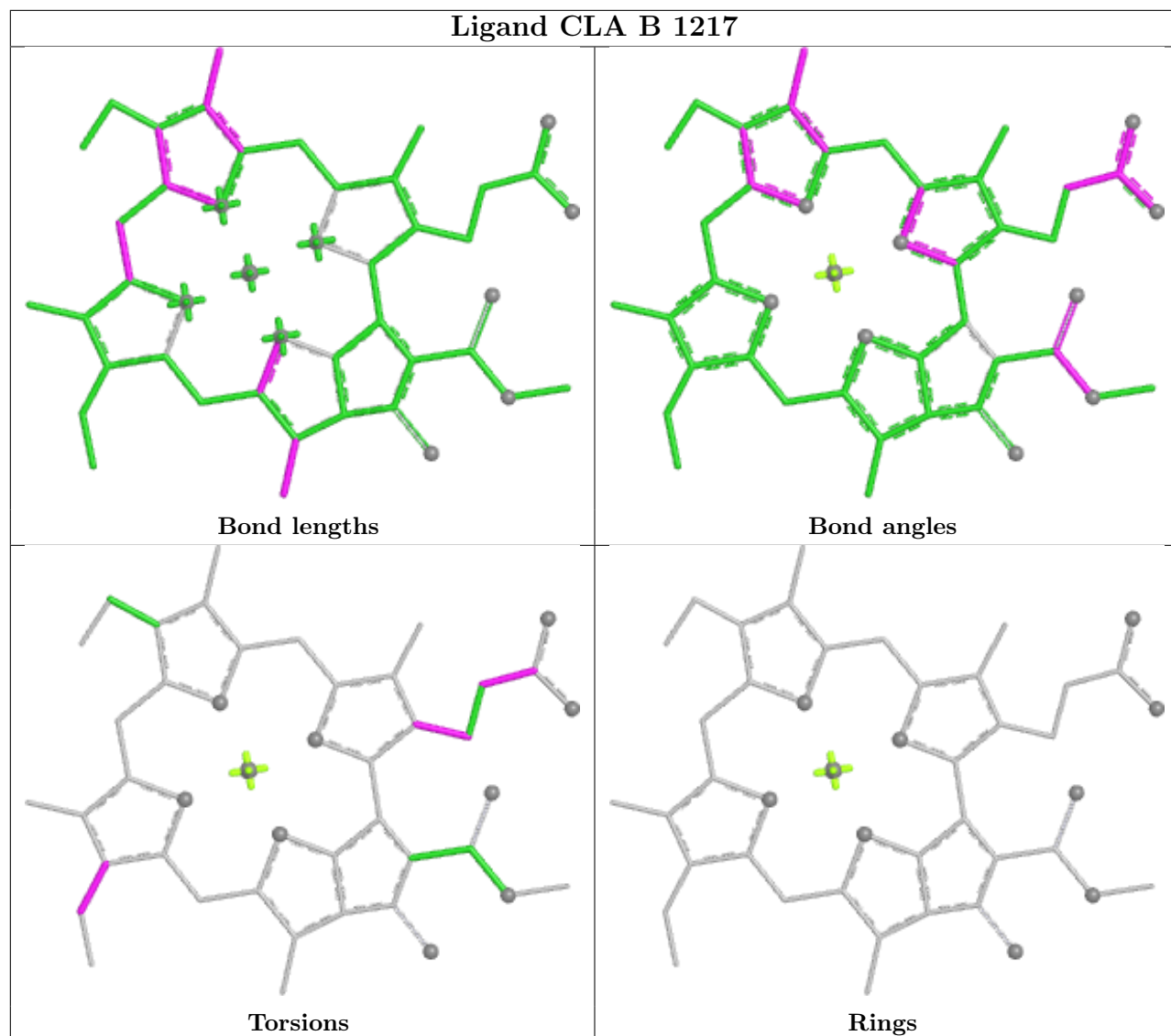
Ligand CHL 1 601

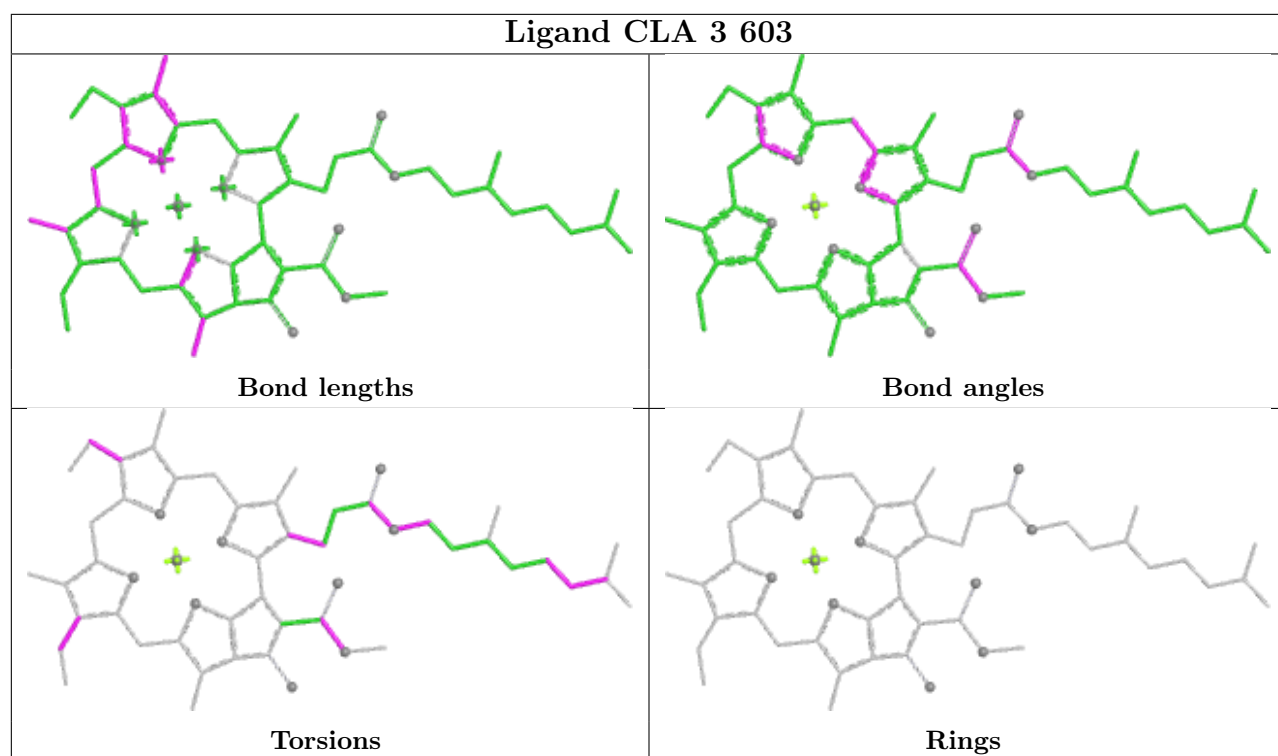


Ligand CLA A 1139

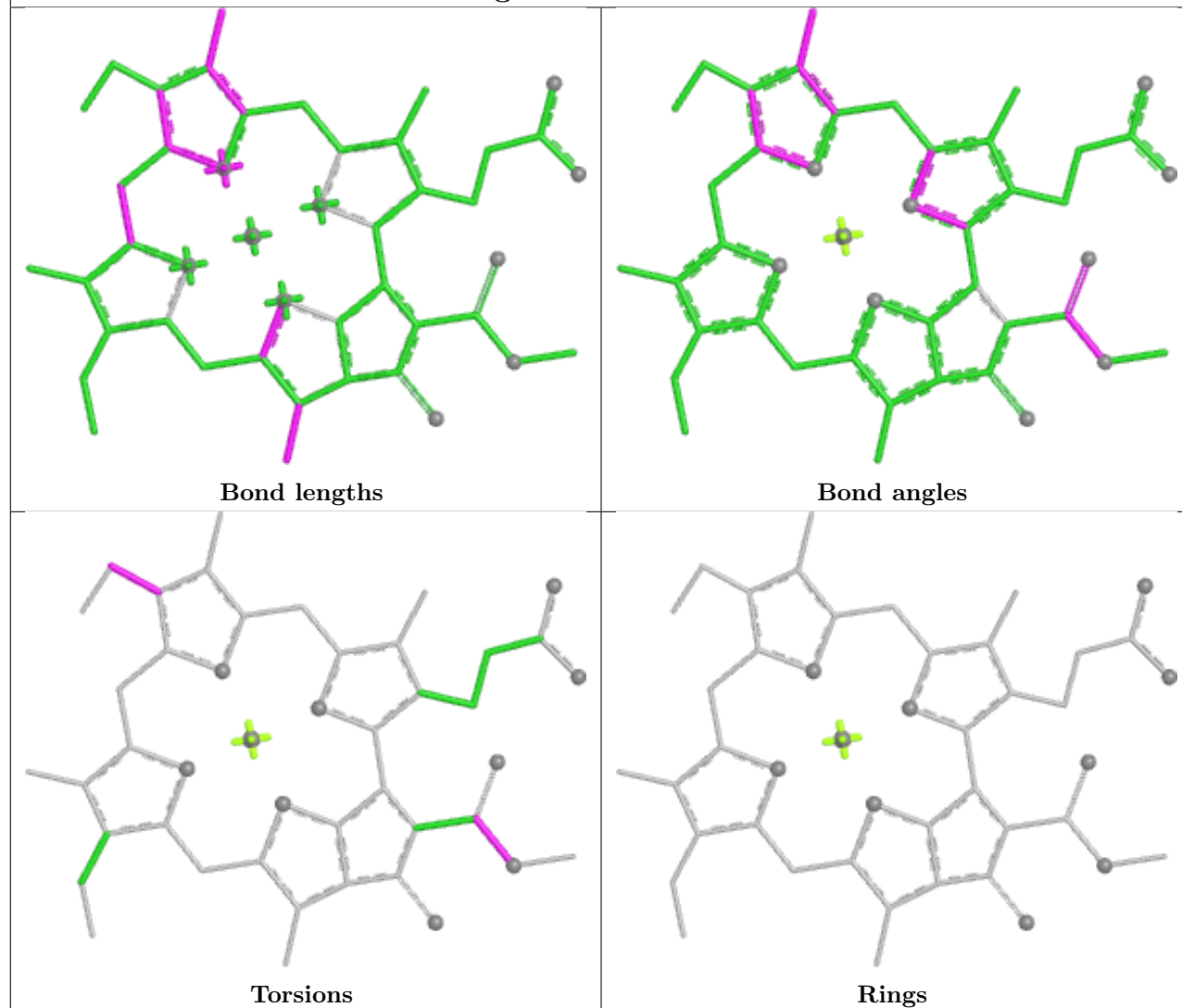




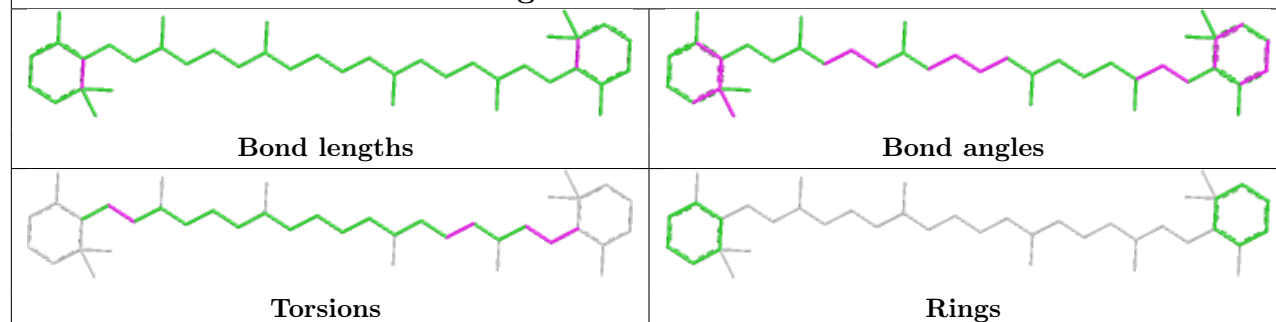


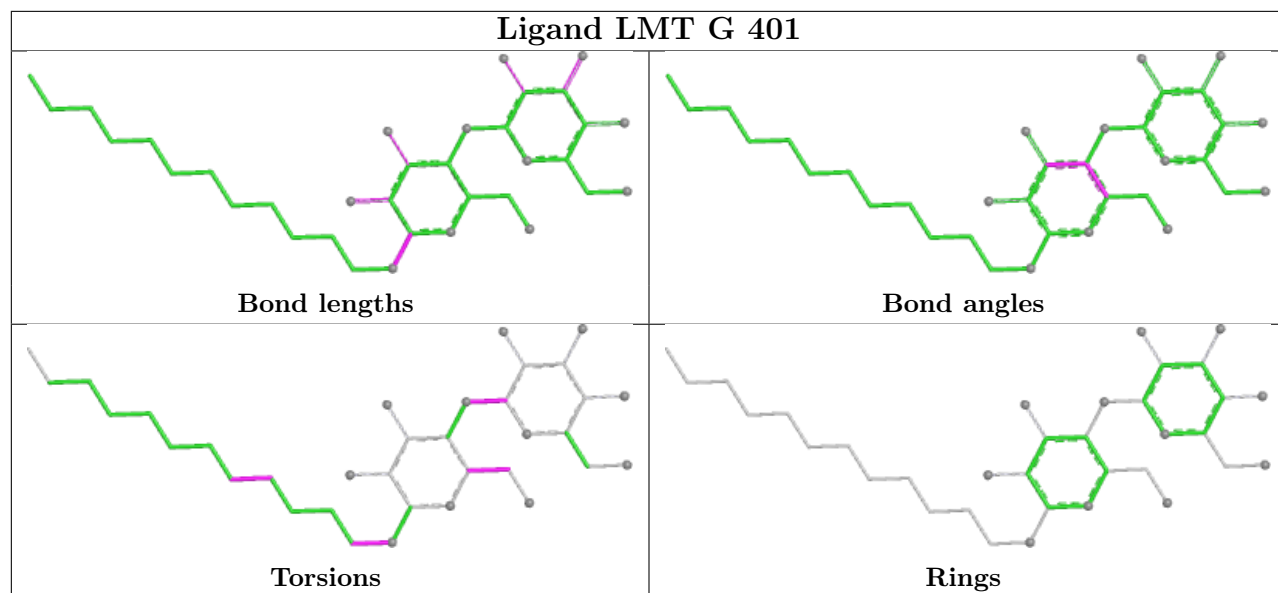


Ligand CLA F 301

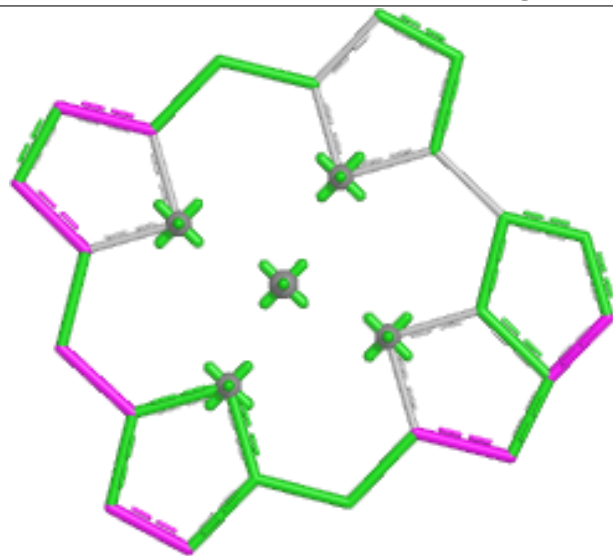


Ligand BCR M 4021

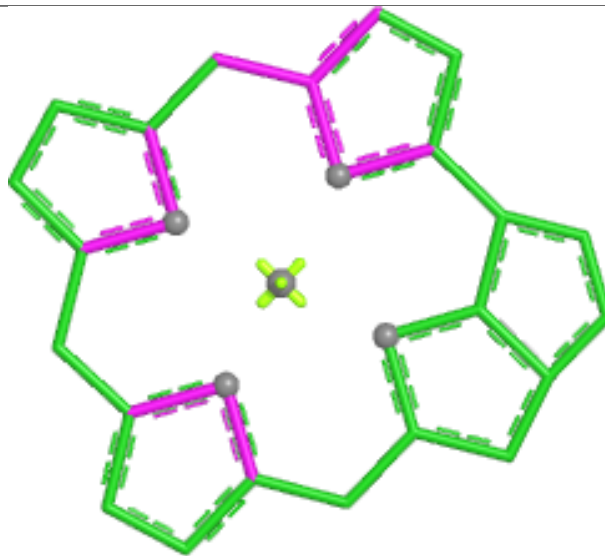




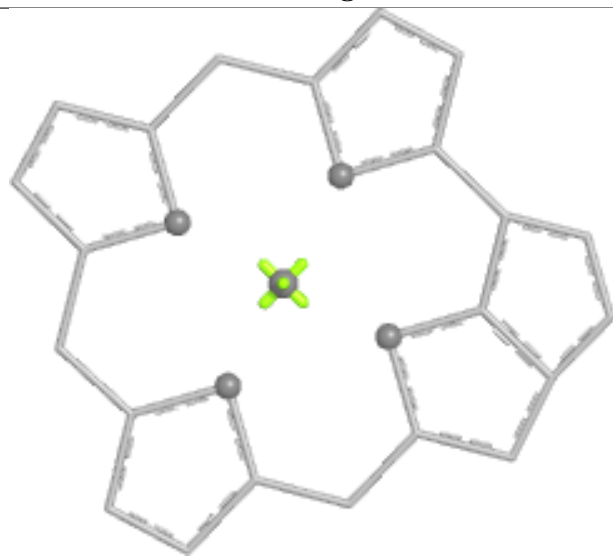
Ligand CLA F 303



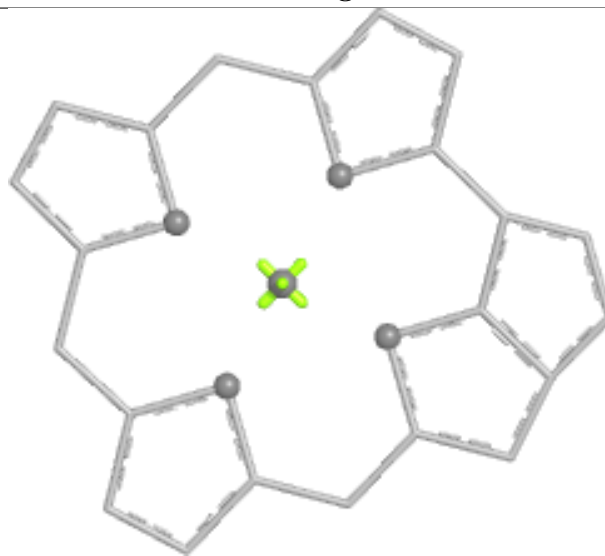
Bond lengths



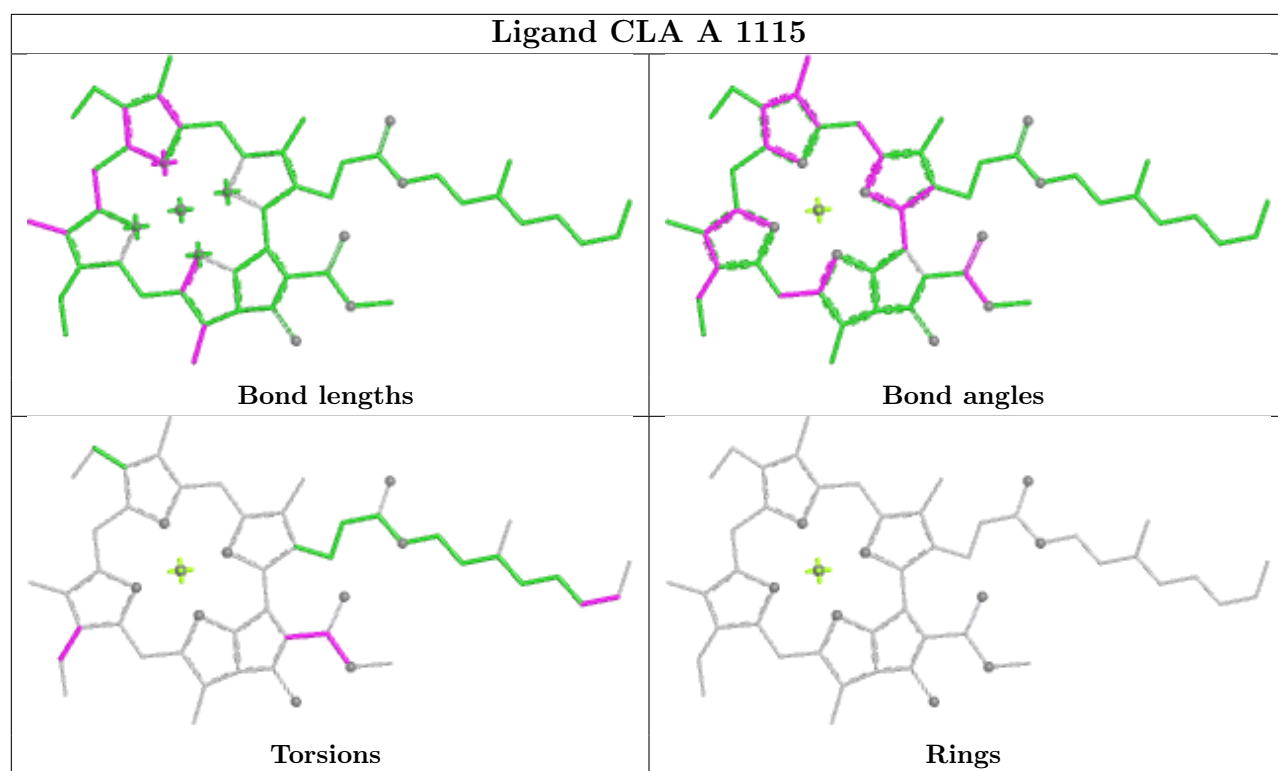
Bond angles

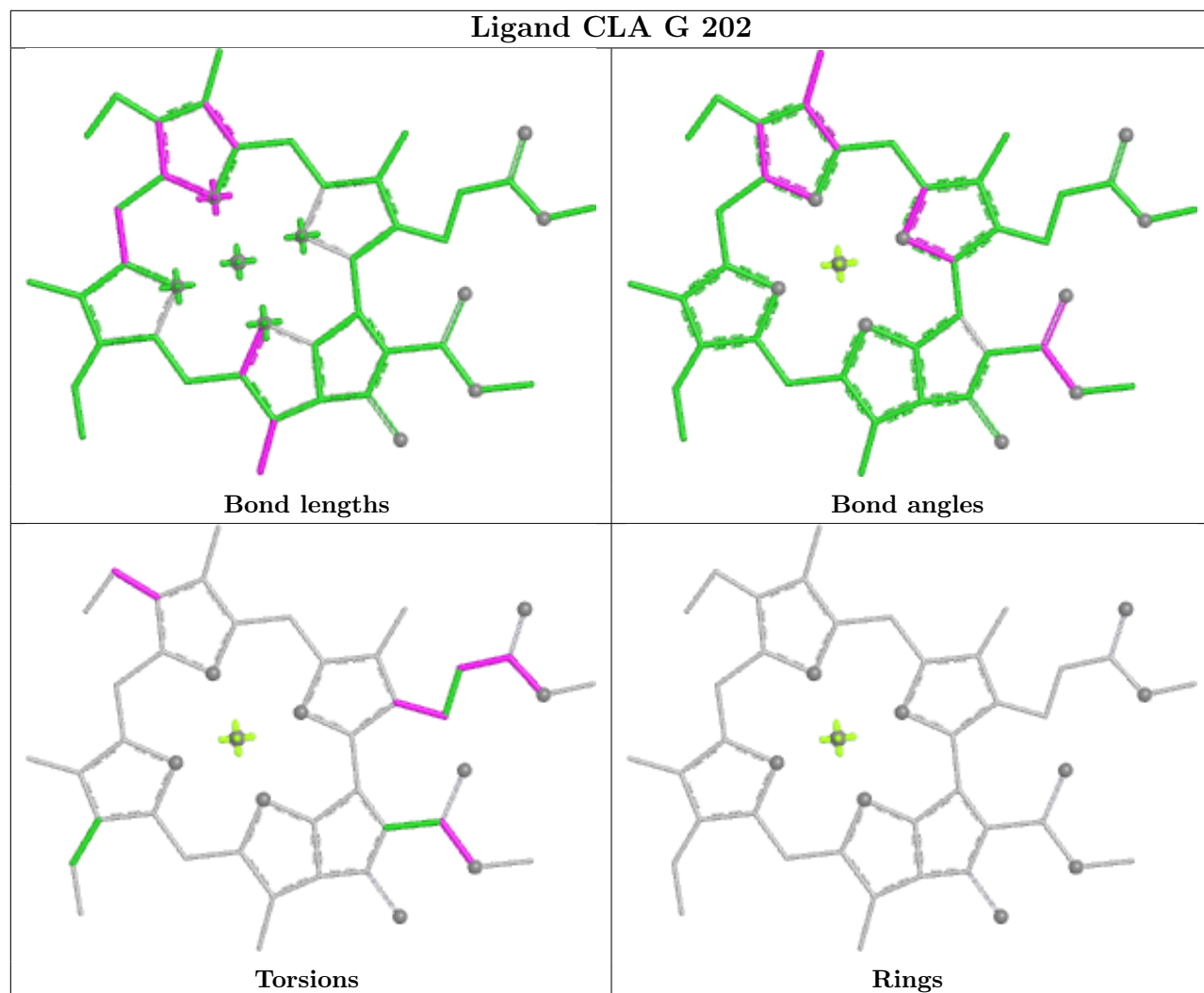


Torsions

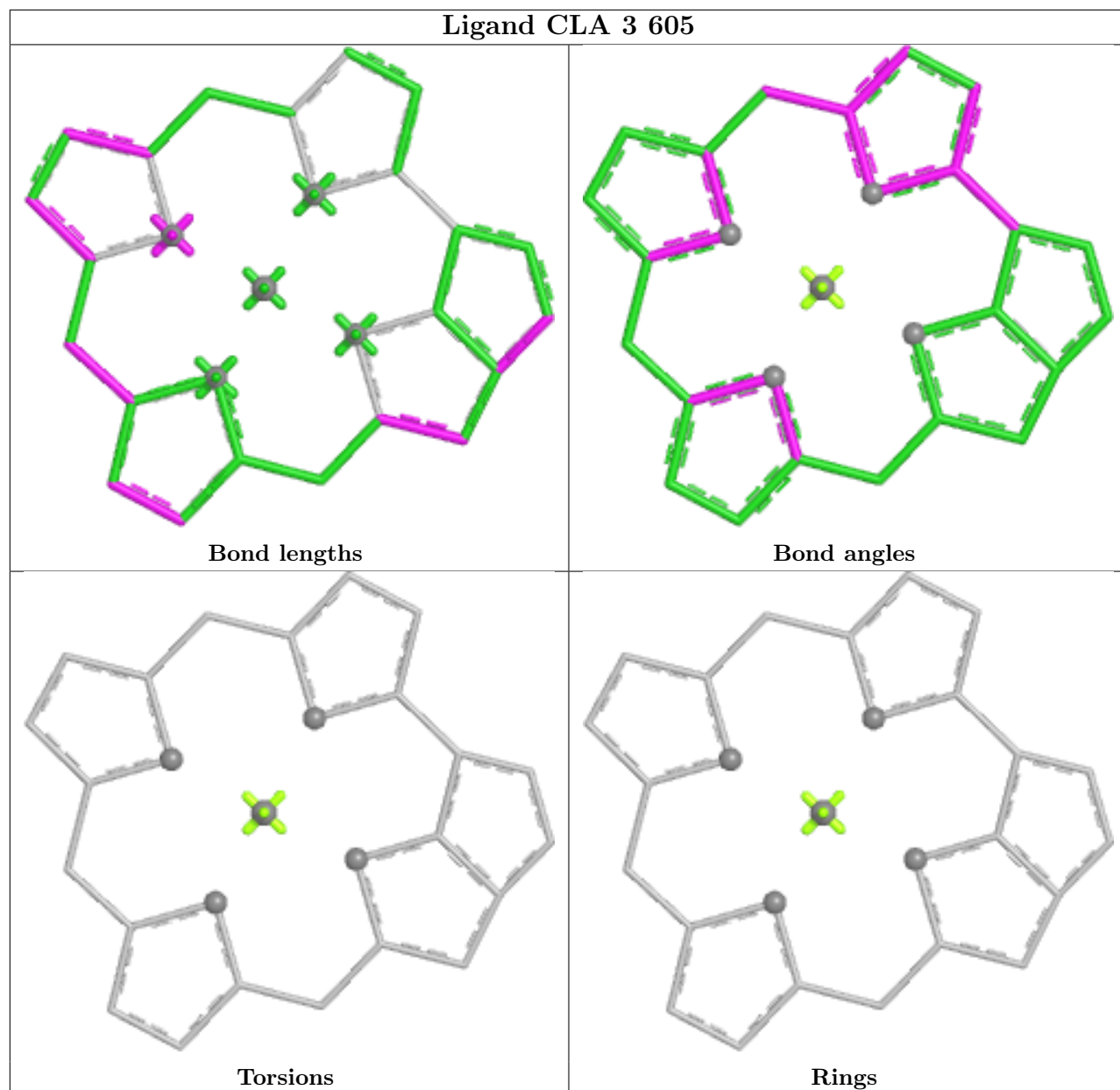


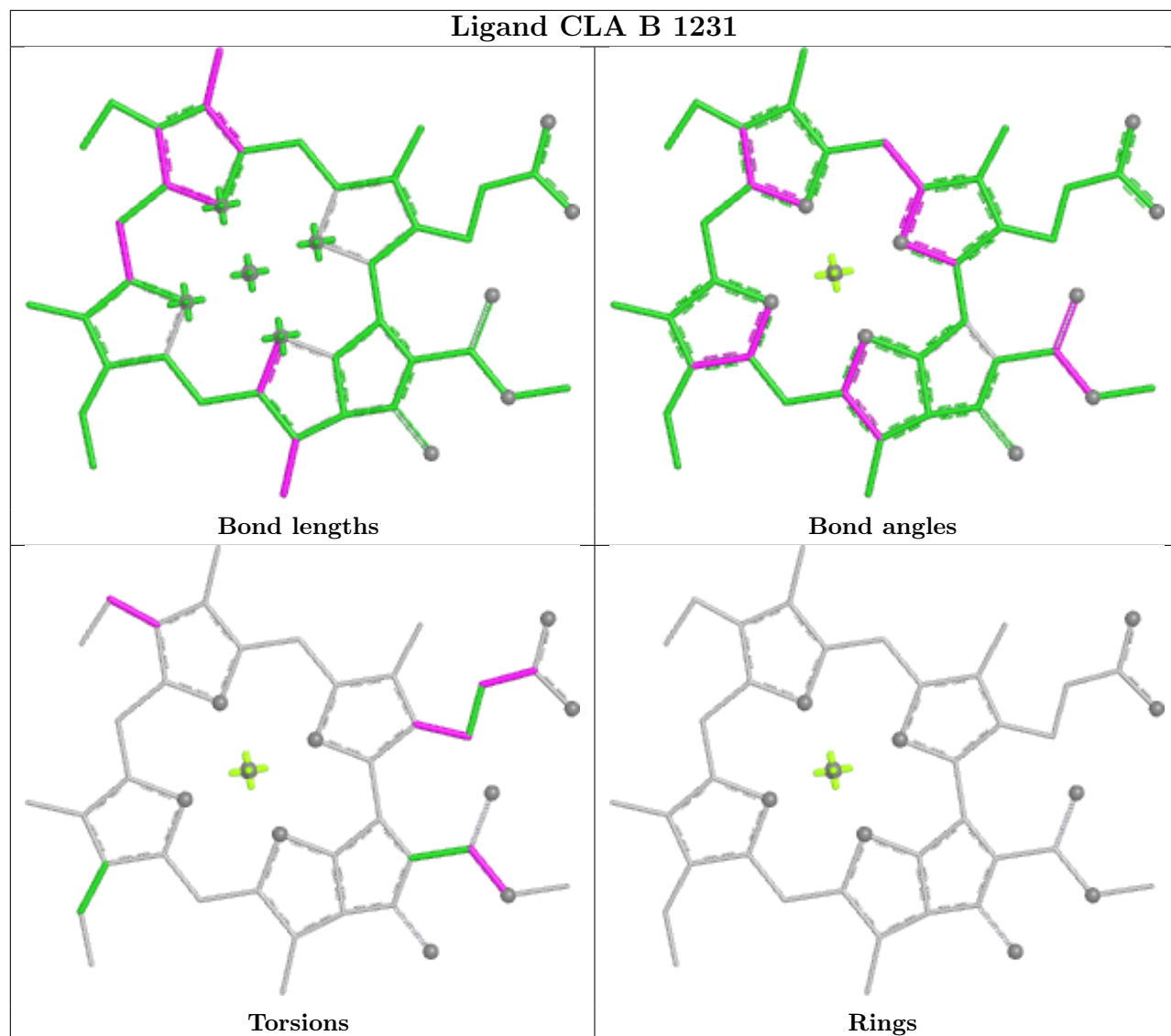
Rings



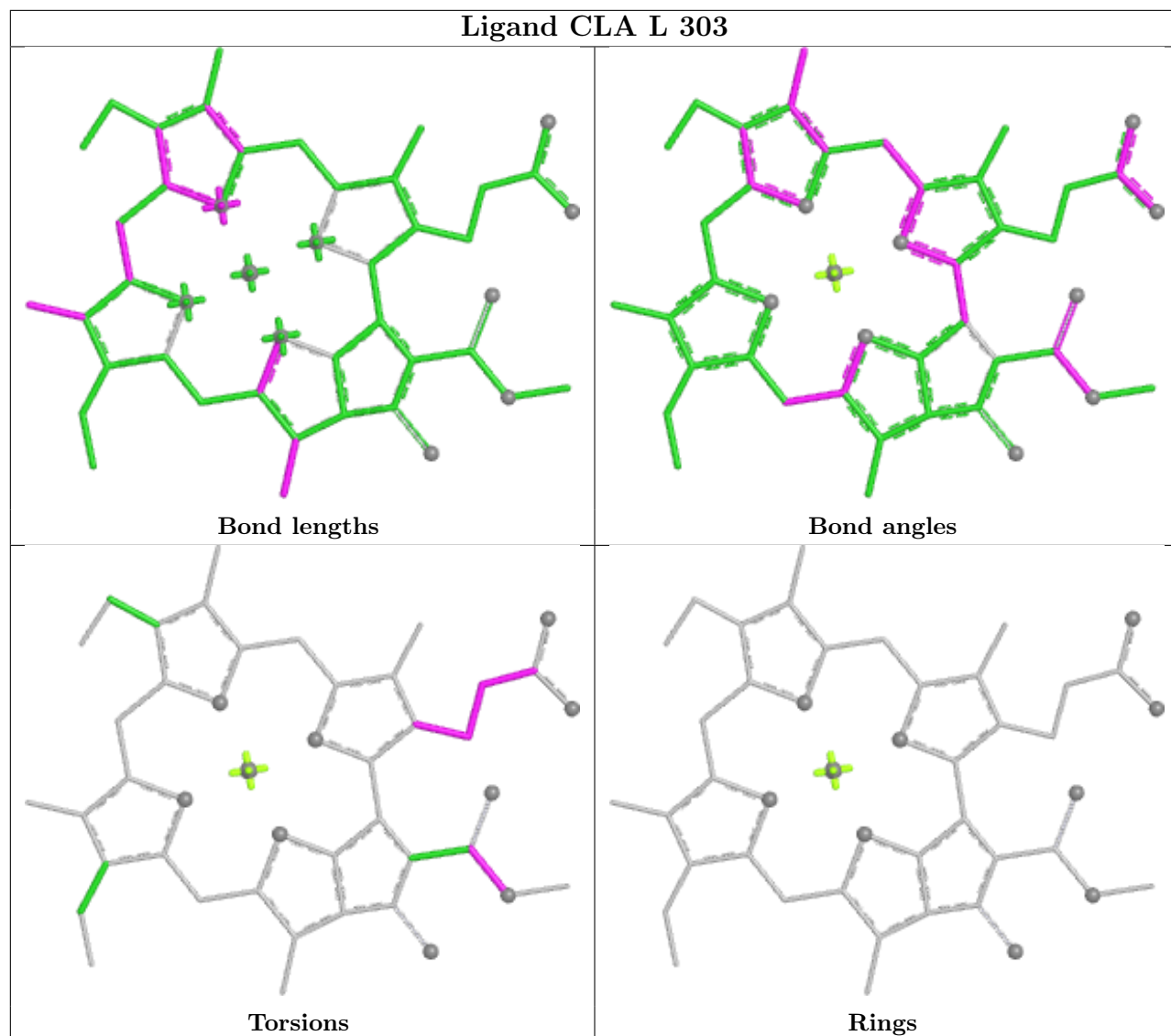


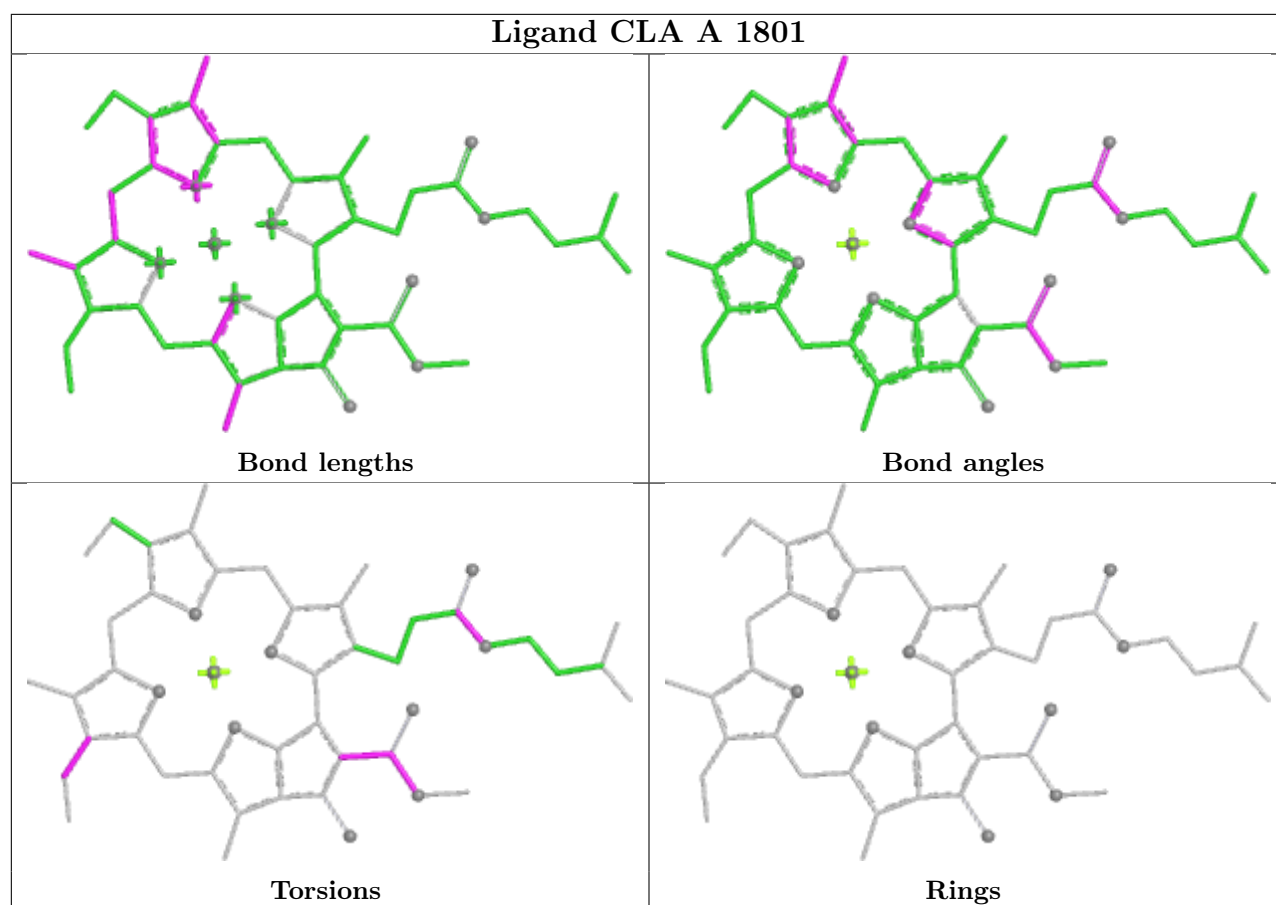
Ligand CLA 3 605



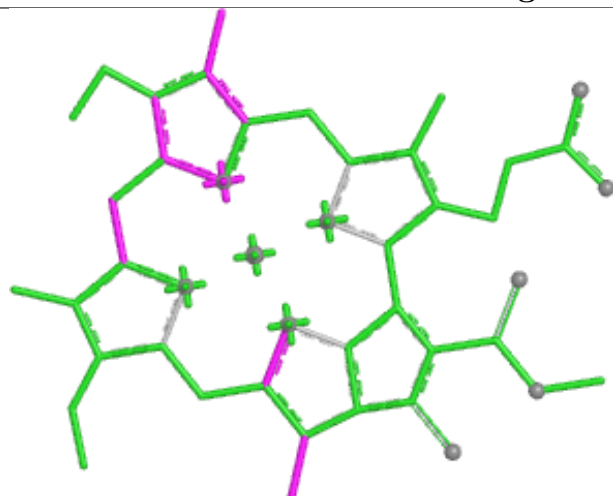


Ligand CLA L 303

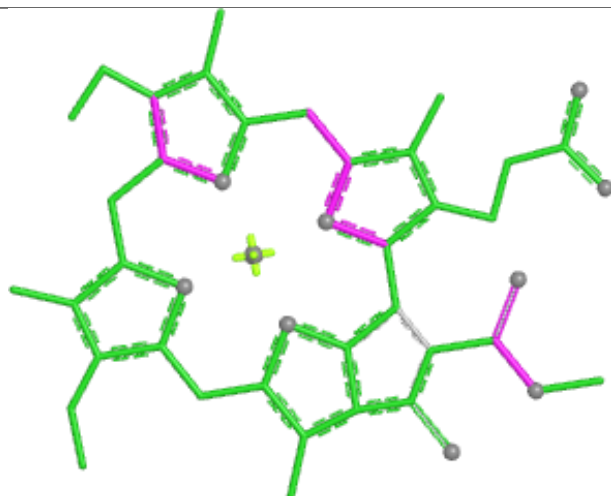




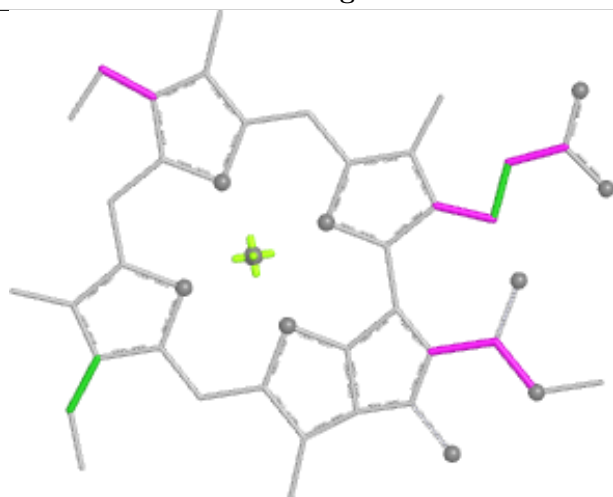
Ligand CLA J 102



Bond lengths



Bond angles

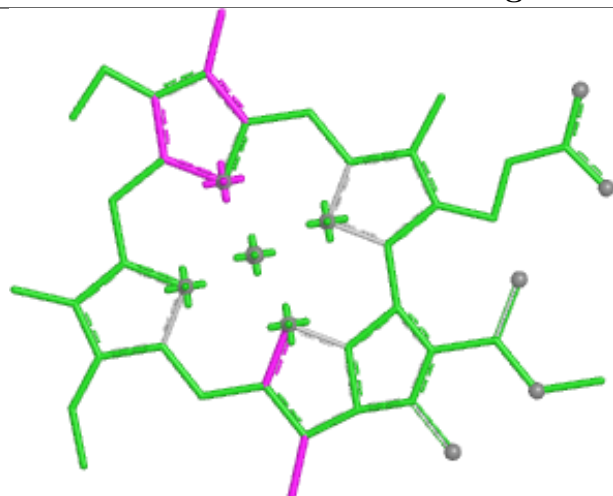


Torsions

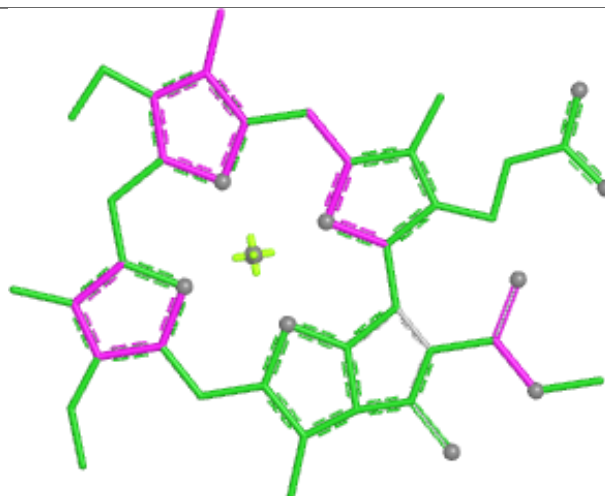


Rings

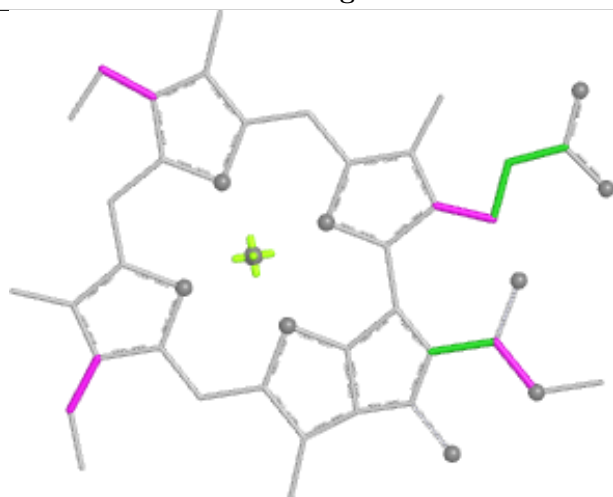
Ligand CLA B 1239



Bond lengths



Bond angles

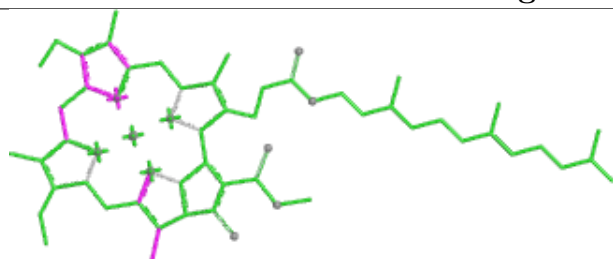


Torsions

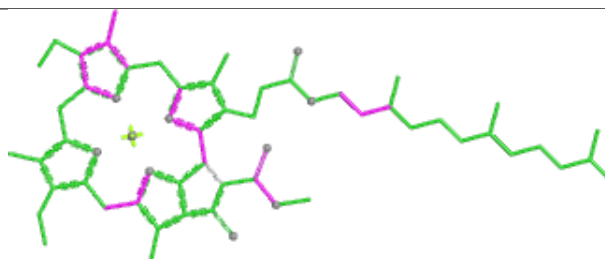


Rings

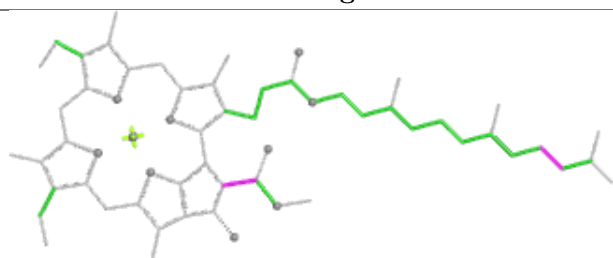
Ligand CLA 4 602



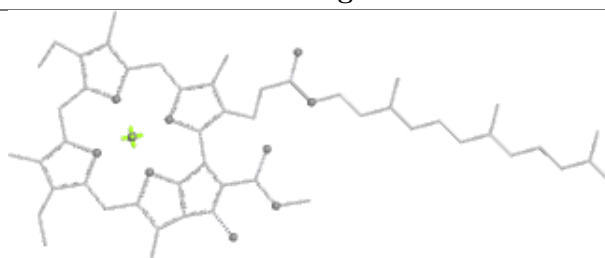
Bond lengths



Bond angles

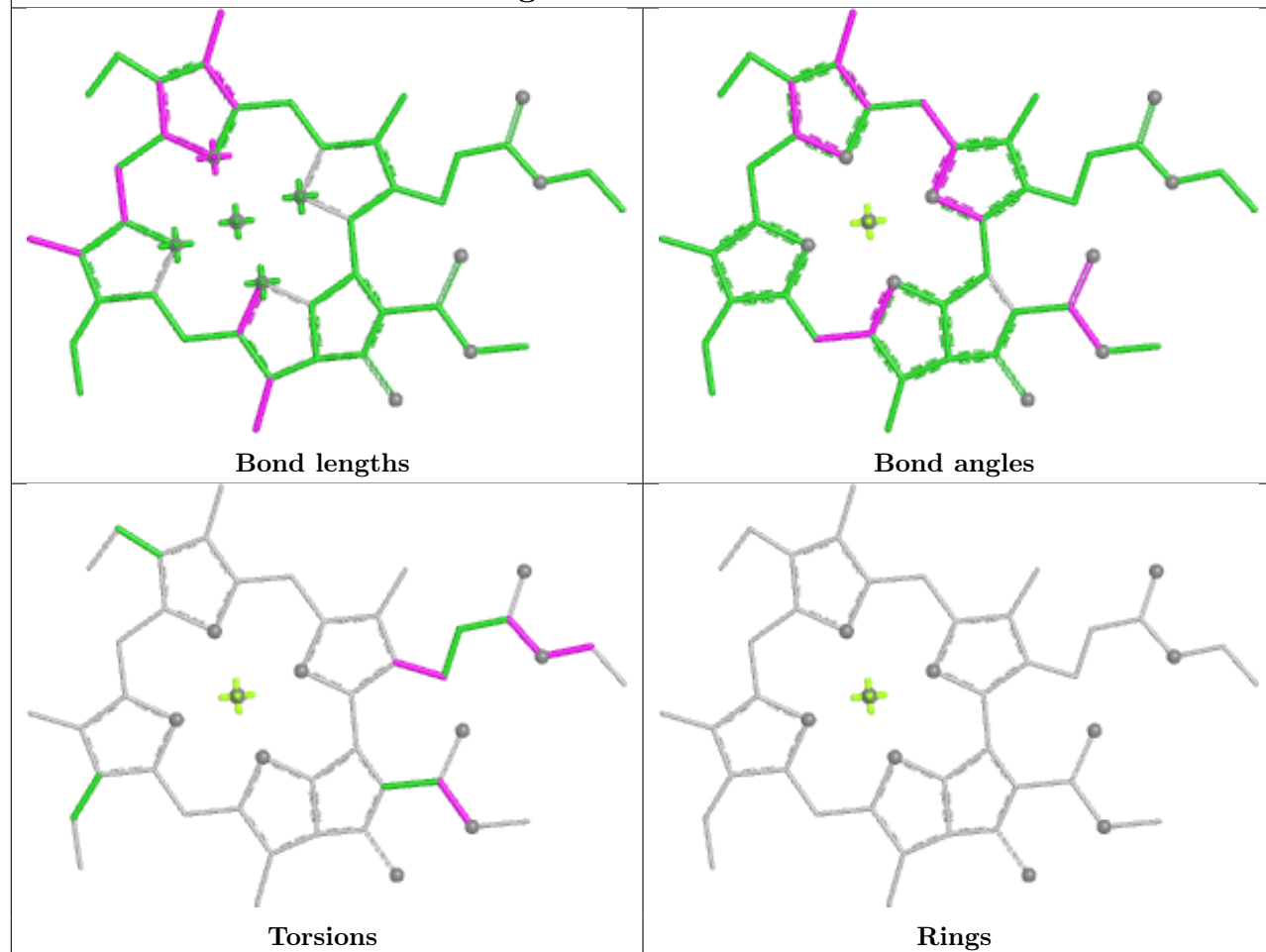


Torsions

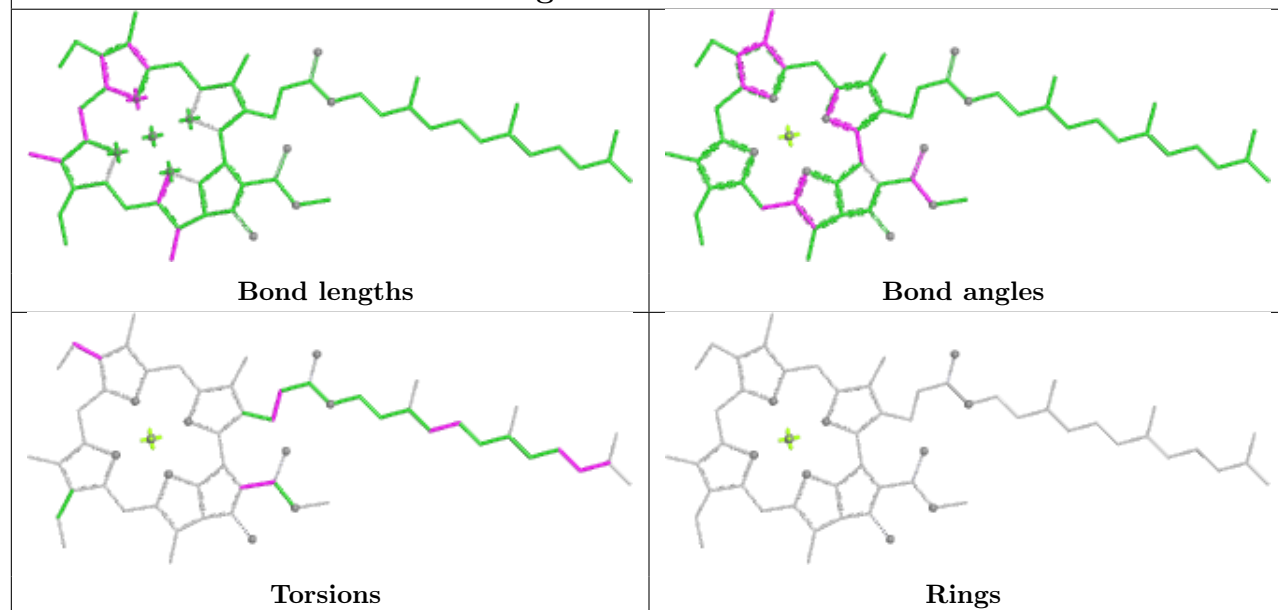


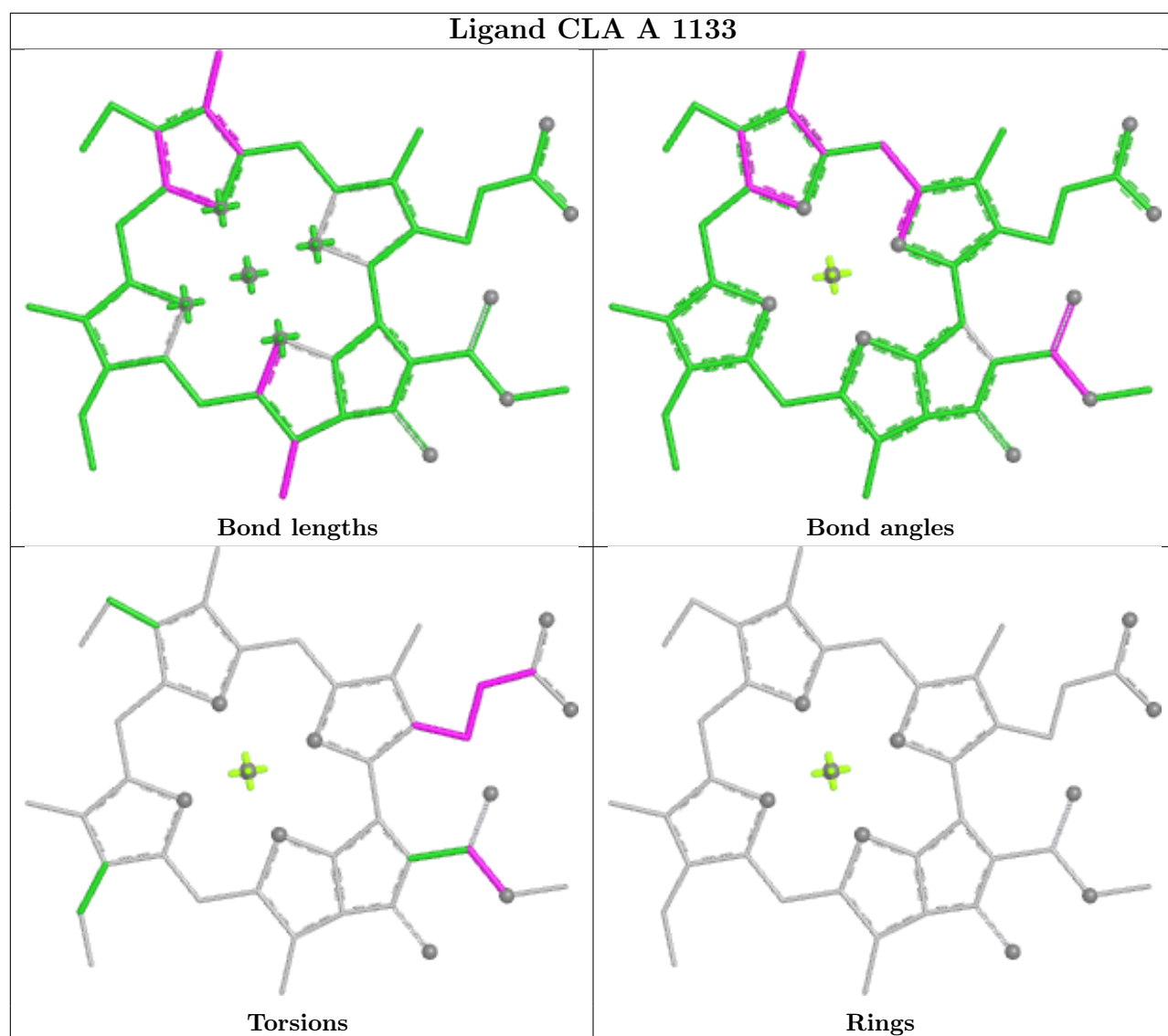
Rings

Ligand CLA B 1206

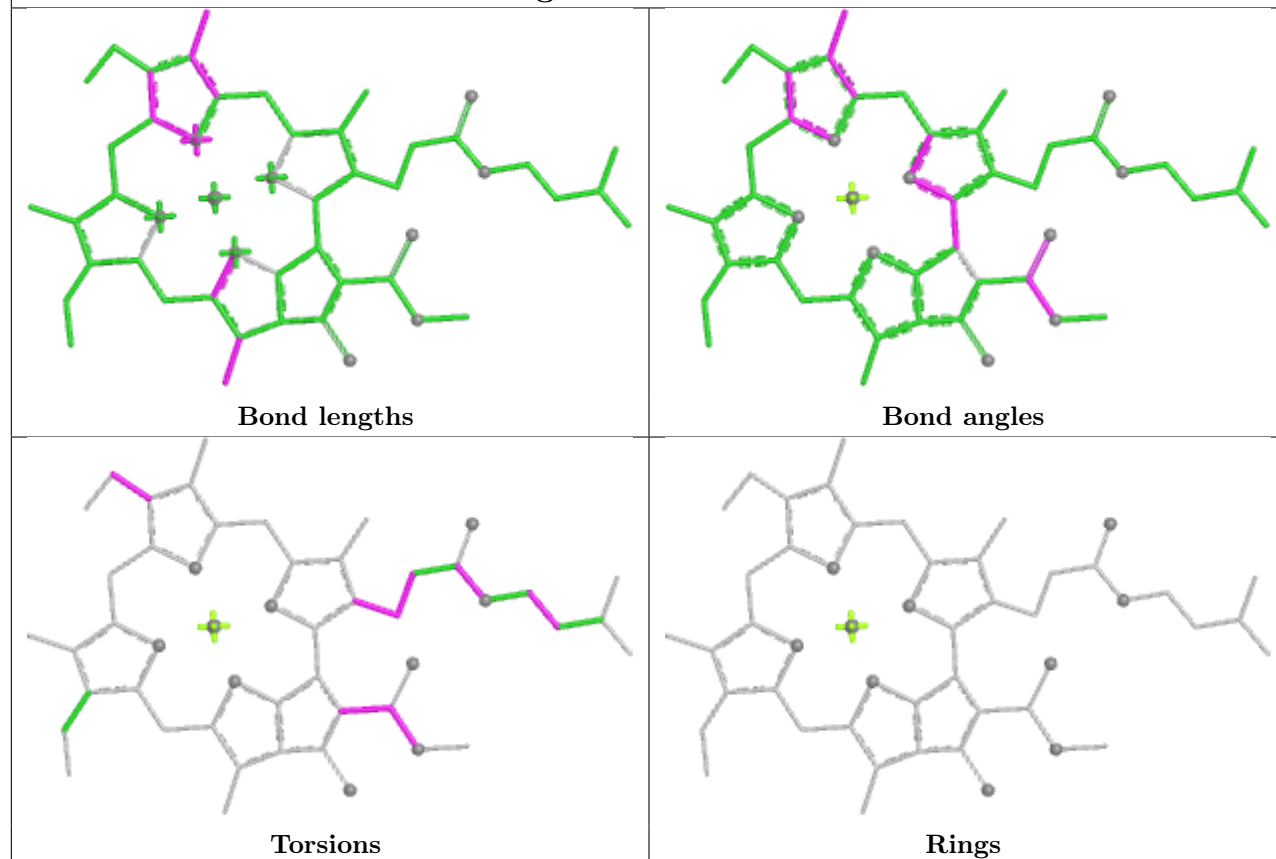


Ligand CLA 3 602

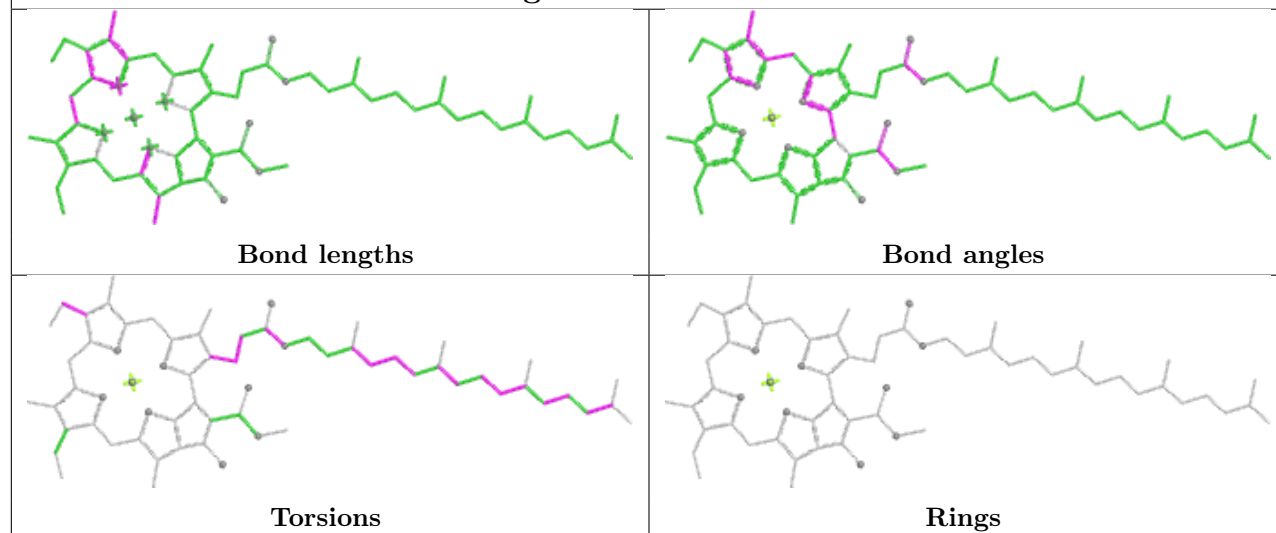




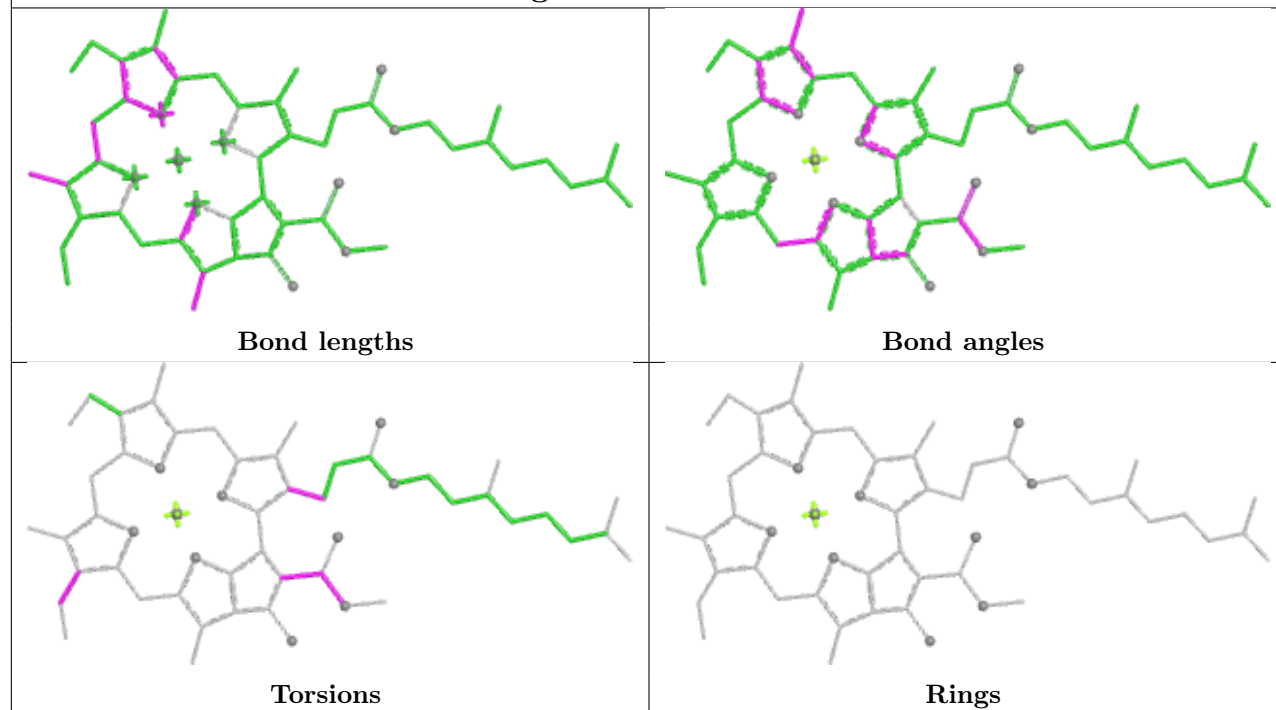
Ligand CLA 4 601



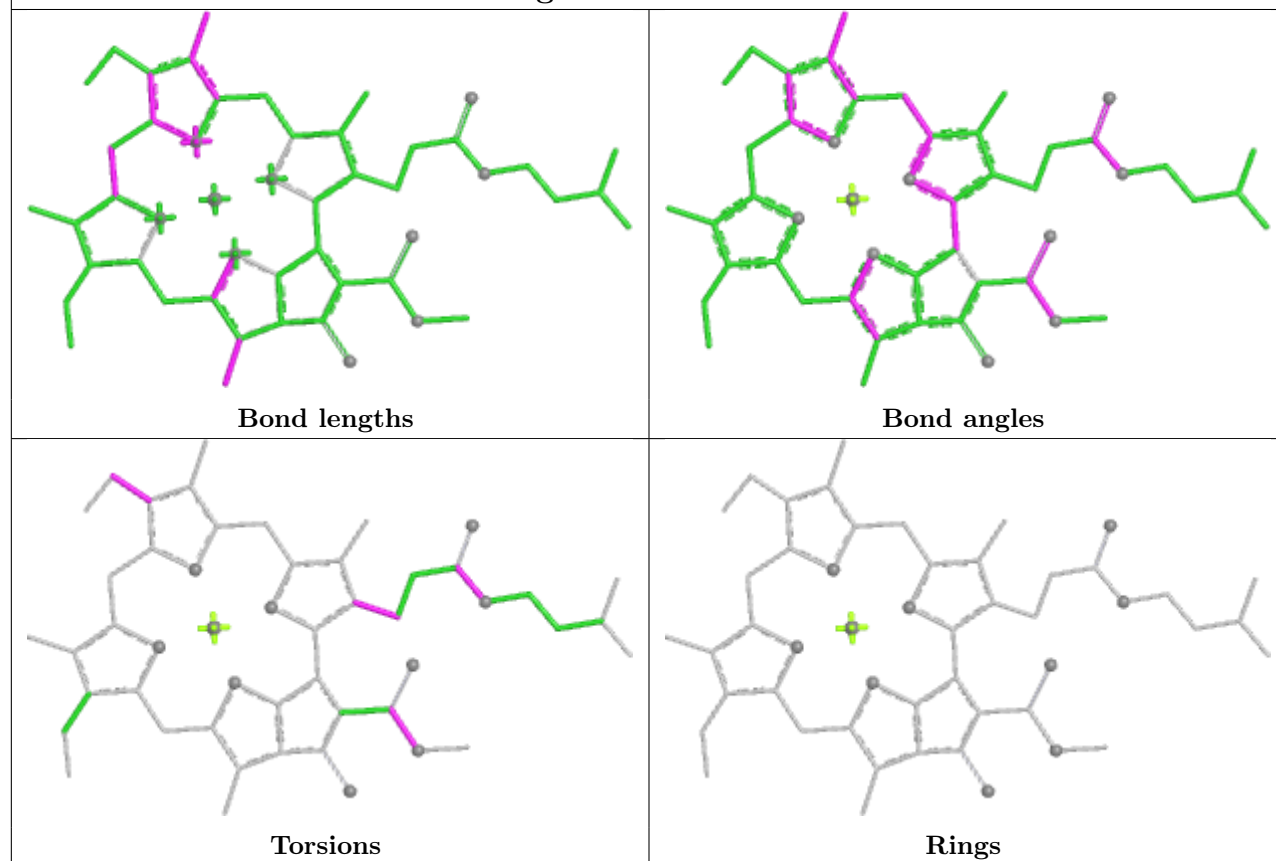
Ligand CLA B 1238

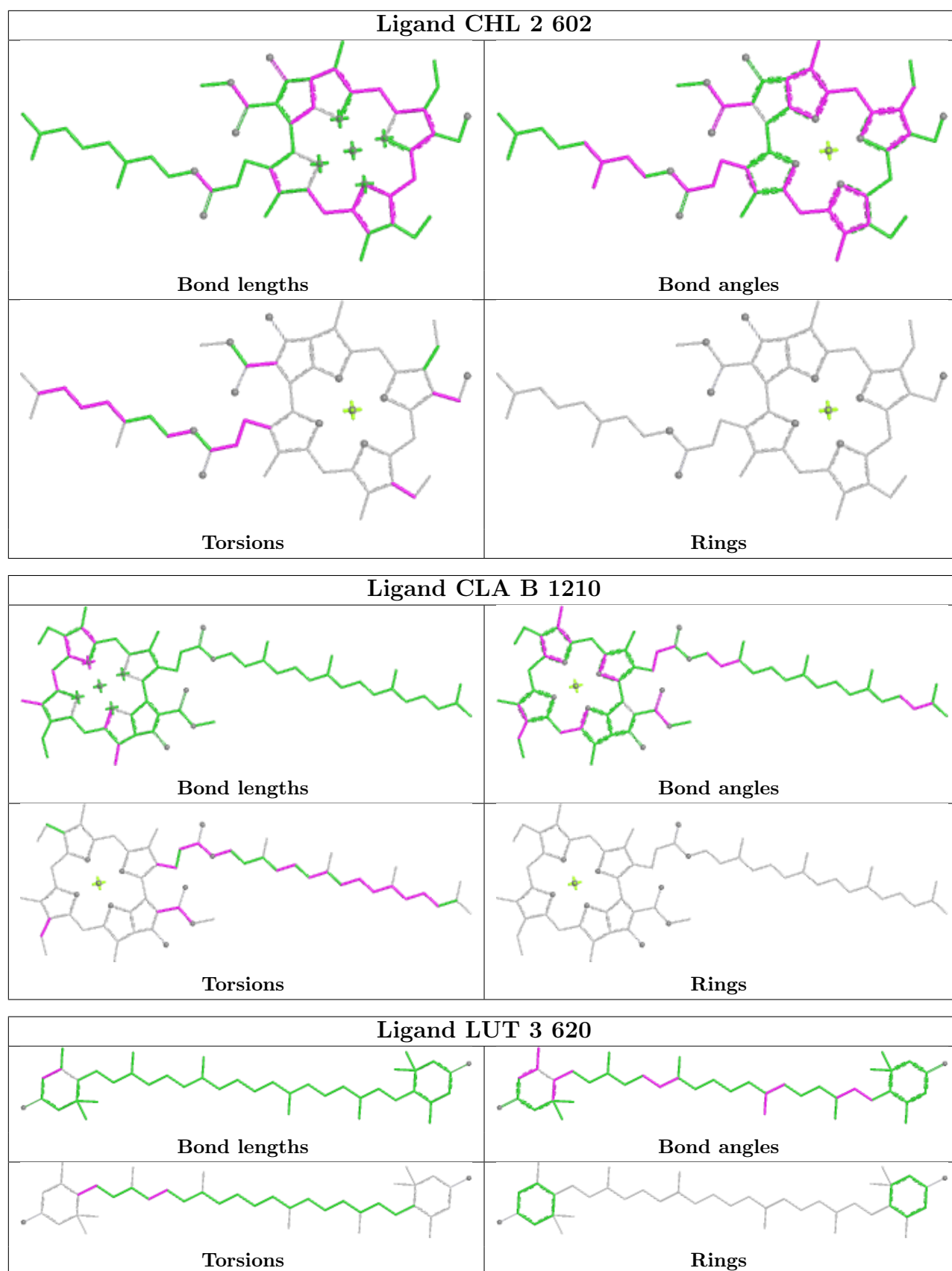


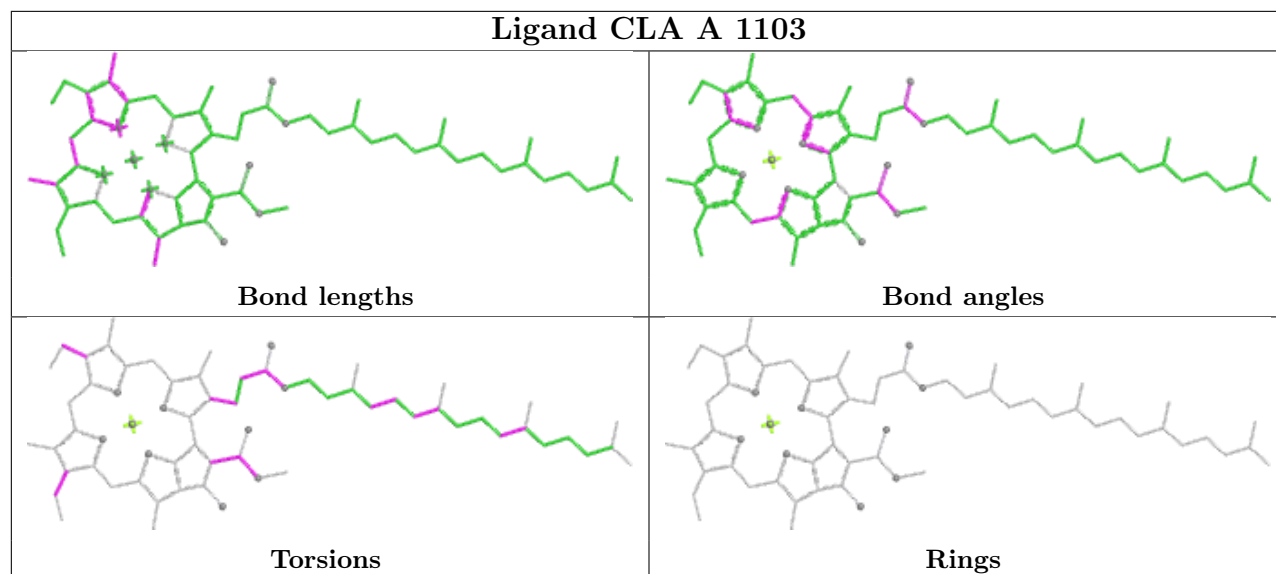
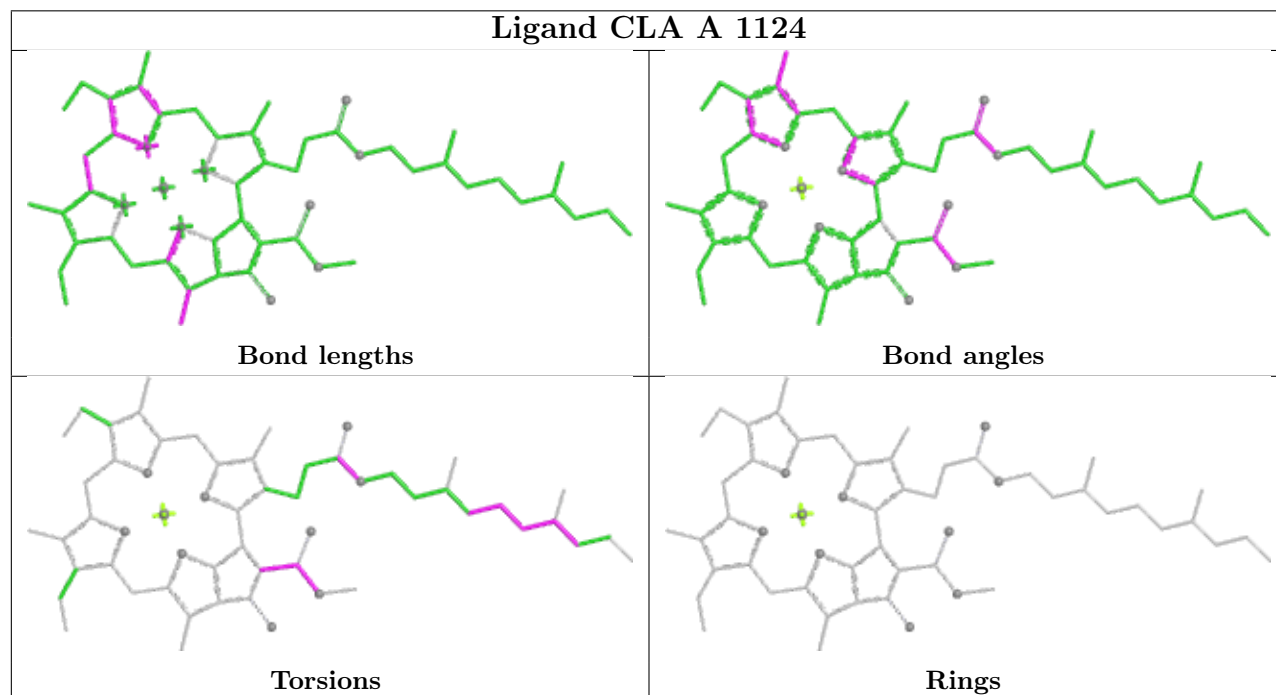
Ligand CLA K 201



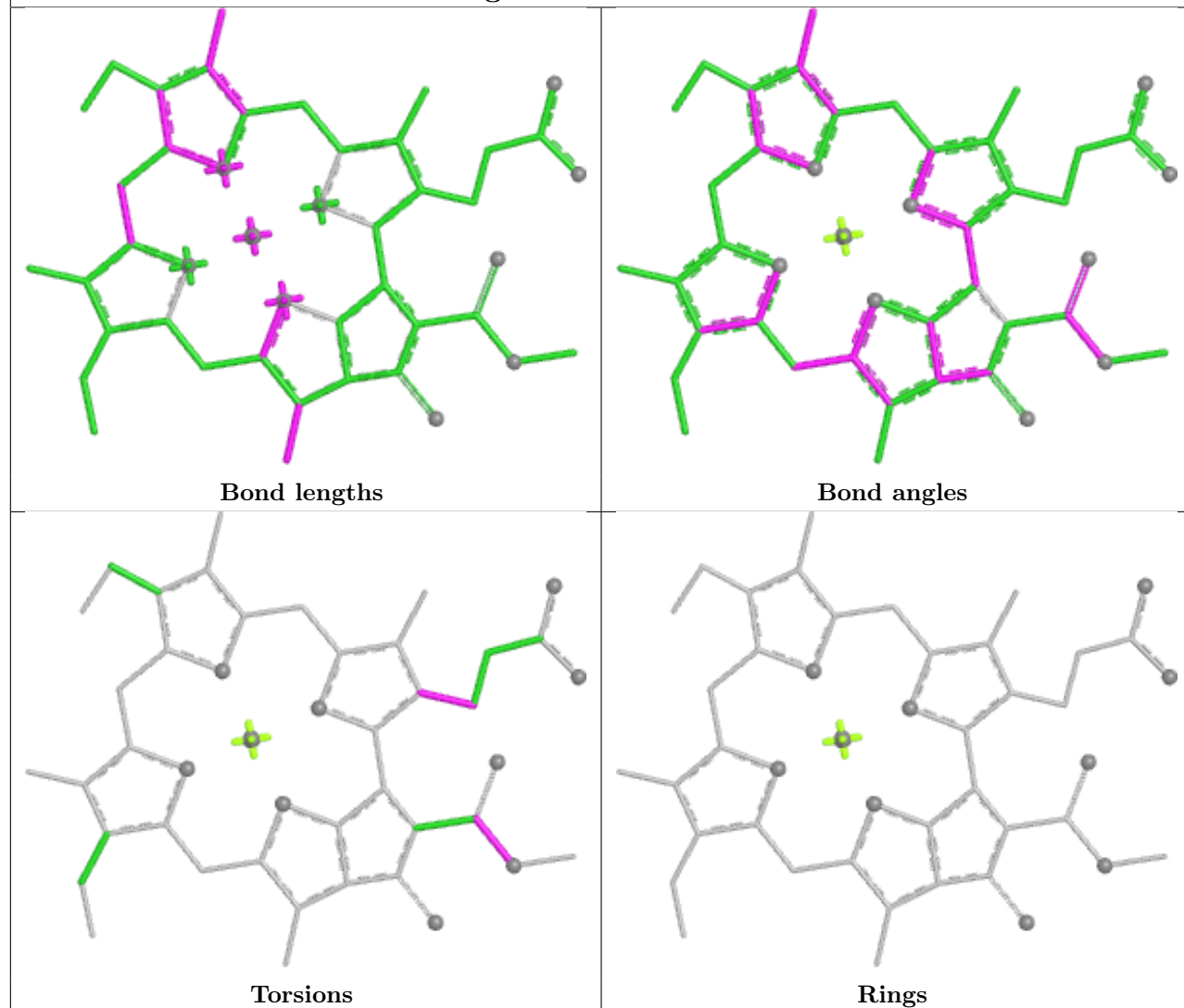
Ligand CLA 3 604



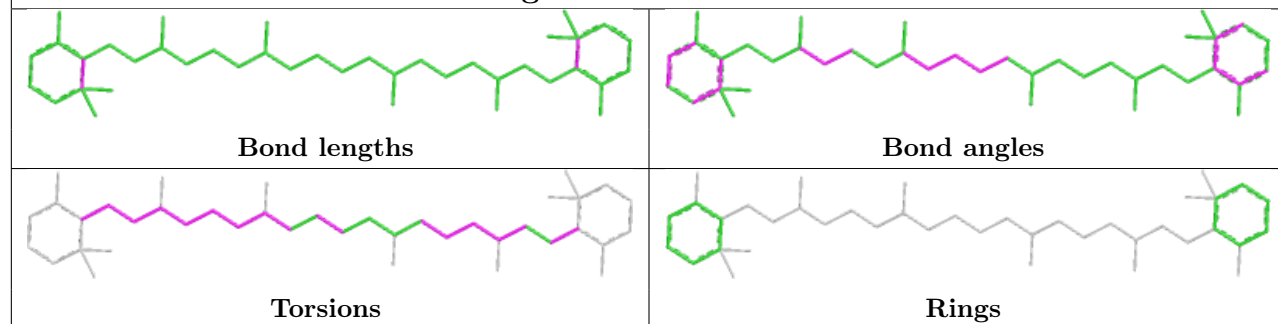


Ligand CLA A 1103**Ligand CLA A 1124**

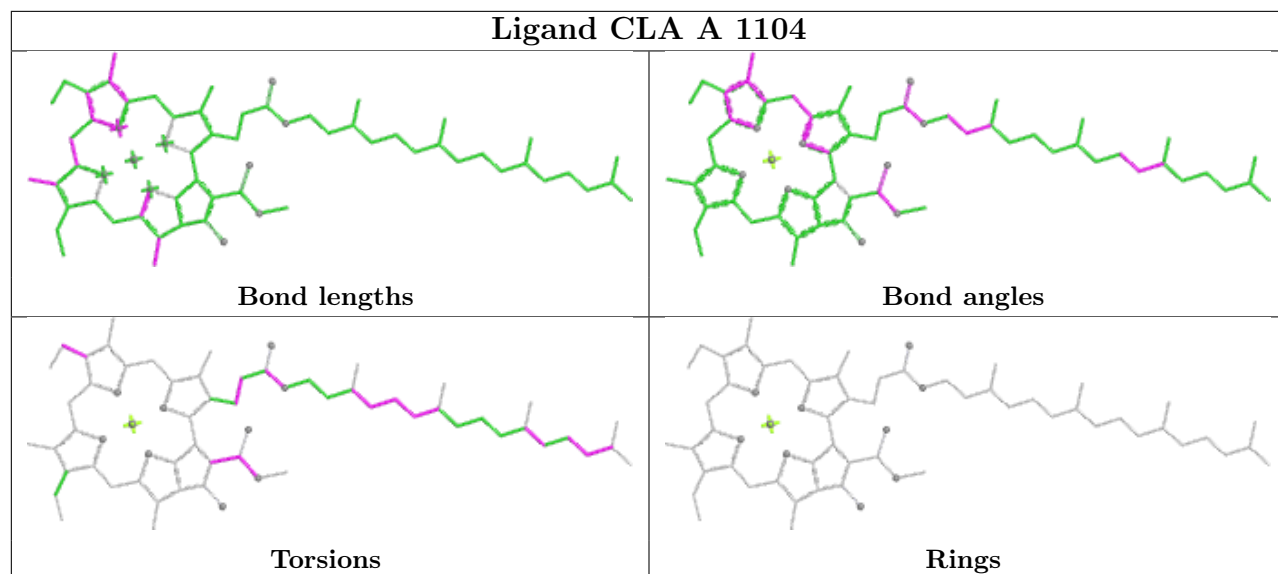
Ligand CLA B 1219



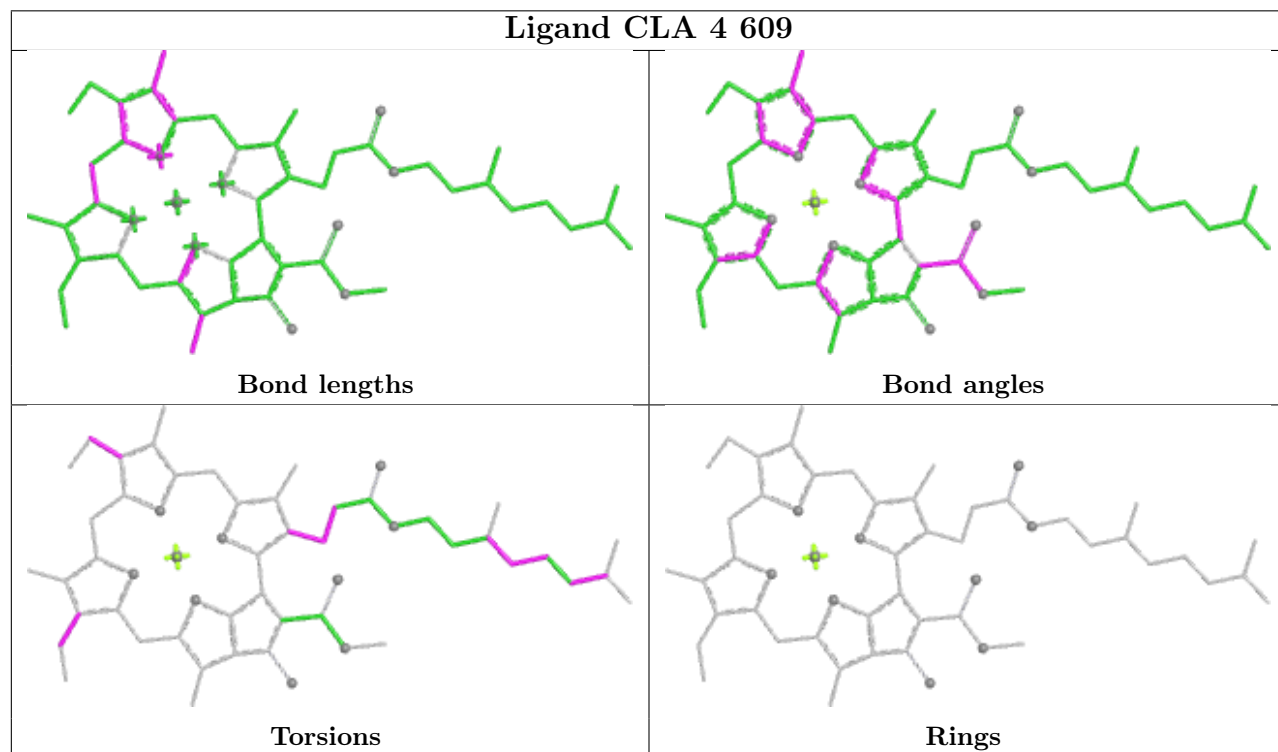
Ligand BCR B 4014



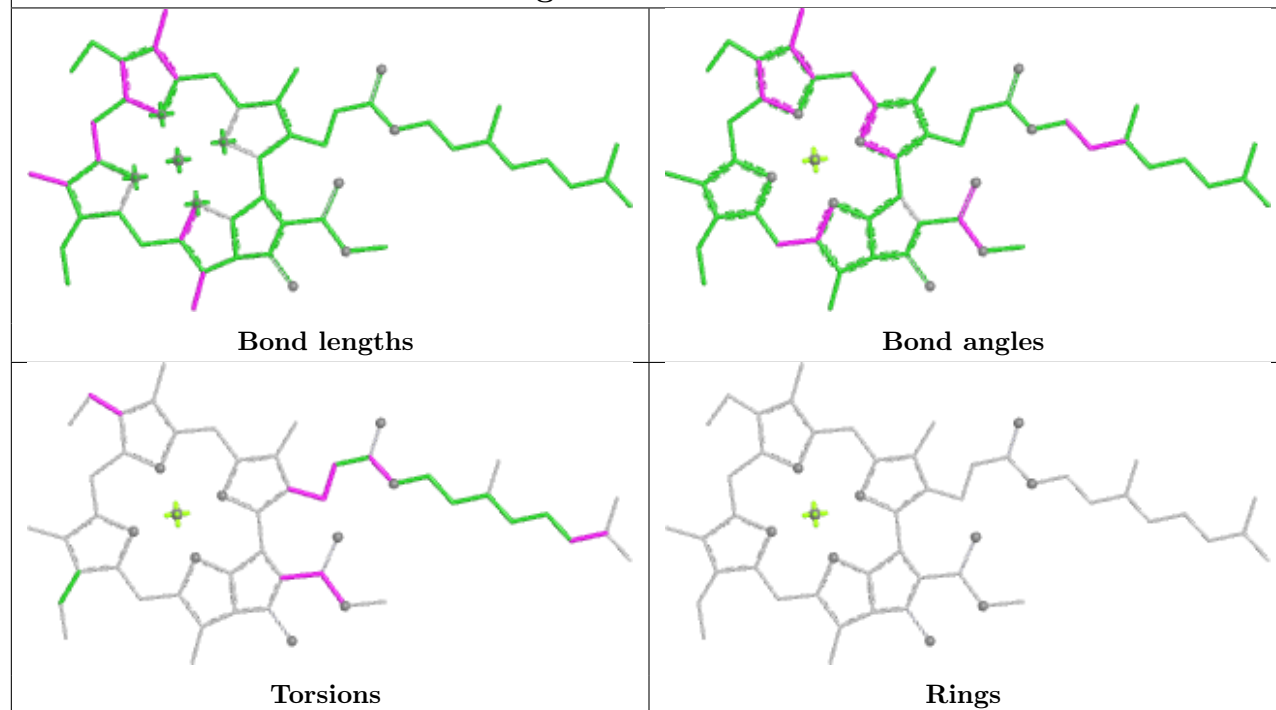
Ligand CLA A 1104



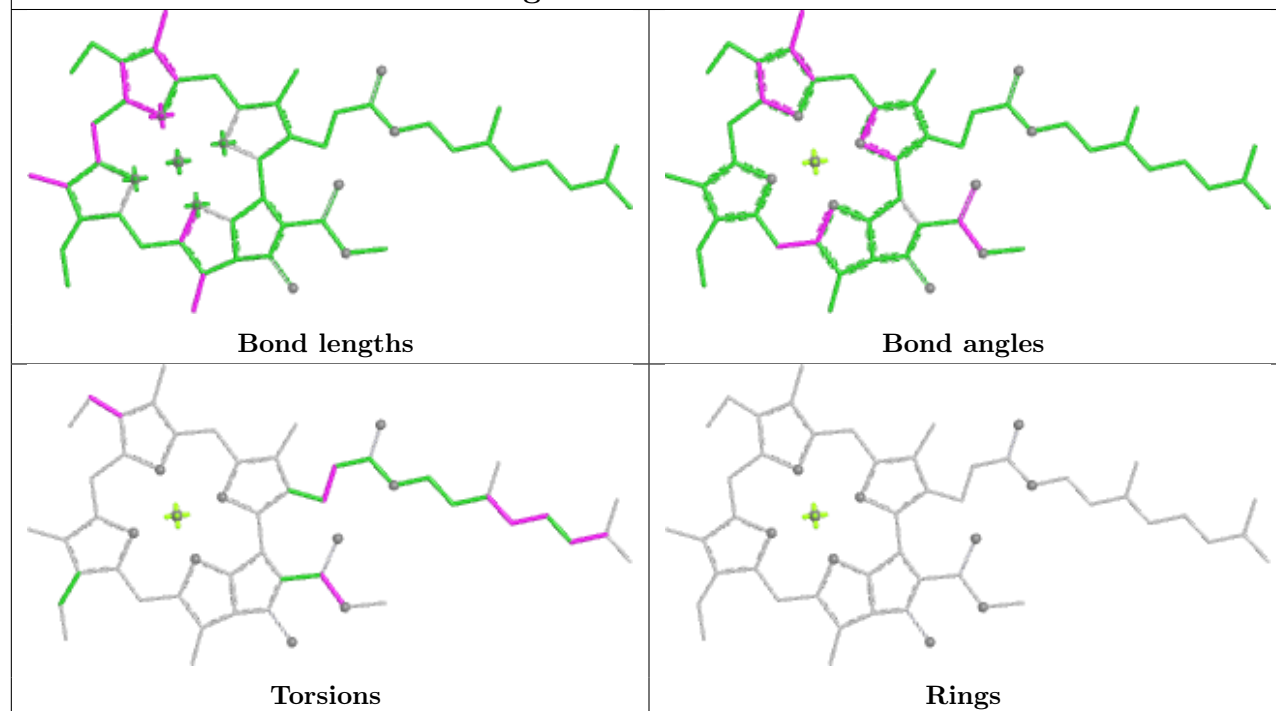
Ligand CLA 4 609

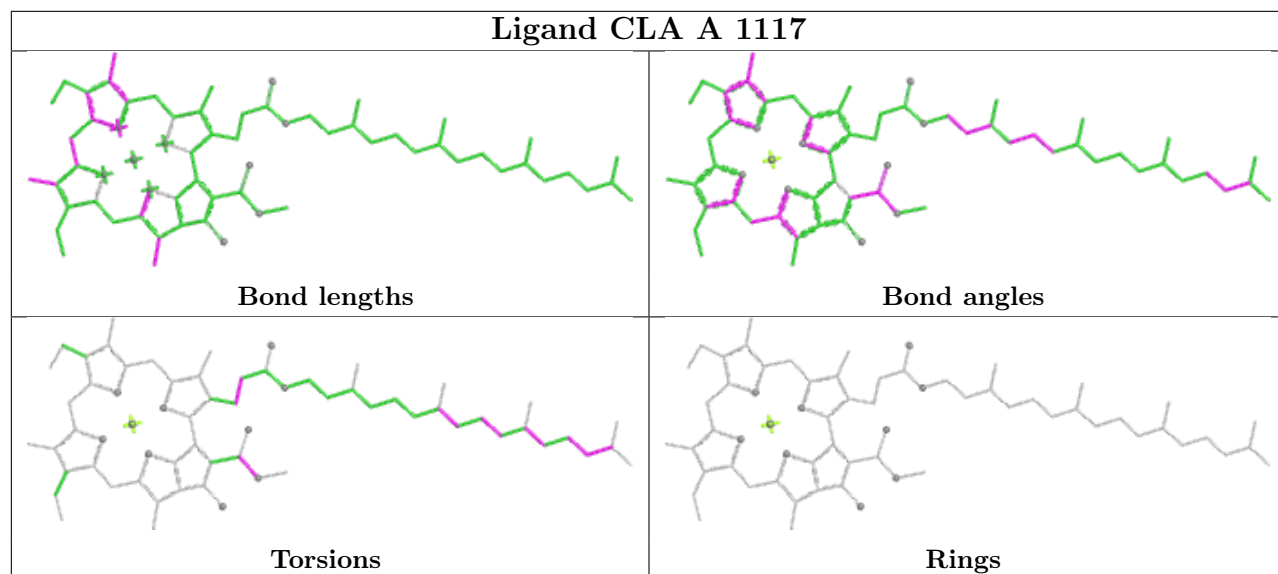
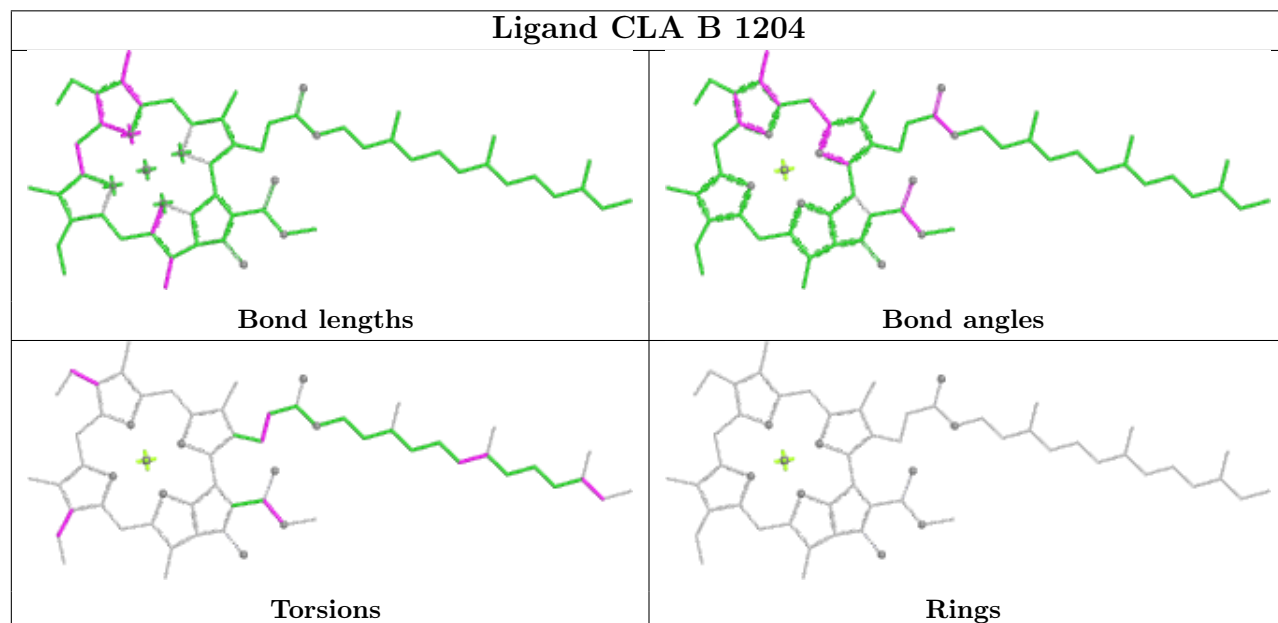


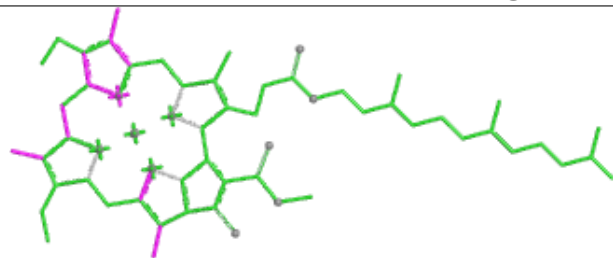
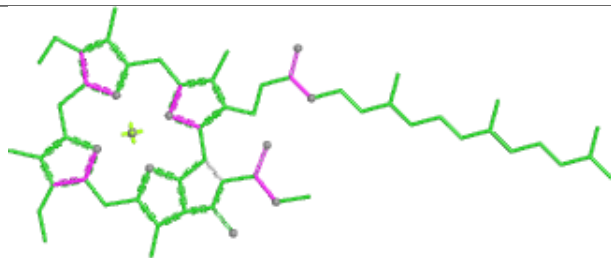
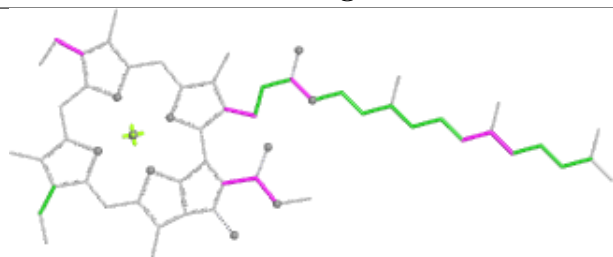
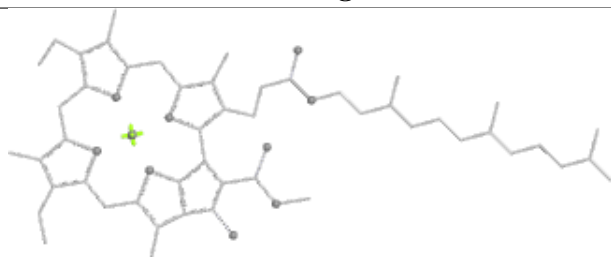
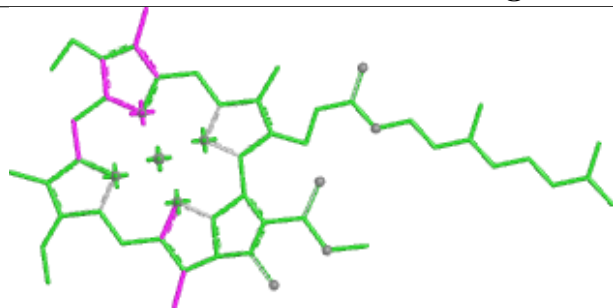
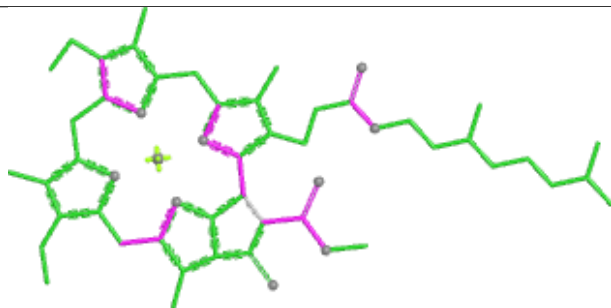
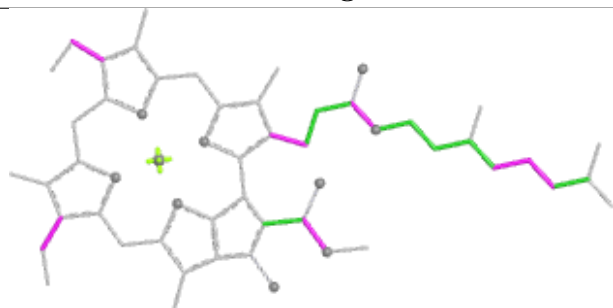
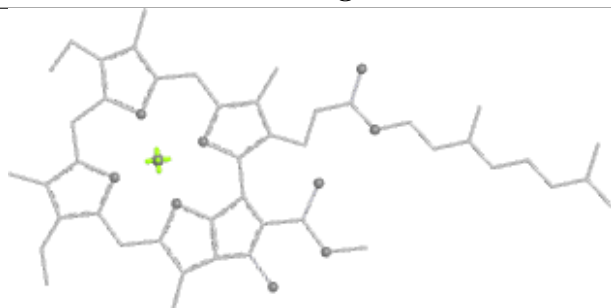
Ligand CLA 4 603

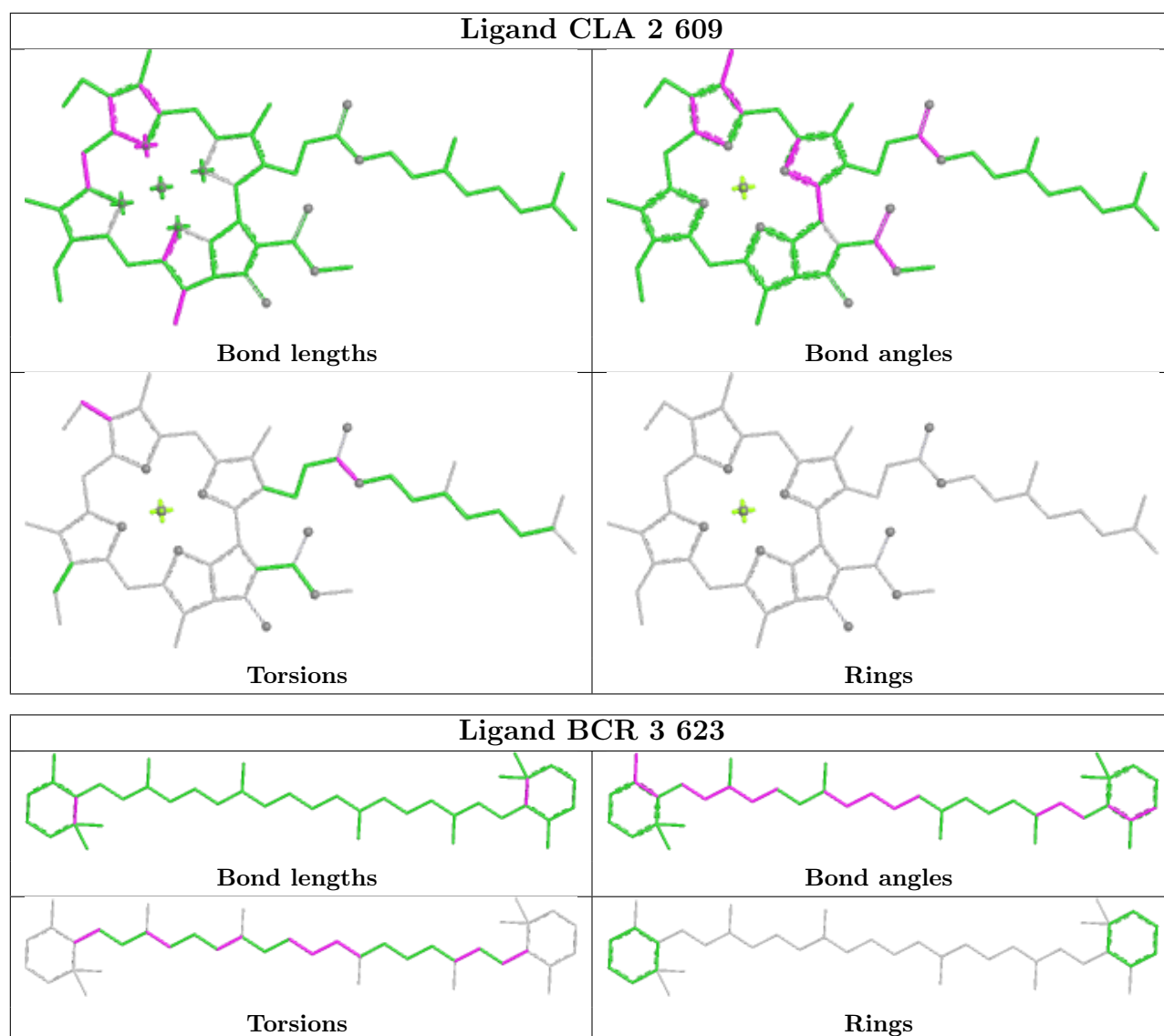


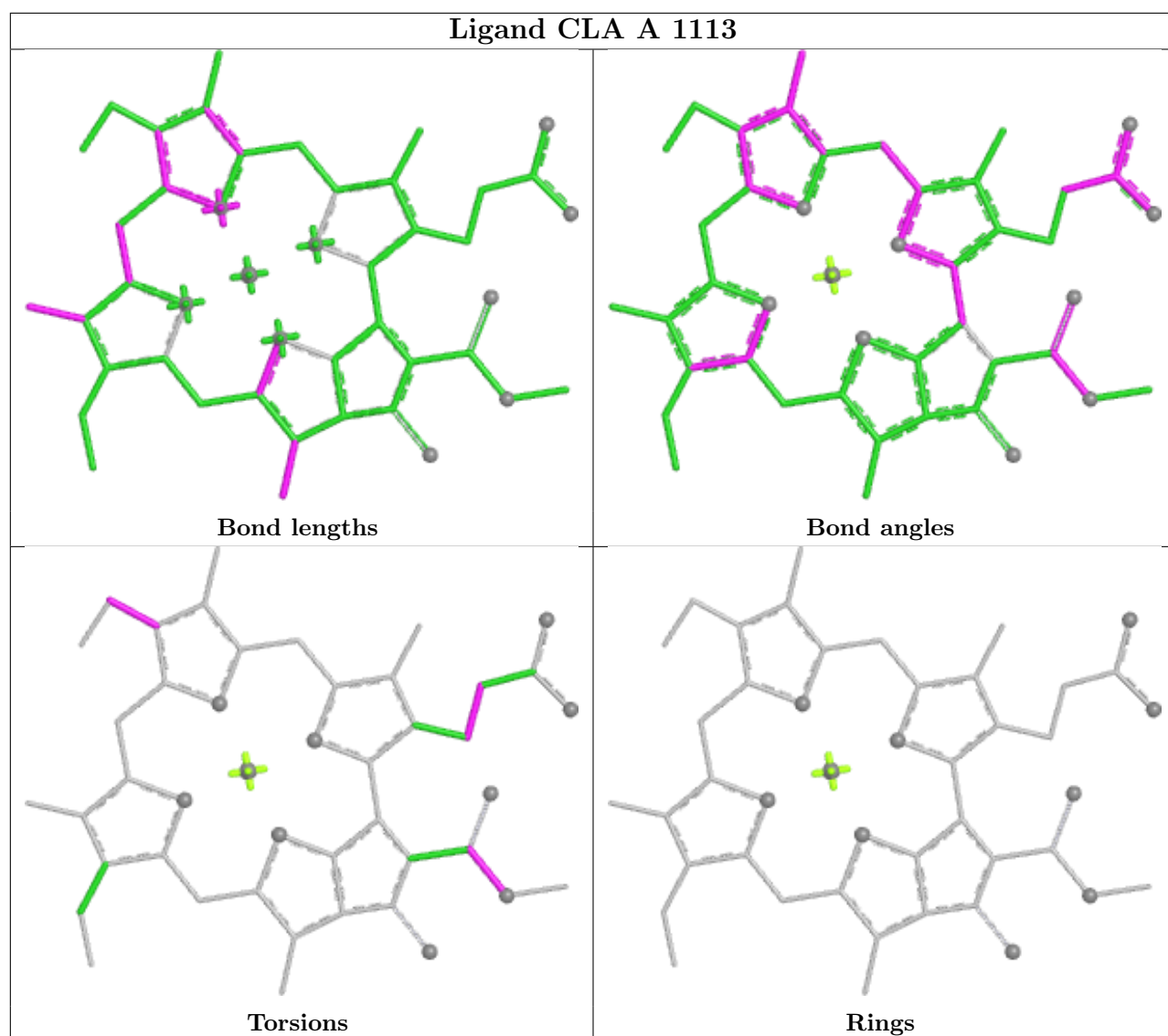
Ligand CLA B 1235



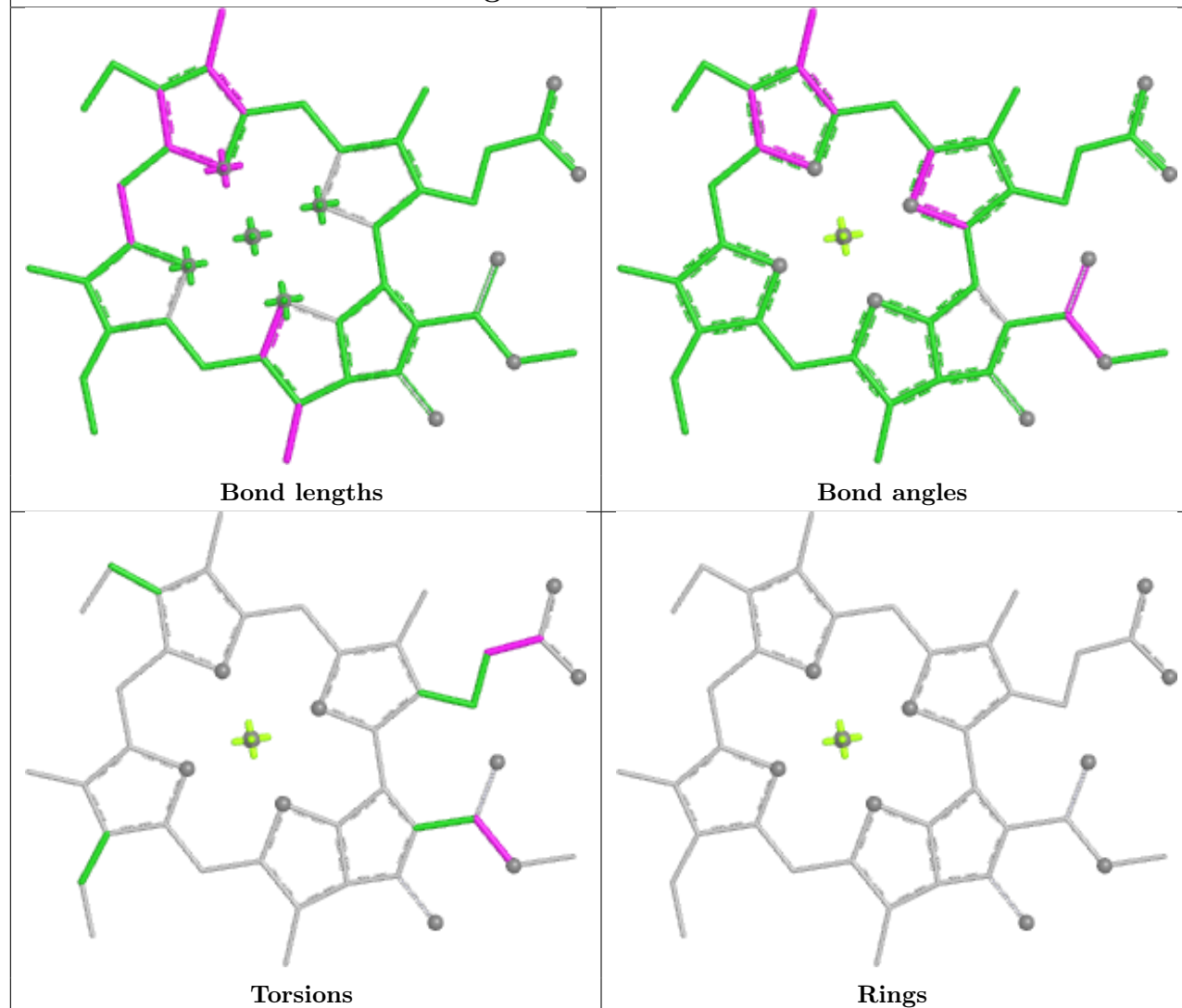
Ligand CLA A 1117**Ligand CLA B 1204**

Ligand CLA A 1122**Bond lengths****Bond angles****Torsions****Rings****Ligand CLA B 1229****Bond lengths****Bond angles****Torsions****Rings**

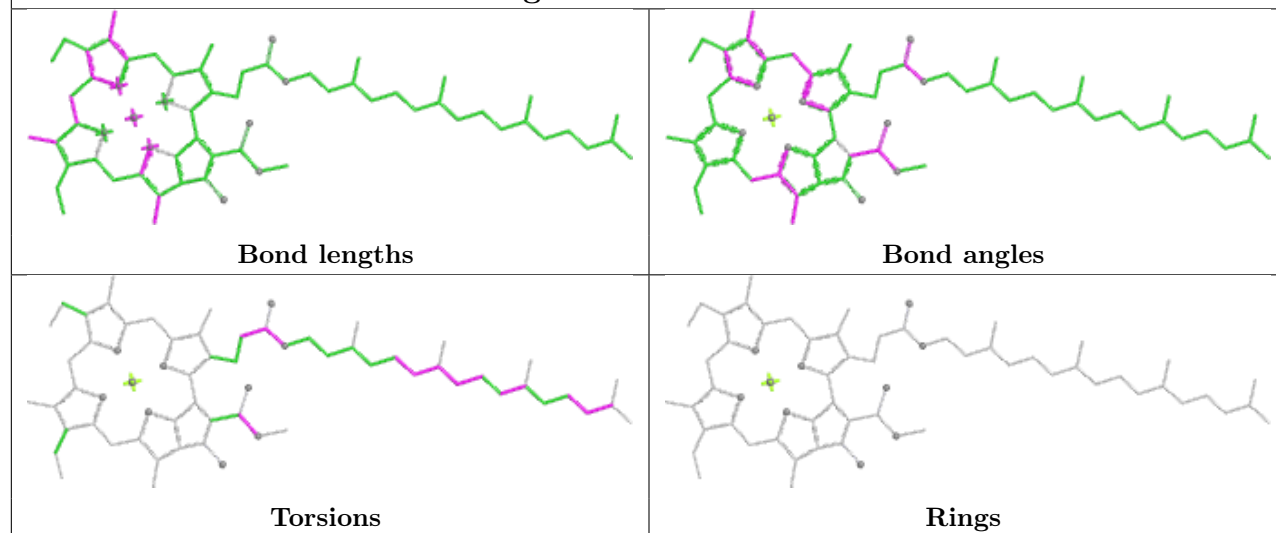


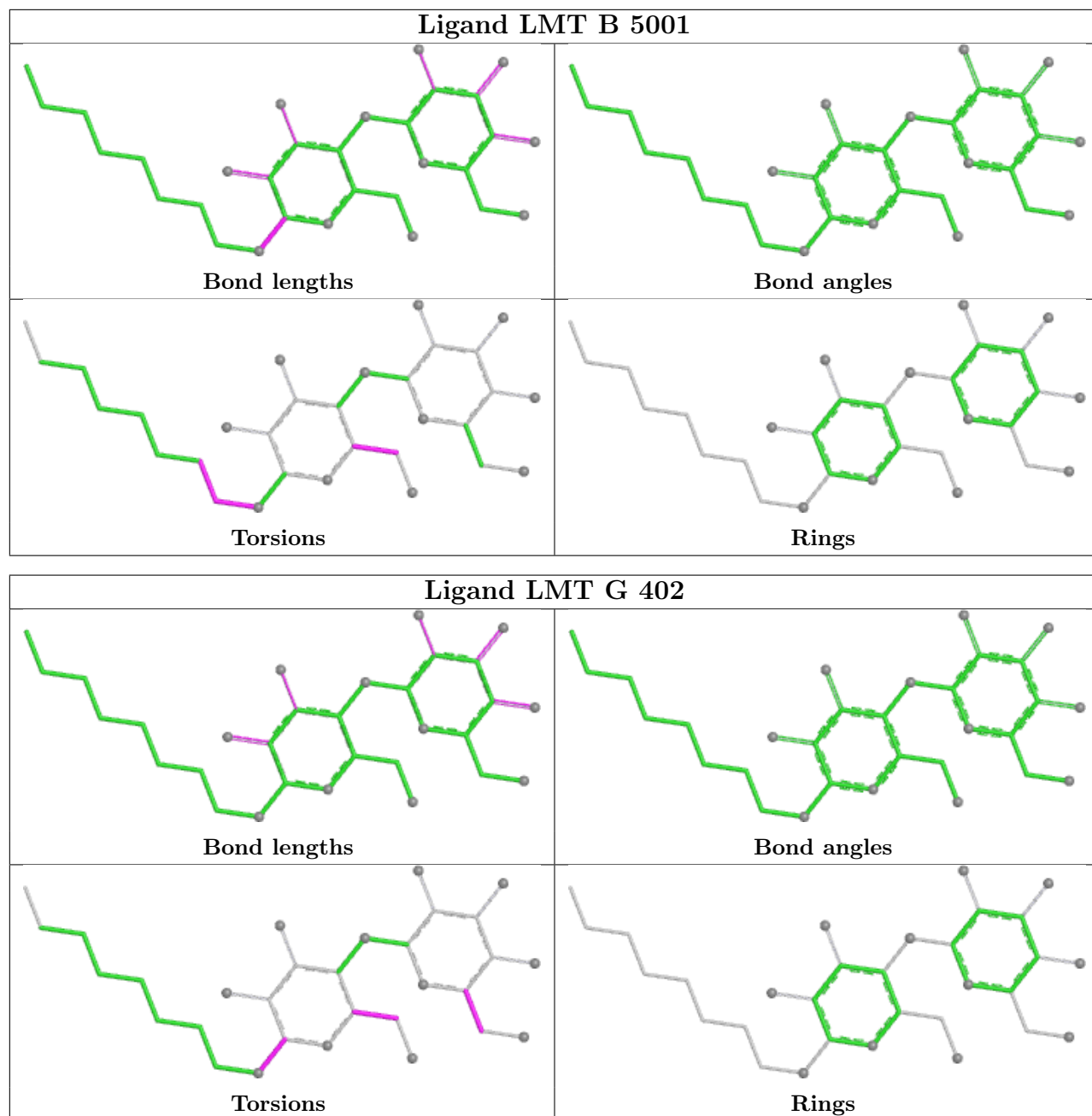


Ligand CLA A 1120

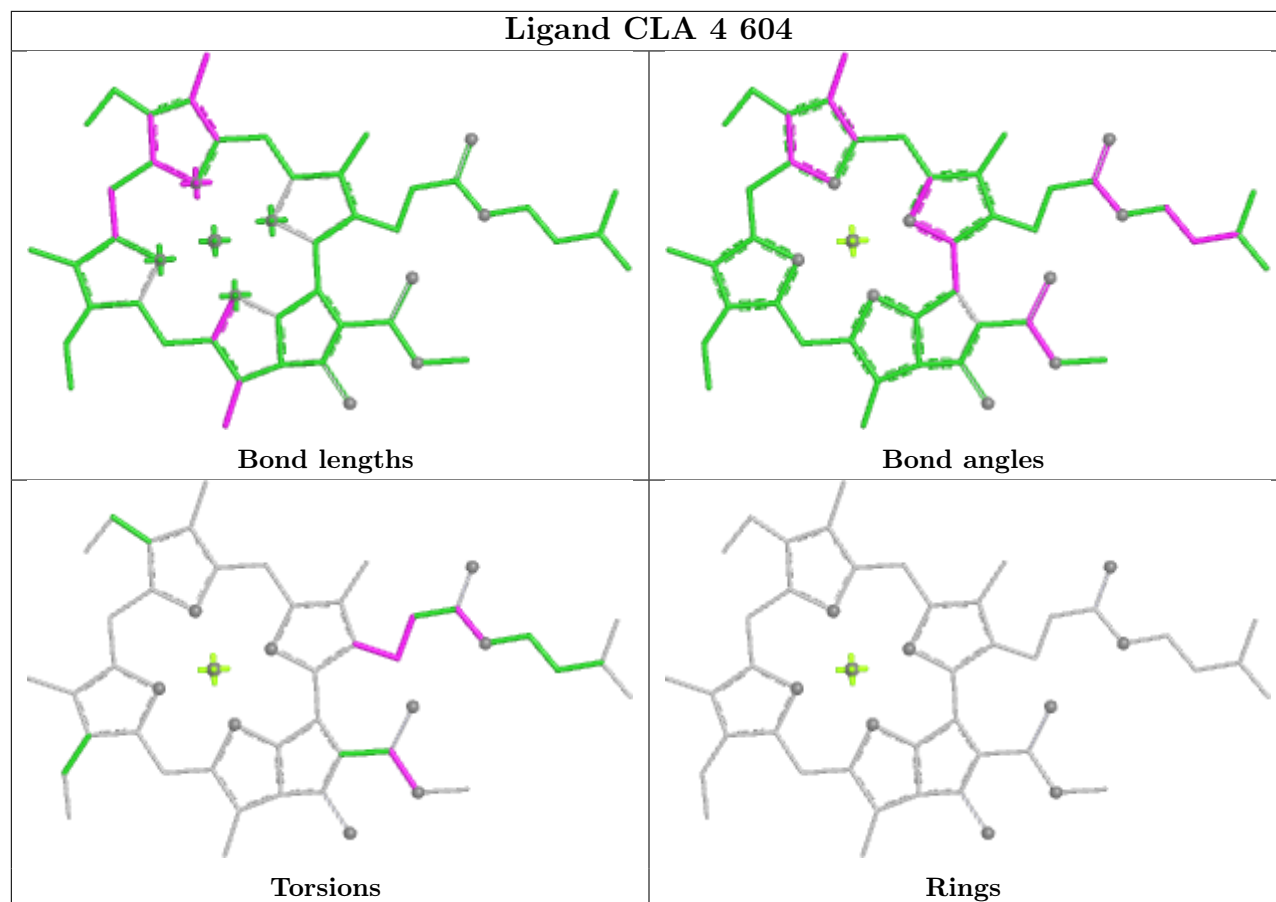


Ligand CLA B 1021

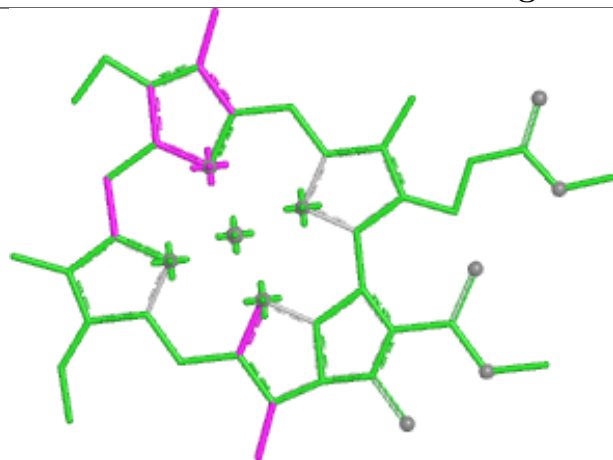




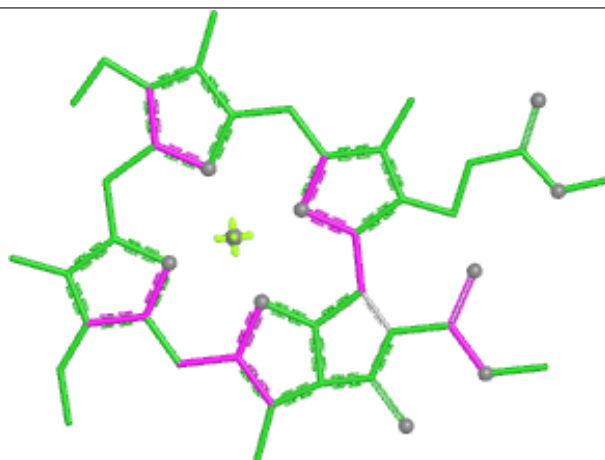
Ligand CLA 4 604



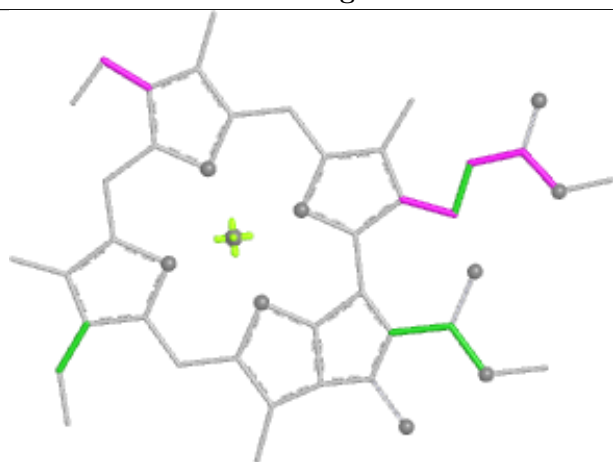
Ligand CLA 1 614



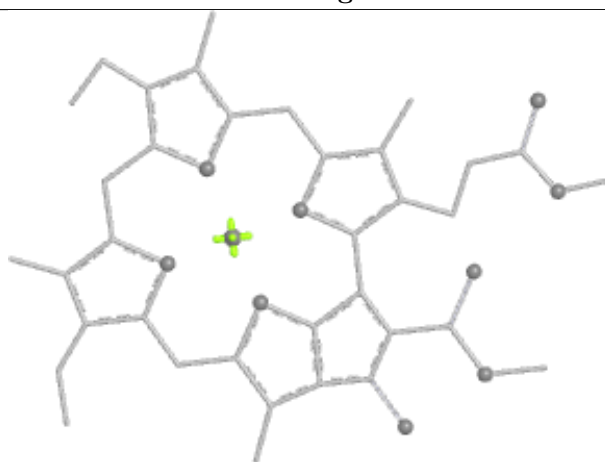
Bond lengths



Bond angles

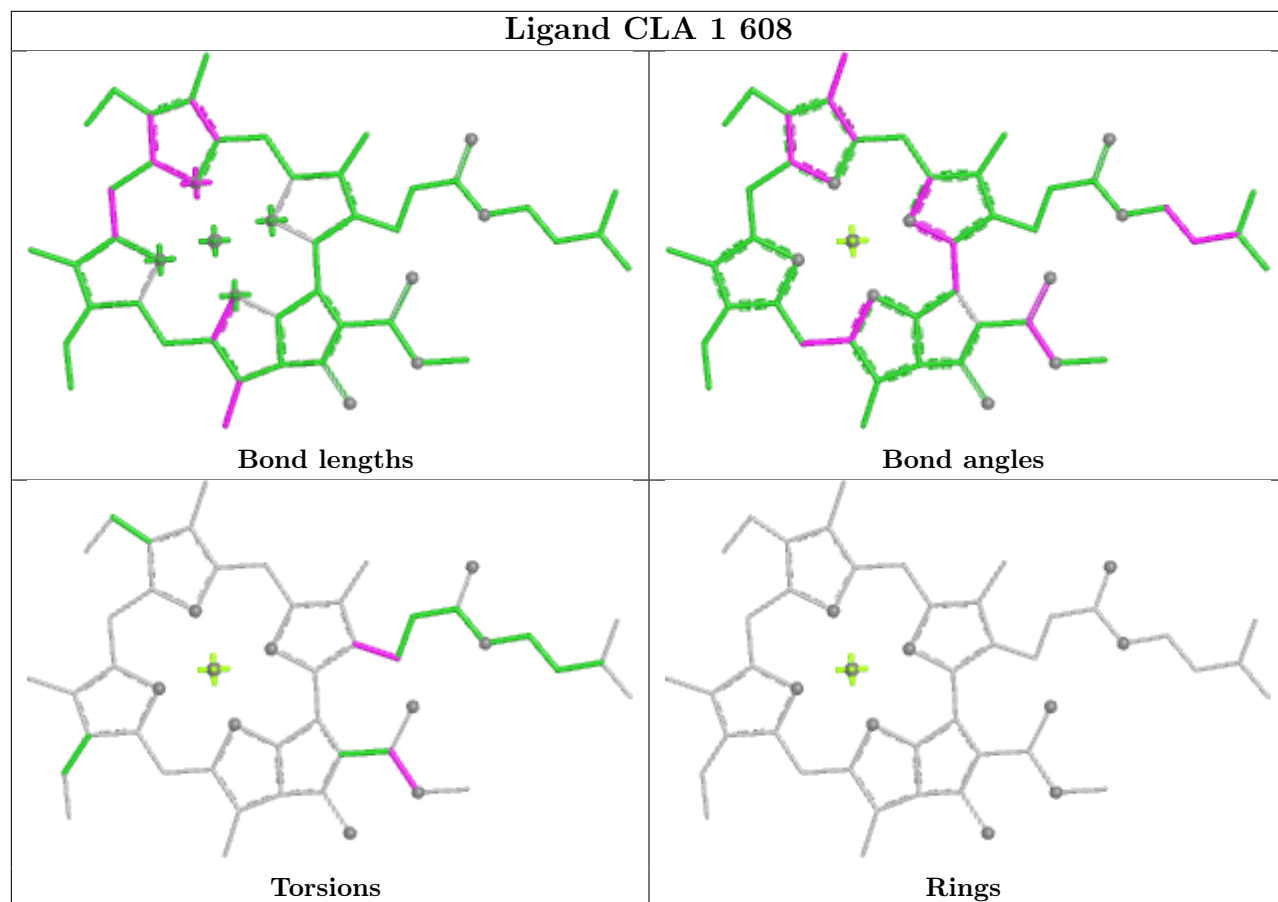


Torsions

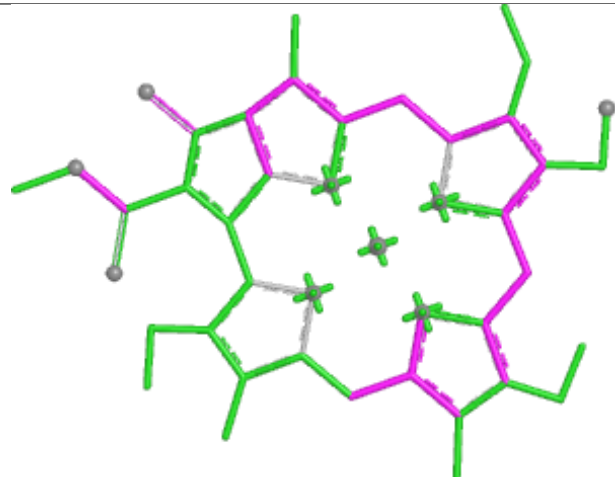


Rings

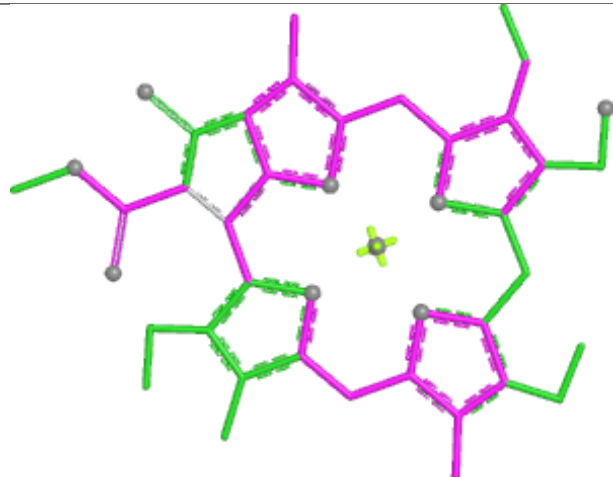
Ligand CLA 1 608



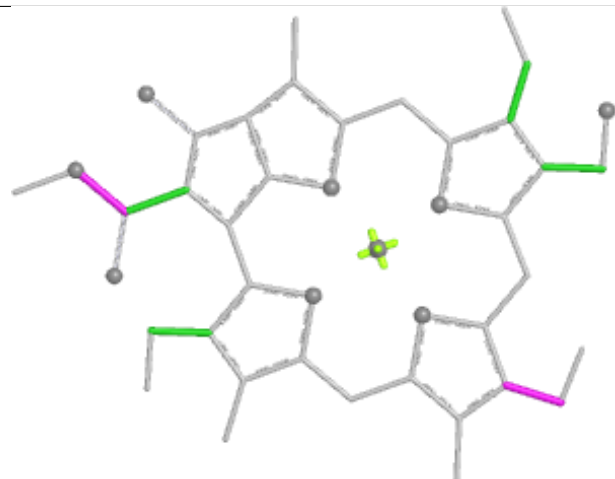
Ligand CHL 4 615



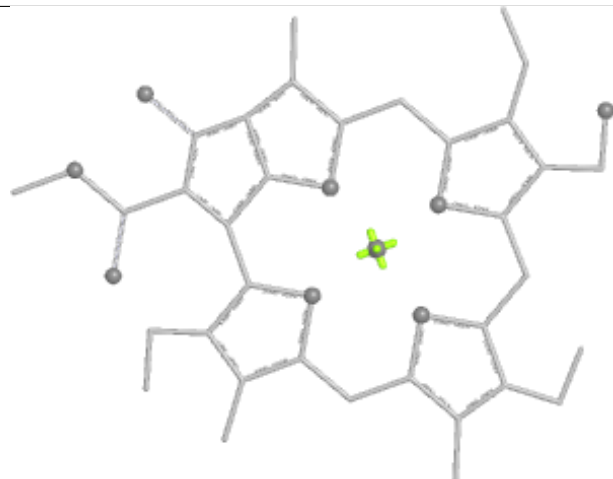
Bond lengths



Bond angles

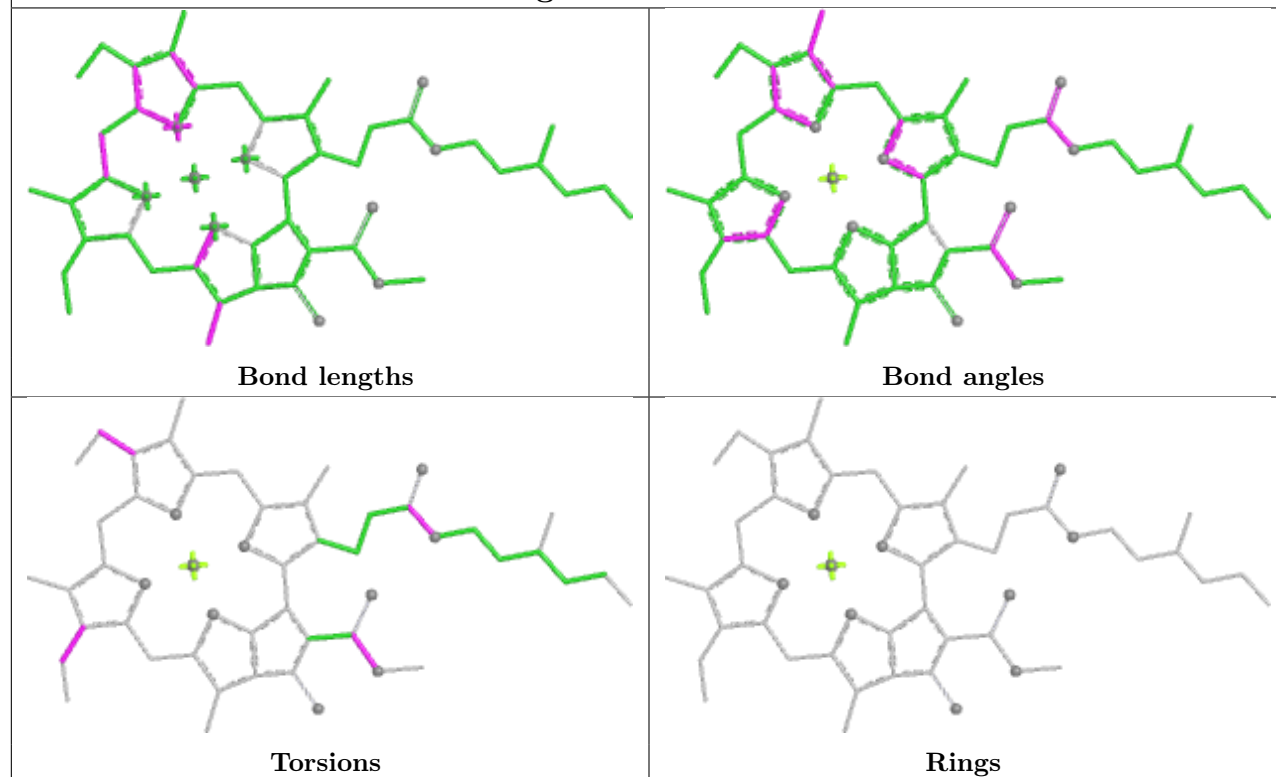


Torsions

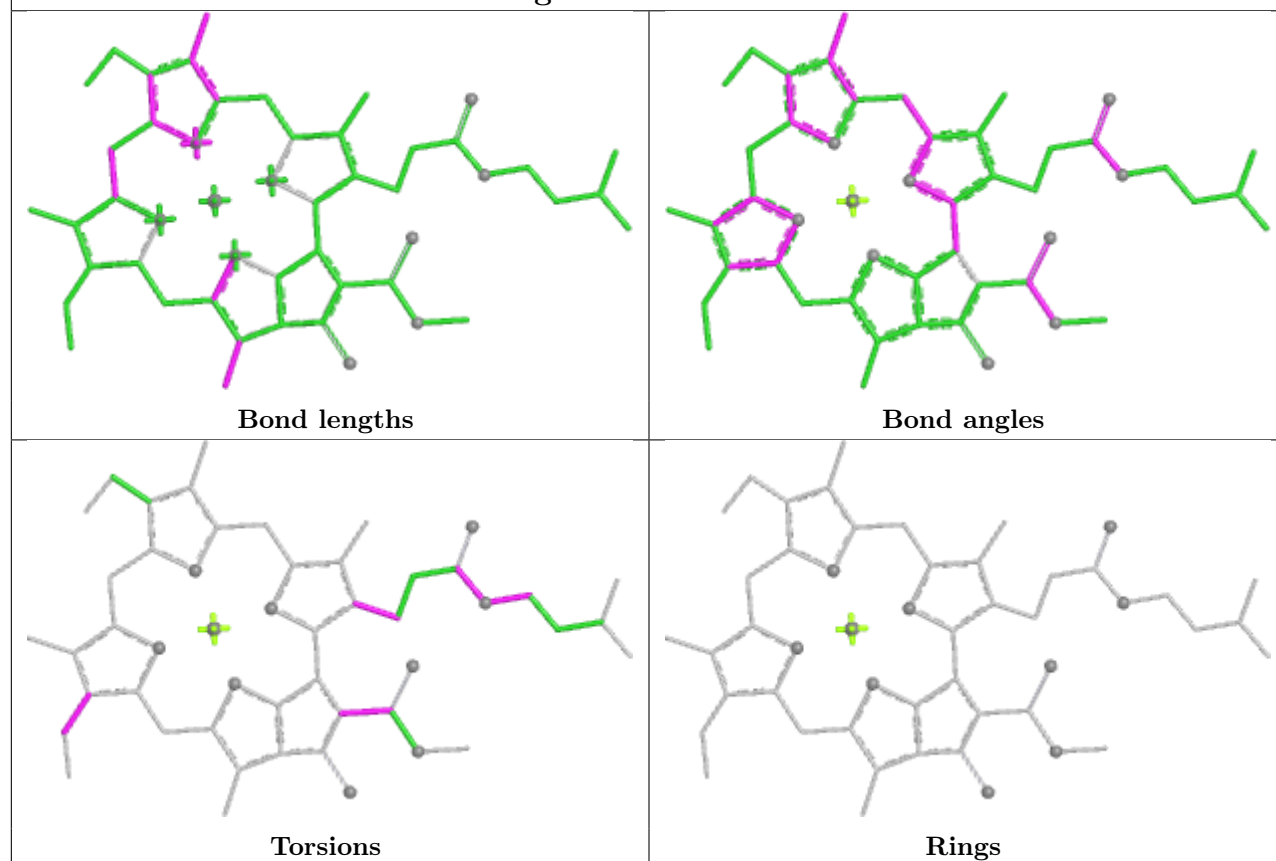


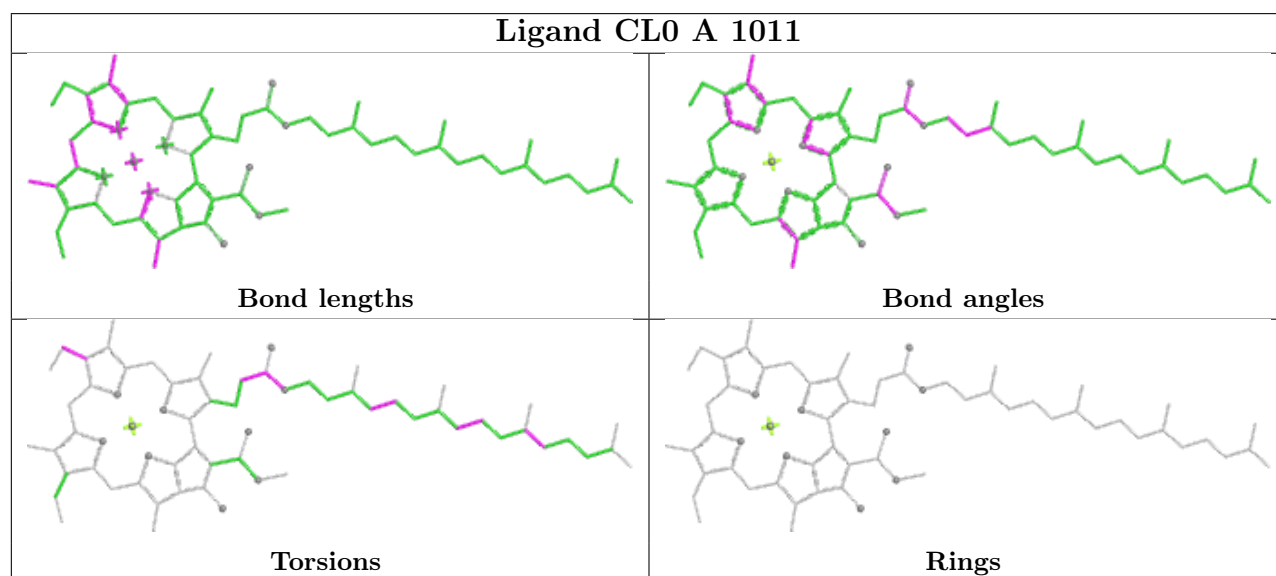
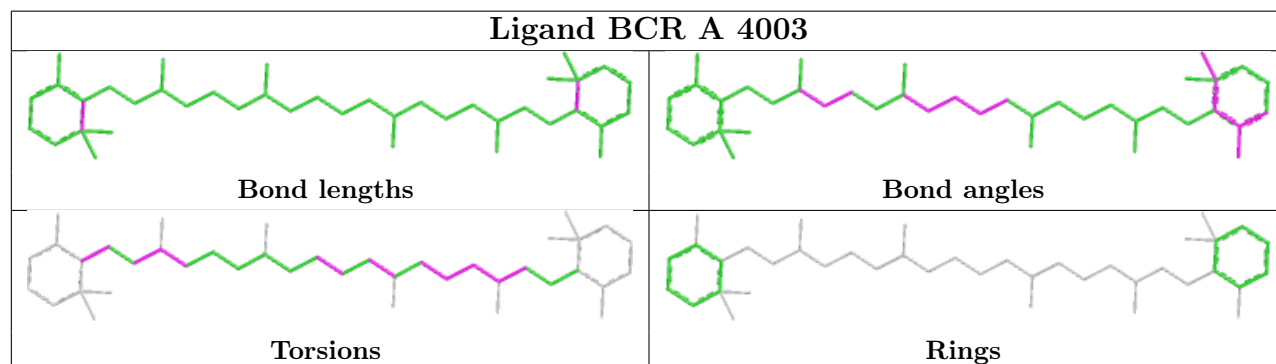
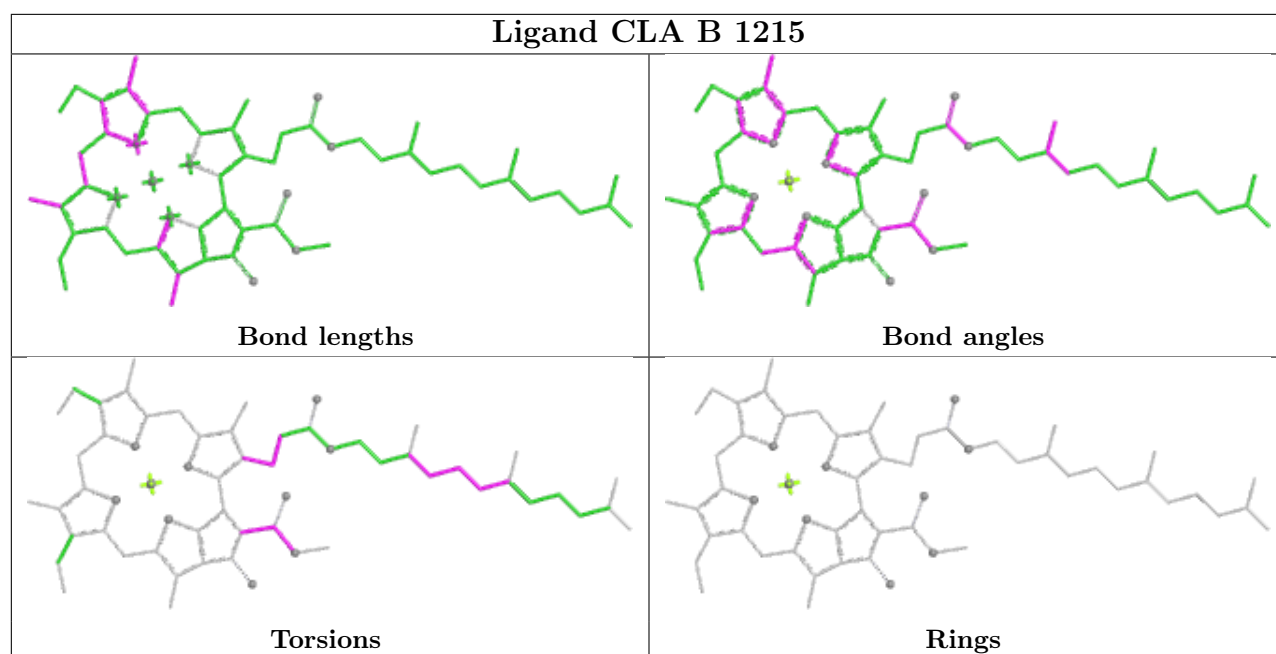
Rings

Ligand CLA 2 612

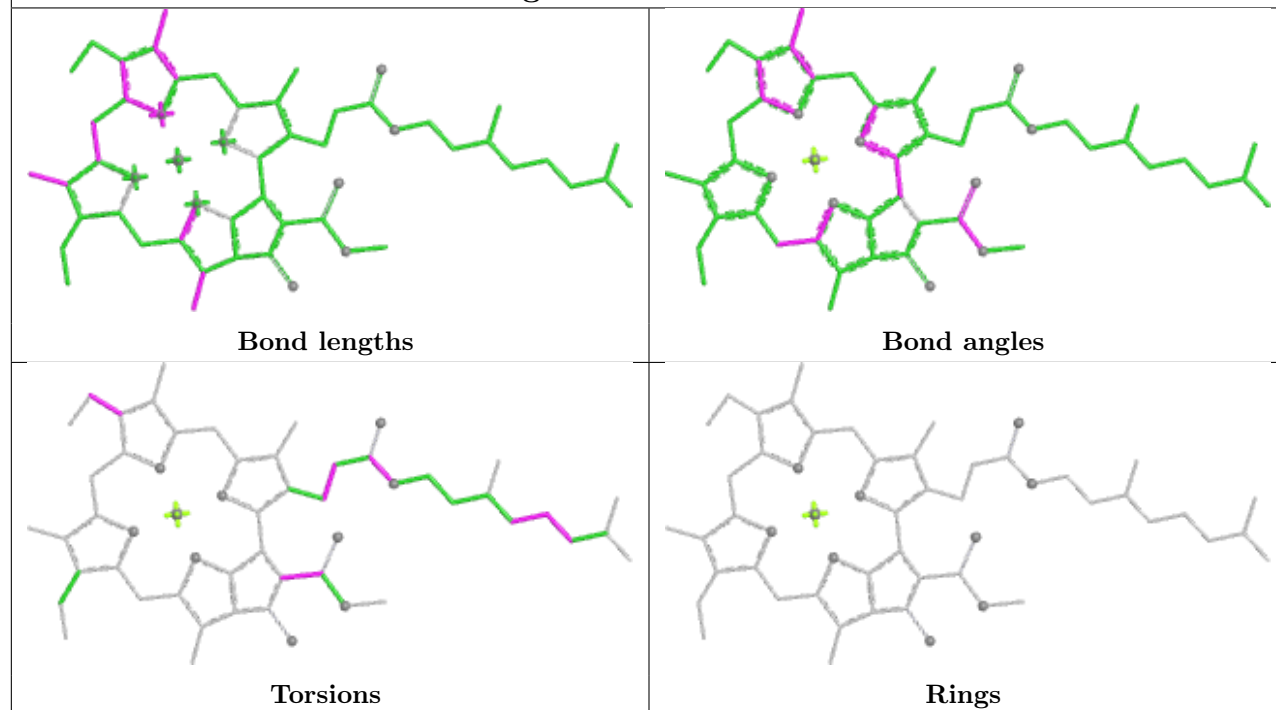


Ligand CLA L 301

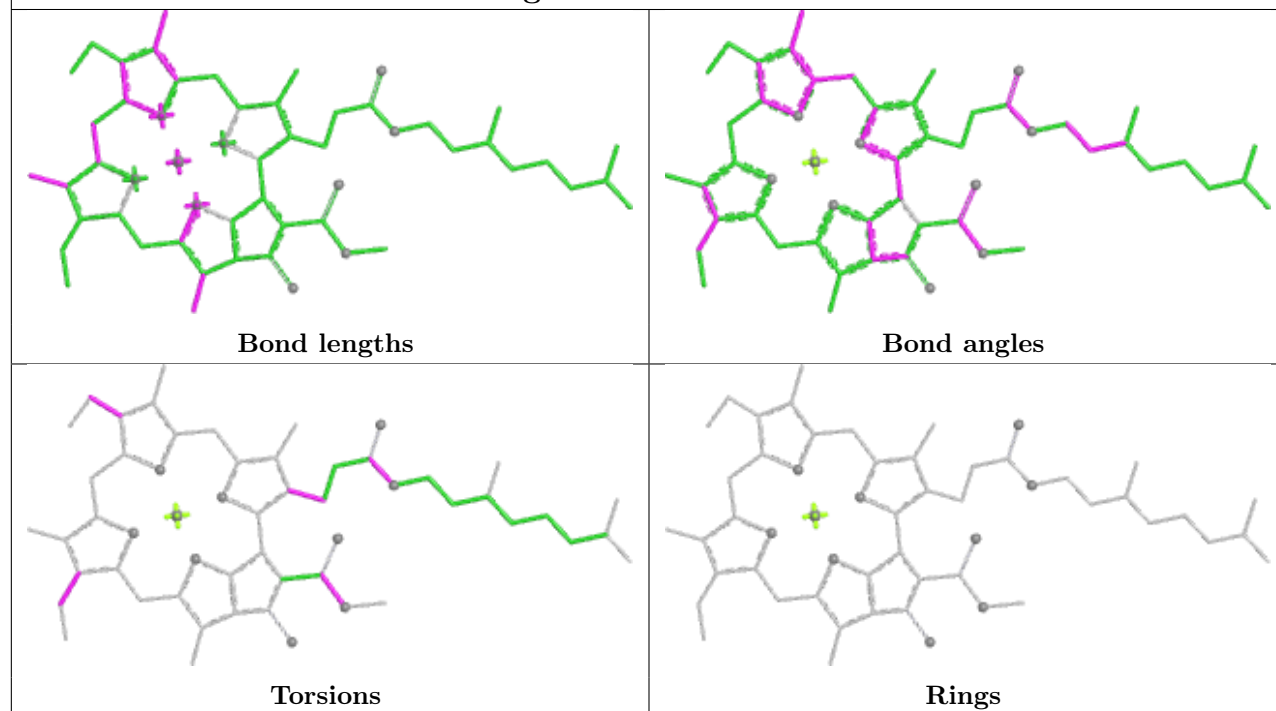




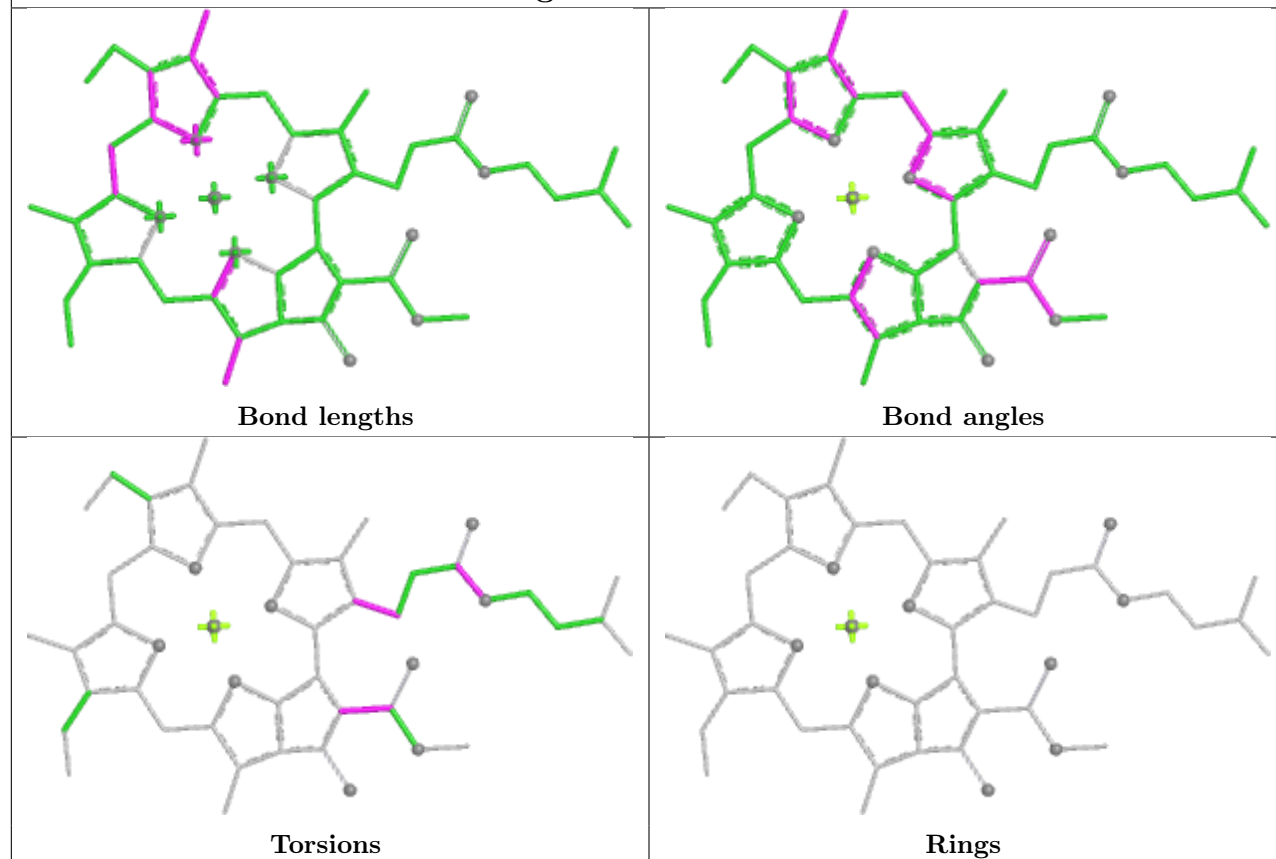
Ligand CLA A 1106



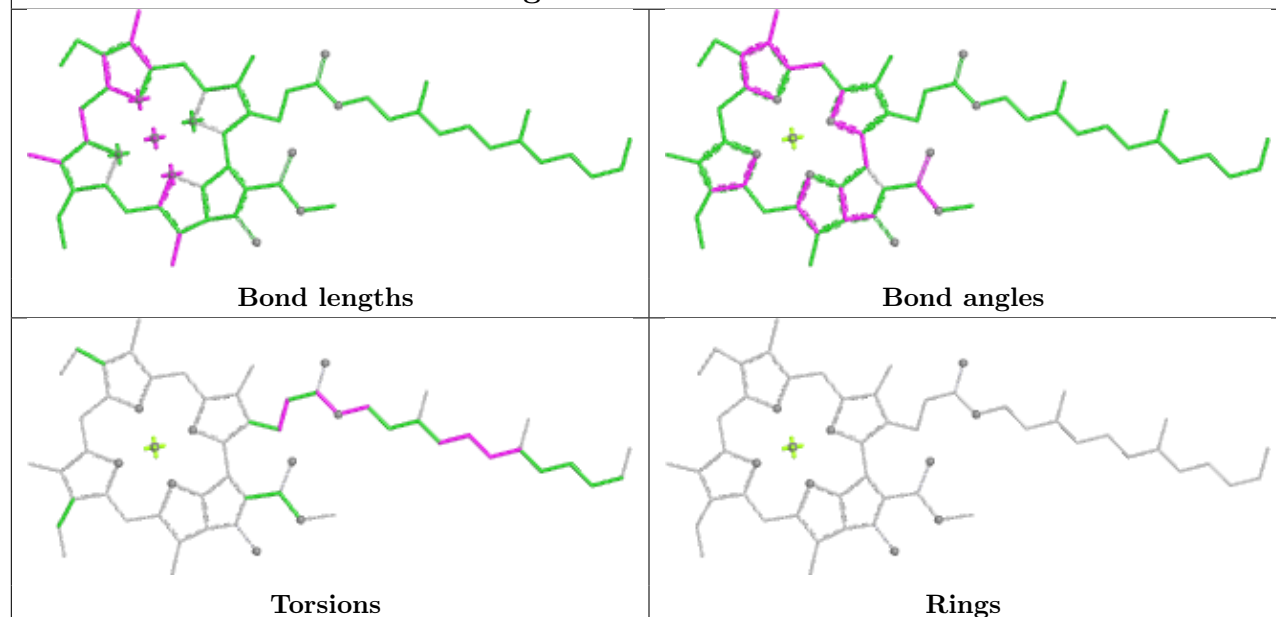
Ligand CLA B 1216

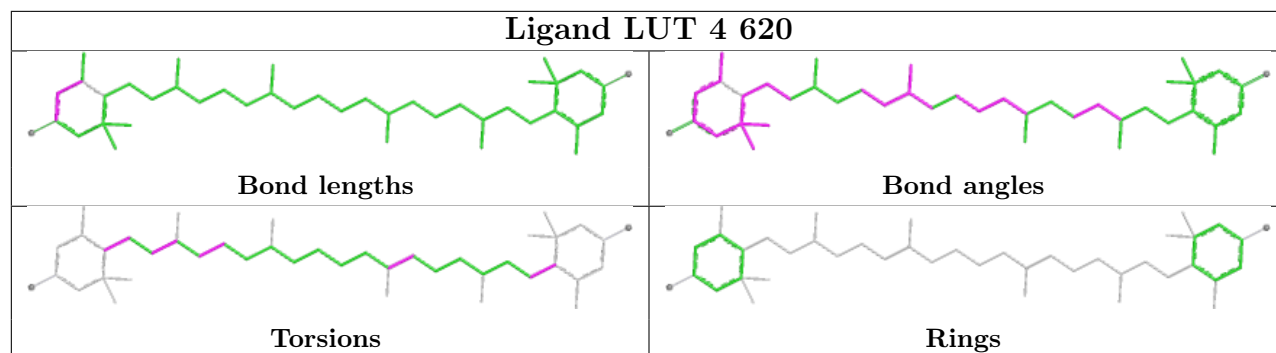


Ligand CLA 2 614



Ligand CLA B 1214





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.

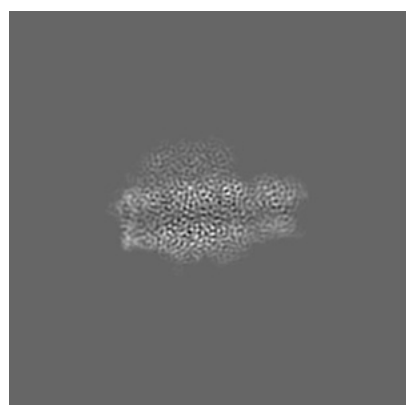
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-23023. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

6.1 Orthogonal projections [i](#)

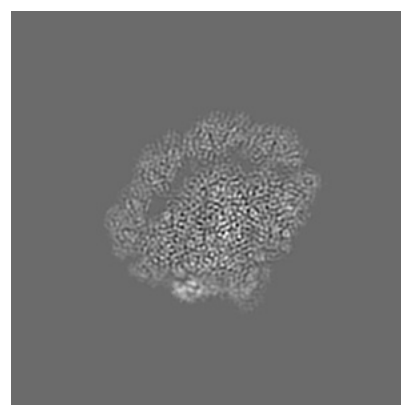
6.1.1 Primary map



X



Y

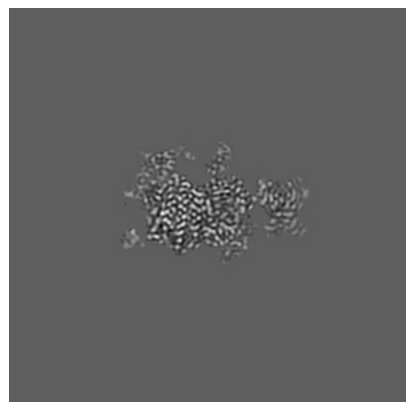


Z

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

6.2 Central slices [i](#)

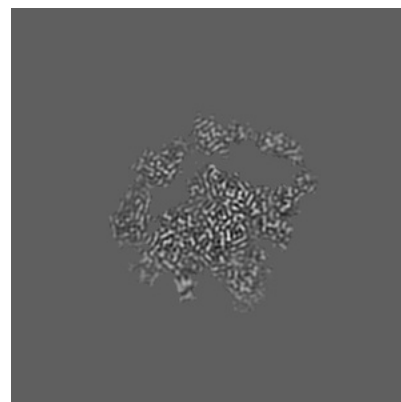
6.2.1 Primary map



X Index: 140



Y Index: 140



Z Index: 140

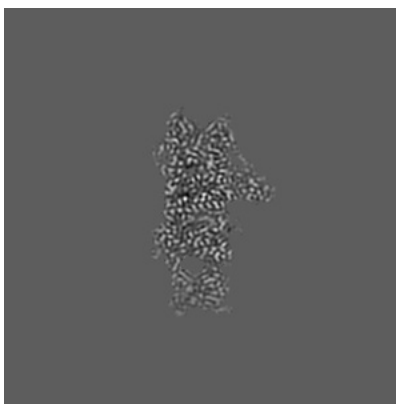
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

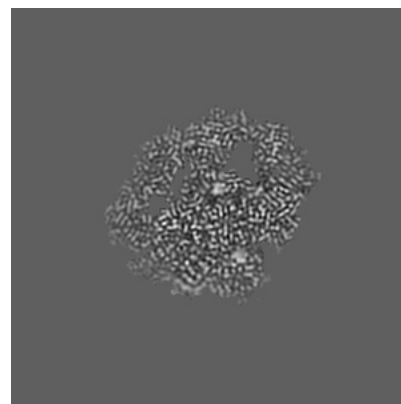
6.3.1 Primary map



X Index: 150



Y Index: 133

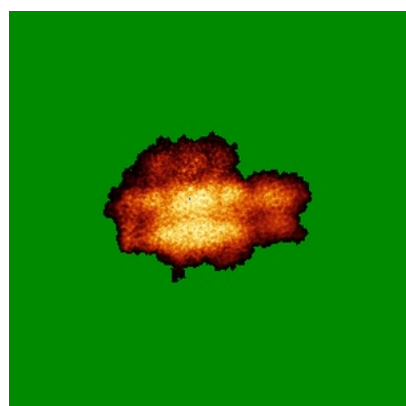


Z Index: 148

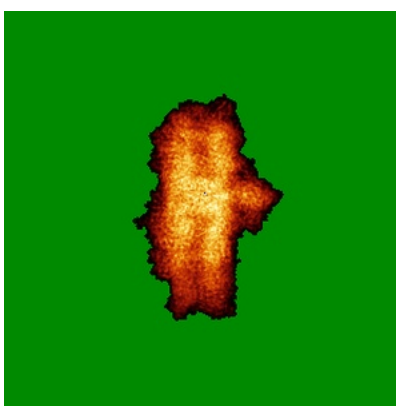
The images above show the largest variance slices of the map in three orthogonal directions.

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

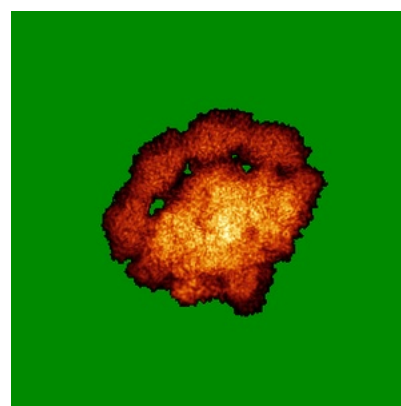
6.4.1 Primary map



X



Y

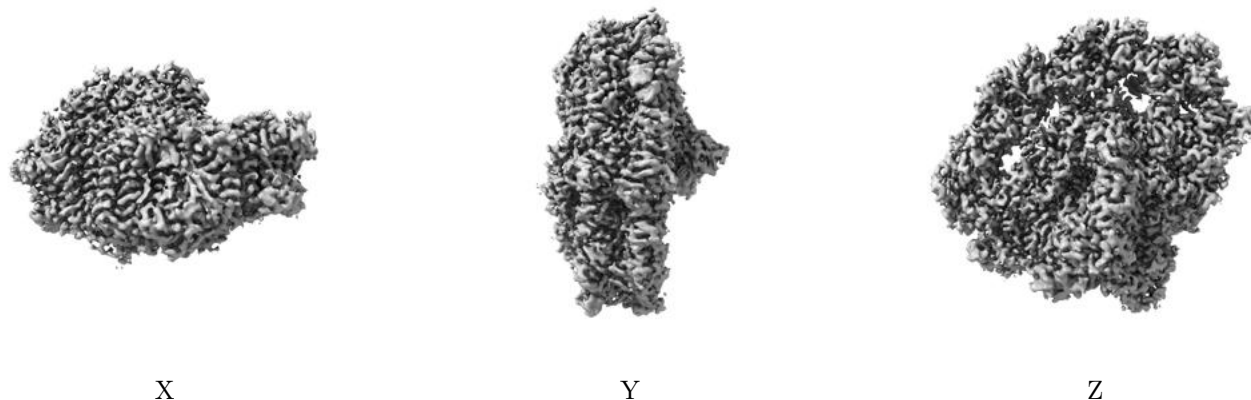


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 1.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

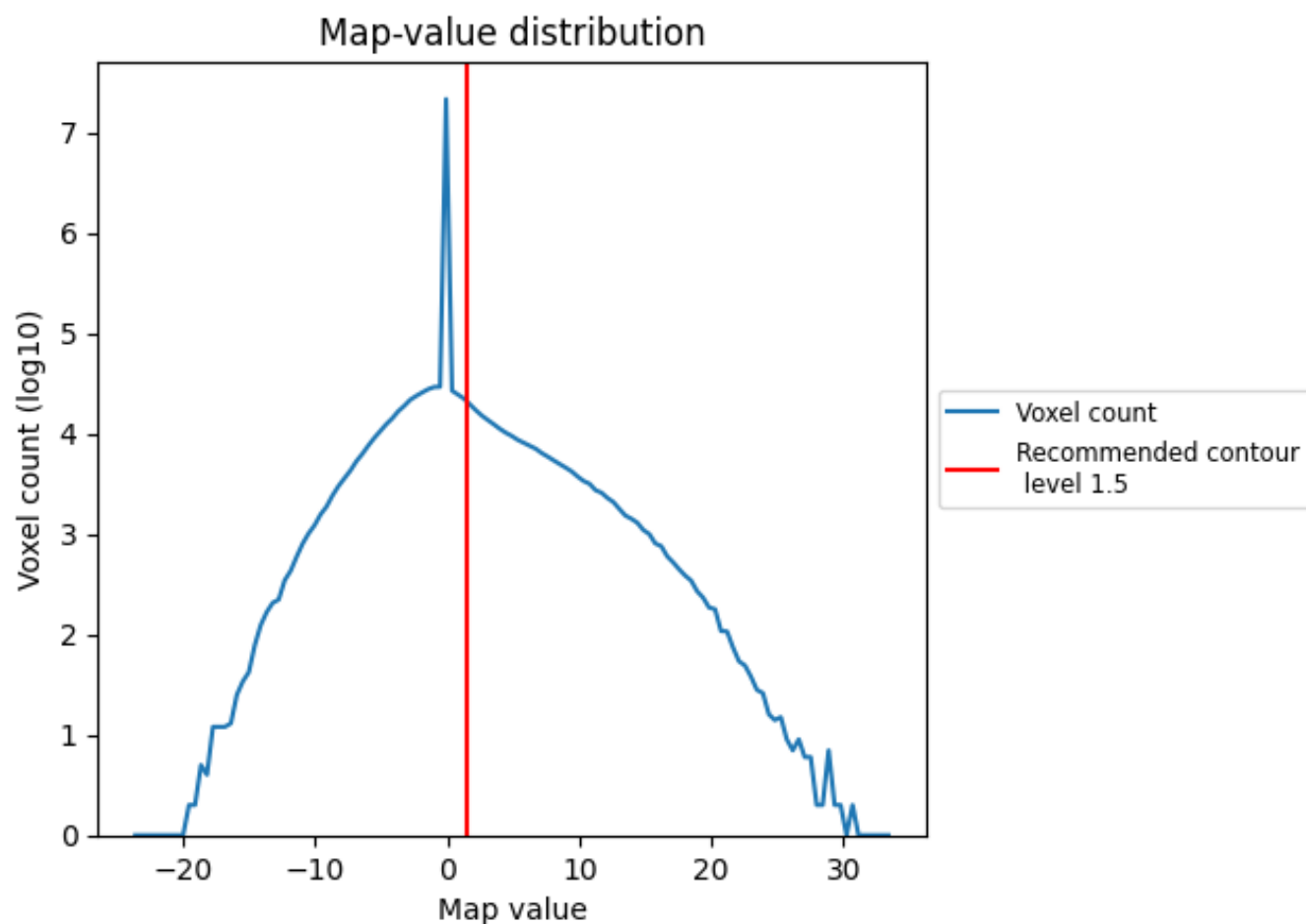
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

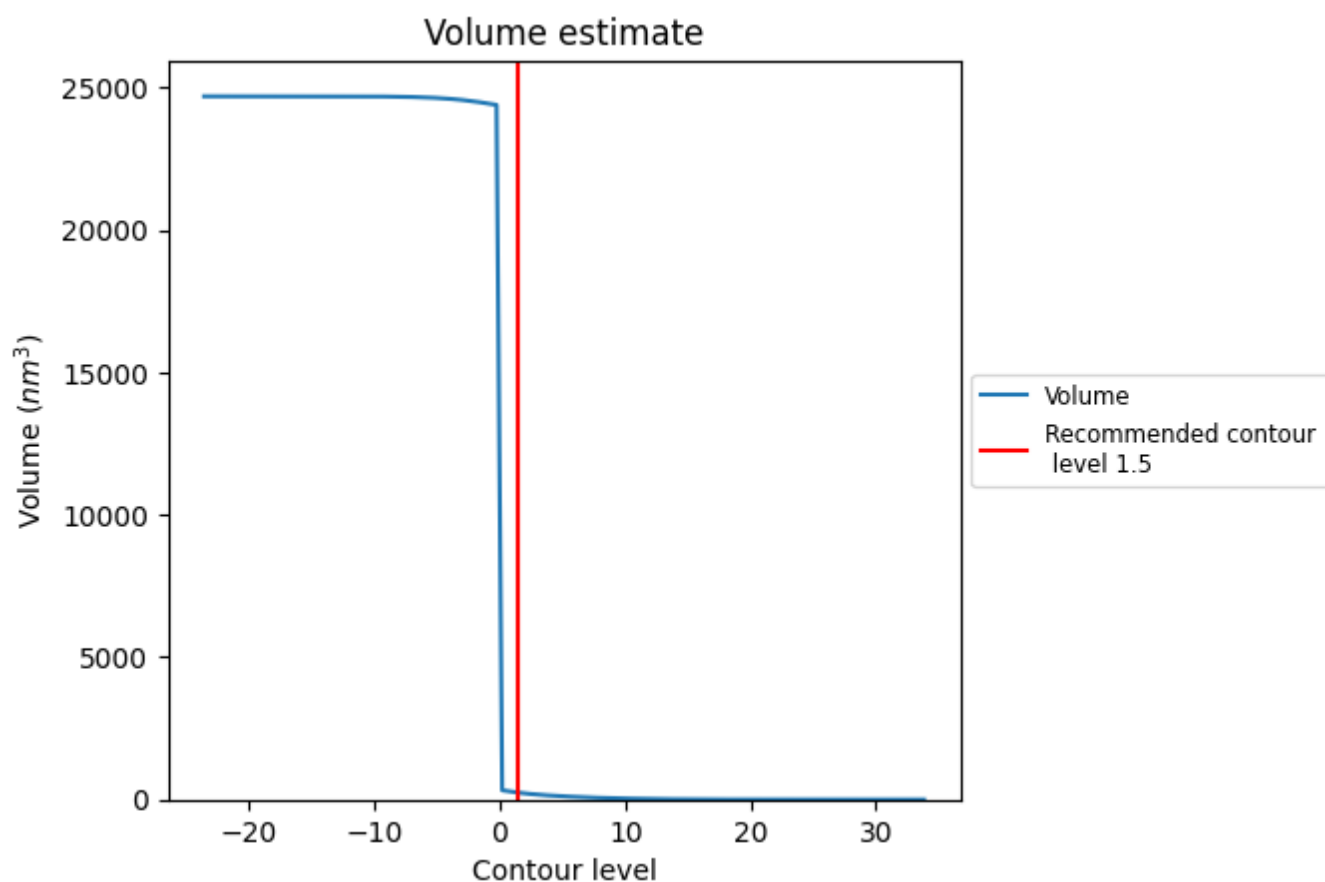
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

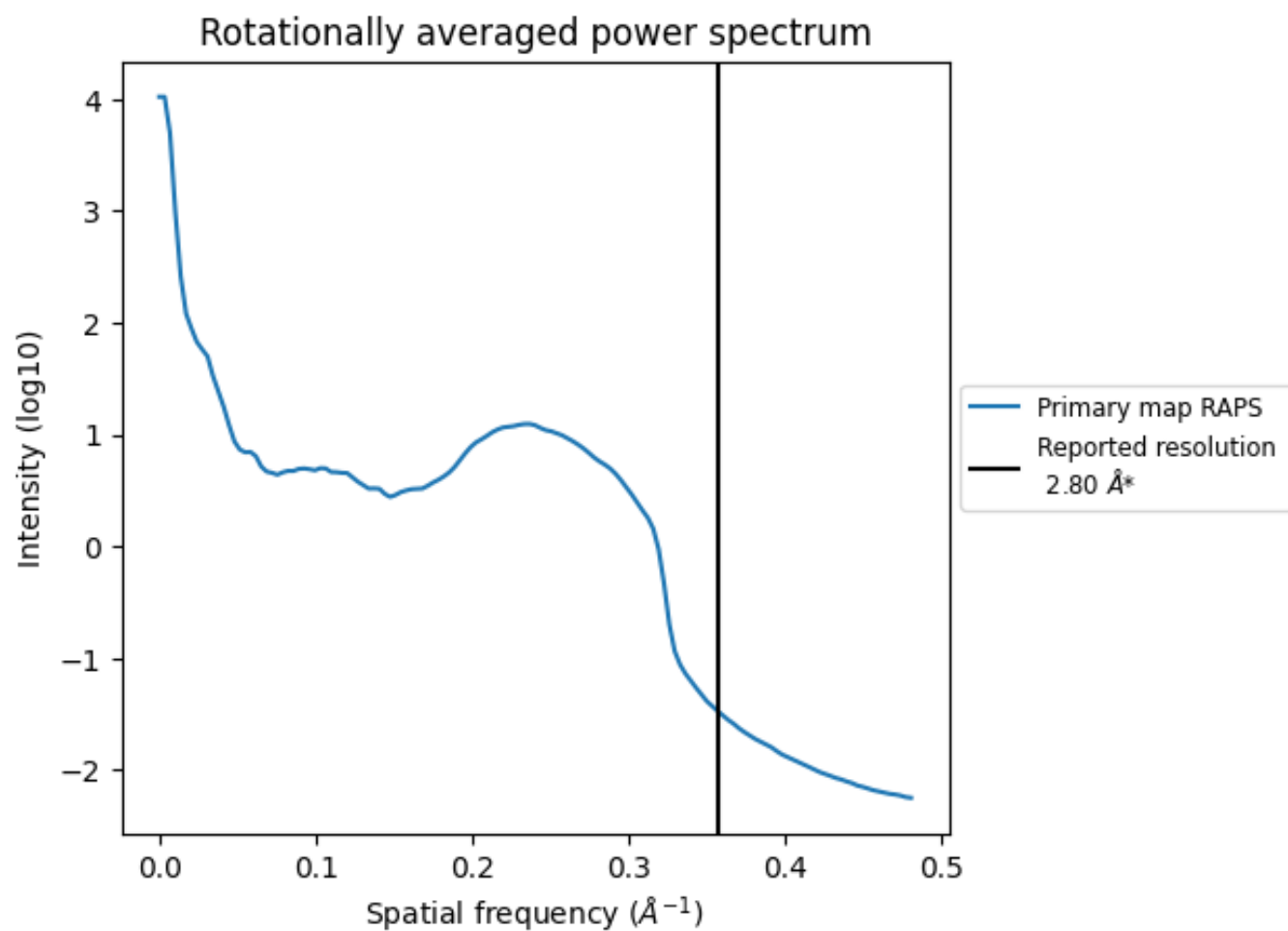
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 242 nm³; this corresponds to an approximate mass of 219 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 0.357 Å⁻¹

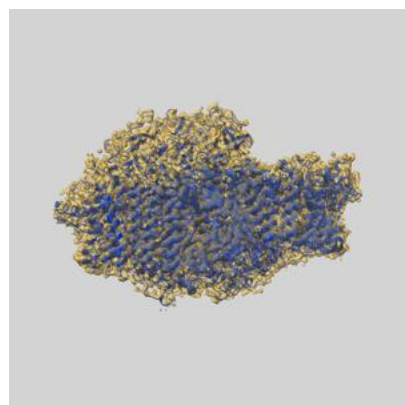
8 Fourier-Shell correlation ⓘ

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

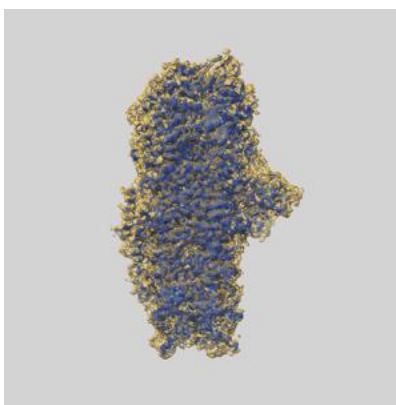
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-23023 and PDB model 7KSQ. Per-residue inclusion information can be found in section 3 on page 24.

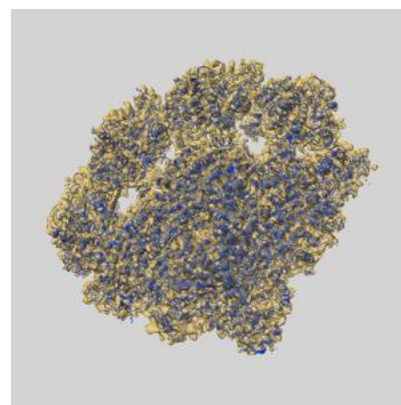
9.1 Map-model overlay [i](#)



X



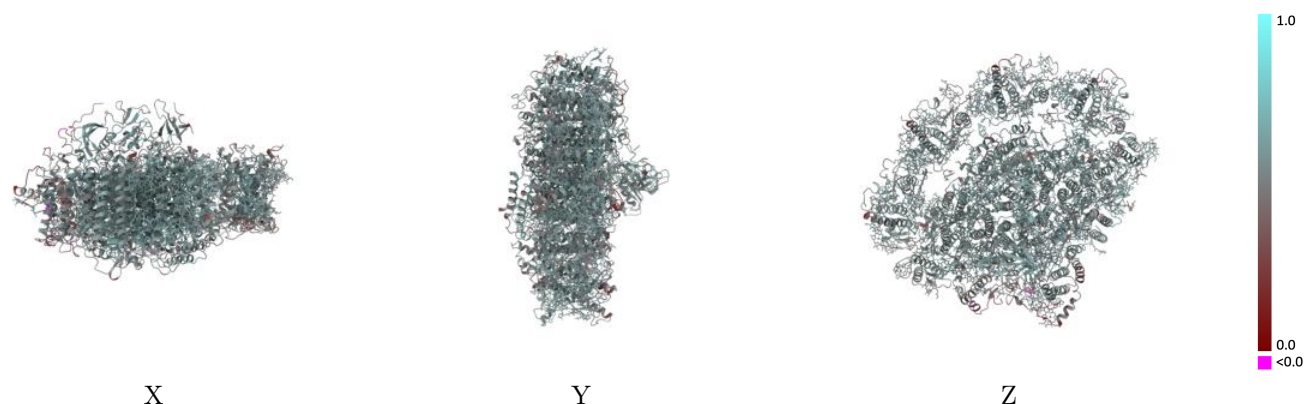
Y



Z

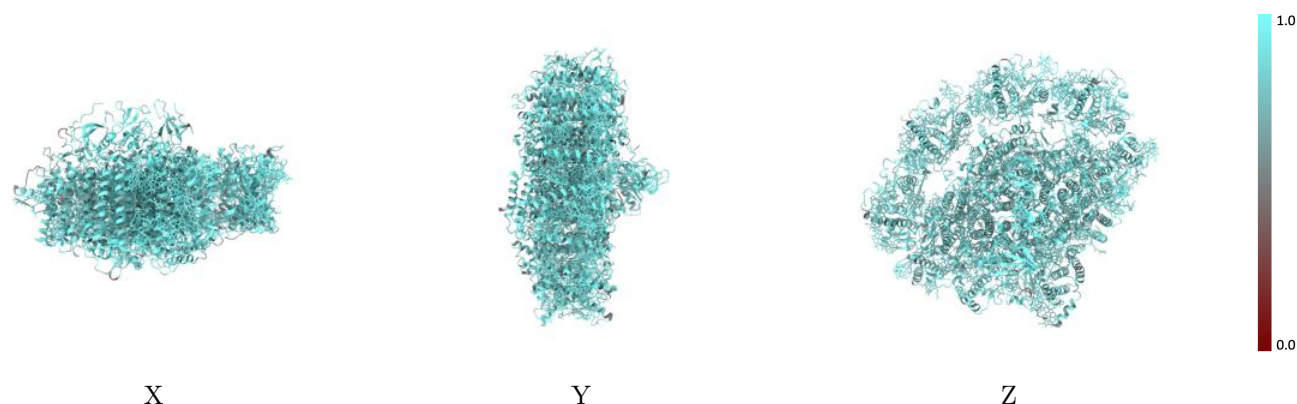
The images above show the 3D surface view of the map at the recommended contour level 1.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



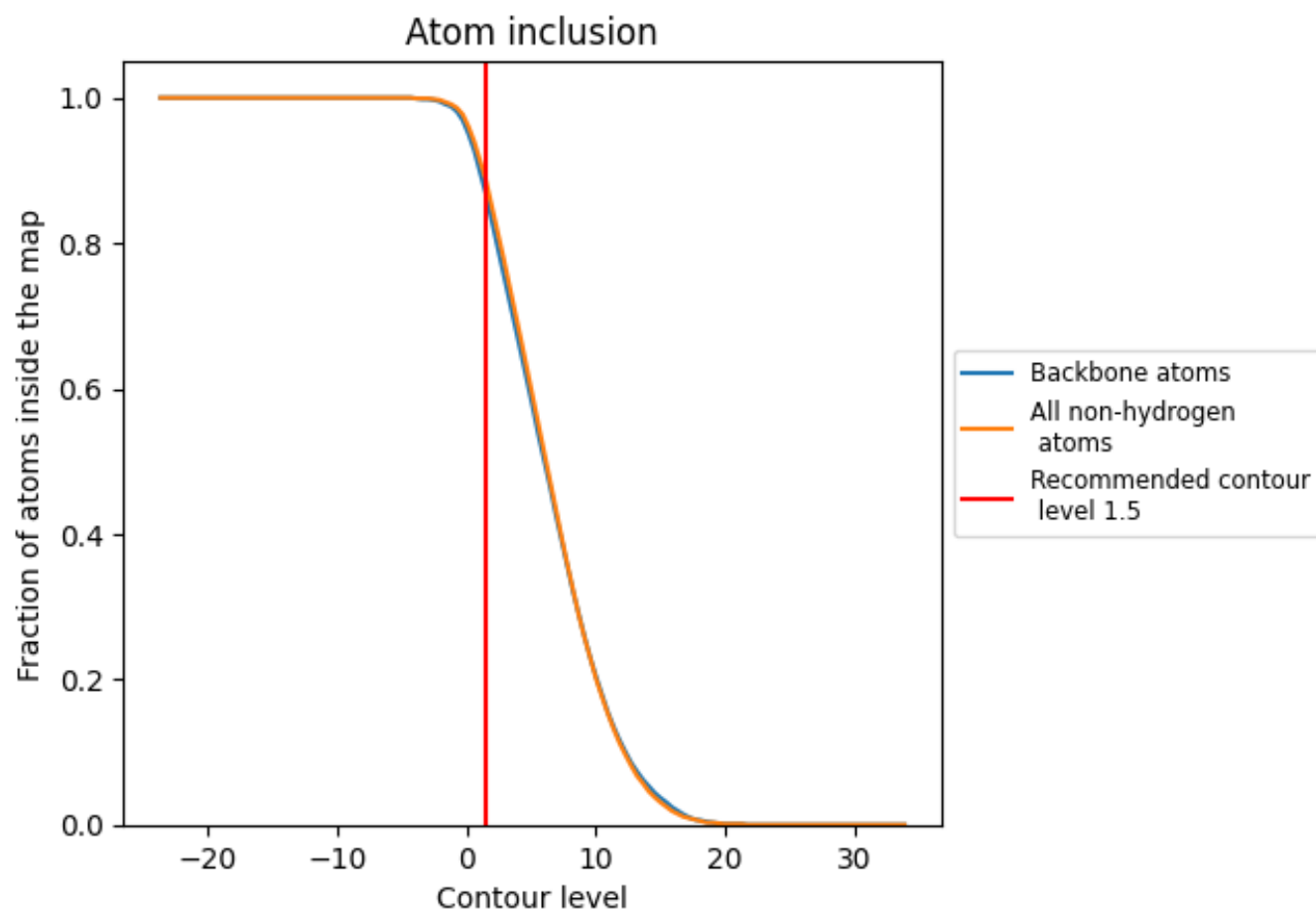
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (1.5).

9.4 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 89% 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 (1.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8880	 0.5440
1	 0.8670	 0.5280
2	 0.8610	 0.5260
3	 0.8620	 0.5330
4	 0.8650	 0.5220
A	 0.9090	 0.5680
B	 0.9180	 0.5730
C	 0.9350	 0.5700
D	 0.8770	 0.5340
E	 0.8740	 0.5380
F	 0.8720	 0.5480
G	 0.8720	 0.5400
H	 0.7220	 0.4090
I	 0.8740	 0.5450
J	 0.8940	 0.5590
K	 0.8310	 0.5070
L	 0.8480	 0.5110
M	 0.8540	 0.5140
O	 0.8950	 0.3850

