



Full wwPDB EM Validation Report ⓘ

Mar 10, 2026 – 05:58 AM UTC

PDB ID : 7EW6 / pdb_00007ew6
EMDB ID : EMD-31348
Title : Barley photosystem I-LHCI-Lhca5 supercomplex
Authors : Wang, W.D.; Shen, L.; Tang, K.; Han, G.Y.; Zhang, X.; Shen, J.R.
Deposited on : 2021-05-24
Resolution : 3.40 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:

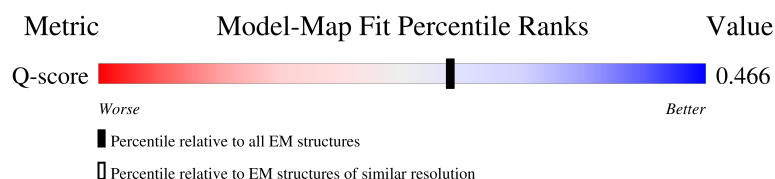
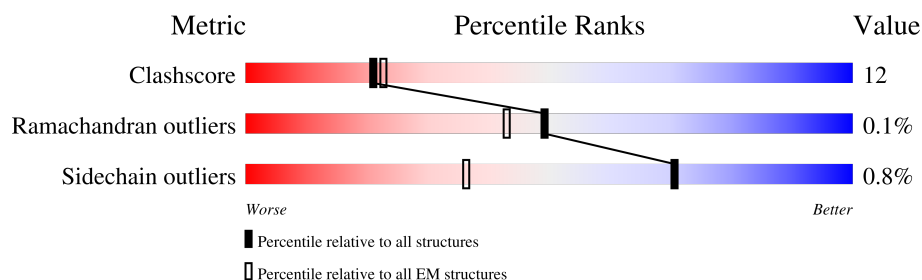
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance

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

The reported resolution of this entry is 3.40 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.



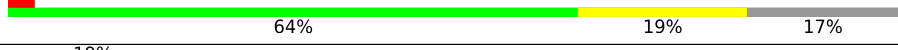
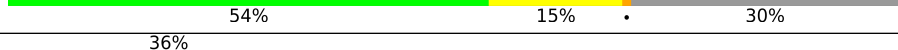
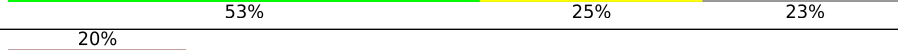
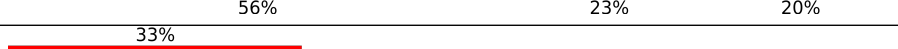
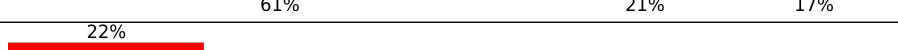
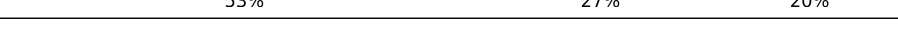
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14717 (2.90 - 3.90)

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	750	
2	B	734	
3	C	81	
4	D	205	

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Mol	Chain	Length	Quality of chain
5	E	147	
6	F	235	
7	H	143	
8	I	36	
9	J	42	
10	K	131	
11	L	209	
12	1	247	
13	2	255	
14	3	269	
15	5	257	

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
16	CL0	A	801	X	-	-	-
17	CLA	1	504	X	-	-	-
17	CLA	1	505	X	-	-	-
17	CLA	1	506	X	-	-	-
17	CLA	1	507	X	-	-	-
17	CLA	1	508	X	-	-	-
17	CLA	1	510	X	-	-	-
17	CLA	1	511	X	-	-	-
17	CLA	1	515	X	-	-	-
17	CLA	2	504	X	-	-	-
17	CLA	2	506	X	-	-	-
17	CLA	2	507	X	-	-	-
17	CLA	2	508	X	-	-	-
17	CLA	2	509	X	-	-	-
17	CLA	2	510	X	-	-	-
17	CLA	2	511	X	-	-	-
17	CLA	2	514	X	-	-	-
17	CLA	3	301	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
17	CLA	3	306	X	-	-	-
17	CLA	3	307	X	-	-	-
17	CLA	3	308	X	-	-	-
17	CLA	3	310	X	-	-	-
17	CLA	3	311	X	-	-	-
17	CLA	3	312	X	-	-	-
17	CLA	3	313	X	-	-	-
17	CLA	3	314	X	-	-	-
17	CLA	3	316	X	-	-	-
17	CLA	3	317	X	-	-	-
17	CLA	3	318	X	-	-	-
17	CLA	5	305	X	-	-	-
17	CLA	5	306	X	-	-	-
17	CLA	5	307	X	-	-	-
17	CLA	5	308	X	-	-	-
17	CLA	5	309	X	-	-	-
17	CLA	5	310	X	-	-	-
17	CLA	5	311	X	-	-	-
17	CLA	5	312	X	-	-	-
17	CLA	5	313	X	-	-	-
17	CLA	5	316	X	-	-	-
17	CLA	A	802	X	-	-	-
17	CLA	A	803	X	-	-	-
17	CLA	A	804	X	-	-	-
17	CLA	A	805	X	-	-	-
17	CLA	A	806	X	-	-	-
17	CLA	A	807	X	-	-	-
17	CLA	A	808	X	-	-	-
17	CLA	A	809	X	-	-	-
17	CLA	A	810	X	-	-	-
17	CLA	A	811	X	-	-	-
17	CLA	A	812	X	-	-	-
17	CLA	A	813	X	-	-	-
17	CLA	A	814	X	-	-	-
17	CLA	A	815	X	-	-	-
17	CLA	A	816	X	-	-	-
17	CLA	A	817	X	-	-	-
17	CLA	A	818	X	-	-	-
17	CLA	A	819	X	-	-	-
17	CLA	A	820	X	-	-	-
17	CLA	A	821	X	-	-	-
17	CLA	A	822	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
17	CLA	A	823	X	-	-	-
17	CLA	A	824	X	-	-	-
17	CLA	A	825	X	-	-	-
17	CLA	A	826	X	-	-	-
17	CLA	A	827	X	-	-	-
17	CLA	A	828	X	-	-	-
17	CLA	A	829	X	-	-	-
17	CLA	A	830	X	-	-	-
17	CLA	A	831	X	-	-	-
17	CLA	A	832	X	-	-	-
17	CLA	A	833	X	-	-	-
17	CLA	A	834	X	-	-	-
17	CLA	A	835	X	-	-	-
17	CLA	A	836	X	-	-	-
17	CLA	A	837	X	-	-	-
17	CLA	A	838	X	-	-	-
17	CLA	A	839	X	-	-	-
17	CLA	A	840	X	-	-	-
17	CLA	A	842	X	-	-	-
17	CLA	A	852	X	-	-	-
17	CLA	B	801	X	-	-	-
17	CLA	B	802	X	-	-	-
17	CLA	B	803	X	-	-	-
17	CLA	B	804	X	-	-	-
17	CLA	B	805	X	-	-	-
17	CLA	B	806	X	-	-	-
17	CLA	B	807	X	-	-	-
17	CLA	B	808	X	-	-	-
17	CLA	B	809	X	-	-	-
17	CLA	B	810	X	-	-	-
17	CLA	B	811	X	-	-	-
17	CLA	B	812	X	-	-	-
17	CLA	B	813	X	-	-	-
17	CLA	B	814	X	-	-	-
17	CLA	B	815	X	-	-	-
17	CLA	B	816	X	-	-	-
17	CLA	B	817	X	-	-	-
17	CLA	B	818	X	-	-	-
17	CLA	B	819	X	-	-	-
17	CLA	B	820	X	-	-	-
17	CLA	B	821	X	-	-	-
17	CLA	B	822	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
17	CLA	B	823	X	-	-	-
17	CLA	B	824	X	-	-	-
17	CLA	B	825	X	-	-	-
17	CLA	B	826	X	-	-	-
17	CLA	B	827	X	-	-	-
17	CLA	B	828	X	-	-	-
17	CLA	B	829	X	-	-	-
17	CLA	B	830	X	-	-	-
17	CLA	B	831	X	-	-	-
17	CLA	B	832	X	-	-	-
17	CLA	B	833	X	-	-	-
17	CLA	B	834	X	-	-	-
17	CLA	B	835	X	-	-	-
17	CLA	B	837	X	-	-	-
17	CLA	B	838	X	-	-	-
17	CLA	B	839	X	-	-	-
17	CLA	B	840	X	-	-	-
17	CLA	B	841	X	-	-	-
17	CLA	B	842	X	-	-	-
17	CLA	F	802	X	-	-	-
17	CLA	F	803	X	-	-	-
17	CLA	J	101	X	-	-	-
17	CLA	K	201	X	-	-	-
17	CLA	K	202	X	-	-	-
17	CLA	K	203	X	-	-	-
17	CLA	K	205	X	-	-	-
17	CLA	L	301	X	-	-	-
17	CLA	L	302	X	-	-	-
17	CLA	L	303	X	-	-	-
17	CLA	L	304	X	-	-	-
25	CHL	1	512	X	-	-	-
25	CHL	1	514	X	-	-	-
25	CHL	1	517	X	-	-	-
25	CHL	2	512	X	-	-	-
25	CHL	2	513	X	-	-	-
25	CHL	2	515	X	-	-	-
25	CHL	2	516	X	-	-	-
25	CHL	3	302	X	-	-	-
25	CHL	3	315	X	-	-	-
25	CHL	5	314	X	-	-	-
25	CHL	5	315	X	-	-	-
25	CHL	5	317	X	-	-	-

2 Entry composition

There are 26 unique types of molecules in this entry. The entry contains 32973 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
			5813	3812	983	1000	18		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	733	Total	C	N	O	S	0	0
			5849	3834	995	1006	14		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	81	Total	C	N	O	S	0	0
			610	376	105	117	12		

- Molecule 4 is a protein called Photosystem I reaction center subunit II, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	142	Total	C	N	O	S	0	0
			1113	716	193	201	3		

- Molecule 5 is a protein called Photosystem I reaction center subunit IV, chloroplastic.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	E	68	Total	C	N	O	0	0
			538	341	98	99		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	158	Total	C	N	O	S	0	0
			1203	774	208	218	3		

- Molecule 7 is a protein called Photosystem I reaction center subunit VI, chloroplastic.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	H	61	Total	C	N	O	0	0
			454	303	76	75		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
8	I	30	Total	C	N	O	0	0
			232	161	35	36		

- Molecule 9 is a protein called Photosystem I reaction center subunit IX.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	42	Total	C	N	O	S	0	0
			333	228	51	53	1		

- Molecule 10 is a protein called Photosystem I reaction center subunit psaK, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	K	84	Total	C	N	O	S	0	0
			565	359	94	108	4		

- Molecule 11 is a protein called Photosystem I reaction center subunit XI, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	L	146	Total	C	N	O	S	0	0
			1088	716	174	197	1		

- Molecule 12 is a protein called Chlorophyll a-b binding protein Lhca1.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	1	191	Total	C	N	O	S	0	0
			1422	921	239	258	4		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	73	PHE	UNK	conflict	UNP A0A287WC32
1	74	GLU	UNK	conflict	UNP A0A287WC32
1	75	ARG	UNK	conflict	UNP A0A287WC32

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	2	203	Total	C	N	O	S	0	0
			1561	1018	257	283	3		

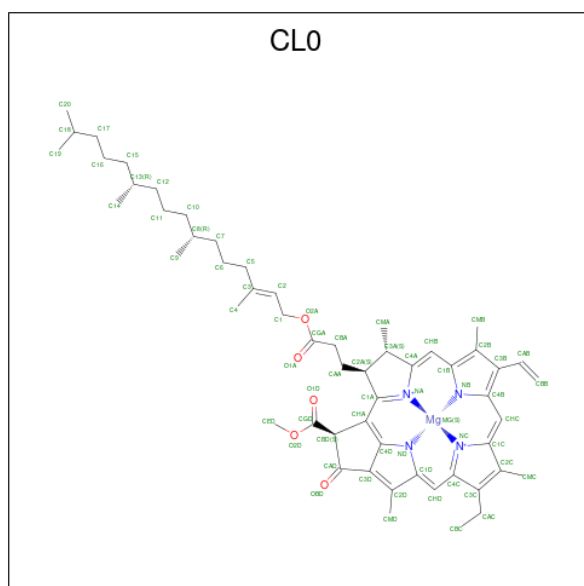
- Molecule 14 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	3	222	Total	C	N	O	S	0	0
			1629	1063	271	292	3		

- Molecule 15 is a protein called Chlorophyll a-b binding protein Lhca5.

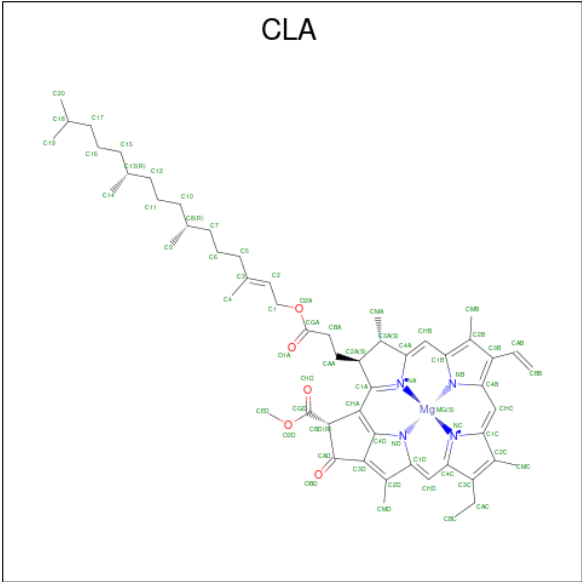
Mol	Chain	Residues	Atoms					AltConf	Trace
15	5	205	Total	C	N	O	S	0	0
			1486	962	247	270	7		

- Molecule 16 is CHLOROPHYLL A ISOMER (CCD ID: CL0) (formula: $C_{55}H_{72}MgN_4O_5$).



Mol	Chain	Residues	Atoms					AltConf
16	A	1	Total	C	Mg	N	O	0
			61	52	1	4	4	

- Molecule 17 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



Mol	Chain	Residues	Atoms					AltConf
17	A	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
17	A	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
17	A	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
17	A	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
17	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	A	1	Total	C	Mg	N	O	0
			39	32	1	4	2	
17	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	A	1	Total	C	Mg	N	O	0
			39	32	1	4	2	
17	A	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
17	A	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
17	A	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
17	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
17	A	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
17	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
17	A	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
17	A	1	Total	C	Mg	N	O	0
			39	32	1	4	2	
17	A	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
17	A	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
17	A	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
17	A	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
17	A	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
17	A	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
17	A	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
17	A	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
17	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
17	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	A	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
17	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
17	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
17	A	1	Total	C	Mg	N	O	0
			63	53	1	4	5	
17	A	1	Total	C	Mg	N	O	0
			45	37	1	4	3	
17	A	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
17	A	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
17	A	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
17	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
17	A	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
17	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	A	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
17	A	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
17	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
17	A	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
17	B	1	Total	C	Mg	N	O	0
			39	31	1	4	3	
17	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
17	B	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
17	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
17	B	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
17	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
17	B	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
17	B	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
17	B	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
17	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
17	B	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
17	B	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
17	B	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
17	B	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
17	B	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
17	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			42	34	1	4	3	

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Mol	Chain	Residues	Atoms					AltConf
17	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
17	B	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
17	F	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
17	F	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
17	J	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
17	K	1	Total	C	Mg	N	O	0
			37	31	1	4	1	
17	K	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
17	K	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
17	K	1	Total	C	Mg	N	O	0
			39	31	1	4	3	
17	L	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
17	L	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
17	L	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
17	L	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
17	1	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
17	1	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
17	1	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
17	1	1	Total	C	Mg	N	O	0
			42	34	1	4	3	

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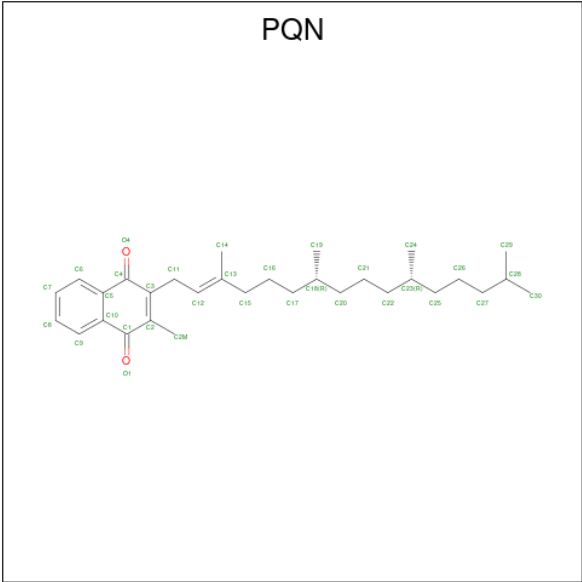
Mol	Chain	Residues	Atoms					AltConf
17	1	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
17	1	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
17	1	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
17	1	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
17	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	1	1	Total	C	Mg	N	O	0
			44	35	1	4	4	
17	2	1	Total	C	Mg	N	O	0
			36	30	1	4	1	
17	2	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
17	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	2	1	Total	C	Mg	N	O	0
			49	41	1	4	3	
17	2	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
17	2	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
17	2	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
17	2	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
17	2	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
17	3	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
17	3	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
17	3	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
17	3	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
17	3	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
17	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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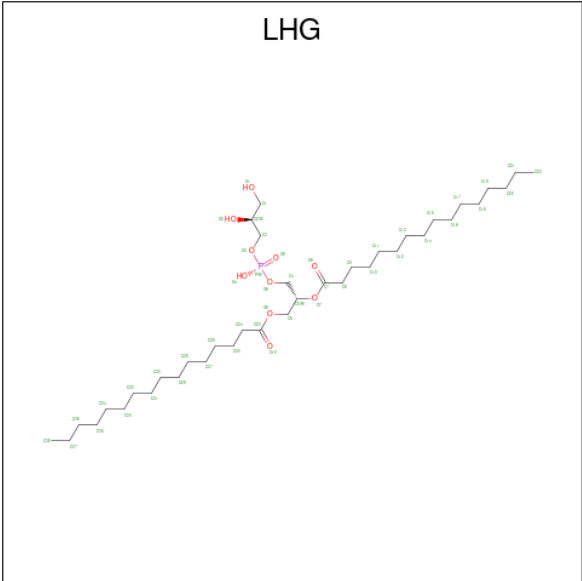
Mol	Chain	Residues	Atoms					AltConf
17	3	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
17	3	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
17	3	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
17	3	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
17	3	1	Total	C	Mg	N	O	0
			37	31	1	4	1	
17	3	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
17	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
17	5	1	Total	C	Mg	N	O	0
			38	30	1	4	3	
17	5	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
17	5	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	5	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
17	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
17	5	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
17	5	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
17	5	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
17	5	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
17	5	1	Total	C	Mg	N	O	0
			41	33	1	4	3	

- Molecule 18 is PHYLLOQUINONE (CCD ID: PQN) (formula: C₃₁H₄₆O₂).



Mol	Chain	Residues	Atoms			AltConf
18	A	1	Total	C	O	0
			33	31	2	
18	B	1	Total	C	O	0
			30	28	2	

- Molecule 19 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$).



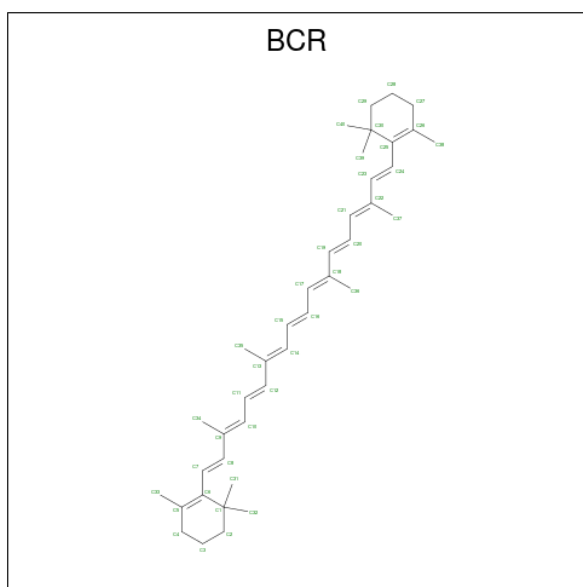
Mol	Chain	Residues	Atoms				AltConf
19	A	1	Total	C	O	P	0
			49	38	10	1	

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Mol	Chain	Residues	Atoms				AltConf
19	A	1	Total	C	O	P	0
			30	19	10	1	
19	B	1	Total	C	O	P	0
			38	27	10	1	
19	1	1	Total	C	O	P	0
			49	38	10	1	
19	2	1	Total	C	O	P	0
			35	24	10	1	

- Molecule 20 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).



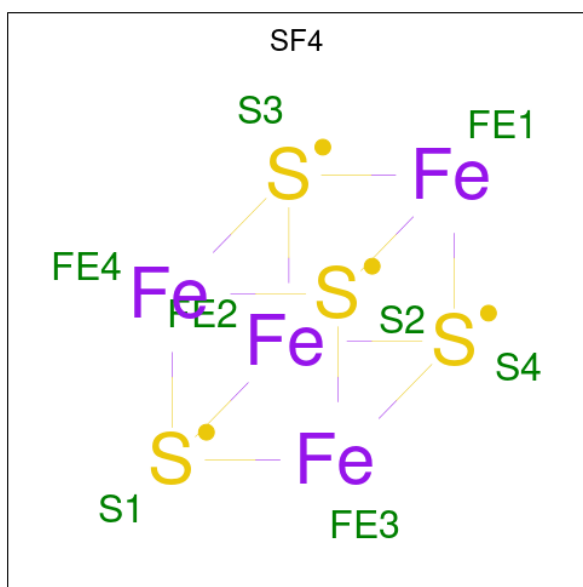
Mol	Chain	Residues	Atoms		AltConf
20	A	1	Total	C	0
			40	40	
20	A	1	Total	C	0
			40	40	
20	A	1	Total	C	0
			40	40	
20	A	1	Total	C	0
			40	40	
20	A	1	Total	C	0
			39	39	
20	A	1	Total	C	0
			40	40	
20	A	1	Total	C	0
			40	40	

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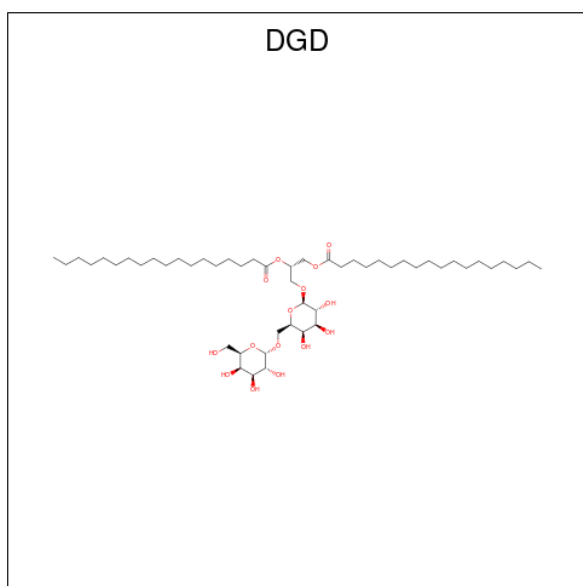
Mol	Chain	Residues	Atoms	AltConf
20	B	1	Total C 40 40	0
20	B	1	Total C 40 40	0
20	B	1	Total C 40 40	0
20	B	1	Total C 40 40	0
20	B	1	Total C 40 40	0
20	B	1	Total C 40 40	0
20	B	1	Total C 40 40	0
20	F	1	Total C 40 40	0
20	F	1	Total C 40 40	0
20	I	1	Total C 40 40	0
20	J	1	Total C 40 40	0
20	K	1	Total C 40 40	0
20	L	1	Total C 40 40	0
20	L	1	Total C 40 40	0
20	1	1	Total C 19 19	0
20	2	1	Total C 40 40	0
20	3	1	Total C 40 40	0
20	5	1	Total C 40 40	0

- Molecule 21 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



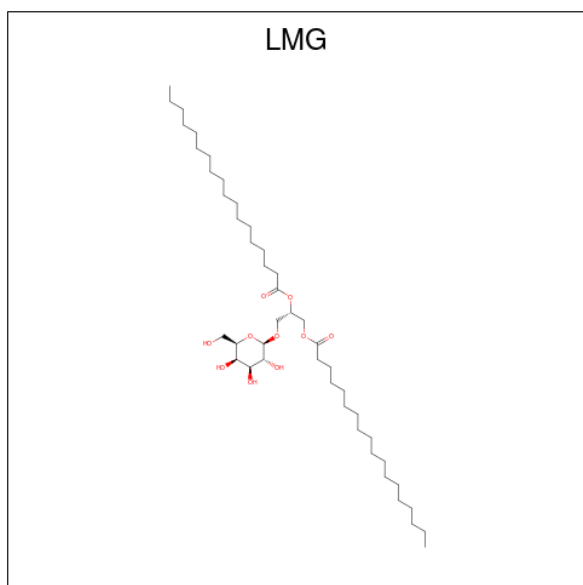
Mol	Chain	Residues	Atoms			AltConf
21	A	1	Total	Fe	S	0
			8	4	4	
21	C	1	Total	Fe	S	0
			8	4	4	
21	C	1	Total	Fe	S	0
			8	4	4	

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



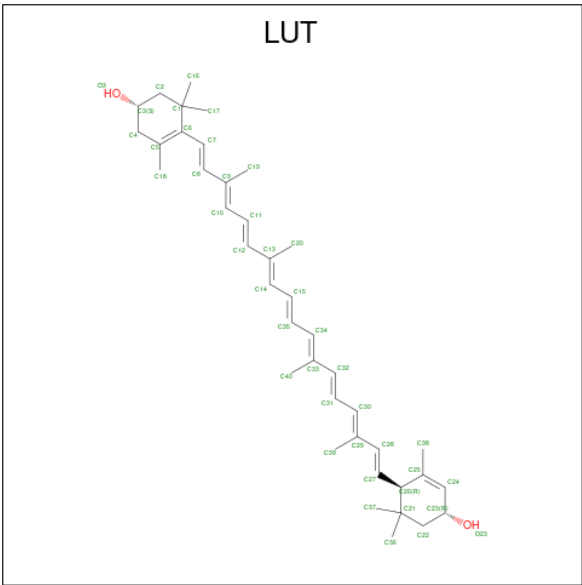
Mol	Chain	Residues	Atoms			AltConf
22	B	1	Total	C	O	0
			59	44	15	
22	J	1	Total	C	O	0
			66	51	15	

- Molecule 23 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



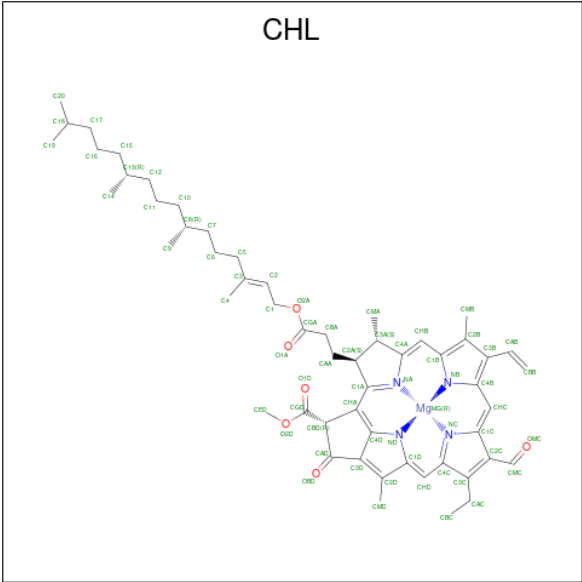
Mol	Chain	Residues	Atoms			AltConf
23	F	1	Total	C	O	0
			30	20	10	
23	F	1	Total	C	O	0
			45	35	10	
23	2	1	Total	C	O	0
			16	9	7	
23	2	1	Total	C	O	0
			36	26	10	
23	5	1	Total	C	O	0
			32	22	10	

- Molecule 24 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (CCD ID: LUT) (formula: $C_{40}H_{56}O_2$).



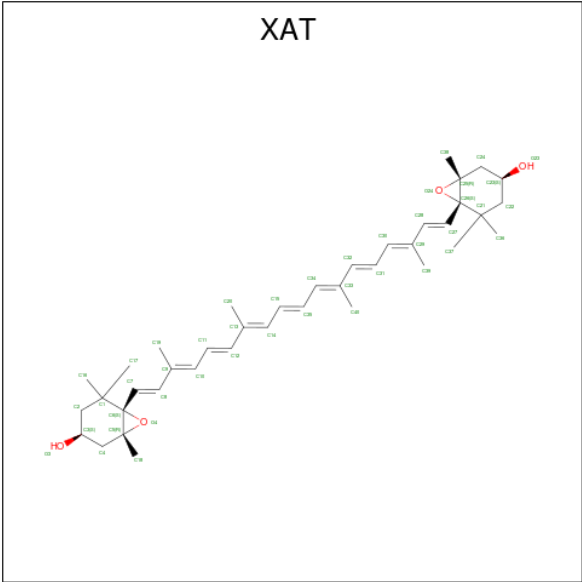
Mol	Chain	Residues	Atoms			AltConf
24	1	1	Total	C	O	0
			42	40	2	
24	1	1	Total	C	O	0
			42	40	2	
24	2	1	Total	C	O	0
			42	40	2	
24	3	1	Total	C	O	0
			42	40	2	
24	3	1	Total	C	O	0
			42	40	2	
24	5	1	Total	C	O	0
			42	40	2	

- Molecule 25 is CHLOROPHYLL B (CCD ID: CHL) (formula: C₅₅H₇₀MgN₄O₆).



Mol	Chain	Residues	Atoms					AltConf
25	1	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
25	1	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
25	1	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
25	2	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
25	2	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
25	2	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
25	2	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
25	3	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
25	3	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
25	5	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
25	5	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
25	5	1	Total	C	Mg	N	O	0
			40	31	1	4	4	

- Molecule 26 is (3S,5R,6S,3'S,5'R,6'S)-5,6,5',6'-DIEPOXY-5,6,5',6'- TETRAHYDRO-BETA ,BETA-CAROTENE-3,3'-DIOL (CCD ID: XAT) (formula: C₄₀H₅₆O₄).

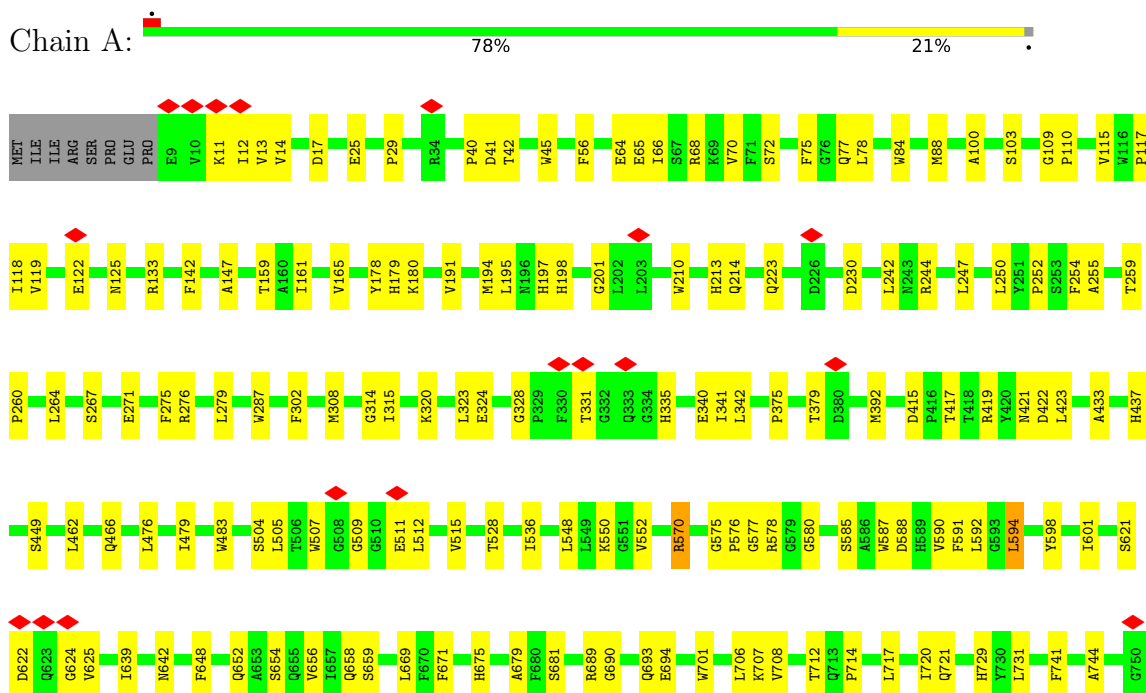


Mol	Chain	Residues	Atoms			AltConf
26	2	1	Total	C	O	0
			44	40	4	
26	5	1	Total	C	O	0
			44	40	4	

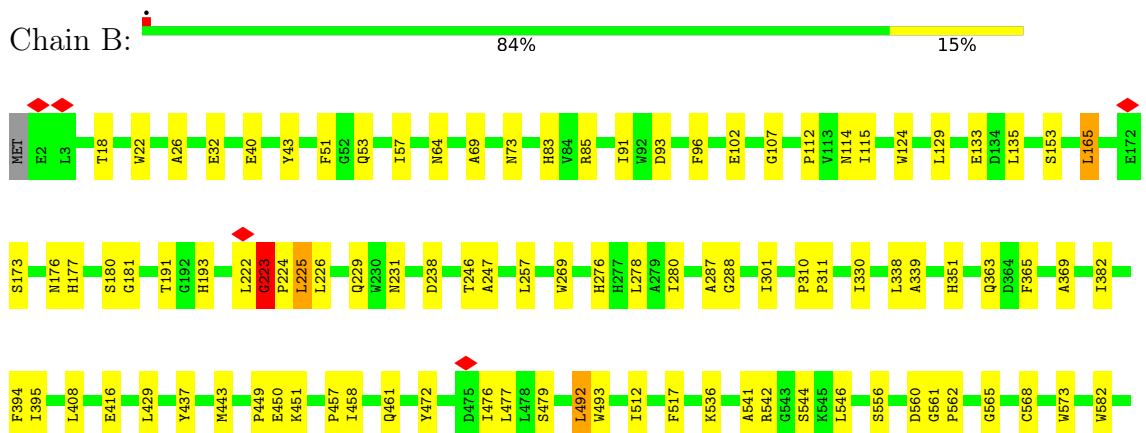
3 Residue-property plots

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

- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

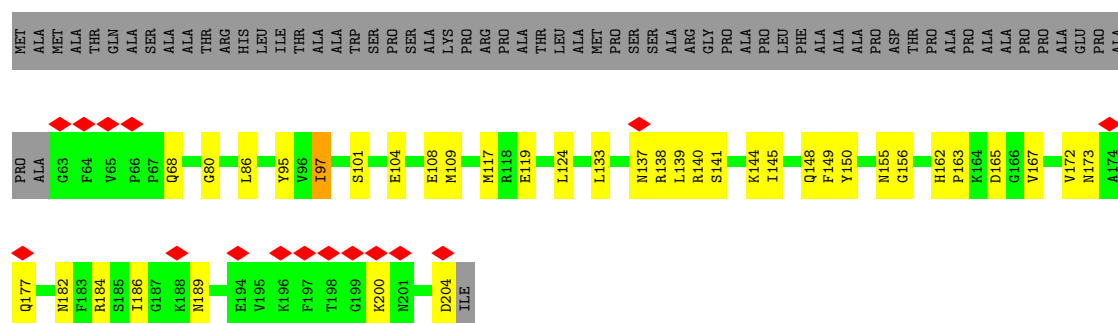




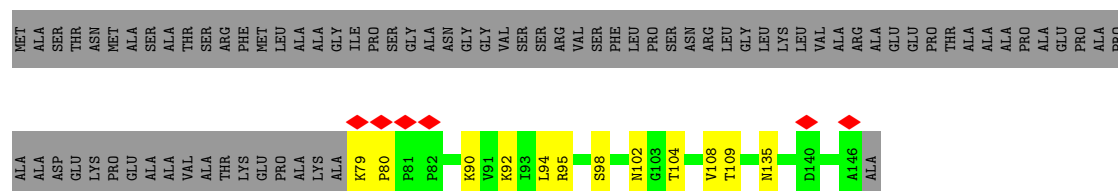
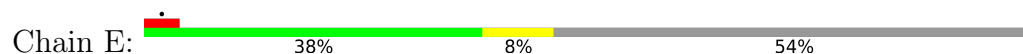
• Molecule 3: Photosystem I iron-sulfur center



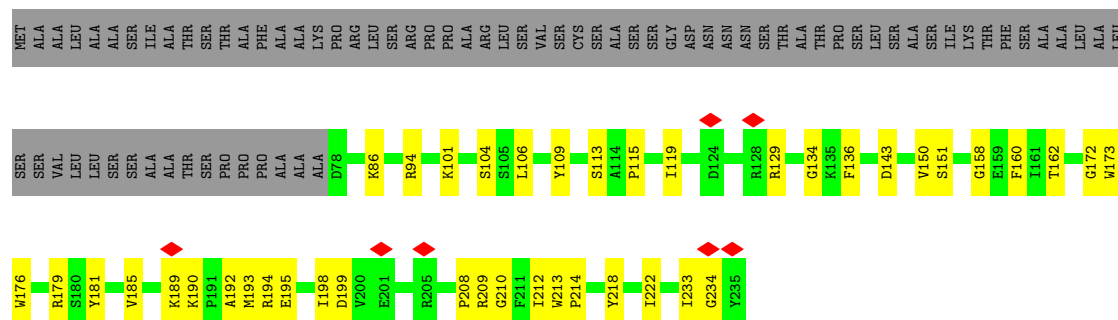
• Molecule 4: Photosystem I reaction center subunit II, chloroplastic



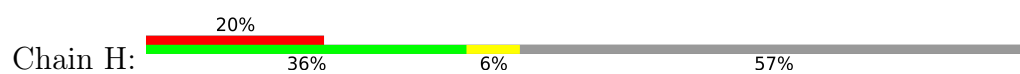
• Molecule 5: Photosystem I reaction center subunit IV, chloroplastic



• Molecule 6: Photosystem I reaction center subunit III, chloroplastic



• Molecule 7: Photosystem I reaction center subunit VI, chloroplastic



MET ALA SER LEU VAL ALA VAL GLN PRO ALA ALA VAL LYS LEU GLY ASP ILE SER SER ILE GLY ARG LYS LEU ALA VAL ARG PRO SER SER ALA VAL SER SER THR ARG ALA ALA GLY ALA VAL VAL ALA LYS TYR GLY LYS SER TYR PHE ASP ASP



- Molecule 8: Photosystem I reaction center subunit VIII

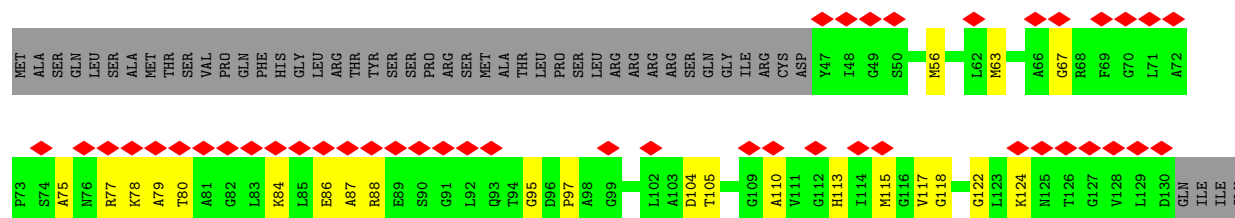


MET THR ASP LEU N3 S6 L11 L14 V15 F16 P17 A18 I19 T22 K32 ILE VAL

- Molecule 9: Photosystem I reaction center subunit IX



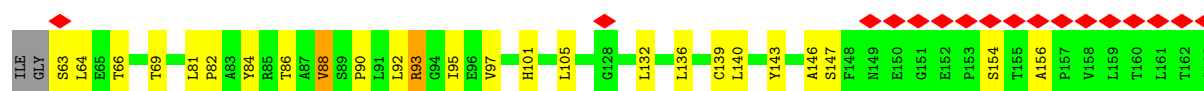
- Molecule 10: Photosystem I reaction center subunit psaK, chloroplastic



- Molecule 11: Photosystem I reaction center subunit XI, chloroplastic

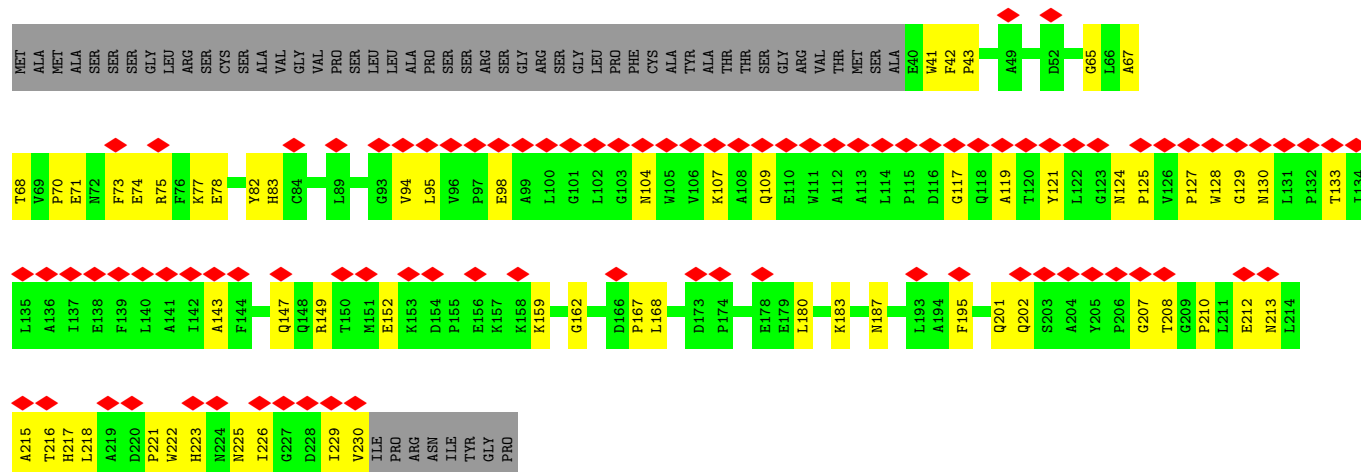


MET ALA THR ALA TYR ALA PRO MET MET SER GLN VAL MET LYS GLY LEU ALA CYS SER LYS PRO ARG GLY MET SER GLY ALA SER LEU THR ARG ARG PRO ARG ARG PHE VAL VAL LYS ALA VAL LYS ASP LYS ASP PRO LYS THR TYR GLN VAL VAL GLN PRO ILE ASN GLY ASP PRO PHE

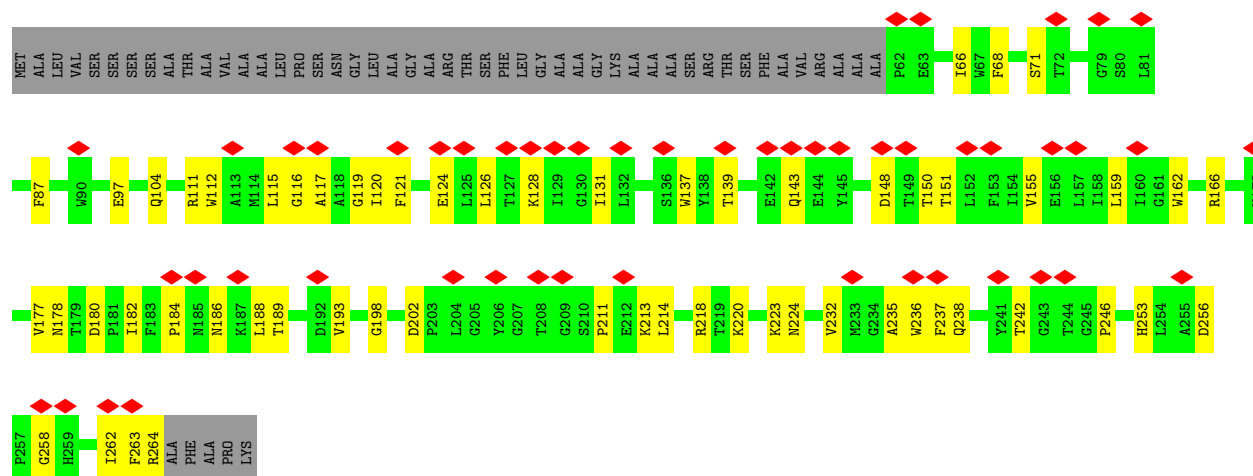




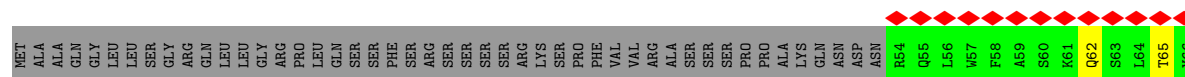
• Molecule 12: Chlorophyll a-b binding protein Lhca1

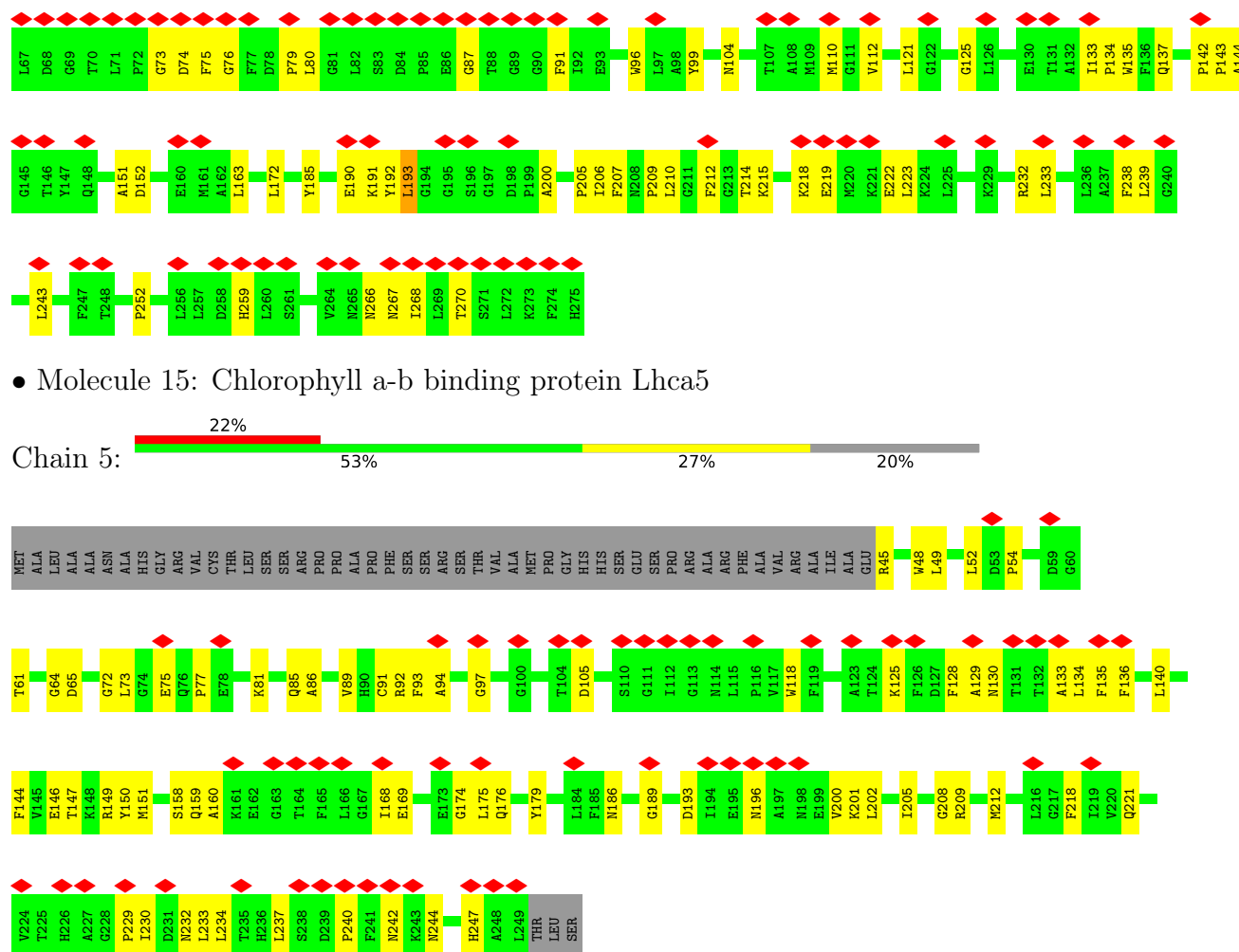


• Molecule 13: Chlorophyll a-b binding protein, chloroplastic



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





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	103844	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 ($e^-/\text{\AA}^2$)	50	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	5.056	Depositor
Minimum map value	-2.079	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.082	Depositor
Recommended contour level	0.72	Depositor
Map size (Å)	575.08, 575.08, 575.08	wwPDB
Map dimensions	440, 440, 440	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.307, 1.307, 1.307	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.64	0/6010	0.42	0/8202
2	B	0.66	0/6058	0.45	3/8273 (0.0%)
3	C	0.65	0/621	0.49	0/840
4	D	0.53	0/1142	0.52	0/1542
5	E	0.52	0/551	0.44	0/751
6	F	0.54	0/1229	0.42	0/1664
7	H	0.34	0/467	0.38	0/631
8	I	0.53	0/238	0.41	0/324
9	J	0.58	0/343	0.59	2/467 (0.4%)
10	K	0.38	0/571	0.43	0/775
11	L	0.51	0/1120	0.42	0/1534
12	1	0.28	0/1467	0.37	0/2008
13	2	0.36	0/1616	0.39	0/2215
14	3	0.34	0/1682	0.43	0/2295
15	5	0.40	0/1527	0.49	1/2085 (0.0%)
All	All	0.55	0/24642	0.44	6/33606 (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

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	223	GLY	CA-C-N	8.07	129.93	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	223	GLY	C-N-CA	8.07	129.93	119.84
15	5	61	THR	N-CA-C	-7.20	106.42	114.62
2	B	223	GLY	N-CA-C	-5.92	100.26	112.34
9	J	34	PRO	O-C-N	-5.63	116.27	123.14
9	J	35	ASP	N-CA-CB	5.09	119.10	110.49

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	222	LEU	Mainchain

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	5813	0	5633	125	0
2	B	5849	0	5600	94	0
3	C	610	0	597	23	0
4	D	1113	0	1113	32	0
5	E	538	0	537	8	0
6	F	1203	0	1199	42	0
7	H	454	0	487	7	0
8	I	232	0	254	5	0
9	J	333	0	347	11	0
10	K	565	0	557	19	0
11	L	1088	0	1079	29	0
12	1	1422	0	1324	52	0
13	2	1561	0	1485	59	0
14	3	1629	0	1496	43	0
15	5	1486	0	1389	59	0
16	A	61	0	62	2	0
17	1	471	0	375	29	0
17	2	454	0	383	20	0
17	3	590	0	442	24	0
17	5	468	0	375	17	0
17	A	2024	0	1724	52	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	B	2118	0	1848	66	0
17	F	83	0	60	3	0
17	J	42	0	31	2	0
17	K	157	0	107	6	0
17	L	193	0	152	6	0
18	A	33	0	46	2	0
18	B	30	0	37	1	0
19	1	49	0	74	5	0
19	2	35	0	40	2	0
19	A	79	0	104	7	0
19	B	38	0	46	0	0
20	1	19	0	26	3	0
20	2	40	0	56	4	0
20	3	40	0	56	4	0
20	5	40	0	56	5	0
20	A	279	0	389	18	0
20	B	280	0	392	19	0
20	F	80	0	112	4	0
20	I	40	0	56	4	0
20	J	40	0	56	1	0
20	K	40	0	56	2	0
20	L	80	0	112	10	0
21	A	8	0	0	0	0
21	C	16	0	0	1	0
22	B	59	0	79	4	0
22	J	66	0	96	3	0
23	2	52	0	55	3	0
23	5	32	0	34	1	0
23	F	75	0	90	3	0
24	1	84	0	112	11	0
24	2	42	0	56	8	0
24	3	84	0	112	12	0
24	5	42	0	56	8	0
25	1	129	0	83	5	0
25	2	174	0	110	13	0
25	3	90	0	60	1	0
25	5	133	0	80	8	0
26	2	44	0	56	7	0
26	5	44	0	56	5	0
All	All	32973	0	31505	768	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 12.

All (768) 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)
6:F:181:TYR:CE1	6:F:185:VAL:CG1	2.51	0.92
6:F:181:TYR:HE1	6:F:185:VAL:CG1	1.82	0.92
6:F:181:TYR:CE1	6:F:185:VAL:HG11	2.07	0.88
6:F:181:TYR:CE1	6:F:185:VAL:HG13	2.18	0.78
2:B:124:TRP:CZ2	2:B:124:TRP:CD2	2.75	0.74
10:K:95:GLY:C	17:K:201:CLA:H3A	2.13	0.73
15:5:129:ALA:HB1	15:5:134:LEU:HD11	1.71	0.73
2:B:26:ALA:HB2	22:B:850:DGD:HA42	1.72	0.71
17:A:821:CLA:HAA2	10:K:79:ALA:HB3	1.73	0.71
9:J:10:VAL:HG13	9:J:12:PRO:HD2	1.72	0.71
5:E:92:LYS:NZ	5:E:102:ASN:OD1	2.23	0.70
14:3:219:GLU:O	14:3:223:LEU:N	2.24	0.70
12:1:128:TRP:HE1	17:1:515:CLA:CAD	2.06	0.69
12:1:83:HIS:HD2	24:1:502:LUT:H35	1.58	0.69
13:2:186:ASN:HB3	25:2:516:CHL:C1D	2.23	0.68
11:L:156:ALA:HB2	11:L:172:GLN:HG3	1.76	0.68
4:D:104:GLU:N	4:D:104:GLU:OE1	2.27	0.68
15:5:135:PHE:HB2	25:5:314:CHL:HBC1	1.75	0.67
14:3:112:VAL:HG11	24:3:303:LUT:H12	1.77	0.66
17:B:807:CLA:H51	22:B:850:DGD:HB71	1.76	0.66
12:1:67:ALA:HB1	12:1:73:PHE:HD1	1.60	0.66
1:A:570:ARG:NH2	19:A:843:LHG:O10	2.29	0.66
1:A:40:PRO:HG2	6:F:192:ALA:HB1	1.77	0.66
6:F:181:TYR:HE1	6:F:185:VAL:HG11	1.48	0.66
17:B:826:CLA:HMA1	20:B:848:BCR:H14C	1.78	0.65
14:3:209:PRO:HD2	24:3:303:LUT:H23	1.79	0.65
1:A:264:LEU:HD21	10:K:117:VAL:HG22	1.78	0.65
11:L:88:VAL:HG23	11:L:93:ARG:HD3	1.78	0.65
12:1:98:GLU:HG2	12:1:104:ASN:HA	1.79	0.65
2:B:476:ILE:HG22	2:B:477:LEU:H	1.62	0.64
15:5:48:TRP:H	15:5:48:TRP:CD1	2.15	0.64
15:5:118:TRP:HE1	15:5:229:PRO:HD3	1.63	0.64
17:B:823:CLA:HAB	17:B:842:CLA:HED1	1.80	0.64
12:1:149:ARG:HA	17:1:513:CLA:HBC3	1.80	0.64
1:A:275:PHE:HE2	17:A:817:CLA:HBB1	1.63	0.64
17:A:806:CLA:H41	19:A:843:LHG:H271	1.80	0.64
25:1:517:CHL:HED1	15:5:147:THR:HB	1.79	0.64
2:B:238:ASP:HB2	2:B:269:TRP:HZ3	1.62	0.63
12:1:229:ILE:HG13	12:1:230:VAL:H	1.63	0.63
4:D:167:VAL:HG21	4:D:173:ASN:HD21	1.64	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:1:119:ALA:H	12:1:129:GLY:HA3	1.63	0.63
13:2:186:ASN:HB3	25:2:516:CHL:C2D	2.29	0.63
1:A:314:GLY:HA2	10:K:88:ARG:HH22	1.63	0.63
22:J:103:DGD:O5E	22:J:103:DGD:O4E	2.09	0.63
12:1:183:LYS:O	12:1:187:ASN:ND2	2.24	0.63
1:A:341:ILE:HG22	1:A:419:ARG:HB3	1.79	0.63
2:B:339:ALA:HB2	20:B:848:BCR:H372	1.79	0.63
10:K:63:MET:HE1	10:K:115:MET:HB2	1.79	0.63
13:2:258:GLY:HA3	14:3:151:ALA:HA	1.81	0.62
14:3:268:ILE:HD11	17:3:308:CLA:H11	1.81	0.62
24:3:303:LUT:O23	17:3:306:CLA:O1A	2.16	0.62
1:A:117:PRO:HB3	1:A:122:GLU:HB3	1.79	0.62
1:A:694:GLU:OE1	2:B:536:LYS:NZ	2.29	0.62
17:B:805:CLA:HBC3	17:B:830:CLA:H41	1.82	0.62
15:5:209:ARG:NH1	17:5:308:CLA:O2D	2.33	0.62
2:B:223:GLY:O	2:B:226:LEU:N	2.33	0.61
2:B:124:TRP:HB3	2:B:129:LEU:HD12	1.81	0.61
1:A:65:GLU:N	1:A:65:GLU:OE1	2.33	0.61
2:B:330:ILE:HG21	17:B:806:CLA:HAC1	1.83	0.61
15:5:85:GLN:OE1	15:5:85:GLN:N	2.34	0.61
15:5:176:GLN:NE2	15:5:193:ASP:O	2.35	0.60
6:F:213:TRP:CD1	6:F:214:PRO:HD3	2.37	0.60
13:2:104:GLN:HE21	13:2:193:VAL:HG12	1.65	0.60
1:A:331:THR:HG21	19:A:844:LHG:HC11	1.82	0.60
13:2:166:ARG:NH2	13:2:177:VAL:O	2.34	0.60
2:B:133:GLU:N	2:B:133:GLU:OE1	2.34	0.59
14:3:112:VAL:HG11	24:3:303:LUT:H10	1.84	0.59
15:5:212:MET:HE1	17:5:308:CLA:HAB	1.84	0.59
17:A:802:CLA:CGA	17:A:802:CLA:H3A	2.32	0.59
2:B:721:TYR:HB2	17:B:803:CLA:HED3	1.83	0.59
13:2:220:LYS:O	13:2:224:ASN:ND2	2.31	0.59
1:A:244:ARG:NH2	1:A:255:ALA:O	2.36	0.59
2:B:191:THR:HG21	2:B:278:LEU:HB2	1.85	0.58
2:B:85:ARG:HB3	2:B:115:ILE:HD12	1.85	0.58
1:A:656:VAL:HG21	1:A:741:PHE:HA	1.85	0.58
1:A:656:VAL:HG22	1:A:744:ALA:HB3	1.85	0.58
12:1:229:ILE:HG13	12:1:230:VAL:N	2.18	0.58
1:A:279:LEU:HG	1:A:505:LEU:HD23	1.85	0.58
17:A:815:CLA:HED2	17:A:815:CLA:H2A	1.85	0.58
2:B:257:LEU:HD21	2:B:493:TRP:HE3	1.67	0.58
5:E:108:VAL:HG23	5:E:109:THR:HG22	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:I:3:ASN:O	8:I:6:SER:OG	2.21	0.58
3:C:62:PHE:O	3:C:63:LEU:HG	2.03	0.58
1:A:267:SER:O	1:A:267:SER:OG	2.17	0.57
17:A:838:CLA:H91	17:F:802:CLA:HBC3	1.85	0.57
3:C:1:MET:N	3:C:45:THR:OG1	2.37	0.57
6:F:190:LYS:HE2	6:F:193:MET:HG2	1.85	0.57
13:2:139:THR:O	13:2:143:GLN:NE2	2.32	0.57
17:B:818:CLA:H8	17:B:835:CLA:H11	1.85	0.57
15:5:75:GLU:N	15:5:75:GLU:OE1	2.37	0.57
20:A:845:BCR:H383	20:A:853:BCR:H10C	1.86	0.57
15:5:240:PRO:O	15:5:244:ASN:ND2	2.38	0.57
1:A:75:PHE:CZ	17:3:301:CLA:HBB1	2.40	0.57
1:A:476:LEU:HB2	1:A:528:THR:HG23	1.87	0.57
1:A:466:GLN:OE1	1:A:466:GLN:N	2.36	0.57
6:F:106:LEU:HB2	6:F:119:ILE:HG21	1.87	0.57
4:D:155:ASN:OD1	4:D:156:GLY:N	2.38	0.56
4:D:162:HIS:HB3	4:D:163:PRO:HD3	1.87	0.56
17:3:308:CLA:CGA	17:3:308:CLA:HBD	2.35	0.56
13:2:166:ARG:CZ	25:2:516:CHL:HMC	2.35	0.56
17:A:840:CLA:HBB2	20:L:305:BCR:H372	1.87	0.56
2:B:83:HIS:HA	7:H:143:ILE:HB	1.86	0.56
17:L:302:CLA:C1B	17:L:303:CLA:HED1	2.35	0.56
19:2:517:LHG:HC91	19:2:517:LHG:H281	1.87	0.56
15:5:196:ASN:O	15:5:200:VAL:N	2.30	0.56
4:D:68:GLN:HB3	4:D:150:TYR:OH	2.06	0.56
11:L:82:PRO:O	11:L:93:ARG:NH1	2.38	0.56
24:1:501:LUT:H32	17:1:504:CLA:CAB	2.36	0.56
14:3:79:PRO:HD2	24:3:304:LUT:H23	1.87	0.56
1:A:64:GLU:OE2	1:A:68:ARG:NH2	2.38	0.56
15:5:234:LEU:HD23	15:5:237:LEU:HD21	1.87	0.56
17:2:509:CLA:H12	25:2:515:CHL:CAD	2.35	0.56
23:5:301:LMG:O5	23:5:301:LMG:O4	2.23	0.56
13:2:115:LEU:O	13:2:119:GLY:N	2.38	0.56
1:A:507:TRP:O	1:A:509:GLY:N	2.38	0.56
15:5:91:CYS:HB2	15:5:208:GLY:HA3	1.88	0.56
15:5:233:LEU:HD23	15:5:237:LEU:HD23	1.88	0.56
1:A:247:LEU:HB3	1:A:254:PHE:HD2	1.70	0.55
1:A:717:LEU:HD23	1:A:721:GLN:HG2	1.88	0.55
6:F:173:TRP:CD1	6:F:210:GLY:HA3	2.41	0.55
12:1:82:TYR:CE1	17:1:513:CLA:HMD1	2.41	0.55
19:1:516:LHG:H241	25:1:517:CHL:C1C	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:B:812:CLA:O1D	17:B:812:CLA:H2A	2.06	0.55
1:A:585:SER:OG	1:A:588:ASP:OD2	2.25	0.55
15:5:218:PHE:HE1	24:5:303:LUT:H41	1.70	0.55
6:F:198:ILE:O	9:J:9:SER:OG	2.25	0.55
4:D:137:ASN:OD1	4:D:140:ARG:NH2	2.25	0.55
12:1:217:HIS:HB2	17:1:506:CLA:HAA2	1.90	0.55
15:5:125:LYS:HE3	15:5:129:ALA:H	1.72	0.55
11:L:136:LEU:HD13	20:L:305:BCR:H401	1.88	0.54
15:5:169:GLU:OE1	15:5:169:GLU:N	2.39	0.54
16:A:801:CL0:H13	17:B:802:CLA:OBD	2.08	0.54
15:5:221:GLN:HB3	15:5:232:ASN:ND2	2.21	0.54
13:2:121:PHE:CE2	24:2:501:LUT:H28	2.43	0.54
1:A:276:ARG:HD2	1:A:287:TRP:CD1	2.42	0.54
17:3:313:CLA:C1B	17:3:313:CLA:H2	2.38	0.54
19:1:516:LHG:H162	19:1:516:LHG:H282	1.89	0.54
13:2:214:LEU:O	13:2:218:ARG:N	2.27	0.54
2:B:18:THR:HG23	2:B:696:LYS:O	2.08	0.54
14:3:267:ASN:OD1	14:3:270:THR:OG1	2.26	0.54
1:A:11:LYS:HG3	1:A:13:VAL:HG23	1.90	0.54
17:A:831:CLA:O1D	17:A:831:CLA:H2A	2.08	0.53
4:D:108:GLU:OE2	4:D:138:ARG:NH1	2.41	0.53
13:2:180:ASP:HB2	13:2:186:ASN:HB2	1.89	0.53
14:3:73:GLY:O	14:3:232:ARG:NH2	2.38	0.53
17:L:304:CLA:HBC3	17:L:304:CLA:HHD	1.89	0.53
2:B:450:GLU:OE2	6:F:129:ARG:NH2	2.30	0.53
1:A:133:ARG:NH1	6:F:109:TYR:OH	2.41	0.53
2:B:73:ASN:ND2	2:B:107:GLY:O	2.27	0.53
14:3:135:TRP:CD1	14:3:252:PRO:HG3	2.44	0.53
17:5:308:CLA:HBB1	17:5:308:CLA:HMB3	1.90	0.53
4:D:80:GLY:C	11:L:64:LEU:HD21	2.34	0.53
1:A:392:MET:HG3	1:A:601:ILE:HD12	1.91	0.53
11:L:199:LEU:HD13	17:L:304:CLA:HED2	1.89	0.53
1:A:588:ASP:HA	1:A:591:PHE:HB3	1.89	0.53
17:B:816:CLA:HBC3	20:B:844:BCR:H391	1.90	0.53
4:D:141:SER:O	4:D:144:LYS:NZ	2.41	0.53
12:1:167:PRO:HD2	24:1:501:LUT:H23	1.91	0.53
24:5:303:LUT:H3	17:5:307:CLA:HMA2	1.91	0.53
1:A:275:PHE:CE2	17:A:817:CLA:HBB1	2.44	0.53
1:A:504:SER:OG	1:A:505:LEU:N	2.40	0.53
17:B:811:CLA:HHC	17:B:811:CLA:HBB1	1.90	0.53
12:1:43:PRO:HD2	25:1:517:CHL:O1D	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:61:ASP:HA	5:E:135:ASN:HD22	1.73	0.53
15:5:92:ARG:NH1	25:5:315:CHL:OBD	2.40	0.53
14:3:62:GLN:O	14:3:65:THR:OG1	2.27	0.52
2:B:363:GLN:OE1	2:B:363:GLN:N	2.42	0.52
1:A:210:TRP:NE1	1:A:214:GLN:OE1	2.42	0.52
16:A:801:CL0:CMB	17:B:802:CLA:OBD	2.57	0.52
2:B:338:LEU:HD22	2:B:382:ILE:HG23	1.90	0.52
15:5:174:GLY:HA3	15:5:179:TYR:O	2.10	0.52
17:A:803:CLA:C4D	9:J:12:PRO:HG3	2.40	0.52
12:1:82:TYR:HE1	17:1:513:CLA:HMD1	1.73	0.52
12:1:202:GLN:OE1	12:1:207:GLY:N	2.41	0.52
17:5:310:CLA:H12	25:5:317:CHL:C3D	2.40	0.52
13:2:258:GLY:O	14:3:152:ASP:N	2.30	0.52
15:5:158:SER:O	15:5:158:SER:OG	2.22	0.52
17:A:810:CLA:HBB1	17:A:810:CLA:HMB3	1.91	0.52
17:B:822:CLA:H11	20:B:844:BCR:HC22	1.92	0.52
2:B:582:TRP:CH2	17:B:802:CLA:HAB	2.45	0.52
13:2:111:ARG:HH11	25:2:513:CHL:CAD	2.23	0.52
4:D:109:MET:HE1	4:D:124:LEU:HD21	1.91	0.51
6:F:86:LYS:HB3	6:F:134:GLY:O	2.10	0.51
1:A:25:GLU:HB2	17:A:810:CLA:HAA2	1.91	0.51
25:5:315:CHL:HHC	25:5:315:CHL:HBB1	1.90	0.51
12:1:143:ALA:O	12:1:147:GLN:N	2.41	0.51
17:B:806:CLA:HMB1	17:B:806:CLA:HBB1	1.91	0.51
24:3:303:LUT:H26	17:3:306:CLA:H12	1.92	0.51
2:B:449:PRO:HG2	6:F:94:ARG:HH11	1.75	0.51
2:B:658:ALA:HB3	17:B:804:CLA:HBB2	1.93	0.51
17:B:808:CLA:HAA2	17:B:810:CLA:HED1	1.92	0.51
20:I:101:BCR:H382	20:I:101:BCR:H23C	1.93	0.51
11:L:203:ASP:OD1	11:L:203:ASP:N	2.43	0.51
13:2:162:TRP:CH2	20:2:503:BCR:H321	2.46	0.51
17:3:314:CLA:O1D	17:3:314:CLA:H2A	2.11	0.51
1:A:340:GLU:OE1	1:A:340:GLU:N	2.42	0.51
17:3:311:CLA:H2A	17:3:311:CLA:HED2	1.93	0.51
4:D:184:ARG:NH1	4:D:189:ASN:OD1	2.40	0.51
13:2:104:GLN:NE2	13:2:193:VAL:HG12	2.25	0.51
17:3:314:CLA:C1B	17:3:314:CLA:H52	2.41	0.51
2:B:394:PHE:O	2:B:542:ARG:NH1	2.44	0.51
2:B:461:GLN:HG2	2:B:472:TYR:CZ	2.46	0.51
2:B:556:SER:HG	2:B:573:TRP:CG	2.29	0.51
12:1:195:PHE:CE2	24:1:502:LUT:H34	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:3:214:THR:HG23	14:3:215:LYS:H	1.75	0.51
2:B:369:ALA:HB1	2:B:725:LEU:HD11	1.92	0.51
2:B:658:ALA:O	17:B:804:CLA:HAB	2.11	0.51
6:F:101:LYS:O	6:F:104:SER:OG	2.20	0.51
25:2:513:CHL:HHC	25:2:513:CHL:HBB1	1.92	0.51
12:1:221:PRO:O	12:1:225:ASN:ND2	2.44	0.50
15:5:105:ASP:HB3	15:5:230:ILE:HD12	1.93	0.50
1:A:415:ASP:OD1	1:A:417:THR:OG1	2.28	0.50
25:2:515:CHL:HBA2	25:2:515:CHL:HBD	1.92	0.50
15:5:233:LEU:HD12	24:5:303:LUT:H163	1.92	0.50
17:A:827:CLA:C4A	17:A:827:CLA:HBA2	2.41	0.50
4:D:97:ILE:HG13	4:D:148:GLN:O	2.12	0.50
20:A:851:BCR:H331	17:J:101:CLA:HBC3	1.93	0.50
17:F:802:CLA:C4B	9:J:22:LEU:HD21	2.41	0.50
17:1:507:CLA:H2A	17:1:507:CLA:HED2	1.94	0.50
19:1:516:LHG:H241	25:1:517:CHL:NC	2.26	0.50
1:A:656:VAL:O	1:A:659:SER:OG	2.26	0.50
2:B:32:GLU:OE1	2:B:32:GLU:N	2.44	0.50
15:5:179:TYR:HB3	17:5:305:CLA:O1D	2.11	0.50
17:B:820:CLA:HMB2	17:B:825:CLA:HMA3	1.93	0.50
13:2:116:GLY:HA2	26:2:502:XAT:H161	1.94	0.50
1:A:56:PHE:CD2	17:A:805:CLA:HMC2	2.47	0.50
15:5:144:PHE:CE2	20:5:302:BCR:H12C	2.47	0.50
1:A:331:THR:HB	1:A:423:LEU:HD21	1.94	0.50
3:C:52:LYS:HE3	3:C:67:VAL:HB	1.94	0.50
6:F:218:TYR:CZ	6:F:222:ILE:HD11	2.47	0.50
14:3:193:LEU:HD12	25:3:315:CHL:CMC	2.41	0.50
17:A:816:CLA:CHD	17:A:817:CLA:HBB2	2.42	0.50
17:A:838:CLA:HAB	17:A:838:CLA:H122	1.93	0.49
13:2:246:PRO:O	24:2:501:LUT:O23	2.26	0.49
14:3:210:LEU:HD23	14:3:212:PHE:HE1	1.77	0.49
1:A:230:ASP:N	1:A:230:ASP:OD1	2.45	0.49
1:A:421:ASN:OD1	1:A:422:ASP:N	2.45	0.49
6:F:172:GLY:O	6:F:176:TRP:N	2.31	0.49
13:2:182:ILE:O	13:2:184:PRO:HD3	2.12	0.49
24:3:303:LUT:C15	17:3:307:CLA:HBB1	2.41	0.49
2:B:560:ASP:OD1	3:C:52:LYS:NZ	2.45	0.49
4:D:95:TYR:HD2	4:D:150:TYR:O	1.94	0.49
2:B:301:ILE:HG23	17:B:820:CLA:HED2	1.95	0.49
6:F:194:ARG:HH21	6:F:199:ASP:HB2	1.77	0.49
1:A:320:LYS:NZ	1:A:324:GLU:OE2	2.33	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:177:HIS:O	2:B:181:GLY:N	2.43	0.49
7:H:88:PHE:CG	11:L:95:ILE:HD13	2.48	0.49
12:1:78:GLU:HG2	12:1:82:TYR:CE2	2.47	0.49
13:2:236:TRP:CZ3	25:2:512:CHL:HHB	2.47	0.49
14:3:137:GLN:HG2	14:3:144:ALA:O	2.12	0.49
1:A:147:ALA:HB2	1:A:375:PRO:HD2	1.94	0.49
17:A:820:CLA:HMB1	17:A:820:CLA:HBB1	1.94	0.49
2:B:91:ILE:HB	2:B:112:PRO:HB2	1.95	0.49
2:B:276:HIS:CE1	2:B:280:ILE:HD13	2.46	0.49
22:B:850:DGD:O1B	22:B:850:DGD:HB42	2.13	0.49
13:2:112:TRP:CD1	17:2:514:CLA:HMD3	2.48	0.49
13:2:202:ASP:OD1	17:2:504:CLA:HBD	2.12	0.49
13:2:263:PHE:C	13:2:264:ARG:HD3	2.38	0.49
2:B:43:TYR:CZ	2:B:330:ILE:HD11	2.47	0.49
2:B:687:LEU:HD23	11:L:84:TYR:HE1	1.77	0.49
20:1:503:BCR:H333	17:1:509:CLA:C1B	2.43	0.49
15:5:97:GLY:HA2	26:5:304:XAT:H181	1.95	0.49
1:A:72:SER:OG	1:A:178:TYR:HB2	2.13	0.48
10:K:77:ARG:HA	10:K:87:ALA:HA	1.94	0.48
14:3:266:ASN:HD21	17:3:313:CLA:HED3	1.78	0.48
1:A:328:GLY:HA3	19:A:844:LHG:HC32	1.94	0.48
2:B:694:ARG:NH1	11:L:146:ALA:O	2.46	0.48
1:A:110:PRO:HB3	1:A:142:PHE:CD2	2.48	0.48
2:B:180:SER:HB3	2:B:288:GLY:HA3	1.95	0.48
3:C:28:MET:HB3	4:D:172:VAL:HG12	1.95	0.48
13:2:66:ILE:HG22	13:2:68:PHE:H	1.77	0.48
13:2:87:PHE:HE2	26:2:502:XAT:H383	1.77	0.48
13:2:112:TRP:HD1	17:2:514:CLA:HMD3	1.78	0.48
2:B:351:HIS:ND1	17:B:818:CLA:OBD	2.47	0.48
20:A:846:BCR:H341	20:A:846:BCR:H11C	1.73	0.48
2:B:687:LEU:HD21	11:L:81:LEU:HD11	1.95	0.48
13:2:120:ILE:O	13:2:124:GLU:HG2	2.13	0.48
17:A:836:CLA:HHC	17:A:836:CLA:HBB1	1.96	0.48
3:C:32:ASP:OD1	3:C:32:ASP:N	2.45	0.48
13:2:117:ALA:HB1	24:2:501:LUT:H32	1.96	0.48
1:A:259:THR:HG23	1:A:260:PRO:HD3	1.94	0.48
1:A:577:GLY:O	1:A:580:GLY:N	2.39	0.48
22:J:103:DGD:HO4E	22:J:103:DGD:HO5E	1.60	0.48
13:2:166:ARG:NH2	13:2:177:VAL:HG12	2.29	0.48
2:B:93:ASP:HB3	2:B:96:PHE:CD1	2.49	0.48
12:1:71:GLU:OE1	12:1:71:GLU:N	2.38	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:2:211:PRO:C	13:2:213:LYS:H	2.20	0.48
1:A:575:GLY:HA2	2:B:562:PRO:HD3	1.95	0.48
14:3:218:LYS:O	14:3:222:GLU:N	2.30	0.48
20:A:848:BCR:H15C	20:A:848:BCR:H351	1.74	0.47
2:B:457:PRO:HB3	2:B:517:PHE:HB2	1.95	0.47
3:C:43:PRO:HB2	4:D:177:GLN:HE21	1.78	0.47
20:F:801:BCR:C10	17:F:802:CLA:HAB	2.44	0.47
10:K:84:LYS:HB2	17:K:205:CLA:HMD2	1.96	0.47
17:3:306:CLA:H92	17:3:306:CLA:H61	1.74	0.47
1:A:118:ILE:HG13	20:A:851:BCR:H322	1.95	0.47
2:B:684:ARG:HE	11:L:63:SER:HB3	1.78	0.47
17:1:510:CLA:H2A	17:1:510:CLA:O2D	2.14	0.47
3:C:32:ASP:O	3:C:37:LYS:NZ	2.47	0.47
24:1:502:LUT:H383	17:1:509:CLA:C3B	2.45	0.47
17:A:852:CLA:H101	9:J:18:TRP:CZ3	2.49	0.47
15:5:45:ARG:HH21	15:5:54:PRO:HG3	1.79	0.47
20:A:853:BCR:C12	20:K:204:BCR:H333	2.45	0.47
2:B:365:PHE:CD2	2:B:734:GLY:HA2	2.50	0.47
20:B:844:BCR:H351	20:B:844:BCR:H15C	1.60	0.47
12:1:215:ALA:HA	12:1:218:LEU:HB2	1.97	0.47
1:A:118:ILE:HG22	1:A:119:VAL:HG13	1.97	0.47
17:A:803:CLA:H2A	17:A:803:CLA:O2D	2.15	0.47
13:2:236:TRP:HZ3	25:2:512:CHL:HHB	1.80	0.47
20:2:503:BCR:H361	20:2:503:BCR:H21C	1.95	0.47
14:3:185:TYR:HA	14:3:190:GLU:OE2	2.15	0.47
20:5:302:BCR:HC8	20:5:302:BCR:H311	1.96	0.47
2:B:229:GLN:C	2:B:231:ASN:H	2.22	0.47
4:D:104:GLU:OE2	4:D:119:GLU:HB2	2.15	0.47
11:L:105:LEU:HD12	11:L:132:LEU:HD23	1.96	0.47
13:2:97:GLU:OE2	23:2:518:LMG:O2	2.28	0.47
15:5:64:GLY:H	15:5:202:LEU:HD13	1.79	0.47
1:A:223:GLN:HE22	1:A:250:LEU:HD22	1.79	0.47
1:A:340:GLU:HG2	1:A:419:ARG:HH11	1.79	0.47
18:A:841:PQN:H193	18:A:841:PQN:H211	1.70	0.47
2:B:310:PRO:HG3	17:B:842:CLA:HBD	1.97	0.47
2:B:658:ALA:CB	17:B:804:CLA:HBB2	2.44	0.47
4:D:149:PHE:CZ	4:D:162:HIS:HB2	2.50	0.47
6:F:194:ARG:NH2	23:F:805:LMG:O3	2.37	0.47
1:A:195:LEU:HG	17:A:824:CLA:HMD2	1.96	0.47
6:F:181:TYR:O	6:F:181:TYR:CD1	2.67	0.47
1:A:689:ARG:NH2	2:B:565:GLY:O	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:B:818:CLA:H91	17:B:818:CLA:H111	1.71	0.46
11:L:139:CYS:CB	20:L:305:BCR:H19C	2.45	0.46
13:2:159:LEU:HB3	20:2:503:BCR:C15	2.44	0.46
1:A:721:GLN:HB2	19:A:843:LHG:HC42	1.96	0.46
2:B:676:GLU:HG2	3:C:81:TYR:HE1	1.80	0.46
6:F:181:TYR:CD1	6:F:181:TYR:C	2.85	0.46
10:K:118:GLY:HA3	17:K:202:CLA:C2C	2.46	0.46
12:1:167:PRO:HG2	17:1:513:CLA:H122	1.97	0.46
13:2:121:PHE:HE1	13:2:235:ALA:HB2	1.79	0.46
17:B:817:CLA:H2A	17:B:817:CLA:HED3	1.96	0.46
7:H:106:LEU:HD13	8:I:19:ILE:HG12	1.97	0.46
12:1:78:GLU:HB2	12:1:159:LYS:HE2	1.98	0.46
12:1:117:GLY:O	12:1:130:ASN:HA	2.16	0.46
17:2:506:CLA:H192	17:2:506:CLA:H161	1.74	0.46
19:2:517:LHG:H301	19:2:517:LHG:H112	1.97	0.46
20:3:305:BCR:H11C	20:3:305:BCR:H341	1.79	0.46
15:5:86:ALA:N	17:5:316:CLA:HED2	2.30	0.46
4:D:163:PRO:C	4:D:165:ASP:H	2.23	0.46
13:2:112:TRP:CE2	25:2:513:CHL:HED2	2.51	0.46
14:3:74:ASP:OD1	14:3:76:GLY:N	2.41	0.46
20:3:305:BCR:H272	17:3:311:CLA:C1C	2.46	0.46
12:1:223:HIS:HA	15:5:130:ASN:ND2	2.30	0.46
17:2:508:CLA:OBD	17:2:514:CLA:H2	2.15	0.46
1:A:197:HIS:O	1:A:201:GLY:N	2.44	0.46
1:A:247:LEU:HB3	1:A:254:PHE:CD2	2.50	0.46
1:A:335:HIS:CE1	19:A:844:LHG:HC12	2.50	0.46
2:B:64:ASN:ND2	17:B:828:CLA:HED1	2.30	0.46
17:1:506:CLA:HHC	17:1:506:CLA:HBB1	1.96	0.46
24:2:501:LUT:H11	24:2:501:LUT:H191	1.73	0.46
17:2:505:CLA:HMD2	17:2:510:CLA:H52	1.97	0.46
17:A:805:CLA:H2	17:A:805:CLA:H62	1.77	0.46
3:C:27:GLU:OE2	4:D:176:ARG:HD3	2.16	0.46
12:1:41:TRP:CD2	12:1:42:PHE:HB2	2.50	0.46
17:3:308:CLA:H12	17:3:313:CLA:CAD	2.46	0.46
1:A:29:PRO:HA	17:A:803:CLA:HBC1	1.97	0.46
12:1:104:ASN:OD1	12:1:107:LYS:HG2	2.16	0.46
15:5:49:LEU:HD23	15:5:52:LEU:HB2	1.97	0.46
1:A:714:PRO:HB3	17:A:852:CLA:HMC3	1.98	0.46
17:A:827:CLA:H141	17:A:827:CLA:H161	1.73	0.46
2:B:176:ASN:HB3	17:B:821:CLA:HMD1	1.97	0.46
10:K:63:MET:O	10:K:67:GLY:N	2.42	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:L:303:CLA:CHA	17:L:303:CLA:HBA1	2.45	0.46
10:K:80:THR:HG23	10:K:86:GLU:HG3	1.98	0.46
1:A:707:LYS:HB2	6:F:179:ARG:HH12	1.81	0.45
3:C:8:TYR:HE1	4:D:182:ASN:HD22	1.64	0.45
12:1:95:LEU:HD11	12:1:210:PRO:HB2	1.97	0.45
2:B:718:ILE:HG23	17:B:828:CLA:HAB	1.97	0.45
12:1:222:TRP:HB3	15:5:128:PHE:O	2.16	0.45
14:3:238:PHE:CD2	24:3:304:LUT:H12	2.52	0.45
15:5:72:GLY:HA2	15:5:75:GLU:OE2	2.16	0.45
13:2:189:THR:HG1	13:2:198:GLY:H	1.62	0.45
25:2:512:CHL:C4C	23:2:519:LMG:H312	2.45	0.45
14:3:110:MET:O	17:3:311:CLA:HAB	2.15	0.45
20:3:305:BCR:H15C	20:3:305:BCR:H351	1.64	0.45
2:B:287:ALA:HB2	17:B:820:CLA:HBC2	1.98	0.45
2:B:662:MET:O	2:B:666:SER:OG	2.32	0.45
20:B:846:BCR:H371	20:B:846:BCR:H24C	1.62	0.45
24:2:501:LUT:H35	24:2:501:LUT:H401	1.74	0.45
15:5:221:GLN:HB3	15:5:232:ASN:HD22	1.80	0.45
1:A:125:ASN:O	1:A:133:ARG:NH2	2.50	0.45
1:A:594:LEU:HD13	1:A:594:LEU:HA	1.83	0.45
17:B:838:CLA:H112	17:B:838:CLA:H142	1.71	0.45
6:F:213:TRP:CG	6:F:214:PRO:HD3	2.52	0.45
17:2:508:CLA:H2	17:2:508:CLA:HED3	1.98	0.45
15:5:242:ASN:HA	15:5:247:HIS:CE1	2.51	0.45
1:A:621:SER:OG	1:A:625:VAL:N	2.50	0.45
20:A:851:BCR:H15C	20:A:851:BCR:H351	1.72	0.45
20:1:503:BCR:C10	17:1:515:CLA:H3A	2.47	0.45
13:2:166:ARG:NE	25:2:513:CHL:OMC	2.48	0.45
14:3:74:ASP:HA	17:3:309:CLA:O1D	2.16	0.45
2:B:676:GLU:HG2	3:C:81:TYR:CE1	2.52	0.45
10:K:78:LYS:O	10:K:86:GLU:HB2	2.16	0.45
1:A:507:TRP:CH2	17:A:835:CLA:HED1	2.51	0.45
17:A:825:CLA:H141	17:A:835:CLA:H52	1.98	0.45
17:L:301:CLA:HMB3	17:L:301:CLA:HBB1	1.98	0.45
13:2:180:ASP:CB	13:2:186:ASN:HB2	2.46	0.45
17:2:507:CLA:H93	17:2:507:CLA:H62	1.83	0.45
1:A:12:ILE:O	1:A:14:VAL:HG13	2.16	0.45
2:B:609:PHE:O	2:B:613:SER:OG	2.33	0.45
2:B:615:TYR:OH	2:B:621:ARG:NH2	2.50	0.45
17:B:833:CLA:HBC1	17:B:838:CLA:H192	1.98	0.45
8:I:14:LEU:C	8:I:17:PRO:HD2	2.41	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:1:162:GLY:N	17:1:504:CLA:OBD	2.33	0.45
13:2:178:ASN:HB2	13:2:188:LEU:HB2	1.99	0.45
1:A:706:LEU:O	6:F:179:ARG:NH1	2.50	0.45
2:B:91:ILE:HD11	2:B:114:ASN:OD1	2.16	0.45
17:1:511:CLA:HED1	15:5:133:ALA:HB1	1.98	0.45
19:1:516:LHG:H242	19:1:516:LHG:H131	1.99	0.45
17:5:309:CLA:HMB3	17:5:309:CLA:HBB1	1.98	0.45
1:A:576:PRO:HD3	2:B:561:GLY:HA2	1.98	0.44
1:A:642:ASN:HB2	2:B:651:LEU:HD11	1.99	0.44
1:A:701:TRP:CE3	2:B:416:GLU:HB3	2.52	0.44
17:A:805:CLA:H162	17:A:805:CLA:H122	1.74	0.44
17:A:829:CLA:H62	17:A:829:CLA:H41	1.72	0.44
20:A:853:BCR:H15C	20:A:853:BCR:H351	1.74	0.44
17:B:824:CLA:HBA2	20:B:847:BCR:H16C	1.97	0.44
11:L:140:LEU:HD23	20:L:305:BCR:H23C	1.98	0.44
12:1:74:GLU:OE2	12:1:75:ARG:HG3	2.17	0.44
12:1:152:GLU:HB3	17:1:513:CLA:HBC1	1.99	0.44
17:1:511:CLA:O2D	17:1:511:CLA:H2A	2.17	0.44
13:2:223:LYS:HD3	17:2:510:CLA:O1D	2.18	0.44
17:2:508:CLA:HBA1	17:2:508:CLA:H3A	1.71	0.44
17:B:806:CLA:HBC2	17:B:830:CLA:HMA1	1.99	0.44
4:D:167:VAL:HB	4:D:173:ASN:OD1	2.17	0.44
6:F:212:ILE:HD12	15:5:73:LEU:HD22	2.00	0.44
13:2:162:TRP:HH2	20:2:503:BCR:H321	1.81	0.44
24:5:303:LUT:H15	24:5:303:LUT:H201	1.82	0.44
17:A:836:CLA:H3A	17:A:836:CLA:HBA2	1.76	0.44
20:A:849:BCR:H24C	20:A:849:BCR:H371	1.75	0.44
10:K:56:MET:HE1	10:K:113:HIS:HA	1.98	0.44
19:1:516:LHG:H151	19:1:516:LHG:H262	1.99	0.44
14:3:267:ASN:HB3	17:3:308:CLA:OBD	2.18	0.44
17:3:308:CLA:H43	17:3:313:CLA:OBD	2.18	0.44
2:B:173:SER:O	2:B:177:HIS:ND1	2.38	0.44
2:B:655:LEU:HD13	17:B:801:CLA:HAA1	2.00	0.44
18:B:843:PQN:H171	20:B:849:BCR:H382	2.00	0.44
3:C:15:THR:HG22	3:C:28:MET:HE3	1.98	0.44
13:2:256:ASP:OD1	13:2:256:ASP:N	2.50	0.44
17:2:505:CLA:HED2	17:2:510:CLA:H61	1.99	0.44
14:3:99:TYR:HE1	14:3:200:ALA:HA	1.82	0.44
15:5:175:LEU:HD13	15:5:175:LEU:HA	1.89	0.44
20:5:302:BCR:H352	20:5:302:BCR:H10C	2.00	0.44
17:B:833:CLA:H61	20:F:804:BCR:HC32	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:I:11:LEU:HD23	8:I:11:LEU:HA	1.83	0.44
12:1:229:ILE:HD13	17:1:506:CLA:HMD2	2.00	0.44
14:3:104:ASN:HA	17:3:316:CLA:HMD2	1.98	0.44
1:A:449:SER:HB3	1:A:536:ILE:HD13	1.98	0.44
1:A:570:ARG:HB3	1:A:587:TRP:HB2	1.98	0.44
2:B:193:HIS:HB2	17:B:815:CLA:CHC	2.48	0.44
2:B:225:LEU:HD22	20:B:844:BCR:H292	2.00	0.44
17:B:811:CLA:HHC	17:B:811:CLA:CBB	2.48	0.44
20:B:844:BCR:H24C	20:B:844:BCR:H371	1.72	0.44
4:D:97:ILE:HB	4:D:149:PHE:HB3	2.00	0.44
20:F:804:BCR:H11C	20:F:804:BCR:H341	1.67	0.44
20:A:845:BCR:H20C	20:A:845:BCR:H361	1.77	0.44
14:3:191:LYS:HE2	14:3:192:TYR:CZ	2.53	0.44
1:A:41:ASP:OD1	1:A:42:THR:N	2.44	0.44
1:A:379:THR:HG21	1:A:515:VAL:HB	1.99	0.44
1:A:693:GLN:HG2	2:B:546:LEU:HD22	1.98	0.44
2:B:40:GLU:HG2	2:B:165:LEU:HD23	2.00	0.44
2:B:477:LEU:C	2:B:479:SER:H	2.26	0.44
20:B:845:BCR:H15C	20:B:845:BCR:H351	1.69	0.44
11:L:97:VAL:HG13	11:L:101:HIS:CE1	2.53	0.44
14:3:91:PHE:HA	14:3:96:TRP:CD1	2.53	0.44
14:3:192:TYR:HD1	14:3:205:PRO:HD2	1.83	0.44
17:5:307:CLA:NA	17:5:307:CLA:H12	2.33	0.44
17:B:828:CLA:H2A	17:B:828:CLA:O1D	2.18	0.43
20:1:503:BCR:H341	20:1:503:BCR:H11C	1.67	0.43
13:2:232:VAL:HG21	26:2:502:XAT:H12	2.00	0.43
26:5:304:XAT:H183	17:5:310:CLA:C3B	2.48	0.43
2:B:102:GLU:CD	7:H:133:LEU:HD12	2.42	0.43
2:B:124:TRP:CZ2	2:B:124:TRP:NE1	2.86	0.43
17:B:802:CLA:H91	17:B:802:CLA:H111	1.74	0.43
17:B:820:CLA:CMB	17:B:825:CLA:HMA3	2.48	0.43
17:B:824:CLA:HAB	17:B:831:CLA:HMD2	2.00	0.43
11:L:66:THR:H	11:L:69:THR:HG22	1.83	0.43
24:2:501:LUT:H12	17:2:504:CLA:CAB	2.47	0.43
24:3:304:LUT:H35	24:3:304:LUT:H401	1.67	0.43
15:5:234:LEU:O	15:5:237:LEU:HG	2.19	0.43
1:A:84:TRP:O	1:A:88:MET:HG2	2.18	0.43
1:A:259:THR:CG2	1:A:260:PRO:HD3	2.48	0.43
2:B:246:THR:OG1	2:B:247:ALA:N	2.32	0.43
2:B:443:MET:HG3	2:B:451:LYS:O	2.18	0.43
5:E:79:LYS:N	5:E:80:PRO:HD2	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:90:LYS:HE3	5:E:104:THR:HG21	2.00	0.43
11:L:194:TRP:CE3	20:L:306:BCR:H333	2.54	0.43
26:5:304:XAT:H15	26:5:304:XAT:H201	1.85	0.43
1:A:213:HIS:HB2	17:A:813:CLA:C1C	2.48	0.43
20:B:848:BCR:H11C	20:B:848:BCR:H341	1.86	0.43
7:H:108:GLY:O	7:H:111:SER:OG	2.27	0.43
10:K:105:THR:CB	17:K:201:CLA:HAB	2.48	0.43
20:L:305:BCR:H15C	20:L:305:BCR:H351	1.82	0.43
12:1:128:TRP:HB2	12:1:133:THR:HG21	2.00	0.43
24:1:501:LUT:H15	24:1:501:LUT:H201	1.90	0.43
24:1:501:LUT:H161	24:1:501:LUT:H8	1.99	0.43
2:B:276:HIS:HB2	17:B:818:CLA:C1B	2.47	0.43
4:D:109:MET:HE3	4:D:109:MET:HB3	1.83	0.43
7:H:125:LEU:HD23	7:H:128:LYS:HB2	2.01	0.43
13:2:120:ILE:HG13	26:2:502:XAT:C16	2.48	0.43
17:5:307:CLA:H12	17:5:307:CLA:HBA2	1.80	0.43
17:A:805:CLA:H112	17:A:805:CLA:H91	1.70	0.43
17:A:808:CLA:H202	17:A:808:CLA:H161	1.87	0.43
2:B:43:TYR:CE2	2:B:330:ILE:HD11	2.54	0.43
20:B:852:BCR:H15C	20:B:852:BCR:H351	1.65	0.43
6:F:158:GLY:HA2	6:F:162:THR:HB	2.01	0.43
20:I:101:BCR:H15C	20:I:101:BCR:H351	1.79	0.43
12:1:127:PRO:HG2	12:1:128:TRP:CE3	2.54	0.43
1:A:17:ASP:HA	1:A:179:HIS:O	2.18	0.43
1:A:40:PRO:HA	1:A:45:TRP:CG	2.54	0.43
1:A:669:LEU:HB3	17:B:802:CLA:H62	2.01	0.43
1:A:712:THR:OG1	6:F:195:GLU:OE1	2.33	0.43
20:A:853:BCR:H20C	20:A:853:BCR:H361	1.80	0.43
3:C:28:MET:O	4:D:176:ARG:HD2	2.19	0.43
6:F:233:ILE:HG13	6:F:234:GLY:N	2.32	0.43
11:L:64:LEU:HD23	11:L:64:LEU:HA	1.71	0.43
1:A:159:THR:HG22	17:A:813:CLA:CGA	2.49	0.43
1:A:654:SER:O	1:A:658:GLN:HG2	2.18	0.43
2:B:53:GLN:O	2:B:53:GLN:NE2	2.50	0.43
2:B:582:TRP:HH2	17:B:802:CLA:HAB	1.81	0.43
4:D:200:LYS:HD2	4:D:204:ASP:C	2.44	0.43
6:F:113:SER:OG	6:F:115:PRO:HD2	2.19	0.43
17:L:301:CLA:H62	17:L:301:CLA:H41	1.75	0.43
12:1:94:VAL:HG12	12:1:95:LEU:HD22	1.99	0.43
15:5:149:ARG:HA	25:5:315:CHL:HAC2	2.00	0.43
15:5:218:PHE:CE1	24:5:303:LUT:H41	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:100:ALA:O	1:A:103:SER:OG	2.31	0.43
1:A:252:PRO:HG2	1:A:271:GLU:OE1	2.18	0.43
17:A:816:CLA:C4A	17:A:816:CLA:HBA2	2.48	0.43
20:A:845:BCR:H11C	20:A:845:BCR:H341	1.87	0.43
17:B:837:CLA:HBC2	17:B:837:CLA:HHD	2.00	0.43
7:H:129:LYS:HE3	7:H:129:LYS:HB2	1.86	0.43
11:L:64:LEU:O	11:L:69:THR:HG21	2.19	0.43
11:L:175:GLU:O	11:L:179:GLN:HG2	2.18	0.43
12:1:42:PHE:CE1	25:1:517:CHL:HED3	2.54	0.43
12:1:82:TYR:CE2	12:1:149:ARG:HD2	2.54	0.43
12:1:201:GLN:HB3	12:1:213:ASN:ND2	2.33	0.43
15:5:159:GLN:HG2	25:5:315:CHL:HMC	2.01	0.43
1:A:88:MET:HE1	17:A:808:CLA:H2A	2.00	0.43
6:F:181:TYR:OH	6:F:194:ARG:O	2.35	0.43
12:1:124:ASN:HA	12:1:125:PRO:HD3	1.94	0.43
12:1:168:LEU:O	12:1:168:LEU:HD23	2.19	0.43
13:2:253:HIS:ND1	17:2:506:CLA:HAA2	2.34	0.43
1:A:77:GLN:O	1:A:77:GLN:NE2	2.52	0.42
1:A:109:GLY:HA2	1:A:110:PRO:HD3	1.92	0.42
1:A:598:TYR:HB2	1:A:731:LEU:HD11	2.01	0.42
4:D:86:LEU:HA	4:D:86:LEU:HD23	1.75	0.42
6:F:94:ARG:NH2	6:F:143:ASP:O	2.51	0.42
12:1:149:ARG:HA	17:1:513:CLA:CBC	2.49	0.42
17:2:505:CLA:O1D	17:2:505:CLA:H12	2.19	0.42
15:5:65:ASP:HA	17:5:308:CLA:O1D	2.19	0.42
1:A:17:ASP:OD1	1:A:180:LYS:HD3	2.19	0.42
1:A:78:LEU:HD12	1:A:78:LEU:HA	1.84	0.42
1:A:576:PRO:HD2	3:C:52:LYS:HG2	2.00	0.42
17:A:806:CLA:H91	17:A:806:CLA:H112	1.75	0.42
6:F:208:PRO:HG3	23:F:806:LMG:H111	2.00	0.42
9:J:31:ARG:NH2	17:J:101:CLA:O1D	2.53	0.42
12:1:109:GLN:NE2	24:1:502:LUT:H372	2.34	0.42
17:1:509:CLA:HMA2	17:1:515:CLA:C3C	2.48	0.42
13:2:236:TRP:HD1	13:2:237:PHE:CD1	2.38	0.42
13:2:237:PHE:HB2	17:2:506:CLA:HAC2	2.01	0.42
17:2:510:CLA:H12	17:2:510:CLA:HBA1	1.81	0.42
14:3:259:HIS:CG	17:3:308:CLA:HAA2	2.54	0.42
15:5:146:GLU:HG3	17:5:316:CLA:C4B	2.50	0.42
1:A:191:VAL:HA	1:A:194:MET:HB2	2.00	0.42
1:A:507:TRP:CZ2	17:A:826:CLA:HMC2	2.53	0.42
20:A:848:BCR:H20C	20:A:848:BCR:H361	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:L:306:BCR:H15C	20:L:306:BCR:H351	1.70	0.42
12:1:77:LYS:HB2	12:1:159:LYS:NZ	2.34	0.42
13:2:126:LEU:O	13:2:131:ILE:HG22	2.19	0.42
2:B:458:ILE:HG21	6:F:151:SER:HB3	2.00	0.42
20:B:849:BCR:H20C	20:B:849:BCR:H361	1.84	0.42
3:C:25:VAL:HG13	3:C:44:ARG:O	2.18	0.42
6:F:136:PHE:CD2	9:J:40:PRO:HG3	2.53	0.42
9:J:8:LEU:HD23	9:J:13:VAL:HG11	2.01	0.42
12:1:70:PRO:HA	12:1:73:PHE:HB3	2.02	0.42
15:5:77:PRO:O	15:5:81:LYS:HG2	2.19	0.42
15:5:89:VAL:HG21	15:5:149:ARG:NH1	2.35	0.42
15:5:93:PHE:CE2	17:5:316:CLA:HAC2	2.54	0.42
15:5:212:MET:HE1	17:5:308:CLA:CAB	2.49	0.42
1:A:314:GLY:HA2	10:K:88:ARG:NH2	2.34	0.42
17:A:806:CLA:H161	17:A:828:CLA:HBB2	2.00	0.42
2:B:22:TRP:CG	2:B:704:GLN:HE22	2.36	0.42
2:B:69:ALA:HB2	2:B:135:LEU:HD12	2.01	0.42
17:B:841:CLA:O1D	17:B:841:CLA:H2A	2.19	0.42
11:L:81:LEU:HB2	11:L:82:PRO:HD2	2.01	0.42
25:2:512:CHL:C1A	23:2:519:LMG:H152	2.49	0.42
14:3:233:LEU:CD2	24:3:303:LUT:H11	2.49	0.42
20:A:846:BCR:H20C	20:A:846:BCR:H361	1.89	0.42
3:C:27:GLU:OE1	3:C:44:ARG:NH2	2.52	0.42
3:C:58:CYS:HA	21:C:102:SF4:S4	2.59	0.42
13:2:148:ASP:OD2	13:2:150:THR:OG1	2.36	0.42
1:A:13:VAL:HA	14:3:87:GLY:HA2	2.02	0.42
1:A:161:ILE:O	1:A:165:VAL:HG23	2.20	0.42
1:A:308:MET:HE1	17:A:820:CLA:C1D	2.50	0.42
1:A:511:GLU:OE1	1:A:512:LEU:HG	2.19	0.42
1:A:690:GLY:N	2:B:568:CYS:O	2.52	0.42
20:A:851:BCR:H321	20:A:851:BCR:HC8	2.00	0.42
17:B:824:CLA:HED3	17:B:824:CLA:H2A	2.01	0.42
20:B:847:BCR:H341	20:B:847:BCR:H11C	1.73	0.42
17:1:506:CLA:HHC	17:1:506:CLA:CBB	2.49	0.42
15:5:94:ALA:HB2	26:5:304:XAT:C13	2.50	0.42
15:5:136:PHE:O	15:5:140:LEU:HG	2.19	0.42
1:A:302:PHE:HE1	17:A:820:CLA:HAB	1.85	0.42
1:A:592:LEU:HA	1:A:592:LEU:HD23	1.86	0.42
1:A:671:PHE:CE2	1:A:675:HIS:HE1	2.36	0.42
17:B:832:CLA:HMB1	17:B:832:CLA:HBB1	2.01	0.42
6:F:181:TYR:CD1	6:F:185:VAL:HG13	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:L:140:LEU:HB3	11:L:181:THR:HG22	2.02	0.42
12:1:65:GLY:O	12:1:68:THR:HG23	2.19	0.42
14:3:210:LEU:HD23	14:3:212:PHE:CE1	2.55	0.42
1:A:75:PHE:HZ	17:3:301:CLA:HBB1	1.84	0.42
1:A:621:SER:HG	1:A:624:GLY:H	1.65	0.42
1:A:622:ASP:N	1:A:622:ASP:OD1	2.51	0.42
19:A:843:LHG:H242	19:A:843:LHG:H272	1.75	0.42
2:B:64:ASN:HD21	17:B:828:CLA:HED1	1.84	0.42
17:B:813:CLA:HBA1	17:B:813:CLA:H3A	1.72	0.42
10:K:110:ALA:HA	20:K:204:BCR:C11	2.50	0.42
11:L:143:TYR:O	11:L:147:SER:OG	2.35	0.42
17:1:506:CLA:HBA2	17:1:506:CLA:H3A	1.77	0.42
17:2:506:CLA:C4C	17:2:506:CLA:H51	2.50	0.42
26:5:304:XAT:H173	26:5:304:XAT:H3	1.71	0.42
1:A:323:LEU:O	1:A:335:HIS:HB2	2.20	0.42
1:A:648:PHE:O	1:A:652:GLN:HB2	2.20	0.42
18:A:841:PQN:H222	18:A:841:PQN:H262	1.77	0.42
6:F:136:PHE:CE2	9:J:40:PRO:HG3	2.54	0.42
14:3:163:LEU:O	20:3:305:BCR:H16C	2.20	0.42
20:A:846:BCR:H351	20:A:846:BCR:H15C	1.78	0.41
17:B:815:CLA:H91	17:B:815:CLA:H112	1.88	0.41
10:K:122:GLY:HA2	10:K:124:LYS:NZ	2.34	0.41
12:1:208:THR:HG21	12:1:213:ASN:HD21	1.85	0.41
12:1:212:GLU:O	12:1:216:THR:OG1	2.32	0.41
15:5:160:ALA:HB1	15:5:168:ILE:O	2.19	0.41
1:A:242:LEU:HD23	1:A:242:LEU:HA	1.82	0.41
1:A:550:LYS:HD3	2:B:670:TYR:HE1	1.85	0.41
1:A:681:SER:HB3	1:A:729:HIS:HB2	2.03	0.41
17:B:822:CLA:C1D	20:B:844:BCR:H323	2.49	0.41
6:F:150:VAL:HG12	6:F:160:PHE:HB2	2.02	0.41
10:K:97:PRO:HD3	17:K:201:CLA:CAA	2.50	0.41
11:L:92:LEU:HA	11:L:95:ILE:HG22	2.01	0.41
24:1:502:LUT:H11	24:1:502:LUT:H191	1.92	0.41
1:A:314:GLY:HA3	10:K:75:ALA:HB1	2.02	0.41
1:A:342:LEU:HA	1:A:342:LEU:HD23	1.73	0.41
17:B:822:CLA:CAD	20:B:844:BCR:HC41	2.50	0.41
5:E:94:LEU:HD13	5:E:94:LEU:HA	1.89	0.41
13:2:87:PHE:HB3	17:2:507:CLA:CAD	2.50	0.41
13:2:121:PHE:CD2	24:2:501:LUT:H28	2.55	0.41
24:3:304:LUT:H15	24:3:304:LUT:H201	1.94	0.41
15:5:150:TYR:CD2	15:5:151:MET:HE2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:5:174:GLY:O	15:5:175:LEU:HB2	2.20	0.41
20:5:302:BCR:H351	20:5:302:BCR:H15C	1.73	0.41
1:A:223:GLN:NE2	1:A:250:LEU:HD22	2.35	0.41
1:A:315:ILE:HB	17:A:821:CLA:HMD3	2.02	0.41
2:B:429:LEU:HA	2:B:429:LEU:HD23	1.80	0.41
2:B:492:LEU:HD13	2:B:492:LEU:HA	1.76	0.41
17:B:808:CLA:H2	20:I:101:BCR:HC31	2.03	0.41
17:B:811:CLA:H2A	17:B:811:CLA:O1D	2.21	0.41
20:B:844:BCR:H11C	20:B:844:BCR:H341	1.71	0.41
14:3:142:PRO:N	14:3:143:PRO:HD2	2.35	0.41
20:5:302:BCR:C37	25:5:317:CHL:HHB	2.50	0.41
1:A:66:ILE:O	1:A:70:VAL:HG13	2.20	0.41
1:A:194:MET:SD	1:A:198:HIS:CE1	3.13	0.41
1:A:679:ALA:HB3	17:A:802:CLA:HBB2	2.01	0.41
17:A:820:CLA:H92	17:A:820:CLA:H62	1.89	0.41
17:A:827:CLA:H151	20:J:102:BCR:H351	2.02	0.41
2:B:310:PRO:HA	2:B:311:PRO:HD3	1.93	0.41
3:C:27:GLU:OE1	3:C:44:ARG:NH1	2.54	0.41
11:L:154:SER:HB2	11:L:168:ALA:HB1	2.02	0.41
12:1:226:ILE:HB	17:1:506:CLA:H11	2.01	0.41
14:3:239:LEU:HD12	14:3:239:LEU:HA	1.88	0.41
15:5:186:ASN:ND2	15:5:189:GLY:HA2	2.35	0.41
1:A:548:LEU:O	1:A:552:VAL:HG23	2.21	0.41
22:B:850:DGD:O6D	22:B:850:DGD:O3D	2.37	0.41
3:C:62:PHE:HD2	4:D:186:ILE:HG21	1.86	0.41
6:F:209:ARG:HH22	15:5:72:GLY:HA3	1.84	0.41
9:J:25:LEU:O	9:J:29:ILE:HG13	2.21	0.41
26:2:502:XAT:H35	26:2:502:XAT:H401	1.81	0.41
17:3:309:CLA:O2D	17:3:309:CLA:H2A	2.21	0.41
17:3:311:CLA:C4A	17:3:311:CLA:HBA2	2.51	0.41
24:5:303:LUT:H11	24:5:303:LUT:H191	1.93	0.41
17:A:827:CLA:H143	17:A:827:CLA:H111	1.84	0.41
2:B:53:GLN:HE21	2:B:57:ILE:HG13	1.86	0.41
5:E:95:ARG:HD2	5:E:98:SER:HB2	2.02	0.41
12:1:180:LEU:C	17:1:504:CLA:HMA1	2.46	0.41
13:2:120:ILE:HG12	13:2:137:TRP:CG	2.55	0.41
13:2:128:LYS:HA	13:2:128:LYS:HD2	1.91	0.41
15:5:200:VAL:HG12	17:5:305:CLA:HMA1	2.02	0.41
1:A:41:ASP:OD1	1:A:45:TRP:HB2	2.21	0.41
17:B:826:CLA:H102	17:B:838:CLA:H2	2.01	0.41
17:B:838:CLA:H192	17:B:838:CLA:H162	1.76	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:B:838:CLA:H151	20:F:804:BCR:H402	2.02	0.41
6:F:212:ILE:HD12	15:5:73:LEU:HD13	2.02	0.41
17:1:510:CLA:HBA1	17:1:510:CLA:H3A	1.69	0.41
13:2:68:PHE:HD2	13:2:71:SER:HB3	1.85	0.41
14:3:80:LEU:N	24:3:304:LUT:O23	2.54	0.41
1:A:694:GLU:OE2	2:B:544:SER:OG	2.28	0.41
20:A:847:BCR:H371	20:A:847:BCR:H24C	1.82	0.41
2:B:193:HIS:HB2	17:B:815:CLA:C1C	2.51	0.41
2:B:395:ILE:HD11	2:B:541:ALA:HB1	2.03	0.41
17:B:806:CLA:HBC2	17:B:830:CLA:CMA	2.51	0.41
17:B:807:CLA:H61	17:B:807:CLA:H93	1.73	0.41
17:B:811:CLA:HBA2	17:B:811:CLA:HBD	2.03	0.41
17:B:815:CLA:H112	17:B:815:CLA:H142	1.85	0.41
20:B:844:BCR:H20C	20:B:844:BCR:H361	1.80	0.41
4:D:101:SER:OG	4:D:117:MET:SD	2.66	0.41
4:D:104:GLU:CD	4:D:119:GLU:HB2	2.46	0.41
4:D:133:LEU:HA	4:D:133:LEU:HD12	1.84	0.41
5:E:135:ASN:N	5:E:135:ASN:OD1	2.52	0.41
20:L:305:BCR:C8	20:L:305:BCR:H331	2.50	0.41
24:1:502:LUT:H201	24:1:502:LUT:H15	1.74	0.41
26:2:502:XAT:H15	26:2:502:XAT:H201	1.83	0.41
17:2:506:CLA:HBB1	17:2:506:CLA:HMB1	2.03	0.41
14:3:121:LEU:O	14:3:125:GLY:N	2.54	0.41
14:3:243:LEU:HD13	14:3:243:LEU:HA	1.95	0.41
25:5:314:CHL:CMC	25:5:317:CHL:HHC	2.50	0.41
1:A:479:ILE:O	1:A:483:TRP:N	2.48	0.41
3:C:3:HIS:ND1	3:C:69:LEU:HA	2.36	0.41
12:1:121:TYR:CE1	17:1:509:CLA:H2	2.56	0.41
17:A:836:CLA:C1A	17:A:836:CLA:CGA	2.99	0.40
2:B:51:PHE:HB2	2:B:153:SER:HB3	2.03	0.40
17:B:811:CLA:HAC2	20:I:101:BCR:H373	2.03	0.40
10:K:124:LYS:HE3	17:K:202:CLA:HMA3	2.03	0.40
24:1:502:LUT:H12	17:1:507:CLA:CBB	2.50	0.40
13:2:238:GLN:OE1	24:2:501:LUT:H24	2.22	0.40
1:A:433:ALA:O	1:A:437:HIS:ND1	2.40	0.40
17:A:806:CLA:H193	17:A:806:CLA:HED2	2.02	0.40
17:A:806:CLA:H203	17:A:806:CLA:H162	1.71	0.40
17:A:831:CLA:H12	17:A:831:CLA:H52	1.97	0.40
4:D:139:LEU:HB3	4:D:145:ILE:CG2	2.52	0.40
6:F:189:LYS:HG3	6:F:190:LYS:N	2.36	0.40
8:I:19:ILE:HA	8:I:22:THR:HG22	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:J:8:LEU:HD23	9:J:8:LEU:HA	1.93	0.40
22:J:103:DGD:HAG2	22:J:103:DGD:HAN1	1.76	0.40
13:2:238:GLN:O	13:2:242:THR:OG1	2.26	0.40
24:5:303:LUT:H401	24:5:303:LUT:H35	1.61	0.40
1:A:462:LEU:HD22	2:B:96:PHE:HA	2.03	0.40
17:A:804:CLA:H62	17:A:804:CLA:H2	1.80	0.40
17:A:831:CLA:H192	20:L:305:BCR:H10C	2.02	0.40
20:A:845:BCR:H351	20:A:845:BCR:H15C	1.72	0.40
2:B:408:LEU:HD12	2:B:408:LEU:HA	1.81	0.40
3:C:10:THR:HB	3:C:64:SER:OG	2.21	0.40
6:F:209:ARG:NH1	23:F:806:LMG:O5	2.55	0.40
13:2:151:THR:O	13:2:155:VAL:HG23	2.21	0.40
24:5:303:LUT:H183	17:5:307:CLA:C3B	2.51	0.40
1:A:115:VAL:HG22	1:A:125:ASN:OD1	2.21	0.40
2:B:472:TYR:OH	2:B:512:ILE:O	2.39	0.40
17:B:804:CLA:CGA	17:B:804:CLA:H3A	2.44	0.40
4:D:139:LEU:O	4:D:145:ILE:HG22	2.20	0.40
11:L:84:TYR:O	11:L:86:THR:HG23	2.22	0.40
11:L:90:PRO:HA	11:L:93:ARG:HG3	2.03	0.40
11:L:136:LEU:HA	11:L:136:LEU:HD23	1.88	0.40
20:L:305:BCR:H11C	20:L:305:BCR:H341	1.74	0.40
12:1:226:ILE:HG21	17:1:506:CLA:H42	2.04	0.40
14:3:74:ASP:OD1	14:3:75:PHE:N	2.53	0.40
14:3:206:ILE:HG23	14:3:207:PHE:CD1	2.57	0.40
15:5:201:LYS:O	15:5:205:ILE:HG12	2.21	0.40
17:B:807:CLA:H152	17:B:807:CLA:H111	1.90	0.40
17:1:506:CLA:H41	17:1:506:CLA:H62	1.83	0.40
13:2:87:PHE:CE2	26:2:502:XAT:H383	2.56	0.40
13:2:120:ILE:HG23	13:2:137:TRP:CD1	2.56	0.40
14:3:133:ILE:HG22	14:3:134:PRO:O	2.22	0.40
14:3:172:LEU:HD12	17:3:316:CLA:HMA2	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	740/750 (99%)	690 (93%)	50 (7%)	0	100	100
2	B	731/734 (100%)	688 (94%)	42 (6%)	1 (0%)	48	78
3	C	79/81 (98%)	70 (89%)	9 (11%)	0	100	100
4	D	140/205 (68%)	118 (84%)	22 (16%)	0	100	100
5	E	66/147 (45%)	61 (92%)	5 (8%)	0	100	100
6	F	156/235 (66%)	150 (96%)	6 (4%)	0	100	100
7	H	59/143 (41%)	58 (98%)	1 (2%)	0	100	100
8	I	28/36 (78%)	28 (100%)	0	0	100	100
9	J	40/42 (95%)	37 (92%)	2 (5%)	1 (2%)	4	21
10	K	82/131 (63%)	73 (89%)	9 (11%)	0	100	100
11	L	144/209 (69%)	135 (94%)	9 (6%)	0	100	100
12	1	189/247 (76%)	179 (95%)	10 (5%)	0	100	100
13	2	201/255 (79%)	185 (92%)	16 (8%)	0	100	100
14	3	220/269 (82%)	195 (89%)	25 (11%)	0	100	100
15	5	203/257 (79%)	173 (85%)	30 (15%)	0	100	100
All	All	3078/3741 (82%)	2840 (92%)	236 (8%)	2 (0%)	49	78

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	223	GLY
9	J	36	ALA

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	592/608 (97%)	585 (99%)	7 (1%)	63	72

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	594/601 (99%)	589 (99%)	5 (1%)	73	77
3	C	70/71 (99%)	69 (99%)	1 (1%)	59	70
4	D	119/160 (74%)	118 (99%)	1 (1%)	73	77
5	E	58/112 (52%)	58 (100%)	0	100	100
6	F	120/183 (66%)	120 (100%)	0	100	100
7	H	48/110 (44%)	48 (100%)	0	100	100
8	I	26/33 (79%)	26 (100%)	0	100	100
9	J	35/36 (97%)	35 (100%)	0	100	100
10	K	52/102 (51%)	51 (98%)	1 (2%)	50	66
11	L	112/166 (68%)	110 (98%)	2 (2%)	51	67
12	1	134/196 (68%)	134 (100%)	0	100	100
13	2	156/194 (80%)	155 (99%)	1 (1%)	78	80
14	3	147/216 (68%)	146 (99%)	1 (1%)	76	78
15	5	139/202 (69%)	139 (100%)	0	100	100
All	All	2402/2990 (80%)	2383 (99%)	19 (1%)	70	77

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	570	ARG
1	A	578	ARG
1	A	590	VAL
1	A	594	LEU
1	A	639	ILE
1	A	708	VAL
1	A	720	ILE
2	B	165	LEU
2	B	224	PRO
2	B	225	LEU
2	B	437	TYR
2	B	492	LEU
3	C	47	ASP
4	D	97	ILE
10	K	104	ASP
11	L	88	VAL
11	L	93	ARG
13	2	262	ILE

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Mol	Chain	Res	Type
14	3	193	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	238	HIS
1	A	317	HIS
2	B	193	HIS
2	B	196	HIS
2	B	235	GLN
2	B	308	HIS
2	B	627	ASN
2	B	630	GLN
2	B	633	ASN
4	D	68	GLN
4	D	177	GLN
4	D	182	ASN
9	J	30	ASN
11	L	121	HIS
14	3	266	ASN
15	5	244	ASN

5.3.3 RNA [i](#)

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](#)

199 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
17	CLA	1	515	-	48,52,73	1.50	11 (22%)	58,87,113	1.41	5 (8%)
17	CLA	A	802	-	62,66,73	1.25	9 (14%)	73,104,113	1.35	5 (6%)
17	CLA	B	836	-	46,50,73	1.39	9 (19%)	53,85,113	1.39	4 (7%)
17	CLA	A	832	-	47,53,73	1.37	7 (14%)	59,88,113	1.59	5 (8%)
17	CLA	B	817	-	53,57,73	1.33	9 (16%)	61,93,113	1.47	5 (8%)
17	CLA	A	821	-	46,50,73	1.38	9 (19%)	53,85,113	1.59	7 (13%)
17	CLA	B	815	-	69,73,73	1.21	9 (13%)	82,113,113	1.34	6 (7%)
17	CLA	A	807	-	41,47,73	1.40	9 (21%)	50,80,113	1.58	5 (10%)
17	CLA	B	822	-	51,55,73	1.34	11 (21%)	60,91,113	1.57	6 (10%)
17	CLA	1	509	-	54,58,73	1.30	7 (12%)	64,95,113	1.43	7 (10%)
20	BCR	A	848	-	41,41,41	1.07	2 (4%)	56,56,56	2.00	11 (19%)
17	CLA	A	835	-	55,59,73	1.33	8 (14%)	64,96,113	1.62	7 (10%)
24	LUT	3	304	-	42,43,43	0.90	2 (4%)	51,60,60	1.65	10 (19%)
17	CLA	K	201	-	41,45,73	1.43	10 (24%)	50,78,113	1.51	6 (12%)
17	CLA	2	514	-	59,63,73	1.23	9 (15%)	70,101,113	1.37	5 (7%)
17	CLA	A	818	-	44,48,73	1.38	7 (15%)	51,82,113	1.57	7 (13%)
17	CLA	3	317	-	45,49,73	1.40	10 (22%)	54,84,113	1.57	9 (16%)
17	CLA	B	832	-	47,51,73	1.31	7 (14%)	55,86,113	1.44	4 (7%)
17	CLA	5	316	-	45,49,73	1.35	8 (17%)	54,84,113	1.56	7 (12%)
19	LHG	1	516	17	48,48,48	0.91	2 (4%)	51,54,54	1.18	5 (9%)
17	CLA	B	818	-	63,67,73	1.19	7 (11%)	74,105,113	1.45	8 (10%)
17	CLA	3	310	-	49,53,73	1.34	8 (16%)	58,89,113	1.45	6 (10%)
17	CLA	B	810	2	44,48,73	1.38	9 (20%)	51,82,113	1.63	8 (15%)
17	CLA	B	813	-	47,51,73	1.41	7 (14%)	55,86,113	1.49	5 (9%)
17	CLA	B	814	-	45,49,73	1.45	10 (22%)	54,84,113	1.58	10 (18%)
25	CHL	2	516	13	38,51,74	4.01	17 (44%)	32,86,114	2.73	11 (34%)
17	CLA	A	819	-	44,48,73	1.40	7 (15%)	51,82,113	1.54	5 (9%)
17	CLA	3	307	-	44,48,73	1.51	9 (20%)	51,82,113	1.39	4 (7%)
17	CLA	3	313	-	52,56,73	1.33	7 (13%)	61,92,113	1.51	5 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	CLA	A	833	-	44,48,73	1.38	9 (20%)	51,82,113	1.59	6 (11%)
17	CLA	B	821	-	54,58,73	1.34	8 (14%)	64,95,113	1.49	5 (7%)
23	LMG	F	806	-	45,45,55	0.95	2 (4%)	53,53,63	1.08	5 (9%)
25	CHL	3	302	13	41,55,74	4.01	21 (51%)	35,91,114	2.49	12 (34%)
17	CLA	A	837	-	45,49,73	1.42	11 (24%)	54,84,113	1.65	9 (16%)
17	CLA	B	833	-	69,73,73	1.15	8 (11%)	82,113,113	1.42	7 (8%)
17	CLA	2	507	13	52,56,73	1.61	9 (17%)	60,91,113	1.68	8 (13%)
20	BCR	5	302	-	41,41,41	0.86	1 (2%)	56,56,56	1.95	12 (21%)
23	LMG	5	301	-	32,32,55	1.18	2 (6%)	40,40,63	1.16	3 (7%)
17	CLA	J	101	9	46,50,73	1.37	8 (17%)	53,85,113	1.49	4 (7%)
17	CLA	A	825	-	63,67,73	1.25	9 (14%)	74,105,113	1.34	5 (6%)
24	LUT	1	502	-	42,43,43	0.92	2 (4%)	51,60,60	1.81	12 (23%)
25	CHL	1	514	-	35,49,74	4.49	18 (51%)	30,83,114	2.36	10 (33%)
24	LUT	5	303	-	42,43,43	0.92	2 (4%)	51,60,60	2.12	14 (27%)
17	CLA	B	828	-	45,49,73	1.38	9 (20%)	54,84,113	1.59	9 (16%)
20	BCR	J	102	-	41,41,41	0.98	2 (4%)	56,56,56	2.19	21 (37%)
17	CLA	A	840	-	45,49,73	1.44	10 (22%)	54,84,113	1.51	5 (9%)
17	CLA	A	810	17	58,62,73	1.27	11 (18%)	68,99,113	1.50	6 (8%)
17	CLA	2	511	-	44,48,73	1.40	10 (22%)	51,82,113	1.74	6 (11%)
20	BCR	B	844	-	41,41,41	0.83	1 (2%)	56,56,56	2.60	17 (30%)
17	CLA	A	808	1	69,73,73	1.15	8 (11%)	82,113,113	1.34	7 (8%)
17	CLA	A	803	-	45,49,73	1.40	9 (20%)	54,84,113	1.63	7 (12%)
17	CLA	A	839	-	46,50,73	1.39	8 (17%)	53,85,113	1.57	5 (9%)
17	CLA	1	510	19	50,54,73	1.31	10 (20%)	59,90,113	1.42	5 (8%)
24	LUT	3	303	-	42,43,43	0.85	1 (2%)	51,60,60	1.66	12 (23%)
25	CHL	2	512	-	41,54,74	3.89	18 (43%)	36,90,114	2.75	11 (30%)
26	XAT	2	502	-	41,47,47	1.16	4 (9%)	54,74,74	2.78	19 (35%)
17	CLA	A	811	-	44,48,73	1.39	7 (15%)	51,82,113	1.55	7 (13%)
19	LHG	A	844	17	29,29,48	1.21	3 (10%)	32,35,54	1.21	3 (9%)
17	CLA	B	842	-	61,65,73	1.22	10 (16%)	72,103,113	1.34	4 (5%)
20	BCR	A	851	-	41,41,41	0.90	1 (2%)	56,56,56	2.18	18 (32%)
19	LHG	2	517	17	34,34,48	1.07	2 (5%)	37,40,54	1.23	5 (13%)
17	CLA	3	312	-	45,49,73	1.41	9 (20%)	54,84,113	1.46	6 (11%)
20	BCR	A	846	-	41,41,41	0.99	1 (2%)	56,56,56	2.07	18 (32%)
17	CLA	A	823	-	58,62,73	1.35	10 (17%)	65,99,113	1.38	7 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	CLA	B	825	-	46,50,73	1.37	8 (17%)	53,85,113	1.46	7 (13%)
17	CLA	B	834	-	49,53,73	1.35	7 (14%)	58,89,113	1.52	7 (12%)
17	CLA	5	309	-	49,53,73	1.39	10 (20%)	58,89,113	1.45	7 (12%)
20	BCR	B	852	-	41,41,41	1.21	2 (4%)	56,56,56	2.05	17 (30%)
17	CLA	B	816	-	47,51,73	1.37	7 (14%)	55,86,113	1.50	4 (7%)
17	CLA	2	505	-	56,60,73	1.21	9 (16%)	65,97,113	1.45	6 (9%)
17	CLA	B	840	-	45,49,73	1.37	8 (17%)	54,84,113	1.62	6 (11%)
20	BCR	3	305	-	41,41,41	0.90	2 (4%)	56,56,56	1.99	15 (26%)
17	CLA	B	837	-	54,58,73	1.31	9 (16%)	64,95,113	1.46	8 (12%)
17	CLA	3	306	-	56,60,73	1.32	7 (12%)	69,97,113	1.60	7 (10%)
25	CHL	5	314	-	41,55,74	4.00	19 (46%)	35,91,114	2.51	13 (37%)
22	DGD	J	103	-	67,67,67	0.83	2 (2%)	81,81,81	1.11	4 (4%)
17	CLA	F	803	-	45,49,73	1.39	9 (20%)	54,84,113	1.48	5 (9%)
18	PQN	B	843	-	31,31,34	1.38	2 (6%)	39,41,45	1.52	6 (15%)
17	CLA	A	804	17	56,60,73	1.27	8 (14%)	65,97,113	1.43	4 (6%)
25	CHL	3	315	-	37,51,74	3.96	19 (51%)	30,86,114	2.97	11 (36%)
17	CLA	1	505	-	46,50,73	1.41	7 (15%)	53,85,113	1.42	4 (7%)
25	CHL	5	315	-	40,54,74	3.94	20 (50%)	34,90,114	2.38	13 (38%)
17	CLA	B	819	-	45,49,73	1.43	8 (17%)	54,84,113	1.63	7 (12%)
17	CLA	A	812	-	46,50,73	1.37	8 (17%)	53,85,113	1.57	8 (15%)
17	CLA	K	202	-	45,49,73	1.38	9 (20%)	54,84,113	1.53	6 (11%)
17	CLA	A	852	-	61,65,73	1.26	9 (14%)	72,103,113	1.32	6 (8%)
20	BCR	I	101	-	41,41,41	1.19	2 (4%)	56,56,56	2.09	16 (28%)
17	CLA	A	816	-	63,67,73	1.21	7 (11%)	74,105,113	1.42	7 (9%)
20	BCR	2	503	-	41,41,41	0.92	1 (2%)	56,56,56	3.71	27 (48%)
17	CLA	A	805	-	68,72,73	1.21	10 (14%)	80,111,113	1.46	9 (11%)
17	CLA	B	835	-	64,68,73	1.21	9 (14%)	76,107,113	1.38	6 (7%)
17	CLA	A	814	-	46,50,73	1.39	10 (21%)	53,85,113	1.55	5 (9%)
20	BCR	A	853	-	41,41,41	0.99	2 (4%)	56,56,56	2.25	18 (32%)
20	BCR	B	846	-	41,41,41	1.01	2 (4%)	56,56,56	2.29	18 (32%)
17	CLA	A	827	-	69,73,73	1.20	9 (13%)	82,113,113	1.36	8 (9%)
20	BCR	B	845	-	41,41,41	1.04	1 (2%)	56,56,56	2.07	16 (28%)
17	CLA	A	817	-	42,47,73	1.65	12 (28%)	49,81,113	1.63	5 (10%)
25	CHL	5	317	-	34,48,74	3.89	18 (52%)	32,82,114	2.84	13 (40%)
20	BCR	B	848	-	41,41,41	1.00	2 (4%)	56,56,56	1.99	16 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	CLA	5	308	-	64,68,73	1.23	9 (14%)	76,107,113	1.41	7 (9%)
17	CLA	B	811	-	59,63,73	1.29	9 (15%)	70,101,113	1.39	6 (8%)
17	CLA	A	830	-	54,58,73	1.30	7 (12%)	64,95,113	1.50	5 (7%)
17	CLA	2	508	-	51,55,73	1.38	8 (15%)	60,91,113	1.32	4 (6%)
21	SF4	C	101	3	0,12,12	-	-	-	-	-
23	LMG	2	518	-	16,16,55	0.48	0	22,22,63	0.99	2 (9%)
17	CLA	5	311	-	46,50,73	1.32	8 (17%)	53,85,113	1.56	5 (9%)
17	CLA	B	802	-	68,72,73	1.18	10 (14%)	80,111,113	1.33	8 (10%)
22	DGD	B	850	-	60,60,67	0.88	2 (3%)	74,74,81	1.40	11 (14%)
17	CLA	A	842	19	54,58,73	1.30	10 (18%)	64,95,113	1.40	6 (9%)
17	CLA	A	809	1	40,47,73	1.46	8 (20%)	43,80,113	1.43	3 (6%)
20	BCR	A	849	-	40,40,41	1.05	2 (5%)	54,54,56	1.88	13 (24%)
17	CLA	B	805	-	45,49,73	1.39	9 (20%)	54,84,113	1.55	6 (11%)
17	CLA	5	312	-	50,54,73	1.34	9 (18%)	59,90,113	1.34	4 (6%)
19	LHG	B	851	-	37,37,48	1.09	2 (5%)	40,43,54	1.19	4 (10%)
17	CLA	A	826	-	64,68,73	1.23	8 (12%)	76,107,113	1.41	7 (9%)
17	CLA	1	506	-	59,63,73	1.26	8 (13%)	70,101,113	1.39	6 (8%)
17	CLA	A	831	-	67,71,73	1.29	13 (19%)	81,110,113	1.39	8 (9%)
17	CLA	B	829	-	44,48,73	1.40	7 (15%)	51,82,113	1.60	7 (13%)
17	CLA	B	823	-	46,50,73	1.39	10 (21%)	53,85,113	1.50	4 (7%)
23	LMG	2	519	-	36,36,55	1.10	2 (5%)	44,44,63	1.38	8 (18%)
19	LHG	A	843	-	48,48,48	0.90	3 (6%)	51,54,54	1.30	5 (9%)
17	CLA	F	802	-	46,50,73	1.40	10 (21%)	53,85,113	1.49	4 (7%)
17	CLA	1	507	12	46,50,73	1.34	8 (17%)	53,85,113	1.52	5 (9%)
24	LUT	2	501	-	42,43,43	0.89	1 (2%)	51,60,60	2.06	14 (27%)
20	BCR	1	503	-	19,19,41	0.66	0	26,26,56	2.04	7 (26%)
16	CL0	A	801	-	55,69,73	2.41	6 (10%)	58,107,113	2.27	15 (25%)
20	BCR	F	801	-	41,41,41	0.98	2 (4%)	56,56,56	2.11	17 (30%)
17	CLA	1	513	-	69,73,73	1.18	9 (13%)	82,113,113	1.26	6 (7%)
20	BCR	L	305	-	41,41,41	0.95	1 (2%)	56,56,56	2.15	17 (30%)
17	CLA	3	316	-	41,45,73	1.36	8 (19%)	50,78,113	1.58	6 (12%)
17	CLA	B	804	-	69,73,73	1.19	9 (13%)	82,113,113	1.32	4 (4%)
20	BCR	B	849	-	41,41,41	1.06	2 (4%)	56,56,56	2.01	16 (28%)
25	CHL	2	513	-	32,48,74	4.05	15 (46%)	27,81,114	2.56	15 (55%)
17	CLA	2	506	-	69,73,73	1.14	7 (10%)	82,113,113	1.39	5 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	CLA	5	305	-	41,46,73	1.52	10 (24%)	50,79,113	1.72	10 (20%)
17	CLA	1	504	-	45,49,73	1.40	9 (20%)	52,84,113	1.42	5 (9%)
17	CLA	3	318	-	49,53,73	1.40	8 (16%)	60,89,113	1.45	7 (11%)
17	CLA	A	806	1	69,73,73	1.19	7 (10%)	82,113,113	1.31	5 (6%)
17	CLA	B	826	-	66,70,73	1.17	7 (10%)	78,109,113	1.36	8 (10%)
17	CLA	L	304	-	49,53,73	1.32	9 (18%)	58,89,113	1.67	9 (15%)
17	CLA	5	307	15	69,73,73	1.16	8 (11%)	82,113,113	1.25	5 (6%)
17	CLA	B	806	-	42,47,73	1.46	9 (21%)	50,80,113	1.56	7 (14%)
17	CLA	B	824	-	49,53,73	1.40	9 (18%)	58,89,113	1.41	5 (8%)
17	CLA	5	313	15	44,48,73	1.38	7 (15%)	51,82,113	1.53	5 (9%)
25	CHL	2	515	-	40,53,74	4.06	18 (45%)	35,89,114	2.69	13 (37%)
17	CLA	L	303	-	56,60,73	1.26	9 (16%)	65,97,113	1.59	8 (12%)
17	CLA	3	308	-	59,63,73	1.18	8 (13%)	70,101,113	1.44	7 (10%)
21	SF4	C	102	3	0,12,12	-	-	-	-	-
17	CLA	1	511	-	50,54,73	1.36	9 (18%)	59,90,113	1.46	5 (8%)
17	CLA	B	801	-	69,73,73	1.21	11 (15%)	82,113,113	1.29	7 (8%)
17	CLA	1	508	-	44,48,73	1.38	8 (18%)	51,82,113	1.46	7 (13%)
17	CLA	B	838	-	69,73,73	1.18	9 (13%)	82,113,113	1.36	7 (8%)
17	CLA	A	834	1	45,49,73	1.41	9 (20%)	54,84,113	1.47	7 (12%)
24	LUT	1	501	-	42,43,43	0.87	2 (4%)	51,60,60	1.77	12 (23%)
17	CLA	A	813	-	49,53,73	1.34	9 (18%)	58,89,113	1.48	5 (8%)
17	CLA	2	510	19	64,68,73	1.18	10 (15%)	76,107,113	1.38	7 (9%)
17	CLA	3	309	-	43,48,73	1.57	10 (23%)	52,82,113	1.58	6 (11%)
20	BCR	A	847	-	41,41,41	0.94	2 (4%)	56,56,56	2.01	20 (35%)
26	XAT	5	304	-	41,47,47	1.26	5 (12%)	54,74,74	2.43	19 (35%)
20	BCR	B	847	-	41,41,41	1.02	2 (4%)	56,56,56	2.35	20 (35%)
17	CLA	B	827	-	45,49,73	1.38	10 (22%)	54,84,113	1.64	10 (18%)
20	BCR	K	204	-	41,41,41	1.00	2 (4%)	56,56,56	2.02	16 (28%)
17	CLA	A	822	-	45,49,73	1.37	8 (17%)	54,84,113	1.61	6 (11%)
17	CLA	5	306	-	43,48,73	1.38	7 (16%)	51,83,113	1.56	5 (9%)
17	CLA	L	301	-	60,64,73	1.24	11 (18%)	71,102,113	1.35	7 (9%)
17	CLA	2	509	-	54,58,73	1.27	8 (14%)	64,95,113	1.48	6 (9%)
25	CHL	1	512	-	41,55,74	4.09	18 (43%)	35,91,114	2.29	13 (37%)
23	LMG	F	805	-	30,30,55	1.23	2 (6%)	38,38,63	1.20	3 (7%)
20	BCR	L	306	-	41,41,41	0.85	1 (2%)	56,56,56	1.97	18 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	CLA	B	807	2	69,73,73	1.21	9 (13%)	82,113,113	1.30	6 (7%)
17	CLA	3	314	14	59,63,73	1.23	9 (15%)	70,101,113	1.43	7 (10%)
17	CLA	A	829	-	59,63,73	1.29	8 (13%)	70,101,113	1.46	8 (11%)
17	CLA	2	504	13	37,44,73	1.52	8 (21%)	48,76,113	1.67	7 (14%)
17	CLA	B	841	-	58,62,73	1.27	10 (17%)	68,99,113	1.41	7 (10%)
25	CHL	1	517	12	35,49,74	4.09	19 (54%)	30,83,114	3.11	14 (46%)
17	CLA	B	831	-	47,51,73	1.41	8 (17%)	55,86,113	1.46	4 (7%)
17	CLA	A	838	-	69,73,73	1.21	8 (11%)	82,113,113	1.33	9 (10%)
17	CLA	3	301	-	45,49,73	1.39	9 (20%)	54,84,113	1.58	7 (12%)
17	CLA	B	839	-	51,55,73	1.32	8 (15%)	60,91,113	1.54	7 (11%)
18	PQN	A	841	-	34,34,34	1.41	2 (5%)	43,45,45	1.26	5 (11%)
21	SF4	A	850	2,1	0,12,12	-	-	-	-	-
17	CLA	A	836	-	59,63,73	1.29	9 (15%)	70,101,113	1.50	7 (10%)
17	CLA	A	820	-	61,65,73	1.21	6 (9%)	72,103,113	1.51	10 (13%)
17	CLA	A	824	-	44,48,73	1.39	7 (15%)	51,82,113	1.52	5 (9%)
17	CLA	B	812	-	58,62,73	1.37	10 (17%)	71,100,113	1.43	8 (11%)
17	CLA	A	828	-	45,49,73	1.39	7 (15%)	54,84,113	1.51	6 (11%)
17	CLA	A	815	-	49,53,73	1.41	9 (18%)	58,89,113	1.42	5 (8%)
17	CLA	B	809	-	44,48,73	1.40	8 (18%)	51,82,113	1.51	5 (9%)
17	CLA	L	302	-	44,48,73	1.40	6 (13%)	50,82,113	1.61	6 (12%)
17	CLA	5	310	-	54,58,73	1.29	8 (14%)	64,95,113	1.41	7 (10%)
17	CLA	B	820	-	57,61,73	1.30	9 (15%)	67,98,113	1.35	6 (8%)
17	CLA	K	203	-	44,48,73	1.38	8 (18%)	51,82,113	1.51	5 (9%)
17	CLA	B	830	-	60,64,73	1.32	11 (18%)	71,102,113	1.34	5 (7%)
17	CLA	3	311	-	54,58,73	1.24	7 (12%)	64,95,113	1.57	8 (12%)
17	CLA	B	808	-	56,60,73	1.31	9 (16%)	65,97,113	1.48	7 (10%)
20	BCR	A	845	-	41,41,41	1.12	2 (4%)	56,56,56	2.29	19 (33%)
17	CLA	K	205	10	42,47,73	1.44	8 (19%)	48,81,113	1.57	5 (10%)
17	CLA	B	803	-	69,73,73	1.19	7 (10%)	82,113,113	1.30	7 (8%)
20	BCR	F	804	-	41,41,41	1.00	1 (2%)	56,56,56	1.98	17 (30%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	1	515	-	1/1/10/20	5/15/87/115	-
17	CLA	A	802	-	1/1/13/20	10/31/107/115	-
17	CLA	B	836	-	-	5/12/88/115	-
17	CLA	A	832	-	1/1/10/20	5/13/89/115	-
17	CLA	B	817	-	1/1/11/20	7/20/96/115	-
17	CLA	A	821	-	1/1/10/20	2/12/88/115	-
17	CLA	B	815	-	1/1/15/20	10/39/115/115	-
17	CLA	A	807	-	1/1/8/20	3/7/79/115	-
17	CLA	B	822	-	1/1/11/20	4/18/94/115	-
17	CLA	1	509	-	-	4/21/97/115	-
20	BCR	A	848	-	-	6/29/63/63	0/2/2/2
17	CLA	A	835	-	1/1/12/20	10/23/99/115	-
24	LUT	3	304	-	-	2/29/67/67	0/2/2/2
17	CLA	K	201	-	1/1/8/20	2/4/76/115	-
17	CLA	2	514	-	1/1/13/20	9/27/103/115	-
17	CLA	A	818	-	1/1/9/20	2/10/82/115	-
17	CLA	3	317	-	1/1/10/20	2/10/86/115	-
17	CLA	B	832	-	1/1/10/20	3/13/89/115	-
17	CLA	5	316	-	1/1/10/20	2/10/86/115	-
19	LHG	1	516	17	-	23/53/53/53	-
17	CLA	B	818	-	1/1/13/20	14/32/108/115	-
17	CLA	3	310	-	1/1/11/20	4/15/91/115	-
17	CLA	B	810	2	1/1/9/20	0/10/82/115	-
17	CLA	B	813	-	1/1/10/20	2/13/89/115	-
17	CLA	B	814	-	1/1/10/20	4/10/86/115	-
25	CHL	2	516	13	3/3/15/26	8/13/109/137	-
17	CLA	A	819	-	1/1/9/20	4/10/82/115	-
17	CLA	3	307	-	1/1/9/20	4/10/82/115	-
17	CLA	3	313	-	1/1/11/20	7/19/95/115	-
17	CLA	A	833	-	1/1/9/20	1/10/82/115	-
17	CLA	B	821	-	1/1/12/20	4/21/97/115	-
25	CHL	3	302	13	3/3/16/26	2/17/115/137	-
23	LMG	F	806	-	-	18/40/60/70	0/1/1/1
17	CLA	A	837	-	1/1/10/20	2/10/86/115	-
17	CLA	B	833	-	1/1/15/20	3/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	2	507	13	2/2/11/20	3/16/88/115	-
20	BCR	5	302	-	-	7/29/63/63	0/2/2/2
23	LMG	5	301	-	-	7/27/47/70	0/1/1/1
17	CLA	J	101	9	1/1/10/20	7/12/88/115	-
17	CLA	A	825	-	1/1/13/20	8/32/108/115	-
24	LUT	1	502	-	-	3/29/67/67	0/2/2/2
25	CHL	1	514	-	3/3/14/26	4/10/104/137	-
24	LUT	5	303	-	-	2/29/67/67	0/2/2/2
17	CLA	B	828	-	1/1/10/20	2/10/86/115	-
20	BCR	J	102	-	-	2/29/63/63	0/2/2/2
17	CLA	A	840	-	1/1/10/20	4/10/86/115	-
17	CLA	A	810	17	1/1/12/20	5/26/102/115	-
17	CLA	2	511	-	1/1/9/20	2/10/82/115	-
20	BCR	B	844	-	-	4/29/63/63	0/2/2/2
17	CLA	A	808	1	1/1/15/20	8/39/115/115	-
17	CLA	A	803	-	1/1/10/20	3/10/86/115	-
17	CLA	A	839	-	1/1/10/20	4/12/88/115	-
17	CLA	1	510	19	1/1/11/20	8/17/93/115	-
25	CHL	2	512	-	3/3/16/26	5/17/113/137	-
24	LUT	3	303	-	-	2/29/67/67	0/2/2/2
26	XAT	2	502	-	-	6/31/93/93	0/4/4/4
17	CLA	A	811	-	1/1/9/20	2/10/82/115	-
19	LHG	A	844	17	-	11/34/34/53	-
17	CLA	B	842	-	1/1/13/20	14/30/106/115	-
20	BCR	A	851	-	-	6/29/63/63	0/2/2/2
19	LHG	2	517	17	-	3/39/39/53	-
17	CLA	3	312	-	1/1/10/20	6/10/86/115	-
20	BCR	A	846	-	-	7/29/63/63	0/2/2/2
17	CLA	A	823	-	1/1/12/20	14/27/99/115	-
17	CLA	B	825	-	1/1/10/20	2/12/88/115	-
17	CLA	B	834	-	1/1/11/20	8/15/91/115	-
17	CLA	5	309	-	1/1/11/20	6/15/91/115	-
20	BCR	B	852	-	-	4/29/63/63	0/2/2/2
17	CLA	B	816	-	1/1/10/20	4/13/89/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	2	505	-	-	13/24/100/115	-
17	CLA	B	840	-	1/1/10/20	3/10/86/115	-
20	BCR	3	305	-	-	7/29/63/63	0/2/2/2
17	CLA	B	837	-	1/1/12/20	4/21/97/115	-
17	CLA	3	306	-	1/1/13/20	12/23/99/115	-
25	CHL	5	314	-	3/3/16/26	9/17/115/137	-
22	DGD	J	103	-	-	26/55/95/95	0/2/2/2
17	CLA	F	803	-	1/1/10/20	4/10/86/115	-
18	PQN	B	843	-	-	8/20/40/43	0/2/2/2
17	CLA	A	804	17	1/1/12/20	4/24/100/115	-
25	CHL	3	315	-	3/3/15/26	3/12/110/137	-
17	CLA	1	505	-	1/1/10/20	4/12/88/115	-
25	CHL	5	315	-	3/3/16/26	6/15/113/137	-
17	CLA	B	819	-	1/1/10/20	0/10/86/115	-
17	CLA	A	812	-	1/1/10/20	2/12/88/115	-
17	CLA	K	202	-	1/1/10/20	5/10/86/115	-
17	CLA	A	852	-	1/1/13/20	10/30/106/115	-
20	BCR	I	101	-	-	4/29/63/63	0/2/2/2
17	CLA	A	816	-	1/1/13/20	12/31/107/115	-
20	BCR	2	503	-	-	8/29/63/63	0/2/2/2
17	CLA	A	805	-	1/1/14/20	17/38/114/115	-
17	CLA	B	835	-	1/1/14/20	6/33/109/115	-
17	CLA	A	814	-	1/1/10/20	2/12/88/115	-
20	BCR	A	853	-	-	2/29/63/63	0/2/2/2
20	BCR	B	846	-	-	5/29/63/63	0/2/2/2
17	CLA	A	827	-	1/1/15/20	16/39/115/115	-
20	BCR	B	845	-	-	6/29/63/63	0/2/2/2
17	CLA	A	817	-	1/1/9/20	2/4/82/115	-
25	CHL	5	317	-	3/3/14/26	4/8/102/137	-
20	BCR	B	848	-	-	2/29/63/63	0/2/2/2
17	CLA	5	308	-	1/1/14/20	14/33/109/115	-
17	CLA	B	811	-	1/1/13/20	9/27/103/115	-
17	CLA	A	830	-	1/1/12/20	1/21/97/115	-
17	CLA	2	508	-	1/1/11/20	3/17/93/115	-
21	SF4	C	101	3	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	LMG	2	518	-	-	3/7/27/70	0/1/1/1
17	CLA	5	311	-	1/1/10/20	3/12/88/115	-
17	CLA	B	802	-	1/1/14/20	6/37/113/115	-
22	DGD	B	850	-	-	20/48/88/95	0/2/2/2
17	CLA	A	842	19	1/1/12/20	10/21/97/115	-
17	CLA	A	809	1	1/1/9/20	3/6/84/115	-
20	BCR	A	849	-	-	2/27/61/63	0/2/2/2
17	CLA	B	805	-	1/1/10/20	4/10/86/115	-
17	CLA	5	312	-	1/1/11/20	7/17/93/115	-
19	LHG	B	851	-	-	17/42/42/53	-
17	CLA	A	826	-	1/1/14/20	12/33/109/115	-
17	CLA	1	506	-	1/1/13/20	9/27/103/115	-
17	CLA	A	831	-	1/1/14/20	14/35/111/115	-
17	CLA	B	829	-	1/1/9/20	2/10/82/115	-
17	CLA	B	823	-	1/1/10/20	4/12/88/115	-
23	LMG	2	519	-	-	14/31/51/70	0/1/1/1
19	LHG	A	843	-	-	12/53/53/53	-
17	CLA	F	802	-	1/1/10/20	4/12/88/115	-
17	CLA	1	507	12	1/1/10/20	3/12/88/115	-
24	LUT	2	501	-	-	0/29/67/67	0/2/2/2
20	BCR	1	503	-	-	4/11/28/63	0/1/1/2
16	CL0	A	801	-	3/3/18/25	6/33/125/135	-
20	BCR	F	801	-	-	6/29/63/63	0/2/2/2
17	CLA	1	513	-	-	18/39/115/115	-
20	BCR	L	305	-	-	8/29/63/63	0/2/2/2
17	CLA	3	316	-	1/1/8/20	0/4/76/115	-
17	CLA	B	804	-	1/1/15/20	14/39/115/115	-
25	CHL	2	513	-	3/3/13/26	7/10/100/137	-
20	BCR	B	849	-	-	2/29/63/63	0/2/2/2
17	CLA	2	506	-	1/1/15/20	13/39/115/115	-
17	CLA	5	305	-	1/1/9/20	0/8/80/115	-
17	CLA	1	504	-	1/1/10/20	3/10/86/115	-
17	CLA	3	318	-	1/1/11/20	6/15/91/115	-
17	CLA	A	806	1	1/1/15/20	19/39/115/115	-
17	CLA	B	826	-	1/1/14/20	8/36/112/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	L	304	-	1/1/11/20	6/15/91/115	-
17	CLA	5	307	15	1/1/15/20	17/39/115/115	-
17	CLA	B	806	-	1/1/8/20	2/10/79/115	-
17	CLA	B	824	-	1/1/11/20	6/15/91/115	-
17	CLA	5	313	15	1/1/9/20	4/10/82/115	-
25	CHL	2	515	-	3/3/16/26	5/15/111/137	-
17	CLA	L	303	-	1/1/12/20	10/24/100/115	-
17	CLA	3	308	-	1/1/13/20	12/27/103/115	-
21	SF4	C	102	3	-	-	0/6/5/5
17	CLA	1	511	-	1/1/11/20	6/17/93/115	-
17	CLA	B	801	-	1/1/15/20	8/39/115/115	-
17	CLA	1	508	-	1/1/9/20	2/10/82/115	-
17	CLA	B	838	-	1/1/15/20	2/39/115/115	-
17	CLA	A	834	1	1/1/10/20	3/10/86/115	-
24	LUT	1	501	-	-	2/29/67/67	0/2/2/2
17	CLA	A	813	-	1/1/11/20	8/15/91/115	-
17	CLA	2	510	19	1/1/14/20	14/33/109/115	-
17	CLA	3	309	-	-	2/10/86/115	-
20	BCR	A	847	-	-	2/29/63/63	0/2/2/2
26	XAT	5	304	-	-	2/31/93/93	0/4/4/4
20	BCR	B	847	-	-	5/29/63/63	0/2/2/2
17	CLA	B	827	-	1/1/10/20	2/10/86/115	-
20	BCR	K	204	-	-	8/29/63/63	0/2/2/2
17	CLA	A	822	-	1/1/10/20	4/10/86/115	-
17	CLA	5	306	-	1/1/10/20	4/8/84/115	-
17	CLA	L	301	-	1/1/13/20	4/29/105/115	-
17	CLA	2	509	-	1/1/12/20	7/21/97/115	-
25	CHL	1	512	-	3/3/16/26	8/17/115/137	-
23	LMG	F	805	-	-	4/25/45/70	0/1/1/1
20	BCR	L	306	-	-	6/29/63/63	0/2/2/2
17	CLA	B	807	2	1/1/15/20	7/39/115/115	-
17	CLA	3	314	14	1/1/13/20	13/27/103/115	-
17	CLA	A	829	-	1/1/13/20	5/27/103/115	-
17	CLA	2	504	13	1/1/7/20	2/4/73/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	B	841	-	1/1/12/20	11/26/102/115	-
25	CHL	1	517	12	3/3/14/26	5/10/104/137	-
17	CLA	B	831	-	1/1/10/20	2/13/89/115	-
17	CLA	A	838	-	1/1/15/20	13/39/115/115	-
17	CLA	3	301	-	1/1/10/20	4/10/86/115	-
17	CLA	B	839	-	1/1/11/20	5/18/94/115	-
18	PQN	A	841	-	-	13/23/43/43	0/2/2/2
21	SF4	A	850	2,1	-	-	0/6/5/5
17	CLA	A	836	-	1/1/13/20	10/27/103/115	-
17	CLA	A	820	-	1/1/13/20	10/30/106/115	-
17	CLA	A	824	-	1/1/9/20	4/10/82/115	-
17	CLA	B	812	-	1/1/13/20	7/25/101/115	-
17	CLA	A	828	-	1/1/10/20	2/10/86/115	-
17	CLA	A	815	-	1/1/11/20	4/15/91/115	-
17	CLA	B	809	-	1/1/9/20	4/10/82/115	-
17	CLA	L	302	-	1/1/9/20	2/10/82/115	-
17	CLA	5	310	-	1/1/12/20	8/21/97/115	-
17	CLA	B	820	-	1/1/12/20	7/25/101/115	-
17	CLA	K	203	-	1/1/9/20	5/10/82/115	-
17	CLA	B	830	-	1/1/13/20	10/29/105/115	-
17	CLA	3	311	-	1/1/12/20	9/21/97/115	-
17	CLA	B	808	-	1/1/12/20	5/24/100/115	-
20	BCR	A	845	-	-	4/29/63/63	0/2/2/2
17	CLA	K	205	10	1/1/9/20	2/8/80/115	-
17	CLA	B	803	-	1/1/15/20	16/39/115/115	-
20	BCR	F	804	-	-	2/29/63/63	0/2/2/2

All (1487) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	1	514	CHL	C2C-C3C	11.16	1.47	1.36
25	2	516	CHL	C1D-C2D	10.32	1.51	1.39
25	1	512	CHL	C2C-C3C	10.25	1.46	1.36
25	1	512	CHL	C1D-C2D	10.22	1.51	1.39
25	1	517	CHL	C1D-C2D	10.13	1.51	1.39
25	1	514	CHL	C1D-C2D	10.12	1.51	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	2	515	CHL	C2C-C3C	10.07	1.46	1.36
25	5	314	CHL	C1D-C2D	10.04	1.51	1.39
25	2	512	CHL	C1D-C2D	10.03	1.51	1.39
25	2	513	CHL	C2C-C3C	10.01	1.46	1.36
25	5	317	CHL	C1D-C2D	10.00	1.50	1.39
25	5	314	CHL	C2C-C3C	9.89	1.45	1.36
25	2	515	CHL	C1D-C2D	9.81	1.50	1.39
25	3	302	CHL	C2C-C3C	9.72	1.45	1.36
25	2	513	CHL	C1D-C2D	9.69	1.50	1.39
16	A	801	CL0	C1A-CHA	9.66	1.51	1.40
25	5	315	CHL	C1D-C2D	9.57	1.50	1.39
25	1	517	CHL	C2C-C3C	9.45	1.45	1.36
25	3	315	CHL	C1D-C2D	9.40	1.50	1.39
25	3	315	CHL	C2C-C3C	9.39	1.45	1.36
25	2	516	CHL	C2C-C3C	9.32	1.45	1.36
16	A	801	CL0	C1D-C2D	9.25	1.50	1.39
25	2	512	CHL	C2C-C3C	9.22	1.45	1.36
25	3	302	CHL	C1D-C2D	9.12	1.49	1.39
25	5	315	CHL	C2C-C3C	9.04	1.45	1.36
16	A	801	CL0	C1B-C2B	8.74	1.49	1.39
25	1	512	CHL	C1B-C2B	8.32	1.49	1.39
25	5	314	CHL	C1B-C2B	8.25	1.48	1.39
25	1	514	CHL	C1B-C2B	8.24	1.48	1.39
25	2	515	CHL	C1B-C2B	8.22	1.48	1.39
25	3	302	CHL	C1B-C2B	8.15	1.48	1.39
25	5	315	CHL	C1B-C2B	8.01	1.48	1.39
25	2	512	CHL	C1B-C2B	8.00	1.48	1.39
25	1	514	CHL	C3B-C4B	7.70	1.48	1.41
25	1	517	CHL	C1B-C2B	7.58	1.48	1.39
25	2	515	CHL	C4B-C3B	7.52	1.48	1.39
25	1	512	CHL	C3B-C4B	7.41	1.48	1.41
25	5	317	CHL	C3B-C4B	7.36	1.48	1.41
25	2	516	CHL	C1B-C2B	7.36	1.47	1.39
25	3	315	CHL	C1B-C2B	7.35	1.47	1.39
25	5	314	CHL	C3B-C4B	7.22	1.48	1.41
25	2	513	CHL	C1B-C2B	7.17	1.47	1.39
25	5	317	CHL	C1B-C2B	7.15	1.47	1.39
25	3	302	CHL	C3B-C4B	7.07	1.48	1.41
25	1	512	CHL	C1A-CHA	7.06	1.48	1.40
25	3	302	CHL	C1A-CHA	7.04	1.48	1.40
25	5	314	CHL	C1A-CHA	7.01	1.48	1.40
25	2	513	CHL	C3B-C4B	7.00	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	841	PQN	C3-C2	6.86	1.47	1.35
25	1	514	CHL	C1A-CHA	6.84	1.48	1.39
25	3	315	CHL	C3B-C4B	6.84	1.48	1.41
25	2	512	CHL	C4B-C3B	6.77	1.47	1.39
25	1	517	CHL	C3B-C4B	6.72	1.47	1.41
25	2	516	CHL	C3A-C2A	-6.68	1.48	1.54
25	2	512	CHL	C1A-CHA	6.66	1.47	1.40
25	5	315	CHL	C1A-CHA	6.65	1.47	1.40
25	2	516	CHL	C1A-CHA	6.61	1.47	1.40
17	2	507	CLA	C2-C3	6.59	1.52	1.33
25	5	315	CHL	C3B-C4B	6.57	1.47	1.41
25	5	317	CHL	C1A-CHA	6.46	1.47	1.40
25	5	315	CHL	C3D-C4D	-6.44	1.31	1.41
25	2	515	CHL	C3A-C2A	-6.43	1.49	1.54
18	B	843	PQN	C3-C2	6.32	1.46	1.35
25	2	516	CHL	C4B-C3B	6.20	1.46	1.39
25	2	513	CHL	C1A-CHA	6.18	1.47	1.39
25	1	517	CHL	C1A-CHA	6.01	1.47	1.39
25	2	515	CHL	C1A-CHA	5.93	1.46	1.40
25	2	516	CHL	C3D-C4D	-5.72	1.32	1.41
25	1	514	CHL	C3D-C4D	-5.72	1.32	1.41
25	1	517	CHL	C3D-C4D	-5.72	1.32	1.41
25	2	515	CHL	C3D-C4D	-5.69	1.32	1.41
25	3	302	CHL	C3D-C4D	-5.63	1.32	1.41
25	2	512	CHL	C3A-C2A	-5.57	1.49	1.54
25	3	315	CHL	C3D-C4D	-5.55	1.33	1.41
25	5	317	CHL	C3D-C4D	-5.52	1.33	1.41
25	2	512	CHL	C3D-C4D	-5.50	1.33	1.41
25	3	302	CHL	C3A-C2A	-5.46	1.50	1.54
25	1	514	CHL	CHC-C4B	5.44	1.48	1.39
25	5	314	CHL	C3D-C4D	-5.41	1.33	1.41
25	3	315	CHL	C1A-CHA	5.40	1.46	1.40
25	2	516	CHL	CHB-C4A	-5.36	1.32	1.38
25	3	302	CHL	CHB-C4A	-5.36	1.32	1.38
25	1	512	CHL	C3D-C4D	-5.31	1.33	1.41
25	1	514	CHL	CHD-C4C	5.28	1.49	1.39
25	2	513	CHL	CHB-C4A	-5.21	1.32	1.38
25	1	514	CHL	C3B-C2B	5.21	1.47	1.40
25	1	514	CHL	OBD-CAD	5.20	1.29	1.22
25	2	512	CHL	O2D-CGD	5.20	1.46	1.33
25	5	314	CHL	CHB-C4A	-5.16	1.32	1.38
25	1	514	CHL	CHD-C1D	5.16	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	1	512	CHL	O2D-CGD	5.13	1.45	1.33
25	5	315	CHL	C3A-C2A	-5.04	1.50	1.54
25	1	514	CHL	C3D-C2D	5.04	1.48	1.39
25	1	512	CHL	OBD-CAD	5.01	1.28	1.22
25	2	515	CHL	CHB-C4A	-5.00	1.32	1.38
25	2	513	CHL	O2D-CGD	5.00	1.45	1.33
25	5	317	CHL	O2D-CGD	4.99	1.45	1.33
25	2	515	CHL	O2D-CGD	4.98	1.45	1.33
25	1	517	CHL	O2D-CGD	4.97	1.45	1.33
25	3	315	CHL	O2D-CGD	4.97	1.45	1.33
25	5	314	CHL	O2D-CGD	4.95	1.45	1.33
25	1	512	CHL	C3B-C2B	4.94	1.47	1.40
25	1	514	CHL	CHB-C1B	4.93	1.47	1.39
25	3	315	CHL	CHC-C4B	4.90	1.47	1.39
25	2	516	CHL	O2D-CGD	4.87	1.45	1.33
25	3	315	CHL	OBD-CAD	4.86	1.28	1.22
25	1	517	CHL	CHC-C4B	4.86	1.47	1.39
25	5	317	CHL	CHC-C4B	4.84	1.47	1.39
25	3	315	CHL	CHB-C4A	-4.83	1.32	1.38
25	1	512	CHL	CHC-C4B	4.81	1.47	1.39
25	1	514	CHL	O2D-CGD	4.80	1.45	1.33
25	1	512	CHL	CHB-C1B	4.74	1.47	1.39
25	1	512	CHL	CHD-C1D	4.73	1.47	1.39
25	3	302	CHL	OBD-CAD	4.73	1.28	1.22
25	2	515	CHL	CHD-C4C	4.72	1.48	1.39
25	1	512	CHL	CHD-C4C	4.72	1.48	1.39
25	2	515	CHL	CHC-C4B	4.70	1.47	1.39
25	1	514	CHL	CHC-C1C	4.69	1.48	1.39
25	5	314	CHL	CHC-C4B	4.66	1.47	1.39
25	2	512	CHL	CHB-C4A	-4.63	1.33	1.38
25	3	302	CHL	O2D-CGD	4.62	1.44	1.33
25	5	314	CHL	OBD-CAD	4.62	1.28	1.22
25	2	516	CHL	OBD-CAD	4.61	1.28	1.22
25	5	317	CHL	CHD-C4C	4.61	1.48	1.39
25	2	515	CHL	CHD-C1D	4.60	1.47	1.39
25	5	314	CHL	C3B-C2B	4.60	1.46	1.40
25	5	315	CHL	O2D-CGD	4.59	1.44	1.33
25	5	315	CHL	CHB-C4A	-4.57	1.33	1.38
25	2	516	CHL	CHD-C4C	4.54	1.48	1.39
25	3	302	CHL	C3B-C2B	4.54	1.46	1.40
25	5	314	CHL	CHD-C4C	4.53	1.48	1.39
25	2	515	CHL	O2A-CGA	4.53	1.45	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	5	315	CHL	CHB-C1B	4.52	1.46	1.39
25	3	315	CHL	C3A-C2A	-4.52	1.50	1.54
25	1	512	CHL	CHB-C4A	-4.50	1.33	1.38
25	2	512	CHL	CHD-C4C	4.50	1.48	1.39
25	2	512	CHL	CHC-C4B	4.50	1.46	1.39
25	2	512	CHL	OBD-CAD	4.50	1.28	1.22
25	2	516	CHL	CHD-C1D	4.49	1.46	1.39
25	1	517	CHL	CHD-C1D	4.49	1.46	1.39
25	5	315	CHL	O2A-CGA	4.48	1.45	1.30
25	2	512	CHL	CHD-C1D	4.47	1.46	1.39
25	2	513	CHL	CHC-C4B	4.46	1.46	1.39
25	3	302	CHL	CHD-C1D	4.46	1.46	1.39
25	5	317	CHL	CHD-C1D	4.46	1.46	1.39
25	1	512	CHL	C3D-C2D	4.45	1.47	1.39
25	5	317	CHL	C2C-C3C	4.44	1.46	1.37
25	5	317	CHL	OBD-CAD	4.44	1.28	1.22
25	5	317	CHL	C3B-C2B	4.42	1.46	1.40
25	5	315	CHL	OBD-CAD	4.42	1.28	1.22
25	1	517	CHL	OBD-CAD	4.42	1.28	1.22
25	1	517	CHL	CHB-C4A	-4.42	1.33	1.38
25	5	317	CHL	C3D-C2D	4.41	1.47	1.39
25	3	302	CHL	CHD-C4C	4.41	1.47	1.39
16	A	801	CL0	C3A-C4A	-4.38	1.47	1.50
25	3	315	CHL	CHB-C1B	4.38	1.46	1.39
25	2	513	CHL	CHB-C1B	4.37	1.46	1.39
25	3	302	CHL	CHC-C4B	4.37	1.46	1.39
17	3	309	CLA	C1B-C2B	4.37	1.48	1.41
23	F	805	LMG	O8-C28	4.36	1.46	1.33
25	1	517	CHL	C3B-C2B	4.36	1.46	1.40
25	2	512	CHL	CHB-C1B	4.35	1.46	1.39
25	3	315	CHL	CHC-C1C	4.35	1.47	1.39
23	5	301	LMG	O8-C28	4.34	1.46	1.33
25	5	315	CHL	CHD-C1D	4.34	1.46	1.39
25	2	515	CHL	OBD-CAD	4.33	1.28	1.22
19	A	844	LHG	O8-C23	4.32	1.45	1.33
25	1	517	CHL	CHC-C1C	4.32	1.47	1.39
25	2	512	CHL	O2A-CGA	4.31	1.46	1.33
25	5	315	CHL	CHD-C4C	4.31	1.47	1.39
25	2	513	CHL	CHD-C1D	4.31	1.46	1.39
17	3	309	CLA	C3B-C4B	4.30	1.48	1.39
25	1	517	CHL	CHD-C4C	4.30	1.47	1.39
25	1	512	CHL	CHC-C1C	4.29	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	1	517	CHL	CHB-C1B	4.29	1.46	1.39
25	3	302	CHL	CHC-C1C	4.28	1.47	1.39
25	3	302	CHL	C3D-C2D	4.28	1.46	1.39
25	2	516	CHL	CHC-C4B	4.28	1.46	1.39
25	5	314	CHL	CHD-C1D	4.28	1.46	1.39
25	2	513	CHL	CHD-C4C	4.27	1.47	1.39
25	5	314	CHL	C3D-C2D	4.25	1.46	1.39
19	B	851	LHG	O8-C23	4.25	1.45	1.33
25	5	314	CHL	CHB-C1B	4.25	1.46	1.39
19	B	851	LHG	O7-C7	4.25	1.46	1.34
25	5	314	CHL	O2A-CGA	4.24	1.46	1.33
17	A	817	CLA	O1D-CGD	4.23	1.36	1.20
25	1	512	CHL	C3A-C2A	-4.22	1.51	1.54
25	2	515	CHL	CHB-C1B	4.20	1.46	1.39
25	2	512	CHL	CHC-C1C	4.19	1.47	1.39
25	1	512	CHL	O2A-CGA	4.16	1.45	1.33
25	3	302	CHL	CHB-C1B	4.16	1.46	1.39
23	2	519	LMG	O8-C28	4.16	1.45	1.33
19	1	516	LHG	O8-C23	4.15	1.45	1.33
22	B	850	DGD	O1G-C1A	4.15	1.45	1.33
25	3	315	CHL	C3D-C2D	4.14	1.46	1.39
22	J	103	DGD	O1G-C1A	4.13	1.45	1.33
25	5	314	CHL	C3A-C2A	-4.09	1.51	1.54
25	5	315	CHL	C3B-C2B	4.08	1.45	1.40
23	2	519	LMG	O7-C10	4.05	1.45	1.34
25	5	314	CHL	CHC-C1C	4.05	1.47	1.39
23	5	301	LMG	O7-C10	4.04	1.45	1.34
25	5	317	CHL	CHB-C1B	4.03	1.46	1.39
23	F	805	LMG	O7-C10	4.03	1.45	1.34
25	2	515	CHL	C3D-C2D	4.02	1.46	1.39
25	3	302	CHL	O2A-CGA	4.01	1.45	1.33
25	2	516	CHL	CHC-C1C	4.01	1.47	1.39
22	J	103	DGD	O2G-C1B	4.01	1.45	1.34
17	5	305	CLA	C3B-C4B	4.01	1.48	1.39
19	A	843	LHG	O8-C23	4.00	1.45	1.33
25	2	516	CHL	CHB-C1B	4.00	1.46	1.39
20	I	101	BCR	C30-C25	-3.99	1.48	1.53
25	5	315	CHL	CHC-C4B	3.99	1.46	1.39
25	1	514	CHL	CHB-C4A	-3.97	1.33	1.38
25	3	315	CHL	CHD-C4C	3.94	1.46	1.39
19	2	517	LHG	O8-C23	3.93	1.44	1.33
25	2	516	CHL	C3D-C2D	3.93	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	2	513	CHL	C3B-C2B	3.93	1.45	1.40
23	F	806	LMG	O8-C28	3.92	1.44	1.33
25	2	515	CHL	CHC-C1C	3.91	1.46	1.39
23	F	806	LMG	O7-C10	3.91	1.45	1.34
25	2	513	CHL	CHC-C1C	3.90	1.46	1.39
19	2	517	LHG	O7-C7	3.89	1.45	1.34
20	I	101	BCR	C1-C6	-3.84	1.48	1.53
19	1	516	LHG	O7-C7	3.83	1.45	1.34
25	5	317	CHL	CHC-C1C	3.83	1.46	1.39
20	B	852	BCR	C30-C25	-3.80	1.48	1.53
25	3	315	CHL	C3B-C2B	3.80	1.45	1.40
25	1	517	CHL	C3D-C2D	3.79	1.46	1.39
25	2	512	CHL	C3D-C2D	3.77	1.46	1.39
17	B	812	CLA	CAB-C3B	-3.76	1.43	1.50
19	A	844	LHG	O7-C7	3.75	1.44	1.34
20	B	845	BCR	C30-C25	-3.73	1.49	1.53
17	5	305	CLA	C1B-C2B	3.70	1.47	1.41
18	A	841	PQN	C10-C5	3.70	1.46	1.40
17	1	511	CLA	C1D-ND	3.70	1.42	1.37
25	3	315	CHL	CHD-C1D	3.68	1.45	1.39
19	A	843	LHG	O7-C7	3.68	1.44	1.34
25	5	315	CHL	CBD-CGD	-3.66	1.47	1.52
22	B	850	DGD	O2G-C1B	3.65	1.44	1.34
16	A	801	CL0	C4B-C3B	3.62	1.43	1.39
17	1	515	CLA	CAD-C3D	-3.62	1.45	1.50
25	5	315	CHL	CHC-C1C	3.62	1.46	1.39
20	F	804	BCR	C1-C6	-3.61	1.49	1.53
17	3	307	CLA	C4B-NB	3.59	1.42	1.37
20	A	845	BCR	C1-C6	-3.56	1.49	1.53
17	A	829	CLA	CMB-C2B	-3.55	1.43	1.50
20	A	845	BCR	C30-C25	-3.49	1.49	1.53
17	1	513	CLA	C1D-ND	3.45	1.42	1.37
17	2	508	CLA	C1D-ND	3.44	1.42	1.37
17	3	307	CLA	C1D-ND	3.42	1.42	1.37
25	5	315	CHL	C3D-C2D	3.42	1.45	1.39
20	B	847	BCR	C30-C25	-3.41	1.49	1.53
17	A	831	CLA	CAB-C3B	-3.41	1.43	1.50
17	3	312	CLA	C1D-ND	3.38	1.42	1.37
17	1	504	CLA	C1D-ND	3.36	1.42	1.37
18	B	843	PQN	C10-C5	3.35	1.46	1.40
17	A	823	CLA	C2A-C1A	-3.35	1.50	1.53
17	1	513	CLA	C4B-NB	3.33	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B	852	BCR	C1-C6	-3.31	1.49	1.53
17	B	813	CLA	C1D-ND	3.30	1.42	1.37
17	2	504	CLA	C1D-ND	3.30	1.42	1.37
25	5	317	CHL	CHB-C4A	-3.30	1.33	1.38
17	3	313	CLA	C1D-ND	3.30	1.42	1.37
17	1	509	CLA	C1D-ND	3.29	1.42	1.37
26	5	304	XAT	O24-C25	-3.29	1.42	1.46
17	K	202	CLA	C1D-ND	3.27	1.42	1.37
20	A	846	BCR	C1-C6	-3.25	1.49	1.53
17	A	838	CLA	C1D-ND	3.24	1.42	1.37
17	L	302	CLA	C1D-ND	3.23	1.42	1.37
17	3	306	CLA	C1D-ND	3.23	1.42	1.37
26	5	304	XAT	C22-C21	-3.23	1.49	1.54
25	3	302	CHL	CBD-CGD	-3.23	1.48	1.52
17	1	515	CLA	C1D-ND	3.22	1.42	1.37
17	B	830	CLA	CMB-C2B	-3.20	1.44	1.50
17	B	821	CLA	C1D-ND	3.20	1.42	1.37
17	F	802	CLA	C1D-ND	3.20	1.42	1.37
17	B	829	CLA	CMB-C2B	-3.19	1.44	1.50
17	A	815	CLA	C1D-ND	3.18	1.42	1.37
17	3	307	CLA	C1B-C2B	3.18	1.50	1.43
17	J	101	CLA	C1D-ND	3.17	1.42	1.37
17	2	509	CLA	C1D-ND	3.17	1.42	1.37
17	A	836	CLA	CMB-C2B	-3.16	1.44	1.50
17	3	313	CLA	C4B-NB	3.14	1.42	1.37
17	3	318	CLA	CAB-C3B	-3.14	1.44	1.50
17	2	507	CLA	C1D-ND	3.13	1.42	1.37
17	1	505	CLA	C4B-NB	3.12	1.42	1.37
17	3	310	CLA	C4B-NB	3.12	1.42	1.37
17	5	312	CLA	C1D-ND	3.12	1.42	1.37
17	B	814	CLA	C1B-NB	-3.12	1.33	1.37
17	K	205	CLA	C4B-NB	3.11	1.42	1.37
25	3	315	CHL	CBD-CGD	-3.10	1.48	1.52
20	B	844	BCR	C30-C25	-3.10	1.49	1.53
20	B	848	BCR	C30-C25	-3.09	1.49	1.53
20	K	204	BCR	C30-C25	-3.08	1.49	1.53
17	2	511	CLA	C1D-ND	3.06	1.41	1.37
17	A	823	CLA	C1D-ND	3.06	1.41	1.37
17	A	826	CLA	C1B-NB	-3.05	1.33	1.37
17	5	310	CLA	C1D-ND	3.05	1.41	1.37
17	5	307	CLA	C1D-ND	3.04	1.41	1.37
20	A	849	BCR	C30-C25	-3.04	1.49	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	1	506	CLA	C1D-ND	3.03	1.41	1.37
25	2	513	CHL	C3D-C2D	3.02	1.46	1.37
17	1	505	CLA	C1D-ND	3.02	1.41	1.37
17	A	818	CLA	CMB-C2B	-3.01	1.44	1.50
17	F	803	CLA	C1D-ND	3.00	1.41	1.37
17	B	815	CLA	CMB-C2B	-3.00	1.44	1.50
20	L	306	BCR	C1-C6	-3.00	1.49	1.53
17	1	508	CLA	C1D-ND	2.99	1.41	1.37
17	1	510	CLA	C4B-NB	2.99	1.41	1.37
17	3	310	CLA	C1D-ND	2.99	1.41	1.37
17	3	308	CLA	C1D-ND	2.99	1.41	1.37
17	A	809	CLA	C2D-C1D	2.99	1.47	1.42
17	K	205	CLA	C1D-ND	2.97	1.41	1.37
17	B	820	CLA	CMB-C2B	-2.97	1.44	1.50
17	A	803	CLA	C1D-ND	2.97	1.41	1.37
17	B	815	CLA	CMC-C2C	-2.97	1.44	1.50
17	A	835	CLA	C1B-NB	-2.97	1.34	1.37
17	A	835	CLA	CMC-C2C	-2.96	1.44	1.50
17	2	506	CLA	C1D-ND	2.96	1.41	1.37
17	3	314	CLA	C4B-NB	2.96	1.41	1.37
17	B	826	CLA	C1B-NB	-2.95	1.34	1.37
17	A	825	CLA	C1D-ND	2.93	1.41	1.37
17	B	830	CLA	C4B-NB	2.93	1.41	1.37
17	B	813	CLA	CMD-C2D	-2.92	1.44	1.50
20	3	305	BCR	C30-C25	-2.92	1.50	1.53
17	B	838	CLA	C1D-ND	2.92	1.41	1.37
17	1	506	CLA	C4B-NB	2.92	1.41	1.37
17	A	812	CLA	C1B-NB	-2.91	1.34	1.37
17	A	830	CLA	C1B-NB	-2.91	1.34	1.37
17	A	842	CLA	C1D-ND	2.91	1.41	1.37
17	A	817	CLA	C3A-C2A	-2.90	1.52	1.54
20	B	846	BCR	C30-C25	-2.89	1.50	1.53
20	L	305	BCR	C30-C25	-2.87	1.50	1.53
17	3	312	CLA	C4B-NB	2.87	1.41	1.37
17	5	309	CLA	C1D-ND	2.87	1.41	1.37
20	A	848	BCR	C1-C6	-2.87	1.50	1.53
17	B	806	CLA	C1D-ND	2.86	1.41	1.37
17	B	831	CLA	C1D-ND	2.86	1.41	1.37
17	3	317	CLA	C1D-ND	2.85	1.41	1.37
20	A	849	BCR	C1-C6	-2.85	1.50	1.53
17	A	824	CLA	CMB-C2B	-2.85	1.44	1.50
17	3	306	CLA	CAB-C3B	-2.85	1.44	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	2	510	CLA	C4B-NB	2.85	1.41	1.37
24	1	501	LUT	C22-C21	-2.85	1.51	1.54
17	3	301	CLA	CMB-C2B	-2.84	1.44	1.50
17	B	837	CLA	MG-NB	-2.84	2.00	2.05
25	1	514	CHL	CBD-CGD	-2.83	1.48	1.52
20	J	102	BCR	C1-C6	-2.83	1.50	1.53
17	A	834	CLA	C1D-ND	2.83	1.41	1.37
17	A	833	CLA	CMB-C2B	-2.83	1.45	1.50
17	A	826	CLA	CMC-C2C	-2.83	1.45	1.50
17	A	821	CLA	C4B-NB	2.83	1.41	1.37
17	A	817	CLA	CMB-C2B	-2.83	1.45	1.50
17	B	820	CLA	CMC-C2C	-2.82	1.45	1.50
17	A	805	CLA	MG-NB	-2.82	2.00	2.05
17	3	318	CLA	C1D-ND	2.82	1.41	1.37
17	B	809	CLA	C1D-ND	2.82	1.41	1.37
17	B	836	CLA	C1D-ND	2.81	1.41	1.37
17	1	508	CLA	C4B-NB	2.81	1.41	1.37
17	B	810	CLA	CMC-C2C	-2.81	1.45	1.50
17	B	833	CLA	C1D-ND	2.81	1.41	1.37
17	B	830	CLA	CMC-C2C	-2.80	1.45	1.50
17	L	303	CLA	CMB-C2B	-2.80	1.45	1.50
17	B	809	CLA	CMD-C2D	-2.79	1.45	1.50
17	5	308	CLA	C1D-ND	2.79	1.41	1.37
17	5	313	CLA	C1D-ND	2.79	1.41	1.37
20	K	204	BCR	C1-C6	-2.79	1.50	1.53
17	A	819	CLA	CMB-C2B	-2.78	1.45	1.50
17	A	802	CLA	C1D-ND	2.78	1.41	1.37
24	5	303	LUT	C1-C6	-2.78	1.50	1.53
17	3	310	CLA	C1B-C2B	2.78	1.49	1.43
17	A	819	CLA	C1B-NB	-2.78	1.34	1.37
17	B	816	CLA	CMD-C2D	-2.78	1.45	1.50
20	A	853	BCR	C1-C6	-2.78	1.50	1.53
17	3	316	CLA	C4B-NB	2.78	1.41	1.37
17	B	821	CLA	CMD-C2D	-2.77	1.45	1.50
17	B	838	CLA	CMB-C2B	-2.77	1.45	1.50
17	2	507	CLA	C4B-NB	2.77	1.41	1.37
17	B	836	CLA	C4B-NB	2.77	1.41	1.37
17	A	820	CLA	CMB-C2B	-2.77	1.45	1.50
17	B	816	CLA	C1D-ND	2.77	1.41	1.37
17	B	803	CLA	CMC-C2C	-2.77	1.45	1.50
20	A	848	BCR	C30-C25	-2.77	1.50	1.53
17	A	816	CLA	C1D-ND	2.77	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	B	801	CLA	CMC-C2C	-2.77	1.45	1.50
17	A	811	CLA	MG-NB	-2.77	2.00	2.05
17	A	811	CLA	CMD-C2D	-2.76	1.45	1.50
17	A	810	CLA	CMB-C2B	-2.76	1.45	1.50
17	K	203	CLA	MG-NB	-2.76	2.00	2.05
17	5	310	CLA	C4B-NB	2.76	1.41	1.37
17	B	827	CLA	CMD-C2D	-2.76	1.45	1.50
17	B	821	CLA	C4B-NB	2.76	1.41	1.37
17	5	306	CLA	C1D-ND	2.75	1.41	1.37
17	B	812	CLA	CMB-C2B	-2.75	1.45	1.50
17	A	812	CLA	CMC-C2C	-2.75	1.45	1.50
17	J	101	CLA	C4B-NB	2.75	1.41	1.37
17	B	813	CLA	C1B-NB	-2.74	1.34	1.37
17	A	832	CLA	CMB-C2B	-2.74	1.45	1.50
17	B	842	CLA	C1D-ND	2.74	1.41	1.37
17	1	515	CLA	C4B-NB	2.74	1.41	1.37
17	B	802	CLA	C1D-ND	2.74	1.41	1.37
17	B	835	CLA	C1D-ND	2.74	1.41	1.37
26	5	304	XAT	O4-C5	-2.74	1.42	1.46
17	A	838	CLA	CMD-C2D	-2.74	1.45	1.50
17	A	831	CLA	C1B-NB	-2.74	1.34	1.37
17	3	317	CLA	C4B-NB	2.73	1.41	1.37
17	A	816	CLA	MG-NB	-2.73	2.00	2.05
17	1	509	CLA	C4B-NB	2.73	1.41	1.37
17	B	834	CLA	CMB-C2B	-2.72	1.45	1.50
17	B	814	CLA	CMD-C2D	-2.71	1.45	1.50
26	2	502	XAT	O4-C5	-2.71	1.42	1.46
17	A	816	CLA	CMD-C2D	-2.71	1.45	1.50
17	B	824	CLA	CMD-C2D	-2.71	1.45	1.50
17	A	852	CLA	C1D-ND	2.71	1.41	1.37
17	B	824	CLA	CMB-C2B	-2.71	1.45	1.50
17	A	829	CLA	C1B-NB	-2.71	1.34	1.37
17	1	505	CLA	C1B-C2B	2.71	1.49	1.43
17	B	810	CLA	MG-NB	-2.71	2.00	2.05
17	B	817	CLA	C1D-ND	2.70	1.41	1.37
17	F	803	CLA	MG-NB	-2.70	2.00	2.05
17	B	811	CLA	CMB-C2B	-2.70	1.45	1.50
17	B	820	CLA	C4B-NB	2.70	1.41	1.37
17	A	829	CLA	MG-NB	-2.70	2.00	2.05
17	3	309	CLA	C1D-ND	2.70	1.41	1.37
17	5	310	CLA	C1B-C2B	2.70	1.49	1.43
17	B	809	CLA	CMB-C2B	-2.70	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	B	839	CLA	C1D-ND	2.70	1.41	1.37
17	5	316	CLA	C1D-ND	2.70	1.41	1.37
17	B	819	CLA	CMD-C2D	-2.70	1.45	1.50
17	B	823	CLA	C1D-ND	2.70	1.41	1.37
17	A	814	CLA	CMD-C2D	-2.69	1.45	1.50
17	B	806	CLA	CMD-C2D	-2.69	1.45	1.50
17	1	511	CLA	MG-NB	-2.69	2.00	2.05
17	A	852	CLA	CMB-C2B	-2.69	1.45	1.50
17	B	834	CLA	C1D-ND	2.69	1.41	1.37
17	A	835	CLA	CMB-C2B	-2.69	1.45	1.50
25	3	315	CHL	CHA-CBD	-2.69	1.48	1.51
17	A	815	CLA	MG-NB	-2.69	2.00	2.05
17	2	510	CLA	C1D-ND	2.69	1.41	1.37
17	L	304	CLA	CMD-C2D	-2.68	1.45	1.50
17	B	819	CLA	CMB-C2B	-2.68	1.45	1.50
17	A	809	CLA	CMC-C2C	-2.68	1.45	1.50
17	K	201	CLA	C4B-NB	2.68	1.41	1.37
17	B	831	CLA	CMB-C2B	-2.68	1.45	1.50
17	B	822	CLA	C4B-NB	2.68	1.41	1.37
17	A	817	CLA	MG-NB	-2.67	2.00	2.05
20	A	847	BCR	C30-C25	-2.67	1.50	1.53
17	A	831	CLA	CMC-C2C	-2.67	1.45	1.50
17	B	803	CLA	MG-NB	-2.67	2.00	2.05
17	B	806	CLA	MG-NB	-2.67	2.00	2.05
17	B	823	CLA	MG-NB	-2.67	2.00	2.05
17	A	830	CLA	CMB-C2B	-2.67	1.45	1.50
17	B	831	CLA	CMD-C2D	-2.66	1.45	1.50
17	2	506	CLA	CMB-C2B	-2.66	1.45	1.50
17	B	813	CLA	CMB-C2B	-2.66	1.45	1.50
17	A	828	CLA	CMD-C2D	-2.66	1.45	1.50
17	B	816	CLA	CMC-C2C	-2.66	1.45	1.50
17	A	838	CLA	CMB-C2B	-2.66	1.45	1.50
17	1	510	CLA	C3B-C4B	2.66	1.50	1.42
17	A	818	CLA	MG-NB	-2.66	2.00	2.05
17	B	839	CLA	MG-NB	-2.66	2.00	2.05
17	B	801	CLA	MG-NB	-2.66	2.00	2.05
17	A	834	CLA	CMB-C2B	-2.65	1.45	1.50
17	A	836	CLA	CMD-C2D	-2.65	1.45	1.50
17	B	808	CLA	MG-NB	-2.65	2.00	2.05
17	A	840	CLA	MG-NB	-2.65	2.00	2.05
17	A	822	CLA	C1D-ND	2.65	1.41	1.37
17	3	306	CLA	C4B-C3B	2.65	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	B	805	CLA	CMB-C2B	-2.65	1.45	1.50
17	A	826	CLA	MG-NB	-2.65	2.00	2.05
17	A	806	CLA	CMC-C2C	-2.65	1.45	1.50
17	B	838	CLA	CMD-C2D	-2.65	1.45	1.50
17	B	842	CLA	C4B-NB	2.65	1.41	1.37
17	1	504	CLA	MG-NB	-2.65	2.00	2.05
17	A	806	CLA	CMB-C2B	-2.65	1.45	1.50
17	B	826	CLA	CMD-C2D	-2.65	1.45	1.50
17	1	510	CLA	C1D-ND	2.65	1.41	1.37
17	B	813	CLA	CMC-C2C	-2.64	1.45	1.50
17	B	807	CLA	CMC-C2C	-2.64	1.45	1.50
17	3	314	CLA	C1D-ND	2.64	1.41	1.37
17	B	808	CLA	CMD-C2D	-2.64	1.45	1.50
17	A	805	CLA	C1D-ND	2.64	1.41	1.37
17	1	515	CLA	CMD-C2D	-2.64	1.45	1.50
17	B	829	CLA	MG-NB	-2.64	2.00	2.05
17	B	814	CLA	CMC-C2C	-2.64	1.45	1.50
17	A	804	CLA	CMD-C2D	-2.64	1.45	1.50
17	5	305	CLA	CMC-C2C	-2.64	1.45	1.50
17	A	832	CLA	CMD-C2D	-2.64	1.45	1.50
17	A	824	CLA	MG-NB	-2.64	2.00	2.05
17	B	803	CLA	CMD-C2D	-2.63	1.45	1.50
17	5	312	CLA	C4B-NB	2.63	1.41	1.37
17	B	806	CLA	CMC-C2C	-2.63	1.45	1.50
17	A	807	CLA	CMB-C2B	-2.63	1.45	1.50
17	B	830	CLA	MG-NB	-2.63	2.00	2.05
17	B	827	CLA	CMB-C2B	-2.63	1.45	1.50
17	A	806	CLA	C1B-NB	-2.63	1.34	1.37
17	A	831	CLA	MG-NB	-2.63	2.00	2.05
17	A	823	CLA	CMB-C2B	-2.63	1.45	1.50
17	A	837	CLA	CMD-C2D	-2.63	1.45	1.50
17	B	807	CLA	CMB-C2B	-2.63	1.45	1.50
17	A	825	CLA	CMD-C2D	-2.63	1.45	1.50
17	A	828	CLA	C1D-ND	2.63	1.41	1.37
17	A	842	CLA	C4B-NB	2.62	1.41	1.37
17	K	203	CLA	C1B-C2B	2.62	1.49	1.43
17	2	507	CLA	MG-NB	-2.62	2.00	2.05
17	A	830	CLA	CMD-C2D	-2.62	1.45	1.50
17	A	825	CLA	MG-NB	-2.62	2.00	2.05
17	B	811	CLA	CMC-C2C	-2.62	1.45	1.50
17	A	822	CLA	MG-NB	-2.62	2.00	2.05
17	A	824	CLA	CMD-C2D	-2.61	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	K	203	CLA	CMD-C2D	-2.61	1.45	1.50
17	A	819	CLA	C1D-ND	2.61	1.41	1.37
17	A	803	CLA	CMB-C2B	-2.61	1.45	1.50
17	B	803	CLA	CMB-C2B	-2.61	1.45	1.50
17	B	804	CLA	CMD-C2D	-2.61	1.45	1.50
17	A	833	CLA	CMD-C2D	-2.61	1.45	1.50
20	A	853	BCR	C30-C25	-2.61	1.50	1.53
17	A	802	CLA	CMB-C2B	-2.61	1.45	1.50
17	A	823	CLA	CMC-C2C	-2.61	1.45	1.50
20	F	801	BCR	C30-C25	-2.60	1.50	1.53
17	B	824	CLA	MG-NB	-2.60	2.00	2.05
25	1	517	CHL	CBD-CGD	-2.60	1.49	1.52
17	1	509	CLA	C1B-C2B	2.60	1.49	1.43
17	5	308	CLA	MG-NB	-2.60	2.00	2.05
17	A	839	CLA	C4B-NB	2.60	1.41	1.37
17	B	816	CLA	CMB-C2B	-2.60	1.45	1.50
17	1	507	CLA	C1D-ND	2.60	1.41	1.37
17	B	826	CLA	MG-NB	-2.59	2.00	2.05
17	2	514	CLA	C1D-ND	2.59	1.41	1.37
17	B	842	CLA	MG-NB	-2.59	2.00	2.05
17	B	802	CLA	MG-NB	-2.59	2.00	2.05
17	1	513	CLA	C1B-C2B	2.59	1.49	1.43
17	A	826	CLA	CMD-C2D	-2.59	1.45	1.50
17	B	840	CLA	CMD-C2D	-2.59	1.45	1.50
17	A	807	CLA	C1D-ND	2.59	1.41	1.37
17	1	508	CLA	C1B-C2B	2.59	1.49	1.43
17	B	833	CLA	MG-NB	-2.59	2.00	2.05
17	A	827	CLA	MG-NB	-2.59	2.00	2.05
17	A	823	CLA	CMD-C2D	-2.59	1.45	1.50
17	3	313	CLA	C1B-C2B	2.59	1.49	1.43
17	2	504	CLA	MG-NB	-2.59	2.00	2.05
17	A	840	CLA	CMB-C2B	-2.59	1.45	1.50
17	3	311	CLA	C1D-ND	2.59	1.41	1.37
17	5	311	CLA	C4B-NB	2.59	1.41	1.37
17	A	811	CLA	CMC-C2C	-2.59	1.45	1.50
17	B	807	CLA	CMD-C2D	-2.59	1.45	1.50
17	A	833	CLA	CMC-C2C	-2.58	1.45	1.50
17	B	825	CLA	CMD-C2D	-2.58	1.45	1.50
17	B	830	CLA	CMD-C2D	-2.58	1.45	1.50
17	A	803	CLA	CMD-C2D	-2.58	1.45	1.50
17	A	827	CLA	CMD-C2D	-2.58	1.45	1.50
17	1	510	CLA	C1B-C2B	2.58	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	A	820	CLA	C1D-ND	2.58	1.41	1.37
17	2	507	CLA	C1B-C2B	2.58	1.49	1.43
17	B	834	CLA	MG-NB	-2.58	2.00	2.05
17	A	821	CLA	CMD-C2D	-2.58	1.45	1.50
17	B	840	CLA	CMB-C2B	-2.58	1.45	1.50
17	3	318	CLA	C1B-C2B	2.57	1.49	1.43
17	3	318	CLA	MG-NB	-2.57	2.00	2.05
17	5	308	CLA	CMC-C2C	-2.57	1.45	1.50
17	A	829	CLA	CMC-C2C	-2.57	1.45	1.50
17	5	307	CLA	C1B-C2B	2.57	1.49	1.43
17	A	803	CLA	MG-NB	-2.57	2.00	2.05
17	B	824	CLA	C1D-ND	2.57	1.41	1.37
17	A	828	CLA	MG-NB	-2.57	2.00	2.05
17	B	819	CLA	MG-NB	-2.57	2.00	2.05
20	A	851	BCR	C1-C6	-2.57	1.50	1.53
17	A	824	CLA	C1B-NB	-2.57	1.34	1.37
17	B	834	CLA	CMC-C2C	-2.57	1.45	1.50
17	L	301	CLA	CMB-C2B	-2.57	1.45	1.50
17	B	813	CLA	MG-NB	-2.57	2.00	2.05
17	A	822	CLA	C4B-NB	2.56	1.41	1.37
17	A	837	CLA	C4B-NB	2.56	1.41	1.37
25	5	317	CHL	C3A-C4A	-2.56	1.49	1.50
17	B	814	CLA	C1D-ND	2.56	1.41	1.37
20	B	849	BCR	C30-C25	-2.56	1.50	1.53
17	3	301	CLA	C1D-ND	2.56	1.41	1.37
17	A	831	CLA	CMD-C2D	-2.56	1.45	1.50
17	L	304	CLA	C1D-ND	2.56	1.41	1.37
17	A	839	CLA	CMD-C2D	-2.56	1.45	1.50
20	A	847	BCR	C1-C6	-2.56	1.50	1.53
17	A	806	CLA	MG-NB	-2.56	2.00	2.05
17	2	508	CLA	CMD-C2D	-2.56	1.45	1.50
17	5	305	CLA	CMD-C2D	-2.56	1.45	1.50
17	3	311	CLA	MG-NB	-2.56	2.00	2.05
17	A	810	CLA	C1D-ND	2.56	1.41	1.37
17	A	852	CLA	CMC-C2C	-2.56	1.45	1.50
17	B	817	CLA	CMC-C2C	-2.56	1.45	1.50
17	A	835	CLA	MG-NB	-2.55	2.00	2.05
17	B	822	CLA	CMD-C2D	-2.55	1.45	1.50
17	2	505	CLA	C1D-ND	2.55	1.41	1.37
17	A	809	CLA	C1B-C2B	2.55	1.49	1.43
17	B	802	CLA	CMB-C2B	-2.55	1.45	1.50
17	B	804	CLA	MG-NB	-2.55	2.00	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	3	312	CLA	C1B-C2B	2.55	1.49	1.43
17	B	819	CLA	C1D-ND	2.55	1.41	1.37
17	B	816	CLA	MG-NB	-2.55	2.00	2.05
17	2	504	CLA	CMB-C2B	-2.55	1.45	1.50
17	5	307	CLA	C4B-NB	2.55	1.41	1.37
17	A	852	CLA	CMD-C2D	-2.54	1.45	1.50
17	A	807	CLA	MG-NB	-2.54	2.00	2.05
17	B	826	CLA	CMC-C2C	-2.54	1.45	1.50
17	A	815	CLA	C1B-C2B	2.54	1.49	1.43
25	2	513	CHL	CAD-C3D	-2.54	1.48	1.51
26	2	502	XAT	O24-C25	-2.54	1.42	1.46
17	B	835	CLA	CMB-C2B	-2.54	1.45	1.50
17	B	817	CLA	MG-NB	-2.54	2.00	2.05
17	B	815	CLA	CMD-C2D	-2.54	1.45	1.50
17	A	828	CLA	CMB-C2B	-2.54	1.45	1.50
17	B	809	CLA	C1B-NB	-2.54	1.34	1.37
17	B	825	CLA	MG-NB	-2.54	2.00	2.05
17	K	201	CLA	MG-NB	-2.53	2.00	2.05
17	3	314	CLA	C1B-C2B	2.53	1.49	1.43
17	A	811	CLA	C1B-NB	-2.53	1.34	1.37
17	A	816	CLA	CMC-C2C	-2.53	1.45	1.50
17	B	814	CLA	MG-NB	-2.53	2.00	2.05
17	B	801	CLA	CMB-C2B	-2.53	1.45	1.50
17	A	825	CLA	C1B-NB	-2.53	1.34	1.37
17	B	825	CLA	CMC-C2C	-2.53	1.45	1.50
17	B	805	CLA	C1B-NB	-2.52	1.34	1.37
17	B	810	CLA	C1B-C2B	2.52	1.49	1.43
17	5	309	CLA	MG-NB	-2.52	2.00	2.05
17	A	840	CLA	C1B-C2B	2.52	1.49	1.43
17	B	810	CLA	CMB-C2B	-2.52	1.45	1.50
17	B	832	CLA	CMB-C2B	-2.52	1.45	1.50
20	B	847	BCR	C1-C6	-2.52	1.50	1.53
17	B	811	CLA	MG-NB	-2.52	2.00	2.05
17	B	815	CLA	MG-NB	-2.52	2.00	2.05
17	2	504	CLA	C1B-C2B	2.52	1.49	1.43
17	A	838	CLA	MG-NB	-2.51	2.00	2.05
17	5	312	CLA	MG-NB	-2.51	2.00	2.05
17	A	821	CLA	CMB-C2B	-2.51	1.45	1.50
17	A	813	CLA	MG-NB	-2.51	2.00	2.05
17	A	813	CLA	CMD-C2D	-2.51	1.45	1.50
17	A	839	CLA	CMC-C2C	-2.51	1.45	1.50
17	B	823	CLA	CMD-C2D	-2.51	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	A	840	CLA	CMD-C2D	-2.51	1.45	1.50
17	3	301	CLA	CMC-C2C	-2.51	1.45	1.50
17	B	830	CLA	C1D-ND	2.51	1.41	1.37
17	B	836	CLA	CMB-C2B	-2.51	1.45	1.50
17	3	317	CLA	C1B-C2B	2.51	1.49	1.43
17	A	812	CLA	MG-NB	-2.51	2.00	2.05
17	B	802	CLA	CMC-C2C	-2.51	1.45	1.50
17	2	511	CLA	C1B-C2B	2.50	1.49	1.43
17	A	835	CLA	CMD-C2D	-2.50	1.45	1.50
17	A	808	CLA	C1D-ND	2.50	1.41	1.37
17	B	822	CLA	CMB-C2B	-2.50	1.45	1.50
17	A	808	CLA	MG-NB	-2.50	2.00	2.05
17	B	837	CLA	CMC-C2C	-2.50	1.45	1.50
17	1	507	CLA	MG-NB	-2.50	2.00	2.05
17	L	301	CLA	MG-NB	-2.50	2.00	2.05
17	A	827	CLA	CMC-C2C	-2.50	1.45	1.50
17	B	837	CLA	CMB-C2B	-2.50	1.45	1.50
17	A	808	CLA	CMB-C2B	-2.50	1.45	1.50
17	1	504	CLA	CMC-C2C	-2.49	1.45	1.50
17	A	802	CLA	C1B-NB	-2.49	1.34	1.37
17	A	815	CLA	CMB-C2B	-2.49	1.45	1.50
17	B	837	CLA	CMD-C2D	-2.49	1.45	1.50
17	3	311	CLA	CMB-C2B	-2.49	1.45	1.50
17	B	827	CLA	CMC-C2C	-2.49	1.45	1.50
17	2	508	CLA	C4B-NB	2.49	1.41	1.37
17	A	808	CLA	CMC-C2C	-2.49	1.45	1.50
17	B	804	CLA	CMB-C2B	-2.49	1.45	1.50
17	2	511	CLA	C4B-NB	2.49	1.41	1.37
17	B	841	CLA	MG-NB	-2.49	2.00	2.05
17	B	804	CLA	CMC-C2C	-2.49	1.45	1.50
17	A	821	CLA	CMC-C2C	-2.48	1.45	1.50
17	L	301	CLA	C1D-ND	2.48	1.41	1.37
17	F	802	CLA	CMD-C2D	-2.48	1.45	1.50
17	3	307	CLA	C3B-C4B	2.48	1.50	1.42
17	B	823	CLA	C1B-NB	-2.48	1.34	1.37
17	A	805	CLA	CMB-C2B	-2.48	1.45	1.50
17	A	832	CLA	C1D-ND	2.48	1.41	1.37
17	A	830	CLA	MG-NB	-2.48	2.00	2.05
17	A	810	CLA	CMD-C2D	-2.48	1.45	1.50
17	5	306	CLA	MG-NB	-2.48	2.00	2.05
17	B	831	CLA	C4B-NB	2.48	1.41	1.37
17	B	840	CLA	C1B-NB	-2.48	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	B	804	CLA	C1D-ND	2.48	1.41	1.37
17	A	818	CLA	C1D-ND	2.47	1.41	1.37
17	A	839	CLA	C1D-ND	2.47	1.41	1.37
17	B	808	CLA	C4B-NB	2.47	1.41	1.37
17	B	806	CLA	CMB-C2B	-2.47	1.45	1.50
17	3	306	CLA	CMD-C2D	-2.47	1.45	1.50
17	B	835	CLA	CMC-C2C	-2.47	1.45	1.50
17	B	838	CLA	CMC-C2C	-2.47	1.45	1.50
17	B	833	CLA	C1B-NB	-2.47	1.34	1.37
17	B	829	CLA	C1D-ND	2.47	1.41	1.37
17	B	811	CLA	CMD-C2D	-2.47	1.45	1.50
17	B	841	CLA	CMD-C2D	-2.47	1.45	1.50
17	1	511	CLA	C1B-C2B	2.47	1.48	1.43
17	5	308	CLA	CMD-C2D	-2.47	1.45	1.50
17	A	829	CLA	CMD-C2D	-2.47	1.45	1.50
17	B	822	CLA	C1D-ND	2.47	1.41	1.37
17	K	202	CLA	C1B-C2B	2.47	1.48	1.43
17	B	801	CLA	CMD-C2D	-2.47	1.45	1.50
17	B	808	CLA	C1D-ND	2.47	1.41	1.37
17	B	817	CLA	CMB-C2B	-2.46	1.45	1.50
17	B	812	CLA	MG-NB	-2.46	2.00	2.05
17	A	837	CLA	MG-NB	-2.46	2.00	2.05
17	2	514	CLA	C4B-NB	2.46	1.41	1.37
17	A	833	CLA	MG-NB	-2.46	2.00	2.05
17	B	835	CLA	C1B-C2B	2.46	1.48	1.43
17	B	808	CLA	CMB-C2B	-2.46	1.45	1.50
17	B	818	CLA	CMB-C2B	-2.46	1.45	1.50
26	2	502	XAT	C2-C1	-2.46	1.50	1.54
17	B	841	CLA	CMB-C2B	-2.46	1.45	1.50
17	5	306	CLA	C4B-NB	2.46	1.41	1.37
17	A	821	CLA	MG-ND	-2.46	2.00	2.05
17	3	314	CLA	MG-NB	-2.46	2.00	2.05
17	A	822	CLA	CMD-C2D	-2.46	1.45	1.50
17	A	809	CLA	CMB-C2B	-2.45	1.45	1.50
17	F	802	CLA	C4B-NB	2.45	1.41	1.37
17	2	507	CLA	CMB-C2B	-2.45	1.45	1.50
17	B	827	CLA	C1D-ND	2.45	1.41	1.37
17	A	816	CLA	C1B-C2B	2.45	1.48	1.43
17	A	813	CLA	CMC-C2C	-2.45	1.45	1.50
17	2	514	CLA	C1B-C2B	2.45	1.48	1.43
17	B	812	CLA	CMD-C2D	-2.45	1.45	1.50
17	B	835	CLA	MG-NB	-2.45	2.00	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	A	831	CLA	CMB-C2B	-2.45	1.45	1.50
17	A	802	CLA	CMC-C2C	-2.45	1.45	1.50
17	A	837	CLA	CMC-C2C	-2.45	1.45	1.50
17	B	820	CLA	MG-NB	-2.45	2.00	2.05
17	L	301	CLA	CMD-C2D	-2.44	1.45	1.50
17	3	313	CLA	CMD-C2D	-2.44	1.45	1.50
17	A	840	CLA	C1D-ND	2.44	1.41	1.37
17	B	801	CLA	C1B-NB	-2.44	1.34	1.37
17	A	812	CLA	CMD-C2D	-2.44	1.45	1.50
17	A	839	CLA	MG-NB	-2.44	2.00	2.05
17	A	820	CLA	CMD-C2D	-2.44	1.45	1.50
17	1	515	CLA	MG-NB	-2.44	2.00	2.05
17	A	821	CLA	C1B-C2B	2.44	1.48	1.43
20	B	849	BCR	C1-C6	-2.44	1.50	1.53
17	B	807	CLA	C1B-NB	-2.44	1.34	1.37
17	B	802	CLA	CMD-C2D	-2.44	1.45	1.50
17	K	201	CLA	C1D-ND	2.44	1.41	1.37
17	J	101	CLA	C1B-C2B	2.44	1.48	1.43
17	5	310	CLA	CMC-C2C	-2.44	1.45	1.50
17	B	821	CLA	CMB-C2B	-2.44	1.45	1.50
17	2	508	CLA	CMB-C2B	-2.44	1.45	1.50
17	3	306	CLA	C4B-NB	2.44	1.41	1.37
17	5	311	CLA	C1D-ND	2.44	1.41	1.37
17	A	805	CLA	CMC-C2C	-2.44	1.45	1.50
17	A	811	CLA	C1B-C2B	2.44	1.48	1.43
17	B	812	CLA	CMC-C2C	-2.44	1.45	1.50
17	A	834	CLA	C4B-NB	2.44	1.41	1.37
17	1	504	CLA	C4B-NB	2.44	1.41	1.37
17	2	508	CLA	MG-NB	-2.44	2.01	2.05
17	A	842	CLA	C1B-C2B	2.44	1.48	1.43
17	1	506	CLA	C1B-C2B	2.44	1.48	1.43
17	A	834	CLA	MG-NB	-2.44	2.01	2.05
17	B	815	CLA	C1D-ND	2.44	1.41	1.37
17	A	837	CLA	C1D-ND	2.43	1.41	1.37
17	2	505	CLA	C4B-NB	2.43	1.41	1.37
17	A	819	CLA	MG-NB	-2.43	2.01	2.05
17	B	832	CLA	MG-NB	-2.43	2.01	2.05
17	B	817	CLA	CMD-C2D	-2.43	1.45	1.50
17	1	506	CLA	CMB-C2B	-2.43	1.45	1.50
17	B	819	CLA	C1B-NB	-2.43	1.34	1.37
17	B	821	CLA	C1B-C2B	2.43	1.48	1.43
17	2	514	CLA	MG-NB	-2.43	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	B	837	CLA	C1B-NB	-2.43	1.34	1.37
17	B	821	CLA	C3B-C4B	2.43	1.49	1.42
17	A	819	CLA	CMC-C2C	-2.43	1.45	1.50
17	L	301	CLA	CMC-C2C	-2.43	1.45	1.50
17	B	822	CLA	C1B-C2B	2.43	1.48	1.43
17	B	812	CLA	C1B-NB	-2.43	1.34	1.37
17	A	804	CLA	C1B-C2B	2.43	1.48	1.43
17	A	806	CLA	C1D-ND	2.43	1.41	1.37
17	3	318	CLA	C4B-C3B	2.42	1.48	1.43
24	1	502	LUT	C1-C6	-2.42	1.50	1.53
17	1	515	CLA	C1B-C2B	2.42	1.48	1.43
17	F	802	CLA	CMC-C2C	-2.42	1.45	1.50
17	A	814	CLA	CMC-C2C	-2.42	1.45	1.50
17	A	805	CLA	CMD-C2D	-2.42	1.45	1.50
17	B	839	CLA	CMC-C2C	-2.42	1.45	1.50
17	A	842	CLA	CHC-C1C	2.42	1.43	1.38
26	5	304	XAT	C2-C1	-2.42	1.50	1.54
17	A	804	CLA	MG-NB	-2.42	2.01	2.05
17	A	832	CLA	MG-NB	-2.42	2.01	2.05
17	5	306	CLA	C1B-C2B	2.42	1.48	1.43
17	A	825	CLA	CMC-C2C	-2.42	1.45	1.50
17	A	814	CLA	CMB-C2B	-2.42	1.45	1.50
17	B	811	CLA	C1D-ND	2.42	1.41	1.37
17	B	817	CLA	C1B-C2B	2.42	1.48	1.43
17	A	820	CLA	CMC-C2C	-2.41	1.45	1.50
17	A	826	CLA	CMB-C2B	-2.41	1.45	1.50
17	B	823	CLA	CMB-C2B	-2.41	1.45	1.50
17	A	810	CLA	CMC-C2C	-2.41	1.45	1.50
17	B	808	CLA	CMC-C2C	-2.41	1.45	1.50
17	B	802	CLA	C1B-C2B	2.41	1.48	1.43
17	5	311	CLA	C3B-C4B	2.41	1.49	1.42
17	B	818	CLA	MG-NB	-2.41	2.01	2.05
17	A	831	CLA	C1D-ND	2.41	1.41	1.37
17	B	819	CLA	CMC-C2C	-2.41	1.45	1.50
17	A	840	CLA	CMC-C2C	-2.41	1.45	1.50
17	5	313	CLA	CMB-C2B	-2.41	1.45	1.50
17	B	840	CLA	MG-NB	-2.41	2.01	2.05
17	K	203	CLA	CMC-C2C	-2.41	1.45	1.50
17	2	509	CLA	CMB-C2B	-2.41	1.45	1.50
17	B	807	CLA	MG-NB	-2.41	2.01	2.05
17	B	829	CLA	CMD-C2D	-2.41	1.45	1.50
17	2	507	CLA	CMD-C2D	-2.41	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	A	812	CLA	CMB-C2B	-2.40	1.45	1.50
17	5	309	CLA	CMD-C2D	-2.40	1.45	1.50
17	F	802	CLA	MG-NB	-2.40	2.01	2.05
17	B	838	CLA	MG-NB	-2.40	2.01	2.05
17	L	302	CLA	C1B-C2B	2.40	1.48	1.43
17	A	827	CLA	CMB-C2B	-2.40	1.45	1.50
17	B	831	CLA	CMC-C2C	-2.40	1.45	1.50
17	2	511	CLA	MG-NB	-2.40	2.01	2.05
17	A	817	CLA	CHC-C1C	2.40	1.43	1.38
17	B	812	CLA	C1D-ND	2.40	1.41	1.37
17	B	837	CLA	C1D-ND	2.40	1.41	1.37
17	5	311	CLA	CMB-C2B	-2.40	1.45	1.50
17	5	316	CLA	CMD-C2D	-2.40	1.45	1.50
17	3	316	CLA	C1B-C2B	2.40	1.48	1.43
17	A	806	CLA	CMD-C2D	-2.40	1.45	1.50
17	5	313	CLA	C1B-C2B	2.40	1.48	1.43
17	B	820	CLA	CMD-C2D	-2.40	1.45	1.50
17	B	842	CLA	CMC-C2C	-2.40	1.45	1.50
24	3	304	LUT	C22-C21	-2.40	1.51	1.54
17	A	813	CLA	C1B-C2B	2.40	1.48	1.43
17	2	508	CLA	C1B-C2B	2.40	1.48	1.43
17	B	828	CLA	CMC-C2C	-2.39	1.45	1.50
17	A	852	CLA	MG-NB	-2.39	2.01	2.05
17	B	831	CLA	MG-NB	-2.39	2.01	2.05
17	A	802	CLA	CMD-C2D	-2.39	1.45	1.50
17	B	839	CLA	CMD-C2D	-2.39	1.45	1.50
17	A	807	CLA	CMC-C2C	-2.39	1.45	1.50
17	B	840	CLA	CMC-C2C	-2.39	1.45	1.50
20	3	305	BCR	C1-C6	-2.39	1.50	1.53
17	A	811	CLA	CMB-C2B	-2.39	1.45	1.50
17	3	311	CLA	C1B-NB	-2.39	1.34	1.37
17	A	803	CLA	CMC-C2C	-2.39	1.45	1.50
17	B	805	CLA	CMC-C2C	-2.39	1.45	1.50
17	B	804	CLA	C1B-C2B	2.39	1.48	1.43
24	3	303	LUT	C22-C21	-2.39	1.51	1.54
17	A	821	CLA	MG-NB	-2.39	2.01	2.05
17	A	823	CLA	MG-NB	-2.39	2.01	2.05
17	3	317	CLA	MG-NB	-2.39	2.01	2.05
17	B	839	CLA	C1B-NB	-2.39	1.34	1.37
25	1	517	CHL	CHA-CBD	-2.39	1.48	1.51
17	B	818	CLA	CMD-C2D	-2.38	1.45	1.50
17	A	840	CLA	C1B-NB	-2.38	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	2	510	CLA	C1B-C2B	2.38	1.48	1.43
17	K	202	CLA	CHC-C1C	2.38	1.43	1.38
17	A	809	CLA	MG-NB	-2.38	2.01	2.05
20	F	801	BCR	C1-C6	-2.38	1.50	1.53
17	1	509	CLA	CMD-C2D	-2.38	1.45	1.50
17	L	302	CLA	CMB-C2B	-2.38	1.45	1.50
17	B	842	CLA	C1B-C2B	2.38	1.48	1.43
24	2	501	LUT	C1-C6	-2.38	1.50	1.53
17	B	818	CLA	CMC-C2C	-2.38	1.45	1.50
17	3	307	CLA	CHC-C1C	2.38	1.43	1.38
17	A	804	CLA	CMB-C2B	-2.38	1.45	1.50
17	A	836	CLA	C1D-ND	2.38	1.41	1.37
17	5	309	CLA	CMB-C2B	-2.38	1.45	1.50
17	3	311	CLA	CMD-C2D	-2.38	1.45	1.50
17	B	828	CLA	C1B-NB	-2.38	1.34	1.37
17	A	814	CLA	C1B-C2B	2.38	1.48	1.43
17	A	839	CLA	C1B-C2B	2.38	1.48	1.43
17	A	819	CLA	CMD-C2D	-2.38	1.45	1.50
17	B	803	CLA	C1D-ND	2.38	1.41	1.37
17	B	820	CLA	C1D-ND	2.38	1.41	1.37
17	L	304	CLA	CMC-C2C	-2.37	1.45	1.50
25	2	515	CHL	CBD-CGD	-2.37	1.49	1.52
17	B	824	CLA	C1B-C2B	2.37	1.48	1.43
17	A	816	CLA	C1B-NB	-2.37	1.34	1.37
17	B	824	CLA	CMC-C2C	-2.37	1.45	1.50
17	F	803	CLA	C4B-NB	2.37	1.41	1.37
17	B	823	CLA	CMC-C2C	-2.37	1.45	1.50
17	A	818	CLA	CMC-C2C	-2.37	1.45	1.50
17	2	510	CLA	MG-NB	-2.37	2.01	2.05
17	B	828	CLA	MG-NB	-2.37	2.01	2.05
17	1	505	CLA	CMB-C2B	-2.37	1.45	1.50
17	A	820	CLA	MG-NB	-2.37	2.01	2.05
17	A	812	CLA	C1D-ND	2.37	1.41	1.37
17	1	513	CLA	MG-NB	-2.36	2.01	2.05
17	B	828	CLA	C1B-C2B	2.36	1.48	1.43
17	1	509	CLA	MG-NB	-2.36	2.01	2.05
17	K	205	CLA	CHC-C1C	2.36	1.43	1.38
17	A	814	CLA	C1D-ND	2.36	1.41	1.37
17	L	302	CLA	C4B-NB	2.36	1.41	1.37
17	B	814	CLA	CMB-C2B	-2.36	1.45	1.50
24	5	303	LUT	C22-C21	-2.36	1.51	1.54
17	2	505	CLA	CMC-C2C	-2.36	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	K	201	CLA	CMC-C2C	-2.36	1.45	1.50
17	5	316	CLA	CMB-C2B	-2.36	1.45	1.50
17	A	838	CLA	CMC-C2C	-2.36	1.45	1.50
17	B	816	CLA	C1B-NB	-2.36	1.34	1.37
17	5	316	CLA	MG-NB	-2.36	2.01	2.05
17	A	842	CLA	CMC-C2C	-2.36	1.45	1.50
17	5	309	CLA	C1B-C2B	2.36	1.48	1.43
17	5	316	CLA	C1B-C2B	2.36	1.48	1.43
16	A	801	CL0	O2A-CGA	-2.36	1.31	1.42
17	A	833	CLA	C1D-ND	2.35	1.41	1.37
17	A	818	CLA	C1B-NB	-2.35	1.34	1.37
17	B	836	CLA	CMC-C2C	-2.35	1.45	1.50
17	5	308	CLA	CMB-C2B	-2.35	1.45	1.50
17	K	202	CLA	C4B-NB	2.35	1.41	1.37
17	A	825	CLA	CMB-C2B	-2.35	1.45	1.50
17	1	504	CLA	MG-ND	-2.35	2.01	2.05
17	A	810	CLA	MG-NB	-2.35	2.01	2.05
17	B	828	CLA	C3A-C2A	-2.35	1.52	1.54
17	A	828	CLA	C1B-C2B	2.35	1.48	1.43
17	B	826	CLA	C1D-ND	2.35	1.40	1.37
17	A	827	CLA	C1B-NB	-2.35	1.34	1.37
17	A	824	CLA	C1D-ND	2.35	1.40	1.37
17	2	506	CLA	C4B-NB	2.35	1.40	1.37
17	B	823	CLA	C1B-C2B	2.35	1.48	1.43
17	1	511	CLA	C4B-NB	2.34	1.40	1.37
17	3	301	CLA	C4B-NB	2.34	1.40	1.37
17	B	822	CLA	CMC-C2C	-2.34	1.46	1.50
17	L	304	CLA	MG-NB	-2.34	2.01	2.05
17	B	829	CLA	CMC-C2C	-2.34	1.46	1.50
17	5	310	CLA	MG-NB	-2.34	2.01	2.05
17	3	307	CLA	CMD-C2D	-2.34	1.46	1.50
17	5	307	CLA	MG-NB	-2.34	2.01	2.05
17	A	832	CLA	C1B-NB	-2.34	1.34	1.37
17	5	309	CLA	C1B-NB	-2.34	1.34	1.37
17	B	842	CLA	CMD-C2D	-2.34	1.46	1.50
17	2	514	CLA	CMB-C2B	-2.34	1.46	1.50
17	F	802	CLA	CMB-C2B	-2.34	1.46	1.50
17	3	316	CLA	CMB-C2B	-2.34	1.46	1.50
17	A	817	CLA	C1B-NB	-2.34	1.34	1.37
17	B	841	CLA	C1D-ND	2.33	1.40	1.37
17	B	833	CLA	CMD-C2D	-2.33	1.46	1.50
17	A	831	CLA	C4B-C3B	2.33	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	F	803	CLA	CMC-C2C	-2.33	1.46	1.50
17	3	308	CLA	C1B-C2B	2.33	1.48	1.43
17	B	801	CLA	C1D-ND	2.33	1.40	1.37
17	B	836	CLA	CMD-C2D	-2.33	1.46	1.50
17	A	808	CLA	CMD-C2D	-2.33	1.46	1.50
17	K	205	CLA	CMB-C2B	-2.33	1.46	1.50
17	3	309	CLA	MG-NB	-2.33	2.01	2.05
17	A	830	CLA	C1D-ND	2.33	1.40	1.37
17	A	813	CLA	CMB-C2B	-2.33	1.46	1.50
17	A	852	CLA	C4B-NB	2.33	1.40	1.37
17	B	810	CLA	C1B-NB	-2.33	1.34	1.37
17	B	817	CLA	MG-ND	-2.33	2.01	2.05
17	B	811	CLA	C1B-NB	-2.33	1.34	1.37
17	A	832	CLA	CMC-C2C	-2.33	1.46	1.50
17	A	839	CLA	CMB-C2B	-2.33	1.46	1.50
17	5	313	CLA	MG-NB	-2.33	2.01	2.05
17	A	836	CLA	C1B-NB	-2.32	1.34	1.37
17	B	833	CLA	C1B-C2B	2.32	1.48	1.43
17	A	815	CLA	CMD-C2D	-2.32	1.46	1.50
17	B	805	CLA	MG-NB	-2.32	2.01	2.05
17	2	508	CLA	CHC-C1C	2.32	1.43	1.38
17	B	812	CLA	C4B-C3B	2.32	1.48	1.43
17	L	303	CLA	C4B-NB	2.32	1.40	1.37
17	A	842	CLA	CMB-C2B	-2.32	1.46	1.50
17	B	832	CLA	CMC-C2C	-2.32	1.46	1.50
17	2	514	CLA	CMD-C2D	-2.32	1.46	1.50
17	5	313	CLA	CMD-C2D	-2.32	1.46	1.50
17	2	506	CLA	CMD-C2D	-2.32	1.46	1.50
24	3	304	LUT	C1-C6	-2.32	1.50	1.53
25	5	314	CHL	CBD-CGD	-2.32	1.49	1.52
17	1	506	CLA	CMC-C2C	-2.31	1.46	1.50
17	3	301	CLA	CMD-C2D	-2.31	1.46	1.50
17	2	511	CLA	CMB-C2B	-2.31	1.46	1.50
17	F	803	CLA	C1B-C2B	2.31	1.48	1.43
17	5	311	CLA	C1B-C2B	2.31	1.48	1.43
17	A	815	CLA	C1B-NB	-2.31	1.34	1.37
17	A	822	CLA	C1B-C2B	2.31	1.48	1.43
17	3	306	CLA	C2C-C1C	2.31	1.45	1.40
17	B	831	CLA	C1B-C2B	2.31	1.48	1.43
17	A	852	CLA	C1B-C2B	2.31	1.48	1.43
20	J	102	BCR	C30-C25	-2.31	1.50	1.53
17	A	830	CLA	CMC-C2C	-2.31	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	B	821	CLA	MG-NB	-2.31	2.01	2.05
17	3	301	CLA	C1B-NB	-2.31	1.34	1.37
17	B	824	CLA	C4B-NB	2.30	1.40	1.37
17	1	513	CLA	CMD-C2D	-2.30	1.46	1.50
17	5	312	CLA	C1B-C2B	2.30	1.48	1.43
17	3	314	CLA	C3B-C4B	2.30	1.49	1.42
17	A	837	CLA	C3A-C2A	-2.30	1.52	1.54
17	B	841	CLA	CMC-C2C	-2.30	1.46	1.50
17	K	205	CLA	C3B-C4B	2.30	1.49	1.42
17	A	818	CLA	CMD-C2D	-2.30	1.46	1.50
17	A	837	CLA	CMB-C2B	-2.30	1.46	1.50
17	A	802	CLA	MG-NB	-2.30	2.01	2.05
17	K	202	CLA	MG-NB	-2.30	2.01	2.05
17	K	205	CLA	C1B-C2B	2.30	1.48	1.43
17	B	832	CLA	CMD-C2D	-2.30	1.46	1.50
17	A	817	CLA	CMC-C2C	-2.30	1.46	1.50
20	B	848	BCR	C1-C6	-2.30	1.50	1.53
17	B	804	CLA	C1B-NB	-2.30	1.34	1.37
17	A	815	CLA	MG-ND	-2.30	2.01	2.05
17	5	311	CLA	MG-NB	-2.30	2.01	2.05
17	A	822	CLA	CMB-C2B	-2.30	1.46	1.50
17	B	833	CLA	CMB-C2B	-2.30	1.46	1.50
17	B	835	CLA	CMD-C2D	-2.30	1.46	1.50
17	J	101	CLA	CHC-C1C	2.30	1.43	1.38
17	5	313	CLA	C4B-NB	2.29	1.40	1.37
17	3	313	CLA	C3B-C4B	2.29	1.49	1.42
17	2	511	CLA	CMD-C2D	-2.29	1.46	1.50
17	L	302	CLA	MG-NB	-2.29	2.01	2.05
17	5	312	CLA	CMB-C2B	-2.29	1.46	1.50
17	F	803	CLA	CMD-C2D	-2.29	1.46	1.50
17	K	202	CLA	CMD-C2D	-2.29	1.46	1.50
17	A	803	CLA	C4B-NB	2.29	1.40	1.37
17	1	510	CLA	CMB-C2B	-2.29	1.46	1.50
17	1	507	CLA	C4B-NB	2.29	1.40	1.37
17	2	504	CLA	CMC-C2C	-2.29	1.46	1.50
17	1	507	CLA	CMB-C2B	-2.29	1.46	1.50
17	A	814	CLA	C4B-NB	2.29	1.40	1.37
17	B	809	CLA	MG-NB	-2.29	2.01	2.05
17	B	827	CLA	MG-NB	-2.29	2.01	2.05
17	3	317	CLA	CMC-C2C	-2.29	1.46	1.50
17	A	836	CLA	CMC-C2C	-2.28	1.46	1.50
17	A	817	CLA	MG-ND	-2.28	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	3	301	CLA	MG-NB	-2.28	2.01	2.05
17	3	312	CLA	C3B-C4B	2.28	1.49	1.42
17	B	808	CLA	C1B-C2B	2.28	1.48	1.43
17	A	805	CLA	C1B-NB	-2.28	1.34	1.37
17	B	802	CLA	C4B-NB	2.28	1.40	1.37
17	1	507	CLA	C1B-C2B	2.28	1.48	1.43
17	A	833	CLA	C3B-C4B	2.28	1.49	1.42
17	B	812	CLA	C1B-C2B	2.28	1.48	1.43
17	L	303	CLA	C1D-ND	2.28	1.40	1.37
17	1	508	CLA	MG-NB	-2.28	2.01	2.05
17	B	841	CLA	C1B-NB	-2.28	1.34	1.37
17	1	508	CLA	CMD-C2D	-2.28	1.46	1.50
20	B	846	BCR	C1-C6	-2.28	1.50	1.53
17	A	828	CLA	CMC-C2C	-2.27	1.46	1.50
17	3	307	CLA	CMC-C2C	-2.27	1.46	1.50
17	5	316	CLA	CMC-C2C	-2.27	1.46	1.50
17	3	308	CLA	MG-NB	-2.27	2.01	2.05
17	B	836	CLA	MG-NB	-2.27	2.01	2.05
17	B	832	CLA	C1B-C2B	2.27	1.48	1.43
17	B	822	CLA	MG-NB	-2.27	2.01	2.05
17	A	815	CLA	CMC-C2C	-2.27	1.46	1.50
17	A	824	CLA	CMC-C2C	-2.27	1.46	1.50
17	5	307	CLA	CMB-C2B	-2.27	1.46	1.50
17	B	821	CLA	CMC-C2C	-2.27	1.46	1.50
17	L	303	CLA	MG-NB	-2.26	2.01	2.05
17	A	831	CLA	C1B-C2B	2.26	1.48	1.43
17	B	810	CLA	CMD-C2D	-2.26	1.46	1.50
17	B	825	CLA	C1B-C2B	2.26	1.48	1.43
17	1	504	CLA	C1B-C2B	2.26	1.48	1.43
17	A	834	CLA	CMD-C2D	-2.26	1.46	1.50
17	3	306	CLA	C1B-C2B	2.26	1.48	1.43
17	B	805	CLA	CHC-C1C	2.26	1.43	1.38
17	B	834	CLA	C4B-NB	2.26	1.40	1.37
17	J	101	CLA	MG-NB	-2.26	2.01	2.05
17	A	825	CLA	MG-ND	-2.26	2.01	2.05
17	B	839	CLA	C4B-NB	2.26	1.40	1.37
17	B	834	CLA	CMD-C2D	-2.26	1.46	1.50
17	1	510	CLA	MG-NB	-2.26	2.01	2.05
17	A	809	CLA	CBD-CGD	-2.26	1.49	1.51
17	A	804	CLA	C1D-ND	2.26	1.40	1.37
17	A	807	CLA	CMD-C2D	-2.25	1.46	1.50
17	B	837	CLA	CHC-C1C	2.25	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	3	310	CLA	CMB-C2B	-2.25	1.46	1.50
17	K	201	CLA	MG-ND	-2.25	2.01	2.05
17	5	305	CLA	C1D-ND	2.25	1.40	1.37
17	A	810	CLA	C1B-NB	-2.25	1.34	1.37
17	B	806	CLA	C1B-C2B	2.25	1.48	1.43
17	B	823	CLA	C4B-NB	2.25	1.40	1.37
17	3	314	CLA	CMD-C2D	-2.25	1.46	1.50
17	K	201	CLA	CHC-C1C	2.25	1.43	1.38
17	B	840	CLA	C1D-ND	2.25	1.40	1.37
17	K	203	CLA	C1D-ND	2.25	1.40	1.37
17	A	817	CLA	CMD-C2D	-2.25	1.46	1.50
17	B	822	CLA	CHC-C1C	2.25	1.43	1.38
17	B	815	CLA	CHC-C1C	2.25	1.43	1.38
17	1	507	CLA	CMC-C2C	-2.25	1.46	1.50
17	F	802	CLA	C1B-C2B	2.24	1.48	1.43
17	1	505	CLA	CHC-C1C	2.24	1.43	1.38
17	3	311	CLA	CMC-C2C	-2.24	1.46	1.50
17	A	826	CLA	C1D-ND	2.24	1.40	1.37
17	3	307	CLA	MG-NB	-2.24	2.01	2.05
17	2	509	CLA	C3B-C4B	2.24	1.49	1.42
17	2	507	CLA	CHC-C1C	2.24	1.43	1.38
17	2	510	CLA	CMD-C2D	-2.24	1.46	1.50
17	B	825	CLA	C1D-ND	2.24	1.40	1.37
17	B	803	CLA	C1B-C2B	2.24	1.48	1.43
17	2	509	CLA	MG-NB	-2.24	2.01	2.05
17	1	510	CLA	CMC-C2C	-2.24	1.46	1.50
17	K	202	CLA	CMB-C2B	-2.24	1.46	1.50
17	1	505	CLA	C3B-C4B	2.24	1.49	1.42
17	B	828	CLA	CMB-C2B	-2.23	1.46	1.50
17	2	505	CLA	CMB-C2B	-2.23	1.46	1.50
17	5	305	CLA	C1B-NB	-2.23	1.34	1.37
17	B	826	CLA	CMB-C2B	-2.23	1.46	1.50
17	B	805	CLA	C4B-NB	2.23	1.40	1.37
17	2	504	CLA	CMD-C2D	-2.23	1.46	1.50
17	A	813	CLA	C1D-ND	2.23	1.40	1.37
17	A	826	CLA	CHC-C1C	2.23	1.43	1.38
17	B	825	CLA	CMB-C2B	-2.23	1.46	1.50
17	F	803	CLA	CMB-C2B	-2.23	1.46	1.50
17	5	312	CLA	CMD-C2D	-2.23	1.46	1.50
17	B	837	CLA	C1B-C2B	2.23	1.48	1.43
17	B	839	CLA	C1B-C2B	2.23	1.48	1.43
17	B	809	CLA	CMC-C2C	-2.23	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	1	506	CLA	MG-NB	-2.23	2.01	2.05
17	B	832	CLA	MG-ND	-2.23	2.01	2.05
17	B	839	CLA	CMB-C2B	-2.23	1.46	1.50
17	K	201	CLA	CMB-C2B	-2.22	1.46	1.50
17	A	836	CLA	CHC-C1C	2.22	1.42	1.38
17	2	510	CLA	MG-ND	-2.22	2.01	2.05
17	3	317	CLA	CMB-C2B	-2.22	1.46	1.50
17	L	303	CLA	CMC-C2C	-2.22	1.46	1.50
17	5	309	CLA	CMC-C2C	-2.22	1.46	1.50
17	B	810	CLA	C4B-NB	2.22	1.40	1.37
17	K	201	CLA	C3B-C4B	2.22	1.49	1.42
17	A	807	CLA	C1B-NB	-2.22	1.34	1.37
17	2	506	CLA	MG-NB	-2.22	2.01	2.05
17	1	504	CLA	C3B-C4B	2.22	1.49	1.42
17	3	309	CLA	CMC-C2C	-2.22	1.46	1.50
17	A	825	CLA	C4B-NB	2.21	1.40	1.37
17	B	838	CLA	C4B-NB	2.21	1.40	1.37
17	B	836	CLA	CHC-C1C	2.21	1.42	1.38
17	L	303	CLA	CMD-C2D	-2.21	1.46	1.50
17	5	306	CLA	CMB-C2B	-2.21	1.46	1.50
17	A	822	CLA	CMC-C2C	-2.21	1.46	1.50
17	B	817	CLA	C4B-NB	2.21	1.40	1.37
17	A	802	CLA	C1B-C2B	2.21	1.48	1.43
17	1	507	CLA	CMD-C2D	-2.20	1.46	1.50
17	K	202	CLA	C3B-C4B	2.20	1.49	1.42
17	5	308	CLA	C1B-C2B	2.20	1.48	1.43
25	2	516	CHL	CBD-CGD	-2.20	1.49	1.52
17	3	310	CLA	C3B-C4B	2.20	1.49	1.42
17	B	802	CLA	C3B-C4B	2.20	1.49	1.42
17	B	824	CLA	C1B-NB	-2.20	1.35	1.37
17	2	514	CLA	CMC-C2C	-2.20	1.46	1.50
17	B	841	CLA	C1B-C2B	2.20	1.48	1.43
17	2	508	CLA	C3B-C4B	2.20	1.49	1.42
17	L	303	CLA	C3B-C4B	2.20	1.49	1.42
17	2	509	CLA	C1B-C2B	2.20	1.48	1.43
17	A	814	CLA	CAC-C3C	-2.20	1.45	1.51
17	3	317	CLA	C3B-C4B	2.20	1.49	1.42
17	A	827	CLA	MG-ND	-2.20	2.01	2.05
17	3	317	CLA	CMD-C2D	-2.20	1.46	1.50
17	A	814	CLA	MG-NB	-2.20	2.01	2.05
17	B	819	CLA	C3A-C2A	-2.20	1.52	1.54
17	B	822	CLA	C3B-C4B	2.20	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	1	508	CLA	CHC-C1C	2.20	1.42	1.38
17	A	833	CLA	C1B-C2B	2.20	1.48	1.43
17	B	829	CLA	C1B-NB	-2.20	1.35	1.37
17	2	514	CLA	MG-ND	-2.20	2.01	2.05
17	3	312	CLA	MG-NB	-2.19	2.01	2.05
17	A	829	CLA	MG-ND	-2.19	2.01	2.05
25	5	315	CHL	CHA-CBD	-2.19	1.49	1.51
25	3	302	CHL	CHA-CBD	-2.19	1.49	1.51
25	5	317	CHL	CBD-CGD	-2.19	1.49	1.52
17	1	515	CLA	C3B-C4B	2.19	1.49	1.42
17	A	820	CLA	C3B-C4B	2.19	1.49	1.42
17	B	801	CLA	C1B-C2B	2.19	1.48	1.43
17	A	836	CLA	CAA-C2A	-2.19	1.50	1.54
19	A	844	LHG	O7-C5	-2.19	1.41	1.46
17	B	829	CLA	MG-ND	-2.19	2.01	2.05
17	5	305	CLA	CMB-C2B	-2.19	1.45	1.50
17	2	511	CLA	CMC-C2C	-2.19	1.46	1.50
17	A	810	CLA	C1B-C2B	2.19	1.48	1.43
17	B	820	CLA	CHC-C1C	2.19	1.42	1.38
17	B	807	CLA	MG-ND	-2.19	2.01	2.05
17	2	510	CLA	C3B-C4B	2.19	1.49	1.42
17	2	504	CLA	C4B-NB	2.19	1.40	1.37
17	1	511	CLA	CMD-C2D	-2.18	1.46	1.50
17	F	802	CLA	C3B-C4B	2.18	1.49	1.42
17	1	509	CLA	C3B-C4B	2.18	1.49	1.42
17	3	316	CLA	C3B-C4B	2.18	1.49	1.42
17	5	308	CLA	C3B-C4B	2.18	1.49	1.42
17	A	840	CLA	C4B-NB	2.18	1.40	1.37
24	1	502	LUT	C22-C21	-2.18	1.52	1.54
17	B	827	CLA	CHC-C1C	2.18	1.42	1.38
17	B	825	CLA	MG-ND	-2.18	2.01	2.05
17	A	839	CLA	MG-ND	-2.18	2.01	2.05
17	3	311	CLA	C3B-C4B	2.18	1.49	1.42
17	B	815	CLA	C1B-C2B	2.18	1.48	1.43
17	B	812	CLA	C3B-C2B	-2.18	1.35	1.44
17	5	309	CLA	C4B-NB	2.18	1.40	1.37
17	B	832	CLA	C1B-NB	-2.18	1.35	1.37
17	J	101	CLA	CMD-C2D	-2.18	1.46	1.50
17	A	837	CLA	MG-ND	-2.18	2.01	2.05
17	B	831	CLA	C1B-NB	-2.18	1.35	1.37
17	L	304	CLA	C1B-C2B	2.18	1.48	1.43
17	B	818	CLA	C4B-NB	2.18	1.40	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	5	308	CLA	C4B-NB	2.18	1.40	1.37
17	2	505	CLA	MG-NB	-2.18	2.01	2.05
17	2	506	CLA	C1B-C2B	2.18	1.48	1.43
17	1	506	CLA	C3B-C4B	2.17	1.49	1.42
17	J	101	CLA	CMB-C2B	-2.17	1.46	1.50
17	B	824	CLA	C3B-C4B	2.17	1.49	1.42
17	A	852	CLA	C3B-C4B	2.17	1.49	1.42
17	A	808	CLA	C1B-NB	-2.17	1.35	1.37
17	A	803	CLA	C1B-C2B	2.17	1.48	1.43
17	5	312	CLA	CMC-C2C	-2.17	1.46	1.50
17	A	836	CLA	C4B-NB	2.17	1.40	1.37
17	B	842	CLA	CMB-C2B	-2.17	1.46	1.50
17	3	314	CLA	CHC-C1C	2.17	1.42	1.38
17	5	310	CLA	CMD-C2D	-2.17	1.46	1.50
17	2	505	CLA	C1B-C2B	2.17	1.48	1.43
17	L	301	CLA	CAC-C3C	-2.17	1.45	1.51
17	B	836	CLA	C1B-C2B	2.17	1.48	1.43
17	B	801	CLA	CAC-C3C	-2.17	1.45	1.51
17	A	834	CLA	C1B-C2B	2.17	1.48	1.43
17	5	305	CLA	MG-NB	-2.17	2.01	2.05
17	B	835	CLA	C3B-C4B	2.16	1.49	1.42
17	2	510	CLA	CHC-C1C	2.16	1.42	1.38
17	3	317	CLA	CHC-C1C	2.16	1.42	1.38
17	5	312	CLA	C3B-C4B	2.16	1.49	1.42
17	B	842	CLA	C3B-C4B	2.16	1.49	1.42
17	B	830	CLA	CAC-C3C	-2.16	1.45	1.51
17	B	811	CLA	CAA-C2A	-2.16	1.50	1.54
17	5	311	CLA	CMD-C2D	-2.16	1.46	1.50
17	A	813	CLA	C3B-C4B	2.16	1.49	1.42
20	2	503	BCR	C1-C6	-2.16	1.51	1.53
17	3	316	CLA	MG-NB	-2.16	2.01	2.05
17	2	507	CLA	CMC-C2C	-2.16	1.46	1.50
17	A	810	CLA	C4B-NB	2.16	1.40	1.37
17	B	828	CLA	CHC-C1C	2.16	1.42	1.38
25	2	512	CHL	CBD-CGD	-2.16	1.49	1.52
17	B	808	CLA	CAB-C3B	-2.16	1.41	1.47
17	B	838	CLA	MG-ND	-2.16	2.01	2.05
17	B	840	CLA	C1B-C2B	2.16	1.48	1.43
17	B	811	CLA	CMA-C3A	-2.16	1.48	1.53
17	B	833	CLA	C4B-NB	2.16	1.40	1.37
17	5	313	CLA	CMC-C2C	-2.15	1.46	1.50
17	B	805	CLA	CMD-C2D	-2.15	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	A	809	CLA	C4B-NB	2.15	1.40	1.37
17	2	505	CLA	CHC-C1C	2.15	1.42	1.38
17	L	304	CLA	CMB-C2B	-2.15	1.46	1.50
17	3	318	CLA	CMD-C2D	-2.15	1.46	1.50
17	A	823	CLA	C4B-NB	2.15	1.40	1.37
17	L	301	CLA	C1B-C2B	2.15	1.48	1.43
17	A	819	CLA	CHC-C1C	2.15	1.42	1.38
17	A	802	CLA	CHC-C1C	2.15	1.42	1.38
19	A	843	LHG	O7-C5	-2.15	1.41	1.46
17	1	515	CLA	CMC-C2C	-2.15	1.46	1.50
17	A	810	CLA	C3B-C4B	2.15	1.49	1.42
17	B	828	CLA	MG-ND	-2.15	2.01	2.05
17	A	840	CLA	CHC-C1C	2.15	1.42	1.38
17	B	823	CLA	CHC-C1C	2.15	1.42	1.38
17	A	837	CLA	C1B-NB	-2.15	1.35	1.37
17	B	814	CLA	CHC-C1C	2.15	1.42	1.38
17	A	804	CLA	CMC-C2C	-2.15	1.46	1.50
17	K	203	CLA	CMB-C2B	-2.14	1.46	1.50
17	3	312	CLA	CMB-C2B	-2.14	1.46	1.50
17	3	309	CLA	CAA-C2A	-2.14	1.49	1.54
17	B	841	CLA	CHC-C1C	2.14	1.42	1.38
17	K	203	CLA	MG-ND	-2.14	2.01	2.05
17	B	838	CLA	C1B-C2B	2.14	1.48	1.43
17	1	504	CLA	CHC-C1C	2.14	1.42	1.38
17	B	815	CLA	MG-ND	-2.14	2.01	2.05
17	2	509	CLA	CMD-C2D	-2.14	1.46	1.50
17	A	815	CLA	C4B-NB	2.14	1.40	1.37
17	L	304	CLA	C1B-NB	-2.14	1.35	1.37
17	5	310	CLA	CHC-C1C	2.14	1.42	1.38
17	A	833	CLA	MG-ND	-2.14	2.01	2.05
17	A	821	CLA	C1B-NB	-2.14	1.35	1.37
17	3	313	CLA	CHC-C1C	2.14	1.42	1.38
17	A	822	CLA	C1B-NB	-2.14	1.35	1.37
17	B	840	CLA	C4B-NB	2.14	1.40	1.37
17	B	833	CLA	CMC-C2C	-2.14	1.46	1.50
17	5	307	CLA	CMD-C2D	-2.14	1.46	1.50
17	L	301	CLA	MG-ND	-2.14	2.01	2.05
17	A	824	CLA	C3B-C4B	2.14	1.49	1.42
17	B	827	CLA	C1B-C2B	2.14	1.48	1.43
17	3	309	CLA	CMD-C2D	-2.13	1.46	1.50
17	3	312	CLA	CMC-C2C	-2.13	1.46	1.50
26	2	502	XAT	C22-C21	-2.13	1.51	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	F	803	CLA	C3B-C4B	2.13	1.48	1.42
17	1	511	CLA	C3B-C4B	2.13	1.48	1.42
17	B	807	CLA	C1D-ND	2.13	1.40	1.37
17	3	301	CLA	C3B-C4B	2.13	1.48	1.42
17	A	817	CLA	C1D-ND	2.13	1.40	1.37
17	A	837	CLA	CHC-C1C	2.13	1.42	1.38
17	1	510	CLA	CMD-C2D	-2.13	1.46	1.50
17	B	814	CLA	MG-ND	-2.13	2.01	2.05
17	3	314	CLA	CMB-C2B	-2.12	1.46	1.50
17	A	842	CLA	C3B-C4B	2.12	1.48	1.42
17	B	807	CLA	CAC-C3C	-2.12	1.45	1.51
17	L	301	CLA	CHC-C1C	2.12	1.42	1.38
17	B	801	CLA	MG-ND	-2.12	2.01	2.05
17	A	817	CLA	CAB-C3B	-2.12	1.41	1.47
17	B	835	CLA	CHC-C1C	2.12	1.42	1.38
17	A	811	CLA	C1D-ND	2.12	1.40	1.37
17	2	505	CLA	C1B-NB	-2.12	1.35	1.37
17	K	205	CLA	CMD-C2D	-2.12	1.46	1.50
17	A	842	CLA	MG-NB	-2.12	2.01	2.05
17	1	505	CLA	CMC-C2C	-2.12	1.46	1.50
17	A	828	CLA	MG-ND	-2.12	2.01	2.05
17	5	316	CLA	C4B-NB	2.12	1.40	1.37
17	1	504	CLA	CMB-C2B	-2.12	1.46	1.50
17	3	313	CLA	CMB-C2B	-2.12	1.46	1.50
17	A	852	CLA	C1B-NB	-2.12	1.35	1.37
17	A	827	CLA	C1B-C2B	2.12	1.48	1.43
17	5	305	CLA	CHC-C1C	2.12	1.42	1.38
26	5	304	XAT	C22-C23	-2.11	1.49	1.52
17	K	205	CLA	MG-NB	-2.11	2.01	2.05
17	5	309	CLA	CHC-C1C	2.11	1.42	1.38
17	B	814	CLA	C1B-C2B	2.11	1.48	1.43
17	B	818	CLA	C1D-ND	2.11	1.40	1.37
17	B	835	CLA	C4B-NB	2.11	1.40	1.37
17	1	513	CLA	CMB-C2B	-2.11	1.46	1.50
17	J	101	CLA	C3B-C4B	2.11	1.48	1.42
17	A	826	CLA	C1B-C2B	2.11	1.48	1.43
17	A	818	CLA	MG-ND	-2.11	2.01	2.05
17	A	810	CLA	CHC-C1C	2.11	1.42	1.38
17	B	837	CLA	MG-ND	-2.11	2.01	2.05
17	2	510	CLA	CMB-C2B	-2.11	1.46	1.50
17	3	308	CLA	CMC-C2C	-2.11	1.46	1.50
17	1	506	CLA	CHC-C1C	2.11	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	5	308	CLA	CHC-C1C	2.11	1.42	1.38
17	1	511	CLA	CMB-C2B	-2.11	1.46	1.50
17	1	515	CLA	CHC-C1C	2.10	1.42	1.38
17	B	806	CLA	C1B-NB	-2.10	1.35	1.37
17	L	302	CLA	CMC-C2C	-2.10	1.46	1.50
17	A	834	CLA	CMC-C2C	-2.10	1.46	1.50
17	3	308	CLA	CMD-C2D	-2.10	1.46	1.50
17	A	827	CLA	C1D-ND	2.10	1.40	1.37
17	B	804	CLA	CAC-C3C	-2.10	1.45	1.51
17	1	508	CLA	CMB-C2B	-2.10	1.46	1.50
17	2	505	CLA	MG-ND	-2.10	2.01	2.05
17	B	836	CLA	C3B-C4B	2.10	1.48	1.42
17	B	827	CLA	C1B-NB	-2.10	1.35	1.37
17	B	806	CLA	CAC-C3C	-2.10	1.45	1.51
17	F	802	CLA	C1B-NB	-2.10	1.35	1.37
17	K	201	CLA	C1B-C2B	2.09	1.48	1.43
17	1	513	CLA	CHC-C1C	2.09	1.42	1.38
17	B	842	CLA	C1B-NB	-2.09	1.35	1.37
17	A	813	CLA	C4B-NB	2.09	1.40	1.37
17	2	511	CLA	CHC-C1C	2.09	1.42	1.38
17	A	832	CLA	C1B-C2B	2.09	1.48	1.43
17	A	842	CLA	CMD-C2D	-2.09	1.46	1.50
17	5	306	CLA	CMD-C2D	-2.09	1.46	1.50
17	A	812	CLA	MG-ND	-2.09	2.01	2.05
17	A	821	CLA	CHC-C1C	2.09	1.42	1.38
17	1	508	CLA	C3B-C4B	2.09	1.48	1.42
17	B	818	CLA	C1B-C2B	2.09	1.48	1.43
17	B	809	CLA	CAC-C3C	-2.09	1.45	1.51
17	1	511	CLA	CMC-C2C	-2.09	1.46	1.50
17	L	303	CLA	C1B-C2B	2.08	1.48	1.43
17	A	806	CLA	MG-ND	-2.08	2.01	2.05
17	A	833	CLA	C1B-NB	-2.08	1.35	1.37
17	1	507	CLA	C1B-NB	-2.08	1.35	1.37
17	1	510	CLA	CHC-C1C	2.08	1.42	1.38
17	1	511	CLA	CHC-C1C	2.08	1.42	1.38
17	A	838	CLA	CHC-C1C	2.08	1.42	1.38
17	A	803	CLA	C1B-NB	-2.08	1.35	1.37
17	3	310	CLA	CMC-C2C	-2.08	1.46	1.50
17	B	830	CLA	CAB-C3B	-2.08	1.41	1.47
17	B	819	CLA	C1B-C2B	2.08	1.48	1.43
17	A	802	CLA	C3B-C4B	2.08	1.48	1.42
17	1	513	CLA	CMC-C2C	-2.08	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	A	840	CLA	C3B-C4B	2.08	1.48	1.42
17	3	310	CLA	CMD-C2D	-2.08	1.46	1.50
17	3	316	CLA	CHC-C1C	2.08	1.42	1.38
17	2	511	CLA	CAC-C3C	-2.08	1.45	1.51
17	A	838	CLA	C1B-NB	-2.08	1.35	1.37
17	A	810	CLA	CAC-C3C	-2.07	1.45	1.51
17	2	511	CLA	C1B-NB	-2.07	1.35	1.37
17	5	312	CLA	C1B-NB	-2.07	1.35	1.37
17	B	822	CLA	CAC-C3C	-2.07	1.45	1.51
17	B	827	CLA	MG-ND	-2.07	2.01	2.05
20	5	302	BCR	C1-C6	-2.07	1.51	1.53
17	B	804	CLA	MG-ND	-2.07	2.01	2.05
17	B	841	CLA	CAA-C2A	-2.07	1.50	1.54
17	A	805	CLA	CAA-C2A	-2.07	1.50	1.54
17	5	307	CLA	CHC-C1C	2.07	1.42	1.38
17	2	506	CLA	CMC-C2C	-2.07	1.46	1.50
17	A	830	CLA	C1B-C2B	2.07	1.48	1.43
17	A	805	CLA	CMA-C3A	-2.07	1.48	1.53
17	2	509	CLA	CHC-C1C	2.07	1.42	1.38
17	A	808	CLA	C4B-NB	2.07	1.40	1.37
17	B	808	CLA	C1B-NB	-2.07	1.35	1.37
17	B	813	CLA	CAC-C3C	-2.07	1.45	1.51
17	5	311	CLA	CMC-C2C	-2.07	1.46	1.50
17	A	838	CLA	MG-ND	-2.07	2.01	2.05
17	A	812	CLA	CHC-C1C	2.06	1.42	1.38
17	1	513	CLA	C3B-C4B	2.06	1.48	1.42
17	5	307	CLA	C3B-C4B	2.06	1.48	1.42
17	A	805	CLA	C1B-C2B	2.06	1.48	1.43
17	A	804	CLA	C3B-C4B	2.06	1.48	1.42
17	B	830	CLA	C1B-NB	-2.06	1.35	1.37
17	L	301	CLA	C1B-NB	-2.06	1.35	1.37
17	3	309	CLA	C1B-NB	-2.06	1.35	1.37
17	B	801	CLA	C4B-NB	2.06	1.40	1.37
17	A	809	CLA	C1B-NB	-2.06	1.35	1.37
17	A	835	CLA	MG-ND	-2.06	2.01	2.05
17	A	827	CLA	CAA-C2A	-2.06	1.50	1.54
17	A	807	CLA	C1B-C2B	2.06	1.48	1.43
17	B	809	CLA	CHC-C1C	2.06	1.42	1.38
17	A	836	CLA	MG-NB	-2.06	2.01	2.05
17	3	308	CLA	MG-ND	-2.06	2.01	2.05
17	A	816	CLA	C4B-NB	2.06	1.40	1.37
17	3	318	CLA	C4B-NB	2.06	1.40	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	A	829	CLA	C3B-C4B	2.06	1.48	1.42
17	B	803	CLA	C1B-NB	-2.06	1.35	1.37
17	2	504	CLA	C3B-C4B	2.06	1.48	1.42
17	1	509	CLA	CMC-C2C	-2.05	1.46	1.50
17	2	510	CLA	CMC-C2C	-2.05	1.46	1.50
17	B	811	CLA	C3B-C4B	2.05	1.48	1.42
17	B	834	CLA	C1B-C2B	2.05	1.47	1.43
17	B	830	CLA	MG-ND	-2.05	2.01	2.05
17	K	201	CLA	CMD-C2D	-2.05	1.46	1.50
17	B	842	CLA	MG-ND	-2.05	2.01	2.05
17	5	310	CLA	C3B-C4B	2.05	1.48	1.42
25	1	517	CHL	C2A-C3A	-2.05	1.49	1.55
17	B	814	CLA	CAC-C3C	-2.05	1.45	1.51
17	B	802	CLA	MG-ND	-2.05	2.01	2.05
17	5	305	CLA	MG-ND	-2.05	2.01	2.05
17	3	312	CLA	CMD-C2D	-2.05	1.46	1.50
17	A	831	CLA	C3B-C2B	-2.05	1.36	1.44
17	A	831	CLA	CAA-C2A	-2.05	1.50	1.54
17	A	829	CLA	C4B-NB	2.05	1.40	1.37
17	B	805	CLA	C1D-ND	2.05	1.40	1.37
17	B	807	CLA	C1B-C2B	2.05	1.47	1.43
17	A	834	CLA	C1B-NB	-2.04	1.35	1.37
17	B	816	CLA	C1B-C2B	2.04	1.47	1.43
17	A	803	CLA	MG-ND	-2.04	2.01	2.05
17	5	309	CLA	C3B-C4B	2.04	1.48	1.42
17	B	823	CLA	C3B-C4B	2.04	1.48	1.42
17	A	814	CLA	C1B-NB	-2.04	1.35	1.37
17	1	515	CLA	MG-ND	-2.04	2.01	2.05
17	B	820	CLA	MG-ND	-2.04	2.01	2.05
17	1	510	CLA	MG-ND	-2.04	2.01	2.05
17	3	316	CLA	CMC-C2C	-2.04	1.46	1.50
17	B	817	CLA	CAB-C3B	-2.04	1.41	1.47
17	L	304	CLA	MG-ND	-2.04	2.01	2.05
17	3	318	CLA	CMB-C2B	-2.04	1.46	1.50
17	5	306	CLA	CMC-C2C	-2.04	1.46	1.50
17	3	308	CLA	C3B-C4B	2.04	1.48	1.42
17	A	813	CLA	CHC-C1C	2.04	1.42	1.38
17	A	825	CLA	C3B-C4B	2.04	1.48	1.42
17	2	514	CLA	C1B-NB	-2.03	1.35	1.37
17	A	823	CLA	CHC-C1C	2.03	1.42	1.38
17	3	316	CLA	C1D-ND	2.03	1.40	1.37
17	B	802	CLA	CHC-C1C	2.03	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	B	830	CLA	C1B-C2B	2.03	1.47	1.43
17	K	202	CLA	CMC-C2C	-2.03	1.46	1.50
25	3	302	CHL	CMC-C2C	2.03	1.49	1.44
17	3	314	CLA	CMC-C2C	-2.03	1.46	1.50
17	1	515	CLA	CMB-C2B	-2.03	1.46	1.50
17	A	842	CLA	MG-ND	-2.03	2.01	2.05
17	3	301	CLA	C1B-C2B	2.03	1.47	1.43
17	B	805	CLA	C1B-C2B	2.03	1.47	1.43
17	B	841	CLA	C3B-C4B	2.03	1.48	1.42
17	A	808	CLA	CAC-C3C	-2.03	1.45	1.51
17	A	807	CLA	MG-ND	-2.02	2.01	2.05
17	B	827	CLA	C3B-C4B	2.02	1.48	1.42
17	A	817	CLA	CBD-CGD	-2.02	1.49	1.51
17	L	301	CLA	C4B-NB	2.02	1.40	1.37
17	A	807	CLA	C4B-NB	2.02	1.40	1.37
17	B	838	CLA	C1B-NB	-2.02	1.35	1.37
17	2	509	CLA	CMC-C2C	-2.02	1.46	1.50
17	B	815	CLA	CAC-C3C	-2.02	1.45	1.51
17	A	804	CLA	CHC-C1C	2.02	1.42	1.38
17	B	810	CLA	C1D-ND	2.02	1.40	1.37
17	A	835	CLA	C1B-C2B	2.02	1.47	1.43
17	B	825	CLA	C4B-NB	2.02	1.40	1.37
17	B	801	CLA	CHC-C1C	2.02	1.42	1.38
17	B	806	CLA	C4B-NB	2.02	1.40	1.37
17	K	203	CLA	C1B-NB	-2.02	1.35	1.37
17	3	317	CLA	MG-ND	-2.01	2.01	2.05
17	3	312	CLA	MG-ND	-2.01	2.01	2.05
17	F	802	CLA	CHC-C1C	2.01	1.42	1.38
17	A	823	CLA	C3B-C4B	2.01	1.48	1.42
17	B	810	CLA	CAC-C3C	-2.01	1.45	1.51
17	A	831	CLA	C4B-NB	2.01	1.40	1.37
17	B	820	CLA	C3B-C4B	2.01	1.48	1.42
17	A	837	CLA	C1B-C2B	2.01	1.47	1.43
17	A	814	CLA	CAB-C3B	-2.01	1.42	1.47
17	3	307	CLA	CMB-C2B	-2.01	1.46	1.50
17	A	805	CLA	CAC-C3C	-2.01	1.45	1.51
17	A	823	CLA	C1B-C2B	2.01	1.47	1.43
17	5	316	CLA	CHC-C1C	2.01	1.42	1.38
17	3	308	CLA	CHC-C1C	2.01	1.42	1.38
24	1	501	LUT	C1-C6	-2.01	1.51	1.53
17	L	303	CLA	CHC-C1C	2.01	1.42	1.38
17	A	834	CLA	CHC-C1C	2.01	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	A	831	CLA	CAC-C3C	-2.01	1.46	1.51
17	A	835	CLA	CHC-C1C	2.01	1.42	1.38
17	B	826	CLA	CAC-C3C	-2.00	1.46	1.51
25	1	514	CHL	CHA-CBD	-2.00	1.49	1.51
17	F	803	CLA	MG-ND	-2.00	2.01	2.05
17	L	304	CLA	CHC-C1C	2.00	1.42	1.38
17	3	310	CLA	MG-NB	-2.00	2.01	2.05
17	3	309	CLA	CHC-C1C	2.00	1.42	1.38
17	B	822	CLA	C1B-NB	-2.00	1.35	1.37
17	3	309	CLA	MG-ND	-2.00	2.01	2.05
17	B	828	CLA	CMD-C2D	-2.00	1.46	1.50

All (1612) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	2	503	BCR	C40-C30-C25	-13.10	89.71	110.24
16	A	801	CL0	C1B-CHB-C4A	10.79	130.77	120.23
25	3	302	CHL	O2D-CGD-CBD	9.95	121.88	110.95
25	1	517	CHL	C1B-CHB-C4A	9.43	127.39	121.32
25	2	512	CHL	C1B-CHB-C4A	9.38	127.36	121.32
25	2	515	CHL	O2D-CGD-CBD	9.27	121.13	110.95
25	1	517	CHL	O2D-CGD-CBD	9.27	121.13	110.95
25	5	317	CHL	CHA-C1A-C2A	-9.12	120.36	133.83
20	2	503	BCR	C40-C30-C39	-9.08	82.63	108.63
20	2	503	BCR	C20-C21-C22	-9.01	114.64	127.28
25	3	315	CHL	O2D-CGD-CBD	8.89	120.72	110.95
25	1	514	CHL	O2D-CGD-CBD	8.61	120.41	110.95
25	2	516	CHL	C1B-CHB-C4A	8.54	126.81	121.32
25	5	314	CHL	O2D-CGD-CBD	8.23	120.00	110.95
17	3	308	CLA	C4A-NA-C1A	8.17	110.41	106.68
20	B	847	BCR	C15-C14-C13	-8.11	115.90	127.28
17	A	810	CLA	C4A-NA-C1A	8.08	110.37	106.68
25	2	512	CHL	O2D-CGD-CBD	7.97	119.70	110.95
17	A	835	CLA	C4A-NA-C1A	7.94	110.30	106.68
25	5	317	CHL	O2D-CGD-CBD	7.94	119.67	110.95
25	1	512	CHL	O2D-CGD-CBD	7.88	119.61	110.95
17	2	511	CLA	C4A-NA-C1A	7.83	110.25	106.68
17	A	832	CLA	C4A-NA-C1A	7.80	110.24	106.68
25	5	315	CHL	O2D-CGD-CBD	7.73	119.44	110.95
17	B	804	CLA	C4A-NA-C1A	7.69	110.19	106.68
17	L	303	CLA	C4A-NA-C1A	7.66	110.17	106.68
17	A	820	CLA	C4A-NA-C1A	7.63	110.16	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	3	306	CLA	C4A-NA-C1A	7.63	110.16	106.68
25	3	315	CHL	C1B-CHB-C4A	7.57	126.19	121.32
17	B	839	CLA	C4A-NA-C1A	7.55	110.12	106.68
17	2	506	CLA	C4A-NA-C1A	7.52	110.11	106.68
17	2	509	CLA	C4A-NA-C1A	7.50	110.10	106.68
17	A	821	CLA	C4A-NA-C1A	7.48	110.09	106.68
20	B	844	BCR	C7-C8-C9	-7.47	115.18	126.23
17	A	830	CLA	C4A-NA-C1A	7.46	110.08	106.68
17	3	313	CLA	C4A-NA-C1A	7.46	110.08	106.68
24	5	303	LUT	C26-C27-C28	-7.44	113.00	124.58
17	B	822	CLA	C4A-NA-C1A	7.42	110.06	106.68
17	A	839	CLA	C4A-NA-C1A	7.42	110.06	106.68
17	5	311	CLA	C4A-NA-C1A	7.40	110.06	106.68
17	L	302	CLA	C4A-NA-C1A	7.40	110.06	106.68
25	2	516	CHL	O2D-CGD-CBD	7.38	119.05	110.95
17	2	504	CLA	C4A-NA-C1A	7.36	110.04	106.68
17	3	311	CLA	C4A-NA-C1A	7.32	110.02	106.68
17	A	836	CLA	C4A-NA-C1A	7.25	109.99	106.68
17	B	816	CLA	C4A-NA-C1A	7.22	109.97	106.68
17	B	821	CLA	C4A-NA-C1A	7.20	109.96	106.68
17	B	840	CLA	C4A-NA-C1A	7.19	109.96	106.68
17	3	301	CLA	C4A-NA-C1A	7.19	109.96	106.68
20	A	853	BCR	C24-C23-C22	-7.18	115.61	126.23
17	A	816	CLA	C4A-NA-C1A	7.18	109.95	106.68
17	B	838	CLA	C4A-NA-C1A	7.15	109.94	106.68
26	2	502	XAT	C38-C25-C26	-7.15	110.54	122.30
17	A	822	CLA	C4A-NA-C1A	7.13	109.93	106.68
17	A	808	CLA	C4A-NA-C1A	7.13	109.93	106.68
17	B	818	CLA	C4A-NA-C1A	7.12	109.93	106.68
20	B	844	BCR	C20-C21-C22	-7.07	117.36	127.28
20	B	846	BCR	C7-C8-C9	-7.05	115.80	126.23
17	A	802	CLA	C4A-NA-C1A	7.04	109.89	106.68
17	3	310	CLA	C4A-NA-C1A	7.03	109.89	106.68
20	F	801	BCR	C24-C23-C22	-7.01	115.86	126.23
25	2	513	CHL	C1B-CHB-C4A	7.00	125.83	121.32
26	2	502	XAT	C18-C5-C6	-6.99	110.80	122.30
17	3	316	CLA	C4A-NA-C1A	6.97	109.86	106.68
17	5	306	CLA	C4A-NA-C1A	6.95	109.85	106.68
17	A	828	CLA	C4A-NA-C1A	6.94	109.85	106.68
17	B	832	CLA	C4A-NA-C1A	6.91	109.83	106.68
17	B	817	CLA	C4A-NA-C1A	6.91	109.83	106.68
17	5	316	CLA	C4A-NA-C1A	6.90	109.83	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	1	507	CLA	C4A-NA-C1A	6.85	109.81	106.68
20	B	844	BCR	C15-C14-C13	-6.84	117.69	127.28
17	2	510	CLA	C4A-NA-C1A	6.84	109.80	106.68
17	2	505	CLA	C4A-NA-C1A	6.83	109.80	106.68
17	3	318	CLA	C4A-NA-C1A	6.81	109.79	106.68
17	B	833	CLA	C4A-NA-C1A	6.79	109.78	106.68
17	1	506	CLA	C4A-NA-C1A	6.76	109.76	106.68
17	B	812	CLA	C4A-NA-C1A	6.76	109.76	106.68
26	2	502	XAT	C11-C10-C9	-6.74	117.82	127.28
17	B	835	CLA	C4A-NA-C1A	6.73	109.75	106.68
17	A	805	CLA	C4A-NA-C1A	6.72	109.74	106.68
17	B	814	CLA	C4A-NA-C1A	6.71	109.74	106.68
17	3	314	CLA	C4A-NA-C1A	6.71	109.74	106.68
17	A	803	CLA	C4A-NA-C1A	6.69	109.73	106.68
17	B	829	CLA	C4A-NA-C1A	6.67	109.72	106.68
26	5	304	XAT	C38-C25-C26	-6.66	111.34	122.30
17	A	807	CLA	C4A-NA-C1A	6.66	109.72	106.68
17	A	809	CLA	C4A-NA-C1A	6.65	109.71	106.68
20	B	845	BCR	C7-C8-C9	-6.61	116.46	126.23
17	A	814	CLA	C4A-NA-C1A	6.61	109.69	106.68
17	3	317	CLA	C4A-NA-C1A	6.60	109.69	106.68
17	B	808	CLA	C4A-NA-C1A	6.60	109.69	106.68
17	1	511	CLA	C4A-NA-C1A	6.59	109.69	106.68
17	B	841	CLA	C4A-NA-C1A	6.59	109.69	106.68
17	5	310	CLA	C4A-NA-C1A	6.59	109.68	106.68
17	A	840	CLA	C4A-NA-C1A	6.58	109.68	106.68
17	F	803	CLA	C4A-NA-C1A	6.57	109.68	106.68
25	2	515	CHL	C1B-CHB-C4A	6.56	125.54	121.32
17	1	505	CLA	C4A-NA-C1A	6.54	109.66	106.68
17	A	827	CLA	C4A-NA-C1A	6.53	109.66	106.68
17	2	514	CLA	C4A-NA-C1A	6.53	109.66	106.68
17	F	802	CLA	C4A-NA-C1A	6.52	109.65	106.68
20	2	503	BCR	C24-C23-C22	-6.51	116.60	126.23
17	A	804	CLA	C4A-NA-C1A	6.51	109.65	106.68
17	B	823	CLA	C4A-NA-C1A	6.51	109.65	106.68
17	A	842	CLA	C4A-NA-C1A	6.50	109.64	106.68
17	B	807	CLA	C4A-NA-C1A	6.50	109.64	106.68
17	B	831	CLA	C4A-NA-C1A	6.50	109.64	106.68
24	5	303	LUT	C35-C34-C33	-6.49	118.17	127.28
17	B	809	CLA	C4A-NA-C1A	6.47	109.63	106.68
17	A	806	CLA	C4A-NA-C1A	6.47	109.63	106.68
17	5	308	CLA	C4A-NA-C1A	6.47	109.63	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	L	304	CLA	C4A-NA-C1A	6.44	109.61	106.68
17	3	309	CLA	C4A-NA-C1A	6.42	109.61	106.68
17	1	510	CLA	C4A-NA-C1A	6.41	109.60	106.68
17	5	307	CLA	C4A-NA-C1A	6.40	109.60	106.68
17	A	811	CLA	C4A-NA-C1A	6.40	109.60	106.68
17	1	509	CLA	C4A-NA-C1A	6.39	109.59	106.68
17	B	819	CLA	C4A-NA-C1A	6.38	109.59	106.68
17	B	803	CLA	C4A-NA-C1A	6.37	109.58	106.68
17	A	826	CLA	C4A-NA-C1A	6.35	109.58	106.68
17	B	813	CLA	C4A-NA-C1A	6.35	109.58	106.68
17	A	813	CLA	C4A-NA-C1A	6.34	109.57	106.68
17	A	837	CLA	C4A-NA-C1A	6.33	109.57	106.68
17	A	817	CLA	C4A-NA-C1A	6.32	109.56	106.68
17	A	831	CLA	C4A-NA-C1A	6.31	109.56	106.68
17	A	852	CLA	C4A-NA-C1A	6.31	109.56	106.68
17	B	810	CLA	C4A-NA-C1A	6.29	109.55	106.68
17	B	827	CLA	C4A-NA-C1A	6.29	109.55	106.68
17	K	201	CLA	C4A-NA-C1A	6.28	109.54	106.68
17	B	802	CLA	C4A-NA-C1A	6.26	109.53	106.68
20	2	503	BCR	C15-C14-C13	6.26	136.05	127.28
17	B	825	CLA	C4A-NA-C1A	6.23	109.52	106.68
17	A	833	CLA	C4A-NA-C1A	6.22	109.52	106.68
17	1	513	CLA	C4A-NA-C1A	6.22	109.52	106.68
25	2	516	CHL	CHA-C1A-C2A	-6.22	118.70	133.31
17	A	834	CLA	C4A-NA-C1A	6.21	109.51	106.68
17	B	842	CLA	C4A-NA-C1A	6.21	109.51	106.68
17	B	834	CLA	C4A-NA-C1A	6.17	109.50	106.68
17	2	507	CLA	C4A-NA-C1A	6.16	109.49	106.68
17	1	508	CLA	C4A-NA-C1A	6.15	109.48	106.68
17	A	825	CLA	C4A-NA-C1A	6.14	109.48	106.68
25	3	315	CHL	CHA-C1A-C2A	-6.13	118.91	133.31
20	2	503	BCR	C40-C30-C29	-6.12	85.44	108.95
20	A	848	BCR	C28-C27-C26	-6.12	103.14	114.06
26	5	304	XAT	C18-C5-C6	-6.12	112.24	122.30
17	5	312	CLA	C4A-NA-C1A	6.11	109.47	106.68
17	B	811	CLA	C4A-NA-C1A	6.11	109.47	106.68
17	A	838	CLA	C4A-NA-C1A	6.09	109.46	106.68
17	B	837	CLA	C4A-NA-C1A	6.09	109.46	106.68
20	B	846	BCR	C24-C23-C22	-6.09	117.23	126.23
17	K	202	CLA	C4A-NA-C1A	6.08	109.45	106.68
17	L	301	CLA	C4A-NA-C1A	6.08	109.45	106.68
17	5	313	CLA	C4A-NA-C1A	6.06	109.44	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	A	812	CLA	C4A-NA-C1A	6.05	109.44	106.68
17	B	806	CLA	C4A-NA-C1A	6.05	109.44	106.68
17	B	828	CLA	C4A-NA-C1A	6.05	109.44	106.68
20	J	102	BCR	C28-C27-C26	-6.03	103.30	114.06
17	A	829	CLA	C4A-NA-C1A	6.03	109.43	106.68
17	J	101	CLA	C4A-NA-C1A	6.03	109.43	106.68
17	A	815	CLA	C4A-NA-C1A	6.02	109.43	106.68
17	K	205	CLA	C4A-NA-C1A	6.02	109.42	106.68
17	B	805	CLA	C4A-NA-C1A	6.01	109.42	106.68
25	2	512	CHL	CHA-C1A-C2A	-5.99	119.23	133.31
17	B	815	CLA	C4A-NA-C1A	5.99	109.41	106.68
17	3	307	CLA	C4A-NA-C1A	5.99	109.41	106.68
20	L	305	BCR	C28-C27-C26	-5.98	103.39	114.06
17	3	312	CLA	C4A-NA-C1A	5.95	109.39	106.68
17	1	504	CLA	C4A-NA-C1A	5.93	109.39	106.68
17	A	824	CLA	C4A-NA-C1A	5.92	109.38	106.68
17	B	830	CLA	C4A-NA-C1A	5.92	109.38	106.68
25	2	515	CHL	CHA-C1A-C2A	-5.91	119.43	133.31
20	3	305	BCR	C15-C14-C13	-5.91	118.99	127.28
20	B	846	BCR	C15-C14-C13	-5.91	118.99	127.28
17	B	836	CLA	C4A-NA-C1A	5.90	109.37	106.68
17	K	203	CLA	C4A-NA-C1A	5.86	109.35	106.68
17	5	309	CLA	C4A-NA-C1A	5.86	109.35	106.68
20	1	503	BCR	C11-C10-C9	-5.86	119.06	127.28
20	B	844	BCR	C11-C10-C9	-5.83	119.10	127.28
26	5	304	XAT	O4-C5-C4	5.83	118.95	113.49
17	A	818	CLA	C4A-NA-C1A	5.82	109.33	106.68
20	A	848	BCR	C24-C23-C22	-5.79	117.67	126.23
17	A	819	CLA	C4A-NA-C1A	5.79	109.32	106.68
17	B	826	CLA	C4A-NA-C1A	5.79	109.32	106.68
26	2	502	XAT	O24-C25-C38	5.78	121.51	115.05
25	5	314	CHL	CHA-C1A-C2A	-5.78	119.74	133.31
17	B	820	CLA	C4A-NA-C1A	5.78	109.31	106.68
17	2	508	CLA	C4A-NA-C1A	5.78	109.31	106.68
20	2	503	BCR	C39-C30-C25	5.77	119.29	110.24
20	A	845	BCR	C15-C14-C13	-5.76	119.19	127.28
20	B	852	BCR	C7-C8-C9	-5.76	117.71	126.23
24	1	502	LUT	C15-C14-C13	-5.75	119.21	127.28
17	5	305	CLA	C4A-NA-C1A	5.68	109.27	106.68
20	B	844	BCR	C24-C23-C22	-5.68	117.83	126.23
20	B	844	BCR	C16-C17-C18	-5.67	119.33	127.28
17	A	823	CLA	C4A-NA-C1A	5.66	109.26	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	849	BCR	C7-C8-C9	-5.65	117.87	126.23
20	2	503	BCR	C15-C16-C17	-5.64	111.98	123.52
17	B	824	CLA	C4A-NA-C1A	5.62	109.24	106.68
20	A	845	BCR	C16-C17-C18	-5.61	119.41	127.28
20	A	851	BCR	C15-C14-C13	-5.58	119.45	127.28
26	2	502	XAT	O4-C5-C18	5.58	121.28	115.05
20	I	101	BCR	C24-C23-C22	-5.51	118.08	126.23
20	B	852	BCR	C15-C14-C13	-5.50	119.56	127.28
20	L	305	BCR	C16-C17-C18	-5.48	119.59	127.28
20	F	801	BCR	C28-C27-C26	-5.47	104.30	114.06
20	F	804	BCR	C11-C10-C9	-5.46	119.63	127.28
24	2	501	LUT	C26-C27-C28	-5.44	116.11	124.58
17	B	801	CLA	C4A-NA-C1A	5.44	109.16	106.68
25	1	512	CHL	CHA-C1A-C2A	-5.42	120.58	133.31
20	K	204	BCR	C16-C17-C18	-5.40	119.70	127.28
20	B	849	BCR	C20-C21-C22	-5.37	119.75	127.28
26	5	304	XAT	O24-C25-C24	5.35	118.50	113.49
17	1	515	CLA	C4A-NA-C1A	5.35	109.12	106.68
25	5	315	CHL	CHA-C1A-C2A	-5.34	120.77	133.31
20	5	302	BCR	C33-C5-C6	-5.24	118.76	124.48
20	F	801	BCR	C20-C21-C22	-5.24	119.93	127.28
20	A	847	BCR	C15-C14-C13	-5.23	119.94	127.28
20	A	853	BCR	C28-C27-C26	-5.21	104.76	114.06
25	2	513	CHL	O2D-CGD-CBD	5.20	119.93	111.43
20	A	845	BCR	C33-C5-C6	-5.16	118.85	124.48
20	2	503	BCR	C16-C15-C14	5.15	134.06	123.52
26	2	502	XAT	O4-C5-C4	5.14	118.31	113.49
16	A	801	CL0	CHA-C1A-C2A	-5.11	126.28	133.83
20	A	845	BCR	C20-C21-C22	-5.09	120.14	127.28
25	5	314	CHL	C1B-CHB-C4A	5.09	124.60	121.32
20	A	846	BCR	C16-C17-C18	-5.07	120.17	127.28
24	1	502	LUT	C26-C27-C28	-5.03	116.75	124.58
20	B	847	BCR	C7-C8-C9	-5.01	118.82	126.23
25	3	302	CHL	CHA-C1A-C2A	-4.98	121.61	133.31
20	I	101	BCR	C20-C21-C22	-4.98	120.29	127.28
24	3	304	LUT	C35-C34-C33	-4.96	120.32	127.28
20	L	306	BCR	C15-C14-C13	-4.89	120.43	127.28
24	2	501	LUT	C7-C8-C9	-4.89	119.01	126.23
24	1	501	LUT	C18-C5-C6	-4.86	119.19	124.48
19	A	843	LHG	O7-C7-C8	4.85	121.96	111.48
20	B	849	BCR	C24-C23-C22	-4.84	119.07	126.23
23	2	519	LMG	O7-C10-C11	4.84	121.95	111.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	5	302	BCR	C7-C8-C9	-4.84	119.08	126.23
20	A	846	BCR	C11-C10-C9	-4.83	120.50	127.28
18	B	843	PQN	C11-C12-C13	-4.82	118.53	126.83
17	2	507	CLA	C4-C3-C2	-4.81	110.14	122.23
20	B	847	BCR	C15-C16-C17	-4.79	113.72	123.52
20	A	846	BCR	C24-C23-C22	-4.77	119.17	126.23
20	J	102	BCR	C16-C17-C18	-4.72	120.66	127.28
24	3	303	LUT	C26-C27-C28	-4.71	117.25	124.58
24	2	501	LUT	C15-C14-C13	-4.71	120.68	127.28
20	3	305	BCR	C24-C23-C22	-4.68	119.31	126.23
17	2	507	CLA	C5-C3-C2	-4.67	110.69	123.13
20	A	851	BCR	C28-C27-C26	-4.65	105.76	114.06
20	B	845	BCR	C15-C14-C13	-4.64	120.77	127.28
20	A	848	BCR	C20-C21-C22	-4.61	120.81	127.28
20	K	204	BCR	C28-C27-C26	-4.61	105.84	114.06
20	A	851	BCR	C38-C26-C25	-4.60	119.46	124.48
17	A	805	CLA	CAA-C2A-C3A	-4.60	100.58	113.00
20	B	846	BCR	C16-C17-C18	-4.58	120.85	127.28
20	B	848	BCR	C15-C14-C13	-4.55	120.90	127.28
20	L	305	BCR	C11-C10-C9	-4.54	120.91	127.28
20	F	804	BCR	C15-C14-C13	-4.53	120.92	127.28
20	B	848	BCR	C24-C23-C22	-4.53	119.53	126.23
26	5	304	XAT	C26-C27-C28	-4.53	116.41	125.99
20	B	849	BCR	C16-C17-C18	-4.52	120.93	127.28
20	A	849	BCR	C20-C21-C22	-4.50	120.96	127.28
20	K	204	BCR	C20-C21-C22	-4.48	121.00	127.28
20	A	845	BCR	C38-C26-C25	-4.48	119.60	124.48
20	B	845	BCR	C30-C25-C26	-4.47	116.53	122.64
16	A	801	CL0	C1C-CHC-C4B	4.47	132.06	116.07
20	B	847	BCR	C11-C10-C9	-4.47	121.01	127.28
20	B	848	BCR	C38-C26-C25	-4.46	119.61	124.48
25	5	317	CHL	CHB-C4A-NA	4.46	126.47	121.83
20	2	503	BCR	C33-C5-C6	-4.43	119.65	124.48
20	J	102	BCR	C3-C4-C5	-4.42	106.18	114.06
20	A	851	BCR	C3-C4-C5	-4.42	106.18	114.06
20	A	848	BCR	C15-C14-C13	-4.42	121.08	127.28
17	A	817	CLA	CAA-C2A-C3A	-4.41	106.11	116.23
20	K	204	BCR	C38-C26-C25	-4.41	119.67	124.48
20	I	101	BCR	C7-C8-C9	-4.39	119.74	126.23
24	1	501	LUT	C35-C34-C33	-4.38	121.14	127.28
17	L	304	CLA	CAC-C3C-C4C	4.37	130.48	124.79
24	3	304	LUT	C21-C26-C27	-4.36	107.81	112.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	846	BCR	C15-C14-C13	-4.36	121.17	127.28
25	1	517	CHL	CHA-C1A-NA	4.35	126.04	122.15
23	5	301	LMG	O7-C10-C11	4.35	120.89	111.48
19	B	851	LHG	O7-C7-C8	4.34	120.88	111.48
20	J	102	BCR	C15-C14-C13	-4.34	121.19	127.28
24	1	501	LUT	C26-C27-C28	-4.32	117.85	124.58
20	3	305	BCR	C38-C26-C25	-4.31	119.78	124.48
20	B	845	BCR	C33-C5-C6	-4.29	119.80	124.48
24	2	501	LUT	C11-C10-C9	-4.29	121.27	127.28
20	L	306	BCR	C24-C23-C22	-4.28	119.90	126.23
24	5	303	LUT	C18-C5-C6	-4.28	119.81	124.48
20	1	503	BCR	C33-C5-C6	-4.28	119.81	124.48
22	B	850	DGD	O2G-C1B-C2B	4.20	120.57	111.48
20	A	853	BCR	C16-C17-C18	-4.20	121.39	127.28
17	A	829	CLA	O2D-CGD-O1D	-4.18	115.70	123.85
20	B	852	BCR	C33-C5-C6	-4.18	119.92	124.48
25	5	315	CHL	C1B-CHB-C4A	4.17	124.00	121.32
20	L	305	BCR	C7-C8-C9	-4.16	120.08	126.23
20	A	845	BCR	C24-C23-C22	-4.15	120.09	126.23
20	2	503	BCR	C30-C25-C26	-4.15	116.97	122.64
26	2	502	XAT	C31-C30-C29	-4.13	121.49	127.28
20	A	851	BCR	C16-C17-C18	-4.12	121.50	127.28
24	2	501	LUT	C35-C34-C33	-4.12	121.50	127.28
26	2	502	XAT	C26-C27-C28	-4.10	117.31	125.99
24	5	303	LUT	C15-C14-C13	-4.09	121.54	127.28
19	1	516	LHG	O7-C7-C8	4.08	120.30	111.48
20	B	852	BCR	C38-C26-C25	-4.07	120.04	124.48
20	3	305	BCR	C11-C10-C9	-4.07	121.57	127.28
20	A	853	BCR	C20-C21-C22	-4.07	121.58	127.28
20	A	853	BCR	C27-C26-C25	-4.06	117.22	122.70
17	A	836	CLA	O2D-CGD-O1D	-4.04	115.98	123.85
23	F	805	LMG	O7-C10-C11	4.04	120.22	111.48
20	F	801	BCR	C16-C17-C18	-4.04	121.62	127.28
24	3	304	LUT	C26-C27-C28	-4.02	118.32	124.58
16	A	801	CL0	CHB-C4A-NA	4.02	126.02	121.83
20	L	306	BCR	C1-C6-C5	-4.01	117.16	122.64
19	A	844	LHG	O7-C7-C8	3.99	120.10	111.48
20	B	844	BCR	C3-C4-C5	-3.98	106.95	114.06
20	A	849	BCR	C24-C23-C22	-3.96	120.37	126.23
19	2	517	LHG	O7-C7-C8	3.96	120.06	111.48
20	A	846	BCR	C20-C21-C22	-3.96	121.72	127.28
16	A	801	CL0	C1-C2-C3	-3.95	119.73	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	I	101	BCR	C15-C14-C13	-3.94	121.75	127.28
20	5	302	BCR	C15-C14-C13	-3.93	121.77	127.28
17	A	833	CLA	O2D-CGD-O1D	-3.90	116.25	123.85
20	K	204	BCR	C33-C5-C6	-3.90	120.23	124.48
20	F	804	BCR	C7-C8-C9	-3.88	120.50	126.23
20	2	503	BCR	C29-C30-C25	3.87	116.07	110.44
20	A	853	BCR	C2-C1-C6	3.87	116.06	110.44
20	L	305	BCR	C38-C26-C25	-3.86	120.27	124.48
20	B	849	BCR	C3-C4-C5	-3.84	107.20	114.06
17	3	306	CLA	C1-C2-C3	-3.83	119.92	126.20
20	B	852	BCR	C28-C27-C26	-3.83	107.23	114.06
26	5	304	XAT	C10-C11-C12	-3.82	112.12	123.20
20	A	853	BCR	C15-C14-C13	-3.82	121.92	127.28
20	B	848	BCR	C15-C16-C17	-3.82	115.71	123.52
20	B	847	BCR	C33-C5-C6	-3.82	120.32	124.48
20	A	851	BCR	C33-C5-C6	-3.82	120.32	124.48
17	B	828	CLA	O2D-CGD-O1D	-3.80	116.45	123.85
24	3	303	LUT	C31-C30-C29	-3.80	121.95	127.28
20	B	848	BCR	C7-C8-C9	-3.79	120.62	126.23
20	I	101	BCR	C16-C17-C18	-3.78	121.97	127.28
17	2	504	CLA	CBD-CHA-C1A	3.78	132.04	128.03
17	B	829	CLA	C3A-C2A-C1A	-3.78	102.43	106.30
20	2	503	BCR	C23-C22-C21	3.77	124.94	119.01
26	2	502	XAT	C24-C23-C22	-3.77	103.73	110.79
17	A	819	CLA	O2D-CGD-O1D	-3.77	116.51	123.85
20	A	847	BCR	C16-C17-C18	-3.75	122.02	127.28
20	J	102	BCR	C20-C21-C22	-3.74	122.03	127.28
22	J	103	DGD	O2G-C1B-C2B	3.74	119.57	111.48
20	A	845	BCR	C28-C27-C26	-3.73	107.40	114.06
20	B	849	BCR	C33-C5-C6	-3.73	120.41	124.48
26	2	502	XAT	C35-C34-C33	-3.73	122.05	127.28
17	A	837	CLA	CAA-C2A-C3A	-3.73	107.68	116.23
20	L	305	BCR	C3-C4-C5	-3.72	107.42	114.06
17	K	202	CLA	CAA-C2A-C3A	-3.71	107.72	116.23
22	B	850	DGD	C4D-C3D-C2D	-3.71	104.31	110.83
20	A	847	BCR	C8-C7-C6	-3.71	117.09	127.00
20	F	804	BCR	C28-C27-C26	-3.71	107.44	114.06
20	A	848	BCR	C38-C26-C25	-3.70	120.44	124.48
26	2	502	XAT	O24-C25-C24	3.70	116.96	113.49
20	A	845	BCR	C30-C25-C26	-3.69	117.59	122.64
20	3	305	BCR	C33-C5-C6	-3.69	120.46	124.48
26	5	304	XAT	O24-C25-C38	3.68	119.17	115.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	K	202	CLA	O2D-CGD-O1D	-3.68	116.68	123.85
20	1	503	BCR	C7-C8-C9	-3.68	120.79	126.23
20	2	503	BCR	C39-C30-C29	3.68	123.08	108.95
18	B	843	PQN	C2M-C2-C3	-3.67	118.42	124.45
17	3	314	CLA	O2D-CGD-O1D	-3.66	116.73	123.85
25	2	513	CHL	C2A-C3A-C4A	-3.66	101.14	103.53
20	B	848	BCR	C33-C5-C6	-3.65	120.50	124.48
20	5	302	BCR	C38-C26-C25	-3.64	120.51	124.48
17	A	838	CLA	O2D-CGD-O1D	-3.64	116.76	123.85
17	B	819	CLA	CAA-C2A-C3A	-3.64	107.89	116.23
20	A	853	BCR	C29-C30-C25	3.64	115.72	110.44
17	B	810	CLA	C3A-C2A-C1A	-3.63	102.59	106.30
20	B	847	BCR	C38-C26-C25	-3.63	120.53	124.48
26	5	304	XAT	O4-C5-C18	3.62	119.10	115.05
20	I	101	BCR	C11-C10-C9	-3.61	122.21	127.28
18	A	841	PQN	C11-C12-C13	-3.61	120.62	126.83
17	B	822	CLA	O2D-CGD-O1D	-3.60	116.85	123.85
17	K	205	CLA	C3B-C4B-NB	-3.59	107.32	110.53
17	L	304	CLA	O2D-CGD-O1D	-3.59	116.87	123.85
20	A	848	BCR	C33-C5-C6	-3.58	120.57	124.48
17	A	839	CLA	O2D-CGD-O1D	-3.57	116.89	123.85
20	L	305	BCR	C15-C14-C13	-3.57	122.27	127.28
26	2	502	XAT	C4-C3-C2	-3.57	104.12	110.79
17	A	814	CLA	O2D-CGD-O1D	-3.57	116.90	123.85
25	3	315	CHL	CBC-CAC-C3C	-3.57	107.77	112.87
17	L	303	CLA	O2D-CGD-O1D	-3.55	116.93	123.85
20	B	845	BCR	C28-C27-C26	-3.55	107.73	114.06
19	1	516	LHG	O8-C23-C24	3.55	122.66	111.83
17	B	834	CLA	C3B-C4B-NB	-3.54	107.37	110.53
17	2	505	CLA	C3B-C4B-NB	-3.54	107.37	110.53
23	F	806	LMG	O7-C10-C11	3.54	119.14	111.48
20	J	102	BCR	C24-C23-C22	-3.54	121.00	126.23
22	B	850	DGD	C2G-O2G-C1B	-3.54	109.33	117.80
17	B	808	CLA	C3B-C4B-NB	-3.54	107.37	110.53
26	2	502	XAT	C8-C9-C10	3.53	124.56	119.01
25	5	314	CHL	CBC-CAC-C3C	-3.53	107.82	112.87
20	5	302	BCR	C16-C17-C18	-3.53	122.33	127.28
17	A	830	CLA	O2D-CGD-O1D	-3.53	116.98	123.85
17	B	815	CLA	O2D-CGD-O1D	-3.53	116.98	123.85
17	A	803	CLA	O2D-CGD-O1D	-3.51	117.01	123.85
17	B	826	CLA	O2D-CGD-O1D	-3.51	117.01	123.85
17	B	820	CLA	C3B-C4B-NB	-3.51	107.40	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	847	BCR	C3-C4-C5	-3.51	107.80	114.06
17	A	835	CLA	O2D-CGD-O1D	-3.51	117.02	123.85
17	A	813	CLA	C3B-C4B-NB	-3.50	107.41	110.53
17	K	203	CLA	C3A-C2A-C1A	-3.50	102.72	106.30
20	A	847	BCR	C33-C5-C6	-3.49	120.67	124.48
17	5	305	CLA	CMB-C2B-C1B	-3.49	122.47	125.94
22	J	103	DGD	C1E-O6E-C5E	3.49	120.53	113.72
25	1	514	CHL	C2A-C3A-C4A	-3.48	101.26	103.53
20	L	306	BCR	C28-C27-C26	-3.48	107.85	114.06
17	A	818	CLA	O2D-CGD-O1D	-3.48	117.07	123.85
20	2	503	BCR	C7-C8-C9	-3.48	121.09	126.23
17	A	812	CLA	C3B-C4B-NB	-3.47	107.43	110.53
26	5	304	XAT	C38-C25-C24	3.47	118.14	114.24
20	F	804	BCR	C11-C12-C13	-3.47	116.85	126.36
17	A	836	CLA	O2D-CGD-CBD	3.47	117.29	111.23
24	5	303	LUT	C7-C8-C9	-3.47	121.11	126.23
20	2	503	BCR	C38-C26-C25	-3.47	120.70	124.48
17	5	305	CLA	O2D-CGD-O1D	-3.46	117.11	123.85
20	2	503	BCR	C12-C13-C14	-3.46	113.57	119.01
20	B	844	BCR	C28-C27-C26	-3.46	107.89	114.06
20	A	853	BCR	C3-C4-C5	-3.46	107.89	114.06
25	3	315	CHL	O1D-CGD-CBD	-3.45	119.49	124.72
20	B	844	BCR	C11-C12-C13	-3.44	116.92	126.36
17	A	812	CLA	O2D-CGD-O1D	-3.44	117.15	123.85
20	J	102	BCR	C38-C26-C25	-3.44	120.73	124.48
17	A	824	CLA	C3A-C2A-C1A	-3.44	102.78	106.30
20	A	848	BCR	C16-C17-C18	-3.43	122.47	127.28
17	A	826	CLA	O2D-CGD-O1D	-3.42	117.19	123.85
20	K	204	BCR	C3-C4-C5	-3.42	107.96	114.06
17	B	802	CLA	O2D-CGD-O1D	-3.42	117.20	123.85
17	A	833	CLA	C3A-C2A-C1A	-3.41	102.81	106.30
20	A	847	BCR	C20-C21-C22	-3.41	122.50	127.28
20	I	101	BCR	C30-C25-C26	-3.41	117.98	122.64
17	B	801	CLA	O2D-CGD-O1D	-3.41	117.22	123.85
20	F	801	BCR	C33-C5-C6	-3.41	120.77	124.48
20	B	847	BCR	C23-C24-C25	-3.41	117.90	127.00
20	5	302	BCR	C11-C10-C9	-3.40	122.50	127.28
20	B	849	BCR	C10-C11-C12	-3.40	113.35	123.20
20	B	848	BCR	C3-C4-C5	-3.39	108.00	114.06
17	A	831	CLA	O2D-CGD-O1D	-3.39	117.25	123.85
20	L	306	BCR	C33-C5-C6	-3.39	120.79	124.48
17	A	827	CLA	C1-C2-C3	-3.38	120.65	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	A	804	CLA	O2D-CGD-O1D	-3.38	117.26	123.85
17	B	815	CLA	C3B-C4B-NB	-3.38	107.51	110.53
17	5	305	CLA	CHB-C1B-C2B	-3.38	123.36	130.51
20	A	846	BCR	C33-C5-C6	-3.38	120.80	124.48
17	B	808	CLA	O2D-CGD-O1D	-3.38	117.28	123.85
20	B	846	BCR	C8-C9-C10	3.38	124.32	119.01
17	5	313	CLA	C3B-C4B-NB	-3.37	107.52	110.53
17	1	506	CLA	O2D-CGD-O1D	-3.37	117.28	123.85
17	B	816	CLA	C3B-C4B-NB	-3.37	107.53	110.53
17	K	201	CLA	C3B-C4B-NB	-3.37	107.53	110.53
17	A	825	CLA	O2D-CGD-O1D	-3.37	117.30	123.85
20	3	305	BCR	C16-C17-C18	-3.37	122.56	127.28
20	A	849	BCR	C3-C4-C5	-3.37	108.06	114.06
26	5	304	XAT	C15-C14-C13	-3.35	122.58	127.28
17	A	823	CLA	O2D-CGD-O1D	-3.35	117.34	123.85
17	K	205	CLA	C3A-C2A-C1A	-3.34	102.89	106.30
19	1	516	LHG	C5-O7-C7	-3.34	109.81	117.80
20	L	305	BCR	C20-C21-C22	-3.33	122.60	127.28
20	B	847	BCR	C12-C13-C14	3.33	124.24	119.01
17	A	827	CLA	O2D-CGD-O1D	-3.33	117.38	123.85
17	A	819	CLA	C3A-C2A-C1A	-3.32	102.90	106.30
17	A	832	CLA	CBD-CHA-C1A	3.32	132.39	127.38
17	5	313	CLA	C3A-C2A-C1A	-3.32	102.91	106.30
17	A	806	CLA	C1-C2-C3	-3.31	120.77	126.20
20	2	503	BCR	C10-C11-C12	-3.31	113.61	123.20
17	B	810	CLA	O2D-CGD-O1D	-3.31	117.41	123.85
17	B	827	CLA	O2D-CGD-O1D	-3.30	117.42	123.85
17	B	841	CLA	O2D-CGD-O1D	-3.30	117.42	123.85
20	A	847	BCR	C3-C4-C5	-3.30	108.17	114.06
17	1	510	CLA	O2D-CGD-O1D	-3.29	117.44	123.85
24	3	304	LUT	C7-C8-C9	-3.29	121.36	126.23
17	A	826	CLA	C1-C2-C3	-3.29	120.80	126.20
22	B	850	DGD	O1G-C1A-C2A	3.29	121.87	111.83
20	5	302	BCR	C34-C9-C10	-3.29	117.49	122.82
17	1	507	CLA	C3B-C4B-NB	-3.29	107.60	110.53
17	B	838	CLA	O2D-CGD-O1D	-3.28	117.45	123.85
25	1	517	CHL	CBC-CAC-C3C	-3.28	108.18	112.87
20	2	503	BCR	C21-C20-C19	3.28	132.69	123.20
17	A	811	CLA	O2D-CGD-O1D	-3.28	117.47	123.85
20	B	845	BCR	C16-C17-C18	-3.27	122.69	127.28
17	A	817	CLA	C3B-C4B-NB	-3.27	107.61	110.53
25	5	314	CHL	OMC-CMC-C2C	-3.25	119.47	125.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	849	BCR	C28-C27-C26	-3.25	108.25	114.06
17	2	511	CLA	O2D-CGD-O1D	-3.25	117.52	123.85
20	F	801	BCR	C20-C19-C18	-3.25	117.45	126.36
17	J	101	CLA	O2D-CGD-O1D	-3.25	117.52	123.85
17	A	836	CLA	C3B-C4B-NB	-3.24	107.63	110.53
24	3	303	LUT	C10-C11-C12	-3.24	113.81	123.20
17	A	837	CLA	O2D-CGD-O1D	-3.24	117.54	123.85
17	A	806	CLA	C3B-C4B-NB	-3.23	107.65	110.53
17	B	803	CLA	O2D-CGD-O1D	-3.23	117.57	123.85
17	B	812	CLA	O2D-CGD-O1D	-3.23	117.57	123.85
17	A	817	CLA	CMA-C3A-C2A	-3.22	108.83	116.23
17	5	311	CLA	C3B-C4B-NB	-3.22	107.65	110.53
17	B	817	CLA	O2D-CGD-O1D	-3.22	117.58	123.85
20	A	851	BCR	C2-C1-C6	3.22	115.11	110.44
17	2	505	CLA	O2D-CGD-O1D	-3.21	117.59	123.85
17	3	309	CLA	CHB-C1B-C2B	-3.20	123.73	130.51
20	B	846	BCR	C1-C6-C5	-3.20	118.26	122.64
24	1	502	LUT	C18-C5-C6	-3.20	120.99	124.48
20	A	847	BCR	C33-C5-C4	3.20	120.41	113.60
17	K	202	CLA	C3B-C4B-NB	-3.19	107.68	110.53
20	B	844	BCR	C38-C26-C25	-3.19	121.00	124.48
17	3	317	CLA	C3B-C4B-NB	-3.19	107.69	110.53
17	B	833	CLA	C1-C2-C3	-3.19	120.98	126.20
17	B	840	CLA	CAA-C2A-C3A	-3.18	108.94	116.23
20	5	302	BCR	C8-C9-C10	3.18	124.01	119.01
17	3	301	CLA	C3B-C4B-NB	-3.17	107.70	110.53
17	2	509	CLA	C3B-C4B-NB	-3.17	107.70	110.53
20	A	851	BCR	C20-C21-C22	-3.17	122.84	127.28
17	A	803	CLA	CAA-C2A-C3A	-3.16	108.98	116.23
17	A	842	CLA	O2D-CGD-O1D	-3.16	117.69	123.85
25	2	515	CHL	CBC-CAC-C3C	-3.16	108.35	112.87
17	3	301	CLA	CAA-C2A-C3A	-3.16	108.99	116.23
17	B	821	CLA	C3B-C4B-NB	-3.15	107.71	110.53
17	A	818	CLA	C3A-C2A-C1A	-3.15	103.07	106.30
17	B	805	CLA	CAA-C2A-C3A	-3.15	109.00	116.23
17	A	842	CLA	C3B-C4B-NB	-3.15	107.72	110.53
20	K	204	BCR	C15-C14-C13	-3.15	122.86	127.28
20	I	101	BCR	C33-C5-C6	-3.15	121.05	124.48
17	3	306	CLA	C1C-NC-C4C	3.15	108.12	106.68
17	A	823	CLA	C3B-C4B-NB	-3.15	107.72	110.53
17	B	842	CLA	C3B-C4B-NB	-3.15	107.72	110.53
17	B	819	CLA	O2D-CGD-O1D	-3.15	117.72	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	2	501	LUT	C18-C5-C6	-3.14	121.05	124.48
17	3	316	CLA	CAA-C2A-C3A	-3.14	109.02	116.23
17	A	803	CLA	C3B-C4B-NB	-3.14	107.73	110.53
17	3	308	CLA	C3B-C4B-NB	-3.14	107.73	110.53
20	A	845	BCR	C38-C26-C27	3.14	120.29	113.60
20	B	846	BCR	C33-C5-C6	-3.14	121.06	124.48
19	A	843	LHG	O8-C23-C24	3.13	121.39	111.83
17	B	832	CLA	O2D-CGD-O1D	-3.13	117.75	123.85
25	2	515	CHL	O1D-CGD-CBD	-3.13	119.98	124.72
17	A	807	CLA	CBD-CHA-C1A	3.13	131.34	128.03
17	A	808	CLA	C3B-C4B-NB	-3.12	107.74	110.53
17	A	813	CLA	O2D-CGD-O1D	-3.12	117.78	123.85
17	B	824	CLA	C3B-C4B-NB	-3.12	107.75	110.53
17	B	818	CLA	O2D-CGD-O1D	-3.12	117.78	123.85
25	2	513	CHL	C3D-C4D-ND	3.11	116.58	110.42
17	A	822	CLA	O2D-CGD-O1D	-3.11	117.79	123.85
17	5	305	CLA	C3A-C2A-C1A	-3.11	103.12	106.30
17	5	306	CLA	C3B-C4B-NB	-3.11	107.75	110.53
17	1	515	CLA	C3B-C4B-NB	-3.11	107.76	110.53
25	1	514	CHL	C1B-CHB-C4A	-3.10	119.33	121.32
25	3	315	CHL	C1C-CHC-C4B	3.10	127.16	116.07
17	A	852	CLA	C3B-C4B-NB	-3.10	107.77	110.53
18	A	841	PQN	C2M-C2-C3	-3.09	119.36	124.45
17	A	822	CLA	CAA-C2A-C3A	-3.09	109.13	116.23
17	A	835	CLA	C1-C2-C3	-3.09	121.13	126.20
17	B	805	CLA	C3B-C4B-NB	-3.09	107.77	110.53
18	B	843	PQN	C11-C3-C2	-3.09	119.59	124.89
17	B	814	CLA	O2D-CGD-O1D	-3.09	117.83	123.85
17	B	837	CLA	CAC-C3C-C4C	3.09	128.81	124.79
19	2	517	LHG	O8-C23-C24	3.09	121.25	111.83
20	A	846	BCR	C7-C8-C9	-3.09	121.67	126.23
25	1	512	CHL	OMC-CMC-C2C	-3.09	119.76	125.12
17	B	827	CLA	CAA-C2A-C3A	-3.08	109.16	116.23
17	A	825	CLA	C3B-C4B-NB	-3.08	107.78	110.53
25	5	317	CHL	C4C-C3C-C2C	-3.08	101.32	108.42
20	L	306	BCR	C16-C17-C18	-3.08	122.96	127.28
17	1	510	CLA	C3B-C4B-NB	-3.08	107.78	110.53
25	2	513	CHL	C1C-CHC-C4B	3.07	127.05	116.07
17	A	838	CLA	C3B-C4B-NB	-3.07	107.79	110.53
17	1	513	CLA	O2D-CGD-O1D	-3.07	117.88	123.85
17	A	829	CLA	C3B-C4B-NB	-3.06	107.79	110.53
20	2	503	BCR	C37-C22-C21	-3.06	117.86	122.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	B	823	CLA	C3B-C4B-NB	-3.06	107.80	110.53
17	B	842	CLA	O2D-CGD-O1D	-3.06	117.89	123.85
20	5	302	BCR	C35-C13-C12	3.06	122.76	118.09
25	2	513	CHL	CHA-C1A-NA	3.06	124.89	122.15
17	2	507	CLA	C3B-C4B-NB	-3.05	107.81	110.53
17	B	811	CLA	C3B-C4B-NB	-3.05	107.81	110.53
25	3	302	CHL	O1D-CGD-CBD	-3.05	120.10	124.72
25	2	516	CHL	C1C-CHC-C4B	3.04	126.95	116.07
17	A	807	CLA	C3A-C2A-C1A	-3.04	103.19	106.30
20	A	845	BCR	C11-C10-C9	-3.04	123.01	127.28
17	B	809	CLA	C3B-C4B-NB	-3.04	107.82	110.53
17	2	504	CLA	C3A-C4A-CHB	-3.04	120.19	123.91
17	B	811	CLA	CAA-C2A-C3A	-3.03	104.80	113.00
20	B	846	BCR	C3-C4-C5	-3.03	108.65	114.06
17	B	830	CLA	O2D-CGD-O1D	-3.03	117.94	123.85
17	A	819	CLA	C3B-C4B-NB	-3.03	107.82	110.53
17	B	839	CLA	O2D-CGD-O1D	-3.03	117.95	123.85
20	B	852	BCR	C3-C4-C5	-3.02	108.66	114.06
16	A	801	CL0	CBC-CAC-C3C	-3.02	108.55	112.87
26	5	304	XAT	C24-C23-C22	-3.02	105.15	110.79
17	3	311	CLA	C1-C2-C3	-3.02	121.88	126.76
20	B	849	BCR	C15-C14-C13	-3.01	123.05	127.28
20	A	851	BCR	C38-C26-C27	3.01	120.02	113.60
17	L	301	CLA	C3B-C4B-NB	-3.01	107.84	110.53
17	L	301	CLA	O2D-CGD-O1D	-3.01	117.99	123.85
25	3	302	CHL	O2D-CGD-O1D	-3.01	117.99	123.85
26	5	304	XAT	C18-C5-C4	3.01	117.62	114.24
20	J	102	BCR	C33-C5-C6	-3.01	121.20	124.48
25	5	317	CHL	C1B-CHB-C4A	3.00	123.17	120.23
17	3	317	CLA	O2D-CGD-O1D	-3.00	118.01	123.85
17	B	836	CLA	C3B-C4B-NB	-3.00	107.85	110.53
20	J	102	BCR	C38-C26-C27	3.00	119.98	113.60
19	A	843	LHG	C5-O7-C7	-3.00	110.63	117.80
17	5	305	CLA	C1B-NB-C4B	2.99	108.41	106.31
17	B	804	CLA	O2D-CGD-O1D	-2.99	118.03	123.85
17	B	833	CLA	O2D-CGD-O1D	-2.99	118.03	123.85
17	L	303	CLA	CHB-C4A-NA	2.99	128.71	124.40
17	B	802	CLA	O2D-CGD-CBD	2.99	116.45	111.23
20	3	305	BCR	C3-C4-C5	-2.99	108.73	114.06
20	B	844	BCR	C33-C5-C6	-2.98	121.23	124.48
17	3	317	CLA	CAA-C2A-C3A	-2.98	109.39	116.23
17	B	809	CLA	O2D-CGD-O1D	-2.98	118.05	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	1	505	CLA	C3B-C4B-NB	-2.98	107.87	110.53
17	A	832	CLA	CHB-C4A-NA	2.98	128.69	124.40
20	A	847	BCR	C38-C26-C25	-2.98	121.24	124.48
20	B	852	BCR	C16-C17-C18	-2.98	123.11	127.28
17	2	514	CLA	C3B-C4B-NB	-2.97	107.88	110.53
25	5	315	CHL	OMC-CMC-C2C	-2.97	119.96	125.12
20	L	306	BCR	C33-C5-C4	2.97	119.93	113.60
17	B	807	CLA	O2D-CGD-O1D	-2.97	118.06	123.85
20	B	848	BCR	C20-C21-C22	-2.97	123.11	127.28
24	3	303	LUT	C18-C5-C6	-2.97	121.24	124.48
17	A	840	CLA	C3B-C4B-NB	-2.97	107.88	110.53
25	1	517	CHL	C1C-CHC-C4B	2.96	126.68	116.07
25	3	315	CHL	OMC-CMC-C2C	-2.96	119.97	125.12
17	A	820	CLA	C3B-C4B-NB	-2.96	107.89	110.53
17	B	813	CLA	O2D-CGD-O1D	-2.96	118.08	123.85
17	A	839	CLA	C3B-C4B-NB	-2.96	107.89	110.53
25	5	317	CHL	C1C-CHC-C4B	2.96	126.66	116.07
17	1	506	CLA	C3B-C4B-NB	-2.96	107.89	110.53
16	A	801	CL0	C4C-CHD-C1D	2.96	126.64	116.07
24	5	303	LUT	C16-C1-C6	-2.95	105.61	110.24
17	A	816	CLA	C3B-C4B-NB	-2.95	107.90	110.53
20	B	848	BCR	C11-C10-C9	-2.95	123.14	127.28
20	3	305	BCR	C7-C8-C9	-2.95	121.88	126.23
17	A	814	CLA	C3B-C4B-NB	-2.95	107.90	110.53
20	2	503	BCR	C36-C18-C19	2.94	122.58	118.09
17	5	313	CLA	O2D-CGD-O1D	-2.94	118.12	123.85
17	B	835	CLA	C3B-C4B-NB	-2.94	107.91	110.53
17	A	820	CLA	O2D-CGD-O1D	-2.94	118.13	123.85
17	B	836	CLA	O2D-CGD-O1D	-2.94	118.13	123.85
25	5	314	CHL	C1C-CHC-C4B	2.93	126.56	116.07
24	1	502	LUT	C3-C4-C5	-2.93	104.88	112.18
17	3	318	CLA	O2D-CGD-O1D	-2.93	118.14	123.85
20	B	852	BCR	C24-C23-C22	-2.93	121.90	126.23
24	2	501	LUT	C30-C31-C32	-2.93	114.71	123.20
26	5	304	XAT	C6-C7-C8	-2.93	119.80	125.99
17	F	803	CLA	CAA-C2A-C3A	-2.93	109.52	116.23
25	5	315	CHL	O1D-CGD-CBD	-2.92	120.29	124.72
17	1	506	CLA	C1-C2-C3	-2.92	121.41	126.20
25	3	302	CHL	C1C-CHC-C4B	2.92	126.53	116.07
17	A	805	CLA	C3B-C4B-NB	-2.92	107.92	110.53
17	B	827	CLA	C3B-C4B-NB	-2.92	107.92	110.53
23	F	806	LMG	O8-C28-C29	2.92	120.73	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	1	504	CLA	C3B-C4B-NB	-2.92	107.92	110.53
17	5	310	CLA	O2D-CGD-O1D	-2.92	118.17	123.85
17	3	309	CLA	CMB-C2B-C1B	-2.92	123.04	125.94
17	K	201	CLA	CHB-C4A-NA	2.92	128.61	124.40
22	B	850	DGD	O6D-C1D-O3G	-2.91	103.16	110.04
17	B	835	CLA	O2D-CGD-O1D	-2.91	118.18	123.85
26	5	304	XAT	C4-C3-C2	-2.91	105.34	110.79
17	5	307	CLA	C3B-C4B-NB	-2.91	107.93	110.53
20	B	846	BCR	C38-C26-C25	-2.91	121.31	124.48
17	F	802	CLA	O2D-CGD-O1D	-2.91	118.19	123.85
17	3	314	CLA	C3B-C4B-NB	-2.91	107.94	110.53
17	A	840	CLA	O2D-CGD-O1D	-2.91	118.19	123.85
20	A	849	BCR	C15-C14-C13	-2.90	123.20	127.28
17	B	821	CLA	O2D-CGD-O1D	-2.90	118.19	123.85
17	A	816	CLA	O2D-CGD-O1D	-2.90	118.20	123.85
25	1	514	CHL	O1D-CGD-CBD	-2.90	120.32	124.72
25	2	512	CHL	C1C-CHC-C4B	2.90	126.45	116.07
20	3	305	BCR	C20-C21-C22	-2.90	123.21	127.28
17	B	804	CLA	C3B-C4B-NB	-2.90	107.94	110.53
25	2	515	CHL	C1C-CHC-C4B	2.90	126.43	116.07
24	5	303	LUT	C35-C15-C14	-2.89	117.60	123.52
19	A	844	LHG	C5-O7-C7	-2.89	110.88	117.80
17	3	313	CLA	O2D-CGD-O1D	-2.89	118.22	123.85
24	1	502	LUT	C8-C7-C6	-2.89	119.28	127.00
17	B	807	CLA	C3B-C4B-NB	-2.88	107.95	110.53
20	K	204	BCR	C7-C8-C9	-2.88	121.97	126.23
17	2	511	CLA	CHB-C4A-NA	2.88	128.56	124.40
17	B	841	CLA	C3B-C4B-NB	-2.88	107.96	110.53
26	2	502	XAT	C38-C25-C24	2.88	117.48	114.24
17	B	818	CLA	C3B-C4B-NB	-2.88	107.96	110.53
17	2	510	CLA	C3B-C4B-NB	-2.88	107.96	110.53
17	1	511	CLA	C3B-C4B-NB	-2.87	107.97	110.53
17	B	835	CLA	C1-C2-C3	-2.87	121.49	126.20
25	2	515	CHL	OMC-CMC-C2C	-2.87	120.14	125.12
20	B	845	BCR	C27-C26-C25	-2.87	118.83	122.70
17	A	821	CLA	O2D-CGD-O1D	-2.87	118.27	123.85
24	1	501	LUT	C7-C8-C9	-2.87	122.00	126.23
20	L	305	BCR	C29-C30-C25	2.87	114.60	110.44
24	3	303	LUT	C15-C35-C34	-2.87	117.66	123.52
22	B	850	DGD	C1D-O6D-C5D	2.86	119.31	113.72
17	B	822	CLA	C3B-C4B-NB	-2.86	107.97	110.53
17	3	309	CLA	O2D-CGD-O1D	-2.86	118.28	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	846	BCR	C38-C26-C25	-2.86	121.36	124.48
17	J	101	CLA	C3B-C4B-NB	-2.86	107.98	110.53
17	A	834	CLA	C3B-C4B-NB	-2.86	107.98	110.53
17	B	828	CLA	CAA-C2A-C3A	-2.86	109.68	116.23
17	B	824	CLA	O2D-CGD-O1D	-2.85	118.30	123.85
22	B	850	DGD	O2G-C1B-O1B	-2.85	117.04	123.70
17	5	308	CLA	CMB-C2B-C1B	-2.85	121.08	125.42
20	F	801	BCR	C10-C11-C12	-2.85	114.95	123.20
17	A	810	CLA	C3B-C4B-NB	-2.85	107.99	110.53
17	1	509	CLA	O2D-CGD-O1D	-2.84	118.31	123.85
20	B	852	BCR	C38-C26-C27	2.84	119.66	113.60
17	B	806	CLA	C3B-C4B-NB	-2.84	107.99	110.53
17	B	819	CLA	C3B-C4B-NB	-2.84	107.99	110.53
17	B	831	CLA	C3B-C4B-NB	-2.84	107.99	110.53
17	2	508	CLA	O2D-CGD-O1D	-2.84	118.31	123.85
20	F	804	BCR	C16-C17-C18	-2.84	123.29	127.28
17	2	511	CLA	C3A-C2A-C1A	-2.84	103.39	106.30
24	2	501	LUT	C3-C4-C5	-2.84	105.11	112.18
17	A	820	CLA	CHB-C4A-NA	2.84	128.50	124.40
17	F	802	CLA	C3B-C4B-NB	-2.84	108.00	110.53
26	2	502	XAT	C15-C14-C13	-2.84	123.30	127.28
17	A	834	CLA	O2D-CGD-O1D	-2.84	118.33	123.85
17	2	511	CLA	O2D-CGD-CBD	2.84	116.19	111.23
17	A	811	CLA	C3A-C2A-C1A	-2.84	103.40	106.30
17	B	840	CLA	C3B-C4B-NB	-2.84	108.00	110.53
20	K	204	BCR	C10-C11-C12	-2.83	114.99	123.20
25	3	315	CHL	CMA-C3A-C4A	-2.83	108.51	114.61
17	2	507	CLA	C3A-C2A-C1A	-2.83	103.41	106.30
17	5	312	CLA	O2D-CGD-O1D	-2.83	118.35	123.85
17	B	834	CLA	O2D-CGD-O1D	-2.83	118.35	123.85
17	L	302	CLA	C2A-C3A-C4A	-2.82	103.24	106.24
20	B	847	BCR	C28-C27-C26	-2.82	109.02	114.06
20	J	102	BCR	C11-C10-C9	-2.82	123.32	127.28
20	A	851	BCR	C7-C8-C9	-2.82	122.06	126.23
17	3	306	CLA	O2D-CGD-O1D	-2.82	118.36	123.85
25	5	315	CHL	C1C-CHC-C4B	2.82	126.14	116.07
25	1	517	CHL	O1D-CGD-CBD	-2.82	120.45	124.72
20	L	305	BCR	C38-C26-C27	2.81	119.59	113.60
17	1	511	CLA	O2D-CGD-O1D	-2.81	118.37	123.85
17	B	817	CLA	C3B-C4B-NB	-2.81	108.02	110.53
17	A	829	CLA	O2D-CGD-CBD	2.81	116.15	111.23
20	F	804	BCR	C38-C26-C25	-2.81	121.42	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	A	839	CLA	CHB-C4A-NA	2.81	128.46	124.40
20	L	306	BCR	C21-C20-C19	-2.81	115.06	123.20
17	B	829	CLA	C3B-C4B-NB	-2.81	108.02	110.53
20	A	847	BCR	C4-C5-C6	-2.81	118.91	122.70
17	A	803	CLA	O2D-CGD-CBD	2.80	116.13	111.23
17	A	835	CLA	CHB-C4A-NA	2.80	128.44	124.40
17	B	822	CLA	CHB-C4A-NA	2.80	128.44	124.40
20	B	845	BCR	C8-C9-C10	2.80	123.41	119.01
17	B	831	CLA	O2D-CGD-O1D	-2.80	118.40	123.85
24	3	303	LUT	C22-C23-C24	2.80	115.34	111.18
17	A	840	CLA	CAA-C2A-C3A	-2.80	109.82	116.23
17	B	838	CLA	O2D-CGD-CBD	2.80	116.12	111.23
17	3	311	CLA	O2D-CGD-O1D	-2.80	118.41	123.85
17	A	807	CLA	C3B-C4B-NB	-2.79	108.04	110.53
17	A	830	CLA	C3B-C4B-NB	-2.79	108.04	110.53
20	L	306	BCR	C38-C26-C25	-2.79	121.44	124.48
19	2	517	LHG	C5-O7-C7	-2.79	111.12	117.80
20	A	848	BCR	C38-C26-C27	2.79	119.54	113.60
25	1	517	CHL	O2D-CGD-O1D	-2.79	118.42	123.85
17	5	316	CLA	CAA-C2A-C3A	-2.79	109.84	116.23
20	F	804	BCR	C21-C20-C19	-2.79	115.12	123.20
17	B	837	CLA	O2D-CGD-O1D	-2.79	118.42	123.85
20	A	847	BCR	C7-C8-C9	-2.78	122.12	126.23
25	1	514	CHL	OMC-CMC-C2C	-2.78	120.29	125.12
17	3	306	CLA	CHB-C4A-NA	2.78	128.41	124.40
25	1	512	CHL	CBC-CAC-C3C	-2.78	108.89	112.87
16	A	801	CL0	C6-C5-C3	-2.78	106.69	113.47
20	B	846	BCR	C34-C9-C10	-2.78	118.31	122.82
17	B	823	CLA	O2D-CGD-O1D	-2.78	118.44	123.85
17	3	301	CLA	O2D-CGD-O1D	-2.78	118.44	123.85
17	B	814	CLA	CAA-C2A-C3A	-2.78	109.86	116.23
17	B	829	CLA	O2D-CGD-O1D	-2.78	118.44	123.85
17	1	515	CLA	O2D-CGD-O1D	-2.78	118.44	123.85
16	A	801	CL0	O2D-CGD-CBD	2.78	120.71	113.90
17	1	511	CLA	CHB-C4A-NA	2.78	128.41	124.40
17	A	834	CLA	CAA-C2A-C3A	-2.78	109.87	116.23
17	B	826	CLA	C3B-C4B-NB	-2.77	108.05	110.53
20	B	847	BCR	C33-C5-C4	2.77	119.51	113.60
17	L	303	CLA	C3B-C4B-NB	-2.77	108.06	110.53
23	F	805	LMG	O8-C28-C29	2.77	119.56	111.15
17	1	508	CLA	C3A-C2A-C1A	-2.77	103.47	106.30
17	3	308	CLA	CHB-C4A-NA	2.77	128.39	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	2	506	CLA	C3B-C4B-NB	-2.76	108.06	110.53
20	J	102	BCR	C29-C30-C25	2.76	114.45	110.44
25	1	514	CHL	CBC-CAC-C3C	-2.76	108.92	112.87
25	5	317	CHL	CAC-C3C-C4C	2.76	129.70	124.73
22	B	850	DGD	O3G-C3G-C2G	-2.76	104.11	110.82
20	A	851	BCR	C29-C30-C25	2.76	114.44	110.44
17	1	504	CLA	O2D-CGD-O1D	-2.76	118.48	123.85
20	A	847	BCR	C24-C23-C22	-2.76	122.16	126.23
17	A	837	CLA	CMB-C2B-C1B	-2.75	121.23	125.42
17	A	831	CLA	C1-C2-C3	-2.75	121.69	126.20
17	3	312	CLA	C3B-C4B-NB	-2.75	108.07	110.53
17	A	828	CLA	C3B-C4B-NB	-2.75	108.08	110.53
24	2	501	LUT	C18-C5-C4	2.75	119.47	114.42
17	A	837	CLA	C3B-C4B-NB	-2.75	108.08	110.53
17	B	806	CLA	O2D-CGD-O1D	-2.75	118.50	123.85
17	B	830	CLA	C3B-C4B-NB	-2.75	108.08	110.53
17	5	308	CLA	O2D-CGD-O1D	-2.75	118.50	123.85
17	2	509	CLA	CHB-C4A-NA	2.74	128.36	124.40
20	B	846	BCR	C33-C5-C4	2.74	119.44	113.60
20	B	847	BCR	C36-C18-C19	2.74	122.28	118.09
25	2	516	CHL	CMB-C2B-C3B	2.74	130.43	124.69
17	1	507	CLA	O2D-CGD-O1D	-2.74	118.52	123.85
17	A	802	CLA	C3B-C4B-NB	-2.74	108.09	110.53
17	3	313	CLA	CHB-C4A-NA	2.74	128.35	124.40
20	I	101	BCR	C28-C27-C26	-2.74	109.17	114.06
20	B	847	BCR	C1-C6-C5	-2.74	118.90	122.64
25	3	302	CHL	CBC-CAC-C3C	-2.73	108.96	112.87
17	F	803	CLA	C3B-C4B-NB	-2.73	108.09	110.53
17	A	842	CLA	C1-C2-C3	-2.73	122.34	126.76
20	A	847	BCR	C11-C10-C9	-2.73	123.45	127.28
25	1	512	CHL	C1C-CHC-C4B	2.73	125.84	116.07
17	B	833	CLA	CHB-C4A-NA	2.73	128.34	124.40
20	I	101	BCR	C15-C16-C17	-2.73	117.93	123.52
20	B	846	BCR	C35-C13-C14	-2.73	118.39	122.82
20	B	847	BCR	C35-C13-C14	-2.73	118.40	122.82
17	1	505	CLA	O2D-CGD-O1D	-2.72	118.54	123.85
20	A	853	BCR	C32-C1-C6	-2.72	105.97	110.24
17	A	811	CLA	O2D-CGD-CBD	2.72	115.99	111.23
20	B	847	BCR	C1-C6-C7	2.72	123.04	115.65
23	2	519	LMG	C7-O1-C1	-2.72	107.96	113.80
19	A	843	LHG	C6-C5-C4	-2.72	105.44	111.78
17	3	316	CLA	C3B-C4B-NB	-2.72	108.10	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	1	502	LUT	C15-C35-C34	-2.72	117.95	123.52
20	F	804	BCR	C29-C30-C25	2.72	114.39	110.44
20	B	847	BCR	C21-C20-C19	-2.72	115.33	123.20
17	L	304	CLA	CHB-C4A-NA	2.72	128.32	124.40
17	B	825	CLA	O2D-CGD-O1D	-2.71	118.57	123.85
20	B	849	BCR	C37-C22-C21	-2.71	118.42	122.82
20	L	306	BCR	C3-C4-C5	-2.71	109.22	114.06
17	A	815	CLA	O2D-CGD-O1D	-2.71	118.57	123.85
17	B	825	CLA	CHB-C4A-NA	2.71	128.31	124.40
24	3	303	LUT	C20-C13-C12	2.71	122.23	118.09
20	B	844	BCR	C15-C16-C17	-2.71	117.98	123.52
17	A	818	CLA	C3B-C4B-NB	-2.71	108.11	110.53
17	B	819	CLA	CMA-C3A-C2A	-2.71	110.02	116.23
17	B	811	CLA	O2D-CGD-O1D	-2.70	118.59	123.85
17	A	822	CLA	C3B-C4B-NB	-2.70	108.12	110.53
17	B	803	CLA	C3B-C4B-NB	-2.70	108.12	110.53
17	A	810	CLA	O2D-CGD-O1D	-2.70	118.59	123.85
20	A	846	BCR	C30-C25-C26	-2.70	118.95	122.64
20	A	851	BCR	C23-C24-C25	-2.70	119.79	127.00
20	B	852	BCR	C34-C9-C10	-2.69	118.45	122.82
17	B	805	CLA	CHB-C4A-NA	2.69	128.29	124.40
17	3	312	CLA	CAA-C2A-C3A	-2.69	110.06	116.23
20	A	846	BCR	C28-C27-C26	-2.69	109.26	114.06
19	B	851	LHG	O8-C23-C24	2.69	120.04	111.83
20	A	853	BCR	C38-C26-C27	2.69	119.33	113.60
20	B	848	BCR	C21-C20-C19	-2.69	115.41	123.20
17	B	821	CLA	CHB-C4A-NA	2.69	128.28	124.40
20	A	849	BCR	C28-C27-C26	-2.69	109.27	114.06
17	5	310	CLA	C1-C2-C3	-2.69	122.42	126.76
17	K	203	CLA	O2D-CGD-O1D	-2.68	118.62	123.85
17	B	835	CLA	CHB-C4A-NA	2.68	128.27	124.40
20	I	101	BCR	C10-C11-C12	-2.67	115.45	123.20
17	A	803	CLA	CHB-C4A-NA	2.67	128.26	124.40
17	B	805	CLA	CMA-C3A-C2A	-2.67	110.10	116.23
20	K	204	BCR	C38-C26-C27	2.67	119.29	113.60
20	F	804	BCR	C3-C4-C5	-2.67	109.29	114.06
20	5	302	BCR	C21-C20-C19	-2.67	115.46	123.20
17	1	510	CLA	CHB-C4A-NA	2.67	128.25	124.40
20	A	849	BCR	C38-C26-C25	-2.67	121.57	124.48
17	A	804	CLA	C3B-C4B-NB	-2.67	108.15	110.53
20	F	801	BCR	C15-C14-C13	-2.67	123.54	127.28
17	3	306	CLA	CMB-C2B-C3B	2.67	130.62	123.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	849	BCR	C29-C30-C25	2.67	114.31	110.44
20	B	845	BCR	C3-C4-C5	-2.67	109.30	114.06
16	A	801	CL0	O2D-CGD-O1D	-2.66	118.03	124.08
26	2	502	XAT	C19-C9-C10	-2.66	118.51	122.82
17	B	840	CLA	O2D-CGD-O1D	-2.66	118.67	123.85
17	2	510	CLA	O2D-CGD-O1D	-2.66	118.67	123.85
17	3	316	CLA	CHB-C4A-NA	2.66	128.24	124.40
17	3	317	CLA	CHB-C4A-NA	2.66	128.24	124.40
17	A	828	CLA	O2D-CGD-O1D	-2.66	118.68	123.85
24	3	304	LUT	C18-C5-C6	-2.66	121.59	124.48
20	B	846	BCR	C23-C22-C21	2.66	123.19	119.01
17	3	313	CLA	C3B-C4B-NB	-2.65	108.16	110.53
17	2	507	CLA	O2D-CGD-O1D	-2.65	118.68	123.85
20	F	801	BCR	C29-C30-C25	2.65	114.29	110.44
17	B	837	CLA	O2A-CGA-O1A	-2.65	116.99	123.63
17	A	805	CLA	O2D-CGD-O1D	-2.65	118.69	123.85
17	A	833	CLA	O2D-CGD-CBD	2.65	115.86	111.23
17	1	513	CLA	C3B-C4B-NB	-2.65	108.17	110.53
17	A	805	CLA	CHB-C4A-NA	2.65	128.22	124.40
17	L	302	CLA	C3B-C4B-NB	-2.65	108.17	110.53
20	A	846	BCR	C8-C7-C6	-2.65	119.92	127.00
20	B	848	BCR	C33-C5-C4	2.65	119.24	113.60
20	L	306	BCR	C31-C1-C6	-2.64	106.10	110.24
17	B	839	CLA	O2A-CGA-O1A	-2.64	117.02	123.63
17	A	829	CLA	CMB-C2B-C1B	-2.64	121.40	125.42
24	3	304	LUT	C10-C11-C12	-2.64	115.55	123.20
25	5	317	CHL	CMB-C2B-C3B	2.64	129.96	124.68
17	B	812	CLA	C1-C2-C3	-2.64	121.87	126.20
20	I	101	BCR	C36-C18-C19	2.64	122.12	118.09
17	3	311	CLA	CHB-C4A-NA	2.64	128.21	124.40
25	1	517	CHL	C4D-ND-C1D	-2.64	103.22	105.22
17	B	803	CLA	C1-C2-C3	-2.64	121.88	126.20
17	B	818	CLA	CHB-C4A-NA	2.64	128.20	124.40
17	A	836	CLA	O2A-CGA-O1A	-2.63	117.04	123.63
24	3	303	LUT	C27-C28-C29	-2.63	120.67	126.32
25	1	512	CHL	O1D-CGD-CBD	-2.63	120.73	124.72
17	B	837	CLA	C3B-C4B-NB	-2.63	108.18	110.53
17	5	306	CLA	CAA-C2A-C3A	-2.63	110.20	116.23
17	3	311	CLA	CAC-C3C-C4C	2.63	128.21	124.79
17	3	310	CLA	CHB-C4A-NA	2.63	128.19	124.40
25	5	317	CHL	OMC-CMC-C2C	-2.62	120.56	125.12
17	B	820	CLA	O2D-CGD-O1D	-2.62	118.74	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	1	508	CLA	CMB-C2B-C1B	-2.62	121.43	125.42
20	B	844	BCR	C36-C18-C17	-2.62	118.57	122.82
20	A	846	BCR	C33-C5-C4	2.62	119.18	113.60
20	F	804	BCR	C24-C23-C22	-2.62	122.36	126.23
17	3	307	CLA	C3A-C2A-C1A	-2.61	103.63	106.30
17	B	833	CLA	O2A-CGA-O1A	-2.61	117.10	123.63
20	L	306	BCR	C7-C8-C9	-2.61	122.37	126.23
20	L	306	BCR	C4-C5-C6	-2.61	119.18	122.70
24	2	501	LUT	C39-C29-C28	2.61	122.07	118.09
17	A	824	CLA	O2D-CGD-O1D	-2.61	118.78	123.85
17	2	506	CLA	O2D-CGD-O1D	-2.61	118.78	123.85
17	3	317	CLA	CMA-C3A-C2A	-2.60	110.26	116.23
17	B	825	CLA	C3B-C4B-NB	-2.60	108.20	110.53
17	L	303	CLA	O2D-CGD-CBD	2.60	115.78	111.23
18	A	841	PQN	C11-C3-C2	-2.60	120.43	124.89
17	A	852	CLA	O2D-CGD-O1D	-2.60	118.79	123.85
17	5	309	CLA	CMB-C2B-C1B	-2.60	121.46	125.42
20	3	305	BCR	C8-C7-C6	-2.60	120.06	127.00
25	2	512	CHL	O1D-CGD-CBD	-2.60	120.78	124.72
20	J	102	BCR	C2-C1-C6	2.60	114.21	110.44
17	5	309	CLA	CAA-CBA-CGA	-2.60	105.56	112.49
17	B	827	CLA	CMB-C2B-C1B	-2.59	121.47	125.42
17	A	802	CLA	O2D-CGD-O1D	-2.59	118.80	123.85
17	3	314	CLA	CHB-C4A-NA	2.59	128.14	124.40
17	A	821	CLA	CMB-C2B-C1B	-2.59	121.47	125.42
23	2	519	LMG	O7-C10-O9	-2.59	117.65	123.70
24	3	303	LUT	C8-C7-C6	-2.59	120.08	127.00
17	B	807	CLA	CHB-C4A-NA	2.59	128.14	124.40
20	F	804	BCR	C33-C5-C6	-2.59	121.66	124.48
17	2	509	CLA	O2D-CGD-O1D	-2.59	118.81	123.85
23	F	806	LMG	C8-O7-C10	-2.59	111.61	117.80
17	5	310	CLA	CHB-C4A-NA	2.58	128.13	124.40
17	J	101	CLA	CHB-C4A-NA	2.58	128.13	124.40
25	5	315	CHL	CBC-CAC-C3C	-2.58	109.18	112.87
17	B	808	CLA	O2A-CGA-O1A	-2.58	117.18	123.63
19	B	851	LHG	C5-O7-C7	-2.58	111.63	117.80
17	1	504	CLA	CHB-C4A-NA	2.58	128.12	124.40
17	3	307	CLA	O2D-CGD-O1D	-2.58	118.83	123.85
17	A	820	CLA	CMB-C2B-C1B	-2.58	121.50	125.42
17	B	809	CLA	C2A-C1A-CHA	2.57	126.70	122.71
17	B	825	CLA	CMB-C2B-C1B	-2.57	121.50	125.42
17	A	838	CLA	C1-C2-C3	-2.57	121.98	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	A	809	CLA	C3B-C4B-NB	-2.57	108.23	110.53
18	B	843	PQN	C14-C13-C15	2.57	119.69	115.23
17	5	316	CLA	CHB-C4A-NA	2.57	128.10	124.40
20	B	845	BCR	C24-C23-C22	-2.57	122.44	126.23
25	5	315	CHL	CMA-C3A-C4A	-2.57	109.08	114.61
25	5	314	CHL	O2D-CGD-O1D	-2.56	118.86	123.85
25	1	517	CHL	OMC-CMC-C2C	-2.56	120.67	125.12
20	L	305	BCR	C36-C18-C17	-2.56	118.67	122.82
17	B	827	CLA	CHB-C4A-NA	2.56	128.09	124.40
25	1	517	CHL	CMB-C2B-C3B	2.56	129.80	124.68
24	2	501	LUT	C40-C33-C32	2.56	122.00	118.09
20	J	102	BCR	C27-C26-C25	-2.56	119.25	122.70
20	A	847	BCR	C28-C27-C26	-2.56	109.49	114.06
25	2	513	CHL	CMA-C3A-C4A	-2.56	106.54	114.81
20	2	503	BCR	C35-C13-C12	2.56	121.99	118.09
17	B	816	CLA	CHB-C4A-NA	2.56	128.09	124.40
25	5	315	CHL	CMD-C2D-C3D	-2.55	119.58	124.68
17	L	303	CLA	CAA-C2A-C3A	-2.55	106.10	113.00
24	1	502	LUT	C18-C5-C4	2.55	119.11	114.42
17	3	311	CLA	O2A-CGA-O1A	-2.55	117.25	123.63
17	A	818	CLA	O2D-CGD-CBD	2.55	115.69	111.23
25	1	512	CHL	C1B-CHB-C4A	2.55	122.96	121.32
17	B	802	CLA	O2A-CGA-O1A	-2.55	117.25	123.63
25	2	515	CHL	O2D-CGD-O1D	-2.55	118.89	123.85
25	1	514	CHL	CHA-C1A-NA	2.55	124.43	122.15
17	B	806	CLA	C3A-C4A-CHB	-2.55	120.79	123.91
17	B	805	CLA	O2D-CGD-O1D	-2.55	118.89	123.85
20	J	102	BCR	C10-C11-C12	-2.55	115.83	123.20
22	J	103	DGD	O1G-C1A-C2A	2.54	119.59	111.83
20	I	101	BCR	C27-C26-C25	-2.54	119.27	122.70
20	J	102	BCR	C31-C1-C6	-2.54	106.26	110.24
17	A	812	CLA	CMB-C2B-C1B	-2.54	121.55	125.42
20	L	306	BCR	C38-C26-C27	2.54	119.02	113.60
17	2	514	CLA	O2D-CGD-O1D	-2.54	118.90	123.85
20	A	846	BCR	C3-C4-C5	-2.54	109.53	114.06
17	1	505	CLA	CHB-C4A-NA	2.54	128.06	124.40
17	3	308	CLA	C1-C2-C3	-2.54	122.04	126.20
17	2	514	CLA	CHB-C4A-NA	2.53	128.06	124.40
23	2	518	LMG	O6-C1-C2	-2.53	105.17	110.37
17	1	508	CLA	O2D-CGD-O1D	-2.53	118.92	123.85
17	B	822	CLA	O2D-CGD-CBD	2.53	115.66	111.23
20	B	852	BCR	C30-C25-C26	-2.53	119.18	122.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	J	102	BCR	C34-C9-C8	2.53	121.95	118.09
25	5	317	CHL	O1D-CGD-CBD	-2.53	120.89	124.72
17	B	821	CLA	C1-C2-C3	-2.53	122.67	126.76
23	2	519	LMG	O8-C28-C29	2.53	119.54	111.83
17	B	834	CLA	CHB-C4A-NA	2.53	128.05	124.40
17	A	832	CLA	C3B-C4B-NB	-2.53	108.28	110.53
17	1	510	CLA	O2D-CGD-CBD	2.53	115.64	111.23
24	5	303	LUT	C39-C29-C28	2.52	121.94	118.09
25	3	315	CHL	CMB-C2B-C3B	2.52	129.73	124.68
17	5	305	CLA	C2A-C1A-CHA	2.52	126.62	122.71
20	A	849	BCR	C16-C15-C14	-2.52	118.36	123.52
17	B	829	CLA	O2D-CGD-CBD	2.52	115.63	111.23
17	A	833	CLA	C3B-C4B-NB	-2.51	108.28	110.53
17	5	308	CLA	C3B-C4B-NB	-2.51	108.28	110.53
17	3	310	CLA	O2D-CGD-O1D	-2.51	118.95	123.85
17	3	306	CLA	CAB-C3B-C2B	2.51	130.21	123.53
17	5	307	CLA	O2D-CGD-O1D	-2.51	118.96	123.85
17	2	514	CLA	O2A-CGA-O1A	-2.51	117.35	123.63
17	K	205	CLA	O2D-CGD-O1D	-2.51	118.39	124.08
20	B	852	BCR	C23-C24-C25	-2.51	120.30	127.00
17	B	838	CLA	CHB-C4A-NA	2.51	128.02	124.40
17	A	837	CLA	CMA-C3A-C2A	-2.50	110.49	116.23
18	B	843	PQN	C2M-C2-C1	2.50	121.28	116.68
20	A	849	BCR	C10-C11-C12	-2.50	115.95	123.20
20	B	846	BCR	C28-C27-C26	-2.50	109.60	114.06
20	B	844	BCR	C20-C19-C18	-2.50	119.51	126.36
17	B	823	CLA	CHB-C4A-NA	2.50	128.00	124.40
17	B	801	CLA	C1-C2-C3	-2.50	122.11	126.20
17	5	316	CLA	O2D-CGD-O1D	-2.49	118.99	123.85
25	2	512	CHL	OMC-CMC-C2C	-2.49	120.79	125.12
17	A	833	CLA	CHB-C4A-NA	2.49	128.00	124.40
17	5	309	CLA	O2D-CGD-O1D	-2.49	119.00	123.85
25	3	302	CHL	CMB-C2B-C3B	2.49	129.66	124.68
17	B	813	CLA	C3B-C4B-NB	-2.49	108.31	110.53
17	A	810	CLA	CMB-C2B-C1B	-2.49	121.62	125.42
17	5	311	CLA	O2D-CGD-O1D	-2.49	119.00	123.85
20	A	851	BCR	C21-C20-C19	-2.49	115.98	123.20
20	F	801	BCR	C2-C1-C6	2.49	114.06	110.44
17	A	814	CLA	CHB-C4A-NA	2.49	127.99	124.40
17	A	822	CLA	CHB-C4A-NA	2.49	127.99	124.40
17	3	301	CLA	CHB-C4A-NA	2.49	127.99	124.40
17	B	832	CLA	C3B-C4B-NB	-2.49	108.31	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	2	510	CLA	O2A-CGA-O1A	-2.49	117.41	123.63
23	2	519	LMG	O1-C1-C2	2.49	112.05	108.27
20	A	849	BCR	C34-C9-C10	-2.48	118.79	122.82
17	B	814	CLA	CAC-C3C-C4C	2.48	128.02	124.79
17	B	835	CLA	O2A-CGA-O1A	-2.48	117.42	123.63
20	2	503	BCR	C20-C19-C18	2.48	133.17	126.36
20	1	503	BCR	C8-C7-C6	-2.48	120.37	127.00
17	5	306	CLA	CMA-C3A-C2A	-2.48	110.54	116.23
17	5	308	CLA	CHB-C4A-NA	2.48	127.98	124.40
20	A	847	BCR	C1-C6-C5	-2.48	119.25	122.64
17	A	816	CLA	CHB-C4A-NA	2.48	127.97	124.40
24	1	501	LUT	C21-C26-C27	-2.48	109.98	112.83
17	A	827	CLA	CMB-C2B-C1B	-2.47	121.65	125.42
17	2	504	CLA	CAC-C3C-C4C	2.47	128.01	124.79
17	1	507	CLA	CHB-C4A-NA	2.47	127.97	124.40
25	2	512	CHL	CMB-C2B-C3B	2.47	129.87	124.69
17	2	510	CLA	CHB-C4A-NA	2.47	127.97	124.40
17	5	308	CLA	CMB-C2B-C3B	2.47	132.36	126.55
20	L	306	BCR	C30-C25-C26	-2.47	119.26	122.64
17	B	834	CLA	O2A-CGA-O1A	-2.47	116.98	123.33
17	2	510	CLA	CMB-C2B-C1B	-2.47	121.66	125.42
17	B	828	CLA	C3B-C4B-NB	-2.47	108.33	110.53
17	B	817	CLA	CHB-C4A-NA	2.47	127.96	124.40
17	A	831	CLA	O2A-CGA-O1A	-2.47	117.46	123.63
20	5	302	BCR	C35-C13-C14	-2.47	118.82	122.82
17	L	302	CLA	CHB-C4A-NA	2.46	127.93	124.43
16	A	801	CL0	CMB-C2B-C3B	2.46	129.85	124.69
17	5	307	CLA	O2A-CGA-O1A	-2.46	117.47	123.63
20	F	801	BCR	C27-C26-C25	-2.46	119.38	122.70
17	3	311	CLA	O1D-CGD-CBD	2.46	129.36	124.52
17	A	824	CLA	C2A-C1A-CHA	2.46	126.52	122.71
17	A	808	CLA	O2D-CGD-O1D	-2.46	119.07	123.85
25	2	513	CHL	O2D-CGD-O1D	-2.46	119.07	123.85
20	A	853	BCR	C35-C13-C14	-2.45	118.84	122.82
17	3	318	CLA	CAB-C3B-C2B	2.45	130.05	123.53
20	J	102	BCR	C36-C18-C19	2.45	121.83	118.09
23	F	805	LMG	C8-O7-C10	-2.45	111.93	117.80
17	A	827	CLA	C3B-C4B-NB	-2.45	108.35	110.53
17	K	203	CLA	C3B-C4B-NB	-2.45	108.35	110.53
17	K	201	CLA	CHB-C1B-NB	2.45	127.72	124.05
24	1	501	LUT	C30-C31-C32	-2.45	116.11	123.20
24	3	304	LUT	C16-C1-C6	-2.44	106.41	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	B	820	CLA	O2A-CGA-O1A	-2.44	117.51	123.63
17	A	806	CLA	O2D-CGD-O1D	-2.44	119.09	123.85
17	B	841	CLA	CHB-C4A-NA	2.44	127.93	124.40
17	A	828	CLA	CHB-C4A-NA	2.44	127.93	124.40
20	A	851	BCR	C31-C1-C6	-2.44	106.42	110.24
20	B	848	BCR	C36-C18-C19	2.44	121.82	118.09
17	A	831	CLA	CAB-C3B-C2B	2.44	130.02	123.53
17	A	825	CLA	O2A-CGA-O1A	-2.44	117.53	123.63
17	A	830	CLA	O1D-CGD-CBD	2.44	129.32	124.52
25	1	514	CHL	C1C-CHC-C4B	2.44	124.79	116.07
20	A	845	BCR	C8-C7-C6	-2.44	120.49	127.00
17	B	837	CLA	CHB-C4A-NA	2.43	127.91	124.40
25	2	513	CHL	CMD-C2D-C3D	-2.43	120.36	124.94
17	A	810	CLA	CHB-C4A-NA	2.43	127.91	124.40
20	3	305	BCR	C15-C16-C17	-2.43	118.54	123.52
25	5	314	CHL	CMB-C2B-C3B	2.43	129.54	124.68
17	A	828	CLA	CAA-C2A-C3A	-2.43	110.65	116.23
17	1	506	CLA	CHB-C4A-NA	2.43	127.91	124.40
17	B	826	CLA	CHB-C4A-NA	2.43	127.90	124.40
17	B	810	CLA	O2D-CGD-CBD	2.43	115.47	111.23
17	A	806	CLA	CHB-C4A-NA	2.43	127.90	124.40
19	1	516	LHG	O8-C23-O10	-2.42	117.57	123.63
20	L	305	BCR	C39-C30-C25	-2.42	106.44	110.24
17	3	312	CLA	O2D-CGD-O1D	-2.42	119.14	123.85
20	A	847	BCR	C21-C20-C19	-2.42	116.19	123.20
17	B	828	CLA	CMA-C3A-C2A	-2.42	110.68	116.23
17	A	811	CLA	C3B-C4B-NB	-2.42	108.37	110.53
20	A	845	BCR	C10-C11-C12	-2.42	116.20	123.20
17	A	807	CLA	CHB-C4A-NA	2.42	127.89	124.40
20	A	853	BCR	C39-C30-C25	-2.42	106.45	110.24
17	A	831	CLA	CMB-C2B-C3B	2.42	129.95	123.53
17	3	308	CLA	O2D-CGD-O1D	-2.42	119.15	123.85
17	F	803	CLA	CHB-C4A-NA	2.42	127.89	124.40
17	2	504	CLA	CHB-C4A-NA	2.42	127.86	124.43
17	2	505	CLA	CHB-C4A-NA	2.41	127.88	124.40
17	A	821	CLA	O1D-CGD-CBD	2.41	129.28	124.52
24	1	501	LUT	C20-C13-C12	2.41	121.77	118.09
25	3	302	CHL	C1B-CHB-C4A	2.41	122.87	121.32
17	A	832	CLA	O2A-CGA-O1A	-2.41	117.60	123.63
20	A	847	BCR	C34-C9-C8	2.41	121.77	118.09
17	B	812	CLA	CHB-C4A-NA	2.41	127.88	124.40
17	B	839	CLA	CHB-C4A-NA	2.41	127.88	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	1	512	CHL	CMB-C2B-C3B	2.41	129.49	124.68
17	F	802	CLA	CHB-C4A-NA	2.41	127.87	124.40
17	A	838	CLA	CMB-C2B-C1B	-2.40	121.76	125.42
17	L	301	CLA	CMB-C2B-C1B	-2.40	121.76	125.42
17	B	840	CLA	CHB-C4A-NA	2.40	127.86	124.40
17	2	508	CLA	C3B-C4B-NB	-2.40	108.39	110.53
17	B	830	CLA	O1D-CGD-CBD	2.40	129.25	124.52
20	B	849	BCR	C38-C26-C25	-2.40	121.87	124.48
20	A	846	BCR	C38-C26-C27	2.40	118.71	113.60
17	3	316	CLA	CMB-C2B-C1B	-2.40	121.77	125.42
20	A	848	BCR	C8-C7-C6	-2.40	120.60	127.00
17	B	833	CLA	C3B-C4B-NB	-2.39	108.39	110.53
20	A	847	BCR	C15-C16-C17	-2.39	118.62	123.52
17	A	826	CLA	C3B-C4B-NB	-2.39	108.39	110.53
17	1	509	CLA	O2A-CGA-O1A	-2.39	117.64	123.63
17	A	820	CLA	O2D-CGD-CBD	2.39	115.41	111.23
25	5	314	CHL	CMA-C3A-C4A	-2.39	109.46	114.61
25	1	512	CHL	CAC-C3C-C4C	2.39	130.16	124.03
17	A	821	CLA	C3B-C4B-NB	-2.39	108.40	110.53
17	A	820	CLA	O2A-CGA-O1A	-2.39	117.66	123.63
17	2	511	CLA	C3B-C4B-NB	-2.38	108.40	110.53
20	A	845	BCR	C20-C19-C18	-2.38	119.82	126.36
17	5	311	CLA	CHB-C4A-NA	2.38	127.84	124.40
20	B	846	BCR	C4-C5-C6	-2.38	119.49	122.70
17	3	310	CLA	O2A-CGA-O1A	-2.38	117.21	123.33
17	B	827	CLA	CMA-C3A-C2A	-2.38	110.78	116.23
17	B	833	CLA	CMB-C2B-C1B	-2.38	121.80	125.42
20	I	101	BCR	C35-C13-C12	2.38	121.72	118.09
17	L	301	CLA	C1-C2-C3	-2.38	122.30	126.20
17	A	819	CLA	O1D-CGD-CBD	2.38	129.21	124.52
17	3	318	CLA	CHB-C4A-NA	2.38	127.83	124.40
17	A	823	CLA	O1D-CGD-CBD	2.38	129.21	124.52
17	A	802	CLA	CHB-C4A-NA	2.38	127.83	124.40
17	3	301	CLA	O1D-CGD-CBD	2.37	129.20	124.52
23	2	519	LMG	O6-C5-C4	2.37	113.98	109.70
25	1	517	CHL	C2A-C3A-C4A	-2.37	101.98	103.53
20	B	852	BCR	C8-C9-C10	2.37	122.74	119.01
17	A	822	CLA	CMA-C3A-C2A	-2.37	110.79	116.23
20	B	849	BCR	C40-C30-C25	-2.37	106.53	110.24
25	3	302	CHL	CMA-C3A-C4A	-2.37	109.51	114.61
17	L	301	CLA	CHB-C4A-NA	2.37	127.82	124.40
18	B	843	PQN	C11-C3-C4	2.37	121.07	118.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	5	315	CHL	CAC-C3C-C4C	2.37	130.11	124.03
17	1	509	CLA	CHB-C4A-NA	2.37	127.81	124.40
17	A	835	CLA	C3B-C4B-NB	-2.36	108.42	110.53
17	A	802	CLA	CMB-C2B-C1B	-2.36	121.82	125.42
17	A	817	CLA	CHB-C4A-NA	2.36	127.81	124.40
17	B	842	CLA	CHB-C4A-NA	2.36	127.81	124.40
17	B	815	CLA	O2D-CGD-CBD	2.36	115.36	111.23
20	B	846	BCR	C37-C22-C21	-2.36	118.99	122.82
24	1	502	LUT	C30-C31-C32	-2.36	116.36	123.20
24	3	304	LUT	C40-C33-C34	-2.36	118.99	122.82
24	1	501	LUT	C10-C11-C12	-2.36	116.36	123.20
20	B	845	BCR	C29-C28-C27	-2.36	106.09	111.28
25	3	302	CHL	CAC-C3C-C4C	2.36	130.09	124.03
25	5	314	CHL	O1D-CGD-CBD	-2.36	121.15	124.72
24	1	501	LUT	C15-C14-C13	-2.36	123.97	127.28
25	1	514	CHL	O2D-CGD-O1D	-2.36	119.26	123.85
17	A	824	CLA	C3B-C4B-NB	-2.36	108.43	110.53
17	3	308	CLA	O2D-CGD-CBD	2.35	115.34	111.23
17	1	509	CLA	C3B-C4B-NB	-2.35	108.43	110.53
17	B	813	CLA	CHB-C4A-NA	2.35	127.79	124.40
25	2	513	CHL	CMB-C2B-C3B	2.35	129.38	124.68
17	A	829	CLA	O2A-CGA-O1A	-2.35	117.75	123.63
17	B	804	CLA	CHB-C4A-NA	2.35	127.79	124.40
17	A	837	CLA	CHB-C4A-NA	2.35	127.78	124.40
24	2	501	LUT	C21-C26-C27	-2.34	110.13	112.83
17	B	808	CLA	O2D-CGD-CBD	2.34	115.33	111.23
17	5	309	CLA	C3B-C4B-NB	-2.34	108.44	110.53
25	5	315	CHL	O2A-CGA-CBA	2.34	121.40	114.00
17	A	814	CLA	O2D-CGD-CBD	2.34	115.32	111.23
17	A	818	CLA	CMB-C2B-C1B	-2.34	121.86	125.42
20	B	849	BCR	C8-C7-C6	-2.34	120.75	127.00
20	B	847	BCR	C34-C9-C10	-2.34	119.03	122.82
25	1	517	CHL	C2A-C1A-CHA	-2.34	117.96	121.84
17	A	804	CLA	CHB-C4A-NA	2.34	127.77	124.40
17	B	810	CLA	C2D-C1D-ND	-2.34	107.81	110.13
20	L	306	BCR	C27-C26-C25	-2.34	119.55	122.70
17	B	812	CLA	CAA-CBA-CGA	-2.34	106.57	113.21
20	F	801	BCR	C8-C7-C6	-2.34	120.76	127.00
20	J	102	BCR	C8-C7-C6	-2.34	120.76	127.00
20	B	849	BCR	C16-C15-C14	-2.34	118.74	123.52
17	A	809	CLA	CHB-C4A-NA	2.33	127.77	124.40
17	B	814	CLA	CHB-C4A-NA	2.33	127.77	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	3	312	CLA	CHB-C4A-NA	2.33	127.76	124.40
25	1	514	CHL	CMB-C2B-C3B	2.33	129.34	124.68
17	A	835	CLA	O2D-CGD-CBD	2.33	115.30	111.23
20	A	851	BCR	C33-C5-C4	2.33	118.56	113.60
17	B	839	CLA	C3B-C4B-NB	-2.32	108.45	110.53
17	B	818	CLA	O2D-CGD-CBD	2.32	115.29	111.23
17	B	841	CLA	O2A-CGA-O1A	-2.32	117.82	123.63
23	2	519	LMG	C3-C4-C5	2.32	114.44	110.23
20	A	849	BCR	C8-C9-C10	2.32	122.66	119.01
19	A	843	LHG	O7-C7-O9	-2.32	118.28	123.70
17	B	836	CLA	CHB-C4A-NA	2.32	127.75	124.40
17	B	826	CLA	CMB-C2B-C1B	-2.32	121.89	125.42
17	B	801	CLA	CMB-C2B-C1B	-2.32	121.89	125.42
17	2	506	CLA	CHB-C4A-NA	2.32	127.74	124.40
17	A	837	CLA	CMB-C2B-C3B	2.31	131.99	126.55
17	3	314	CLA	O2D-CGD-CBD	2.31	115.27	111.23
24	3	303	LUT	C1-C6-C5	-2.31	119.48	122.64
17	5	312	CLA	C3B-C4B-NB	-2.31	108.47	110.53
17	B	820	CLA	CMB-C2B-C1B	-2.31	121.90	125.42
17	B	834	CLA	CAA-C2A-C3A	-2.31	106.76	113.00
17	A	827	CLA	CMB-C2B-C3B	2.31	131.98	126.55
17	1	509	CLA	CMB-C2B-C1B	-2.31	121.91	125.42
20	K	204	BCR	C2-C1-C6	2.30	113.79	110.44
20	A	846	BCR	C16-C15-C14	-2.30	118.81	123.52
20	A	853	BCR	C33-C5-C6	-2.30	121.97	124.48
17	A	808	CLA	CHB-C4A-NA	2.30	127.72	124.40
17	K	205	CLA	CHB-C4A-NA	2.30	127.72	124.40
20	A	853	BCR	C37-C22-C21	-2.30	119.09	122.82
17	5	310	CLA	O2A-CGA-O1A	-2.30	117.88	123.63
20	1	503	BCR	C34-C9-C10	-2.30	119.09	122.82
16	A	801	CL0	CAB-C3B-C2B	2.30	129.50	124.69
17	A	812	CLA	CHB-C4A-NA	2.30	127.71	124.40
25	5	315	CHL	C4C-CHD-C1D	2.30	124.28	116.07
17	B	838	CLA	C3B-C4B-NB	-2.29	108.48	110.53
24	3	304	LUT	C15-C14-C13	-2.29	124.06	127.28
20	A	845	BCR	C16-C15-C14	-2.29	118.83	123.52
17	A	842	CLA	CHB-C4A-NA	2.29	127.70	124.40
20	B	845	BCR	C21-C20-C19	-2.29	116.58	123.20
26	5	304	XAT	C30-C31-C32	-2.29	116.58	123.20
17	A	808	CLA	C1-C2-C3	-2.28	122.46	126.20
17	B	810	CLA	C3B-C4B-NB	-2.28	108.49	110.53
17	B	819	CLA	O2D-CGD-CBD	2.28	115.22	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	L	305	BCR	C33-C5-C6	-2.28	121.99	124.48
17	A	825	CLA	CHB-C4A-NA	2.28	127.69	124.40
20	J	102	BCR	C23-C24-C25	-2.28	120.90	127.00
17	A	852	CLA	C1-C2-C3	-2.28	122.46	126.20
20	B	845	BCR	C34-C9-C10	-2.28	119.12	122.82
17	B	824	CLA	O2A-CGA-O1A	-2.28	117.47	123.33
17	B	828	CLA	CAC-C3C-C4C	2.28	127.75	124.79
17	A	840	CLA	CHB-C4A-NA	2.28	127.69	124.40
17	3	309	CLA	C1B-NB-C4B	2.28	107.91	106.31
20	B	845	BCR	C10-C11-C12	-2.28	116.61	123.20
17	A	852	CLA	CHB-C4A-NA	2.27	127.68	124.40
17	B	814	CLA	CMA-C3A-C2A	-2.27	111.02	116.23
25	3	315	CHL	C4D-ND-C1D	-2.27	103.49	105.22
17	1	515	CLA	CBD-CHA-C1A	2.27	131.79	127.58
17	A	852	CLA	O2A-CGA-O1A	-2.27	117.95	123.63
20	L	305	BCR	C23-C24-C25	-2.27	120.94	127.00
25	5	317	CHL	O2D-CGD-O1D	-2.27	119.43	123.85
17	B	809	CLA	C3A-C2A-C1A	-2.27	103.98	106.30
17	A	834	CLA	C2A-C3A-C4A	2.27	104.25	101.59
20	1	503	BCR	C33-C5-C4	2.27	118.43	113.60
20	2	503	BCR	C34-C9-C10	-2.27	119.15	122.82
17	B	838	CLA	O2A-CGA-O1A	-2.27	117.96	123.63
17	2	506	CLA	O2A-CGA-O1A	-2.26	117.97	123.63
17	5	316	CLA	C3B-C4B-NB	-2.26	108.51	110.53
17	A	821	CLA	CHB-C4A-NA	2.26	127.66	124.40
17	B	819	CLA	CHB-C4A-NA	2.26	127.66	124.40
20	3	305	BCR	C35-C13-C14	-2.26	119.16	122.82
20	F	804	BCR	C15-C16-C17	-2.25	118.91	123.52
17	L	304	CLA	CMB-C2B-C1B	-2.25	121.99	125.42
16	A	801	CL0	C1-O2A-CGA	2.25	121.57	112.40
17	5	305	CLA	CMB-C2B-C3B	2.25	130.02	124.63
24	1	502	LUT	C38-C25-C24	-2.25	118.03	123.36
17	F	803	CLA	O2D-CGD-O1D	-2.25	119.47	123.85
17	5	310	CLA	CMB-C2B-C1B	-2.25	121.99	125.42
20	A	853	BCR	C31-C1-C6	-2.25	106.71	110.24
17	L	304	CLA	C3B-C4B-NB	-2.25	108.52	110.53
25	2	513	CHL	CED-O2D-CGD	2.25	121.02	115.92
17	2	507	CLA	O1D-CGD-CBD	2.25	128.95	124.52
17	B	820	CLA	CHB-C4A-NA	2.25	127.64	124.40
25	2	516	CHL	C4C-CHD-C1D	2.25	124.10	116.07
17	B	802	CLA	C7-C6-C5	-2.24	109.61	114.47
24	1	501	LUT	C18-C5-C4	2.24	118.55	114.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	B	802	CLA	C3B-C4B-NB	-2.24	108.53	110.53
20	A	851	BCR	C10-C11-C12	-2.24	116.70	123.20
17	1	513	CLA	CHB-C4A-NA	2.24	127.63	124.40
22	B	850	DGD	C3G-C2G-C1G	-2.24	106.56	111.78
17	1	508	CLA	C3B-C4B-NB	-2.24	108.53	110.53
20	B	848	BCR	C39-C30-C25	-2.24	106.73	110.24
17	5	307	CLA	CHB-C4A-NA	2.24	127.63	124.40
17	B	829	CLA	CHB-C4A-NA	2.24	127.63	124.40
17	L	302	CLA	O2D-CGD-O1D	-2.24	119.50	123.85
17	A	803	CLA	CMA-C3A-C2A	-2.24	111.10	116.23
17	A	826	CLA	CHB-C4A-NA	2.23	127.62	124.40
17	B	830	CLA	O2A-CGA-O1A	-2.23	118.04	123.63
17	B	802	CLA	CHB-C4A-NA	2.23	127.62	124.40
17	B	811	CLA	CHB-C4A-NA	2.23	127.62	124.40
17	L	303	CLA	O2A-CGA-O1A	-2.23	118.04	123.63
17	2	504	CLA	C3B-C4B-NB	-2.23	108.54	110.53
25	3	302	CHL	O2A-CGA-CBA	2.23	120.56	112.14
20	A	847	BCR	C11-C12-C13	-2.23	120.25	126.36
20	B	844	BCR	C40-C30-C25	-2.23	106.75	110.24
17	1	507	CLA	O1D-CGD-CBD	2.23	128.91	124.52
23	5	301	LMG	O7-C10-O9	-2.23	118.50	123.70
25	2	512	CHL	O2D-CGD-O1D	-2.23	119.51	123.85
25	5	317	CHL	C4C-CHD-C1D	2.23	124.04	116.07
20	A	845	BCR	C7-C8-C9	-2.23	122.94	126.23
25	2	512	CHL	CAC-C3C-C4C	2.23	129.75	124.03
17	3	312	CLA	CAC-C3C-C4C	2.23	127.69	124.79
17	5	310	CLA	C3B-C4B-NB	-2.22	108.54	110.53
17	A	823	CLA	CHB-C4A-NA	2.22	127.59	124.43
20	I	101	BCR	C16-C15-C14	-2.22	118.97	123.52
20	B	846	BCR	C36-C18-C17	-2.22	119.21	122.82
20	B	852	BCR	C21-C20-C19	-2.22	116.76	123.20
17	3	318	CLA	CMB-C2B-C3B	2.22	129.44	123.53
17	3	314	CLA	C1-C2-C3	-2.22	122.56	126.20
25	2	516	CHL	O1D-CGD-CBD	-2.22	121.36	124.72
20	B	845	BCR	C35-C13-C14	-2.22	119.22	122.82
17	B	816	CLA	O2D-CGD-O1D	-2.22	119.53	123.85
17	B	818	CLA	O2A-CGA-O1A	-2.22	118.08	123.63
22	J	103	DGD	C6D-O5D-C1E	-2.22	109.04	113.80
19	2	517	LHG	O8-C23-O10	-2.22	118.08	123.63
17	3	310	CLA	C3B-C4B-NB	-2.22	108.55	110.53
17	3	318	CLA	C3B-C4B-NB	-2.21	108.03	110.33
20	I	101	BCR	C3-C4-C5	-2.21	110.11	114.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	5	312	CLA	CHB-C4A-NA	2.21	127.59	124.40
20	A	845	BCR	C23-C24-C25	-2.21	121.10	127.00
24	5	303	LUT	C30-C31-C32	-2.21	116.80	123.20
18	A	841	PQN	C14-C13-C15	2.21	119.06	115.23
24	2	501	LUT	C35-C15-C14	-2.21	119.00	123.52
17	B	818	CLA	CMB-C2B-C1B	-2.21	122.06	125.42
24	3	303	LUT	C19-C9-C8	2.21	121.46	118.09
20	F	804	BCR	C31-C1-C6	-2.21	106.78	110.24
17	A	813	CLA	CHB-C4A-NA	2.20	127.58	124.40
23	5	301	LMG	O8-C28-C29	2.20	118.56	111.83
17	B	812	CLA	CAB-C3B-C2B	2.20	129.39	123.53
20	K	204	BCR	C36-C18-C17	-2.20	119.25	122.82
26	5	304	XAT	C31-C30-C29	-2.20	124.19	127.28
20	B	848	BCR	C23-C24-C25	-2.20	121.12	127.00
25	2	513	CHL	CAD-C3D-C4D	2.20	113.65	110.21
25	2	512	CHL	C4C-CHD-C1D	2.20	123.94	116.07
17	A	838	CLA	CHB-C4A-NA	2.20	127.57	124.40
17	A	835	CLA	O2A-CGA-O1A	-2.20	118.13	123.63
25	2	513	CHL	CAC-C3C-C4C	2.20	129.68	124.03
20	F	801	BCR	C35-C13-C12	2.19	121.44	118.09
17	5	316	CLA	CMB-C2B-C1B	-2.19	122.08	125.42
20	J	102	BCR	C21-C20-C19	-2.19	116.84	123.20
22	B	850	DGD	O3G-C1D-C2D	-2.19	104.94	108.27
20	K	204	BCR	C24-C23-C22	-2.19	122.99	126.23
17	A	830	CLA	CHB-C4A-NA	2.19	127.56	124.40
17	2	509	CLA	C1-C2-C3	-2.19	123.22	126.76
17	B	812	CLA	CMB-C2B-C3B	2.19	129.35	123.53
17	L	303	CLA	CMB-C2B-C1B	-2.19	122.08	125.42
17	2	510	CLA	O2D-CGD-CBD	2.19	115.06	111.23
17	3	317	CLA	O2D-CGD-CBD	2.19	115.06	111.23
25	2	516	CHL	O2D-CGD-O1D	-2.19	119.59	123.85
17	A	823	CLA	O2A-CGA-O1A	-2.19	118.16	123.63
20	B	849	BCR	C2-C1-C6	2.19	113.61	110.44
17	1	506	CLA	O2A-CGA-O1A	-2.19	118.16	123.63
17	1	508	CLA	CHB-C4A-NA	2.18	127.55	124.40
17	1	513	CLA	C1-C2-C3	-2.18	122.62	126.20
17	A	818	CLA	C2A-C1A-CHA	2.18	126.10	122.71
25	5	317	CHL	C4A-C3A-C2A	-2.18	99.67	103.96
20	B	847	BCR	C19-C18-C17	-2.18	115.58	119.01
17	B	826	CLA	O2A-CGA-O1A	-2.18	118.17	123.63
17	1	508	CLA	CMB-C2B-C3B	2.18	131.68	126.55
17	5	309	CLA	CHB-C4A-NA	2.18	127.55	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	844	BCR	C35-C13-C14	-2.18	119.29	122.82
17	1	511	CLA	CAA-C2A-C3A	-2.17	107.13	113.00
20	A	849	BCR	C35-C13-C12	2.17	121.41	118.09
20	F	801	BCR	C34-C9-C8	2.17	121.41	118.09
17	B	831	CLA	CHB-C4A-NA	2.17	127.53	124.40
17	A	838	CLA	O2A-CGA-O1A	-2.17	118.20	123.63
17	A	827	CLA	CHB-C4A-NA	2.17	127.53	124.40
20	A	853	BCR	C30-C25-C26	-2.17	119.67	122.64
17	B	822	CLA	CMB-C2B-C1B	-2.17	122.12	125.42
16	A	801	CL0	C4C-C3C-C2C	-2.17	104.81	113.37
17	B	803	CLA	O1D-CGD-CBD	2.16	128.78	124.52
17	3	311	CLA	C3B-C4B-NB	-2.16	108.60	110.53
20	F	804	BCR	C33-C5-C4	2.16	118.20	113.60
17	B	801	CLA	O2D-CGD-CBD	2.16	115.01	111.23
17	1	504	CLA	CMB-C2B-C1B	-2.16	122.13	125.42
25	5	314	CHL	O2A-CGA-CBA	2.16	120.30	112.14
24	1	502	LUT	C16-C1-C6	-2.16	106.86	110.24
20	1	503	BCR	C11-C12-C13	-2.16	120.44	126.36
17	B	827	CLA	O2D-CGD-CBD	2.16	115.00	111.23
17	1	509	CLA	CMB-C2B-C3B	2.16	131.62	126.55
17	A	836	CLA	C3A-C2A-C1A	2.16	104.57	101.34
20	A	851	BCR	C11-C10-C9	-2.16	124.25	127.28
17	B	811	CLA	CMB-C2B-C1B	-2.16	122.14	125.42
20	L	306	BCR	C20-C21-C22	-2.16	124.25	127.28
17	L	304	CLA	O2A-CGA-O1A	-2.16	117.79	123.33
26	5	304	XAT	C19-C9-C8	2.16	121.38	118.09
17	A	805	CLA	C1-C2-C3	-2.15	122.67	126.20
25	2	516	CHL	CMD-C2D-C3D	-2.15	120.38	124.68
25	1	512	CHL	O2D-CGD-O1D	-2.15	119.66	123.85
17	5	316	CLA	CMA-C3A-C2A	-2.15	111.29	116.23
17	B	825	CLA	CMB-C2B-C3B	2.15	131.61	126.55
24	5	303	LUT	C10-C11-C12	-2.15	116.97	123.20
20	L	306	BCR	C34-C9-C8	2.15	121.37	118.09
25	1	512	CHL	O2A-CGA-CBA	2.15	120.27	112.14
20	3	305	BCR	C23-C24-C25	-2.15	121.25	127.00
17	A	820	CLA	CHD-C1D-ND	-2.15	121.78	124.80
17	5	313	CLA	CHB-C4A-NA	2.15	127.50	124.40
17	B	803	CLA	O2A-CGA-O1A	-2.15	118.25	123.63
17	B	824	CLA	CHB-C4A-NA	2.15	127.50	124.40
20	B	848	BCR	C35-C13-C12	2.15	121.37	118.09
20	K	204	BCR	C33-C5-C4	2.15	118.17	113.60
17	5	306	CLA	CHB-C4A-NA	2.15	127.50	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	B	827	CLA	CMB-C2B-C3B	2.15	131.60	126.55
17	A	837	CLA	O2D-CGD-CBD	2.15	114.98	111.23
20	L	305	BCR	C34-C9-C10	-2.14	119.34	122.82
25	2	516	CHL	CMA-C3A-C4A	-2.14	110.00	114.61
25	2	513	CHL	OMC-CMC-C2C	-2.14	121.40	125.12
17	B	810	CLA	C2A-C1A-CHA	2.14	126.03	122.71
25	2	513	CHL	C4C-CHD-C1D	2.14	123.73	116.07
20	K	204	BCR	C23-C24-C25	-2.14	121.28	127.00
20	A	847	BCR	C36-C18-C19	2.14	121.36	118.09
17	B	826	CLA	CMB-C2B-C3B	2.14	131.58	126.55
17	L	304	CLA	CAC-C3C-C2C	-2.14	123.63	127.56
17	3	313	CLA	O2A-CGA-O1A	-2.14	118.28	123.63
17	B	834	CLA	CAA-C2A-C1A	-2.14	104.97	111.97
20	2	503	BCR	C3-C2-C1	-2.14	106.87	114.43
17	A	831	CLA	CHB-C4A-NA	2.14	127.48	124.40
17	5	305	CLA	O1D-CGD-CBD	2.13	128.73	124.52
17	3	309	CLA	CMB-C2B-C3B	2.13	129.74	124.63
17	1	513	CLA	O2D-CGD-CBD	2.13	114.96	111.23
17	3	301	CLA	CMA-C3A-C2A	-2.13	111.34	116.23
26	5	304	XAT	C35-C34-C33	-2.13	124.29	127.28
25	3	302	CHL	C4C-CHD-C1D	2.13	123.70	116.07
17	3	316	CLA	CMA-C3A-C2A	-2.13	111.34	116.23
17	B	806	CLA	CMB-C2B-C1B	-2.13	122.17	125.42
17	B	815	CLA	CHB-C4A-NA	2.13	127.48	124.40
17	K	201	CLA	C2A-C1A-CHA	2.13	127.55	123.86
17	B	815	CLA	O2A-CGA-O1A	-2.13	118.31	123.63
20	A	845	BCR	C39-C30-C25	-2.13	106.91	110.24
17	B	828	CLA	CHB-C4A-NA	2.13	127.47	124.40
17	K	203	CLA	CHB-C4A-NA	2.13	127.47	124.40
17	L	301	CLA	O2A-CGA-O1A	-2.13	118.31	123.63
17	A	827	CLA	O1D-CGD-CBD	2.13	128.71	124.52
25	1	512	CHL	C4C-CHD-C1D	2.13	123.67	116.07
19	A	844	LHG	O8-C23-C24	2.12	118.31	111.83
17	A	839	CLA	O2D-CGD-CBD	2.12	114.94	111.23
17	B	839	CLA	O1D-CGD-CBD	2.12	128.71	124.52
20	L	305	BCR	C16-C15-C14	-2.12	119.18	123.52
17	A	826	CLA	C2D-C1D-ND	-2.12	108.03	110.13
20	F	801	BCR	C16-C15-C14	-2.12	119.19	123.52
17	B	827	CLA	C2A-C3A-C4A	2.12	104.07	101.59
25	5	315	CHL	CMB-C2B-C3B	2.12	128.91	124.68
17	A	826	CLA	O1D-CGD-CBD	2.12	128.69	124.52
17	B	828	CLA	O2D-CGD-CBD	2.12	114.93	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	2	508	CLA	CHB-C4A-NA	2.12	127.45	124.40
20	A	848	BCR	C3-C4-C5	-2.11	110.28	114.06
17	A	813	CLA	O2A-CGA-O1A	-2.11	117.89	123.33
17	A	815	CLA	CHB-C4A-NA	2.11	127.45	124.40
17	B	803	CLA	CHB-C4A-NA	2.11	127.45	124.40
17	A	815	CLA	O2A-CGA-O1A	-2.11	117.90	123.33
24	1	501	LUT	C35-C15-C14	-2.11	119.20	123.52
17	1	515	CLA	CMB-C2B-C1B	-2.11	122.21	125.42
17	A	808	CLA	CMB-C2B-C1B	-2.11	122.21	125.42
17	A	816	CLA	CMB-C2B-C1B	-2.11	122.21	125.42
17	A	834	CLA	CHB-C4A-NA	2.11	127.44	124.40
24	1	502	LUT	C39-C29-C28	2.11	121.31	118.09
26	2	502	XAT	C40-C33-C34	-2.10	119.41	122.82
17	A	838	CLA	O1D-CGD-CBD	2.10	128.67	124.52
25	1	517	CHL	C4C-CHD-C1D	2.10	123.59	116.07
17	A	820	CLA	C1-C2-C3	-2.10	122.75	126.20
17	K	202	CLA	CHB-C4A-NA	2.10	127.43	124.40
20	K	204	BCR	C31-C1-C6	-2.10	106.95	110.24
17	B	807	CLA	C1-C2-C3	-2.10	122.76	126.20
17	A	808	CLA	CAA-C2A-C3A	-2.10	107.33	113.00
26	2	502	XAT	O4-C5-C6	-2.10	57.27	58.93
17	B	807	CLA	CMB-C2B-C1B	-2.10	122.23	125.42
25	2	516	CHL	C4D-ND-C1D	-2.10	103.63	105.22
17	B	814	CLA	C3B-C4B-NB	-2.09	108.66	110.53
17	B	814	CLA	C2A-C3A-C4A	2.09	104.05	101.59
20	A	846	BCR	C27-C26-C25	-2.09	119.87	122.70
17	B	806	CLA	C2A-C1A-CHA	2.09	125.96	122.71
17	A	834	CLA	CMA-C3A-C2A	-2.09	111.43	116.23
17	A	810	CLA	O2A-CGA-O1A	-2.09	118.39	123.63
17	A	811	CLA	CHB-C4A-NA	2.09	127.42	124.40
17	A	820	CLA	CMB-C2B-C3B	2.09	131.47	126.55
17	B	837	CLA	CMB-C2B-C1B	-2.09	122.24	125.42
24	3	304	LUT	C38-C25-C24	-2.09	118.41	123.36
17	A	812	CLA	CMB-C2B-C3B	2.09	131.47	126.55
20	A	845	BCR	C37-C22-C21	-2.09	119.43	122.82
20	J	102	BCR	C15-C16-C17	-2.09	119.25	123.52
20	F	804	BCR	C1-C6-C5	-2.09	119.78	122.64
23	2	518	LMG	O6-C5-C4	2.09	113.31	109.55
25	3	315	CHL	O2D-CGD-O1D	-2.09	119.79	123.85
18	A	841	PQN	C2M-C2-C1	2.09	120.52	116.68
25	5	314	CHL	C4C-CHD-C1D	2.09	123.53	116.07
17	B	825	CLA	C2A-C1A-CHA	2.09	127.49	123.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	A	838	CLA	CMB-C2B-C3B	2.09	131.46	126.55
17	B	839	CLA	CMB-C2B-C1B	-2.08	122.25	125.42
24	3	303	LUT	C12-C13-C14	-2.08	115.73	119.01
20	B	847	BCR	C10-C11-C12	-2.08	117.17	123.20
23	2	519	LMG	C8-O7-C10	-2.08	112.81	117.80
17	B	817	CLA	O2A-CGA-O1A	-2.08	118.42	123.63
25	2	515	CHL	CMD-C2D-C3D	-2.08	120.53	124.68
17	A	812	CLA	O2D-CGD-CBD	2.08	114.87	111.23
17	A	816	CLA	O2A-CGA-O1A	-2.08	118.42	123.63
17	K	201	CLA	CHB-C1B-C2B	-2.08	121.39	127.43
17	K	202	CLA	O2D-CGD-CBD	2.08	114.86	111.23
24	5	303	LUT	C21-C26-C27	-2.08	110.44	112.83
17	2	507	CLA	C4-C3-C5	-2.08	109.25	114.96
20	B	846	BCR	C36-C18-C19	2.07	121.26	118.09
20	2	503	BCR	C38-C26-C27	2.07	118.02	113.60
24	5	303	LUT	C11-C10-C9	-2.07	124.37	127.28
17	B	837	CLA	CHA-C1A-NA	-2.07	121.70	126.39
17	A	821	CLA	CAA-C2A-C1A	-2.07	107.56	112.14
17	A	829	CLA	CHB-C1B-NB	2.07	127.16	124.05
20	B	848	BCR	C8-C7-C6	-2.07	121.47	127.00
17	3	314	CLA	O2A-CGA-O1A	-2.07	118.45	123.63
17	B	828	CLA	O1D-CGD-CBD	2.07	128.60	124.52
19	B	851	LHG	O7-C7-O9	-2.07	118.87	123.70
17	B	832	CLA	CHB-C4A-NA	2.07	127.38	124.40
17	L	302	CLA	CMB-C2B-C1B	-2.07	122.27	125.42
17	A	823	CLA	CMB-C2B-C1B	-2.07	122.27	125.42
17	B	841	CLA	C1-C2-C3	-2.07	122.81	126.20
17	B	841	CLA	O1D-CGD-CBD	2.07	128.59	124.52
24	5	303	LUT	C8-C7-C6	-2.07	121.48	127.00
20	A	853	BCR	C21-C20-C19	-2.06	117.22	123.20
25	2	515	CHL	C4C-CHD-C1D	2.06	123.45	116.07
20	5	302	BCR	C24-C23-C22	-2.06	123.18	126.23
17	B	802	CLA	CMB-C2B-C1B	-2.06	122.28	125.42
20	B	845	BCR	C33-C5-C4	2.06	117.99	113.60
20	F	801	BCR	C3-C4-C5	-2.06	110.39	114.06
17	B	806	CLA	CMB-C2B-C3B	2.06	131.39	126.55
17	B	814	CLA	CHA-C1A-NA	-2.06	121.74	126.39
20	A	849	BCR	C33-C5-C6	-2.06	122.24	124.48
17	A	836	CLA	CHB-C4A-NA	2.06	127.37	124.40
20	A	851	BCR	C30-C25-C24	2.06	121.22	115.65
17	A	812	CLA	CHB-C1B-NB	2.06	127.13	124.05
17	2	509	CLA	O2A-CGA-O1A	-2.05	118.49	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	844	BCR	C23-C24-C25	-2.05	121.51	127.00
17	3	318	CLA	O1D-CGD-CBD	2.05	128.57	124.52
25	1	517	CHL	C3D-C4D-ND	2.05	116.23	112.94
17	A	811	CLA	C2A-C1A-CHA	2.05	125.89	122.71
17	3	307	CLA	C2A-C1A-CHA	2.05	125.89	122.71
25	5	314	CHL	CAC-C3C-C4C	2.05	129.29	124.03
20	A	847	BCR	C23-C24-C25	-2.05	121.53	127.00
20	B	849	BCR	C23-C22-C21	2.05	122.23	119.01
17	A	805	CLA	O1D-CGD-CBD	2.05	128.55	124.52
25	2	512	CHL	CMD-C2D-C3D	-2.05	120.60	124.68
16	A	801	CL0	C4-C3-C5	2.05	118.78	115.23
17	B	838	CLA	CMB-C2B-C1B	-2.04	122.31	125.42
20	B	852	BCR	C20-C21-C22	-2.04	124.41	127.28
20	B	852	BCR	C10-C11-C12	-2.04	117.28	123.20
17	B	810	CLA	C1D-ND-C4D	2.04	107.75	106.31
17	B	801	CLA	CMB-C2B-C3B	2.04	131.35	126.55
17	3	317	CLA	C2A-C3A-C4A	2.04	103.98	101.59
22	B	850	DGD	C6D-O5D-C1E	-2.04	109.42	113.80
20	A	845	BCR	C36-C18-C17	-2.04	119.51	122.82
24	2	501	LUT	C19-C9-C10	-2.04	119.51	122.82
17	3	317	CLA	CHD-C1D-ND	-2.04	121.94	124.80
23	F	806	LMG	C9-C8-C7	-2.04	107.04	111.78
25	2	515	CHL	CMB-C2B-C3B	2.04	128.95	124.69
17	B	812	CLA	O2A-CGA-O1A	-2.04	118.54	123.63
17	B	818	CLA	CMB-C2B-C3B	2.04	131.34	126.55
25	2	515	CHL	CMA-C3A-C4A	-2.03	110.23	114.61
17	B	814	CLA	C2A-C1A-CHA	2.03	127.39	123.86
24	5	303	LUT	C28-C29-C30	-2.03	115.81	119.01
17	5	305	CLA	CHB-C1B-NB	2.03	127.10	124.05
17	3	308	CLA	C3A-C2A-C1A	2.03	104.38	101.34
26	2	502	XAT	C40-C33-C32	2.03	121.19	118.09
17	3	310	CLA	O1A-CGA-CBA	2.03	129.53	123.09
24	1	502	LUT	C35-C34-C33	-2.03	124.43	127.28
17	2	504	CLA	C2A-C1A-CHA	2.03	125.86	122.71
17	B	801	CLA	O2A-CGA-O1A	-2.03	118.56	123.63
23	F	806	LMG	O8-C28-O10	-2.03	118.56	123.63
17	5	309	CLA	CMB-C2B-C3B	2.03	131.31	126.55
17	5	311	CLA	CMB-C2B-C1B	-2.03	122.33	125.42
17	A	805	CLA	CAA-C2A-C1A	-2.03	105.34	111.97
17	B	808	CLA	CHB-C4A-NA	2.02	127.32	124.40
20	A	846	BCR	C21-C20-C19	-2.02	117.33	123.20
17	B	808	CLA	CHD-C1D-ND	-2.02	121.96	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	B	813	CLA	C2D-C1D-ND	-2.02	108.12	110.13
17	A	829	CLA	CHB-C4A-NA	2.02	127.32	124.40
17	2	505	CLA	C1-C2-C3	-2.02	122.89	126.20
20	L	305	BCR	C37-C22-C21	-2.02	119.54	122.82
25	2	515	CHL	O2A-CGA-CBA	2.02	120.38	114.00
20	A	848	BCR	C27-C26-C25	-2.02	119.98	122.70
17	A	805	CLA	O2A-CGA-O1A	-2.02	118.59	123.63
17	5	308	CLA	CAC-C3C-C4C	2.01	127.41	124.79
25	1	512	CHL	CED-O2D-CGD	2.01	120.48	115.92
19	1	516	LHG	O7-C7-O9	-2.01	119.00	123.70
20	B	847	BCR	C30-C25-C26	-2.01	119.89	122.64
20	2	503	BCR	C28-C29-C30	-2.01	107.31	114.43
20	A	846	BCR	C37-C22-C21	-2.01	119.56	122.82
17	B	829	CLA	C2A-C1A-CHA	2.01	125.83	122.71
17	2	505	CLA	CHB-C1B-NB	2.01	127.06	124.05
17	A	842	CLA	O2A-CGA-O1A	-2.01	118.60	123.63
17	A	828	CLA	CMA-C3A-C2A	-2.01	111.63	116.23
17	B	840	CLA	CMB-C2B-C1B	-2.01	122.36	125.42
17	A	816	CLA	CMB-C2B-C3B	2.01	131.27	126.55
17	A	815	CLA	CMB-C2B-C1B	-2.01	122.37	125.42
20	3	305	BCR	C40-C30-C25	-2.00	107.10	110.24
17	A	831	CLA	C3B-C4B-NB	-2.00	108.25	110.33
20	F	804	BCR	C37-C22-C23	2.00	121.15	118.09
24	1	501	LUT	C8-C7-C6	-2.00	121.65	127.00
17	B	826	CLA	O2D-CGD-CBD	2.00	114.73	111.23
20	3	305	BCR	C36-C18-C19	2.00	121.15	118.09
17	L	304	CLA	O1D-CGD-CBD	2.00	128.47	124.52
20	F	801	BCR	C37-C22-C21	-2.00	119.57	122.82
26	5	304	XAT	C35-C15-C14	-2.00	119.42	123.52
19	2	517	LHG	O7-C7-O9	-2.00	119.03	123.70
20	B	852	BCR	C35-C13-C14	-2.00	119.58	122.82

All (171) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
16	A	801	CL0	ND
16	A	801	CL0	NA
16	A	801	CL0	NC
17	A	802	CLA	ND
17	A	803	CLA	ND
17	A	804	CLA	ND
17	A	805	CLA	ND

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Mol	Chain	Res	Type	Atom
17	A	806	CLA	ND
17	A	807	CLA	ND
17	A	808	CLA	ND
17	A	809	CLA	ND
17	A	810	CLA	ND
17	A	811	CLA	ND
17	A	812	CLA	ND
17	A	813	CLA	ND
17	A	814	CLA	ND
17	A	815	CLA	ND
17	A	816	CLA	ND
17	A	817	CLA	ND
17	A	818	CLA	ND
17	A	819	CLA	ND
17	A	820	CLA	ND
17	A	821	CLA	ND
17	A	822	CLA	ND
17	A	823	CLA	ND
17	A	824	CLA	ND
17	A	825	CLA	ND
17	A	826	CLA	ND
17	A	827	CLA	ND
17	A	828	CLA	ND
17	A	829	CLA	ND
17	A	830	CLA	ND
17	A	831	CLA	ND
17	A	832	CLA	ND
17	A	833	CLA	ND
17	A	834	CLA	ND
17	A	835	CLA	ND
17	A	836	CLA	ND
17	A	837	CLA	ND
17	A	838	CLA	ND
17	A	839	CLA	ND
17	A	840	CLA	ND
17	A	842	CLA	ND
17	A	852	CLA	ND
17	B	801	CLA	ND
17	B	802	CLA	ND
17	B	803	CLA	ND
17	B	804	CLA	ND
17	B	805	CLA	ND

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Mol	Chain	Res	Type	Atom
17	B	806	CLA	ND
17	B	807	CLA	ND
17	B	808	CLA	ND
17	B	809	CLA	ND
17	B	810	CLA	ND
17	B	811	CLA	ND
17	B	812	CLA	ND
17	B	813	CLA	ND
17	B	814	CLA	ND
17	B	815	CLA	ND
17	B	816	CLA	ND
17	B	817	CLA	ND
17	B	818	CLA	ND
17	B	819	CLA	ND
17	B	820	CLA	ND
17	B	821	CLA	ND
17	B	822	CLA	ND
17	B	823	CLA	ND
17	B	824	CLA	ND
17	B	825	CLA	ND
17	B	826	CLA	ND
17	B	827	CLA	ND
17	B	828	CLA	ND
17	B	829	CLA	ND
17	B	830	CLA	ND
17	B	831	CLA	ND
17	B	832	CLA	ND
17	B	833	CLA	ND
17	B	834	CLA	ND
17	B	835	CLA	ND
17	B	837	CLA	ND
17	B	838	CLA	ND
17	B	839	CLA	ND
17	B	840	CLA	ND
17	B	841	CLA	ND
17	B	842	CLA	ND
17	F	802	CLA	ND
17	F	803	CLA	ND
17	J	101	CLA	ND
17	K	201	CLA	ND
17	K	202	CLA	ND
17	K	203	CLA	ND

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Mol	Chain	Res	Type	Atom
17	K	205	CLA	ND
17	L	301	CLA	ND
17	L	302	CLA	ND
17	L	303	CLA	ND
17	L	304	CLA	ND
17	1	504	CLA	ND
17	1	505	CLA	ND
17	1	506	CLA	ND
17	1	507	CLA	ND
17	1	508	CLA	ND
17	1	510	CLA	ND
17	1	511	CLA	ND
17	1	515	CLA	ND
17	2	504	CLA	ND
17	2	506	CLA	ND
17	2	507	CLA	ND
17	2	507	CLA	C8
17	2	508	CLA	ND
17	2	509	CLA	ND
17	2	510	CLA	ND
17	2	511	CLA	ND
17	2	514	CLA	ND
17	3	301	CLA	ND
17	3	306	CLA	ND
17	3	307	CLA	ND
17	3	308	CLA	ND
17	3	310	CLA	ND
17	3	311	CLA	ND
17	3	312	CLA	ND
17	3	313	CLA	ND
17	3	314	CLA	ND
17	3	316	CLA	ND
17	3	317	CLA	ND
17	3	318	CLA	ND
17	5	305	CLA	ND
17	5	306	CLA	ND
17	5	307	CLA	ND
17	5	308	CLA	ND
17	5	309	CLA	ND
17	5	310	CLA	ND
17	5	311	CLA	ND
17	5	312	CLA	ND

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Mol	Chain	Res	Type	Atom
17	5	313	CLA	ND
17	5	316	CLA	ND
25	1	512	CHL	ND
25	1	512	CHL	NA
25	1	512	CHL	NC
25	1	514	CHL	ND
25	1	514	CHL	NA
25	1	514	CHL	NC
25	1	517	CHL	ND
25	1	517	CHL	NA
25	1	517	CHL	NC
25	2	512	CHL	ND
25	2	512	CHL	NA
25	2	512	CHL	NC
25	2	513	CHL	ND
25	2	513	CHL	NA
25	2	513	CHL	NC
25	2	515	CHL	ND
25	2	515	CHL	NA
25	2	515	CHL	NC
25	2	516	CHL	ND
25	2	516	CHL	NA
25	2	516	CHL	NC
25	3	302	CHL	ND
25	3	302	CHL	NA
25	3	302	CHL	NC
25	3	315	CHL	ND
25	3	315	CHL	NA
25	3	315	CHL	NC
25	5	314	CHL	ND
25	5	314	CHL	NA
25	5	314	CHL	NC
25	5	315	CHL	ND
25	5	315	CHL	NA
25	5	315	CHL	NC
25	5	317	CHL	ND
25	5	317	CHL	NA
25	5	317	CHL	NC

All (1228) torsion outliers are listed below:

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Mol	Chain	Res	Type	Atoms
16	A	801	CL0	CHA-CBD-CGD-O2D
17	A	802	CLA	C6-C7-C8-C9
17	A	803	CLA	CHA-CBD-CGD-O2D
17	A	804	CLA	C1A-C2A-CAA-CBA
17	A	804	CLA	C3A-C2A-CAA-CBA
17	A	805	CLA	C1A-C2A-CAA-CBA
17	A	805	CLA	CAD-CBD-CGD-O2D
17	A	806	CLA	CAD-CBD-CGD-O2D
17	A	807	CLA	CAD-CBD-CGD-O2D
17	A	808	CLA	CHA-CBD-CGD-O1D
17	A	808	CLA	CHA-CBD-CGD-O2D
17	A	809	CLA	C1A-C2A-CAA-CBA
17	A	809	CLA	C2B-C3B-CAB-CBB
17	A	809	CLA	C4B-C3B-CAB-CBB
17	A	815	CLA	CHA-CBD-CGD-O1D
17	A	815	CLA	CHA-CBD-CGD-O2D
17	A	816	CLA	CBD-CGD-O2D-CED
17	A	821	CLA	C1A-C2A-CAA-CBA
17	A	821	CLA	C3A-C2A-CAA-CBA
17	A	822	CLA	CBD-CGD-O2D-CED
17	A	823	CLA	C1A-C2A-CAA-CBA
17	A	823	CLA	C2B-C3B-CAB-CBB
17	A	823	CLA	C4B-C3B-CAB-CBB
17	A	827	CLA	CBD-CGD-O2D-CED
17	A	831	CLA	CAD-CBD-CGD-O1D
17	A	831	CLA	CAD-CBD-CGD-O2D
17	A	831	CLA	CBD-CGD-O2D-CED
17	A	835	CLA	CAD-CBD-CGD-O1D
17	A	835	CLA	CAD-CBD-CGD-O2D
17	A	835	CLA	C2-C3-C5-C6
17	A	840	CLA	C2B-C3B-CAB-CBB
17	A	840	CLA	C4B-C3B-CAB-CBB
17	A	842	CLA	C1A-C2A-CAA-CBA
17	A	842	CLA	C3A-C2A-CAA-CBA
17	A	842	CLA	C2B-C3B-CAB-CBB
17	A	842	CLA	C4B-C3B-CAB-CBB
17	A	842	CLA	CHA-CBD-CGD-O1D
17	A	842	CLA	CHA-CBD-CGD-O2D
17	A	842	CLA	CBD-CGD-O2D-CED
17	A	852	CLA	CBD-CGD-O2D-CED
17	B	804	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
17	B	804	CLA	CBD-CGD-O2D-CED
17	B	805	CLA	CBD-CGD-O2D-CED
17	B	806	CLA	CAD-CBD-CGD-O1D
17	B	806	CLA	CAD-CBD-CGD-O2D
17	B	808	CLA	C2B-C3B-CAB-CBB
17	B	808	CLA	C4B-C3B-CAB-CBB
17	B	809	CLA	CHA-CBD-CGD-O1D
17	B	809	CLA	CHA-CBD-CGD-O2D
17	B	811	CLA	C1A-C2A-CAA-CBA
17	B	811	CLA	CAD-CBD-CGD-O1D
17	B	811	CLA	CAD-CBD-CGD-O2D
17	B	812	CLA	CBD-CGD-O2D-CED
17	B	815	CLA	CBD-CGD-O2D-CED
17	B	816	CLA	CHA-CBD-CGD-O1D
17	B	816	CLA	CHA-CBD-CGD-O2D
17	B	817	CLA	CBD-CGD-O2D-CED
17	B	818	CLA	C1A-C2A-CAA-CBA
17	B	818	CLA	C3A-C2A-CAA-CBA
17	B	822	CLA	CHA-CBD-CGD-O1D
17	B	822	CLA	CHA-CBD-CGD-O2D
17	B	823	CLA	C1A-C2A-CAA-CBA
17	B	823	CLA	C3A-C2A-CAA-CBA
17	B	824	CLA	C1A-C2A-CAA-CBA
17	B	824	CLA	C3A-C2A-CAA-CBA
17	B	825	CLA	CHA-CBD-CGD-O1D
17	B	825	CLA	CHA-CBD-CGD-O2D
17	B	826	CLA	C11-C12-C13-C14
17	B	832	CLA	CBD-CGD-O2D-CED
17	B	834	CLA	C1A-C2A-CAA-CBA
17	B	834	CLA	C2B-C3B-CAB-CBB
17	B	834	CLA	C4B-C3B-CAB-CBB
17	B	834	CLA	CHA-CBD-CGD-O1D
17	B	834	CLA	CHA-CBD-CGD-O2D
17	B	835	CLA	CBD-CGD-O2D-CED
17	B	836	CLA	C3A-C2A-CAA-CBA
17	B	839	CLA	CHA-CBD-CGD-O1D
17	B	839	CLA	CHA-CBD-CGD-O2D
17	B	842	CLA	C1A-C2A-CAA-CBA
17	B	842	CLA	C3A-C2A-CAA-CBA
17	J	101	CLA	C4B-C3B-CAB-CBB
17	K	201	CLA	C2B-C3B-CAB-CBB
17	K	201	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
17	K	202	CLA	C2B-C3B-CAB-CBB
17	K	202	CLA	C4B-C3B-CAB-CBB
17	K	203	CLA	CHA-CBD-CGD-O1D
17	K	203	CLA	CHA-CBD-CGD-O2D
17	K	203	CLA	CBD-CGD-O2D-CED
17	K	205	CLA	C2B-C3B-CAB-CBB
17	K	205	CLA	C4B-C3B-CAB-CBB
17	L	303	CLA	C1A-C2A-CAA-CBA
17	L	303	CLA	C3-C5-C6-C7
17	L	304	CLA	CHA-CBD-CGD-O1D
17	L	304	CLA	CHA-CBD-CGD-O2D
17	1	505	CLA	C1A-C2A-CAA-CBA
17	1	505	CLA	C3A-C2A-CAA-CBA
17	1	506	CLA	C1A-C2A-CAA-CBA
17	1	506	CLA	C3A-C2A-CAA-CBA
17	1	507	CLA	CBD-CGD-O2D-CED
17	1	508	CLA	CBD-CGD-O2D-CED
17	1	510	CLA	C1A-C2A-CAA-CBA
17	1	510	CLA	C3A-C2A-CAA-CBA
17	1	510	CLA	CBD-CGD-O2D-CED
17	1	511	CLA	CBA-CGA-O2A-C1
17	1	511	CLA	CBD-CGD-O2D-CED
17	1	513	CLA	C4B-C3B-CAB-CBB
17	2	505	CLA	CBD-CGD-O2D-CED
17	2	505	CLA	C3-C5-C6-C7
17	2	509	CLA	C1A-C2A-CAA-CBA
17	2	510	CLA	CBA-CGA-O2A-C1
17	2	511	CLA	C2B-C3B-CAB-CBB
17	2	511	CLA	C4B-C3B-CAB-CBB
17	3	306	CLA	C1A-C2A-CAA-CBA
17	3	306	CLA	C3A-C2A-CAA-CBA
17	3	306	CLA	C2-C1-O2A-CGA
17	3	306	CLA	CBD-CGD-O2D-CED
17	3	308	CLA	CBD-CGD-O2D-CED
17	3	309	CLA	CBD-CGD-O2D-CED
17	3	311	CLA	CBD-CGD-O2D-CED
17	3	312	CLA	CBD-CGD-O2D-CED
17	3	313	CLA	CBD-CGD-O2D-CED
17	5	307	CLA	CBA-CGA-O2A-C1
17	5	307	CLA	O1A-CGA-O2A-C1
17	5	308	CLA	CHA-CBD-CGD-O1D
17	5	308	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
17	5	312	CLA	CBD-CGD-O2D-CED
17	5	313	CLA	CAD-CBD-CGD-O1D
17	5	313	CLA	CAD-CBD-CGD-O2D
19	A	843	LHG	C3-O3-P-O4
19	A	843	LHG	C3-O3-P-O6
19	A	844	LHG	C3-O3-P-O6
19	A	844	LHG	C4-O6-P-O3
19	A	844	LHG	C4-O6-P-O4
19	A	844	LHG	C4-O6-P-O5
19	B	851	LHG	C4-O6-P-O3
19	B	851	LHG	C4-O6-P-O4
19	1	516	LHG	C3-O3-P-O6
19	1	516	LHG	C4-O6-P-O3
19	1	516	LHG	C4-O6-P-O5
19	2	517	LHG	C4-O6-P-O5
20	A	845	BCR	C21-C22-C23-C24
20	A	848	BCR	C23-C24-C25-C26
20	A	851	BCR	C5-C6-C7-C8
20	B	845	BCR	C21-C22-C23-C24
20	B	845	BCR	C37-C22-C23-C24
20	B	847	BCR	C1-C6-C7-C8
20	B	847	BCR	C5-C6-C7-C8
20	B	849	BCR	C21-C22-C23-C24
20	B	849	BCR	C37-C22-C23-C24
20	F	801	BCR	C17-C18-C19-C20
20	F	801	BCR	C37-C22-C23-C24
20	I	101	BCR	C21-C22-C23-C24
20	I	101	BCR	C37-C22-C23-C24
20	I	101	BCR	C23-C24-C25-C26
20	I	101	BCR	C23-C24-C25-C30
20	K	204	BCR	C23-C24-C25-C26
20	L	305	BCR	C17-C18-C19-C20
20	L	305	BCR	C36-C18-C19-C20
20	L	305	BCR	C21-C22-C23-C24
20	L	305	BCR	C37-C22-C23-C24
20	2	503	BCR	C21-C22-C23-C24
20	5	302	BCR	C1-C6-C7-C8
20	5	302	BCR	C5-C6-C7-C8
20	5	302	BCR	C11-C12-C13-C14
22	B	850	DGD	C2B-C1B-O2G-C2G
22	B	850	DGD	O1B-C1B-O2G-C2G
22	J	103	DGD	C2E-C1E-O5D-C6D

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Mol	Chain	Res	Type	Atoms
22	J	103	DGD	O6E-C1E-O5D-C6D
23	2	519	LMG	O9-C10-O7-C8
24	1	501	LUT	C1-C6-C7-C8
24	1	501	LUT	C5-C6-C7-C8
25	1	512	CHL	C1C-C2C-CMC-OMC
25	1	512	CHL	C3C-C2C-CMC-OMC
25	1	517	CHL	C1C-C2C-CMC-OMC
25	1	517	CHL	C3C-C2C-CMC-OMC
25	2	513	CHL	C4C-C3C-CAC-CBC
25	2	513	CHL	CHA-CBD-CGD-O1D
25	2	515	CHL	C3C-C2C-CMC-OMC
25	2	516	CHL	C1A-C2A-CAA-CBA
25	2	516	CHL	CAD-CBD-CGD-O1D
25	2	516	CHL	CAD-CBD-CGD-O2D
25	5	314	CHL	C1C-C2C-CMC-OMC
25	5	314	CHL	C3C-C2C-CMC-OMC
25	5	315	CHL	C1C-C2C-CMC-OMC
25	5	315	CHL	C3C-C2C-CMC-OMC
25	5	315	CHL	CHA-CBD-CGD-O2D
25	5	317	CHL	C1C-C2C-CMC-OMC
25	5	317	CHL	C3C-C2C-CMC-OMC
26	2	502	XAT	C5-C6-C7-C8
26	2	502	XAT	O4-C6-C7-C8
26	2	502	XAT	C7-C8-C9-C10
26	2	502	XAT	C7-C8-C9-C19
26	2	502	XAT	C27-C28-C29-C30
17	B	836	CLA	O1D-CGD-O2D-CED
17	2	509	CLA	O1D-CGD-O2D-CED
17	A	806	CLA	O1D-CGD-O2D-CED
17	A	852	CLA	O1D-CGD-O2D-CED
17	B	803	CLA	O1D-CGD-O2D-CED
17	B	804	CLA	O1D-CGD-O2D-CED
17	B	812	CLA	O1D-CGD-O2D-CED
17	B	832	CLA	O1D-CGD-O2D-CED
17	3	301	CLA	O1D-CGD-O2D-CED
17	3	306	CLA	O1D-CGD-O2D-CED
17	3	308	CLA	O1D-CGD-O2D-CED
17	3	312	CLA	O1D-CGD-O2D-CED
17	3	317	CLA	O1D-CGD-O2D-CED
17	5	307	CLA	O1D-CGD-O2D-CED
17	A	806	CLA	CBD-CGD-O2D-CED
17	A	813	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
17	A	815	CLA	CBD-CGD-O2D-CED
17	A	820	CLA	CBD-CGD-O2D-CED
17	B	803	CLA	CBD-CGD-O2D-CED
17	B	811	CLA	CBD-CGD-O2D-CED
17	B	814	CLA	CBD-CGD-O2D-CED
17	B	816	CLA	CBD-CGD-O2D-CED
17	B	820	CLA	CBD-CGD-O2D-CED
17	B	823	CLA	CBD-CGD-O2D-CED
17	B	836	CLA	CBD-CGD-O2D-CED
17	F	802	CLA	CBD-CGD-O2D-CED
17	1	506	CLA	CBD-CGD-O2D-CED
17	1	509	CLA	CBD-CGD-O2D-CED
17	1	513	CLA	CBD-CGD-O2D-CED
17	1	515	CLA	CBD-CGD-O2D-CED
17	2	509	CLA	CBD-CGD-O2D-CED
17	3	301	CLA	CBD-CGD-O2D-CED
17	3	307	CLA	CBD-CGD-O2D-CED
17	3	317	CLA	CBD-CGD-O2D-CED
17	5	307	CLA	CBD-CGD-O2D-CED
17	5	309	CLA	CBD-CGD-O2D-CED
25	2	513	CHL	CBD-CGD-O2D-CED
25	5	315	CHL	CBD-CGD-O2D-CED
17	L	303	CLA	O1A-CGA-O2A-C1
17	1	509	CLA	O1A-CGA-O2A-C1
17	2	510	CLA	O1A-CGA-O2A-C1
17	A	816	CLA	O1D-CGD-O2D-CED
17	B	815	CLA	O1D-CGD-O2D-CED
17	A	820	CLA	O1D-CGD-O2D-CED
17	1	513	CLA	O1D-CGD-O2D-CED
17	3	307	CLA	O1D-CGD-O2D-CED
17	5	309	CLA	O1D-CGD-O2D-CED
17	1	509	CLA	CBA-CGA-O2A-C1
17	2	514	CLA	CBD-CGD-O2D-CED
17	A	831	CLA	O1A-CGA-O2A-C1
17	3	308	CLA	O1A-CGA-O2A-C1
17	5	310	CLA	O1A-CGA-O2A-C1
23	F	806	LMG	O10-C28-O8-C9
17	1	511	CLA	O1A-CGA-O2A-C1
17	A	831	CLA	O1D-CGD-O2D-CED
17	A	827	CLA	O1D-CGD-O2D-CED
17	B	817	CLA	O1D-CGD-O2D-CED
17	B	835	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
17	1	507	CLA	O1D-CGD-O2D-CED
17	1	508	CLA	O1D-CGD-O2D-CED
17	1	511	CLA	O1D-CGD-O2D-CED
17	2	505	CLA	O1D-CGD-O2D-CED
17	A	810	CLA	CBD-CGD-O2D-CED
17	A	828	CLA	CBD-CGD-O2D-CED
17	1	510	CLA	O1D-CGD-O2D-CED
17	3	318	CLA	CBA-CGA-O2A-C1
17	3	318	CLA	O1A-CGA-O2A-C1
17	B	807	CLA	C3-C5-C6-C7
17	B	811	CLA	C3-C5-C6-C7
17	B	841	CLA	C3-C5-C6-C7
17	3	306	CLA	C3-C5-C6-C7
18	A	841	PQN	C13-C15-C16-C17
17	A	831	CLA	CBA-CGA-O2A-C1
17	A	835	CLA	CBA-CGA-O2A-C1
17	L	303	CLA	CBA-CGA-O2A-C1
17	3	308	CLA	CBA-CGA-O2A-C1
22	J	103	DGD	C2A-C1A-O1G-C1G
23	F	806	LMG	C29-C28-O8-C9
17	L	304	CLA	CBD-CGD-O2D-CED
17	2	507	CLA	CBD-CGD-O2D-CED
17	5	316	CLA	CBD-CGD-O2D-CED
25	2	516	CHL	CBD-CGD-O2D-CED
25	3	315	CHL	CBD-CGD-O2D-CED
23	2	519	LMG	C11-C10-O7-C8
17	L	304	CLA	C2C-C3C-CAC-CBC
17	A	822	CLA	O1D-CGD-O2D-CED
17	A	842	CLA	O1D-CGD-O2D-CED
17	B	805	CLA	O1D-CGD-O2D-CED
17	B	823	CLA	O1D-CGD-O2D-CED
17	K	203	CLA	O1D-CGD-O2D-CED
17	1	515	CLA	O1D-CGD-O2D-CED
17	3	309	CLA	O1D-CGD-O2D-CED
17	3	311	CLA	O1D-CGD-O2D-CED
17	5	312	CLA	O1D-CGD-O2D-CED
17	2	514	CLA	O1A-CGA-O2A-C1
17	3	313	CLA	O1D-CGD-O2D-CED
17	A	836	CLA	C4-C3-C5-C6
17	B	818	CLA	C4-C3-C5-C6
17	B	841	CLA	C4-C3-C5-C6
17	5	307	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
17	B	818	CLA	C2-C3-C5-C6
17	5	307	CLA	C2-C3-C5-C6
17	5	308	CLA	CBD-CGD-O2D-CED
17	B	816	CLA	O1D-CGD-O2D-CED
17	A	831	CLA	C2A-CAA-CBA-CGA
17	A	836	CLA	C3-C5-C6-C7
17	B	835	CLA	C3-C5-C6-C7
17	3	314	CLA	C3-C5-C6-C7
17	A	816	CLA	CBA-CGA-O2A-C1
17	B	822	CLA	CBA-CGA-O2A-C1
17	B	830	CLA	CBA-CGA-O2A-C1
17	5	310	CLA	CBA-CGA-O2A-C1
20	2	503	BCR	C13-C14-C15-C16
17	B	818	CLA	O1A-CGA-O2A-C1
17	2	506	CLA	O1A-CGA-O2A-C1
22	J	103	DGD	O1A-C1A-O1G-C1G
17	B	820	CLA	O1D-CGD-O2D-CED
17	1	509	CLA	O1D-CGD-O2D-CED
25	5	315	CHL	O1D-CGD-O2D-CED
25	1	512	CHL	CBD-CGD-O2D-CED
22	B	850	DGD	C5B-C6B-C7B-C8B
17	J	101	CLA	C2C-C3C-CAC-CBC
19	1	516	LHG	O2-C2-C3-O3
17	A	813	CLA	O1D-CGD-O2D-CED
17	B	811	CLA	O1D-CGD-O2D-CED
17	1	506	CLA	O1D-CGD-O2D-CED
25	2	513	CHL	O1D-CGD-O2D-CED
17	B	818	CLA	CBA-CGA-O2A-C1
17	2	506	CLA	CBA-CGA-O2A-C1
17	2	514	CLA	CBA-CGA-O2A-C1
17	A	816	CLA	O1A-CGA-O2A-C1
17	A	835	CLA	O1A-CGA-O2A-C1
17	F	802	CLA	O1D-CGD-O2D-CED
17	3	318	CLA	CBD-CGD-O2D-CED
17	A	815	CLA	O1D-CGD-O2D-CED
17	2	506	CLA	CBD-CGD-O2D-CED
17	2	510	CLA	CBD-CGD-O2D-CED
17	5	310	CLA	CBD-CGD-O2D-CED
23	2	519	LMG	O6-C5-C6-O5
17	A	820	CLA	CBA-CGA-O2A-C1
17	L	303	CLA	C4-C3-C5-C6
17	3	308	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
17	B	841	CLA	C2-C3-C5-C6
17	B	830	CLA	O1A-CGA-O2A-C1
17	B	824	CLA	CBD-CGD-O2D-CED
17	F	803	CLA	CBD-CGD-O2D-CED
25	2	512	CHL	C2A-CAA-CBA-CGA
17	L	304	CLA	C4C-C3C-CAC-CBC
17	A	828	CLA	O1D-CGD-O2D-CED
17	B	822	CLA	O1A-CGA-O2A-C1
22	J	103	DGD	O6D-C1D-O3G-C3G
23	F	806	LMG	O6-C1-O1-C7
17	B	814	CLA	O1D-CGD-O2D-CED
17	3	314	CLA	CBA-CGA-O2A-C1
19	B	851	LHG	C24-C23-O8-C6
17	A	802	CLA	CBD-CGD-O2D-CED
17	A	824	CLA	CBD-CGD-O2D-CED
17	A	826	CLA	CBD-CGD-O2D-CED
17	B	834	CLA	CBD-CGD-O2D-CED
17	1	504	CLA	CBD-CGD-O2D-CED
17	J	101	CLA	C4C-C3C-CAC-CBC
17	2	514	CLA	O1D-CGD-O2D-CED
17	A	811	CLA	CBD-CGD-O2D-CED
17	A	825	CLA	CBD-CGD-O2D-CED
17	A	820	CLA	O1A-CGA-O2A-C1
19	B	851	LHG	O10-C23-O8-C6
17	A	810	CLA	CBA-CGA-O2A-C1
17	A	836	CLA	CBA-CGA-O2A-C1
17	B	812	CLA	CBA-CGA-O2A-C1
17	B	842	CLA	CBA-CGA-O2A-C1
17	L	301	CLA	CBA-CGA-O2A-C1
17	5	308	CLA	CBA-CGA-O2A-C1
17	3	310	CLA	CBD-CGD-O2D-CED
17	A	810	CLA	O1D-CGD-O2D-CED
17	L	304	CLA	O1D-CGD-O2D-CED
17	A	836	CLA	C2-C3-C5-C6
17	L	303	CLA	C2-C3-C5-C6
17	3	308	CLA	C2-C3-C5-C6
17	A	852	CLA	C3-C5-C6-C7
17	B	830	CLA	CBD-CGD-O2D-CED
17	A	826	CLA	C6-C7-C8-C9
17	A	827	CLA	C14-C13-C15-C16
17	A	838	CLA	C11-C12-C13-C14
17	B	818	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
17	2	506	CLA	C11-C12-C13-C14
18	A	841	PQN	C19-C18-C20-C21
18	B	843	PQN	C19-C18-C20-C21
25	3	315	CHL	O1D-CGD-O2D-CED
23	F	806	LMG	C2-C1-O1-C7
17	L	301	CLA	O1A-CGA-O2A-C1
17	J	101	CLA	CBD-CGD-O2D-CED
20	A	845	BCR	C37-C22-C23-C24
20	A	847	BCR	C7-C8-C9-C34
20	A	853	BCR	C37-C22-C23-C24
20	B	844	BCR	C7-C8-C9-C34
20	F	801	BCR	C36-C18-C19-C20
20	L	305	BCR	C7-C8-C9-C34
20	2	503	BCR	C37-C22-C23-C24
20	3	305	BCR	C7-C8-C9-C34
20	5	302	BCR	C11-C12-C13-C35
26	2	502	XAT	C27-C28-C29-C39
20	A	847	BCR	C7-C8-C9-C10
20	A	853	BCR	C21-C22-C23-C24
20	B	844	BCR	C7-C8-C9-C10
20	F	801	BCR	C21-C22-C23-C24
20	L	305	BCR	C7-C8-C9-C10
23	2	519	LMG	C4-C5-C6-O5
25	5	314	CHL	C2A-CAA-CBA-CGA
17	1	510	CLA	CBA-CGA-O2A-C1
16	A	801	CL0	CAA-CBA-CGA-O2A
17	3	306	CLA	CBA-CGA-O2A-C1
17	2	514	CLA	C2-C1-O2A-CGA
17	2	507	CLA	O1D-CGD-O2D-CED
22	J	103	DGD	O6E-C5E-C6E-O5E
17	A	805	CLA	C10-C11-C12-C13
17	2	506	CLA	C15-C16-C17-C18
17	2	510	CLA	C5-C6-C7-C8
17	A	806	CLA	C6-C7-C8-C10
18	A	841	PQN	C18-C20-C21-C22
18	B	843	PQN	C15-C16-C17-C18
23	2	519	LMG	C28-C29-C30-C31
17	A	810	CLA	O1A-CGA-O2A-C1
17	3	306	CLA	O1A-CGA-O2A-C1
17	5	308	CLA	O1A-CGA-O2A-C1
17	A	805	CLA	C8-C10-C11-C12
17	B	802	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
17	B	802	CLA	C15-C16-C17-C18
17	2	514	CLA	C5-C6-C7-C8
17	A	808	CLA	C2A-CAA-CBA-CGA
17	A	823	CLA	C2A-CAA-CBA-CGA
17	B	801	CLA	C2A-CAA-CBA-CGA
17	3	308	CLA	C2A-CAA-CBA-CGA
17	3	314	CLA	C2A-CAA-CBA-CGA
25	2	516	CHL	O1D-CGD-O2D-CED
17	2	507	CLA	C5-C6-C7-C8
17	5	308	CLA	C10-C11-C12-C13
17	A	836	CLA	O1A-CGA-O2A-C1
17	B	842	CLA	O1A-CGA-O2A-C1
17	B	842	CLA	C3-C5-C6-C7
17	3	308	CLA	C3-C5-C6-C7
23	2	518	LMG	O6-C1-O1-C7
17	A	838	CLA	C5-C6-C7-C8
17	B	838	CLA	C5-C6-C7-C8
17	3	308	CLA	C5-C6-C7-C8
17	5	308	CLA	C5-C6-C7-C8
19	B	851	LHG	O2-C2-C3-O3
17	B	812	CLA	O1A-CGA-O2A-C1
17	B	835	CLA	C5-C6-C7-C8
17	5	316	CLA	O1D-CGD-O2D-CED
17	A	823	CLA	C5-C6-C7-C8
17	5	307	CLA	C10-C11-C12-C13
17	K	202	CLA	CBD-CGD-O2D-CED
17	3	314	CLA	O1A-CGA-O2A-C1
22	B	850	DGD	O6D-C5D-C6D-O5D
17	5	308	CLA	O1D-CGD-O2D-CED
25	1	512	CHL	O1D-CGD-O2D-CED
17	A	827	CLA	C10-C11-C12-C13
17	B	818	CLA	C5-C6-C7-C8
17	B	826	CLA	C8-C10-C11-C12
17	3	306	CLA	C5-C6-C7-C8
17	A	804	CLA	CBA-CGA-O2A-C1
17	A	825	CLA	CBA-CGA-O2A-C1
17	A	838	CLA	CBD-CGD-O2D-CED
17	2	510	CLA	C3-C5-C6-C7
17	3	318	CLA	O1D-CGD-O2D-CED
17	A	827	CLA	C8-C10-C11-C12
17	B	837	CLA	C2C-C3C-CAC-CBC
23	F	806	LMG	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
23	F	805	LMG	O9-C10-O7-C8
17	A	827	CLA	C2A-CAA-CBA-CGA
17	A	805	CLA	C5-C6-C7-C8
17	A	802	CLA	C5-C6-C7-C8
17	A	806	CLA	C13-C15-C16-C17
17	B	803	CLA	C10-C11-C12-C13
25	2	516	CHL	C2A-CAA-CBA-CGA
17	A	829	CLA	C4-C3-C5-C6
22	B	850	DGD	C4D-C5D-C6D-O5D
23	F	805	LMG	C11-C10-O7-C8
23	F	806	LMG	C11-C10-O7-C8
23	F	806	LMG	O9-C10-O7-C8
19	1	516	LHG	C23-C24-C25-C26
17	1	506	CLA	C6-C7-C8-C9
17	5	307	CLA	C16-C17-C18-C20
20	A	848	BCR	C37-C22-C23-C24
20	A	851	BCR	C37-C22-C23-C24
20	K	204	BCR	C37-C22-C23-C24
20	L	306	BCR	C11-C12-C13-C35
20	1	503	BCR	C7-C8-C9-C34
20	3	305	BCR	C37-C22-C23-C24
26	5	304	XAT	C27-C28-C29-C39
20	A	848	BCR	C21-C22-C23-C24
20	K	204	BCR	C21-C22-C23-C24
20	1	503	BCR	C7-C8-C9-C10
20	3	305	BCR	C7-C8-C9-C10
20	3	305	BCR	C21-C22-C23-C24
17	B	802	CLA	C2A-CAA-CBA-CGA
17	B	821	CLA	C2A-CAA-CBA-CGA
17	2	509	CLA	C2A-CAA-CBA-CGA
17	5	308	CLA	C2A-CAA-CBA-CGA
25	3	302	CHL	CBA-CGA-O2A-C1
17	A	829	CLA	C5-C6-C7-C8
19	A	844	LHG	O1-C1-C2-C3
17	B	824	CLA	O1D-CGD-O2D-CED
17	5	310	CLA	O1D-CGD-O2D-CED
17	A	823	CLA	C6-C7-C8-C9
17	2	510	CLA	C11-C12-C13-C14
17	3	308	CLA	C6-C7-C8-C9
17	3	314	CLA	C6-C7-C8-C9
17	5	308	CLA	C11-C12-C13-C14
17	B	834	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
17	2	510	CLA	O1D-CGD-O2D-CED
17	F	803	CLA	O1D-CGD-O2D-CED
22	J	103	DGD	C2B-C1B-O2G-C2G
17	2	506	CLA	O1D-CGD-O2D-CED
17	2	505	CLA	CBA-CGA-O2A-C1
17	A	831	CLA	C15-C16-C17-C18
17	B	842	CLA	CBD-CGD-O2D-CED
17	3	314	CLA	C2-C1-O2A-CGA
17	5	310	CLA	C2-C1-O2A-CGA
17	2	510	CLA	C11-C12-C13-C15
17	3	314	CLA	C6-C7-C8-C10
23	5	301	LMG	C11-C12-C13-C14
25	1	512	CHL	CBA-CGA-O2A-C1
25	2	512	CHL	CBA-CGA-O2A-C1
17	1	504	CLA	O1D-CGD-O2D-CED
17	A	804	CLA	O1A-CGA-O2A-C1
17	A	825	CLA	O1A-CGA-O2A-C1
22	J	103	DGD	O1B-C1B-O2G-C2G
17	A	817	CLA	C4B-C3B-CAB-CBB
17	A	822	CLA	C4B-C3B-CAB-CBB
17	A	834	CLA	C4B-C3B-CAB-CBB
17	B	803	CLA	C4B-C3B-CAB-CBB
17	B	815	CLA	C4B-C3B-CAB-CBB
17	B	836	CLA	C4B-C3B-CAB-CBB
17	B	841	CLA	C4B-C3B-CAB-CBB
17	F	802	CLA	C4B-C3B-CAB-CBB
17	2	508	CLA	C4B-C3B-CAB-CBB
17	2	514	CLA	C4B-C3B-CAB-CBB
17	5	313	CLA	C4B-C3B-CAB-CBB
22	J	103	DGD	C1A-C2A-C3A-C4A
25	5	314	CHL	CBA-CGA-O2A-C1
17	3	308	CLA	C6-C7-C8-C10
17	5	308	CLA	C11-C12-C13-C15
17	A	824	CLA	O1D-CGD-O2D-CED
17	5	307	CLA	C2A-CAA-CBA-CGA
17	B	842	CLA	C8-C10-C11-C12
19	A	843	LHG	C27-C28-C29-C30
19	A	844	LHG	C7-C8-C9-C10
22	J	103	DGD	C7B-C8B-C9B-CAB
23	2	519	LMG	C11-C12-C13-C14
17	A	805	CLA	C3A-C2A-CAA-CBA
17	A	852	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
17	B	834	CLA	C3A-C2A-CAA-CBA
17	L	303	CLA	C3A-C2A-CAA-CBA
17	3	310	CLA	C3A-C2A-CAA-CBA
17	3	318	CLA	C3A-C2A-CAA-CBA
17	5	309	CLA	C3A-C2A-CAA-CBA
25	2	516	CHL	C3A-C2A-CAA-CBA
25	5	314	CHL	C3A-C2A-CAA-CBA
17	A	802	CLA	O1D-CGD-O2D-CED
17	A	806	CLA	C5-C6-C7-C8
17	A	806	CLA	C15-C16-C17-C18
23	F	806	LMG	C28-C29-C30-C31
17	A	823	CLA	C6-C7-C8-C10
23	F	806	LMG	C12-C13-C14-C15
17	B	821	CLA	CBD-CGD-O2D-CED
19	1	516	LHG	C1-C2-C3-O3
17	A	842	CLA	CBA-CGA-O2A-C1
17	3	311	CLA	CBA-CGA-O2A-C1
17	A	826	CLA	C3-C5-C6-C7
17	A	831	CLA	C13-C15-C16-C17
19	1	516	LHG	C34-C35-C36-C37
22	B	850	DGD	CDB-CEB-CFB-CGB
17	2	505	CLA	O1A-CGA-O2A-C1
17	A	822	CLA	C2B-C3B-CAB-CBB
17	A	834	CLA	C2B-C3B-CAB-CBB
17	B	836	CLA	C2B-C3B-CAB-CBB
17	B	841	CLA	C2B-C3B-CAB-CBB
17	F	802	CLA	C2B-C3B-CAB-CBB
17	J	101	CLA	C2B-C3B-CAB-CBB
17	1	511	CLA	C2B-C3B-CAB-CBB
17	1	513	CLA	C2B-C3B-CAB-CBB
17	5	313	CLA	C2B-C3B-CAB-CBB
20	A	848	BCR	C23-C24-C25-C30
20	A	851	BCR	C1-C6-C7-C8
20	A	851	BCR	C23-C24-C25-C26
20	A	851	BCR	C23-C24-C25-C30
20	K	204	BCR	C23-C24-C25-C30
20	L	306	BCR	C23-C24-C25-C26
20	L	306	BCR	C23-C24-C25-C30
20	1	503	BCR	C1-C6-C7-C8
20	1	503	BCR	C5-C6-C7-C8
20	2	503	BCR	C1-C6-C7-C8
20	2	503	BCR	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
20	3	305	BCR	C1-C6-C7-C8
20	3	305	BCR	C5-C6-C7-C8
19	B	851	LHG	C29-C30-C31-C32
25	1	514	CHL	CBD-CGD-O2D-CED
23	5	301	LMG	C29-C28-O8-C9
22	J	103	DGD	C6B-C7B-C8B-C9B
17	A	826	CLA	O1D-CGD-O2D-CED
17	A	816	CLA	C2A-CAA-CBA-CGA
17	5	312	CLA	C2A-CAA-CBA-CGA
17	B	841	CLA	C5-C6-C7-C8
19	A	843	LHG	C14-C15-C16-C17
17	A	805	CLA	C13-C15-C16-C17
17	A	831	CLA	C5-C6-C7-C8
17	A	829	CLA	C2-C3-C5-C6
17	3	311	CLA	O1A-CGA-O2A-C1
17	B	807	CLA	C6-C7-C8-C9
19	A	843	LHG	C31-C32-C33-C34
23	2	518	LMG	C2-C1-O1-C7
17	A	842	CLA	O1A-CGA-O2A-C1
17	A	818	CLA	CBD-CGD-O2D-CED
19	A	844	LHG	C8-C7-O7-C5
19	1	516	LHG	C8-C7-O7-C5
17	A	806	CLA	C10-C11-C12-C13
17	1	510	CLA	O1A-CGA-O2A-C1
19	1	516	LHG	C9-C10-C11-C12
18	A	841	PQN	C25-C26-C27-C28
19	1	516	LHG	C7-C8-C9-C10
22	J	103	DGD	C5D-C6D-O5D-C1E
17	A	820	CLA	C2A-CAA-CBA-CGA
17	1	506	CLA	C6-C7-C8-C10
17	5	307	CLA	C16-C17-C18-C19
18	A	841	PQN	C26-C27-C28-C30
17	L	303	CLA	CBD-CGD-O2D-CED
25	5	317	CHL	CBD-CGD-O2D-CED
19	1	516	LHG	C14-C15-C16-C17
17	5	308	CLA	C8-C10-C11-C12
19	B	851	LHG	C9-C10-C11-C12
19	A	844	LHG	O9-C7-O7-C5
17	A	836	CLA	C6-C7-C8-C9
22	B	850	DGD	C2B-C3B-C4B-C5B
22	J	103	DGD	CEA-CFA-CGA-CHA
17	A	827	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
17	B	807	CLA	C15-C16-C17-C18
19	A	843	LHG	C29-C30-C31-C32
17	A	811	CLA	O1D-CGD-O2D-CED
17	A	825	CLA	O1D-CGD-O2D-CED
17	B	833	CLA	C5-C6-C7-C8
17	L	301	CLA	C4-C3-C5-C6
17	B	817	CLA	C2A-CAA-CBA-CGA
17	5	310	CLA	C2A-CAA-CBA-CGA
17	B	829	CLA	CBD-CGD-O2D-CED
17	3	310	CLA	O1D-CGD-O2D-CED
17	B	830	CLA	O1D-CGD-O2D-CED
19	A	843	LHG	C10-C11-C12-C13
17	A	836	CLA	C6-C7-C8-C10
23	5	301	LMG	O10-C28-O8-C9
17	A	852	CLA	C1A-C2A-CAA-CBA
17	B	804	CLA	C1A-C2A-CAA-CBA
17	B	820	CLA	C1A-C2A-CAA-CBA
17	B	821	CLA	C1A-C2A-CAA-CBA
17	3	308	CLA	C1A-C2A-CAA-CBA
17	3	310	CLA	C1A-C2A-CAA-CBA
17	3	313	CLA	C1A-C2A-CAA-CBA
17	3	314	CLA	C1A-C2A-CAA-CBA
17	5	309	CLA	C1A-C2A-CAA-CBA
19	1	516	LHG	O9-C7-O7-C5
17	A	805	CLA	C6-C7-C8-C10
17	B	803	CLA	C12-C13-C15-C16
17	B	807	CLA	C12-C13-C15-C16
17	B	826	CLA	C11-C12-C13-C15
17	B	830	CLA	C6-C7-C8-C10
17	5	307	CLA	C12-C13-C15-C16
17	A	805	CLA	C2-C3-C5-C6
17	A	835	CLA	CBD-CGD-O2D-CED
17	B	808	CLA	C2A-CAA-CBA-CGA
17	2	506	CLA	C2A-CAA-CBA-CGA
17	3	306	CLA	C2A-CAA-CBA-CGA
17	A	805	CLA	C6-C7-C8-C9
17	A	808	CLA	C11-C12-C13-C14
17	A	816	CLA	C6-C7-C8-C9
17	B	807	CLA	C14-C13-C15-C16
17	B	830	CLA	C6-C7-C8-C9
17	A	825	CLA	C5-C6-C7-C8
23	5	301	LMG	O6-C5-C6-O5

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Mol	Chain	Res	Type	Atoms
17	A	839	CLA	CBD-CGD-O2D-CED
22	B	850	DGD	C4A-C5A-C6A-C7A
23	F	805	LMG	C13-C14-C15-C16
17	J	101	CLA	O1D-CGD-O2D-CED
22	J	103	DGD	O1G-C1G-C2G-C3G
22	J	103	DGD	C1G-C2G-C3G-O3G
23	F	806	LMG	C11-C12-C13-C14
17	A	806	CLA	CBA-CGA-O2A-C1
23	2	519	LMG	C29-C28-O8-C9
18	A	841	PQN	C26-C27-C28-C29
25	5	314	CHL	CHA-CBD-CGD-O1D
25	5	314	CHL	CHA-CBD-CGD-O2D
20	B	847	BCR	C11-C12-C13-C35
17	B	841	CLA	C6-C7-C8-C9
20	B	847	BCR	C11-C12-C13-C14
23	F	806	LMG	C38-C39-C40-C41
17	A	832	CLA	CBA-CGA-O2A-C1
17	B	804	CLA	CBA-CGA-O2A-C1
17	3	313	CLA	O2A-C1-C2-C3
17	A	816	CLA	C3-C5-C6-C7
25	1	514	CHL	C3C-C2C-CMC-OMC
17	A	838	CLA	O1D-CGD-O2D-CED
17	A	827	CLA	C13-C15-C16-C17
17	A	823	CLA	CBD-CGD-O2D-CED
17	A	805	CLA	C4-C3-C5-C6
22	J	103	DGD	C6A-C7A-C8A-C9A
22	B	850	DGD	CCB-CDB-CEB-CFB
17	A	829	CLA	CBA-CGA-O2A-C1
22	B	850	DGD	C3B-C4B-C5B-C6B
16	A	801	CL0	C3-C5-C6-C7
17	B	818	CLA	C8-C10-C11-C12
17	A	825	CLA	C11-C12-C13-C14
17	A	805	CLA	C16-C17-C18-C19
17	B	808	CLA	CBA-CGA-O2A-C1
17	1	506	CLA	CBA-CGA-O2A-C1
25	2	515	CHL	C1C-C2C-CMC-OMC
17	A	837	CLA	CBD-CGD-O2D-CED
19	2	517	LHG	C7-C8-C9-C10
17	5	307	CLA	C8-C10-C11-C12
25	3	302	CHL	O1A-CGA-O2A-C1
17	A	806	CLA	C4-C3-C5-C6
17	A	827	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
17	A	852	CLA	C4-C3-C5-C6
17	2	506	CLA	C4-C3-C5-C6
17	A	838	CLA	C11-C10-C8-C9
17	2	510	CLA	C11-C10-C8-C9
17	5	307	CLA	C14-C13-C15-C16
25	1	514	CHL	O1D-CGD-O2D-CED
17	A	806	CLA	O1A-CGA-O2A-C1
17	A	814	CLA	C4B-C3B-CAB-CBB
17	A	852	CLA	C4B-C3B-CAB-CBB
17	B	805	CLA	C4B-C3B-CAB-CBB
17	1	511	CLA	C4B-C3B-CAB-CBB
17	3	301	CLA	C4B-C3B-CAB-CBB
17	5	307	CLA	C4B-C3B-CAB-CBB
17	5	312	CLA	C4B-C3B-CAB-CBB
22	B	850	DGD	C4B-C5B-C6B-C7B
22	J	103	DGD	CFA-CGA-CHA-CIA
17	A	802	CLA	C6-C7-C8-C10
17	A	808	CLA	C11-C12-C13-C15
17	A	816	CLA	C6-C7-C8-C10
17	B	818	CLA	C11-C10-C8-C7
17	1	513	CLA	C12-C13-C15-C16
17	2	510	CLA	C11-C10-C8-C7
18	B	843	PQN	C17-C18-C20-C21
18	A	841	PQN	C15-C16-C17-C18
17	K	202	CLA	O1D-CGD-O2D-CED
17	A	813	CLA	C3A-C2A-CAA-CBA
17	A	826	CLA	C3A-C2A-CAA-CBA
17	B	813	CLA	C3A-C2A-CAA-CBA
17	B	830	CLA	C4-C3-C5-C6
25	2	515	CHL	C3A-C2A-CAA-CBA
17	1	513	CLA	C5-C6-C7-C8
17	2	506	CLA	C2-C3-C5-C6
17	A	831	CLA	C10-C11-C12-C13
17	1	506	CLA	O1A-CGA-O2A-C1
17	A	838	CLA	CBA-CGA-O2A-C1
17	B	833	CLA	C3-C5-C6-C7
17	A	806	CLA	C16-C17-C18-C19
17	A	827	CLA	C16-C17-C18-C19
17	B	803	CLA	C15-C16-C17-C18
24	1	502	LUT	C7-C8-C9-C19
17	A	835	CLA	C4-C3-C5-C6
17	A	832	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
17	B	804	CLA	O1A-CGA-O2A-C1
25	1	512	CHL	O1A-CGA-O2A-C1
17	A	802	CLA	C8-C10-C11-C12
17	B	803	CLA	C4-C3-C5-C6
25	2	513	CHL	C2C-C3C-CAC-CBC
25	2	513	CHL	CHA-CBD-CGD-O2D
19	B	851	LHG	O6-C4-C5-O7
17	3	301	CLA	C2B-C3B-CAB-CBB
17	5	307	CLA	C2B-C3B-CAB-CBB
20	A	845	BCR	C1-C6-C7-C8
20	B	844	BCR	C1-C6-C7-C8
20	K	204	BCR	C1-C6-C7-C8
24	3	303	LUT	C1-C6-C7-C8
19	1	516	LHG	C11-C10-C9-C8
17	B	830	CLA	C3-C5-C6-C7
22	J	103	DGD	C4B-C5B-C6B-C7B
17	2	506	CLA	C13-C15-C16-C17
25	5	317	CHL	O1D-CGD-O2D-CED
23	2	519	LMG	O1-C7-C8-O7
23	5	301	LMG	O1-C7-C8-O7
19	A	843	LHG	C23-C24-C25-C26
23	F	806	LMG	C10-C11-C12-C13
17	2	510	CLA	C10-C11-C12-C13
18	A	841	PQN	C20-C21-C22-C23
17	A	806	CLA	C2-C3-C5-C6
17	A	852	CLA	C2-C3-C5-C6
17	B	830	CLA	C2-C3-C5-C6
25	2	512	CHL	O1A-CGA-O2A-C1
22	B	850	DGD	C6A-C7A-C8A-C9A
17	1	513	CLA	C14-C13-C15-C16
17	B	842	CLA	O1D-CGD-O2D-CED
23	2	519	LMG	O10-C28-O8-C9
17	B	829	CLA	O1D-CGD-O2D-CED
22	B	850	DGD	CEB-CFB-CGB-CHB
17	J	101	CLA	C1A-C2A-CAA-CBA
17	1	504	CLA	C1A-C2A-CAA-CBA
17	1	507	CLA	C1A-C2A-CAA-CBA
17	B	815	CLA	C2A-CAA-CBA-CGA
17	B	815	CLA	CBA-CGA-O2A-C1
17	B	803	CLA	C2-C3-C5-C6
17	5	311	CLA	CBD-CGD-O2D-CED
17	B	839	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
17	3	306	CLA	C6-C7-C8-C9
19	A	843	LHG	C35-C36-C37-C38
17	B	818	CLA	CBD-CGD-O2D-CED
25	1	517	CHL	CBD-CGD-O2D-CED
20	B	852	BCR	C37-C22-C23-C24
20	K	204	BCR	C11-C12-C13-C35
20	2	503	BCR	C7-C8-C9-C34
17	A	806	CLA	C12-C13-C15-C16
17	A	838	CLA	C11-C10-C8-C7
17	B	803	CLA	C6-C7-C8-C10
17	2	508	CLA	O2A-C1-C2-C3
20	L	306	BCR	C11-C12-C13-C14
26	5	304	XAT	C27-C28-C29-C30
25	5	314	CHL	O1A-CGA-O2A-C1
19	1	516	LHG	C28-C29-C30-C31
17	B	804	CLA	O2A-C1-C2-C3
22	J	103	DGD	C1G-C2G-O2G-C1B
17	A	829	CLA	O1A-CGA-O2A-C1
17	A	827	CLA	C16-C17-C18-C20
17	B	808	CLA	O1A-CGA-O2A-C1
17	B	803	CLA	CAA-CBA-CGA-O2A
19	1	516	LHG	C4-C5-C6-O8
17	B	828	CLA	CBD-CGD-O2D-CED
17	A	806	CLA	C16-C17-C18-C20
22	J	103	DGD	O1G-C1G-C2G-O2G
17	A	806	CLA	C14-C13-C15-C16
17	A	831	CLA	C11-C10-C8-C9
17	B	802	CLA	C6-C7-C8-C9
17	B	803	CLA	C6-C7-C8-C9
17	3	313	CLA	CBA-CGA-O2A-C1
17	A	823	CLA	C3A-C2A-CAA-CBA
22	J	103	DGD	C4E-C5E-C6E-O5E
17	A	838	CLA	O1A-CGA-O2A-C1
17	B	815	CLA	O1A-CGA-O2A-C1
17	1	513	CLA	C2-C1-O2A-CGA
17	A	808	CLA	C15-C16-C17-C18
17	A	835	CLA	O1D-CGD-O2D-CED
18	B	843	PQN	C14-C13-C15-C16
22	J	103	DGD	C3A-C4A-C5A-C6A
17	B	839	CLA	O1A-CGA-O2A-C1
17	B	837	CLA	C4C-C3C-CAC-CBC
25	2	516	CHL	C4C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
17	A	839	CLA	O1D-CGD-O2D-CED
19	A	843	LHG	C30-C31-C32-C33
22	J	103	DGD	C9B-CAB-CBB-CCB
16	A	801	CL0	C2-C1-O2A-CGA
20	A	846	BCR	C7-C8-C9-C34
20	F	801	BCR	C7-C8-C9-C34
24	3	304	LUT	C7-C8-C9-C19
17	A	819	CLA	C4B-C3B-CAB-CBB
17	A	826	CLA	C1A-C2A-CAA-CBA
17	A	835	CLA	C1A-C2A-CAA-CBA
17	A	839	CLA	C4B-C3B-CAB-CBB
17	B	820	CLA	C4B-C3B-CAB-CBB
17	F	803	CLA	C4B-C3B-CAB-CBB
17	2	505	CLA	C1A-C2A-CAA-CBA
17	2	505	CLA	C4B-C3B-CAB-CBB
17	3	307	CLA	C4B-C3B-CAB-CBB
17	3	312	CLA	C4B-C3B-CAB-CBB
17	3	318	CLA	C1A-C2A-CAA-CBA
17	5	306	CLA	C4B-C3B-CAB-CBB
17	B	821	CLA	O1D-CGD-O2D-CED
17	5	312	CLA	CAA-CBA-CGA-O2A
24	3	304	LUT	C7-C8-C9-C10
25	1	512	CHL	C2A-CAA-CBA-CGA
17	1	513	CLA	C13-C15-C16-C17
19	B	851	LHG	O6-C4-C5-C6
17	B	826	CLA	C6-C7-C8-C10
18	A	841	PQN	C17-C18-C20-C21
17	1	513	CLA	C16-C17-C18-C20
17	3	306	CLA	C6-C7-C8-C10
17	A	840	CLA	CBD-CGD-O2D-CED
17	3	313	CLA	O1A-CGA-O2A-C1
17	A	835	CLA	C3A-C2A-CAA-CBA
17	B	811	CLA	C3A-C2A-CAA-CBA
17	2	505	CLA	C3A-C2A-CAA-CBA
17	L	303	CLA	O1D-CGD-O2D-CED
17	A	838	CLA	C2A-CAA-CBA-CGA
17	B	820	CLA	C2C-C3C-CAC-CBC
17	A	837	CLA	O1D-CGD-O2D-CED
17	B	818	CLA	O1D-CGD-O2D-CED
17	B	817	CLA	C1-C2-C3-C4
19	2	517	LHG	C23-C24-C25-C26
22	J	103	DGD	O2G-C2G-C3G-O3G

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Mol	Chain	Res	Type	Atoms
17	A	832	CLA	O2A-C1-C2-C3
17	5	311	CLA	O1D-CGD-O2D-CED
23	2	519	LMG	O1-C7-C8-C9
23	2	519	LMG	C7-C8-C9-O8
23	5	301	LMG	O1-C7-C8-C9
18	A	841	PQN	C14-C13-C15-C16
18	B	843	PQN	C12-C13-C15-C16
17	A	812	CLA	CAD-CBD-CGD-O2D
17	A	813	CLA	CAD-CBD-CGD-O2D
17	A	819	CLA	CAD-CBD-CGD-O2D
17	A	823	CLA	CAD-CBD-CGD-O2D
17	A	824	CLA	CAD-CBD-CGD-O2D
17	B	812	CLA	CAD-CBD-CGD-O2D
17	B	814	CLA	CAD-CBD-CGD-O2D
17	B	827	CLA	CAD-CBD-CGD-O2D
17	B	837	CLA	CAD-CBD-CGD-O2D
17	B	841	CLA	CAD-CBD-CGD-O2D
17	2	505	CLA	CAD-CBD-CGD-O2D
17	3	312	CLA	CAD-CBD-CGD-O2D
25	3	315	CHL	C1A-C2A-CAA-CBA
17	A	823	CLA	O1D-CGD-O2D-CED
19	1	516	LHG	C24-C23-O8-C6
17	B	803	CLA	C8-C10-C11-C12
16	A	801	CL0	CAD-CBD-CGD-O2D
17	A	803	CLA	CHA-CBD-CGD-O1D
17	A	805	CLA	CAD-CBD-CGD-O1D
17	A	806	CLA	CAD-CBD-CGD-O1D
17	A	810	CLA	CHA-CBD-CGD-O1D
17	A	812	CLA	CAD-CBD-CGD-O1D
17	A	813	CLA	CAD-CBD-CGD-O1D
17	A	819	CLA	CAD-CBD-CGD-O1D
17	A	823	CLA	CAD-CBD-CGD-O1D
17	A	824	CLA	CAD-CBD-CGD-O1D
17	B	812	CLA	CAD-CBD-CGD-O1D
17	B	814	CLA	CAD-CBD-CGD-O1D
17	B	827	CLA	CAD-CBD-CGD-O1D
17	B	831	CLA	CHA-CBD-CGD-O1D
17	B	831	CLA	CHA-CBD-CGD-O2D
17	B	837	CLA	CAD-CBD-CGD-O1D
17	B	841	CLA	CAD-CBD-CGD-O1D
17	K	202	CLA	CHA-CBD-CGD-O2D
17	2	505	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
17	3	311	CLA	CHA-CBD-CGD-O1D
17	3	311	CLA	CHA-CBD-CGD-O2D
17	3	312	CLA	CAD-CBD-CGD-O1D
17	5	306	CLA	CHA-CBD-CGD-O2D
19	A	843	LHG	C3-O3-P-O5
19	A	844	LHG	C3-O3-P-O5
19	B	851	LHG	C3-O3-P-O4
19	B	851	LHG	C3-O3-P-O5
19	B	851	LHG	C3-O3-P-O6
19	1	516	LHG	C3-O3-P-O5
20	B	847	BCR	C19-C20-C21-C22
25	2	512	CHL	CHA-CBD-CGD-O1D
25	2	512	CHL	CHA-CBD-CGD-O2D
25	5	315	CHL	CHA-CBD-CGD-O1D
17	A	808	CLA	C3-C5-C6-C7
22	B	850	DGD	C3A-C4A-C5A-C6A
17	3	314	CLA	C4-C3-C5-C6
17	A	817	CLA	C2B-C3B-CAB-CBB
17	A	839	CLA	C2B-C3B-CAB-CBB
17	A	852	CLA	C2B-C3B-CAB-CBB
17	B	803	CLA	C2B-C3B-CAB-CBB
17	B	815	CLA	C2B-C3B-CAB-CBB
17	2	508	CLA	C2B-C3B-CAB-CBB
17	2	514	CLA	C2B-C3B-CAB-CBB
17	3	307	CLA	C2B-C3B-CAB-CBB
17	5	312	CLA	C2B-C3B-CAB-CBB
20	A	846	BCR	C23-C24-C25-C26
25	2	513	CHL	CAD-CBD-CGD-O2D
19	B	851	LHG	C2-C3-O3-P
19	1	516	LHG	C2-C3-O3-P
20	A	846	BCR	C37-C22-C23-C24
20	B	846	BCR	C7-C8-C9-C34
17	1	513	CLA	C15-C16-C17-C18
17	1	513	CLA	C16-C17-C18-C19
19	1	516	LHG	O10-C23-O8-C6
22	B	850	DGD	C1A-C2A-C3A-C4A
23	F	806	LMG	C9-C8-O7-C10
20	2	503	BCR	C18-C19-C20-C21
20	5	302	BCR	C10-C11-C12-C13
17	A	805	CLA	C11-C10-C8-C9
17	B	807	CLA	C11-C10-C8-C9
17	A	838	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
23	2	519	LMG	C14-C15-C16-C17
17	B	820	CLA	C5-C6-C7-C8
25	1	517	CHL	O1D-CGD-O2D-CED
18	B	843	PQN	C13-C15-C16-C17
17	A	840	CLA	O1D-CGD-O2D-CED
20	B	848	BCR	C36-C18-C19-C20
23	F	806	LMG	C8-C7-O1-C1
17	B	802	CLA	C8-C10-C11-C12
17	B	804	CLA	C13-C15-C16-C17
20	L	306	BCR	C19-C20-C21-C22
19	1	516	LHG	C11-C12-C13-C14
17	B	840	CLA	C4B-C3B-CAB-CBB
17	2	504	CLA	C4B-C3B-CAB-CBB
17	B	801	CLA	C16-C17-C18-C19
19	B	851	LHG	C7-C8-C9-C10
17	B	811	CLA	C4-C3-C5-C6
17	1	513	CLA	C4-C3-C5-C6
17	B	801	CLA	C8-C10-C11-C12
17	A	805	CLA	C12-C13-C15-C16
17	B	804	CLA	C11-C10-C8-C7
17	5	307	CLA	C11-C10-C8-C7
17	3	314	CLA	C2-C3-C5-C6
20	A	849	BCR	C11-C10-C9-C34
20	B	845	BCR	C11-C10-C9-C34
20	B	846	BCR	C11-C10-C9-C34
20	B	846	BCR	C20-C21-C22-C37
20	B	852	BCR	C11-C10-C9-C34
20	F	804	BCR	C35-C13-C14-C15
20	5	302	BCR	C11-C10-C9-C34
22	B	850	DGD	C2G-C1G-O1G-C1A
17	A	826	CLA	C2-C1-O2A-CGA
19	A	843	LHG	C11-C12-C13-C14
22	J	103	DGD	CDA-CEA-CFA-CGA
20	B	848	BCR	C17-C18-C19-C20
24	1	502	LUT	C7-C8-C9-C10
18	A	841	PQN	C12-C13-C15-C16
17	3	311	CLA	C2A-CAA-CBA-CGA
17	A	820	CLA	C6-C7-C8-C9
17	A	827	CLA	C11-C10-C8-C9
17	B	804	CLA	C14-C13-C15-C16
17	B	826	CLA	C11-C10-C8-C9
17	1	513	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
23	2	519	LMG	C7-C8-O7-C10
23	2	519	LMG	C9-C8-O7-C10
17	A	818	CLA	O1D-CGD-O2D-CED
17	A	838	CLA	C3-C5-C6-C7
17	1	515	CLA	CAA-CBA-CGA-O2A
17	A	831	CLA	C11-C12-C13-C15
25	1	512	CHL	CAA-CBA-CGA-O2A
17	A	808	CLA	C1A-C2A-CAA-CBA
17	A	813	CLA	C1A-C2A-CAA-CBA
17	B	801	CLA	C1A-C2A-CAA-CBA
17	B	813	CLA	C1A-C2A-CAA-CBA
17	B	832	CLA	C1A-C2A-CAA-CBA
17	B	839	CLA	C1A-C2A-CAA-CBA
17	2	510	CLA	C1A-C2A-CAA-CBA
20	A	849	BCR	C11-C10-C9-C8
20	B	845	BCR	C11-C10-C9-C8
20	B	846	BCR	C11-C10-C9-C8
20	B	846	BCR	C20-C21-C22-C23
20	B	852	BCR	C11-C10-C9-C8
20	F	804	BCR	C12-C13-C14-C15
20	5	302	BCR	C11-C10-C9-C8
17	A	807	CLA	C2B-C3B-CAB-CBB
17	A	814	CLA	C2B-C3B-CAB-CBB
17	A	819	CLA	C2B-C3B-CAB-CBB
17	B	809	CLA	C2B-C3B-CAB-CBB
17	B	820	CLA	C2B-C3B-CAB-CBB
17	B	824	CLA	C2B-C3B-CAB-CBB
17	F	803	CLA	C2B-C3B-CAB-CBB
17	L	302	CLA	C2B-C3B-CAB-CBB
17	2	504	CLA	C2B-C3B-CAB-CBB
17	2	505	CLA	C2B-C3B-CAB-CBB
17	3	312	CLA	C2B-C3B-CAB-CBB
17	5	306	CLA	C2B-C3B-CAB-CBB
20	A	845	BCR	C5-C6-C7-C8
20	B	844	BCR	C5-C6-C7-C8
20	J	102	BCR	C23-C24-C25-C30
20	K	204	BCR	C5-C6-C7-C8
20	L	305	BCR	C23-C24-C25-C30
24	3	303	LUT	C5-C6-C7-C8
17	B	830	CLA	C11-C10-C8-C9
17	B	842	CLA	C4-C3-C5-C6
17	A	827	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
17	L	301	CLA	C2-C3-C5-C6
17	1	513	CLA	C2-C3-C5-C6
23	F	806	LMG	C29-C30-C31-C32
22	J	103	DGD	C1B-C2B-C3B-C4B
17	1	515	CLA	CAA-CBA-CGA-O1A
17	A	825	CLA	C11-C10-C8-C7
17	A	826	CLA	C6-C7-C8-C10
17	A	838	CLA	C11-C12-C13-C15
17	B	804	CLA	C6-C7-C8-C10
17	B	842	CLA	C11-C10-C8-C7
19	1	516	LHG	O7-C5-C6-O8
17	A	826	CLA	C4-C3-C5-C6
17	B	815	CLA	C4-C3-C5-C6
17	B	811	CLA	C2-C3-C5-C6
17	A	836	CLA	CBD-CGD-O2D-CED
17	A	825	CLA	C11-C10-C8-C9
20	A	846	BCR	C19-C20-C21-C22
17	5	307	CLA	C5-C6-C7-C8
23	2	518	LMG	O1-C7-C8-O7
17	B	801	CLA	C13-C15-C16-C17
17	B	826	CLA	CBA-CGA-O2A-C1
19	A	844	LHG	C24-C23-O8-C6
17	5	311	CLA	C1A-C2A-CAA-CBA
17	B	826	CLA	O1A-CGA-O2A-C1
17	1	510	CLA	CAA-CBA-CGA-O2A
17	1	506	CLA	C4-C3-C5-C6
17	A	805	CLA	CAA-CBA-CGA-O2A
17	A	807	CLA	C4B-C3B-CAB-CBB
17	B	809	CLA	C4B-C3B-CAB-CBB
17	B	824	CLA	C4B-C3B-CAB-CBB
17	L	302	CLA	C4B-C3B-CAB-CBB
17	1	510	CLA	C4B-C3B-CAB-CBB
17	B	801	CLA	C16-C17-C18-C20
25	1	517	CHL	CHA-CBD-CGD-O2D
17	2	505	CLA	C2A-CAA-CBA-CGA
17	A	813	CLA	CAA-CBA-CGA-O2A
25	2	515	CHL	CAA-CBA-CGA-O2A
17	B	801	CLA	C4-C3-C5-C6
23	F	806	LMG	O1-C7-C8-O7
17	A	826	CLA	C2-C3-C5-C6
17	A	823	CLA	C3-C5-C6-C7
17	5	308	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
23	F	806	LMG	C31-C32-C33-C34
17	B	826	CLA	C6-C7-C8-C9
17	1	513	CLA	C11-C12-C13-C14
17	5	308	CLA	C11-C10-C8-C9
17	B	841	CLA	O1A-CGA-O2A-C1
17	1	515	CLA	CHA-CBD-CGD-O2D
17	B	817	CLA	C2-C1-O2A-CGA
17	A	836	CLA	C3A-C2A-CAA-CBA
17	2	514	CLA	C3A-C2A-CAA-CBA
17	A	831	CLA	C3-C5-C6-C7
17	B	841	CLA	CBA-CGA-O2A-C1
17	B	835	CLA	C4-C3-C5-C6
17	A	816	CLA	C2-C3-C5-C6
17	B	828	CLA	O1D-CGD-O2D-CED
18	B	843	PQN	C20-C21-C22-C23
23	F	806	LMG	C7-C8-C9-O8
17	A	802	CLA	O1A-CGA-O2A-C1
17	2	510	CLA	C4-C3-C5-C6
17	3	311	CLA	CAA-CBA-CGA-O2A
17	A	813	CLA	CAA-CBA-CGA-O1A
20	A	846	BCR	C21-C22-C23-C24
20	B	852	BCR	C21-C22-C23-C24
20	F	801	BCR	C7-C8-C9-C10
17	2	506	CLA	C3-C5-C6-C7
17	B	807	CLA	C5-C6-C7-C8
17	B	842	CLA	CAA-CBA-CGA-O2A
17	B	842	CLA	C2-C3-C5-C6
17	A	827	CLA	C12-C13-C15-C16
17	1	513	CLA	C6-C7-C8-C10
18	A	841	PQN	C16-C17-C18-C20
19	A	844	LHG	O10-C23-O8-C6
25	2	515	CHL	CAA-CBA-CGA-O1A
17	A	803	CLA	C2B-C3B-CAB-CBB
17	B	805	CLA	C2B-C3B-CAB-CBB
17	B	840	CLA	C2B-C3B-CAB-CBB
17	5	309	CLA	C2B-C3B-CAB-CBB
20	A	846	BCR	C23-C24-C25-C30
20	A	848	BCR	C1-C6-C7-C8
20	A	848	BCR	C5-C6-C7-C8
20	B	845	BCR	C1-C6-C7-C8
20	B	845	BCR	C5-C6-C7-C8
20	J	102	BCR	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
20	L	305	BCR	C23-C24-C25-C26
20	3	305	BCR	C23-C24-C25-C30
24	1	502	LUT	C1-C6-C7-C8
24	5	303	LUT	C1-C6-C7-C8
24	5	303	LUT	C5-C6-C7-C8
17	B	833	CLA	CAA-CBA-CGA-O2A
17	B	802	CLA	C2-C3-C5-C6
17	A	816	CLA	C2-C1-O2A-CGA
17	B	812	CLA	C2-C1-O2A-CGA
17	B	817	CLA	CAA-CBA-CGA-O2A
17	K	203	CLA	C4C-C3C-CAC-CBC
17	B	804	CLA	C15-C16-C17-C18
17	A	820	CLA	C4-C3-C5-C6
17	A	820	CLA	C2-C3-C5-C6
17	B	835	CLA	C2-C3-C5-C6
19	B	851	LHG	C1-C2-C3-O3
25	1	514	CHL	C1C-C2C-CMC-OMC
17	2	509	CLA	CBA-CGA-O2A-C1
22	B	850	DGD	C8A-C9A-CAA-CBA
17	A	838	CLA	C14-C13-C15-C16
17	B	804	CLA	C6-C7-C8-C9
17	B	818	CLA	C6-C7-C8-C9
17	B	818	CLA	CAA-CBA-CGA-O2A
17	1	505	CLA	C4B-C3B-CAB-CBB
20	A	846	BCR	C7-C8-C9-C10
20	A	851	BCR	C21-C22-C23-C24
20	K	204	BCR	C11-C12-C13-C14
20	L	306	BCR	C21-C22-C23-C24
20	2	503	BCR	C7-C8-C9-C10
17	A	826	CLA	C11-C12-C13-C15
17	A	816	CLA	CAA-CBA-CGA-O2A
17	A	832	CLA	CAA-CBA-CGA-O2A
19	1	516	LHG	O8-C23-C24-C25
17	A	834	CLA	CBD-CGD-O2D-CED
17	L	303	CLA	C2A-CAA-CBA-CGA
17	2	510	CLA	C8-C10-C11-C12
19	B	851	LHG	C26-C27-C28-C29
22	B	850	DGD	C7B-C8B-C9B-CAB
17	A	805	CLA	O1D-CGD-O2D-CED
17	B	815	CLA	C2-C1-O2A-CGA
17	1	513	CLA	C11-C12-C13-C15
17	2	506	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
18	B	843	PQN	C21-C22-C23-C25
17	5	310	CLA	CAA-CBA-CGA-O2A
17	B	803	CLA	CAA-CBA-CGA-O1A
17	A	802	CLA	C2A-CAA-CBA-CGA
17	A	836	CLA	C2A-CAA-CBA-CGA
17	2	509	CLA	O1A-CGA-O2A-C1
17	B	801	CLA	C3A-C2A-CAA-CBA
17	2	509	CLA	C3A-C2A-CAA-CBA
17	3	313	CLA	C3A-C2A-CAA-CBA
17	5	306	CLA	CHA-CBD-CGD-O1D
17	2	506	CLA	C16-C17-C18-C19
17	B	815	CLA	C2-C3-C5-C6
17	B	842	CLA	CAA-CBA-CGA-O1A
17	A	827	CLA	O1A-CGA-O2A-C1
17	A	802	CLA	CBA-CGA-O2A-C1
17	B	817	CLA	CAA-CBA-CGA-O1A
17	A	806	CLA	C2A-CAA-CBA-CGA
17	A	806	CLA	C6-C7-C8-C9
17	A	852	CLA	C6-C7-C8-C9
17	B	803	CLA	C14-C13-C15-C16
17	B	842	CLA	C11-C10-C8-C9
18	A	841	PQN	C16-C17-C18-C19
17	A	802	CLA	CAA-CBA-CGA-O2A
17	A	832	CLA	CAA-CBA-CGA-O1A
17	B	838	CLA	C10-C11-C12-C13
17	A	820	CLA	CAA-CBA-CGA-O2A
17	A	827	CLA	CBA-CGA-O2A-C1
22	B	850	DGD	C2G-C3G-O3G-C1D
17	A	826	CLA	O1A-CGA-O2A-C1
17	3	311	CLA	CAA-CBA-CGA-O1A
17	B	803	CLA	O1A-CGA-O2A-C1
17	3	314	CLA	CBD-CGD-O2D-CED
23	F	805	LMG	O7-C10-C11-C12
19	1	516	LHG	O10-C23-C24-C25
17	A	830	CLA	CAD-CBD-CGD-O2D
17	A	833	CLA	CAD-CBD-CGD-O2D
17	B	804	CLA	CAD-CBD-CGD-O2D
17	B	840	CLA	CAD-CBD-CGD-O2D
17	1	505	CLA	CAD-CBD-CGD-O2D
17	3	314	CLA	CAD-CBD-CGD-O2D
17	5	309	CLA	CAD-CBD-CGD-O2D
17	5	312	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
17	A	823	CLA	C2-C1-O2A-CGA
17	A	816	CLA	CAA-CBA-CGA-O1A
16	A	801	CL0	C1A-C2A-CAA-CBA
25	5	314	CHL	C1A-C2A-CAA-CBA
19	B	851	LHG	C10-C11-C12-C13
17	A	820	CLA	CAA-CBA-CGA-O1A
17	2	505	CLA	CAA-CBA-CGA-O2A
17	5	310	CLA	CAA-CBA-CGA-O1A
23	5	301	LMG	C28-C29-C30-C31
17	3	314	CLA	O1D-CGD-O2D-CED
22	B	850	DGD	C5A-C6A-C7A-C8A

There are no ring outliers.

155 monomers are involved in 369 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	1	515	CLA	3	0
17	A	802	CLA	2	0
17	B	817	CLA	1	0
17	A	821	CLA	2	0
17	B	815	CLA	4	0
17	B	822	CLA	3	0
17	1	509	CLA	4	0
20	A	848	BCR	2	0
17	A	835	CLA	2	0
24	3	304	LUT	5	0
17	K	201	CLA	3	0
17	2	514	CLA	3	0
17	B	832	CLA	1	0
17	5	316	CLA	3	0
19	1	516	LHG	5	0
17	B	818	CLA	4	0
17	B	810	CLA	1	0
17	B	813	CLA	1	0
25	2	516	CHL	3	0
17	3	307	CLA	1	0
17	3	313	CLA	4	0
17	B	821	CLA	1	0
23	F	806	LMG	2	0
17	B	833	CLA	2	0
17	2	507	CLA	2	0
20	5	302	BCR	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	5	301	LMG	1	0
17	J	101	CLA	2	0
17	A	825	CLA	1	0
24	1	502	LUT	7	0
24	5	303	LUT	8	0
17	B	828	CLA	4	0
20	J	102	BCR	1	0
17	A	840	CLA	1	0
17	A	810	CLA	2	0
20	B	844	BCR	9	0
17	A	808	CLA	2	0
17	A	803	CLA	3	0
17	1	510	CLA	2	0
24	3	303	LUT	7	0
25	2	512	CHL	4	0
26	2	502	XAT	7	0
19	A	844	LHG	3	0
17	B	842	CLA	2	0
20	A	851	BCR	4	0
19	2	517	LHG	2	0
20	A	846	BCR	3	0
17	B	825	CLA	2	0
17	5	309	CLA	1	0
20	B	852	BCR	1	0
17	B	816	CLA	1	0
17	2	505	CLA	3	0
20	3	305	BCR	4	0
17	B	837	CLA	1	0
17	3	306	CLA	3	0
25	5	314	CHL	2	0
22	J	103	DGD	3	0
18	B	843	PQN	1	0
17	A	804	CLA	1	0
25	3	315	CHL	1	0
25	5	315	CHL	4	0
17	K	202	CLA	2	0
17	A	852	CLA	2	0
20	I	101	BCR	4	0
17	A	816	CLA	2	0
20	2	503	BCR	4	0
17	A	805	CLA	4	0
17	B	835	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	A	853	BCR	4	0
20	B	846	BCR	1	0
17	A	827	CLA	4	0
20	B	845	BCR	1	0
17	A	817	CLA	3	0
25	5	317	CHL	3	0
20	B	848	BCR	3	0
17	5	308	CLA	5	0
17	B	811	CLA	5	0
17	2	508	CLA	3	0
23	2	518	LMG	1	0
17	B	802	CLA	6	0
22	B	850	DGD	4	0
20	A	849	BCR	1	0
17	B	805	CLA	1	0
17	A	826	CLA	1	0
17	1	506	CLA	8	0
17	A	831	CLA	3	0
17	B	823	CLA	1	0
23	2	519	LMG	2	0
19	A	843	LHG	4	0
17	F	802	CLA	3	0
17	1	507	CLA	2	0
24	2	501	LUT	8	0
20	1	503	BCR	3	0
16	A	801	CL0	2	0
20	F	801	BCR	1	0
17	1	513	CLA	6	0
20	L	305	BCR	8	0
17	3	316	CLA	2	0
17	B	804	CLA	4	0
20	B	849	BCR	2	0
25	2	513	CHL	4	0
17	2	506	CLA	5	0
17	5	305	CLA	2	0
17	1	504	CLA	3	0
17	A	806	CLA	5	0
17	B	826	CLA	2	0
17	L	304	CLA	2	0
17	5	307	CLA	4	0
17	B	806	CLA	4	0
17	B	824	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	2	515	CHL	2	0
17	L	303	CLA	2	0
17	3	308	CLA	6	0
21	C	102	SF4	1	0
17	1	511	CLA	2	0
17	B	801	CLA	1	0
17	B	838	CLA	5	0
24	1	501	LUT	4	0
17	A	813	CLA	2	0
17	2	510	CLA	4	0
17	3	309	CLA	2	0
20	A	847	BCR	1	0
26	5	304	XAT	5	0
20	B	847	BCR	2	0
20	K	204	BCR	2	0
17	L	301	CLA	2	0
17	2	509	CLA	1	0
23	F	805	LMG	1	0
20	L	306	BCR	2	0
17	B	807	CLA	3	0
17	3	314	CLA	2	0
17	A	829	CLA	1	0
17	2	504	CLA	2	0
17	B	841	CLA	1	0
25	1	517	CHL	5	0
17	B	831	CLA	1	0
17	A	838	CLA	2	0
17	3	301	CLA	2	0
18	A	841	PQN	2	0
17	A	836	CLA	3	0
17	A	820	CLA	4	0
17	A	824	CLA	1	0
17	B	812	CLA	1	0
17	A	828	CLA	1	0
17	A	815	CLA	1	0
17	L	302	CLA	1	0
17	5	310	CLA	2	0
17	B	820	CLA	4	0
17	B	830	CLA	3	0
17	3	311	CLA	4	0
17	B	808	CLA	2	0
20	A	845	BCR	4	0

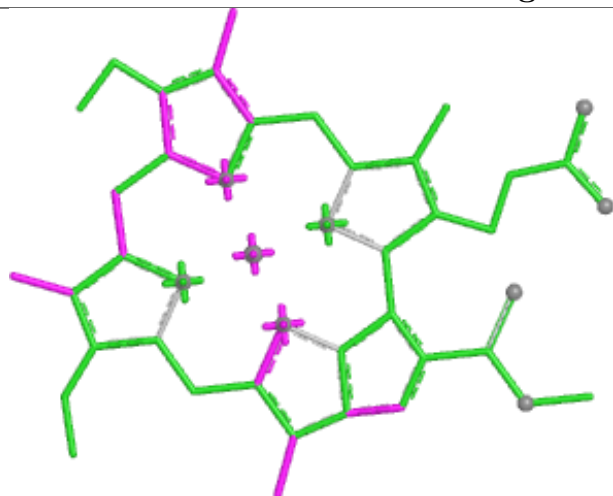
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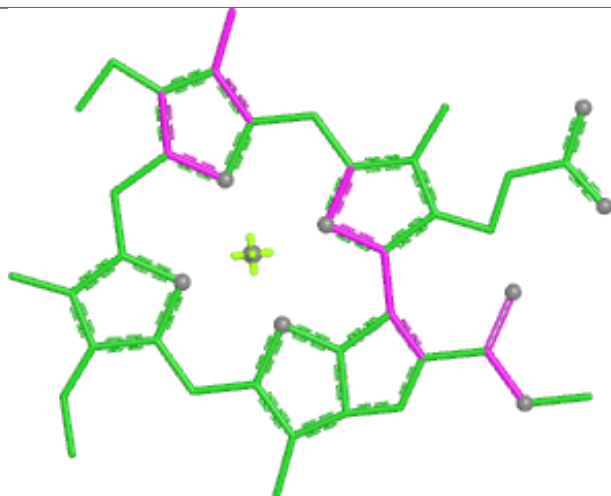
Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	K	205	CLA	1	0
17	B	803	CLA	1	0
20	F	804	BCR	3	0

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

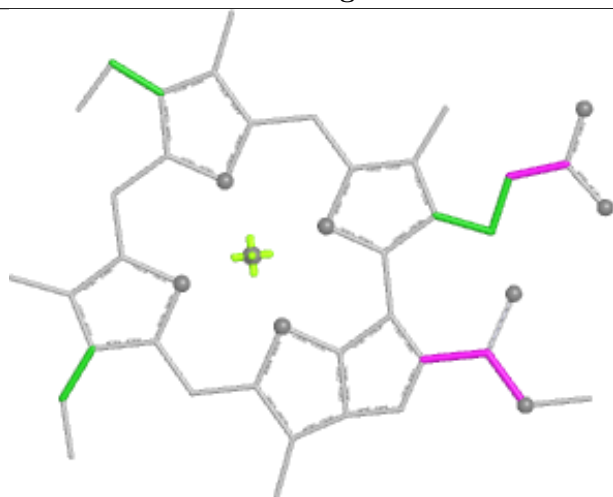
Ligand CLA 1 515



Bond lengths



Bond angles

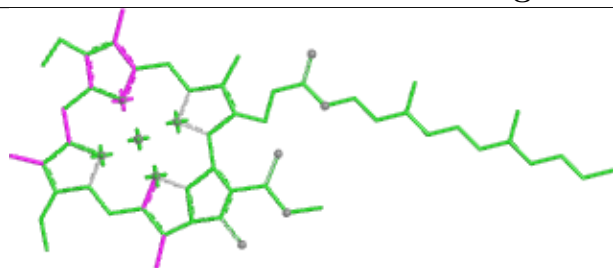


Torsions

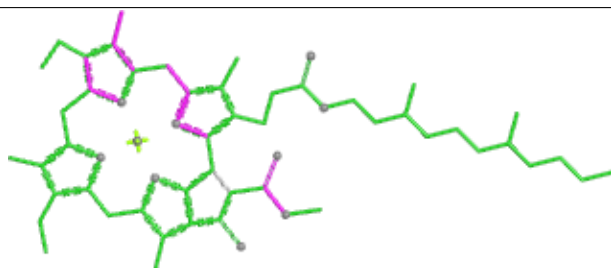


Rings

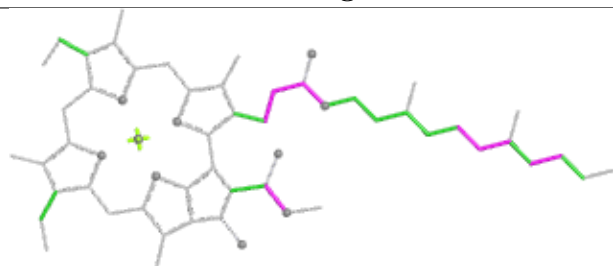
Ligand CLA A 802



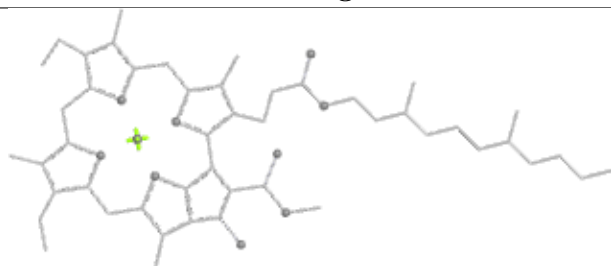
Bond lengths



Bond angles

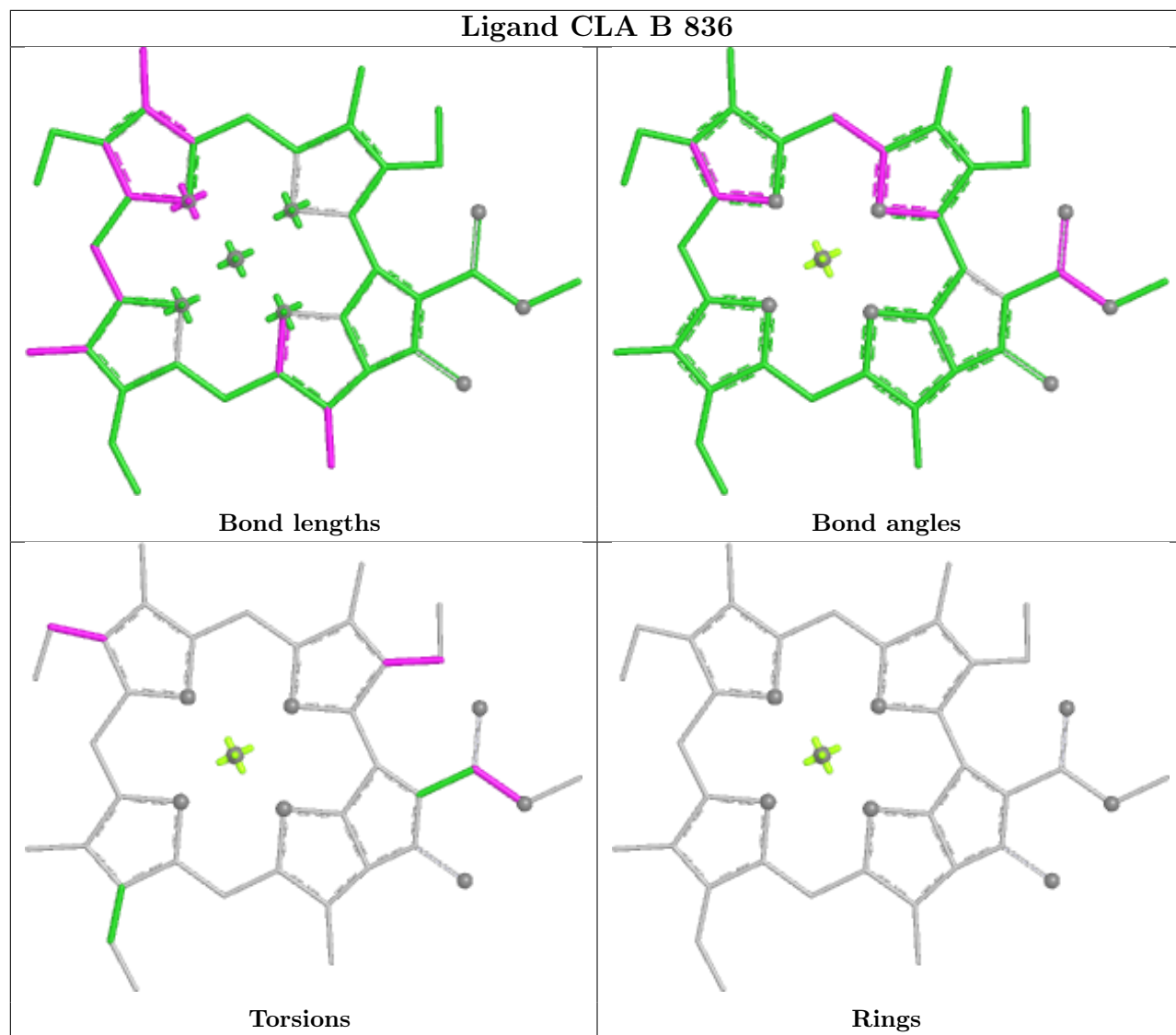


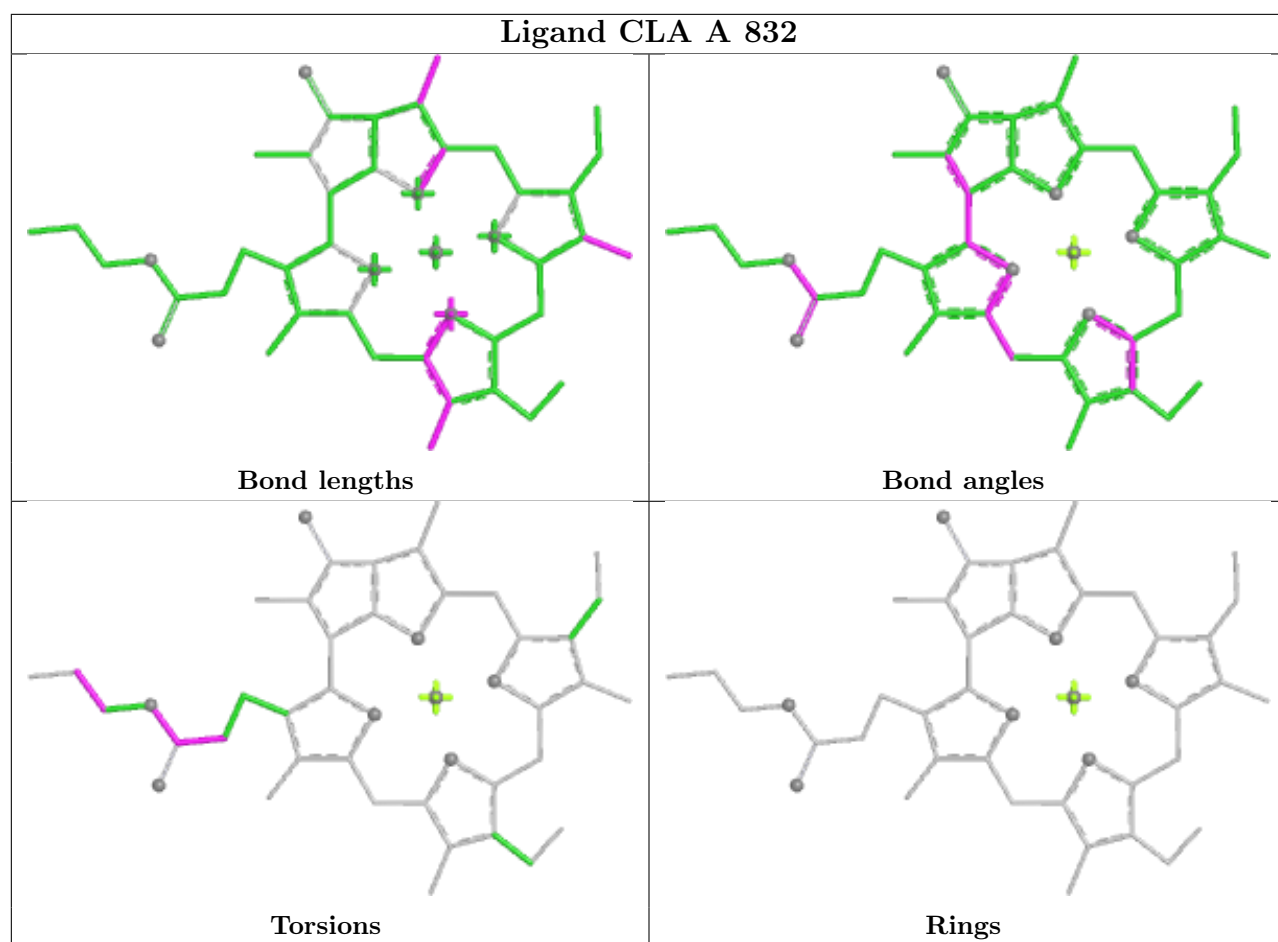
Torsions

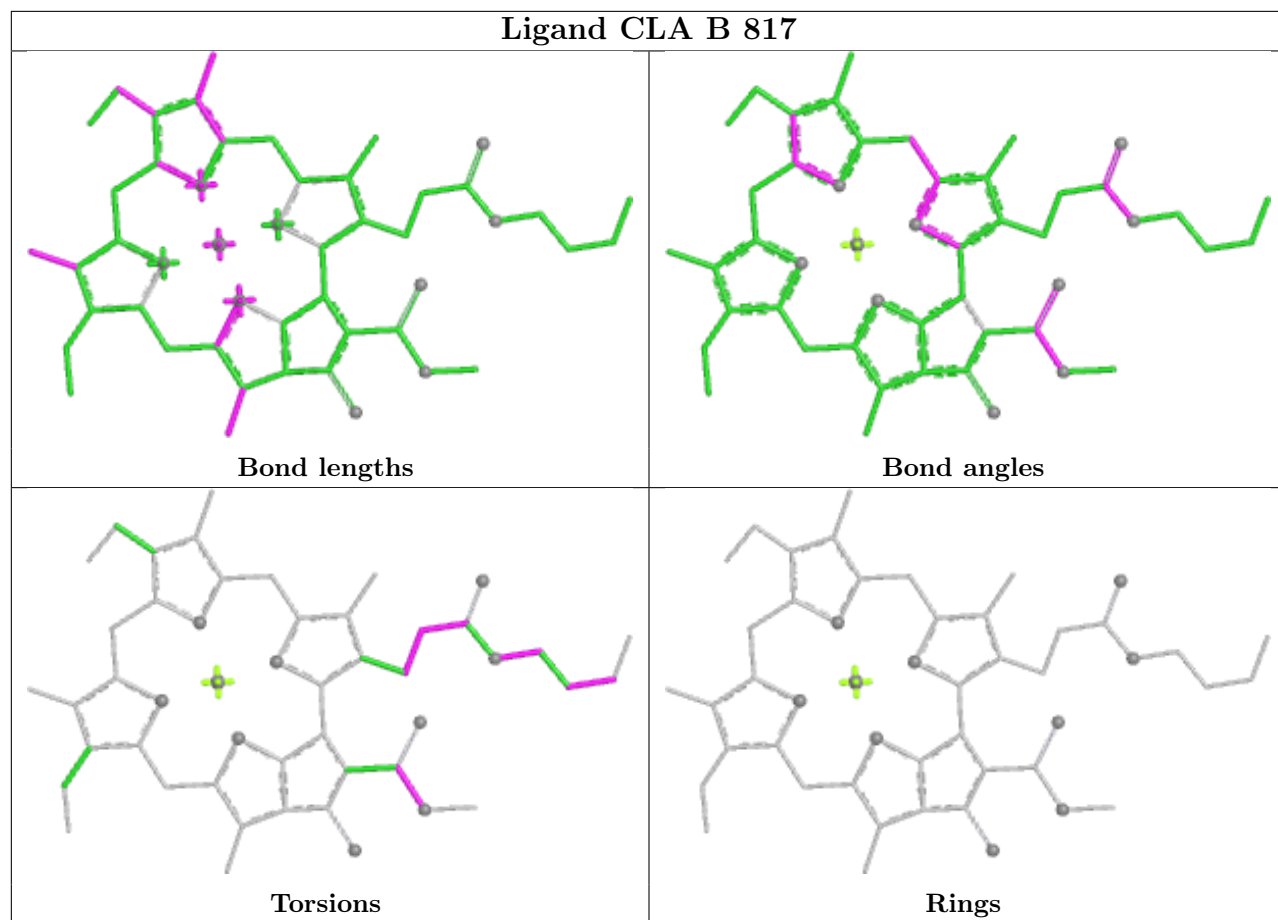


Rings

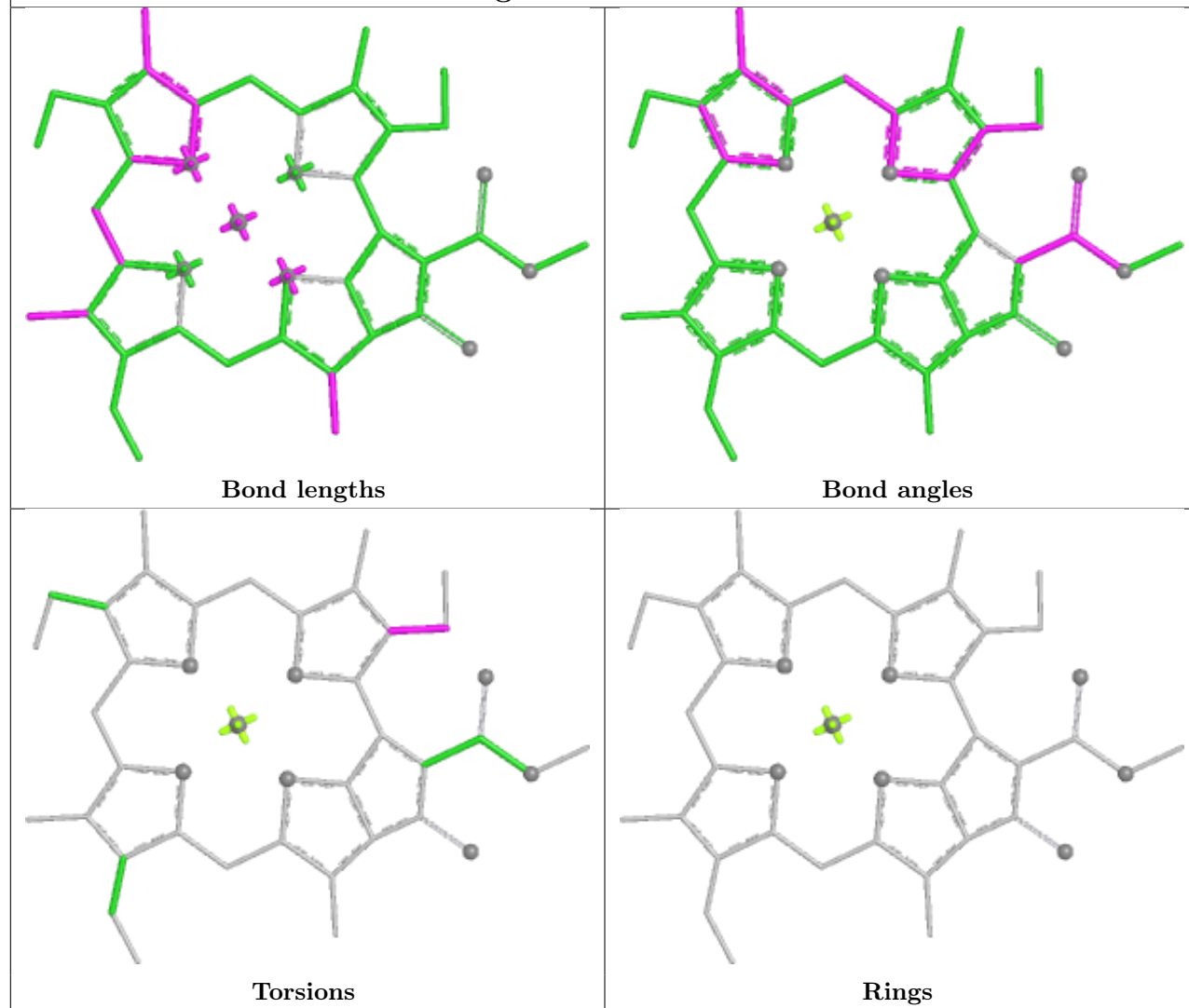
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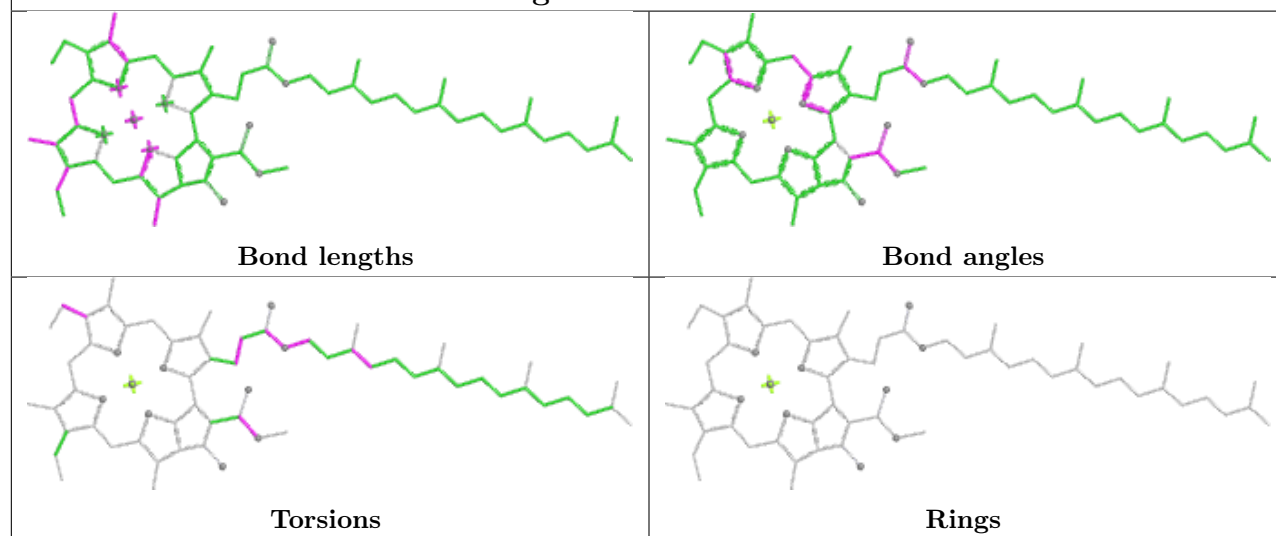




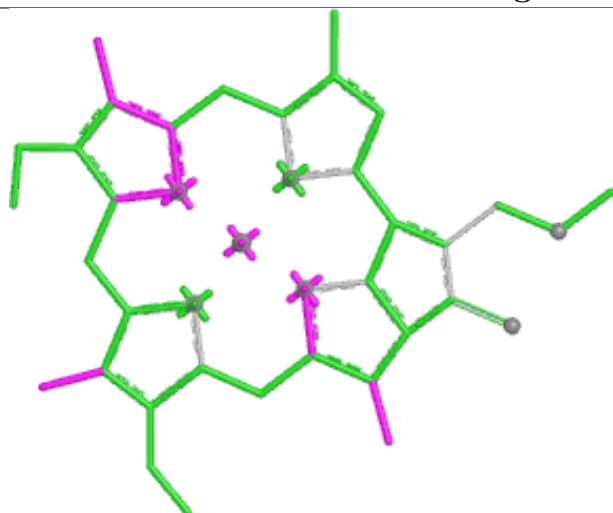
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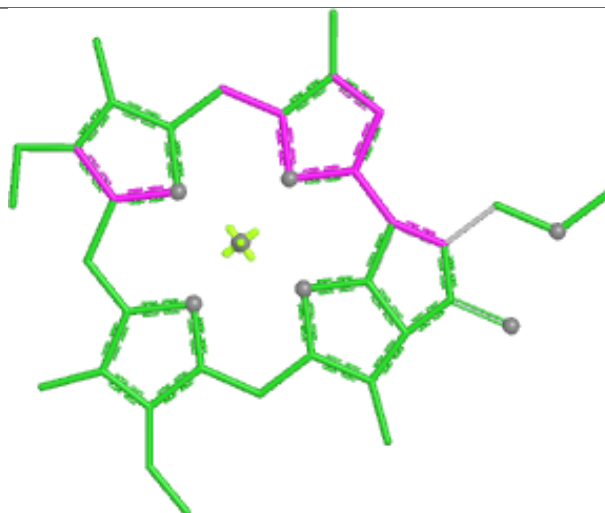
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Ligand CLA A 807



Bond lengths



Bond angles

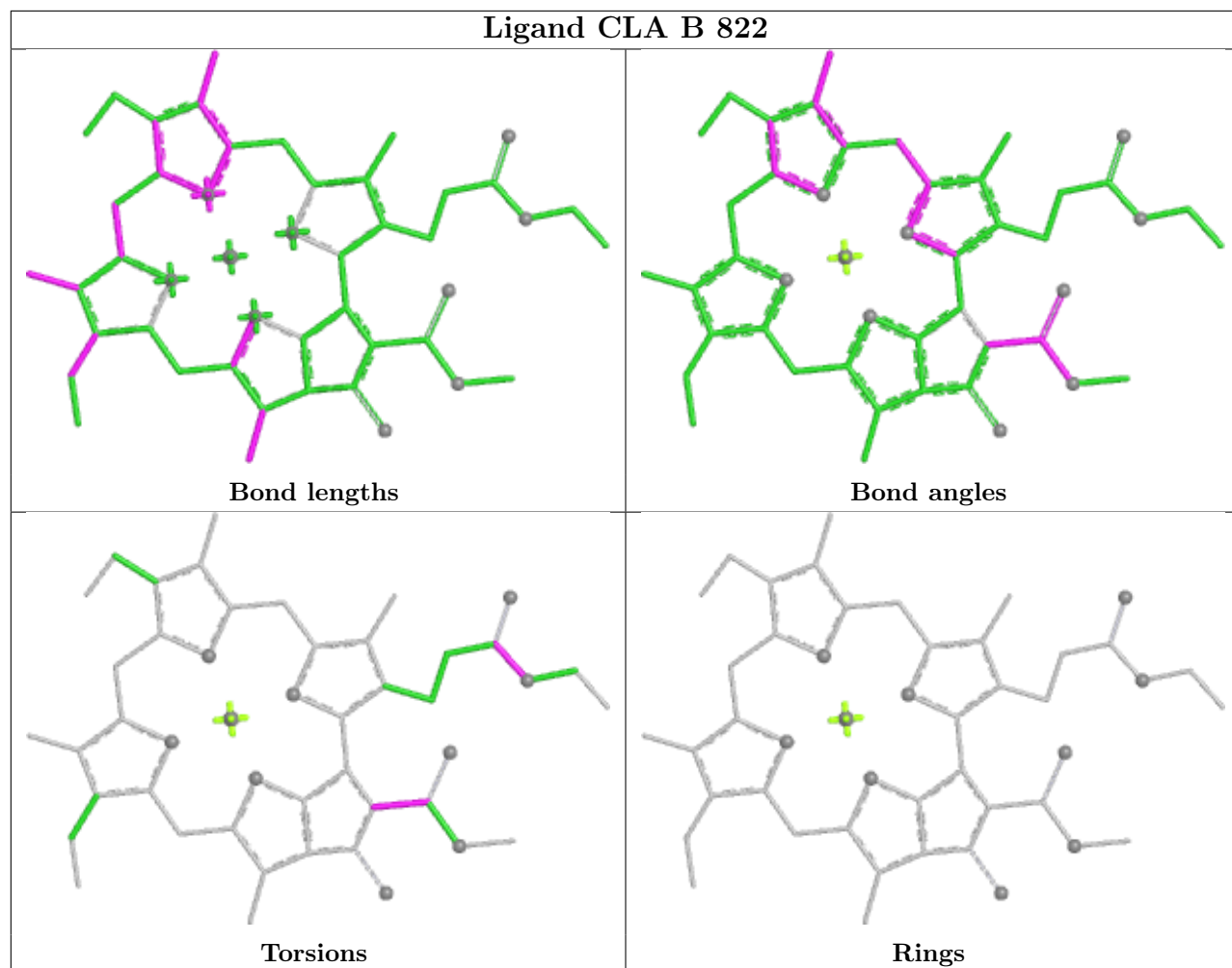


Torsions

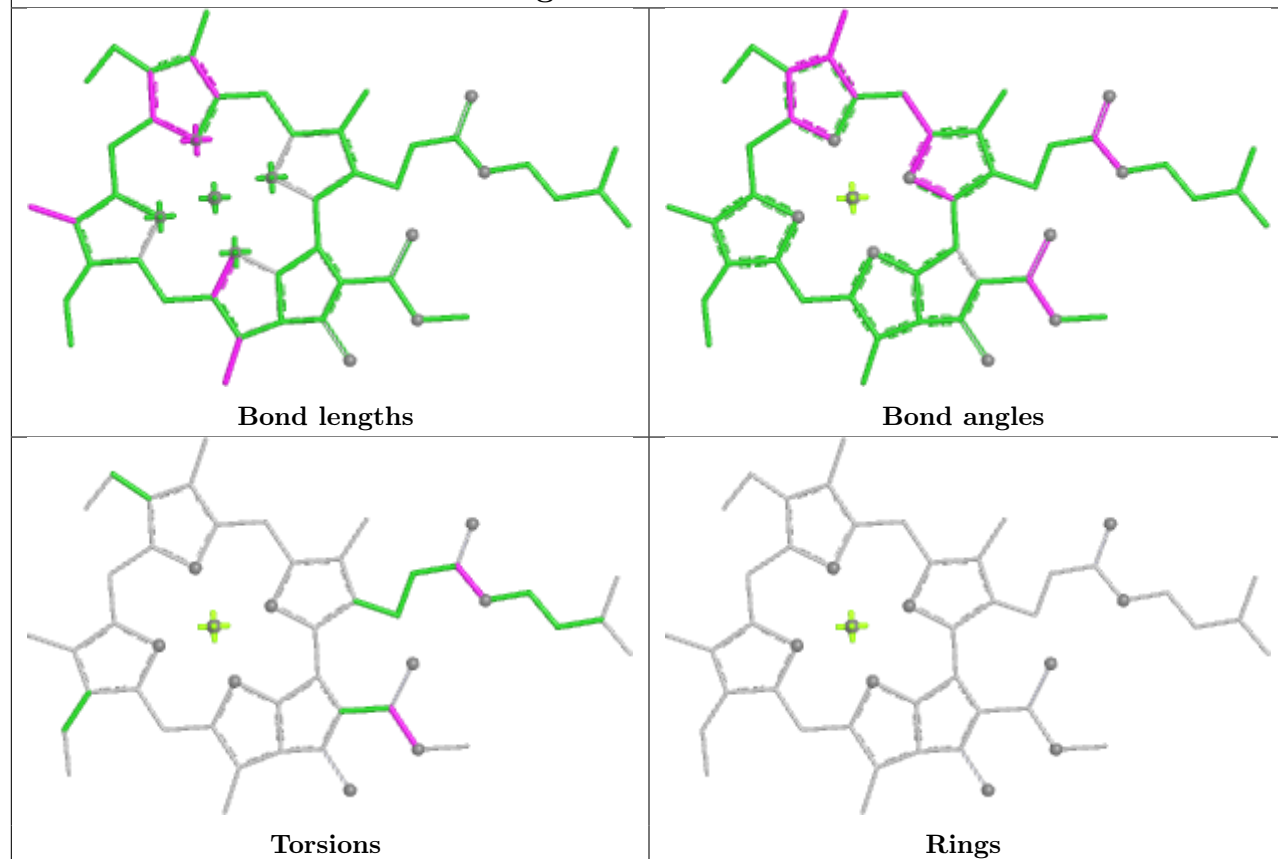


Rings

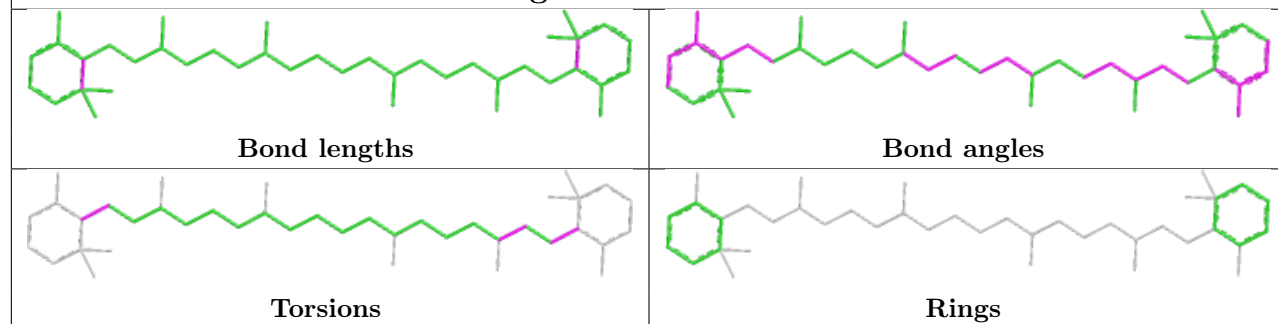
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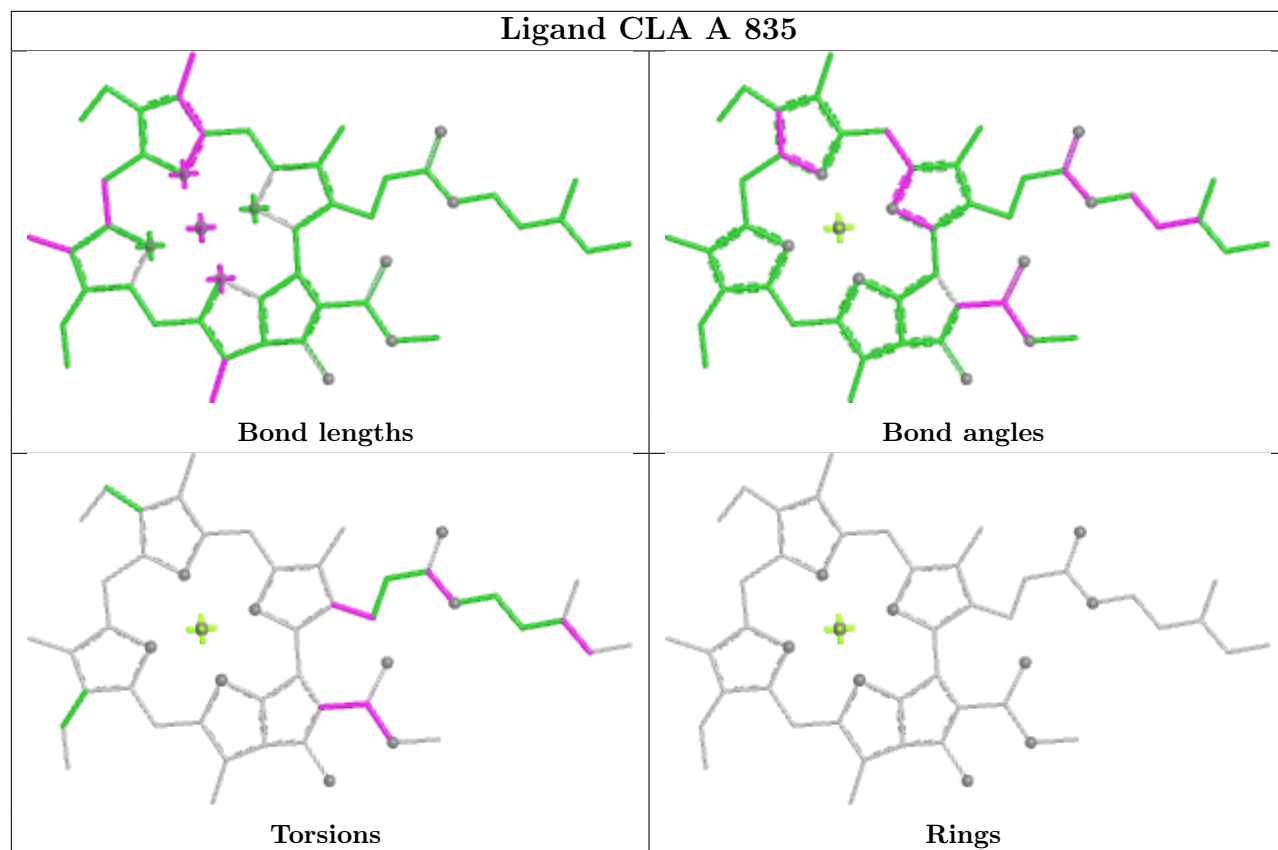
Ligand CLA 1 509



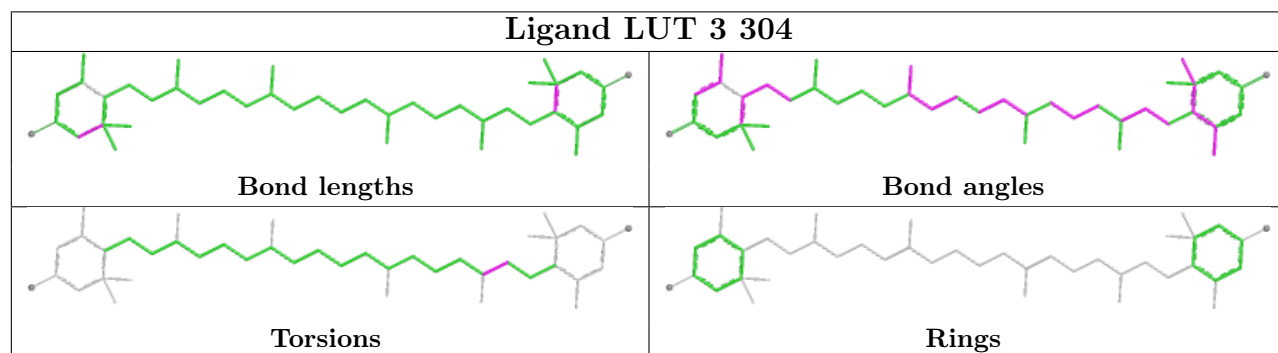
Ligand BCR A 848

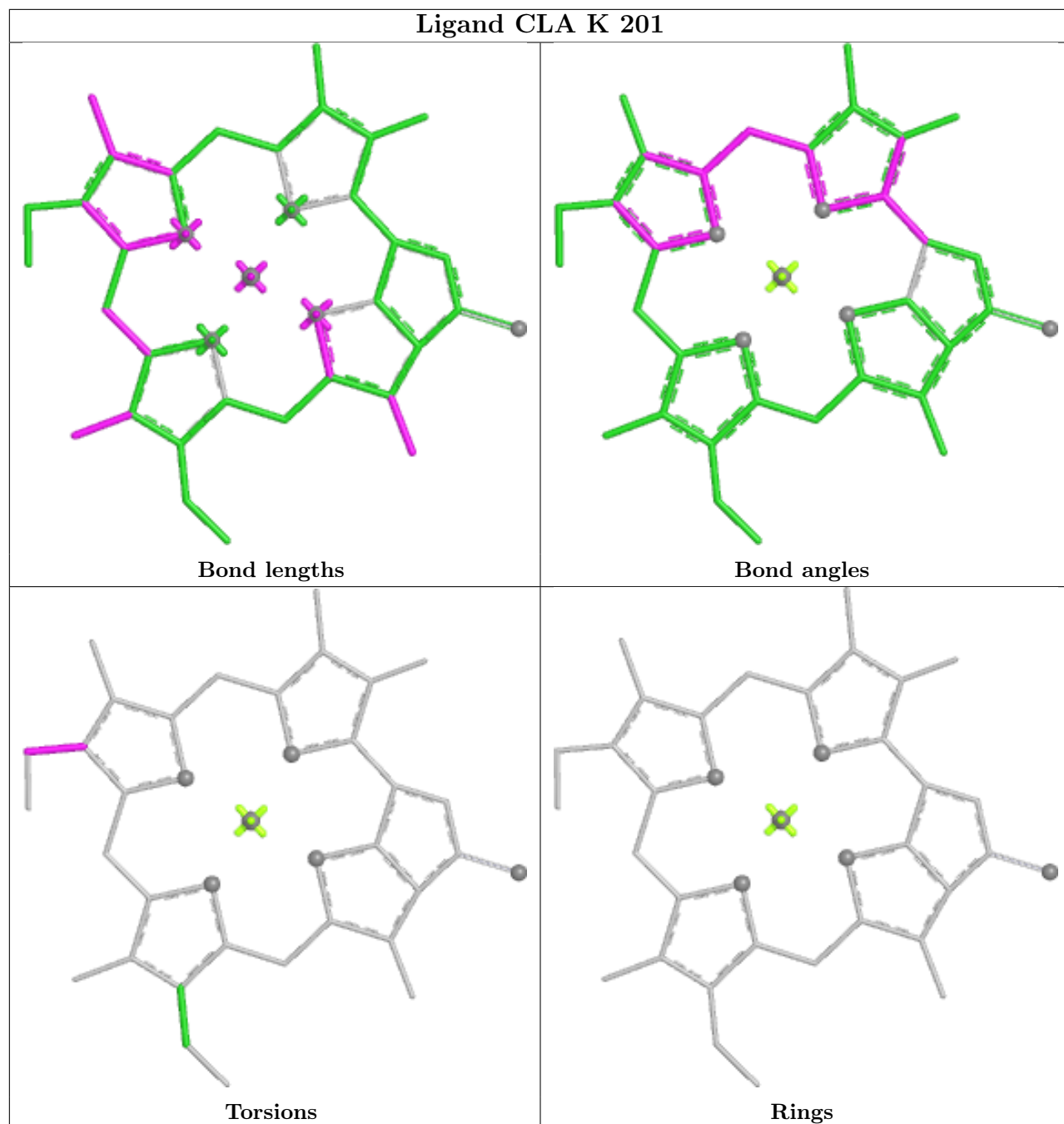


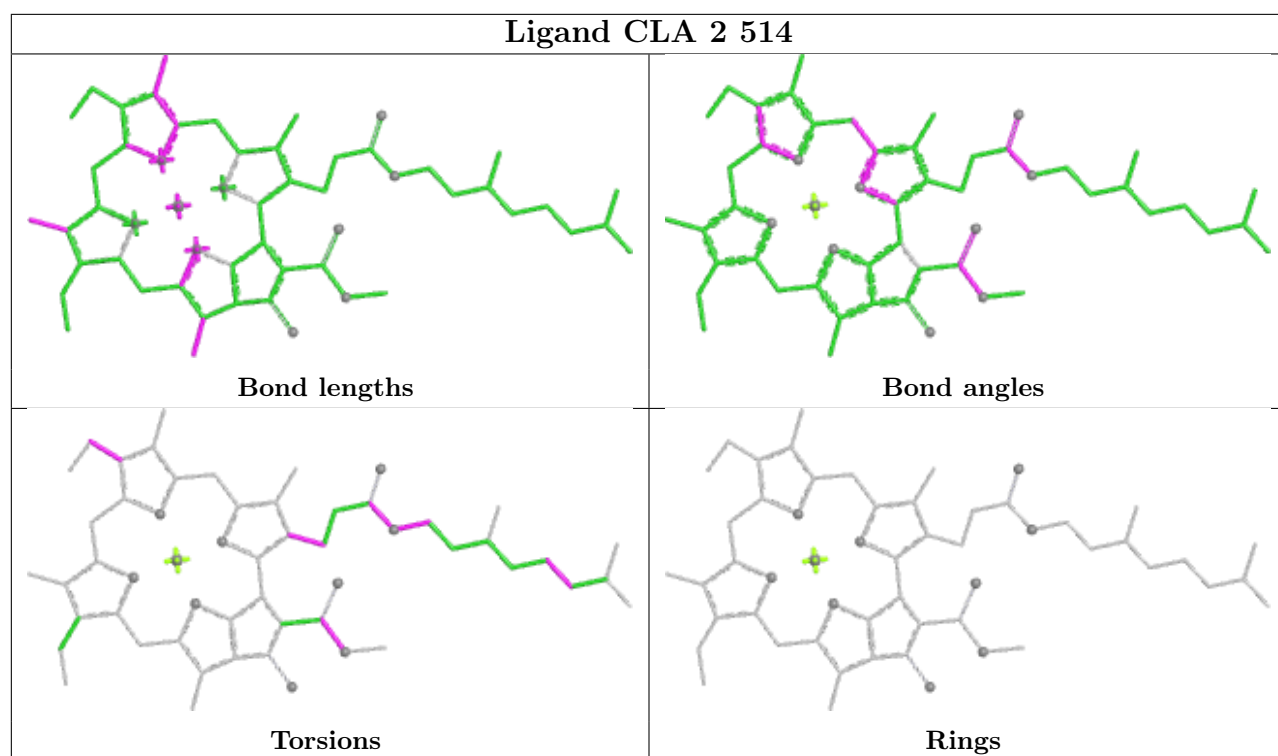
Ligand CLA A 835



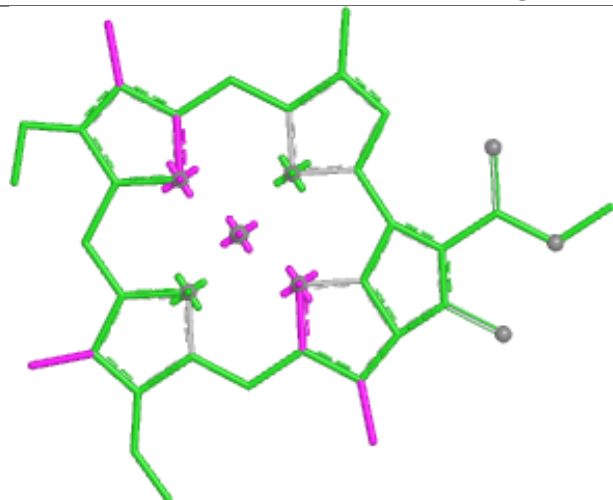
Ligand LUT 3 304



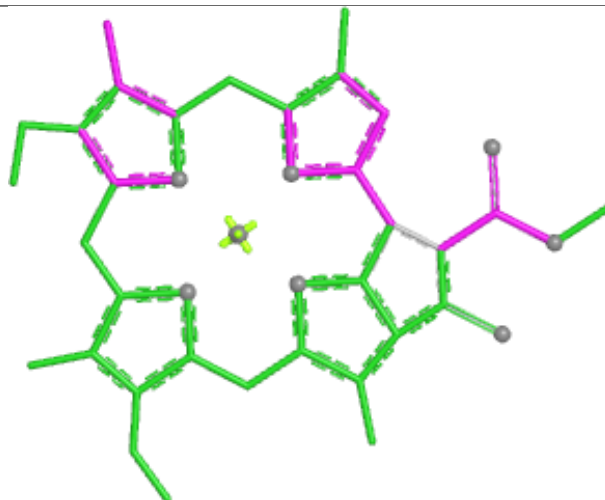




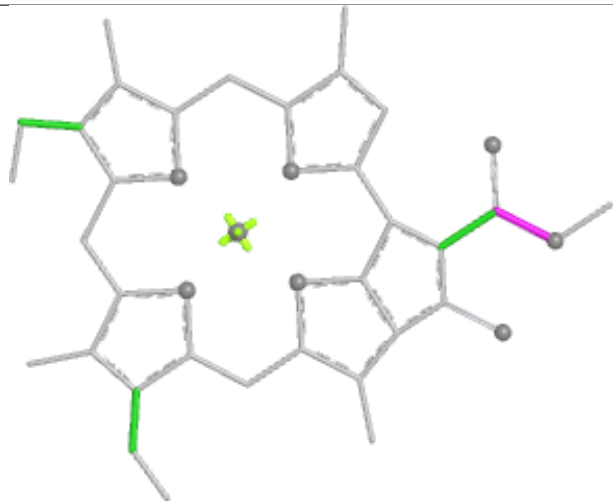
Ligand CLA A 818



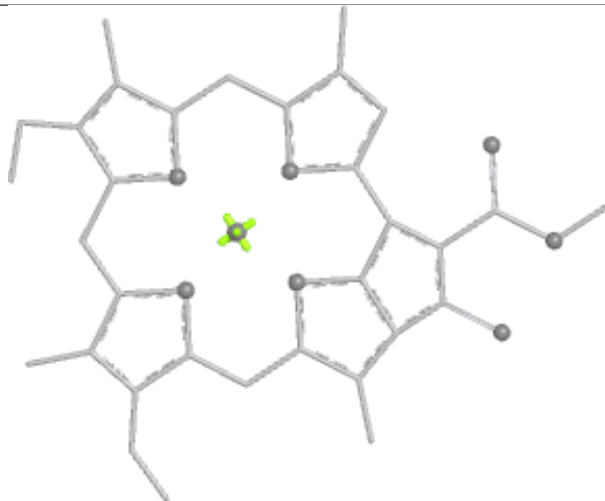
Bond lengths



Bond angles

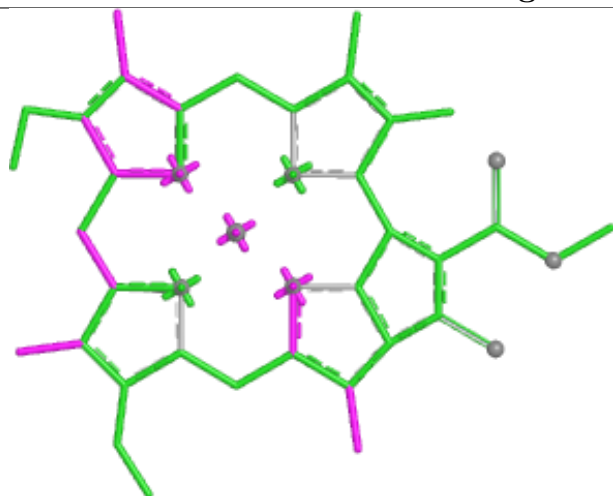


Torsions

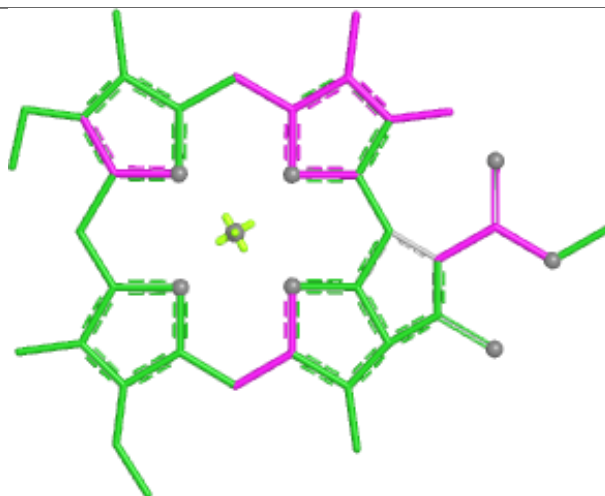


Rings

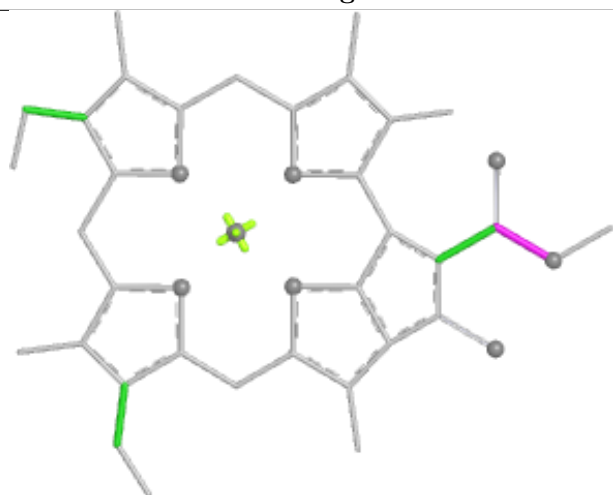
Ligand CLA 3 317



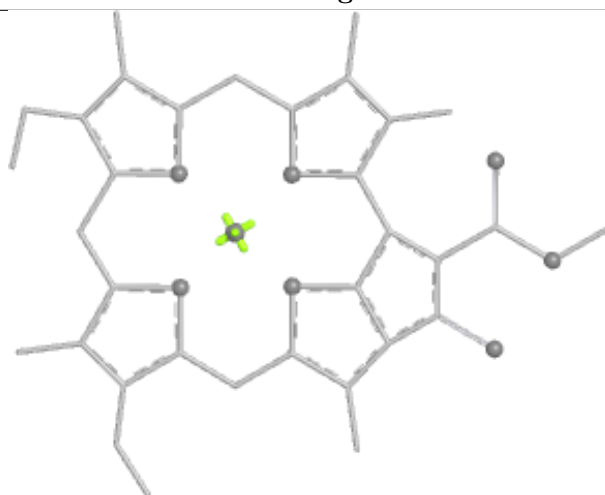
Bond lengths



Bond angles

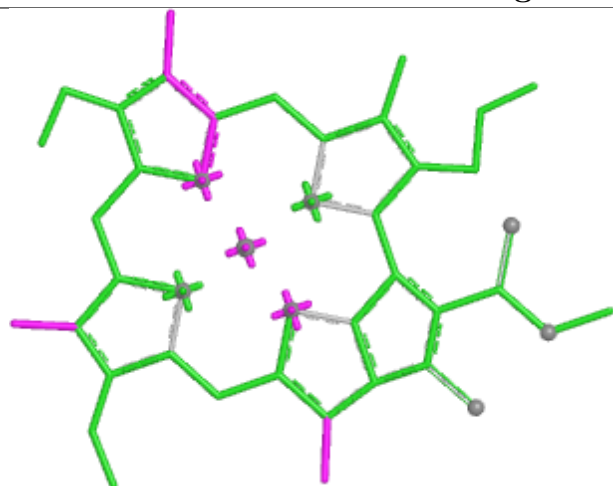


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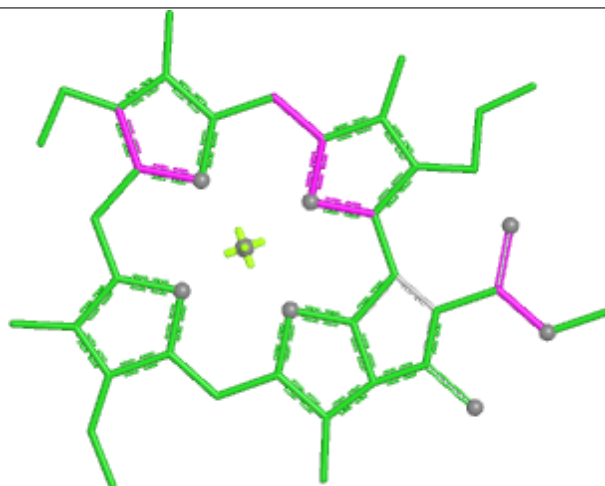


Rings

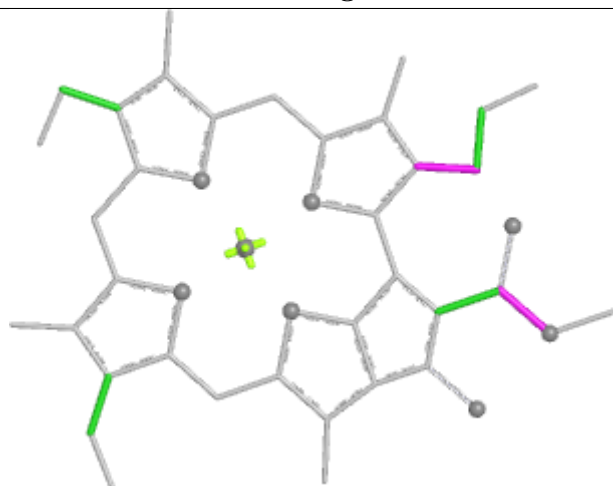
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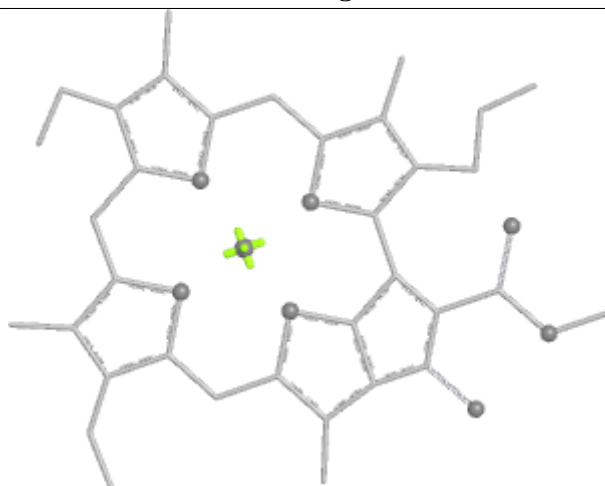
Bond lengths



Bond angles

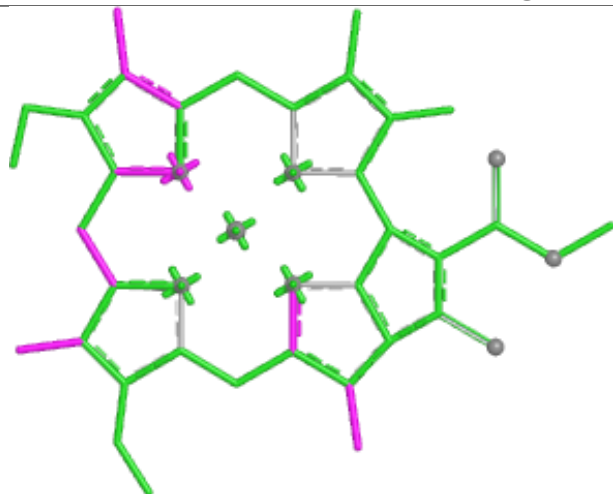


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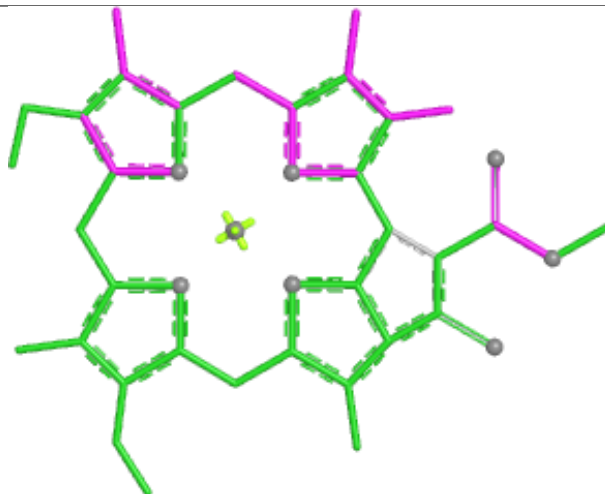


Rings

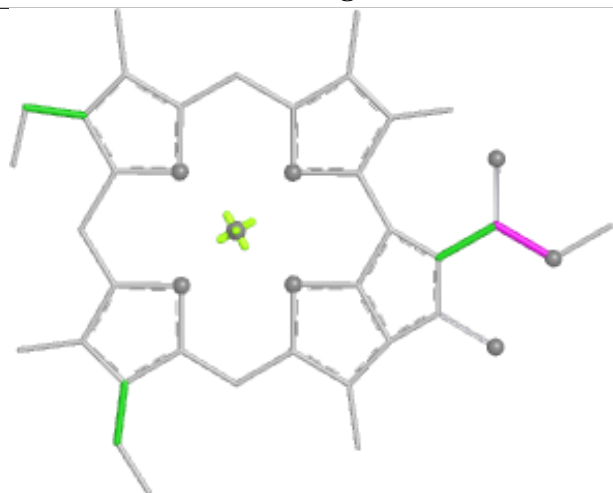
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Bond lengths



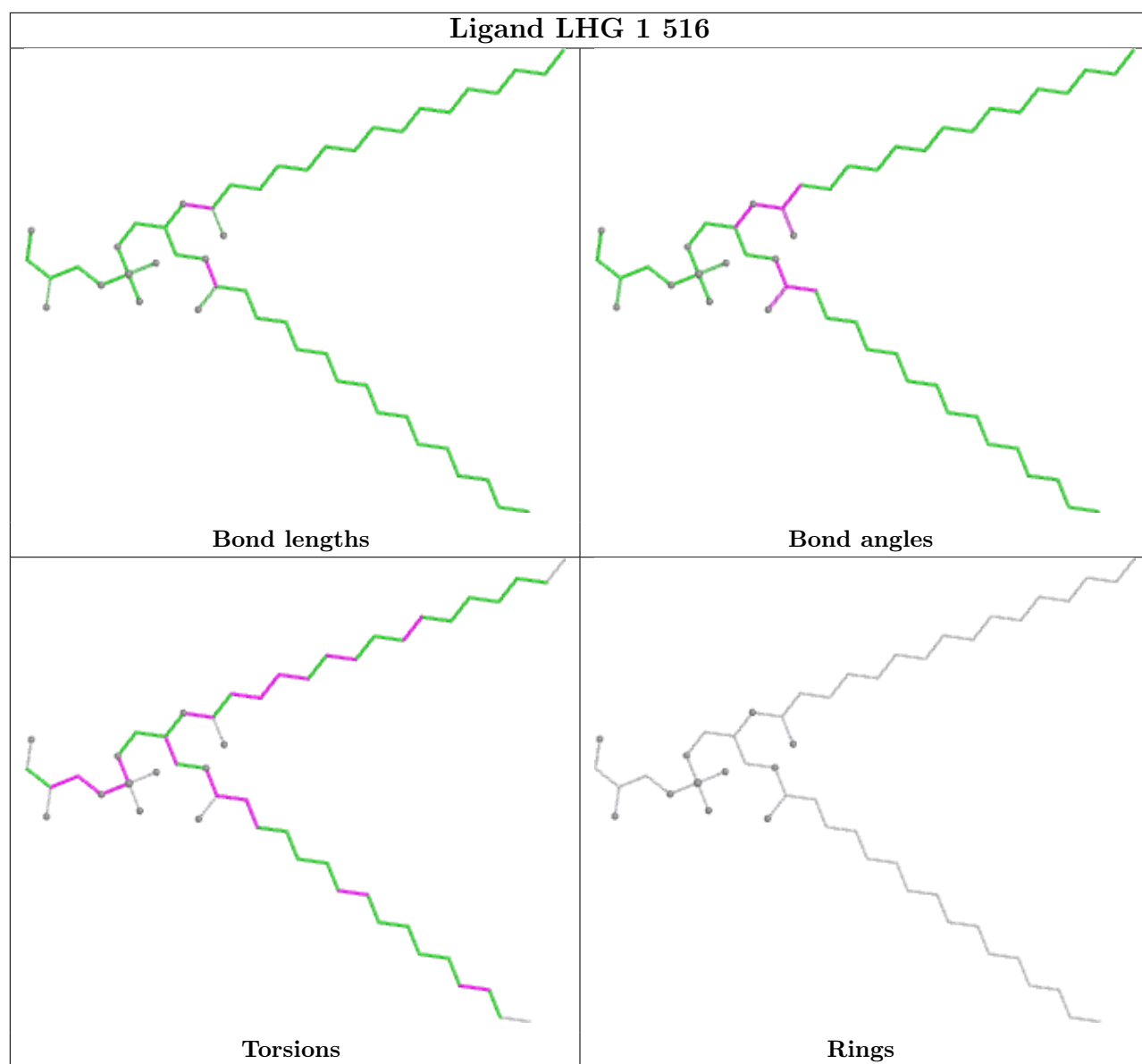
Bond angles



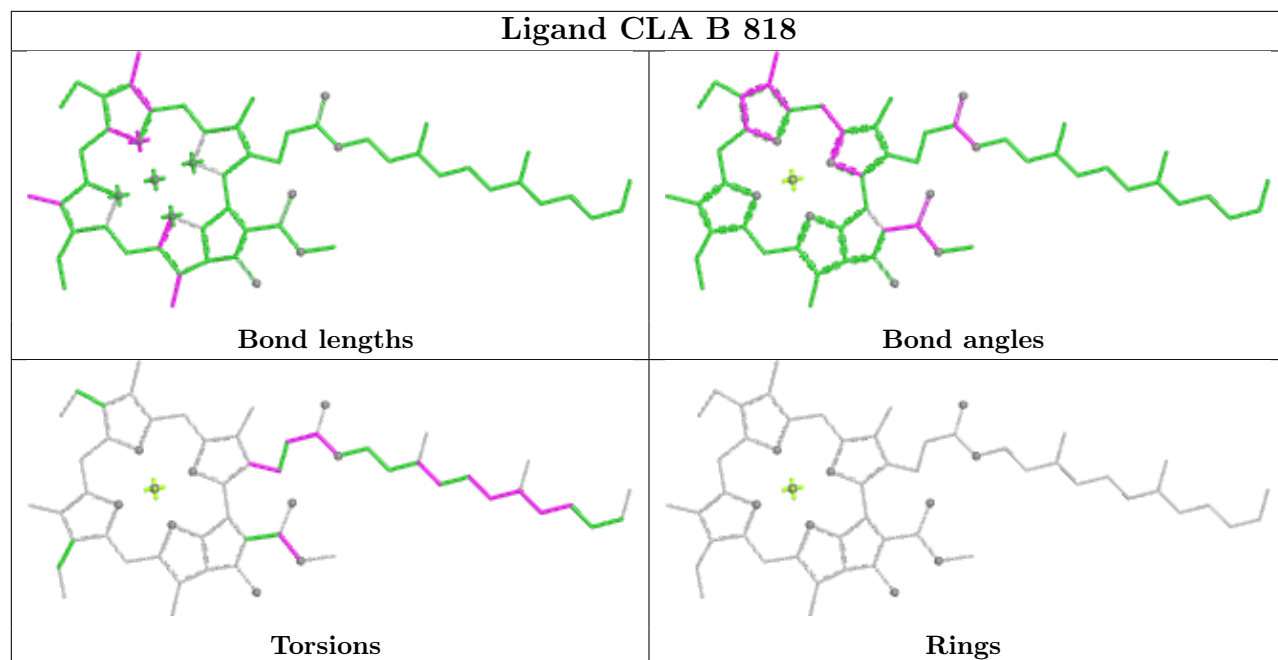
Torsions



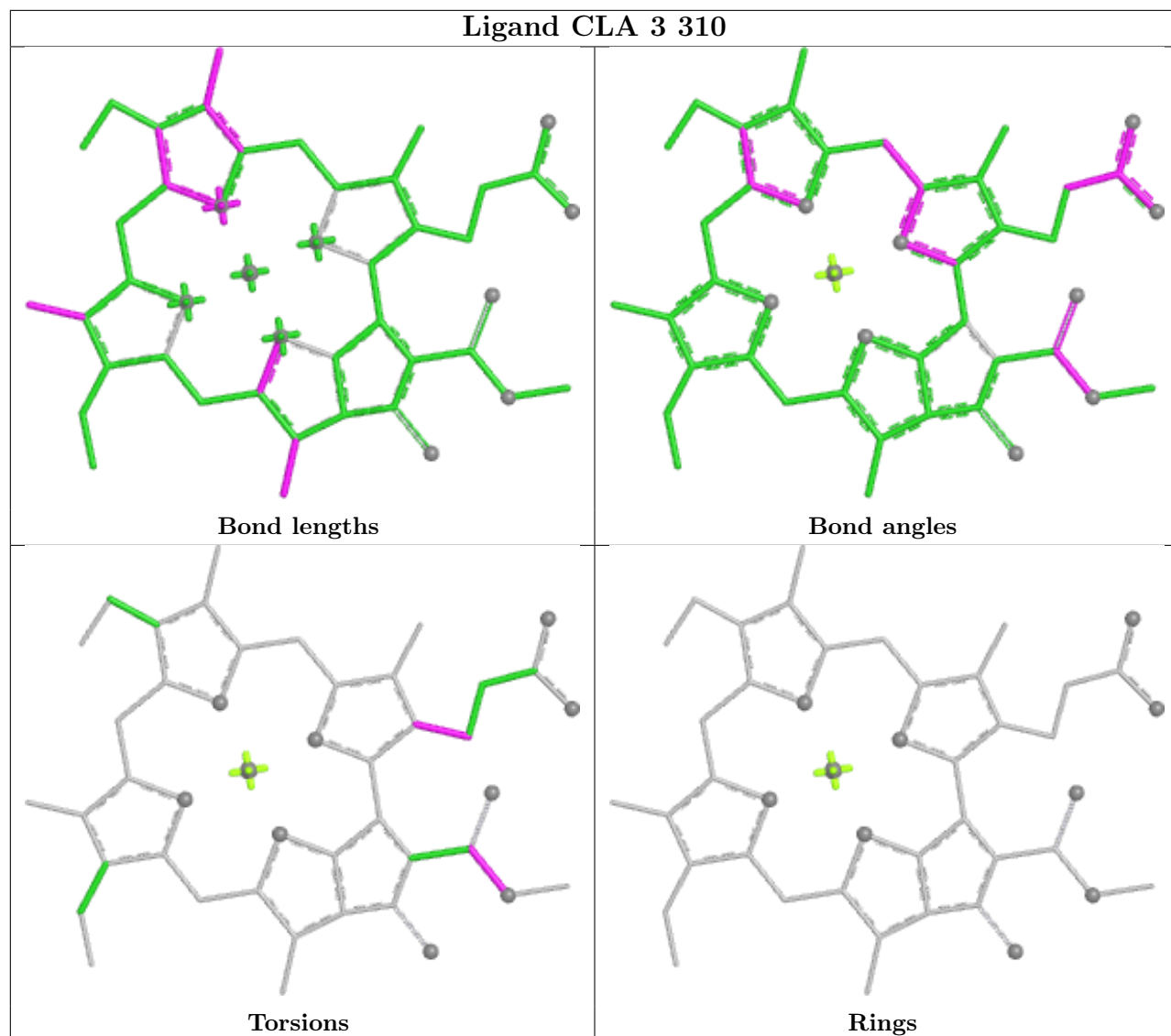
Rings



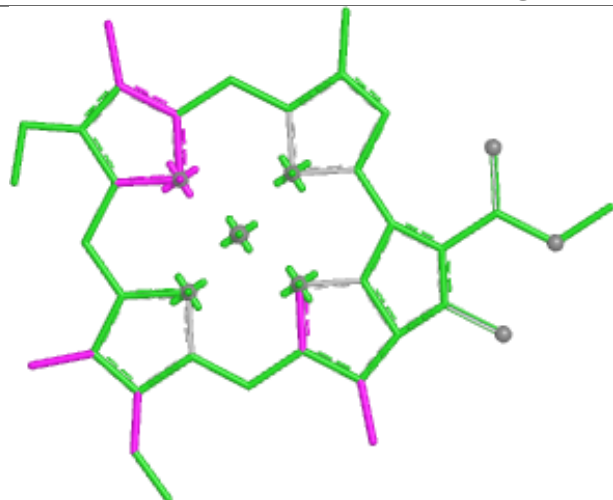
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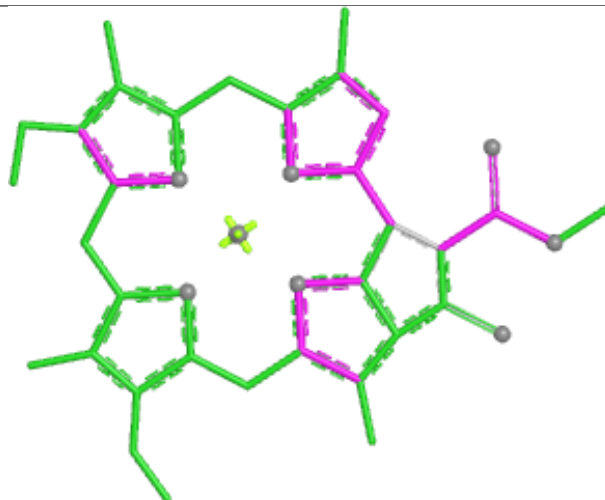
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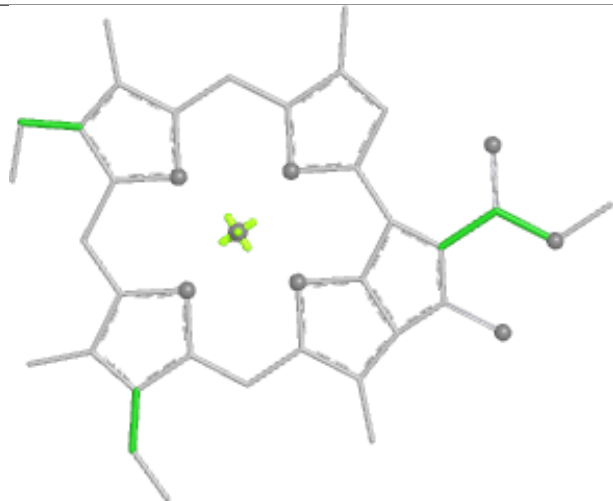
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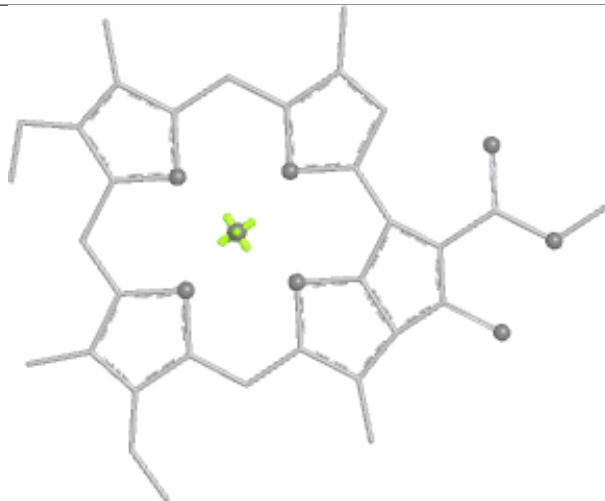
Bond lengths



Bond angles

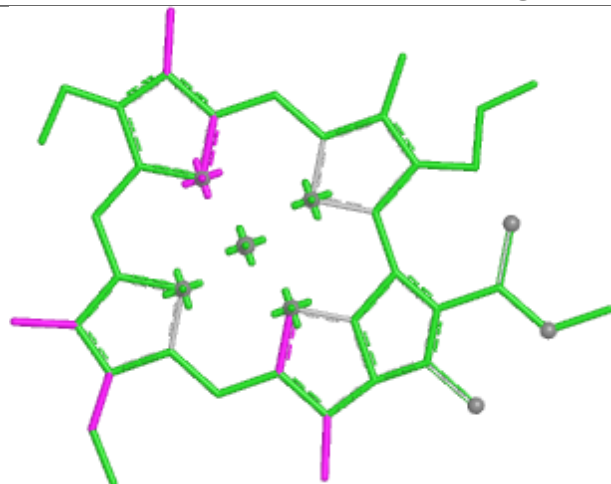


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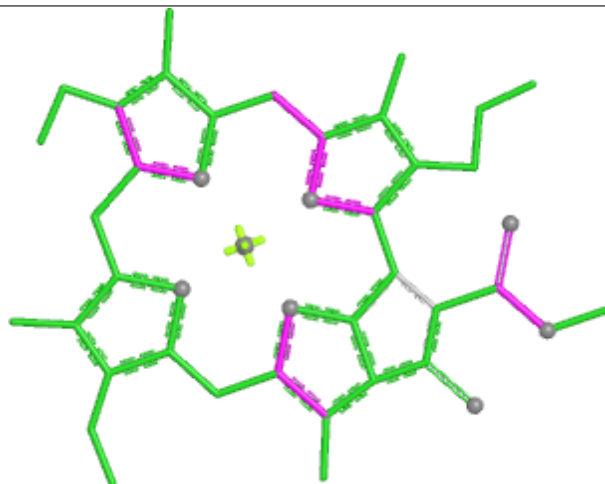


Rings

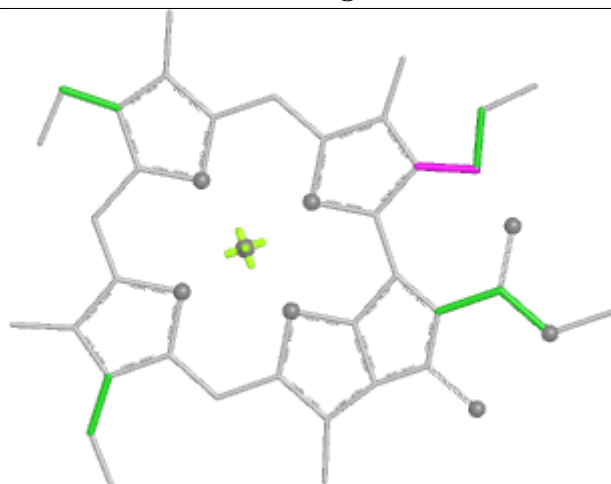
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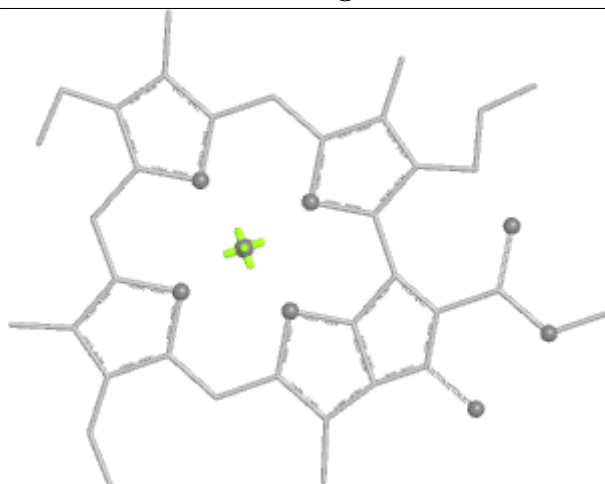
Bond lengths



Bond angles

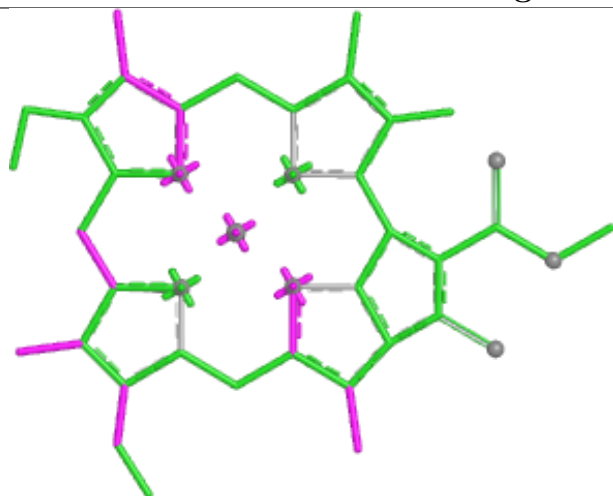


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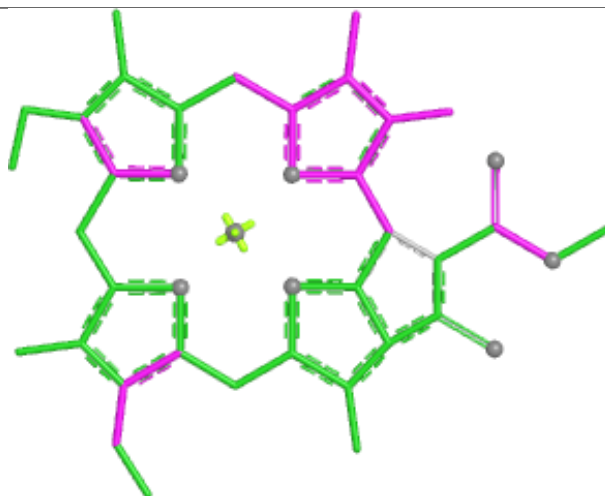


Rings

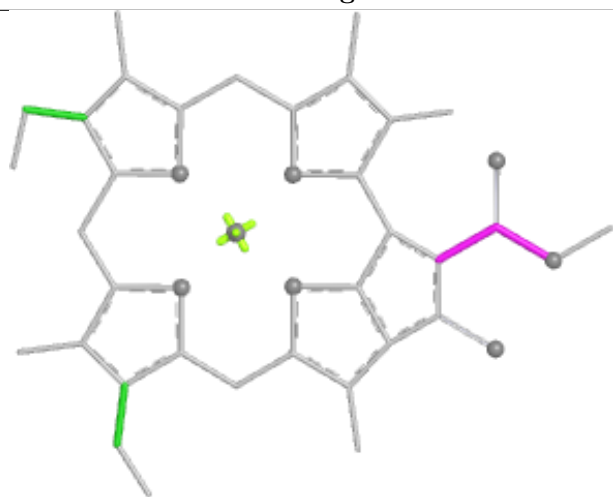
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Bond lengths



Bond angles

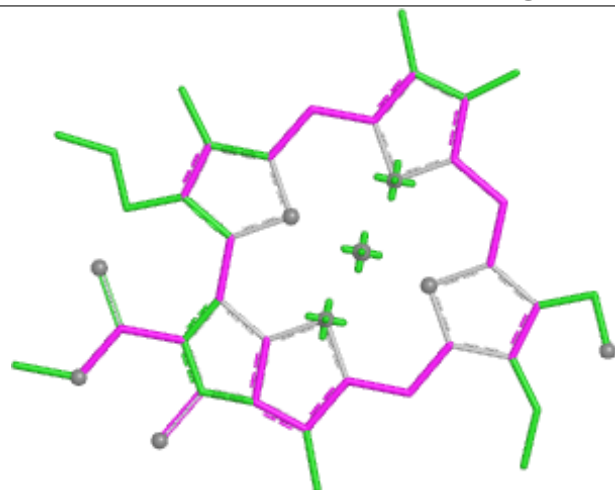


Torsions

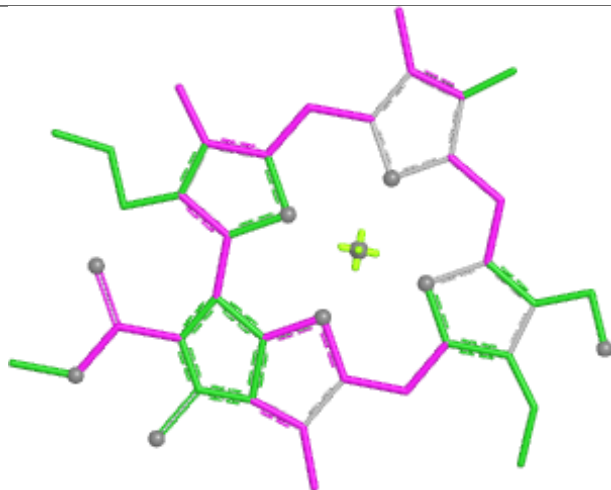


Rings

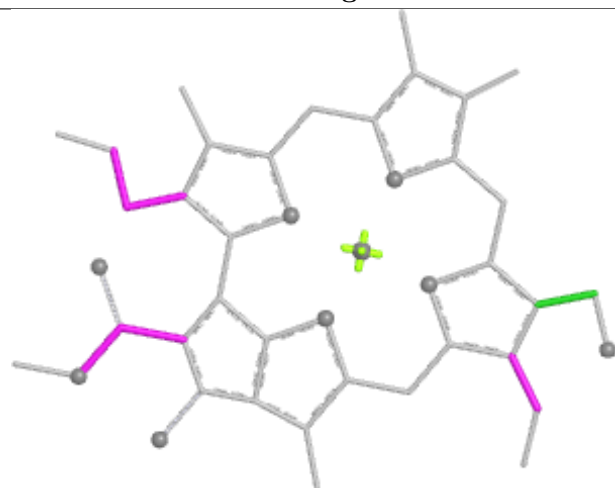
Ligand CHL 2 516



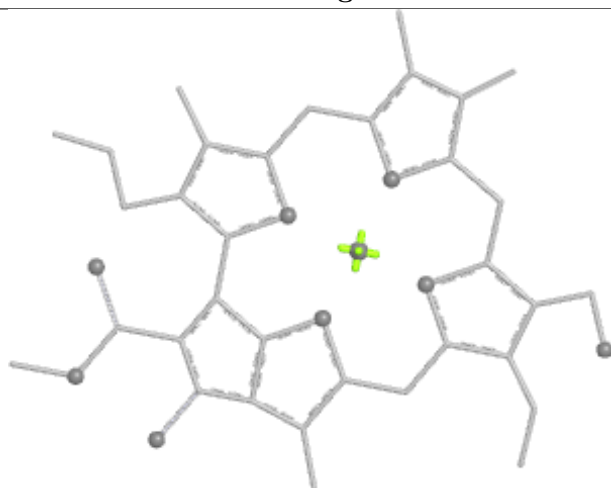
Bond lengths



Bond angles

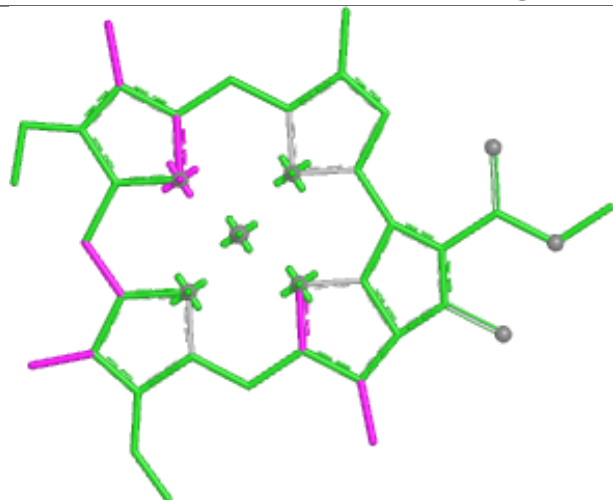


Torsions

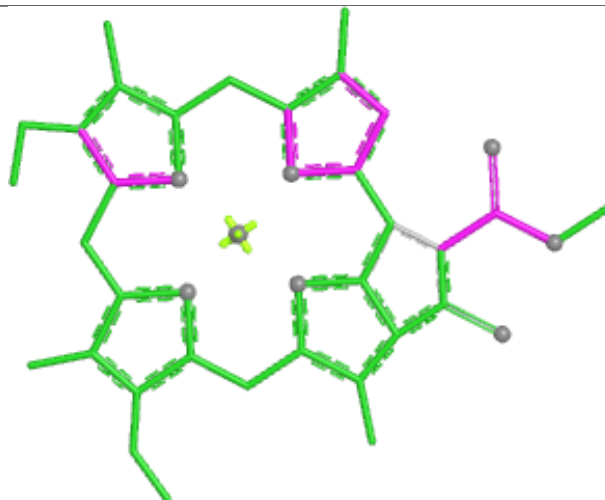


Rings

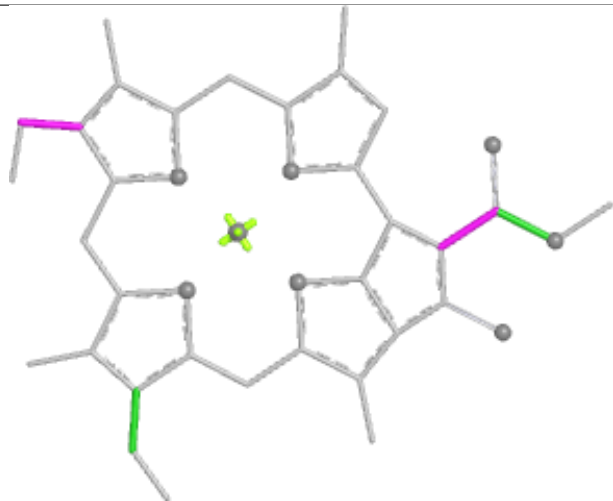
Ligand CLA A 819



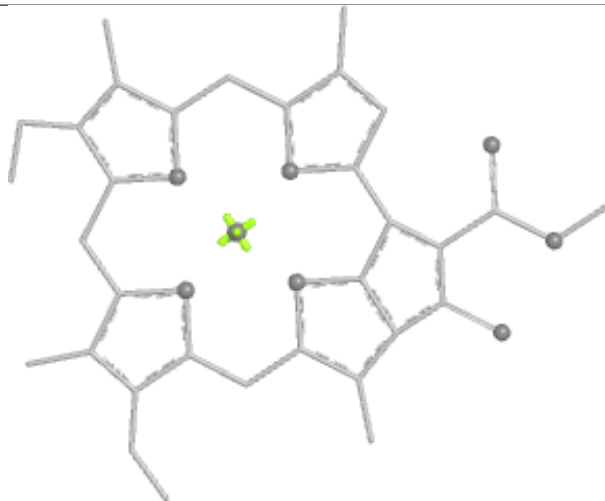
Bond lengths



Bond angles

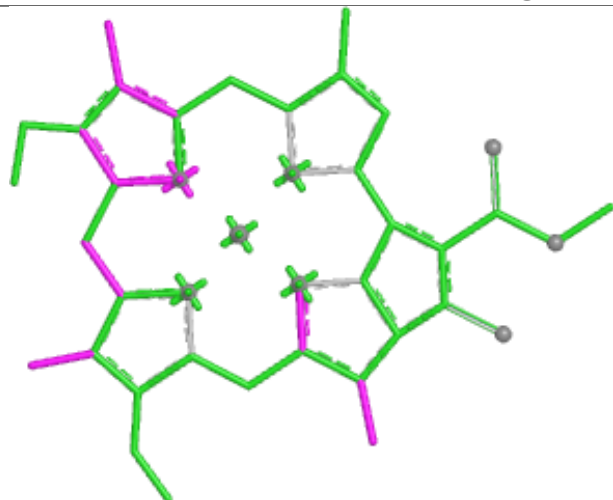


Torsions

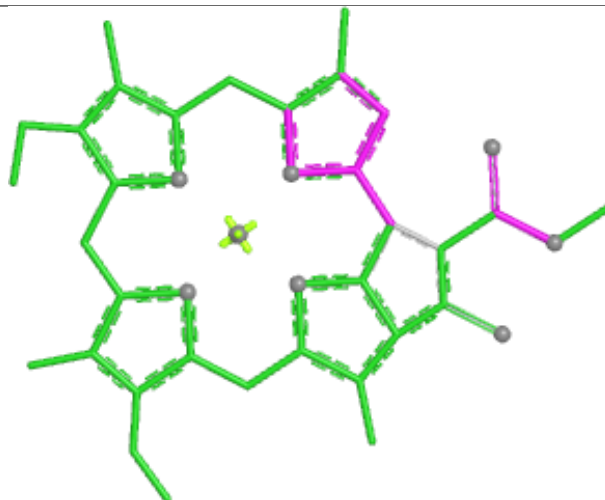


Rings

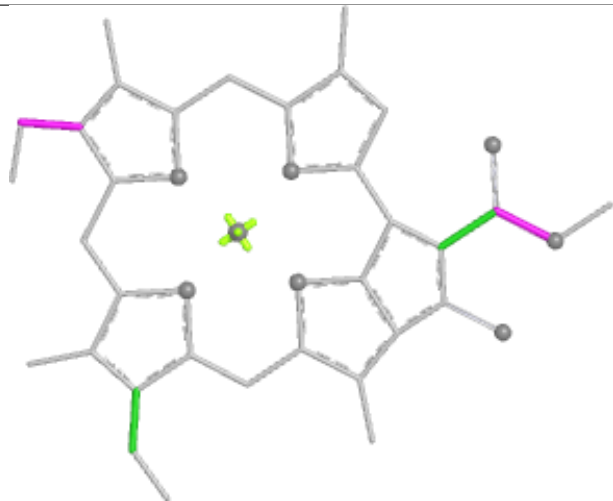
Ligand CLA 3 307



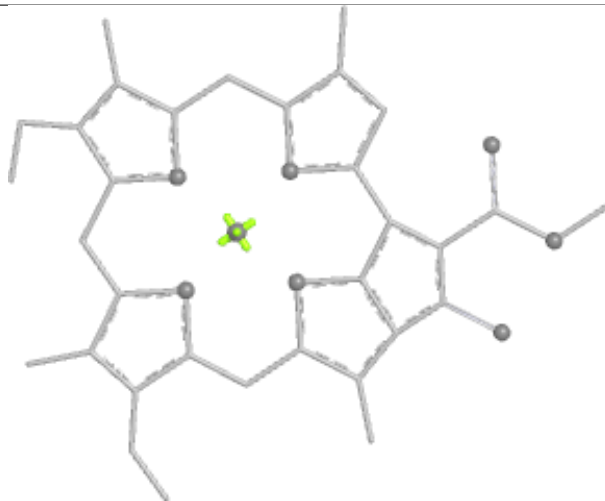
Bond lengths



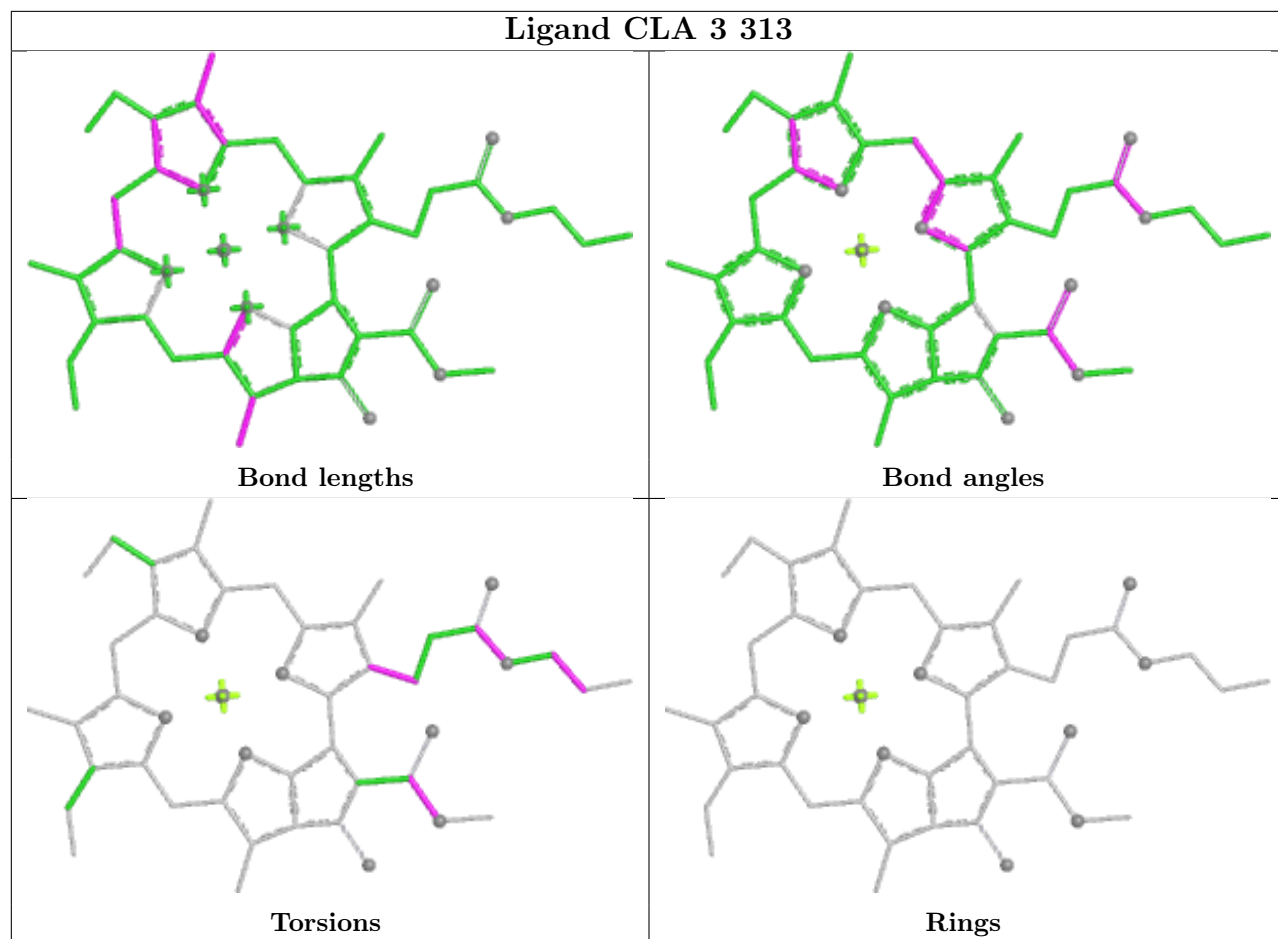
Bond angles



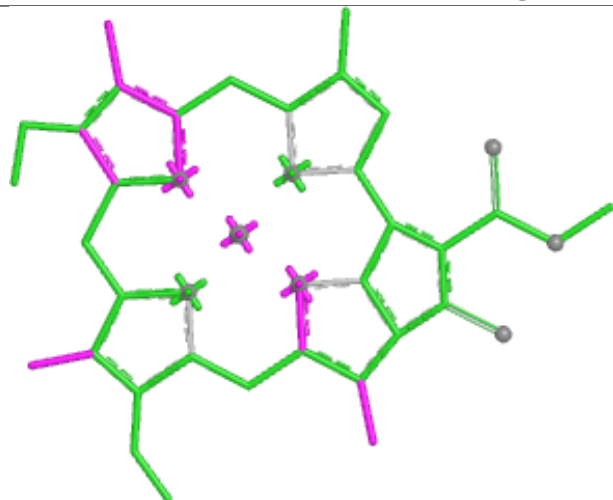
Torsions



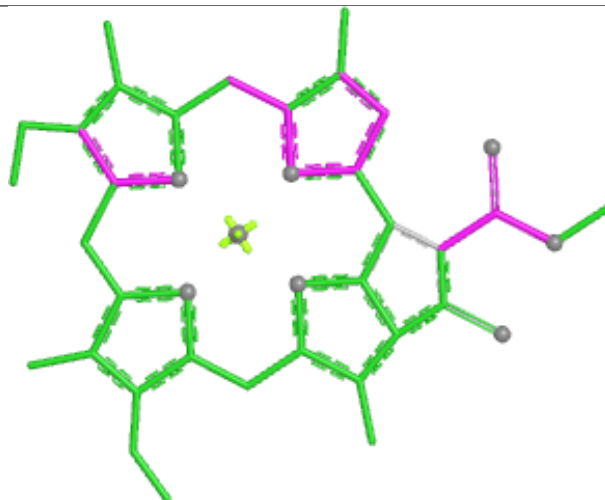
Rings



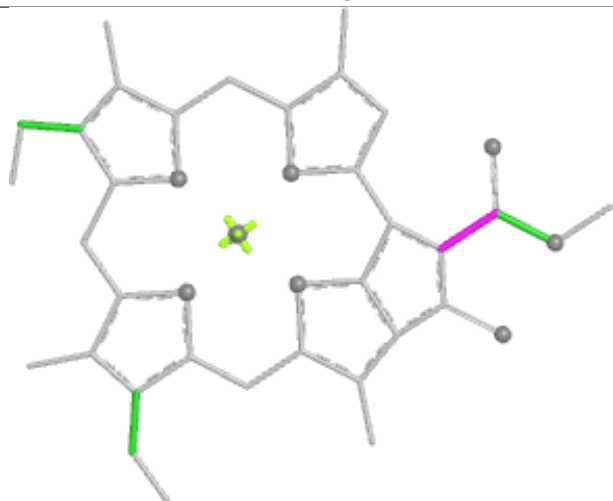
Ligand CLA A 833



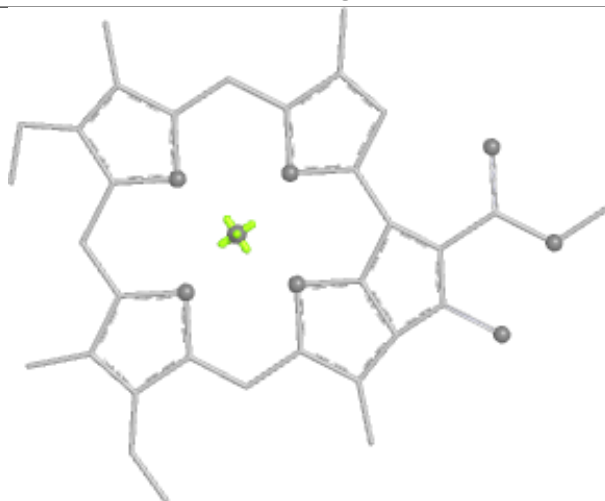
Bond lengths



Bond angles

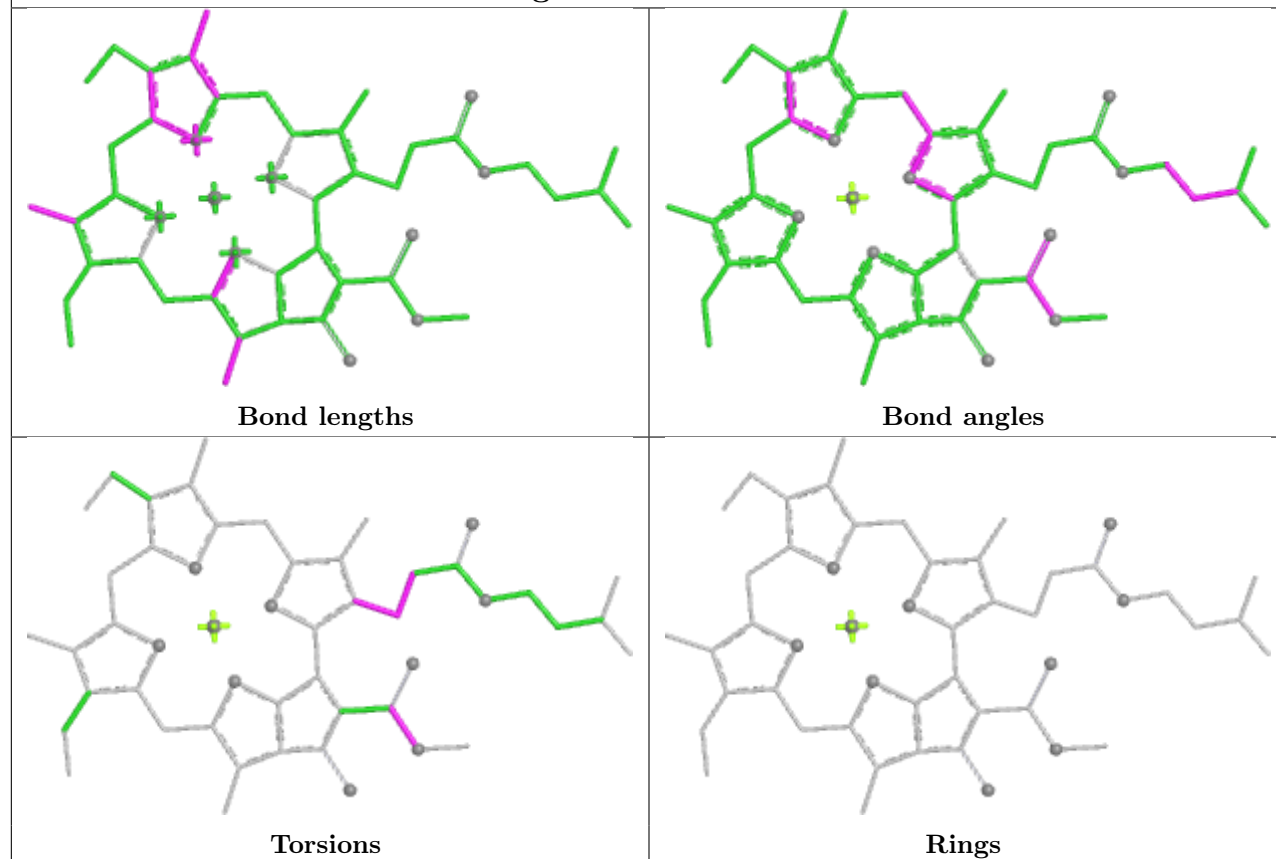


Torsions

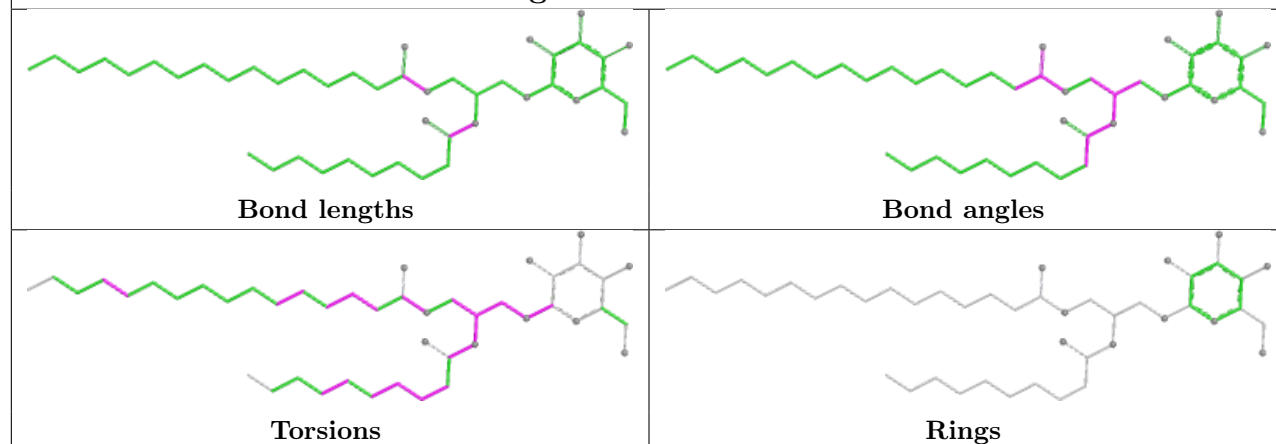


Rings

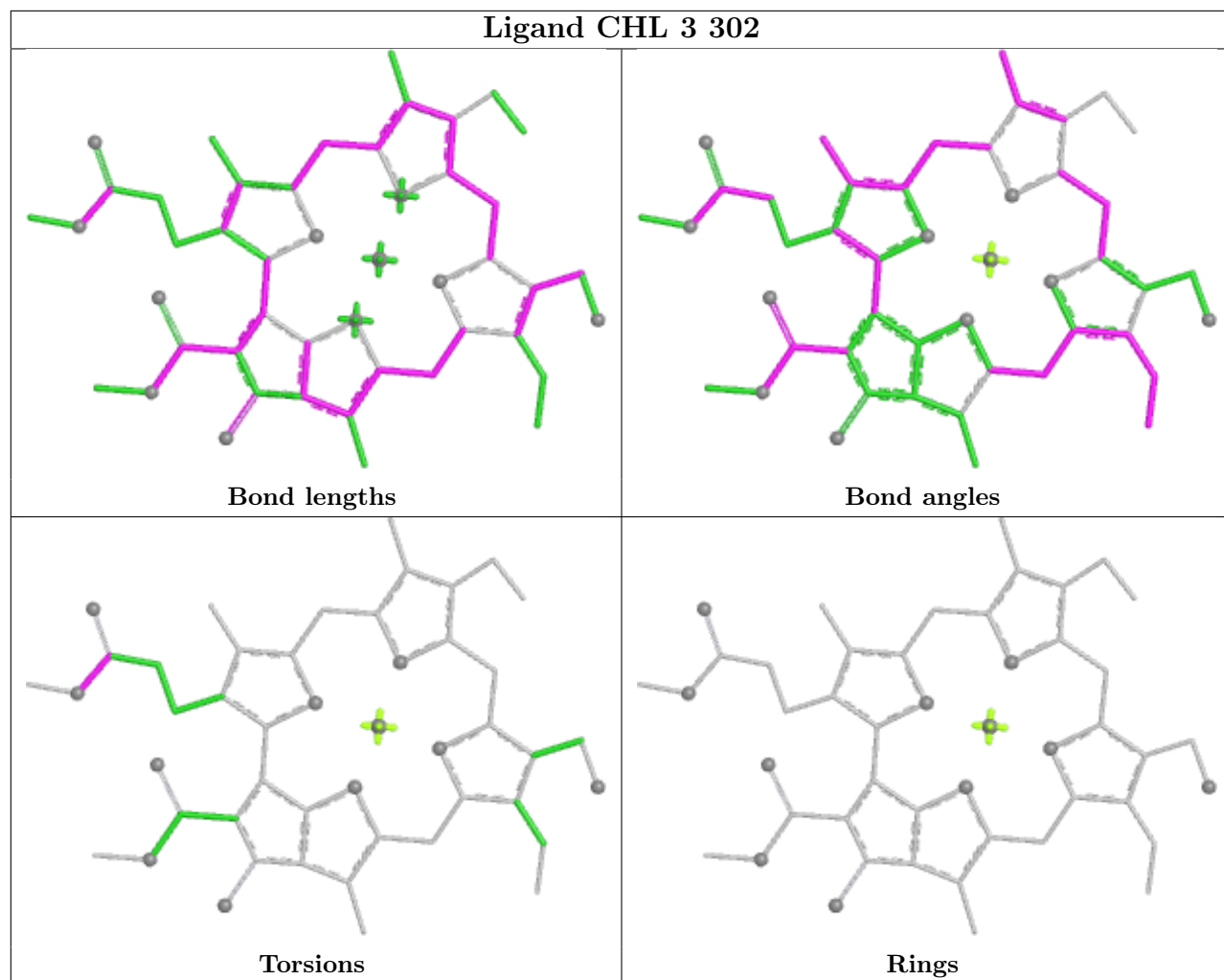
Ligand CLA B 821



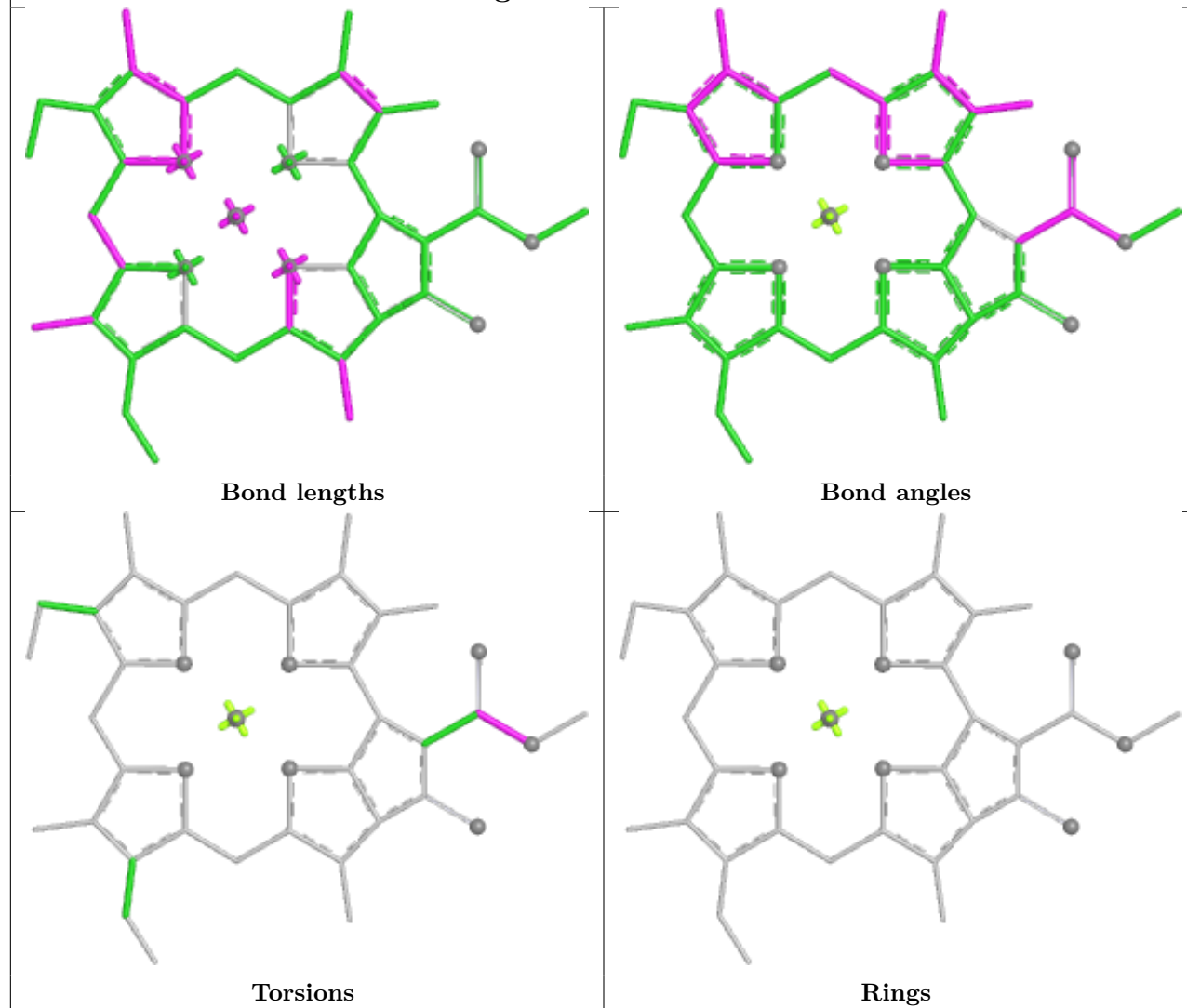
Ligand LMG F 806



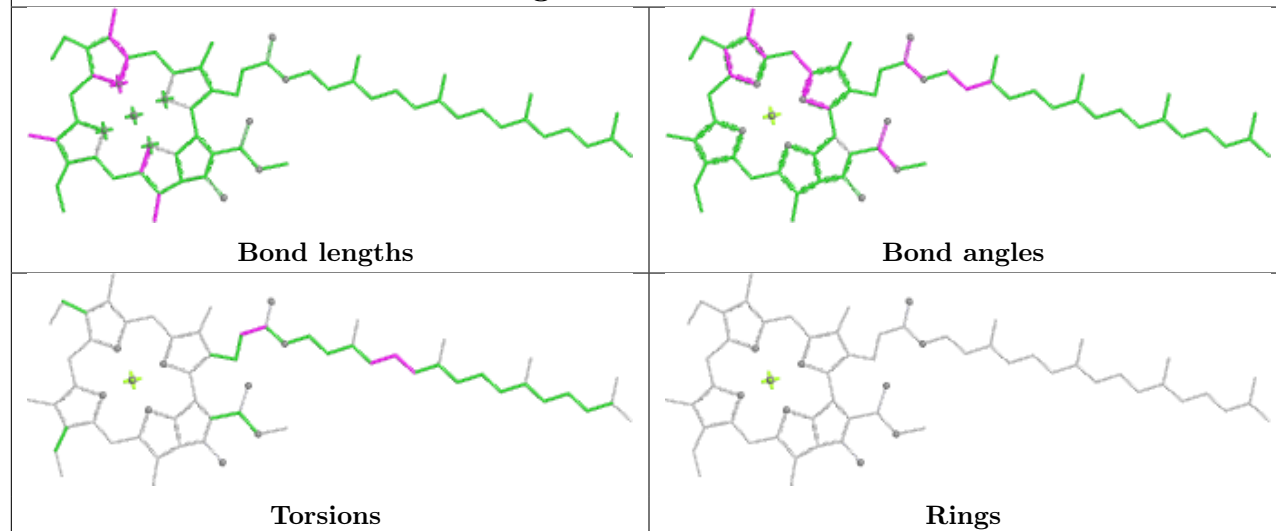
Ligand CHL 3 302

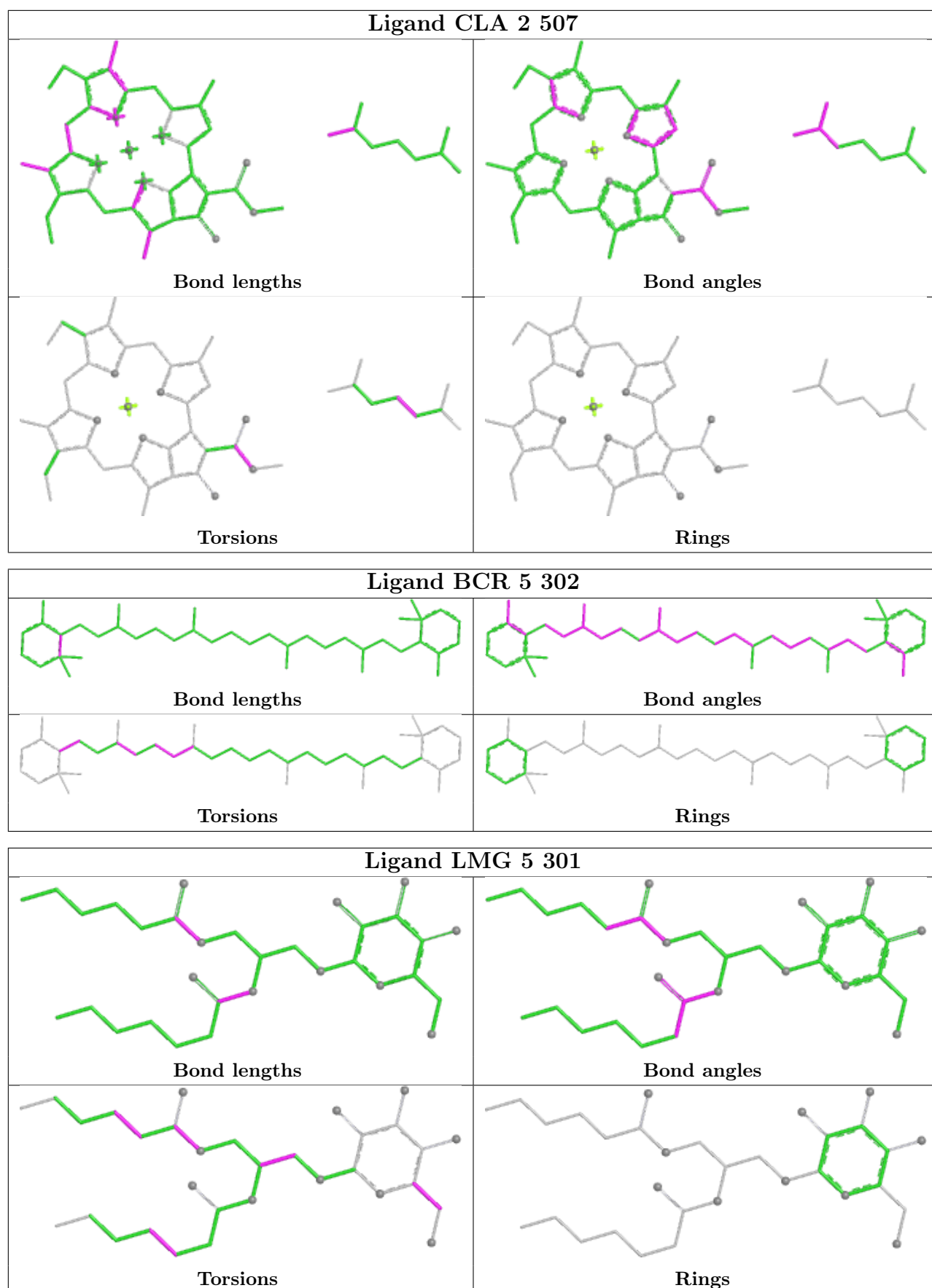


Ligand CLA A 837

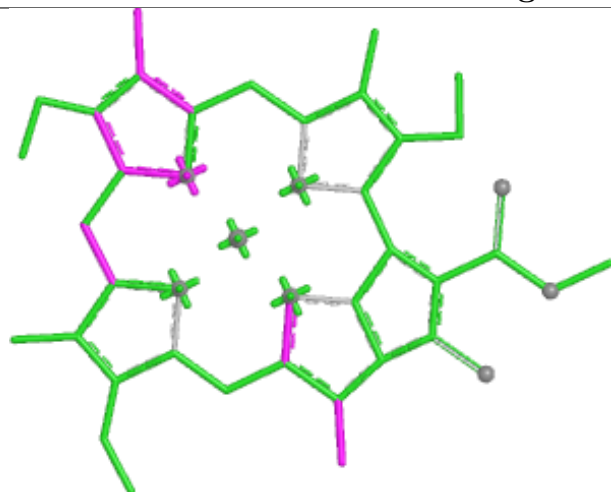


Ligand CLA B 833

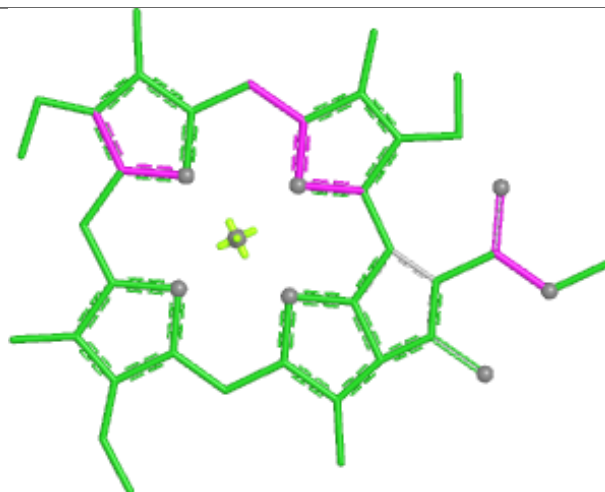




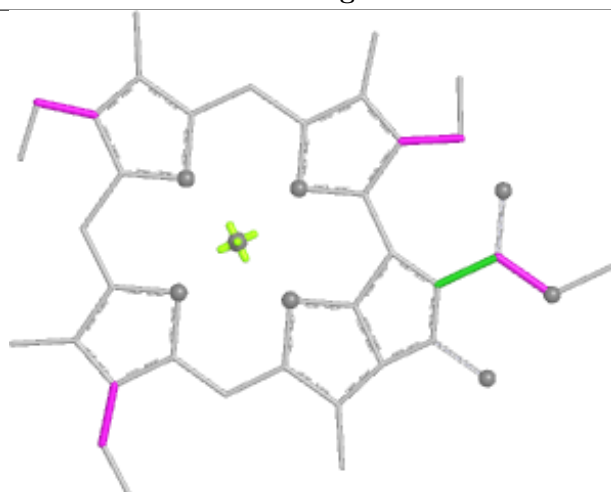
Ligand CLA J 101



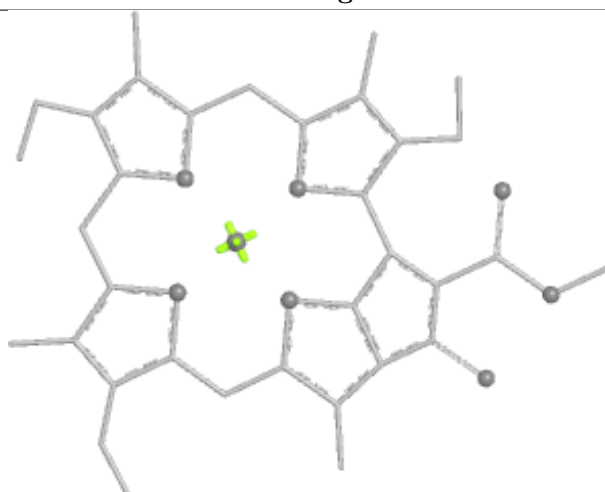
Bond lengths



Bond angles

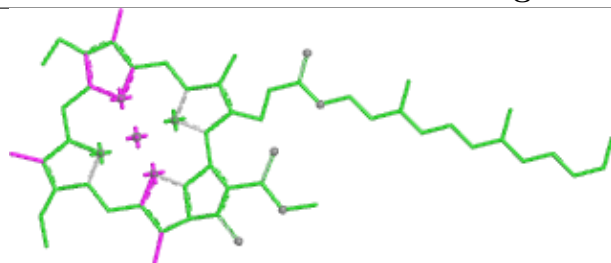


Torsions

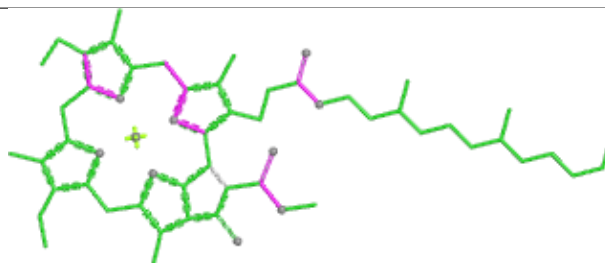


Rings

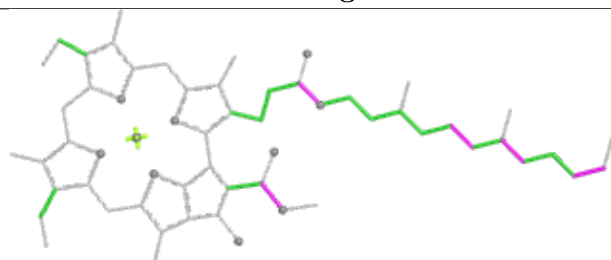
Ligand CLA A 825



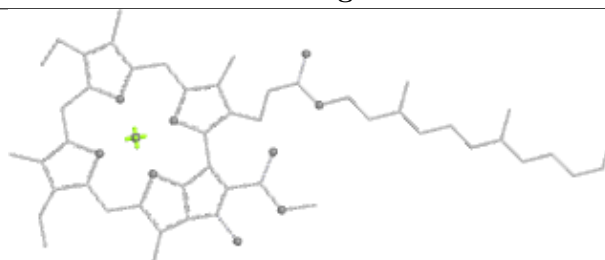
Bond lengths



Bond angles

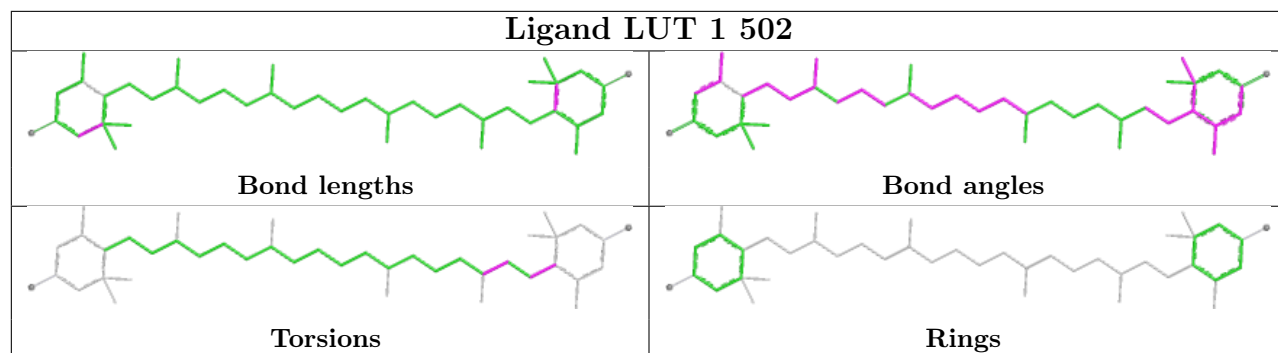


Torsions

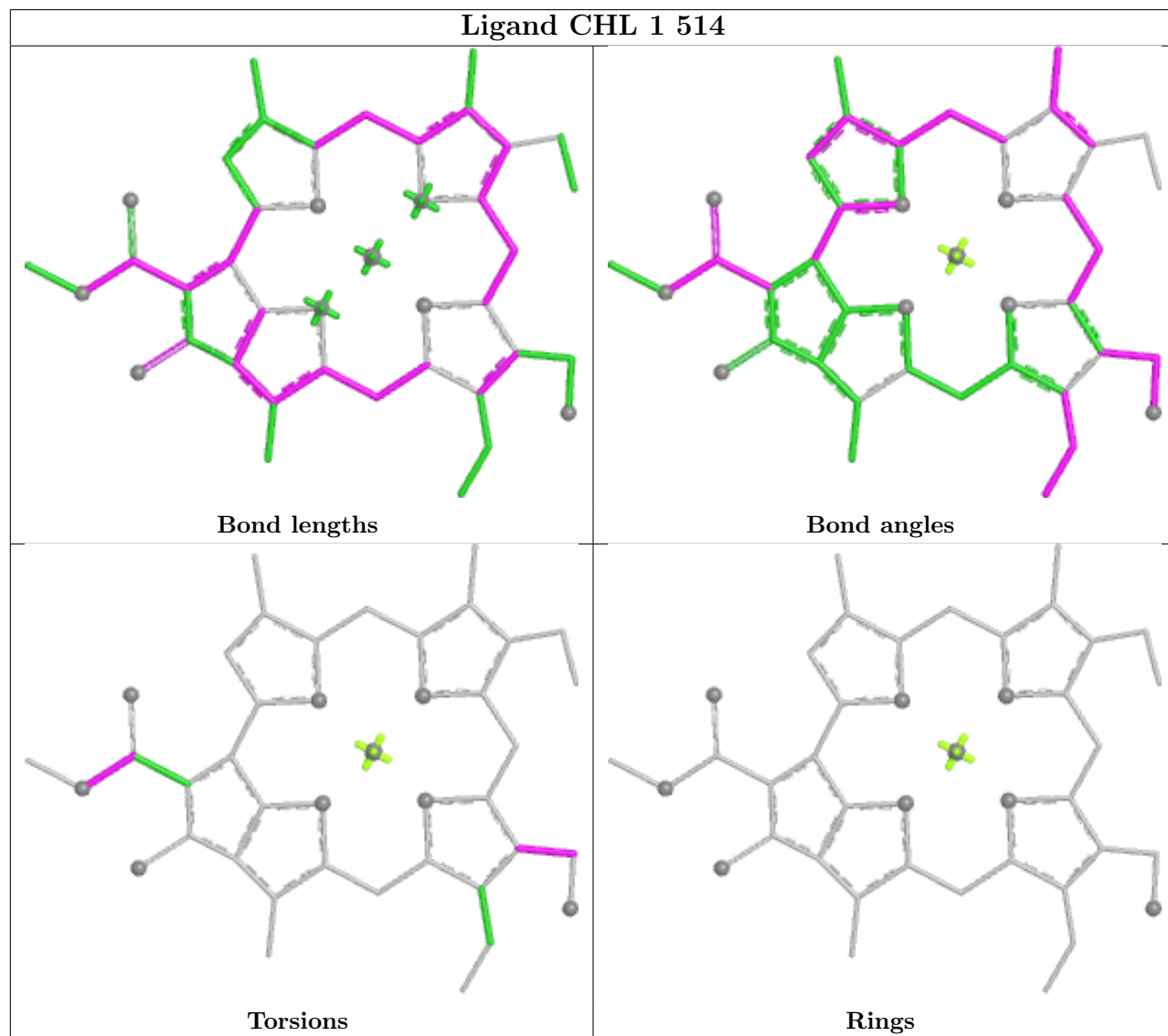


Rings

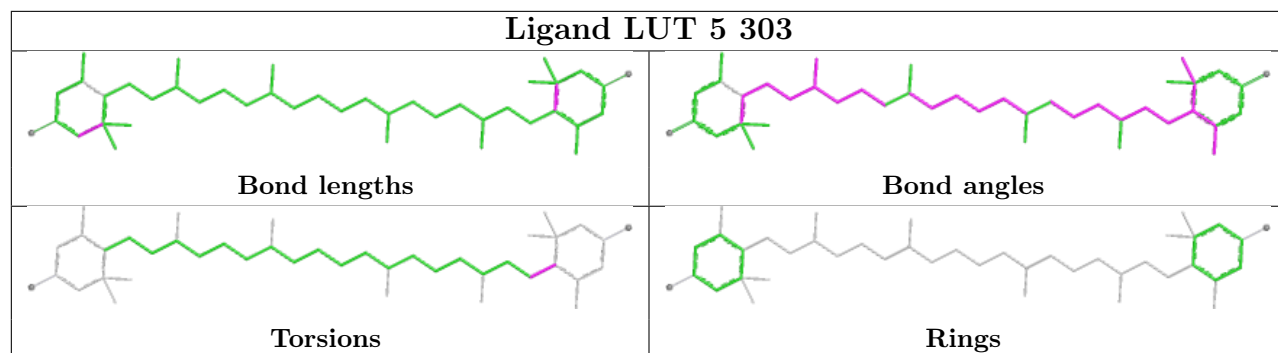
Ligand LUT 1 502



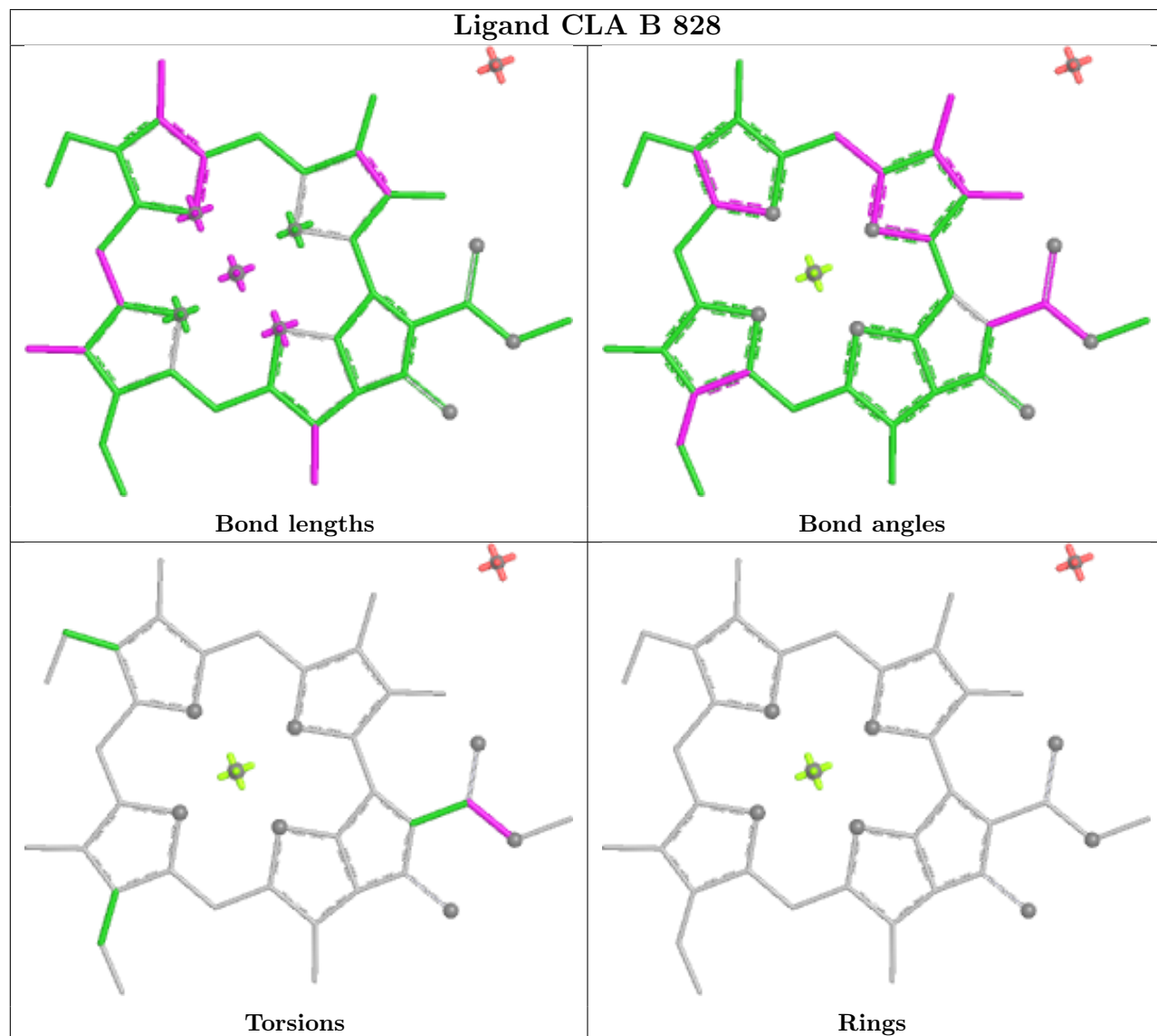
Ligand CHL 1 514



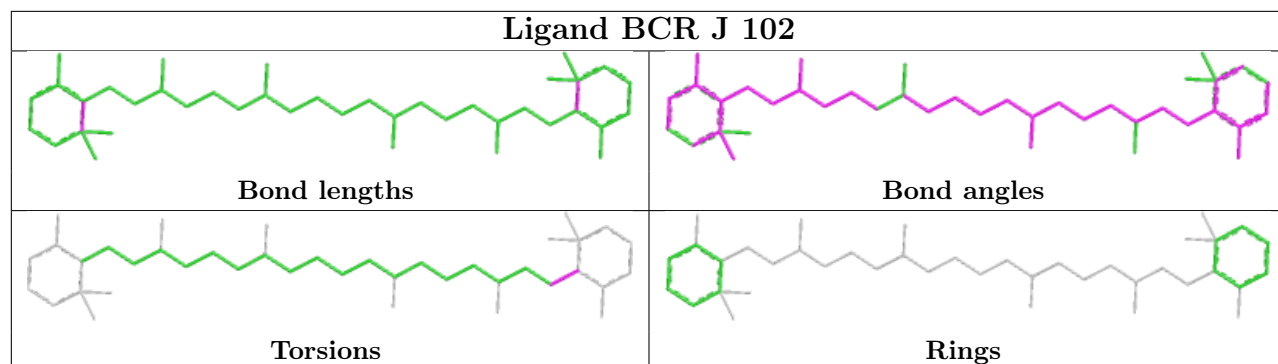
Ligand LUT 5 303



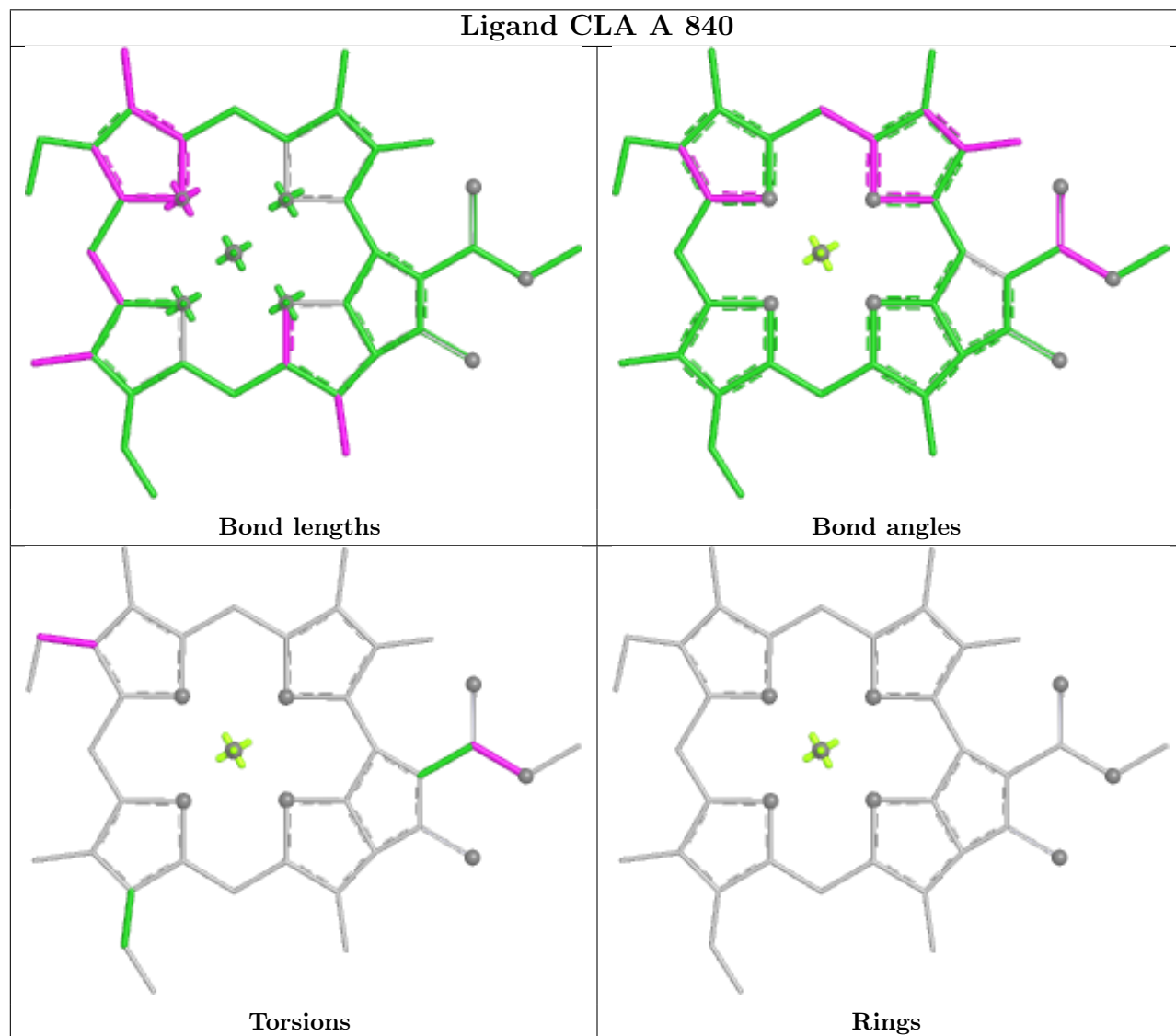
Ligand CLA B 828

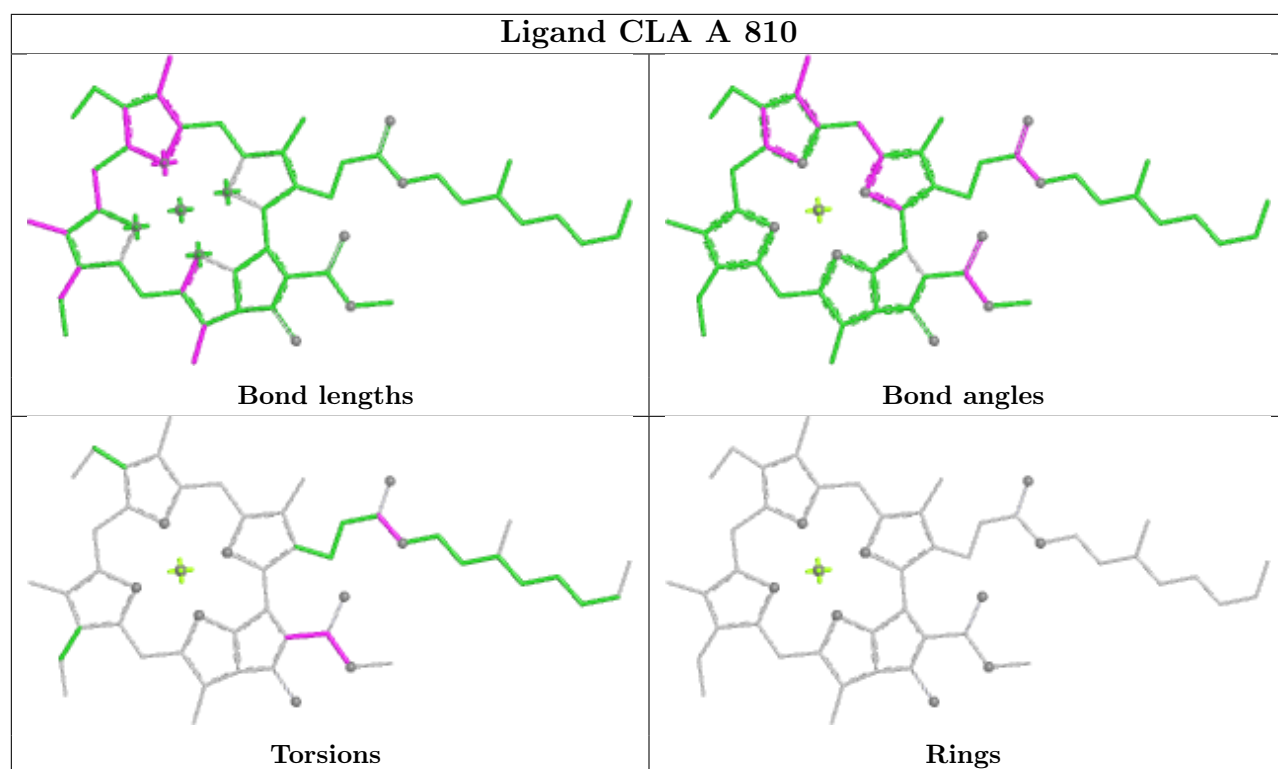


Ligand BCR J 102

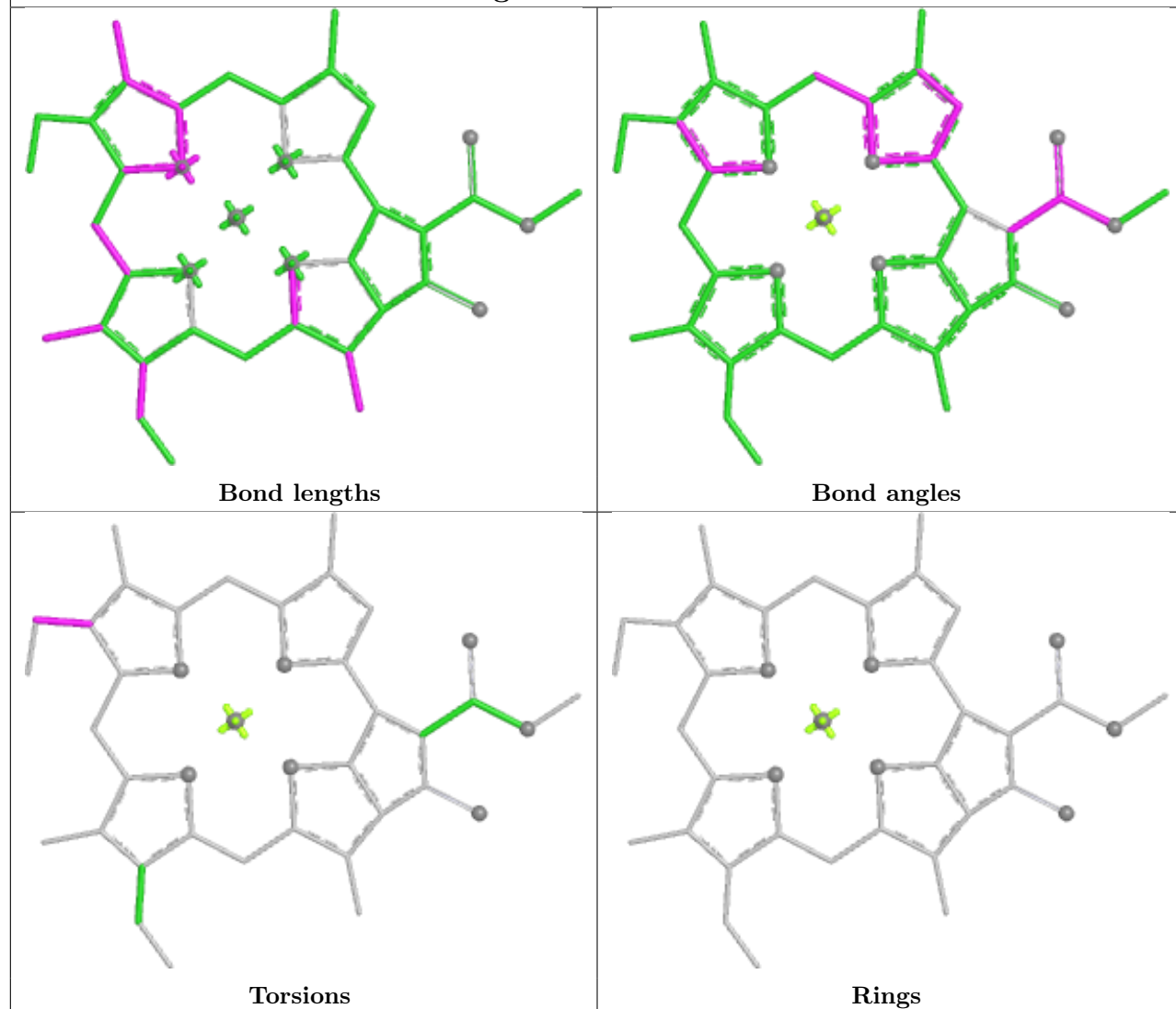


Ligand CLA A 840

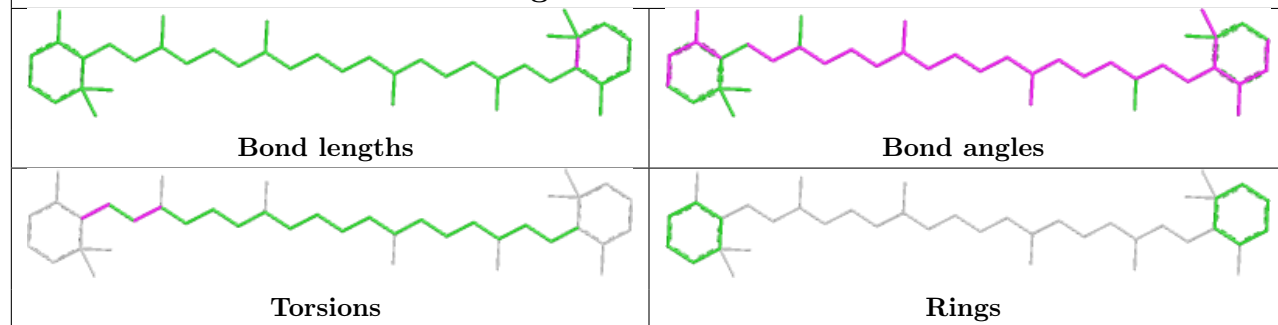


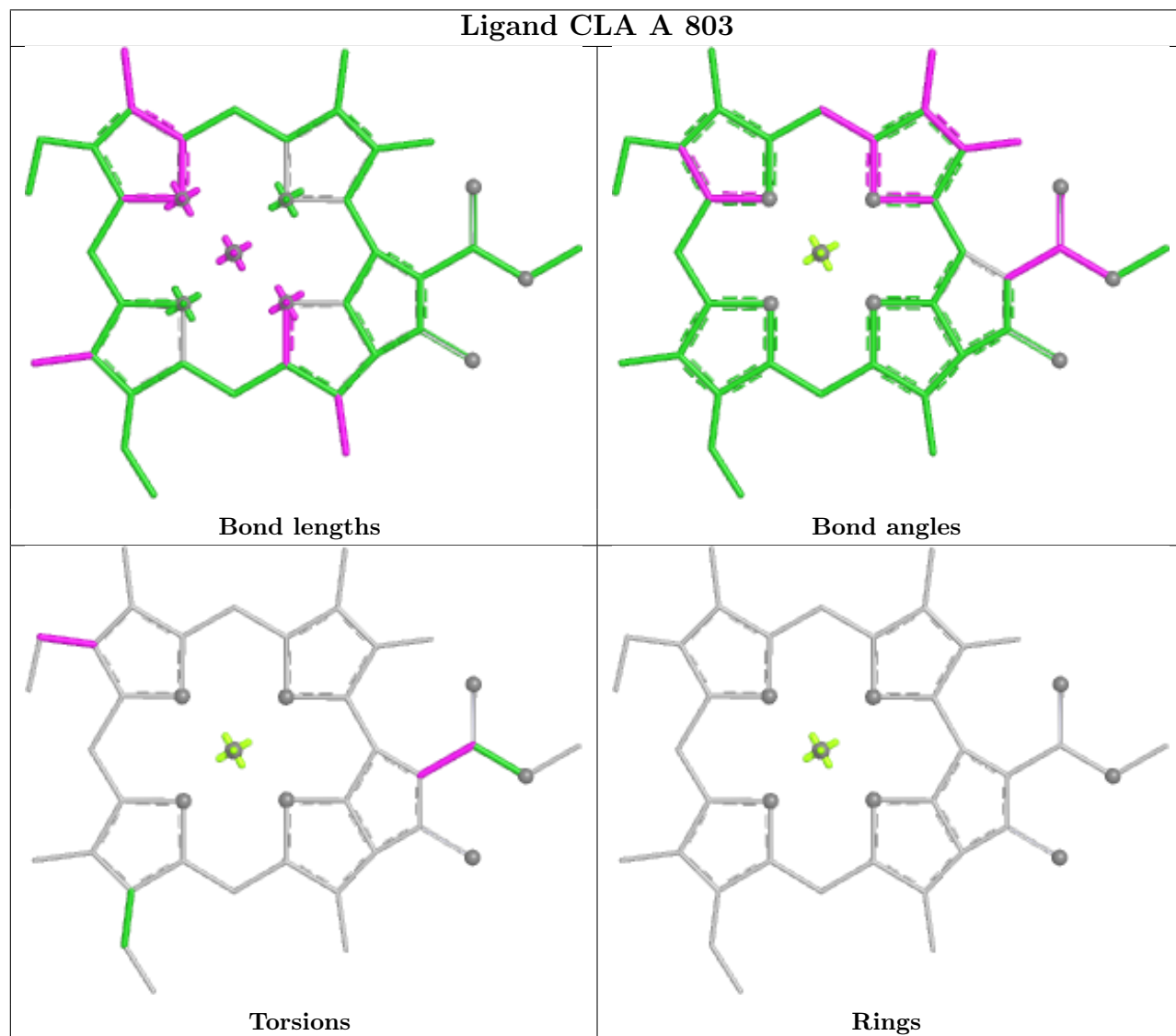
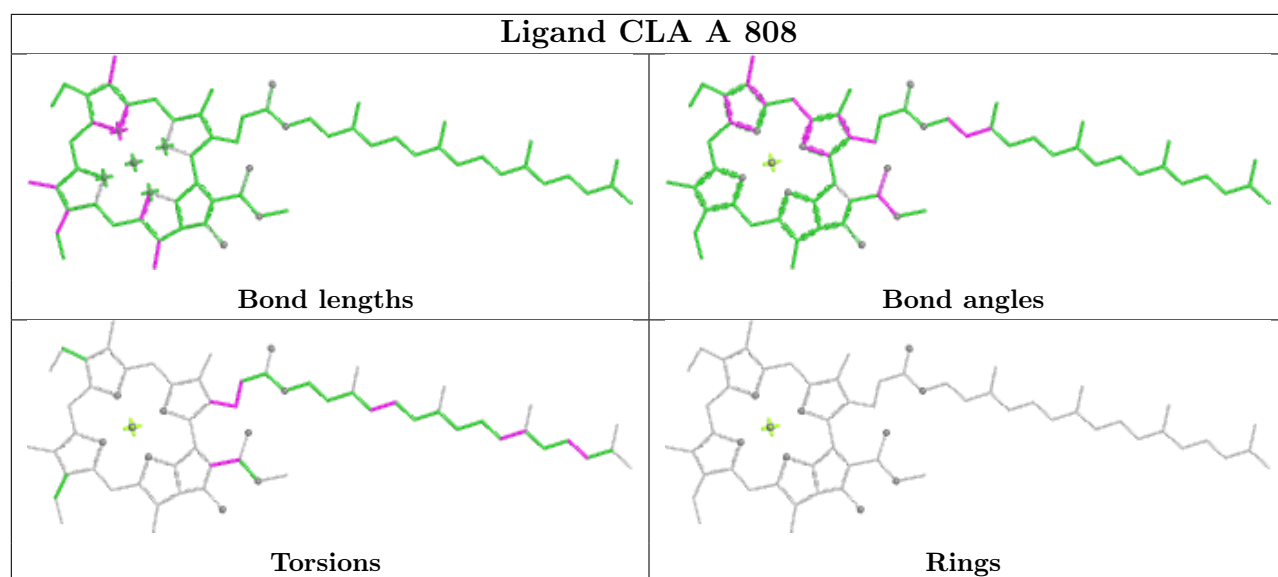


Ligand CLA 2 511

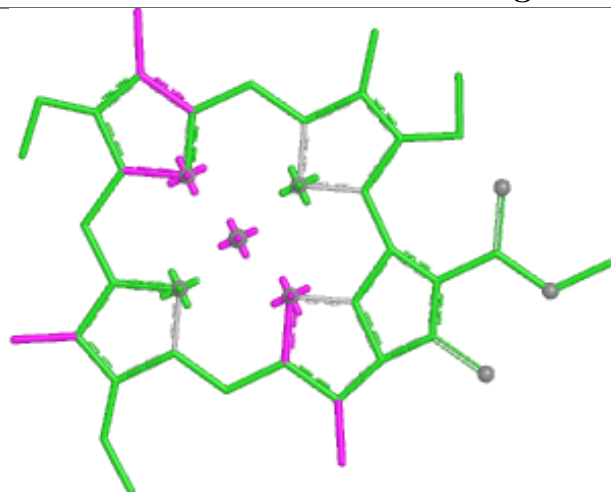


Ligand BCR B 844

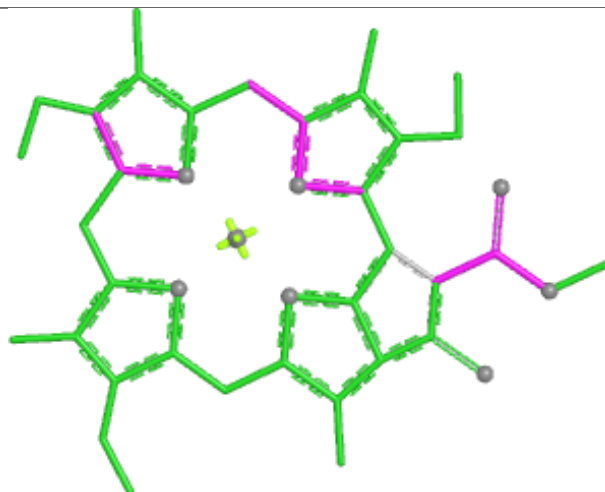




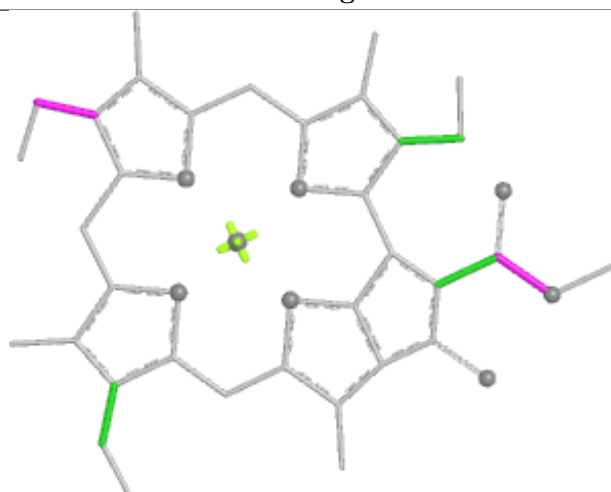
Ligand CLA A 839



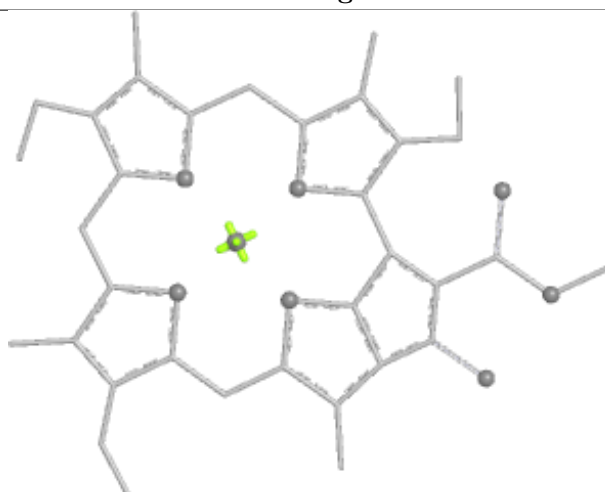
Bond lengths



Bond angles

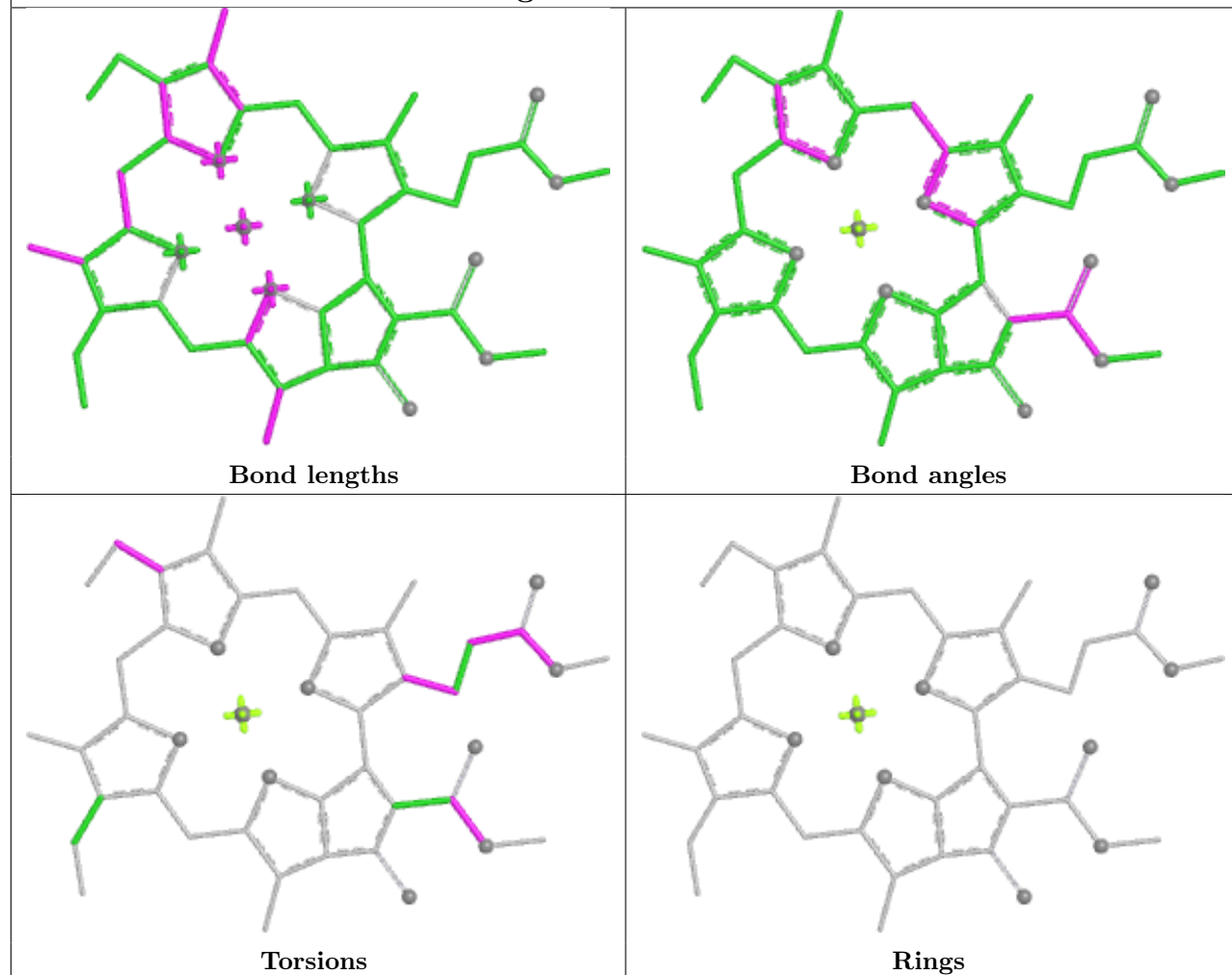


Torsions

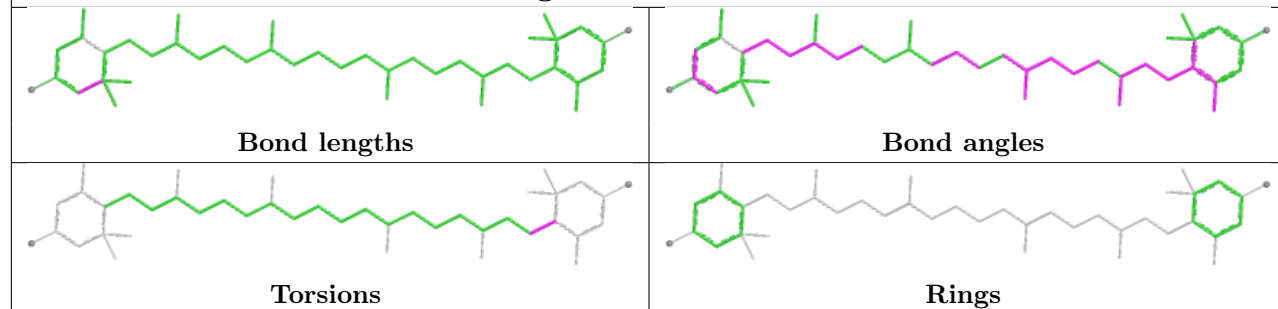


Rings

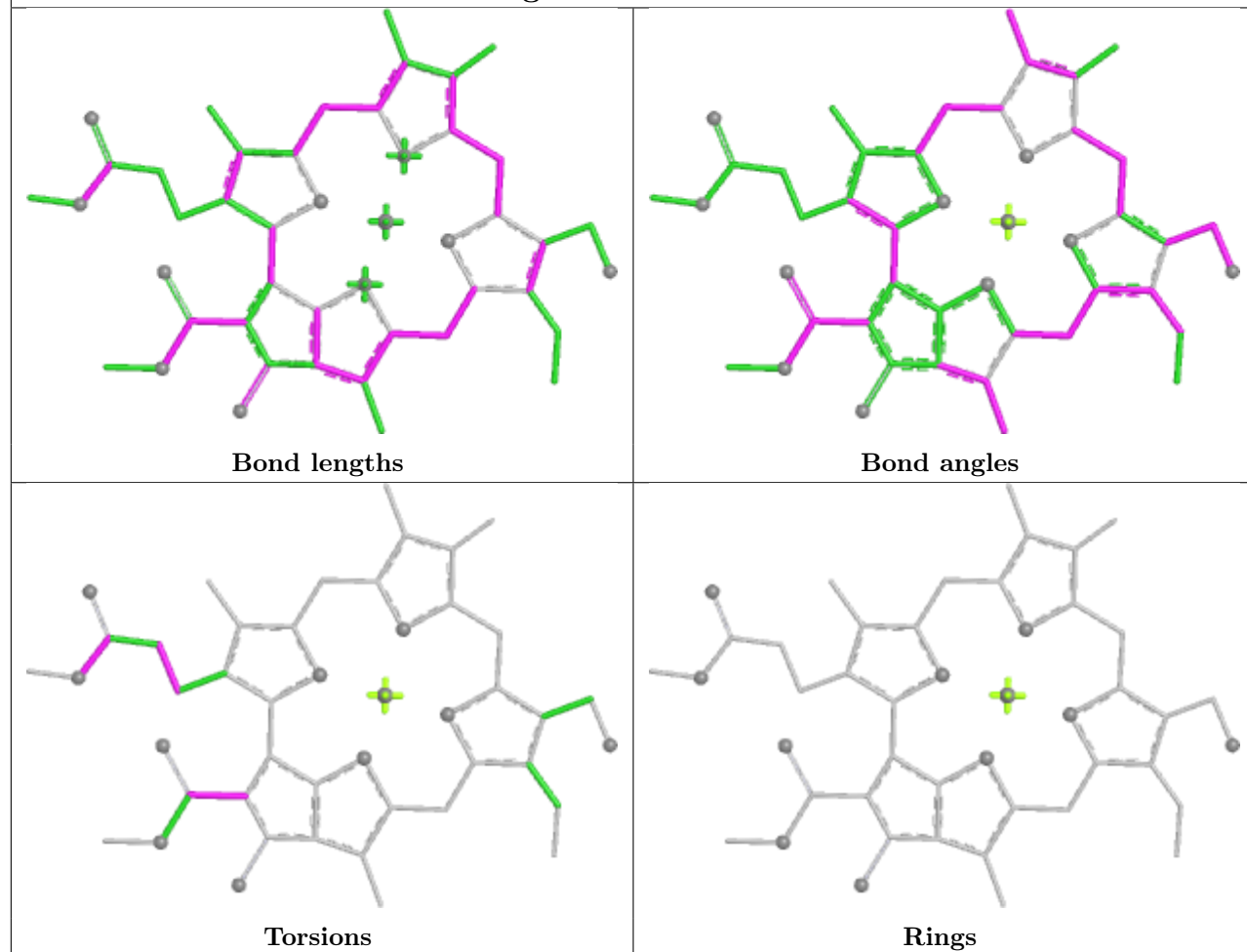
Ligand CLA 1 510



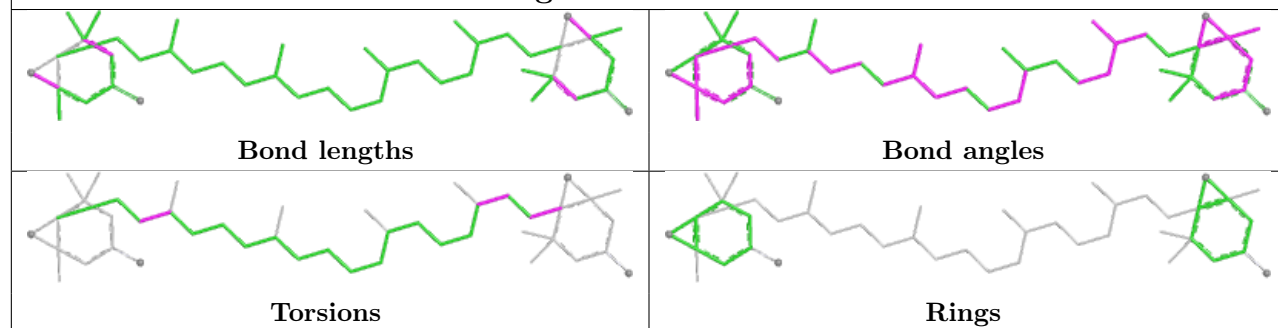
Ligand LUT 3 303



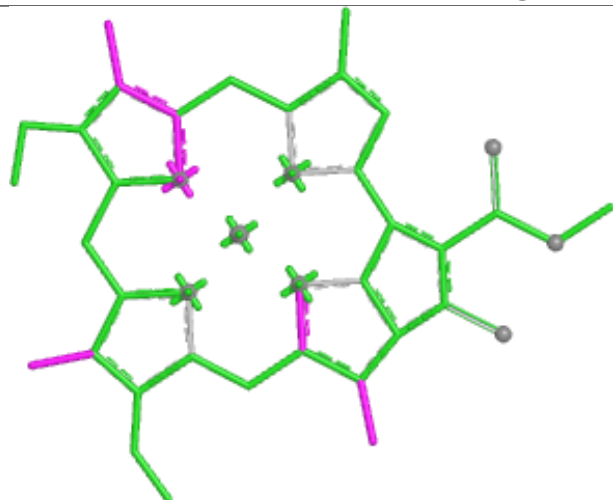
Ligand CHL 2 512



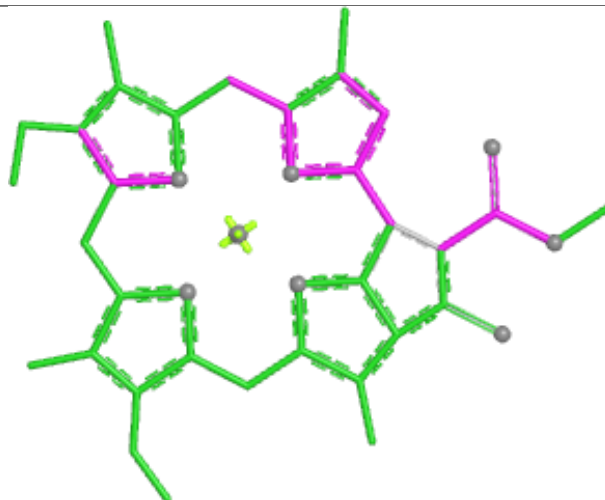
Ligand XAT 2 502



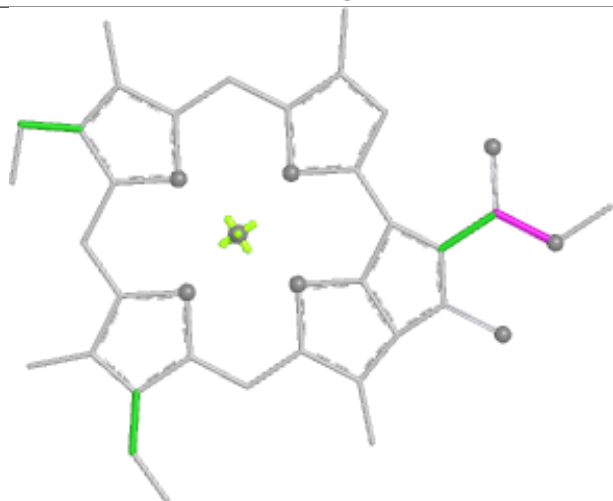
Ligand CLA A 811



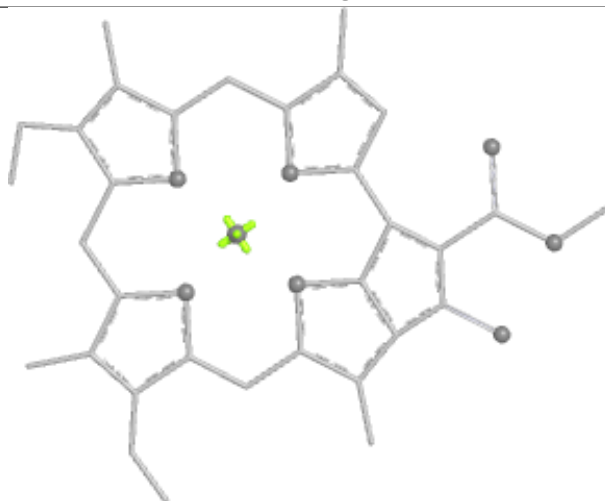
Bond lengths



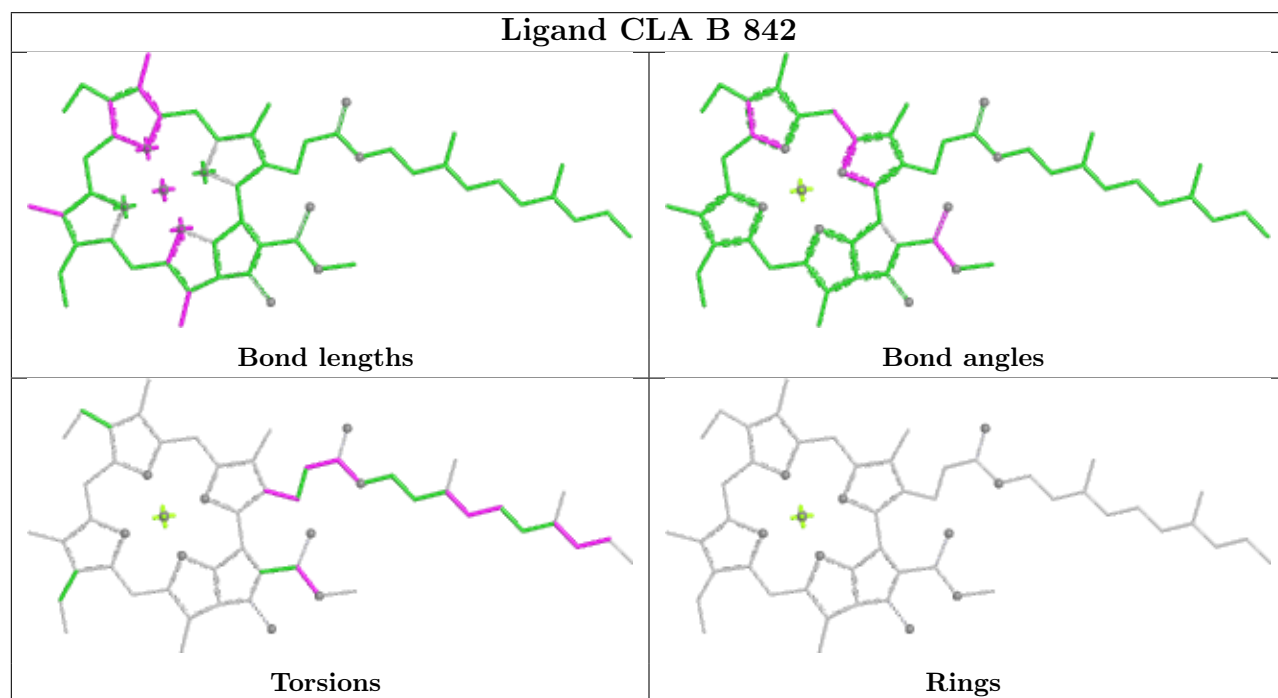
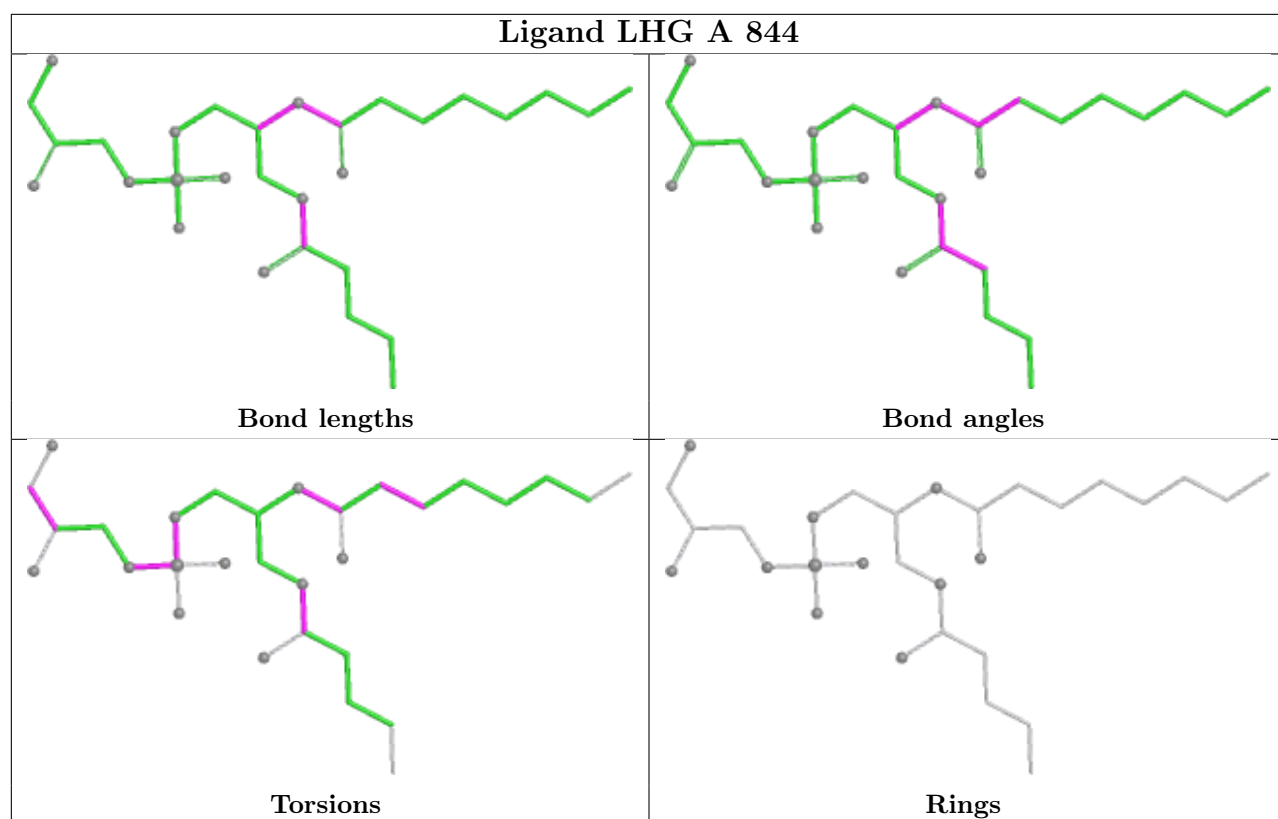
Bond angles

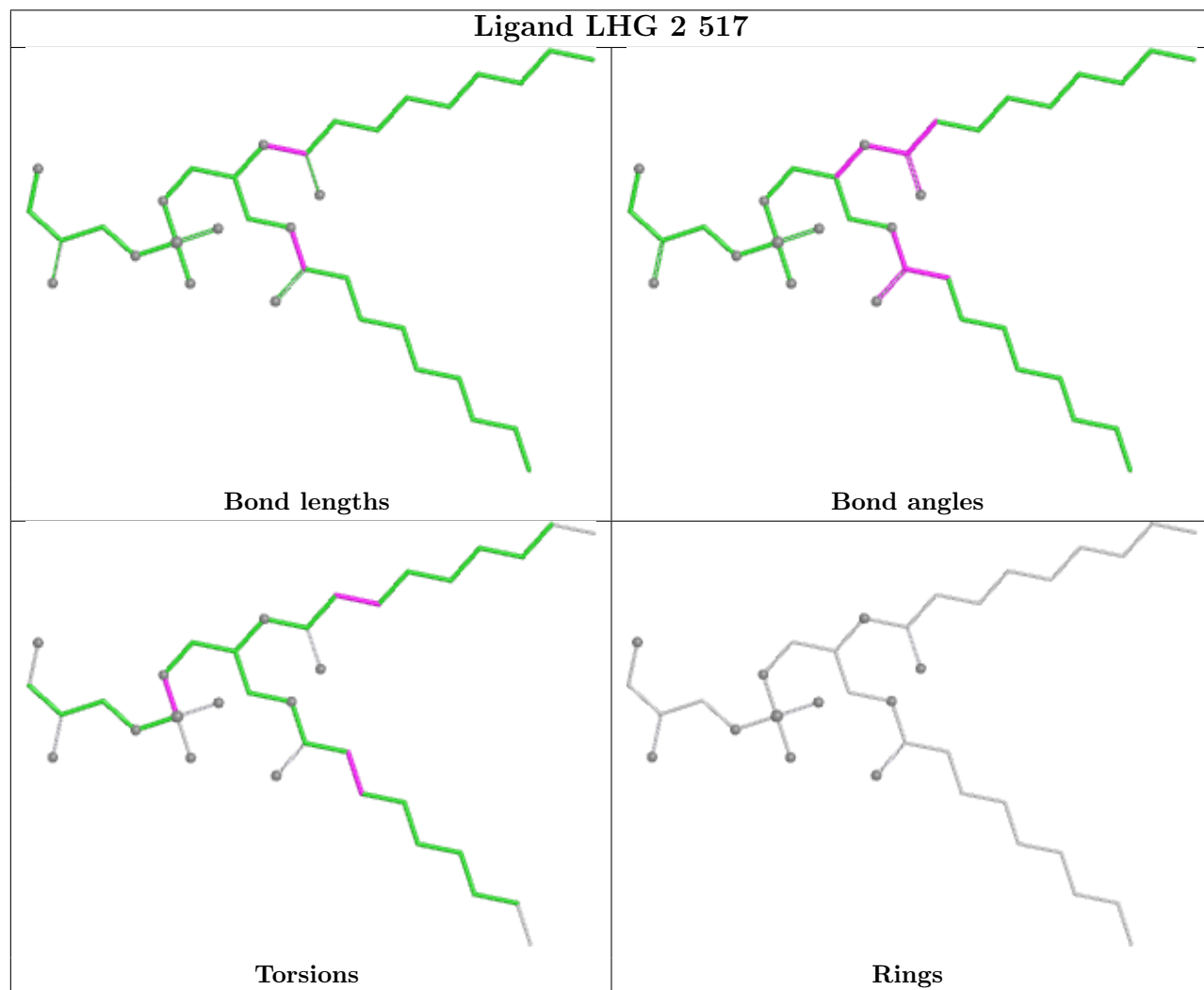
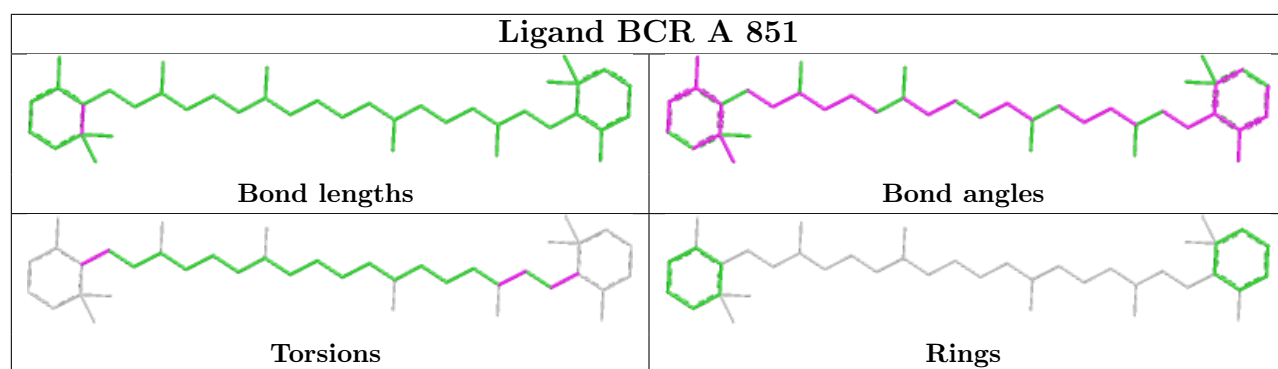


Torsions

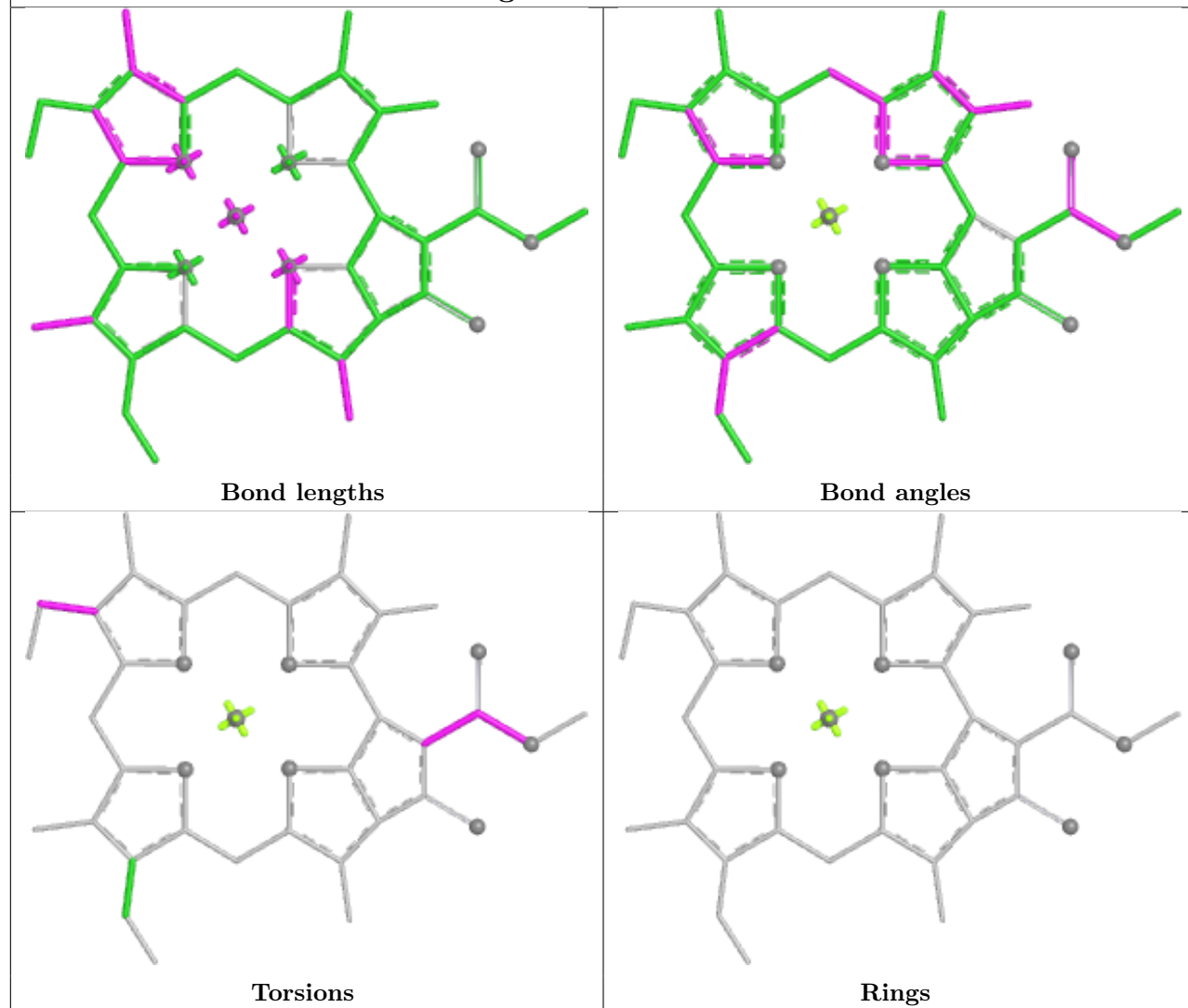


Rings

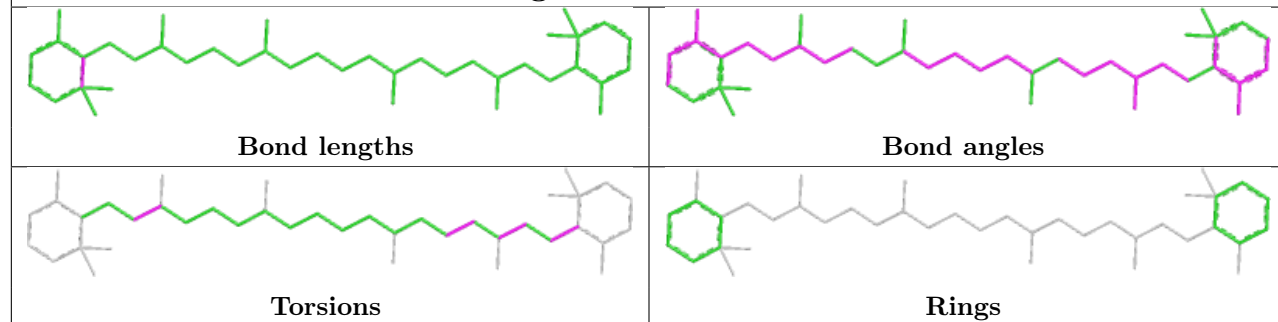


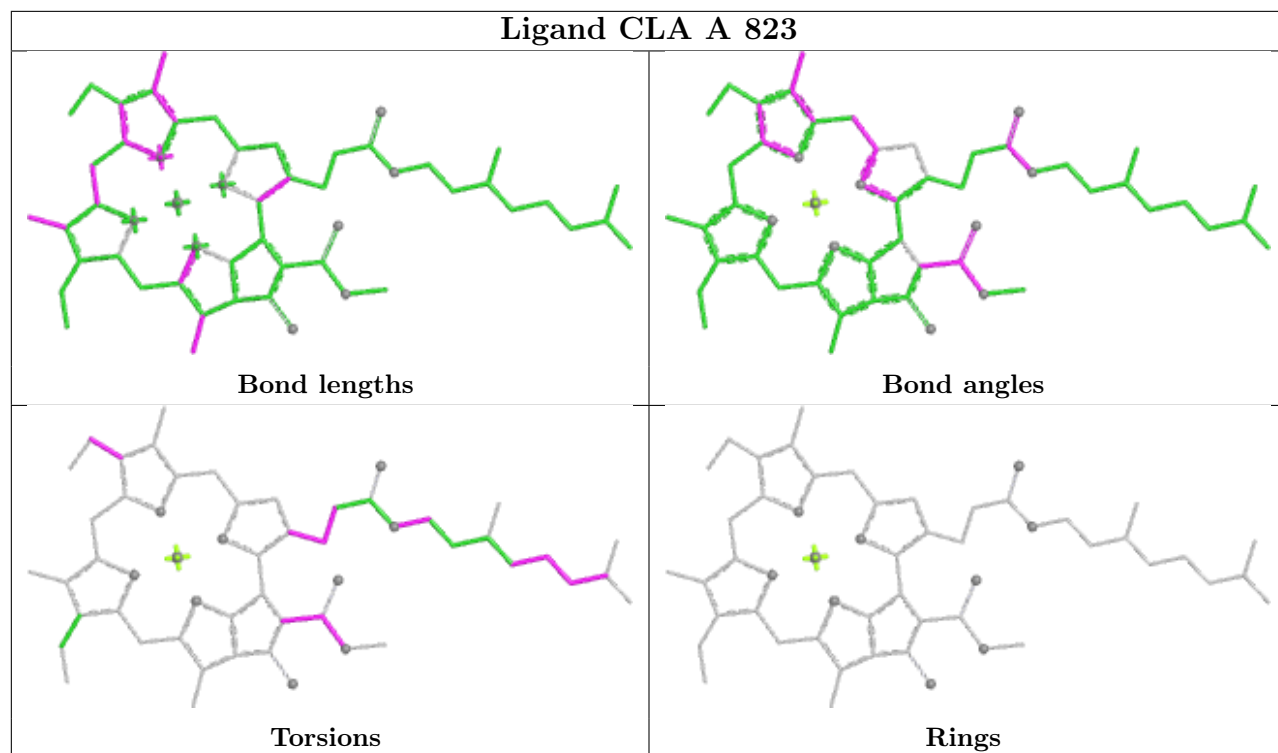


Ligand CLA 3 312

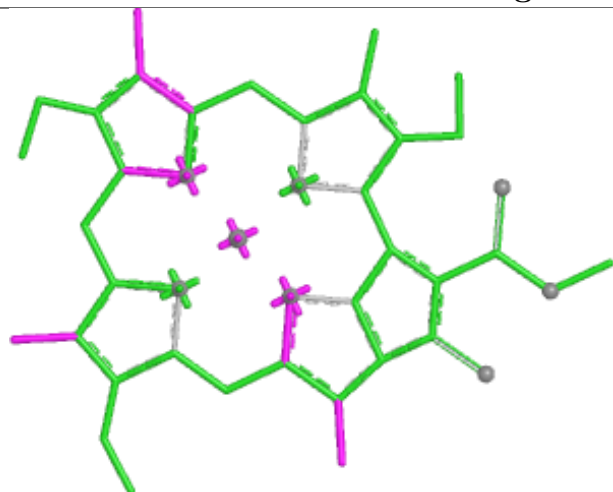


Ligand BCR A 846





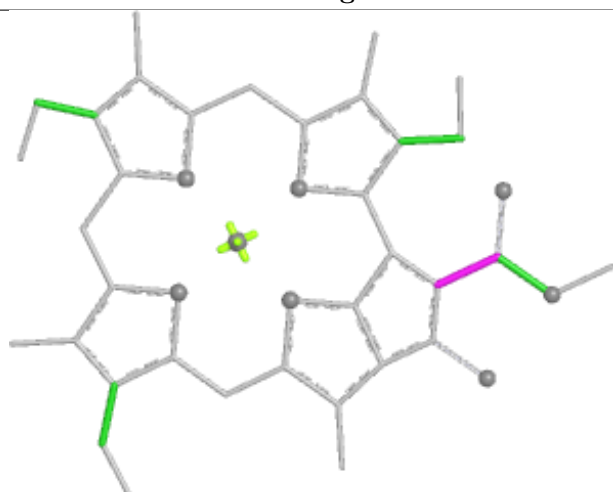
Ligand CLA B 825



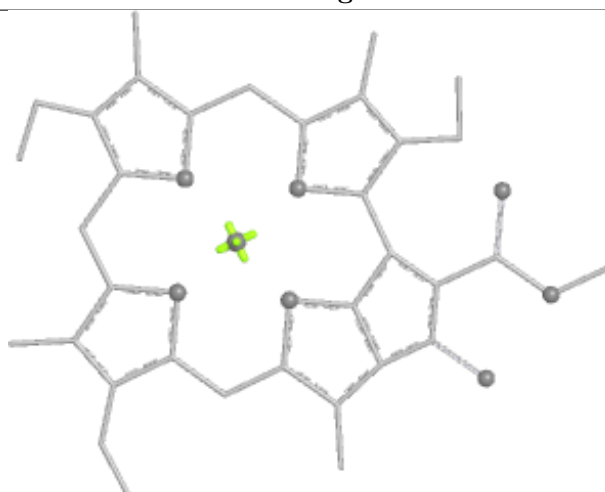
Bond lengths



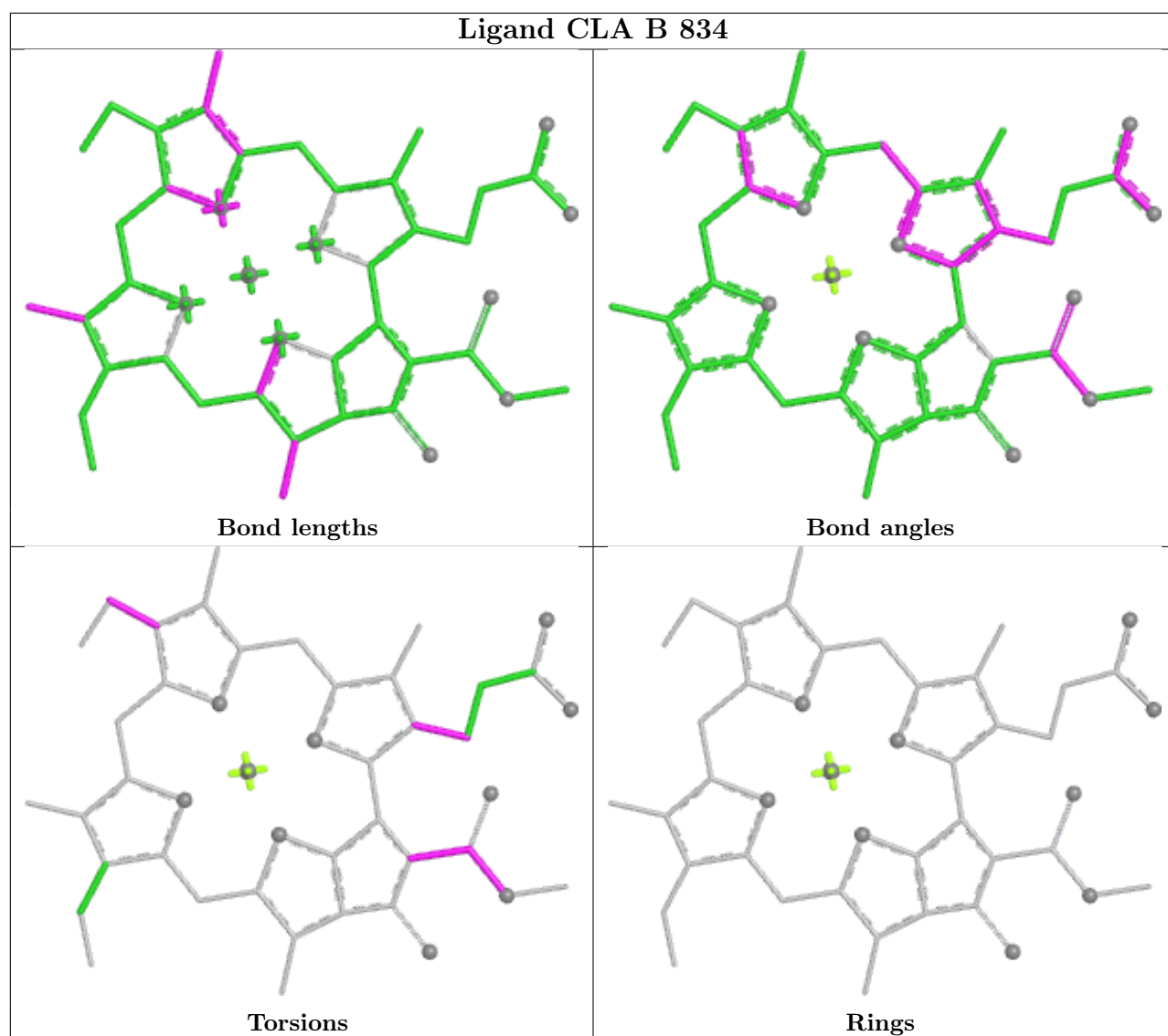
Bond angles



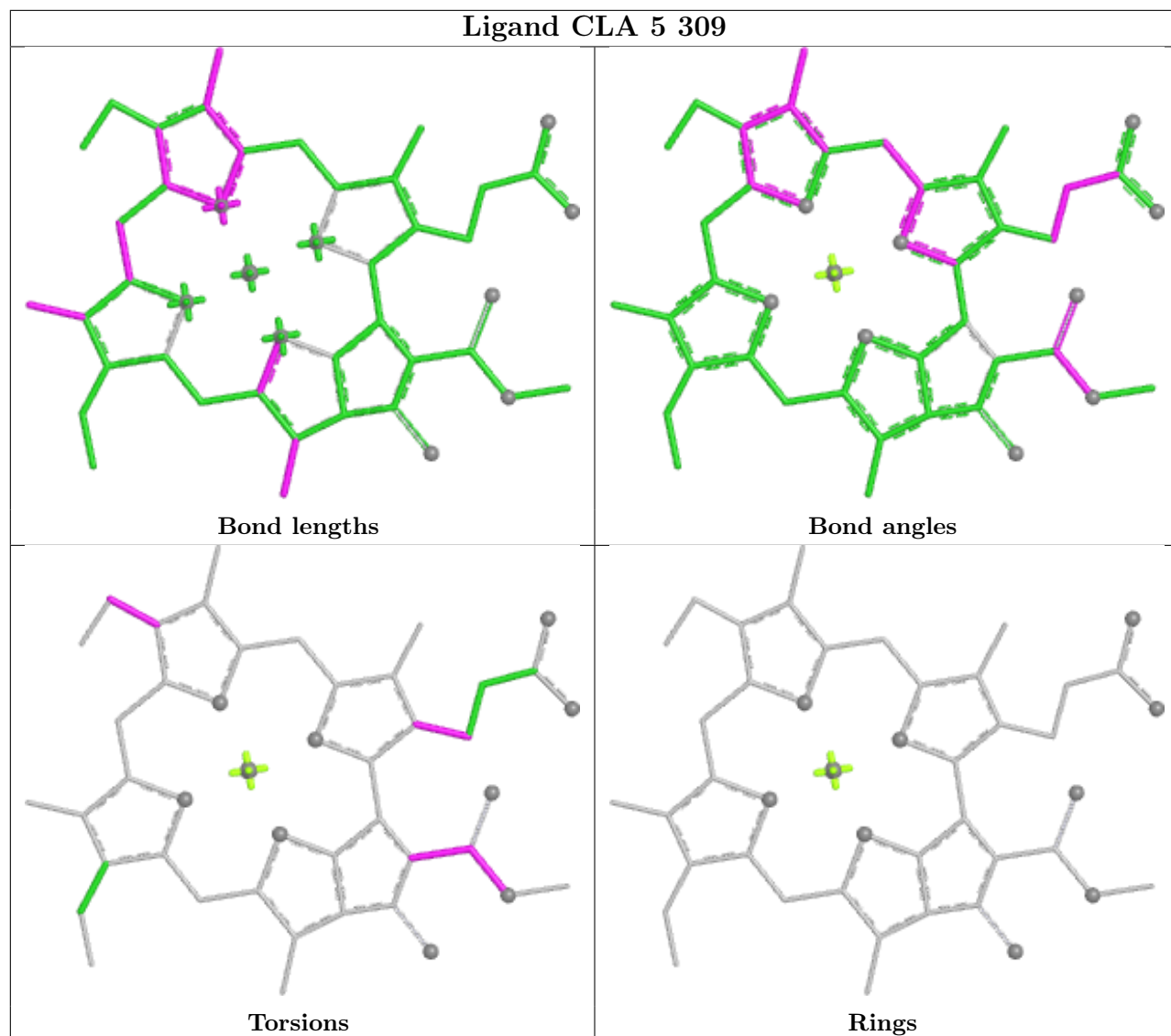
Torsions



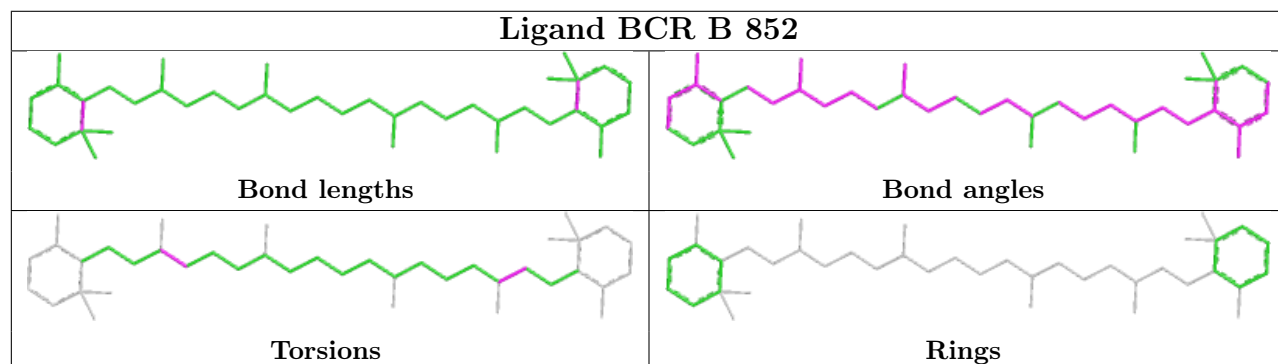
Rings



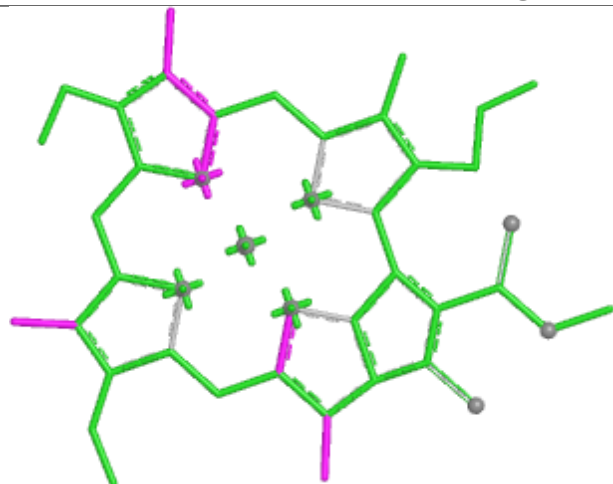
Ligand CLA 5 309



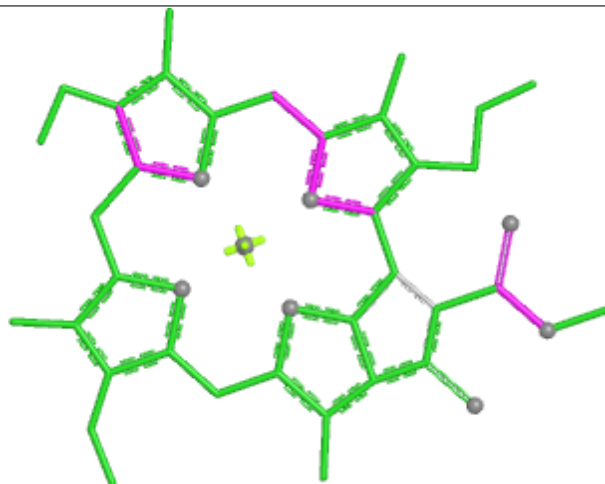
Ligand BCR B 852



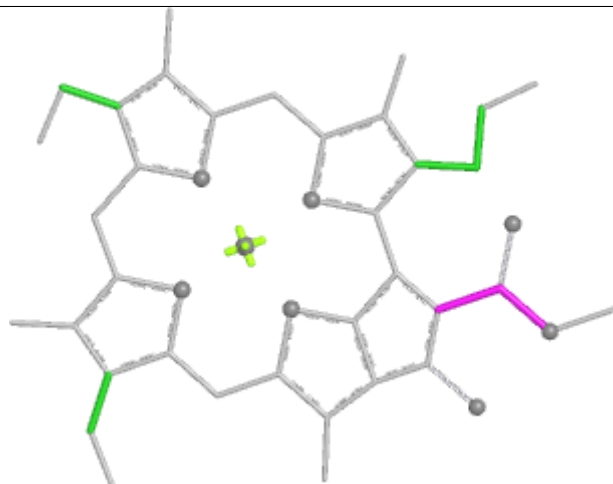
Ligand CLA B 816



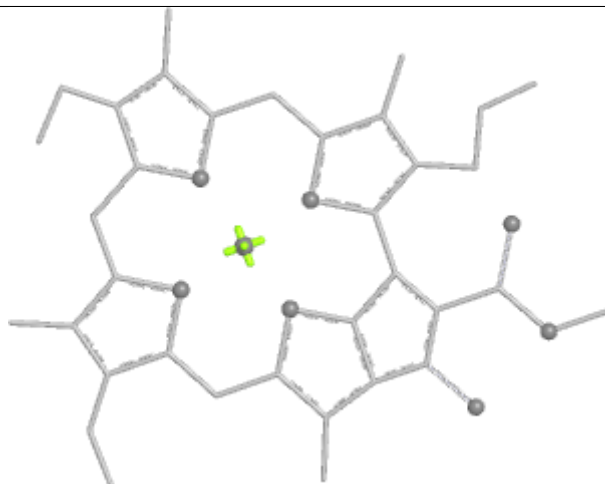
Bond lengths



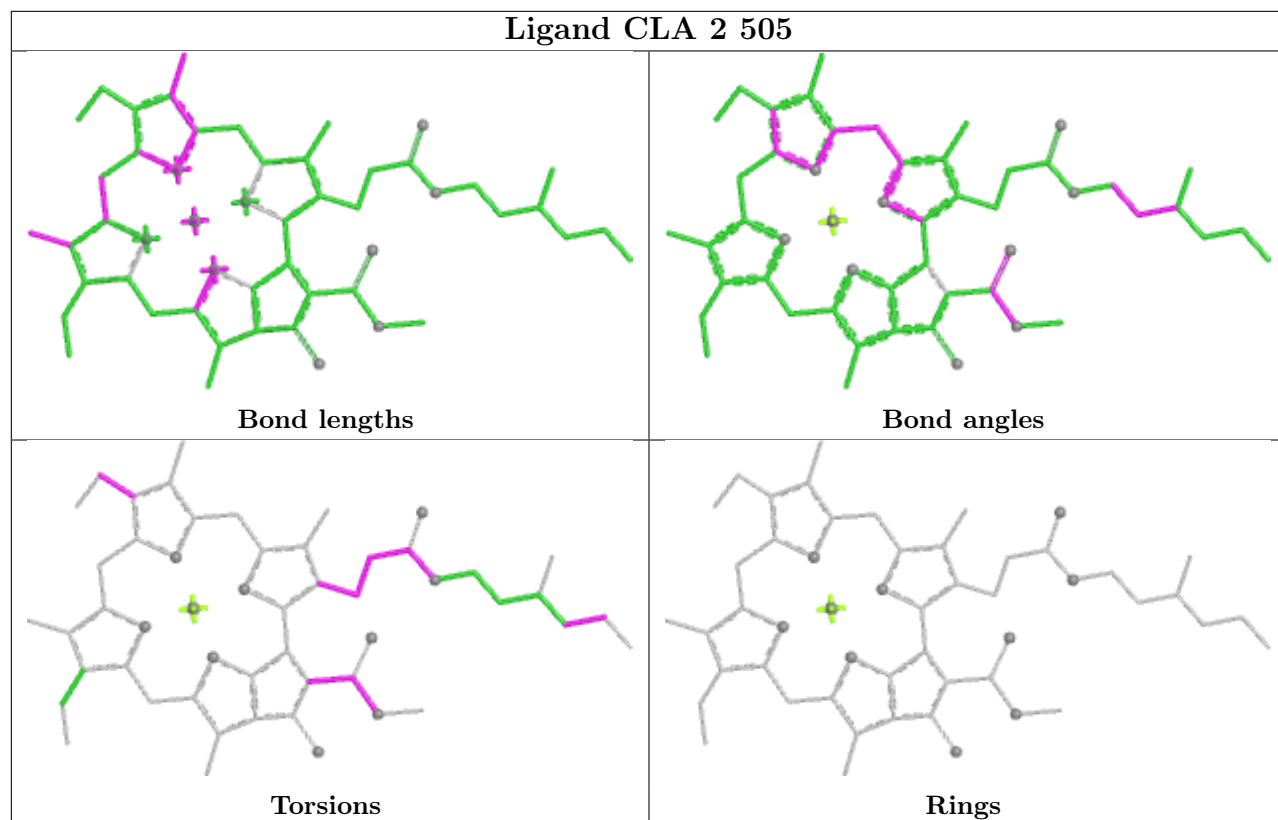
Bond angles



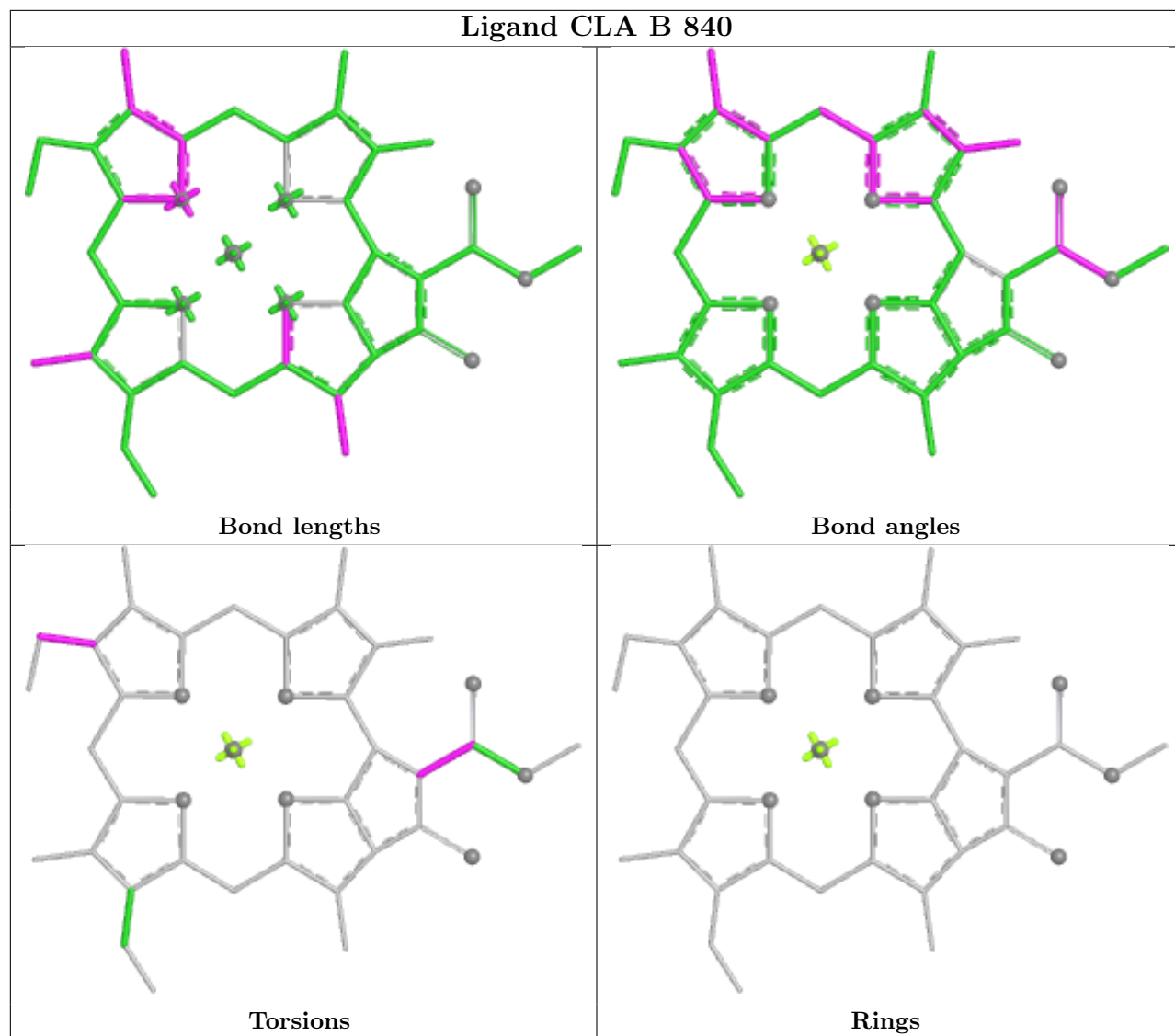
Torsions



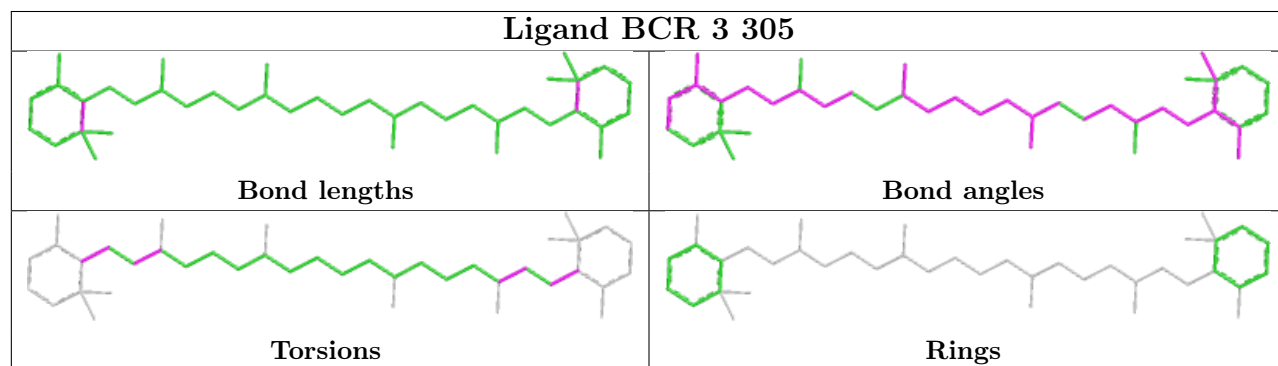
Rings



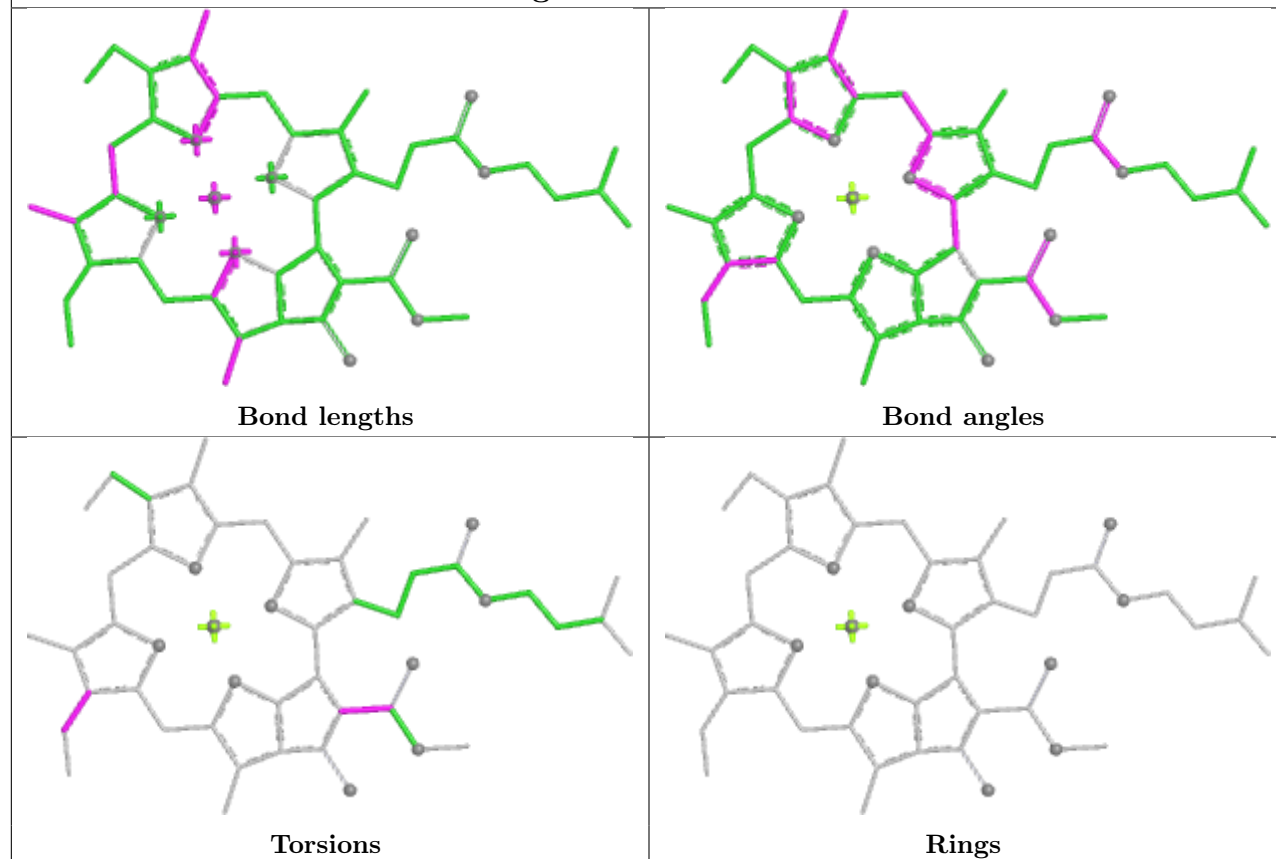
Ligand CLA B 840



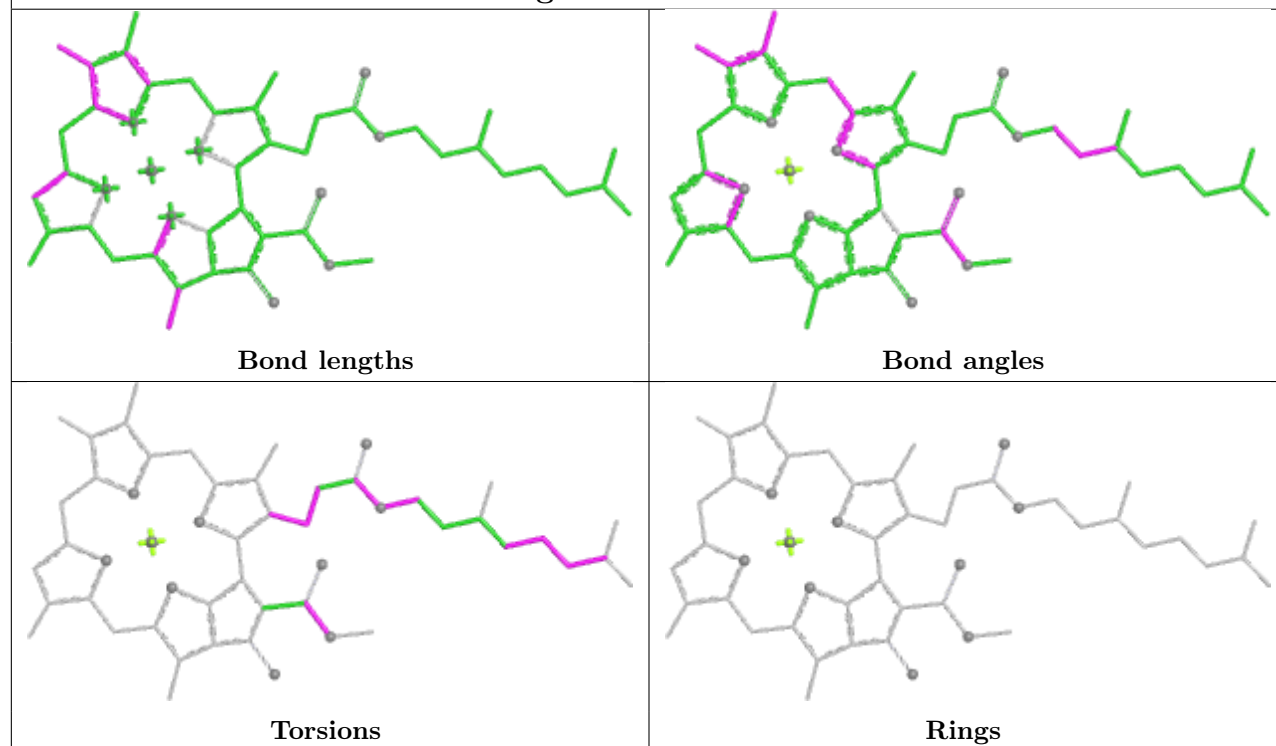
Ligand BCR 3 305



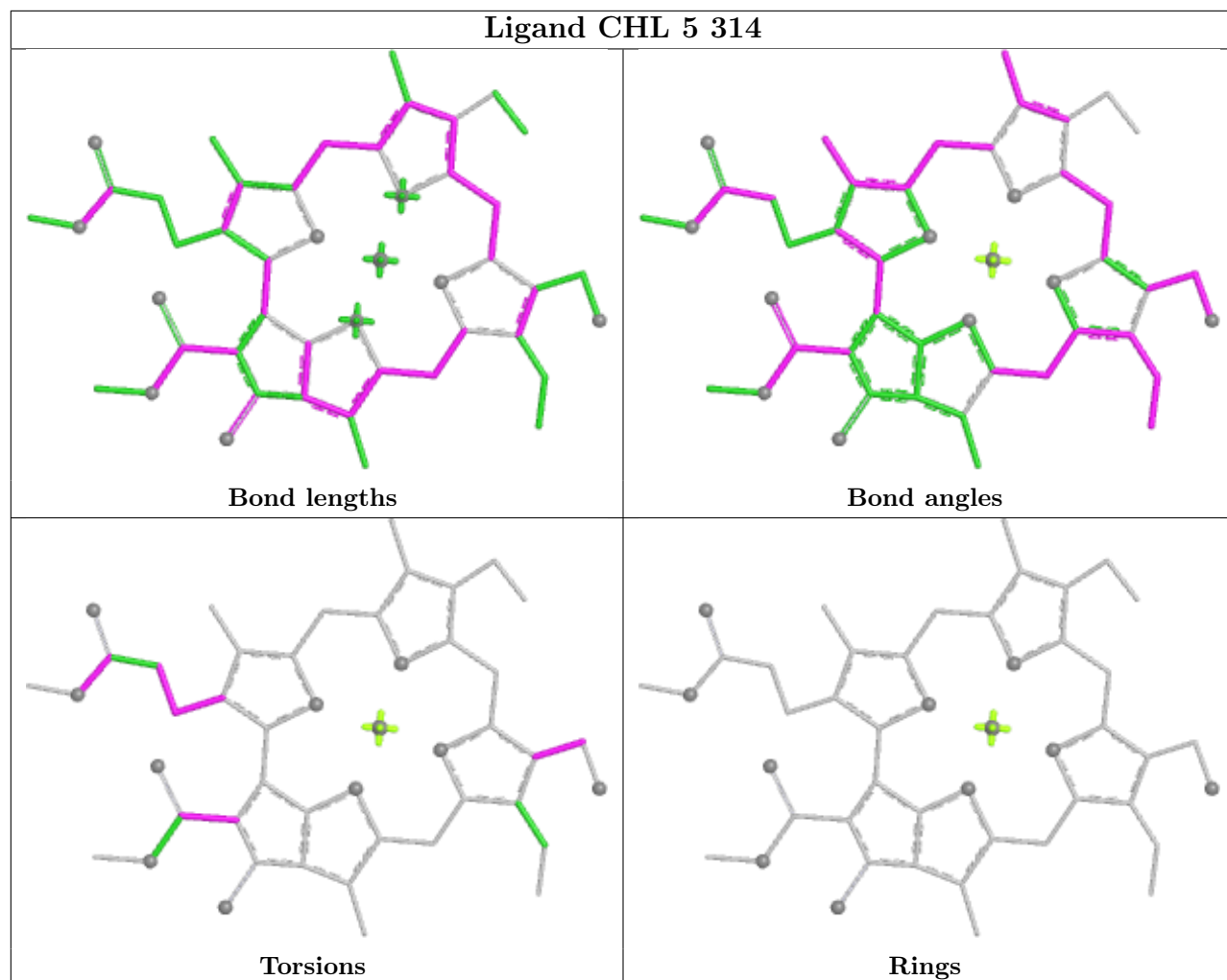
Ligand CLA B 837



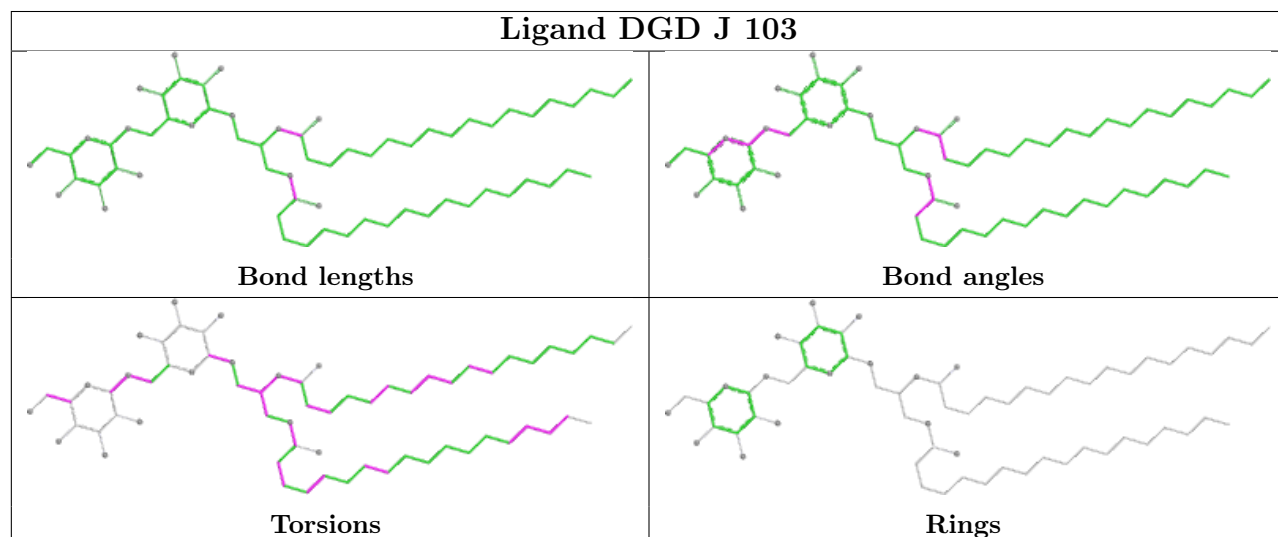
Ligand CLA 3 306



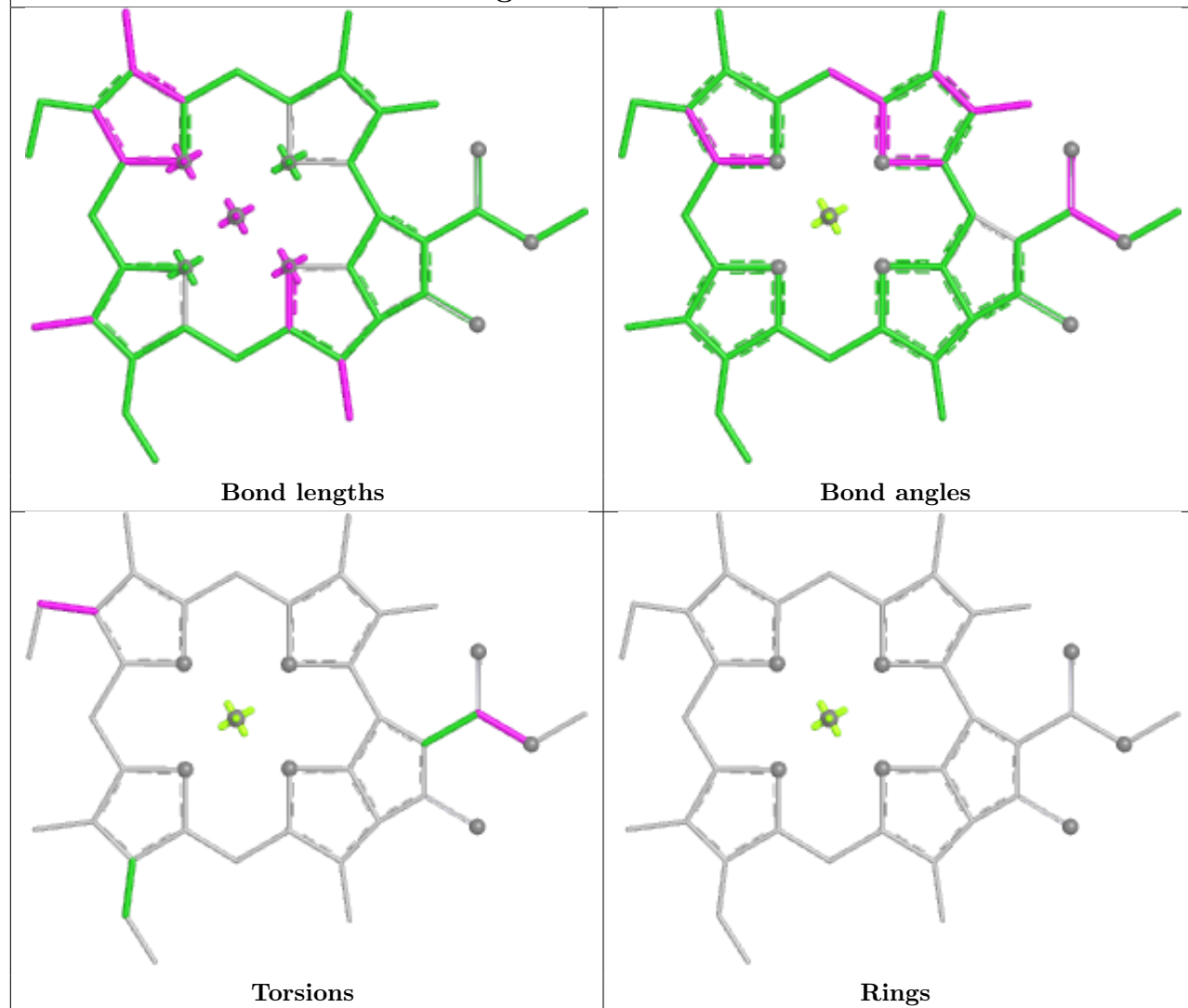
Ligand CHL 5 314



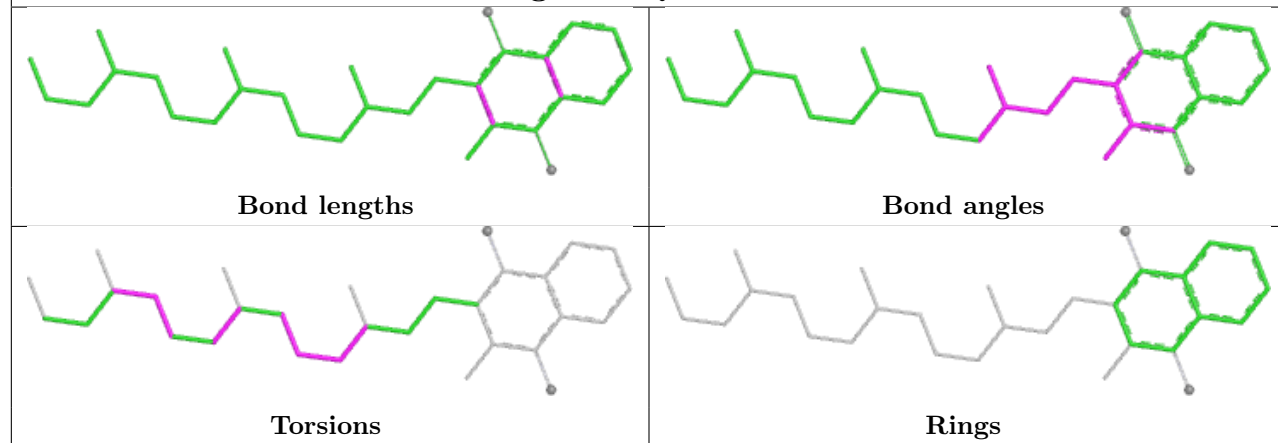
Ligand DGD J 103

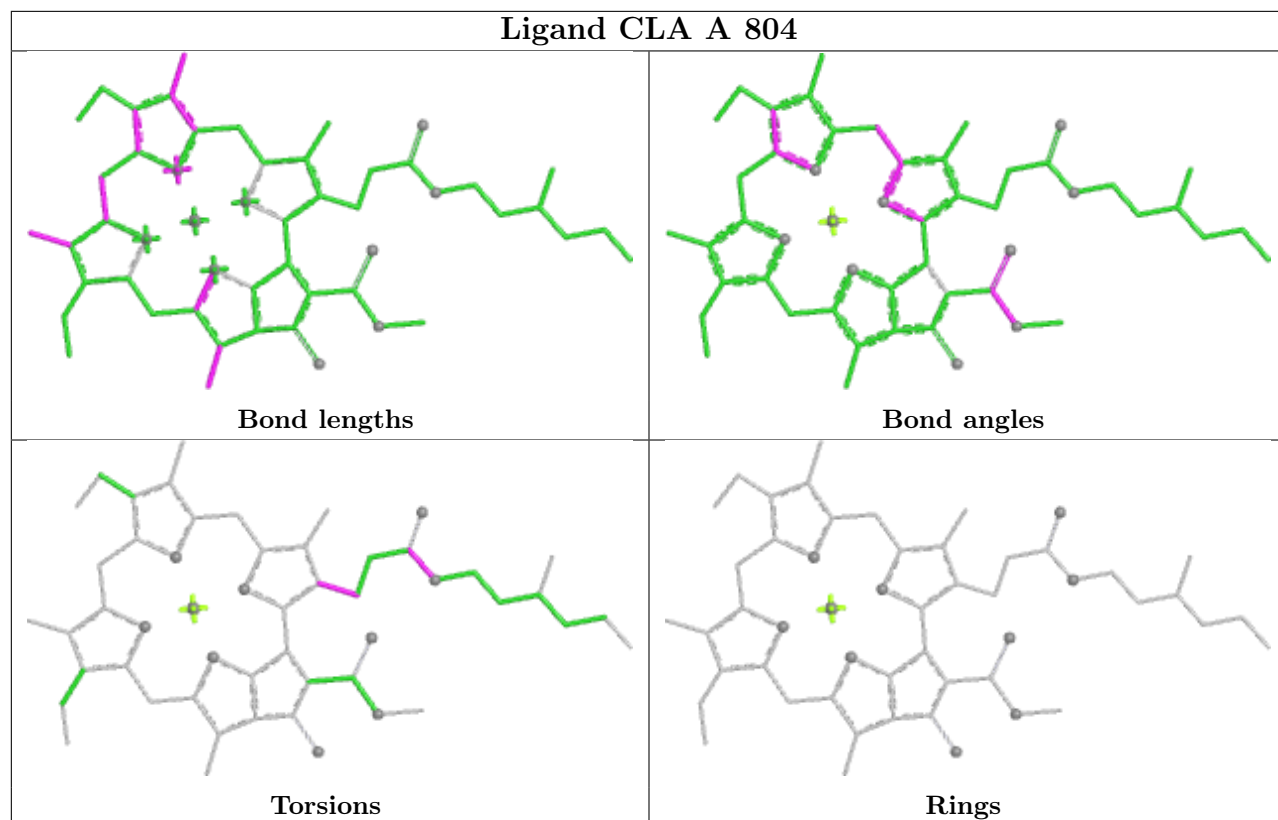


Ligand CLA F 803

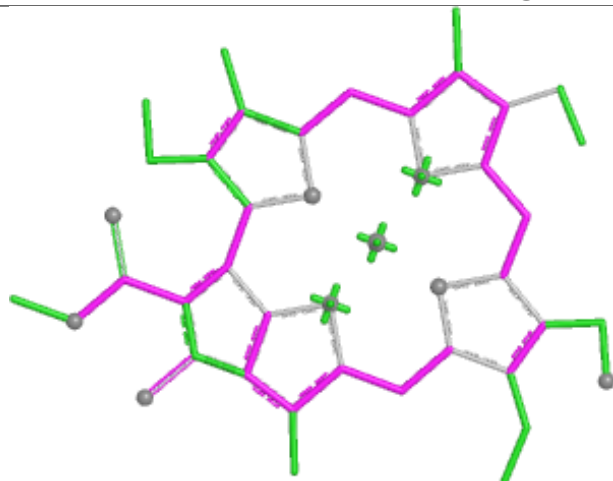


Ligand PQN B 843

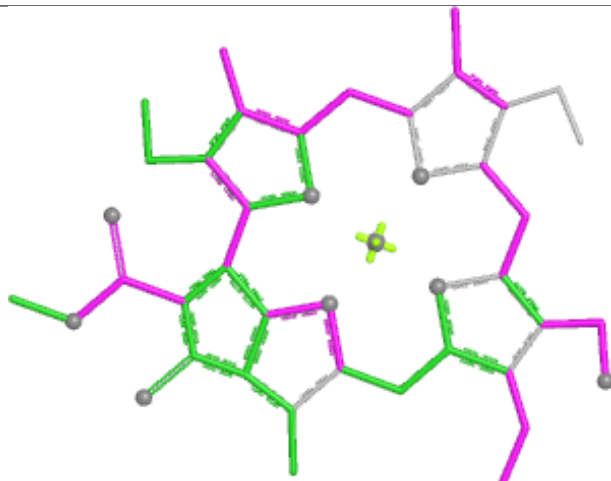




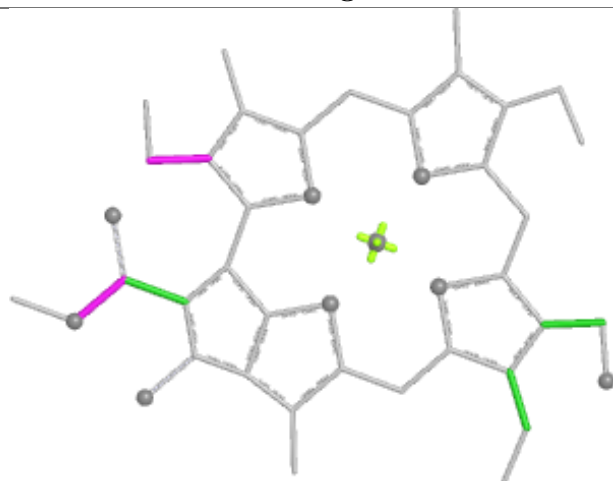
Ligand CHL 3 315



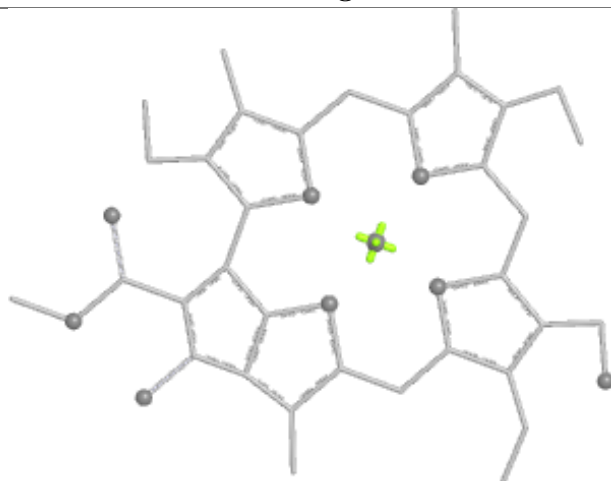
Bond lengths



Bond angles

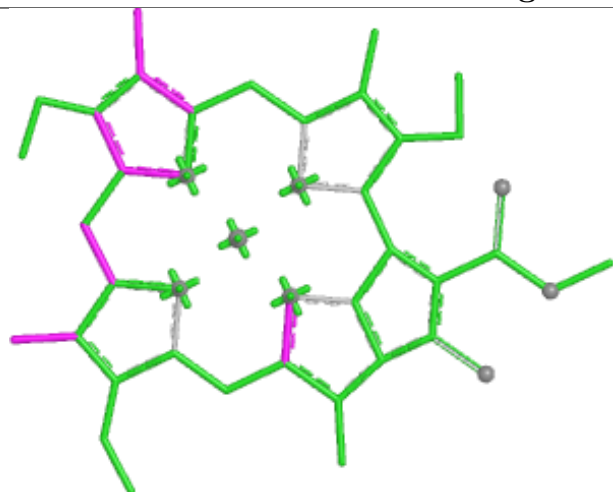


Torsions

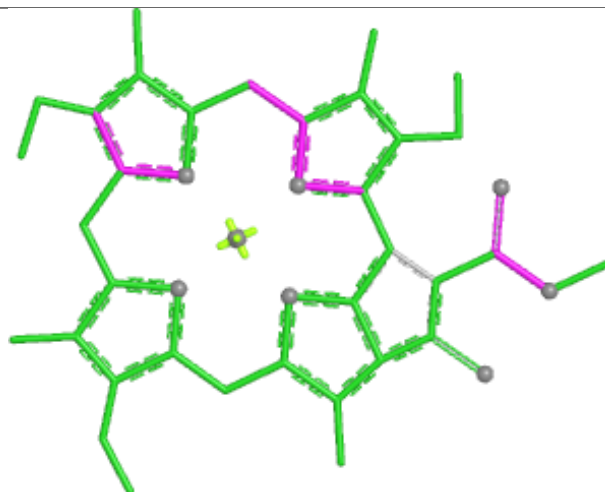


Rings

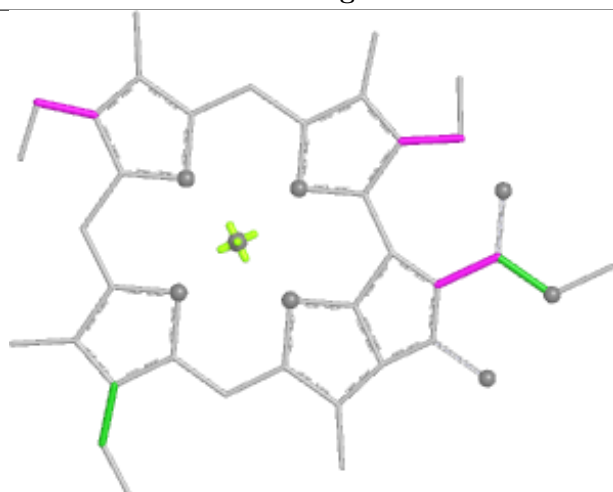
Ligand CLA 1 505



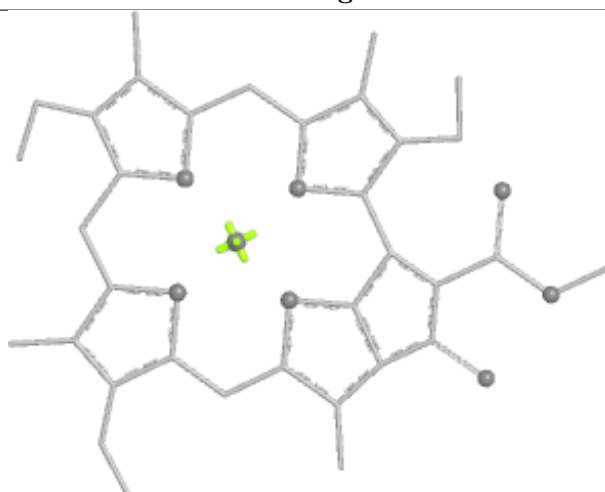
Bond lengths



Bond angles

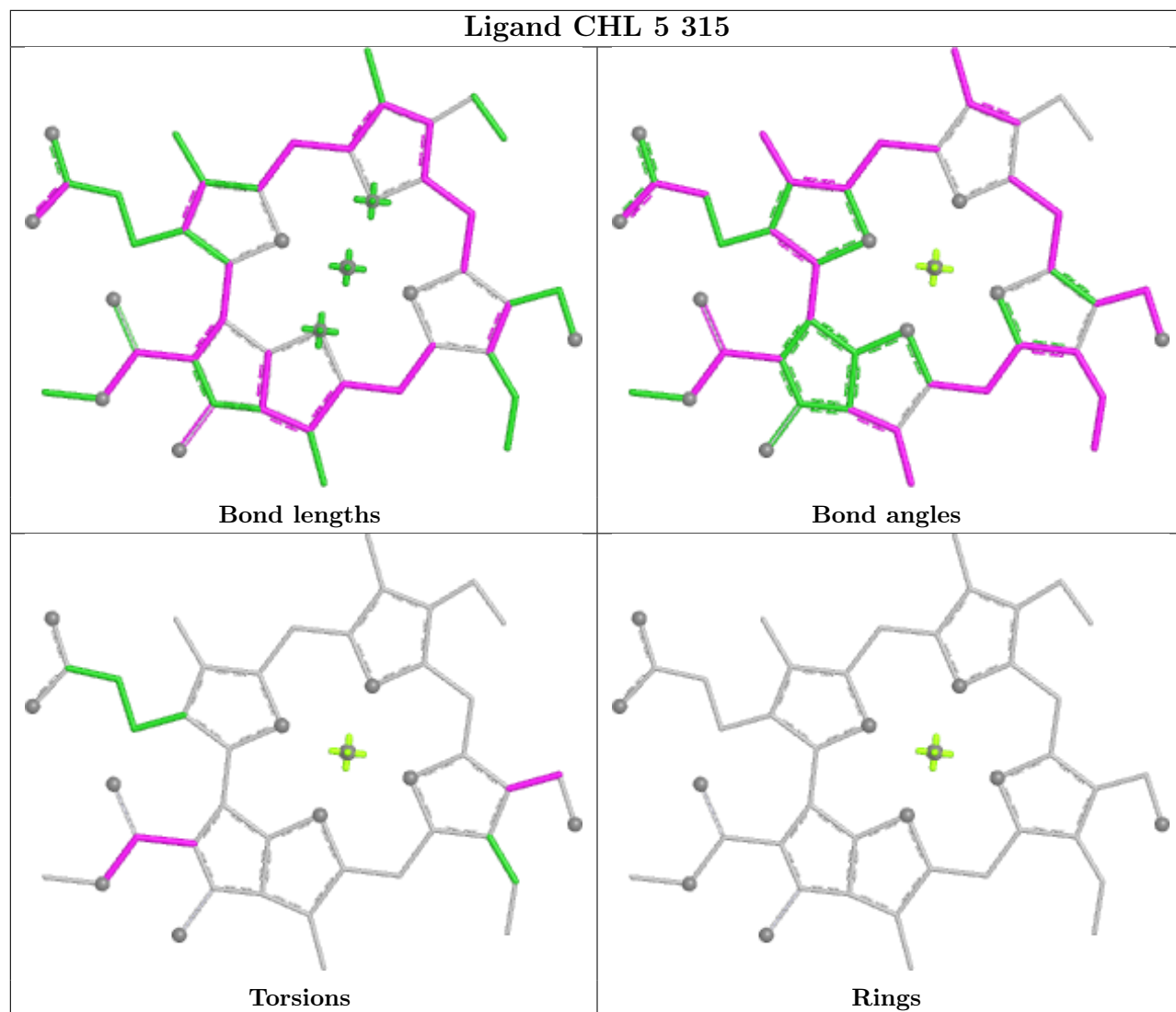


Torsions

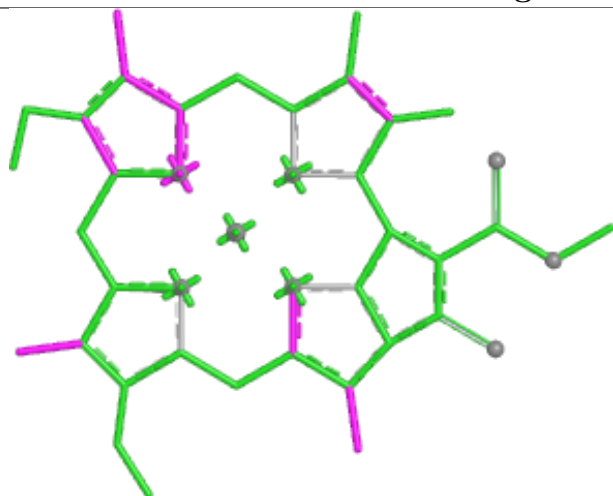


Rings

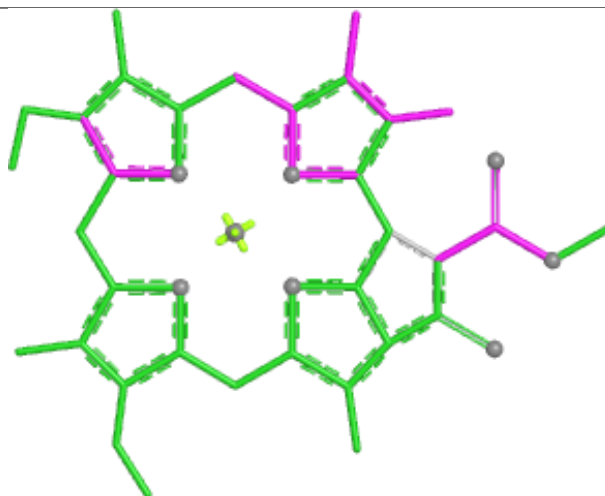
Ligand CHL 5 315



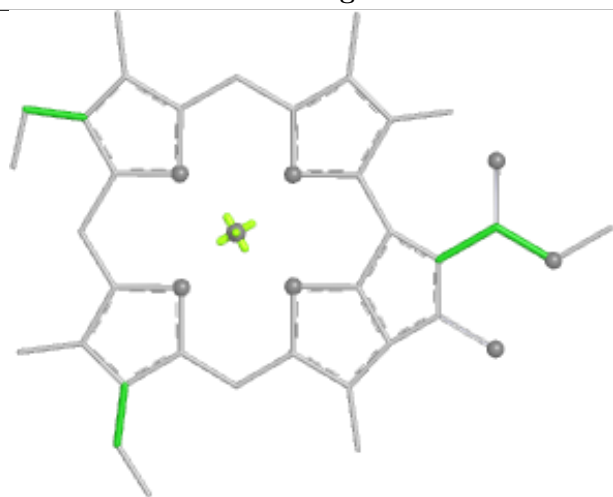
Ligand CLA B 819



Bond lengths



Bond angles

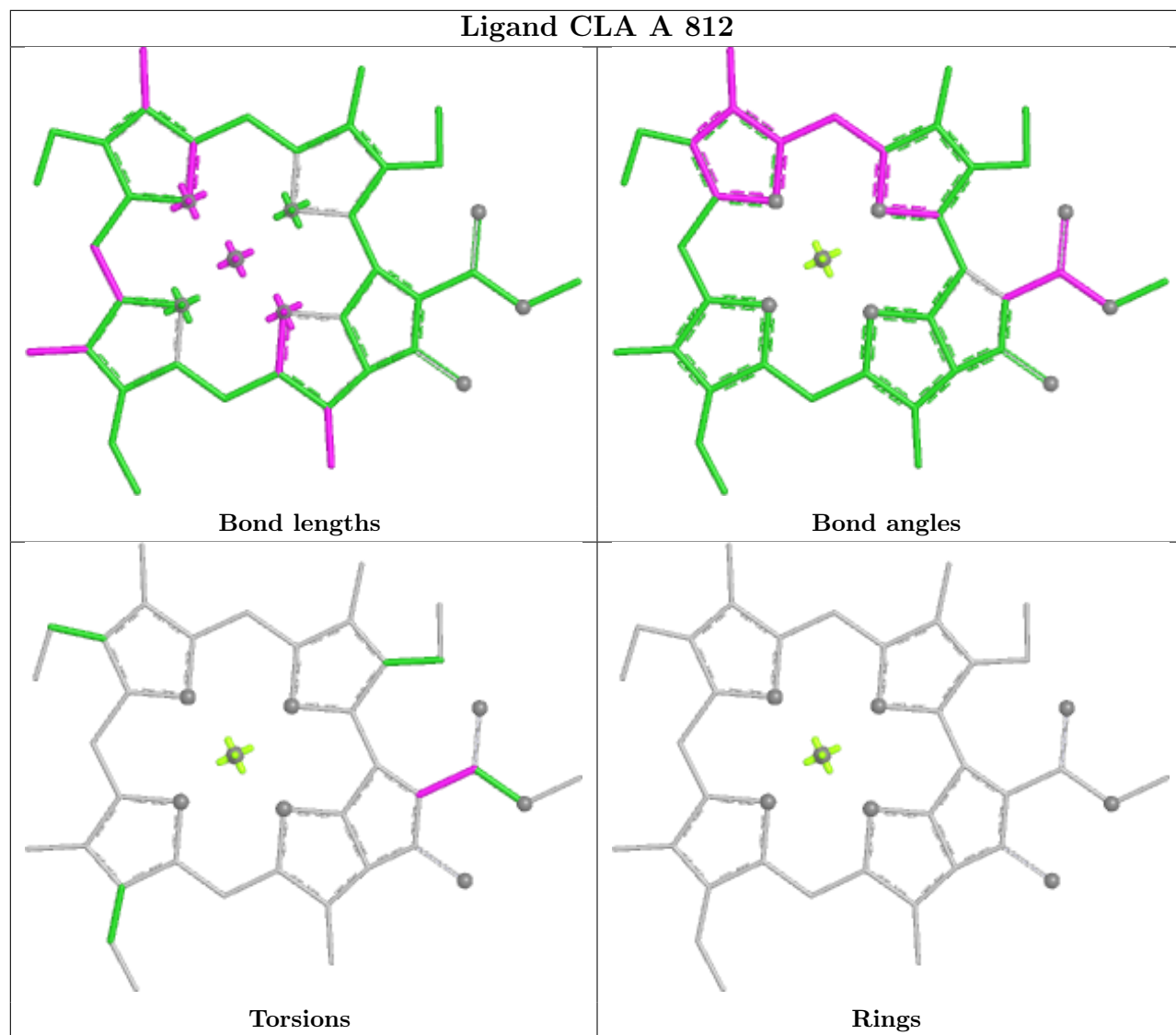


Torsions

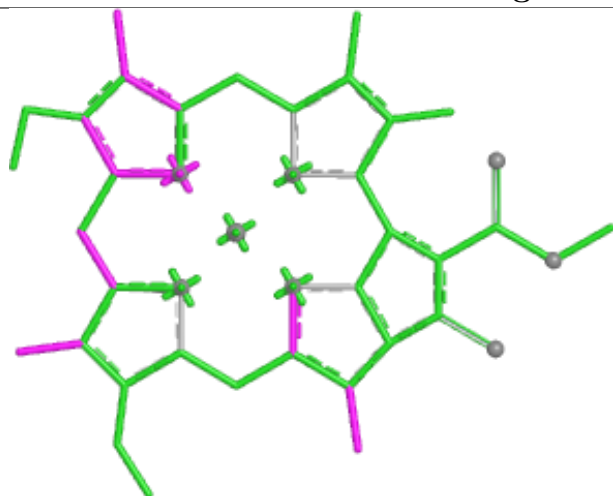


Rings

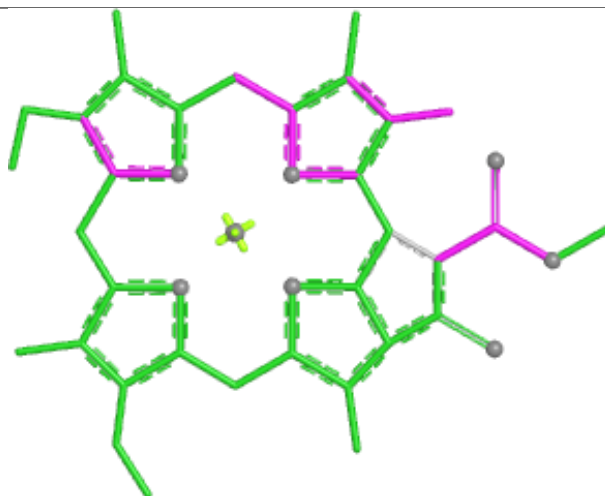
Ligand CLA A 812



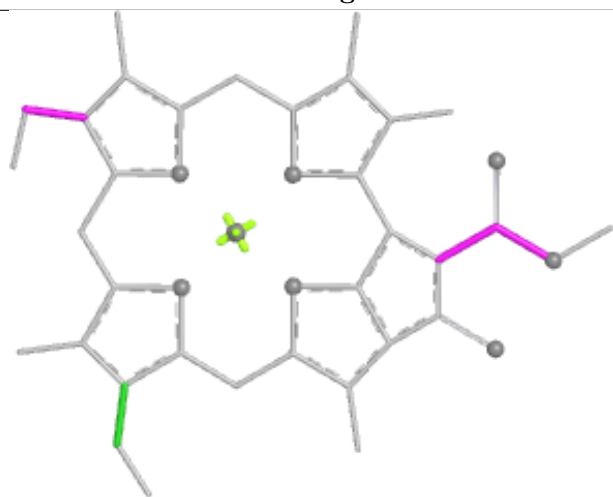
Ligand CLA K 202



Bond lengths



Bond angles

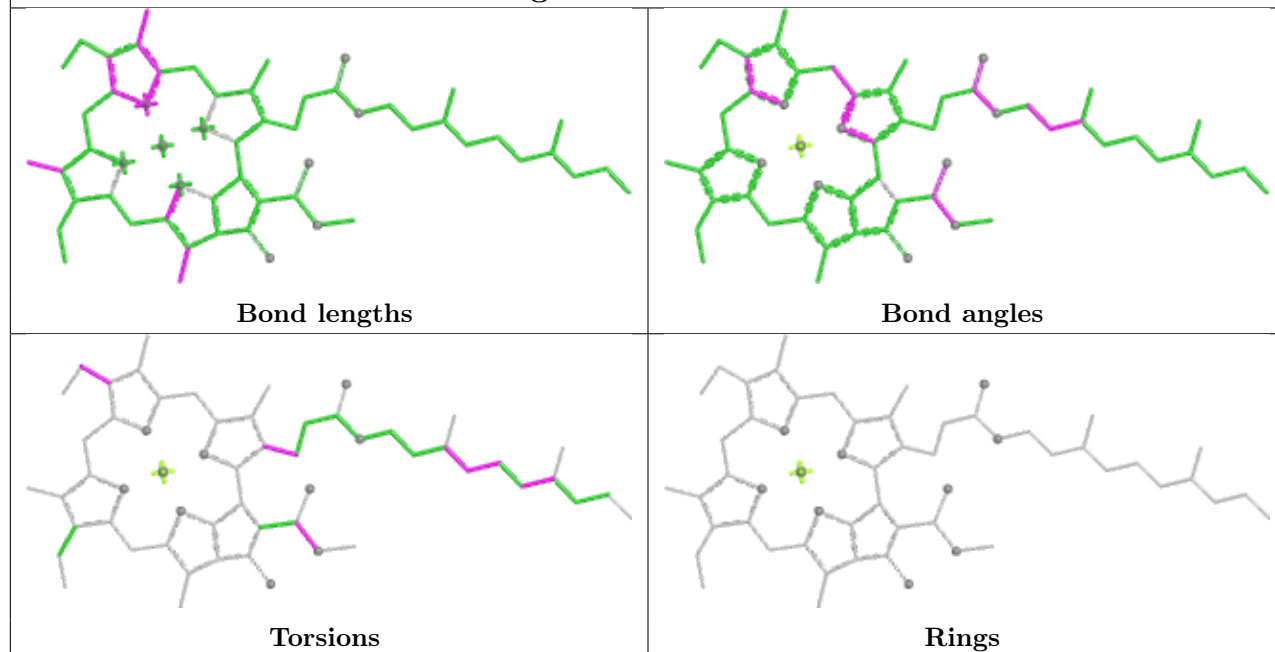


Torsions

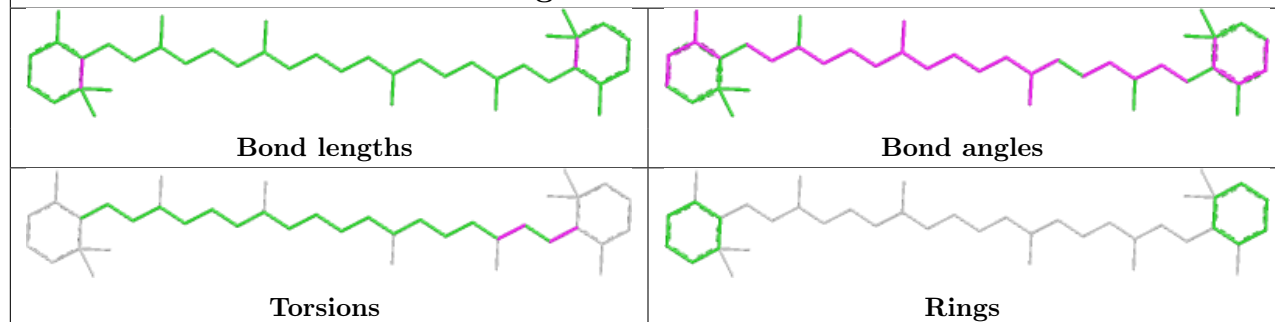


Rings

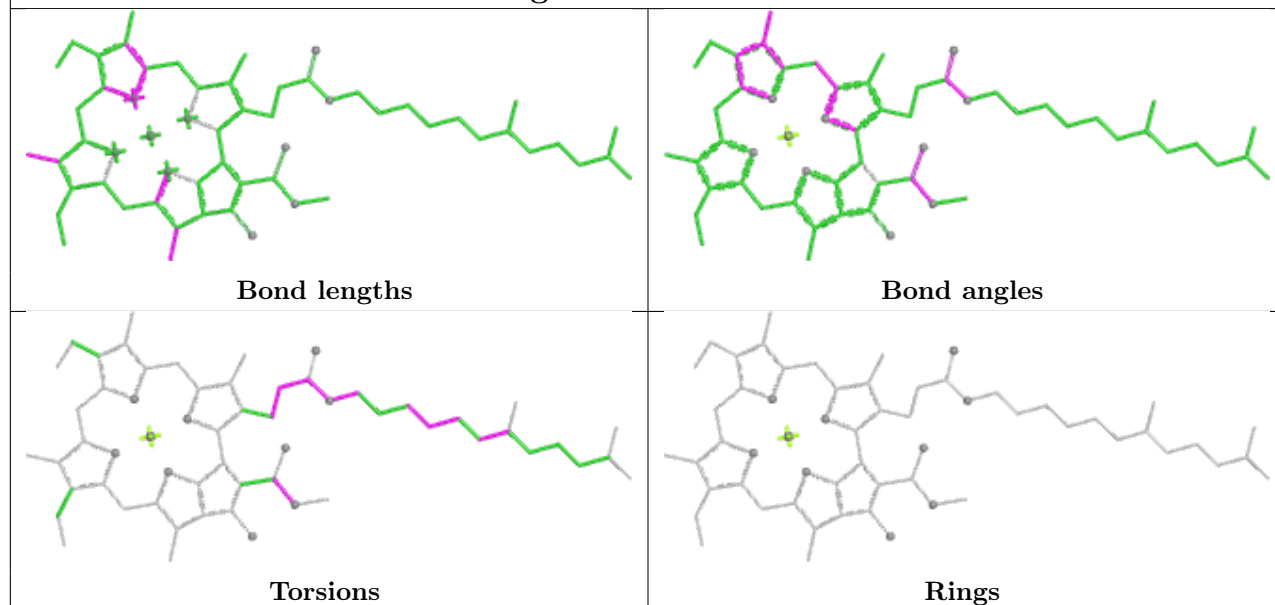
Ligand CLA A 852

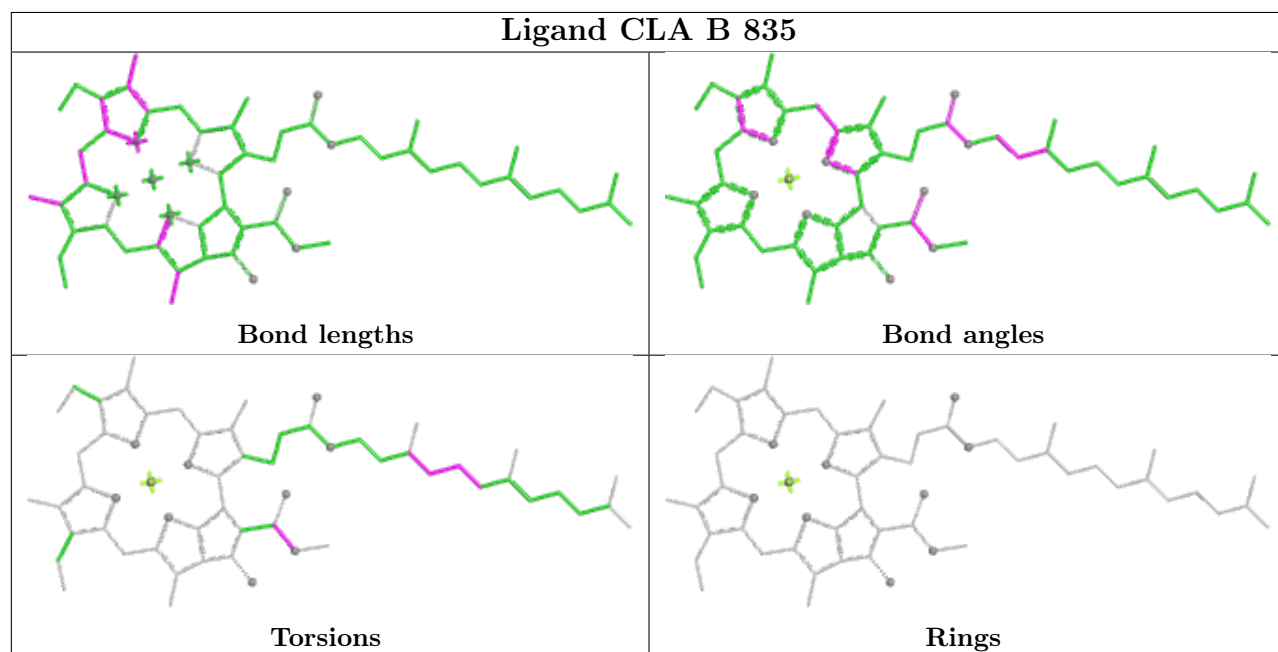
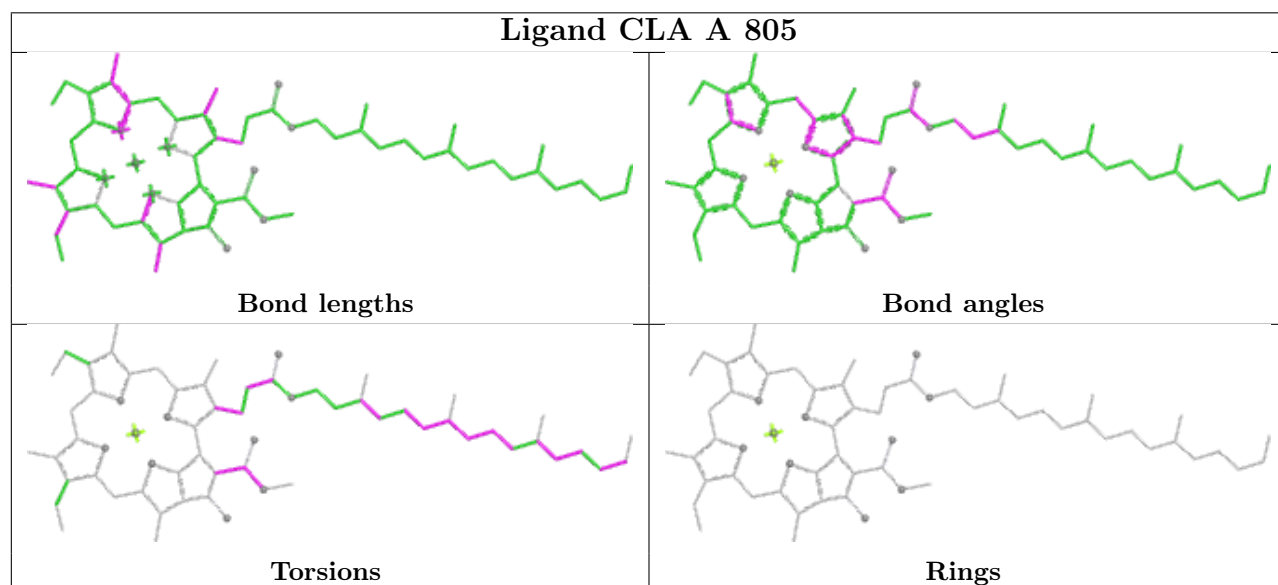
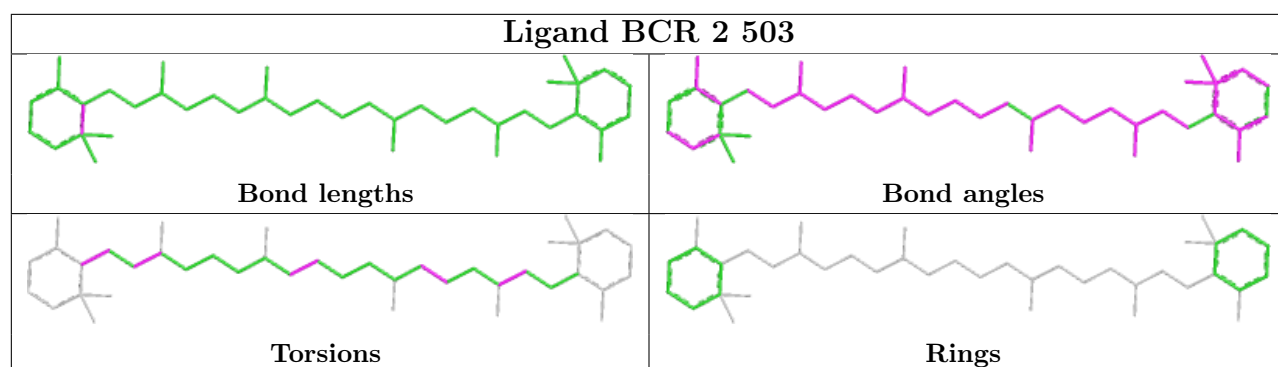


Ligand BCR I 101

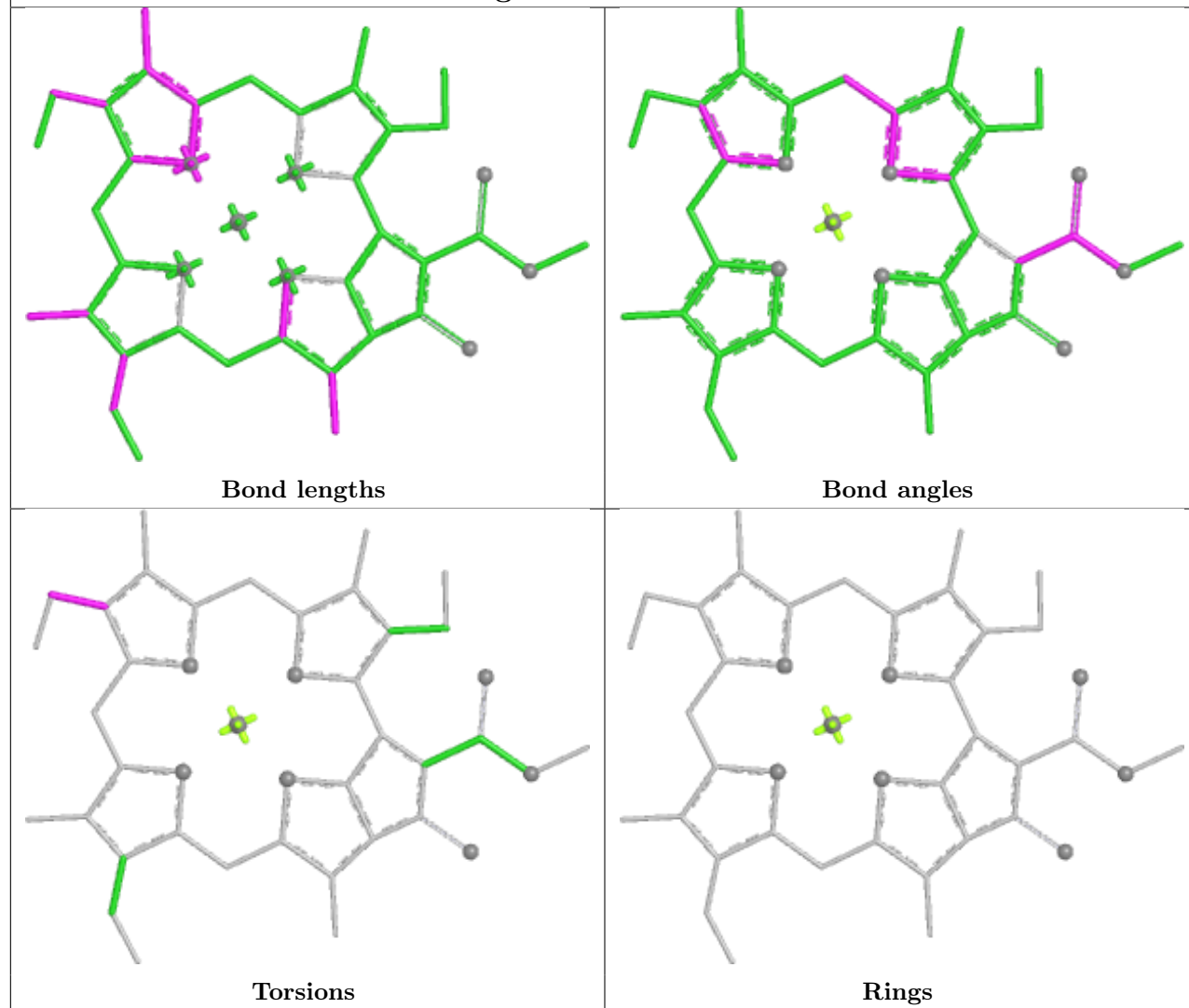


Ligand CLA A 816

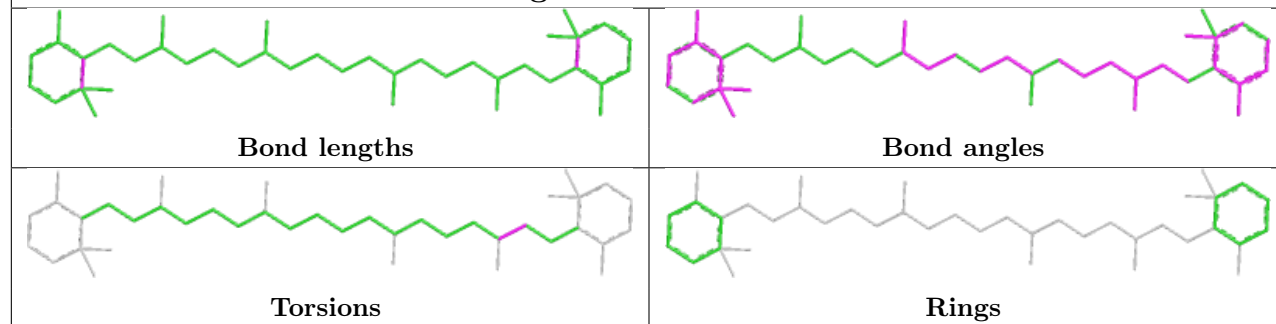


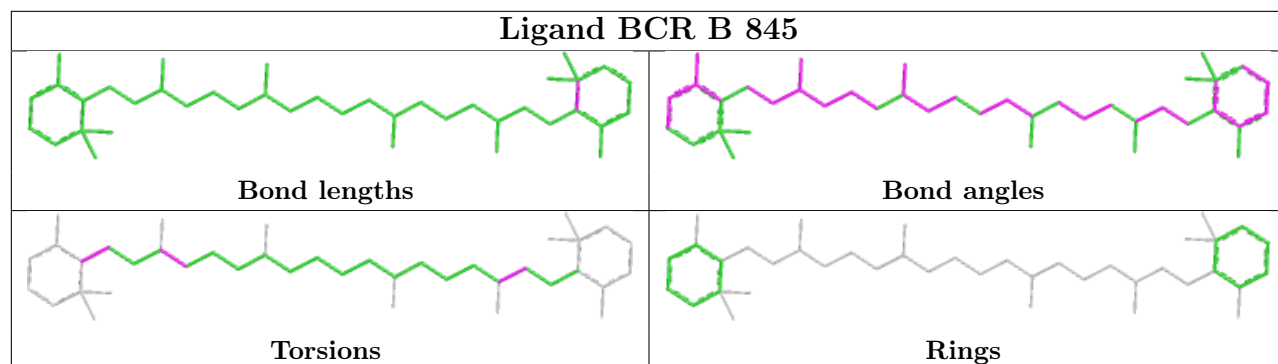
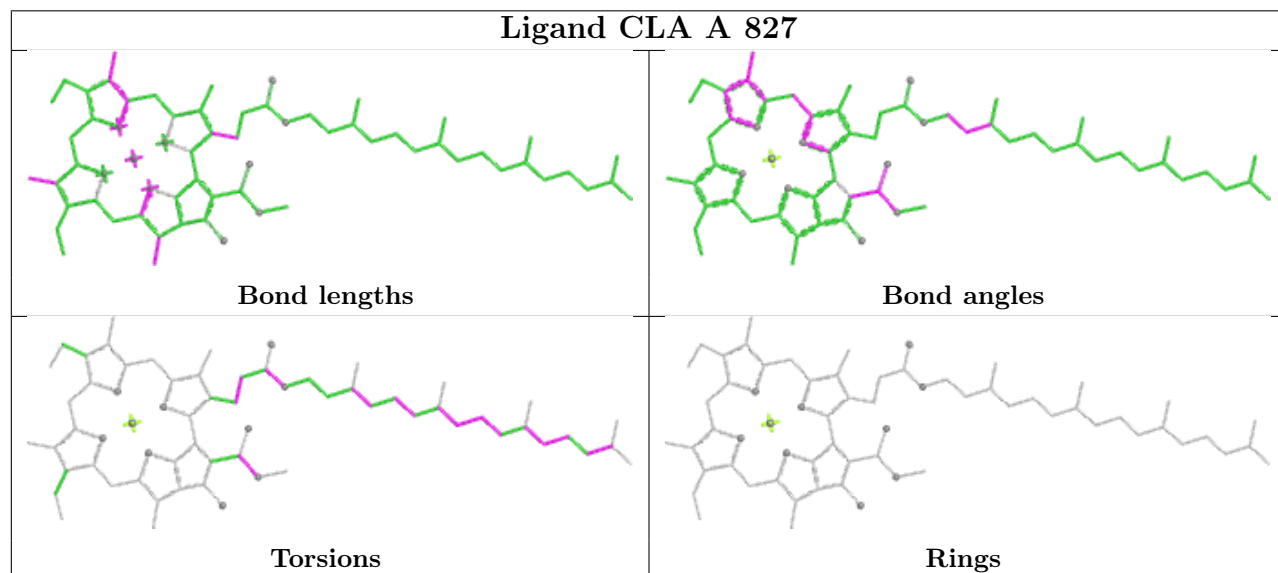
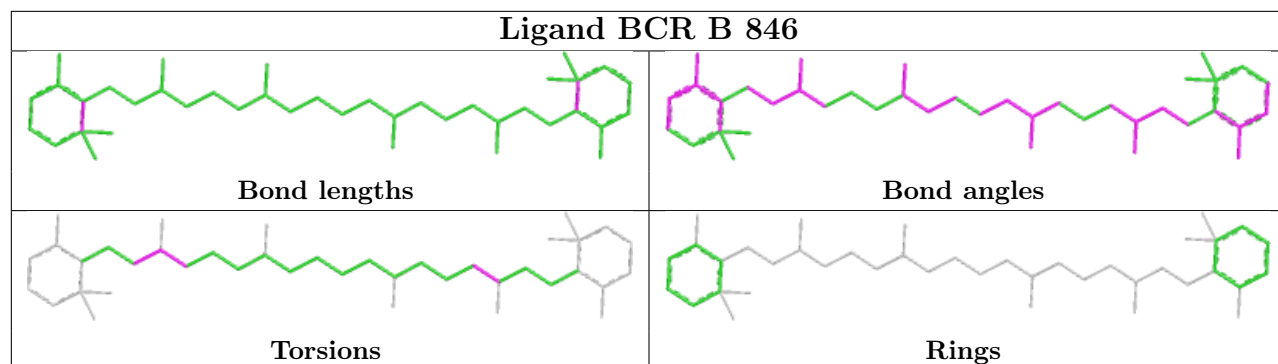


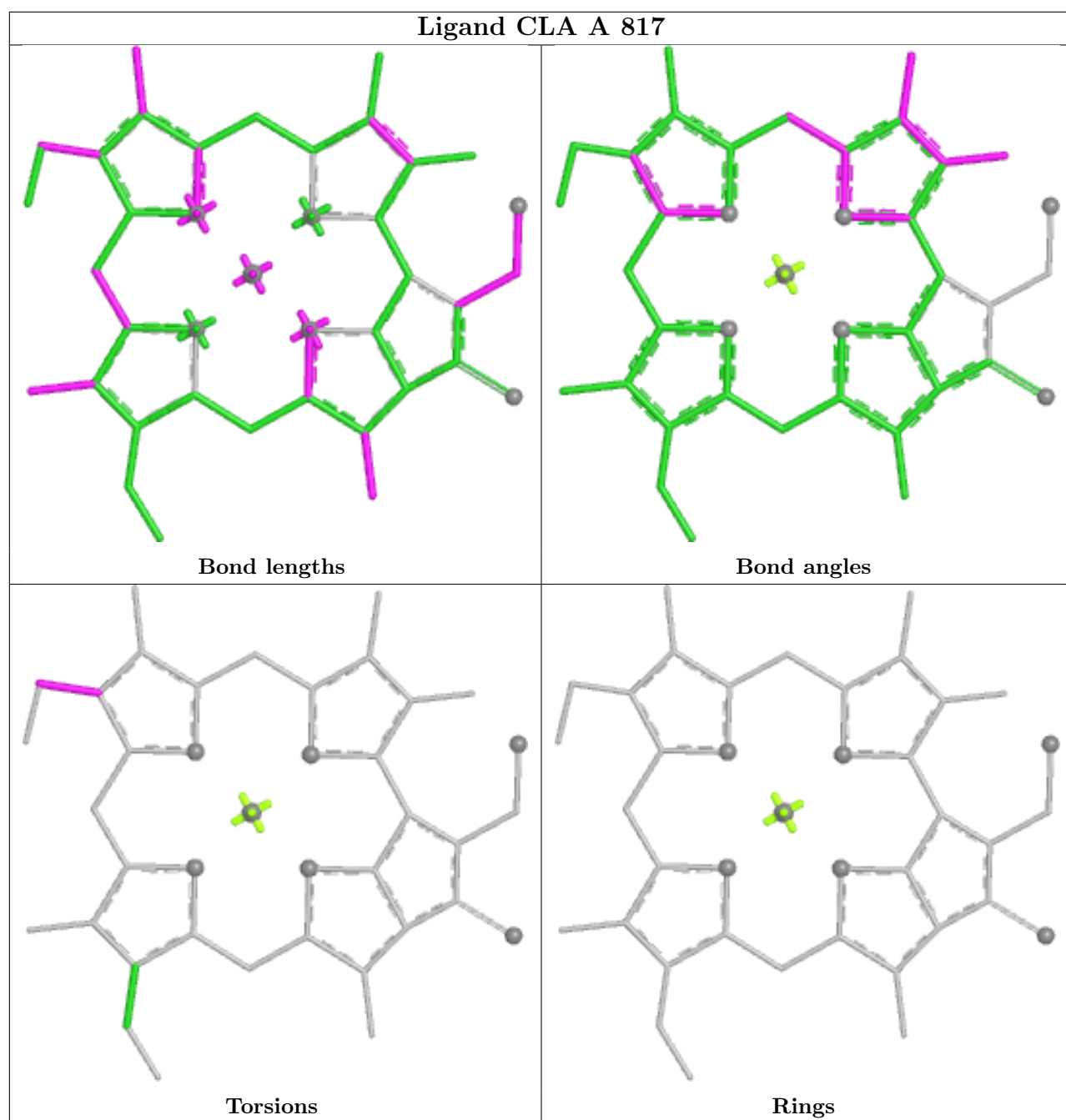
Ligand CLA A 814



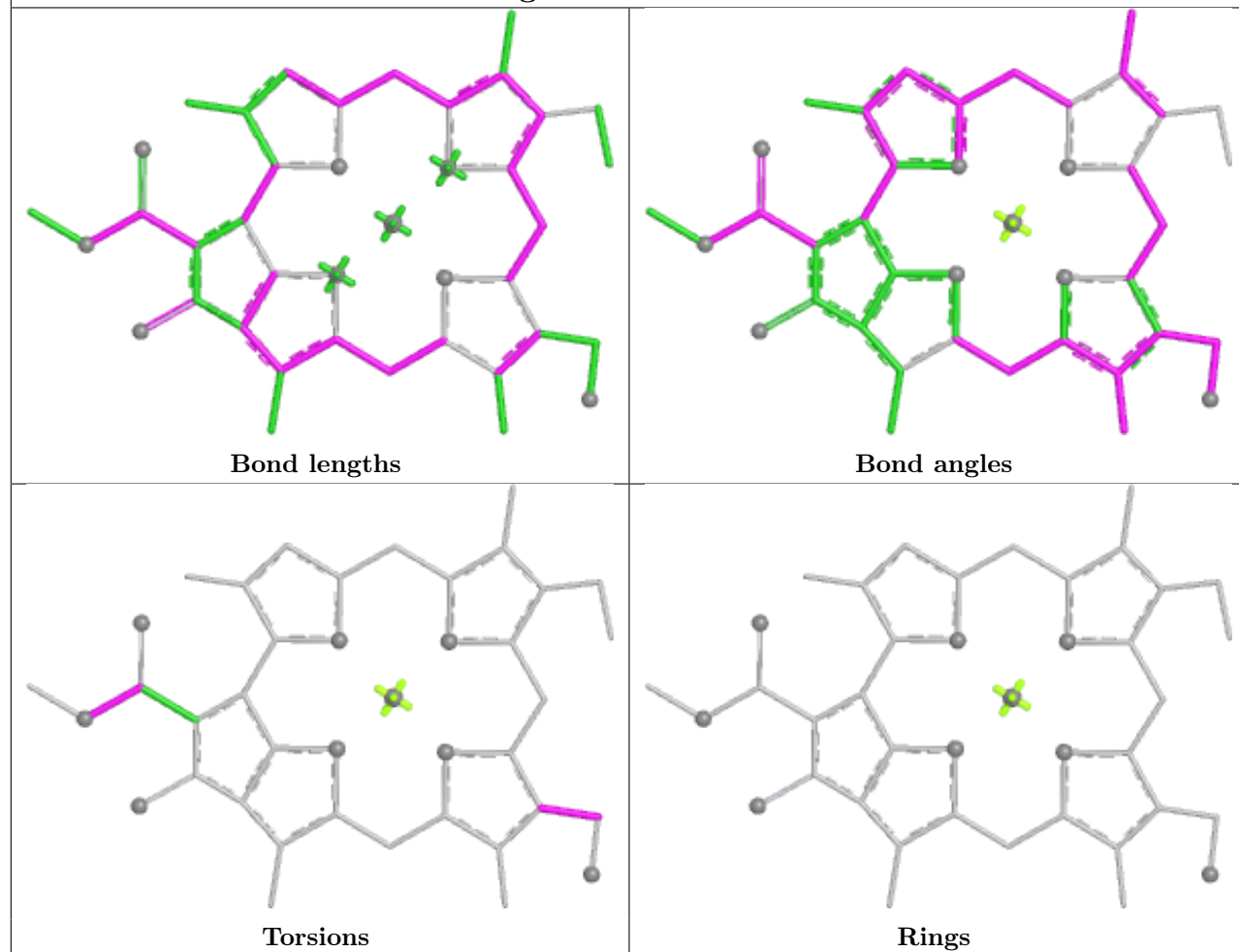
Ligand BCR A 853



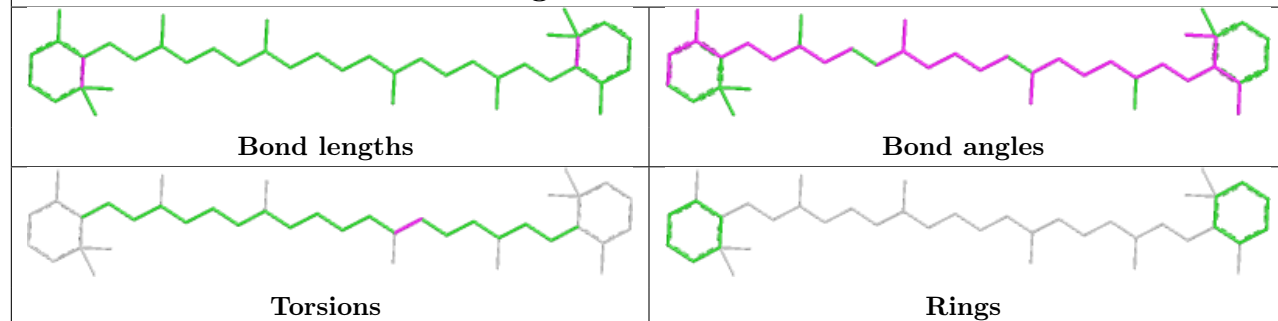




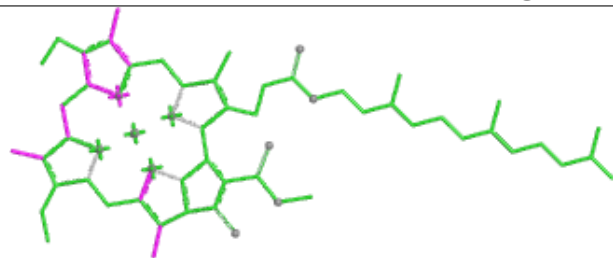
Ligand CHL 5 317



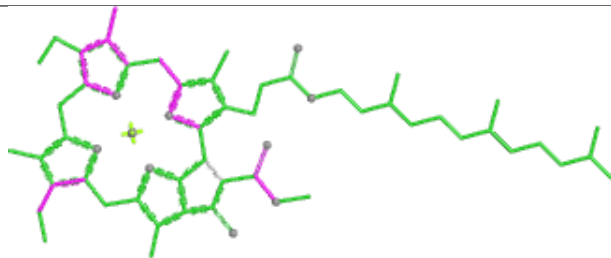
Ligand BCR B 848



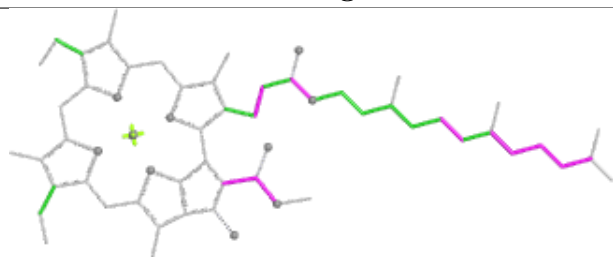
Ligand CLA 5 308



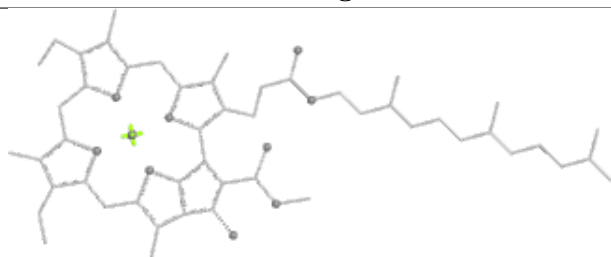
Bond lengths



Bond angles

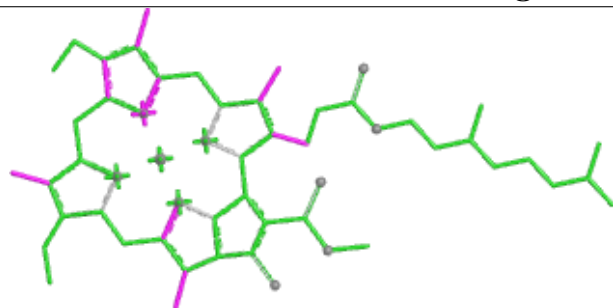


Torsions

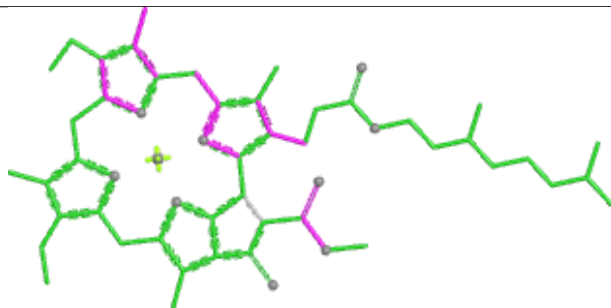


Rings

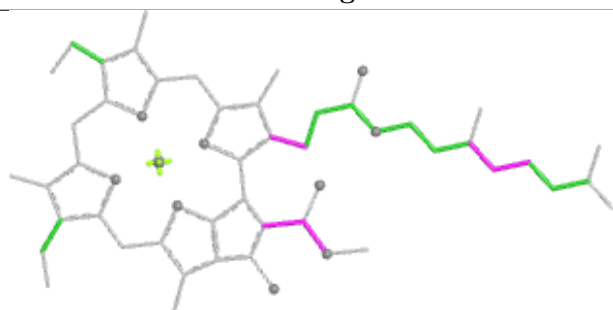
Ligand CLA B 811



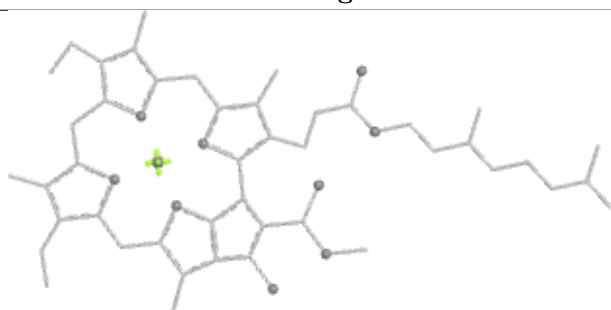
Bond lengths



Bond angles

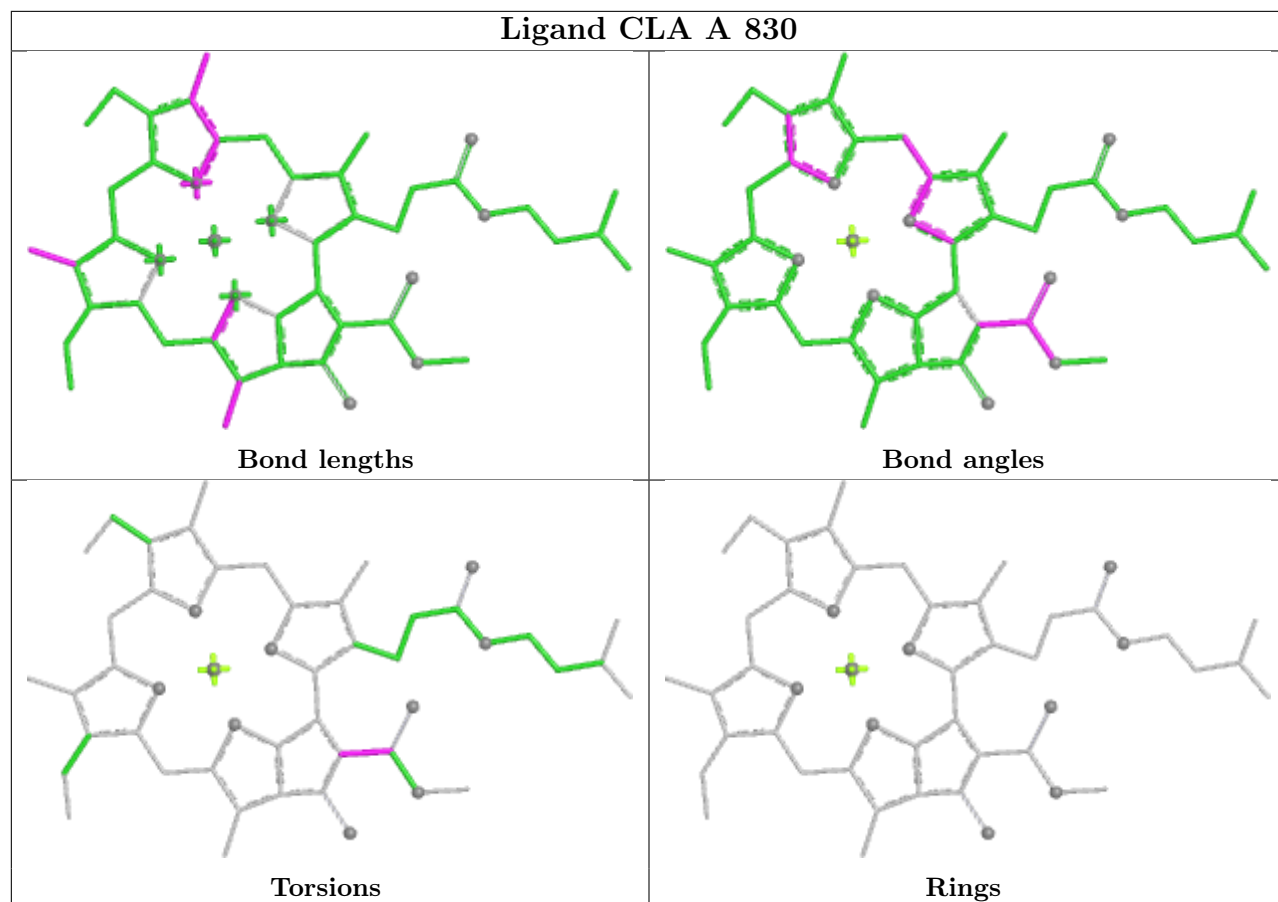


Torsions

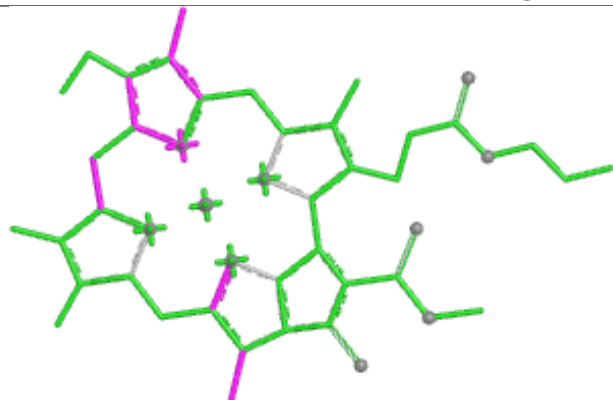


Rings

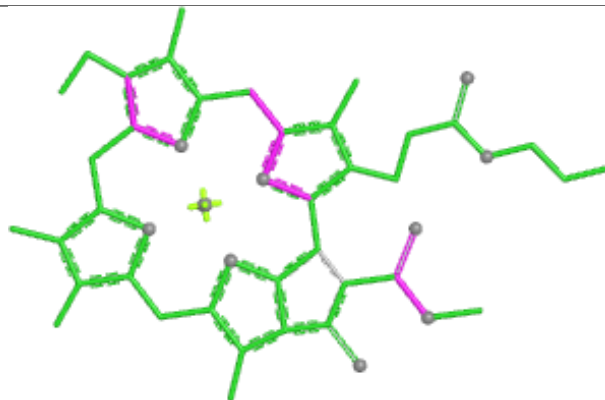
Ligand CLA A 830



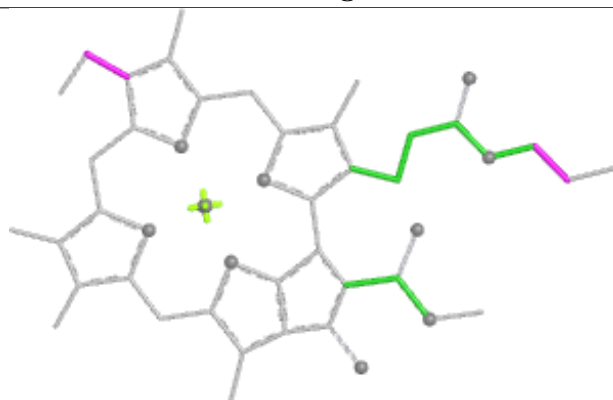
Ligand CLA 2 508



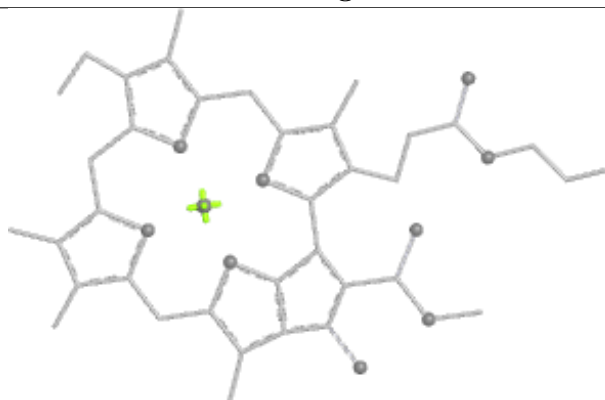
Bond lengths



Bond angles

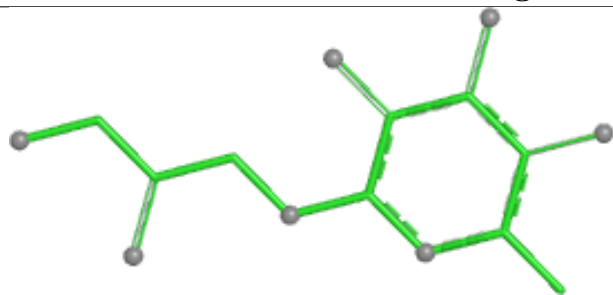


Torsions

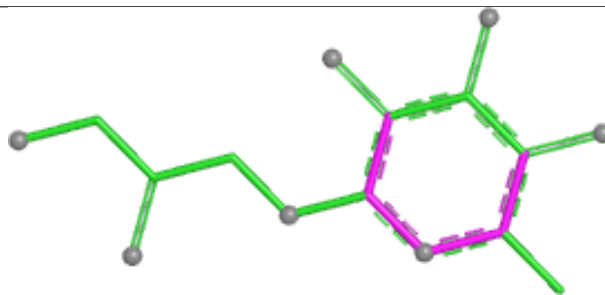


Rings

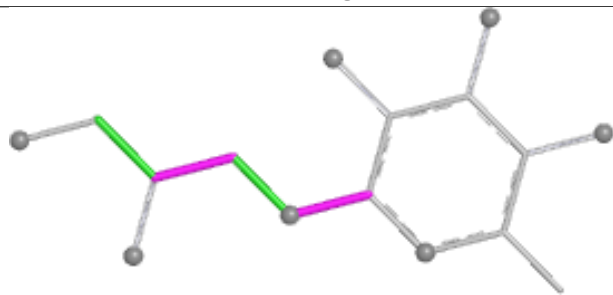
Ligand LMG 2 518



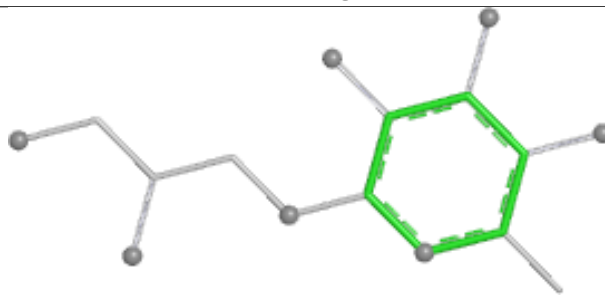
Bond lengths



Bond angles

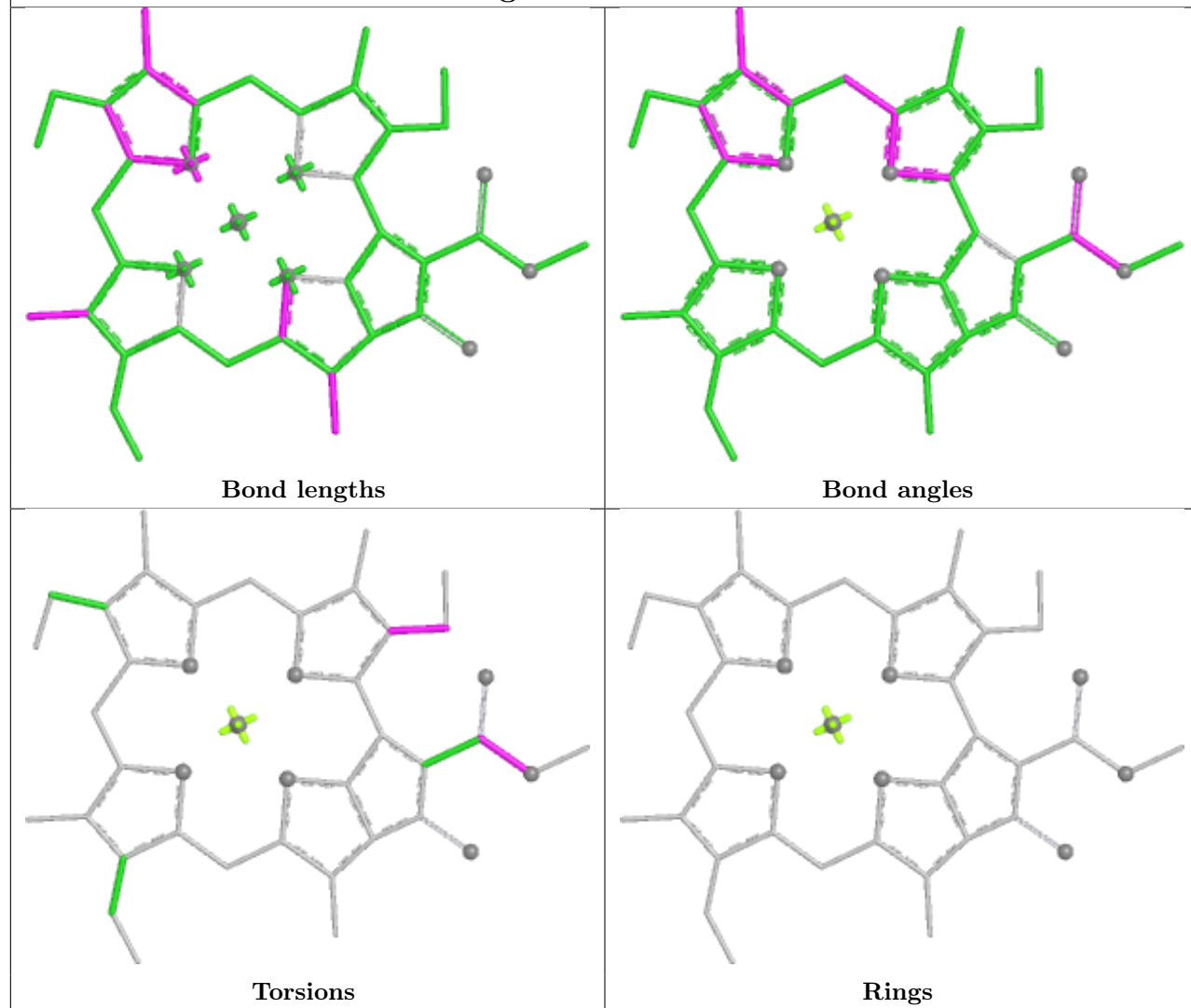


Torsions

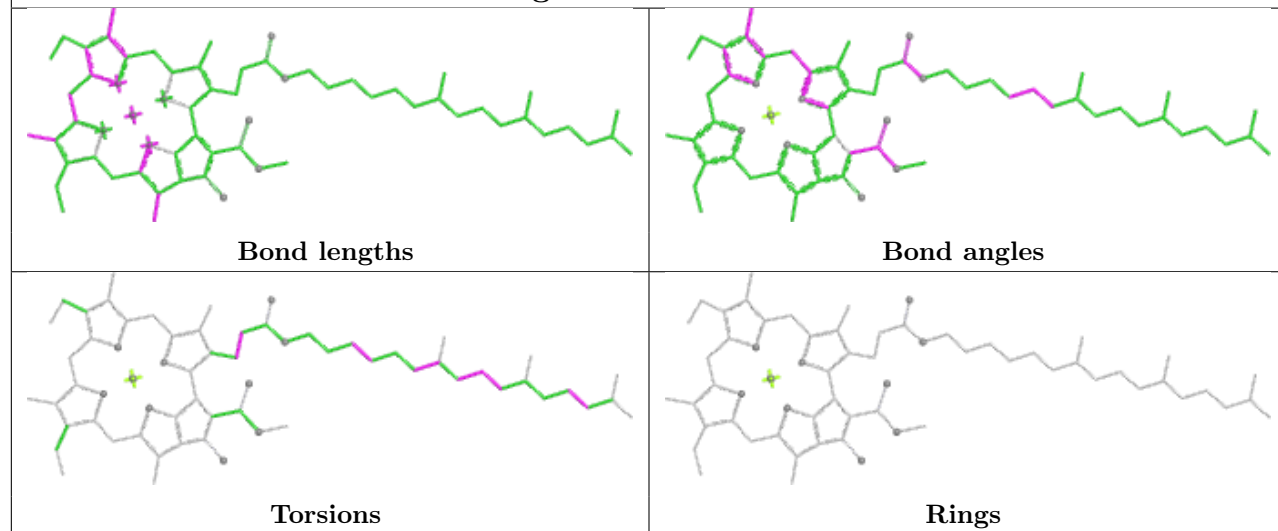


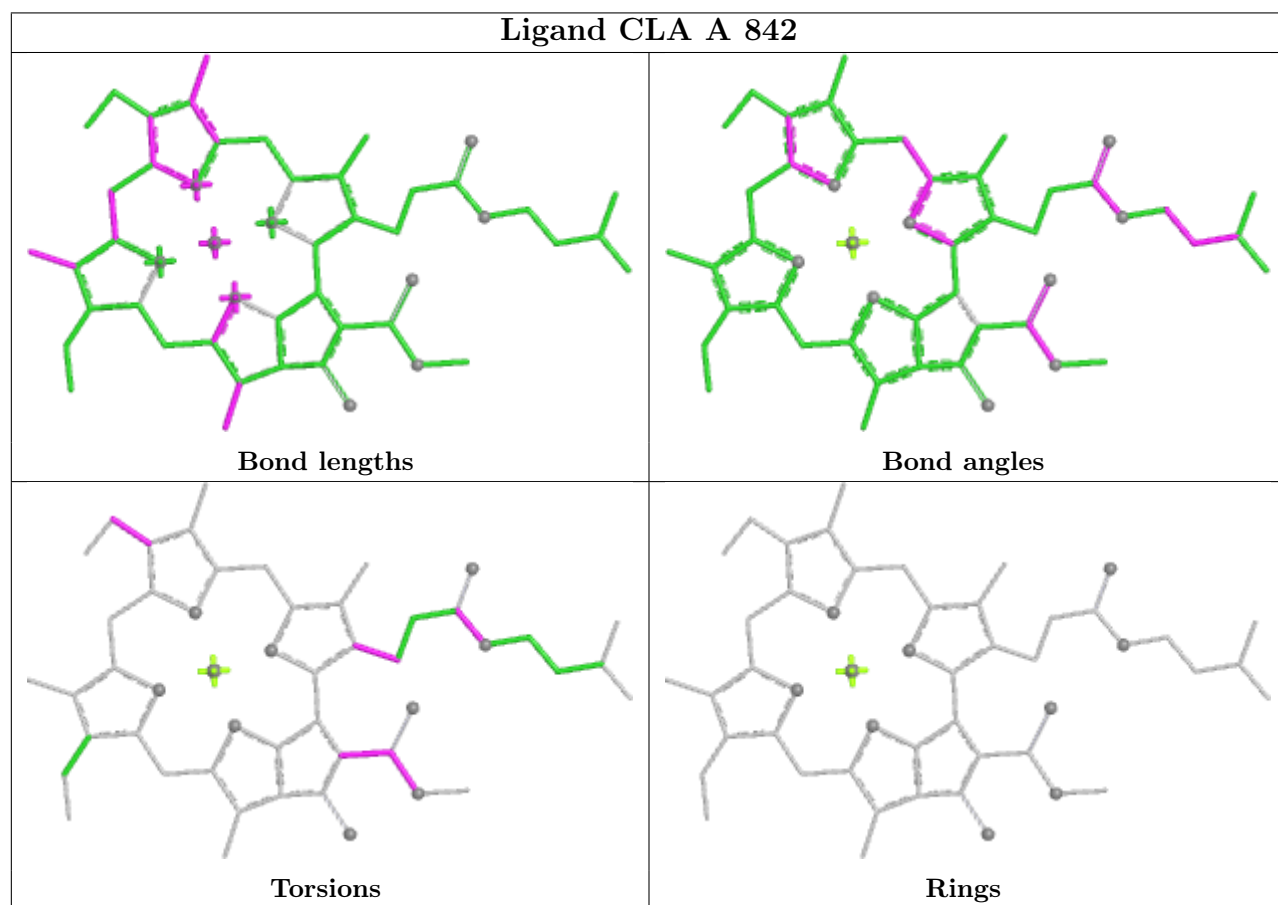
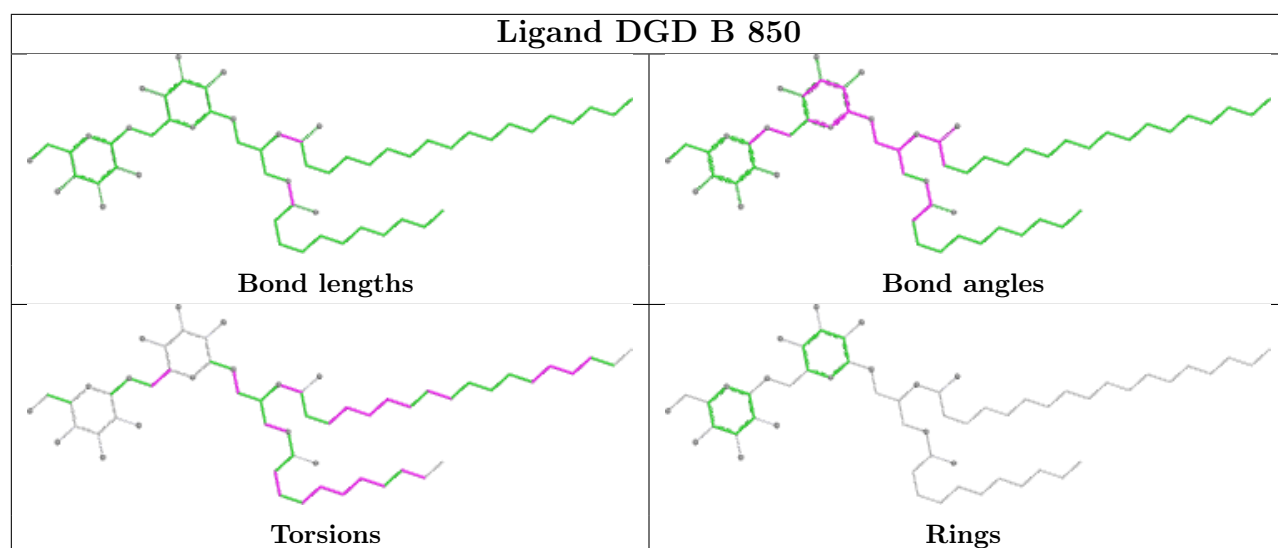
Rings

Ligand CLA 5 311

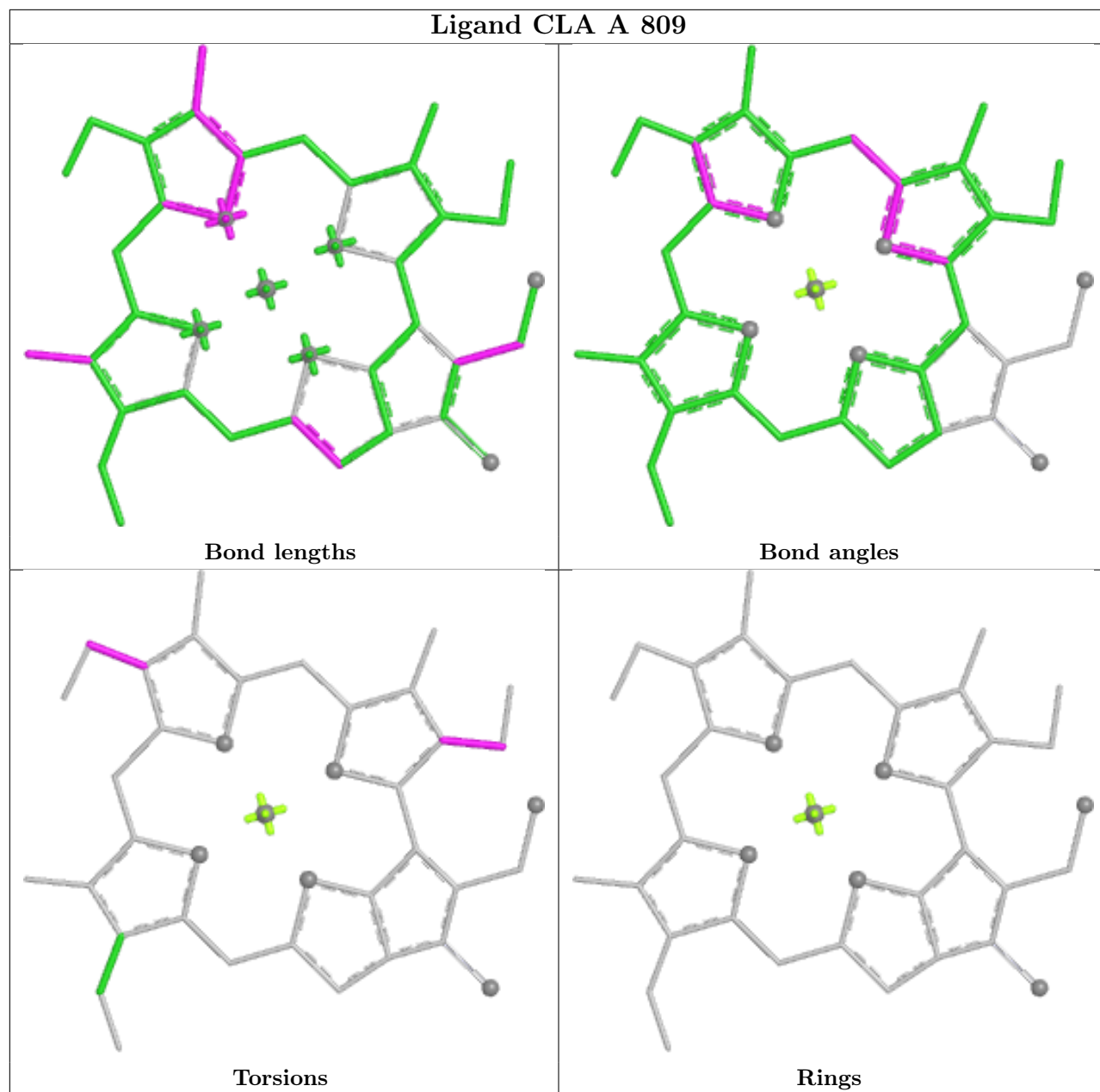


Ligand CLA B 802

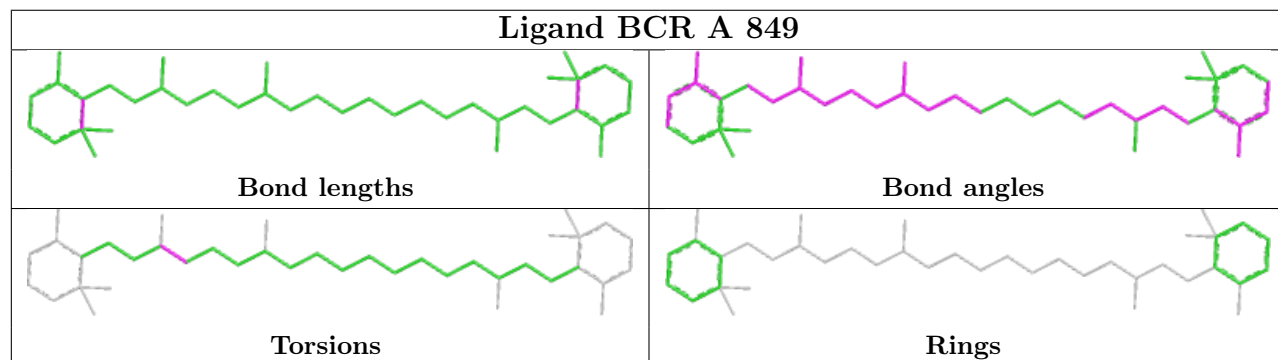




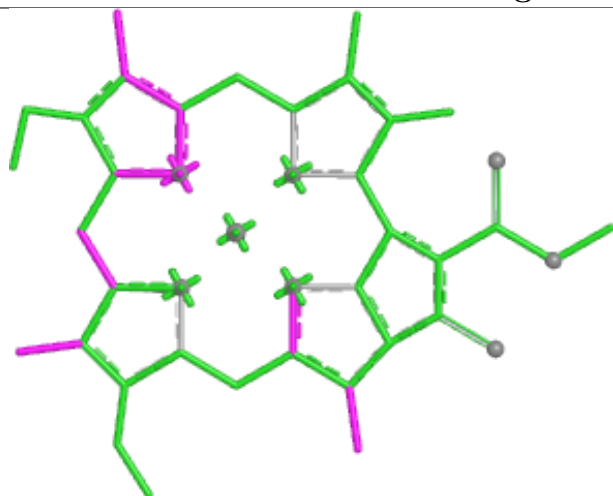
Ligand CLA A 809



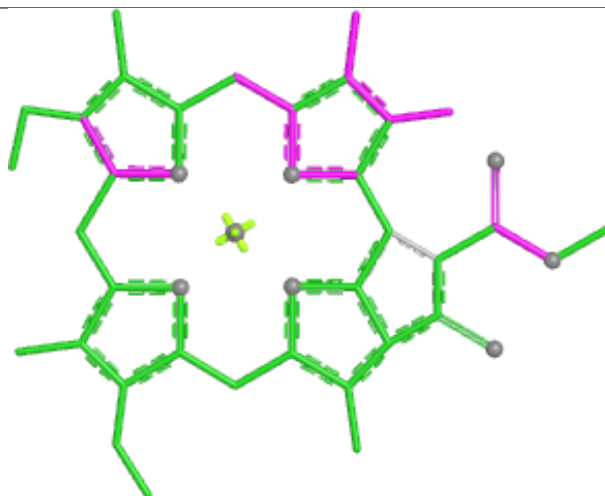
Ligand BCR A 849



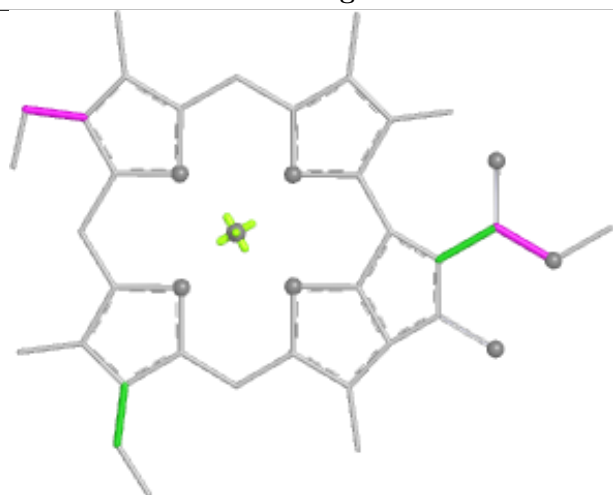
Ligand CLA B 805



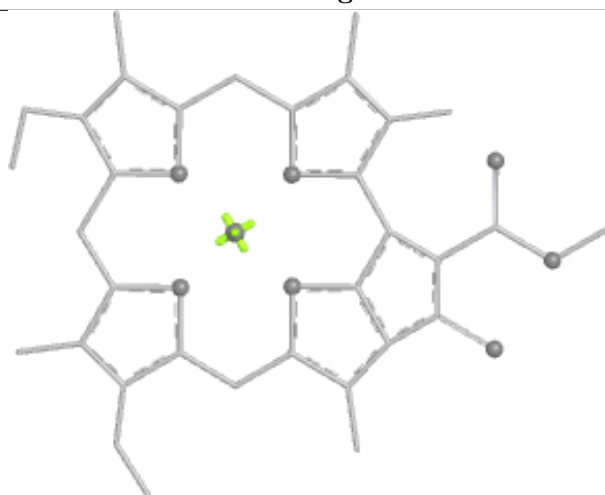
Bond lengths



Bond angles

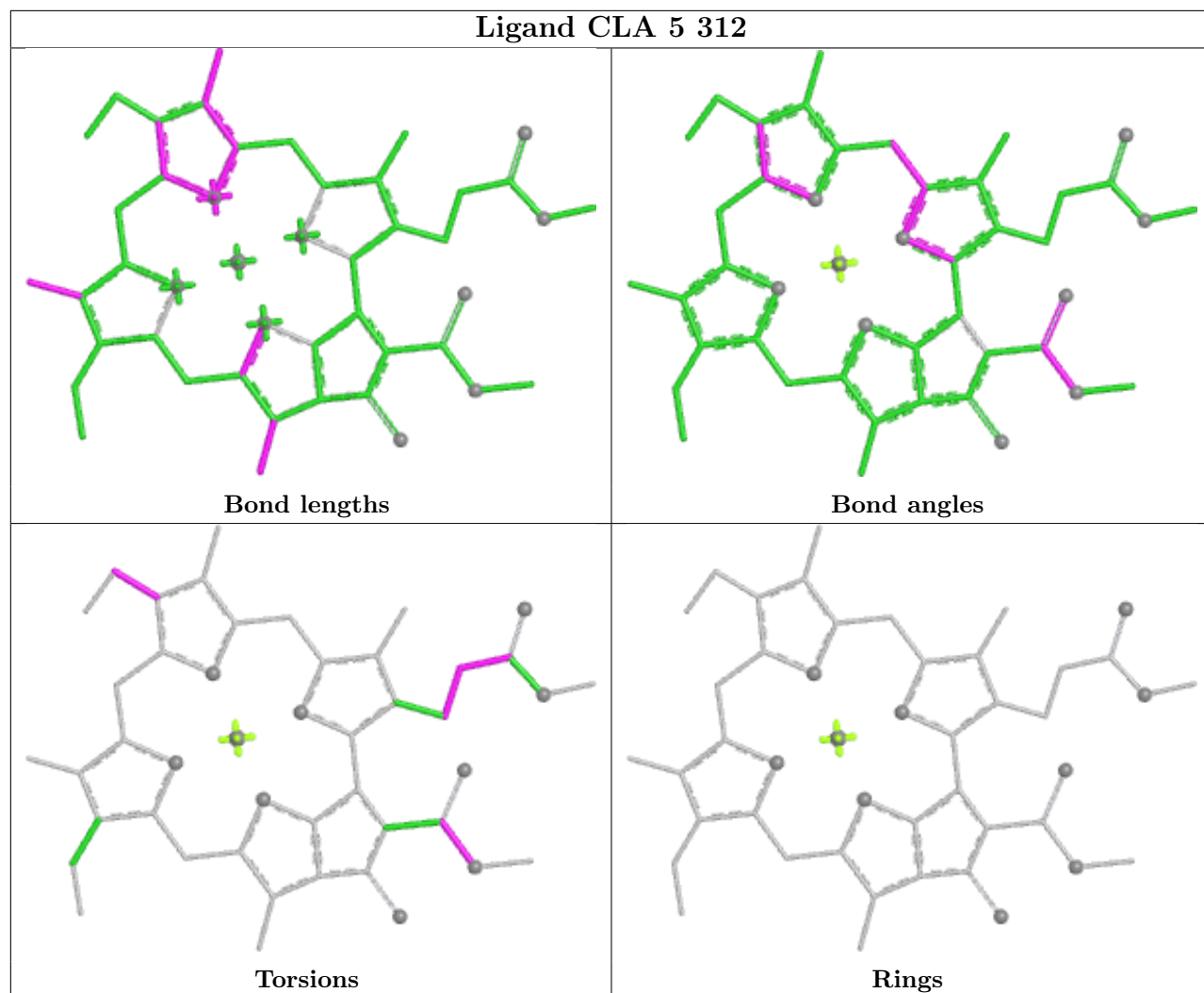


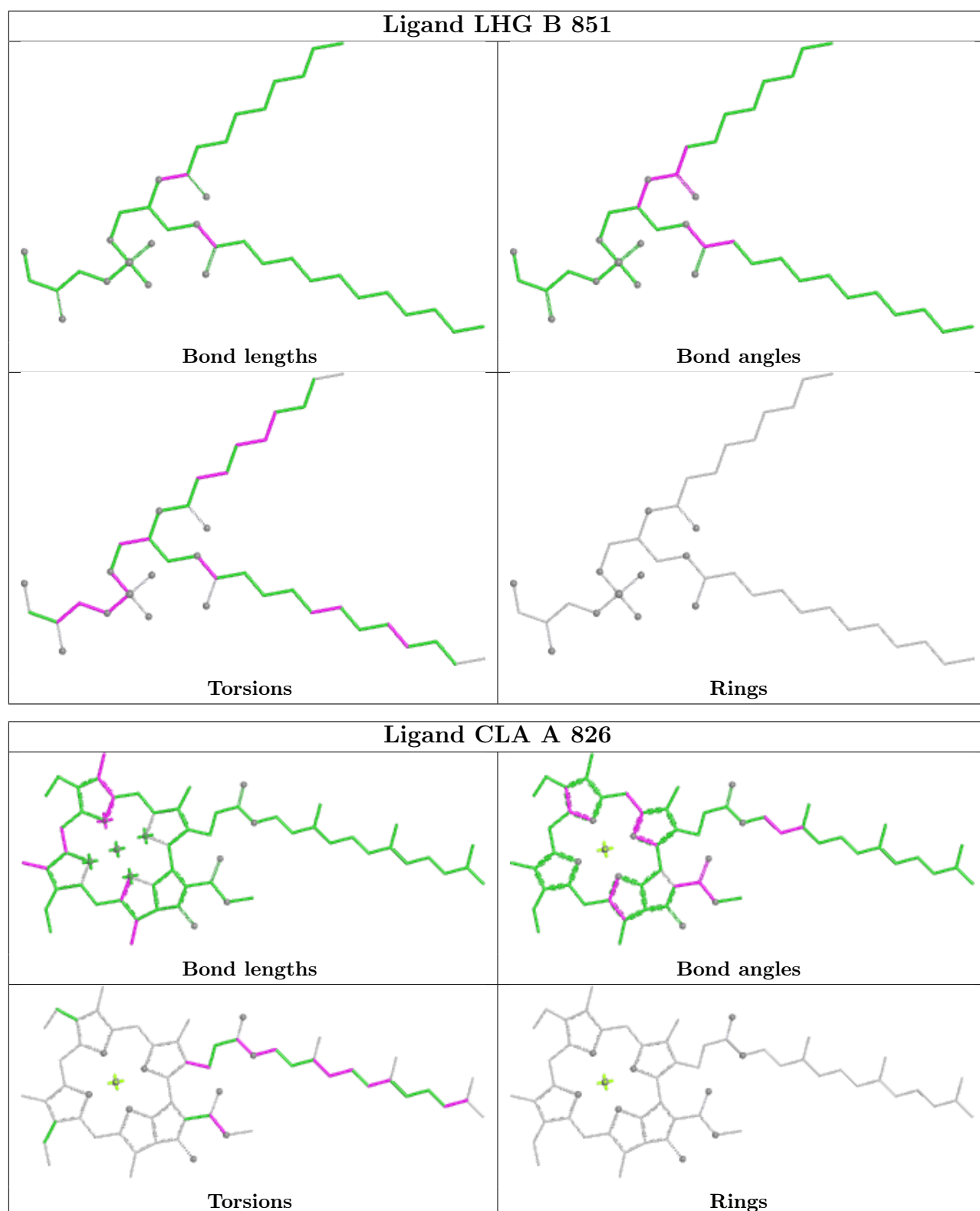
Torsions



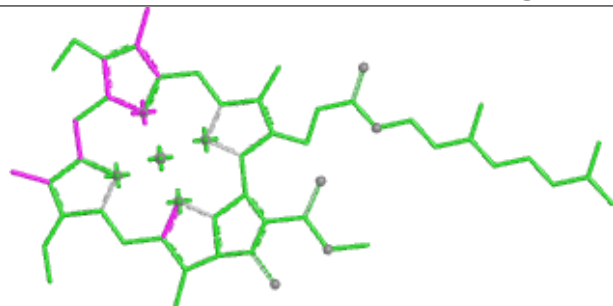
Rings

Ligand CLA 5 312

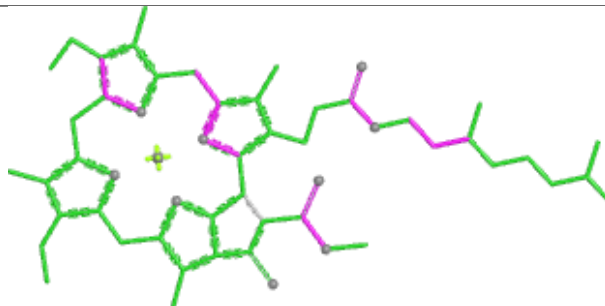




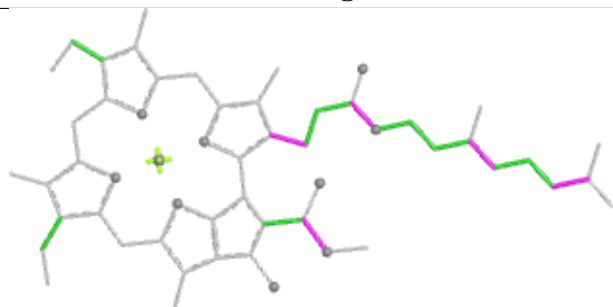
Ligand CLA 1 506



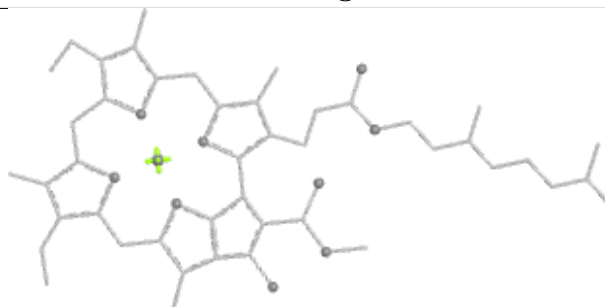
Bond lengths



Bond angles

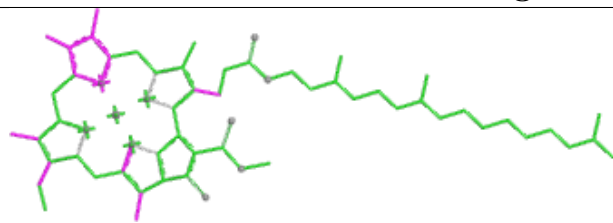


Torsions

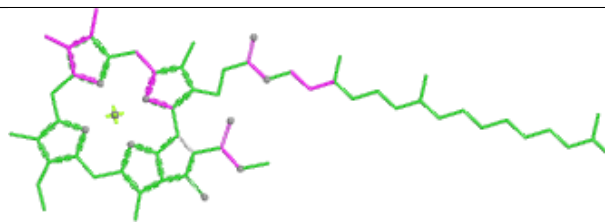


Rings

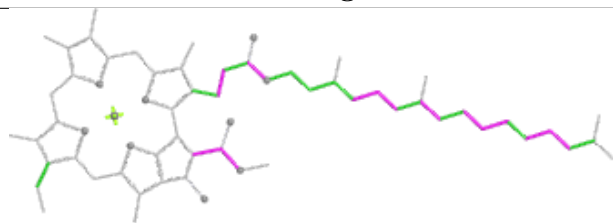
Ligand CLA A 831



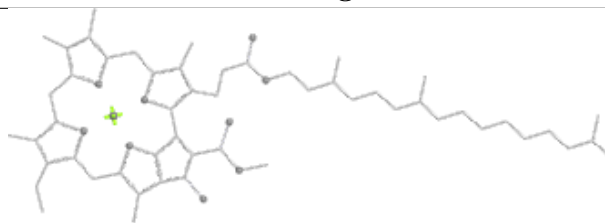
Bond lengths



Bond angles

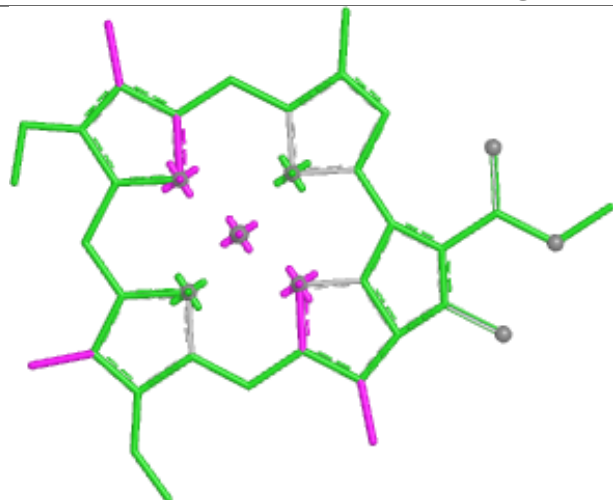


Torsions

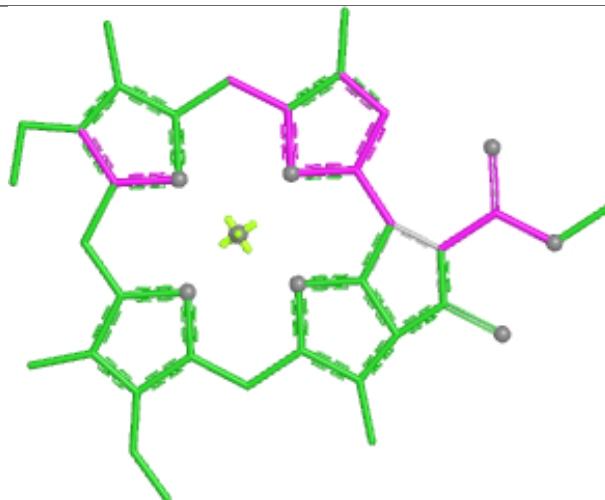


Rings

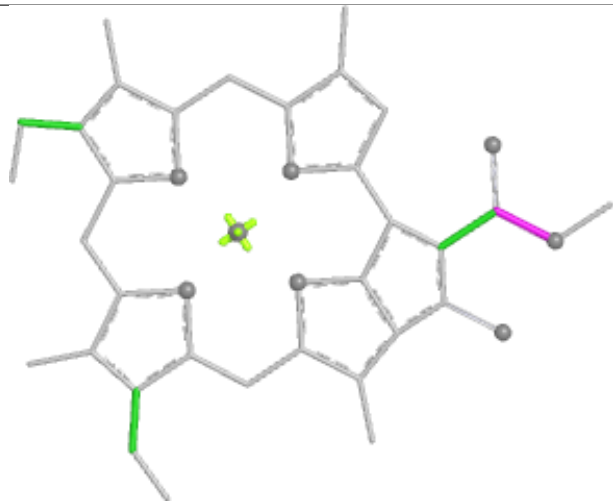
Ligand CLA B 829



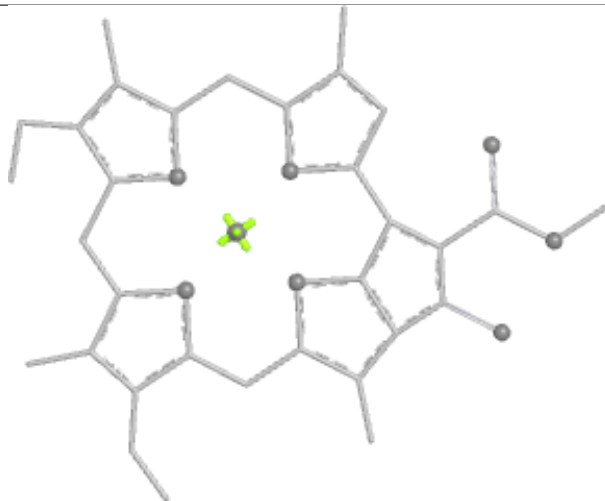
Bond lengths



Bond angles

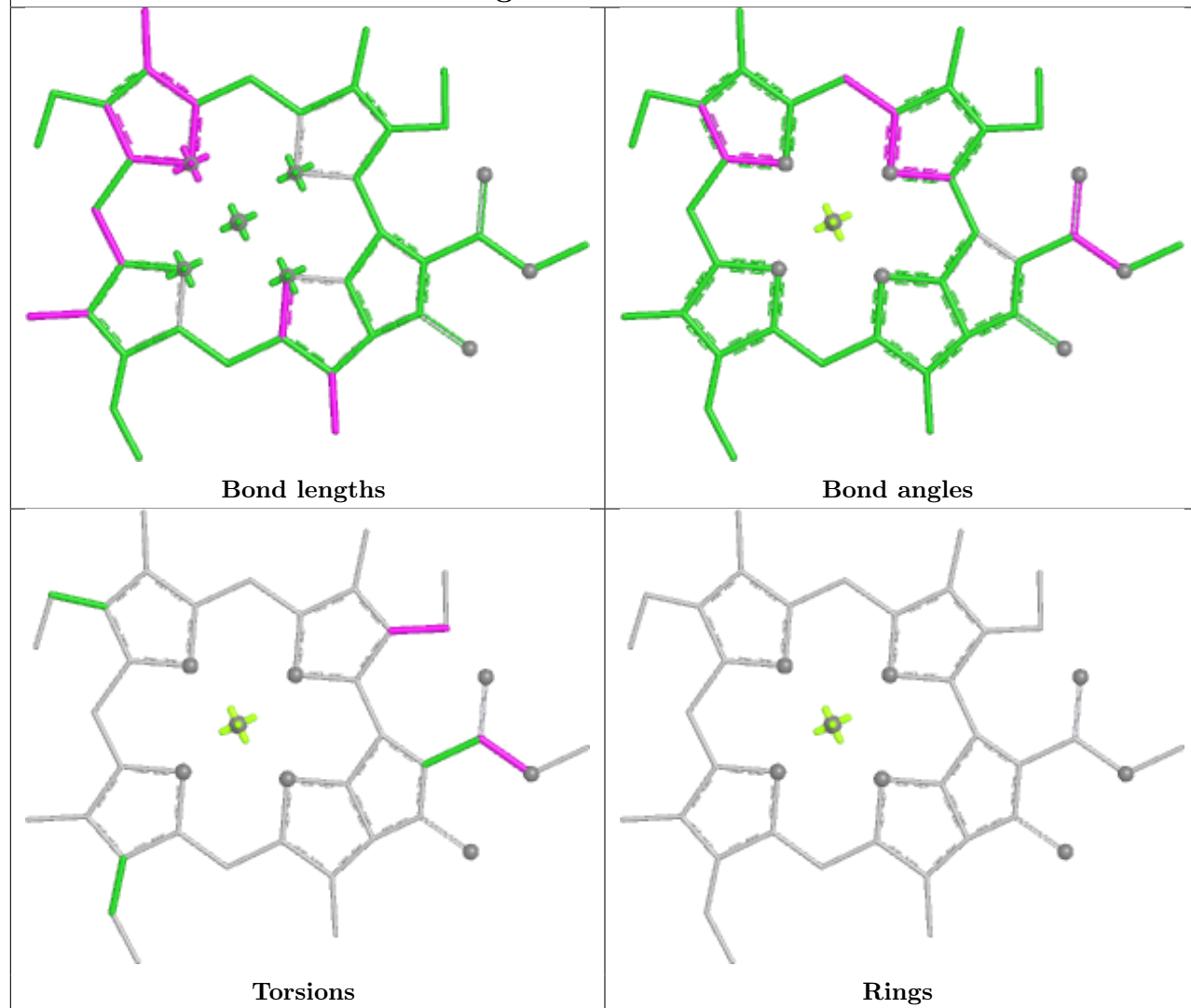


Torsions

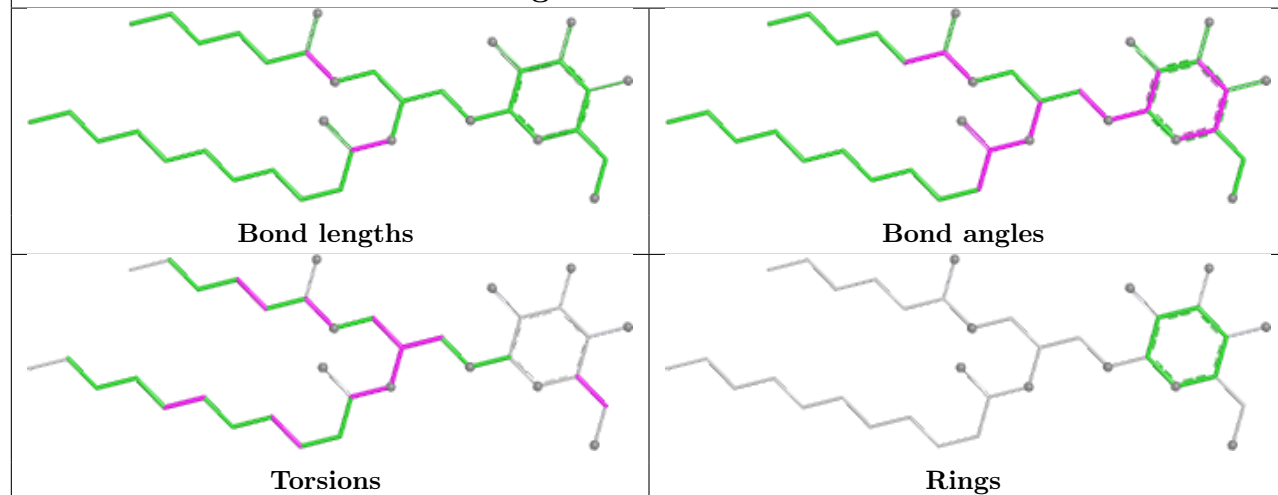


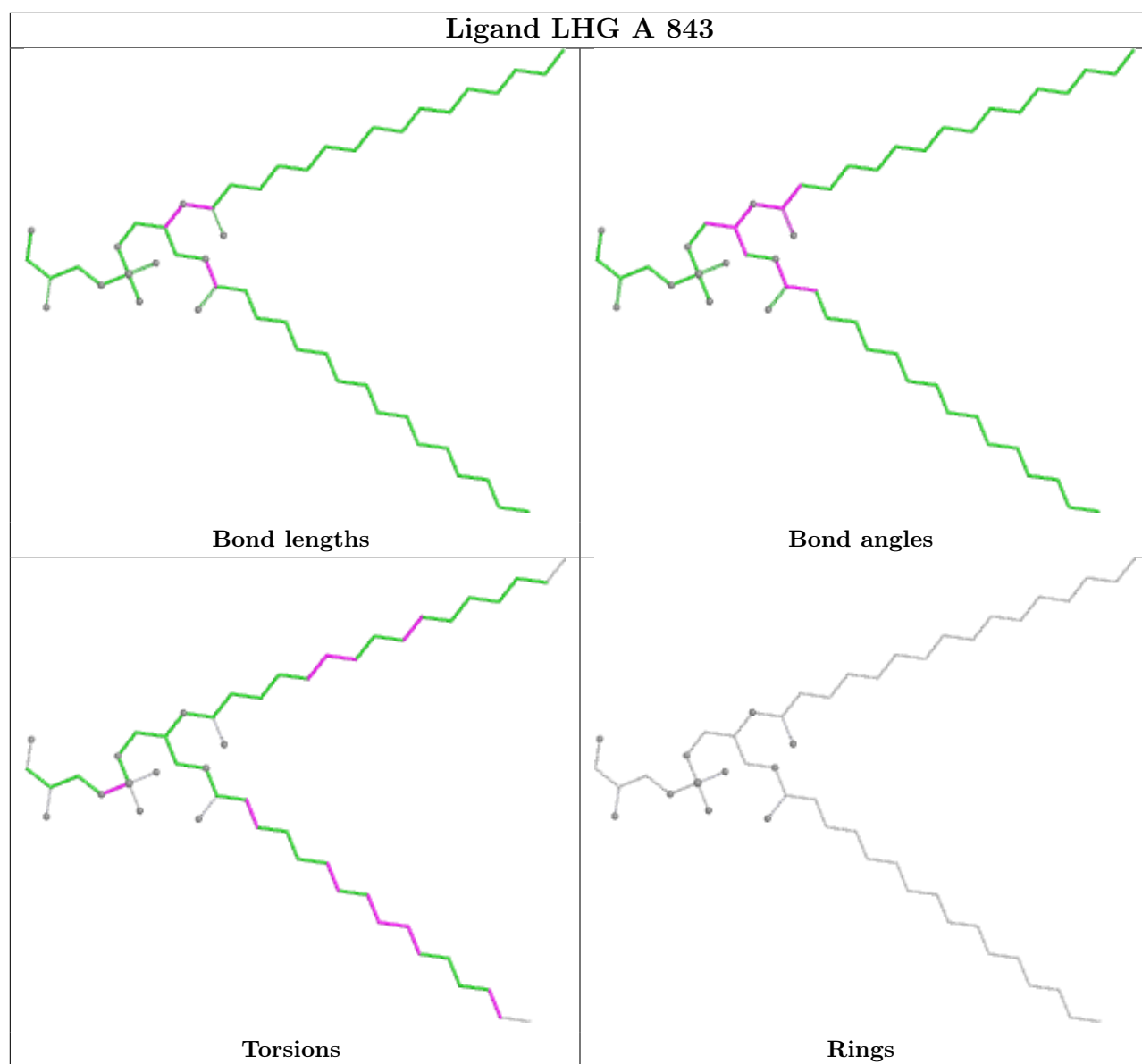
Rings

Ligand CLA B 823

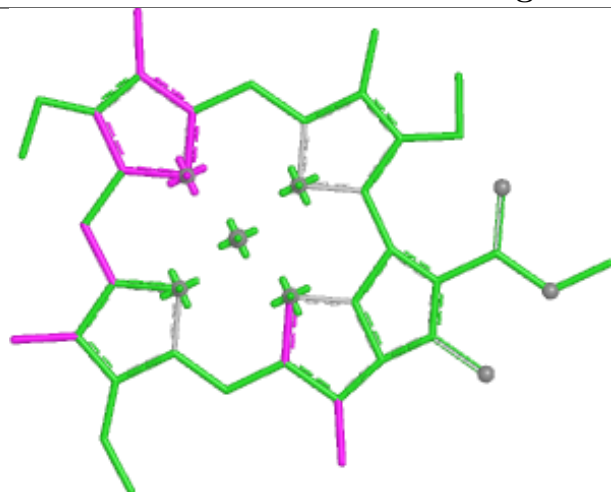


Ligand LMG 2 519

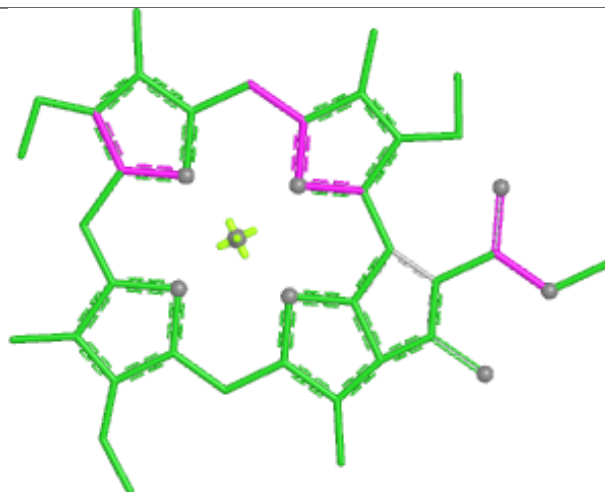




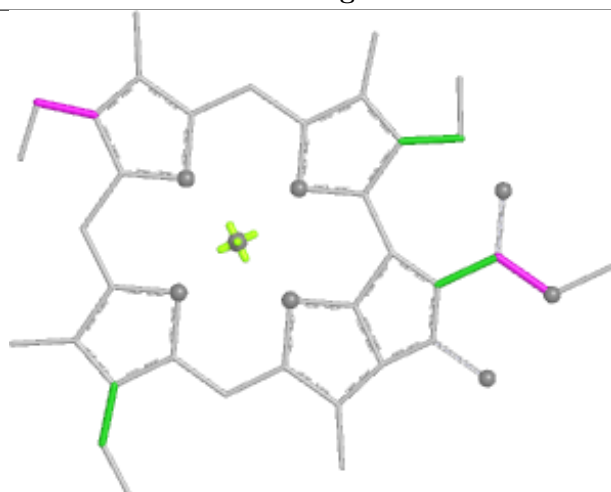
Ligand CLA F 802



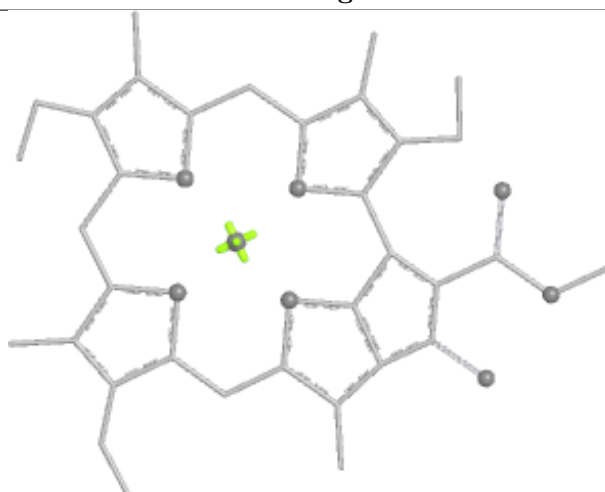
Bond lengths



Bond angles

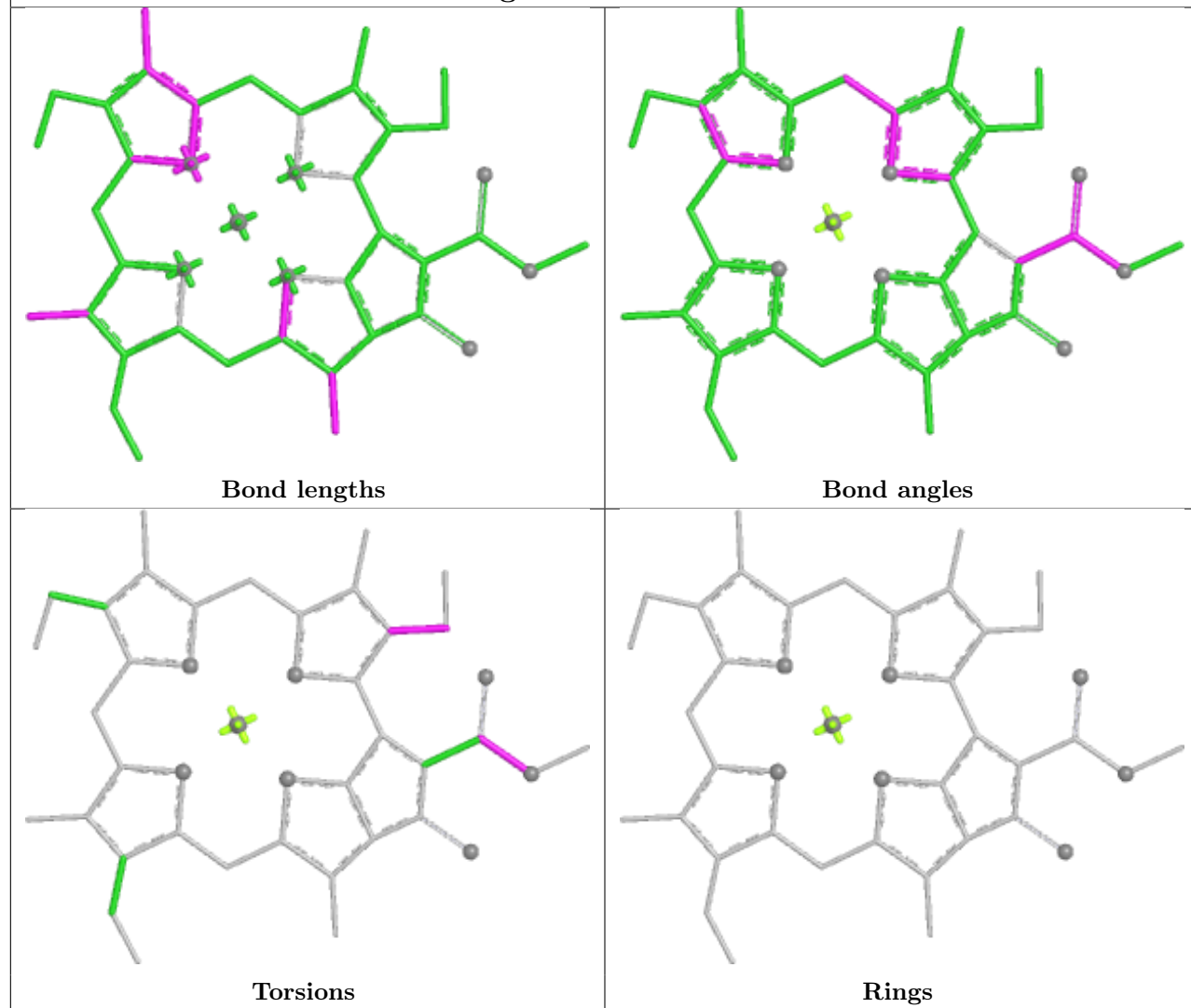


Torsions

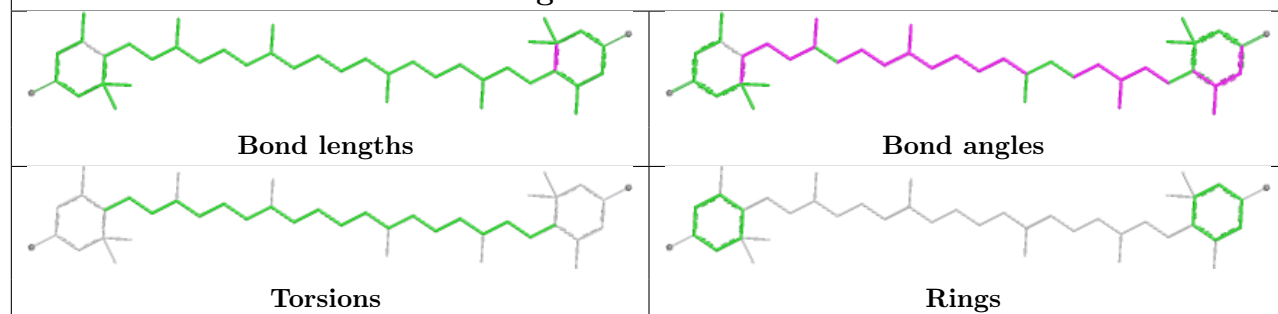


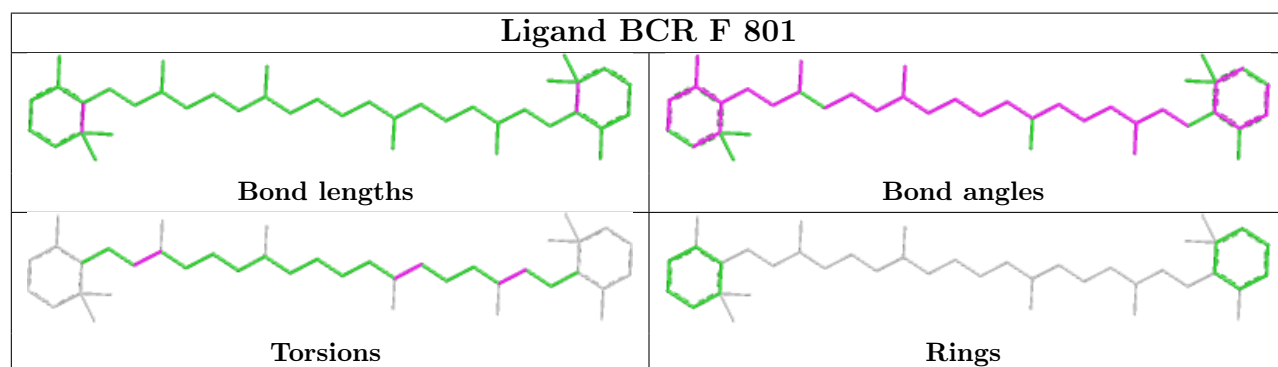
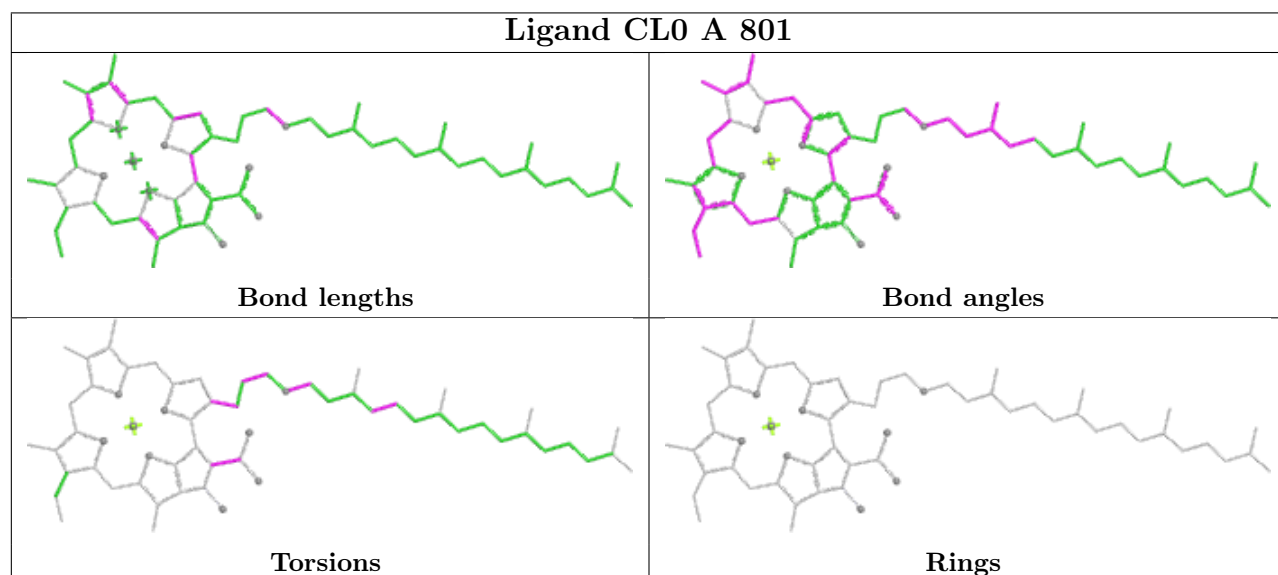
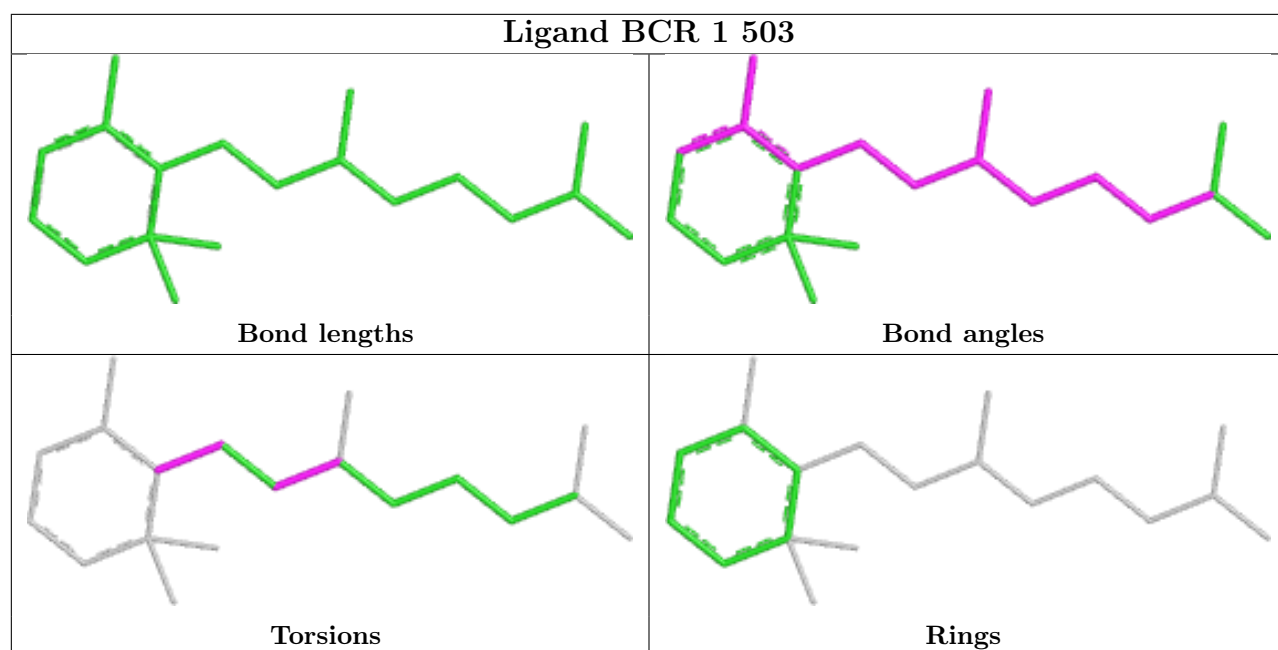
Rings

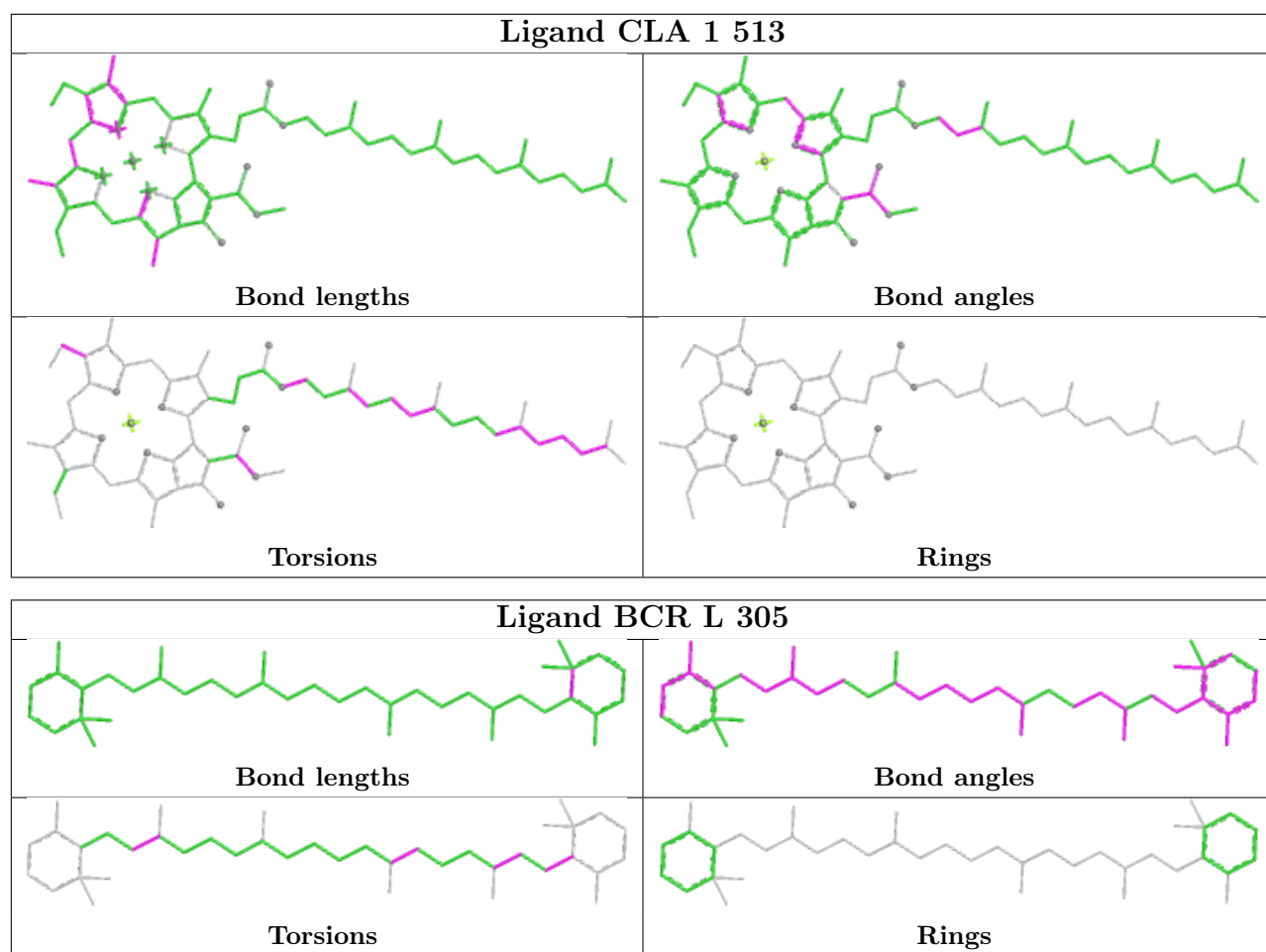
Ligand CLA 1 507



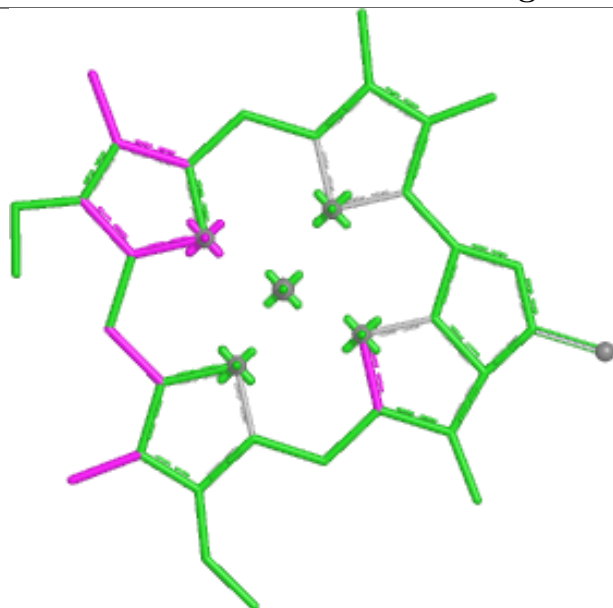
Ligand LUT 2 501



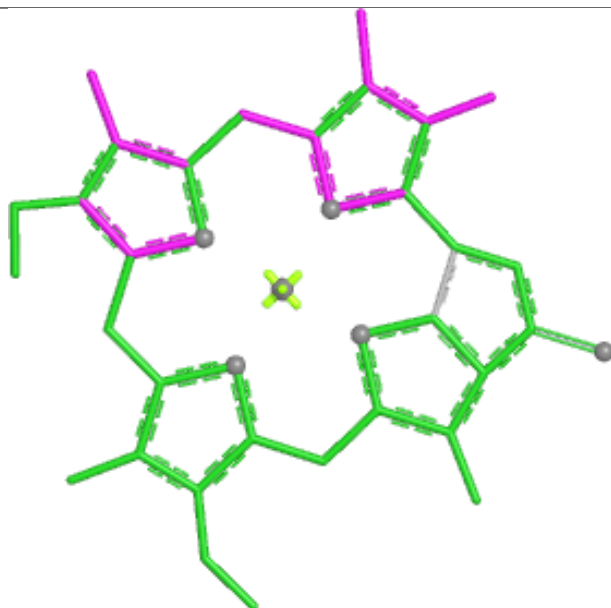




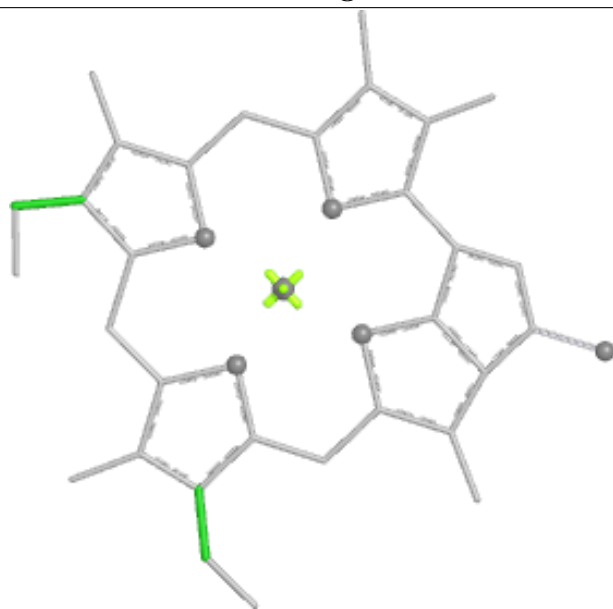
Ligand CLA 3 316



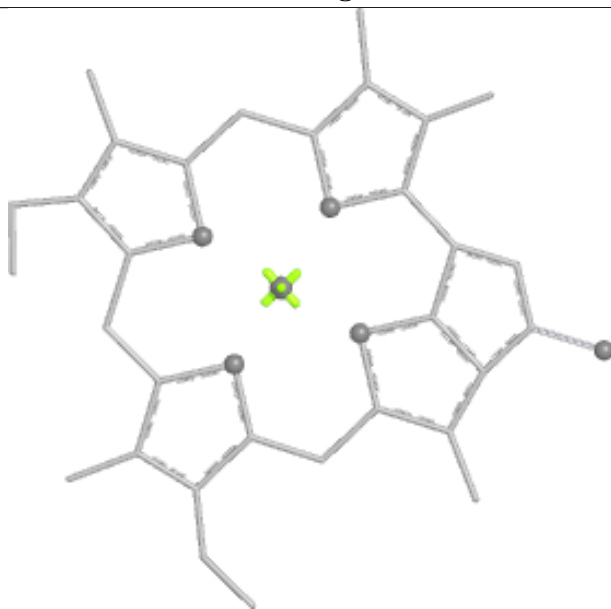
Bond lengths



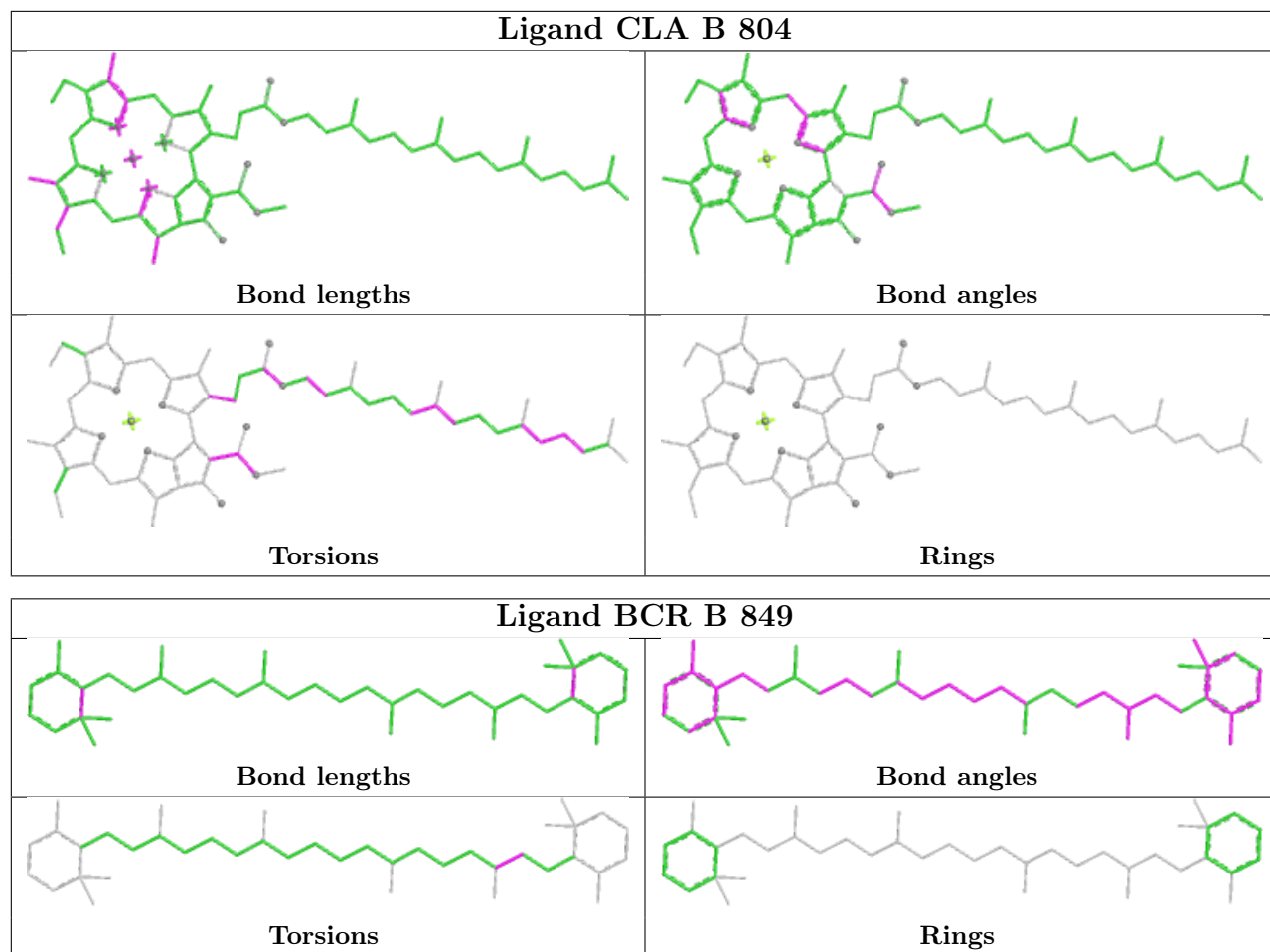
Bond angles



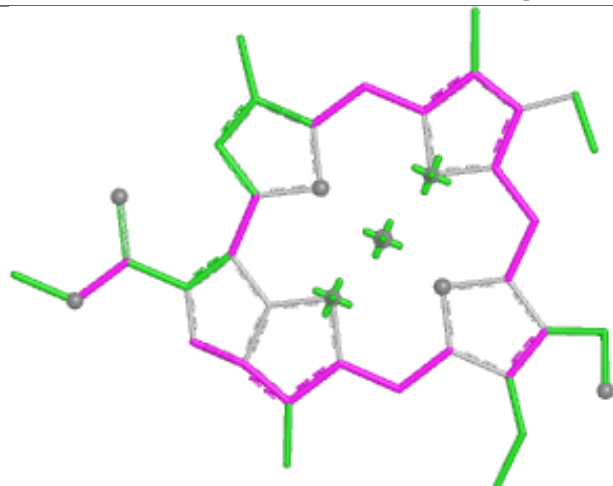
Torsions



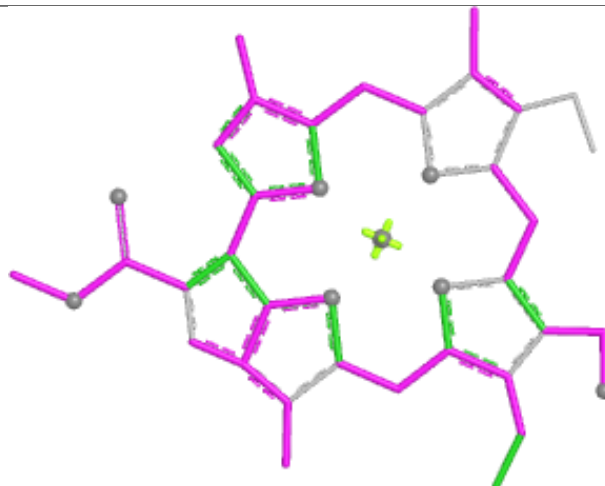
Rings



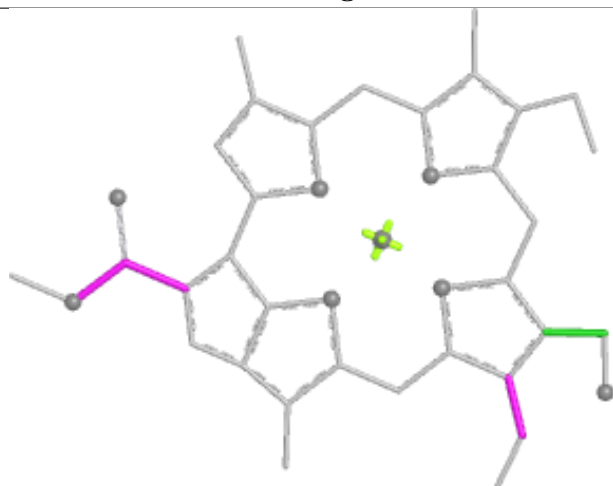
Ligand CHL 2 513



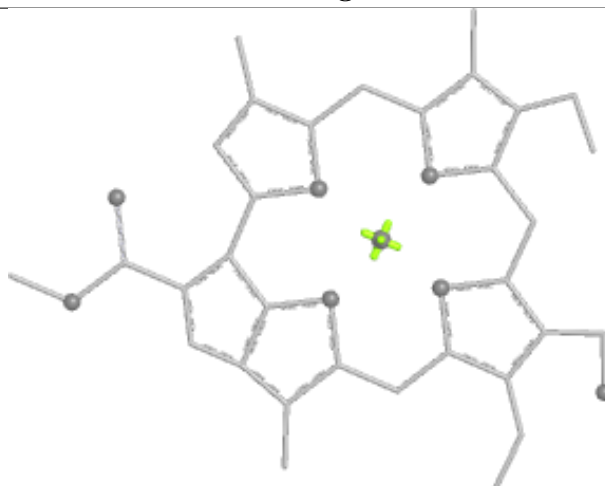
Bond lengths



Bond angles

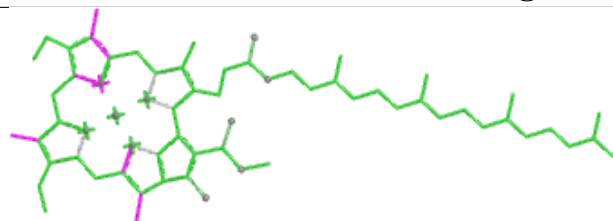


Torsions

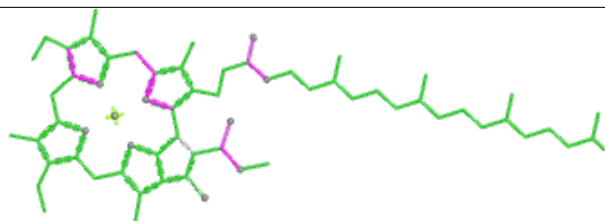


Rings

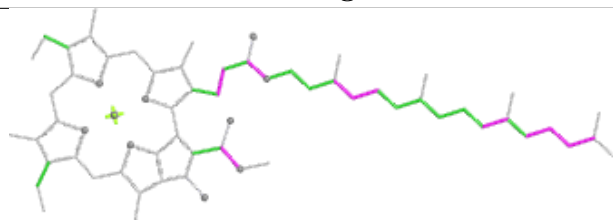
Ligand CLA 2 506



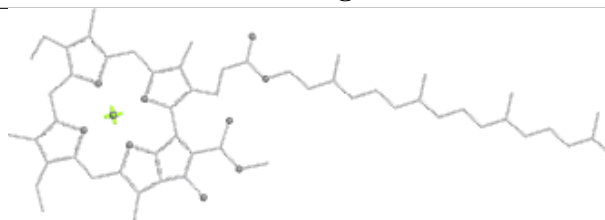
Bond lengths



Bond angles

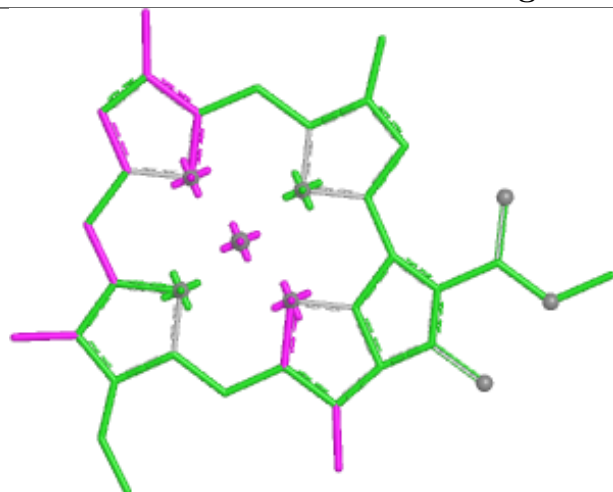


Torsions



Rings

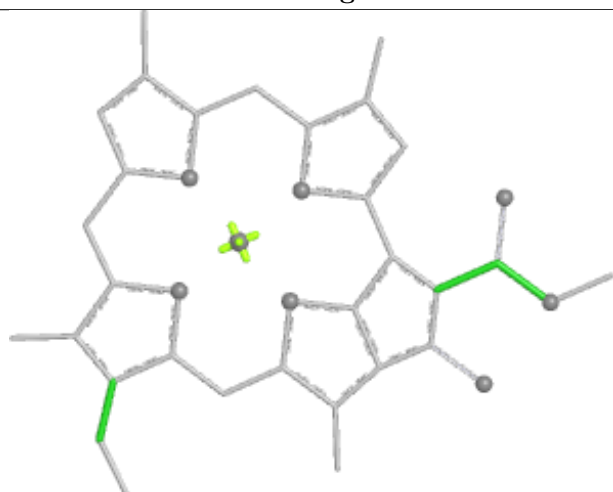
Ligand CLA 5 305



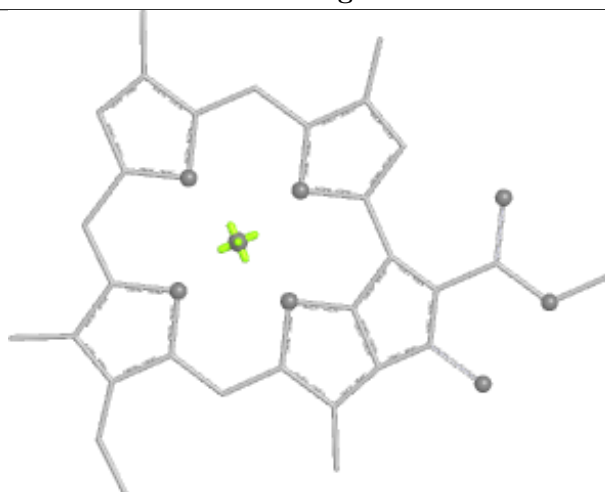
Bond lengths



Bond angles

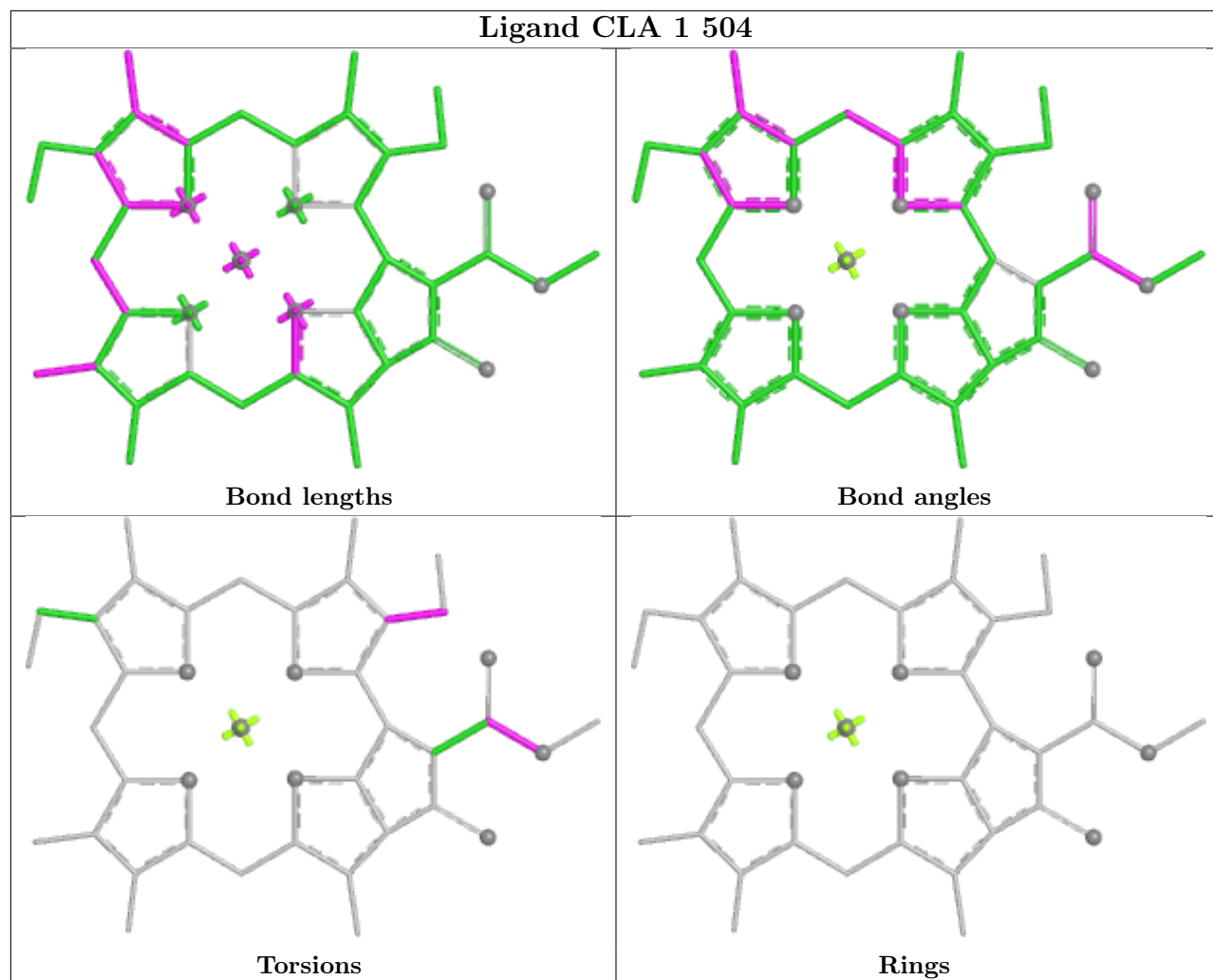


Torsions

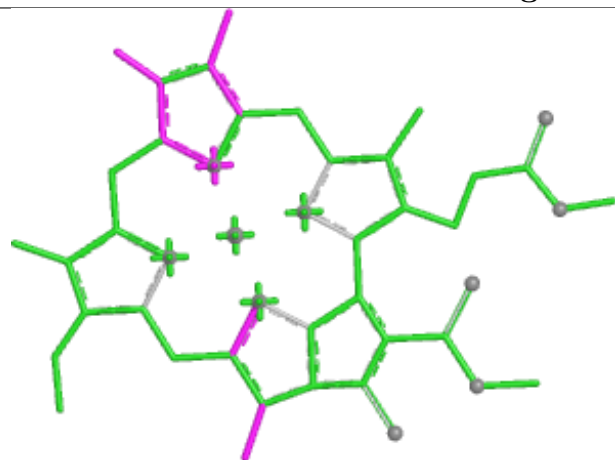


Rings

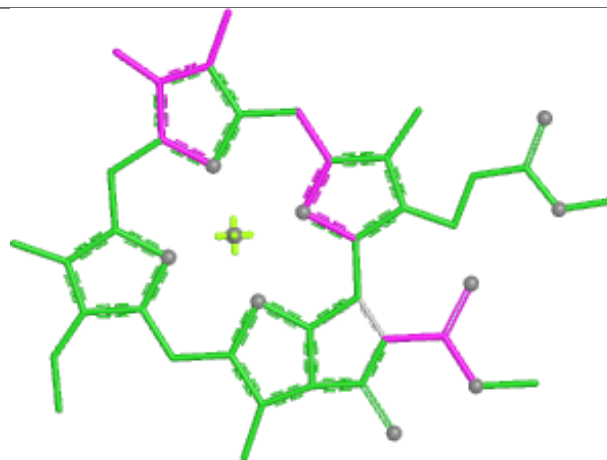
Ligand CLA 1 504



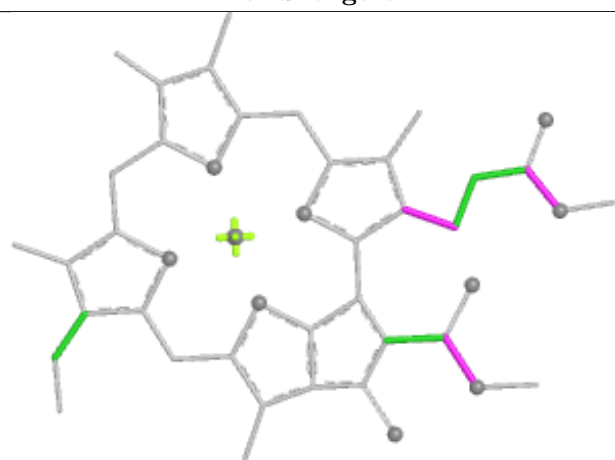
Ligand CLA 3 318



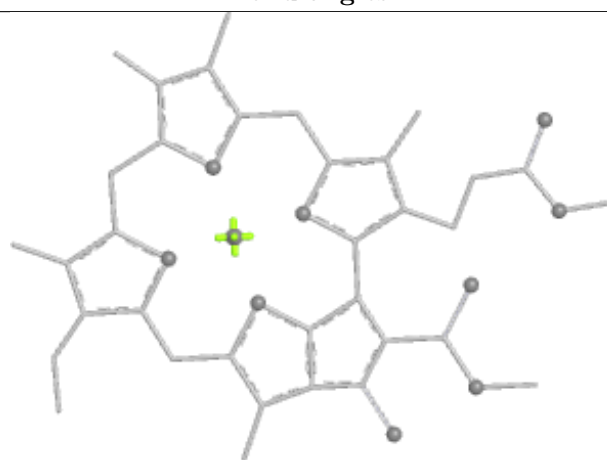
Bond lengths



Bond angles

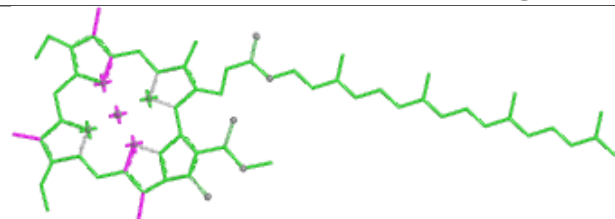


Torsions

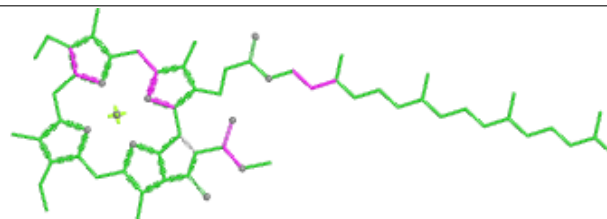


Rings

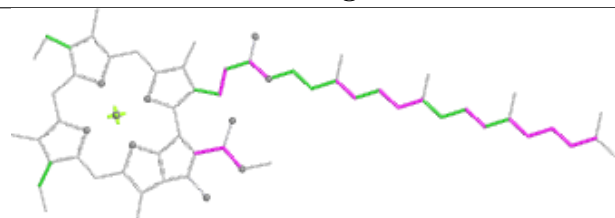
Ligand CLA A 806



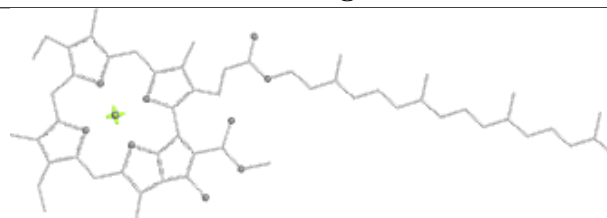
Bond lengths



Bond angles

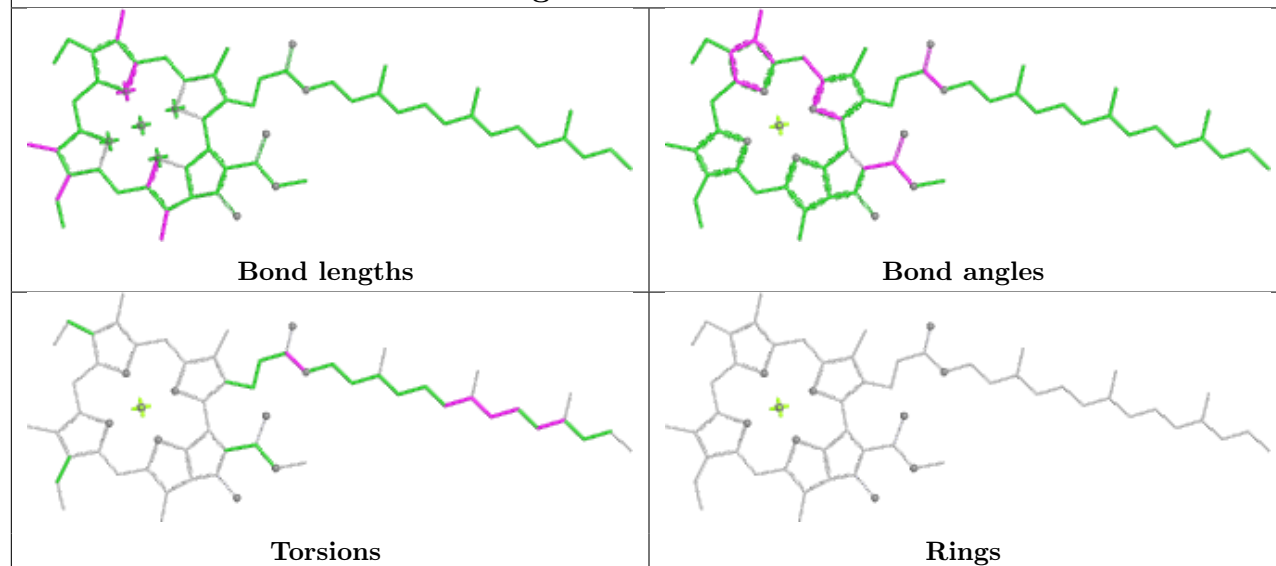


Torsions

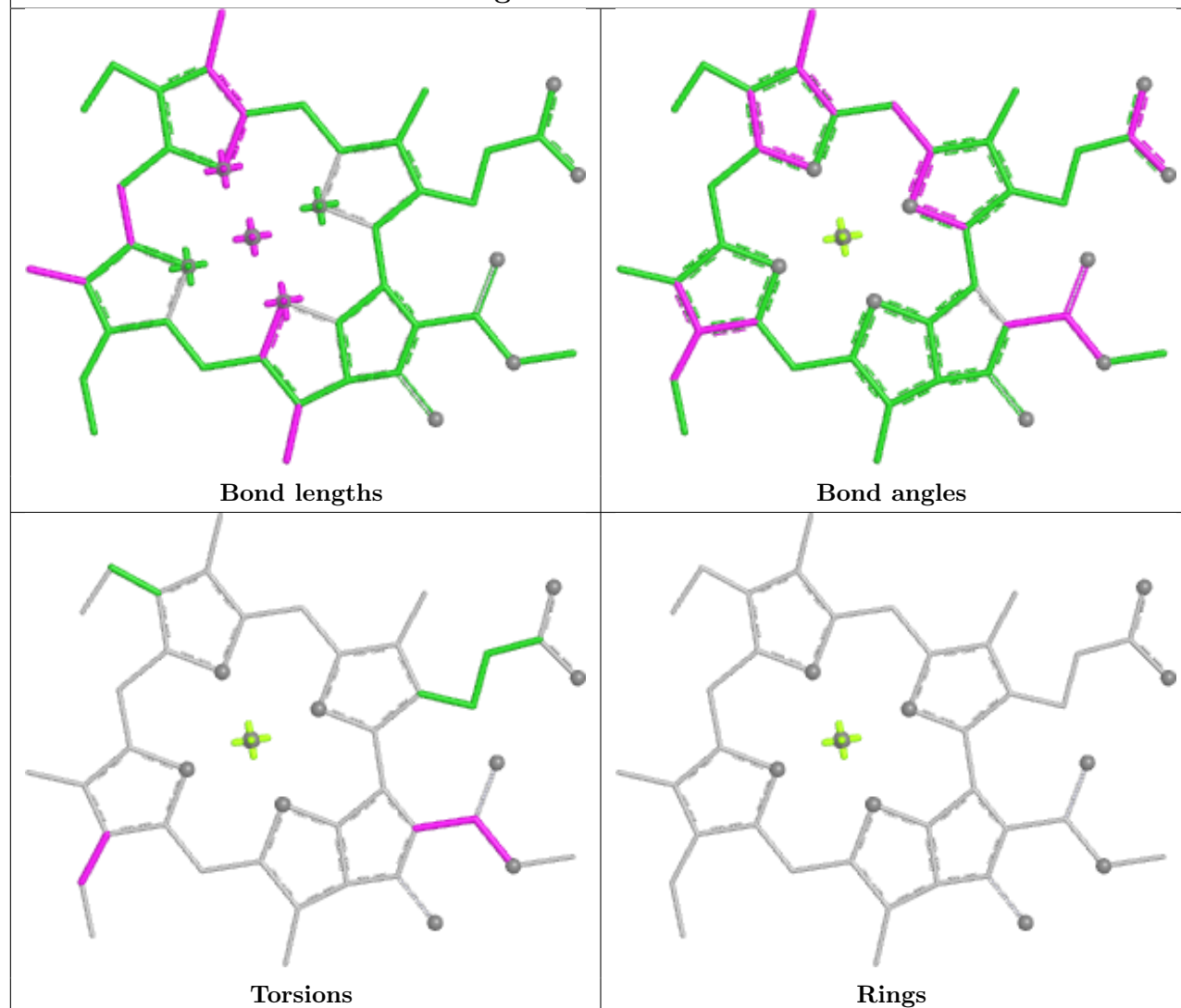


Rings

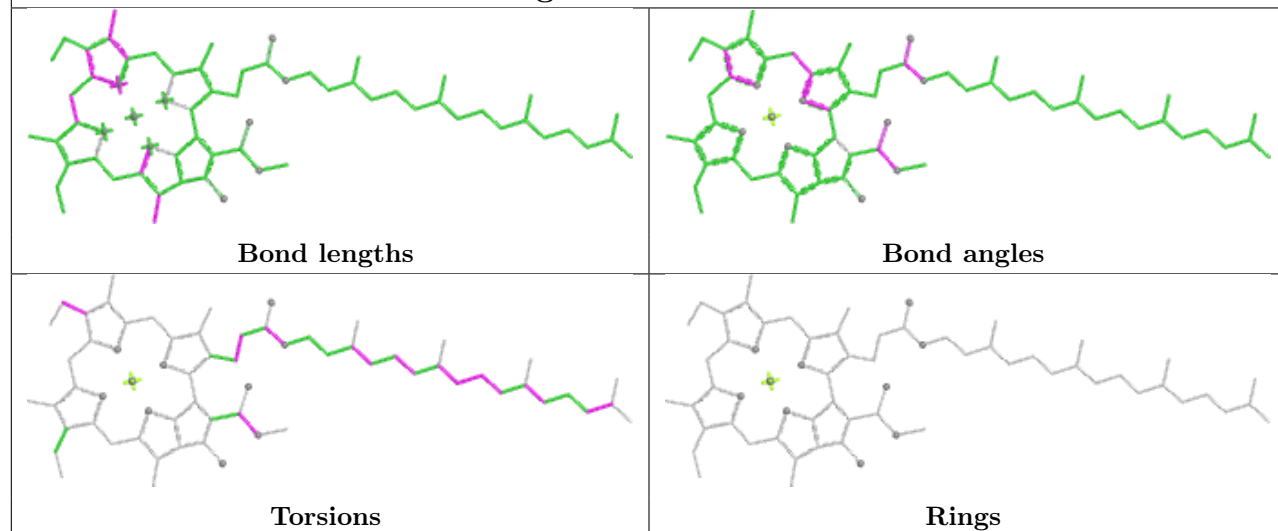
Ligand CLA B 826



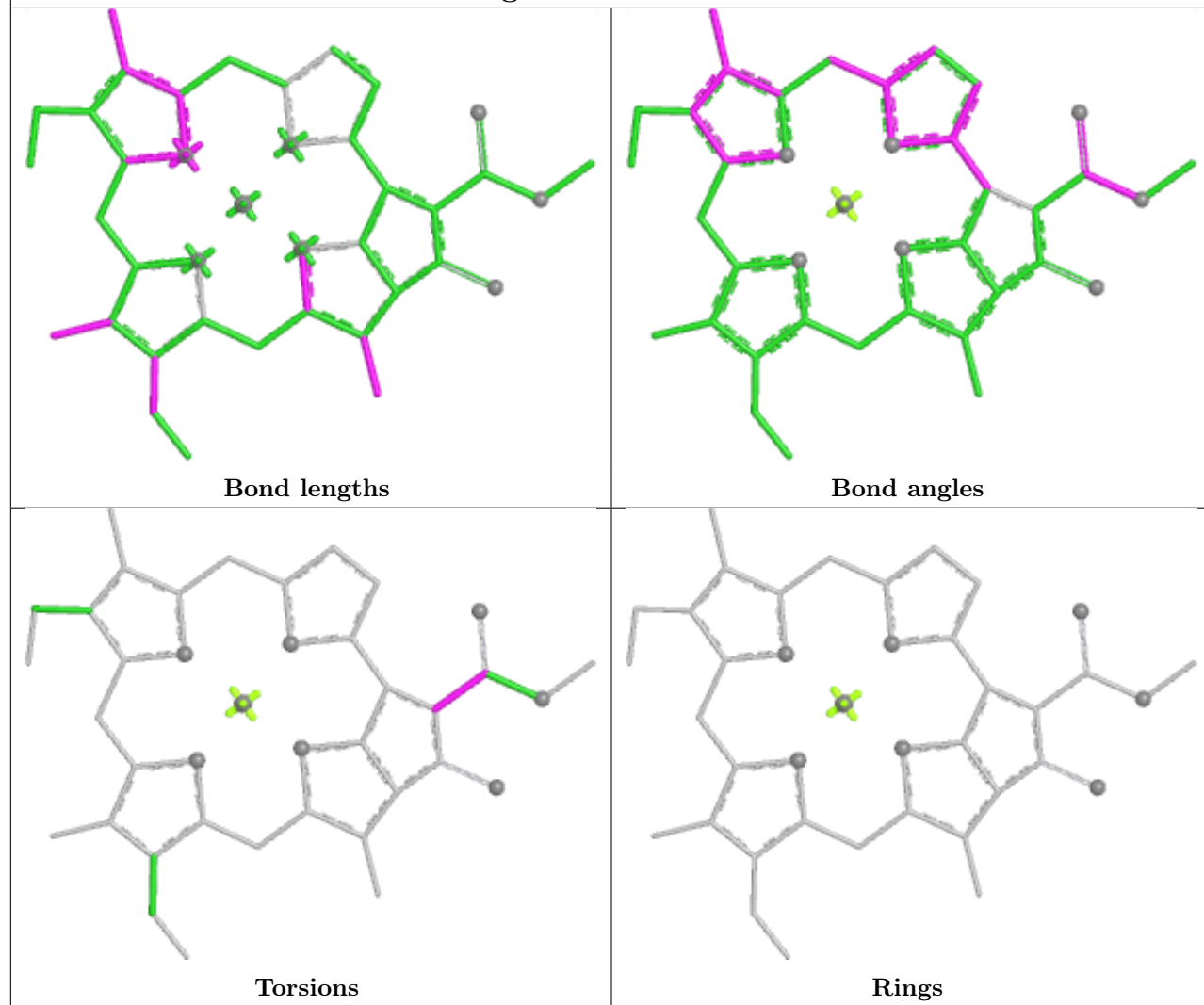
Ligand CLA L 304



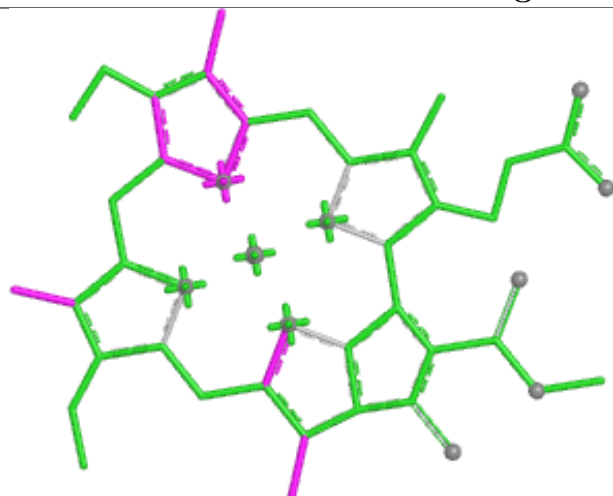
Ligand CLA 5 307



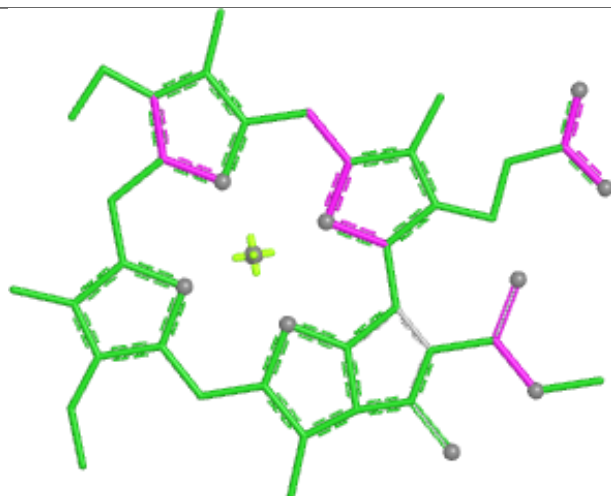
Ligand CLA B 806



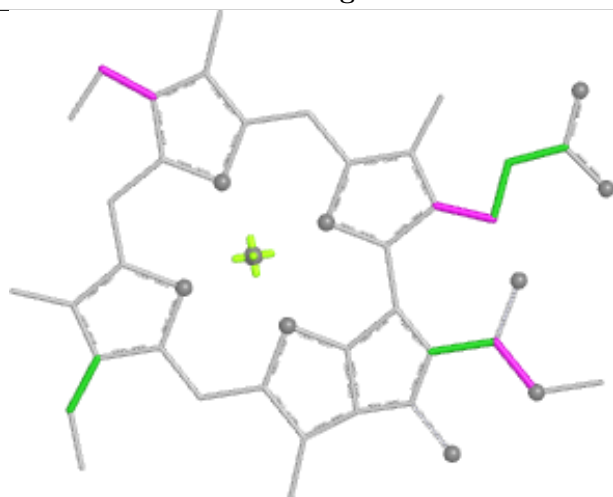
Ligand CLA B 824



Bond lengths



Bond angles

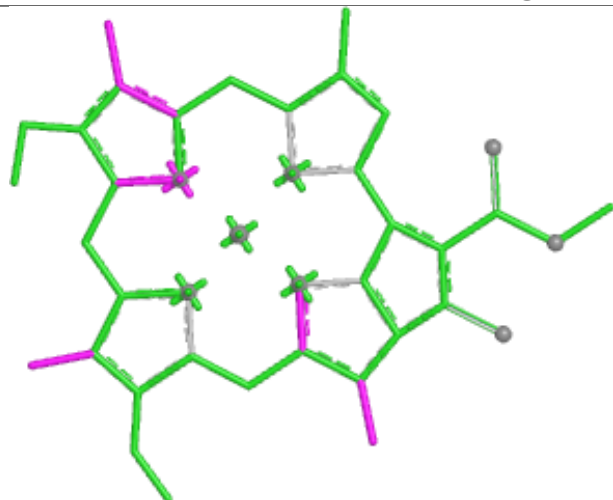


Torsions

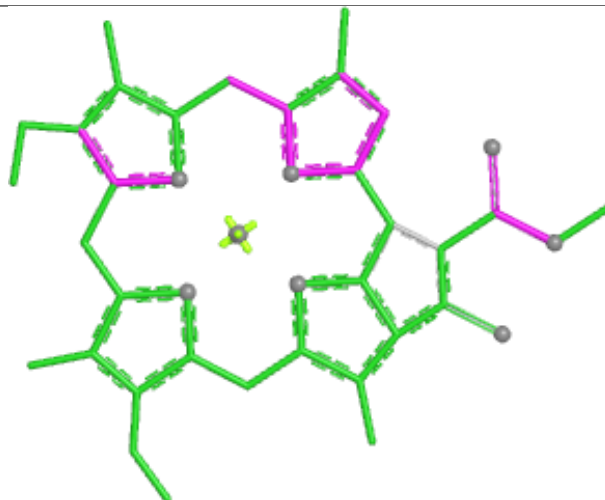


Rings

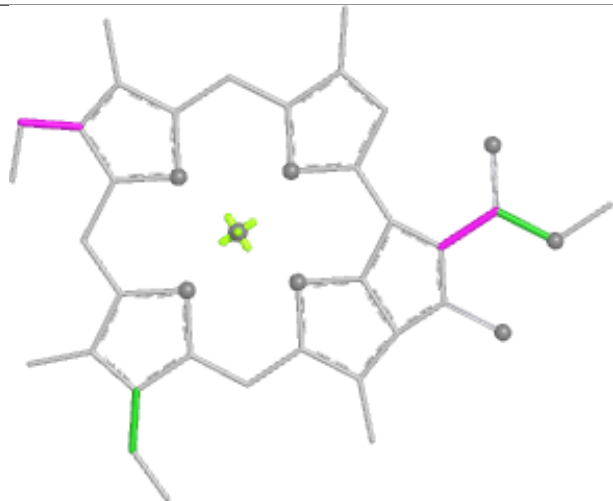
Ligand CLA 5 313



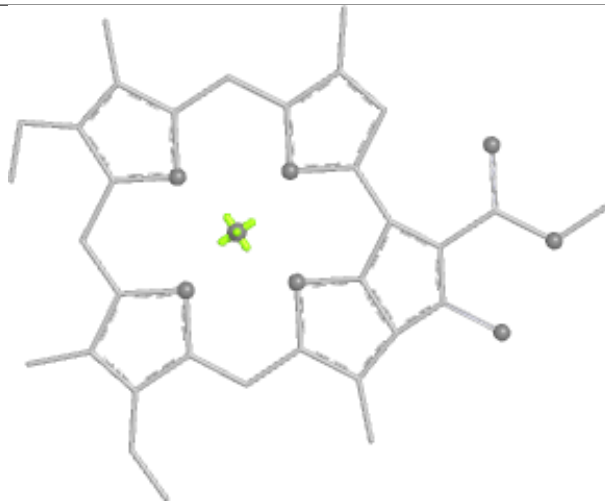
Bond lengths



Bond angles

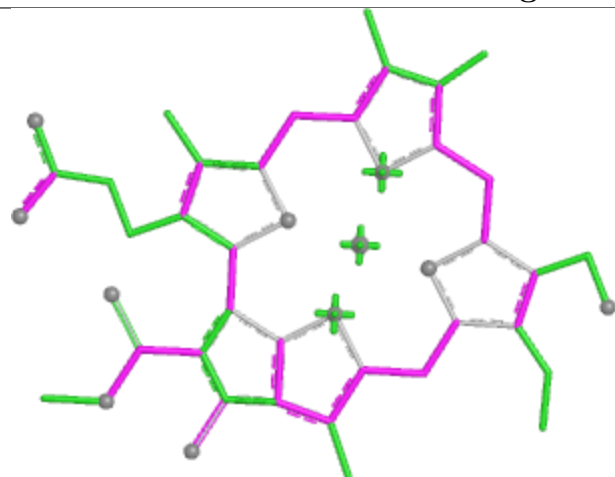


Torsions

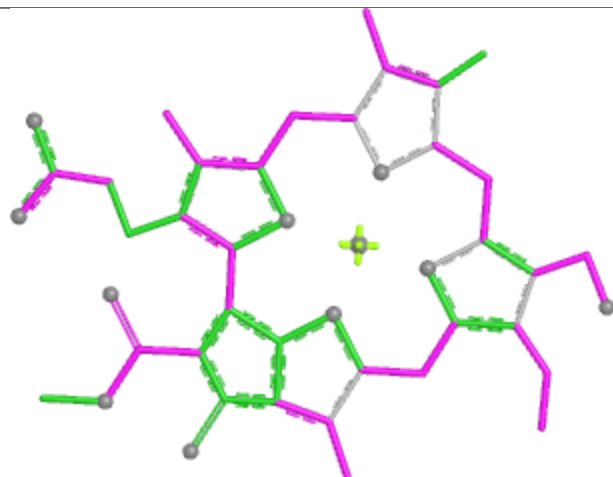


Rings

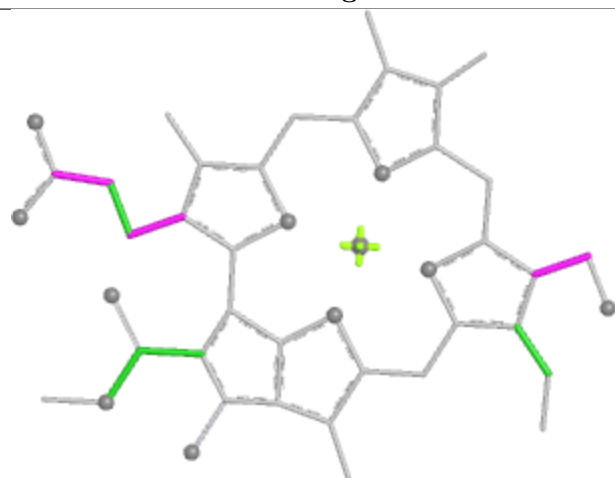
Ligand CHL 2 515



Bond lengths



Bond angles

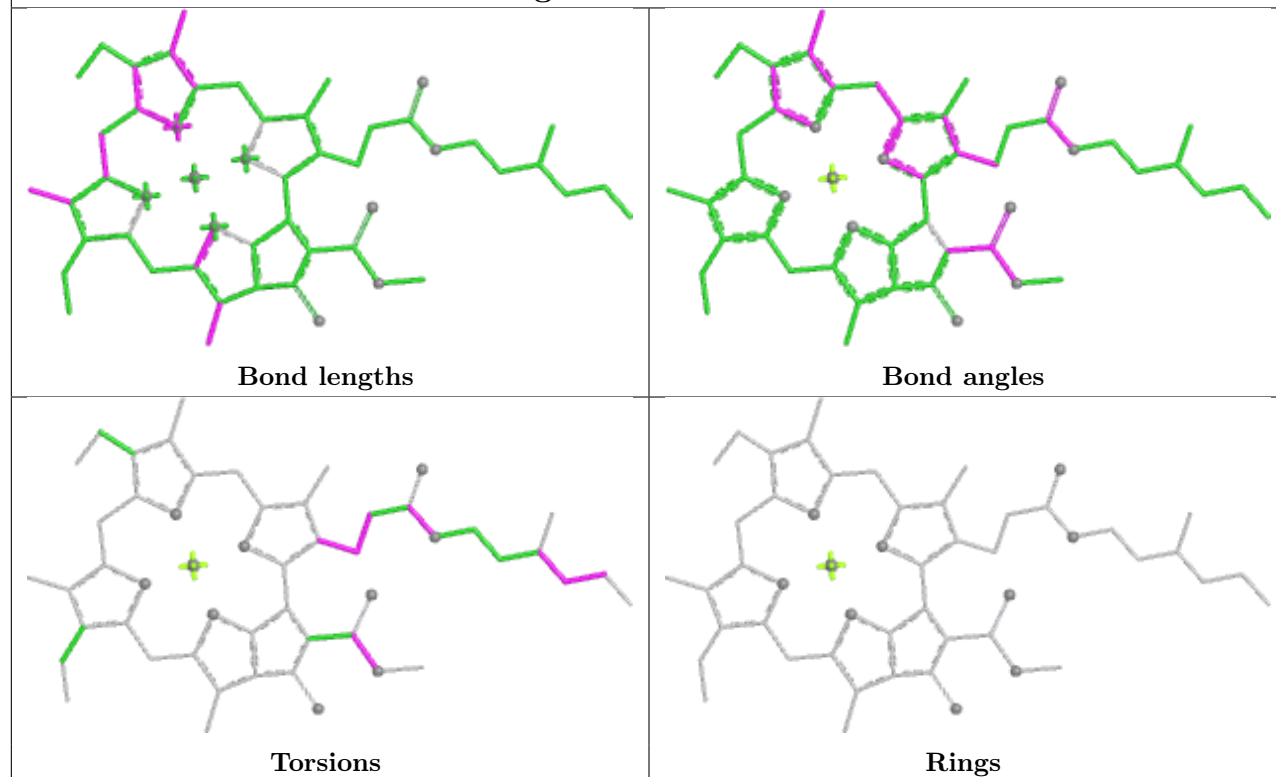


Torsions

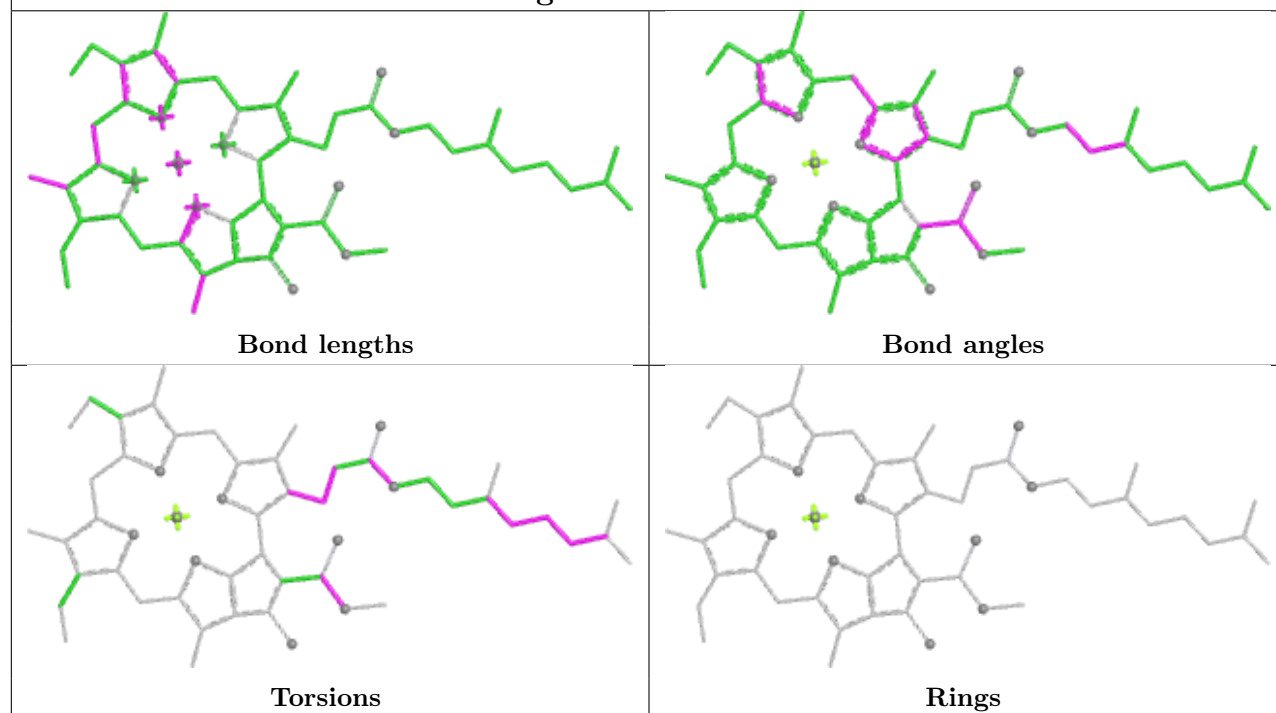


Rings

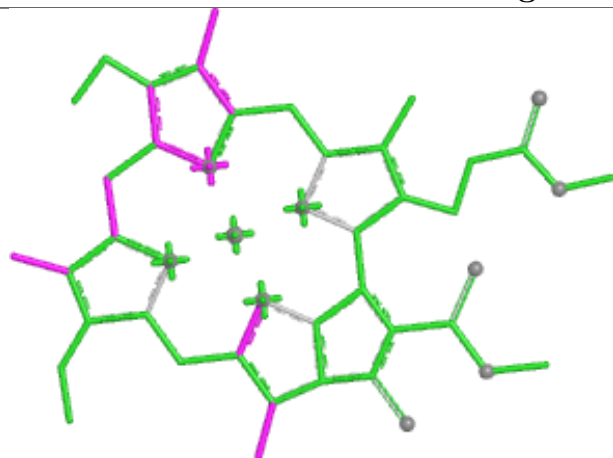
Ligand CLA L 303



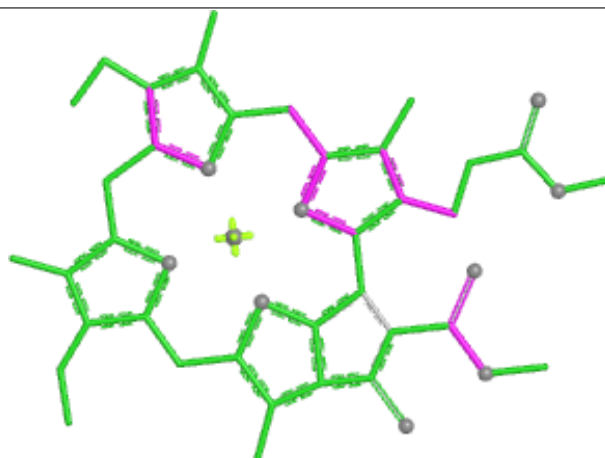
Ligand CLA 3 308



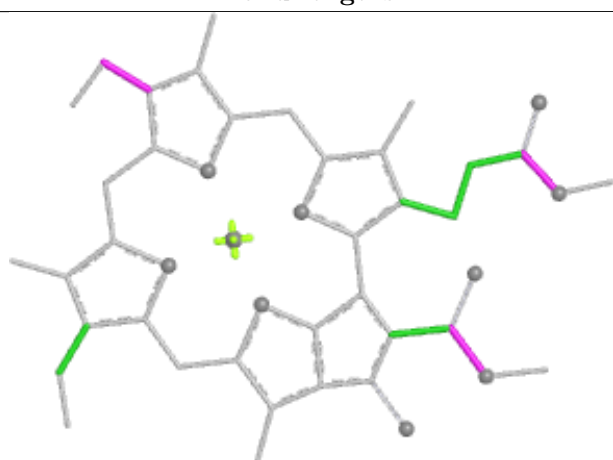
Ligand CLA 1 511



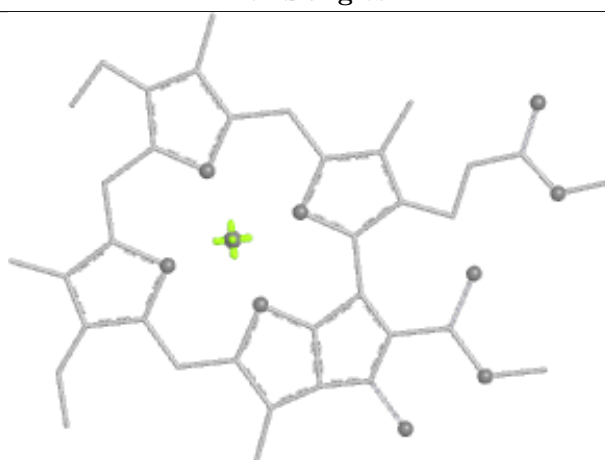
Bond lengths



Bond angles

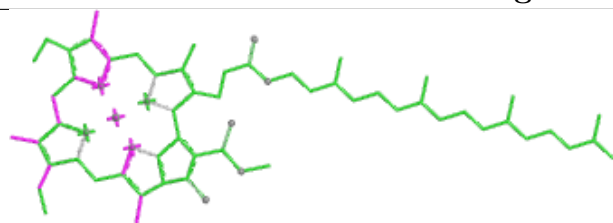


Torsions

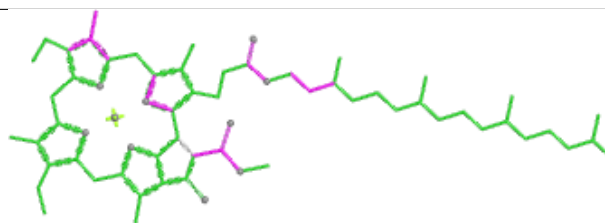


Rings

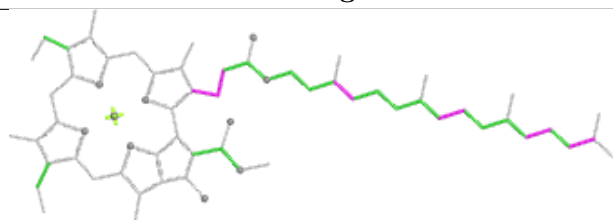
Ligand CLA B 801



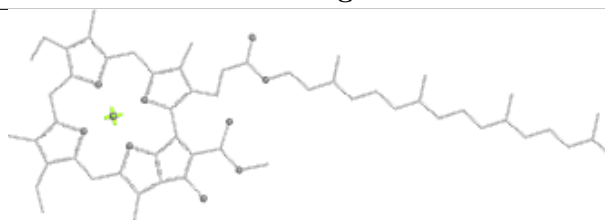
Bond lengths



Bond angles

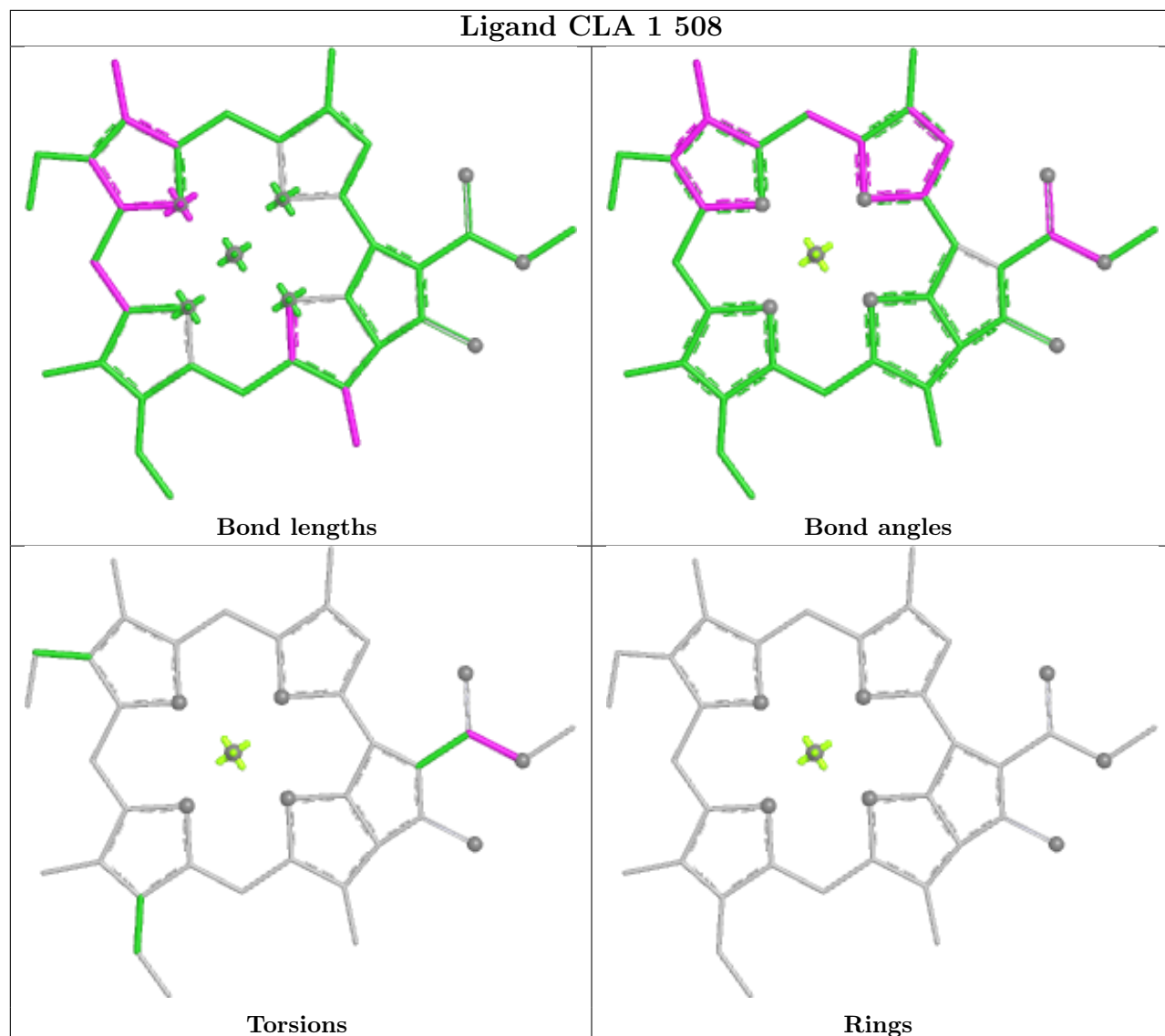


Torsions

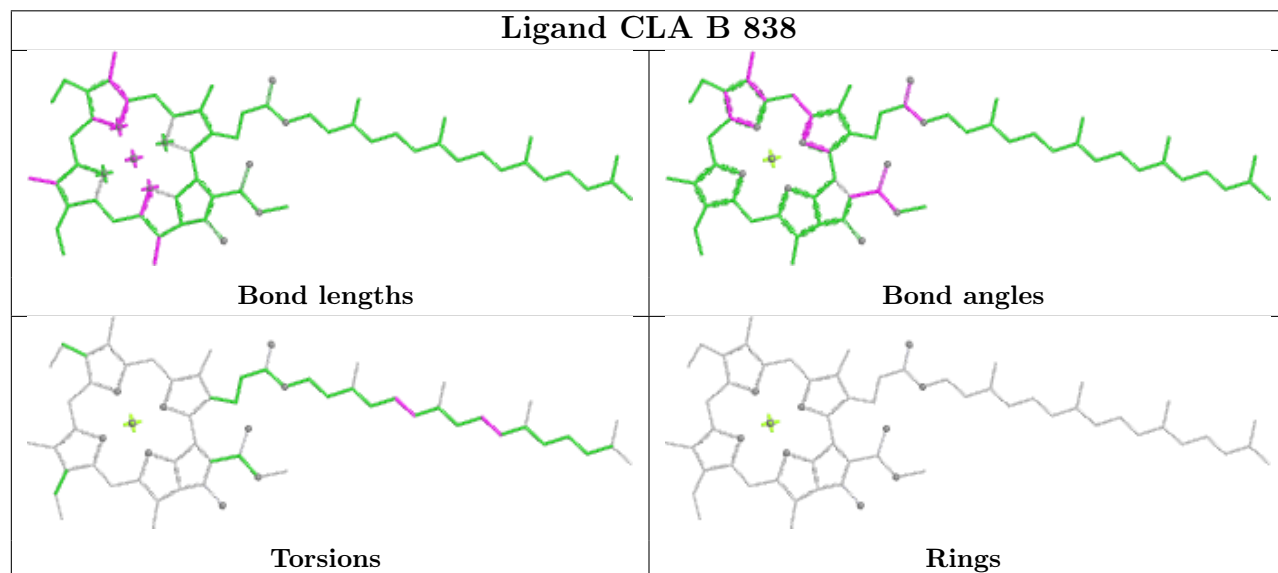


Rings

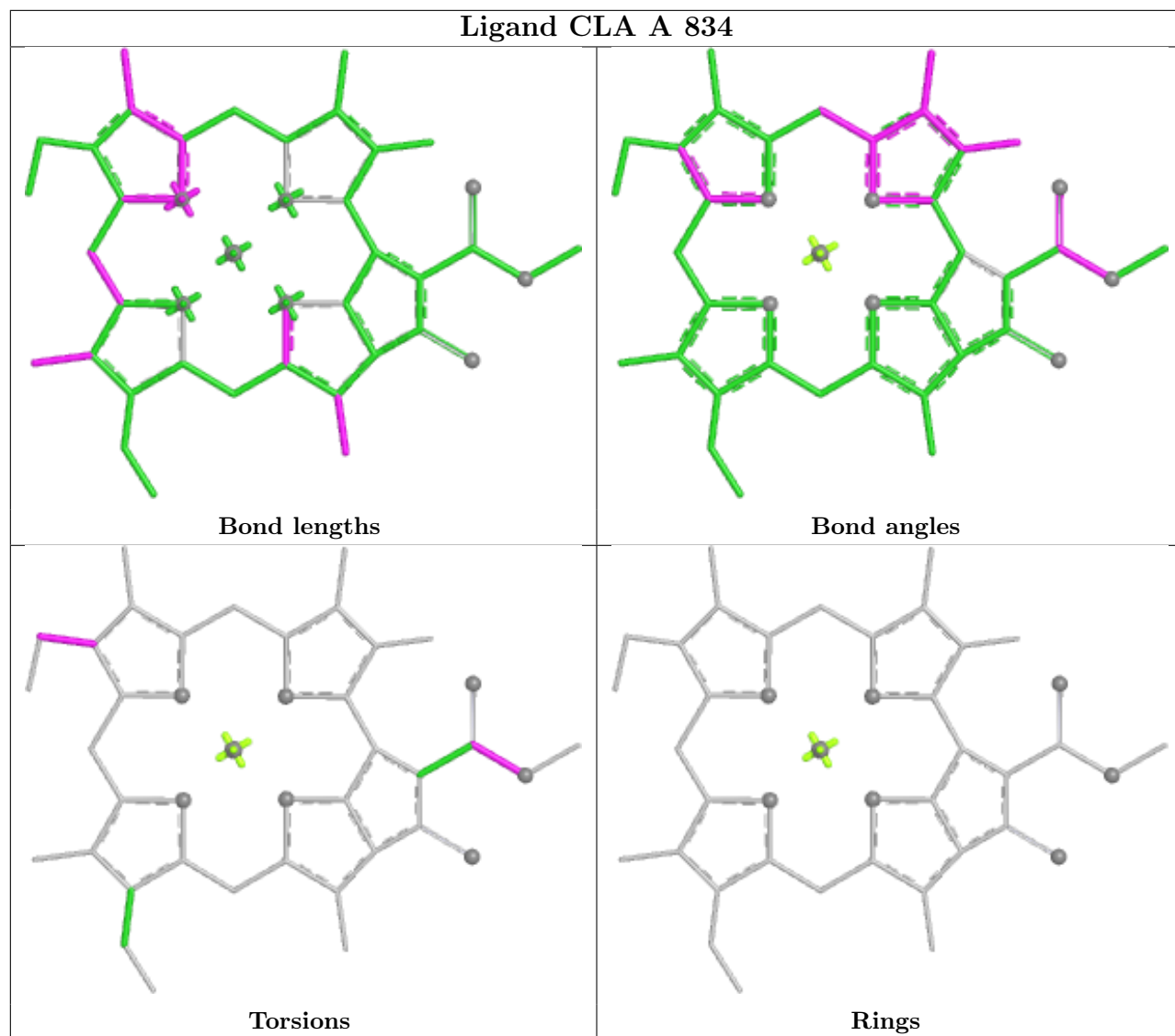
Ligand CLA 1 508



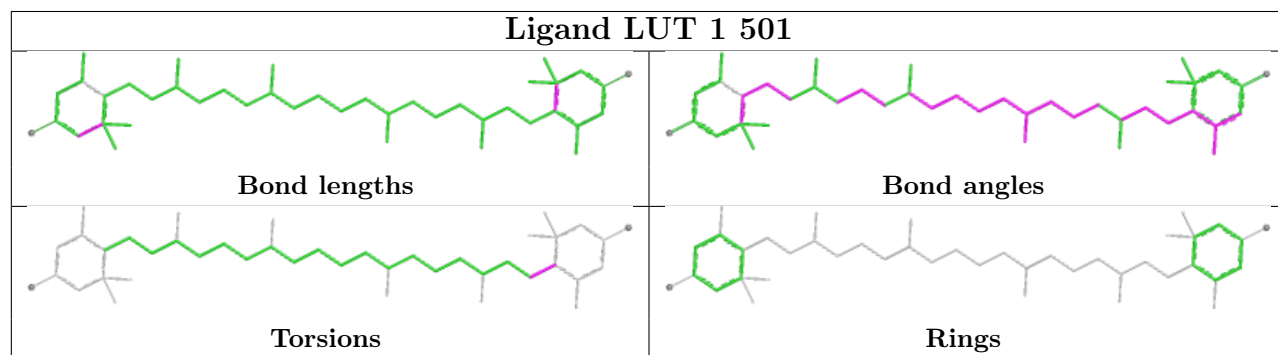
Ligand CLA B 838



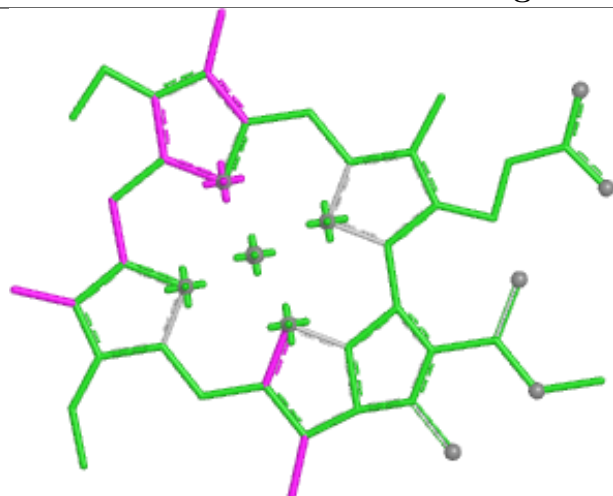
Ligand CLA A 834



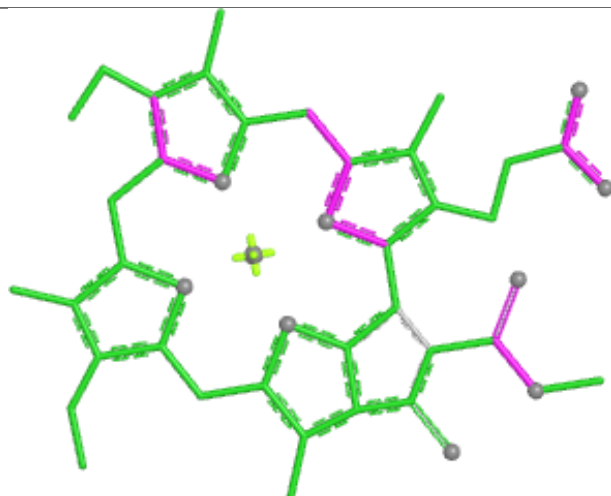
Ligand LUT 1 501



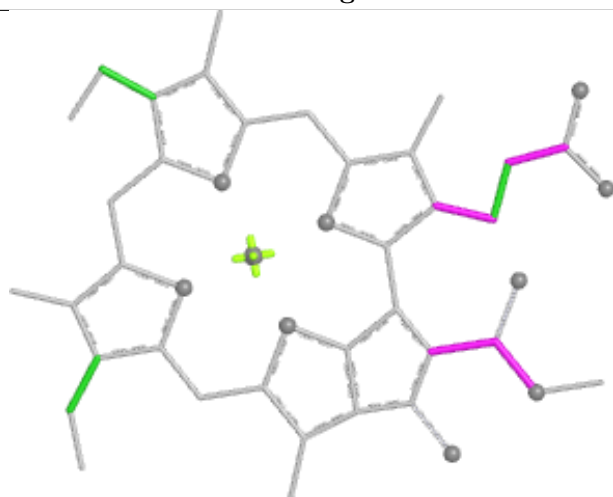
Ligand CLA A 813



Bond lengths



Bond angles

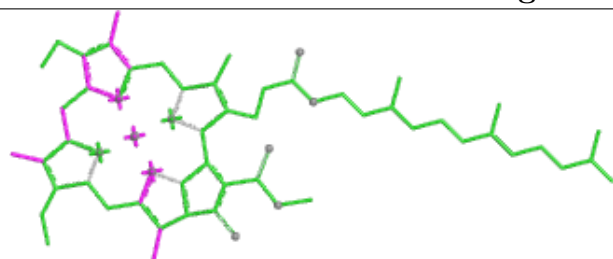


Torsions

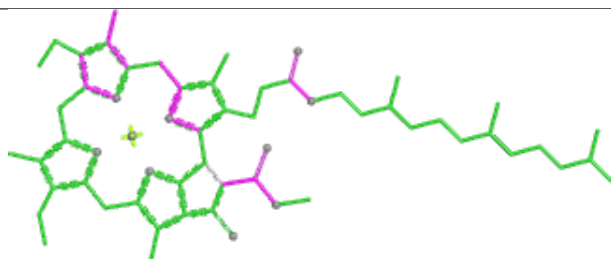


Rings

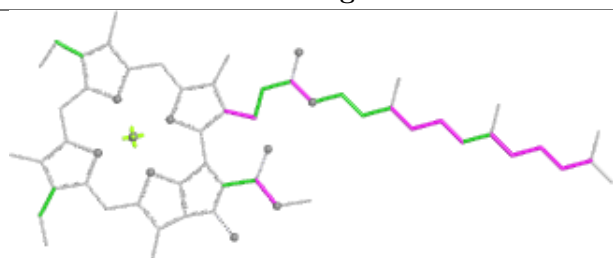
Ligand CLA 2 510



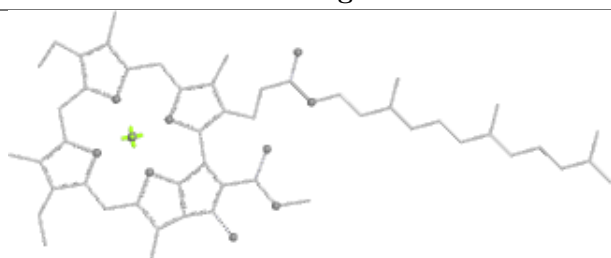
Bond lengths



Bond angles

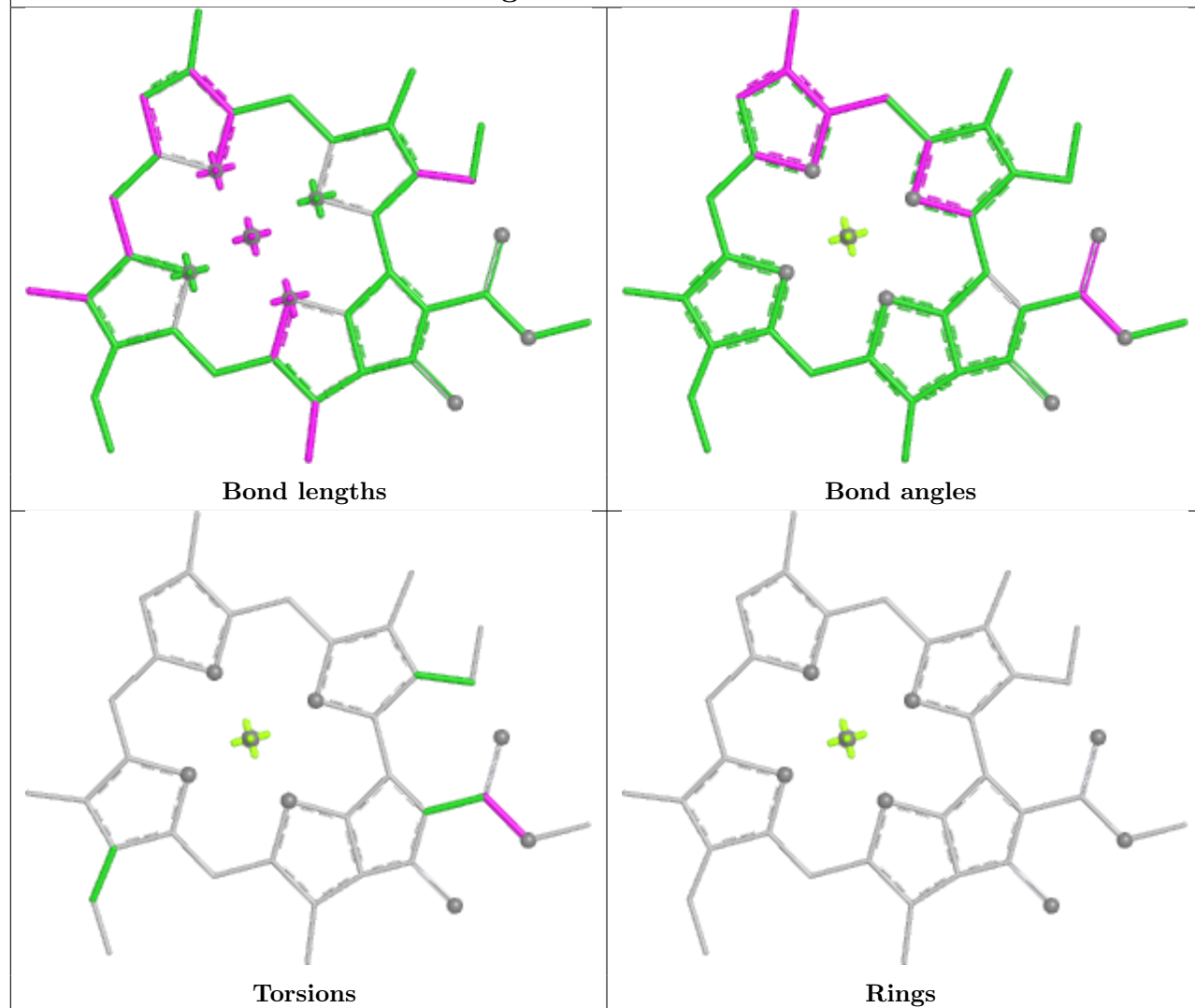


Torsions

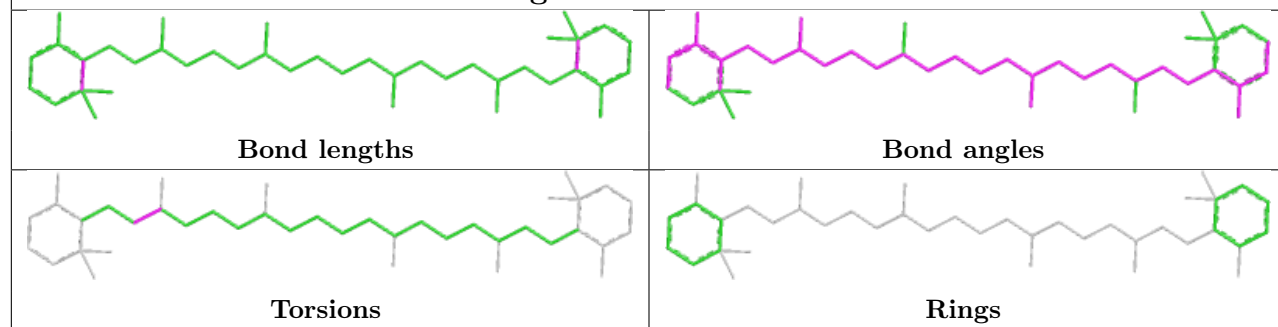


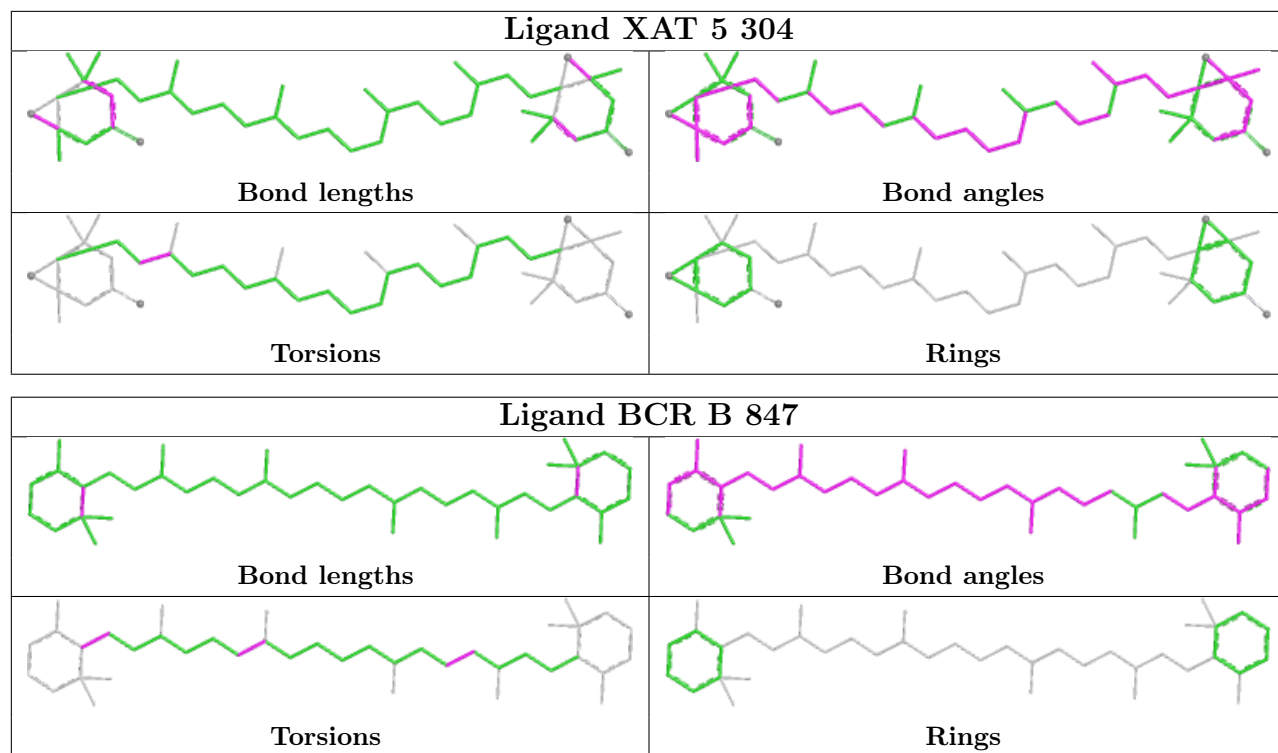
Rings

Ligand CLA 3 309

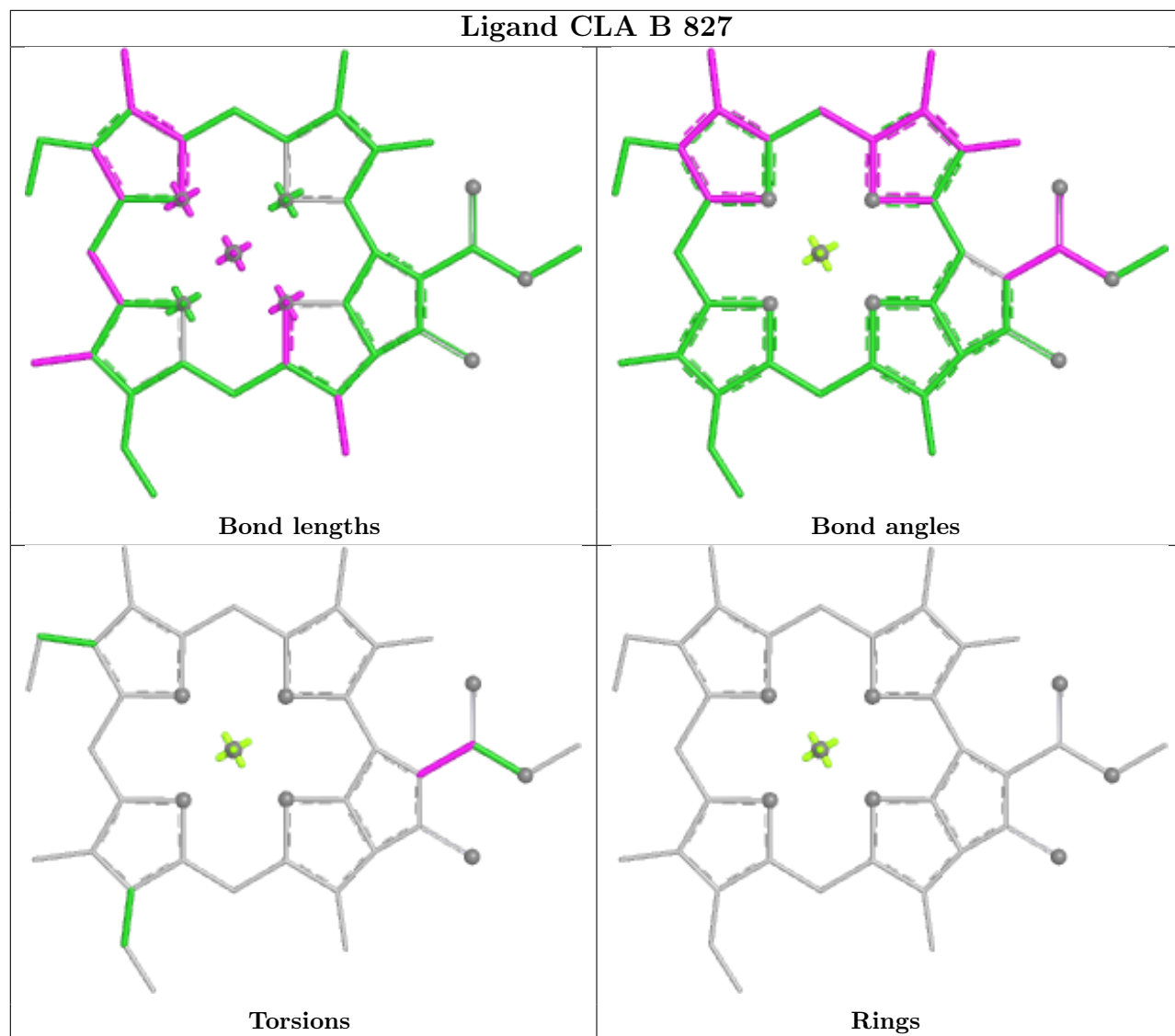


Ligand BCR A 847

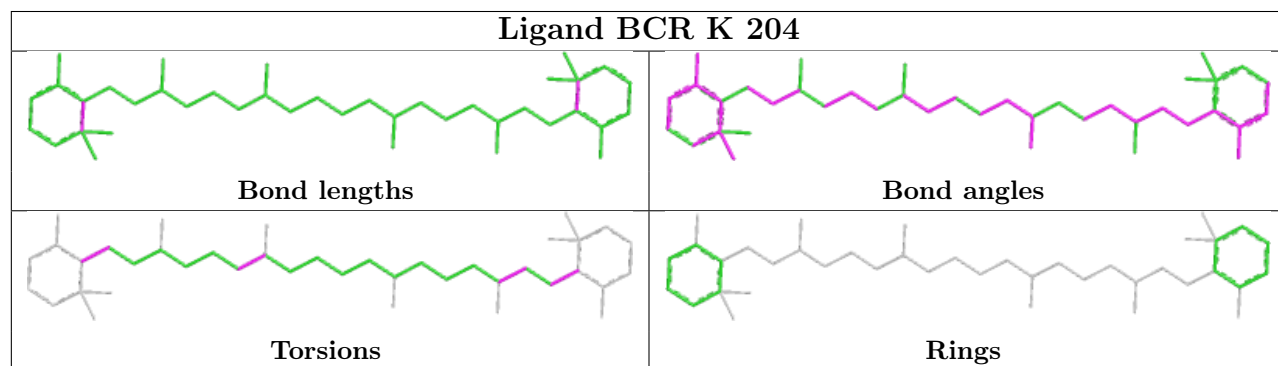




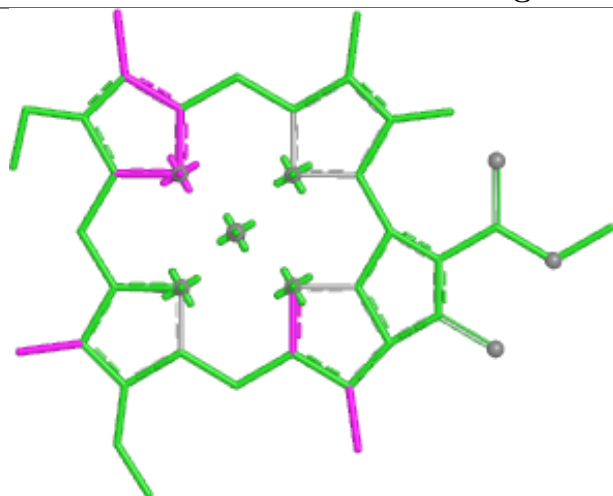
Ligand CLA B 827



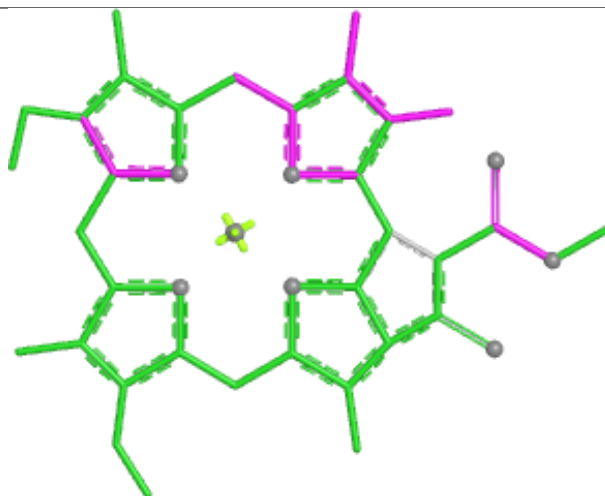
Ligand BCR K 204



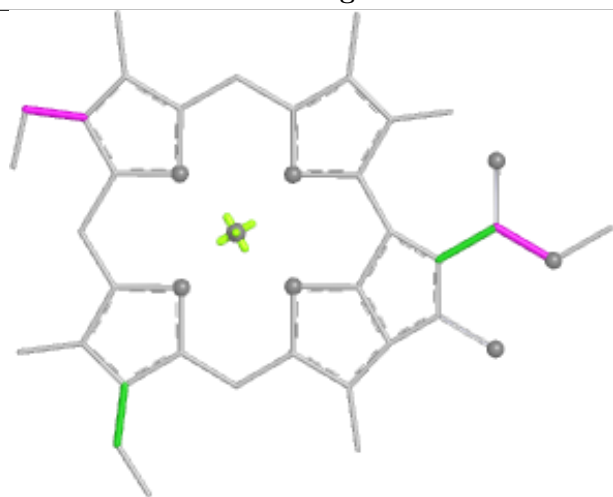
Ligand CLA A 822



Bond lengths



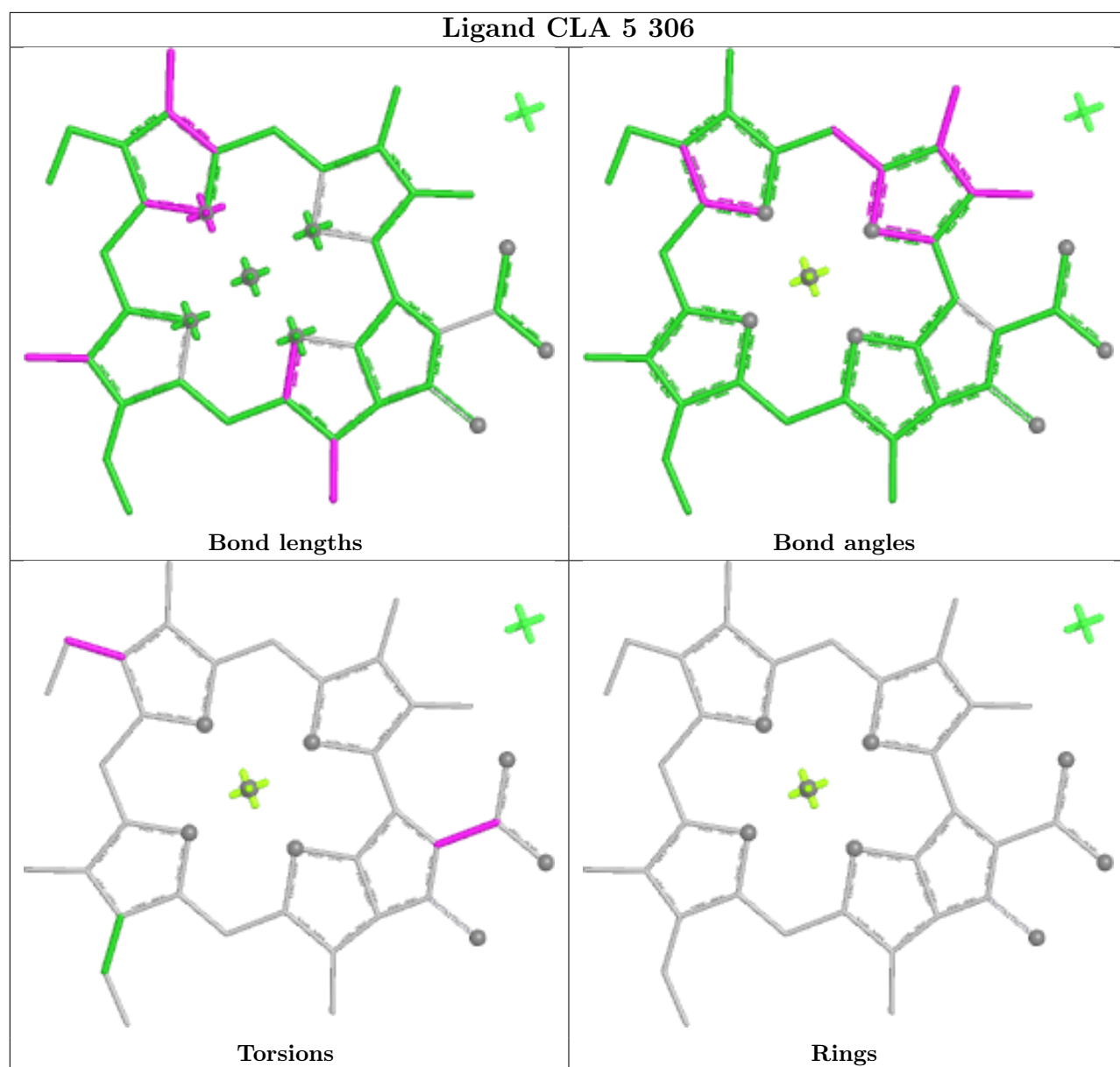
Bond angles



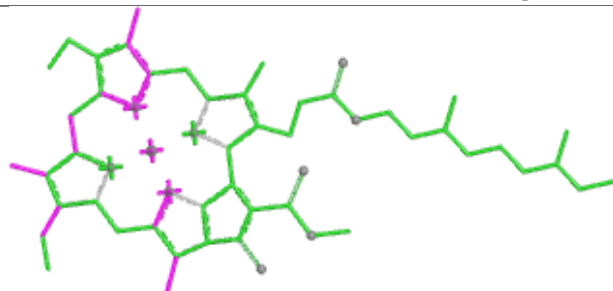
Torsions



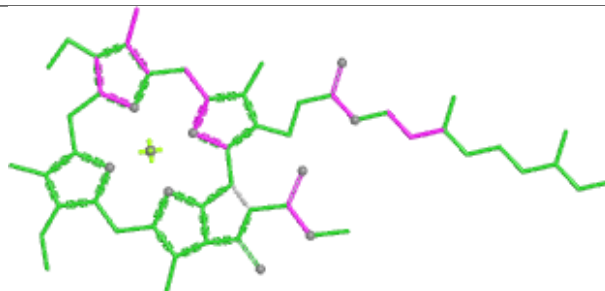
Rings



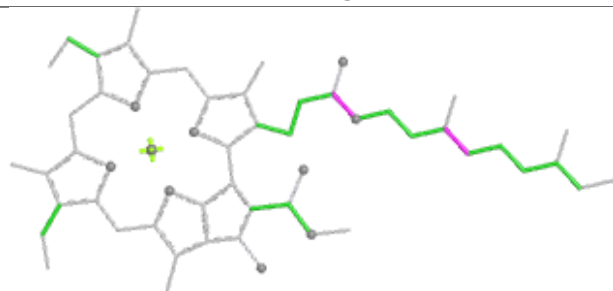
Ligand CLA L 301



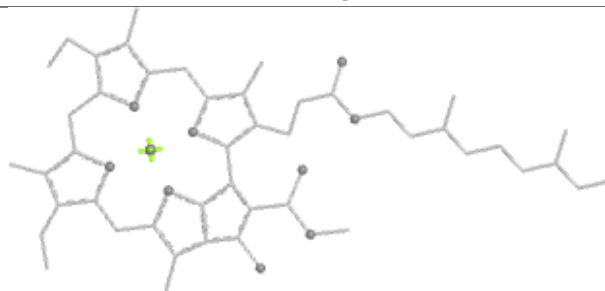
Bond lengths



Bond angles

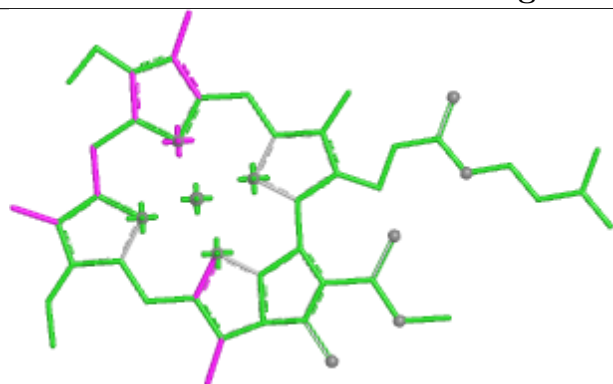


Torsions

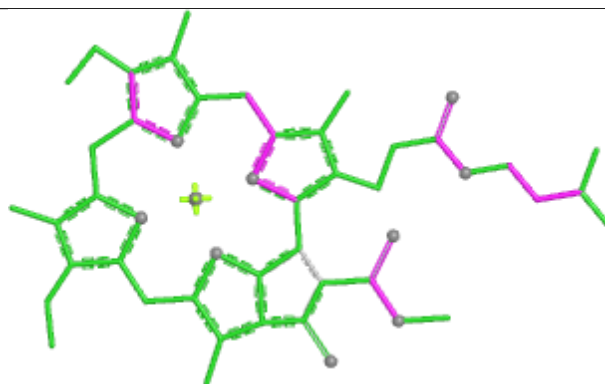


Rings

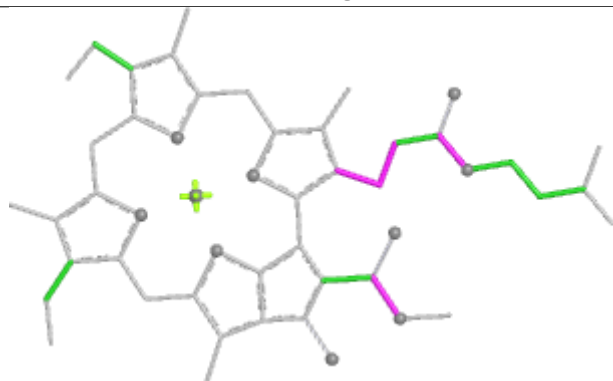
Ligand CLA 2 509



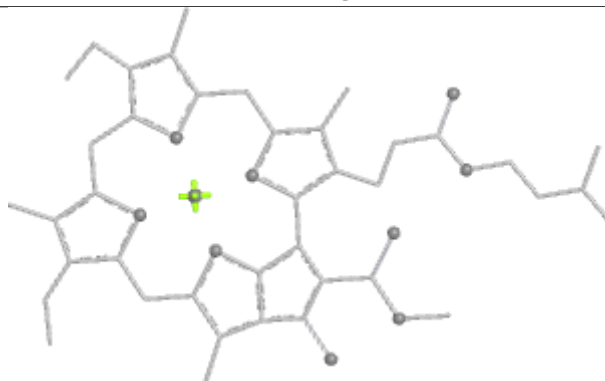
Bond lengths



Bond angles

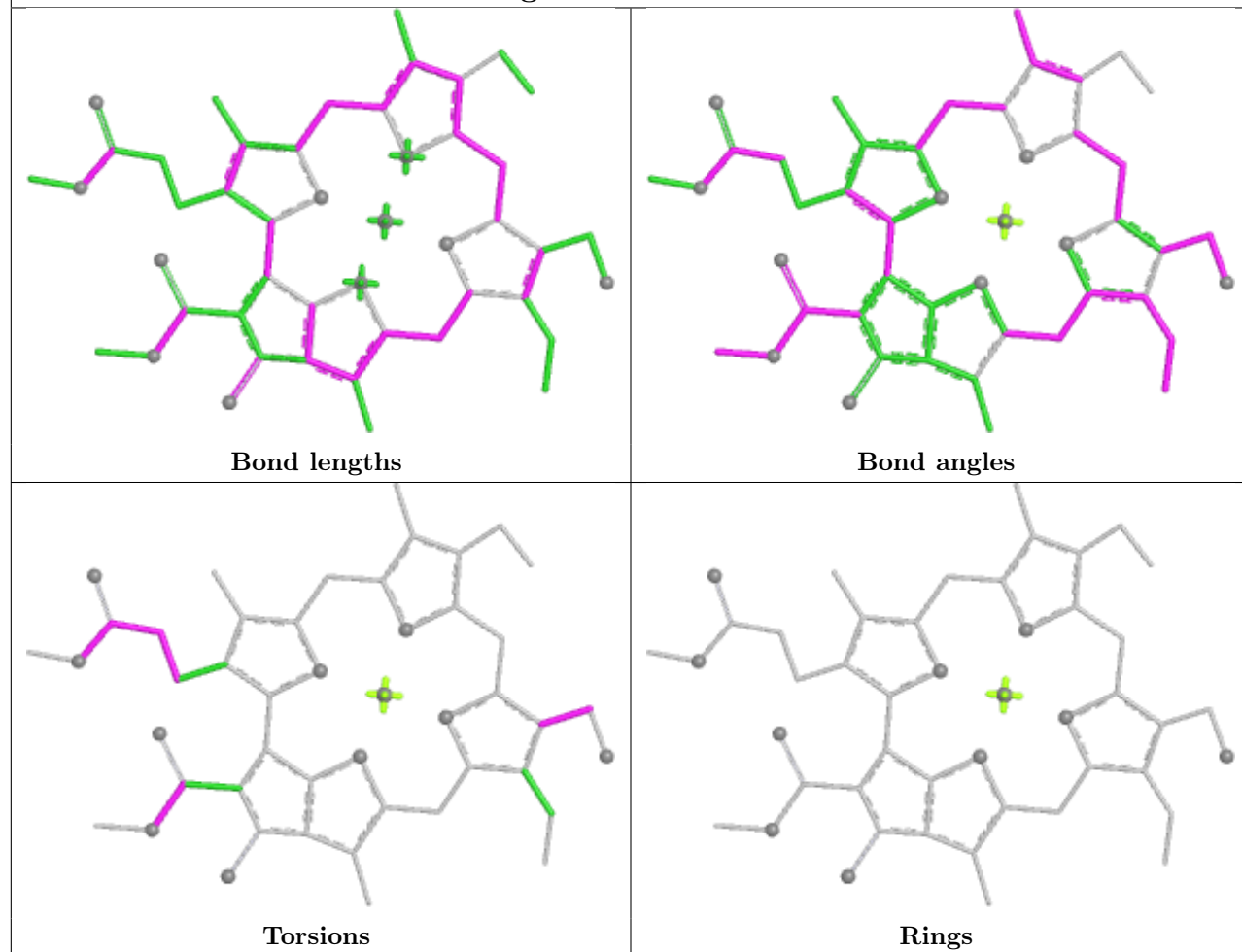


Torsions

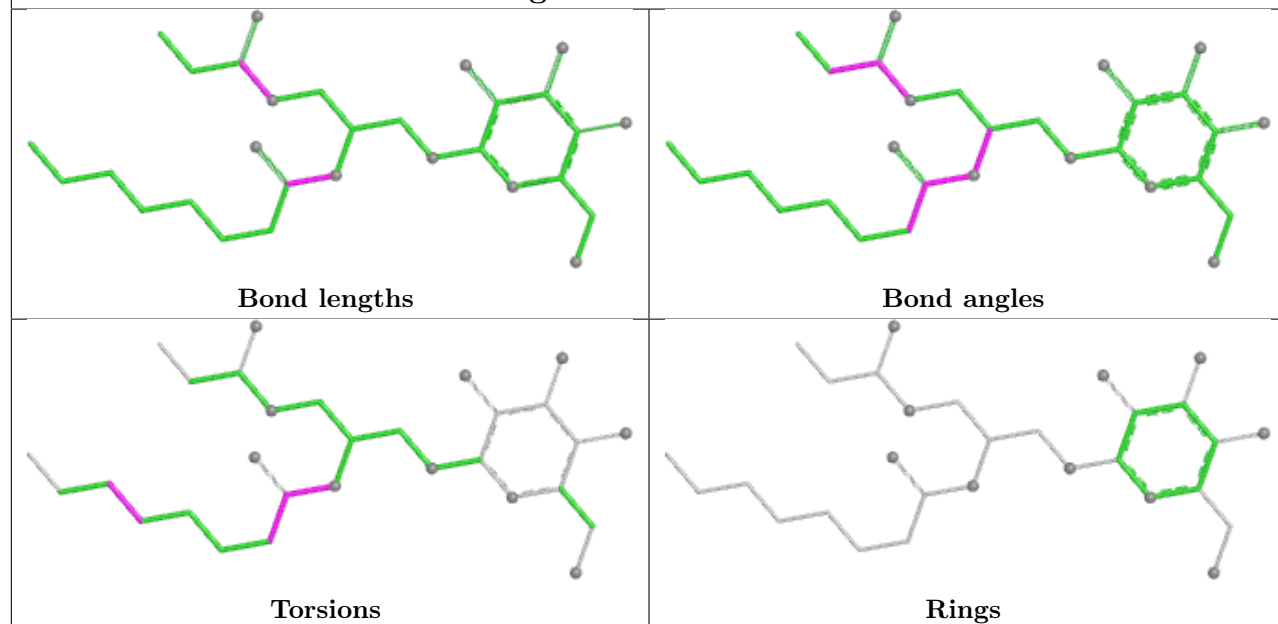


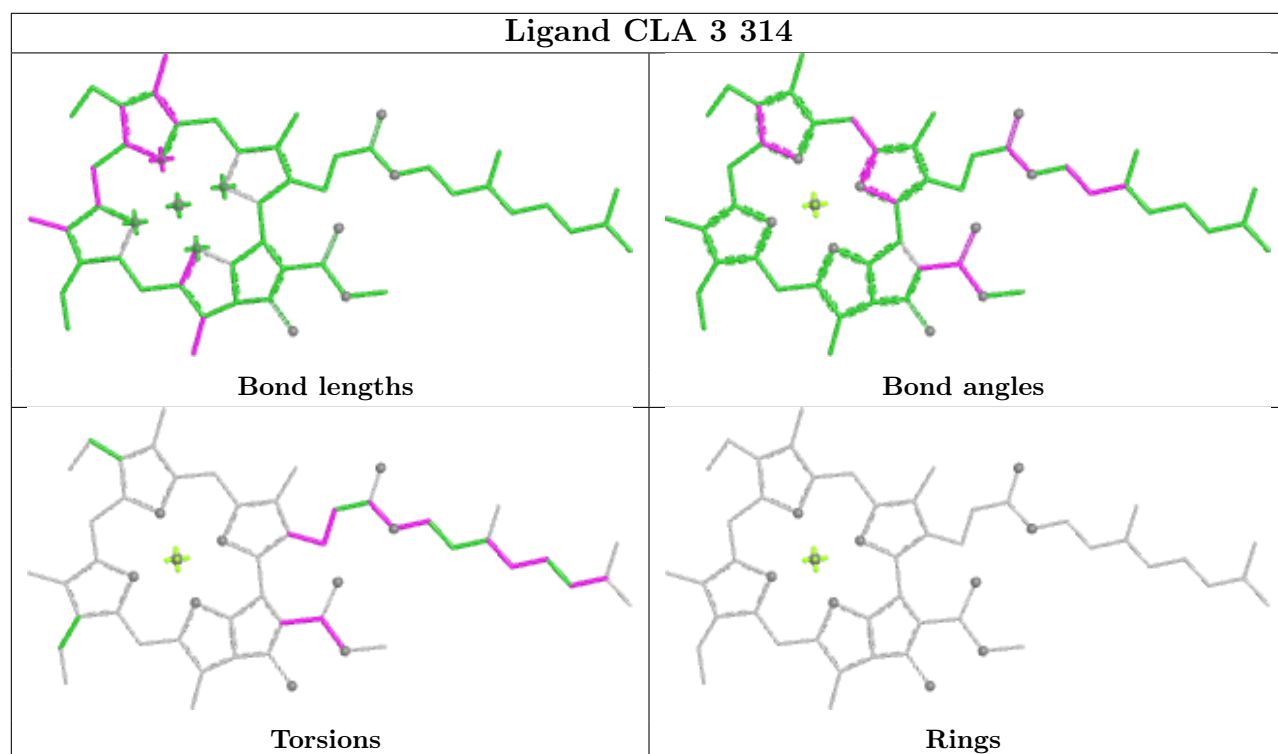
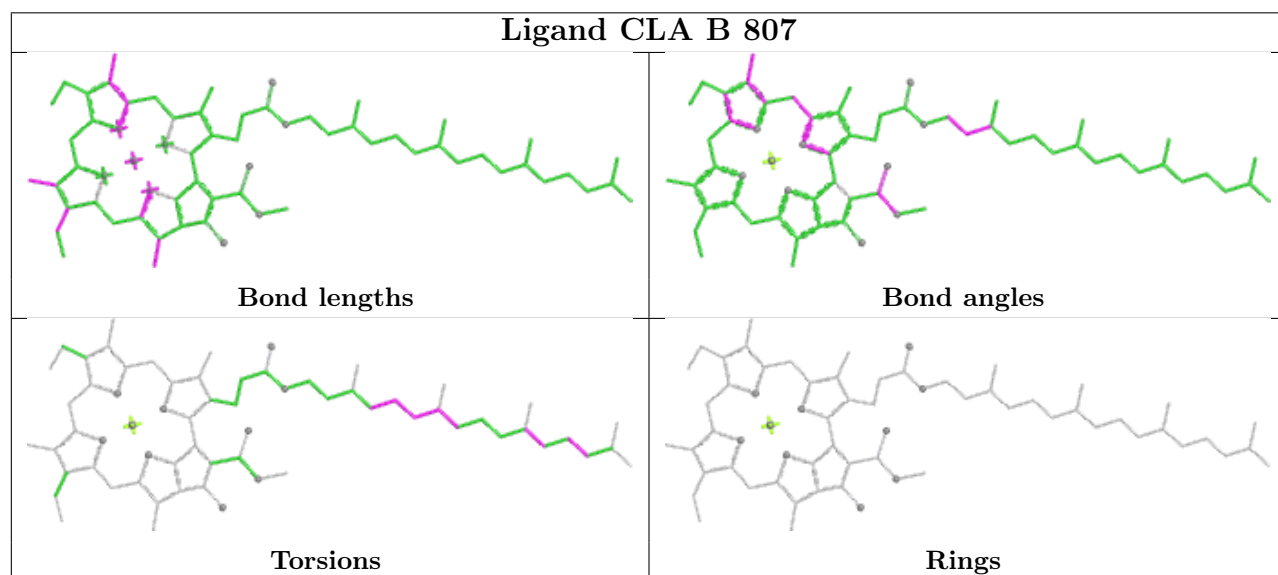
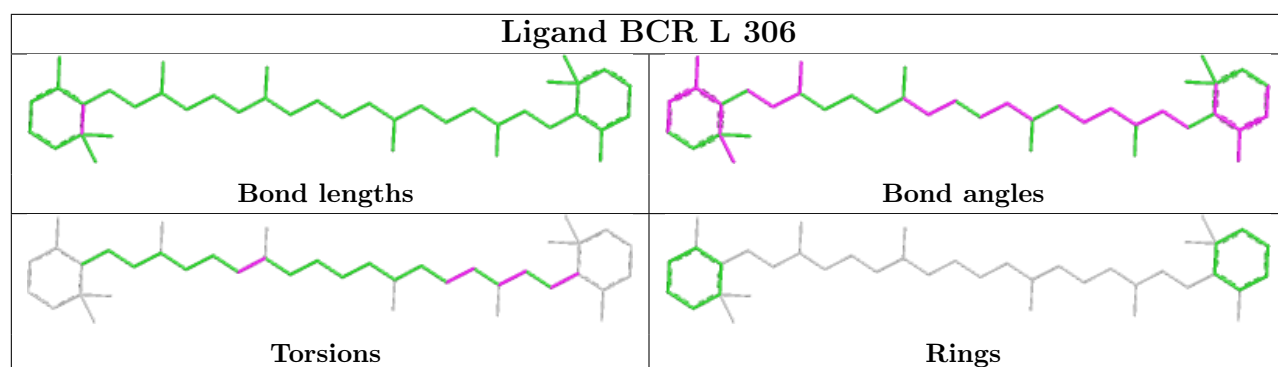
Rings

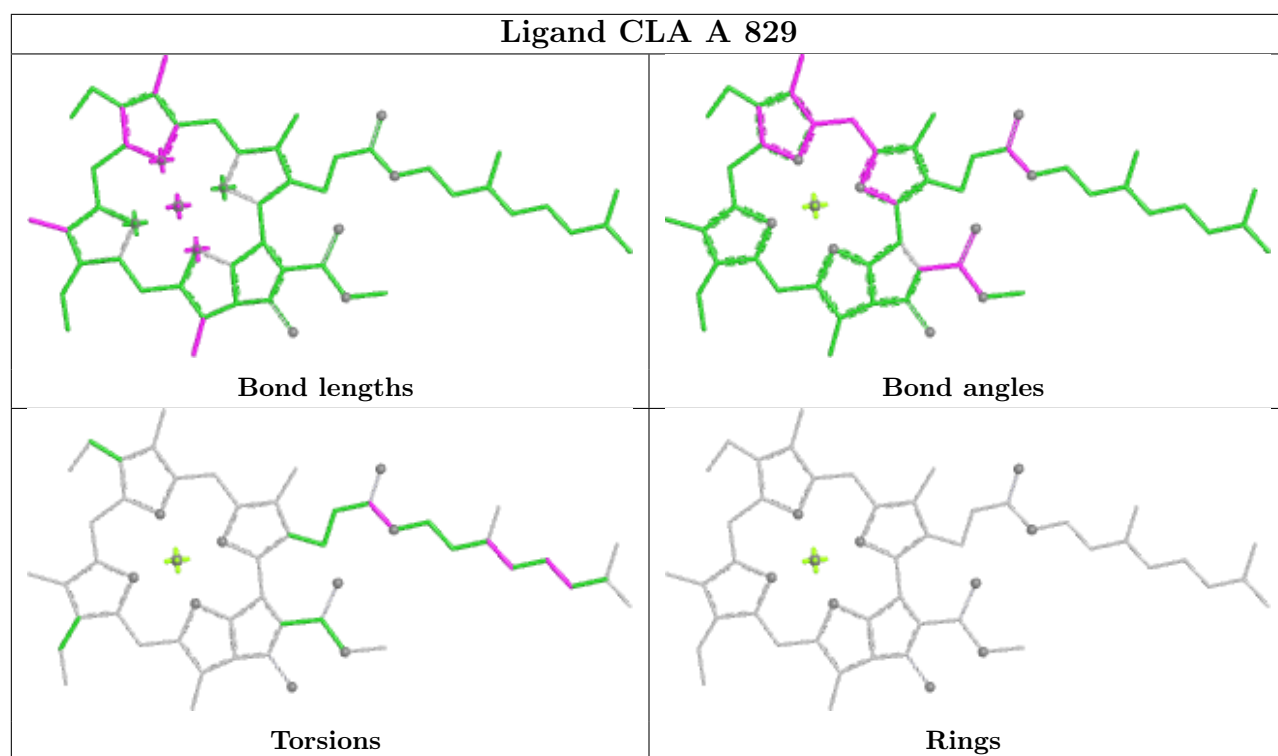
Ligand CHL 1 512



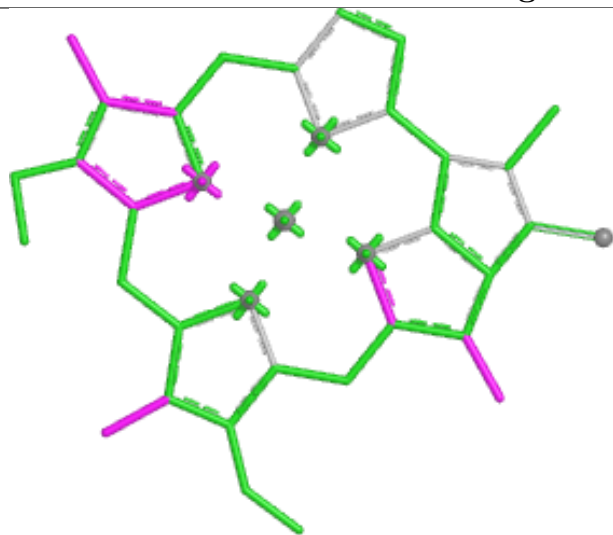
Ligand LMG F 805



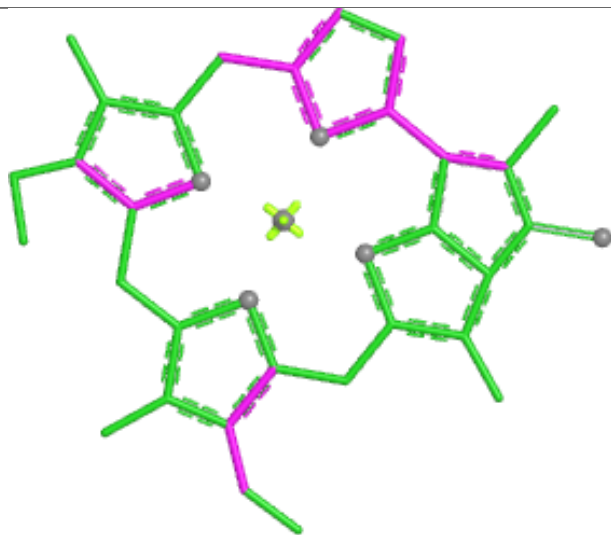




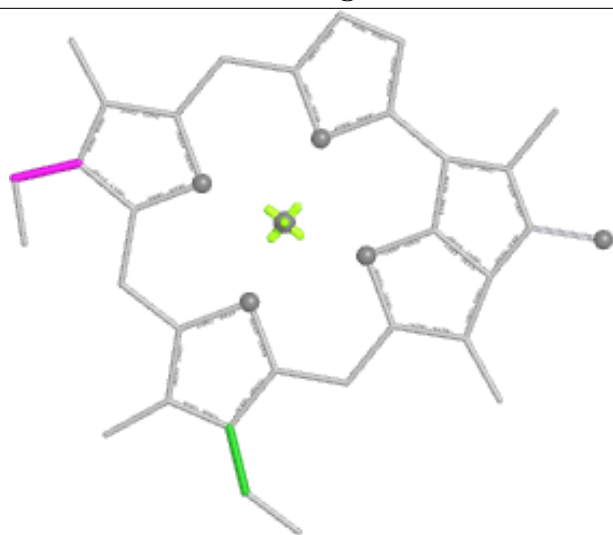
Ligand CLA 2 504



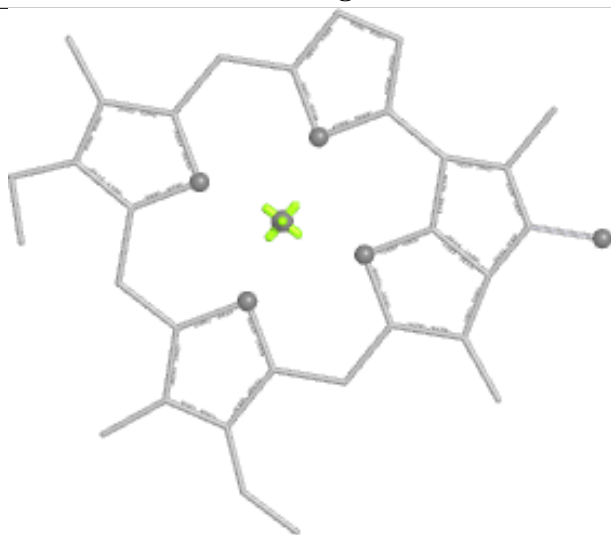
Bond lengths



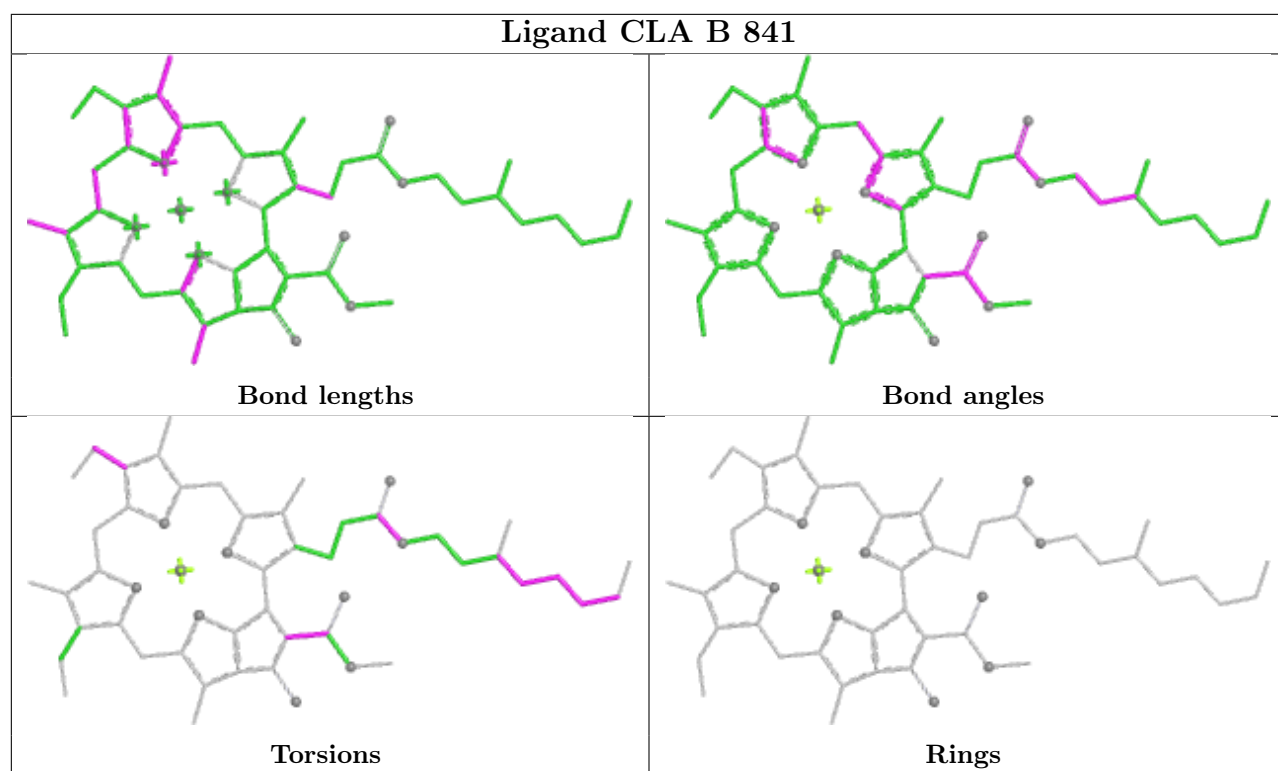
Bond angles



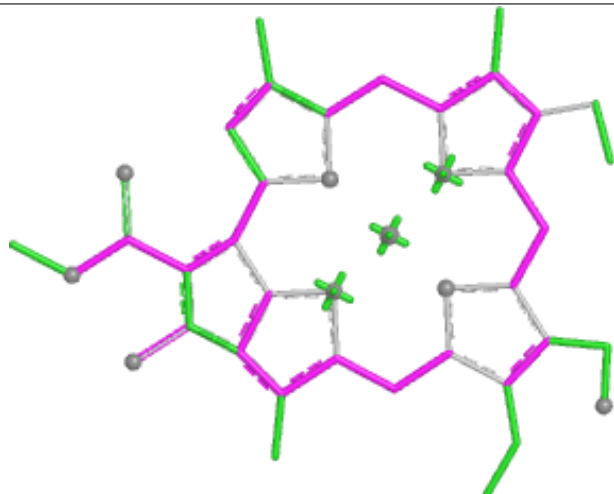
Torsions



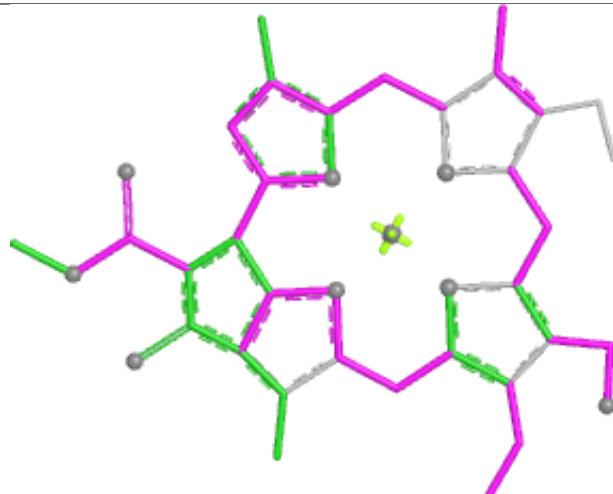
Rings



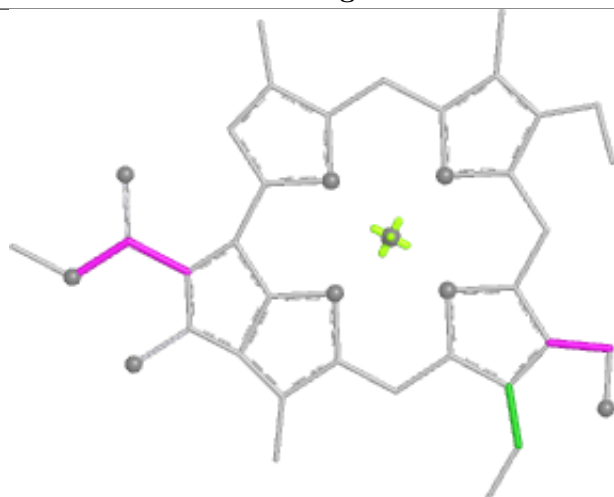
Ligand CHL 1 517



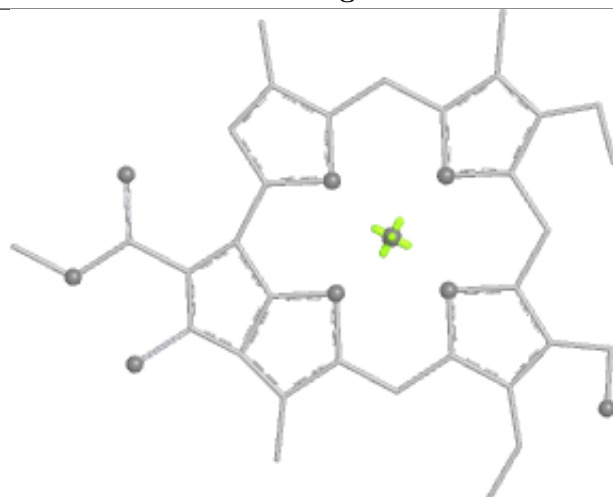
Bond lengths



Bond angles

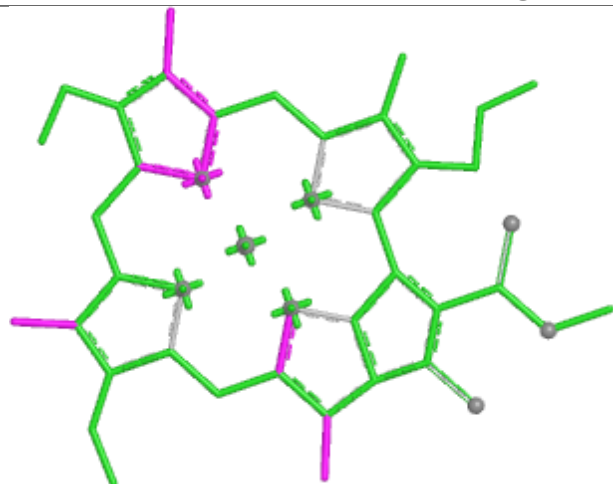


Torsions

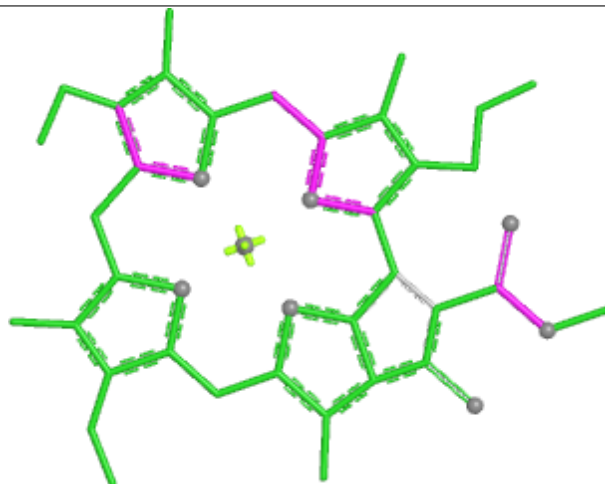


Rings

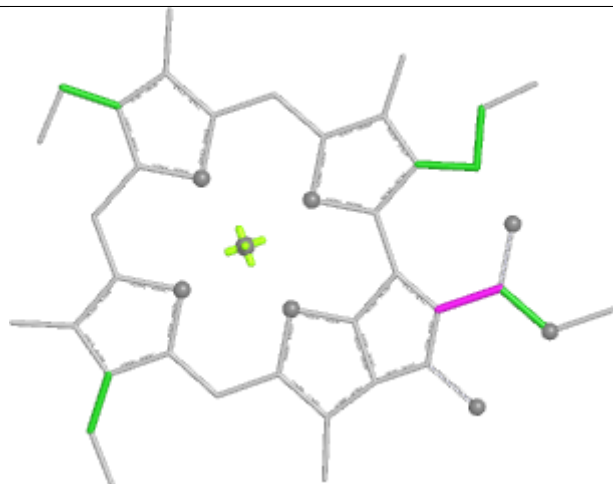
Ligand CLA B 831



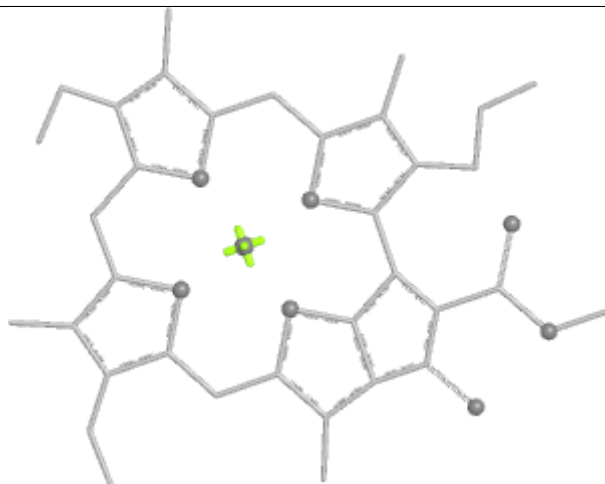
Bond lengths



Bond angles

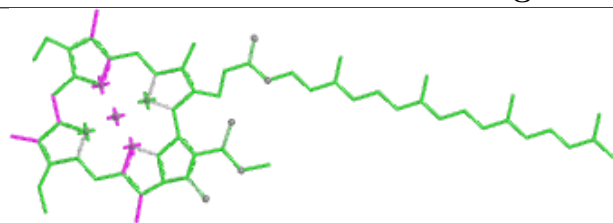


Torsions

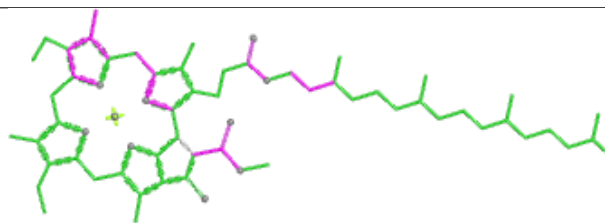


Rings

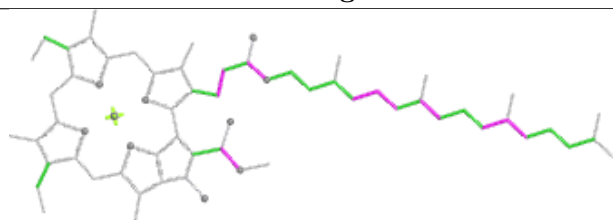
Ligand CLA A 838



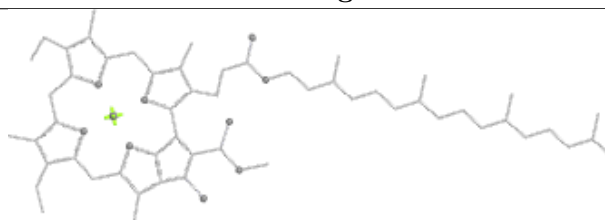
Bond lengths



Bond angles

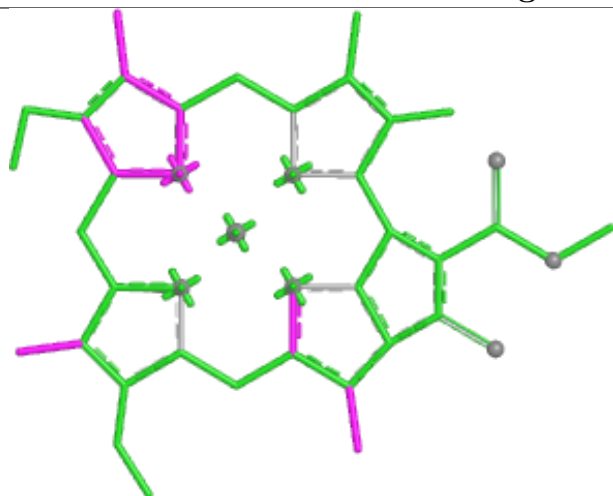


Torsions

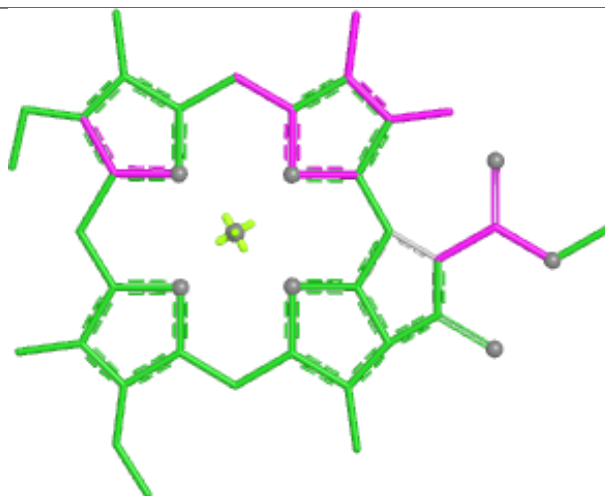


Rings

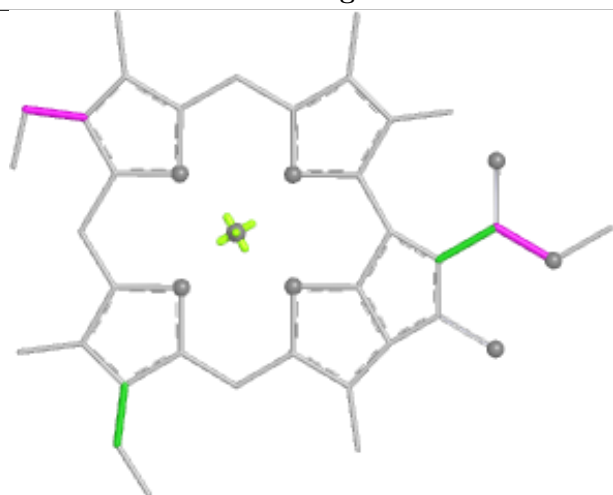
Ligand CLA 3 301



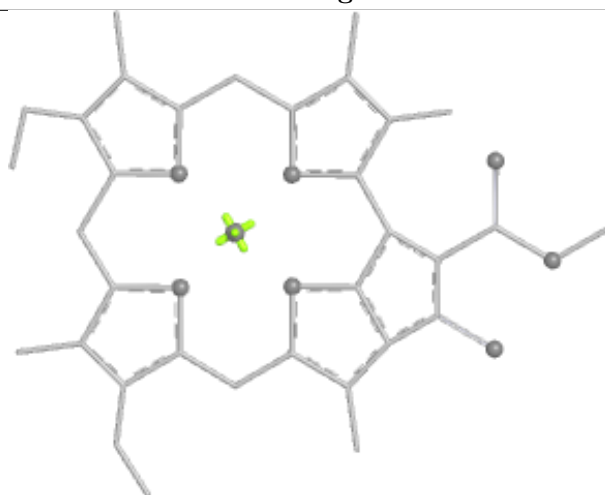
Bond lengths



Bond angles

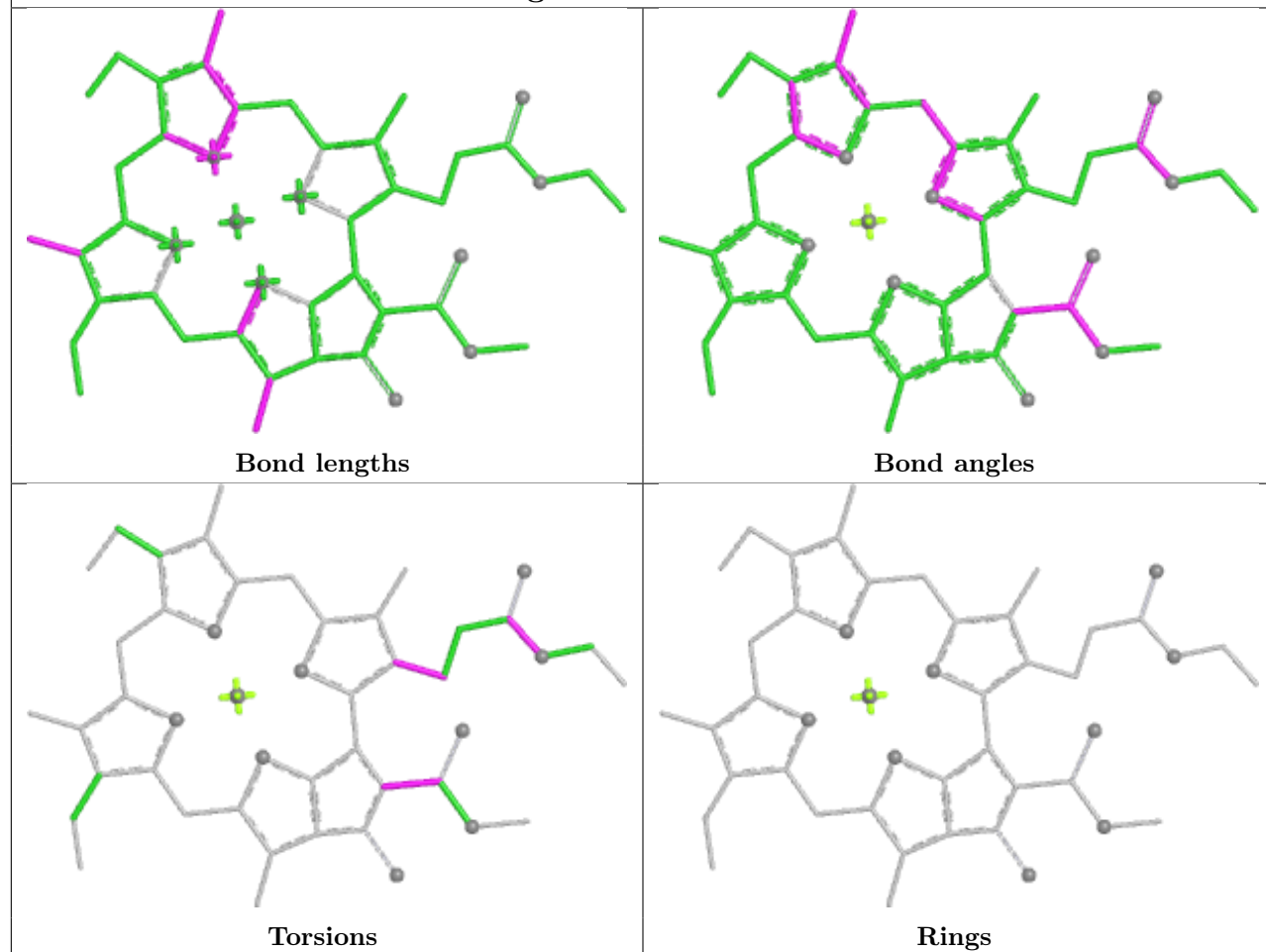


Torsions

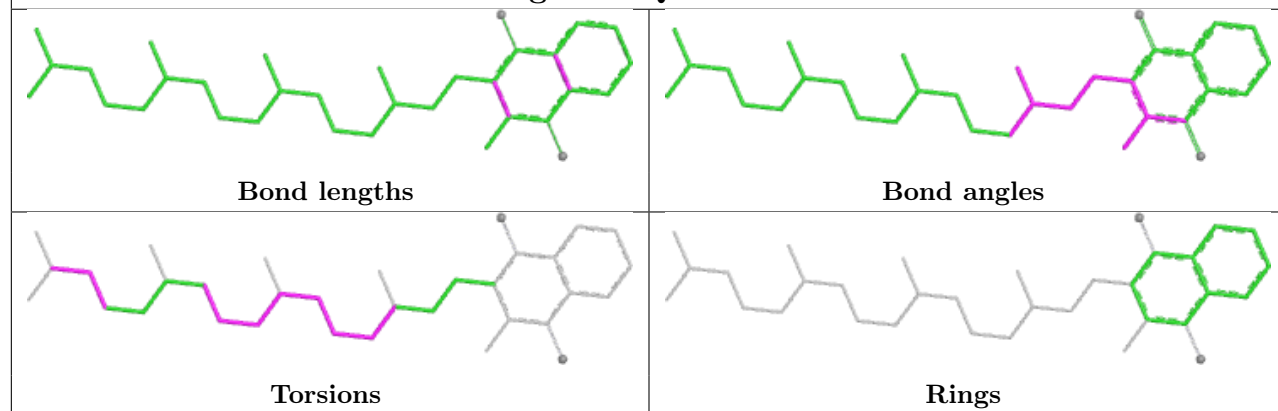


Rings

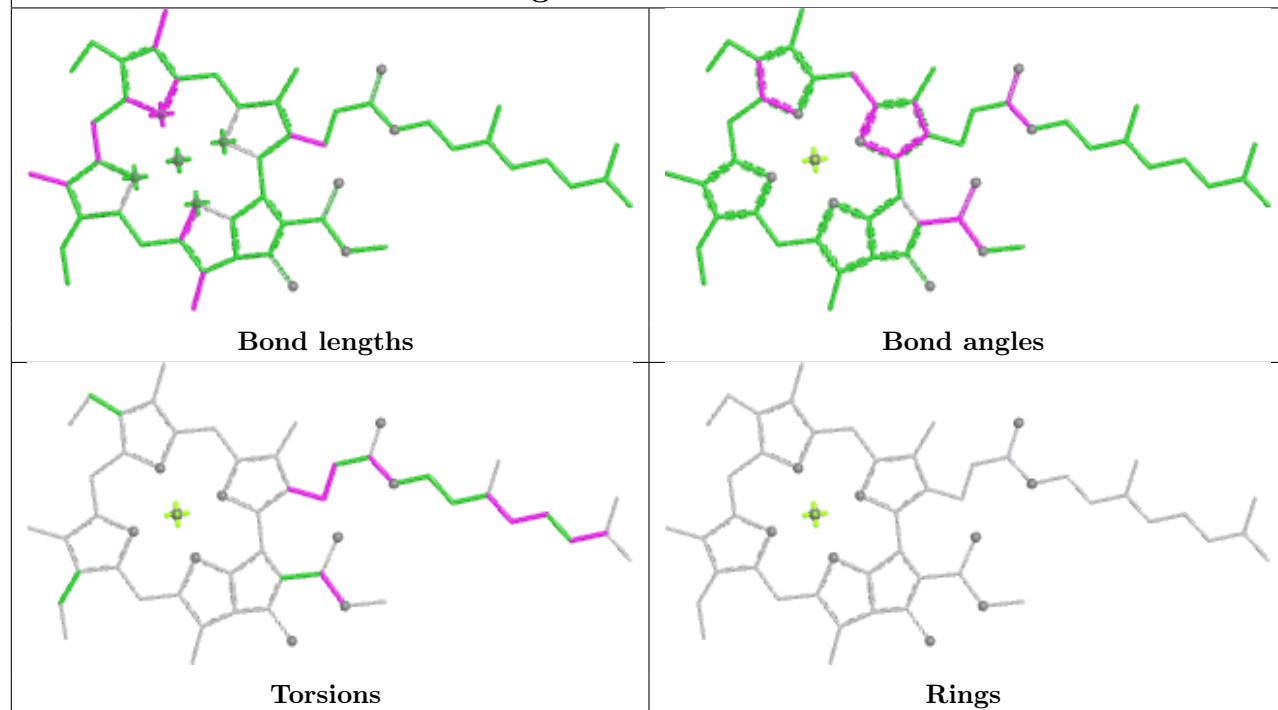
Ligand CLA B 839



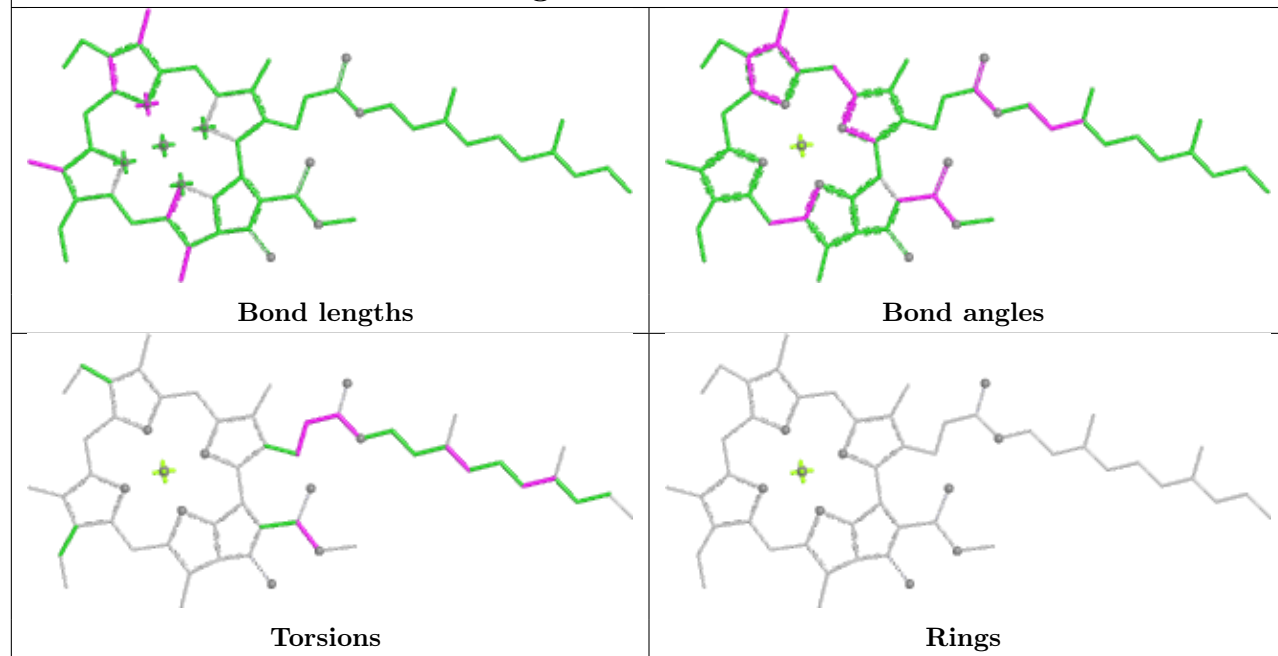
Ligand PQN A 841



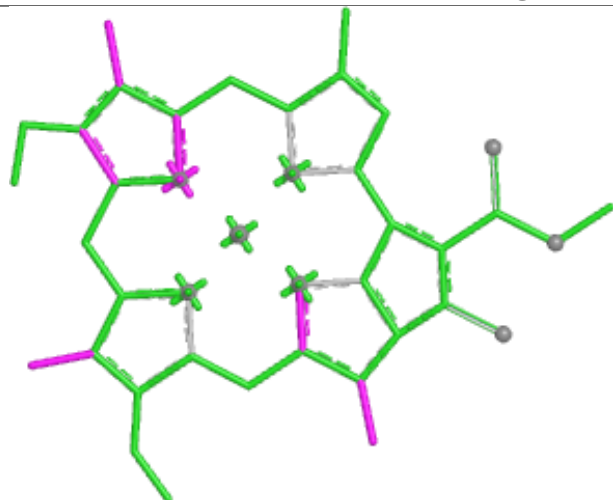
Ligand CLA A 836



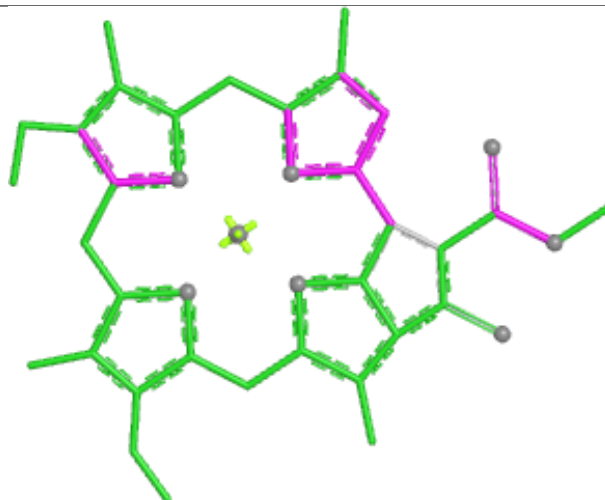
Ligand CLA A 820



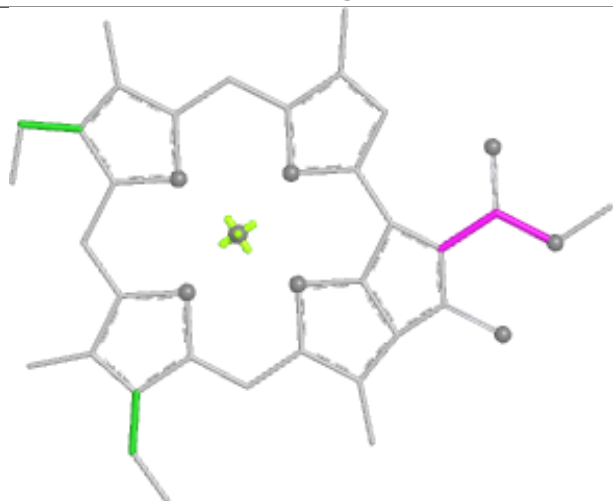
Ligand CLA A 824



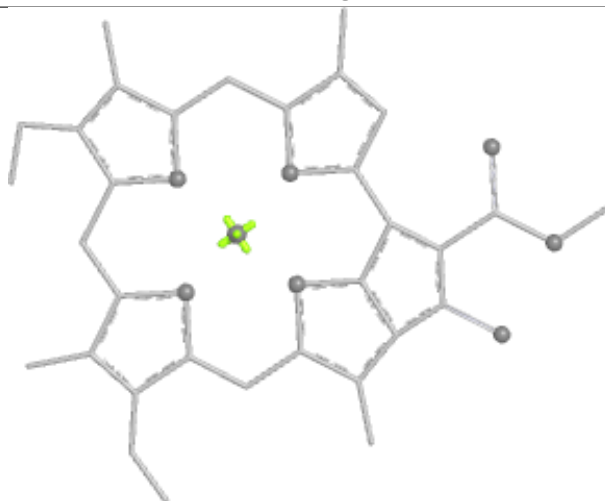
Bond lengths



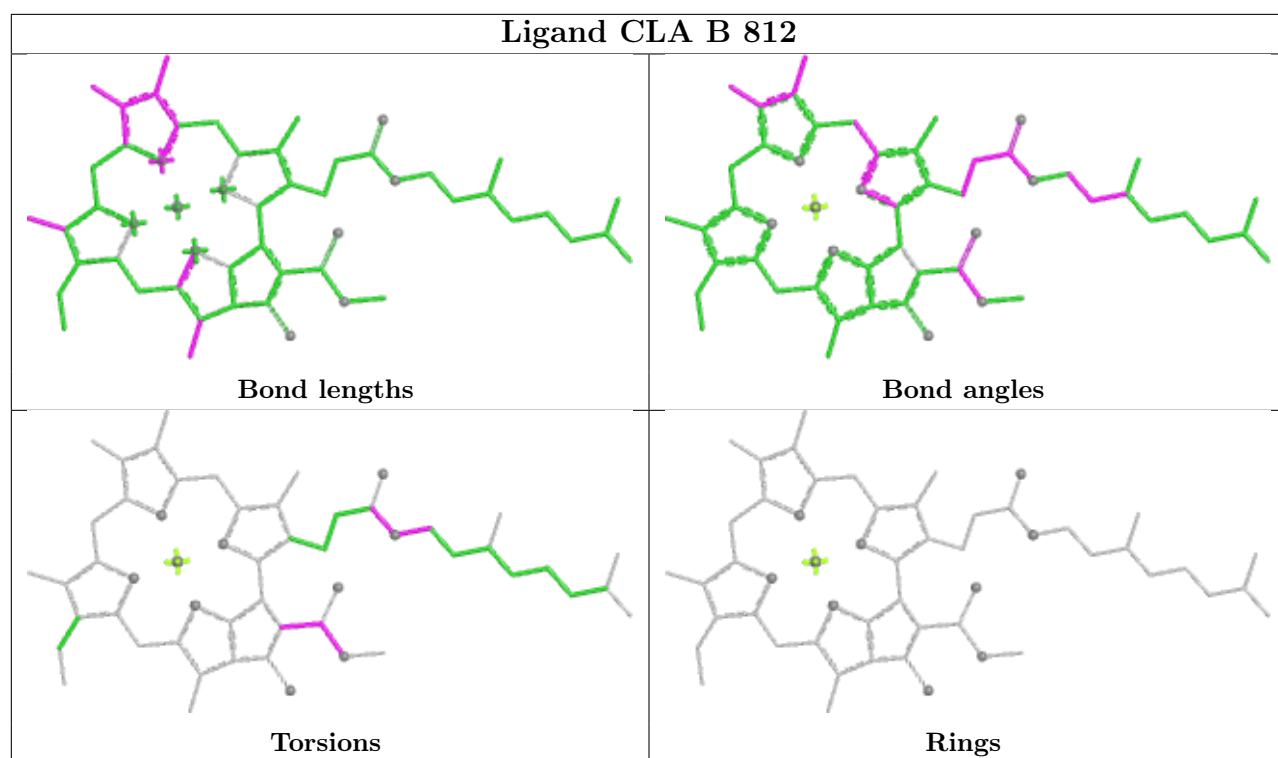
Bond angles



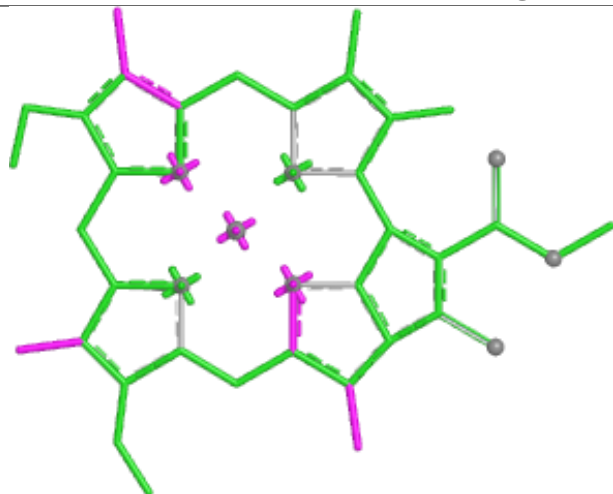
Torsions



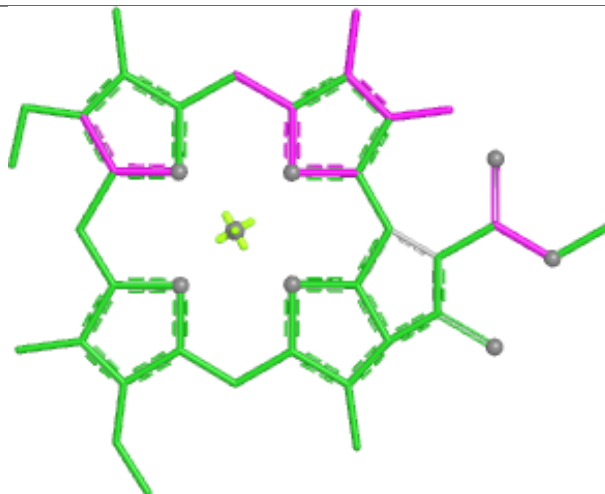
Rings



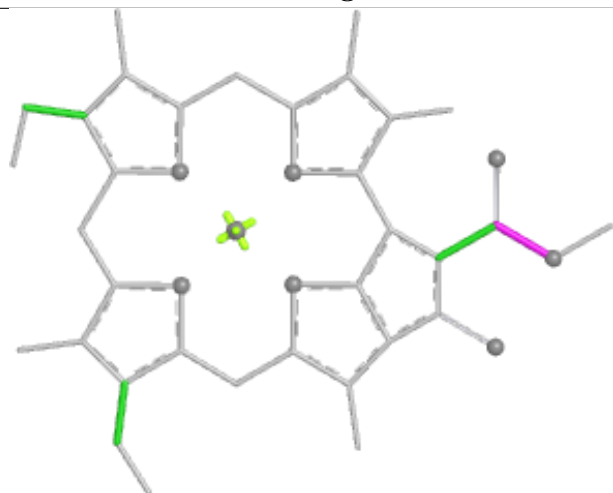
Ligand CLA A 828



Bond lengths



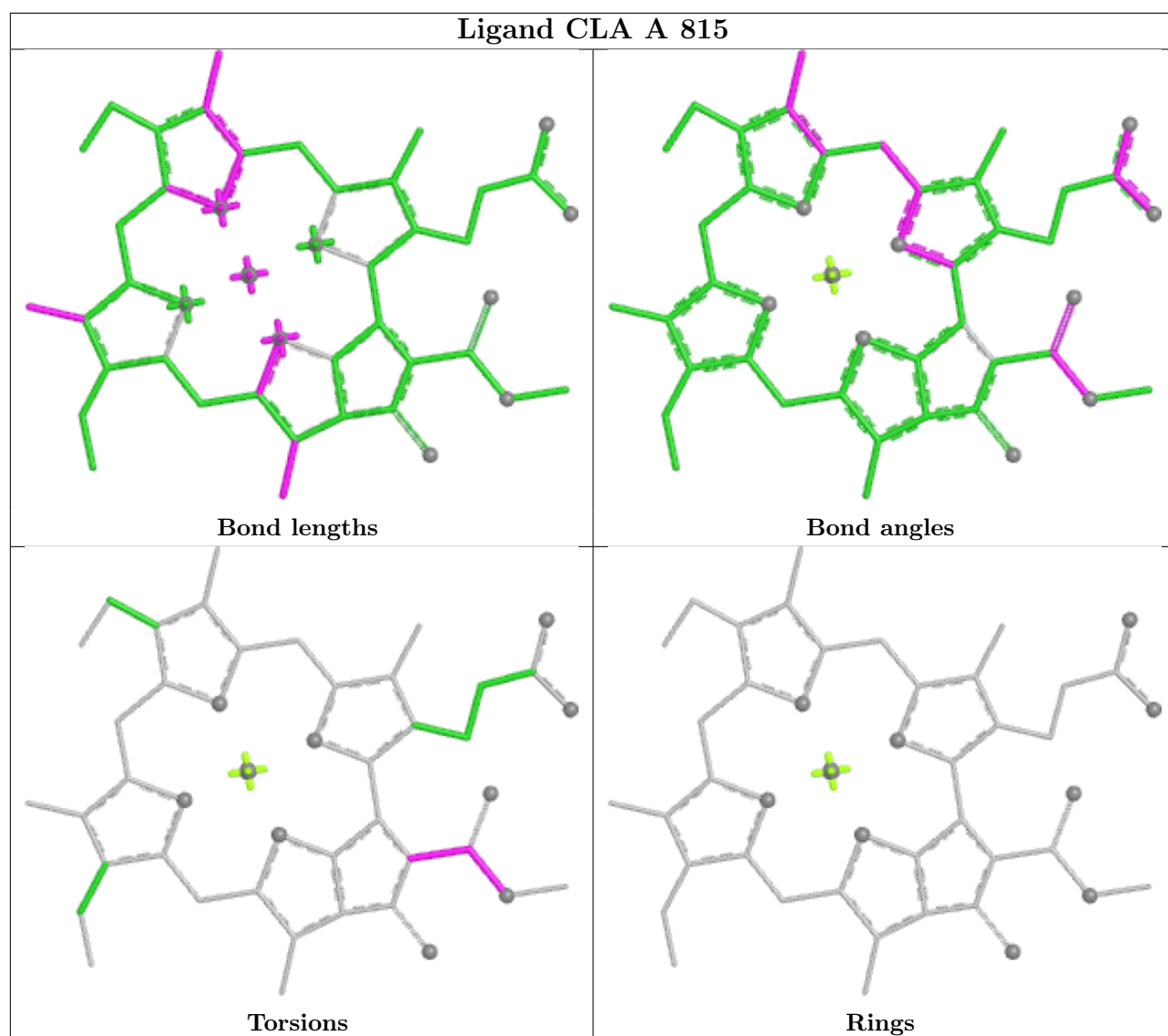
Bond angles



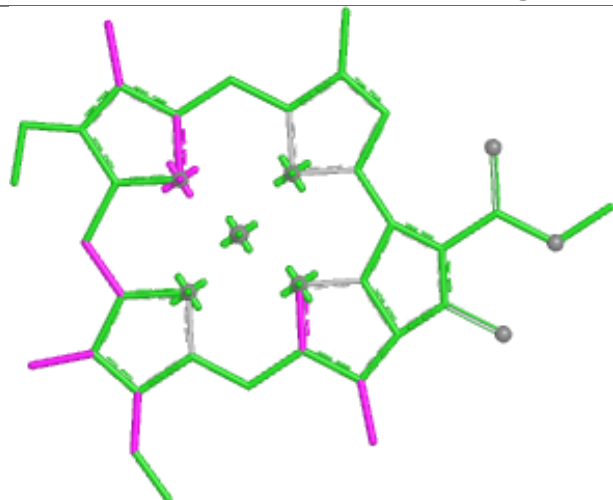
Torsions



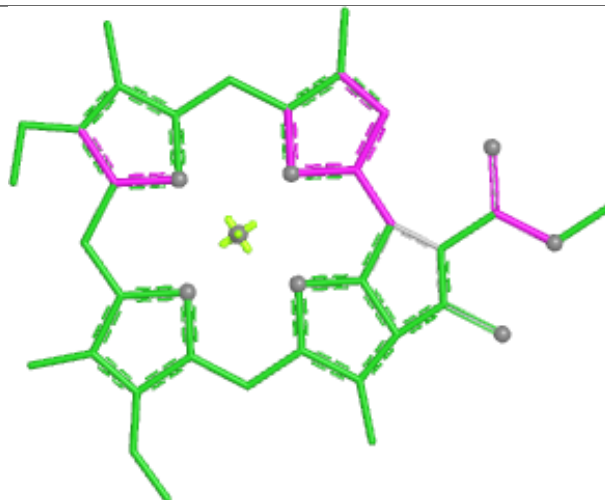
Rings



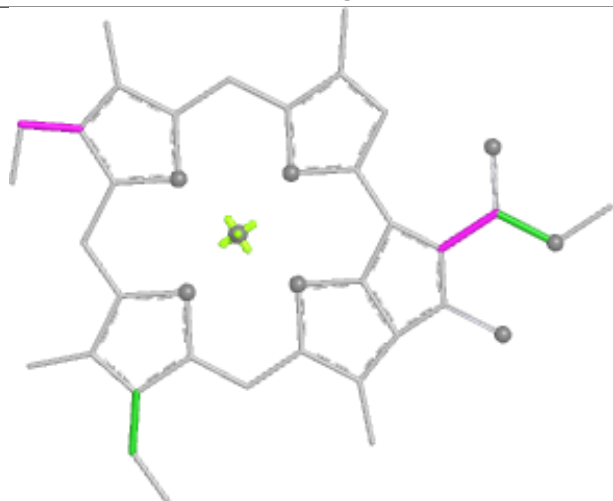
Ligand CLA B 809



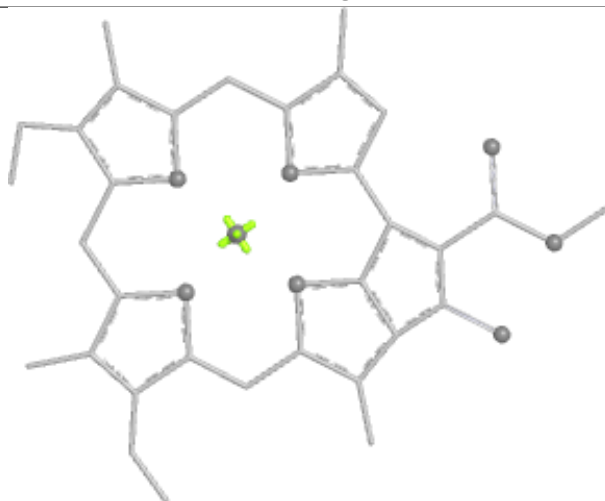
Bond lengths



Bond angles

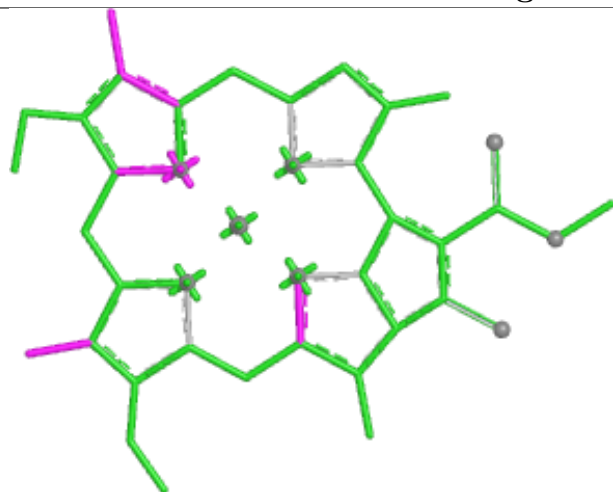


Torsions

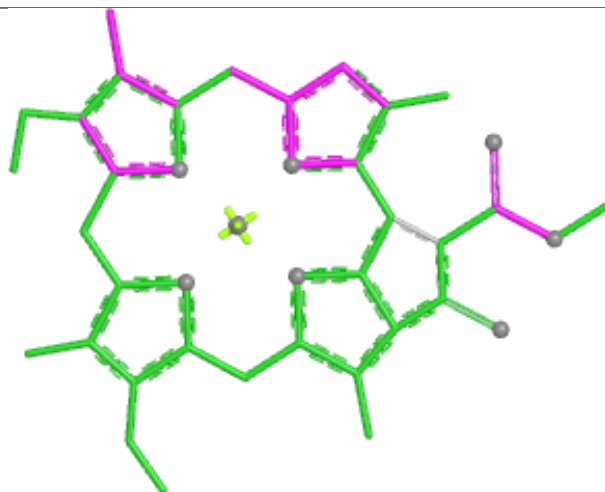


Rings

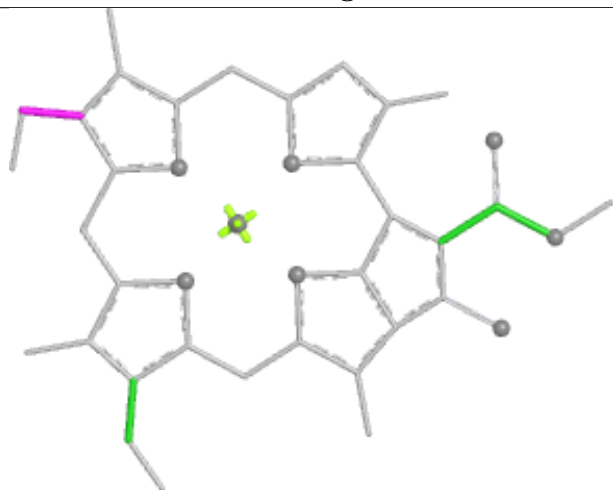
Ligand CLA L 302



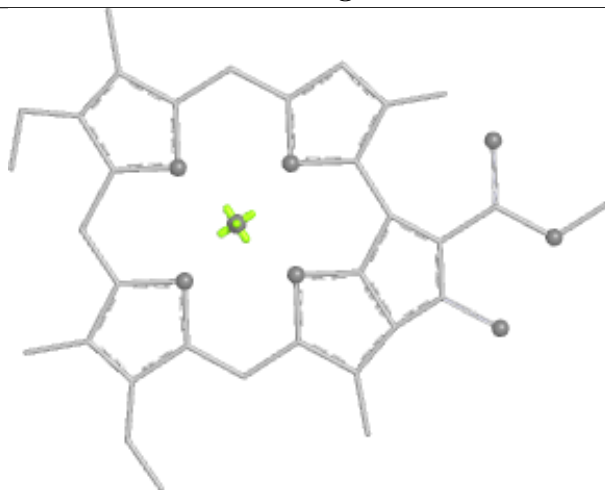
Bond lengths



Bond angles

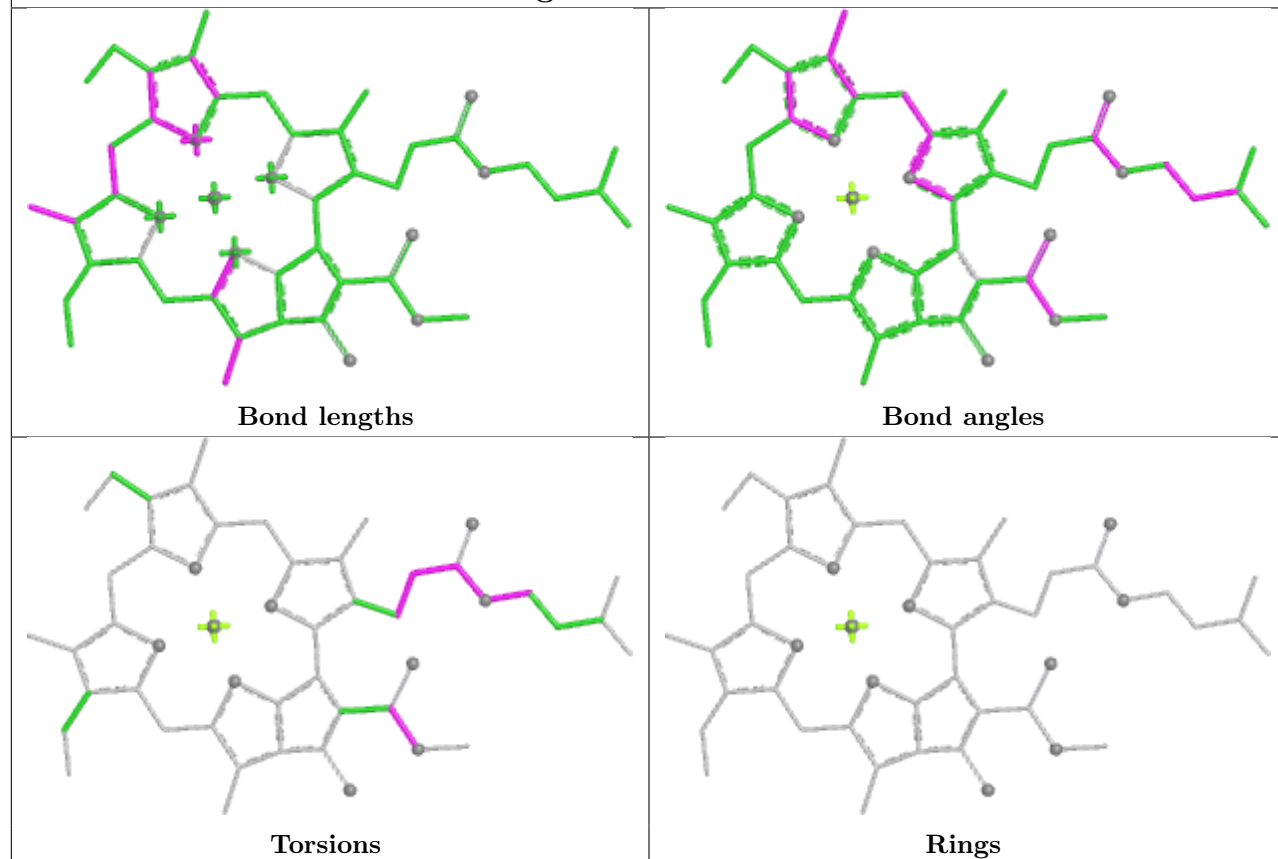


Torsions

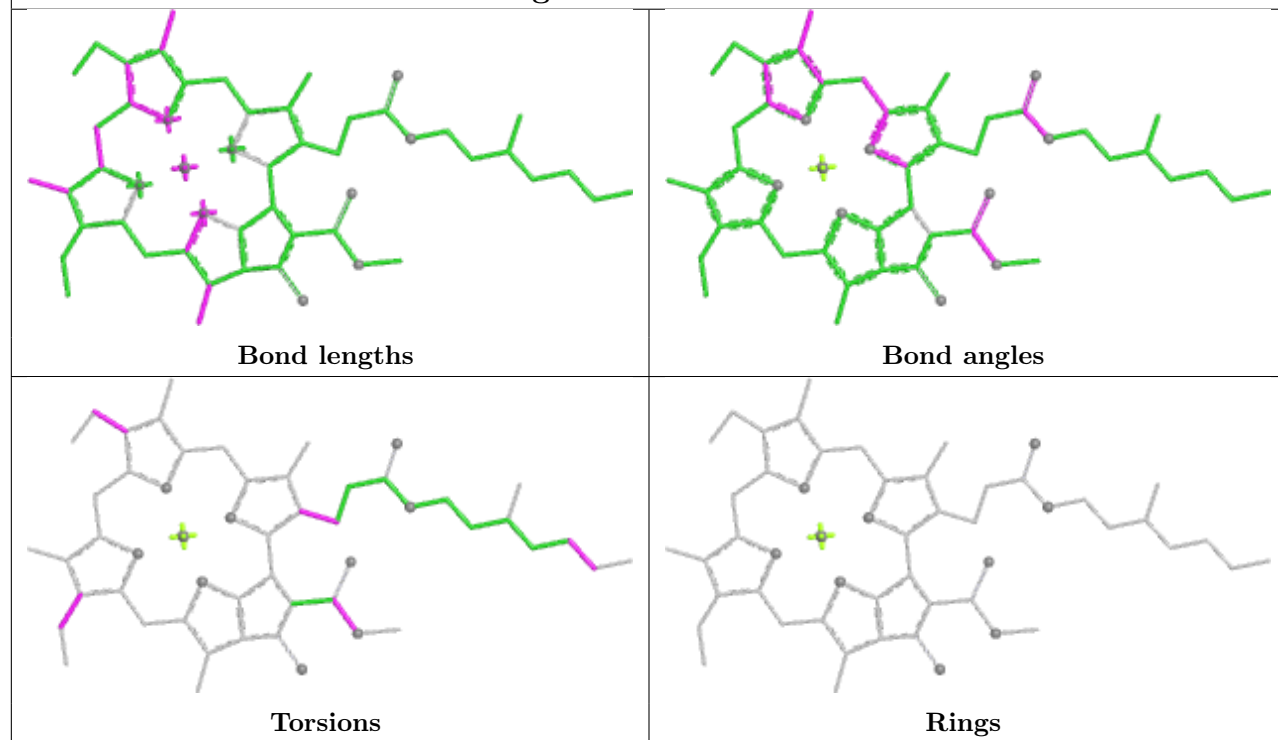


Rings

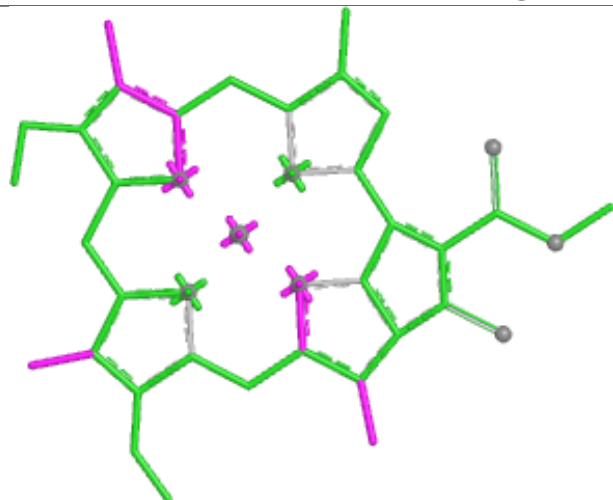
Ligand CLA 5 310



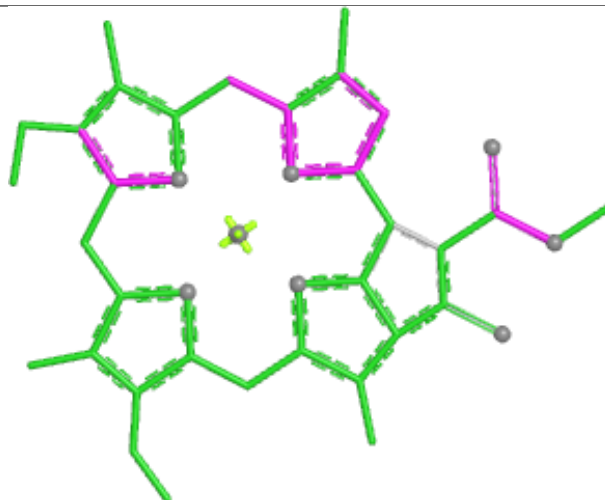
Ligand CLA B 820



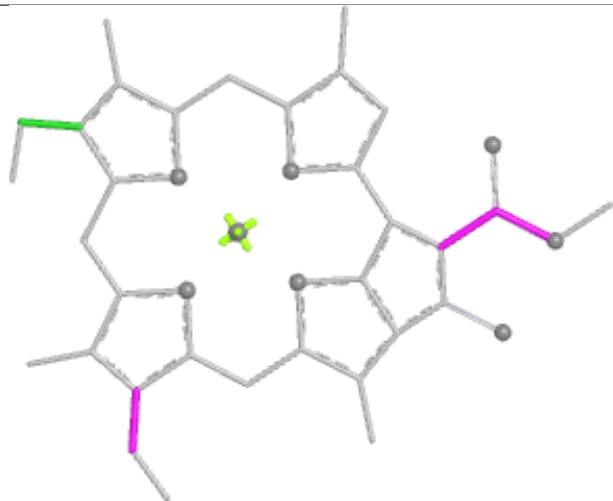
Ligand CLA K 203



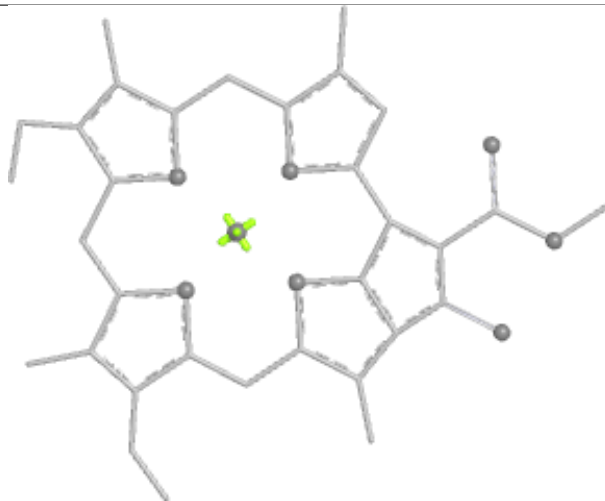
Bond lengths



Bond angles

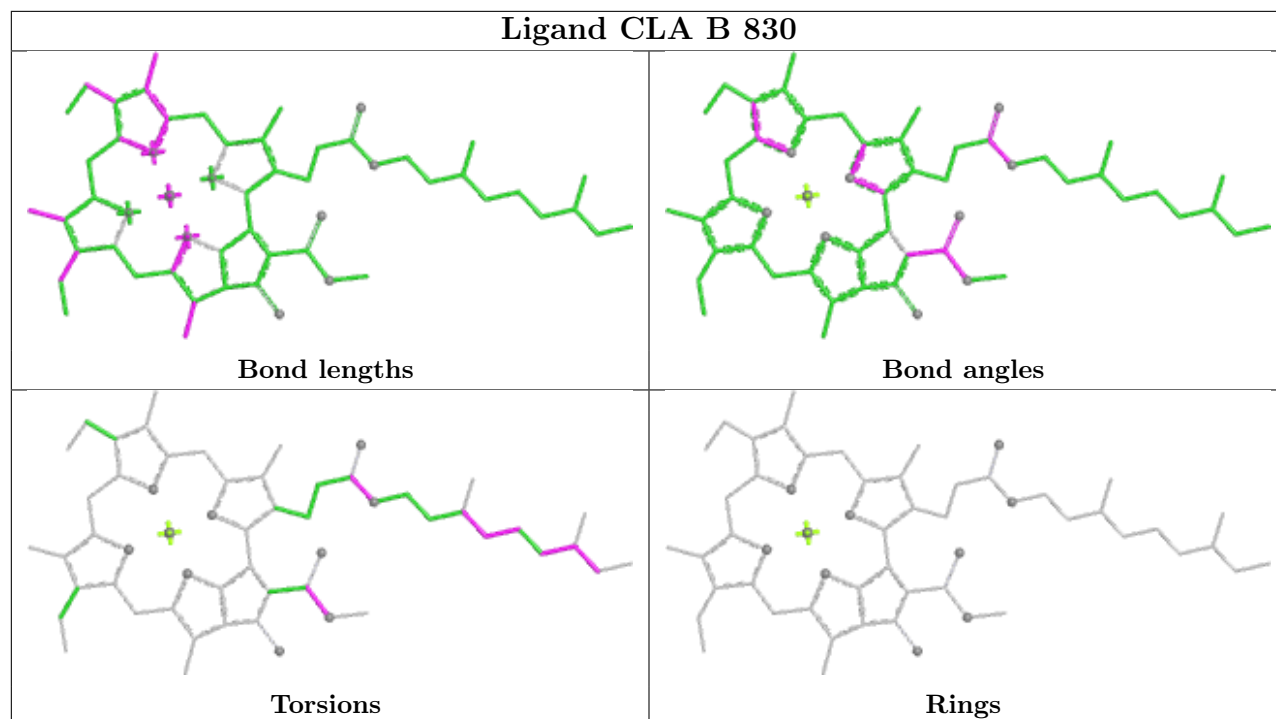


Torsions

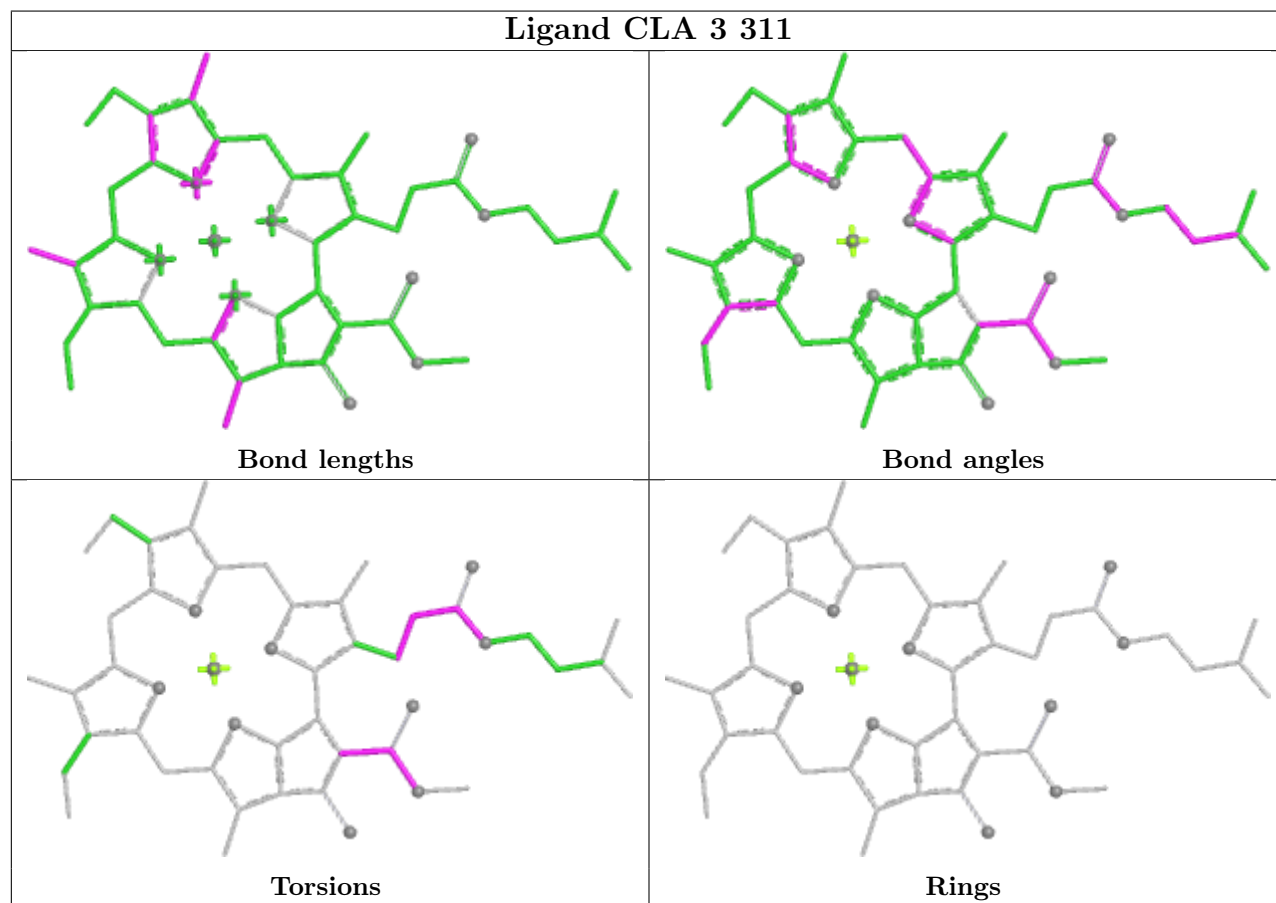


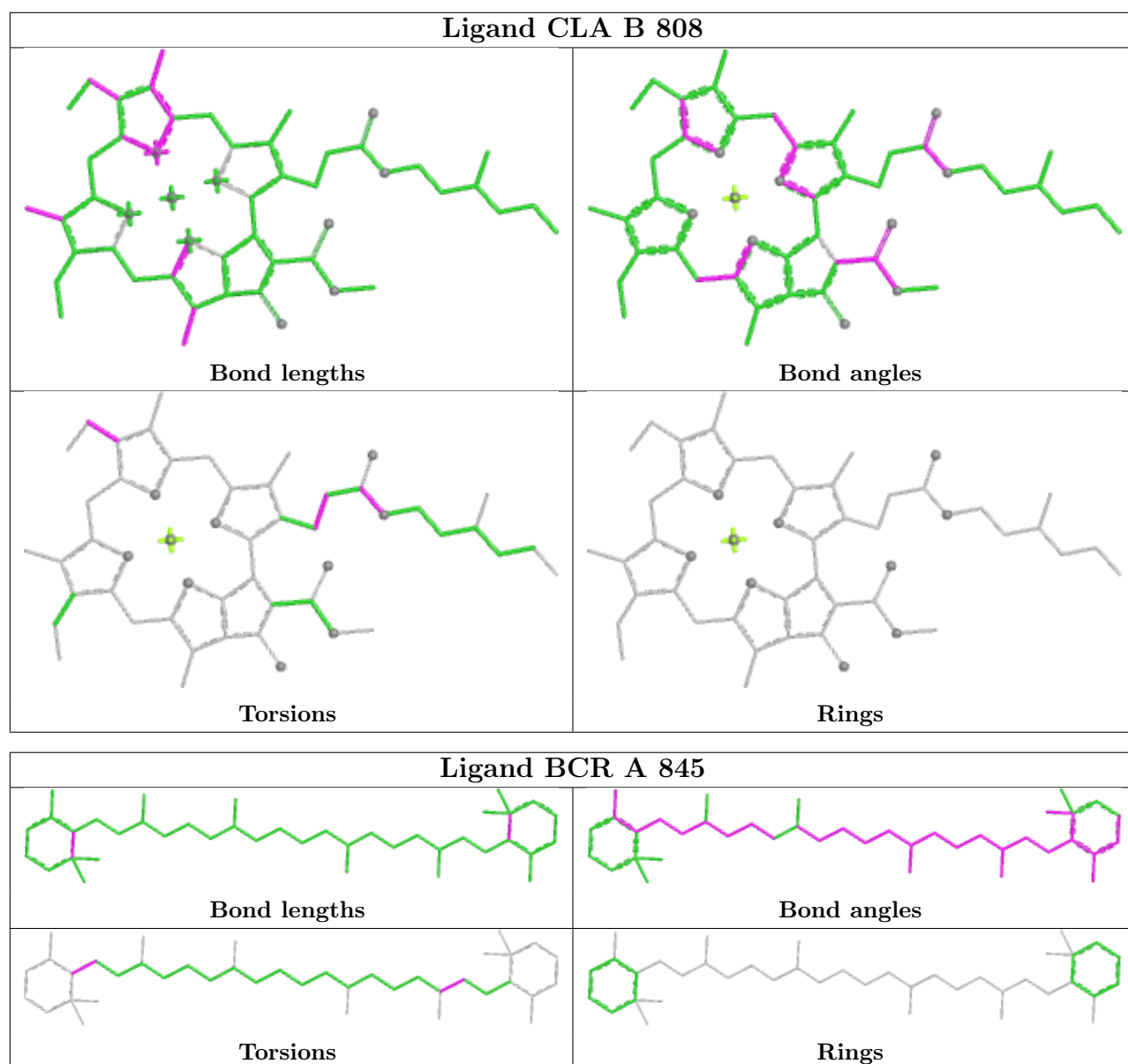
Rings

Ligand CLA B 830

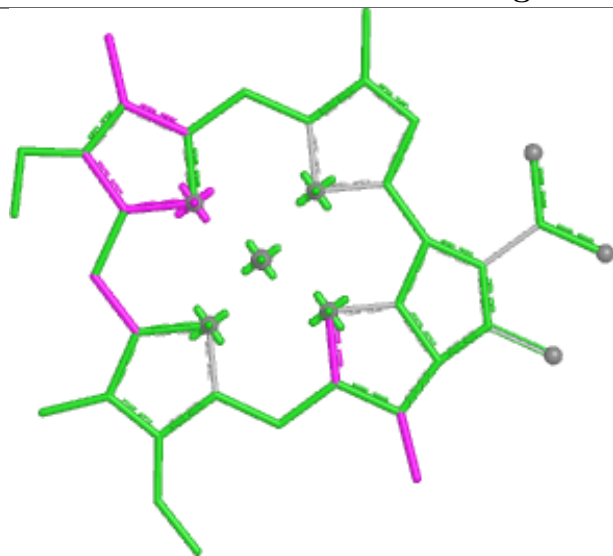


Ligand CLA 3 311

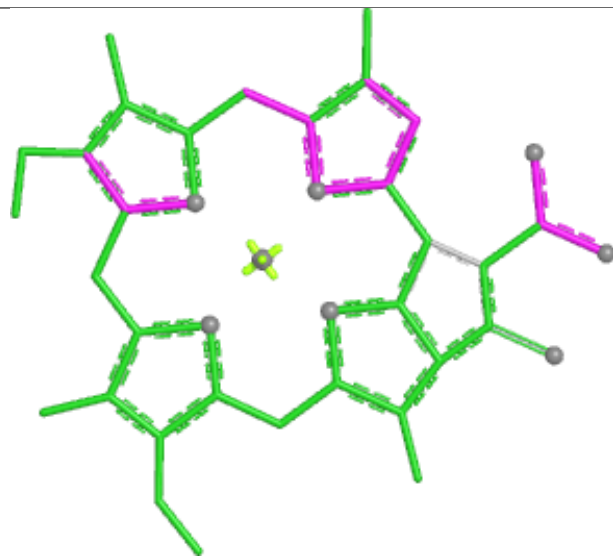




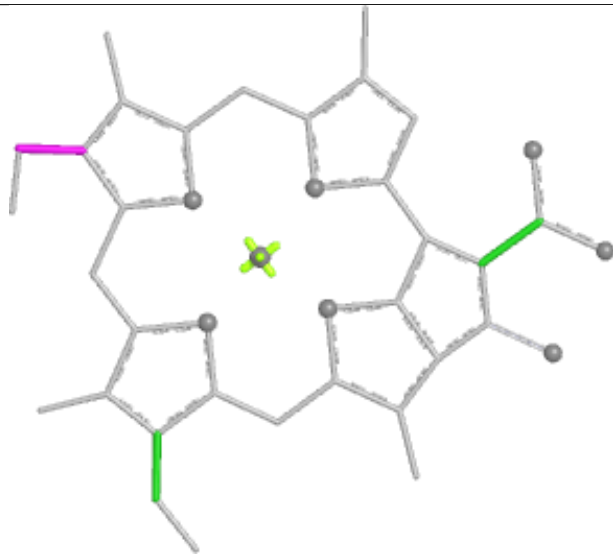
Ligand CLA K 205



Bond lengths



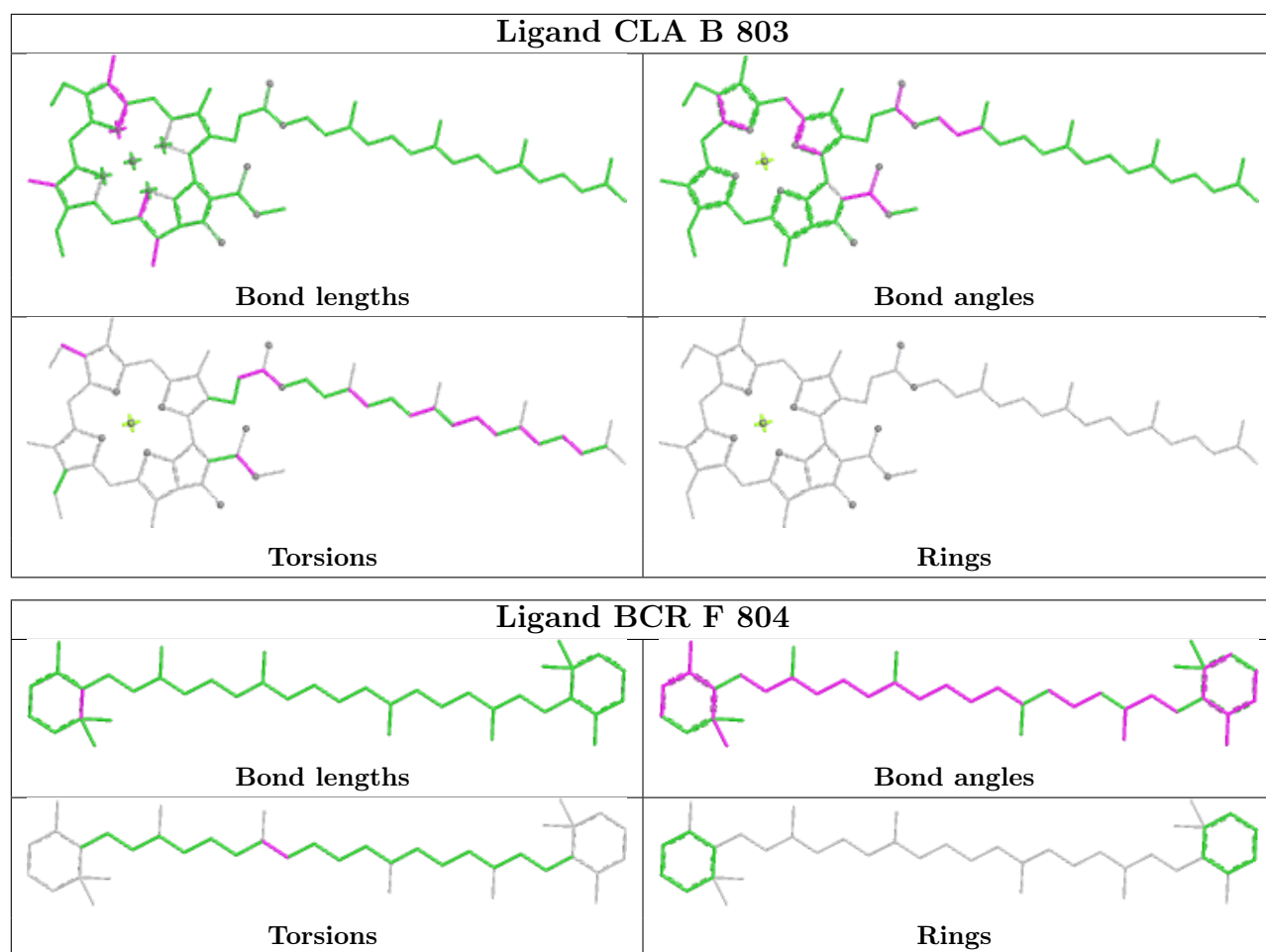
Bond angles



Torsions



Rings



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.

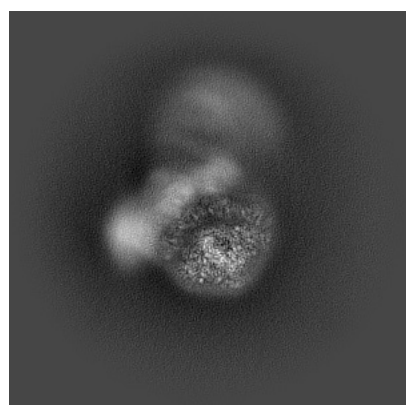
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-31348. These allow visual inspection of the internal detail of the map and identification of artifacts.

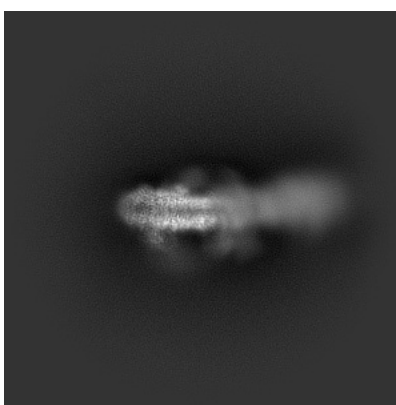
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

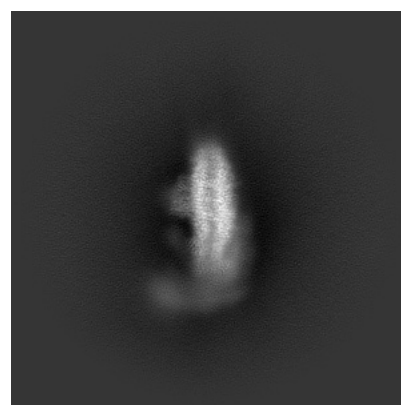
6.1.1 Primary map



X



Y

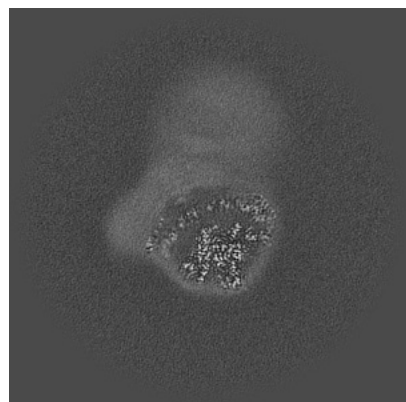


Z

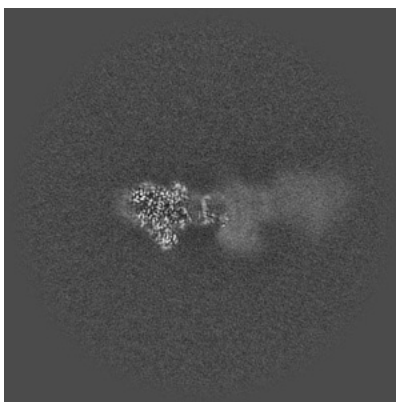
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

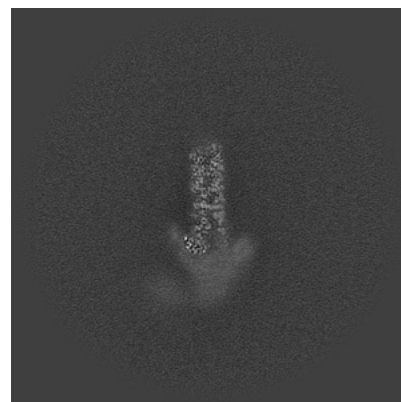
6.2.1 Primary map



X Index: 220



Y Index: 220

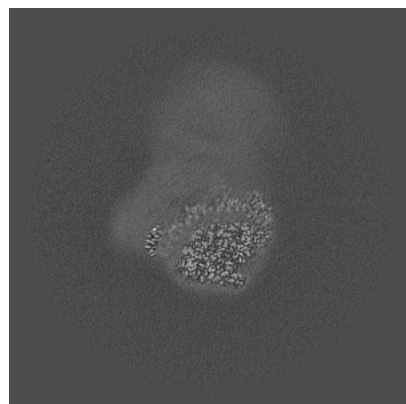


Z Index: 220

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

6.3 Largest variance slices [i](#)

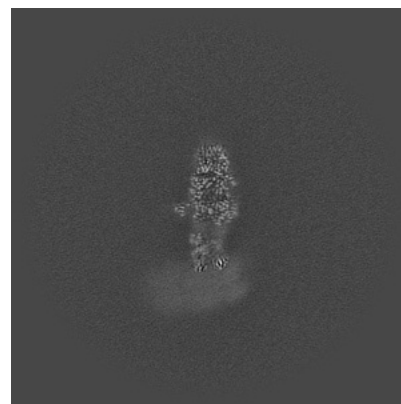
6.3.1 Primary map



X Index: 229



Y Index: 231

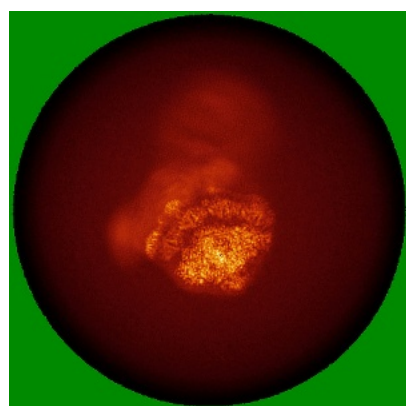


Z Index: 188

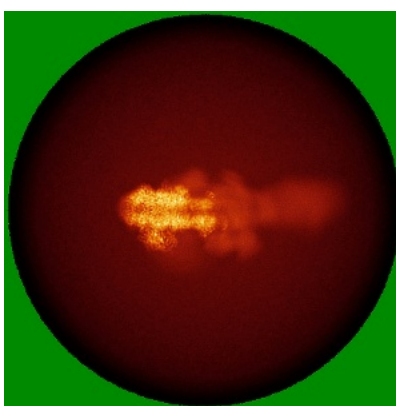
The images above show the largest variance slices of the map in three orthogonal directions.

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

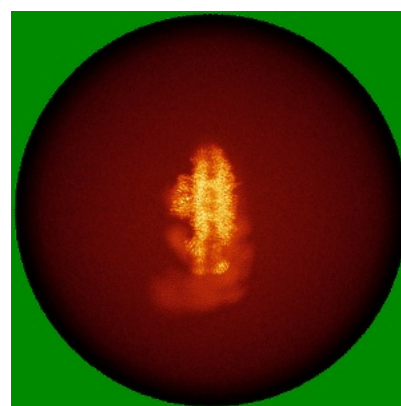
6.4.1 Primary map



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

This section was not generated.

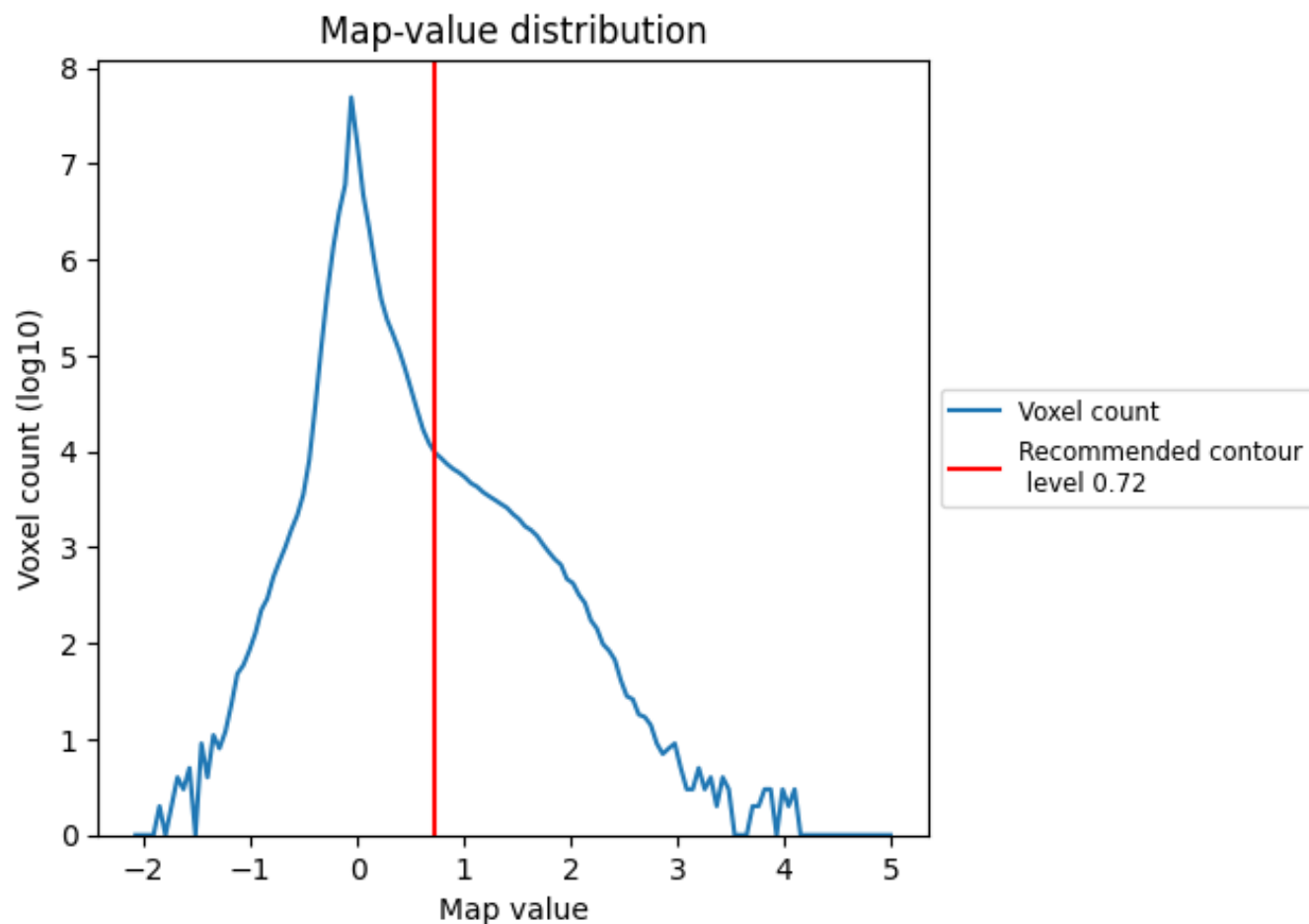
6.6 Mask visualisation

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

7 Map analysis [i](#)

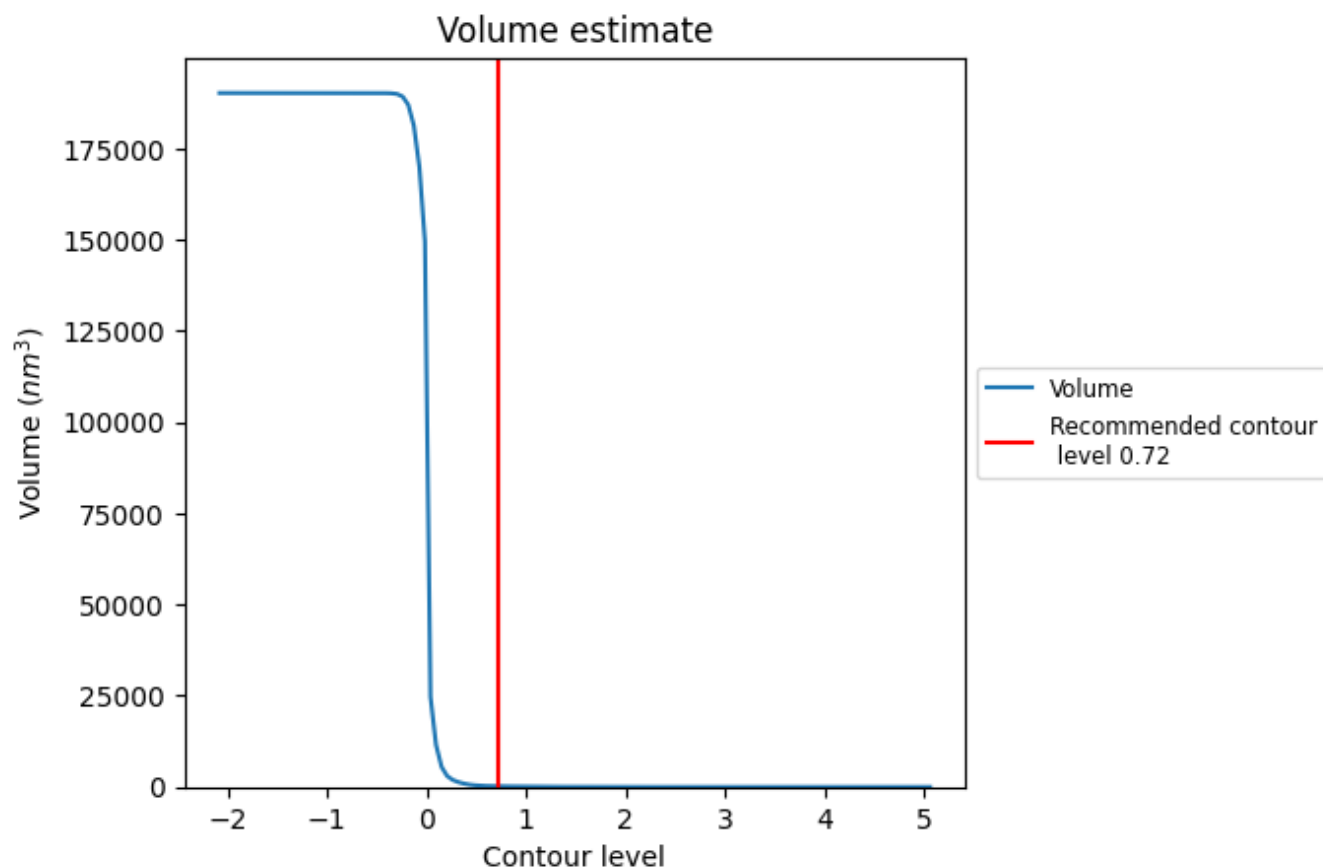
This section contains the results of statistical analysis of the map.

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.

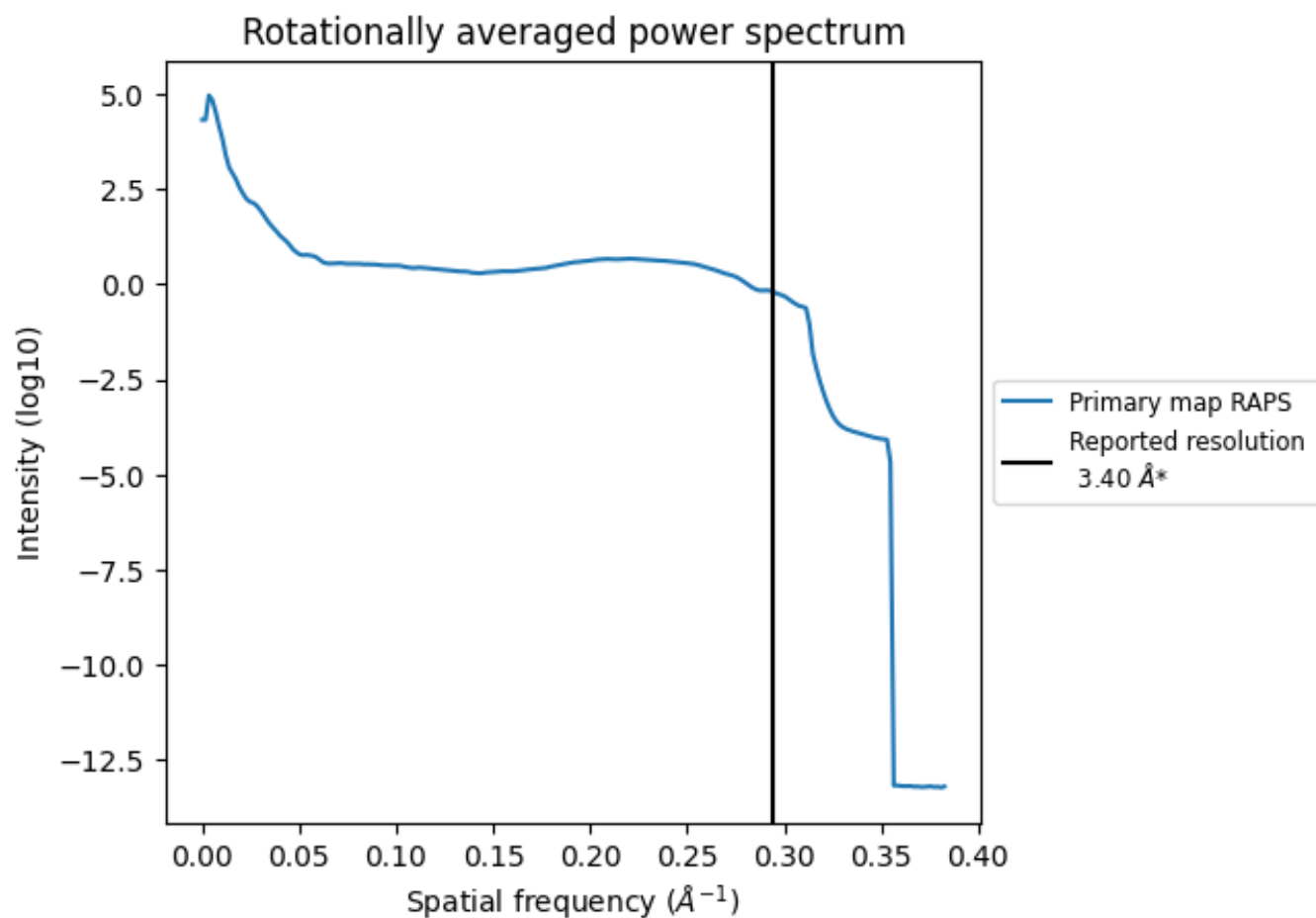
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 189 nm^3 ; this corresponds to an approximate mass of 170 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 $0.294 \text{ \AA}^{-1}$

8 Fourier-Shell correlation ⓘ

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

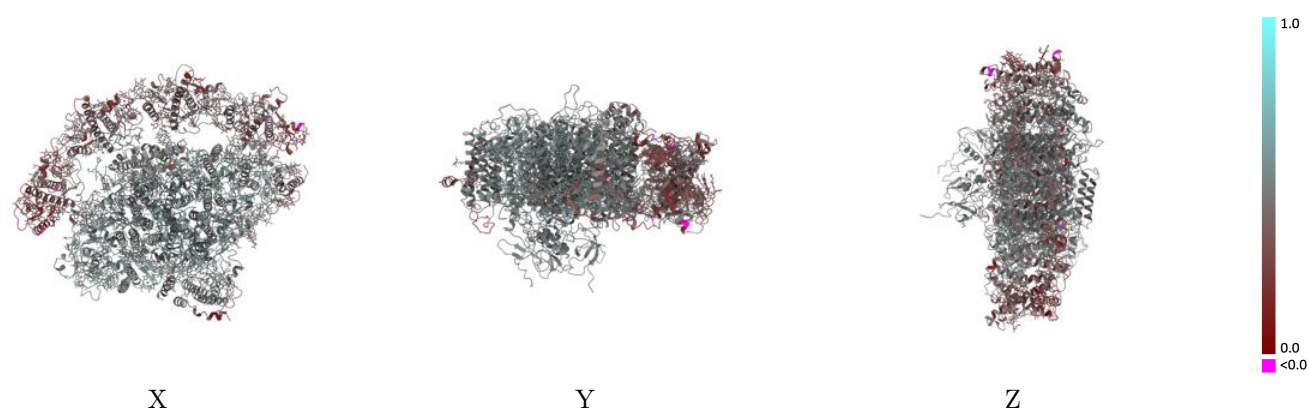
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-31348 and PDB model 7EW6. Per-residue inclusion information can be found in section 3 on page 25.

9.1 Map-model overlay [i](#)

This section was not generated.

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

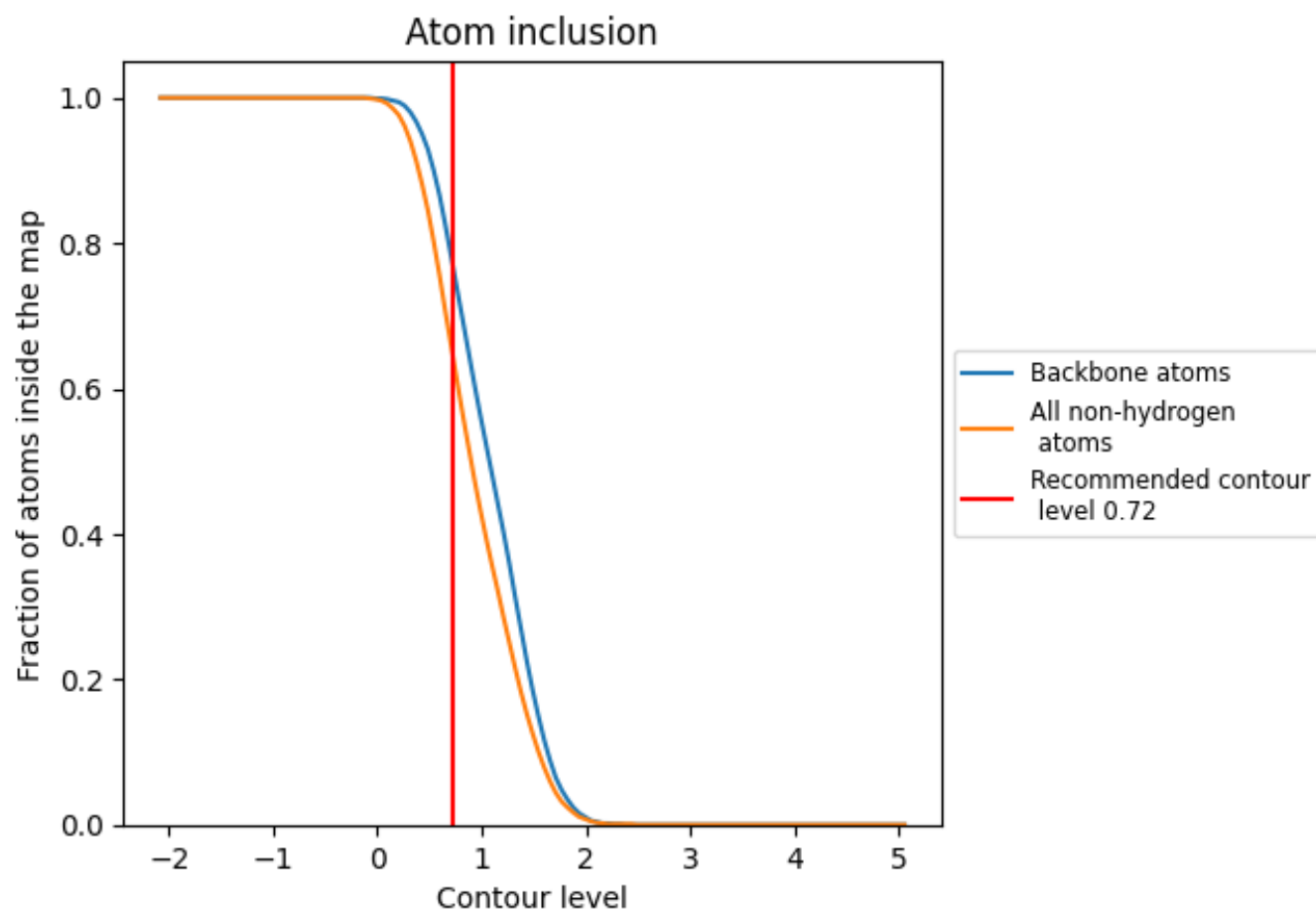


The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 77% of all backbone atoms, 65% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.72) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6480	0.4660
1	0.3980	0.3020
2	0.5250	0.3870
3	0.4570	0.3520
5	0.5640	0.3970
A	0.7350	0.5220
B	0.7690	0.5240
C	0.8610	0.5200
D	0.6940	0.4910
E	0.6980	0.4810
F	0.6450	0.4880
H	0.3740	0.3900
I	0.6750	0.5100
J	0.4840	0.4810
K	0.3900	0.3820
L	0.6170	0.4580

