



Full wwPDB EM Validation Report ⓘ

Apr 6, 2026 – 12:56 AM UTC

PDB ID : 9UH4 / pdb_00009uh4
EMDB ID : EMD-64154
Title : PSI-4 FCPI supercomplex from haptophyte *Chrysotila roscoffensis*
Authors : La Rocca, R.; Tsai, P.-C.; Kato, K.; Nakajima, Y.; Akita, F.; Shen, J.-R.
Deposited on : 2025-04-14
Resolution : 2.12 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

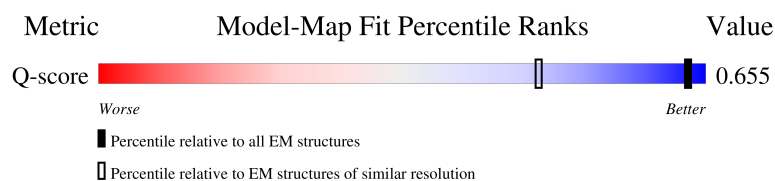
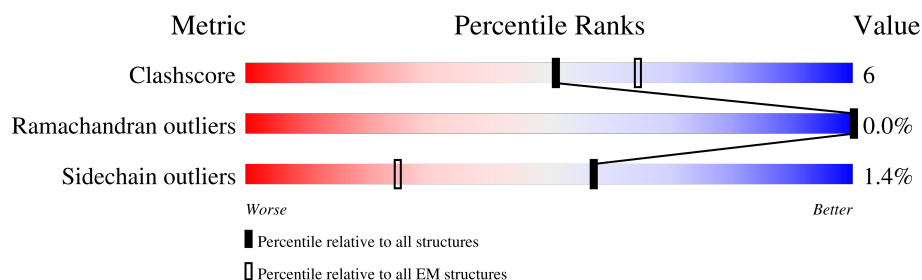
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.12 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.







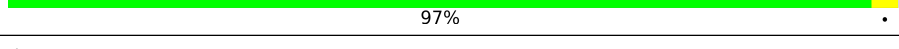
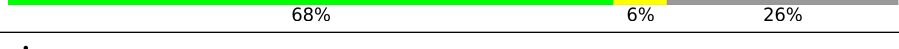
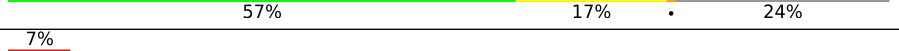
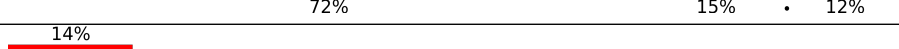
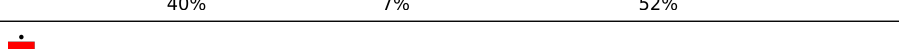
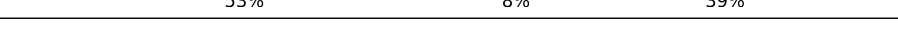
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	2398 (1.64 - 2.62)

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	752	
2	B	734	
3	C	81	
4	D	142	

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Mol	Chain	Length	Quality of chain
5	E	67	
6	F	184	
7	I	35	
8	J	39	
9	L	141	
10	M	29	
11	U	191	
12	G	209	
13	H	169	
14	K	200	
15	k	89	

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	CLA	A	802	X	-	-	-
16	CLA	A	803	X	-	-	-
16	CLA	A	804	X	-	-	-
16	CLA	A	805	X	-	-	-
16	CLA	A	810	X	-	-	-
16	CLA	A	811	X	-	-	-
16	CLA	A	812	X	-	-	-
16	CLA	A	815	X	-	-	-
16	CLA	A	816	X	-	-	-
16	CLA	A	817	X	-	-	-
16	CLA	A	818	X	-	-	-
16	CLA	A	820	X	-	-	-
16	CLA	A	821	X	-	-	-
16	CLA	A	822	X	-	-	-
16	CLA	A	823	X	-	-	-
16	CLA	A	824	X	-	-	-
16	CLA	A	825	X	-	-	-
16	CLA	A	828	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
16	CLA	A	829	X	-	-	-
16	CLA	A	831	X	-	-	-
16	CLA	A	832	X	-	-	-
16	CLA	A	833	X	-	-	-
16	CLA	A	834	X	-	-	-
16	CLA	A	835	X	-	-	-
16	CLA	A	836	X	-	-	-
16	CLA	A	838	X	-	-	-
16	CLA	A	845	X	-	-	-
16	CLA	A	853	X	-	-	-
16	CLA	A	854	X	-	-	-
16	CLA	B	801	X	-	-	-
16	CLA	B	802	X	-	-	-
16	CLA	B	803	X	-	-	-
16	CLA	B	804	X	-	-	-
16	CLA	B	805	X	-	-	-
16	CLA	B	806	X	-	-	-
16	CLA	B	807	X	-	-	-
16	CLA	B	808	X	-	-	-
16	CLA	B	809	X	-	-	-
16	CLA	B	812	X	-	-	-
16	CLA	B	815	X	-	-	-
16	CLA	B	816	X	-	-	-
16	CLA	B	820	X	-	-	-
16	CLA	B	821	X	-	-	-
16	CLA	B	822	X	-	-	-
16	CLA	B	823	X	-	-	-
16	CLA	B	827	X	-	-	-
16	CLA	B	829	X	-	-	-
16	CLA	B	830	X	-	-	-
16	CLA	B	831	X	-	-	-
16	CLA	B	832	X	-	-	-
16	CLA	B	833	X	-	-	-
16	CLA	B	836	X	-	-	-
16	CLA	B	844	X	-	-	-
16	CLA	B	845	X	-	-	-
16	CLA	B	847	X	-	-	-
16	CLA	B	848	X	-	-	-
16	CLA	B	849	X	-	-	-
16	CLA	F	802	X	-	-	-
16	CLA	F	803	X	-	-	-
16	CLA	F	804	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
16	CLA	G	302	X	-	-	-
16	CLA	G	303	X	-	-	-
16	CLA	G	305	X	-	-	-
16	CLA	G	306	X	-	-	-
16	CLA	G	310	X	-	-	-
16	CLA	G	315	X	-	-	-
16	CLA	H	301	X	-	-	-
16	CLA	H	302	X	-	-	-
16	CLA	H	303	X	-	-	-
16	CLA	H	304	X	-	-	-
16	CLA	H	305	X	-	-	-
16	CLA	H	307	X	-	-	-
16	CLA	H	308	X	-	-	-
16	CLA	H	309	X	-	-	-
16	CLA	H	312	X	-	-	-
16	CLA	I	102	X	-	-	-
16	CLA	J	104	X	-	-	-
16	CLA	K	203	X	-	-	-
16	CLA	K	204	X	-	-	-
16	CLA	K	205	X	-	-	-
16	CLA	K	206	X	-	-	-
16	CLA	K	207	X	-	-	-
16	CLA	L	204	X	-	-	-
16	CLA	U	204	X	-	-	-
16	CLA	U	206	X	-	-	-
16	CLA	U	207	X	-	-	-
16	CLA	U	208	X	-	-	-
16	CLA	U	209	X	-	-	-
16	CLA	U	211	X	-	-	-
16	CLA	k	201	X	-	-	-
16	CLA	k	202	X	-	-	-
22	CL0	A	850	X	-	-	-

2 Entry composition [i](#)

There are 28 unique types of molecules in this entry. The entry contains 31069 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 (psaA).

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	741	Total	C	N	O	S	0	0
			5813	3807	984	994	28		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	732	Total	C	N	O	S	0	0
			5805	3823	977	984	21		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	80	Total	C	N	O	S	0	0
			599	366	106	116	11		

- Molecule 4 is a protein called Photosystem I reaction center subunit II (psaD).

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	138	Total	C	N	O	S	0	0
			1092	697	188	204	3		

- Molecule 5 is a protein called Photosystem I reaction center subunit IV (psaE).

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	64	Total	C	N	O	S	0	0
			494	314	86	93	1		

- Molecule 6 is a protein called Photosystem I reaction center subunit III (psaF).

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	161	Total	C	N	O	S	0	0
			1246	802	209	229	6		

- Molecule 7 is a protein called Photosystem I reaction center subunit VIII (psaI).

Mol	Chain	Residues	Atoms					AltConf	Trace
7	I	34	Total	C	N	O	S	0	0
			266	183	35	46	2		

- Molecule 8 is a protein called Photosystem I reaction center subunit IX (psaJ).

Mol	Chain	Residues	Atoms					AltConf	Trace
8	J	39	Total	C	N	O	S	0	0
			305	204	45	54	2		

- Molecule 9 is a protein called Photosystem I reaction center subunit XI (psaL).

Mol	Chain	Residues	Atoms					AltConf	Trace
9	L	140	Total	C	N	O	S	0	0
			1056	693	168	194	1		

- Molecule 10 is a protein called Photosystem I reaction center subunit XII (psaM).

Mol	Chain	Residues	Atoms					AltConf	Trace
10	M	29	Total	C	N	O	S	0	0
			216	144	34	37	1		

- Molecule 11 is a protein called Fucoxanthin chlorophyll a/c binding protein I (FCPI-1).

Mol	Chain	Residues	Atoms					AltConf	Trace
11	U	141	Total	C	N	O	S	0	0
			1082	692	183	198	9		

- Molecule 12 is a protein called Fucoxanthin chlorophyll a/c binding protein VII (FCPI-7).

Mol	Chain	Residues	Atoms					AltConf	Trace
12	G	158	Total	C	N	O	S	0	0
			1201	769	194	229	9		

- Molecule 13 is a protein called Fucoxanthin chlorophyll a/c binding protein VIII (FCPI-8).

Mol	Chain	Residues	Atoms					AltConf	Trace
13	H	149	Total	C	N	O	S	0	0
			1128	725	185	206	12		

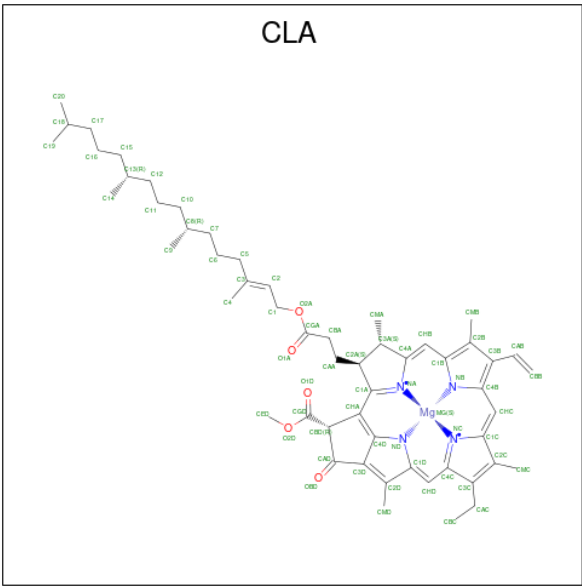
- Molecule 14 is a protein called Fucoxanthin chlorophyll a/c binding protein IX (FCPI-9).

Mol	Chain	Residues	Atoms					AltConf	Trace
14	K	95	Total	C	N	O	S	0	0
			737	488	119	123	7		

- Molecule 15 is a protein called Photosystem I reaction center subunit psaK.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	k	54	Total	C	N	O	S	0	0
			375	245	61	66	3		

- Molecule 16 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
16	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
16	A	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
16	A	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
16	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	A	1	Total 50	C 40	Mg 1	N 4	O 5	0
16	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	A	1	Total 51	C 41	Mg 1	N 4	O 5	0
16	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	A	1	Total 52	C 42	Mg 1	N 4	O 5	0
16	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	A	1	Total 60	C 50	Mg 1	N 4	O 5	0
16	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	B	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
16	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	B	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
16	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
16	B	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
16	B	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
16	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
16	B	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
16	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
16	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	B	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
16	B	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
16	B	1	Total	C	Mg	N	O	0
			63	53	1	4	5	
16	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
16	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
16	B	1	Total	C	Mg	N	O	0
			49	39	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
16	B	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
16	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	B	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
16	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	B	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
16	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	B	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
16	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	B	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
16	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	F	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	F	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
16	F	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
16	I	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	J	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
16	L	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
16	L	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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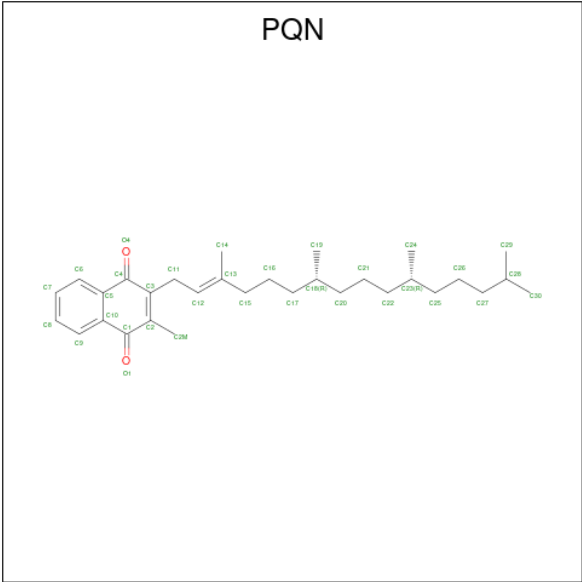
Mol	Chain	Residues	Atoms					AltConf
16	L	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
16	U	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
16	U	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	U	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	U	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	U	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
16	U	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
16	U	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	U	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
16	G	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	G	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
16	G	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	G	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
16	G	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
16	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	G	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
16	G	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
16	G	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
16	G	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	G	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	H	1	Total	C	Mg	N	O	0
			40	32	1	4	3	

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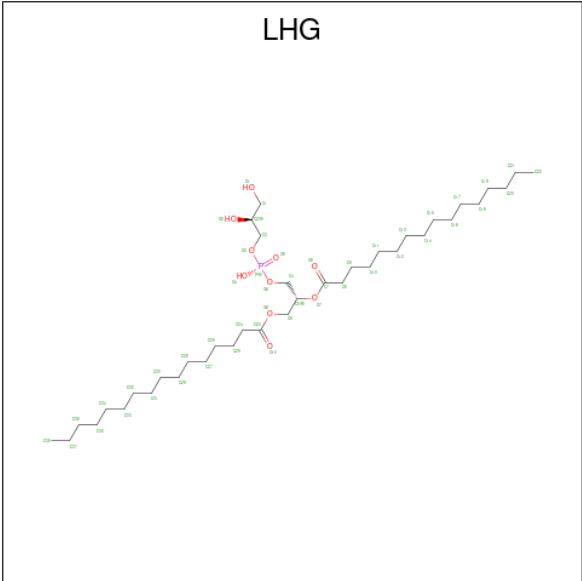
Mol	Chain	Residues	Atoms					AltConf
16	H	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
16	H	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
16	H	1	Total	C	Mg	N	O	0
			44	35	1	4	4	
16	H	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	H	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
16	H	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
16	H	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	K	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
16	K	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
16	K	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	K	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
16	K	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
16	K	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
16	k	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
16	k	1	Total	C	Mg	N	O	0
			55	45	1	4	5	

- Molecule 17 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 18 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P) (labeled as "Ligand of Interest" by depositor).



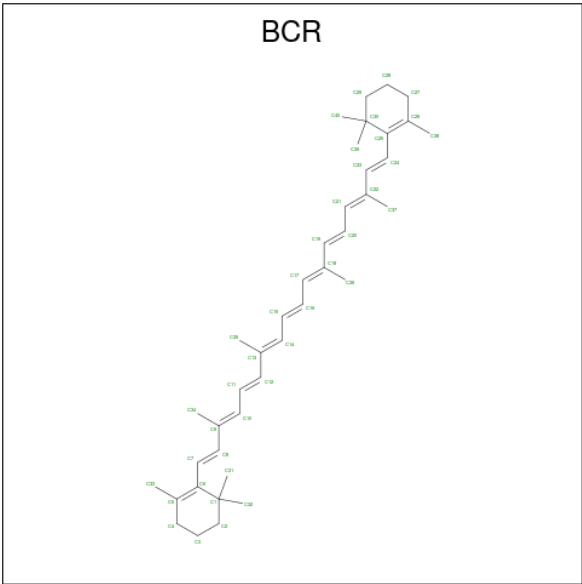
Mol	Chain	Residues	Atoms				AltConf
18	A	1	Total	C	O	P	0
			48	37	10	1	

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Mol	Chain	Residues	Atoms				AltConf
18	A	1	Total	C	O	P	0
			27	16	10	1	
18	G	1	Total	C	O	P	0
			27	16	10	1	

- Molecule 19 is BETA-CAROTENE (CCD ID: BCR) (formula: C₄₀H₅₆) (labeled as "Ligand of Interest" by depositor).



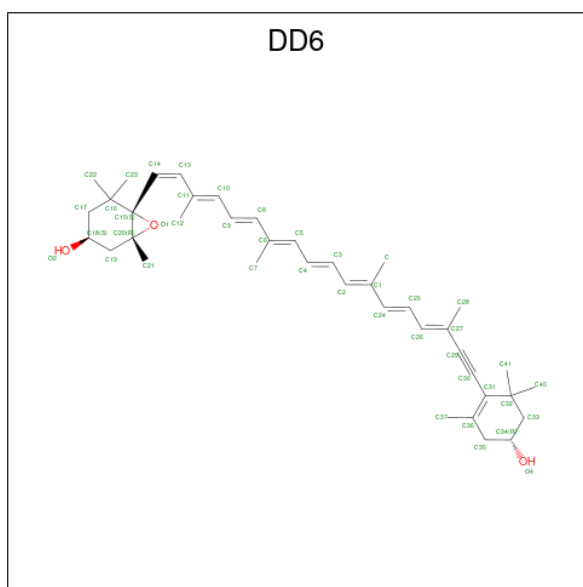
Mol	Chain	Residues	Atoms		AltConf
19	A	1	Total	C	0
			40	40	
19	A	1	Total	C	0
			40	40	
19	A	1	Total	C	0
			40	40	
19	A	1	Total	C	0
			40	40	
19	B	1	Total	C	0
			40	40	
19	B	1	Total	C	0
			40	40	
19	B	1	Total	C	0
			40	40	
19	B	1	Total	C	0
			40	40	

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Mol	Chain	Residues	Atoms	AltConf
19	B	1	Total C 39 39	0
19	F	1	Total C 40 40	0
19	F	1	Total C 40 40	0
19	I	1	Total C 40 40	0
19	I	1	Total C 40 40	0
19	J	1	Total C 40 40	0
19	L	1	Total C 40 40	0
19	L	1	Total C 40 40	0
19	M	1	Total C 40 40	0
19	k	1	Total C 40 40	0

- Molecule 20 is (3S,3'R,5R,6S,7cis)-7',8'-didehydro-5,6-dihydro-5,6-epoxy-beta,beta-carotene-3,3'-diol (CCD ID: DD6) (formula: $C_{40}H_{54}O_3$) (labeled as "Ligand of Interest" by depositor).



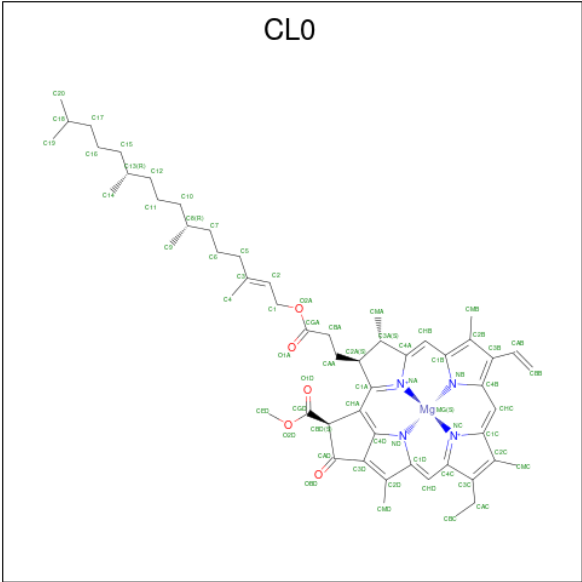
Mol	Chain	Residues	Atoms			AltConf
20	A	1	Total	C	O	0
			43	40	3	
20	J	1	Total	C	O	0
			43	40	3	
20	U	1	Total	C	O	0
			43	40	3	
20	U	1	Total	C	O	0
			43	40	3	
20	U	1	Total	C	O	0
			26	25	1	
20	G	1	Total	C	O	0
			43	40	3	
20	G	1	Total	C	O	0
			27	25	2	
20	G	1	Total	C	O	0
			43	40	3	
20	G	1	Total	C	O	0
			43	40	3	
20	G	1	Total	C	O	0
			43	40	3	
20	H	1	Total	C	O	0
			43	40	3	
20	H	1	Total	C	O	0
			43	40	3	
20	K	1	Total	C	O	0
			43	40	3	

- Molecule 21 is DODECYL-ALPHA-D-MALTOSIDE (CCD ID: LMU) (formula: C₂₄H₄₆O₁₁) (labeled as "Ligand of Interest" by depositor).



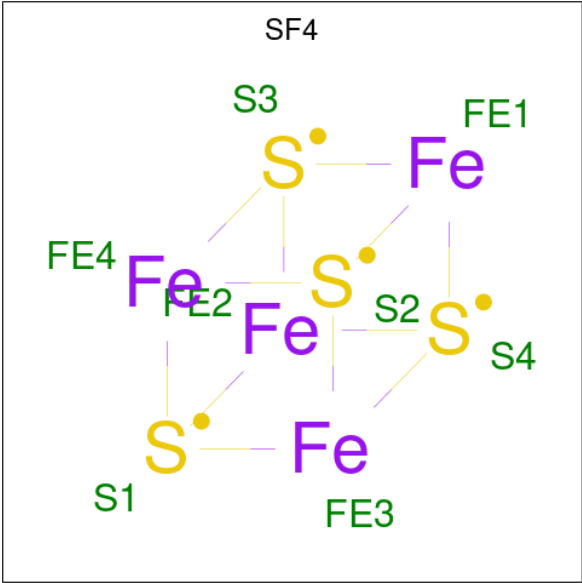
Mol	Chain	Residues	Atoms			AltConf
21	A	1	Total 35	C 24	O 11	0
21	A	1	Total 35	C 24	O 11	0
21	F	1	Total 35	C 24	O 11	0
21	J	1	Total 35	C 24	O 11	0
21	K	1	Total 35	C 24	O 11	0

- Molecule 22 is CHLOROPHYLL A ISOMER (CCD ID: CL0) (formula: $\text{C}_{55}\text{H}_{72}\text{MgN}_4\text{O}_5$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 23 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄) (labeled as "Ligand of Interest" by depositor).



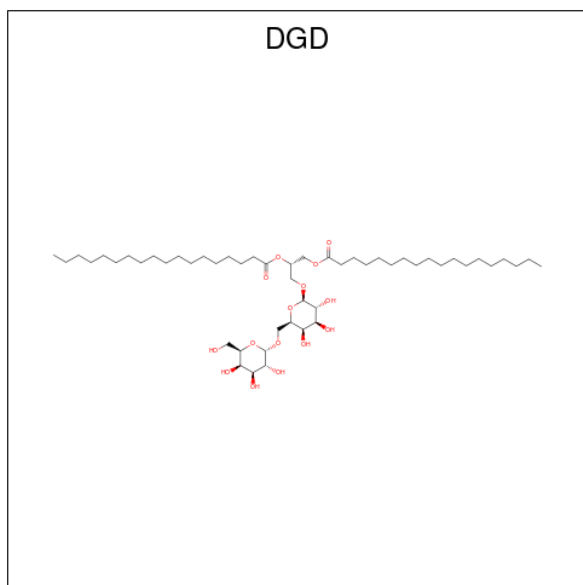
Mol	Chain	Residues	Atoms			AltConf
23	A	1	Total	Fe	S	0
			8	4	4	
23	C	1	Total	Fe	S	0
			8	4	4	

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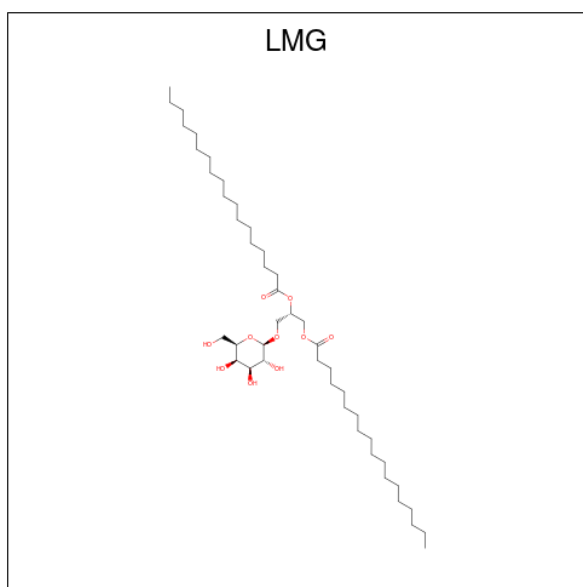
Mol	Chain	Residues	Atoms			AltConf
23	C	1	Total	Fe	S	0
			8	4	4	

- Molecule 24 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$) (labeled as "Ligand of Interest" by depositor).



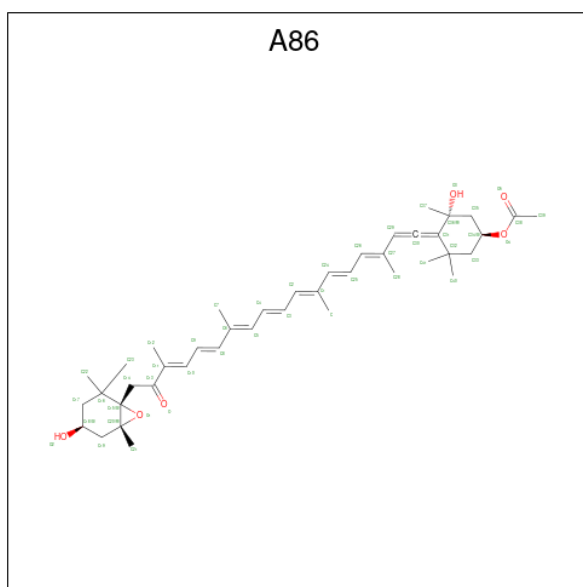
Mol	Chain	Residues	Atoms			AltConf
24	B	1	Total	C	O	0
			60	45	15	

- Molecule 25 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$) (labeled as "Ligand of Interest" by depositor).



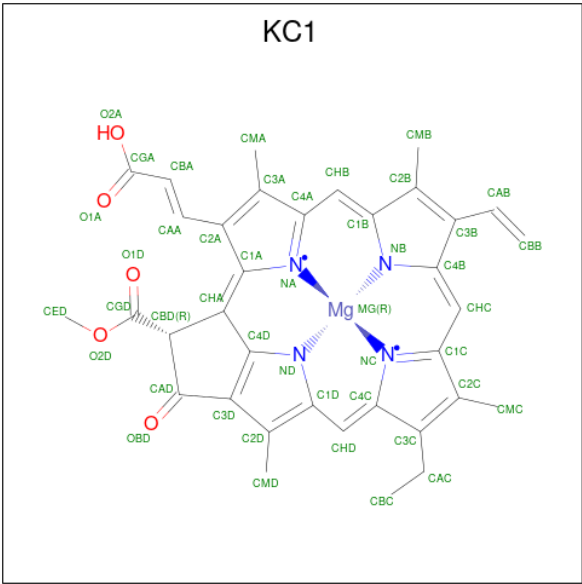
Mol	Chain	Residues	Atoms			AltConf
25	J	1	Total	C	O	0
			39	29	10	
25	U	1	Total	C	O	0
			32	22	10	

- Molecule 26 is (3S,3'S,5R,5'R,6S,6'R,8'R)-3,5'-dihydroxy-8-oxo-6',7'-didehydro-5,5',6,6',7,8-hexahydro-5,6-epoxy-beta,beta-caroten-3'-yl acetate (CCD ID: A86) (formula: C₄₂H₅₈O₆) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
26	U	1	Total	C	O	0
			48	42	6	

- Molecule 27 is Chlorophyll c1 (CCD ID: KC1) (formula: C₃₅H₃₀MgN₄O₅) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
27	U	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

- Molecule 28 is water.

Mol	Chain	Residues	Atoms		AltConf
28	A	132	Total	O	0
			132	132	
28	B	146	Total	O	0
			146	146	
28	C	32	Total	O	0
			32	32	
28	D	19	Total	O	0
			19	19	
28	E	8	Total	O	0
			8	8	
28	F	24	Total	O	0
			24	24	
28	J	1	Total	O	0
			1	1	
28	L	14	Total	O	0
			14	14	
28	M	1	Total	O	0
			1	1	

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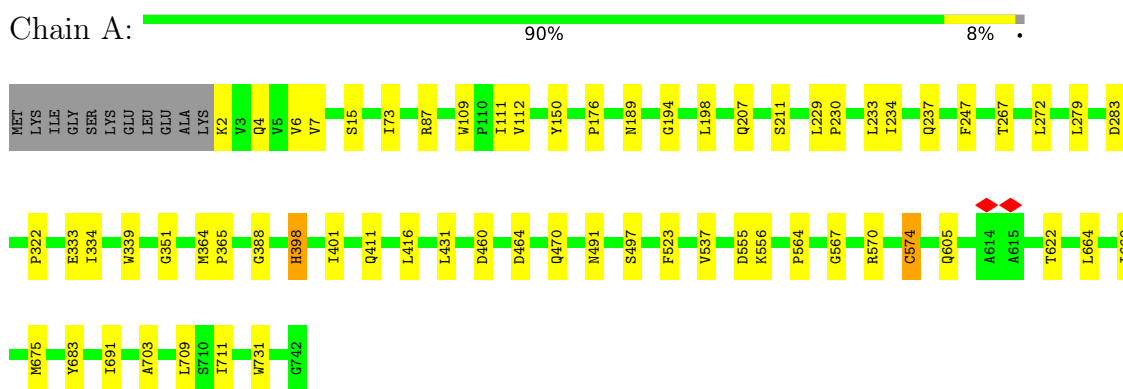
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Mol	Chain	Residues	Atoms		AltConf
28	U	3	Total 3	O 3	0
28	G	5	Total 5	O 5	0
28	H	1	Total 1	O 1	0
28	K	7	Total 7	O 7	0
28	k	2	Total 2	O 2	0

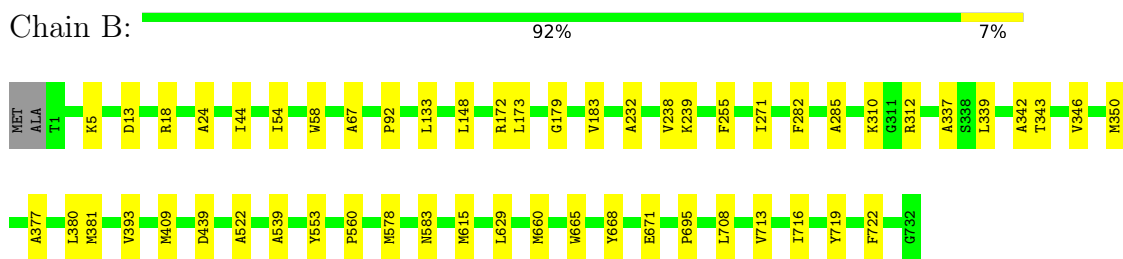
3 Residue-property plots [i](#)

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.

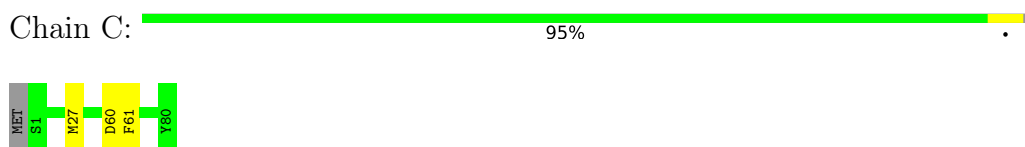
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1 (psaA)



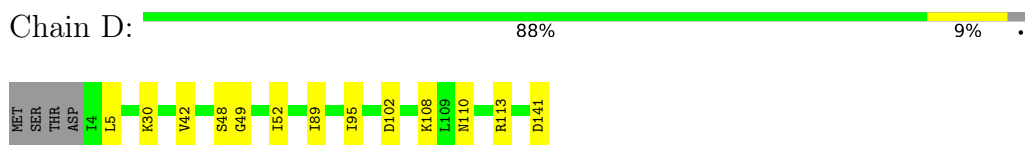
- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2 (psaB)



- Molecule 3: Photosystem I iron-sulfur center (psaC)

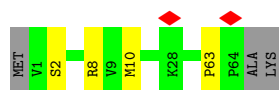


- Molecule 4: Photosystem I reaction center subunit II (psaD)




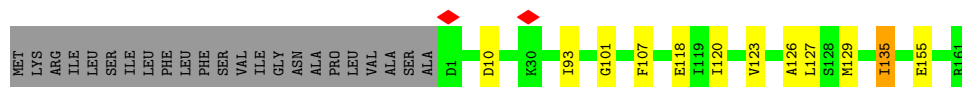
- Molecule 5: Photosystem I reaction center subunit IV (psaE)

Chain E:  90% 6% .




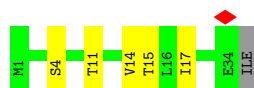
- Molecule 6: Photosystem I reaction center subunit III (psaF)

Chain F:  81% 6% . 12%




- Molecule 7: Photosystem I reaction center subunit VIII (psaI)

Chain I:  83% 14% .




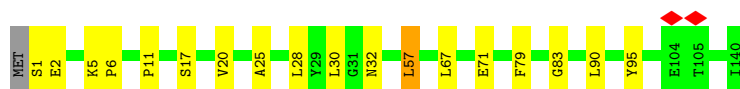
- Molecule 8: Photosystem I reaction center subunit IX (psaJ)

Chain J:  74% 26%



- Molecule 9: Photosystem I reaction center subunit XI (psaL)

Chain L:  87% 12% ..



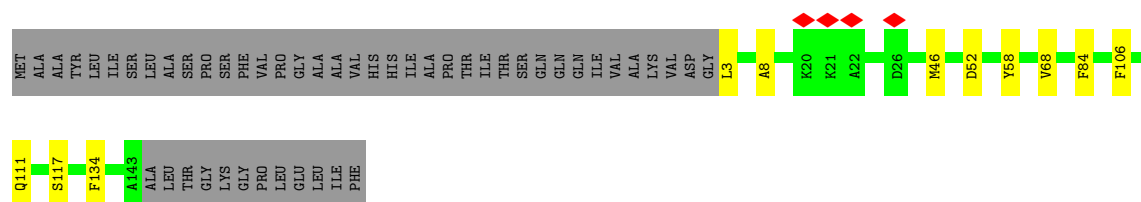
- Molecule 10: Photosystem I reaction center subunit XII (psaM)

Chain M:  97% .



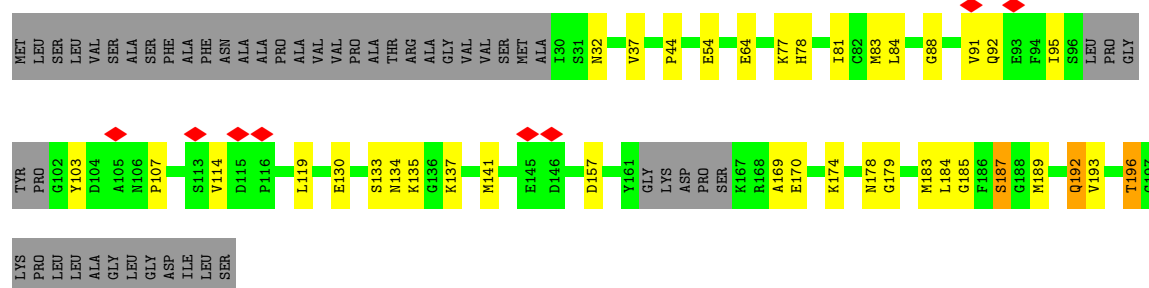
- Molecule 11: Fucoxanthin chlorophyll a/c binding protein I (FCPI-1)

Chain U:  68% 6% 26%



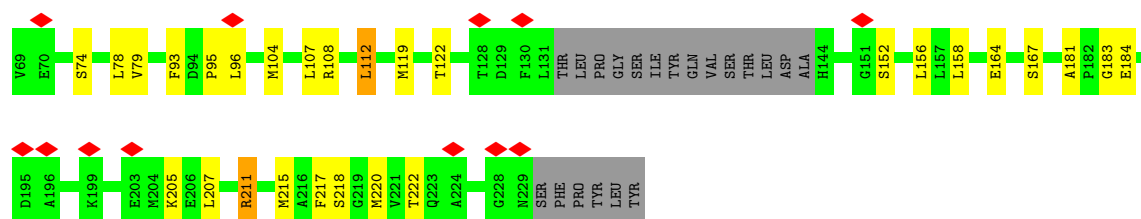
- Molecule 12: Fucoxanthin chlorophyll a/c binding protein VII (FCPI-7)

Chain G: 57% 17% 24%



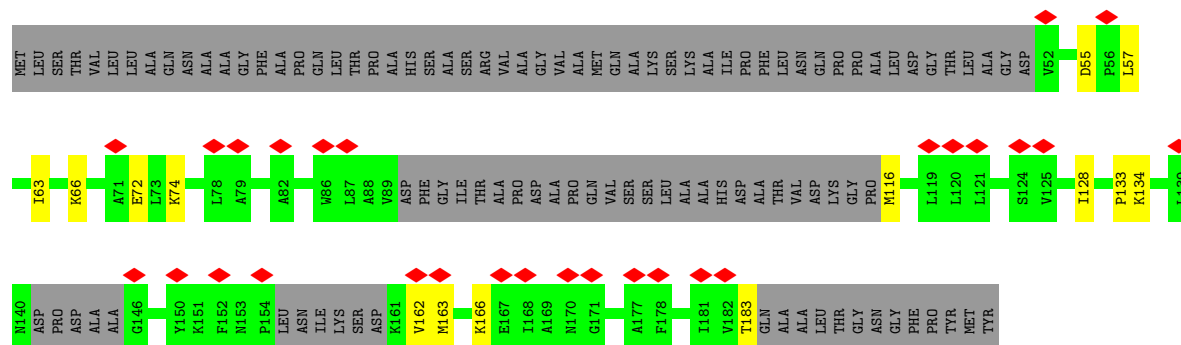
- Molecule 13: Fucoxanthin chlorophyll a/c binding protein VIII (FCPI-8)

Chain H: 7% 72% 15% 12%



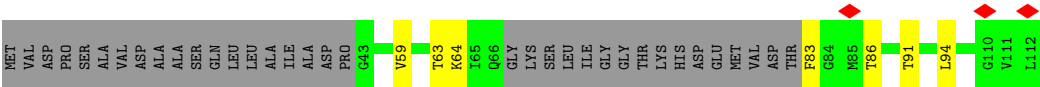
- Molecule 14: Fucoxanthin chlorophyll a/c binding protein IX (FCPI-9)

Chain K: 14% 40% 7% 52%



- Molecule 15: Photosystem I reaction center subunit psaK

Chain k: 53% 8% 39%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	22619	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	165000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.576	Depositor
Minimum map value	-0.256	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.014	Depositor
Recommended contour level	0.065	Depositor
Map size (Å)	436.2, 436.2, 436.2	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.727, 0.727, 0.727	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: A86, DD6, LHG, SF4, CL0, CLA, LMU, LMG, KC1, DGD, PQN, BCR

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.29	0/6007	0.48	1/8185 (0.0%)
2	B	0.30	0/6015	0.50	0/8205
3	C	0.18	0/609	0.41	0/826
4	D	0.30	0/1116	0.52	1/1503 (0.1%)
5	E	0.21	0/505	0.48	0/689
6	F	0.21	0/1275	0.44	0/1728
7	I	0.38	0/273	0.65	0/373
8	J	0.45	0/313	0.82	1/427 (0.2%)
9	L	0.21	0/1081	0.42	0/1470
10	M	0.24	0/218	0.52	0/295
11	U	0.28	0/1109	0.57	1/1499 (0.1%)
12	G	0.33	0/1226	0.70	1/1655 (0.1%)
13	H	0.32	0/1149	0.59	0/1546
14	K	0.33	0/752	0.63	0/1012
15	k	0.17	0/379	0.39	0/514
All	All	0.29	0/22027	0.52	5/29927 (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
13	H	0	1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	J	42	ALA	N-CA-C	-6.01	106.56	114.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	G	169	ALA	N-CA-C	-5.56	108.28	114.62
1	A	398	HIS	CA-CB-CG	-5.33	108.47	113.80
4	D	49	GLY	CA-C-O	-5.18	118.85	122.22
11	U	68	VAL	N-CA-C	-5.13	107.83	112.96

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
13	H	211	ARG	Sidechain

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	5695	47	0
2	B	5805	0	5634	45	0
3	C	599	0	577	2	0
4	D	1092	0	1093	6	0
5	E	494	0	488	2	0
6	F	1246	0	1256	11	0
7	I	266	0	278	3	0
8	J	305	0	310	10	0
9	L	1056	0	1068	17	0
10	M	216	0	234	0	0
11	U	1082	0	1055	8	0
12	G	1201	0	1185	24	0
13	H	1128	0	1131	20	0
14	K	737	0	764	7	0
15	k	375	0	403	5	0
16	A	2540	0	2556	68	0
16	B	2439	0	2456	68	0
16	F	159	0	141	3	0
16	G	561	0	486	16	0
16	H	524	0	475	22	0
16	I	65	0	72	2	0
16	J	42	0	31	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	K	286	0	229	8	0
16	L	164	0	150	4	0
16	U	441	0	417	12	0
16	k	97	0	80	3	0
17	A	33	0	46	3	0
17	B	33	0	46	1	0
18	A	75	0	93	2	0
18	G	27	0	24	2	0
19	A	160	0	224	6	0
19	B	239	0	333	16	0
19	F	80	0	112	0	0
19	I	80	0	112	3	0
19	J	40	0	56	2	0
19	L	80	0	112	3	0
19	M	40	0	56	3	0
19	k	40	0	56	3	0
20	A	43	0	0	0	0
20	G	199	0	0	1	0
20	H	86	0	0	0	0
20	J	43	0	0	0	0
20	K	43	0	0	0	0
20	U	112	0	0	0	0
21	A	70	0	92	2	0
21	F	35	0	46	0	0
21	J	35	0	46	3	0
21	K	35	0	46	0	0
22	A	65	0	72	2	0
23	A	8	0	0	0	0
23	C	16	0	0	0	0
24	B	60	0	81	2	0
25	J	39	0	48	2	0
25	U	32	0	34	2	0
26	U	48	0	0	1	0
27	U	45	0	0	0	0
28	A	132	0	0	2	0
28	B	146	0	0	0	0
28	C	32	0	0	0	0
28	D	19	0	0	0	0
28	E	8	0	0	0	0
28	F	24	0	0	0	0
28	G	5	0	0	0	0
28	H	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	J	1	0	0	0	0
28	K	7	0	0	0	0
28	L	14	0	0	0	0
28	M	1	0	0	0	0
28	U	3	0	0	1	0
28	k	2	0	0	0	0
All	All	31069	0	29999	335	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 6.

All (335) 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)
13:H:122:THR:HA	13:H:220:MET:HE1	1.57	0.86
13:H:112:LEU:HD12	13:H:183:GLY:HA3	1.63	0.81
7:I:17:ILE:HD11	16:I:102:CLA:HAB	1.69	0.75
16:A:822:CLA:H91	19:A:844:BCR:H23C	1.70	0.74
16:A:803:CLA:H72	19:A:842:BCR:HC8	1.71	0.72
13:H:217:PHE:HA	13:H:220:MET:HE3	1.72	0.70
16:A:808:CLA:HBB2	16:A:811:CLA:HMA3	1.75	0.69
13:H:104:MET:HE1	16:H:306:CLA:HMA2	1.76	0.67
16:B:818:CLA:HMD2	19:B:838:BCR:HC7	1.77	0.67
12:G:91:VAL:HG13	12:G:95:ILE:HD13	1.76	0.66
16:H:305:CLA:HBB2	16:H:312:CLA:H151	1.81	0.63
1:A:322:PRO:HB3	9:L:1:SER:HB2	1.79	0.63
13:H:207:LEU:O	13:H:211:ARG:HB2	2.00	0.61
16:B:828:CLA:H111	6:F:93:ILE:HD11	1.83	0.60
8:J:1:MET:HG3	18:G:316:LHG:H241	1.84	0.60
16:A:816:CLA:HBB2	16:A:816:CLA:H151	1.82	0.59
11:U:8:ALA:O	28:U:301:HOH:O	2.17	0.59
1:A:207:GLN:HA	1:A:211:SER:HB2	1.84	0.59
12:G:114:VAL:HG11	12:G:119:LEU:HD11	1.83	0.59
11:U:58:TYR:HE2	16:U:207:CLA:HBA1	1.66	0.59
16:A:845:CLA:HBC2	2:B:583:ASN:HB2	1.85	0.58
2:B:13:ASP:HB3	2:B:18:ARG:HB2	1.86	0.58
16:B:819:CLA:H3A	16:B:836:CLA:HED3	1.85	0.58
13:H:217:PHE:HA	13:H:220:MET:CE	2.33	0.58
2:B:660:MET:HB2	16:B:803:CLA:C1C	2.34	0.57
12:G:91:VAL:HB	16:G:309:CLA:HBC3	1.87	0.57
16:A:836:CLA:H201	9:L:90:LEU:HD23	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:523:PHE:HA	16:A:833:CLA:HED1	1.86	0.56
16:B:819:CLA:HBB2	16:B:836:CLA:H52	1.87	0.56
1:A:491:ASN:HB2	16:A:831:CLA:HED2	1.87	0.56
2:B:393:VAL:HG13	2:B:539:ALA:HB1	1.88	0.56
16:A:831:CLA:HBA2	16:k:202:CLA:H11	1.88	0.55
16:B:849:CLA:H62	9:L:79:PHE:HB3	1.88	0.55
16:A:824:CLA:H91	16:A:826:CLA:H192	1.89	0.55
4:D:108:LYS:O	4:D:113:ARG:NH2	2.40	0.54
12:G:107:PRO:HD2	12:G:193:VAL:HG11	1.89	0.54
16:A:835:CLA:H71	16:A:853:CLA:H171	1.90	0.54
16:B:811:CLA:HBB2	16:B:847:CLA:H61	1.89	0.54
12:G:187:SER:HB2	16:G:308:CLA:HBC2	1.90	0.54
2:B:339:LEU:HB3	2:B:380:LEU:HD13	1.90	0.54
2:B:719:TYR:HB2	16:B:802:CLA:HED2	1.89	0.54
14:K:162:VAL:HG12	14:K:166:LYS:HE3	1.90	0.54
1:A:339:TRP:HB3	16:A:803:CLA:HAC1	1.89	0.53
1:A:416:LEU:HB3	16:A:849:CLA:HMC2	1.91	0.53
9:L:25:ALA:HB2	11:U:106:PHE:HB3	1.90	0.53
16:U:204:CLA:H42	16:U:211:CLA:HED2	1.90	0.53
16:A:845:CLA:HBB	16:B:802:CLA:H202	1.91	0.53
4:D:141:ASP:OD1	4:D:141:ASP:O	2.26	0.53
13:H:181:ALA:HB3	13:H:184:GLU:HB2	1.90	0.53
5:E:2:SER:HB2	5:E:63:PRO:HG3	1.91	0.53
16:B:831:CLA:H122	19:B:841:BCR:H311	1.89	0.53
25:U:201:LMG:H321	16:U:211:CLA:H42	1.91	0.53
16:H:305:CLA:HBB2	16:H:312:CLA:H171	1.91	0.52
16:B:825:CLA:H201	19:B:842:BCR:H11C	1.91	0.52
2:B:255:PHE:HZ	16:B:815:CLA:H71	1.73	0.52
8:J:41:ALA:HB2	21:J:101:LMU:H6'1	1.90	0.52
13:H:164:GLU:HA	13:H:167:SER:HB3	1.91	0.52
16:A:820:CLA:HHC	16:A:820:CLA:HBB1	1.92	0.52
16:k:201:CLA:HHC	16:k:201:CLA:HBB1	1.92	0.52
1:A:234:ILE:HD11	16:A:812:CLA:HAC1	1.91	0.52
16:B:808:CLA:HHC	16:B:808:CLA:HBB1	1.91	0.52
13:H:218:SER:HB3	16:H:312:CLA:H162	1.92	0.52
16:U:211:CLA:HBB1	16:U:211:CLA:HHC	1.91	0.51
13:H:205:LYS:HD2	16:H:302:CLA:HAA2	1.92	0.51
16:A:849:CLA:HHC	16:A:849:CLA:HBB1	1.92	0.51
2:B:346:VAL:O	2:B:350:MET:HB2	2.10	0.51
16:B:836:CLA:HED1	16:B:845:CLA:HHC	1.92	0.51
12:G:88:GLY:O	12:G:92:GLN:HB2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:B:822:CLA:HBB1	16:B:822:CLA:HHC	1.92	0.51
16:B:834:CLA:HHC	16:B:834:CLA:HBB1	1.93	0.51
9:L:32:ASN:HB3	16:L:202:CLA:HAC1	1.93	0.51
16:H:308:CLA:HHC	16:H:308:CLA:HBB1	1.92	0.51
16:H:309:CLA:HHC	16:H:309:CLA:HBB1	1.93	0.51
1:A:279:LEU:HD13	16:A:815:CLA:HMA2	1.92	0.51
6:F:123:VAL:HB	25:J:103:LMG:HC72	1.92	0.51
16:A:847:CLA:H91	19:k:203:BCR:H291	1.91	0.51
16:B:807:CLA:H201	16:B:809:CLA:H192	1.93	0.51
16:A:854:CLA:H42	9:L:20:VAL:HG13	1.93	0.51
2:B:409:MET:HG3	19:B:846:BCR:H402	1.91	0.51
16:B:835:CLA:H193	19:I:101:BCR:H362	1.93	0.51
16:F:804:CLA:HHC	16:F:804:CLA:HBB1	1.92	0.51
16:K:203:CLA:HHC	16:K:203:CLA:HBB1	1.93	0.51
16:K:206:CLA:HHC	16:K:206:CLA:HBB1	1.92	0.50
16:K:205:CLA:HHC	16:K:205:CLA:HBB1	1.91	0.50
16:B:824:CLA:H11	19:B:839:BCR:H393	1.93	0.50
16:B:849:CLA:HHC	16:B:849:CLA:HBB1	1.93	0.50
16:F:802:CLA:HHC	16:F:802:CLA:HBB1	1.93	0.50
16:B:835:CLA:HHC	16:B:835:CLA:HBB1	1.93	0.50
16:G:303:CLA:HHC	16:G:303:CLA:HBB1	1.93	0.50
16:G:309:CLA:HHC	16:G:309:CLA:HBB1	1.92	0.50
16:A:831:CLA:HHC	16:A:831:CLA:HBB1	1.94	0.50
16:B:813:CLA:H143	19:B:839:BCR:HC32	1.93	0.50
8:J:34:PHE:HB3	21:J:101:LMU:H5B	1.94	0.50
2:B:342:ALA:HB2	16:B:820:CLA:H43	1.92	0.50
2:B:312:ARG:HH21	16:B:826:CLA:HBD	1.77	0.49
16:U:205:CLA:H92	16:U:206:CLA:HMA1	1.93	0.49
16:A:820:CLA:HBA2	25:U:201:LMG:H122	1.94	0.49
1:A:703:ALA:N	6:F:118:GLU:OE2	2.42	0.49
8:J:7:THR:OG1	25:J:103:LMG:O5	2.29	0.49
16:G:301:CLA:HHC	16:G:301:CLA:HBB1	1.94	0.49
16:H:302:CLA:HHC	16:H:302:CLA:HBB1	1.94	0.49
16:A:814:CLA:HHC	16:A:814:CLA:HBB1	1.94	0.49
12:G:103:TYR:HA	16:G:309:CLA:HED2	1.95	0.49
16:A:835:CLA:HHC	16:A:835:CLA:HBB1	1.94	0.49
1:A:570:ARG:NH1	28:A:906:HOH:O	2.46	0.49
13:H:152:SER:OG	16:H:308:CLA:OBD	2.31	0.49
16:U:208:CLA:HHC	16:U:208:CLA:HBB1	1.93	0.49
16:H:304:CLA:HBB1	16:H:304:CLA:HHC	1.93	0.49
16:B:807:CLA:HBB1	16:B:808:CLA:H202	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:B:825:CLA:H42	24:B:843:DGD:HB42	1.94	0.49
16:A:809:CLA:HBB2	21:A:848:LMU:H101	1.95	0.49
6:F:107:PHE:HB2	6:F:129:MET:HE1	1.95	0.49
16:A:817:CLA:HHC	16:A:817:CLA:HBB1	1.95	0.48
12:G:77:LYS:O	12:G:81:ILE:HD12	2.13	0.48
16:A:854:CLA:H12	9:L:30:LEU:HD11	1.95	0.48
16:B:807:CLA:H12	7:I:14:VAL:HG21	1.95	0.48
4:D:5:LEU:HD23	4:D:95:ILE:HD13	1.94	0.48
16:A:851:CLA:H172	6:F:101:GLY:HA2	1.95	0.48
16:B:819:CLA:HBB	16:B:836:CLA:O1D	2.12	0.48
1:A:230:PRO:HA	1:A:233:LEU:HD12	1.96	0.48
4:D:102:ASP:OD2	4:D:110:ASN:ND2	2.47	0.48
6:F:127:LEU:HB3	16:G:306:CLA:H41	1.94	0.48
12:G:174:LYS:HD3	16:G:303:CLA:HBD	1.94	0.48
16:A:815:CLA:HHC	16:A:815:CLA:HBB1	1.95	0.48
16:A:818:CLA:H52	16:A:849:CLA:H2	1.95	0.48
1:A:464:ASP:OD1	1:A:470:GLN:NE2	2.45	0.48
2:B:716:ILE:HG22	16:B:823:CLA:H52	1.96	0.48
2:B:522:ALA:HB2	16:B:832:CLA:HMA1	1.94	0.48
1:A:664:LEU:HD11	2:B:615:MET:HB2	1.96	0.48
9:L:5:LYS:NZ	11:U:111:GLN:O	2.46	0.48
14:K:163:MET:SD	16:K:202:CLA:HBB	2.54	0.48
16:A:819:CLA:HAA2	15:k:64:LYS:HE3	1.95	0.47
2:B:393:VAL:HG21	2:B:553:TYR:HB2	1.96	0.47
2:B:713:VAL:HG22	24:B:843:DGD:HBV1	1.96	0.47
16:G:310:CLA:HBA1	16:G:310:CLA:HBD	1.95	0.47
1:A:334:ILE:HG13	1:A:411:GLN:HE22	1.79	0.47
1:A:556:LYS:NZ	2:B:671:GLU:OE2	2.46	0.47
1:A:431:LEU:HD21	1:A:537:VAL:HG12	1.96	0.47
16:U:209:CLA:HHC	16:U:209:CLA:HBB1	1.96	0.47
13:H:107:LEU:HD13	16:H:306:CLA:HBA2	1.96	0.47
2:B:24:ALA:HA	16:B:825:CLA:H43	1.95	0.47
11:U:46:MET:HG2	16:U:207:CLA:HAC1	1.96	0.47
1:A:4:GLN:HG3	1:A:6:VAL:HG13	1.96	0.47
28:A:993:HOH:O	9:L:2:GLU:HB3	2.14	0.47
16:B:824:CLA:HBA2	16:B:824:CLA:H12	1.64	0.47
16:H:306:CLA:H62	16:H:306:CLA:H41	1.66	0.47
16:A:835:CLA:H101	8:J:17:THR:HG23	1.96	0.47
22:A:850:CL0:H35	16:B:801:CLA:O1D	2.15	0.47
16:B:822:CLA:H143	19:B:846:BCR:H20C	1.97	0.47
16:A:813:CLA:HHC	16:A:813:CLA:HBB1	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:A:845:CLA:H41	16:A:845:CLA:H61	1.76	0.46
22:A:850:CL0:O1D	16:B:802:CLA:HBB2	2.15	0.46
16:B:806:CLA:H102	16:B:806:CLA:H152	1.98	0.46
13:H:95:PRO:HB2	14:K:133:PRO:HG2	1.97	0.46
2:B:629:LEU:HD22	2:B:722:PHE:HA	1.97	0.46
2:B:339:LEU:HD11	16:B:805:CLA:H51	1.97	0.46
16:B:835:CLA:H41	16:B:835:CLA:H61	1.68	0.46
2:B:381:MET:HE1	19:B:841:BCR:H361	1.97	0.46
12:G:130:GLU:O	12:G:134:ASN:ND2	2.44	0.45
16:A:851:CLA:H12	16:B:848:CLA:HAA1	1.98	0.45
11:U:134:PHE:HE1	16:U:205:CLA:H202	1.80	0.45
2:B:668:TYR:OH	16:B:803:CLA:OBD	2.31	0.45
16:B:834:CLA:HBB2	17:B:837:PQN:H141	1.97	0.45
12:G:83:MET:HE3	12:G:178:ASN:HB2	1.98	0.45
17:A:837:PQN:H222	17:A:837:PQN:H18	1.69	0.45
7:I:11:THR:O	7:I:15:THR:OG1	2.33	0.45
16:H:303:CLA:H62	16:H:303:CLA:H41	1.78	0.45
16:A:816:CLA:H141	16:A:823:CLA:H193	1.99	0.45
2:B:282:PHE:HE1	16:B:817:CLA:HBB1	1.82	0.45
15:k:63:THR:HG21	15:k:91:THR:HG22	1.97	0.45
2:B:343:THR:HB	2:B:377:ALA:HB2	1.97	0.45
12:G:84:LEU:HD22	16:G:309:CLA:H93	1.99	0.45
1:A:351:GLY:HA2	1:A:388:GLY:HA2	1.97	0.45
2:B:285:ALA:HB2	16:B:817:CLA:HBC2	1.99	0.45
16:B:848:CLA:HHC	16:B:848:CLA:HBB1	1.99	0.45
15:k:83:PHE:HB3	15:k:86:THR:HG23	1.99	0.45
1:A:267:THR:OG1	1:A:283:ASP:OD1	2.30	0.45
19:B:839:BCR:H20C	19:B:839:BCR:H361	1.83	0.45
9:L:6:PRO:HB3	9:L:11:PRO:HA	1.99	0.44
12:G:179:GLY:O	12:G:183:MET:HG3	2.17	0.44
1:A:109:TRP:CD2	16:A:807:CLA:HED3	2.52	0.44
12:G:133:SER:O	12:G:135:LYS:NZ	2.45	0.44
16:G:310:CLA:HBD	16:G:310:CLA:HED2	1.87	0.44
9:L:5:LYS:HG3	9:L:17:SER:HB3	1.98	0.44
16:B:830:CLA:HHC	16:B:830:CLA:HBB1	1.98	0.44
5:E:8:ARG:NH2	6:F:155:GLU:OE1	2.50	0.44
6:F:129:MET:HG3	12:G:141:MET:HE1	2.00	0.44
13:H:156:LEU:HB3	16:H:309:CLA:HBC1	2.00	0.44
13:H:207:LEU:HD12	13:H:207:LEU:HA	1.65	0.44
1:A:111:ILE:HG13	1:A:112:VAL:HG13	1.99	0.44
2:B:578:MET:HG3	2:B:708:LEU:HD21	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:B:834:CLA:H191	9:L:57:LEU:HD11	2.00	0.44
8:J:1:MET:HG3	18:G:316:LHG:C24	2.47	0.44
16:L:202:CLA:H3A	16:L:202:CLA:HBA2	1.78	0.44
1:A:2:LYS:HD2	1:A:2:LYS:HA	1.82	0.44
1:A:7:VAL:HA	1:A:176:PRO:HA	1.99	0.44
16:A:824:CLA:H142	16:A:826:CLA:H18	2.00	0.44
2:B:92:PRO:HB2	16:B:849:CLA:HAA1	2.00	0.44
1:A:574:CYS:HB2	2:B:665:TRP:HB3	2.00	0.44
2:B:232:ALA:HB2	16:B:814:CLA:HMA2	1.99	0.44
12:G:32:ASN:HD22	12:G:32:ASN:HA	1.71	0.44
16:A:828:CLA:HBB1	16:A:829:CLA:HBA1	2.00	0.44
16:B:801:CLA:H122	19:B:842:BCR:H12C	1.99	0.43
16:A:828:CLA:H42	16:A:836:CLA:H2	2.00	0.43
2:B:173:LEU:HD23	2:B:173:LEU:HA	1.82	0.43
16:B:848:CLA:H202	16:B:848:CLA:H161	1.91	0.43
4:D:42:VAL:HG22	4:D:52:ILE:HG12	1.99	0.43
16:H:312:CLA:H12	16:H:312:CLA:HBA2	1.61	0.43
16:K:205:CLA:H12	16:K:205:CLA:H51	1.77	0.43
16:A:851:CLA:H191	6:F:126:ALA:HB1	2.00	0.43
16:B:818:CLA:HBB1	16:B:818:CLA:HHC	1.99	0.43
1:A:237:GLN:NE2	1:A:247:PHE:O	2.50	0.43
16:A:833:CLA:H51	16:A:833:CLA:H11	1.83	0.43
2:B:67:ALA:HB2	2:B:133:LEU:HB2	2.00	0.43
16:B:849:CLA:H12	9:L:67:LEU:HD12	2.00	0.43
16:U:207:CLA:H143	16:U:210:CLA:HBC1	2.00	0.43
14:K:55:ASP:OD1	14:K:55:ASP:O	2.37	0.43
1:A:364:MET:HE3	1:A:364:MET:HB2	1.83	0.43
16:A:833:CLA:H151	16:A:854:CLA:H202	2.00	0.43
19:B:838:BCR:H15C	19:B:838:BCR:H351	1.90	0.43
16:B:849:CLA:H143	9:L:83:GLY:HA2	2.00	0.43
19:L:205:BCR:H20C	19:L:205:BCR:H361	1.79	0.43
12:G:78:HIS:HB3	12:G:183:MET:SD	2.58	0.43
16:G:306:CLA:H152	16:G:306:CLA:H18	1.82	0.43
6:F:120:ILE:HG12	8:J:11:THR:HG22	2.00	0.43
12:G:184:LEU:HD11	16:G:307:CLA:HAC1	2.01	0.43
19:A:844:BCR:H15C	19:A:844:BCR:H351	1.86	0.43
16:H:305:CLA:H3A	16:H:306:CLA:H52	2.01	0.43
1:A:234:ILE:HD12	16:A:812:CLA:HHD	2.01	0.43
17:A:837:PQN:H141	16:F:802:CLA:HBB2	2.01	0.43
16:A:816:CLA:H91	16:A:825:CLA:H162	2.00	0.43
19:J:105:BCR:H15C	19:J:105:BCR:H351	1.91	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:310:LYS:HD3	2:B:310:LYS:HA	1.80	0.42
1:A:272:LEU:HD21	1:A:365:PRO:HD2	2.01	0.42
21:A:855:LMU:H22	21:A:855:LMU:H1'	1.58	0.42
19:L:205:BCR:H15C	19:L:205:BCR:H351	1.86	0.42
12:G:44:PRO:HG2	12:G:64:GLU:HG2	1.99	0.42
12:G:157:ASP:OD1	20:G:311:DD6:O4	2.36	0.42
19:A:843:BCR:H23C	16:A:849:CLA:HBC2	2.00	0.42
16:B:807:CLA:H122	16:B:807:CLA:H161	1.81	0.42
16:B:849:CLA:H41	16:B:849:CLA:H61	1.62	0.42
26:U:202:A86:C5	16:U:207:CLA:H2	2.49	0.42
16:H:302:CLA:H12	16:H:302:CLA:H52	1.87	0.42
14:K:128:ILE:HG12	16:K:203:CLA:HMB2	2.00	0.42
2:B:148:LEU:HD21	19:M:101:BCR:H342	2.02	0.42
2:B:172:ARG:HB2	16:B:844:CLA:HBC2	2.02	0.42
16:B:813:CLA:H92	16:B:813:CLA:H61	1.91	0.42
11:U:3:LEU:HD12	11:U:3:LEU:HA	1.95	0.42
16:G:308:CLA:CAD	16:H:308:CLA:H3A	2.50	0.42
13:H:207:LEU:HG	13:H:211:ARG:NH2	2.34	0.42
14:K:116:MET:HB3	16:K:206:CLA:HBC3	2.00	0.42
19:k:203:BCR:H20C	19:k:203:BCR:H361	1.84	0.42
19:B:846:BCR:H24C	19:B:846:BCR:H371	1.84	0.42
9:L:28:LEU:O	9:L:32:ASN:ND2	2.52	0.42
15:k:59:VAL:HG11	15:k:94:LEU:HB3	2.02	0.42
2:B:54:ILE:HD11	19:M:101:BCR:HC8	2.01	0.42
3:C:60:ASP:HA	3:C:61:PHE:HA	1.87	0.42
1:A:364:MET:HG3	1:A:497:SER:HB2	2.01	0.42
1:A:567:GLY:HA2	2:B:560:PRO:HD3	2.02	0.42
1:A:605:GLN:HB3	1:A:622:THR:HG23	2.02	0.42
16:A:824:CLA:H102	16:A:824:CLA:H61	1.88	0.42
16:A:828:CLA:H192	16:B:835:CLA:HBD	2.01	0.42
2:B:58:TRP:HA	16:B:807:CLA:HBB2	2.02	0.42
19:B:842:BCR:H20C	19:B:842:BCR:H361	1.88	0.42
1:A:564:PRO:HB3	1:A:711:ILE:HB	2.01	0.42
18:A:839:LHG:H282	18:A:839:LHG:H312	1.82	0.42
19:B:840:BCR:H20C	19:B:840:BCR:H361	1.88	0.42
19:I:103:BCR:H361	9:L:95:TYR:HB2	2.01	0.42
1:A:683:TYR:CE2	16:A:801:CLA:HMD1	2.55	0.42
2:B:238:VAL:HG23	2:B:239:LYS:HG2	2.02	0.42
8:J:22:ILE:HG23	16:J:104:CLA:HBB2	2.02	0.42
13:H:93:PHE:HD2	16:H:306:CLA:C1D	2.33	0.42
19:k:203:BCR:H11C	19:k:203:BCR:H341	1.95	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:271:ILE:HG23	16:B:816:CLA:HMA3	2.01	0.41
1:A:731:TRP:NE1	16:A:824:CLA:O1A	2.47	0.41
19:A:844:BCR:H20C	19:A:844:BCR:H361	1.85	0.41
12:G:54:GLU:H	12:G:54:GLU:HG3	1.60	0.41
1:A:229:LEU:HD22	16:A:814:CLA:HED1	2.02	0.41
16:B:806:CLA:H192	16:B:806:CLA:H71	2.02	0.41
19:J:105:BCR:H20C	19:J:105:BCR:H361	1.83	0.41
16:A:806:CLA:H12	16:A:806:CLA:HBA2	1.62	0.41
16:A:854:CLA:H72	16:L:203:CLA:H12	2.01	0.41
2:B:179:GLY:HA2	2:B:183:VAL:HB	2.02	0.41
1:A:555:ASP:OD1	1:A:555:ASP:N	2.53	0.41
18:A:839:LHG:H141	18:A:839:LHG:H112	1.85	0.41
16:A:853:CLA:H91	16:A:853:CLA:H112	1.80	0.41
2:B:5:LYS:HB2	2:B:5:LYS:HE2	1.81	0.41
8:J:23:THR:HA	8:J:26:PHE:CE2	2.55	0.41
13:H:78:LEU:HD11	14:K:133:PRO:HB2	2.02	0.41
16:L:204:CLA:HED2	16:L:204:CLA:HBD	1.89	0.41
16:k:202:CLA:H11	16:k:202:CLA:H51	1.88	0.41
16:I:102:CLA:H93	9:L:79:PHE:CE2	2.56	0.41
13:H:108:ARG:NH2	16:H:306:CLA:O1D	2.54	0.41
13:H:215:MET:HE2	16:H:306:CLA:HMC3	2.03	0.41
1:A:333:GLU:HB2	1:A:411:GLN:HE21	1.86	0.41
16:A:854:CLA:H91	16:A:854:CLA:H112	1.86	0.41
2:B:255:PHE:CG	16:B:815:CLA:HMB2	2.55	0.41
16:B:829:CLA:H62	16:B:829:CLA:H101	1.89	0.41
16:B:831:CLA:H51	16:B:831:CLA:H11	1.83	0.41
3:C:27:MET:HE3	3:C:27:MET:HB3	1.89	0.41
19:I:101:BCR:H15C	19:I:101:BCR:H351	1.89	0.41
19:M:101:BCR:H15C	19:M:101:BCR:H351	1.84	0.41
12:G:185:GLY:O	12:G:189:MET:HG3	2.21	0.41
1:A:87:ARG:HD2	1:A:150:TYR:OH	2.21	0.41
1:A:189:ASN:HB3	16:A:817:CLA:HMD1	2.03	0.41
1:A:460:ASP:HB3	16:A:829:CLA:HED3	2.02	0.41
16:A:808:CLA:HBA1	16:A:810:CLA:HMD2	2.03	0.41
16:A:828:CLA:CAD	19:L:201:BCR:H10C	2.51	0.41
2:B:695:PRO:HB3	16:B:834:CLA:C1C	2.51	0.41
4:D:30:LYS:HG2	4:D:89:ILE:HB	2.03	0.41
1:A:73:ILE:HD11	16:A:809:CLA:H121	2.03	0.40
1:A:669:ILE:HD13	1:A:669:ILE:HA	1.92	0.40
1:A:675:MET:HB2	16:A:801:CLA:C1C	2.51	0.40
1:A:691:ILE:HD13	16:A:851:CLA:HMD2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:G:170:GLU:HG3	16:G:302:CLA:HED1	2.04	0.40
16:A:816:CLA:H72	16:A:816:CLA:H111	1.82	0.40
16:A:849:CLA:H152	16:A:849:CLA:H112	1.81	0.40
2:B:44:ILE:HG21	16:B:805:CLA:H192	2.03	0.40
6:F:135:ILE:H	6:F:135:ILE:HG13	1.67	0.40
15:k:59:VAL:O	15:k:63:THR:HG23	2.21	0.40
1:A:398:HIS:HA	1:A:401:ILE:HD12	2.03	0.40
1:A:709:LEU:HD21	17:A:837:PQN:H151	2.02	0.40
16:K:205:CLA:H41	16:K:205:CLA:H61	1.91	0.40
1:A:194:GLY:O	1:A:198:LEU:HB2	2.21	0.40
16:A:830:CLA:HHC	16:A:830:CLA:HAB	1.95	0.40
19:A:843:BCR:H362	16:A:849:CLA:HBA2	2.03	0.40
16:A:851:CLA:HAA2	16:B:827:CLA:HMB2	2.03	0.40
16:G:303:CLA:HAA1	16:G:304:CLA:HBB1	2.03	0.40
16:A:811:CLA:H102	16:A:811:CLA:H61	1.85	0.40
2:B:337:ALA:HB2	19:B:841:BCR:H372	2.04	0.40
19:B:839:BCR:H19C	16:B:844:CLA:H43	2.04	0.40
8:J:41:ALA:HB2	21:J:101:LMU:C6B	2.51	0.40
11:U:84:PHE:HZ	16:U:207:CLA:H162	1.86	0.40
12:G:192:GLN:O	12:G:196:THR:OG1	2.27	0.40
16:H:312:CLA:H93	16:H:312:CLA:H111	1.77	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	739/752 (98%)	723 (98%)	16 (2%)	0	100	100
2	B	730/734 (100%)	713 (98%)	17 (2%)	0	100	100
3	C	78/81 (96%)	77 (99%)	1 (1%)	0	100	100
4	D	136/142 (96%)	131 (96%)	4 (3%)	1 (1%)	18	15

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	E	62/67 (92%)	60 (97%)	2 (3%)	0	100	100
6	F	159/184 (86%)	157 (99%)	2 (1%)	0	100	100
7	I	32/35 (91%)	30 (94%)	2 (6%)	0	100	100
8	J	37/39 (95%)	37 (100%)	0	0	100	100
9	L	138/141 (98%)	136 (99%)	2 (1%)	0	100	100
10	M	27/29 (93%)	27 (100%)	0	0	100	100
11	U	139/191 (73%)	135 (97%)	4 (3%)	0	100	100
12	G	152/209 (73%)	142 (93%)	10 (7%)	0	100	100
13	H	145/169 (86%)	143 (99%)	2 (1%)	0	100	100
14	K	87/200 (44%)	85 (98%)	2 (2%)	0	100	100
15	k	50/89 (56%)	50 (100%)	0	0	100	100
All	All	2711/3062 (88%)	2646 (98%)	64 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	48	SER

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	603/612 (98%)	601 (100%)	2 (0%)	86	91
2	B	590/591 (100%)	589 (100%)	1 (0%)	87	92
3	C	68/69 (99%)	68 (100%)	0	100	100
4	D	118/122 (97%)	118 (100%)	0	100	100
5	E	53/55 (96%)	52 (98%)	1 (2%)	50	57
6	F	133/152 (88%)	131 (98%)	2 (2%)	57	65
7	I	31/32 (97%)	30 (97%)	1 (3%)	34	37

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	J	32/32 (100%)	32 (100%)	0	100	100
9	L	111/112 (99%)	109 (98%)	2 (2%)	51	59
10	M	21/21 (100%)	20 (95%)	1 (5%)	23	22
11	U	110/148 (74%)	108 (98%)	2 (2%)	51	59
12	G	130/167 (78%)	125 (96%)	5 (4%)	29	30
13	H	119/137 (87%)	112 (94%)	7 (6%)	18	15
14	K	77/153 (50%)	70 (91%)	7 (9%)	9	6
15	k	38/65 (58%)	38 (100%)	0	100	100
All	All	2234/2468 (90%)	2203 (99%)	31 (1%)	57	67

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	SER
1	A	574	CYS
2	B	439	ASP
5	E	10	MET
6	F	10	ASP
6	F	135	ILE
7	I	4	SER
9	L	57	LEU
9	L	71	GLU
10	M	22	ILE
11	U	52	ASP
11	U	117	SER
12	G	37	VAL
12	G	137	LYS
12	G	187	SER
12	G	192	GLN
12	G	196	THR
13	H	74	SER
13	H	79	VAL
13	H	96	LEU
13	H	112	LEU
13	H	119	MET
13	H	158	LEU
13	H	222	THR
14	K	57	LEU
14	K	63	ILE

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Mol	Chain	Res	Type
14	K	66	LYS
14	K	72	GLU
14	K	74	LYS
14	K	134	LYS
14	K	183	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	249	GLN
1	A	377	GLN
1	A	432	ASN
2	B	39	ASN
2	B	112	ASN
2	B	169	ASN
2	B	227	ASN
2	B	264	GLN
2	B	641	GLN
3	C	3	ASN
4	D	99	HIS
4	D	118	ASN
6	F	15	ASN
6	F	122	ASN
9	L	32	ASN
11	U	122	GLN
12	G	32	ASN
12	G	178	ASN
13	H	172	GLN
13	H	229	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

180 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$
16	CLA	A	817	1	49,53,73	1.40	7 (14%)	58,89,113	1.16	5 (8%)
16	CLA	B	807	2	69,73,73	1.18	7 (10%)	82,113,113	0.90	3 (3%)
21	LMU	F	806	-	36,36,36	1.21	2 (5%)	47,47,47	0.97	2 (4%)
16	CLA	A	803	1	69,73,73	1.14	6 (8%)	82,113,113	0.93	4 (4%)
16	CLA	A	807	1	59,63,73	1.28	8 (13%)	70,101,113	1.07	6 (8%)
16	CLA	B	833	2	51,55,73	1.39	6 (11%)	60,91,113	1.01	5 (8%)
16	CLA	F	804	6	50,54,73	1.37	7 (14%)	59,90,113	1.08	4 (6%)
20	DD6	G	313	-	40,45,45	1.39	8 (20%)	51,67,67	1.50	7 (13%)
16	CLA	A	818	28	69,73,73	1.16	7 (10%)	82,113,113	0.87	3 (3%)
16	CLA	A	823	1	69,73,73	1.26	8 (11%)	82,113,113	0.88	3 (3%)
16	CLA	B	803	-	69,73,73	1.16	7 (10%)	82,113,113	0.91	4 (4%)
16	CLA	B	824	2	69,73,73	1.21	7 (10%)	82,113,113	0.96	5 (6%)
16	CLA	A	821	28	69,73,73	1.20	8 (11%)	82,113,113	0.98	5 (6%)
16	CLA	B	815	2	63,67,73	1.21	7 (11%)	74,105,113	0.94	4 (5%)
20	DD6	K	208	-	40,45,45	1.29	7 (17%)	51,67,67	1.55	9 (17%)
20	DD6	H	310	-	40,45,45	1.34	7 (17%)	51,67,67	1.62	10 (19%)
19	BCR	k	203	-	41,41,41	1.10	2 (4%)	56,56,56	1.37	9 (16%)
16	CLA	U	207	-	69,73,73	1.13	6 (8%)	82,113,113	1.04	7 (8%)
16	CLA	B	844	2	69,73,73	1.21	7 (10%)	82,113,113	0.89	3 (3%)
19	BCR	B	838	-	41,41,41	1.08	2 (4%)	56,56,56	1.19	6 (10%)
16	CLA	A	810	1	58,62,73	1.28	7 (12%)	68,99,113	1.03	5 (7%)
16	CLA	B	827	2	53,57,73	1.37	7 (13%)	61,93,113	0.97	3 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
16	CLA	K	206	28	44,48,73	1.49	8 (18%)	51,82,113	1.27	5 (9%)
16	CLA	A	825	1	69,73,73	1.23	7 (10%)	82,113,113	0.91	3 (3%)
16	CLA	K	202	14	46,50,73	1.40	8 (17%)	53,85,113	1.02	4 (7%)
16	CLA	A	812	1	49,53,73	1.42	5 (10%)	58,89,113	1.20	6 (10%)
16	CLA	H	308	13	45,49,73	1.40	6 (13%)	54,84,113	1.23	6 (11%)
16	CLA	A	808	1	60,64,73	1.30	7 (11%)	71,102,113	0.92	3 (4%)
19	BCR	B	846	-	40,40,41	1.08	2 (5%)	54,54,56	1.33	9 (16%)
19	BCR	M	101	-	41,41,41	1.07	2 (4%)	56,56,56	1.28	5 (8%)
16	CLA	B	814	2	59,63,73	1.34	6 (10%)	70,101,113	1.07	4 (5%)
16	CLA	B	812	2	58,62,73	1.28	7 (12%)	68,99,113	0.97	4 (5%)
16	CLA	G	303	-	49,53,73	1.41	8 (16%)	58,89,113	1.14	4 (6%)
16	CLA	G	309	-	60,64,73	1.24	7 (11%)	71,102,113	1.02	5 (7%)
16	CLA	G	304	12	47,51,73	1.38	6 (12%)	55,86,113	1.13	5 (9%)
19	BCR	I	103	-	41,41,41	1.08	2 (4%)	56,56,56	1.24	4 (7%)
16	CLA	A	854	1	69,73,73	1.16	7 (10%)	82,113,113	0.90	5 (6%)
16	CLA	A	831	1	49,53,73	1.37	5 (10%)	58,89,113	1.13	4 (6%)
23	SF4	C	102	3	0,12,12	-	-	-	-	-
16	CLA	H	312	-	69,73,73	1.09	5 (7%)	82,113,113	0.93	5 (6%)
16	CLA	B	832	2	69,73,73	1.18	7 (10%)	82,113,113	0.89	4 (4%)
16	CLA	U	211	11	56,60,73	1.36	7 (12%)	65,97,113	1.05	5 (7%)
16	CLA	H	302	13	64,68,73	1.24	8 (12%)	76,107,113	1.04	4 (5%)
20	DD6	J	102	-	40,45,45	1.34	8 (20%)	51,67,67	1.60	9 (17%)
20	DD6	G	311	-	40,45,45	1.27	8 (20%)	51,67,67	1.43	7 (13%)
20	DD6	U	203	-	40,45,45	1.34	6 (15%)	51,67,67	1.73	13 (25%)
16	CLA	A	853	1	69,73,73	1.14	7 (10%)	82,113,113	0.91	5 (6%)
16	CLA	K	207	-	50,54,73	1.34	6 (12%)	59,90,113	1.06	4 (6%)
16	CLA	A	814	28	49,53,73	1.40	7 (14%)	58,89,113	1.08	4 (6%)
16	CLA	G	305	12	65,69,73	1.17	6 (9%)	77,108,113	1.08	7 (9%)
17	PQN	A	837	-	34,34,34	0.40	0	43,45,45	0.58	1 (2%)
16	CLA	B	826	2	54,58,73	1.38	6 (11%)	64,95,113	0.96	4 (6%)
16	CLA	B	805	2	69,73,73	1.15	7 (10%)	82,113,113	0.90	4 (4%)
16	CLA	K	204	14	49,53,73	1.53	7 (14%)	58,89,113	0.98	3 (5%)
16	CLA	H	309	13	49,53,73	1.41	7 (14%)	58,89,113	1.11	4 (6%)
19	BCR	L	201	-	41,41,41	1.11	2 (4%)	56,56,56	1.20	4 (7%)
16	CLA	B	816	2	64,68,73	1.23	7 (10%)	76,107,113	0.92	4 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
16	CLA	A	832	1	55,59,73	1.34	8 (14%)	64,96,113	1.04	4 (6%)
16	CLA	U	208	11	50,54,73	1.35	7 (14%)	59,90,113	1.14	5 (8%)
20	DD6	A	846	-	40,45,45	1.30	6 (15%)	51,67,67	1.48	9 (17%)
16	CLA	B	819	2	57,61,73	1.25	7 (12%)	67,98,113	0.99	5 (7%)
16	CLA	B	813	2	63,67,73	1.25	8 (12%)	74,105,113	0.90	4 (5%)
16	CLA	B	822	2	69,73,73	1.25	7 (10%)	82,113,113	0.94	4 (4%)
16	CLA	A	851	1	69,73,73	1.20	7 (10%)	82,113,113	0.89	4 (4%)
19	BCR	B	840	-	41,41,41	1.06	3 (7%)	56,56,56	1.25	6 (10%)
16	CLA	B	801	28	69,73,73	1.18	7 (10%)	82,113,113	0.92	3 (3%)
16	CLA	B	829	28	69,73,73	1.16	7 (10%)	82,113,113	0.91	4 (4%)
16	CLA	A	833	1	69,73,73	1.21	6 (8%)	82,113,113	0.92	4 (4%)
22	CL0	A	850	1	58,73,73	0.96	5 (8%)	60,113,113	1.86	10 (16%)
16	CLA	A	820	1	55,59,73	1.36	8 (14%)	64,96,113	1.11	5 (7%)
16	CLA	G	315	12	49,53,73	1.33	5 (10%)	58,89,113	1.24	6 (10%)
16	CLA	H	305	13	49,53,73	1.50	7 (14%)	58,89,113	0.95	3 (5%)
16	CLA	A	835	1	69,73,73	1.20	7 (10%)	82,113,113	0.94	3 (3%)
16	CLA	A	813	1	54,58,73	1.37	7 (12%)	64,95,113	1.04	5 (7%)
16	CLA	H	304	13	47,52,73	1.39	8 (17%)	55,87,113	1.11	4 (7%)
19	BCR	B	839	-	41,41,41	1.06	2 (4%)	56,56,56	1.24	7 (12%)
27	KC1	U	213	11	49,53,53	1.63	11 (22%)	61,89,89	0.91	3 (4%)
16	CLA	B	808	2	69,73,73	1.23	7 (10%)	82,113,113	0.87	2 (2%)
16	CLA	U	206	11	49,53,73	1.38	7 (14%)	58,89,113	1.01	4 (6%)
20	DD6	U	214	-	24,26,45	2.38	6 (25%)	29,35,67	1.51	5 (17%)
16	CLA	A	802	1	59,63,73	1.24	7 (11%)	70,101,113	0.94	4 (5%)
16	CLA	U	209	-	46,50,73	1.39	6 (13%)	53,85,113	1.12	6 (11%)
16	CLA	K	205	14	62,66,73	1.20	7 (11%)	73,104,113	1.20	9 (12%)
16	CLA	B	820	28	67,71,73	1.21	7 (10%)	79,110,113	1.01	6 (7%)
16	CLA	F	802	28	69,73,73	1.18	7 (10%)	82,113,113	0.96	4 (4%)
18	LHG	A	839	-	47,47,48	0.64	1 (2%)	50,53,54	1.27	6 (12%)
16	CLA	B	802	2	69,73,73	1.26	7 (10%)	82,113,113	0.79	3 (3%)
16	CLA	A	824	1	66,70,73	1.20	7 (10%)	78,109,113	1.00	4 (5%)
17	PQN	B	837	-	34,34,34	0.42	0	43,45,45	0.55	1 (2%)
16	CLA	B	848	2	69,73,73	1.26	8 (11%)	82,113,113	1.01	4 (4%)
16	CLA	A	826	1	69,73,73	1.28	8 (11%)	82,113,113	0.82	2 (2%)
20	DD6	U	212	-	40,45,45	1.30	7 (17%)	51,67,67	1.70	12 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
16	CLA	A	827	1	54,58,73	1.39	6 (11%)	64,95,113	0.97	4 (6%)
16	CLA	A	847	1	64,68,73	1.30	7 (10%)	76,107,113	0.92	4 (5%)
16	CLA	G	306	12	69,73,73	1.25	7 (10%)	82,113,113	0.86	3 (3%)
20	DD6	G	312	-	25,28,45	1.47	6 (24%)	32,42,67	1.60	5 (15%)
19	BCR	A	842	-	41,41,41	1.09	2 (4%)	56,56,56	1.16	4 (7%)
16	CLA	A	819	1	47,51,73	1.43	7 (14%)	55,86,113	1.07	4 (7%)
16	CLA	B	821	28	59,63,73	1.22	6 (10%)	70,101,113	0.94	4 (5%)
16	CLA	J	104	8	46,50,73	1.41	6 (13%)	53,85,113	1.05	4 (7%)
16	CLA	L	202	9	53,57,73	1.35	6 (11%)	61,93,113	1.12	5 (8%)
16	CLA	A	805	1	53,57,73	1.38	6 (11%)	61,93,113	1.00	4 (6%)
16	CLA	B	817	28	69,73,73	1.19	7 (10%)	82,113,113	0.99	5 (6%)
16	CLA	A	801	-	69,73,73	1.16	8 (11%)	82,113,113	0.87	4 (4%)
16	CLA	U	204	28	65,69,73	1.19	7 (10%)	77,108,113	0.96	5 (6%)
16	CLA	A	809	1	66,70,73	1.24	7 (10%)	78,109,113	0.86	3 (3%)
16	CLA	B	849	2	69,73,73	1.18	7 (10%)	82,113,113	0.96	4 (4%)
16	CLA	B	834	28	69,73,73	1.18	7 (10%)	82,113,113	0.96	5 (6%)
20	DD6	G	317	-	40,45,45	1.25	8 (20%)	51,67,67	1.45	8 (15%)
16	CLA	B	835	2	69,73,73	1.24	8 (11%)	82,113,113	0.97	4 (4%)
16	CLA	A	829	1	69,73,73	1.20	7 (10%)	82,113,113	0.89	3 (3%)
23	SF4	A	852	2,1	0,12,12	-	-	-	-	-
19	BCR	I	101	-	41,41,41	1.07	2 (4%)	56,56,56	1.27	6 (10%)
16	CLA	B	809	2	69,73,73	1.19	9 (13%)	82,113,113	0.91	4 (4%)
16	CLA	A	834	1	69,73,73	1.27	6 (8%)	82,113,113	0.92	4 (4%)
19	BCR	J	105	-	41,41,41	1.06	2 (4%)	56,56,56	1.23	4 (7%)
16	CLA	I	102	-	69,73,73	1.16	7 (10%)	82,113,113	0.98	5 (6%)
16	CLA	H	307	-	62,66,73	1.20	7 (11%)	73,104,113	0.94	4 (5%)
16	CLA	A	811	1	69,73,73	1.20	7 (10%)	82,113,113	0.90	3 (3%)
21	LMU	A	855	-	36,36,36	0.55	1 (2%)	47,47,47	0.99	2 (4%)
16	CLA	B	828	2	62,66,73	1.26	7 (11%)	73,104,113	1.00	5 (6%)
16	CLA	A	836	28	69,73,73	1.15	7 (10%)	82,113,113	0.95	3 (3%)
20	DD6	G	314	-	40,45,45	1.31	8 (20%)	51,67,67	1.50	9 (17%)
26	A86	U	202	-	47,50,50	1.36	6 (12%)	51,76,76	1.39	7 (13%)
16	CLA	B	811	2	59,63,73	1.25	6 (10%)	70,101,113	0.99	4 (5%)
16	CLA	A	822	28	69,73,73	1.12	6 (8%)	82,113,113	0.93	4 (4%)
16	CLA	L	203	9	69,73,73	1.14	6 (8%)	82,113,113	0.87	4 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
16	CLA	B	836	-	61,65,73	1.26	6 (9%)	72,103,113	1.05	5 (6%)
24	DGD	B	843	-	61,61,67	0.92	2 (3%)	75,75,81	1.11	6 (8%)
19	BCR	A	843	-	41,41,41	1.10	2 (4%)	56,56,56	1.23	5 (8%)
16	CLA	F	803	-	52,56,73	1.36	8 (15%)	61,92,113	1.16	5 (8%)
19	BCR	B	842	-	41,41,41	1.08	2 (4%)	56,56,56	1.18	5 (8%)
16	CLA	A	830	1	54,58,73	1.33	6 (11%)	64,95,113	0.97	3 (4%)
16	CLA	A	804	1	69,73,73	1.16	7 (10%)	82,113,113	0.90	4 (4%)
16	CLA	G	308	-	59,63,73	1.25	7 (11%)	70,101,113	1.05	6 (8%)
16	CLA	U	205	11	69,73,73	1.19	7 (10%)	82,113,113	0.96	3 (3%)
16	CLA	B	830	28	49,53,73	1.41	7 (14%)	58,89,113	1.12	4 (6%)
25	LMG	U	201	-	32,32,55	0.94	1 (3%)	40,40,63	1.22	6 (15%)
16	CLA	A	816	1	69,73,73	1.17	7 (10%)	82,113,113	0.94	4 (4%)
16	CLA	B	825	2	69,73,73	1.25	7 (10%)	82,113,113	0.87	3 (3%)
23	SF4	C	101	3	0,12,12	-	-	-	-	-
16	CLA	A	845	28	69,73,73	1.16	7 (10%)	82,113,113	0.90	3 (3%)
16	CLA	B	804	2	49,53,73	1.44	7 (14%)	58,89,113	1.05	4 (6%)
16	CLA	B	823	2	69,73,73	1.23	7 (10%)	82,113,113	0.94	4 (4%)
16	CLA	G	301	12	49,53,73	1.38	6 (12%)	58,89,113	1.06	4 (6%)
20	DD6	H	311	-	40,45,45	1.31	7 (17%)	51,67,67	1.53	10 (19%)
16	CLA	A	806	1	69,73,73	1.15	6 (8%)	82,113,113	1.00	5 (6%)
16	CLA	U	210	11	69,73,73	1.14	5 (7%)	82,113,113	0.93	5 (6%)
16	CLA	G	310	12	49,53,73	1.42	7 (14%)	58,89,113	1.09	4 (6%)
16	CLA	K	203	14	59,63,73	1.25	7 (11%)	70,101,113	1.02	4 (5%)
25	LMG	J	103	-	39,39,55	0.86	1 (2%)	47,47,63	1.28	4 (8%)
21	LMU	A	848	-	36,36,36	0.50	1 (2%)	47,47,47	0.98	2 (4%)
21	LMU	J	101	-	36,36,36	0.41	0	47,47,47	0.97	2 (4%)
16	CLA	B	810	2	58,62,73	1.40	9 (15%)	71,100,113	0.94	4 (5%)
19	BCR	A	844	-	41,41,41	1.10	2 (4%)	56,56,56	1.25	6 (10%)
16	CLA	B	847	2	56,60,73	1.27	6 (10%)	65,97,113	1.00	4 (6%)
19	BCR	A	841	-	41,41,41	1.03	2 (4%)	56,56,56	1.26	3 (5%)
16	CLA	A	849	1	69,73,73	1.19	6 (8%)	82,113,113	1.01	5 (6%)
19	BCR	F	805	-	41,41,41	1.04	2 (4%)	56,56,56	1.24	6 (10%)
16	CLA	A	838	18	56,60,73	1.28	7 (12%)	65,97,113	1.08	5 (7%)
18	LHG	A	840	16	26,26,48	0.84	0	29,32,54	1.33	3 (10%)
16	CLA	A	815	1	69,73,73	1.21	7 (10%)	82,113,113	0.95	4 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
16	CLA	H	301	-	44,48,73	1.45	6 (13%)	51,82,113	1.36	7 (13%)
16	CLA	G	302	-	45,49,73	1.47	7 (15%)	54,84,113	1.03	3 (5%)
19	BCR	B	841	-	41,41,41	1.08	2 (4%)	56,56,56	1.29	5 (8%)
16	CLA	H	303	13	65,69,73	1.20	5 (7%)	77,108,113	1.05	5 (6%)
16	CLA	B	831	2	62,66,73	1.31	7 (11%)	73,104,113	0.98	3 (4%)
16	CLA	B	818	2	50,54,73	1.38	7 (14%)	59,90,113	1.10	4 (6%)
16	CLA	k	201	15	46,50,73	1.43	5 (10%)	53,85,113	1.19	5 (9%)
16	CLA	k	202	28	59,63,73	1.31	7 (11%)	70,101,113	0.97	3 (4%)
16	CLA	L	204	28	54,58,73	1.34	8 (14%)	64,95,113	1.10	6 (9%)
19	BCR	L	205	-	41,41,41	1.06	2 (4%)	56,56,56	1.26	6 (10%)
16	CLA	A	828	1	69,73,73	1.23	6 (8%)	82,113,113	0.90	3 (3%)
21	LMU	K	201	-	36,36,36	1.19	2 (5%)	47,47,47	1.39	5 (10%)
16	CLA	B	806	2	69,73,73	1.20	7 (10%)	82,113,113	0.90	4 (4%)
19	BCR	F	801	-	41,41,41	1.06	2 (4%)	56,56,56	1.23	3 (5%)
16	CLA	H	306	13	69,73,73	1.20	8 (11%)	82,113,113	1.09	5 (6%)
16	CLA	B	845	2	69,73,73	1.21	7 (10%)	82,113,113	0.87	3 (3%)
16	CLA	G	307	12	64,68,73	1.16	6 (9%)	76,107,113	0.97	4 (5%)
18	LHG	G	316	-	26,26,48	0.35	0	29,32,54	0.43	0

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
16	CLA	A	817	1	1/1/11/20	2/15/91/115	-
16	CLA	B	807	2	1/1/15/20	3/39/115/115	-
21	LMU	F	806	-	-	7/21/61/61	0/2/2/2
16	CLA	A	803	1	1/1/15/20	4/39/115/115	-
16	CLA	B	833	2	1/1/11/20	1/18/94/115	-
16	CLA	A	807	1	-	5/27/103/115	-
16	CLA	F	804	6	1/1/11/20	4/17/93/115	-
20	DD6	G	313	-	-	6/26/80/80	0/3/3/3
16	CLA	A	818	28	1/1/15/20	2/39/115/115	-
16	CLA	A	823	1	1/1/15/20	2/39/115/115	-
16	CLA	B	803	-	1/1/15/20	4/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	CLA	B	824	2	-	3/39/115/115	-
16	CLA	A	821	28	1/1/15/20	7/39/115/115	-
16	CLA	B	815	2	1/1/13/20	2/32/108/115	-
20	DD6	K	208	-	-	10/26/80/80	0/3/3/3
20	DD6	H	310	-	-	15/26/80/80	0/3/3/3
19	BCR	k	203	-	-	10/29/63/63	0/2/2/2
16	CLA	U	207	-	1/1/15/20	3/39/115/115	-
16	CLA	B	844	2	1/1/15/20	4/39/115/115	-
19	BCR	B	838	-	-	9/29/63/63	0/2/2/2
16	CLA	A	810	1	1/1/12/20	3/26/102/115	-
16	CLA	B	827	2	1/1/11/20	3/20/96/115	-
16	CLA	K	206	28	1/1/9/20	0/10/82/115	-
16	CLA	A	825	1	1/1/15/20	6/39/115/115	-
16	CLA	K	202	14	-	0/12/88/115	-
16	CLA	A	812	1	1/1/11/20	1/15/91/115	-
16	CLA	H	308	13	1/1/10/20	2/10/86/115	-
16	CLA	A	808	1	-	0/29/105/115	-
19	BCR	B	846	-	-	17/27/61/63	0/2/2/2
19	BCR	M	101	-	-	8/29/63/63	0/2/2/2
16	CLA	B	814	2	-	7/27/103/115	-
16	CLA	B	812	2	1/1/12/20	1/26/102/115	-
16	CLA	G	303	-	1/1/11/20	4/15/91/115	-
16	CLA	G	309	-	-	6/29/105/115	-
16	CLA	G	304	12	-	4/13/89/115	-
19	BCR	I	103	-	-	11/29/63/63	0/2/2/2
16	CLA	A	854	1	1/1/15/20	5/39/115/115	-
16	CLA	A	831	1	1/1/11/20	2/15/91/115	-
23	SF4	C	102	3	-	-	0/6/5/5
16	CLA	H	312	-	1/1/15/20	20/39/115/115	-
16	CLA	U	211	11	1/1/12/20	4/24/100/115	-
16	CLA	H	302	13	1/1/14/20	3/33/109/115	-
16	CLA	B	832	2	1/1/15/20	2/39/115/115	-
20	DD6	J	102	-	-	5/26/80/80	0/3/3/3
20	DD6	G	311	-	-	7/26/80/80	0/3/3/3
20	DD6	U	203	-	-	10/26/80/80	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	CLA	A	853	1	1/1/15/20	10/39/115/115	-
16	CLA	K	207	-	1/1/11/20	4/17/93/115	-
16	CLA	A	814	28	-	3/15/91/115	-
16	CLA	G	305	12	1/1/14/20	13/35/111/115	-
17	PQN	A	837	-	-	3/23/43/43	0/2/2/2
16	CLA	B	826	2	-	0/21/97/115	-
16	CLA	B	805	2	1/1/15/20	6/39/115/115	-
16	CLA	K	204	14	1/1/11/20	5/15/91/115	-
16	CLA	H	309	13	1/1/11/20	4/15/91/115	-
19	BCR	L	201	-	-	10/29/63/63	0/2/2/2
16	CLA	B	816	2	1/1/14/20	0/33/109/115	-
16	CLA	A	832	1	1/1/12/20	1/23/99/115	-
16	CLA	U	208	11	1/1/11/20	4/17/93/115	-
20	DD6	A	846	-	-	9/26/80/80	0/3/3/3
16	CLA	B	819	2	-	2/25/101/115	-
16	CLA	B	813	2	-	3/32/108/115	-
16	CLA	B	822	2	1/1/15/20	0/39/115/115	-
16	CLA	A	851	1	-	3/39/115/115	-
19	BCR	B	840	-	-	5/29/63/63	0/2/2/2
16	CLA	B	801	28	1/1/15/20	2/39/115/115	-
16	CLA	B	829	28	1/1/15/20	1/39/115/115	-
16	CLA	A	833	1	1/1/15/20	0/39/115/115	-
22	CL0	A	850	1	2/2/20/25	6/37/135/135	-
16	CLA	A	820	1	1/1/12/20	3/23/99/115	-
16	CLA	G	315	12	1/1/11/20	3/15/91/115	-
16	CLA	H	305	13	1/1/11/20	2/15/91/115	-
16	CLA	A	835	1	1/1/15/20	1/39/115/115	-
16	CLA	A	813	1	-	1/21/97/115	-
16	CLA	H	304	13	1/1/10/20	1/14/90/115	-
19	BCR	B	839	-	-	9/29/63/63	0/2/2/2
27	KC1	U	213	11	-	1/15/71/71	-
16	CLA	B	808	2	1/1/15/20	5/39/115/115	-
16	CLA	U	206	11	1/1/11/20	2/15/91/115	-
20	DD6	U	214	-	-	3/14/37/80	0/1/1/3
16	CLA	A	802	1	1/1/13/20	3/27/103/115	-
16	CLA	U	209	-	1/1/10/20	0/12/88/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	CLA	K	205	14	1/1/13/20	3/31/107/115	-
16	CLA	B	820	28	1/1/14/20	5/37/113/115	-
16	CLA	F	802	28	1/1/15/20	1/39/115/115	-
18	LHG	A	839	-	-	18/52/52/53	-
16	CLA	B	802	2	1/1/15/20	1/39/115/115	-
16	CLA	A	824	1	1/1/14/20	3/36/112/115	-
17	PQN	B	837	-	-	1/23/43/43	0/2/2/2
16	CLA	B	848	2	1/1/15/20	4/39/115/115	-
16	CLA	A	826	1	-	2/39/115/115	-
20	DD6	U	212	-	-	14/26/80/80	0/3/3/3
16	CLA	A	827	1	-	3/21/97/115	-
16	CLA	G	306	12	1/1/15/20	9/39/115/115	-
16	CLA	A	847	1	-	4/33/109/115	-
20	DD6	G	312	-	-	5/19/50/80	0/2/2/3
19	BCR	A	842	-	-	10/29/63/63	0/2/2/2
16	CLA	A	819	1	-	0/13/89/115	-
16	CLA	B	821	28	1/1/13/20	3/27/103/115	-
16	CLA	J	104	8	1/1/10/20	3/12/88/115	-
16	CLA	L	202	9	-	6/20/96/115	-
16	CLA	A	805	1	1/1/11/20	2/20/96/115	-
16	CLA	B	817	28	-	5/39/115/115	-
16	CLA	U	204	28	1/1/14/20	10/35/111/115	-
16	CLA	A	801	-	-	1/39/115/115	-
16	CLA	B	849	2	1/1/15/20	5/39/115/115	-
16	CLA	A	809	1	-	0/36/112/115	-
16	CLA	B	834	28	-	4/39/115/115	-
20	DD6	G	317	-	-	12/26/80/80	0/3/3/3
16	CLA	B	835	2	-	7/39/115/115	-
16	CLA	A	829	1	1/1/15/20	2/39/115/115	-
23	SF4	A	852	2,1	-	-	0/6/5/5
19	BCR	I	101	-	-	5/29/63/63	0/2/2/2
16	CLA	B	809	2	1/1/15/20	4/39/115/115	-
16	CLA	A	834	1	1/1/15/20	6/39/115/115	-
19	BCR	J	105	-	-	8/29/63/63	0/2/2/2
16	CLA	I	102	-	1/1/15/20	4/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	CLA	H	307	-	1/1/13/20	6/31/107/115	-
16	CLA	A	811	1	1/1/15/20	3/39/115/115	-
21	LMU	A	855	-	-	8/21/61/61	0/2/2/2
16	CLA	B	828	2	-	5/31/107/115	-
16	CLA	A	836	28	1/1/15/20	4/39/115/115	-
20	DD6	G	314	-	-	11/26/80/80	0/3/3/3
26	A86	U	202	-	-	15/34/90/90	0/3/3/3
16	CLA	B	811	2	-	6/27/103/115	-
16	CLA	A	822	28	1/1/15/20	2/39/115/115	-
16	CLA	L	203	9	-	0/39/115/115	-
16	CLA	B	836	-	1/1/13/20	4/30/106/115	-
24	DGD	B	843	-	-	27/49/89/95	0/2/2/2
19	BCR	A	843	-	-	4/29/63/63	0/2/2/2
16	CLA	F	803	-	1/1/11/20	3/19/95/115	-
19	BCR	B	842	-	-	7/29/63/63	0/2/2/2
16	CLA	A	830	1	-	0/21/97/115	-
16	CLA	A	804	1	1/1/15/20	9/39/115/115	-
16	CLA	G	308	-	-	2/27/103/115	-
16	CLA	U	205	11	-	3/39/115/115	-
16	CLA	B	830	28	1/1/11/20	0/15/91/115	-
25	LMG	U	201	-	-	14/27/47/70	0/1/1/1
16	CLA	A	816	1	1/1/15/20	0/39/115/115	-
16	CLA	B	825	2	-	3/39/115/115	-
23	SF4	C	101	3	-	-	0/6/5/5
16	CLA	A	845	28	1/1/15/20	6/39/115/115	-
16	CLA	B	804	2	1/1/11/20	4/15/91/115	-
16	CLA	B	823	2	1/1/15/20	5/39/115/115	-
16	CLA	G	301	12	-	2/15/91/115	-
20	DD6	H	311	-	-	11/26/80/80	0/3/3/3
16	CLA	A	806	1	-	8/39/115/115	-
16	CLA	G	310	12	1/1/11/20	7/15/91/115	-
16	CLA	K	203	14	1/1/13/20	2/27/103/115	-
16	CLA	U	210	11	-	3/39/115/115	-
25	LMG	J	103	-	-	23/34/54/70	0/1/1/1
21	LMU	A	848	-	-	10/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	LMU	J	101	-	-	9/21/61/61	0/2/2/2
16	CLA	B	810	2	-	0/25/101/115	-
19	BCR	A	844	-	-	9/29/63/63	0/2/2/2
16	CLA	B	847	2	1/1/12/20	7/24/100/115	-
19	BCR	A	841	-	-	7/29/63/63	0/2/2/2
16	CLA	A	849	1	-	7/39/115/115	-
19	BCR	F	805	-	-	11/29/63/63	0/2/2/2
16	CLA	A	838	18	1/1/12/20	3/24/100/115	-
18	LHG	A	840	16	-	5/31/31/53	-
16	CLA	A	815	1	1/1/15/20	4/39/115/115	-
16	CLA	H	301	-	1/1/9/20	1/10/82/115	-
16	CLA	G	302	-	1/1/10/20	1/10/86/115	-
19	BCR	B	841	-	-	6/29/63/63	0/2/2/2
16	CLA	H	303	13	1/1/14/20	4/35/111/115	-
16	CLA	B	831	2	1/1/13/20	1/31/107/115	-
16	CLA	B	818	2	-	1/17/93/115	-
16	CLA	k	201	15	1/1/10/20	0/12/88/115	-
16	CLA	k	202	28	1/1/13/20	3/27/103/115	-
16	CLA	L	204	28	1/1/12/20	5/21/97/115	-
19	BCR	L	205	-	-	8/29/63/63	0/2/2/2
16	CLA	A	828	1	1/1/15/20	3/39/115/115	-
21	LMU	K	201	-	-	12/21/61/61	0/2/2/2
16	CLA	B	806	2	1/1/15/20	5/39/115/115	-
19	BCR	F	801	-	-	8/29/63/63	0/2/2/2
16	CLA	H	306	13	-	6/39/115/115	-
16	CLA	B	845	2	1/1/15/20	3/39/115/115	-
16	CLA	G	307	12	-	5/33/109/115	-
18	LHG	G	316	-	-	22/31/31/53	-

All (1046) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	U	214	DD6	C28-C27	-8.27	1.45	1.50
26	U	202	A86	C13-C11	-6.26	1.37	1.49
16	K	204	CLA	MG-NA	5.17	2.18	2.06
16	B	848	CLA	MG-NA	5.05	2.18	2.06
16	A	826	CLA	MG-NA	5.04	2.18	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	H	305	CLA	MG-NA	5.03	2.18	2.06
20	U	214	DD6	C26-C27	4.94	1.47	1.37
16	G	306	CLA	MG-NA	4.88	2.17	2.06
16	B	831	CLA	MG-NA	4.82	2.17	2.06
16	B	825	CLA	MG-NA	4.80	2.17	2.06
16	A	823	CLA	MG-NA	4.73	2.17	2.06
16	A	823	CLA	C4C-C3C	-4.72	1.37	1.45
16	B	822	CLA	MG-NA	4.71	2.17	2.06
16	A	834	CLA	MG-NA	4.68	2.17	2.06
16	B	823	CLA	MG-NA	4.61	2.17	2.06
16	U	205	CLA	C4C-C3C	-4.61	1.37	1.45
16	B	802	CLA	C4C-C3C	-4.60	1.37	1.45
16	U	211	CLA	MG-NA	4.60	2.17	2.06
16	B	847	CLA	C4C-C3C	-4.57	1.37	1.45
16	B	822	CLA	C4C-C3C	-4.57	1.37	1.45
16	A	815	CLA	C4C-C3C	-4.56	1.37	1.45
16	B	810	CLA	MG-NA	4.56	2.17	2.06
16	G	307	CLA	C4C-C3C	-4.55	1.37	1.45
16	G	301	CLA	C4C-C3C	-4.55	1.37	1.45
16	A	832	CLA	C4C-C3C	-4.54	1.37	1.45
16	A	825	CLA	MG-NA	4.54	2.17	2.06
16	G	304	CLA	C4C-C3C	-4.54	1.37	1.45
16	B	816	CLA	C4C-C3C	-4.53	1.37	1.45
16	U	206	CLA	C4C-C3C	-4.53	1.37	1.45
16	B	804	CLA	C4C-C3C	-4.52	1.37	1.45
16	G	308	CLA	C4C-C3C	-4.52	1.37	1.45
16	B	808	CLA	C4C-C3C	-4.52	1.37	1.45
16	B	818	CLA	C4C-C3C	-4.52	1.37	1.45
16	A	838	CLA	C4C-C3C	-4.51	1.37	1.45
16	k	202	CLA	C4C-C3C	-4.51	1.37	1.45
16	H	304	CLA	C4C-C3C	-4.51	1.37	1.45
16	B	830	CLA	C4C-C3C	-4.51	1.37	1.45
16	B	849	CLA	C4C-C3C	-4.51	1.37	1.45
16	U	211	CLA	C4C-C3C	-4.51	1.37	1.45
16	A	828	CLA	MG-NA	4.51	2.17	2.06
16	B	807	CLA	C4C-C3C	-4.50	1.37	1.45
16	B	813	CLA	C4C-C3C	-4.50	1.37	1.45
16	B	824	CLA	C4C-C3C	-4.50	1.37	1.45
16	A	847	CLA	MG-NA	4.50	2.17	2.06
16	H	303	CLA	C4C-C3C	-4.49	1.37	1.45
16	B	844	CLA	MG-NA	4.49	2.16	2.06
16	A	809	CLA	C4C-C3C	-4.49	1.37	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	U	207	CLA	C4C-C3C	-4.49	1.37	1.45
16	U	209	CLA	C4C-C3C	-4.49	1.37	1.45
16	B	833	CLA	C4C-C3C	-4.49	1.37	1.45
16	A	825	CLA	C4C-C3C	-4.48	1.37	1.45
16	B	828	CLA	C4C-C3C	-4.48	1.37	1.45
16	B	832	CLA	C4C-C3C	-4.48	1.37	1.45
16	A	824	CLA	C4C-C3C	-4.48	1.37	1.45
16	B	814	CLA	MG-NA	4.48	2.16	2.06
16	A	801	CLA	C4C-C3C	-4.48	1.37	1.45
16	B	814	CLA	C4C-C3C	-4.48	1.37	1.45
16	A	806	CLA	C4C-C3C	-4.48	1.37	1.45
16	A	802	CLA	C4C-C3C	-4.48	1.37	1.45
16	A	822	CLA	C4C-C3C	-4.47	1.37	1.45
16	B	804	CLA	MG-NA	4.47	2.16	2.06
16	A	808	CLA	C4C-C3C	-4.47	1.37	1.45
16	A	847	CLA	C4C-C3C	-4.47	1.37	1.45
16	A	818	CLA	C4C-C3C	-4.47	1.37	1.45
16	G	306	CLA	C4C-C3C	-4.47	1.37	1.45
16	L	203	CLA	C4C-C3C	-4.47	1.37	1.45
16	A	813	CLA	C4C-C3C	-4.46	1.37	1.45
16	A	834	CLA	C4C-C3C	-4.46	1.37	1.45
16	B	812	CLA	C4C-C3C	-4.46	1.37	1.45
16	A	805	CLA	C4C-C3C	-4.46	1.37	1.45
16	H	305	CLA	C4C-C3C	-4.46	1.37	1.45
16	A	827	CLA	MG-NA	4.46	2.16	2.06
16	A	828	CLA	C4C-C3C	-4.46	1.37	1.45
16	A	810	CLA	C4C-C3C	-4.46	1.37	1.45
16	B	806	CLA	C4C-C3C	-4.46	1.37	1.45
16	K	205	CLA	C4C-C3C	-4.46	1.37	1.45
16	B	825	CLA	C4C-C3C	-4.45	1.37	1.45
16	A	804	CLA	C4C-C3C	-4.45	1.37	1.45
16	A	820	CLA	C4C-C3C	-4.45	1.37	1.45
16	H	312	CLA	C4C-C3C	-4.45	1.37	1.45
16	A	814	CLA	C4C-C3C	-4.45	1.37	1.45
16	G	302	CLA	C4C-C3C	-4.45	1.37	1.45
16	B	811	CLA	C4C-C3C	-4.44	1.37	1.45
16	B	801	CLA	C4C-C3C	-4.44	1.37	1.45
16	B	845	CLA	C4C-C3C	-4.44	1.37	1.45
16	J	104	CLA	C4C-C3C	-4.44	1.37	1.45
16	B	834	CLA	C4C-C3C	-4.43	1.37	1.45
16	B	823	CLA	C4C-C3C	-4.43	1.37	1.45
16	B	805	CLA	C4C-C3C	-4.43	1.37	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	L	202	CLA	C4C-C3C	-4.43	1.37	1.45
16	A	827	CLA	C4C-C3C	-4.43	1.37	1.45
16	A	812	CLA	MG-NA	4.43	2.16	2.06
16	A	826	CLA	C4C-C3C	-4.43	1.37	1.45
16	F	804	CLA	C4C-C3C	-4.43	1.37	1.45
16	A	803	CLA	C4C-C3C	-4.43	1.37	1.45
16	H	302	CLA	C4C-C3C	-4.43	1.37	1.45
16	U	204	CLA	C4C-C3C	-4.42	1.37	1.45
16	K	204	CLA	C4C-C3C	-4.42	1.37	1.45
16	B	826	CLA	C4C-C3C	-4.42	1.37	1.45
16	I	102	CLA	C4C-C3C	-4.42	1.37	1.45
16	G	305	CLA	C4C-C3C	-4.42	1.37	1.45
16	H	306	CLA	C4C-C3C	-4.42	1.37	1.45
16	B	831	CLA	C4C-C3C	-4.42	1.37	1.45
16	B	835	CLA	C4C-C3C	-4.42	1.37	1.45
16	U	210	CLA	C4C-C3C	-4.42	1.37	1.45
16	B	821	CLA	C4C-C3C	-4.42	1.37	1.45
16	G	303	CLA	C4C-C3C	-4.42	1.37	1.45
16	B	809	CLA	C4C-C3C	-4.41	1.37	1.45
16	F	802	CLA	C4C-C3C	-4.41	1.37	1.45
16	A	833	CLA	C4C-C3C	-4.41	1.37	1.45
16	A	829	CLA	C4C-C3C	-4.41	1.37	1.45
16	A	851	CLA	C4C-C3C	-4.41	1.37	1.45
16	B	827	CLA	C4C-C3C	-4.41	1.37	1.45
16	U	208	CLA	C4C-C3C	-4.41	1.37	1.45
16	A	831	CLA	C4C-C3C	-4.41	1.37	1.45
16	A	836	CLA	C4C-C3C	-4.41	1.37	1.45
24	B	843	DGD	O2G-C1B	4.40	1.46	1.34
16	B	810	CLA	C4C-C3C	-4.40	1.37	1.45
16	B	827	CLA	MG-NA	4.40	2.16	2.06
16	B	803	CLA	C4C-C3C	-4.40	1.37	1.45
16	A	853	CLA	C4C-C3C	-4.40	1.37	1.45
16	K	206	CLA	C4C-C3C	-4.40	1.37	1.45
16	H	307	CLA	C4C-C3C	-4.40	1.37	1.45
16	A	805	CLA	MG-NA	4.40	2.16	2.06
16	A	854	CLA	C4C-C3C	-4.40	1.37	1.45
16	A	835	CLA	C4C-C3C	-4.39	1.37	1.45
16	A	815	CLA	MG-NA	4.39	2.16	2.06
16	A	817	CLA	C4C-C3C	-4.39	1.37	1.45
16	K	203	CLA	C4C-C3C	-4.39	1.37	1.45
16	H	309	CLA	C4C-C3C	-4.39	1.37	1.45
27	U	213	KC1	C4C-C3C	-4.39	1.37	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	A	807	CLA	C4C-C3C	-4.39	1.37	1.45
16	A	816	CLA	C4C-C3C	-4.39	1.37	1.45
16	G	310	CLA	C4C-C3C	-4.39	1.37	1.45
16	A	821	CLA	MG-NA	4.38	2.16	2.06
16	A	845	CLA	C4C-C3C	-4.38	1.37	1.45
16	L	204	CLA	C4C-C3C	-4.38	1.37	1.45
16	H	308	CLA	C4C-C3C	-4.38	1.37	1.45
16	A	811	CLA	C4C-C3C	-4.37	1.37	1.45
16	B	819	CLA	C4C-C3C	-4.36	1.37	1.45
16	B	829	CLA	C4C-C3C	-4.35	1.37	1.45
16	k	201	CLA	C4C-C3C	-4.35	1.37	1.45
16	A	832	CLA	MG-NA	4.35	2.16	2.06
16	B	845	CLA	MG-NA	4.35	2.16	2.06
16	K	202	CLA	C4C-C3C	-4.35	1.37	1.45
16	K	207	CLA	C4C-C3C	-4.35	1.37	1.45
16	G	309	CLA	C4C-C3C	-4.34	1.37	1.45
16	A	833	CLA	MG-NA	4.33	2.16	2.06
16	A	813	CLA	MG-NA	4.33	2.16	2.06
16	B	836	CLA	C4C-C3C	-4.33	1.37	1.45
16	B	817	CLA	C4C-C3C	-4.32	1.37	1.45
16	A	830	CLA	C4C-C3C	-4.32	1.37	1.45
16	B	815	CLA	C4C-C3C	-4.32	1.37	1.45
16	A	811	CLA	MG-NA	4.28	2.16	2.06
16	B	820	CLA	C4C-C3C	-4.28	1.37	1.45
16	G	303	CLA	MG-NA	4.28	2.16	2.06
16	A	809	CLA	MG-NA	4.28	2.16	2.06
16	B	824	CLA	MG-NA	4.27	2.16	2.06
24	B	843	DGD	O1G-C1A	4.26	1.45	1.33
16	A	821	CLA	C4C-C3C	-4.26	1.37	1.45
16	B	844	CLA	C4C-C3C	-4.26	1.37	1.45
16	A	849	CLA	C4C-C3C	-4.25	1.37	1.45
16	A	812	CLA	C4C-C3C	-4.24	1.37	1.45
16	G	315	CLA	C4C-C3C	-4.24	1.37	1.45
16	B	808	CLA	C1C-C2C	-4.24	1.35	1.44
16	A	819	CLA	C4C-C3C	-4.23	1.37	1.45
16	F	803	CLA	MG-NA	4.23	2.16	2.06
16	B	848	CLA	C4C-C3C	-4.23	1.37	1.45
16	B	836	CLA	MG-NA	4.23	2.16	2.06
16	k	201	CLA	C1C-C2C	-4.22	1.35	1.44
16	B	808	CLA	MG-NA	4.22	2.16	2.06
16	A	849	CLA	C1C-C2C	-4.21	1.36	1.44
16	A	803	CLA	C1C-C2C	-4.21	1.36	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	U	210	CLA	C1C-C2C	-4.21	1.36	1.44
16	B	803	CLA	C1C-C2C	-4.21	1.36	1.44
16	B	809	CLA	C1C-C2C	-4.21	1.36	1.44
16	A	808	CLA	MG-NA	4.21	2.16	2.06
16	F	803	CLA	C4C-C3C	-4.20	1.37	1.45
16	k	202	CLA	MG-NA	4.20	2.16	2.06
16	A	823	CLA	C1C-C2C	-4.20	1.36	1.44
16	A	818	CLA	C1C-C2C	-4.19	1.36	1.44
16	B	806	CLA	MG-NA	4.19	2.16	2.06
16	B	835	CLA	C1C-C2C	-4.18	1.36	1.44
16	A	812	CLA	C1C-C2C	-4.18	1.36	1.44
16	B	822	CLA	C1C-C2C	-4.18	1.36	1.44
16	B	833	CLA	MG-NA	4.18	2.16	2.06
16	A	807	CLA	MG-NA	4.18	2.16	2.06
16	A	829	CLA	C1C-C2C	-4.17	1.36	1.44
16	H	301	CLA	C4C-C3C	-4.17	1.38	1.45
16	F	803	CLA	C1C-C2C	-4.16	1.36	1.44
16	L	204	CLA	MG-NA	4.16	2.16	2.06
16	B	826	CLA	MG-NA	4.16	2.16	2.06
16	A	826	CLA	C1C-C2C	-4.15	1.36	1.44
16	H	301	CLA	C1C-C2C	-4.15	1.36	1.44
16	B	820	CLA	C1C-C2C	-4.14	1.36	1.44
16	B	820	CLA	MG-NA	4.13	2.16	2.06
16	A	829	CLA	MG-NA	4.13	2.16	2.06
16	B	835	CLA	MG-NA	4.12	2.16	2.06
16	H	302	CLA	MG-NA	4.12	2.16	2.06
16	A	817	CLA	MG-NA	4.12	2.16	2.06
16	A	819	CLA	MG-NA	4.12	2.16	2.06
16	H	302	CLA	C1C-C2C	-4.11	1.36	1.44
16	H	309	CLA	C1C-C2C	-4.11	1.36	1.44
16	A	853	CLA	C1C-C2C	-4.10	1.36	1.44
16	A	830	CLA	C1C-C2C	-4.10	1.36	1.44
16	G	301	CLA	C1C-C2C	-4.10	1.36	1.44
16	A	851	CLA	C1C-C2C	-4.10	1.36	1.44
16	A	806	CLA	C1C-C2C	-4.10	1.36	1.44
16	A	825	CLA	C1C-C2C	-4.10	1.36	1.44
16	F	802	CLA	MG-NA	4.09	2.16	2.06
16	A	808	CLA	C1C-C2C	-4.08	1.36	1.44
16	H	309	CLA	MG-NA	4.08	2.16	2.06
16	B	807	CLA	MG-NA	4.08	2.16	2.06
16	B	816	CLA	C1C-C2C	-4.08	1.36	1.44
16	A	832	CLA	C1C-C2C	-4.08	1.36	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	A	828	CLA	C1C-C2C	-4.07	1.36	1.44
16	B	802	CLA	C1C-C2C	-4.07	1.36	1.44
16	G	305	CLA	C1C-C2C	-4.07	1.36	1.44
16	A	809	CLA	C1C-C2C	-4.07	1.36	1.44
16	A	807	CLA	C1C-C2C	-4.07	1.36	1.44
16	K	206	CLA	MG-NA	4.07	2.15	2.06
16	B	826	CLA	C1C-C2C	-4.07	1.36	1.44
16	A	836	CLA	C1C-C2C	-4.07	1.36	1.44
16	B	830	CLA	MG-NA	4.07	2.15	2.06
16	A	811	CLA	C1C-C2C	-4.06	1.36	1.44
16	A	804	CLA	C1C-C2C	-4.06	1.36	1.44
16	B	828	CLA	C1C-C2C	-4.06	1.36	1.44
16	B	815	CLA	C1C-C2C	-4.06	1.36	1.44
16	B	819	CLA	C1C-C2C	-4.06	1.36	1.44
16	B	844	CLA	C1C-C2C	-4.06	1.36	1.44
16	U	211	CLA	C1C-C2C	-4.05	1.36	1.44
16	H	312	CLA	C1C-C2C	-4.05	1.36	1.44
16	B	811	CLA	C1C-C2C	-4.05	1.36	1.44
16	B	832	CLA	C1C-C2C	-4.05	1.36	1.44
16	A	822	CLA	C1C-C2C	-4.05	1.36	1.44
16	A	834	CLA	C1C-C2C	-4.05	1.36	1.44
16	B	801	CLA	MG-NA	4.05	2.15	2.06
16	A	847	CLA	C1C-C2C	-4.05	1.36	1.44
16	A	813	CLA	C1C-C2C	-4.05	1.36	1.44
16	A	827	CLA	C1C-C2C	-4.05	1.36	1.44
16	B	845	CLA	C1C-C2C	-4.04	1.36	1.44
16	U	206	CLA	C1C-C2C	-4.04	1.36	1.44
16	B	834	CLA	MG-NA	4.03	2.15	2.06
16	A	817	CLA	C1C-C2C	-4.03	1.36	1.44
16	K	202	CLA	C1C-C2C	-4.03	1.36	1.44
16	B	849	CLA	C1C-C2C	-4.03	1.36	1.44
16	U	207	CLA	C1C-C2C	-4.03	1.36	1.44
16	A	830	CLA	MG-NA	4.03	2.15	2.06
16	A	819	CLA	C1C-C2C	-4.03	1.36	1.44
16	B	805	CLA	C1C-C2C	-4.03	1.36	1.44
16	B	812	CLA	C1C-C2C	-4.03	1.36	1.44
27	U	213	KC1	C3B-C4B	-4.03	1.39	1.46
16	B	817	CLA	C1C-C2C	-4.03	1.36	1.44
27	U	213	KC1	C1C-C2C	-4.03	1.36	1.44
16	L	202	CLA	C1C-C2C	-4.02	1.36	1.44
16	B	816	CLA	MG-NA	4.02	2.15	2.06
16	B	824	CLA	C1C-C2C	-4.02	1.36	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	L	202	CLA	MG-NA	4.02	2.15	2.06
16	B	827	CLA	C1C-C2C	-4.02	1.36	1.44
16	H	308	CLA	C1C-C2C	-4.02	1.36	1.44
16	A	820	CLA	C1C-C2C	-4.01	1.36	1.44
16	B	813	CLA	C1C-C2C	-4.01	1.36	1.44
16	K	204	CLA	C1C-C2C	-4.01	1.36	1.44
16	B	833	CLA	C1C-C2C	-4.01	1.36	1.44
16	H	304	CLA	C1C-C2C	-4.01	1.36	1.44
16	F	802	CLA	C1C-C2C	-4.01	1.36	1.44
16	K	203	CLA	C1C-C2C	-4.01	1.36	1.44
16	B	821	CLA	C1C-C2C	-4.01	1.36	1.44
16	B	829	CLA	C1C-C2C	-4.01	1.36	1.44
16	A	816	CLA	C1C-C2C	-4.00	1.36	1.44
16	B	806	CLA	C1C-C2C	-4.00	1.36	1.44
16	A	835	CLA	C1C-C2C	-4.00	1.36	1.44
16	L	203	CLA	C1C-C2C	-4.00	1.36	1.44
16	K	206	CLA	C1C-C2C	-4.00	1.36	1.44
16	B	802	CLA	MG-NA	4.00	2.15	2.06
16	G	315	CLA	C1C-C2C	-4.00	1.36	1.44
16	A	831	CLA	C1C-C2C	-3.99	1.36	1.44
16	B	836	CLA	C1C-C2C	-3.99	1.36	1.44
16	A	814	CLA	C1C-C2C	-3.99	1.36	1.44
16	G	310	CLA	C1C-C2C	-3.99	1.36	1.44
16	H	307	CLA	C1C-C2C	-3.99	1.36	1.44
16	A	838	CLA	C1C-C2C	-3.99	1.36	1.44
16	A	814	CLA	MG-NA	3.99	2.15	2.06
16	G	306	CLA	C1C-C2C	-3.99	1.36	1.44
16	A	854	CLA	C1C-C2C	-3.99	1.36	1.44
16	A	810	CLA	MG-NA	3.99	2.15	2.06
16	A	801	CLA	C1C-C2C	-3.98	1.36	1.44
16	B	814	CLA	C1C-C2C	-3.98	1.36	1.44
16	B	823	CLA	C1C-C2C	-3.98	1.36	1.44
16	B	810	CLA	C1C-C2C	-3.98	1.36	1.44
16	A	835	CLA	MG-NA	3.98	2.15	2.06
16	A	833	CLA	C1C-C2C	-3.98	1.36	1.44
16	G	308	CLA	C1C-C2C	-3.98	1.36	1.44
16	B	804	CLA	C1C-C2C	-3.97	1.36	1.44
16	G	309	CLA	C1C-C2C	-3.97	1.36	1.44
16	k	202	CLA	C1C-C2C	-3.97	1.36	1.44
16	B	801	CLA	C1C-C2C	-3.97	1.36	1.44
16	A	824	CLA	MG-NA	3.97	2.15	2.06
16	G	302	CLA	C1C-C2C	-3.96	1.36	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	H	301	CLA	MG-NA	3.96	2.15	2.06
16	L	204	CLA	C1C-C2C	-3.96	1.36	1.44
16	F	804	CLA	MG-NA	3.96	2.15	2.06
16	A	845	CLA	C1C-C2C	-3.96	1.36	1.44
16	A	802	CLA	C1C-C2C	-3.96	1.36	1.44
16	B	834	CLA	C1C-C2C	-3.96	1.36	1.44
16	J	104	CLA	C1C-C2C	-3.96	1.36	1.44
16	A	805	CLA	C1C-C2C	-3.96	1.36	1.44
16	B	825	CLA	C1C-C2C	-3.96	1.36	1.44
16	K	207	CLA	C1C-C2C	-3.96	1.36	1.44
16	A	820	CLA	MG-NA	3.96	2.15	2.06
16	U	204	CLA	C1C-C2C	-3.95	1.36	1.44
16	B	828	CLA	MG-NA	3.95	2.15	2.06
16	A	810	CLA	C1C-C2C	-3.95	1.36	1.44
16	F	804	CLA	C1C-C2C	-3.95	1.36	1.44
16	A	821	CLA	C1C-C2C	-3.95	1.36	1.44
16	B	848	CLA	C1C-C2C	-3.95	1.36	1.44
16	U	205	CLA	MG-NA	3.94	2.15	2.06
16	I	102	CLA	MG-NA	3.94	2.15	2.06
16	A	851	CLA	MG-NA	3.93	2.15	2.06
16	B	809	CLA	MG-NA	3.93	2.15	2.06
16	B	847	CLA	C1C-C2C	-3.93	1.36	1.44
16	B	830	CLA	C1C-C2C	-3.93	1.36	1.44
16	G	303	CLA	C1C-C2C	-3.93	1.36	1.44
16	B	802	CLA	MG-NC	3.92	2.15	2.06
16	A	824	CLA	C1C-C2C	-3.92	1.36	1.44
16	B	807	CLA	C1C-C2C	-3.92	1.36	1.44
16	H	303	CLA	C1C-C2C	-3.92	1.36	1.44
16	U	208	CLA	C1C-C2C	-3.92	1.36	1.44
16	B	812	CLA	MG-NA	3.91	2.15	2.06
16	G	304	CLA	C1C-C2C	-3.91	1.36	1.44
16	B	832	CLA	MG-NA	3.90	2.15	2.06
16	B	818	CLA	C1C-C2C	-3.90	1.36	1.44
16	J	104	CLA	MG-NA	3.90	2.15	2.06
16	G	310	CLA	MG-NA	3.90	2.15	2.06
16	G	309	CLA	MG-NA	3.90	2.15	2.06
16	K	205	CLA	C1C-C2C	-3.90	1.36	1.44
16	H	305	CLA	C1C-C2C	-3.89	1.36	1.44
16	I	102	CLA	C1C-C2C	-3.88	1.36	1.44
16	A	815	CLA	C1C-C2C	-3.88	1.36	1.44
16	B	813	CLA	MG-NA	3.87	2.15	2.06
16	B	831	CLA	C1C-C2C	-3.87	1.36	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	H	306	CLA	MG-NA	3.87	2.15	2.06
16	U	209	CLA	C1C-C2C	-3.87	1.36	1.44
16	k	201	CLA	MG-NA	3.86	2.15	2.06
16	G	304	CLA	MG-NA	3.86	2.15	2.06
16	B	818	CLA	MG-NA	3.86	2.15	2.06
16	U	205	CLA	C1C-C2C	-3.85	1.36	1.44
16	A	849	CLA	MG-NA	3.84	2.15	2.06
16	G	307	CLA	C1C-C2C	-3.84	1.36	1.44
16	B	803	CLA	MG-NA	3.83	2.15	2.06
16	B	815	CLA	MG-NA	3.82	2.15	2.06
16	A	854	CLA	MG-NA	3.81	2.15	2.06
16	A	816	CLA	MG-NA	3.80	2.15	2.06
16	B	817	CLA	MG-NA	3.79	2.15	2.06
16	K	207	CLA	MG-NA	3.78	2.15	2.06
16	U	206	CLA	MG-NA	3.77	2.15	2.06
27	U	213	KC1	MG-NA	3.77	2.15	2.06
16	A	845	CLA	MG-NA	3.77	2.15	2.06
16	A	804	CLA	MG-NA	3.77	2.15	2.06
16	G	302	CLA	MG-NA	3.76	2.15	2.06
16	A	834	CLA	MG-NC	3.75	2.15	2.06
16	H	306	CLA	C1C-C2C	-3.75	1.36	1.44
16	G	308	CLA	MG-NA	3.74	2.15	2.06
16	B	829	CLA	MG-NA	3.74	2.15	2.06
16	U	204	CLA	MG-NA	3.73	2.15	2.06
16	B	811	CLA	MG-NA	3.70	2.15	2.06
16	H	303	CLA	MG-NA	3.68	2.15	2.06
16	A	838	CLA	MG-NA	3.66	2.15	2.06
21	F	806	LMU	O5'-C1'	3.62	1.51	1.41
16	K	203	CLA	MG-NA	3.62	2.14	2.06
16	U	208	CLA	MG-NA	3.61	2.14	2.06
19	A	844	BCR	C1-C6	-3.59	1.49	1.53
16	A	801	CLA	MG-NA	3.59	2.14	2.06
16	A	831	CLA	MG-NA	3.59	2.14	2.06
16	H	307	CLA	MG-NA	3.58	2.14	2.06
16	G	301	CLA	MG-NA	3.58	2.14	2.06
19	A	843	BCR	C1-C6	-3.57	1.49	1.53
16	A	836	CLA	MG-NA	3.57	2.14	2.06
16	B	847	CLA	MG-NA	3.57	2.14	2.06
16	A	802	CLA	MG-NA	3.55	2.14	2.06
16	A	853	CLA	MG-NA	3.55	2.14	2.06
20	H	310	DD6	C26-C27	3.54	1.44	1.37
16	A	806	CLA	MG-NA	3.53	2.14	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	B	849	CLA	MG-NA	3.51	2.14	2.06
16	K	204	CLA	MG-NC	3.51	2.14	2.06
16	K	202	CLA	MG-NA	3.49	2.14	2.06
16	B	805	CLA	MG-NA	3.49	2.14	2.06
16	G	315	CLA	MG-NA	3.49	2.14	2.06
27	U	213	KC1	C4A-C3A	-3.48	1.37	1.44
16	U	209	CLA	MG-NA	3.47	2.14	2.06
16	H	305	CLA	MG-NC	3.47	2.14	2.06
19	B	838	BCR	C1-C6	-3.44	1.49	1.53
20	U	214	DD6	C8-C6	-3.43	1.41	1.50
16	H	304	CLA	MG-NA	3.42	2.14	2.06
16	B	819	CLA	MG-NA	3.42	2.14	2.06
20	G	312	DD6	C24-C1	-3.41	1.41	1.50
19	k	203	BCR	C1-C6	-3.38	1.49	1.53
16	U	210	CLA	MG-NA	3.38	2.14	2.06
19	A	842	BCR	C1-C6	-3.37	1.49	1.53
20	G	313	DD6	C28-C27	-3.36	1.48	1.50
20	A	846	DD6	C26-C27	3.35	1.44	1.37
16	A	847	CLA	MG-NC	3.35	2.14	2.06
21	K	201	LMU	O5'-C1'	3.35	1.50	1.41
16	A	818	CLA	MG-NA	3.34	2.14	2.06
27	U	213	KC1	C1B-C2B	-3.34	1.38	1.45
16	B	826	CLA	MG-NC	3.33	2.14	2.06
20	G	313	DD6	C26-C27	3.33	1.44	1.37
16	A	827	CLA	MG-NC	3.32	2.14	2.06
20	U	203	DD6	C26-C27	3.31	1.43	1.37
16	K	205	CLA	MG-NA	3.29	2.14	2.06
16	L	203	CLA	MG-NA	3.28	2.14	2.06
16	B	821	CLA	MG-NA	3.26	2.14	2.06
19	L	201	BCR	C1-C6	-3.25	1.49	1.53
19	B	846	BCR	C1-C6	-3.24	1.49	1.53
20	H	311	DD6	C26-C27	3.23	1.43	1.37
19	J	105	BCR	C30-C25	-3.23	1.49	1.53
19	L	205	BCR	C30-C25	-3.21	1.49	1.53
21	F	806	LMU	O5B-C1B	3.20	1.50	1.41
19	B	839	BCR	C1-C6	-3.20	1.49	1.53
20	K	208	DD6	C26-C27	3.19	1.43	1.37
16	B	814	CLA	MG-NC	3.19	2.13	2.06
16	B	831	CLA	MG-NC	3.19	2.13	2.06
16	A	803	CLA	MG-NA	3.19	2.13	2.06
16	B	810	CLA	MG-NC	3.19	2.13	2.06
16	G	306	CLA	MG-NC	3.18	2.13	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	F	801	BCR	C1-C6	-3.18	1.49	1.53
21	K	201	LMU	O5B-C1B	3.17	1.50	1.41
16	H	308	CLA	MG-NA	3.17	2.13	2.06
19	B	842	BCR	C30-C25	-3.17	1.49	1.53
16	A	828	CLA	MG-NC	3.15	2.13	2.06
19	L	201	BCR	C30-C25	-3.13	1.49	1.53
20	J	102	DD6	C26-C27	3.12	1.43	1.37
16	U	207	CLA	MG-NA	3.11	2.13	2.06
19	I	103	BCR	C1-C6	-3.11	1.49	1.53
16	B	823	CLA	MG-NC	3.08	2.13	2.06
16	G	310	CLA	MG-NC	3.07	2.13	2.06
16	A	822	CLA	MG-NA	3.06	2.13	2.06
16	A	826	CLA	MG-NC	3.06	2.13	2.06
19	B	841	BCR	C1-C6	-3.05	1.49	1.53
16	G	307	CLA	MG-NA	3.05	2.13	2.06
19	M	101	BCR	C30-C25	-3.04	1.49	1.53
20	U	212	DD6	C26-C27	3.04	1.43	1.37
16	B	825	CLA	MG-NC	3.03	2.13	2.06
19	I	103	BCR	C30-C25	-3.03	1.49	1.53
19	F	805	BCR	C1-C6	-3.03	1.49	1.53
16	A	805	CLA	MG-NC	3.00	2.13	2.06
16	B	844	CLA	MG-NC	2.99	2.13	2.06
16	A	851	CLA	MG-NC	2.97	2.13	2.06
19	M	101	BCR	C1-C6	-2.96	1.50	1.53
19	I	101	BCR	C1-C6	-2.96	1.50	1.53
16	H	306	CLA	MG-NC	2.96	2.13	2.06
16	B	845	CLA	MG-NC	2.95	2.13	2.06
19	A	842	BCR	C30-C25	-2.95	1.50	1.53
20	G	314	DD6	C26-C27	2.95	1.43	1.37
19	B	840	BCR	C1-C6	-2.94	1.50	1.53
19	B	842	BCR	C1-C6	-2.93	1.50	1.53
16	B	835	CLA	MG-NC	2.91	2.13	2.06
16	G	305	CLA	MG-NA	2.89	2.13	2.06
22	A	850	CL0	C3B-C4B	-2.88	1.38	1.41
20	G	311	DD6	C26-C27	2.86	1.43	1.37
16	B	848	CLA	MG-NC	2.86	2.13	2.06
19	B	846	BCR	C30-C25	-2.85	1.50	1.53
16	B	817	CLA	C1B-C2B	-2.83	1.36	1.43
16	B	833	CLA	MG-NC	2.82	2.13	2.06
16	A	808	CLA	MG-NC	2.81	2.12	2.06
19	A	841	BCR	C1-C6	-2.80	1.50	1.53
16	A	819	CLA	MG-NC	2.79	2.12	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	A	825	CLA	MG-NC	2.79	2.12	2.06
16	A	820	CLA	MG-NC	2.77	2.12	2.06
20	A	846	DD6	C24-C1	-2.77	1.40	1.46
19	k	203	BCR	C30-C25	-2.75	1.50	1.53
16	B	807	CLA	MG-NC	2.75	2.12	2.06
19	B	841	BCR	C30-C25	-2.74	1.50	1.53
16	A	809	CLA	MG-NC	2.73	2.12	2.06
27	U	213	KC1	C2A-C3A	2.71	1.42	1.37
16	A	821	CLA	MG-NC	2.70	2.12	2.06
16	k	202	CLA	C1D-C2D	-2.69	1.40	1.45
16	A	833	CLA	MG-NC	2.69	2.12	2.06
16	A	811	CLA	MG-NC	2.68	2.12	2.06
19	B	838	BCR	C30-C25	-2.68	1.50	1.53
16	B	813	CLA	MG-NC	2.68	2.12	2.06
20	G	317	DD6	C26-C27	2.68	1.42	1.37
16	A	830	CLA	MG-NC	2.68	2.12	2.06
16	B	804	CLA	MG-NC	2.67	2.12	2.06
16	B	801	CLA	MG-NC	2.67	2.12	2.06
19	J	105	BCR	C1-C6	-2.67	1.50	1.53
16	B	827	CLA	MG-NC	2.67	2.12	2.06
16	G	305	CLA	C1D-C2D	-2.66	1.40	1.45
20	J	102	DD6	C28-C27	-2.66	1.49	1.50
16	B	806	CLA	MG-NC	2.66	2.12	2.06
16	A	835	CLA	MG-NC	2.66	2.12	2.06
16	B	836	CLA	MG-NC	2.66	2.12	2.06
16	U	211	CLA	MG-NC	2.66	2.12	2.06
16	K	206	CLA	MG-NC	2.66	2.12	2.06
19	F	801	BCR	C30-C25	-2.66	1.50	1.53
16	B	845	CLA	C3D-C4D	-2.65	1.38	1.44
16	G	302	CLA	C1D-C2D	-2.65	1.40	1.45
16	A	829	CLA	MG-NC	2.64	2.12	2.06
27	U	213	KC1	MG-NC	2.64	2.12	2.06
16	G	315	CLA	C3D-C4D	-2.64	1.38	1.44
16	B	828	CLA	MG-NC	2.63	2.12	2.06
19	B	840	BCR	C30-C25	-2.62	1.50	1.53
27	U	213	KC1	C1A-CHA	2.62	1.47	1.40
22	A	850	CL0	CHB-C1B	2.62	1.43	1.39
16	B	832	CLA	MG-NC	2.62	2.12	2.06
19	F	805	BCR	C30-C25	-2.62	1.50	1.53
22	A	850	CL0	MG-ND	-2.61	2.00	2.05
16	k	202	CLA	MG-NC	2.61	2.12	2.06
22	A	850	CL0	MG-NB	-2.60	2.00	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	L	202	CLA	MG-NC	2.59	2.12	2.06
16	A	820	CLA	C3D-C4D	-2.59	1.38	1.44
16	B	808	CLA	MG-NC	2.58	2.12	2.06
20	G	314	DD6	C8-C6	-2.58	1.40	1.46
16	A	812	CLA	MG-NC	2.58	2.12	2.06
16	k	201	CLA	C3D-C4D	-2.58	1.38	1.44
16	G	305	CLA	C3D-C4D	-2.57	1.38	1.44
16	B	849	CLA	C3D-C4D	-2.57	1.38	1.44
16	H	312	CLA	C3D-C4D	-2.57	1.38	1.44
20	H	310	DD6	C2-C1	2.56	1.41	1.35
16	A	823	CLA	C1D-C2D	-2.55	1.40	1.45
16	B	825	CLA	C3D-C4D	-2.55	1.38	1.44
19	L	205	BCR	C1-C6	-2.55	1.50	1.53
20	G	314	DD6	C13-C11	-2.55	1.40	1.46
16	B	817	CLA	C3D-C4D	-2.55	1.38	1.44
16	B	830	CLA	C1B-C2B	-2.54	1.37	1.43
19	B	839	BCR	C30-C25	-2.54	1.50	1.53
16	B	819	CLA	C3D-C4D	-2.54	1.38	1.44
20	U	212	DD6	C10-C11	2.54	1.41	1.35
26	U	202	A86	C5-C6	2.53	1.41	1.35
16	F	803	CLA	MG-NC	2.53	2.12	2.06
19	A	843	BCR	C30-C25	-2.53	1.50	1.53
16	A	827	CLA	C3D-C4D	-2.52	1.38	1.44
16	A	803	CLA	C3D-C4D	-2.52	1.38	1.44
20	A	846	DD6	C8-C6	-2.51	1.40	1.46
16	K	203	CLA	C3D-C4D	-2.50	1.38	1.44
16	L	204	CLA	MG-NC	2.50	2.12	2.06
19	A	844	BCR	C30-C25	-2.50	1.50	1.53
16	B	821	CLA	C3D-C4D	-2.50	1.38	1.44
16	U	208	CLA	C3D-C4D	-2.50	1.38	1.44
16	B	802	CLA	C1D-C2D	-2.50	1.40	1.45
16	A	851	CLA	C3D-C4D	-2.49	1.38	1.44
16	B	808	CLA	C1D-C2D	-2.49	1.40	1.45
20	H	310	DD6	C5-C6	2.49	1.41	1.35
20	G	311	DD6	C24-C1	-2.49	1.40	1.46
16	B	824	CLA	MG-NC	2.48	2.12	2.06
16	B	831	CLA	C3D-C4D	-2.48	1.38	1.44
16	H	308	CLA	C3D-C4D	-2.48	1.38	1.44
20	G	314	DD6	C24-C1	-2.48	1.40	1.46
16	A	835	CLA	C3D-C4D	-2.48	1.38	1.44
20	A	846	DD6	C13-C11	-2.48	1.40	1.46
16	U	204	CLA	C3D-C4D	-2.48	1.38	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	B	805	CLA	C3D-C4D	-2.48	1.38	1.44
16	U	207	CLA	C3D-C4D	-2.48	1.38	1.44
16	A	804	CLA	C3D-C4D	-2.47	1.38	1.44
16	G	302	CLA	MG-NC	2.47	2.12	2.06
20	G	317	DD6	C24-C1	-2.46	1.40	1.46
22	A	850	CL0	C3D-C4D	-2.46	1.37	1.41
16	A	807	CLA	MG-NC	2.46	2.12	2.06
16	A	853	CLA	C3D-C4D	-2.46	1.38	1.44
16	A	845	CLA	MG-NC	2.46	2.12	2.06
16	A	822	CLA	C3D-C4D	-2.46	1.38	1.44
16	A	815	CLA	C1B-C2B	-2.45	1.37	1.43
16	B	824	CLA	C3D-C4D	-2.45	1.38	1.44
16	B	812	CLA	C3D-C4D	-2.45	1.38	1.44
16	H	305	CLA	C3D-C4D	-2.45	1.38	1.44
16	B	825	CLA	C1D-C2D	-2.45	1.40	1.45
16	A	818	CLA	C1B-C2B	-2.45	1.37	1.43
16	H	306	CLA	C3D-C4D	-2.45	1.38	1.44
16	H	309	CLA	C3D-C4D	-2.45	1.38	1.44
16	B	829	CLA	C3D-C4D	-2.45	1.38	1.44
16	B	847	CLA	C3D-C4D	-2.45	1.38	1.44
16	G	306	CLA	C3D-C4D	-2.45	1.38	1.44
16	A	824	CLA	MG-NC	2.45	2.12	2.06
26	U	202	A86	C2-C1	2.45	1.41	1.35
16	B	815	CLA	C3D-C4D	-2.45	1.38	1.44
16	H	303	CLA	C1B-C2B	-2.44	1.37	1.43
16	L	203	CLA	C3D-C4D	-2.44	1.38	1.44
20	U	203	DD6	C13-C11	-2.44	1.40	1.46
16	A	813	CLA	C3D-C4D	-2.44	1.38	1.44
16	A	801	CLA	C1D-C2D	-2.44	1.40	1.45
16	B	807	CLA	C3D-C4D	-2.44	1.38	1.44
16	A	815	CLA	C3D-C4D	-2.44	1.38	1.44
16	B	835	CLA	C3D-C4D	-2.44	1.38	1.44
16	A	847	CLA	C3D-C4D	-2.44	1.38	1.44
16	H	304	CLA	C3D-C4D	-2.44	1.38	1.44
16	A	806	CLA	C3D-C4D	-2.44	1.38	1.44
16	B	822	CLA	C1D-C2D	-2.44	1.40	1.45
16	A	832	CLA	MG-NC	2.43	2.12	2.06
16	B	818	CLA	C3D-C4D	-2.43	1.38	1.44
16	B	816	CLA	MG-NC	2.43	2.12	2.06
16	U	206	CLA	C3D-C4D	-2.43	1.38	1.44
16	B	806	CLA	C3D-C4D	-2.43	1.38	1.44
16	B	822	CLA	C3D-C4D	-2.43	1.38	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	B	832	CLA	C3D-C4D	-2.43	1.38	1.44
16	A	816	CLA	C3D-C4D	-2.43	1.38	1.44
16	K	202	CLA	C3D-C4D	-2.43	1.38	1.44
16	U	204	CLA	C1D-C2D	-2.43	1.40	1.45
16	U	205	CLA	C3D-C4D	-2.43	1.38	1.44
16	G	307	CLA	C3D-C4D	-2.43	1.38	1.44
16	A	831	CLA	C3D-C4D	-2.42	1.38	1.44
16	L	204	CLA	C3D-C4D	-2.42	1.38	1.44
16	A	812	CLA	C3D-C4D	-2.42	1.38	1.44
16	B	820	CLA	MG-NC	2.42	2.12	2.06
20	G	312	DD6	C13-C11	-2.42	1.40	1.46
16	A	801	CLA	C1B-C2B	-2.42	1.37	1.43
16	A	802	CLA	C3D-C4D	-2.42	1.38	1.44
16	G	303	CLA	MG-NC	2.42	2.12	2.06
16	A	854	CLA	C3D-C4D	-2.42	1.38	1.44
16	A	818	CLA	C1B-NB	-2.42	1.34	1.37
16	A	829	CLA	C3D-C4D	-2.42	1.38	1.44
16	B	814	CLA	C3D-C4D	-2.42	1.38	1.44
16	A	816	CLA	C1B-C2B	-2.42	1.37	1.43
16	H	303	CLA	C3D-C4D	-2.42	1.38	1.44
16	B	826	CLA	C3D-C4D	-2.42	1.38	1.44
16	A	836	CLA	C3D-C4D	-2.41	1.38	1.44
16	B	833	CLA	C3D-C4D	-2.41	1.38	1.44
20	U	214	DD6	C5-C6	2.41	1.41	1.34
16	J	104	CLA	C3D-C4D	-2.41	1.38	1.44
16	B	827	CLA	C3D-C4D	-2.41	1.38	1.44
16	B	834	CLA	C3D-C4D	-2.41	1.38	1.44
16	H	301	CLA	C3D-C4D	-2.41	1.38	1.44
16	U	205	CLA	MG-NC	2.41	2.12	2.06
20	U	212	DD6	C5-C6	2.41	1.41	1.35
16	B	809	CLA	C3D-C4D	-2.41	1.38	1.44
16	A	818	CLA	C3D-C4D	-2.41	1.38	1.44
16	A	827	CLA	C1D-C2D	-2.41	1.40	1.45
16	A	811	CLA	C3D-C4D	-2.41	1.38	1.44
16	B	810	CLA	C3D-C4D	-2.41	1.38	1.44
16	A	830	CLA	C3D-C4D	-2.40	1.38	1.44
16	B	848	CLA	C3D-C4D	-2.40	1.38	1.44
19	I	101	BCR	C30-C25	-2.40	1.50	1.53
16	B	813	CLA	C3D-C4D	-2.40	1.38	1.44
16	G	308	CLA	C3D-C4D	-2.40	1.38	1.44
16	A	819	CLA	C3D-C4D	-2.40	1.38	1.44
16	B	820	CLA	C3D-C4D	-2.40	1.38	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	A	849	CLA	C3D-C4D	-2.40	1.38	1.44
16	A	823	CLA	C3D-C4D	-2.40	1.38	1.44
16	U	210	CLA	C3D-C4D	-2.40	1.38	1.44
16	U	211	CLA	C3D-C4D	-2.39	1.38	1.44
16	B	830	CLA	C3D-C4D	-2.39	1.38	1.44
16	B	812	CLA	MG-NC	2.39	2.11	2.06
16	B	803	CLA	C1D-C2D	-2.39	1.40	1.45
16	A	801	CLA	C3D-C4D	-2.39	1.38	1.44
20	U	214	DD6	C2-C1	2.39	1.41	1.35
16	A	813	CLA	MG-NC	2.39	2.11	2.06
16	A	832	CLA	C3D-C4D	-2.39	1.38	1.44
16	A	815	CLA	MG-NC	2.39	2.11	2.06
20	G	313	DD6	C5-C6	2.38	1.41	1.35
16	B	808	CLA	C3D-C4D	-2.38	1.38	1.44
16	F	802	CLA	C3D-C4D	-2.38	1.38	1.44
16	A	833	CLA	C3D-C4D	-2.38	1.38	1.44
16	B	828	CLA	C3D-C4D	-2.38	1.38	1.44
16	K	206	CLA	C1D-C2D	-2.38	1.40	1.45
20	G	311	DD6	C8-C6	-2.38	1.40	1.46
19	A	841	BCR	C30-C25	-2.38	1.50	1.53
20	K	208	DD6	C10-C11	2.38	1.41	1.35
16	A	813	CLA	C1B-C2B	-2.38	1.37	1.43
16	G	306	CLA	C1D-C2D	-2.38	1.40	1.45
16	B	845	CLA	C1D-C2D	-2.38	1.40	1.45
16	A	828	CLA	C3D-C4D	-2.38	1.38	1.44
16	A	809	CLA	C1D-C2D	-2.38	1.40	1.45
16	A	824	CLA	C3D-C4D	-2.38	1.38	1.44
16	K	205	CLA	CHB-C1B	2.38	1.44	1.39
16	G	302	CLA	C3D-C4D	-2.37	1.38	1.44
16	K	204	CLA	C3D-C4D	-2.37	1.38	1.44
16	A	809	CLA	C3D-C4D	-2.37	1.38	1.44
16	A	838	CLA	C3D-C4D	-2.37	1.38	1.44
16	B	816	CLA	C3D-C4D	-2.37	1.38	1.44
20	G	312	DD6	C2-C1	2.37	1.41	1.34
16	B	815	CLA	MG-NC	2.37	2.11	2.06
16	A	805	CLA	C3D-C4D	-2.37	1.38	1.44
16	H	306	CLA	C1D-C2D	-2.37	1.40	1.45
16	A	818	CLA	C1D-C2D	-2.37	1.40	1.45
16	G	310	CLA	C3D-C4D	-2.37	1.38	1.44
16	U	211	CLA	C1B-C2B	-2.37	1.37	1.43
16	B	811	CLA	C3D-C4D	-2.37	1.38	1.44
20	K	208	DD6	C5-C6	2.36	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	F	802	CLA	MG-NC	2.36	2.11	2.06
16	G	301	CLA	C3D-C4D	-2.36	1.38	1.44
20	G	313	DD6	C10-C11	2.36	1.41	1.35
16	A	826	CLA	C3D-C4D	-2.36	1.38	1.44
16	A	849	CLA	MG-NC	2.36	2.11	2.06
20	U	203	DD6	C5-C6	2.36	1.41	1.35
16	K	202	CLA	MG-NC	2.36	2.11	2.06
20	U	203	DD6	C2-C1	2.36	1.41	1.35
21	A	855	LMU	O1'-C1'	2.35	1.44	1.40
16	H	307	CLA	C3D-C4D	-2.35	1.38	1.44
20	K	208	DD6	C2-C1	2.35	1.41	1.35
16	A	825	CLA	C3D-C4D	-2.35	1.38	1.44
16	G	304	CLA	C3D-C4D	-2.35	1.38	1.44
16	F	804	CLA	C3D-C4D	-2.35	1.38	1.44
16	H	312	CLA	C1D-C2D	-2.35	1.40	1.45
16	B	823	CLA	C3D-C4D	-2.35	1.38	1.44
16	G	309	CLA	C3D-C4D	-2.35	1.38	1.44
16	A	808	CLA	C3D-C4D	-2.35	1.38	1.44
16	L	202	CLA	C3D-C4D	-2.34	1.38	1.44
16	B	848	CLA	MG-NB	2.34	2.10	2.05
16	A	816	CLA	MG-NC	2.34	2.11	2.06
16	A	823	CLA	MG-NC	2.34	2.11	2.06
16	B	822	CLA	MG-NC	2.34	2.11	2.06
16	B	848	CLA	C1B-C2B	-2.34	1.37	1.43
16	K	205	CLA	C3D-C4D	-2.34	1.38	1.44
16	k	202	CLA	C3D-C4D	-2.34	1.38	1.44
20	G	311	DD6	C13-C11	-2.34	1.41	1.46
16	A	810	CLA	MG-NC	2.34	2.11	2.06
16	B	828	CLA	C1D-C2D	-2.34	1.40	1.45
20	H	311	DD6	C5-C6	2.33	1.41	1.35
16	B	809	CLA	MG-NC	2.33	2.11	2.06
16	B	806	CLA	C1D-C2D	-2.33	1.40	1.45
16	K	207	CLA	C3D-C4D	-2.33	1.39	1.44
16	H	301	CLA	MG-NC	2.33	2.11	2.06
16	B	831	CLA	C1D-C2D	-2.32	1.40	1.45
16	I	102	CLA	C3D-C4D	-2.32	1.39	1.44
16	K	207	CLA	MG-NC	2.32	2.11	2.06
16	A	831	CLA	C1B-C2B	-2.32	1.37	1.43
16	A	807	CLA	C3D-C4D	-2.32	1.39	1.44
16	A	810	CLA	C3D-C4D	-2.32	1.39	1.44
20	G	312	DD6	C8-C6	-2.32	1.41	1.46
16	A	814	CLA	C3D-C4D	-2.32	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	A	820	CLA	C1D-C2D	-2.32	1.40	1.45
16	G	304	CLA	C1B-C2B	-2.32	1.37	1.43
20	U	212	DD6	C2-C1	2.32	1.41	1.35
20	G	317	DD6	C10-C11	2.31	1.41	1.35
16	H	305	CLA	C1D-C2D	-2.31	1.40	1.45
20	G	312	DD6	C5-C6	2.31	1.41	1.35
20	H	310	DD6	C8-C6	-2.31	1.41	1.46
16	K	206	CLA	C1B-C2B	-2.31	1.37	1.43
16	B	844	CLA	C3D-C4D	-2.31	1.39	1.44
16	A	834	CLA	C3D-C4D	-2.31	1.39	1.44
16	G	305	CLA	C1B-C2B	-2.31	1.37	1.43
16	B	802	CLA	C3D-C4D	-2.31	1.39	1.44
16	F	803	CLA	C3D-C4D	-2.30	1.39	1.44
16	B	804	CLA	C3D-C4D	-2.30	1.39	1.44
16	A	802	CLA	MG-NC	2.30	2.11	2.06
16	A	814	CLA	C1B-C2B	-2.30	1.37	1.43
20	G	313	DD6	C2-C1	2.30	1.41	1.35
16	B	823	CLA	C1D-C2D	-2.29	1.40	1.45
20	G	317	DD6	C8-C6	-2.29	1.41	1.46
20	G	317	DD6	C2-C1	2.29	1.41	1.35
20	G	317	DD6	C5-C6	2.29	1.41	1.35
16	A	826	CLA	C1D-C2D	-2.29	1.40	1.45
20	J	102	DD6	C10-C11	2.29	1.41	1.35
16	B	848	CLA	C1D-C2D	-2.29	1.40	1.45
16	U	208	CLA	C1B-C2B	-2.29	1.37	1.43
16	B	807	CLA	C1D-C2D	-2.29	1.40	1.45
20	H	310	DD6	C13-C11	-2.29	1.41	1.46
16	A	838	CLA	MG-NC	2.28	2.11	2.06
16	A	835	CLA	C1B-C2B	-2.28	1.37	1.43
16	B	834	CLA	MG-NC	2.28	2.11	2.06
16	B	829	CLA	MG-NC	2.28	2.11	2.06
16	H	302	CLA	MG-NC	2.28	2.11	2.06
16	A	815	CLA	C1D-C2D	-2.28	1.40	1.45
16	B	819	CLA	C1D-C2D	-2.28	1.40	1.45
16	I	102	CLA	MG-NC	2.28	2.11	2.06
16	A	836	CLA	C1D-C2D	-2.28	1.40	1.45
16	G	303	CLA	C3D-C4D	-2.27	1.39	1.44
16	A	854	CLA	MG-NC	2.27	2.11	2.06
16	A	817	CLA	C3D-C4D	-2.27	1.39	1.44
16	J	104	CLA	MG-NC	2.27	2.11	2.06
20	J	102	DD6	C2-C1	2.27	1.41	1.35
16	B	818	CLA	C1B-C2B	-2.27	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	U	203	DD6	C10-C11	2.27	1.41	1.35
16	B	836	CLA	C3D-C4D	-2.27	1.39	1.44
20	G	317	DD6	C13-C11	-2.27	1.41	1.46
16	A	821	CLA	C3D-C4D	-2.27	1.39	1.44
16	B	811	CLA	C1D-C2D	-2.27	1.40	1.45
16	F	804	CLA	C1B-C2B	-2.27	1.37	1.43
16	H	309	CLA	MG-NC	2.27	2.11	2.06
16	B	822	CLA	C1B-C2B	-2.26	1.37	1.43
16	G	301	CLA	C1B-C2B	-2.26	1.37	1.43
16	U	209	CLA	C3D-C4D	-2.26	1.39	1.44
20	G	313	DD6	C8-C6	-2.26	1.41	1.46
16	B	810	CLA	CAB-C3B	-2.26	1.46	1.50
20	J	102	DD6	C5-C6	2.26	1.41	1.35
20	J	102	DD6	C24-C1	-2.26	1.41	1.46
16	B	817	CLA	C1D-C2D	-2.26	1.40	1.45
16	H	302	CLA	C3D-C4D	-2.26	1.39	1.44
16	B	831	CLA	C1B-C2B	-2.26	1.37	1.43
16	B	820	CLA	C1D-C2D	-2.26	1.40	1.45
16	A	817	CLA	MG-NC	2.26	2.11	2.06
16	B	849	CLA	C1D-C2D	-2.25	1.40	1.45
20	J	102	DD6	C8-C6	-2.25	1.41	1.46
16	B	811	CLA	MG-NC	2.25	2.11	2.06
16	A	814	CLA	MG-NC	2.25	2.11	2.06
16	A	832	CLA	C1D-C2D	-2.25	1.40	1.45
16	B	808	CLA	C1B-C2B	-2.25	1.37	1.43
16	A	811	CLA	C1D-C2D	-2.25	1.40	1.45
16	A	847	CLA	C1D-C2D	-2.25	1.40	1.45
16	U	205	CLA	C1D-C2D	-2.25	1.40	1.45
16	A	819	CLA	C1D-C2D	-2.24	1.40	1.45
16	U	211	CLA	C1D-C2D	-2.24	1.40	1.45
16	A	817	CLA	C1B-C2B	-2.24	1.37	1.43
20	H	311	DD6	C8-C6	-2.24	1.41	1.46
16	A	830	CLA	C1D-C2D	-2.24	1.40	1.45
16	B	844	CLA	C1D-C2D	-2.24	1.40	1.45
20	G	312	DD6	C10-C11	2.24	1.41	1.35
16	A	845	CLA	C3D-C4D	-2.24	1.39	1.44
20	H	311	DD6	C10-C11	2.24	1.41	1.35
16	A	821	CLA	C1D-C2D	-2.24	1.40	1.45
20	H	311	DD6	C2-C1	2.24	1.41	1.35
16	H	302	CLA	C1B-C2B	-2.24	1.37	1.43
16	B	803	CLA	C1B-C2B	-2.23	1.37	1.43
16	H	304	CLA	C1B-C2B	-2.23	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	A	836	CLA	MG-NC	2.23	2.11	2.06
16	A	835	CLA	C1D-C2D	-2.23	1.40	1.45
16	K	203	CLA	C1B-C2B	-2.23	1.37	1.43
16	G	309	CLA	C1B-C2B	-2.23	1.37	1.43
16	U	209	CLA	C1B-C2B	-2.23	1.37	1.43
16	A	849	CLA	C1B-C2B	-2.23	1.37	1.43
16	U	205	CLA	C1B-C2B	-2.23	1.37	1.43
20	G	311	DD6	C10-C11	2.23	1.40	1.35
16	F	802	CLA	C1D-C2D	-2.23	1.40	1.45
16	B	849	CLA	C1B-C2B	-2.23	1.37	1.43
16	F	802	CLA	C1B-C2B	-2.22	1.37	1.43
16	A	825	CLA	C1D-C2D	-2.22	1.40	1.45
16	A	845	CLA	C1D-C2D	-2.22	1.40	1.45
20	U	203	DD6	C8-C6	-2.22	1.41	1.46
16	H	308	CLA	C1B-C2B	-2.22	1.37	1.43
20	H	311	DD6	C24-C1	-2.22	1.41	1.46
16	B	813	CLA	C1D-C2D	-2.21	1.41	1.45
16	U	206	CLA	MG-NC	2.21	2.11	2.06
16	B	803	CLA	MG-NC	2.21	2.11	2.06
16	B	826	CLA	C1D-C2D	-2.21	1.41	1.45
16	B	830	CLA	MG-NC	2.21	2.11	2.06
16	B	835	CLA	C1D-C2D	-2.21	1.41	1.45
18	A	839	LHG	O7-C5	-2.21	1.41	1.46
16	A	853	CLA	MG-NC	2.21	2.11	2.06
16	A	817	CLA	C1D-C2D	-2.21	1.41	1.45
16	J	104	CLA	C1D-C2D	-2.21	1.41	1.45
16	K	204	CLA	C1D-C2D	-2.20	1.41	1.45
16	B	809	CLA	C1D-C2D	-2.20	1.41	1.45
16	B	802	CLA	CHB-C1B	2.20	1.44	1.39
16	L	203	CLA	C1D-C2D	-2.20	1.41	1.45
20	G	313	DD6	C13-C11	-2.20	1.41	1.46
16	G	309	CLA	MG-NC	2.20	2.11	2.06
16	B	834	CLA	C1B-C2B	-2.20	1.38	1.43
16	H	305	CLA	C1B-C2B	-2.20	1.38	1.43
16	A	810	CLA	C1D-C2D	-2.20	1.41	1.45
16	B	801	CLA	C1B-C2B	-2.20	1.38	1.43
16	H	302	CLA	C1D-C2D	-2.20	1.41	1.45
16	B	819	CLA	MG-NC	2.20	2.11	2.06
16	B	804	CLA	C1D-C2D	-2.20	1.41	1.45
16	A	824	CLA	C1D-C2D	-2.20	1.41	1.45
16	B	835	CLA	C1B-C2B	-2.19	1.38	1.43
20	H	311	DD6	C13-C11	-2.19	1.41	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	B	805	CLA	MG-NC	2.19	2.11	2.06
16	G	301	CLA	C1D-C2D	-2.19	1.41	1.45
20	G	311	DD6	C5-C6	2.19	1.40	1.35
27	U	213	KC1	C3B-C2B	2.19	1.41	1.37
16	A	828	CLA	C1D-C2D	-2.19	1.41	1.45
16	U	204	CLA	MG-NC	2.19	2.11	2.06
20	K	208	DD6	C8-C6	-2.19	1.41	1.46
16	H	309	CLA	C1B-C2B	-2.19	1.38	1.43
16	K	206	CLA	C3D-C4D	-2.19	1.39	1.44
16	B	849	CLA	MG-NC	2.18	2.11	2.06
20	G	313	DD6	C24-C1	-2.18	1.41	1.46
16	B	816	CLA	C1D-C2D	-2.18	1.41	1.45
20	H	310	DD6	C10-C11	2.18	1.40	1.35
16	B	803	CLA	C3D-C4D	-2.18	1.39	1.44
16	A	814	CLA	C1D-C2D	-2.18	1.41	1.45
16	I	102	CLA	C1B-C2B	-2.18	1.38	1.43
16	H	312	CLA	C1B-C2B	-2.18	1.38	1.43
20	K	208	DD6	C13-C11	-2.18	1.41	1.46
16	A	820	CLA	C1B-C2B	-2.17	1.38	1.43
16	A	854	CLA	C1D-C2D	-2.17	1.41	1.45
16	A	804	CLA	MG-NC	2.17	2.11	2.06
16	B	814	CLA	C1D-C2D	-2.17	1.41	1.45
16	A	807	CLA	C1D-C2D	-2.17	1.41	1.45
16	B	829	CLA	C1D-C2D	-2.17	1.41	1.45
16	F	803	CLA	C1D-C2D	-2.17	1.41	1.45
16	A	832	CLA	C1B-C2B	-2.17	1.38	1.43
16	G	307	CLA	C1D-C2D	-2.17	1.41	1.45
16	A	851	CLA	C1D-C2D	-2.17	1.41	1.45
16	A	845	CLA	C1B-C2B	-2.16	1.38	1.43
20	J	102	DD6	C13-C11	-2.16	1.41	1.46
16	B	832	CLA	C1D-C2D	-2.16	1.41	1.45
16	F	804	CLA	MG-NC	2.16	2.11	2.06
16	L	204	CLA	C1D-C2D	-2.16	1.41	1.45
16	A	808	CLA	C1D-C2D	-2.16	1.41	1.45
16	B	830	CLA	C1D-C2D	-2.15	1.41	1.45
16	B	810	CLA	MG-NB	2.15	2.10	2.05
16	L	202	CLA	C1D-C2D	-2.15	1.41	1.45
16	B	818	CLA	MG-NC	2.15	2.11	2.06
16	A	834	CLA	C1D-C2D	-2.15	1.41	1.45
16	H	304	CLA	C1D-C2D	-2.15	1.41	1.45
20	K	208	DD6	C24-C1	-2.15	1.41	1.46
16	B	834	CLA	C1D-C2D	-2.15	1.41	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	A	801	CLA	MG-NC	2.15	2.11	2.06
16	B	836	CLA	C1D-C2D	-2.15	1.41	1.45
16	B	809	CLA	C1B-C2B	-2.14	1.38	1.43
20	G	314	DD6	C10-C11	2.14	1.40	1.35
16	B	801	CLA	C3D-C4D	-2.14	1.39	1.44
16	A	829	CLA	C1D-C2D	-2.14	1.41	1.45
16	A	824	CLA	C1B-C2B	-2.14	1.38	1.43
16	G	303	CLA	C1B-C2B	-2.14	1.38	1.43
16	A	853	CLA	C1D-C2D	-2.13	1.41	1.45
16	B	804	CLA	C1B-C2B	-2.13	1.38	1.43
16	G	303	CLA	C1D-C2D	-2.13	1.41	1.45
16	k	201	CLA	C1B-C2B	-2.13	1.38	1.43
25	J	103	LMG	C1-C2	2.13	1.58	1.52
20	G	311	DD6	C25-C26	-2.12	1.36	1.43
16	A	826	CLA	C1B-C2B	-2.12	1.38	1.43
16	B	833	CLA	C1D-C2D	-2.12	1.41	1.45
16	B	820	CLA	C1B-NB	-2.12	1.35	1.37
16	H	307	CLA	MG-NC	2.12	2.11	2.06
16	A	819	CLA	C1B-C2B	-2.12	1.38	1.43
16	B	827	CLA	C1B-C2B	-2.12	1.38	1.43
16	B	813	CLA	C1B-C2B	-2.12	1.38	1.43
16	G	304	CLA	C1D-C2D	-2.12	1.41	1.45
16	A	803	CLA	C1B-C2B	-2.12	1.38	1.43
16	B	813	CLA	MG-NB	2.12	2.10	2.05
16	G	303	CLA	CHB-C1B	2.12	1.44	1.39
16	A	806	CLA	C1D-C2D	-2.12	1.41	1.45
16	G	308	CLA	MG-NC	2.11	2.11	2.06
16	A	826	CLA	C1B-NB	-2.11	1.35	1.37
16	B	805	CLA	C1B-C2B	-2.11	1.38	1.43
16	G	310	CLA	C1D-C2D	-2.11	1.41	1.45
16	A	804	CLA	C1D-C2D	-2.11	1.41	1.45
16	A	838	CLA	CHB-C1B	2.11	1.44	1.39
16	G	307	CLA	CHB-C1B	2.11	1.44	1.39
16	B	827	CLA	C1D-C2D	-2.11	1.41	1.45
16	G	308	CLA	C1D-C2D	-2.10	1.41	1.45
20	G	314	DD6	C5-C6	2.10	1.40	1.35
26	U	202	A86	C8-C6	-2.10	1.41	1.46
16	K	203	CLA	C1D-C2D	-2.10	1.41	1.45
16	B	805	CLA	C1D-C2D	-2.10	1.41	1.45
26	U	202	A86	C24-C1	-2.10	1.41	1.46
16	A	822	CLA	C1B-C2B	-2.09	1.38	1.43
16	B	835	CLA	MG-NB	2.09	2.09	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	G	311	DD6	C2-C1	2.09	1.40	1.35
16	U	209	CLA	C1D-C2D	-2.09	1.41	1.45
16	B	828	CLA	CHB-C1B	2.09	1.44	1.39
16	A	802	CLA	C1B-C2B	-2.09	1.38	1.43
16	A	806	CLA	MG-NC	2.09	2.11	2.06
16	K	205	CLA	C1B-C2B	-2.09	1.38	1.43
16	A	809	CLA	C1B-C2B	-2.09	1.38	1.43
16	A	822	CLA	C1D-C2D	-2.09	1.41	1.45
16	B	815	CLA	C1D-C2D	-2.09	1.41	1.45
16	B	847	CLA	C1D-C2D	-2.09	1.41	1.45
16	G	306	CLA	C1B-C2B	-2.09	1.38	1.43
16	B	809	CLA	C1B-NB	-2.09	1.35	1.37
16	B	824	CLA	C1B-C2B	-2.09	1.38	1.43
16	B	829	CLA	CHB-C1B	2.08	1.44	1.39
16	B	816	CLA	C1B-C2B	-2.08	1.38	1.43
16	H	306	CLA	C1B-C2B	-2.08	1.38	1.43
16	A	833	CLA	C1D-C2D	-2.08	1.41	1.45
16	B	824	CLA	C1D-C2D	-2.08	1.41	1.45
20	G	314	DD6	C2-C1	2.08	1.40	1.35
16	B	801	CLA	C1D-C2D	-2.08	1.41	1.45
16	A	803	CLA	C1D-C2D	-2.08	1.41	1.45
16	L	204	CLA	CHB-C1B	2.08	1.44	1.39
20	G	314	DD6	C25-C26	-2.08	1.36	1.43
16	A	832	CLA	C1B-NB	-2.07	1.35	1.37
16	H	304	CLA	MG-NC	2.07	2.11	2.06
21	A	848	LMU	O1'-C1'	2.07	1.43	1.40
16	U	206	CLA	C1D-C2D	-2.07	1.41	1.45
16	k	202	CLA	CHB-C1B	2.07	1.44	1.39
16	K	204	CLA	C1B-C2B	-2.07	1.38	1.43
16	B	821	CLA	C1B-C2B	-2.07	1.38	1.43
16	B	821	CLA	C1D-C2D	-2.07	1.41	1.45
16	B	823	CLA	CHB-C1B	2.07	1.44	1.39
16	B	810	CLA	C1B-C2B	-2.06	1.38	1.43
16	B	812	CLA	C1D-C2D	-2.06	1.41	1.45
16	A	820	CLA	CHB-C1B	2.06	1.44	1.39
16	B	812	CLA	CHB-C1B	2.06	1.44	1.39
16	K	205	CLA	C1D-C2D	-2.06	1.41	1.45
16	B	807	CLA	C1B-C2B	-2.06	1.38	1.43
16	A	805	CLA	C1D-C2D	-2.06	1.41	1.45
16	U	207	CLA	C1D-C2D	-2.06	1.41	1.45
16	B	817	CLA	C1B-NB	-2.06	1.35	1.37
25	U	201	LMG	O7-C8	-2.06	1.41	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	B	809	CLA	CHB-C1B	2.05	1.44	1.39
16	B	818	CLA	C1D-C2D	-2.05	1.41	1.45
16	U	208	CLA	C1D-C2D	-2.05	1.41	1.45
16	B	825	CLA	C1B-C2B	-2.05	1.38	1.43
16	K	207	CLA	CHB-C1B	2.05	1.44	1.39
16	I	102	CLA	C1D-C2D	-2.05	1.41	1.45
16	F	803	CLA	C1B-C2B	-2.05	1.38	1.43
16	A	836	CLA	CHB-C1B	2.05	1.44	1.39
20	U	212	DD6	C24-C1	-2.05	1.41	1.46
16	B	845	CLA	C1B-C2B	-2.05	1.38	1.43
16	K	203	CLA	MG-NC	2.05	2.11	2.06
16	F	803	CLA	C1B-NB	-2.05	1.35	1.37
16	G	310	CLA	C1B-C2B	-2.05	1.38	1.43
16	A	838	CLA	C1D-C2D	-2.04	1.41	1.45
16	A	853	CLA	C1B-C2B	-2.04	1.38	1.43
16	A	811	CLA	C1B-C2B	-2.04	1.38	1.43
16	G	308	CLA	C1B-C2B	-2.04	1.38	1.43
16	A	821	CLA	C1B-NB	-2.04	1.35	1.37
20	A	846	DD6	C10-C11	2.04	1.40	1.35
20	U	212	DD6	C28-C27	-2.04	1.49	1.50
16	H	307	CLA	CHB-C1B	2.04	1.44	1.39
16	A	801	CLA	C1B-NB	-2.04	1.35	1.37
16	A	823	CLA	C1B-C2B	-2.04	1.38	1.43
16	B	847	CLA	C1B-C2B	-2.04	1.38	1.43
16	A	808	CLA	C1B-C2B	-2.04	1.38	1.43
27	U	213	KC1	C1B-NB	-2.03	1.35	1.37
16	A	802	CLA	C1D-C2D	-2.03	1.41	1.45
16	F	804	CLA	C1D-C2D	-2.03	1.41	1.45
16	H	304	CLA	CHB-C1B	2.03	1.44	1.39
16	K	202	CLA	C1D-C2D	-2.03	1.41	1.45
20	U	212	DD6	C8-C6	-2.03	1.41	1.46
16	G	309	CLA	C1D-C2D	-2.03	1.41	1.45
16	A	813	CLA	C1D-C2D	-2.03	1.41	1.45
16	U	206	CLA	C1B-C2B	-2.03	1.38	1.43
16	U	210	CLA	C1D-C2D	-2.03	1.41	1.45
16	B	806	CLA	CHB-C1B	2.03	1.44	1.39
16	U	208	CLA	MG-NC	2.03	2.11	2.06
16	A	851	CLA	C1B-C2B	-2.03	1.38	1.43
16	A	823	CLA	C1B-NB	-2.02	1.35	1.37
16	U	204	CLA	CHB-C1B	2.02	1.44	1.39
16	U	207	CLA	C1B-C2B	-2.02	1.38	1.43
16	A	816	CLA	C1B-NB	-2.02	1.35	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	H	302	CLA	C1B-NB	-2.02	1.35	1.37
16	H	306	CLA	C1B-NB	-2.02	1.35	1.37
26	U	202	A86	C26-C27	2.02	1.40	1.35
16	K	202	CLA	C1B-NB	-2.02	1.35	1.37
16	H	309	CLA	C1D-C2D	-2.02	1.41	1.45
16	B	815	CLA	C1B-C2B	-2.02	1.38	1.43
20	A	846	DD6	C25-C26	-2.02	1.36	1.43
16	H	307	CLA	C1D-C2D	-2.02	1.41	1.45
16	A	810	CLA	C1B-C2B	-2.02	1.38	1.43
16	K	202	CLA	C1B-C2B	-2.02	1.38	1.43
20	H	310	DD6	C28-C27	-2.02	1.49	1.50
16	B	819	CLA	C1B-C2B	-2.01	1.38	1.43
16	H	308	CLA	C1D-C2D	-2.01	1.41	1.45
16	A	825	CLA	C1B-C2B	-2.01	1.38	1.43
16	B	844	CLA	C1B-C2B	-2.01	1.38	1.43
16	A	807	CLA	C1B-NB	-2.01	1.35	1.37
16	B	832	CLA	C1B-C2B	-2.01	1.38	1.43
16	G	302	CLA	CHB-C1B	2.01	1.43	1.39
19	B	840	BCR	C33-C5	-2.01	1.47	1.50
16	K	206	CLA	CHB-C1B	2.01	1.43	1.39
16	A	821	CLA	C1B-C2B	-2.01	1.38	1.43
20	U	214	DD6	C24-C1	-2.01	1.41	1.46
16	A	804	CLA	C1B-C2B	-2.01	1.38	1.43
16	A	854	CLA	C1B-C2B	-2.01	1.38	1.43
16	A	807	CLA	C1B-C2B	-2.00	1.38	1.43
20	G	317	DD6	C25-C26	-2.00	1.37	1.43
16	A	847	CLA	MG-NB	2.00	2.09	2.05
16	L	204	CLA	C1B-C2B	-2.00	1.38	1.43
16	H	301	CLA	CHB-C1B	2.00	1.43	1.39
16	A	829	CLA	C1B-C2B	-2.00	1.38	1.43
16	L	203	CLA	MG-NC	2.00	2.11	2.06
16	G	315	CLA	CHB-C1B	2.00	1.43	1.39
16	B	810	CLA	C1D-C2D	-2.00	1.41	1.45

All (823) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	850	CL0	C1B-CHB-C4A	9.30	127.30	121.32
20	U	212	DD6	C3-C4-C5	5.22	134.21	123.52
18	A	839	LHG	O4-P-O5	4.37	132.77	112.44
20	U	203	DD6	C4-C3-C2	4.35	132.42	123.52
18	A	840	LHG	O4-P-O5	4.35	132.67	112.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	G	313	DD6	C4-C3-C2	4.30	132.31	123.52
20	H	310	DD6	C3-C4-C5	4.28	132.28	123.52
16	A	838	CLA	C4D-CHA-C1A	4.23	126.29	121.24
26	U	202	A86	C4-C3-C2	4.19	132.10	123.52
20	G	312	DD6	C4-C3-C2	4.18	132.06	123.52
20	H	311	DD6	C3-C4-C5	4.12	131.96	123.52
16	K	205	CLA	C4D-CHA-C1A	4.09	126.12	121.24
19	A	841	BCR	C2-C1-C6	4.09	116.37	110.44
24	B	843	DGD	O2G-C1B-C2B	4.08	120.32	111.48
20	G	317	DD6	C4-C3-C2	4.08	131.86	123.52
16	K	206	CLA	C3A-C2A-C1A	-4.06	102.15	106.30
20	G	311	DD6	C4-C3-C2	4.04	131.79	123.52
19	M	101	BCR	C2-C1-C6	4.00	116.25	110.44
16	G	303	CLA	C4D-CHA-C1A	4.00	126.01	121.24
16	B	807	CLA	C4D-CHA-C1A	3.94	125.94	121.24
20	K	208	DD6	C3-C4-C5	3.94	131.57	123.52
16	K	206	CLA	C4D-CHA-C1A	3.92	125.92	121.24
16	G	305	CLA	CAA-C2A-C3A	-3.91	102.44	113.00
16	B	801	CLA	C4D-CHA-C1A	3.90	125.90	121.24
16	H	301	CLA	C3A-C2A-C1A	-3.90	102.32	106.30
16	B	816	CLA	C4D-CHA-C1A	3.86	125.85	121.24
16	H	301	CLA	C4D-CHA-C1A	3.86	125.85	121.24
20	J	102	DD6	C4-C3-C2	3.86	131.42	123.52
16	B	818	CLA	C4D-CHA-C1A	3.83	125.81	121.24
16	F	804	CLA	C4D-CHA-C1A	3.83	125.81	121.24
16	L	203	CLA	C4D-CHA-C1A	3.82	125.80	121.24
16	A	822	CLA	C4D-CHA-C1A	3.81	125.79	121.24
26	U	202	A86	C3-C4-C5	3.79	131.28	123.52
20	J	102	DD6	C12-C11-C10	-3.79	116.67	122.82
16	A	819	CLA	C4D-CHA-C1A	3.78	125.75	121.24
19	F	801	BCR	C2-C1-C6	3.77	115.91	110.44
16	A	831	CLA	C4D-CHA-C1A	3.76	125.73	121.24
20	H	310	DD6	C4-C3-C2	3.75	131.20	123.52
20	K	208	DD6	C4-C3-C2	3.75	131.18	123.52
16	G	304	CLA	C4D-CHA-C1A	3.74	125.70	121.24
16	G	309	CLA	C4D-CHA-C1A	3.74	125.70	121.24
16	B	836	CLA	C4D-CHA-C1A	3.73	125.69	121.24
20	U	203	DD6	C24-C1-C2	3.72	124.87	119.01
16	B	832	CLA	C4D-CHA-C1A	3.70	125.66	121.24
16	B	844	CLA	C4D-CHA-C1A	3.70	125.66	121.24
20	H	310	DD6	C8-C6-C5	3.69	124.82	119.01
20	J	102	DD6	C13-C11-C10	3.69	124.81	119.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	850	CL0	C3D-C4D-CHA	3.68	114.13	108.54
22	A	850	CL0	C5-C3-C2	3.68	129.42	121.17
16	A	849	CLA	C4D-CHA-C1A	3.67	125.62	121.24
16	A	851	CLA	C4D-CHA-C1A	3.66	125.61	121.24
16	A	811	CLA	C4D-CHA-C1A	3.66	125.61	121.24
16	G	308	CLA	C4D-CHA-C1A	3.66	125.61	121.24
22	A	850	CL0	C1C-CHC-C4B	3.66	129.15	116.07
20	J	102	DD6	C3-C4-C5	3.65	131.00	123.52
16	G	307	CLA	C4D-CHA-C1A	3.65	125.60	121.24
20	G	314	DD6	C8-C6-C5	3.65	124.75	119.01
16	B	814	CLA	C4D-CHA-C1A	3.64	125.59	121.24
20	U	214	DD6	C3-C4-C5	3.63	130.96	123.52
16	A	816	CLA	C4D-CHA-C1A	3.63	125.58	121.24
16	B	848	CLA	C4D-CHA-C1A	3.63	125.58	121.24
16	U	204	CLA	C4D-CHA-C1A	3.63	125.58	121.24
20	U	203	DD6	C3-C4-C5	3.63	130.94	123.52
16	B	830	CLA	C4D-CHA-C1A	3.63	125.57	121.24
16	L	204	CLA	C4D-CHA-C1A	3.63	125.57	121.24
20	U	212	DD6	C8-C6-C5	3.62	124.71	119.01
20	U	214	DD6	C4-C3-C2	3.62	130.93	123.52
16	H	307	CLA	C4D-CHA-C1A	3.62	125.56	121.24
16	B	811	CLA	C4D-CHA-C1A	3.62	125.56	121.24
16	A	828	CLA	C4D-CHA-C1A	3.61	125.55	121.24
16	A	833	CLA	C4D-CHA-C1A	3.61	125.55	121.24
16	B	831	CLA	C4D-CHA-C1A	3.61	125.54	121.24
16	F	803	CLA	C4D-CHA-C1A	3.60	125.54	121.24
16	A	803	CLA	C4D-CHA-C1A	3.60	125.54	121.24
16	B	812	CLA	C4D-CHA-C1A	3.60	125.53	121.24
16	A	834	CLA	C4D-CHA-C1A	3.60	125.53	121.24
16	B	833	CLA	C4D-CHA-C1A	3.58	125.52	121.24
16	B	810	CLA	C4D-CHA-C1A	3.58	125.51	121.24
16	B	815	CLA	C4D-CHA-C1A	3.57	125.50	121.24
16	A	836	CLA	C4D-CHA-C1A	3.56	125.49	121.24
16	B	835	CLA	C4D-CHA-C1A	3.55	125.48	121.24
16	I	102	CLA	C4D-CHA-C1A	3.55	125.48	121.24
16	H	306	CLA	C4D-CHA-C1A	3.54	125.47	121.24
20	G	314	DD6	C24-C1-C2	3.54	124.58	119.01
19	J	105	BCR	C2-C1-C6	3.54	115.58	110.44
16	A	835	CLA	C4D-CHA-C1A	3.54	125.46	121.24
16	A	805	CLA	C4D-CHA-C1A	3.53	125.46	121.24
16	B	814	CLA	CAA-C2A-C3A	-3.53	103.47	113.00
20	G	317	DD6	C12-C11-C10	-3.52	117.11	122.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	F	802	CLA	C4D-CHA-C1A	3.51	125.44	121.24
16	U	208	CLA	C4D-CHA-C1A	3.51	125.43	121.24
20	K	208	DD6	C12-C11-C10	-3.50	117.14	122.82
16	A	813	CLA	C4D-CHA-C1A	3.49	125.41	121.24
16	G	315	CLA	C4D-CHA-C1A	3.49	125.41	121.24
20	A	846	DD6	C12-C11-C10	-3.48	117.18	122.82
16	B	824	CLA	C4D-CHA-C1A	3.47	125.39	121.24
16	G	315	CLA	CHD-C1D-ND	-3.46	119.93	124.80
16	A	853	CLA	C4D-CHA-C1A	3.46	125.37	121.24
19	B	841	BCR	C15-C16-C17	-3.46	116.44	123.52
16	A	820	CLA	C4D-CHA-C1A	3.46	125.37	121.24
16	A	854	CLA	C4D-CHA-C1A	3.46	125.36	121.24
20	H	310	DD6	C12-C11-C10	-3.45	117.22	122.82
16	A	810	CLA	C4D-CHA-C1A	3.45	125.36	121.24
16	B	826	CLA	C4D-CHA-C1A	3.45	125.35	121.24
16	B	827	CLA	C4D-CHA-C1A	3.44	125.35	121.24
16	U	205	CLA	C4D-CHA-C1A	3.43	125.34	121.24
20	G	314	DD6	C12-C11-C10	-3.43	117.26	122.82
16	B	847	CLA	C4D-CHA-C1A	3.43	125.33	121.24
16	A	830	CLA	C4D-CHA-C1A	3.42	125.33	121.24
16	B	845	CLA	C4D-CHA-C1A	3.41	125.31	121.24
19	k	203	BCR	C2-C1-C6	3.41	115.39	110.44
20	G	311	DD6	C12-C11-C10	-3.41	117.29	122.82
20	G	313	DD6	C12-C11-C10	-3.41	117.29	122.82
20	U	203	DD6	C-C1-C2	-3.40	117.30	122.82
16	A	812	CLA	C4D-CHA-C1A	3.39	125.29	121.24
16	B	834	CLA	C4D-CHA-C1A	3.39	125.29	121.24
16	U	206	CLA	C4D-CHA-C1A	3.39	125.29	121.24
16	K	207	CLA	C4D-CHA-C1A	3.39	125.28	121.24
21	K	201	LMU	C2'-C3'-C4'	3.39	117.36	109.68
20	U	212	DD6	C12-C11-C10	-3.38	117.34	122.82
16	A	847	CLA	C4D-CHA-C1A	3.38	125.27	121.24
16	B	829	CLA	C4D-CHA-C1A	3.37	125.27	121.24
16	H	309	CLA	C4D-CHA-C1A	3.37	125.27	121.24
16	A	825	CLA	C4D-CHA-C1A	3.37	125.26	121.24
16	H	303	CLA	C4D-CHA-C1A	3.36	125.25	121.24
16	A	829	CLA	C4D-CHA-C1A	3.35	125.24	121.24
16	H	304	CLA	C4D-CHA-C1A	3.34	125.23	121.24
16	G	315	CLA	CMD-C2D-C1D	3.34	130.61	124.73
16	U	207	CLA	CAA-C2A-C3A	-3.34	103.98	113.00
22	A	850	CL0	C4-C3-C2	-3.33	115.08	123.63
16	k	201	CLA	C4D-CHA-C1A	3.32	125.21	121.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	H	311	DD6	C12-C11-C10	-3.32	117.44	122.82
16	A	808	CLA	C4D-CHA-C1A	3.32	125.20	121.24
16	A	807	CLA	C4A-NA-C1A	3.31	108.19	106.68
20	U	203	DD6	C12-C11-C10	-3.31	117.45	122.82
20	G	317	DD6	C3-C4-C5	3.31	130.29	123.52
16	B	809	CLA	C4D-CHA-C1A	3.31	125.19	121.24
16	A	845	CLA	C4D-CHA-C1A	3.30	125.18	121.24
16	A	824	CLA	C4D-CHA-C1A	3.29	125.17	121.24
16	U	211	CLA	C4D-CHA-C1A	3.29	125.17	121.24
16	A	815	CLA	C4D-CHA-C1A	3.29	125.17	121.24
16	A	817	CLA	C4D-CHA-C1A	3.27	125.15	121.24
16	G	310	CLA	C4D-CHA-C1A	3.27	125.15	121.24
16	L	202	CLA	C4D-CHA-C1A	3.27	125.14	121.24
16	A	806	CLA	C4D-CHA-C1A	3.26	125.14	121.24
16	A	807	CLA	C4D-CHA-C1A	3.26	125.13	121.24
16	k	202	CLA	C4D-CHA-C1A	3.26	125.13	121.24
16	A	827	CLA	C4D-CHA-C1A	3.25	125.12	121.24
16	B	828	CLA	C4D-CHA-C1A	3.24	125.11	121.24
16	A	802	CLA	C4D-CHA-C1A	3.23	125.10	121.24
16	B	805	CLA	C4D-CHA-C1A	3.23	125.10	121.24
16	U	210	CLA	C4D-CHA-C1A	3.23	125.09	121.24
16	K	203	CLA	C4D-CHA-C1A	3.23	125.09	121.24
20	U	212	DD6	C7-C6-C5	-3.22	117.60	122.82
16	G	301	CLA	C4D-CHA-C1A	3.22	125.08	121.24
16	H	306	CLA	O2A-C1-C2	3.21	120.47	108.11
16	H	302	CLA	C4D-CHA-C1A	3.21	125.07	121.24
16	U	207	CLA	C4D-CHA-C1A	3.21	125.07	121.24
16	G	305	CLA	C4D-CHA-C1A	3.21	125.07	121.24
19	I	103	BCR	C27-C26-C25	3.20	127.03	122.70
16	A	832	CLA	C4D-CHA-C1A	3.20	125.06	121.24
20	J	102	DD6	C8-C6-C5	3.19	124.03	119.01
21	K	201	LMU	C1B-O1B-C4'	-3.19	110.42	117.98
16	B	817	CLA	C4D-CHA-C1A	3.19	125.05	121.24
16	B	820	CLA	CHA-C1A-NA	-3.19	119.17	126.39
16	A	814	CLA	C4D-CHA-C1A	3.17	125.03	121.24
20	G	312	DD6	C12-C11-C10	-3.17	117.68	122.82
16	G	302	CLA	C4D-CHA-C1A	3.16	125.02	121.24
16	J	104	CLA	C4D-CHA-C1A	3.16	125.01	121.24
16	A	809	CLA	C4D-CHA-C1A	3.16	125.01	121.24
20	G	314	DD6	C-C1-C2	-3.15	117.71	122.82
16	k	202	CLA	C4A-NA-C1A	3.15	108.12	106.68
16	B	823	CLA	C4D-CHA-C1A	3.15	125.00	121.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	K	205	CLA	O2A-C1-C2	3.14	120.21	108.11
16	K	204	CLA	C4D-CHA-C1A	3.14	124.99	121.24
16	H	306	CLA	C1-O2A-CGA	-3.13	109.08	116.65
20	A	846	DD6	C24-C1-C2	3.12	123.92	119.01
20	H	310	DD6	C24-C1-C2	3.12	123.92	119.01
16	B	806	CLA	C4D-CHA-C1A	3.12	124.97	121.24
16	B	822	CLA	C4D-CHA-C1A	3.12	124.96	121.24
16	A	804	CLA	C4D-CHA-C1A	3.11	124.95	121.24
16	H	305	CLA	C4D-CHA-C1A	3.10	124.94	121.24
16	B	849	CLA	C4D-CHA-C1A	3.10	124.94	121.24
16	A	821	CLA	CHA-C1A-NA	-3.10	119.37	126.39
19	I	103	BCR	C15-C16-C17	-3.10	117.18	123.52
16	B	824	CLA	C1-O2A-CGA	3.10	124.14	116.65
21	K	201	LMU	O5B-C5B-C4B	3.08	115.25	109.70
16	B	813	CLA	C4D-CHA-C1A	3.07	124.91	121.24
19	B	841	BCR	C15-C14-C13	-3.06	122.99	127.28
16	H	312	CLA	CHD-C1D-ND	-3.05	120.51	124.80
16	H	308	CLA	C4D-CHA-C1A	3.04	124.88	121.24
25	J	103	LMG	O6-C1-O1	-3.04	102.86	110.04
20	G	312	DD6	C3-C4-C5	3.03	129.73	123.52
16	H	302	CLA	CHA-C1A-NA	-3.03	119.53	126.39
20	H	310	DD6	C-C1-C2	-3.03	117.91	122.82
20	U	214	DD6	C-C1-C2	-3.02	117.92	122.82
20	G	314	DD6	C7-C6-C5	-3.02	117.92	122.82
16	H	312	CLA	CHA-C1A-NA	-3.02	119.56	126.39
18	A	840	LHG	O8-C23-C24	3.02	120.31	111.15
16	A	822	CLA	CHD-C1D-ND	-3.01	120.56	124.80
19	L	205	BCR	C2-C1-C6	3.00	114.79	110.44
20	A	846	DD6	C4-C3-C2	3.00	129.65	123.52
16	A	823	CLA	C4D-CHA-C1A	2.99	124.81	121.24
20	A	846	DD6	C-C1-C2	-2.99	117.97	122.82
20	A	846	DD6	C30-C29-C27	-2.98	166.09	176.23
20	K	208	DD6	C8-C6-C5	2.98	123.70	119.01
20	G	311	DD6	C3-C4-C5	2.97	129.61	123.52
21	K	201	LMU	C4B-C3B-C2B	2.97	116.04	110.83
20	J	102	DD6	C7-C6-C5	-2.97	118.01	122.82
16	A	803	CLA	CHD-C1D-ND	-2.96	120.63	124.80
20	U	214	DD6	C24-C1-C2	2.96	123.67	119.01
16	A	849	CLA	CHD-C1D-ND	-2.96	120.64	124.80
16	A	818	CLA	C4D-CHA-C1A	2.96	124.77	121.24
16	B	819	CLA	C4D-CHA-C1A	2.95	124.76	121.24
16	K	202	CLA	C4D-CHA-C1A	2.95	124.76	121.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	H	310	DD6	C7-C6-C5	-2.95	118.04	122.82
16	k	202	CLA	CHA-C1A-NA	-2.95	119.72	126.39
16	A	838	CLA	CHD-C1D-ND	-2.95	120.66	124.80
16	G	315	CLA	CHD-C1D-C2D	2.94	131.61	125.49
20	G	311	DD6	C24-C1-C2	2.94	123.63	119.01
24	B	843	DGD	C3G-O3G-C1D	-2.94	107.50	113.80
16	A	810	CLA	C4A-NA-C1A	2.93	108.02	106.68
16	A	817	CLA	C4A-NA-C1A	2.92	108.01	106.68
16	B	823	CLA	CHA-C1A-NA	-2.92	119.77	126.39
16	G	306	CLA	C4D-CHA-C1A	2.92	124.73	121.24
16	A	807	CLA	CHA-C1A-NA	-2.92	119.79	126.39
16	A	845	CLA	CHA-C1A-NA	-2.91	119.80	126.39
16	B	804	CLA	C4D-CHA-C1A	2.91	124.72	121.24
16	U	207	CLA	CHD-C1D-ND	-2.91	120.71	124.80
22	A	850	CL0	C1A-CHA-C4D	2.90	123.83	118.98
20	J	102	DD6	C24-C1-C2	2.90	123.57	119.01
16	U	211	CLA	CHA-C1A-NA	-2.90	119.82	126.39
20	G	313	DD6	C-C1-C2	-2.90	118.12	122.82
20	K	208	DD6	C7-C6-C5	-2.90	118.12	122.82
16	B	836	CLA	CHA-C1A-NA	-2.90	119.83	126.39
16	A	834	CLA	CHA-C1A-NA	-2.89	119.84	126.39
26	U	202	A86	C8-C6-C5	2.89	123.56	119.01
16	A	812	CLA	CHA-C1A-NA	-2.88	119.86	126.39
16	B	802	CLA	CHA-C1A-NA	-2.88	119.87	126.39
21	A	855	LMU	O1'-C1'-C2'	2.88	112.64	108.27
19	L	201	BCR	C27-C26-C25	2.87	126.59	122.70
20	G	311	DD6	C-C1-C2	-2.87	118.16	122.82
16	B	803	CLA	CHA-C1A-NA	-2.87	119.89	126.39
20	G	313	DD6	C24-C1-C2	2.87	123.53	119.01
16	F	803	CLA	CHA-C1A-NA	-2.87	119.90	126.39
26	U	202	A86	C24-C1-C2	2.86	123.52	119.01
16	A	815	CLA	CHA-C1A-NA	-2.86	119.91	126.39
20	J	102	DD6	C-C1-C2	-2.86	118.18	122.82
16	A	831	CLA	CHD-C1D-ND	-2.86	120.77	124.80
16	H	303	CLA	CHD-C1D-ND	-2.86	120.78	124.80
20	U	203	DD6	C8-C6-C5	2.86	123.51	119.01
16	A	817	CLA	CHA-C1A-NA	-2.86	119.92	126.39
16	B	848	CLA	CHA-C1A-NA	-2.86	119.92	126.39
16	A	821	CLA	C4D-CHA-C1A	2.86	124.65	121.24
16	A	825	CLA	CHA-C1A-NA	-2.86	119.92	126.39
16	B	809	CLA	CHA-C1A-NA	-2.85	119.93	126.39
26	U	202	A86	C7-C6-C5	-2.85	118.19	122.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	k	203	BCR	C15-C16-C17	-2.85	117.69	123.52
16	A	801	CLA	CHA-C1A-NA	-2.85	119.94	126.39
16	B	821	CLA	C4D-CHA-C1A	2.85	124.64	121.24
19	M	101	BCR	C15-C16-C17	-2.85	117.70	123.52
20	K	208	DD6	C24-C1-C2	2.84	123.48	119.01
16	B	831	CLA	CHA-C1A-NA	-2.84	119.95	126.39
20	J	102	DD6	C10-C9-C8	2.84	131.43	123.20
16	L	202	CLA	CHA-C1A-NA	-2.84	119.96	126.39
16	K	204	CLA	CHA-C1A-NA	-2.84	119.96	126.39
16	H	312	CLA	C4D-CHA-C1A	2.84	124.63	121.24
16	G	303	CLA	CHA-C1A-NA	-2.84	119.97	126.39
20	U	203	DD6	C7-C6-C5	-2.84	118.22	122.82
19	B	842	BCR	C27-C26-C25	2.84	126.54	122.70
16	B	822	CLA	CHA-C1A-NA	-2.83	119.97	126.39
26	U	202	A86	C-C1-C2	-2.83	118.23	122.82
16	B	806	CLA	CHA-C1A-NA	-2.83	119.98	126.39
19	B	840	BCR	C24-C23-C22	-2.83	122.05	126.23
16	A	828	CLA	CHA-C1A-NA	-2.83	119.99	126.39
16	B	801	CLA	CHA-C1A-NA	-2.83	119.99	126.39
20	A	846	DD6	C3-C4-C5	2.82	129.29	123.52
16	B	818	CLA	CHD-C1D-ND	-2.82	120.83	124.80
16	B	835	CLA	CHA-C1A-NA	-2.82	120.00	126.39
16	B	819	CLA	CHA-C1A-NA	-2.82	120.01	126.39
16	A	827	CLA	CHA-C1A-NA	-2.82	120.01	126.39
16	B	804	CLA	CHA-C1A-NA	-2.81	120.02	126.39
21	K	201	LMU	O5'-C5'-C4'	2.81	115.54	109.72
16	U	209	CLA	CHA-C1A-NA	-2.81	120.02	126.39
16	F	803	CLA	C1-O2A-CGA	2.81	123.46	116.65
20	K	208	DD6	C-C1-C2	-2.81	118.26	122.82
16	G	308	CLA	CHD-C1D-ND	-2.81	120.84	124.80
16	A	832	CLA	CHA-C1A-NA	-2.81	120.03	126.39
16	A	810	CLA	CHA-C1A-NA	-2.81	120.03	126.39
20	G	317	DD6	C7-C6-C5	-2.81	118.27	122.82
16	B	803	CLA	C4D-CHA-C1A	2.81	124.59	121.24
16	A	823	CLA	CHA-C1A-NA	-2.81	120.03	126.39
16	U	210	CLA	CHD-C1D-ND	-2.81	120.85	124.80
16	B	828	CLA	CHA-C1A-NA	-2.81	120.03	126.39
16	A	812	CLA	CHD-C1D-ND	-2.81	120.85	124.80
20	H	310	DD6	C10-C9-C8	2.81	131.33	123.20
20	U	212	DD6	C-C1-C2	-2.80	118.27	122.82
20	G	317	DD6	C8-C6-C5	2.80	123.42	119.01
16	G	305	CLA	CHA-C1A-NA	-2.80	120.04	126.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	A	802	CLA	CHD-C1D-ND	-2.80	120.86	124.80
20	H	311	DD6	C4-C3-C2	2.80	129.25	123.52
16	U	209	CLA	C4D-CHA-C1A	2.80	124.58	121.24
19	I	103	BCR	C15-C14-C13	-2.80	123.36	127.28
20	U	203	DD6	C26-C25-C24	2.79	131.30	123.20
19	L	205	BCR	C27-C26-C25	2.79	126.48	122.70
16	L	204	CLA	CHA-C1A-NA	-2.79	120.07	126.39
20	U	212	DD6	C4-C3-C2	2.79	129.23	123.52
16	H	305	CLA	CHA-C1A-NA	-2.79	120.08	126.39
21	A	848	LMU	O1'-C1'-C2'	2.79	112.51	108.27
16	L	203	CLA	CHD-C1D-ND	-2.79	120.88	124.80
19	M	101	BCR	C15-C14-C13	-2.79	123.37	127.28
16	G	307	CLA	CHD-C1D-ND	-2.79	120.88	124.80
16	G	306	CLA	CHA-C1A-NA	-2.78	120.09	126.39
16	B	833	CLA	CHA-C1A-NA	-2.78	120.10	126.39
16	K	207	CLA	CHA-C1A-NA	-2.78	120.10	126.39
16	B	825	CLA	CHA-C1A-NA	-2.78	120.10	126.39
19	M	101	BCR	C27-C26-C25	2.78	126.45	122.70
16	B	830	CLA	CHA-C1A-NA	-2.77	120.12	126.39
16	B	814	CLA	CHA-C1A-NA	-2.77	120.12	126.39
16	F	802	CLA	CHA-C1A-NA	-2.76	120.13	126.39
25	U	201	LMG	O6-C1-O1	-2.76	103.52	110.04
16	B	834	CLA	CHA-C1A-NA	-2.76	120.14	126.39
16	A	814	CLA	CHA-C1A-NA	-2.76	120.14	126.39
20	G	311	DD6	C7-C6-C5	-2.76	118.34	122.82
16	A	835	CLA	CHA-C1A-NA	-2.76	120.14	126.39
16	B	836	CLA	C4A-NA-C1A	2.76	107.94	106.68
16	G	310	CLA	CHA-C1A-NA	-2.76	120.15	126.39
20	G	314	DD6	C3-C4-C5	2.75	129.15	123.52
16	B	844	CLA	CHA-C1A-NA	-2.75	120.16	126.39
19	F	801	BCR	C27-C26-C25	2.75	126.42	122.70
16	A	824	CLA	CHA-C1A-NA	-2.75	120.16	126.39
16	H	301	CLA	CHD-C1D-ND	-2.75	120.93	124.80
16	A	808	CLA	CHA-C1A-NA	-2.75	120.17	126.39
16	A	806	CLA	CHD-C1D-ND	-2.75	120.93	124.80
16	A	811	CLA	CHA-C1A-NA	-2.75	120.17	126.39
16	B	808	CLA	C4D-CHA-C1A	2.75	124.52	121.24
20	G	311	DD6	C8-C6-C5	2.75	123.33	119.01
16	B	827	CLA	CHA-C1A-NA	-2.75	120.17	126.39
16	A	813	CLA	CHA-C1A-NA	-2.74	120.18	126.39
19	B	841	BCR	C27-C26-C25	2.74	126.41	122.70
16	I	102	CLA	CHA-C1A-NA	-2.74	120.18	126.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	J	101	LMU	C3B-C4B-C5B	2.74	115.20	110.23
16	G	304	CLA	CHD-C1D-ND	-2.74	120.95	124.80
16	A	804	CLA	CHA-C1A-NA	-2.74	120.19	126.39
20	A	846	DD6	C7-C6-C5	-2.74	118.38	122.82
16	G	309	CLA	CHA-C1A-NA	-2.73	120.20	126.39
16	B	845	CLA	CHA-C1A-NA	-2.73	120.20	126.39
17	A	837	PQN	C11-C3-C2	-2.73	120.20	124.89
20	H	311	DD6	C7-C6-C5	-2.73	118.39	122.82
16	A	816	CLA	CHD-C1D-ND	-2.73	120.96	124.80
16	A	854	CLA	CHA-C1A-NA	-2.73	120.21	126.39
19	J	105	BCR	C27-C26-C25	2.73	126.39	122.70
16	B	847	CLA	CHD-C1D-ND	-2.73	120.96	124.80
16	A	818	CLA	CHA-C1A-NA	-2.73	120.21	126.39
16	K	202	CLA	CHD-C1D-ND	-2.73	120.96	124.80
16	A	826	CLA	C4D-CHA-C1A	2.73	124.50	121.24
16	A	830	CLA	CHA-C1A-NA	-2.73	120.22	126.39
20	U	212	DD6	C24-C1-C2	2.73	123.30	119.01
19	k	203	BCR	C27-C26-C25	2.73	126.39	122.70
16	A	847	CLA	CHA-C1A-NA	-2.73	120.22	126.39
19	L	205	BCR	C11-C10-C9	-2.72	123.46	127.28
16	A	819	CLA	CHA-C1A-NA	-2.72	120.22	126.39
16	A	805	CLA	CHA-C1A-NA	-2.72	120.22	126.39
16	U	210	CLA	CHA-C1A-NA	-2.72	120.23	126.39
16	G	302	CLA	CHA-C1A-NA	-2.72	120.23	126.39
16	H	302	CLA	C4A-NA-C1A	2.72	107.92	106.68
16	B	821	CLA	CHD-C1D-ND	-2.71	120.98	124.80
16	H	307	CLA	CHD-C1D-ND	-2.71	120.98	124.80
16	B	811	CLA	CHA-C1A-NA	-2.71	120.25	126.39
16	F	803	CLA	C4A-NA-C1A	2.71	107.92	106.68
16	A	826	CLA	CHA-C1A-NA	-2.71	120.25	126.39
16	B	805	CLA	CHA-C1A-NA	-2.71	120.25	126.39
16	K	203	CLA	CHA-C1A-NA	-2.71	120.26	126.39
16	G	304	CLA	CHA-C1A-NA	-2.71	120.26	126.39
16	B	807	CLA	CHA-C1A-NA	-2.71	120.26	126.39
16	A	820	CLA	CHA-C1A-NA	-2.71	120.26	126.39
16	H	309	CLA	CHA-C1A-NA	-2.71	120.26	126.39
16	G	308	CLA	CHA-C1A-NA	-2.70	120.27	126.39
16	A	836	CLA	CHA-C1A-NA	-2.70	120.27	126.39
16	H	304	CLA	CHA-C1A-NA	-2.70	120.28	126.39
16	L	202	CLA	C4A-NA-C1A	2.70	107.91	106.68
16	B	810	CLA	CHD-C1D-ND	-2.70	121.01	124.80
16	G	305	CLA	CHD-C1D-ND	-2.70	121.01	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	J	104	CLA	CHA-C1A-NA	-2.70	120.28	126.39
19	L	201	BCR	C15-C16-C17	-2.70	118.00	123.52
16	A	851	CLA	CHA-C1A-NA	-2.70	120.29	126.39
19	F	805	BCR	C27-C26-C25	2.69	126.34	122.70
16	L	202	CLA	C1-O2A-CGA	2.69	123.17	116.65
16	A	801	CLA	C4D-CHA-C1A	2.69	124.45	121.24
16	B	847	CLA	CHA-C1A-NA	-2.68	120.31	126.39
16	F	804	CLA	CHA-C1A-NA	-2.68	120.31	126.39
16	B	812	CLA	CHA-C1A-NA	-2.68	120.32	126.39
20	H	311	DD6	C-C1-C2	-2.68	118.47	122.82
19	B	839	BCR	C11-C10-C9	-2.68	123.52	127.28
16	B	824	CLA	CHD-C1D-ND	-2.68	121.03	124.80
19	A	843	BCR	C28-C27-C26	-2.68	109.28	114.06
16	B	829	CLA	CHA-C1A-NA	-2.68	120.32	126.39
16	H	308	CLA	CHD-C1D-ND	-2.68	121.03	124.80
16	U	205	CLA	CHA-C1A-NA	-2.68	120.33	126.39
16	U	206	CLA	CHD-C1D-ND	-2.68	121.03	124.80
16	A	809	CLA	CHA-C1A-NA	-2.68	120.33	126.39
19	J	105	BCR	C24-C23-C22	-2.68	122.28	126.23
20	G	317	DD6	C-C1-C2	-2.68	118.48	122.82
16	K	202	CLA	CHA-C1A-NA	-2.68	120.33	126.39
16	G	301	CLA	CHA-C1A-NA	-2.67	120.34	126.39
16	A	849	CLA	CHA-C1A-NA	-2.67	120.34	126.39
16	B	817	CLA	CHA-C1A-NA	-2.67	120.35	126.39
16	B	813	CLA	CHA-C1A-NA	-2.67	120.35	126.39
16	B	816	CLA	CHD-C1D-ND	-2.67	121.05	124.80
16	k	201	CLA	CHA-C1A-NA	-2.67	120.35	126.39
16	U	208	CLA	CHA-C1A-NA	-2.67	120.36	126.39
16	B	810	CLA	CHA-C1A-NA	-2.66	120.36	126.39
16	B	816	CLA	CHA-C1A-NA	-2.66	120.36	126.39
16	A	832	CLA	C4A-NA-C1A	2.66	107.89	106.68
22	A	850	CL0	C4C-CHD-C1D	2.66	125.58	116.07
16	B	818	CLA	CHA-C1A-NA	-2.66	120.37	126.39
16	A	821	CLA	C4A-NA-C1A	2.66	107.89	106.68
20	H	311	DD6	C8-C6-C5	2.66	123.19	119.01
16	A	838	CLA	CHA-C1A-NA	-2.65	120.38	126.39
16	B	826	CLA	CHA-C1A-NA	-2.65	120.38	126.39
16	K	205	CLA	C1-O2A-CGA	2.65	123.07	116.65
20	G	317	DD6	C24-C1-C2	2.65	123.18	119.01
16	A	833	CLA	CHD-C1D-ND	-2.65	121.08	124.80
16	B	808	CLA	CHA-C1A-NA	-2.65	120.40	126.39
20	A	846	DD6	C8-C6-C5	2.65	123.17	119.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	B	812	CLA	CHD-C1D-ND	-2.65	121.08	124.80
24	B	843	DGD	O3G-C1D-C2D	2.65	112.29	108.27
16	U	206	CLA	CHA-C1A-NA	-2.65	120.40	126.39
16	A	824	CLA	CHD-C1D-ND	-2.65	121.08	124.80
16	I	102	CLA	CHD-C1D-ND	-2.64	121.09	124.80
16	B	830	CLA	CHD-C1D-ND	-2.64	121.09	124.80
16	B	849	CLA	CHA-C1A-NA	-2.64	120.41	126.39
16	U	204	CLA	CHA-C1A-NA	-2.64	120.42	126.39
16	k	201	CLA	CHD-C1D-ND	-2.64	121.09	124.80
19	B	839	BCR	C15-C16-C17	-2.63	118.13	123.52
19	B	840	BCR	C27-C26-C25	2.63	126.26	122.70
20	G	312	DD6	C7-C6-C5	-2.63	118.55	122.82
16	F	804	CLA	CHD-C1D-ND	-2.63	121.10	124.80
16	A	853	CLA	CHD-C1D-ND	-2.63	121.10	124.80
16	B	825	CLA	C4D-CHA-C1A	2.63	124.38	121.24
16	G	309	CLA	CHD-C1D-ND	-2.63	121.10	124.80
16	H	306	CLA	CHA-C1A-NA	-2.63	120.44	126.39
16	G	315	CLA	CHA-C1A-NA	-2.62	120.45	126.39
16	A	831	CLA	CHA-C1A-NA	-2.62	120.45	126.39
16	B	805	CLA	CHD-C1D-ND	-2.62	121.12	124.80
20	H	311	DD6	C24-C1-C2	2.62	123.13	119.01
16	H	301	CLA	CHA-C1A-NA	-2.62	120.37	126.33
16	A	806	CLA	CHA-C1A-NA	-2.62	120.46	126.39
16	B	824	CLA	CHA-C1A-NA	-2.62	120.47	126.39
19	A	842	BCR	C27-C26-C25	2.61	126.24	122.70
16	K	205	CLA	CHA-C1A-NA	-2.61	120.47	126.39
16	A	833	CLA	CHA-C1A-NA	-2.61	120.48	126.39
16	B	815	CLA	CHD-C1D-ND	-2.61	121.13	124.80
16	B	833	CLA	CHD-C1D-ND	-2.61	121.13	124.80
16	G	303	CLA	C4A-NA-C1A	2.61	107.87	106.68
16	A	816	CLA	CHA-C1A-NA	-2.61	120.49	126.39
16	B	832	CLA	CHD-C1D-ND	-2.60	121.14	124.80
16	B	817	CLA	CHD-C1D-ND	-2.60	121.14	124.80
19	A	842	BCR	C15-C16-C17	-2.60	118.20	123.52
16	U	208	CLA	CHD-C1D-ND	-2.60	121.15	124.80
16	B	832	CLA	CHA-C1A-NA	-2.60	120.51	126.39
16	A	813	CLA	CHD-C1D-ND	-2.60	121.15	124.80
16	A	829	CLA	CHA-C1A-NA	-2.60	120.51	126.39
24	B	843	DGD	C1D-O6D-C5D	-2.59	108.65	113.72
16	H	303	CLA	CHA-C1A-NA	-2.59	120.52	126.39
16	H	301	CLA	C4A-NA-C1A	2.59	107.86	106.68
19	L	205	BCR	C3-C4-C5	-2.59	109.43	114.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	B	848	CLA	C4A-NA-C1A	2.59	107.86	106.68
16	U	205	CLA	CHD-C1D-ND	-2.58	121.17	124.80
20	U	203	DD6	C33-C32-C31	2.58	114.57	109.49
16	B	834	CLA	C4A-NA-C1A	2.58	107.86	106.68
19	A	844	BCR	C33-C5-C6	-2.58	121.67	124.48
16	A	804	CLA	CHD-C1D-ND	-2.58	121.18	124.80
16	L	203	CLA	CHA-C1A-NA	-2.57	120.57	126.39
16	K	205	CLA	CHD-C1D-ND	-2.57	121.19	124.80
16	B	829	CLA	CHD-C1D-ND	-2.57	121.19	124.80
16	B	815	CLA	CHA-C1A-NA	-2.57	120.58	126.39
16	H	308	CLA	CHA-C1A-NA	-2.56	120.58	126.39
16	B	813	CLA	CHD-C1D-ND	-2.56	121.19	124.80
16	A	834	CLA	C4A-NA-C1A	2.56	107.85	106.68
16	H	307	CLA	CHA-C1A-NA	-2.56	120.59	126.39
16	H	309	CLA	CHD-C1D-ND	-2.56	121.20	124.80
20	U	203	DD6	O1-C15-C14	-2.56	109.56	116.88
16	B	807	CLA	CHD-C1D-ND	-2.55	121.21	124.80
19	M	101	BCR	C3-C4-C5	-2.55	109.50	114.06
16	G	301	CLA	CHD-C1D-ND	-2.55	121.22	124.80
19	I	101	BCR	C15-C16-C17	-2.55	118.31	123.52
18	A	840	LHG	C11-C10-C9	-2.54	101.50	114.37
16	K	206	CLA	CHA-C1A-NA	-2.54	120.54	126.33
20	G	313	DD6	C7-C6-C5	-2.54	118.70	122.82
17	B	837	PQN	C11-C3-C2	-2.54	120.54	124.89
19	B	838	BCR	C29-C30-C25	2.54	114.13	110.44
16	B	801	CLA	CHD-C1D-ND	-2.54	121.23	124.80
16	H	304	CLA	CHD-C1D-ND	-2.54	121.23	124.80
16	K	203	CLA	CHD-C1D-ND	-2.53	121.24	124.80
16	G	307	CLA	CHA-C1A-NA	-2.53	120.65	126.39
16	B	826	CLA	CHD-C1D-ND	-2.53	121.24	124.80
19	A	842	BCR	C15-C14-C13	-2.53	123.73	127.28
16	K	207	CLA	CHD-C1D-ND	-2.53	121.25	124.80
16	B	817	CLA	C3B-C4B-NB	-2.52	108.28	110.53
16	A	814	CLA	C4A-NA-C1A	2.52	107.83	106.68
16	B	848	CLA	CHD-C1D-ND	-2.52	121.26	124.80
16	B	820	CLA	C4A-NA-C1A	2.51	107.83	106.68
20	G	313	DD6	C3-C4-C5	2.51	128.65	123.52
16	B	821	CLA	CHA-C1A-NA	-2.51	120.71	126.39
16	H	306	CLA	C4B-CHC-C1C	2.51	132.14	126.25
16	A	805	CLA	CHD-C1D-ND	-2.50	121.28	124.80
25	U	201	LMG	O3-C3-C2	-2.50	104.48	110.38
16	B	820	CLA	C4D-CHA-C1A	2.50	124.23	121.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	A	802	CLA	CHA-C1A-NA	-2.50	120.73	126.39
16	U	211	CLA	C4A-NA-C1A	2.50	107.82	106.68
19	B	846	BCR	C24-C23-C22	-2.49	122.55	126.23
16	A	853	CLA	CHA-C1A-NA	-2.49	120.75	126.39
16	A	807	CLA	CHD-C1D-ND	-2.49	121.29	124.80
16	A	803	CLA	CHA-C1A-NA	-2.49	120.75	126.39
21	J	101	LMU	O1'-C1'-C2'	2.49	112.05	108.27
19	I	101	BCR	C2-C1-C6	2.49	114.05	110.44
16	U	207	CLA	CHA-C1A-NA	-2.49	120.76	126.39
20	H	310	DD6	C33-C32-C31	2.48	114.39	109.49
16	A	849	CLA	CHD-C1D-C2D	2.48	130.65	125.49
16	A	819	CLA	CHD-C1D-ND	-2.48	121.31	124.80
16	B	827	CLA	CHD-C1D-ND	-2.48	121.31	124.80
16	A	814	CLA	CHD-C1D-ND	-2.48	121.31	124.80
16	L	204	CLA	CHD-C1D-ND	-2.47	121.33	124.80
16	B	835	CLA	CHD-C1D-ND	-2.47	121.33	124.80
16	F	802	CLA	C4A-NA-C1A	2.47	107.81	106.68
26	U	202	A86	C28-C27-C26	-2.47	118.82	122.82
19	A	841	BCR	C27-C26-C25	2.47	126.03	122.70
18	A	839	LHG	O8-C23-C24	2.47	119.35	111.83
16	A	854	CLA	CHD-C1D-ND	-2.46	121.34	124.80
16	A	829	CLA	CHD-C1D-ND	-2.46	121.34	124.80
19	B	842	BCR	C10-C11-C12	-2.46	116.08	123.20
16	B	814	CLA	CHD-C1D-ND	-2.46	121.35	124.80
16	A	834	CLA	CHD-C1D-ND	-2.45	121.35	124.80
16	B	834	CLA	CHD-C1D-ND	-2.45	121.36	124.80
16	B	849	CLA	CHD-C1D-ND	-2.45	121.36	124.80
16	K	206	CLA	C4A-NA-C1A	2.44	107.79	106.68
16	U	209	CLA	CHD-C1D-ND	-2.44	121.37	124.80
16	A	815	CLA	C3B-C4B-NB	-2.44	108.35	110.53
19	B	846	BCR	C19-C20-C21	-2.43	118.54	123.52
16	A	812	CLA	C4A-NA-C1A	2.43	107.79	106.68
16	U	210	CLA	C4A-NA-C1A	2.43	107.79	106.68
19	J	105	BCR	C15-C16-C17	-2.43	118.55	123.52
20	U	212	DD6	C9-C10-C11	2.43	130.69	127.28
19	B	839	BCR	C33-C5-C6	-2.43	121.83	124.48
16	A	801	CLA	CHD-C1D-ND	-2.43	121.39	124.80
16	A	815	CLA	CHD-C1D-ND	-2.43	121.39	124.80
16	B	803	CLA	CHD-C1D-ND	-2.43	121.39	124.80
16	G	310	CLA	CHD-C1D-ND	-2.43	121.39	124.80
16	A	810	CLA	CHD-C1D-ND	-2.42	121.39	124.80
18	A	839	LHG	C11-C10-C9	-2.42	102.12	114.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	850	CL0	C3C-C4C-NC	-2.42	108.73	114.65
16	A	851	CLA	CHD-C1D-ND	-2.42	121.40	124.80
20	G	314	DD6	C10-C9-C8	2.42	130.21	123.20
16	B	819	CLA	CHD-C1D-ND	-2.42	121.40	124.80
16	A	808	CLA	CHD-C1D-ND	-2.41	121.41	124.80
16	A	812	CLA	CHD-C1D-C2D	2.41	130.51	125.49
19	k	203	BCR	C15-C14-C13	-2.41	123.90	127.28
16	A	820	CLA	CHD-C1D-ND	-2.41	121.41	124.80
16	B	806	CLA	C4A-NA-C1A	2.41	107.78	106.68
16	A	822	CLA	CHA-C1A-NA	-2.41	120.93	126.39
19	B	839	BCR	C15-C14-C13	-2.41	123.90	127.28
16	L	204	CLA	C4A-NA-C1A	2.41	107.78	106.68
16	B	822	CLA	C4A-NA-C1A	2.40	107.78	106.68
16	B	835	CLA	C4A-NA-C1A	2.40	107.78	106.68
22	A	850	CL0	CHA-C1A-C2A	-2.40	127.66	133.31
16	B	811	CLA	CHD-C1D-ND	-2.40	121.42	124.80
20	G	312	DD6	C8-C6-C5	2.40	122.79	119.01
19	F	805	BCR	C11-C10-C9	-2.40	123.91	127.28
20	U	203	DD6	C28-C27-C26	-2.39	119.53	124.18
19	L	201	BCR	C15-C14-C13	-2.39	123.92	127.28
16	J	104	CLA	CHD-C1D-ND	-2.39	121.44	124.80
16	A	836	CLA	CHD-C1D-ND	-2.39	121.44	124.80
19	L	205	BCR	C15-C14-C13	-2.39	123.93	127.28
21	A	848	LMU	C1'-C2'-C3'	2.39	115.03	110.01
20	G	314	DD6	C26-C25-C24	2.38	130.11	123.20
16	B	802	CLA	C4D-CHA-C1A	2.38	124.09	121.24
16	A	825	CLA	CHD-C1D-ND	-2.38	121.45	124.80
19	L	205	BCR	C24-C23-C22	-2.38	122.71	126.23
16	H	312	CLA	CHD-C1D-C2D	2.38	130.44	125.49
20	H	311	DD6	C33-C32-C31	2.38	114.18	109.49
16	A	812	CLA	CMD-C2D-C1D	2.38	128.91	124.73
19	B	846	BCR	C19-C18-C17	-2.37	119.24	124.72
20	K	208	DD6	C13-C11-C10	2.37	122.73	119.01
16	A	847	CLA	CHD-C1D-ND	-2.36	121.47	124.80
16	L	202	CLA	CHD-C1D-ND	-2.36	121.47	124.80
25	U	201	LMG	O1-C1-C2	-2.36	104.68	108.27
16	A	854	CLA	C4A-NA-C1A	2.36	107.76	106.68
19	A	844	BCR	C15-C16-C17	-2.36	118.69	123.52
16	A	832	CLA	CHD-C1D-ND	-2.36	121.49	124.80
19	A	843	BCR	C33-C5-C6	-2.36	121.91	124.48
16	B	804	CLA	CHD-C1D-ND	-2.36	121.49	124.80
19	L	201	BCR	C33-C5-C6	-2.35	121.92	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	F	802	CLA	CHD-C1D-ND	-2.35	121.49	124.80
16	G	303	CLA	CHD-C1D-ND	-2.35	121.50	124.80
16	H	301	CLA	CHD-C1D-C2D	2.34	130.35	125.49
16	A	835	CLA	CHD-C1D-ND	-2.34	121.51	124.80
20	U	212	DD6	C14-C13-C11	2.33	129.15	125.53
16	F	803	CLA	CHD-C1D-ND	-2.33	121.52	124.80
19	F	805	BCR	C2-C1-C6	2.33	113.83	110.44
16	B	828	CLA	CHD-C1D-ND	-2.33	121.52	124.80
16	A	831	CLA	CHD-C1D-C2D	2.32	130.32	125.49
16	A	830	CLA	CHD-C1D-ND	-2.32	121.53	124.80
16	A	803	CLA	CHD-C1D-C2D	2.32	130.32	125.49
19	B	838	BCR	C28-C27-C26	-2.32	109.92	114.06
20	G	313	DD6	C8-C6-C5	2.32	122.66	119.01
16	A	817	CLA	CHD-C1D-ND	-2.32	121.54	124.80
20	U	212	DD6	C28-C27-C26	-2.32	119.68	124.18
16	B	809	CLA	CHD-C1D-ND	-2.32	121.54	124.80
16	B	809	CLA	C4A-NA-C1A	2.31	107.73	106.68
16	k	201	CLA	CMD-C2D-C1D	2.31	128.79	124.73
16	A	823	CLA	C4A-NA-C1A	2.31	107.73	106.68
22	A	850	CL0	C4D-CHA-CBD	-2.31	106.64	108.97
16	A	806	CLA	C1-O2A-CGA	2.30	122.22	116.65
16	A	822	CLA	CHD-C1D-C2D	2.30	130.27	125.49
19	B	838	BCR	C7-C8-C9	-2.30	122.83	126.23
19	k	203	BCR	C11-C10-C9	-2.30	124.06	127.28
21	F	806	LMU	C1B-O1B-C4'	-2.30	112.54	117.98
19	B	842	BCR	C16-C15-C14	-2.29	118.84	123.52
16	A	828	CLA	CHD-C1D-ND	-2.29	121.58	124.80
19	B	840	BCR	C2-C1-C6	2.28	113.76	110.44
16	B	836	CLA	CHD-C1D-ND	-2.28	121.60	124.80
19	k	203	BCR	C2-C3-C4	2.28	116.28	111.28
16	B	811	CLA	C4A-NA-C1A	2.27	107.72	106.68
25	U	201	LMG	O1-C7-C8	-2.27	105.30	110.82
16	A	805	CLA	C4A-NA-C1A	2.27	107.71	106.68
16	A	821	CLA	C1D-ND-C4D	2.26	107.90	106.31
16	A	811	CLA	CHD-C1D-ND	-2.25	121.64	124.80
19	A	844	BCR	C29-C30-C25	2.25	113.71	110.44
16	H	303	CLA	CHD-C1D-C2D	2.25	130.16	125.49
16	k	201	CLA	CHD-C1D-C2D	2.25	130.16	125.49
20	U	203	DD6	C13-C11-C10	2.25	122.54	119.01
16	B	819	CLA	C2A-C1A-CHA	2.24	127.76	123.87
16	A	838	CLA	CHD-C1D-C2D	2.24	130.15	125.49
18	A	839	LHG	O8-C6-C5	-2.24	101.93	108.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	844	BCR	C15-C14-C13	-2.24	124.14	127.28
16	B	818	CLA	CHD-C1D-C2D	2.24	130.14	125.49
16	H	302	CLA	CHD-C1D-ND	-2.24	121.65	124.80
16	B	820	CLA	C2A-C1A-CHA	2.24	127.75	123.87
16	U	207	CLA	CHD-C1D-C2D	2.23	130.13	125.49
16	G	305	CLA	C2A-C1A-CHA	2.23	127.74	123.87
19	B	841	BCR	C2-C1-C6	2.23	113.68	110.44
16	K	205	CLA	C1D-ND-C4D	2.23	107.88	106.31
16	B	821	CLA	CHD-C1D-C2D	2.23	130.12	125.49
16	A	809	CLA	CHD-C1D-ND	-2.22	121.67	124.80
16	A	847	CLA	C4A-NA-C1A	2.22	107.69	106.68
19	B	846	BCR	C29-C30-C25	2.22	113.66	110.44
16	U	210	CLA	CHD-C1D-C2D	2.22	130.10	125.49
27	U	213	KC1	CBA-CAA-C2A	2.21	134.34	125.45
16	A	806	CLA	CHD-C1D-C2D	2.21	130.09	125.49
27	U	213	KC1	C1A-NA-C4A	2.21	107.69	106.68
16	G	304	CLA	CHD-C1D-C2D	2.21	130.08	125.49
19	A	844	BCR	C28-C27-C26	-2.21	110.12	114.06
19	B	846	BCR	C27-C26-C25	2.21	125.69	122.70
25	J	103	LMG	O5-C6-C5	-2.21	103.81	111.33
16	A	845	CLA	CHD-C1D-ND	-2.20	121.70	124.80
24	B	843	DGD	O6E-C5E-C4E	2.20	113.67	109.70
16	B	806	CLA	CHD-C1D-ND	-2.20	121.70	124.80
19	A	843	BCR	C29-C30-C25	2.20	113.64	110.44
16	U	204	CLA	CHD-C1D-ND	-2.20	121.70	124.80
19	B	840	BCR	C31-C1-C6	2.20	113.69	110.24
16	H	307	CLA	CHD-C1D-C2D	2.19	130.05	125.49
16	H	308	CLA	CAA-C2A-C3A	-2.19	111.20	116.23
20	U	212	DD6	C34-C35-C36	2.19	117.63	112.18
16	B	817	CLA	CHD-C1D-C2D	2.19	130.04	125.49
16	G	308	CLA	CHD-C1D-C2D	2.19	130.04	125.49
16	A	816	CLA	CHD-C1D-C2D	2.19	130.04	125.49
20	H	311	DD6	C12-C11-C13	2.19	121.43	118.09
16	G	307	CLA	CHD-C1D-C2D	2.19	130.03	125.49
19	B	846	BCR	C16-C15-C14	-2.18	119.05	123.52
16	B	847	CLA	CHD-C1D-C2D	2.18	130.03	125.49
19	B	846	BCR	C17-C16-C15	-2.18	119.69	124.72
16	I	102	CLA	CHD-C1D-C2D	2.17	130.01	125.49
16	G	315	CLA	CMD-C2D-C3D	-2.17	122.71	127.69
16	J	104	CLA	C4A-NA-C1A	2.17	107.67	106.68
16	G	309	CLA	C4A-NA-C1A	2.17	107.67	106.68
25	J	103	LMG	O3-C3-C2	-2.17	105.26	110.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	G	309	CLA	CHD-C1D-C2D	2.17	130.00	125.49
16	H	308	CLA	CHD-C1D-C2D	2.17	130.00	125.49
19	B	840	BCR	C1-C6-C5	-2.17	119.67	122.64
16	K	205	CLA	CHD-C1D-C2D	2.17	130.00	125.49
19	A	841	BCR	C3-C4-C5	-2.17	110.19	114.06
16	B	828	CLA	CAA-C2A-C3A	-2.17	107.15	113.00
16	A	818	CLA	CHD-C1D-ND	-2.16	121.76	124.80
16	A	802	CLA	CHD-C1D-C2D	2.16	129.98	125.49
19	B	838	BCR	C33-C5-C6	-2.16	122.13	124.48
16	G	308	CLA	C4A-NA-C1A	2.16	107.66	106.68
16	G	305	CLA	C3B-C4B-NB	-2.16	108.61	110.53
16	U	211	CLA	CHD-C1D-ND	-2.15	121.77	124.80
16	B	815	CLA	CHD-C1D-C2D	2.15	129.96	125.49
16	B	812	CLA	CHD-C1D-C2D	2.15	129.96	125.49
16	B	820	CLA	C1D-ND-C4D	2.15	107.82	106.31
16	B	836	CLA	C1D-ND-C4D	2.15	107.82	106.31
16	K	204	CLA	CHD-C1D-ND	-2.15	121.78	124.80
21	F	806	LMU	O5'-C5'-C4'	2.15	114.16	109.72
16	G	302	CLA	CAA-C2A-C3A	-2.15	111.31	116.23
19	I	101	BCR	C15-C14-C13	-2.14	124.27	127.28
19	k	203	BCR	C40-C30-C25	2.14	113.61	110.24
19	B	839	BCR	C27-C26-C25	2.14	125.60	122.70
16	A	807	CLA	CAA-C2A-C1A	2.14	119.00	111.97
16	A	801	CLA	C2A-C1A-CHA	2.14	127.58	123.87
16	G	310	CLA	CAA-C2A-C3A	-2.14	107.22	113.00
16	U	208	CLA	CHD-C1D-C2D	2.14	129.94	125.49
16	B	844	CLA	CHD-C1D-ND	-2.14	121.79	124.80
19	B	842	BCR	C15-C16-C17	-2.14	119.14	123.52
16	H	301	CLA	C2A-C1A-CHA	2.14	126.03	122.71
16	A	821	CLA	C2A-C1A-CHA	2.14	127.58	123.87
24	B	843	DGD	C3G-C2G-C1G	-2.13	106.81	111.78
19	I	101	BCR	C29-C30-C25	2.13	113.54	110.44
16	B	824	CLA	CHD-C1D-C2D	2.13	129.92	125.49
16	B	845	CLA	CHD-C1D-ND	-2.13	121.80	124.80
18	A	839	LHG	C27-C26-C25	-2.13	103.60	114.37
16	U	204	CLA	CAA-CBA-CGA	2.13	119.26	113.21
19	A	843	BCR	C15-C16-C17	-2.13	119.16	123.52
16	H	309	CLA	CHD-C1D-C2D	2.13	129.91	125.49
19	B	839	BCR	C28-C27-C26	-2.13	110.27	114.06
20	G	317	DD6	C13-C11-C10	2.12	122.35	119.01
16	B	828	CLA	C2A-C1A-CHA	2.12	127.55	123.87
20	H	311	DD6	C28-C27-C26	-2.12	120.06	124.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	B	820	CLA	CHD-C1D-ND	-2.12	121.82	124.80
16	B	825	CLA	CHD-C1D-ND	-2.12	121.82	124.80
16	A	819	CLA	C4A-NA-C1A	2.12	107.65	106.68
16	B	831	CLA	C4A-NA-C1A	2.12	107.64	106.68
25	U	201	LMG	O2-C2-C1	-2.12	105.03	110.08
19	B	840	BCR	C15-C16-C17	-2.12	119.19	123.52
16	A	827	CLA	CHD-C1D-ND	-2.12	121.83	124.80
16	U	207	CLA	O2A-C1-C2	2.12	116.25	108.11
16	L	203	CLA	CHD-C1D-C2D	2.12	129.89	125.49
20	G	314	DD6	C4-C3-C2	2.11	127.84	123.52
16	B	823	CLA	CHD-C1D-ND	-2.11	121.83	124.80
19	F	801	BCR	C16-C15-C14	-2.11	119.20	123.52
27	U	213	KC1	C1B-CHB-C4A	2.11	130.50	126.02
19	F	805	BCR	C33-C5-C6	-2.11	122.18	124.48
16	B	805	CLA	CHD-C1D-C2D	2.11	129.88	125.49
16	B	829	CLA	CHD-C1D-C2D	2.11	129.87	125.49
16	F	804	CLA	CHD-C1D-C2D	2.11	129.87	125.49
16	A	817	CLA	C1D-ND-C4D	2.11	107.79	106.31
19	B	841	BCR	C8-C7-C6	-2.10	121.38	127.00
16	U	206	CLA	CHD-C1D-C2D	2.10	129.86	125.49
16	K	206	CLA	CHD-C1D-ND	-2.10	121.84	124.80
16	B	804	CLA	C4A-NA-C1A	2.10	107.64	106.68
16	U	208	CLA	O2D-CGD-CBD	2.10	114.91	111.23
16	B	802	CLA	C2A-C1A-CHA	2.10	127.52	123.87
16	U	209	CLA	C2A-C1A-CHA	2.10	127.52	123.87
16	B	810	CLA	CHD-C1D-C2D	2.10	129.86	125.49
16	K	207	CLA	CHD-C1D-C2D	2.10	129.85	125.49
16	B	819	CLA	CHD-C1D-C2D	2.10	129.85	125.49
16	U	211	CLA	CAA-C2A-C1A	2.10	118.85	111.97
19	F	805	BCR	C40-C30-C25	2.10	113.53	110.24
20	U	212	DD6	C12-C11-C13	2.10	121.29	118.09
19	F	805	BCR	C16-C15-C14	-2.10	119.23	123.52
16	K	205	CLA	C3B-C4B-NB	-2.09	108.66	110.53
16	A	833	CLA	CHD-C1D-C2D	2.09	129.84	125.49
20	U	214	DD6	C41-C32-C31	-2.09	106.77	110.52
16	A	813	CLA	CHD-C1D-C2D	2.09	129.84	125.49
16	B	833	CLA	C4A-NA-C1A	2.09	107.63	106.68
16	U	209	CLA	C1D-ND-C4D	2.09	107.78	106.31
19	B	846	BCR	C33-C5-C6	-2.09	122.20	124.48
16	L	204	CLA	CHD-C1D-C2D	2.09	129.83	125.49
16	A	804	CLA	CHD-C1D-C2D	2.09	129.83	125.49
19	k	203	BCR	C7-C8-C9	-2.09	123.15	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	839	LHG	C18-C17-C16	-2.08	103.83	114.37
16	G	306	CLA	CHD-C1D-ND	-2.08	121.87	124.80
20	H	310	DD6	C13-C11-C10	2.08	122.28	119.01
16	G	308	CLA	C6-C5-C3	2.08	118.54	113.47
16	B	849	CLA	CGD-CBD-CAD	-2.08	104.11	110.85
20	U	203	DD6	C15-C14-C13	2.08	130.39	125.99
16	G	305	CLA	CHD-C1D-C2D	2.08	129.81	125.49
16	U	209	CLA	C3B-C4B-NB	-2.07	108.68	110.53
19	B	838	BCR	C24-C23-C22	-2.07	123.17	126.23
16	B	816	CLA	CHD-C1D-C2D	2.07	129.80	125.49
16	B	830	CLA	CHD-C1D-C2D	2.07	129.79	125.49
19	B	846	BCR	C40-C30-C25	2.07	113.49	110.24
16	A	853	CLA	CHD-C1D-C2D	2.07	129.78	125.49
25	U	201	LMG	O7-C10-O9	-2.06	118.88	123.70
16	G	304	CLA	C3B-C4B-NB	-2.06	108.69	110.53
16	A	807	CLA	CHD-C1D-C2D	2.06	129.78	125.49
16	H	312	CLA	C3B-C4B-NB	-2.06	108.69	110.53
19	A	844	BCR	C27-C26-C25	2.06	125.49	122.70
16	B	803	CLA	C2A-C1A-CHA	2.06	127.44	123.87
16	A	838	CLA	O2D-CGD-CBD	2.06	114.83	111.23
19	B	842	BCR	C2-C1-C6	2.06	113.43	110.44
16	G	301	CLA	CHD-C1D-C2D	2.06	129.76	125.49
16	A	824	CLA	CHD-C1D-C2D	2.05	129.76	125.49
16	H	305	CLA	CHD-C1D-ND	-2.05	121.91	124.80
16	A	849	CLA	C1D-ND-C4D	2.05	107.75	106.31
16	A	820	CLA	CHD-C1D-C2D	2.05	129.75	125.49
16	B	826	CLA	CHD-C1D-C2D	2.05	129.75	125.49
16	B	834	CLA	CHD-C1D-C2D	2.05	129.75	125.49
16	K	202	CLA	CHD-C1D-C2D	2.05	129.75	125.49
16	A	827	CLA	C4A-NA-C1A	2.05	107.61	106.68
19	k	203	BCR	C16-C15-C14	-2.05	119.33	123.52
19	I	101	BCR	C10-C11-C12	-2.05	117.27	123.20
19	B	838	BCR	C15-C16-C17	-2.05	119.33	123.52
16	H	303	CLA	C3B-C4B-NB	-2.04	108.71	110.53
16	U	204	CLA	O2A-C1-C2	2.04	115.97	108.11
19	I	101	BCR	C28-C27-C26	-2.04	110.42	114.06
16	L	204	CLA	O2D-CGD-CBD	2.04	114.79	111.23
19	I	103	BCR	C38-C26-C25	-2.04	122.26	124.48
16	A	820	CLA	O2D-CGD-CBD	2.03	114.78	111.23
25	J	103	LMG	O7-C10-O9	-2.03	118.95	123.70
16	K	203	CLA	CHD-C1D-C2D	2.03	129.72	125.49
16	A	851	CLA	C4A-NA-C1A	2.03	107.61	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	842	BCR	C11-C10-C9	-2.03	124.43	127.28
19	B	839	BCR	C24-C23-C22	-2.03	123.24	126.23
16	U	207	CLA	C3A-C2A-C1A	-2.03	98.30	101.34
16	B	833	CLA	CHD-C1D-C2D	2.03	129.70	125.49
16	H	304	CLA	CHD-C1D-C2D	2.02	129.70	125.49
16	A	853	CLA	CAA-CBA-CGA	-2.02	107.47	113.21
16	I	102	CLA	C1D-ND-C4D	2.02	107.73	106.31
16	A	854	CLA	CHD-C1D-C2D	2.02	129.68	125.49
16	H	308	CLA	O2D-CGD-CBD	2.02	114.75	111.23
16	A	810	CLA	CHD-C1D-C2D	2.02	129.68	125.49
19	A	843	BCR	C7-C8-C9	-2.01	123.26	126.23
21	A	855	LMU	O1B-C4'-C3'	2.01	112.34	107.23
16	B	832	CLA	CHD-C1D-C2D	2.01	129.66	125.49
16	B	823	CLA	CAA-C2A-C1A	2.01	118.56	111.97
16	B	813	CLA	CHD-C1D-C2D	2.01	129.66	125.49
16	K	205	CLA	C4B-CHC-C1C	2.01	130.97	126.25
16	A	813	CLA	C3B-C4B-NB	-2.00	108.74	110.53
20	A	846	DD6	C13-C11-C10	2.00	122.16	119.01
16	B	822	CLA	CHD-C1D-ND	-2.00	121.98	124.80
20	K	208	DD6	C33-C32-C31	2.00	113.43	109.49

All (93) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
16	A	802	CLA	ND
16	A	803	CLA	ND
16	A	804	CLA	ND
16	A	805	CLA	ND
16	A	810	CLA	ND
16	A	811	CLA	ND
16	A	812	CLA	ND
16	A	815	CLA	ND
16	A	816	CLA	ND
16	A	817	CLA	ND
16	A	818	CLA	ND
16	A	820	CLA	ND
16	A	821	CLA	ND
16	A	822	CLA	ND
16	A	823	CLA	ND
16	A	824	CLA	ND
16	A	825	CLA	ND
16	A	828	CLA	ND

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Mol	Chain	Res	Type	Atom
16	A	829	CLA	ND
16	A	831	CLA	ND
16	A	832	CLA	ND
16	A	833	CLA	ND
16	A	834	CLA	ND
16	A	835	CLA	ND
16	A	836	CLA	ND
16	A	838	CLA	ND
16	A	845	CLA	ND
16	A	853	CLA	ND
16	A	854	CLA	ND
16	B	801	CLA	ND
16	B	802	CLA	ND
16	B	803	CLA	ND
16	B	804	CLA	ND
16	B	805	CLA	ND
16	B	806	CLA	ND
16	B	807	CLA	ND
16	B	808	CLA	ND
16	B	809	CLA	ND
16	B	812	CLA	ND
16	B	815	CLA	ND
16	B	816	CLA	ND
16	B	820	CLA	ND
16	B	821	CLA	ND
16	B	822	CLA	ND
16	B	823	CLA	ND
16	B	827	CLA	ND
16	B	829	CLA	ND
16	B	830	CLA	ND
16	B	831	CLA	ND
16	B	832	CLA	ND
16	B	833	CLA	ND
16	B	836	CLA	ND
16	B	844	CLA	ND
16	B	845	CLA	ND
16	B	847	CLA	ND
16	B	848	CLA	ND
16	B	849	CLA	ND
16	F	802	CLA	ND
16	F	803	CLA	ND
16	F	804	CLA	ND

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Mol	Chain	Res	Type	Atom
16	I	102	CLA	ND
16	J	104	CLA	ND
16	L	204	CLA	ND
16	U	204	CLA	ND
16	U	206	CLA	ND
16	U	207	CLA	ND
16	U	208	CLA	ND
16	U	209	CLA	ND
16	U	211	CLA	ND
16	G	302	CLA	ND
16	G	303	CLA	ND
16	G	305	CLA	ND
16	G	306	CLA	ND
16	G	310	CLA	ND
16	G	315	CLA	ND
16	H	301	CLA	ND
16	H	302	CLA	ND
16	H	303	CLA	ND
16	H	304	CLA	ND
16	H	305	CLA	ND
16	H	307	CLA	ND
16	H	308	CLA	ND
16	H	309	CLA	ND
16	H	312	CLA	ND
16	K	203	CLA	ND
16	K	204	CLA	ND
16	K	205	CLA	ND
16	K	206	CLA	ND
16	K	207	CLA	ND
16	k	201	CLA	ND
16	k	202	CLA	ND
22	A	850	CL0	ND
22	A	850	CL0	NC

All (905) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
16	A	804	CLA	C1A-C2A-CAA-CBA
16	A	806	CLA	CBA-CGA-O2A-C1
16	A	806	CLA	O1A-CGA-O2A-C1
16	A	806	CLA	CHA-CBD-CGD-O1D
16	A	806	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
16	A	815	CLA	C3A-C2A-CAA-CBA
16	A	820	CLA	CBD-CGD-O2D-CED
16	A	820	CLA	O1D-CGD-O2D-CED
16	A	826	CLA	CHA-CBD-CGD-O1D
16	A	826	CLA	CHA-CBD-CGD-O2D
16	A	838	CLA	CBD-CGD-O2D-CED
16	A	838	CLA	O1D-CGD-O2D-CED
16	A	845	CLA	C4-C3-C5-C6
16	A	853	CLA	CHA-CBD-CGD-O1D
16	A	853	CLA	CHA-CBD-CGD-O2D
16	B	804	CLA	CHA-CBD-CGD-O1D
16	B	804	CLA	CHA-CBD-CGD-O2D
16	B	808	CLA	CHA-CBD-CGD-O1D
16	B	808	CLA	CHA-CBD-CGD-O2D
16	B	820	CLA	CHA-CBD-CGD-O1D
16	B	820	CLA	CHA-CBD-CGD-O2D
16	B	821	CLA	CHA-CBD-CGD-O1D
16	B	821	CLA	CHA-CBD-CGD-O2D
16	B	824	CLA	CBA-CGA-O2A-C1
16	B	824	CLA	O1A-CGA-O2A-C1
16	B	825	CLA	CHA-CBD-CGD-O1D
16	B	825	CLA	CHA-CBD-CGD-O2D
16	B	828	CLA	CHA-CBD-CGD-O1D
16	B	828	CLA	CHA-CBD-CGD-O2D
16	B	847	CLA	C1A-C2A-CAA-CBA
16	B	847	CLA	C3A-C2A-CAA-CBA
16	B	849	CLA	C1A-C2A-CAA-CBA
16	B	849	CLA	C4-C3-C5-C6
16	F	803	CLA	CBA-CGA-O2A-C1
16	F	803	CLA	O1A-CGA-O2A-C1
16	F	804	CLA	C1A-C2A-CAA-CBA
16	J	104	CLA	CAD-CBD-CGD-O1D
16	J	104	CLA	CAD-CBD-CGD-O2D
16	L	202	CLA	C1A-C2A-CAA-CBA
16	L	202	CLA	CBA-CGA-O2A-C1
16	L	202	CLA	O1A-CGA-O2A-C1
16	L	204	CLA	CBD-CGD-O2D-CED
16	L	204	CLA	O1D-CGD-O2D-CED
16	U	208	CLA	CBD-CGD-O2D-CED
16	U	208	CLA	O1D-CGD-O2D-CED
16	U	210	CLA	CHA-CBD-CGD-O2D
16	G	304	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
16	G	304	CLA	C3A-C2A-CAA-CBA
16	G	305	CLA	C2B-C3B-CAB-CBB
16	G	305	CLA	C4B-C3B-CAB-CBB
16	G	306	CLA	C1A-C2A-CAA-CBA
16	G	306	CLA	C3A-C2A-CAA-CBA
16	G	310	CLA	C1A-C2A-CAA-CBA
16	G	310	CLA	CBD-CGD-O2D-CED
16	G	310	CLA	O1D-CGD-O2D-CED
16	H	303	CLA	CBD-CGD-O2D-CED
16	H	303	CLA	O1D-CGD-O2D-CED
16	H	304	CLA	CAA-CBA-CGA-O1A
16	H	306	CLA	C1A-C2A-CAA-CBA
16	H	306	CLA	C3A-C2A-CAA-CBA
16	H	307	CLA	CHA-CBD-CGD-O1D
16	H	307	CLA	CHA-CBD-CGD-O2D
16	H	308	CLA	CBD-CGD-O2D-CED
16	H	308	CLA	O1D-CGD-O2D-CED
16	H	309	CLA	C1A-C2A-CAA-CBA
16	H	312	CLA	C2B-C3B-CAB-CBB
16	H	312	CLA	C4B-C3B-CAB-CBB
16	H	312	CLA	CBD-CGD-O2D-CED
16	H	312	CLA	O2A-C1-C2-C3
16	H	312	CLA	C1-C2-C3-C4
16	H	312	CLA	C1-C2-C3-C5
16	K	207	CLA	C1A-C2A-CAA-CBA
18	A	840	LHG	C3-O3-P-O5
18	G	316	LHG	C3-O3-P-O4
18	G	316	LHG	C3-O3-P-O5
18	G	316	LHG	C3-O3-P-O6
18	G	316	LHG	C4-O6-P-O3
19	A	841	BCR	C20-C21-C22-C37
19	A	841	BCR	C21-C22-C23-C24
19	A	842	BCR	C7-C8-C9-C10
19	A	842	BCR	C21-C22-C23-C24
19	A	843	BCR	C7-C8-C9-C10
19	A	843	BCR	C7-C8-C9-C34
19	A	844	BCR	C20-C21-C22-C37
19	A	844	BCR	C21-C22-C23-C24
19	B	839	BCR	C6-C7-C8-C9
19	B	839	BCR	C37-C22-C23-C24
19	B	846	BCR	C16-C17-C18-C19
19	B	846	BCR	C20-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
19	B	846	BCR	C20-C21-C22-C37
19	F	801	BCR	C7-C8-C9-C10
19	F	801	BCR	C7-C8-C9-C34
19	F	801	BCR	C37-C22-C23-C24
19	F	805	BCR	C7-C8-C9-C34
19	I	103	BCR	C7-C8-C9-C10
19	I	103	BCR	C7-C8-C9-C34
19	I	103	BCR	C20-C21-C22-C37
19	I	103	BCR	C37-C22-C23-C24
19	I	103	BCR	C23-C24-C25-C26
19	J	105	BCR	C7-C8-C9-C10
19	J	105	BCR	C21-C22-C23-C24
19	J	105	BCR	C37-C22-C23-C24
19	L	201	BCR	C21-C22-C23-C24
19	L	201	BCR	C37-C22-C23-C24
19	L	205	BCR	C22-C23-C24-C25
19	M	101	BCR	C7-C8-C9-C10
19	M	101	BCR	C7-C8-C9-C34
19	k	203	BCR	C6-C7-C8-C9
19	k	203	BCR	C7-C8-C9-C10
19	k	203	BCR	C7-C8-C9-C34
19	k	203	BCR	C10-C11-C12-C13
20	A	846	DD6	C9-C10-C11-C12
20	A	846	DD6	C9-C10-C11-C13
20	A	846	DD6	C10-C11-C13-C14
20	A	846	DD6	C12-C11-C13-C14
20	A	846	DD6	C5-C6-C8-C9
20	A	846	DD6	C7-C6-C8-C9
20	U	203	DD6	C1-C24-C25-C26
20	U	203	DD6	C2-C3-C4-C5
20	U	203	DD6	C3-C4-C5-C6
20	U	212	DD6	C11-C13-C14-C15
20	U	212	DD6	C5-C6-C8-C9
20	U	212	DD6	C7-C6-C8-C9
20	U	214	DD6	C2-C3-C4-C5
20	G	311	DD6	C9-C10-C11-C12
20	G	311	DD6	C9-C10-C11-C13
20	G	311	DD6	C11-C13-C14-C15
20	G	311	DD6	C2-C3-C4-C5
20	G	311	DD6	C4-C5-C6-C7
20	G	311	DD6	C4-C5-C6-C8
20	G	312	DD6	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
20	G	312	DD6	C4-C5-C6-C7
20	G	314	DD6	C2-C1-C24-C25
20	G	314	DD6	C9-C10-C11-C12
20	G	314	DD6	C9-C10-C11-C13
20	G	317	DD6	C-C1-C24-C25
20	G	317	DD6	C2-C1-C24-C25
20	G	317	DD6	C10-C11-C13-C14
20	G	317	DD6	C12-C11-C13-C14
20	G	317	DD6	C24-C25-C26-C27
20	G	317	DD6	C2-C3-C4-C5
20	G	317	DD6	C4-C5-C6-C7
20	H	310	DD6	C9-C10-C11-C12
20	H	310	DD6	C9-C10-C11-C13
20	H	310	DD6	C10-C11-C13-C14
20	H	310	DD6	C12-C11-C13-C14
20	H	310	DD6	C11-C13-C14-C15
20	H	310	DD6	C4-C5-C6-C7
20	H	310	DD6	C4-C5-C6-C8
20	H	310	DD6	C5-C6-C8-C9
20	H	311	DD6	C10-C11-C13-C14
20	H	311	DD6	C12-C11-C13-C14
20	H	311	DD6	C13-C14-C15-O1
20	H	311	DD6	C4-C5-C6-C7
20	H	311	DD6	C4-C5-C6-C8
20	K	208	DD6	C2-C3-C4-C5
20	K	208	DD6	C4-C5-C6-C7
20	K	208	DD6	C4-C5-C6-C8
20	K	208	DD6	C5-C6-C8-C9
20	K	208	DD6	C7-C6-C8-C9
21	A	855	LMU	C2-C1-O1'-C1'
25	J	103	LMG	O6-C1-O1-C7
25	U	201	LMG	C11-C10-O7-C8
26	U	202	A86	C10-C11-C13-O
26	U	202	A86	C12-C11-C13-O
26	U	202	A86	C1-C24-C25-C26
26	U	202	A86	C2-C3-C4-C5
26	U	202	A86	C4-C5-C6-C7
26	U	202	A86	C4-C5-C6-C8
26	U	202	A86	C5-C6-C8-C9
26	U	202	A86	C7-C6-C8-C9
26	U	202	A86	C6-C8-C9-C10
16	H	312	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
26	U	202	A86	C39-C38-O4-C34
21	A	855	LMU	O5B-C1B-O1B-C4'
16	H	312	CLA	O1A-CGA-O2A-C1
16	H	312	CLA	CBA-CGA-O2A-C1
25	U	201	LMG	C4-C5-C6-O5
25	J	103	LMG	O9-C10-O7-C8
25	U	201	LMG	O9-C10-O7-C8
16	B	849	CLA	C3-C5-C6-C7
16	G	307	CLA	C4-C3-C5-C6
16	H	306	CLA	C4-C3-C5-C6
16	A	845	CLA	C2-C3-C5-C6
16	B	835	CLA	C2-C3-C5-C6
16	B	849	CLA	C2-C3-C5-C6
16	H	306	CLA	C2-C3-C5-C6
16	A	836	CLA	C3-C5-C6-C7
19	B	846	BCR	C17-C18-C19-C20
24	B	843	DGD	O6E-C5E-C6E-O5E
19	B	846	BCR	C19-C20-C21-C22
20	U	212	DD6	C24-C25-C26-C27
20	G	313	DD6	C24-C25-C26-C27
16	B	817	CLA	C3-C5-C6-C7
16	B	820	CLA	C3-C5-C6-C7
22	A	850	CL0	CBD-CGD-O2D-CED
18	G	316	LHG	O2-C2-C3-O3
21	A	855	LMU	O5'-C5'-C6'-O6'
25	U	201	LMG	O6-C5-C6-O5
18	A	840	LHG	C8-C7-O7-C5
21	K	201	LMU	O5'-C5'-C6'-O6'
20	H	311	DD6	C2-C3-C4-C5
16	K	203	CLA	C3-C5-C6-C7
24	B	843	DGD	C4E-C5E-C6E-O5E
16	B	835	CLA	C4-C3-C5-C6
16	G	307	CLA	C2-C3-C5-C6
21	A	848	LMU	O5B-C5B-C6B-O6B
21	F	806	LMU	O5'-C5'-C6'-O6'
16	A	825	CLA	C2A-CAA-CBA-CGA
21	A	855	LMU	O5'-C1'-O1'-C1
25	U	201	LMG	O6-C1-O1-C7
25	J	103	LMG	O6-C5-C6-O5
20	U	203	DD6	C1-C2-C3-C4
20	U	203	DD6	C24-C25-C26-C27
20	H	310	DD6	C24-C25-C26-C27

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Mol	Chain	Res	Type	Atoms
18	G	316	LHG	C1-C2-C3-O3
25	J	103	LMG	C29-C28-O8-C9
21	F	806	LMU	C4'-C5'-C6'-O6'
16	H	303	CLA	C4-C3-C5-C6
16	H	303	CLA	C2-C3-C5-C6
16	H	312	CLA	C6-C7-C8-C9
21	A	848	LMU	C4B-C5B-C6B-O6B
26	U	202	A86	O5-C38-O4-C34
21	A	855	LMU	C2'-C1'-O1'-C1
25	J	103	LMG	C2-C1-O1-C7
25	U	201	LMG	C2-C1-O1-C7
18	A	839	LHG	C23-C24-C25-C26
19	A	842	BCR	C7-C8-C9-C34
19	A	844	BCR	C7-C8-C9-C34
19	A	844	BCR	C37-C22-C23-C24
19	B	838	BCR	C7-C8-C9-C34
19	B	838	BCR	C37-C22-C23-C24
19	B	839	BCR	C7-C8-C9-C34
19	B	846	BCR	C7-C8-C9-C34
19	F	805	BCR	C37-C22-C23-C24
19	I	101	BCR	C11-C12-C13-C35
19	J	105	BCR	C7-C8-C9-C34
19	J	105	BCR	C11-C12-C13-C35
19	k	203	BCR	C37-C22-C23-C24
20	G	313	DD6	C-C1-C24-C25
20	G	314	DD6	C-C1-C24-C25
20	G	314	DD6	C12-C11-C13-C14
20	H	310	DD6	C-C1-C24-C25
20	H	310	DD6	C7-C6-C8-C9
19	B	839	BCR	C21-C22-C23-C24
19	B	846	BCR	C7-C8-C9-C10
19	I	103	BCR	C21-C22-C23-C24
20	G	313	DD6	C2-C1-C24-C25
20	H	310	DD6	C2-C1-C24-C25
16	H	312	CLA	C2A-CAA-CBA-CGA
16	A	824	CLA	C10-C11-C12-C13
21	A	855	LMU	C4'-C5'-C6'-O6'
20	A	846	DD6	C3-C4-C5-C6
20	U	214	DD6	C1-C2-C3-C4
20	U	214	DD6	C3-C4-C5-C6
16	B	832	CLA	C13-C15-C16-C17
16	B	814	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
16	G	305	CLA	C2A-CAA-CBA-CGA
16	H	302	CLA	C2A-CAA-CBA-CGA
20	J	102	DD6	C1-C24-C25-C26
20	G	314	DD6	C1-C24-C25-C26
16	A	822	CLA	C13-C15-C16-C17
16	H	312	CLA	C15-C16-C17-C18
16	B	817	CLA	C8-C10-C11-C12
16	B	848	CLA	C13-C15-C16-C17
21	K	201	LMU	O1'-C1-C2-C3
16	A	811	CLA	C10-C11-C12-C13
22	A	850	CL0	O1D-CGD-O2D-CED
16	A	801	CLA	C8-C10-C11-C12
16	B	831	CLA	C5-C6-C7-C8
16	H	312	CLA	C8-C10-C11-C12
18	A	839	LHG	C28-C29-C30-C31
20	A	846	DD6	C1-C2-C3-C4
16	A	845	CLA	C2A-CAA-CBA-CGA
22	A	850	CL0	C3-C5-C6-C7
16	A	824	CLA	C5-C6-C7-C8
16	A	854	CLA	C15-C16-C17-C18
16	A	849	CLA	C4-C3-C5-C6
16	B	844	CLA	C10-C11-C12-C13
21	F	806	LMU	O1'-C1-C2-C3
21	K	201	LMU	C2'-C1'-O1'-C1
19	A	842	BCR	C20-C21-C22-C37
19	B	839	BCR	C20-C21-C22-C37
19	B	842	BCR	C11-C10-C9-C34
19	B	842	BCR	C20-C21-C22-C37
19	B	846	BCR	C35-C13-C14-C15
19	F	805	BCR	C20-C21-C22-C37
19	I	101	BCR	C20-C21-C22-C37
19	k	203	BCR	C16-C17-C18-C36
20	U	212	DD6	C4-C5-C6-C7
20	G	317	DD6	C9-C10-C11-C12
20	H	311	DD6	C9-C10-C11-C12
20	K	208	DD6	C9-C10-C11-C12
26	U	202	A86	C-C1-C2-C3
19	A	842	BCR	C37-C22-C23-C24
20	J	102	DD6	C12-C11-C13-C14
20	U	203	DD6	C-C1-C24-C25
20	U	212	DD6	C12-C11-C13-C14
20	K	208	DD6	C-C1-C24-C25

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Mol	Chain	Res	Type	Atoms
19	B	838	BCR	C7-C8-C9-C10
19	B	839	BCR	C7-C8-C9-C10
20	J	102	DD6	C10-C11-C13-C14
20	U	203	DD6	C2-C1-C24-C25
20	G	314	DD6	C10-C11-C13-C14
25	J	103	LMG	C4-C5-C6-O5
16	A	814	CLA	C2A-CAA-CBA-CGA
16	B	820	CLA	C2A-CAA-CBA-CGA
16	B	834	CLA	C2A-CAA-CBA-CGA
16	B	847	CLA	C2A-CAA-CBA-CGA
16	A	847	CLA	C8-C10-C11-C12
25	J	103	LMG	O10-C28-O8-C9
19	A	841	BCR	C20-C21-C22-C23
19	A	844	BCR	C20-C21-C22-C23
19	I	101	BCR	C20-C21-C22-C23
19	I	103	BCR	C20-C21-C22-C23
19	L	201	BCR	C20-C21-C22-C23
20	U	212	DD6	C4-C5-C6-C8
20	G	312	DD6	C4-C5-C6-C8
20	G	317	DD6	C9-C10-C11-C13
20	G	317	DD6	C4-C5-C6-C8
20	H	311	DD6	C9-C10-C11-C13
20	K	208	DD6	C9-C10-C11-C13
26	U	202	A86	C24-C1-C2-C3
25	J	103	LMG	C11-C10-O7-C8
21	K	201	LMU	C4'-C5'-C6'-O6'
21	A	848	LMU	C1-C2-C3-C4
24	B	843	DGD	C1B-C2B-C3B-C4B
16	K	205	CLA	C2-C1-O2A-CGA
16	B	834	CLA	C16-C17-C18-C20
20	J	102	DD6	C2-C3-C4-C5
20	U	212	DD6	C2-C3-C4-C5
20	G	313	DD6	C2-C3-C4-C5
21	A	848	LMU	C4-C5-C6-C7
18	A	839	LHG	C24-C25-C26-C27
21	A	848	LMU	C7-C8-C9-C10
25	J	103	LMG	C20-C21-C22-C23
16	B	834	CLA	C16-C17-C18-C19
16	B	848	CLA	C15-C16-C17-C18
16	A	807	CLA	C3-C5-C6-C7
16	A	804	CLA	C3A-C2A-CAA-CBA
16	F	804	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
16	G	303	CLA	C3A-C2A-CAA-CBA
16	K	204	CLA	C3A-C2A-CAA-CBA
21	F	806	LMU	C5-C6-C7-C8
20	H	310	DD6	C1-C2-C3-C4
24	B	843	DGD	C3B-C4B-C5B-C6B
18	A	840	LHG	O9-C7-O7-C5
21	A	855	LMU	C2-C3-C4-C5
24	B	843	DGD	C7B-C8B-C9B-CAB
18	A	839	LHG	C10-C11-C12-C13
24	B	843	DGD	CEB-CFB-CGB-CHB
21	A	848	LMU	C11-C10-C9-C8
24	B	843	DGD	C5A-C6A-C7A-C8A
19	A	844	BCR	C1-C6-C7-C8
19	B	839	BCR	C1-C6-C7-C8
19	B	839	BCR	C5-C6-C7-C8
19	I	103	BCR	C23-C24-C25-C30
19	k	203	BCR	C1-C6-C7-C8
16	B	828	CLA	C3-C5-C6-C7
16	L	204	CLA	C2A-CAA-CBA-CGA
19	F	805	BCR	C10-C11-C12-C13
20	U	212	DD6	C1-C24-C25-C26
18	A	839	LHG	C27-C28-C29-C30
25	U	201	LMG	C29-C30-C31-C32
21	K	201	LMU	O5'-C1'-O1'-C1
24	B	843	DGD	O6E-C1E-O5D-C6D
25	J	103	LMG	C13-C14-C15-C16
16	G	306	CLA	C16-C17-C18-C20
20	H	311	DD6	C7-C6-C8-C9
18	A	839	LHG	C9-C10-C11-C12
21	J	101	LMU	C6-C7-C8-C9
16	A	807	CLA	C2A-CAA-CBA-CGA
21	F	806	LMU	C4-C5-C6-C7
24	B	843	DGD	CAB-CBB-CCB-CDB
16	A	823	CLA	C4-C3-C5-C6
16	B	808	CLA	C3-C5-C6-C7
24	B	843	DGD	C4A-C5A-C6A-C7A
25	J	103	LMG	C15-C16-C17-C18
21	J	101	LMU	O5B-C5B-C6B-O6B
25	J	103	LMG	O7-C8-C9-O8
21	J	101	LMU	C7-C8-C9-C10
16	A	853	CLA	C4-C3-C5-C6
16	G	309	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
16	A	823	CLA	C2-C3-C5-C6
18	G	316	LHG	C23-C24-C25-C26
19	B	846	BCR	C15-C16-C17-C18
16	A	813	CLA	C1A-C2A-CAA-CBA
16	A	815	CLA	C1A-C2A-CAA-CBA
16	B	812	CLA	C1A-C2A-CAA-CBA
16	U	204	CLA	C1A-C2A-CAA-CBA
16	G	303	CLA	C1A-C2A-CAA-CBA
16	K	204	CLA	C1A-C2A-CAA-CBA
16	B	835	CLA	C15-C16-C17-C18
18	A	839	LHG	C32-C33-C34-C35
16	H	306	CLA	C13-C15-C16-C17
16	B	823	CLA	C6-C7-C8-C10
16	I	102	CLA	C11-C12-C13-C15
16	G	305	CLA	C11-C10-C8-C7
16	G	305	CLA	C11-C12-C13-C15
24	B	843	DGD	CDB-CEB-CFB-CGB
16	A	853	CLA	C2-C3-C5-C6
18	G	316	LHG	C7-C8-C9-C10
16	A	806	CLA	C2A-CAA-CBA-CGA
17	B	837	PQN	C23-C25-C26-C27
24	B	843	DGD	O1G-C1G-C2G-C3G
25	J	103	LMG	C19-C20-C21-C22
19	B	838	BCR	C20-C21-C22-C37
19	L	205	BCR	C7-C8-C9-C34
20	U	203	DD6	C12-C11-C13-C14
19	L	205	BCR	C7-C8-C9-C10
20	U	203	DD6	C10-C11-C13-C14
20	K	208	DD6	C2-C1-C24-C25
16	U	205	CLA	C8-C10-C11-C12
18	G	316	LHG	O1-C1-C2-C3
25	J	103	LMG	C7-C8-O7-C10
19	B	838	BCR	C10-C11-C12-C13
18	A	839	LHG	C30-C31-C32-C33
19	A	842	BCR	C20-C21-C22-C23
19	B	846	BCR	C12-C13-C14-C15
16	U	205	CLA	C4-C3-C5-C6
16	A	849	CLA	C2-C3-C5-C6
16	U	205	CLA	C2-C3-C5-C6
25	U	201	LMG	O1-C7-C8-O7
25	J	103	LMG	C18-C19-C20-C21
20	G	314	DD6	C11-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
20	G	317	DD6	C11-C13-C14-C15
19	I	101	BCR	C14-C15-C16-C17
16	A	834	CLA	C4-C3-C5-C6
20	J	102	DD6	C27-C29-C30-C31
20	G	317	DD6	C27-C29-C30-C31
16	B	823	CLA	C6-C7-C8-C9
16	U	204	CLA	C6-C7-C8-C9
16	U	204	CLA	C11-C10-C8-C9
16	G	305	CLA	C11-C10-C8-C9
16	G	305	CLA	C11-C12-C13-C14
21	K	201	LMU	C2B-C1B-O1B-C4'
16	B	813	CLA	C5-C6-C7-C8
25	U	201	LMG	C31-C32-C33-C34
16	B	801	CLA	C2A-CAA-CBA-CGA
24	B	843	DGD	C2E-C1E-O5D-C6D
18	G	316	LHG	C8-C7-O7-C5
16	A	825	CLA	C12-C13-C15-C16
16	B	835	CLA	C11-C12-C13-C15
16	U	204	CLA	C6-C7-C8-C10
16	G	306	CLA	C11-C12-C13-C15
21	K	201	LMU	O5B-C1B-O1B-C4'
21	J	101	LMU	O1'-C1-C2-C3
16	A	854	CLA	C4-C3-C5-C6
16	L	202	CLA	C3A-C2A-CAA-CBA
16	U	204	CLA	C3A-C2A-CAA-CBA
19	L	205	BCR	C9-C10-C11-C12
20	G	311	DD6	C24-C25-C26-C27
20	K	208	DD6	C24-C25-C26-C27
16	B	814	CLA	C3-C5-C6-C7
25	U	201	LMG	C12-C13-C14-C15
16	A	820	CLA	C4-C3-C5-C6
16	B	835	CLA	C10-C11-C12-C13
18	G	316	LHG	C4-C5-C6-O8
25	U	201	LMG	O1-C7-C8-C9
21	K	201	LMU	C2-C3-C4-C5
16	G	306	CLA	C16-C17-C18-C19
16	B	811	CLA	C5-C6-C7-C8
25	J	103	LMG	C11-C12-C13-C14
16	A	818	CLA	C4-C3-C5-C6
16	A	821	CLA	C4-C3-C5-C6
16	B	811	CLA	C4-C3-C5-C6
16	A	834	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
25	U	201	LMG	C30-C31-C32-C33
18	G	316	LHG	O6-C4-C5-O7
19	A	841	BCR	C23-C24-C25-C30
19	A	842	BCR	C1-C6-C7-C8
19	A	843	BCR	C1-C6-C7-C8
19	A	844	BCR	C23-C24-C25-C30
19	B	838	BCR	C1-C6-C7-C8
19	B	841	BCR	C23-C24-C25-C30
19	B	846	BCR	C1-C6-C7-C8
19	B	846	BCR	C23-C24-C25-C30
19	F	805	BCR	C1-C6-C7-C8
19	I	103	BCR	C1-C6-C7-C8
19	L	201	BCR	C1-C6-C7-C8
19	L	201	BCR	C23-C24-C25-C30
19	L	205	BCR	C23-C24-C25-C30
19	M	101	BCR	C1-C6-C7-C8
19	M	101	BCR	C23-C24-C25-C30
21	F	806	LMU	C3-C4-C5-C6
16	B	844	CLA	C8-C10-C11-C12
18	G	316	LHG	O7-C5-C6-O8
24	B	843	DGD	C9A-CAA-CBA-CCA
25	J	103	LMG	C14-C15-C16-C17
16	A	806	CLA	C4-C3-C5-C6
20	G	313	DD6	C1-C24-C25-C26
16	A	834	CLA	C2-C3-C5-C6
16	A	825	CLA	C14-C13-C15-C16
16	G	306	CLA	C11-C12-C13-C14
16	H	312	CLA	C11-C10-C8-C9
16	G	305	CLA	C8-C10-C11-C12
25	J	103	LMG	C17-C18-C19-C20
16	A	821	CLA	C2-C3-C5-C6
16	A	854	CLA	C2-C3-C5-C6
16	B	823	CLA	C2-C3-C5-C6
16	B	806	CLA	C10-C11-C12-C13
21	A	848	LMU	C2-C3-C4-C5
19	B	841	BCR	C20-C21-C22-C37
19	J	105	BCR	C20-C21-C22-C37
20	G	312	DD6	C9-C10-C11-C12
18	A	839	LHG	C26-C27-C28-C29
24	B	843	DGD	C3A-C4A-C5A-C6A
18	G	316	LHG	O6-C4-C5-C6
16	G	306	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
17	A	837	PQN	C17-C18-C20-C21
16	U	204	CLA	C10-C11-C12-C13
19	B	841	BCR	C17-C18-C19-C20
19	B	842	BCR	C21-C22-C23-C24
19	F	801	BCR	C21-C22-C23-C24
25	U	201	LMG	C29-C28-O8-C9
16	G	305	CLA	C14-C13-C15-C16
18	G	316	LHG	O9-C7-O7-C5
16	B	823	CLA	C4-C3-C5-C6
16	H	307	CLA	C4-C3-C5-C6
16	B	811	CLA	C2-C3-C5-C6
16	B	811	CLA	O2A-C1-C2-C3
16	I	102	CLA	O2A-C1-C2-C3
21	A	848	LMU	C9-C10-C11-C12
19	B	839	BCR	C20-C21-C22-C23
22	A	850	CL0	C8-C10-C11-C12
21	J	101	LMU	O5'-C1'-O1'-C1
16	A	825	CLA	C4-C3-C5-C6
16	G	309	CLA	C4-C3-C5-C6
24	B	843	DGD	O1G-C1G-C2G-O2G
16	A	804	CLA	C11-C12-C13-C14
21	K	201	LMU	C3-C4-C5-C6
26	U	202	A86	C13-C14-C15-O1
21	A	848	LMU	C3-C4-C5-C6
24	B	843	DGD	C8B-C9B-CAB-CBB
16	H	312	CLA	C16-C17-C18-C19
24	B	843	DGD	C2B-C3B-C4B-C5B
16	A	825	CLA	C2-C3-C5-C6
18	G	316	LHG	C24-C23-O8-C6
20	U	212	DD6	C27-C29-C30-C31
20	G	313	DD6	C27-C29-C30-C31
21	F	806	LMU	C2-C1-O1'-C1'
16	B	823	CLA	C1A-C2A-CAA-CBA
19	B	846	BCR	C22-C23-C24-C25
19	M	101	BCR	C6-C7-C8-C9
20	U	212	DD6	C10-C11-C13-C14
24	B	843	DGD	C6A-C7A-C8A-C9A
24	B	843	DGD	C2A-C1A-O1G-C1G
18	A	839	LHG	C29-C30-C31-C32
18	G	316	LHG	O10-C23-O8-C6
24	B	843	DGD	O1A-C1A-O1G-C1G
16	G	305	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
16	G	306	CLA	C6-C7-C8-C9
21	K	201	LMU	C4B-C5B-C6B-O6B
21	J	101	LMU	C5-C6-C7-C8
20	H	310	DD6	C3-C4-C5-C6
20	H	311	DD6	C3-C4-C5-C6
16	A	805	CLA	C1-C2-C3-C4
16	B	827	CLA	C1-C2-C3-C4
16	A	821	CLA	C8-C10-C11-C12
16	G	308	CLA	C6-C7-C8-C10
25	J	103	LMG	C7-C8-C9-O8
16	A	803	CLA	CAD-CBD-CGD-O2D
16	U	207	CLA	CAD-CBD-CGD-O2D
16	H	312	CLA	C3-C5-C6-C7
16	B	828	CLA	C5-C6-C7-C8
16	A	803	CLA	CAD-CBD-CGD-O1D
16	A	821	CLA	CHA-CBD-CGD-O1D
16	A	821	CLA	CHA-CBD-CGD-O2D
16	A	822	CLA	CHA-CBD-CGD-O1D
16	A	827	CLA	CHA-CBD-CGD-O1D
16	A	827	CLA	CHA-CBD-CGD-O2D
16	A	829	CLA	CHA-CBD-CGD-O1D
16	A	829	CLA	CHA-CBD-CGD-O2D
16	B	813	CLA	CHA-CBD-CGD-O1D
16	B	813	CLA	CHA-CBD-CGD-O2D
16	U	207	CLA	CAD-CBD-CGD-O1D
16	U	210	CLA	CHA-CBD-CGD-O1D
16	G	304	CLA	CHA-CBD-CGD-O1D
16	G	304	CLA	CHA-CBD-CGD-O2D
18	A	839	LHG	C3-O3-P-O5
18	G	316	LHG	C4-O6-P-O5
19	B	841	BCR	C1-C6-C7-C8
19	B	842	BCR	C1-C6-C7-C8
19	F	801	BCR	C1-C6-C7-C8
16	A	815	CLA	CAA-CBA-CGA-O2A
19	M	101	BCR	C37-C22-C23-C24
16	G	305	CLA	C12-C13-C15-C16
16	L	202	CLA	O2A-C1-C2-C3
16	A	818	CLA	C2-C3-C5-C6
16	G	309	CLA	C2-C3-C5-C6
16	A	824	CLA	C14-C13-C15-C16
16	I	102	CLA	C11-C10-C8-C9
16	H	302	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
17	A	837	PQN	C19-C18-C20-C21
16	A	834	CLA	C6-C7-C8-C10
16	G	305	CLA	C6-C7-C8-C10
19	B	846	BCR	C11-C10-C9-C8
21	J	101	LMU	C2-C3-C4-C5
16	G	307	CLA	C11-C12-C13-C15
19	F	801	BCR	C14-C15-C16-C17
21	J	101	LMU	C2'-C1'-O1'-C1
16	B	814	CLA	C4-C3-C5-C6
18	A	839	LHG	C24-C23-O8-C6
16	A	828	CLA	C16-C17-C18-C20
16	H	312	CLA	C16-C17-C18-C20
16	A	804	CLA	C3-C5-C6-C7
16	U	204	CLA	C3-C5-C6-C7
26	U	202	A86	C1-C2-C3-C4
16	A	851	CLA	C4-C3-C5-C6
16	B	814	CLA	C2-C3-C5-C6
18	A	840	LHG	C10-C11-C12-C13
21	K	201	LMU	C2-C1-O1'-C1'
16	B	835	CLA	C11-C12-C13-C14
18	G	316	LHG	C5-C4-O6-P
16	A	804	CLA	C4-C3-C5-C6
16	B	808	CLA	C4-C3-C5-C6
21	A	855	LMU	C3-C4-C5-C6
16	A	851	CLA	C2-C3-C5-C6
16	H	302	CLA	C11-C10-C8-C7
16	G	315	CLA	CAA-CBA-CGA-O2A
16	B	805	CLA	C15-C16-C17-C18
16	A	853	CLA	C3A-C2A-CAA-CBA
16	B	805	CLA	C3A-C2A-CAA-CBA
16	B	814	CLA	C3A-C2A-CAA-CBA
16	B	849	CLA	C3A-C2A-CAA-CBA
16	G	310	CLA	C3A-C2A-CAA-CBA
16	K	207	CLA	C3A-C2A-CAA-CBA
19	B	840	BCR	C20-C21-C22-C37
19	F	801	BCR	C20-C21-C22-C37
19	F	805	BCR	C35-C13-C14-C15
19	L	201	BCR	C11-C10-C9-C34
20	G	314	DD6	C-C1-C2-C3
16	A	807	CLA	C5-C6-C7-C8
16	G	307	CLA	C8-C10-C11-C12
16	B	809	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
16	U	211	CLA	C4-C3-C5-C6
16	B	848	CLA	C2C-C3C-CAC-CBC
16	A	849	CLA	C11-C10-C8-C9
16	B	817	CLA	C14-C13-C15-C16
16	B	844	CLA	C11-C10-C8-C9
16	H	307	CLA	C6-C7-C8-C9
16	A	834	CLA	C13-C15-C16-C17
16	G	303	CLA	CAA-CBA-CGA-O1A
16	U	211	CLA	C2-C3-C5-C6
18	G	316	LHG	O1-C1-C2-O2
16	A	853	CLA	C1A-C2A-CAA-CBA
16	B	805	CLA	C1A-C2A-CAA-CBA
19	B	840	BCR	C20-C21-C22-C23
19	F	805	BCR	C12-C13-C14-C15
19	L	201	BCR	C11-C10-C9-C8
20	G	314	DD6	C24-C1-C2-C3
16	G	315	CLA	CAA-CBA-CGA-O1A
18	A	839	LHG	O6-C4-C5-O7
18	A	840	LHG	O6-C4-C5-O7
16	B	829	CLA	C10-C11-C12-C13
19	A	841	BCR	C1-C6-C7-C8
19	A	841	BCR	C23-C24-C25-C26
19	A	842	BCR	C5-C6-C7-C8
19	A	842	BCR	C23-C24-C25-C30
19	A	843	BCR	C5-C6-C7-C8
19	A	844	BCR	C5-C6-C7-C8
19	A	844	BCR	C23-C24-C25-C26
19	B	838	BCR	C5-C6-C7-C8
19	B	838	BCR	C23-C24-C25-C30
19	B	841	BCR	C5-C6-C7-C8
19	B	841	BCR	C23-C24-C25-C26
19	B	842	BCR	C5-C6-C7-C8
19	B	842	BCR	C23-C24-C25-C30
19	B	846	BCR	C5-C6-C7-C8
19	B	846	BCR	C23-C24-C25-C26
19	F	805	BCR	C5-C6-C7-C8
19	I	103	BCR	C5-C6-C7-C8
19	L	201	BCR	C5-C6-C7-C8
19	L	201	BCR	C23-C24-C25-C26
19	L	205	BCR	C23-C24-C25-C26
19	M	101	BCR	C5-C6-C7-C8
19	k	203	BCR	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
19	k	203	BCR	C23-C24-C25-C30
16	H	309	CLA	CAA-CBA-CGA-O2A
16	B	847	CLA	C4-C3-C5-C6
16	B	808	CLA	C2-C3-C5-C6
16	G	301	CLA	CAA-CBA-CGA-O2A
16	A	804	CLA	C11-C12-C13-C15
16	A	815	CLA	C2A-CAA-CBA-CGA
16	G	309	CLA	C2A-CAA-CBA-CGA
16	K	207	CLA	C2A-CAA-CBA-CGA
17	A	837	PQN	C18-C20-C21-C22
24	B	843	DGD	O2G-C2G-C3G-O3G
16	G	303	CLA	CAA-CBA-CGA-O2A
20	G	312	DD6	C12-C11-C13-C14
16	A	831	CLA	CAA-CBA-CGA-O2A
16	B	806	CLA	C4-C3-C5-C6
16	B	807	CLA	C4-C3-C5-C6
16	A	804	CLA	C2-C3-C5-C6
16	B	809	CLA	C2-C3-C5-C6
16	H	309	CLA	CAA-CBA-CGA-O1A
16	A	845	CLA	C10-C11-C12-C13
16	K	204	CLA	CAA-CBA-CGA-O2A
16	B	805	CLA	C11-C10-C8-C9
20	G	314	DD6	C24-C25-C26-C27
16	G	301	CLA	CAA-CBA-CGA-O1A
24	B	843	DGD	CBB-CCB-CDB-CEB
16	B	801	CLA	C4-C3-C5-C6
18	G	316	LHG	C2-C3-O3-P
16	A	831	CLA	CAA-CBA-CGA-O1A
16	B	803	CLA	C2A-CAA-CBA-CGA
16	B	815	CLA	C10-C11-C12-C13
16	K	204	CLA	CAA-CBA-CGA-O1A
20	A	846	DD6	C27-C29-C30-C31
20	H	310	DD6	C27-C29-C30-C31
16	K	205	CLA	C4-C3-C5-C6
16	B	815	CLA	CAA-CBA-CGA-O2A
16	B	847	CLA	C2-C3-C5-C6
16	A	849	CLA	C10-C11-C12-C13
18	A	839	LHG	C16-C17-C18-C19
21	J	101	LMU	C4-C5-C6-C7
16	U	206	CLA	CAA-CBA-CGA-O2A
16	H	305	CLA	CAA-CBA-CGA-O2A
16	L	204	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
16	A	814	CLA	CAA-CBA-CGA-O2A
16	H	305	CLA	CAA-CBA-CGA-O1A
19	L	201	BCR	C16-C17-C18-C36
20	U	203	DD6	C4-C5-C6-C7
22	A	850	CL0	CHA-CBD-CGD-O2D
18	A	839	LHG	C7-C8-C9-C10
16	A	849	CLA	C8-C10-C11-C12
21	K	201	LMU	C5-C6-C7-C8
25	J	103	LMG	C8-C7-O1-C1
16	A	836	CLA	C2-C1-O2A-CGA
16	B	802	CLA	C2-C1-O2A-CGA
16	B	821	CLA	C2-C1-O2A-CGA
16	H	309	CLA	C3A-C2A-CAA-CBA
16	A	814	CLA	CAA-CBA-CGA-O1A
16	B	807	CLA	C2-C3-C5-C6
16	A	828	CLA	C16-C17-C18-C19
16	A	806	CLA	O2A-C1-C2-C3
16	U	206	CLA	CAA-CBA-CGA-O1A
16	B	827	CLA	O2A-C1-C2-C3
25	J	103	LMG	O1-C7-C8-C9
16	B	828	CLA	C4-C3-C5-C6
20	U	212	DD6	C3-C4-C5-C6
16	B	804	CLA	CAA-CBA-CGA-O1A
16	A	853	CLA	C14-C13-C15-C16
16	B	832	CLA	C14-C13-C15-C16
16	B	804	CLA	CAA-CBA-CGA-O2A
16	H	307	CLA	C2-C3-C5-C6
16	B	805	CLA	C11-C10-C8-C7
16	B	844	CLA	C11-C10-C8-C7
16	A	805	CLA	C2B-C3B-CAB-CBB
16	A	807	CLA	C2B-C3B-CAB-CBB
16	A	810	CLA	C2B-C3B-CAB-CBB
16	A	812	CLA	C2B-C3B-CAB-CBB
16	A	825	CLA	C2B-C3B-CAB-CBB
16	A	832	CLA	C2B-C3B-CAB-CBB
16	A	834	CLA	C2B-C3B-CAB-CBB
16	A	838	CLA	C2B-C3B-CAB-CBB
16	A	845	CLA	C2B-C3B-CAB-CBB
16	A	847	CLA	C2B-C3B-CAB-CBB
16	A	851	CLA	C2B-C3B-CAB-CBB
16	A	853	CLA	C2B-C3B-CAB-CBB
16	A	854	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
16	B	805	CLA	C2B-C3B-CAB-CBB
16	B	811	CLA	C2B-C3B-CAB-CBB
16	B	819	CLA	C2B-C3B-CAB-CBB
16	B	824	CLA	C2B-C3B-CAB-CBB
16	B	825	CLA	C2B-C3B-CAB-CBB
16	B	827	CLA	C2B-C3B-CAB-CBB
16	B	833	CLA	C2B-C3B-CAB-CBB
16	B	836	CLA	C2B-C3B-CAB-CBB
16	B	845	CLA	C2B-C3B-CAB-CBB
16	B	847	CLA	C2B-C3B-CAB-CBB
16	F	803	CLA	C2B-C3B-CAB-CBB
16	J	104	CLA	C2B-C3B-CAB-CBB
16	L	202	CLA	C2B-C3B-CAB-CBB
16	L	204	CLA	C2B-C3B-CAB-CBB
16	U	204	CLA	C2B-C3B-CAB-CBB
16	U	210	CLA	C2B-C3B-CAB-CBB
16	G	302	CLA	C2B-C3B-CAB-CBB
16	G	310	CLA	C2B-C3B-CAB-CBB
16	G	315	CLA	C2B-C3B-CAB-CBB
16	H	301	CLA	C2B-C3B-CAB-CBB
16	H	306	CLA	C2B-C3B-CAB-CBB
16	K	204	CLA	C2B-C3B-CAB-CBB
16	K	207	CLA	C2B-C3B-CAB-CBB
16	k	202	CLA	C2B-C3B-CAB-CBB
19	A	841	BCR	C5-C6-C7-C8
19	A	842	BCR	C23-C24-C25-C26
19	B	838	BCR	C23-C24-C25-C26
19	B	840	BCR	C5-C6-C7-C8
19	B	840	BCR	C23-C24-C25-C26
19	B	840	BCR	C23-C24-C25-C30
19	B	842	BCR	C23-C24-C25-C26
19	F	801	BCR	C5-C6-C7-C8
19	F	805	BCR	C23-C24-C25-C26
19	F	805	BCR	C23-C24-C25-C30
19	I	101	BCR	C5-C6-C7-C8
19	J	105	BCR	C23-C24-C25-C26
19	J	105	BCR	C23-C24-C25-C30
19	L	205	BCR	C1-C6-C7-C8
19	L	205	BCR	C5-C6-C7-C8
19	M	101	BCR	C23-C24-C25-C26
19	k	203	BCR	C23-C24-C25-C26
16	A	849	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
16	B	836	CLA	CAA-CBA-CGA-O2A
18	A	839	LHG	O9-C7-O7-C5
16	K	203	CLA	C2-C1-O2A-CGA
16	U	208	CLA	CAA-CBA-CGA-O2A
24	B	843	DGD	O6D-C1D-O3G-C3G
16	A	817	CLA	CAA-CBA-CGA-O2A
16	G	305	CLA	CBA-CGA-O2A-C1
16	A	806	CLA	C2-C3-C5-C6
16	U	211	CLA	CAA-CBA-CGA-O2A
18	A	839	LHG	O8-C23-C24-C25
16	k	202	CLA	CAA-CBA-CGA-O2A
16	B	817	CLA	C4-C3-C5-C6
16	B	834	CLA	C15-C16-C17-C18
16	K	205	CLA	C2-C3-C5-C6
16	A	811	CLA	CAA-CBA-CGA-O2A
16	B	820	CLA	C14-C13-C15-C16
16	H	307	CLA	C11-C10-C8-C9
16	H	312	CLA	CAA-CBA-CGA-O2A
16	B	835	CLA	C4B-C3B-CAB-CBB
16	F	802	CLA	C1A-C2A-CAA-CBA
16	B	836	CLA	C4-C3-C5-C6
16	B	803	CLA	CAA-CBA-CGA-O2A
16	B	845	CLA	CAA-CBA-CGA-O2A
16	G	306	CLA	CAA-CBA-CGA-O2A
16	G	310	CLA	CAA-CBA-CGA-O2A
20	U	212	DD6	C2-C1-C24-C25
20	H	311	DD6	C5-C6-C8-C9
16	A	821	CLA	CAA-CBA-CGA-O2A
16	B	806	CLA	CAA-CBA-CGA-O2A
16	B	809	CLA	CAA-CBA-CGA-O2A
16	G	309	CLA	CAA-CBA-CGA-O2A
24	B	843	DGD	C2D-C1D-O3G-C3G
16	F	804	CLA	CAA-CBA-CGA-O2A
16	U	204	CLA	CAA-CBA-CGA-O2A
16	A	845	CLA	C2-C1-O2A-CGA
16	A	849	CLA	C2-C1-O2A-CGA
16	A	810	CLA	CAA-CBA-CGA-O2A
16	A	853	CLA	C11-C12-C13-C15
16	B	806	CLA	C2-C3-C5-C6
16	G	307	CLA	C11-C12-C13-C14
16	A	836	CLA	C2A-CAA-CBA-CGA
16	A	847	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
16	G	308	CLA	C5-C6-C7-C8
16	A	804	CLA	C5-C6-C7-C8
16	A	807	CLA	C4-C3-C5-C6
16	B	819	CLA	C3A-C2A-CAA-CBA
16	U	207	CLA	C3A-C2A-CAA-CBA
16	A	853	CLA	C13-C15-C16-C17
16	A	817	CLA	CAA-CBA-CGA-O1A
16	A	836	CLA	C5-C6-C7-C8
16	k	202	CLA	CAA-CBA-CGA-O1A
16	A	802	CLA	CAA-CBA-CGA-O2A
16	U	208	CLA	CAA-CBA-CGA-O1A
16	B	817	CLA	C16-C17-C18-C19
16	B	803	CLA	CAA-CBA-CGA-O1A
16	B	809	CLA	CAA-CBA-CGA-O1A
25	J	103	LMG	O9-C10-C11-C12
20	U	212	DD6	C-C1-C24-C25
16	U	211	CLA	CAA-CBA-CGA-O1A
16	A	854	CLA	C5-C6-C7-C8
16	B	836	CLA	CAA-CBA-CGA-O1A
16	H	312	CLA	C5-C6-C7-C8
24	B	843	DGD	C5D-C6D-O5D-C1E
25	U	201	LMG	C8-C7-O1-C1
16	G	309	CLA	CAA-CBA-CGA-O1A
16	A	804	CLA	CAA-CBA-CGA-O2A
25	J	103	LMG	O7-C10-C11-C12
16	A	803	CLA	C2A-CAA-CBA-CGA
16	B	807	CLA	C2A-CAA-CBA-CGA
21	A	848	LMU	C5-C6-C7-C8
24	B	843	DGD	C1G-C2G-C3G-O3G
16	B	845	CLA	CAA-CBA-CGA-O1A
19	B	846	BCR	C18-C19-C20-C21
16	B	814	CLA	CAA-CBA-CGA-O2A
27	U	213	KC1	C2B-C3B-CAB-CBB
16	B	803	CLA	C3-C5-C6-C7
16	G	310	CLA	CAA-CBA-CGA-O1A
16	A	802	CLA	CAD-CBD-CGD-O2D
16	A	828	CLA	CAD-CBD-CGD-O2D
16	A	835	CLA	CAD-CBD-CGD-O2D
16	B	848	CLA	CAD-CBD-CGD-O2D
16	I	102	CLA	CAD-CBD-CGD-O2D
16	A	811	CLA	CAA-CBA-CGA-O1A
16	A	821	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
19	F	805	BCR	C6-C7-C8-C9
19	I	103	BCR	C22-C23-C24-C25
16	A	827	CLA	C2-C1-O2A-CGA
16	H	312	CLA	CAA-CBA-CGA-O1A
18	A	839	LHG	C34-C35-C36-C37
18	G	316	LHG	C25-C26-C27-C28
16	B	814	CLA	CAA-CBA-CGA-O1A
16	F	804	CLA	CAA-CBA-CGA-O1A
22	A	850	CL0	C5-C6-C7-C8
16	B	811	CLA	CAA-CBA-CGA-O2A
16	A	810	CLA	CAA-CBA-CGA-O1A
16	U	204	CLA	CAA-CBA-CGA-O1A
16	A	803	CLA	CAA-CBA-CGA-O2A
16	A	847	CLA	CAA-CBA-CGA-O2A
16	B	818	CLA	CAA-CBA-CGA-O2A
16	B	847	CLA	CAA-CBA-CGA-O2A
16	A	802	CLA	CAA-CBA-CGA-O1A
16	B	806	CLA	CAA-CBA-CGA-O1A

There are no ring outliers.

138 monomers are involved in 235 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	A	817	CLA	2	0
16	B	807	CLA	5	0
16	A	803	CLA	2	0
16	A	807	CLA	1	0
16	F	804	CLA	1	0
16	A	818	CLA	1	0
16	A	823	CLA	1	0
16	B	803	CLA	2	0
16	B	824	CLA	2	0
16	B	815	CLA	2	0
19	k	203	BCR	3	0
16	U	207	CLA	5	0
16	B	844	CLA	2	0
19	B	838	BCR	2	0
16	A	810	CLA	1	0
16	B	827	CLA	1	0
16	K	206	CLA	2	0
16	A	825	CLA	1	0
16	K	202	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	A	812	CLA	2	0
16	H	308	CLA	3	0
16	A	808	CLA	2	0
19	B	846	BCR	3	0
19	M	101	BCR	3	0
16	B	814	CLA	1	0
16	G	303	CLA	3	0
16	G	309	CLA	4	0
16	G	304	CLA	1	0
19	I	103	BCR	1	0
16	A	854	CLA	5	0
16	A	831	CLA	3	0
16	H	312	CLA	5	0
16	B	832	CLA	1	0
16	U	211	CLA	3	0
16	H	302	CLA	3	0
20	G	311	DD6	1	0
16	A	853	CLA	2	0
16	A	814	CLA	2	0
17	A	837	PQN	3	0
16	B	826	CLA	1	0
16	B	805	CLA	2	0
16	H	309	CLA	2	0
19	L	201	BCR	1	0
16	B	816	CLA	1	0
16	U	208	CLA	1	0
16	B	819	CLA	3	0
16	B	813	CLA	2	0
16	B	822	CLA	2	0
16	A	851	CLA	5	0
19	B	840	BCR	1	0
16	B	801	CLA	2	0
16	B	829	CLA	1	0
16	A	833	CLA	3	0
22	A	850	CL0	2	0
16	A	820	CLA	2	0
16	H	305	CLA	3	0
16	A	835	CLA	3	0
16	A	813	CLA	1	0
16	H	304	CLA	1	0
19	B	839	BCR	4	0
16	B	808	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	U	206	CLA	1	0
16	U	209	CLA	1	0
16	K	205	CLA	3	0
16	B	820	CLA	1	0
16	F	802	CLA	2	0
18	A	839	LHG	2	0
16	B	802	CLA	3	0
16	A	824	CLA	4	0
17	B	837	PQN	1	0
16	B	848	CLA	3	0
16	A	826	CLA	2	0
16	A	847	CLA	1	0
16	G	306	CLA	2	0
19	A	842	BCR	1	0
16	A	819	CLA	1	0
16	J	104	CLA	1	0
16	L	202	CLA	2	0
16	B	817	CLA	2	0
16	A	801	CLA	2	0
16	U	204	CLA	1	0
16	A	809	CLA	2	0
16	B	849	CLA	6	0
16	B	834	CLA	4	0
16	B	835	CLA	4	0
16	A	829	CLA	2	0
19	I	101	BCR	2	0
16	B	809	CLA	1	0
19	J	105	BCR	2	0
16	I	102	CLA	2	0
16	A	811	CLA	2	0
21	A	855	LMU	1	0
16	B	828	CLA	1	0
16	A	836	CLA	2	0
26	U	202	A86	1	0
16	B	811	CLA	1	0
16	A	822	CLA	1	0
16	L	203	CLA	1	0
16	B	836	CLA	4	0
24	B	843	DGD	2	0
19	A	843	BCR	2	0
19	B	842	BCR	3	0
16	A	830	CLA	1	0

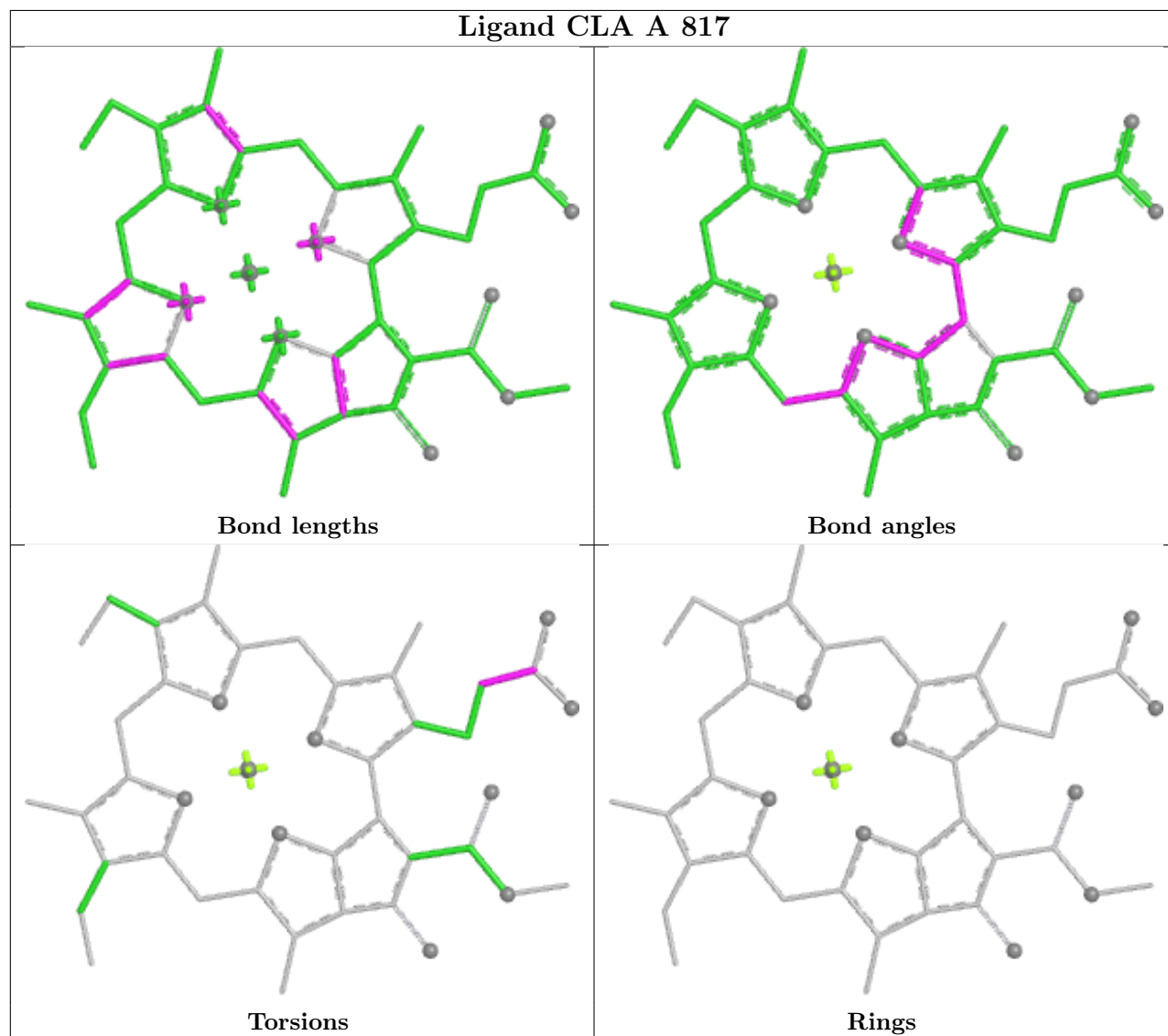
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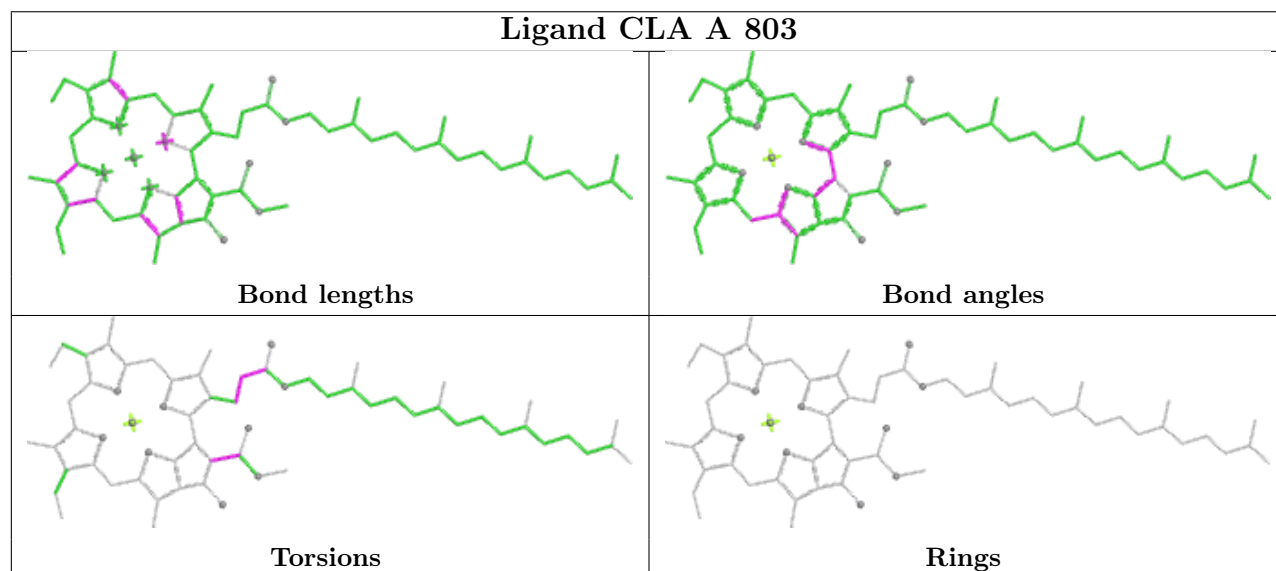
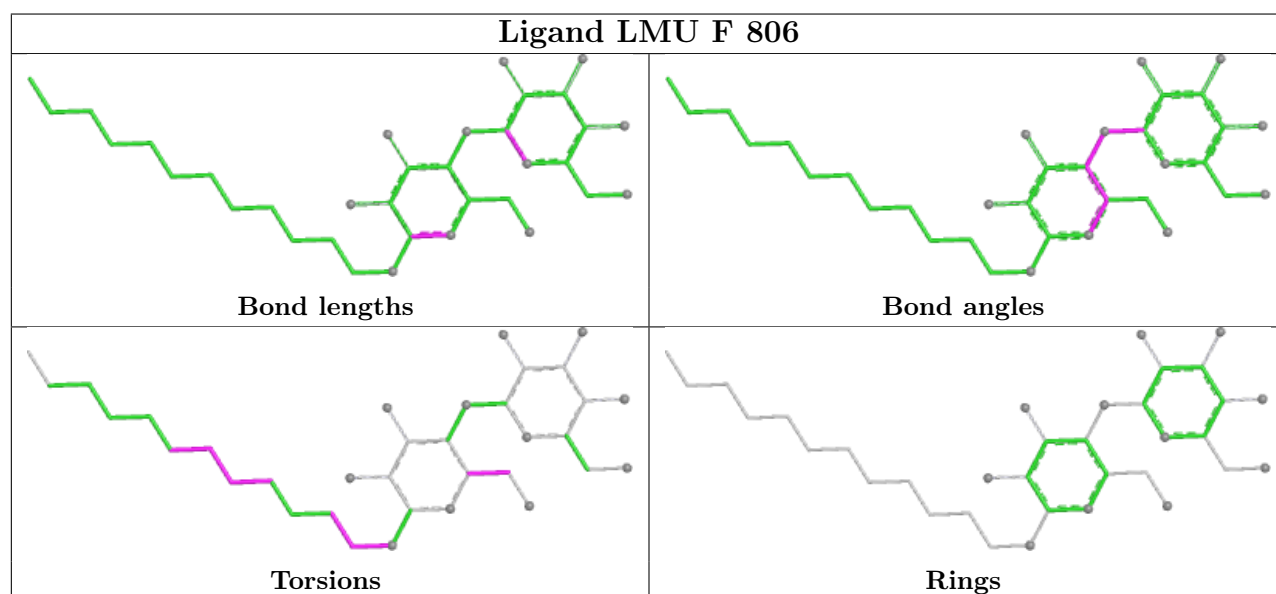
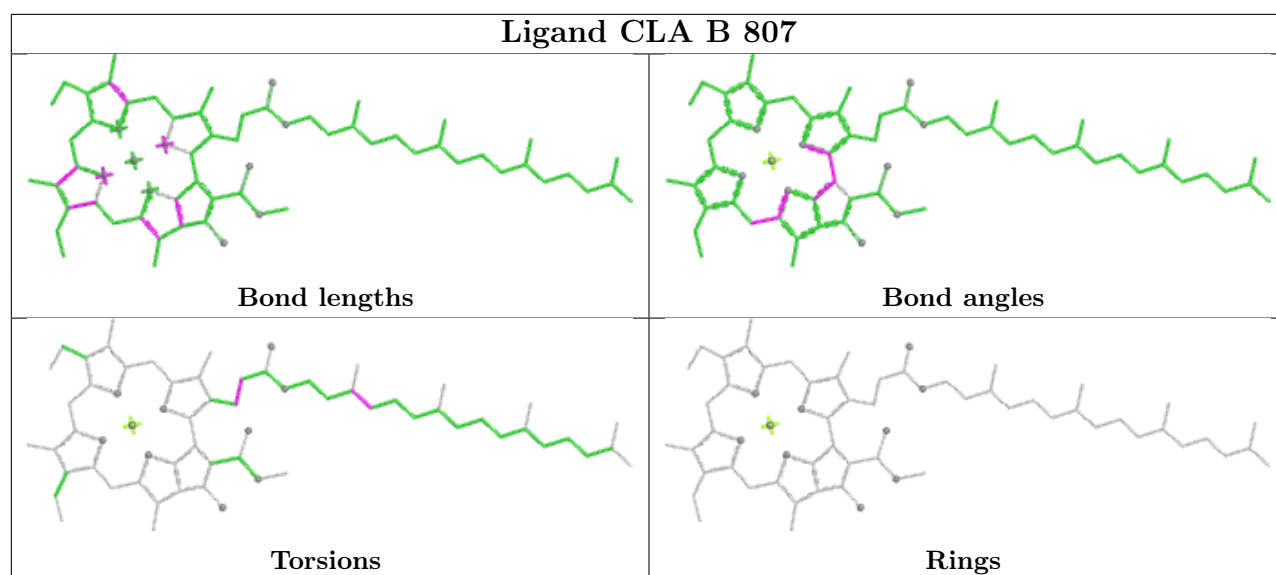
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	G	308	CLA	2	0
16	U	205	CLA	2	0
16	B	830	CLA	1	0
25	U	201	LMG	2	0
16	A	816	CLA	4	0
16	B	825	CLA	3	0
16	A	845	CLA	3	0
16	B	823	CLA	1	0
16	G	301	CLA	1	0
16	A	806	CLA	1	0
16	U	210	CLA	1	0
16	G	310	CLA	2	0
16	K	203	CLA	2	0
25	J	103	LMG	2	0
21	A	848	LMU	1	0
21	J	101	LMU	3	0
19	A	844	BCR	3	0
16	B	847	CLA	1	0
16	A	849	CLA	6	0
16	A	815	CLA	2	0
16	G	302	CLA	1	0
19	B	841	BCR	3	0
16	H	303	CLA	1	0
16	B	831	CLA	2	0
16	B	818	CLA	2	0
16	k	201	CLA	1	0
16	k	202	CLA	2	0
16	L	204	CLA	1	0
19	L	205	BCR	2	0
16	A	828	CLA	4	0
16	B	806	CLA	2	0
16	H	306	CLA	7	0
16	B	845	CLA	1	0
16	G	307	CLA	1	0
18	G	316	LHG	2	0

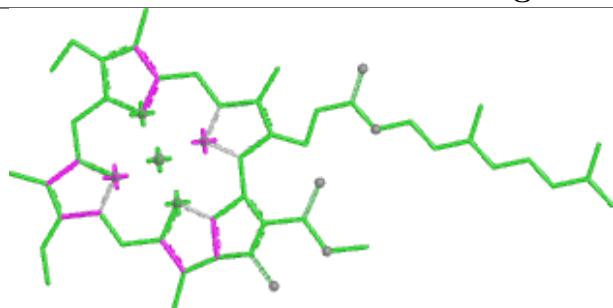
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring

in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

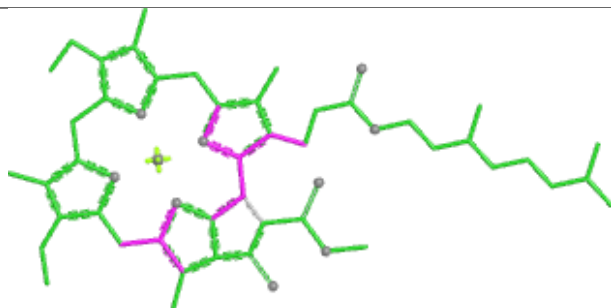




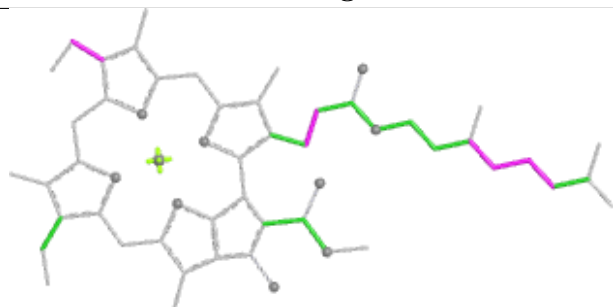
Ligand CLA A 807



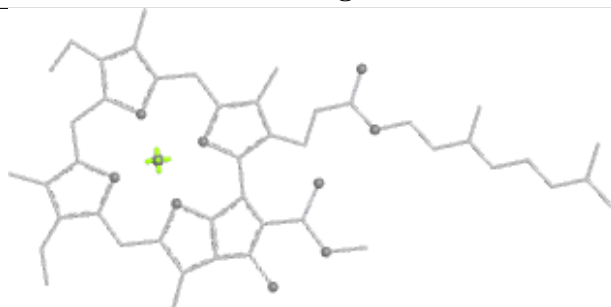
Bond lengths



Bond angles

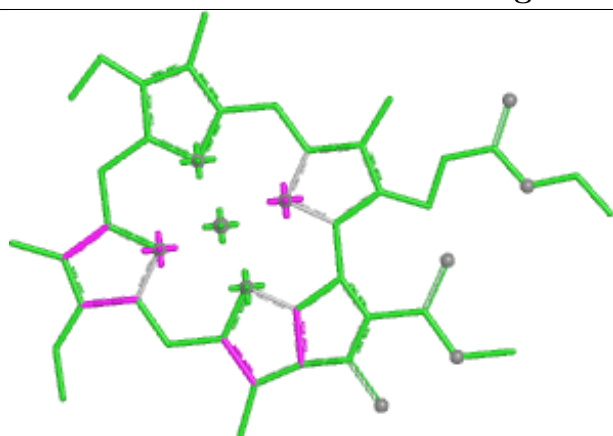


Torsions

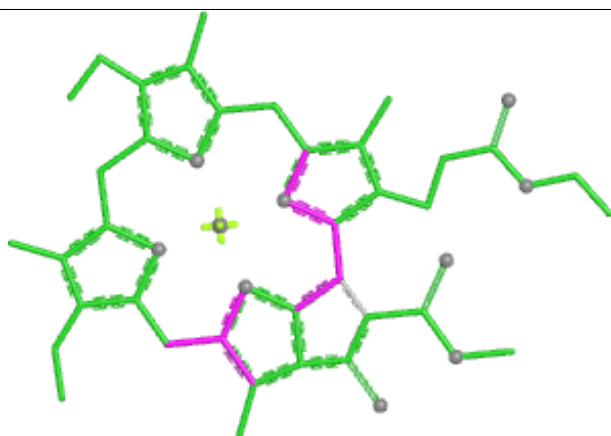


Rings

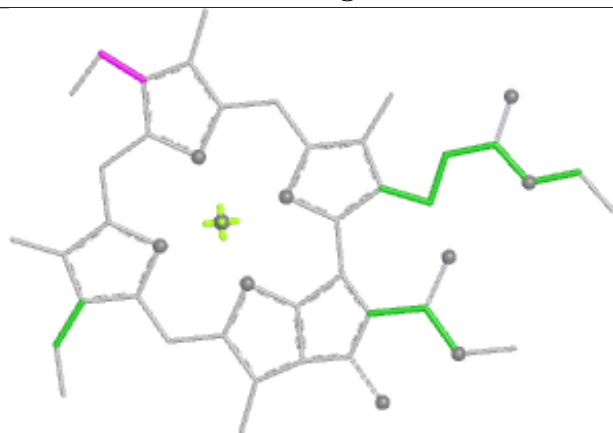
Ligand CLA B 833



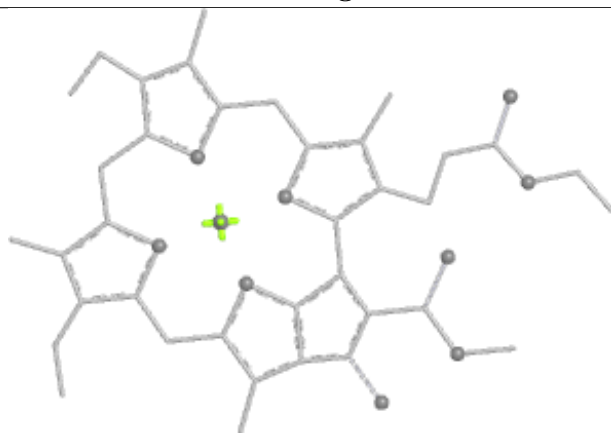
Bond lengths



Bond angles

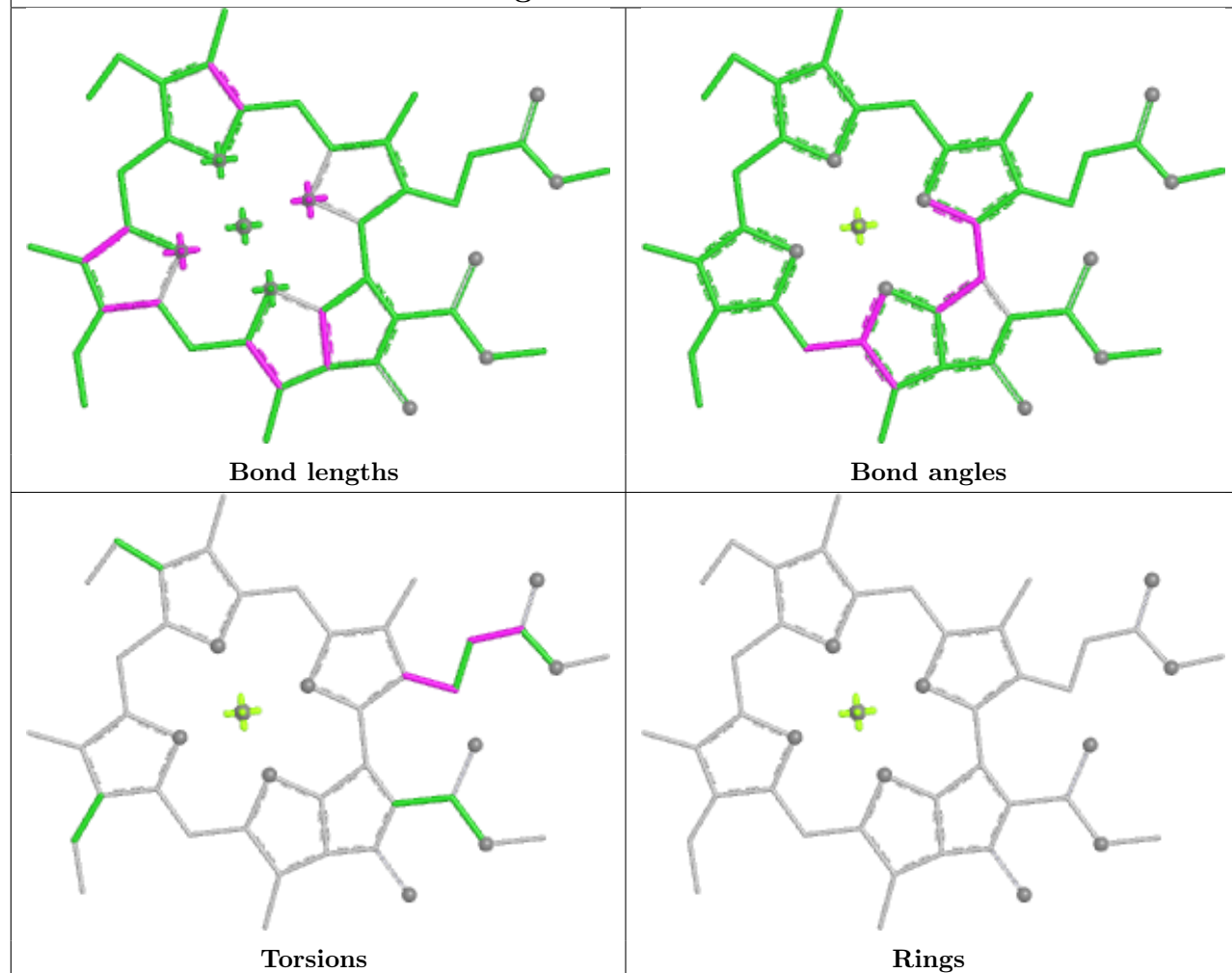


Torsions

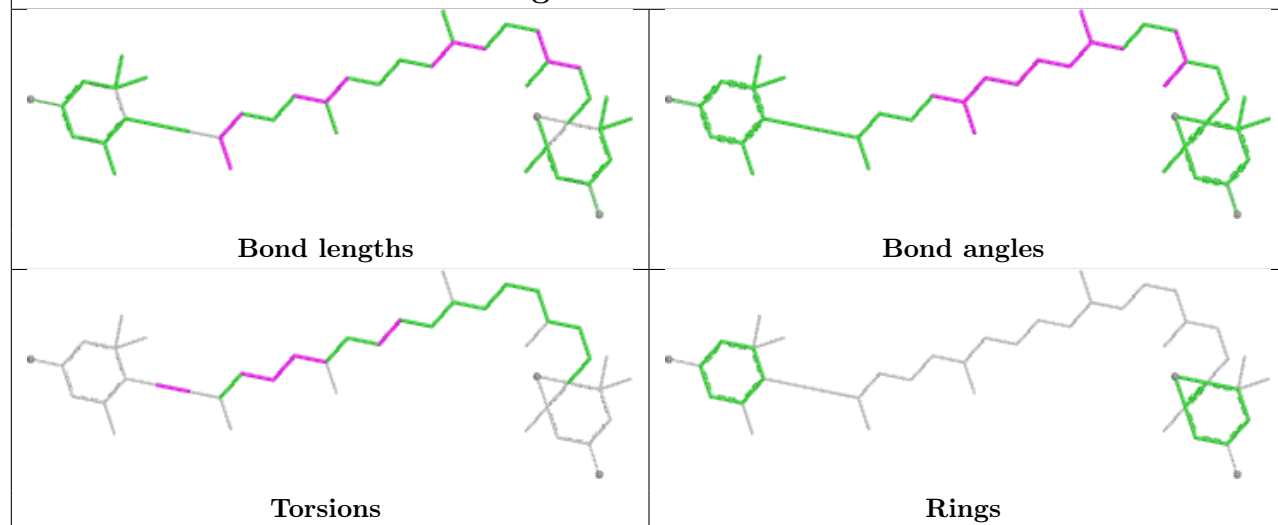


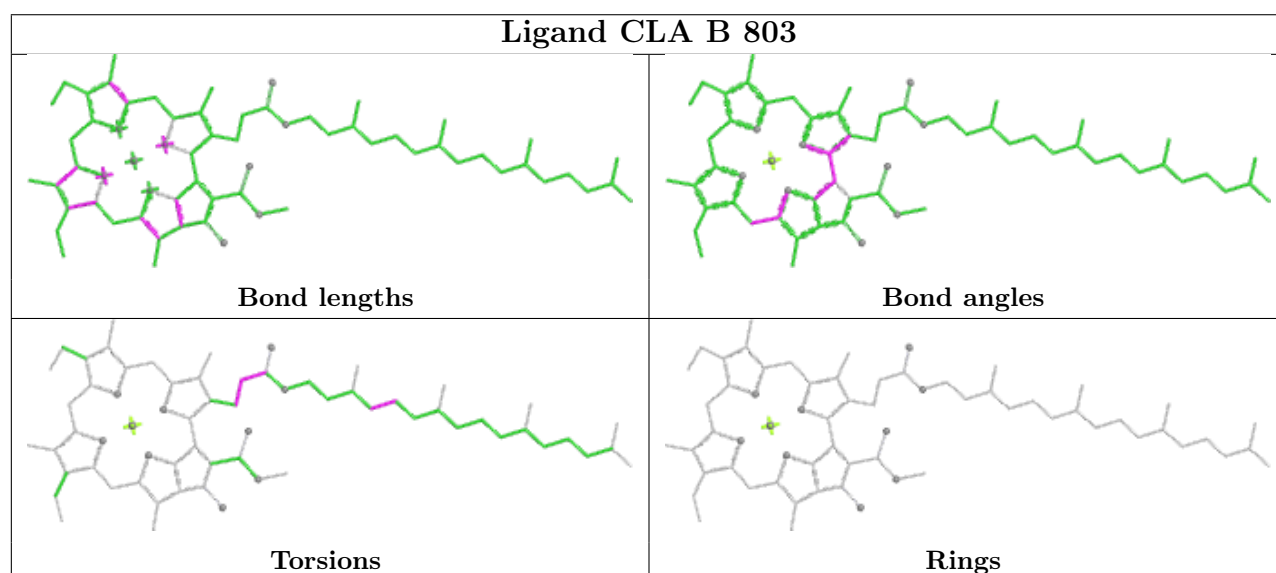
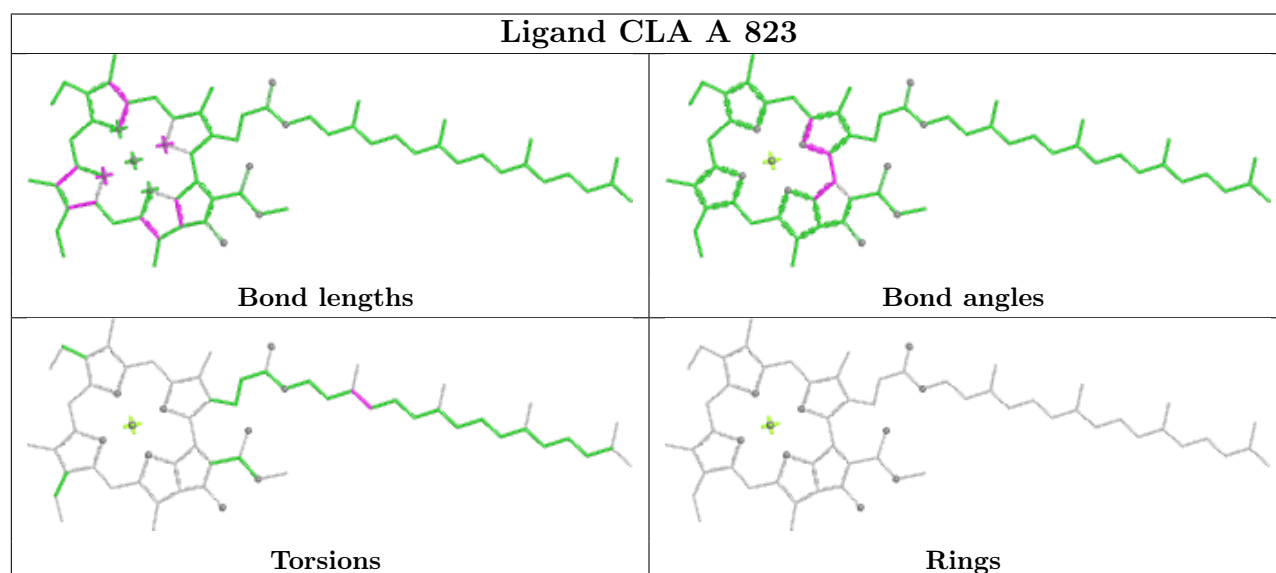
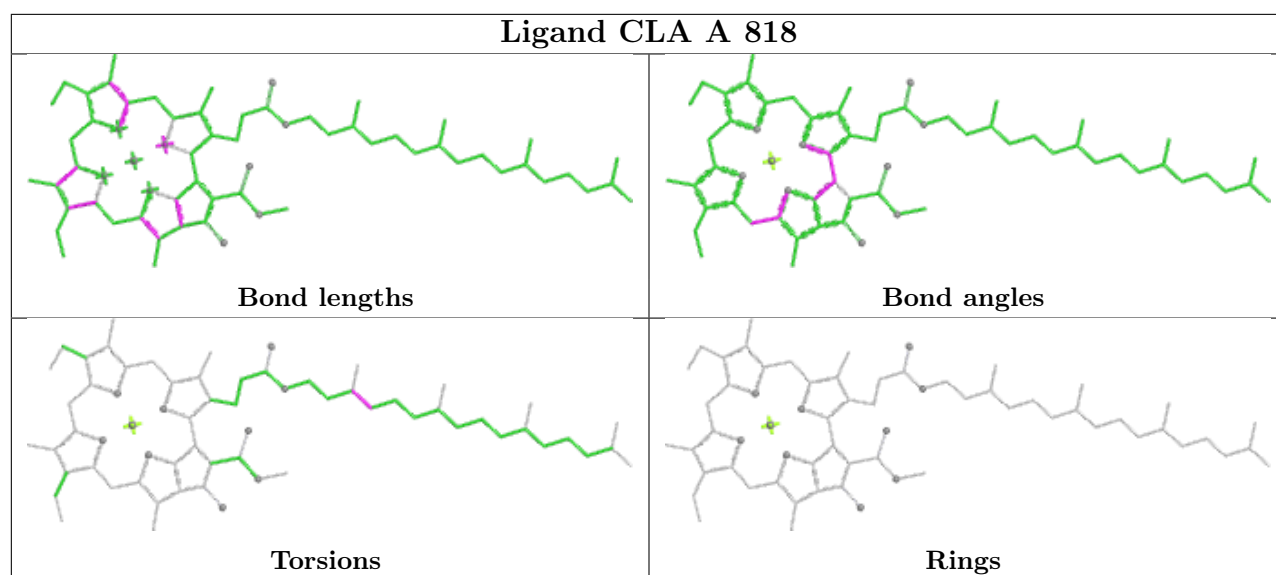
Rings

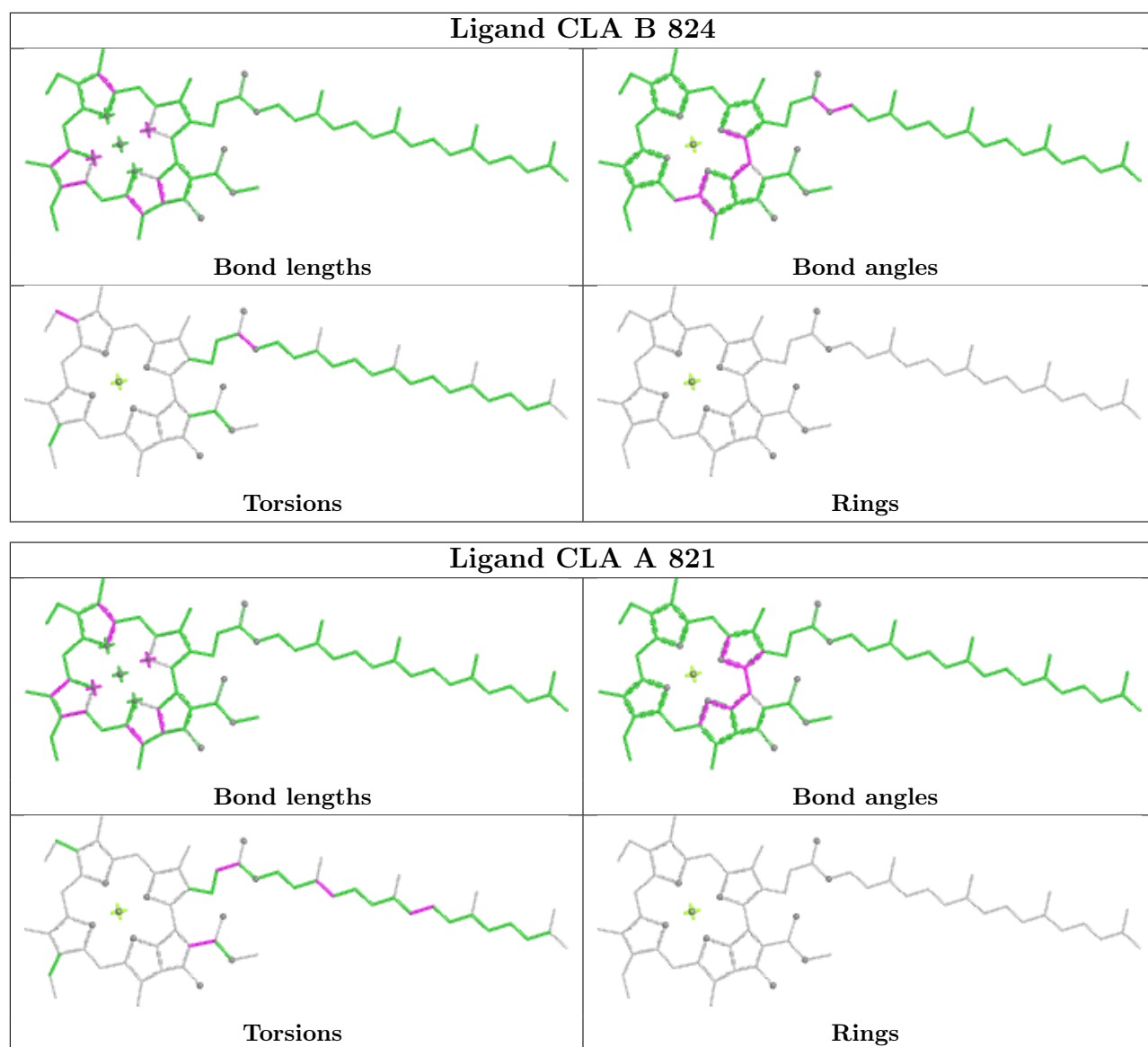
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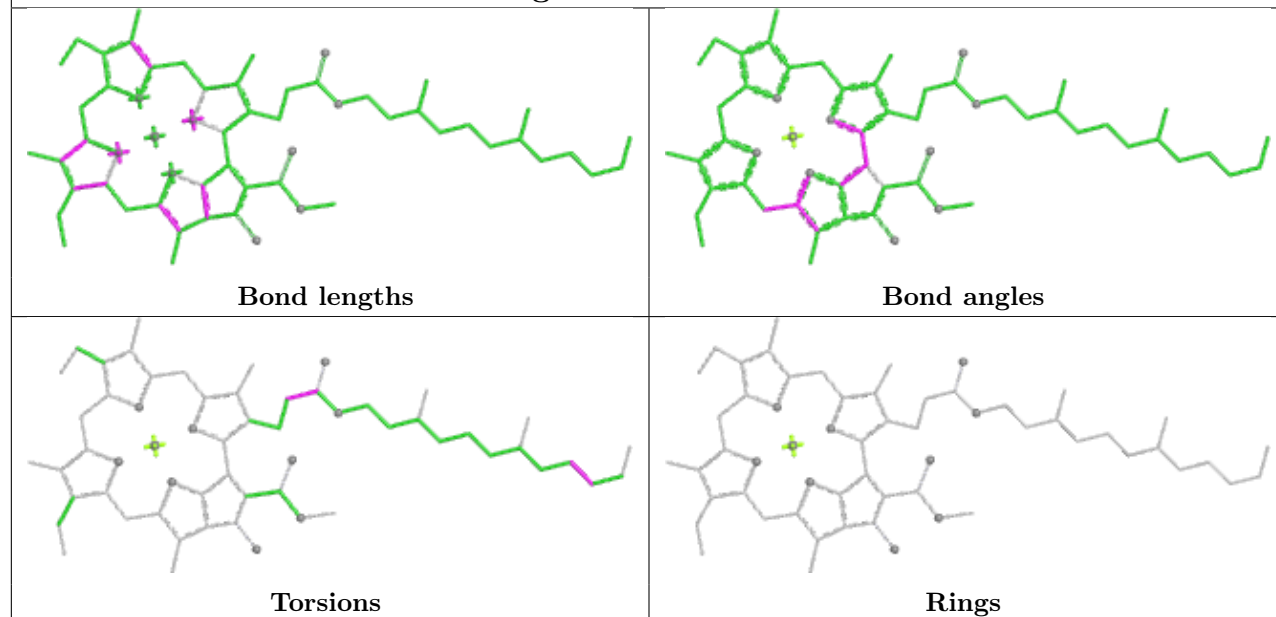
Ligand DD6 G 313



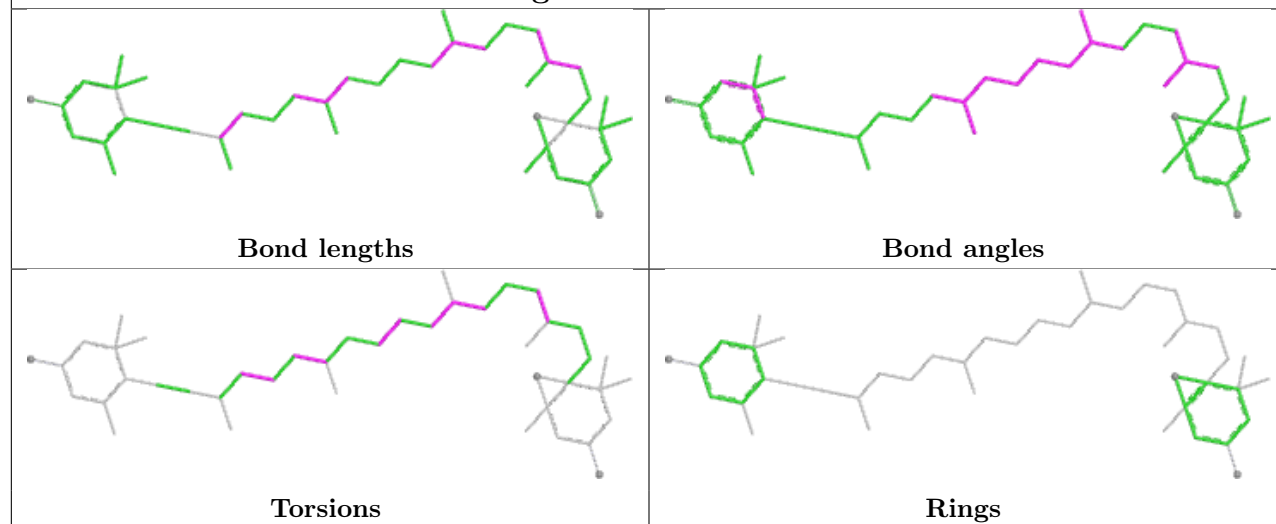




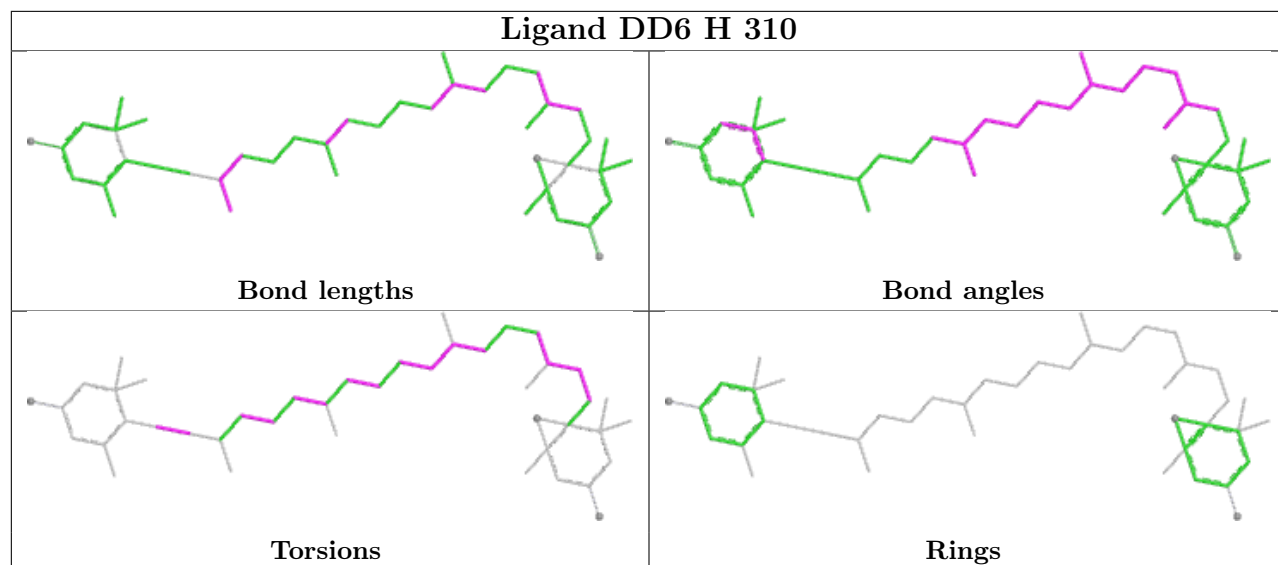
Ligand CLA B 815



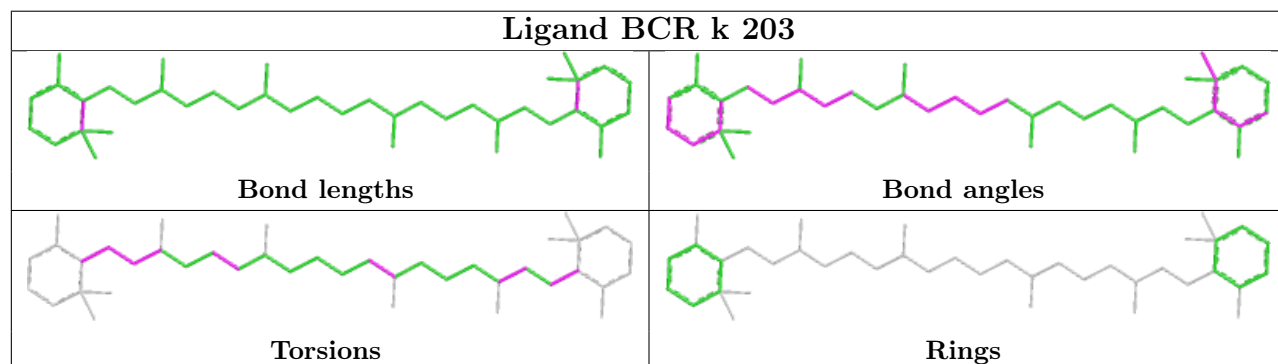
Ligand DD6 K 208



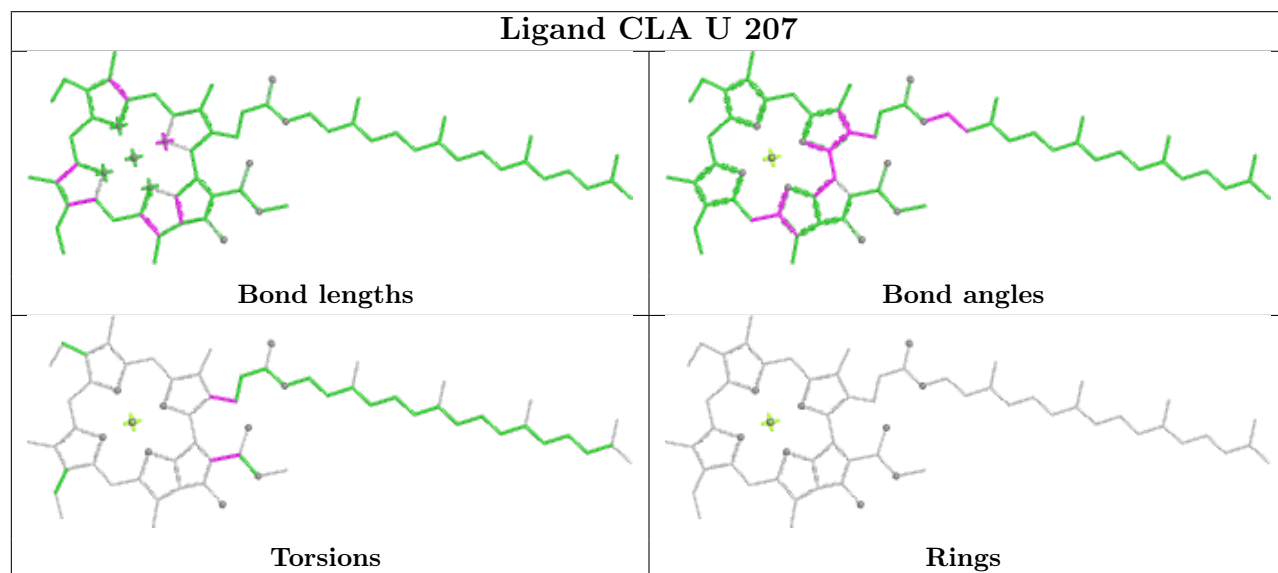
Ligand DD6 H 310

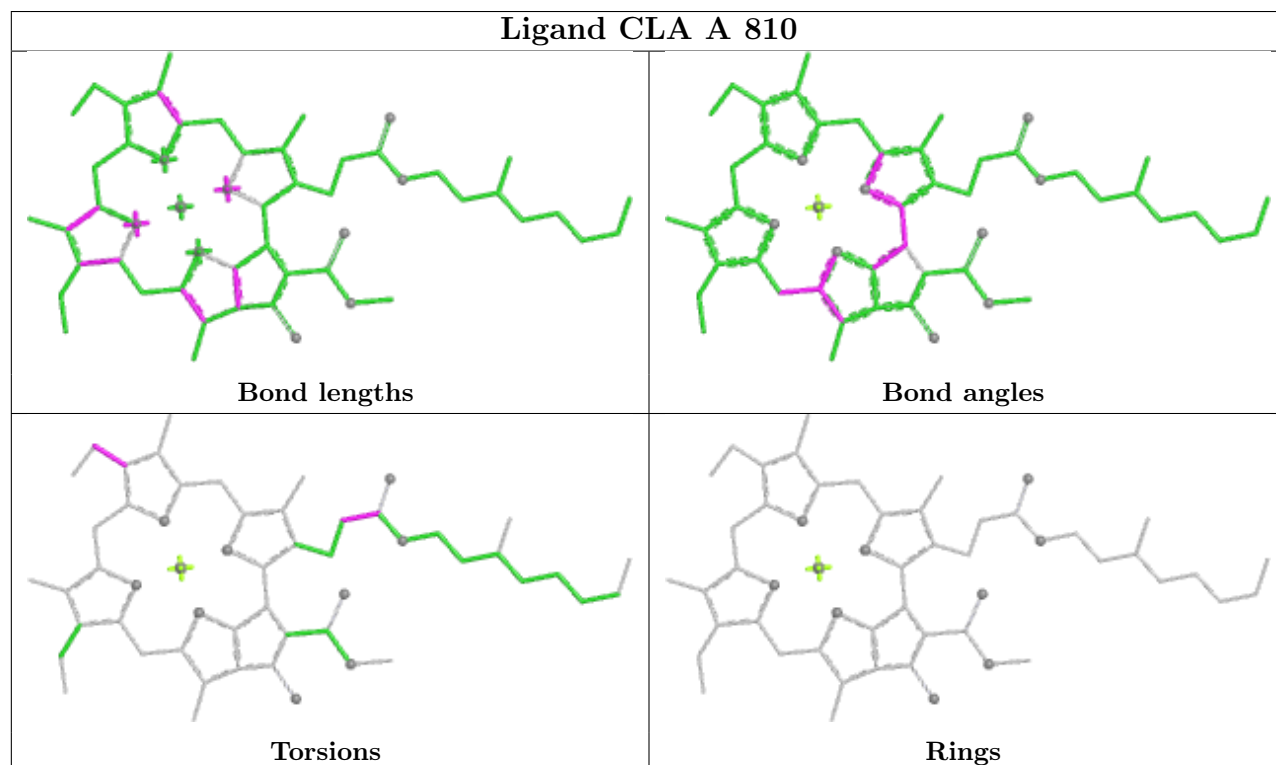
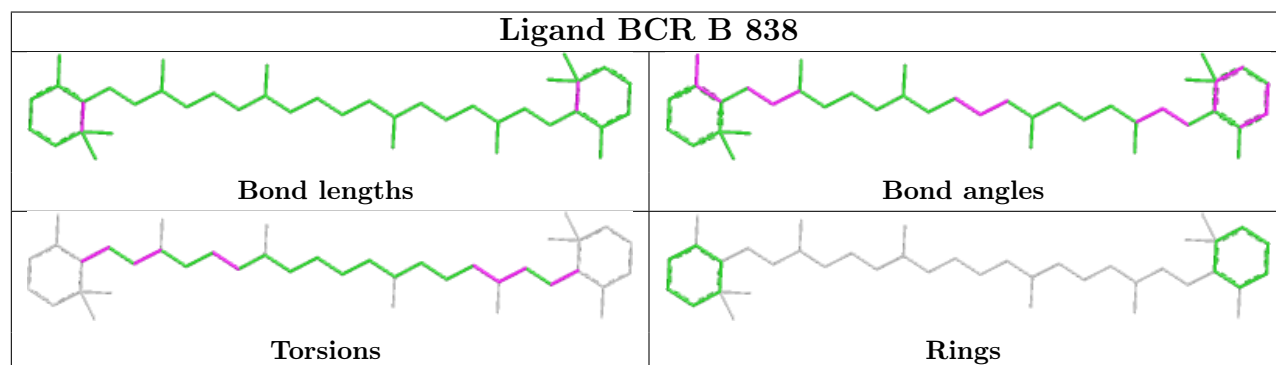
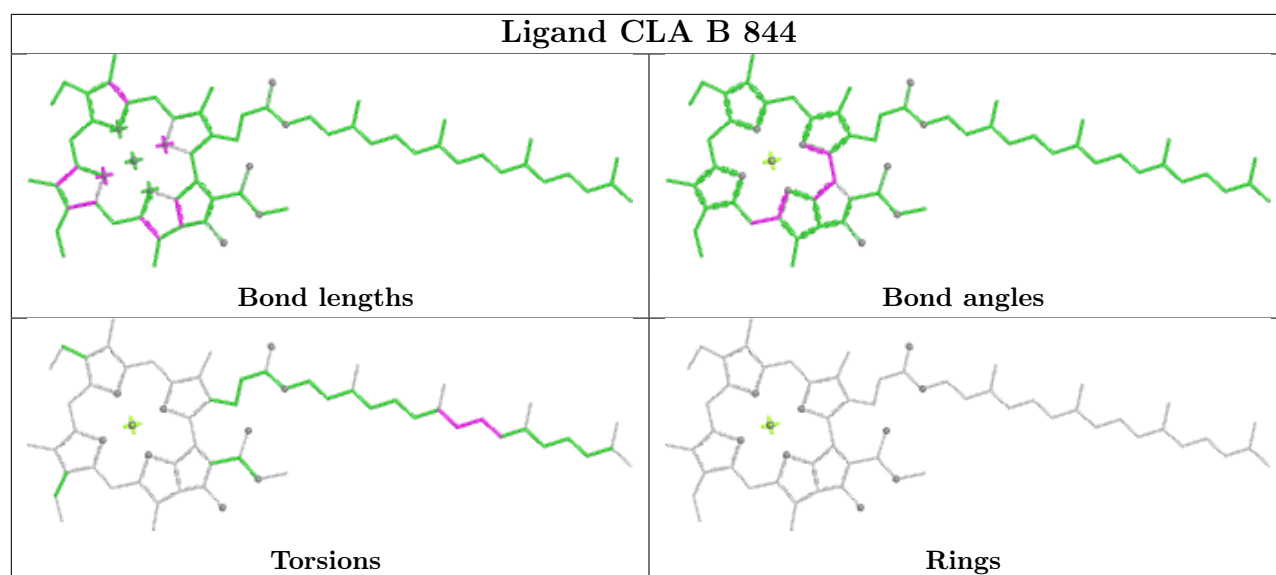


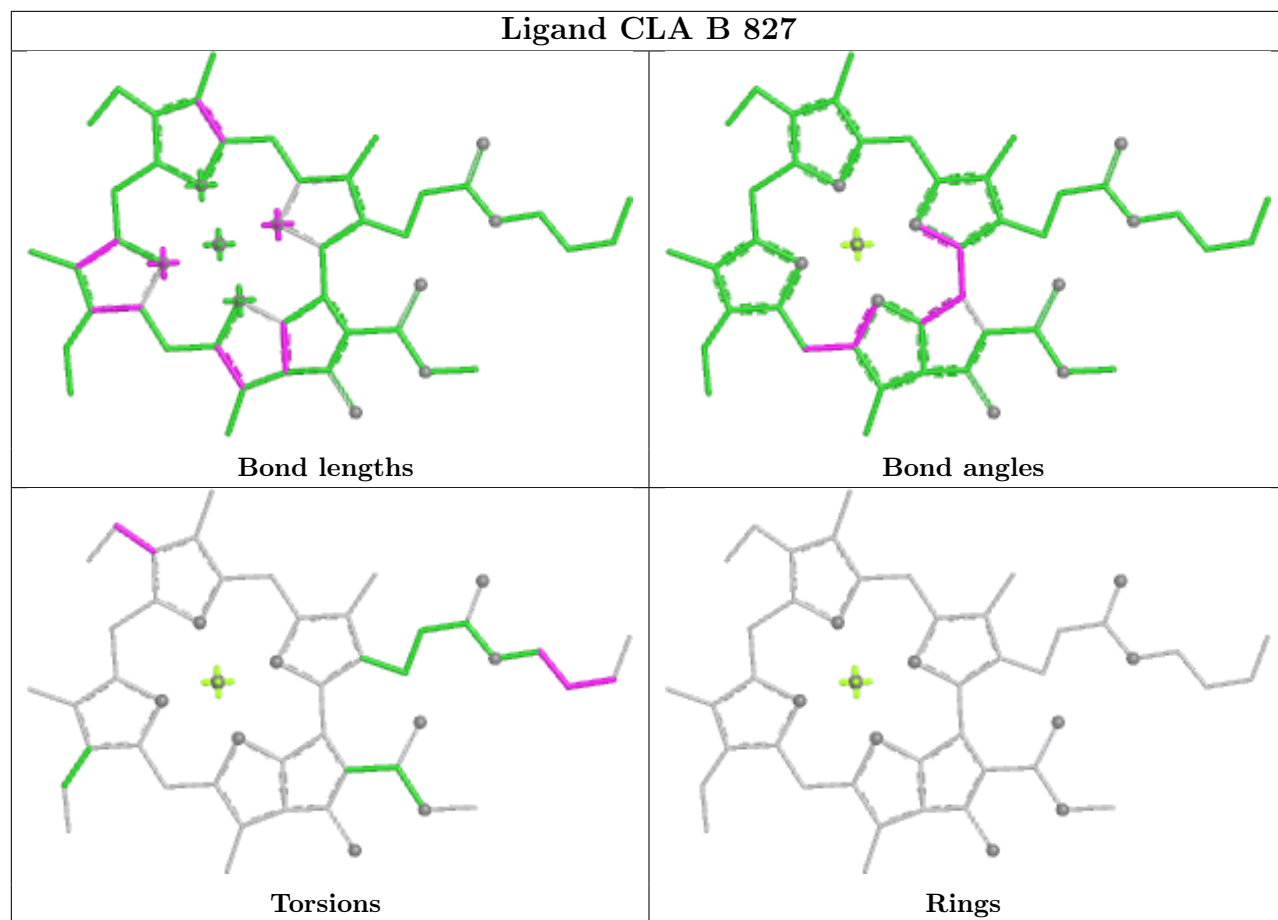
Ligand BCR k 203



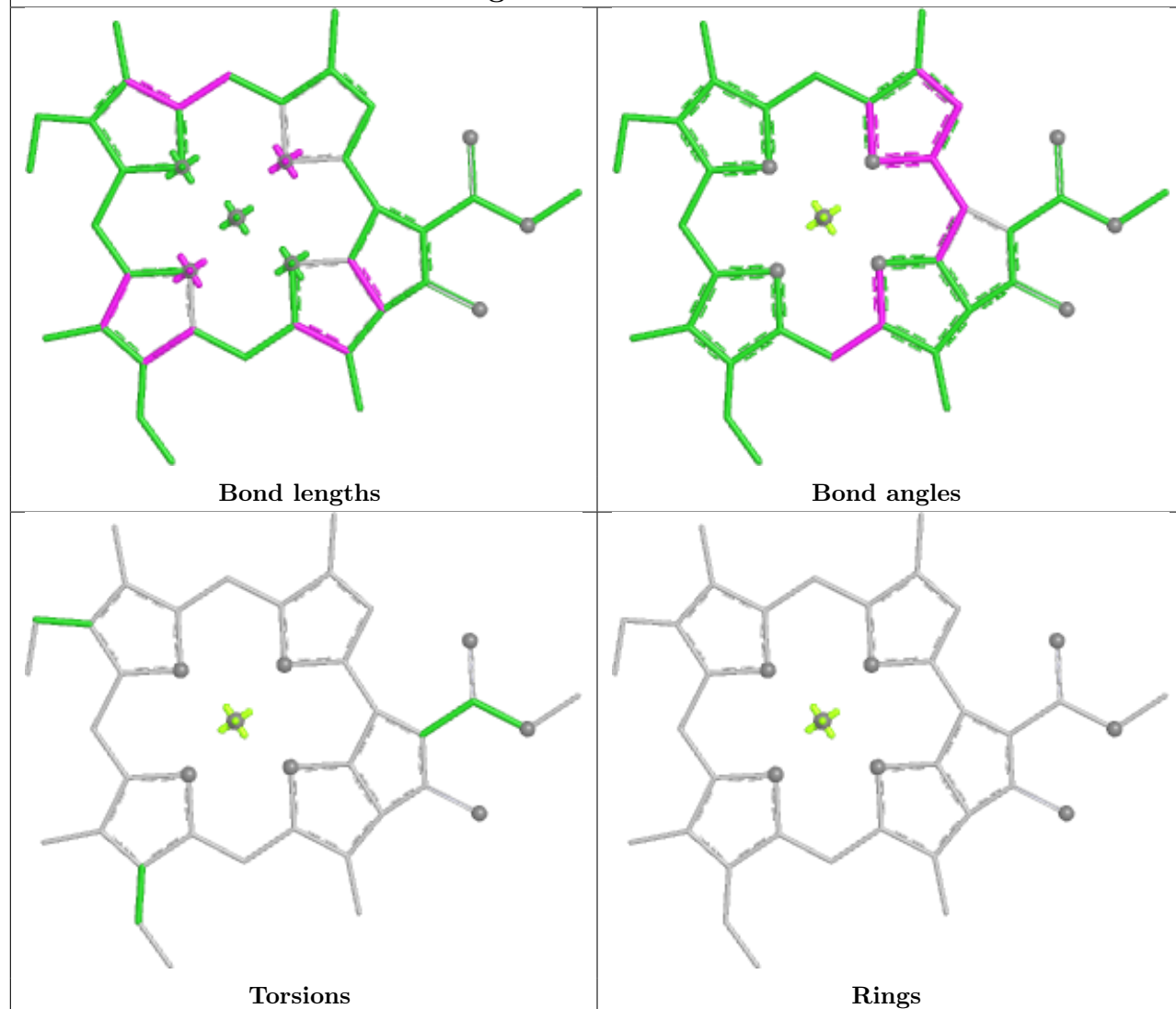
Ligand CLA U 207



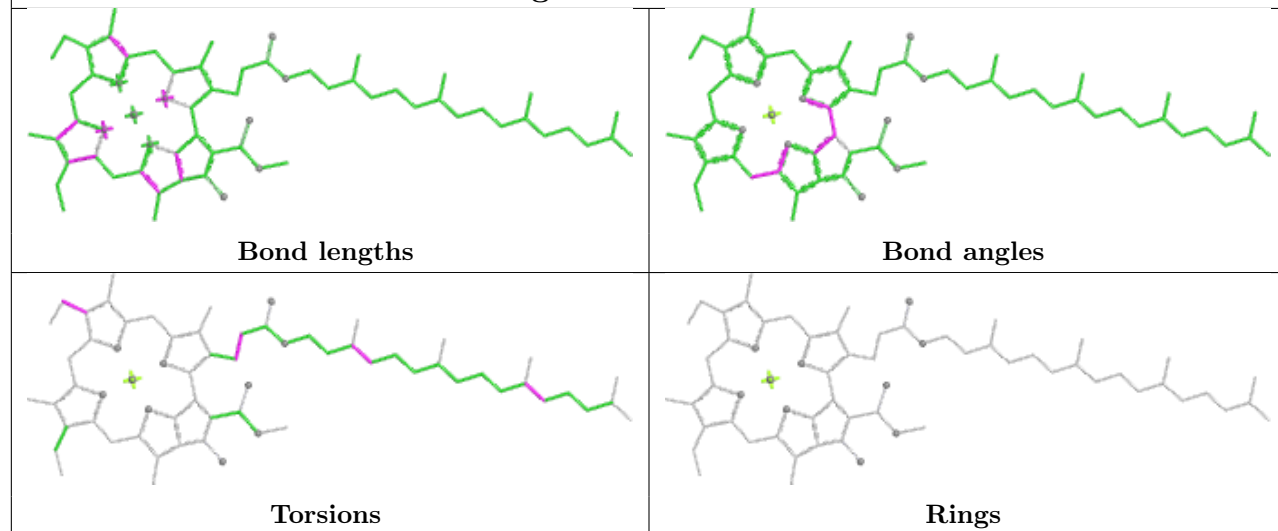


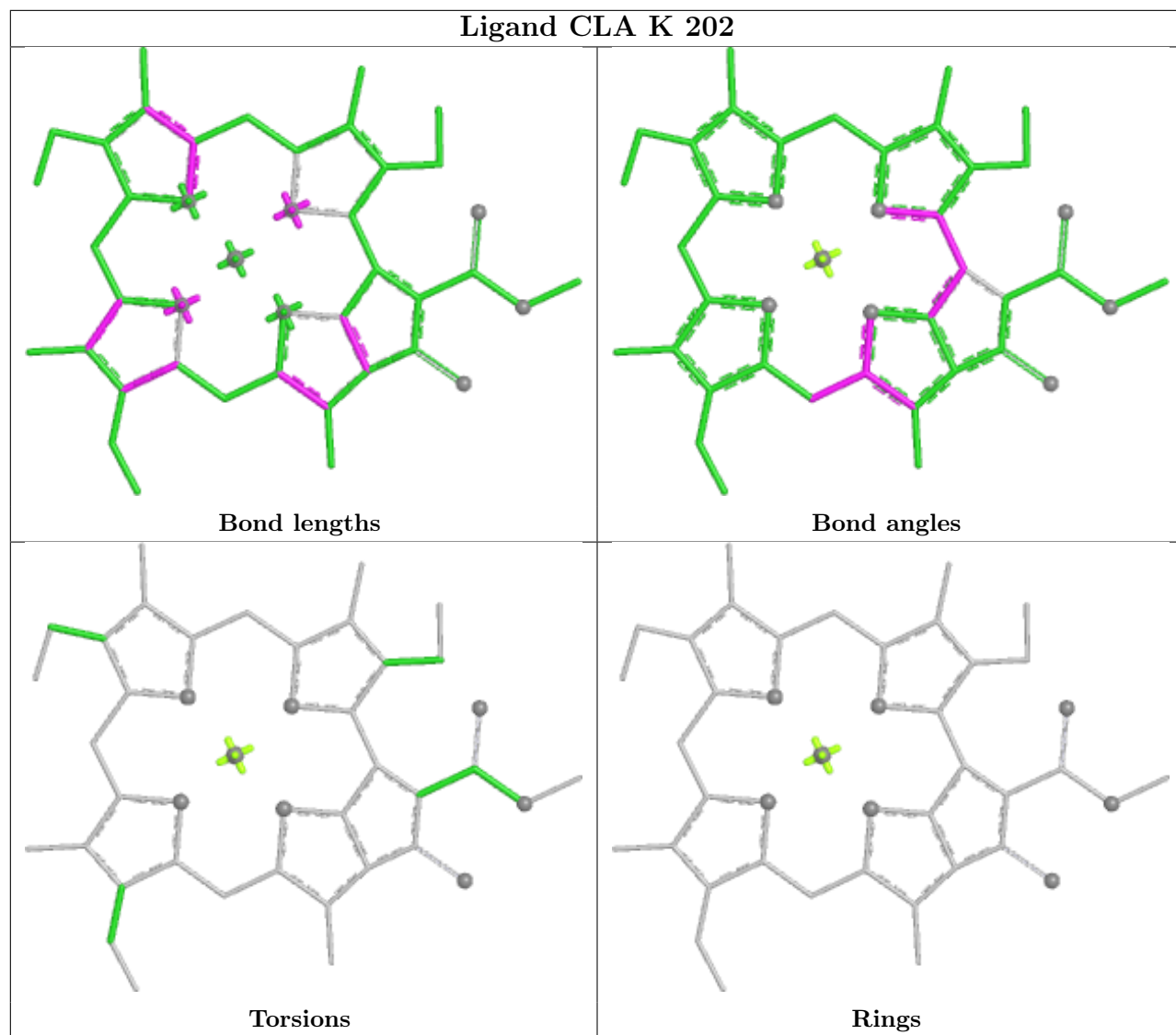


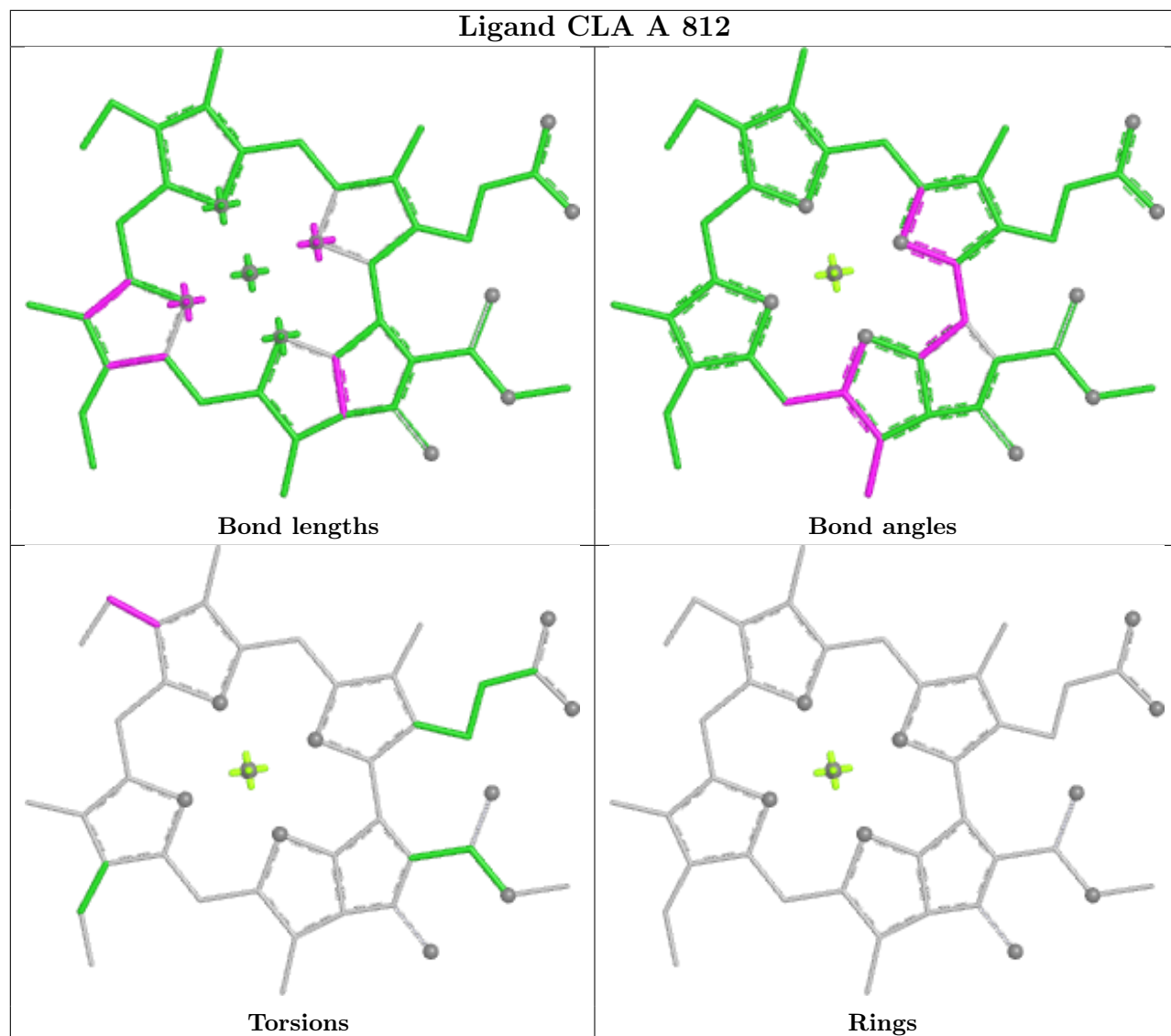
Ligand CLA K 206



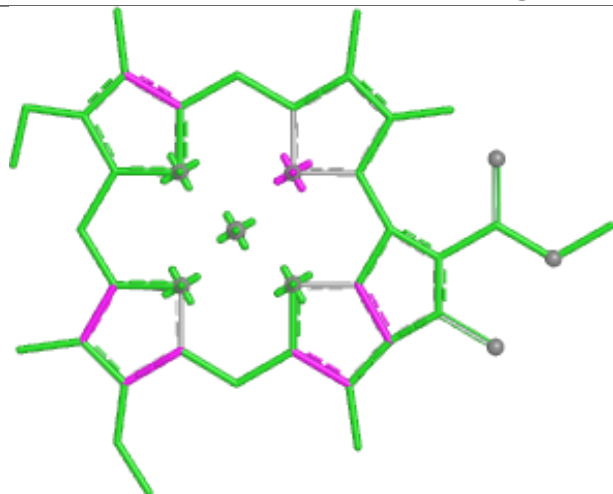
Ligand CLA A 825



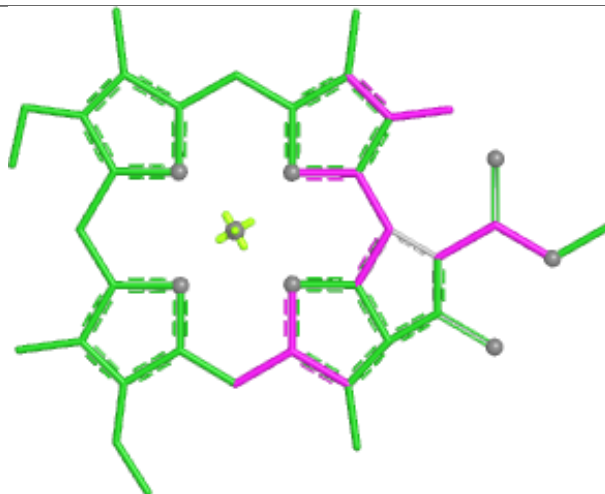




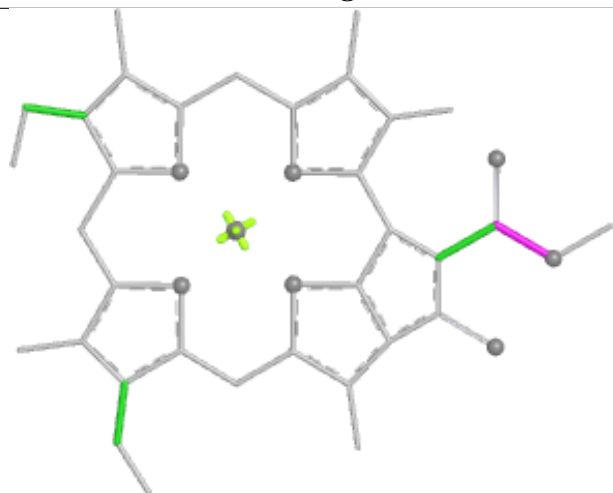
Ligand CLA H 308



Bond lengths



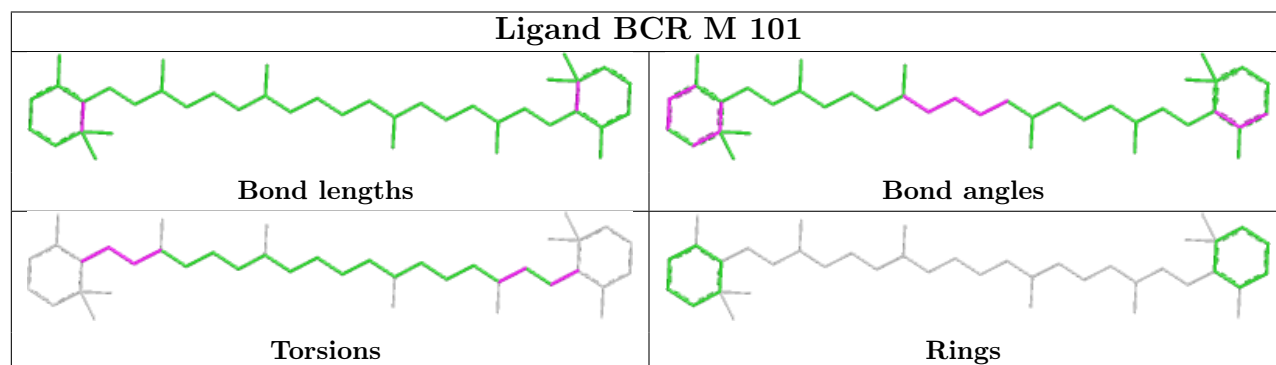
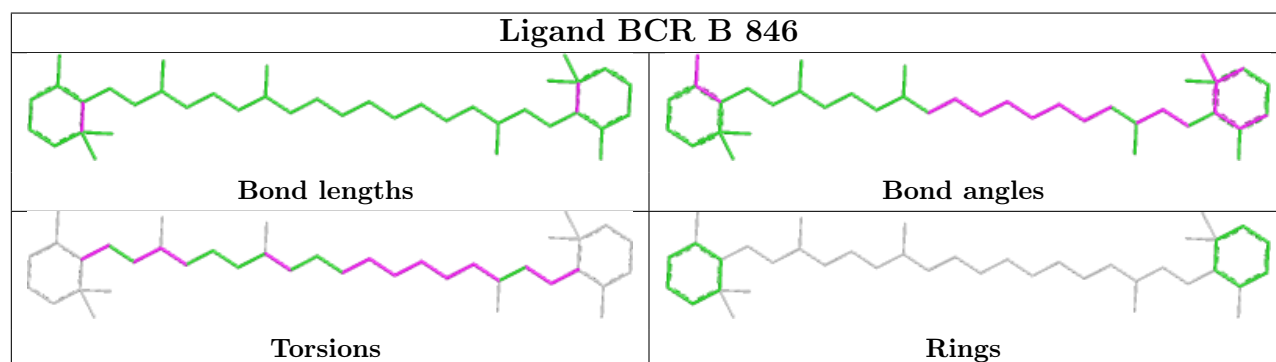
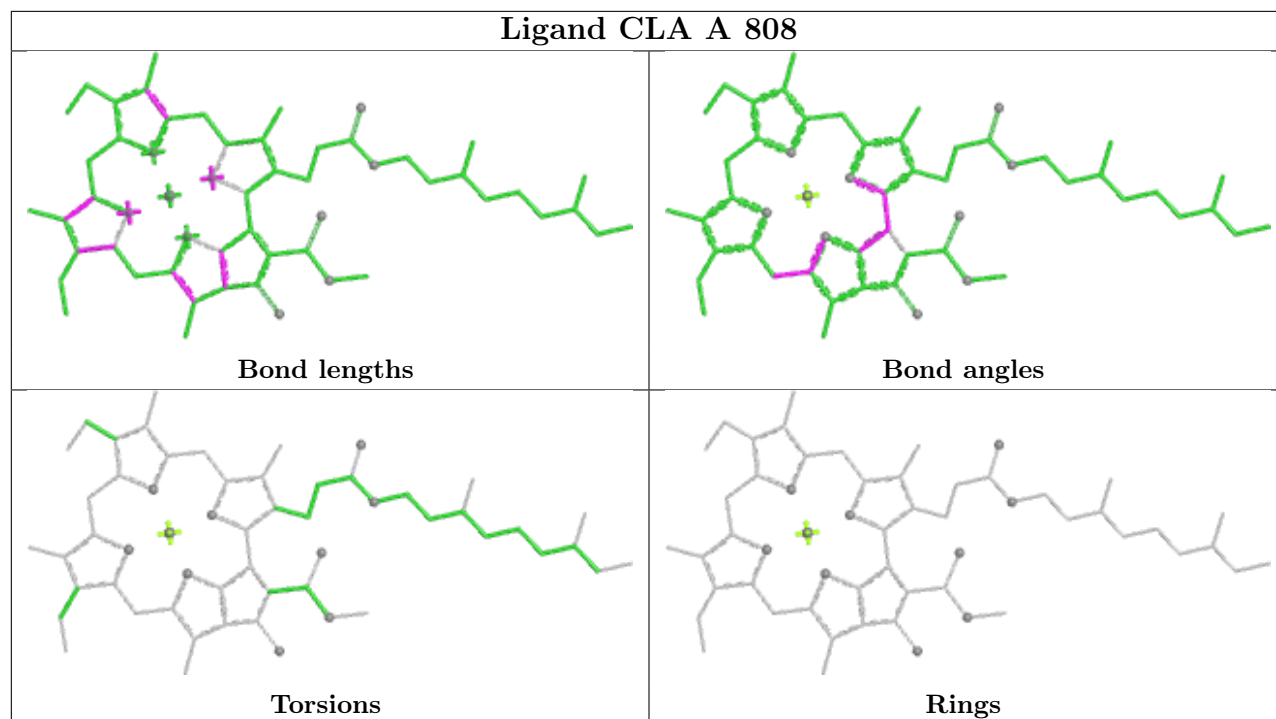
Bond angles



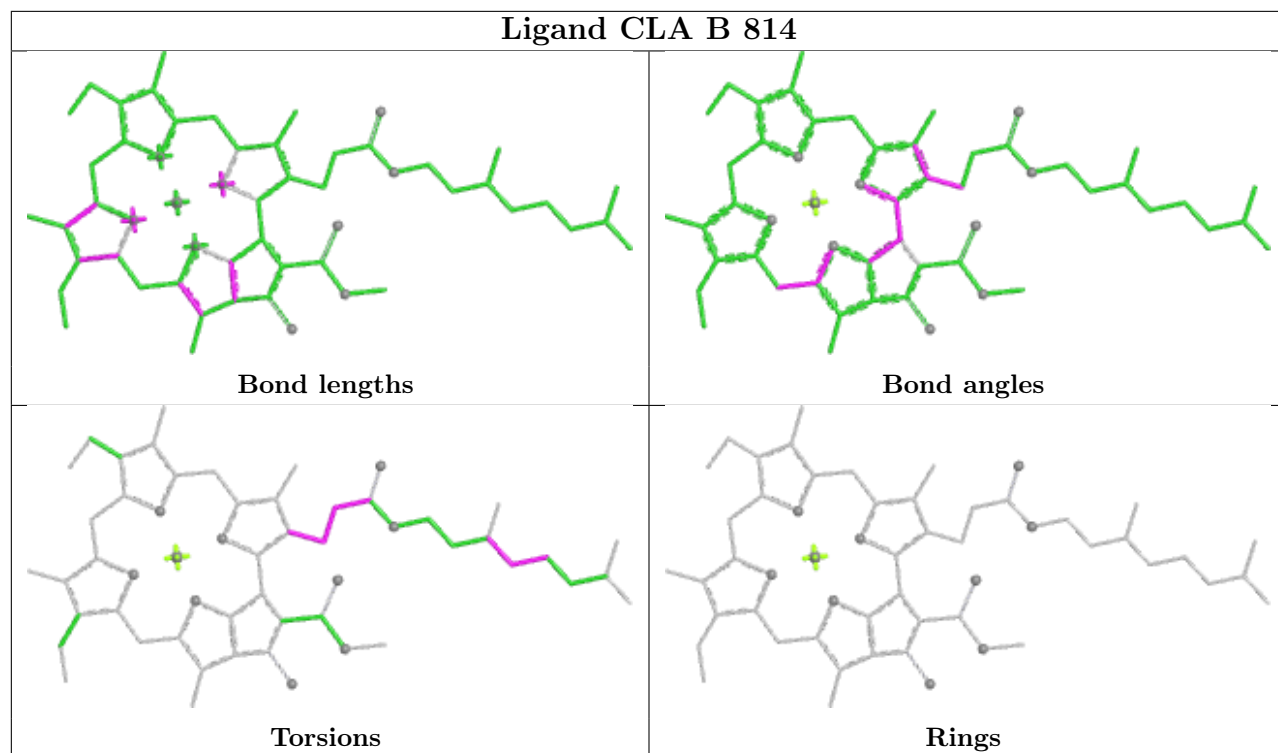
Torsions



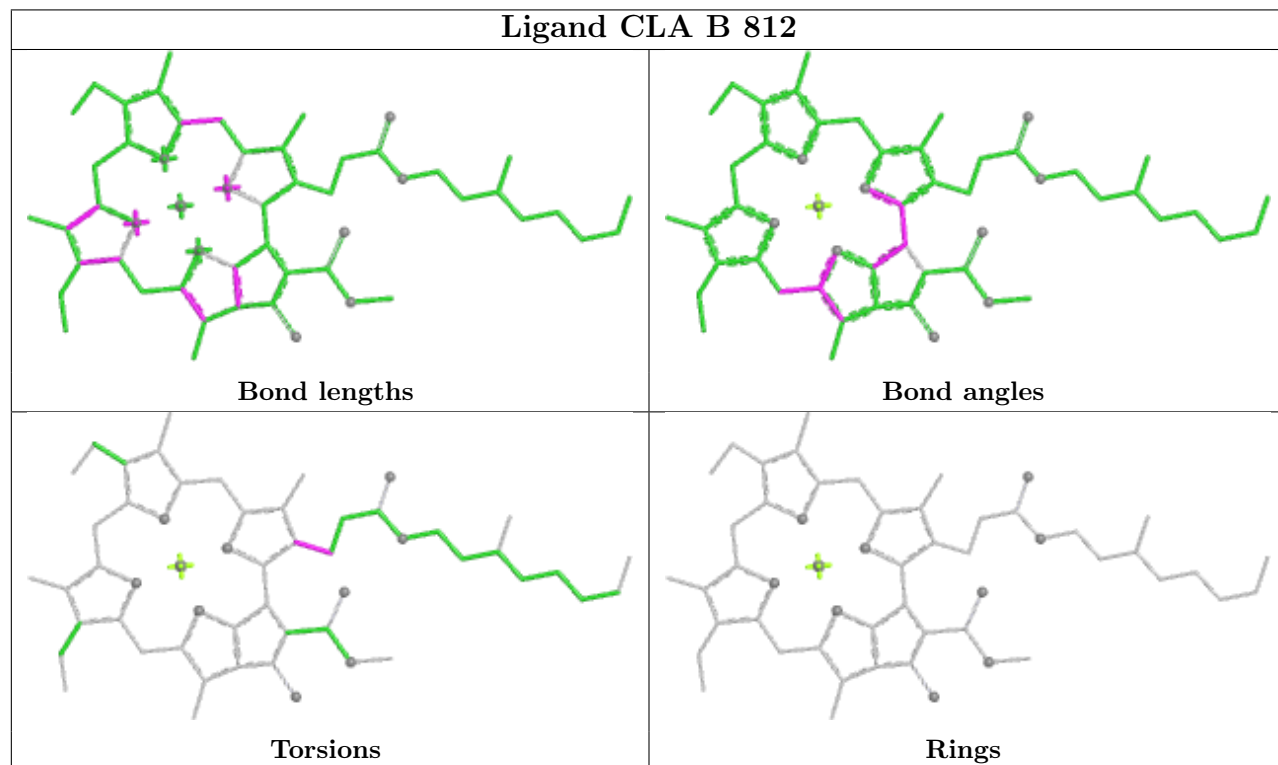
Rings

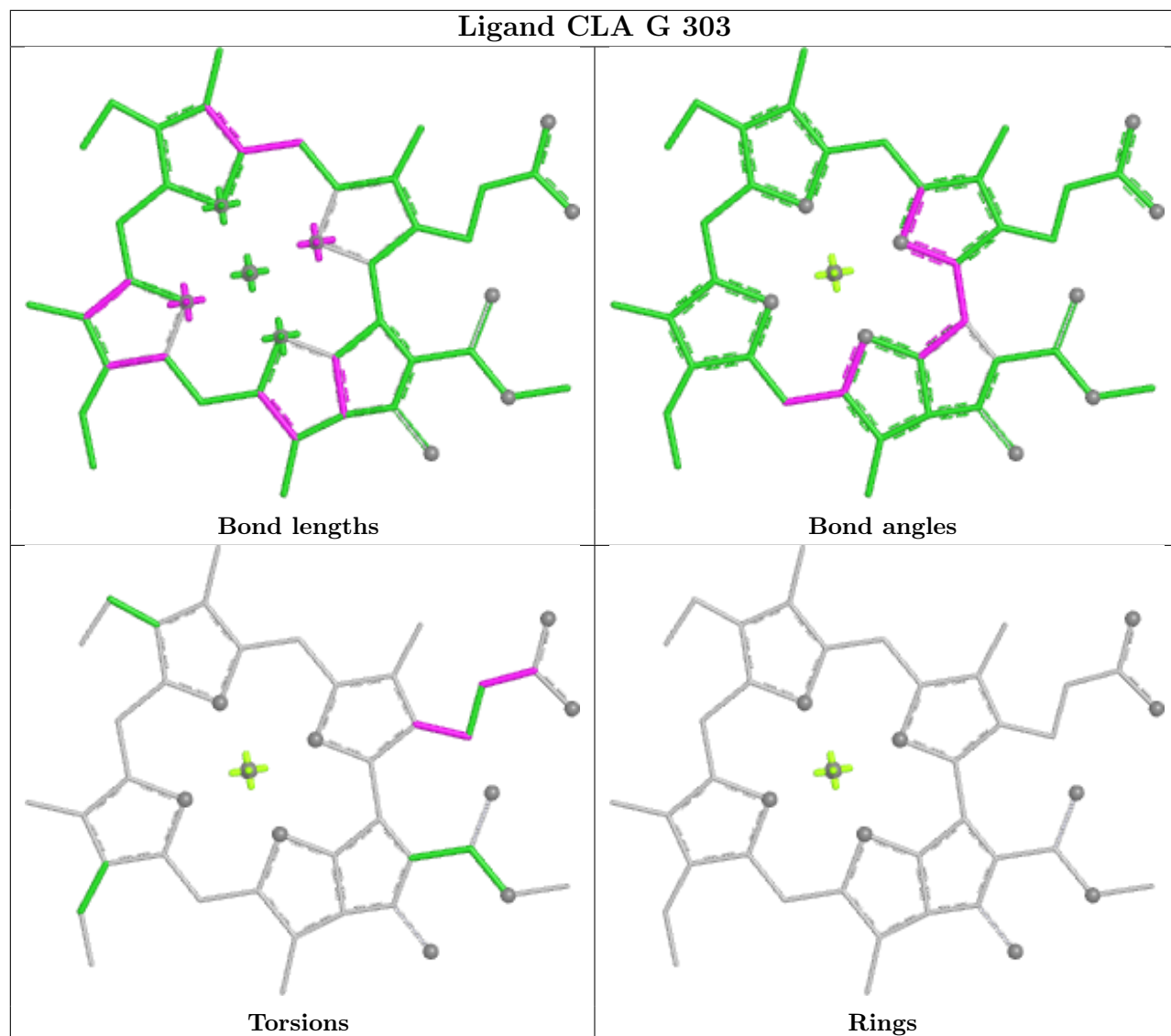


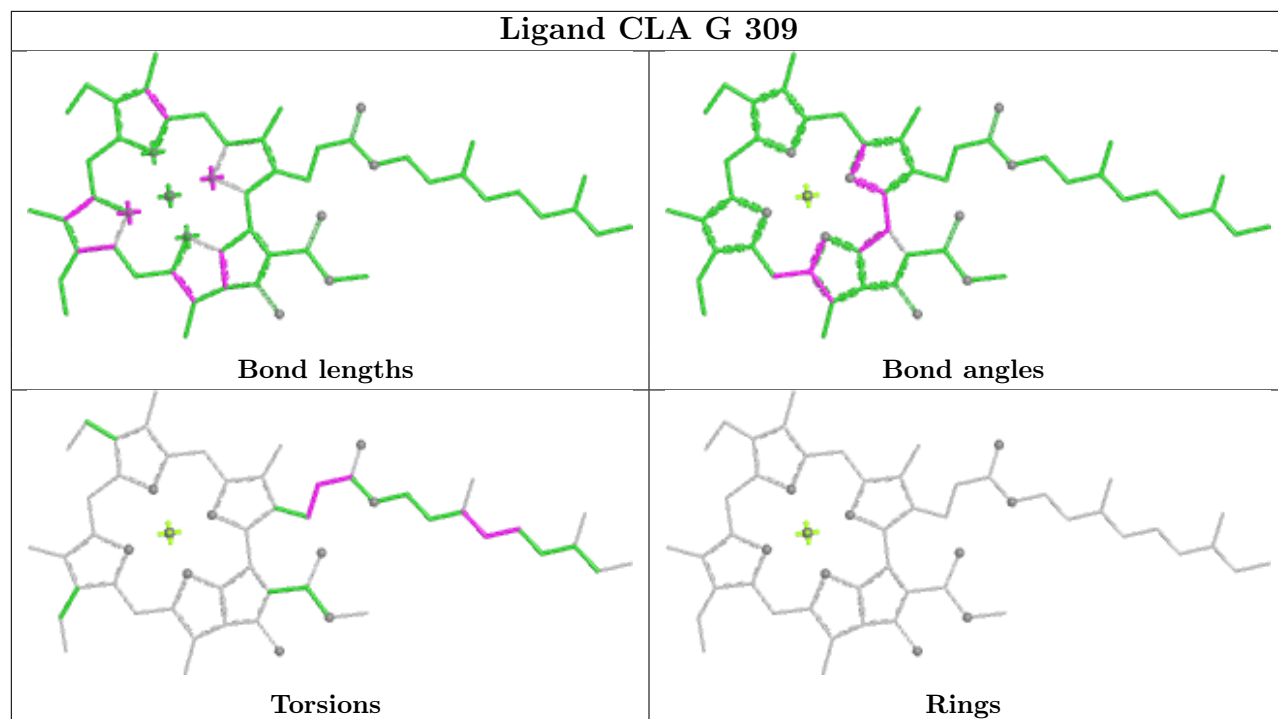
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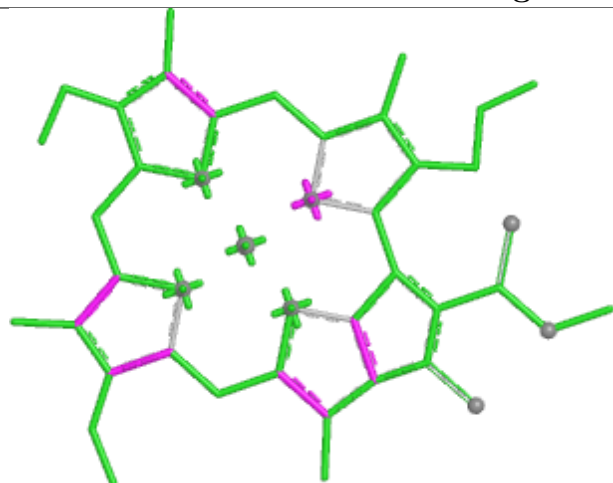
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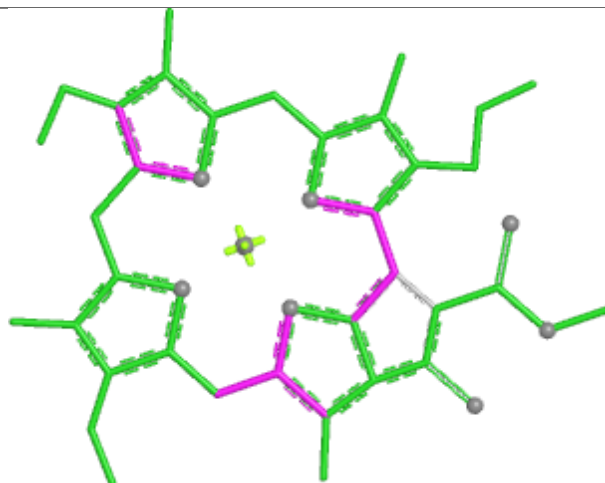




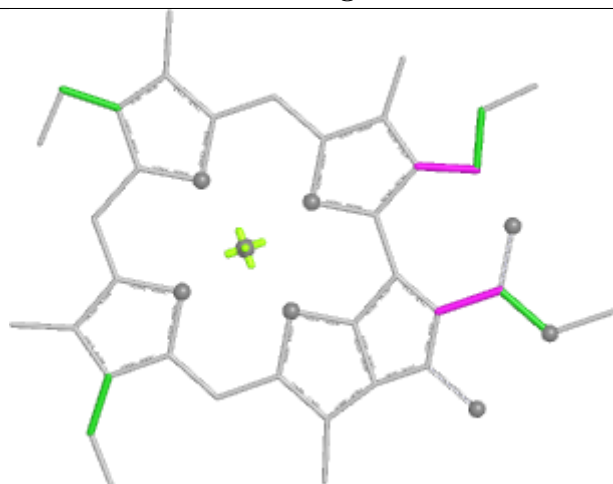
Ligand CLA G 304



Bond lengths



Bond angles

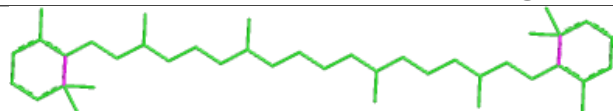


Torsions

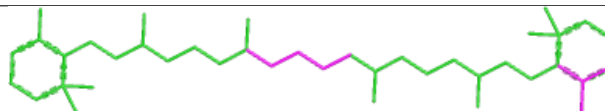


Rings

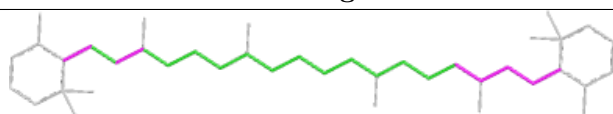
Ligand BCR I 103



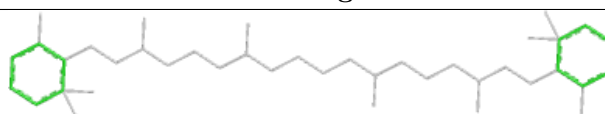
Bond lengths



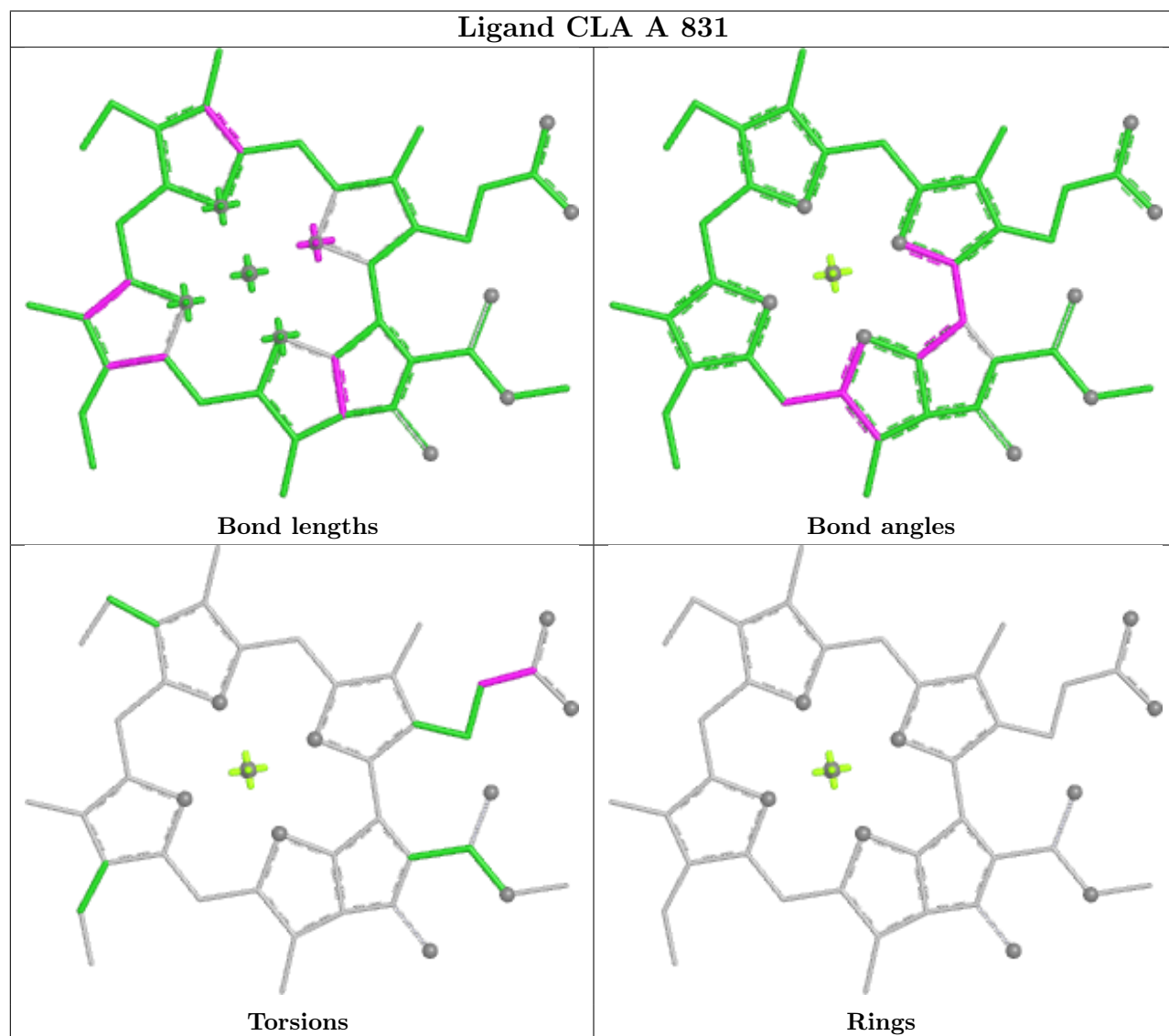
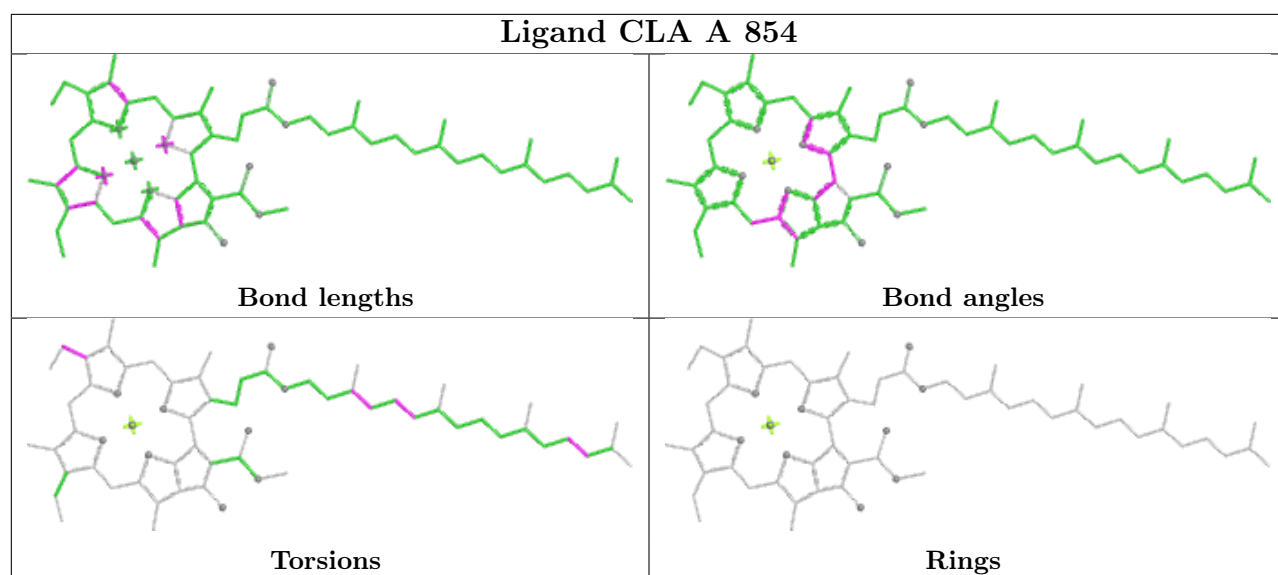
Bond angles

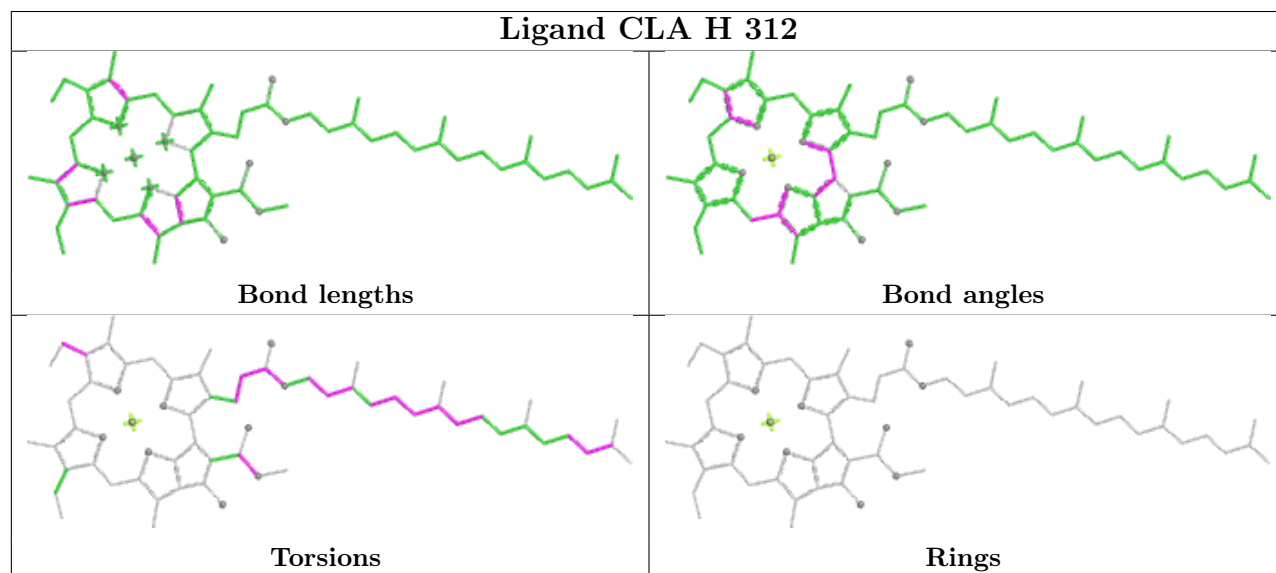
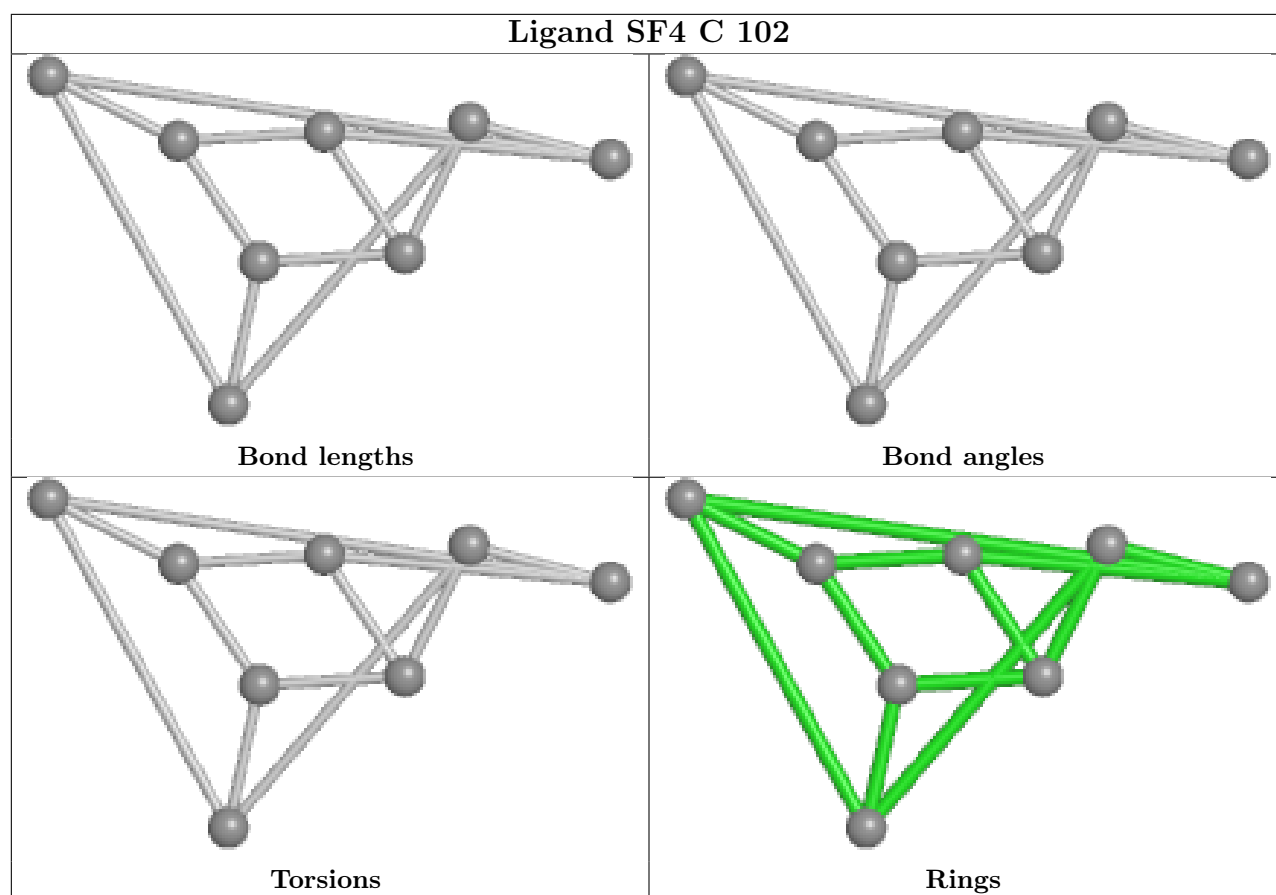


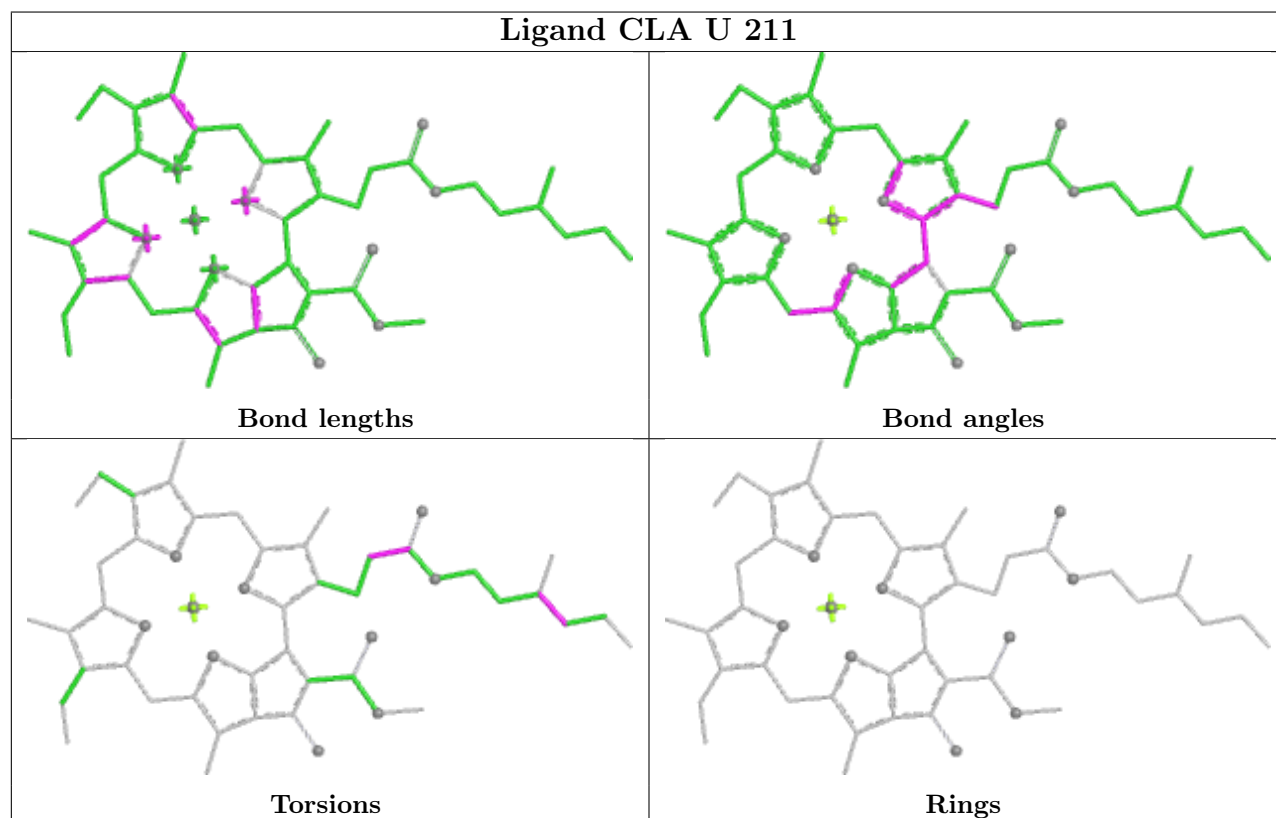
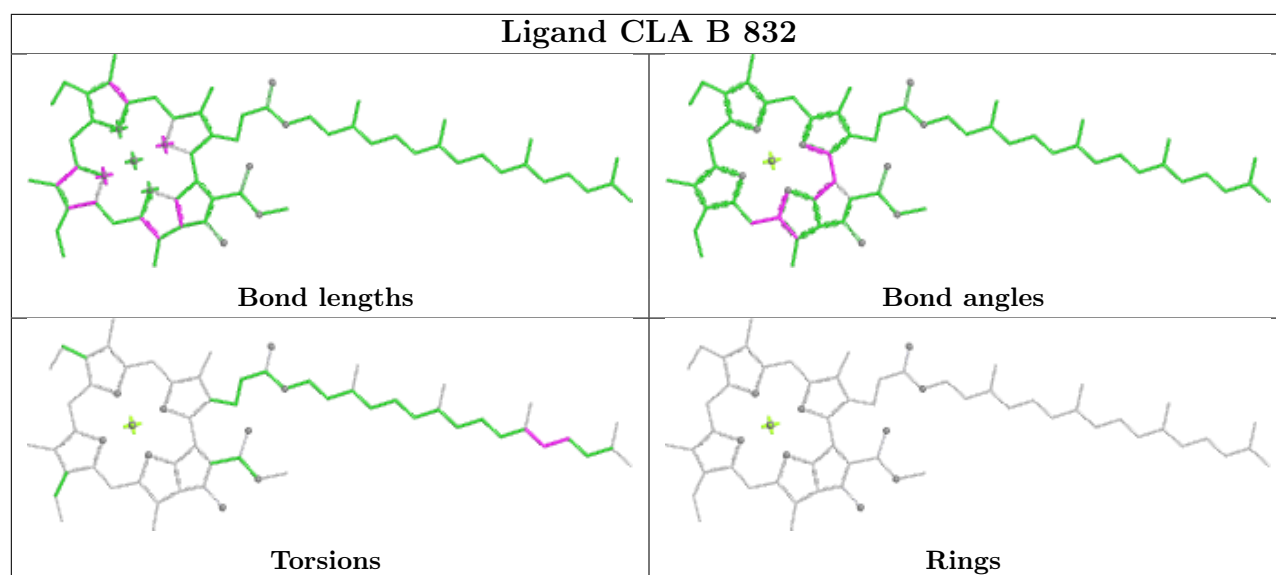
Torsions

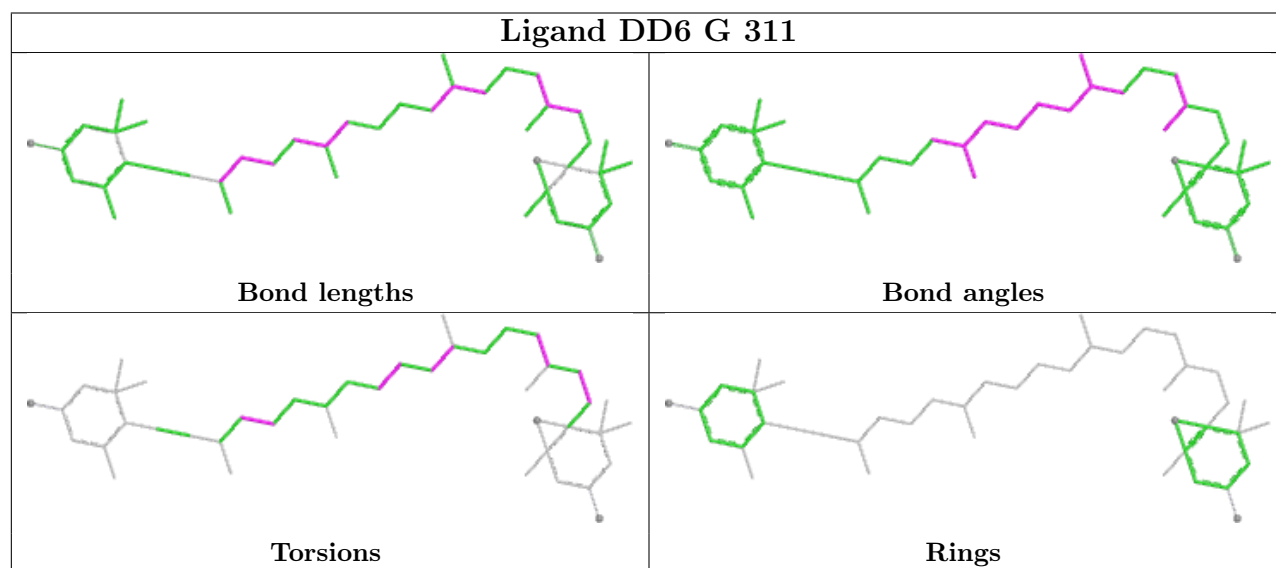
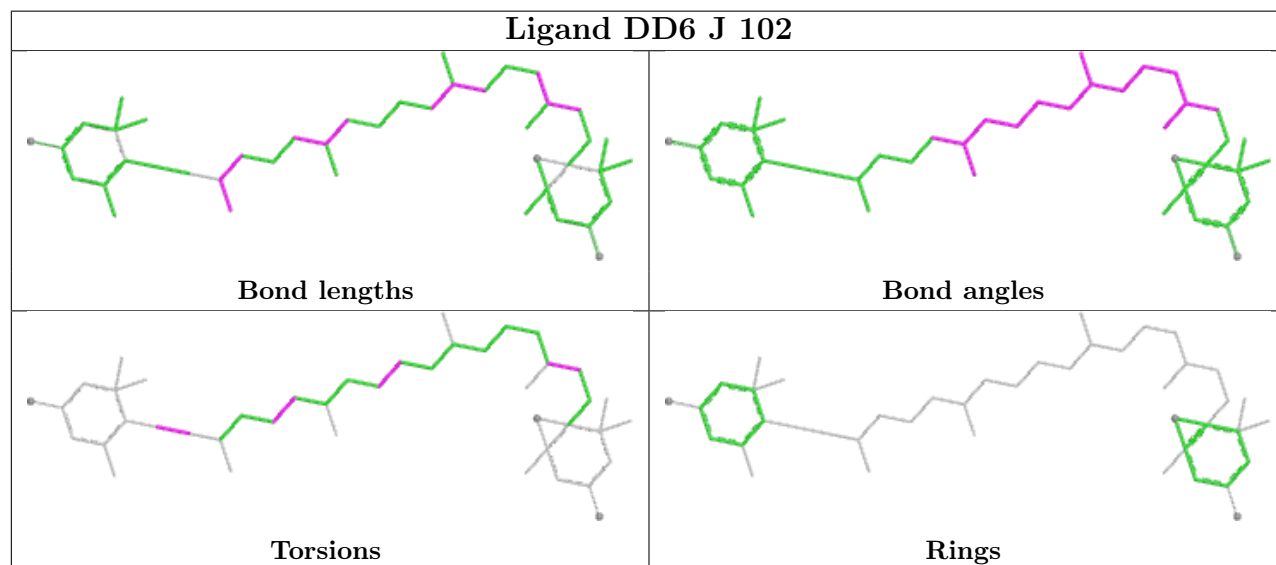
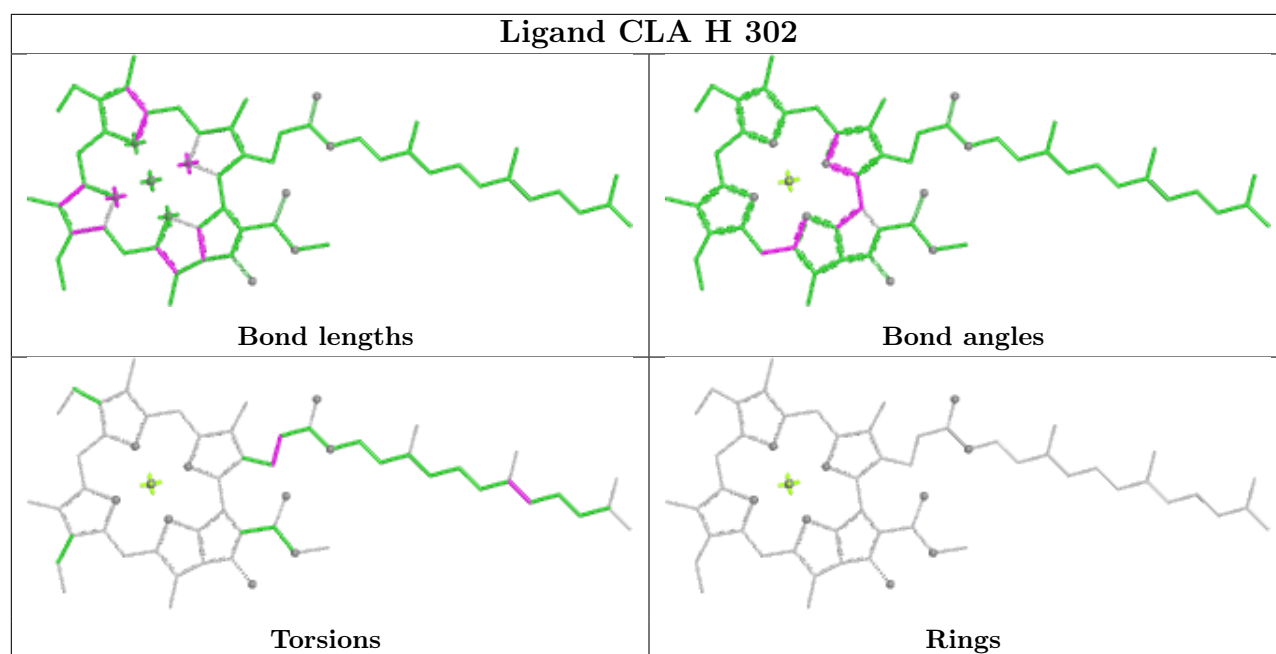


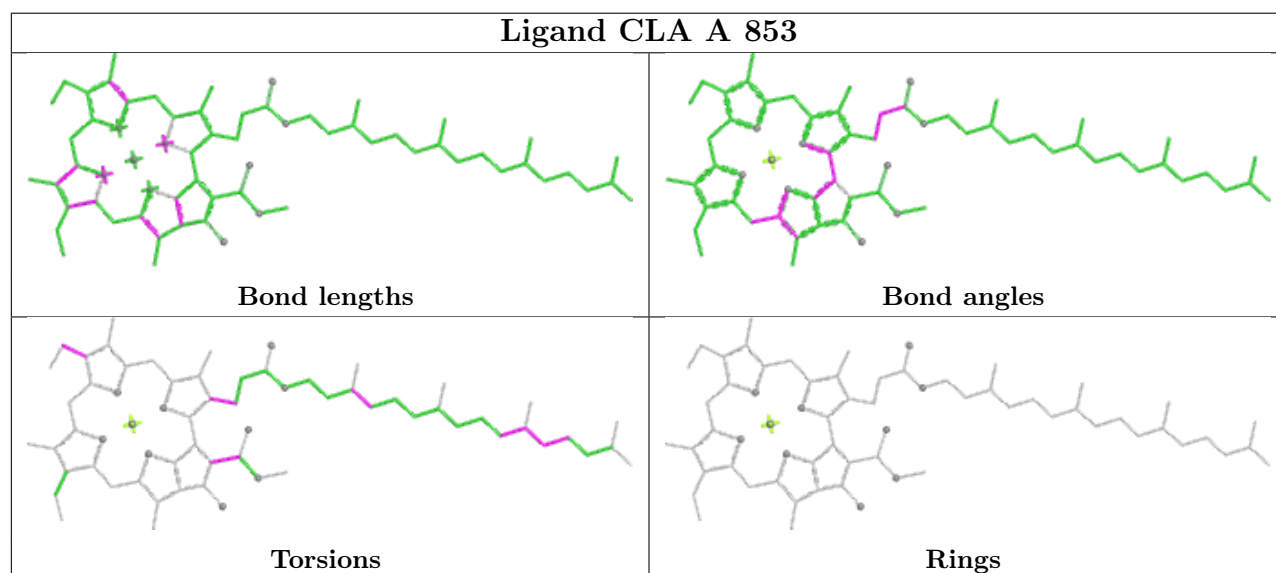
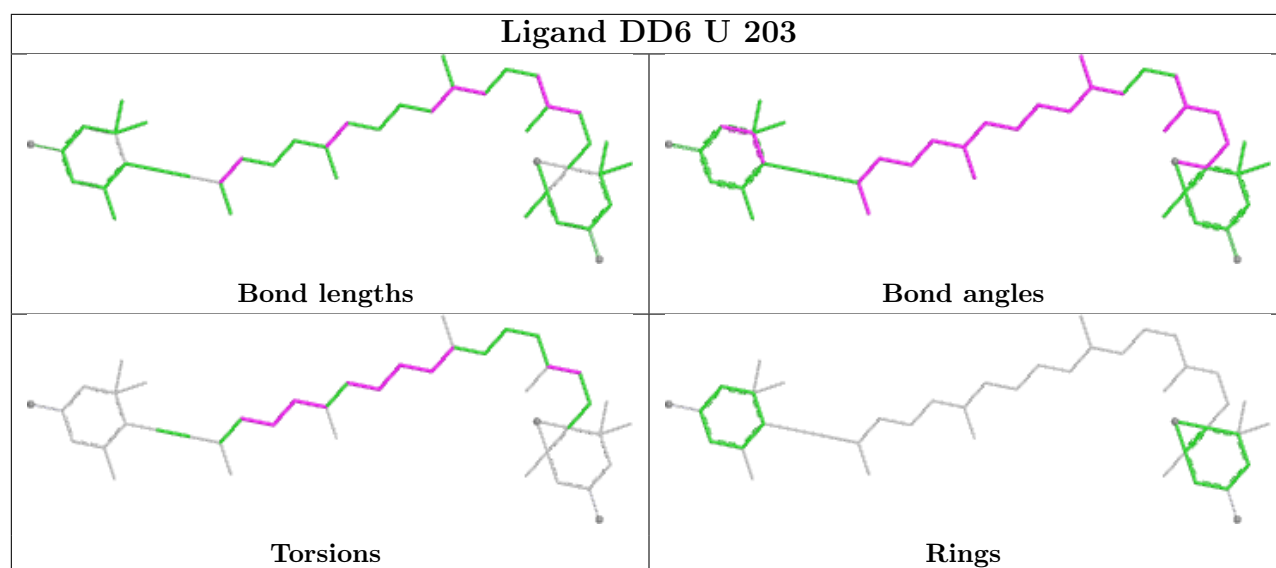
Rings

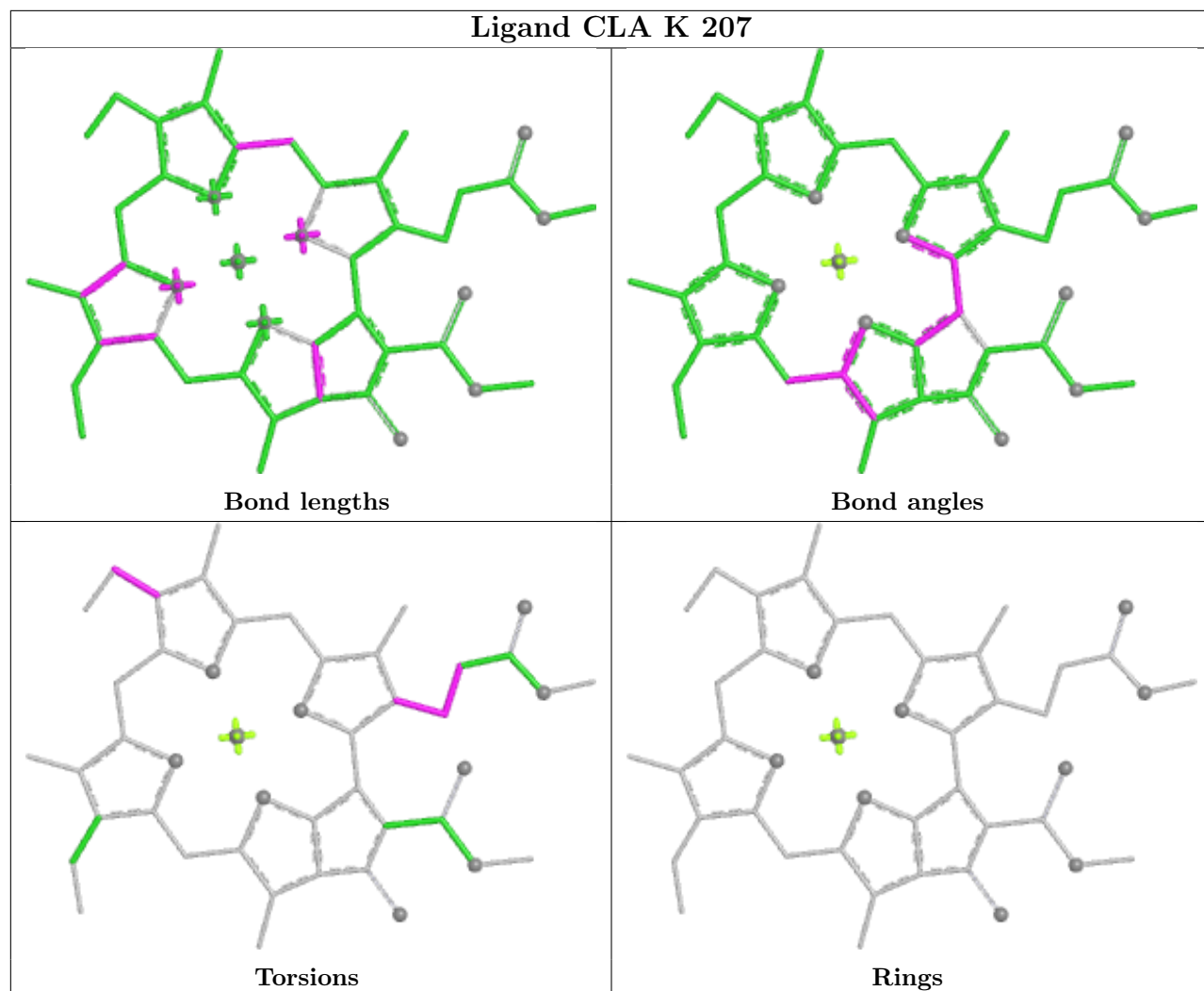




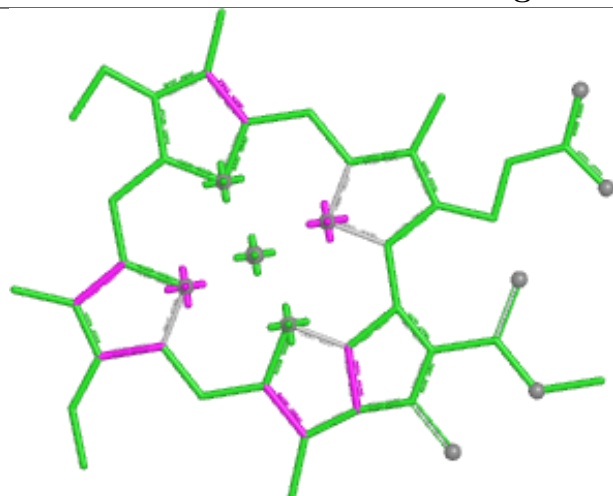




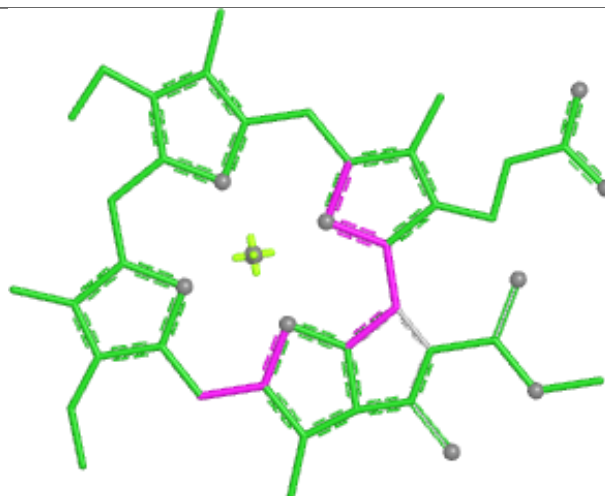




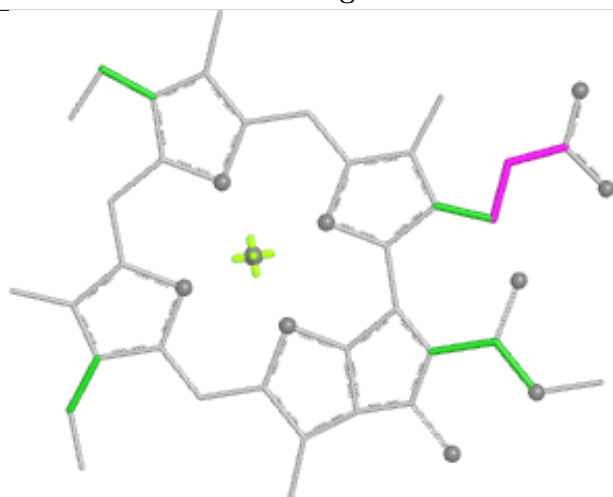
Ligand CLA A 814



Bond lengths



Bond angles

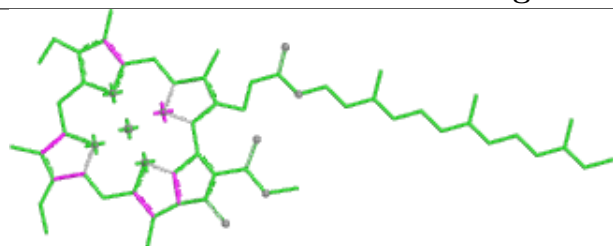


Torsions

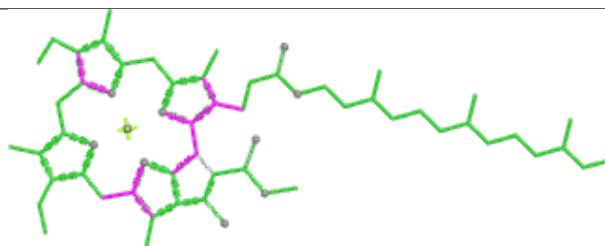


Rings

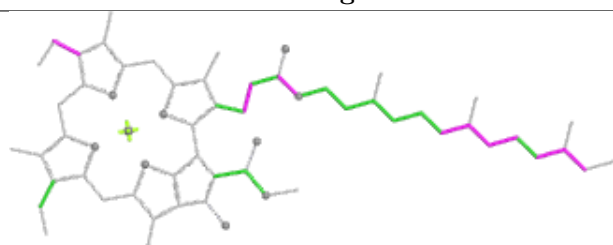
Ligand CLA G 305



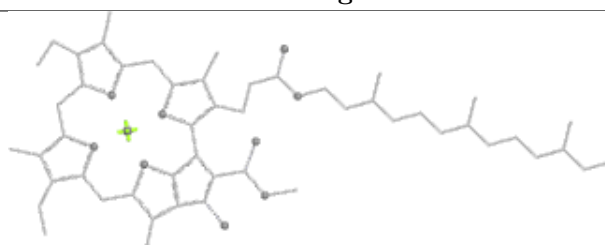
Bond lengths



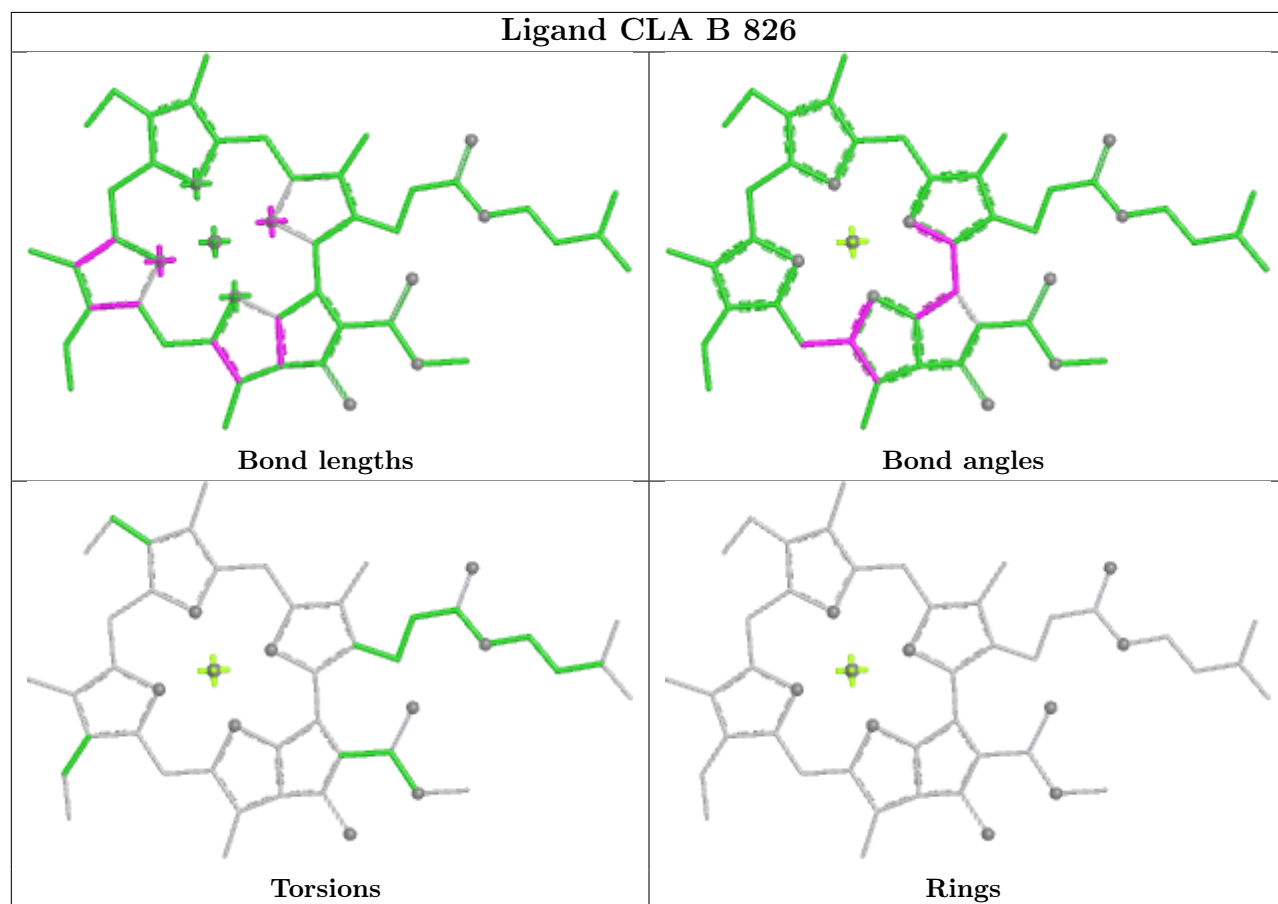
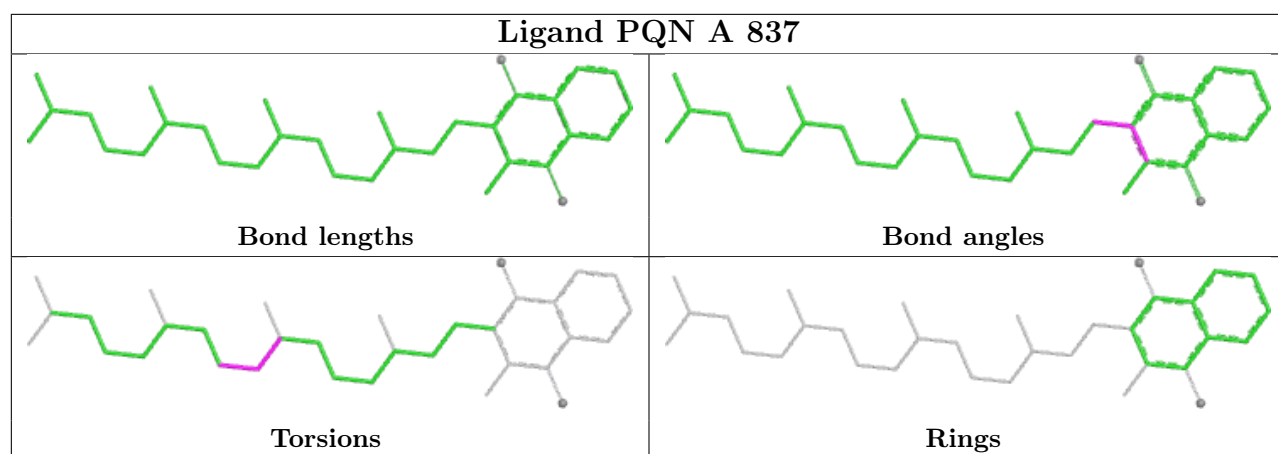
Bond angles

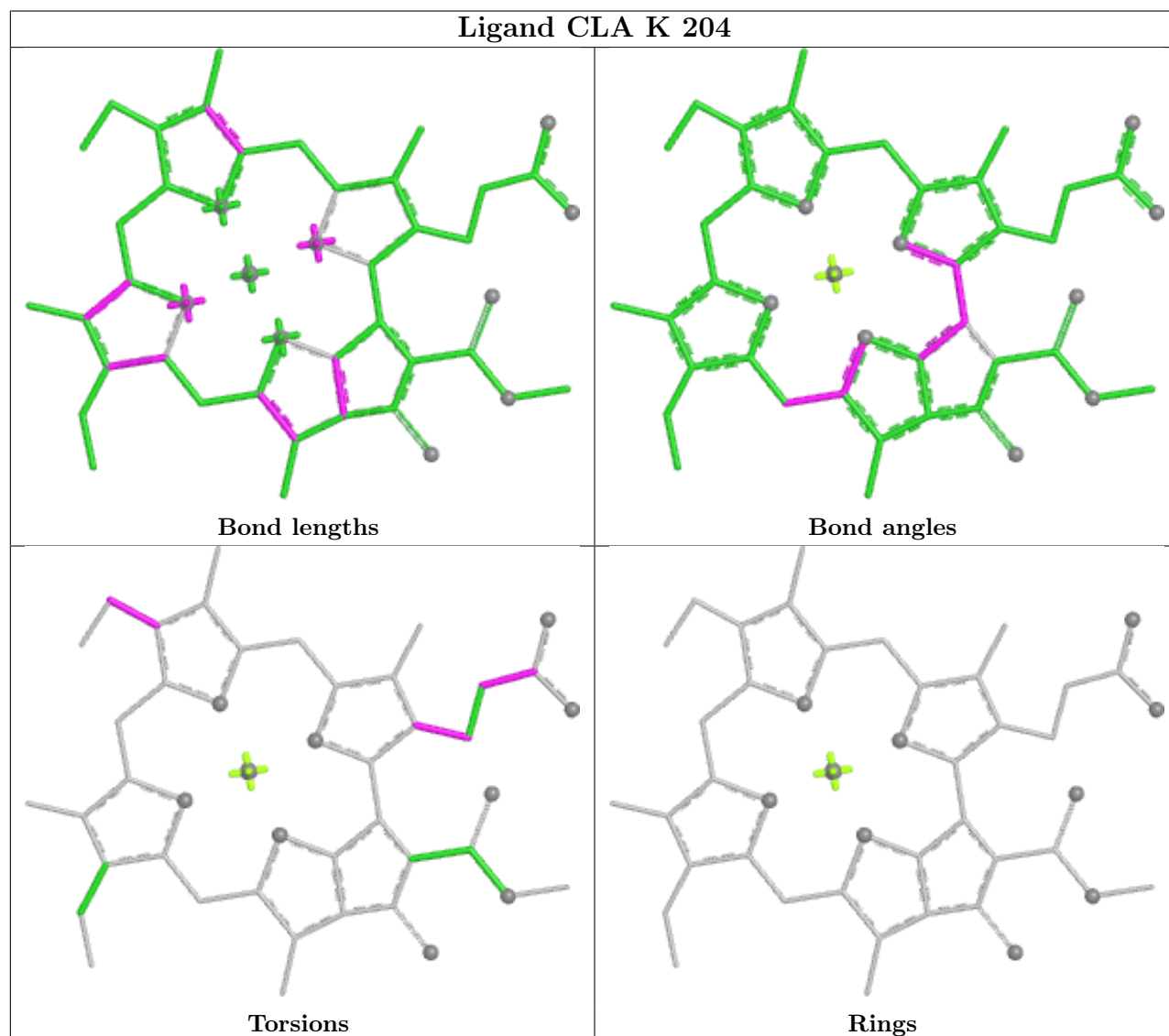
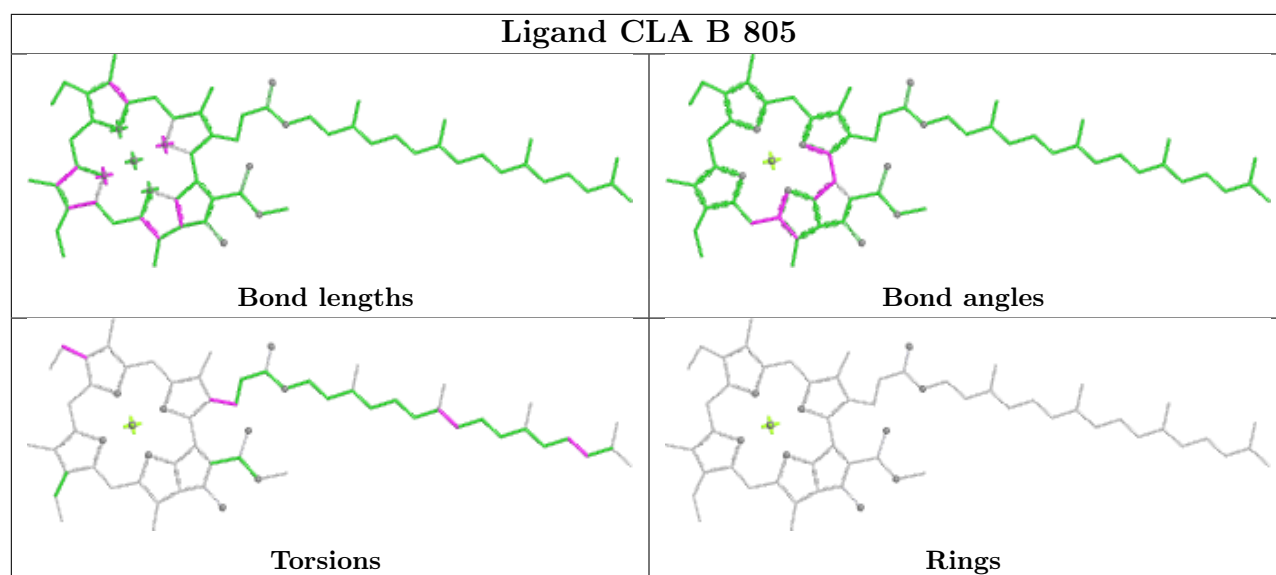


Torsions

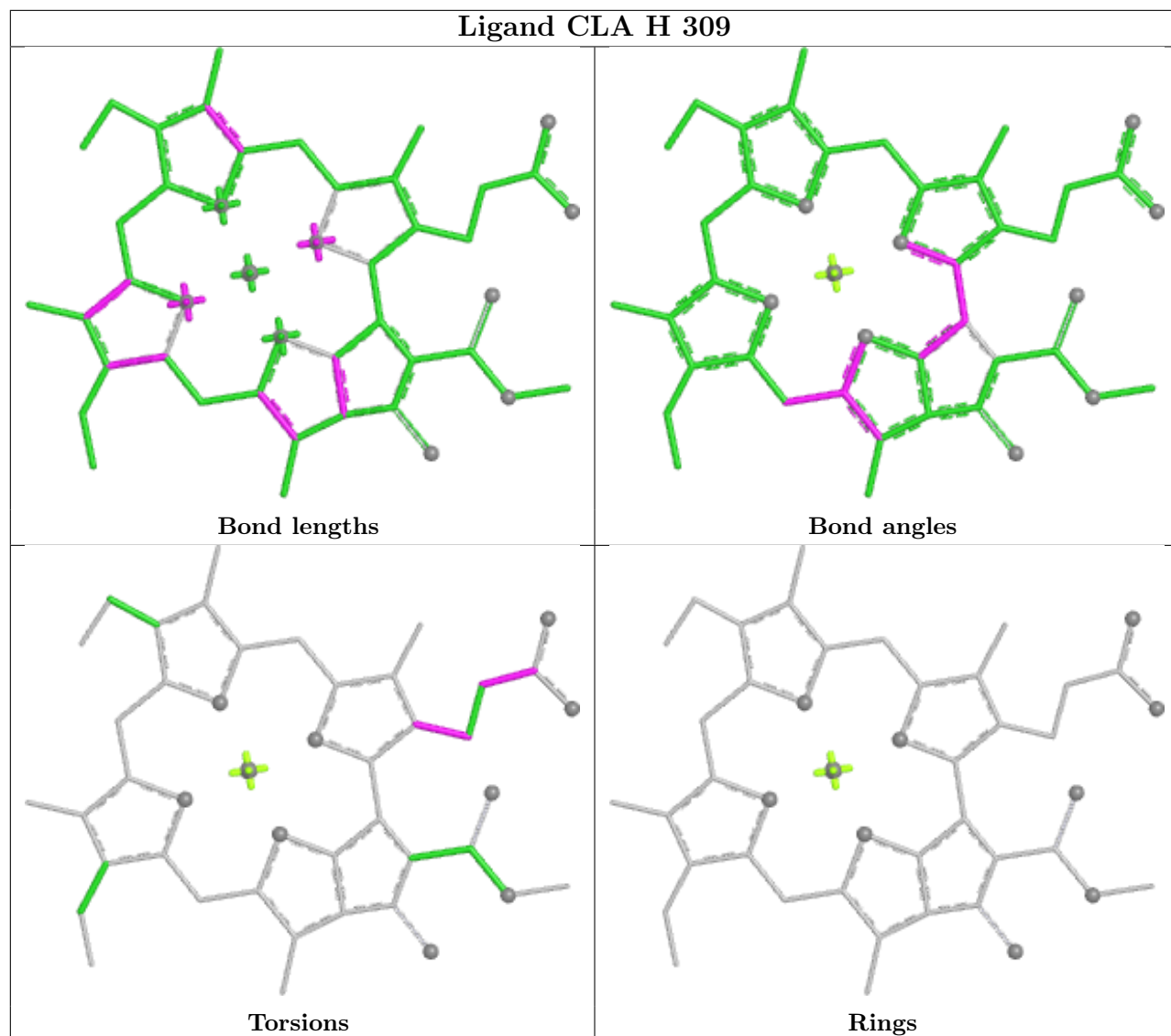


Rings

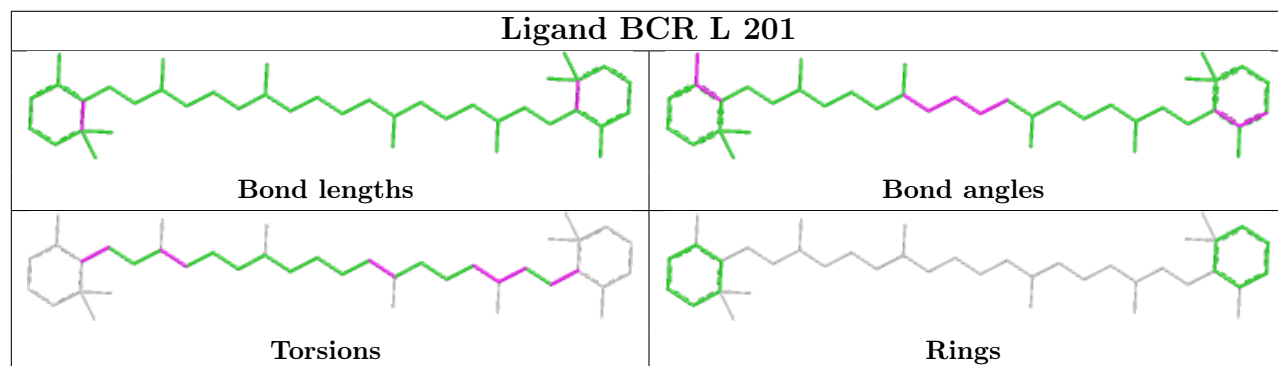




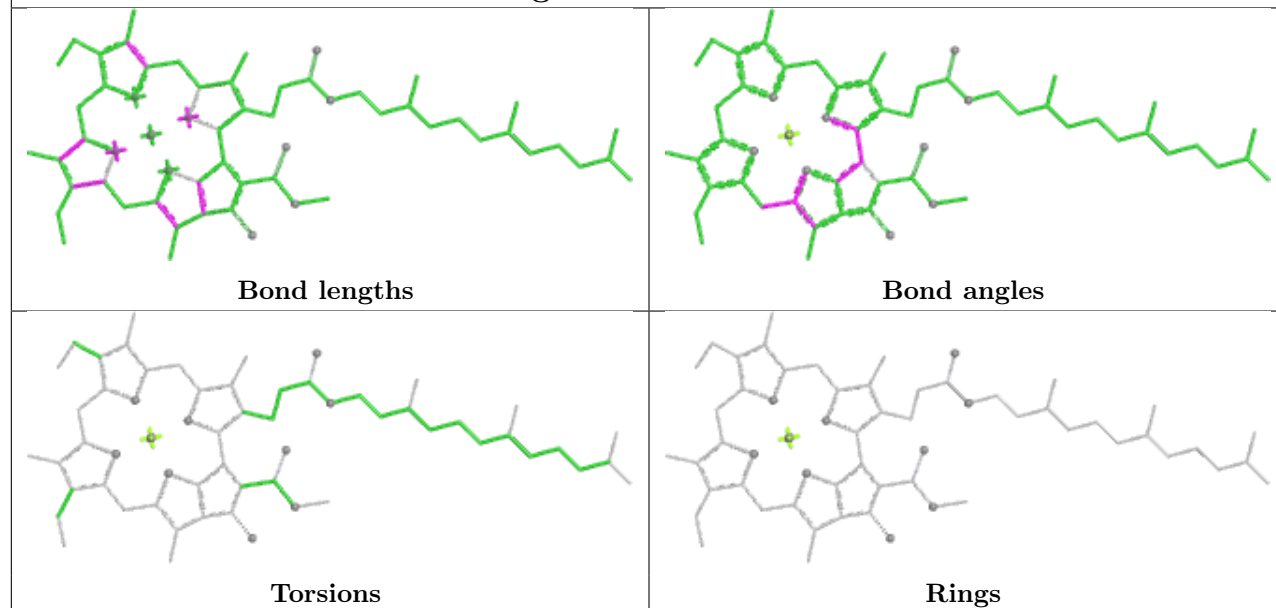
Ligand CLA H 309



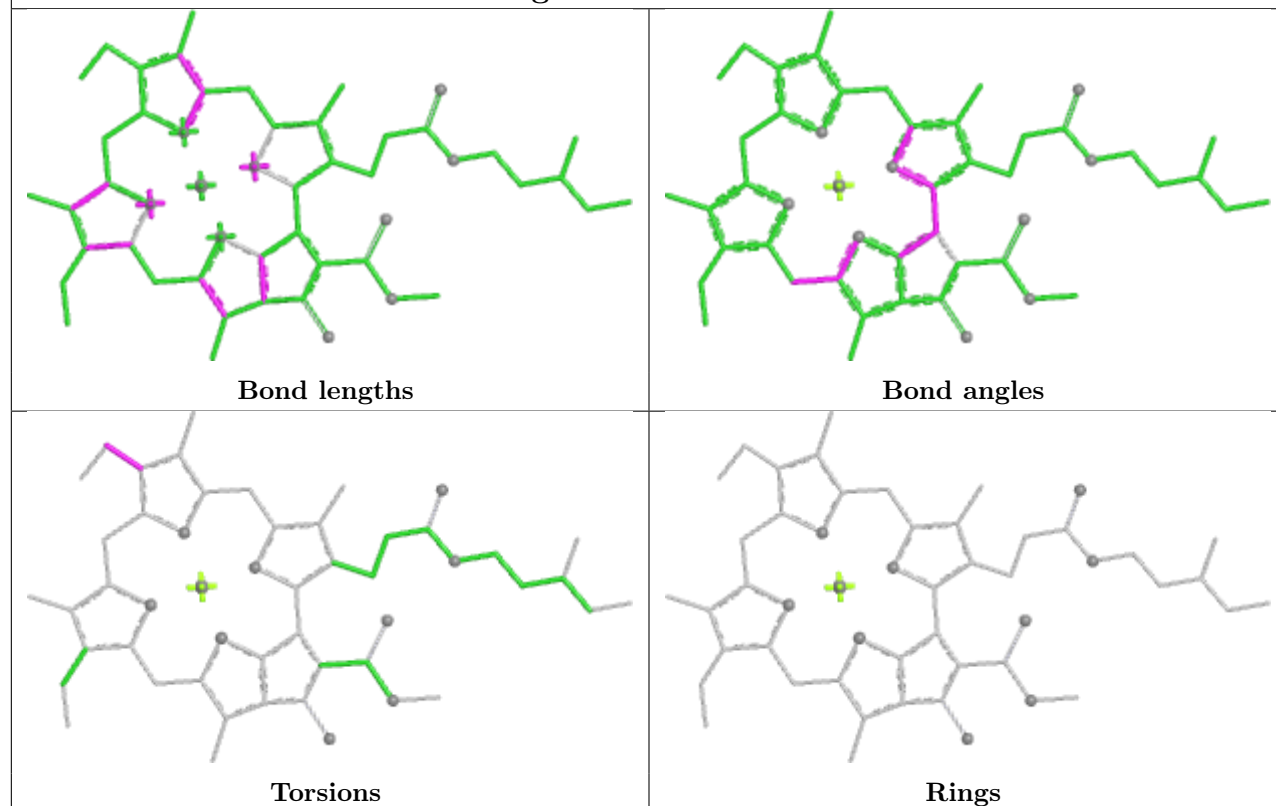
Ligand BCR L 201



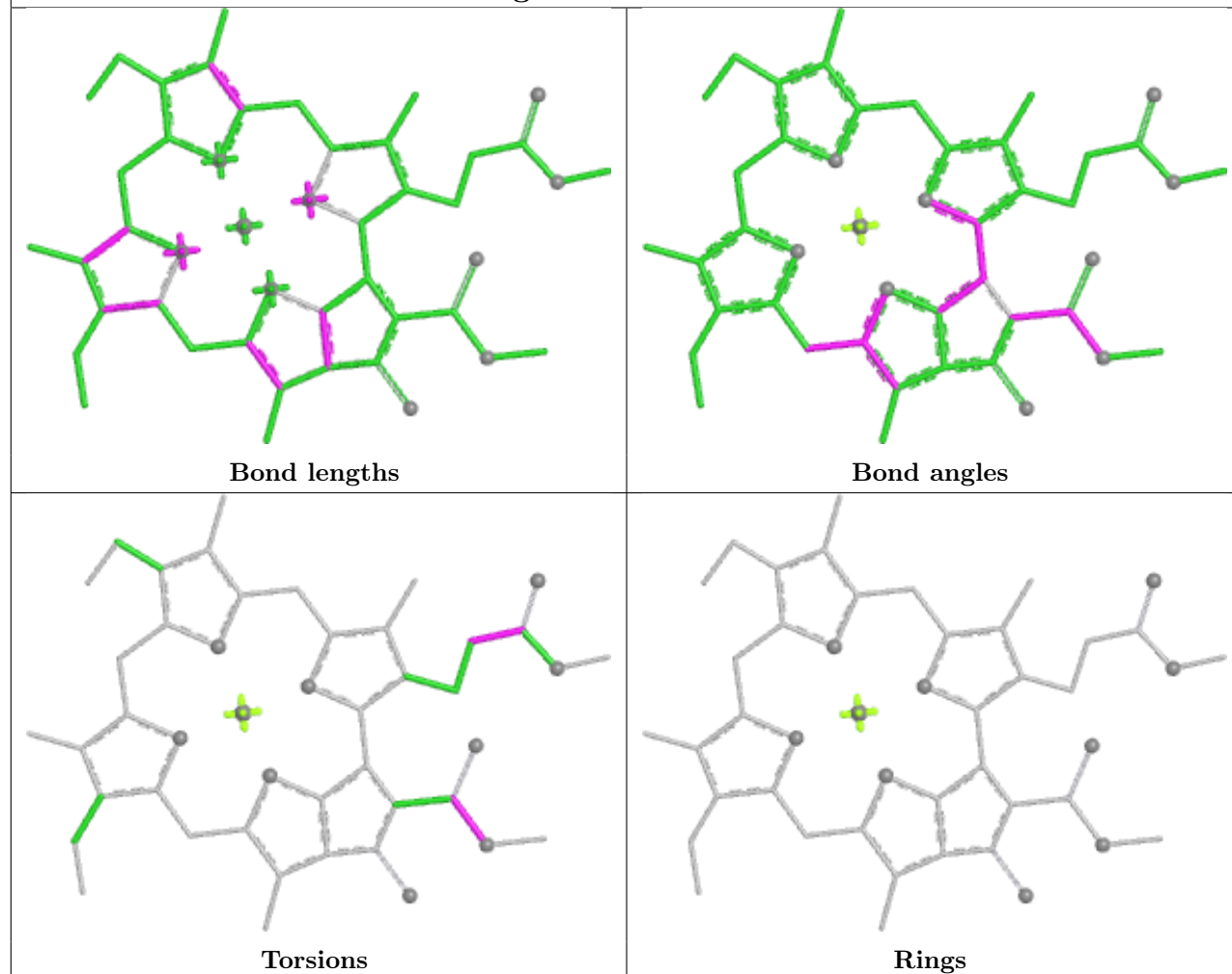
Ligand CLA B 816



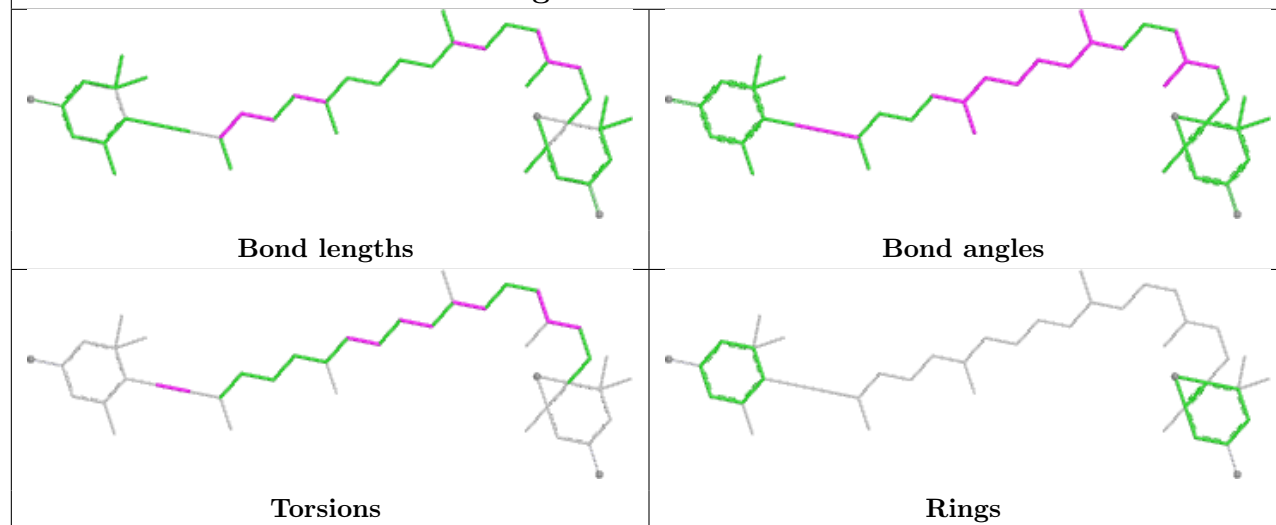
Ligand CLA A 832

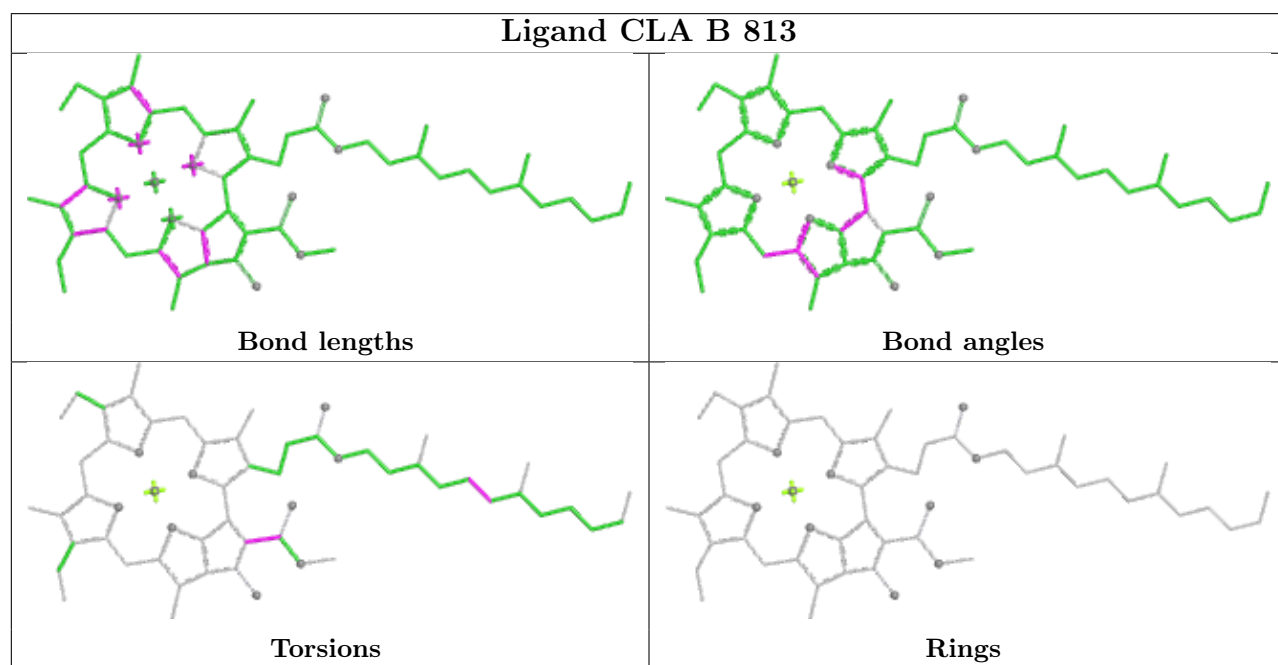
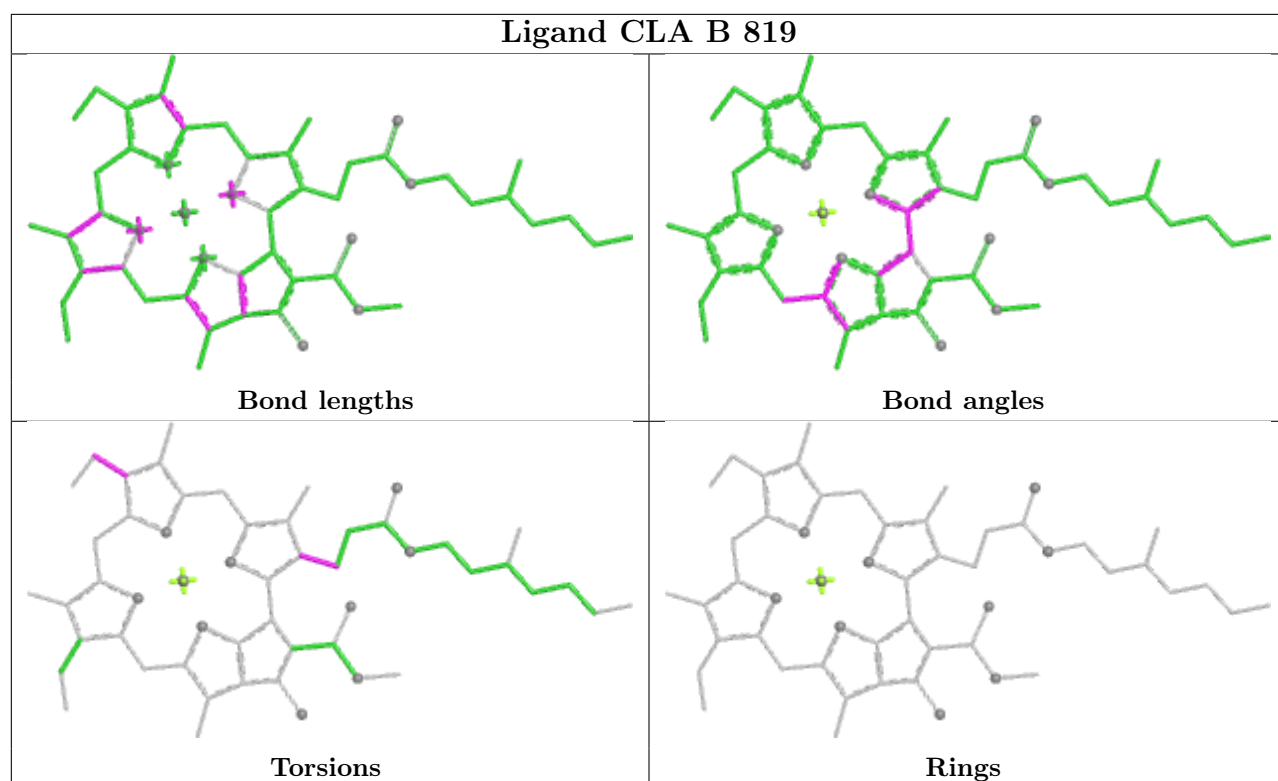


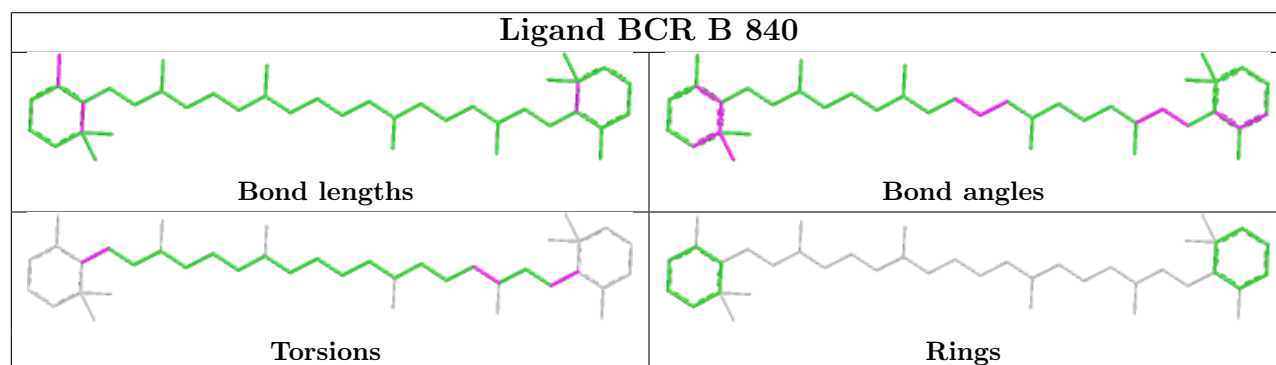
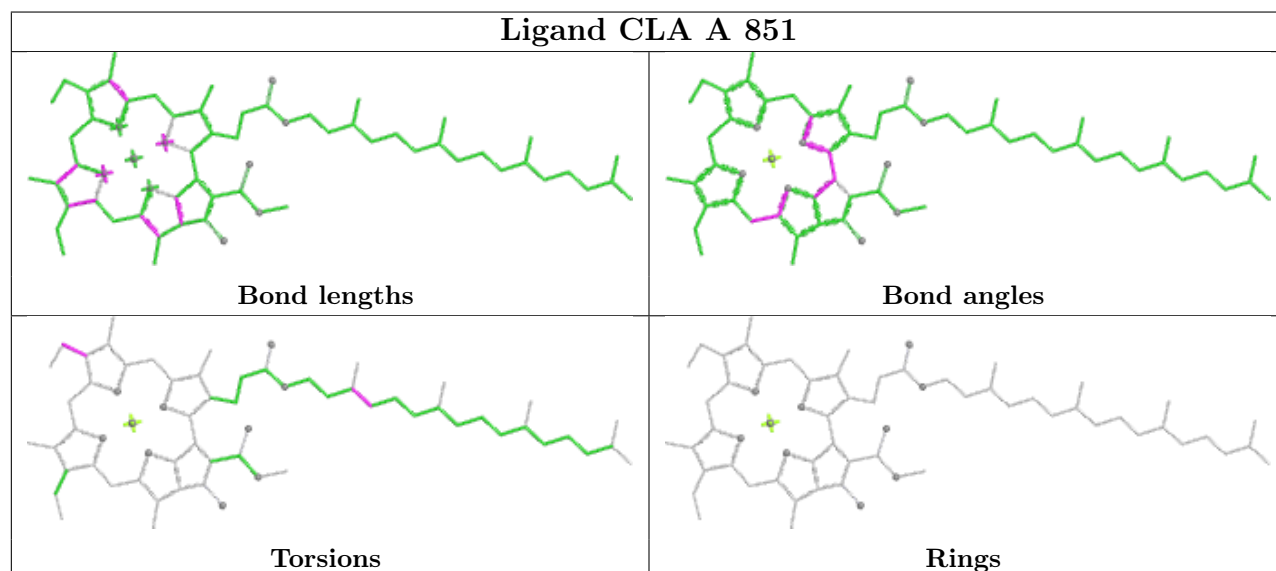
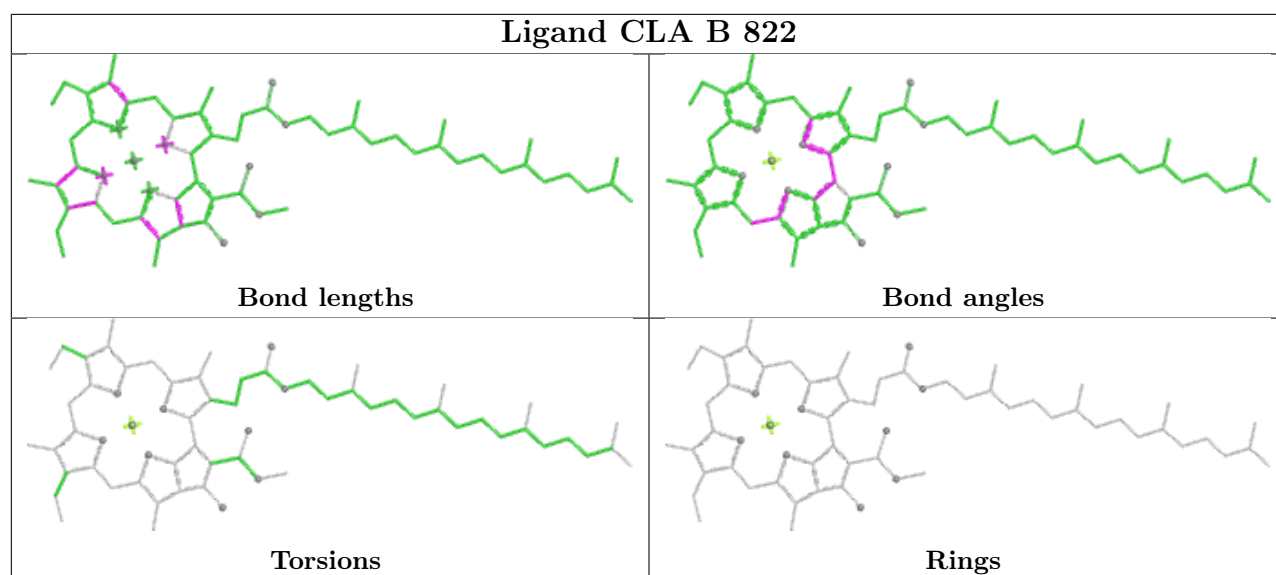
Ligand CLA U 208

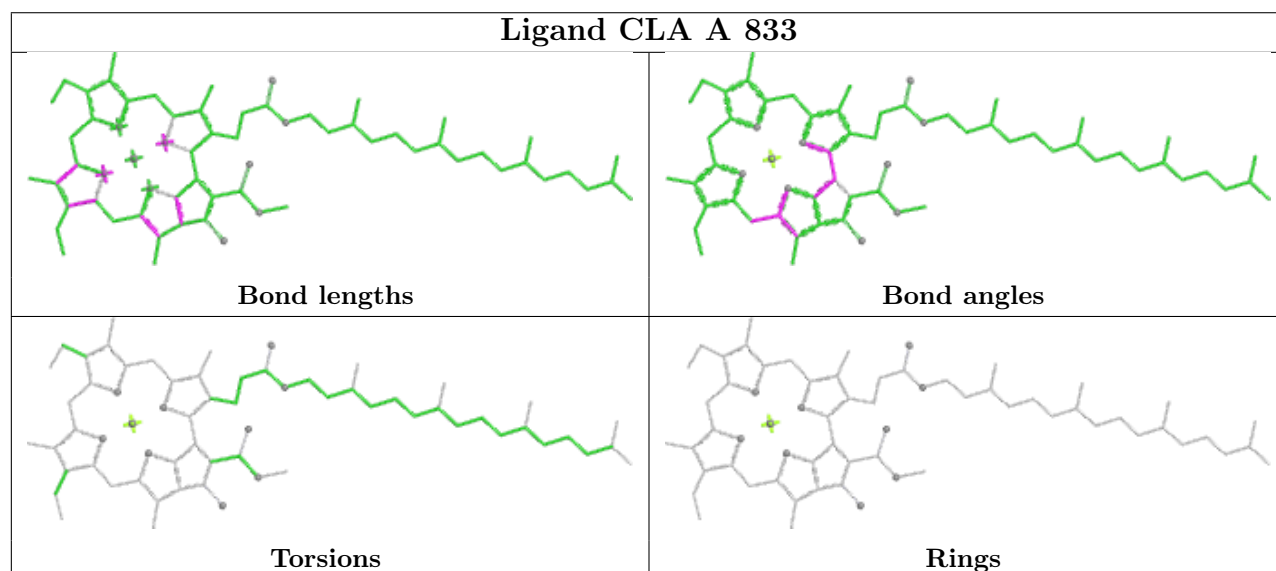
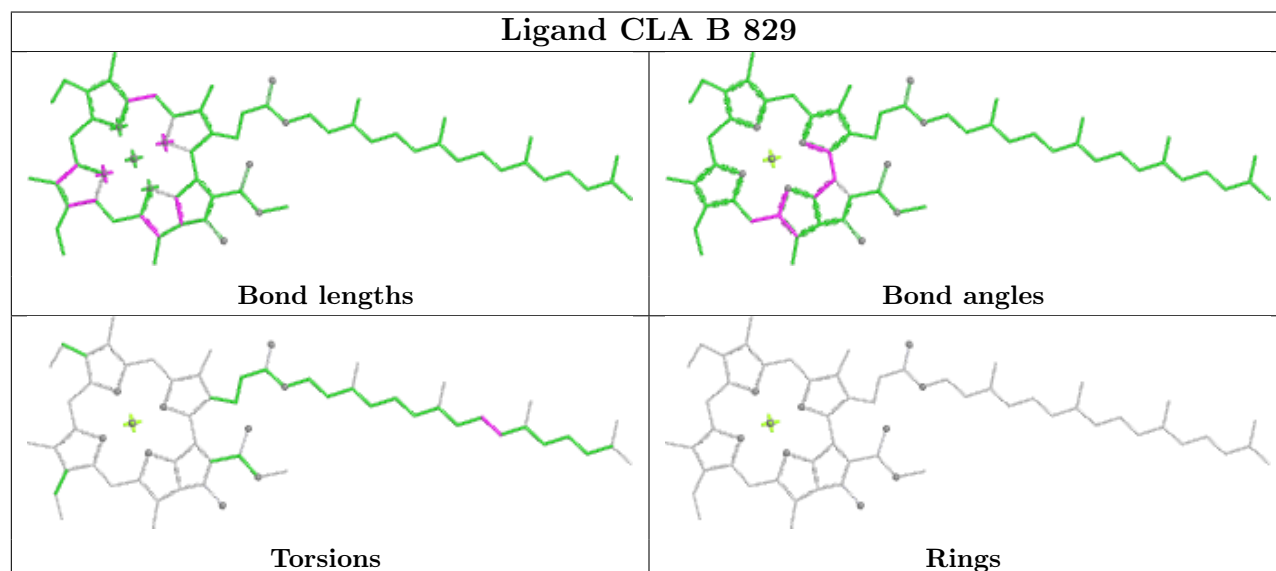
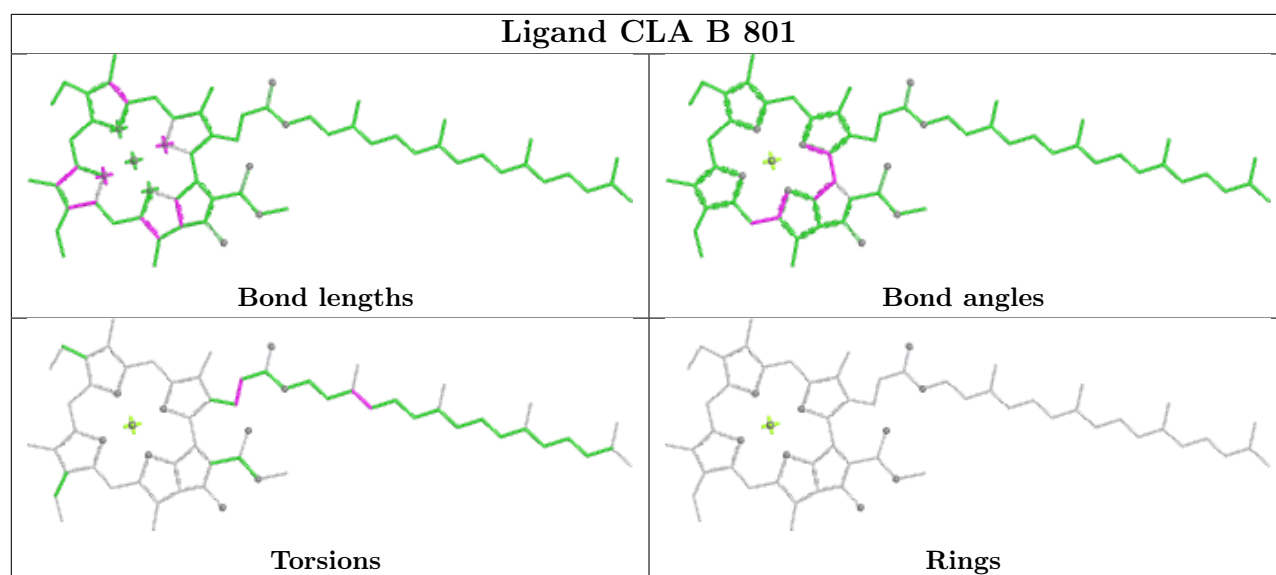


Ligand DD6 A 846

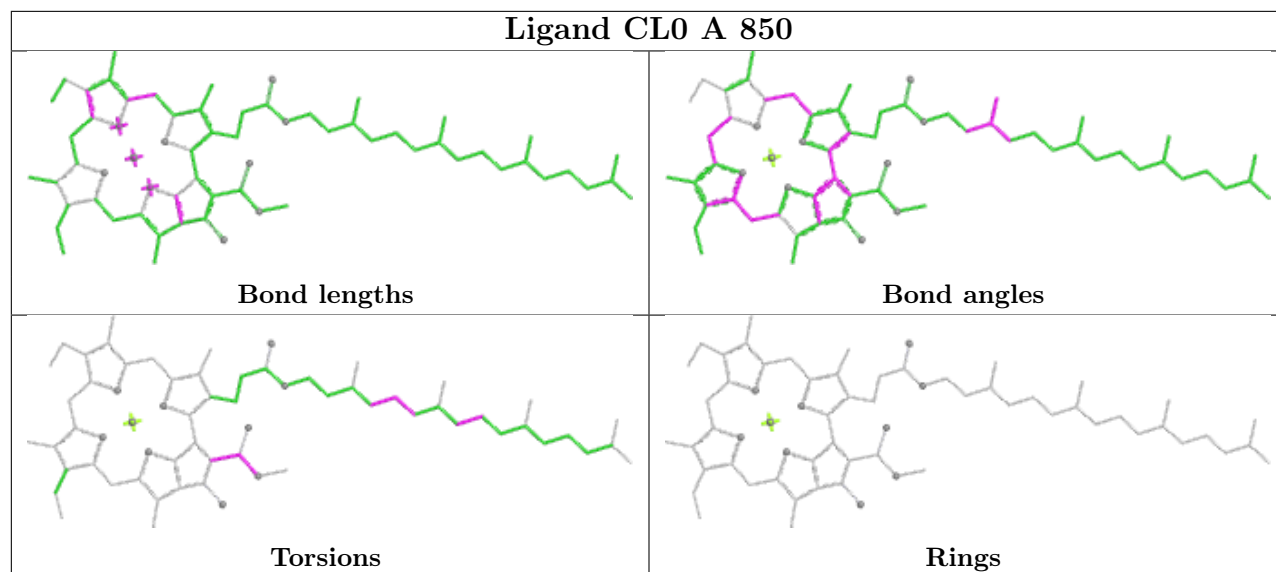




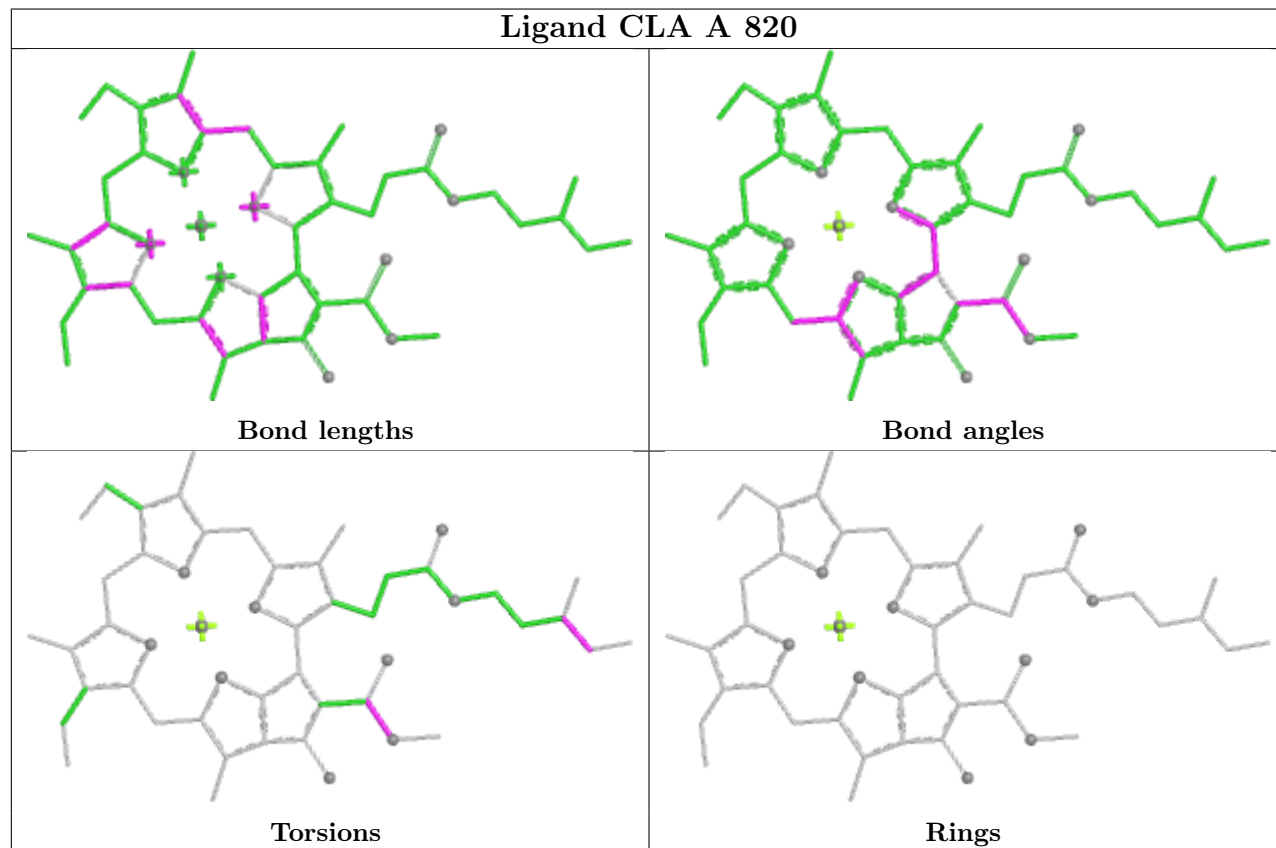


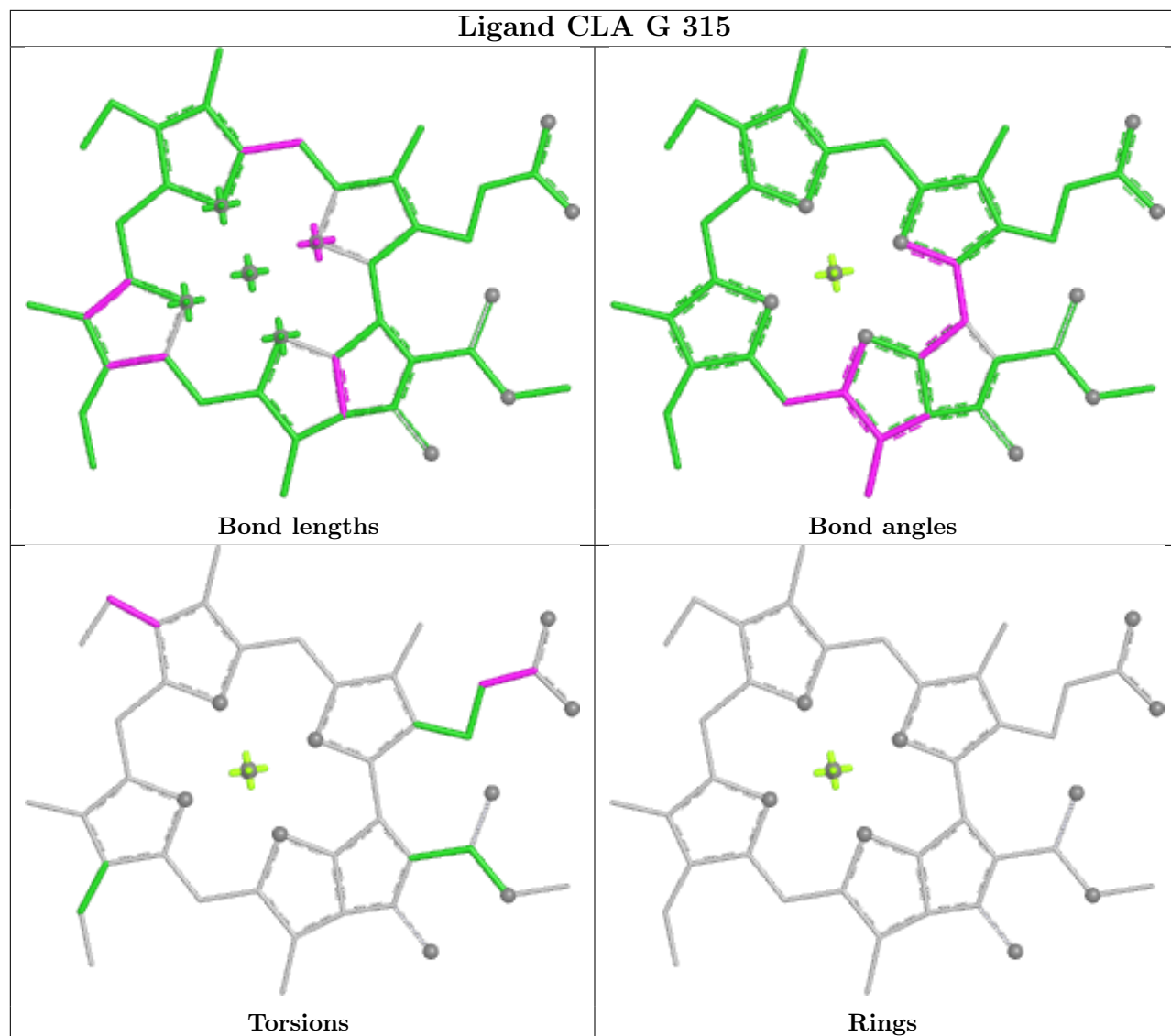


Ligand CL0 A 850

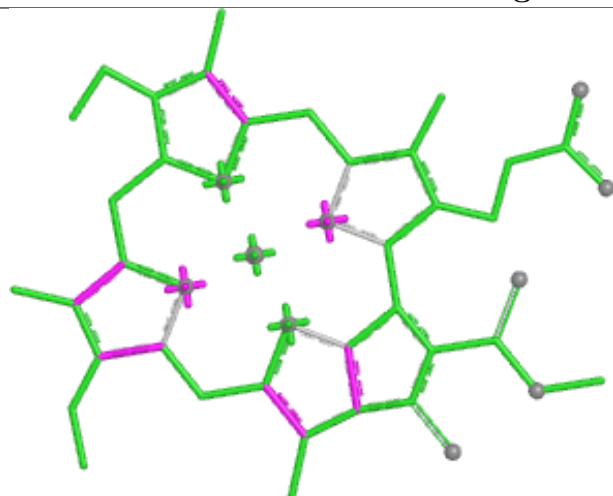


Ligand CLA A 820

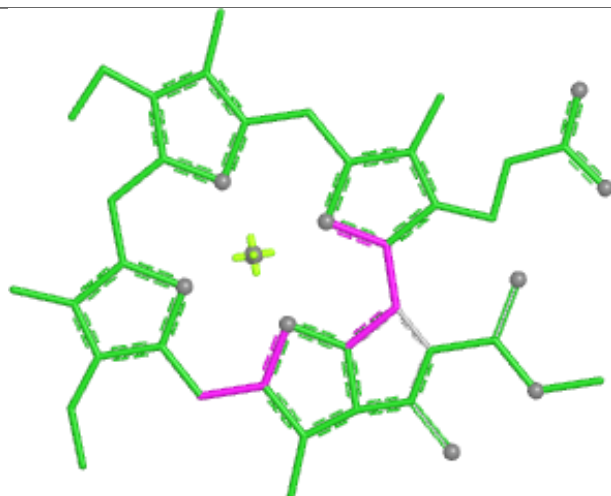




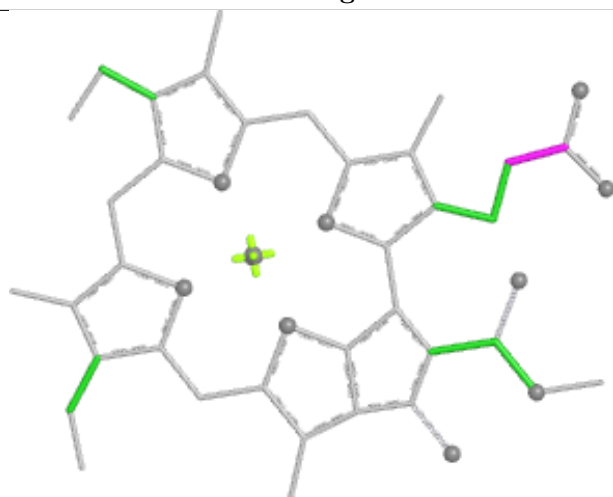
Ligand CLA H 305



Bond lengths



Bond angles

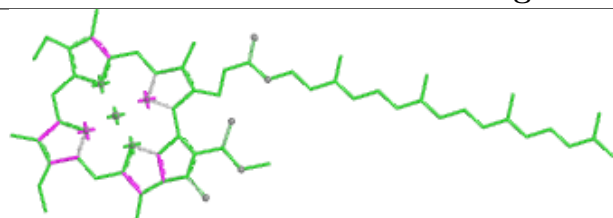


Torsions

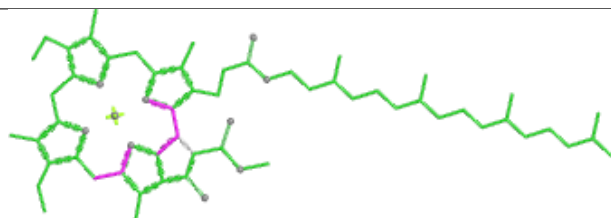


Rings

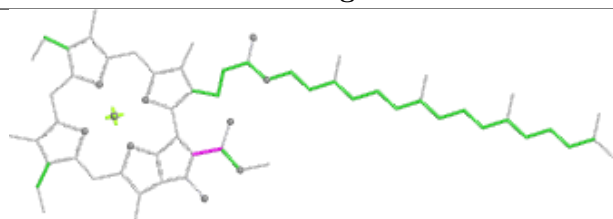
Ligand CLA A 835



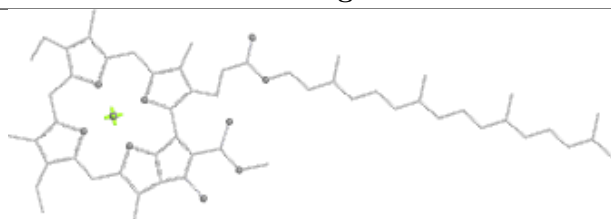
Bond lengths



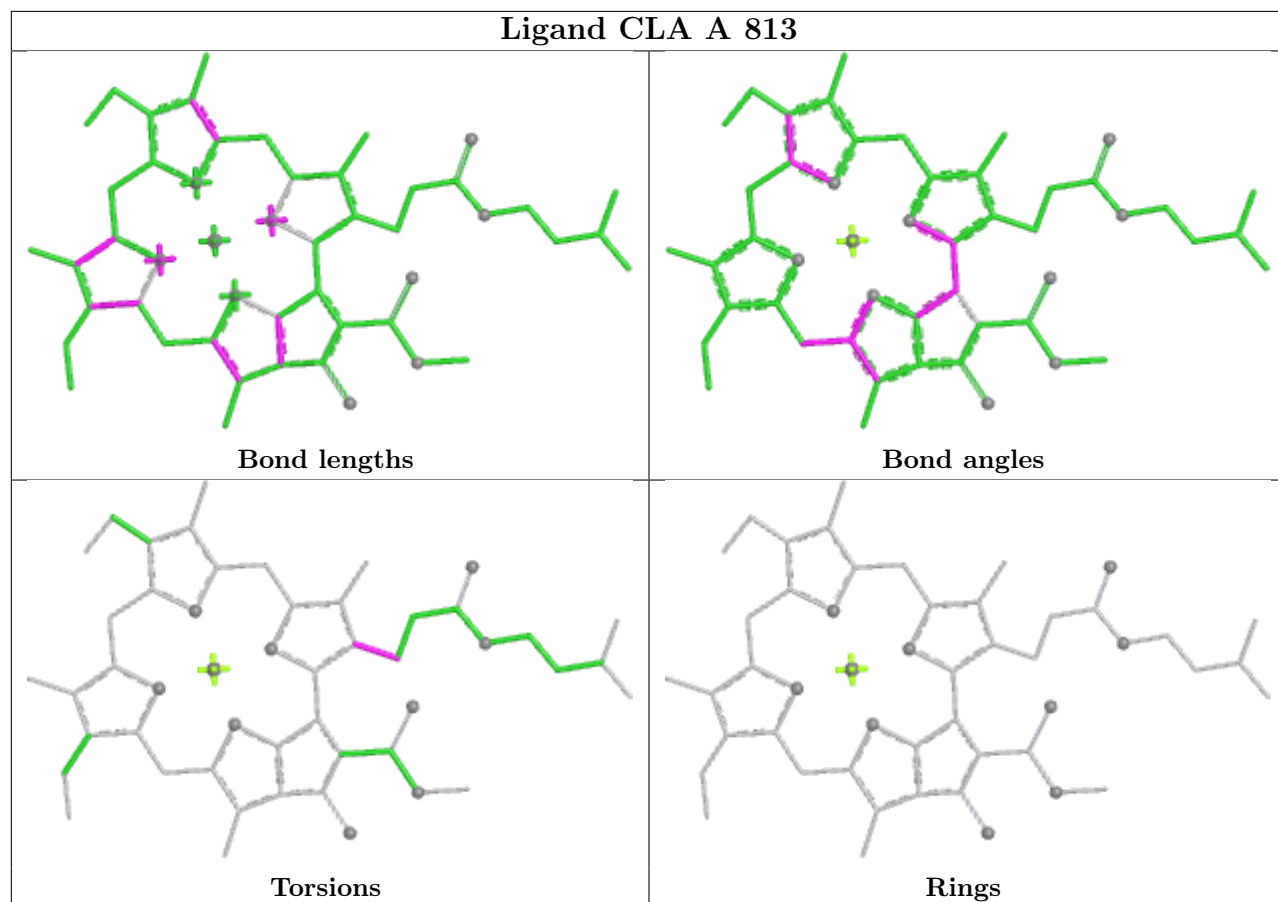
Bond angles

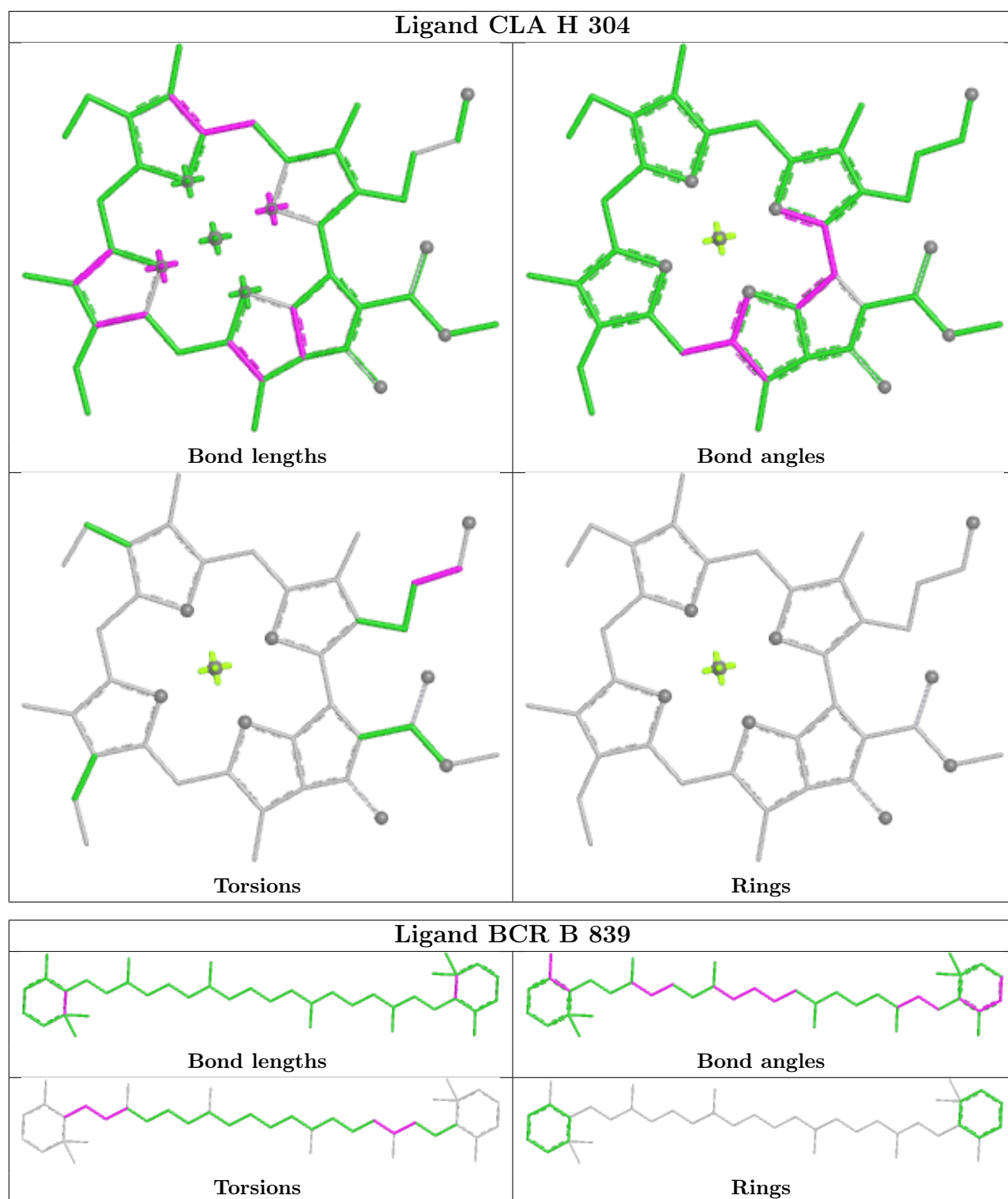


Torsions

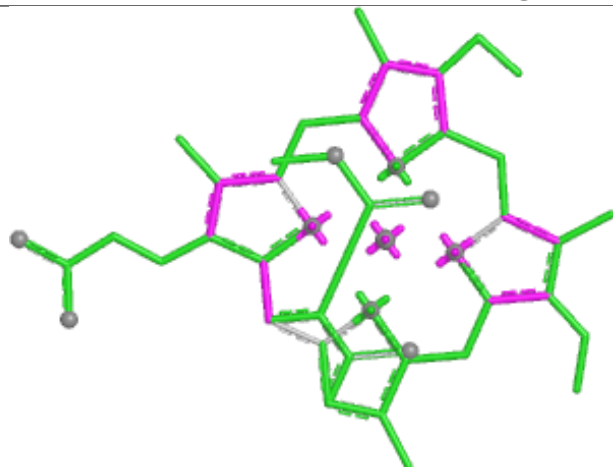


Rings

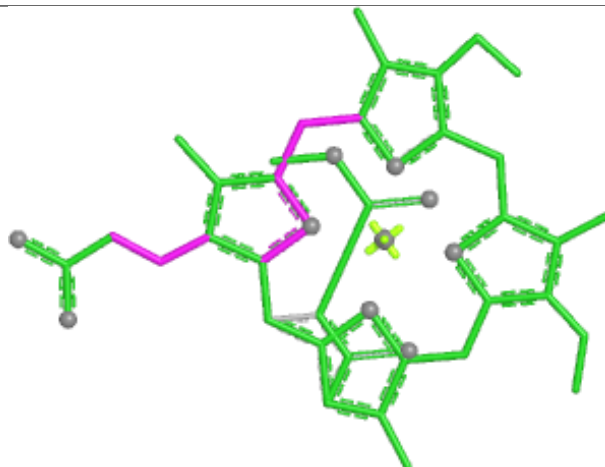




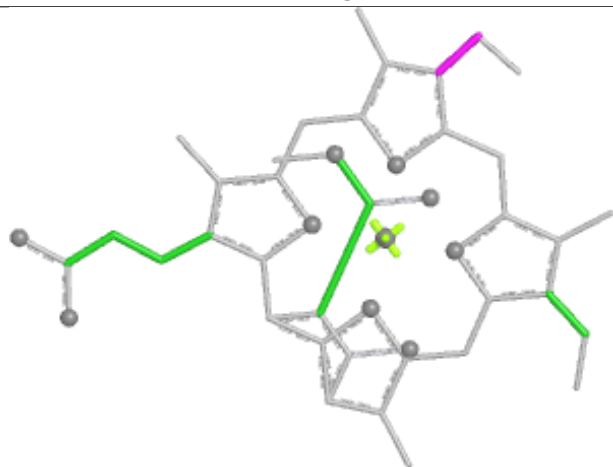
Ligand KC1 U 213



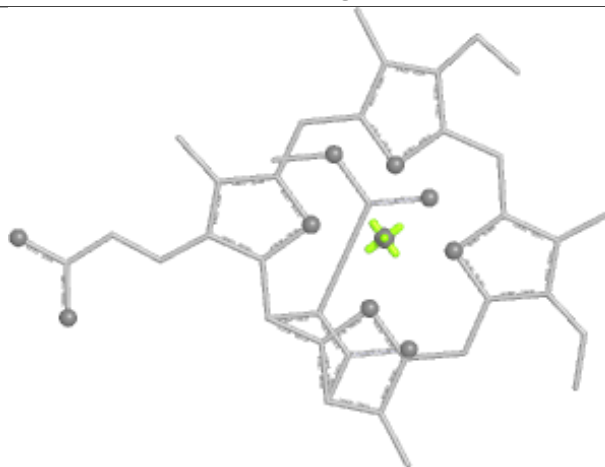
Bond lengths



Bond angles

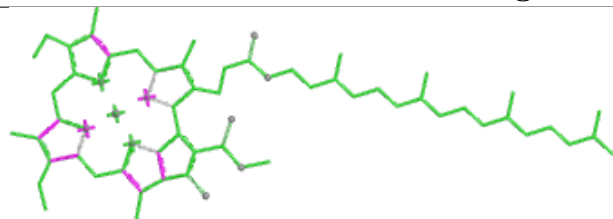


Torsions

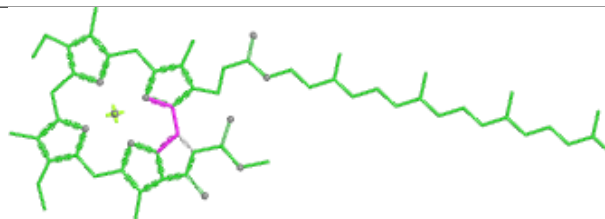


Rings

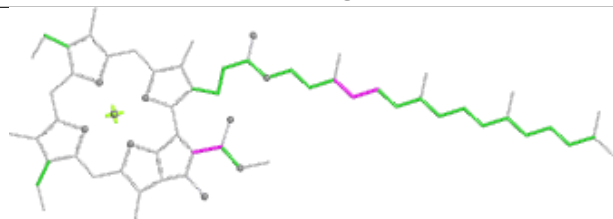
Ligand CLA B 808



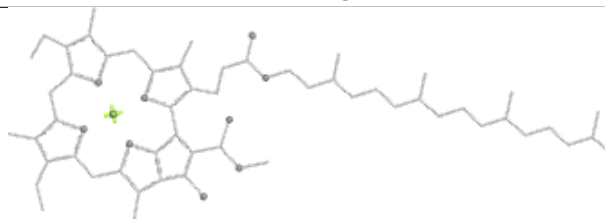
Bond lengths



Bond angles

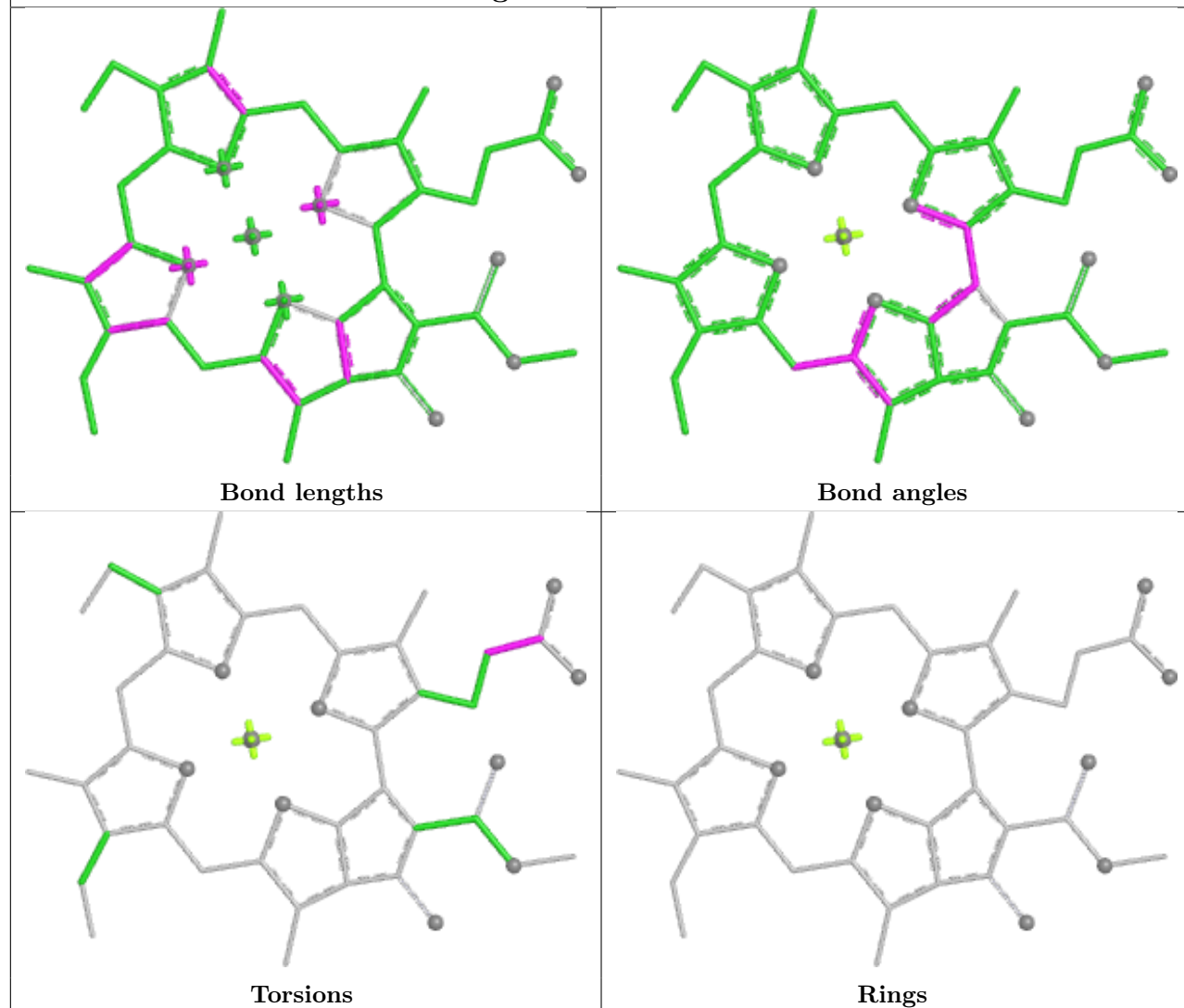


Torsions

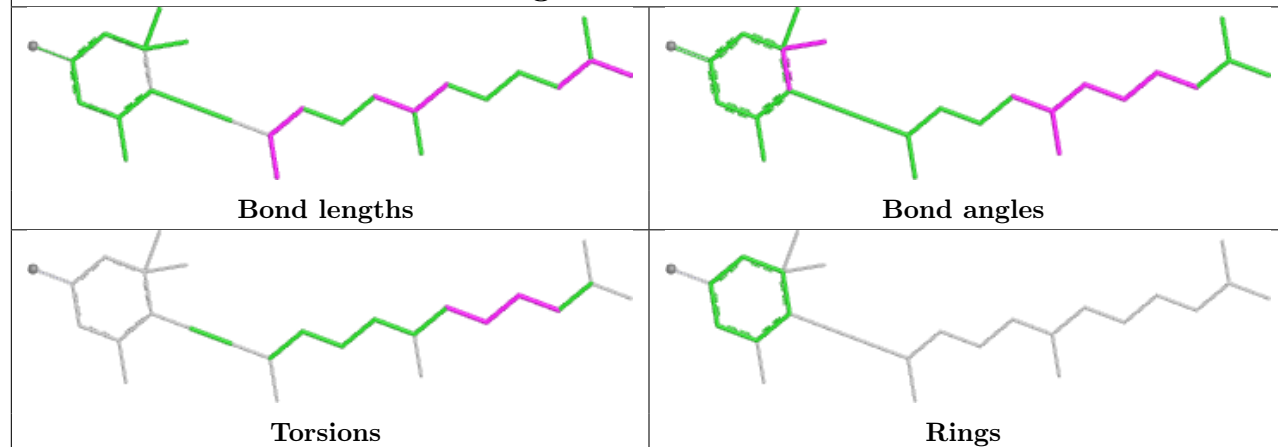


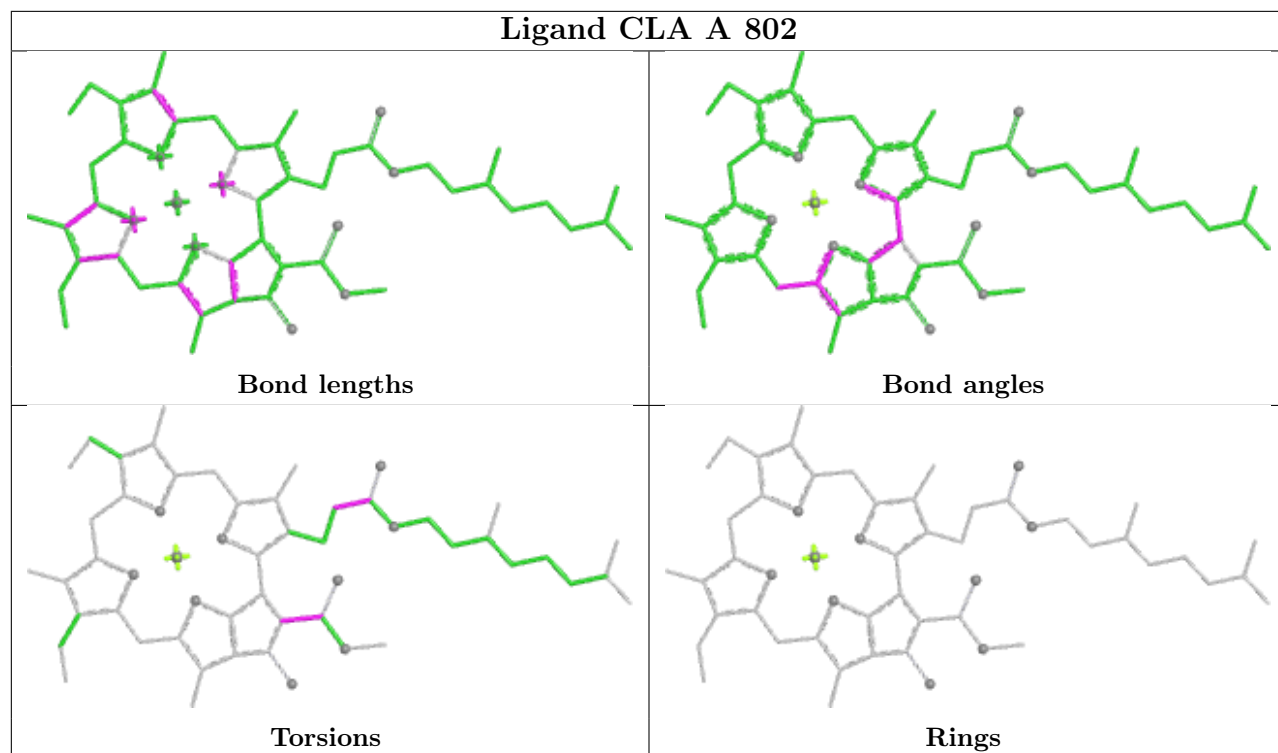
Rings

Ligand CLA U 206

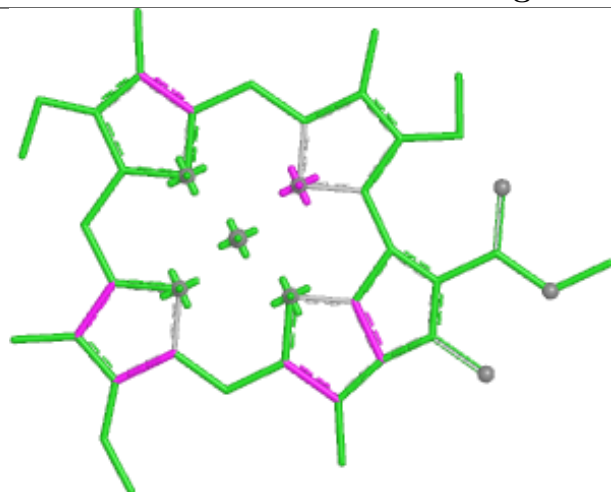


Ligand DD6 U 214

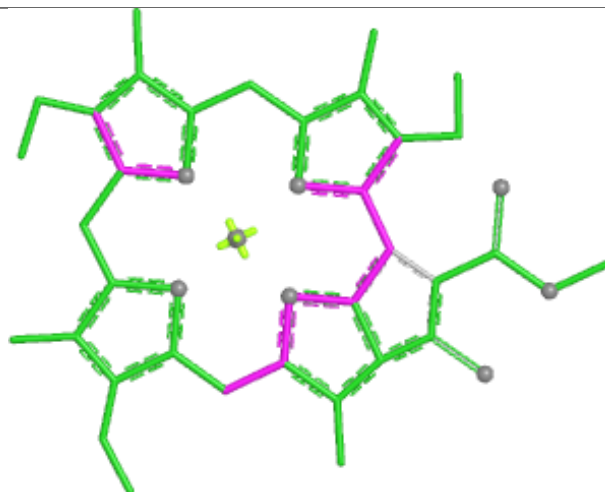




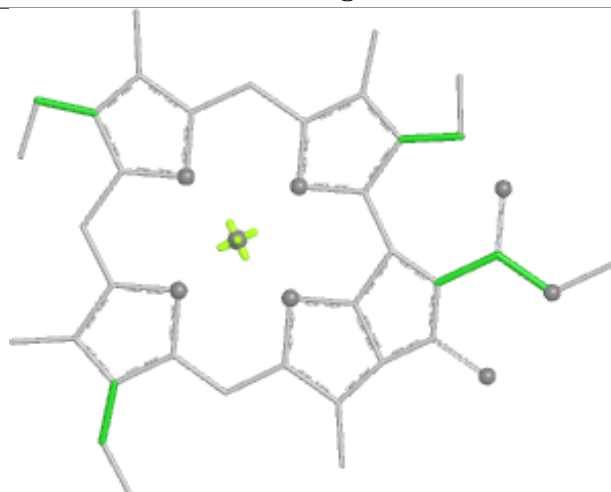
Ligand CLA U 209



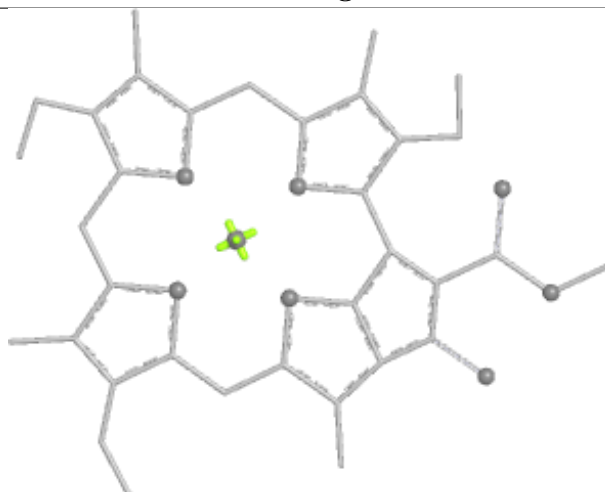
Bond lengths



Bond angles

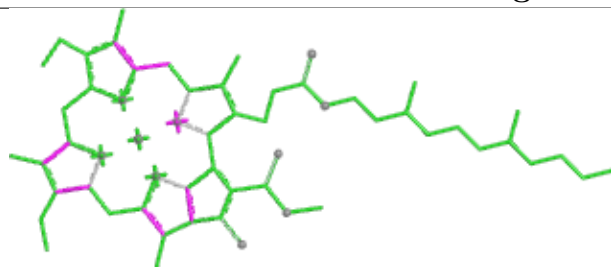


Torsions

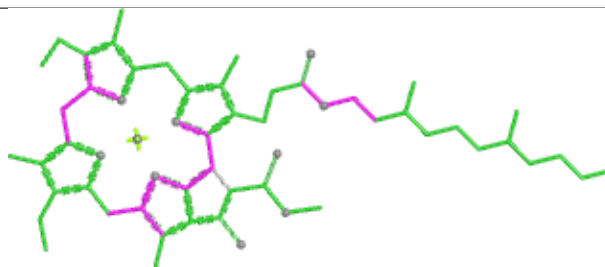


Rings

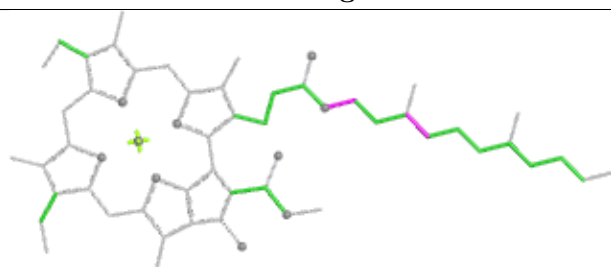
Ligand CLA K 205



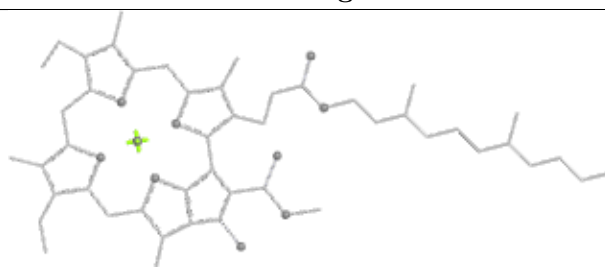
Bond lengths



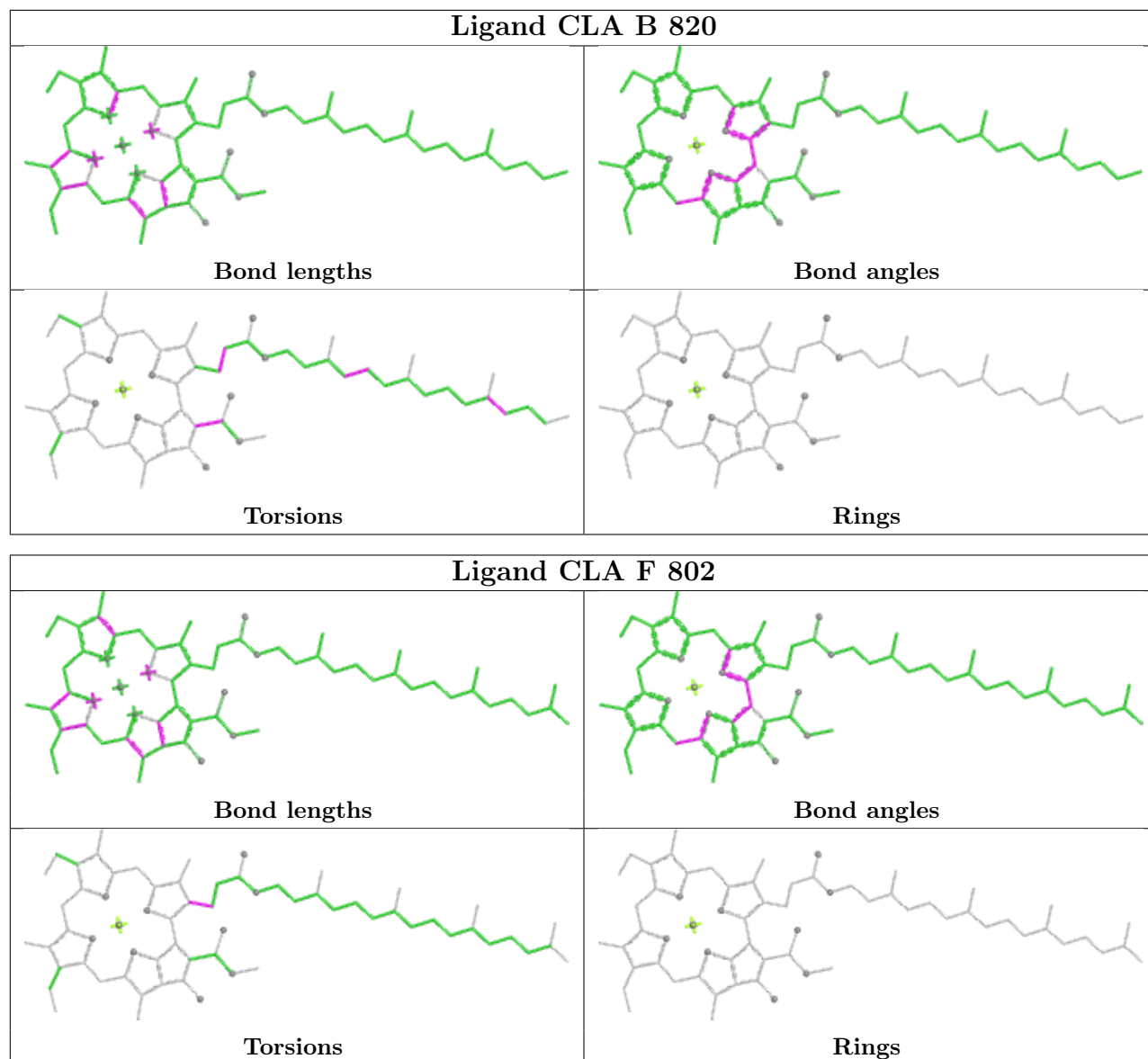
Bond angles

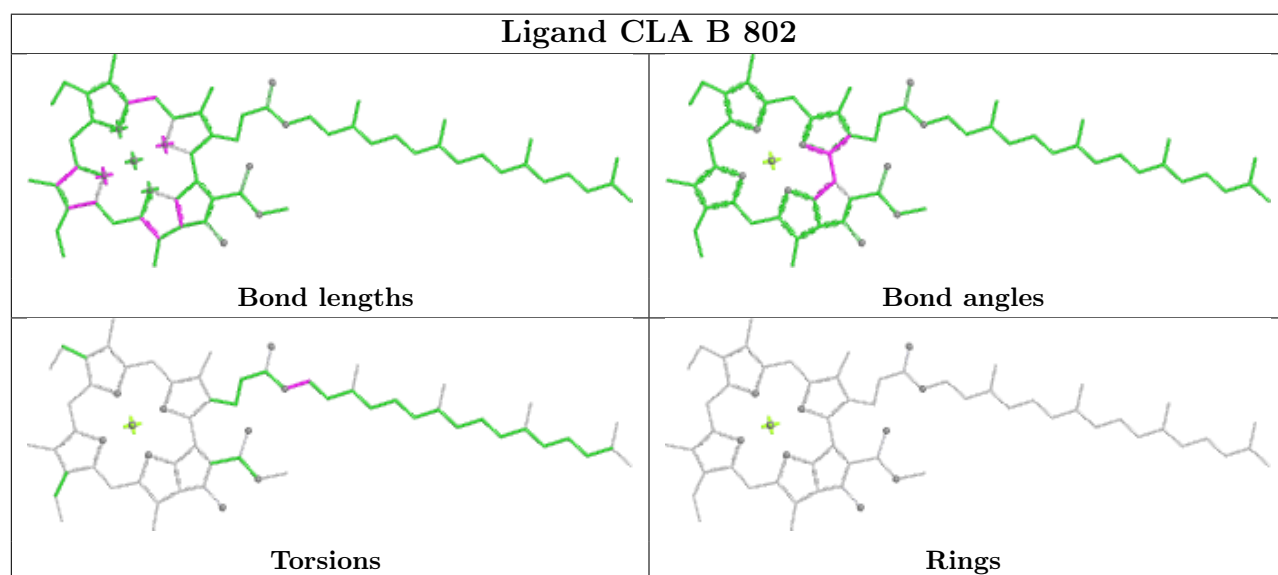
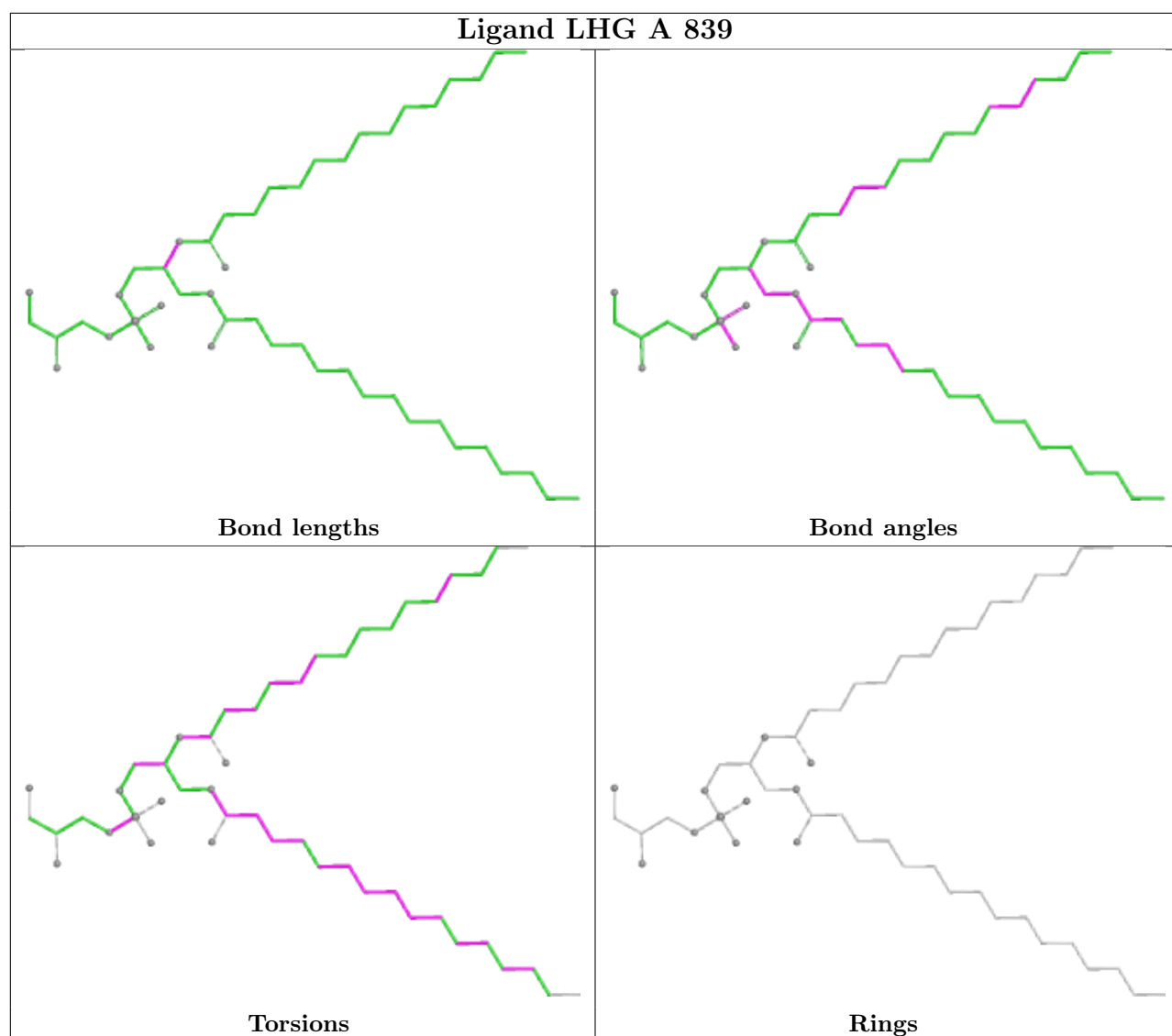


Torsions

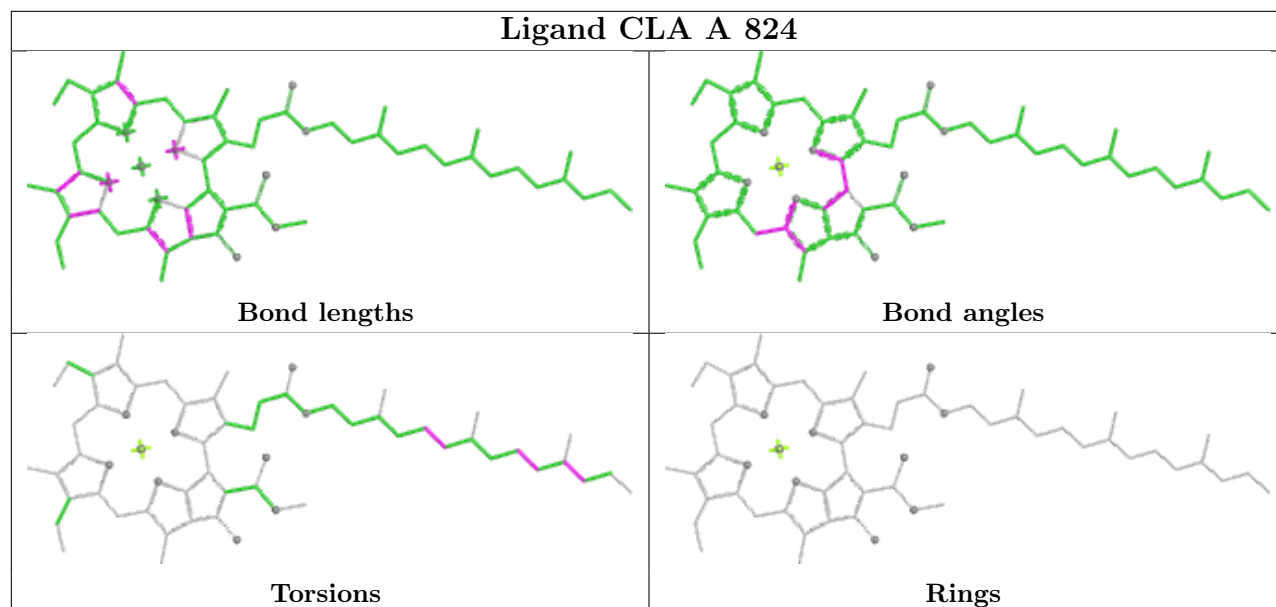


Rings

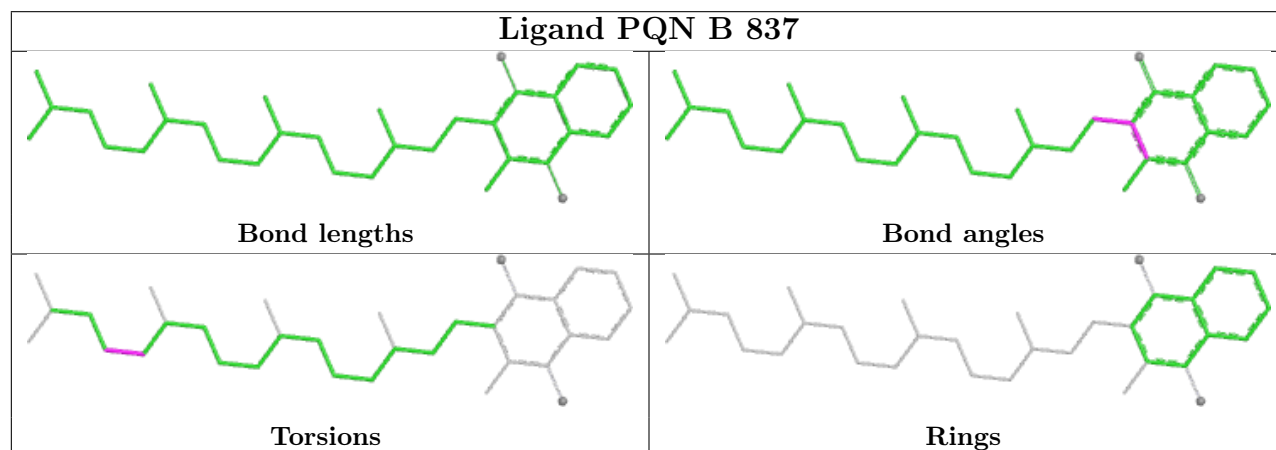




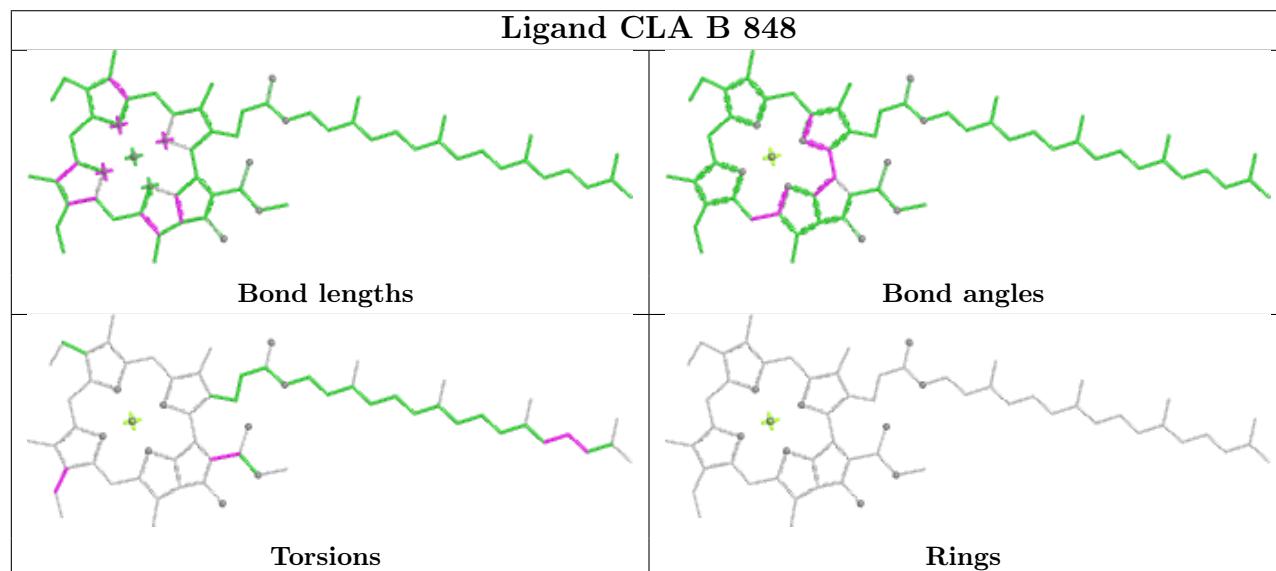
Ligand CLA A 824

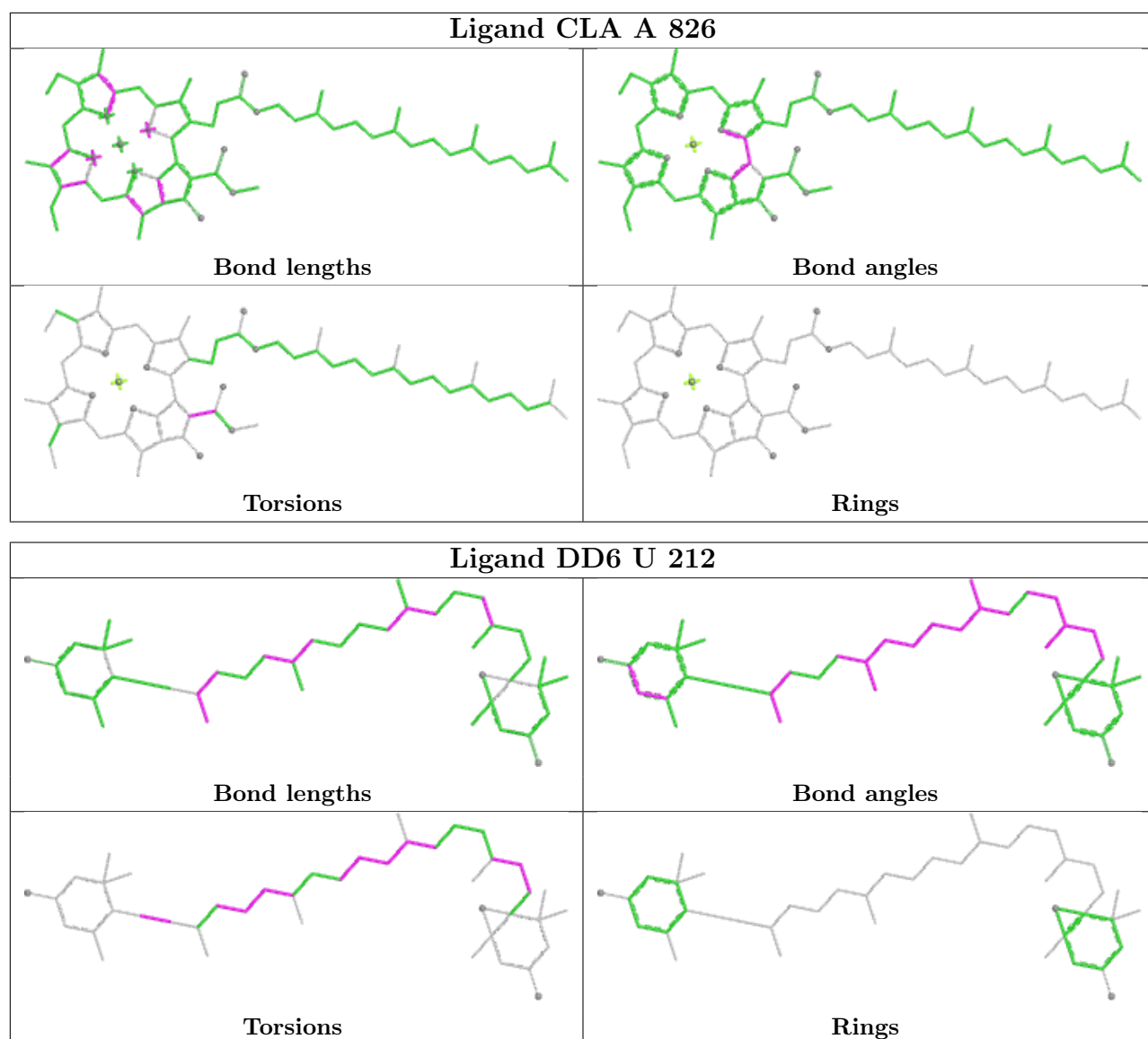


Ligand PQN B 837

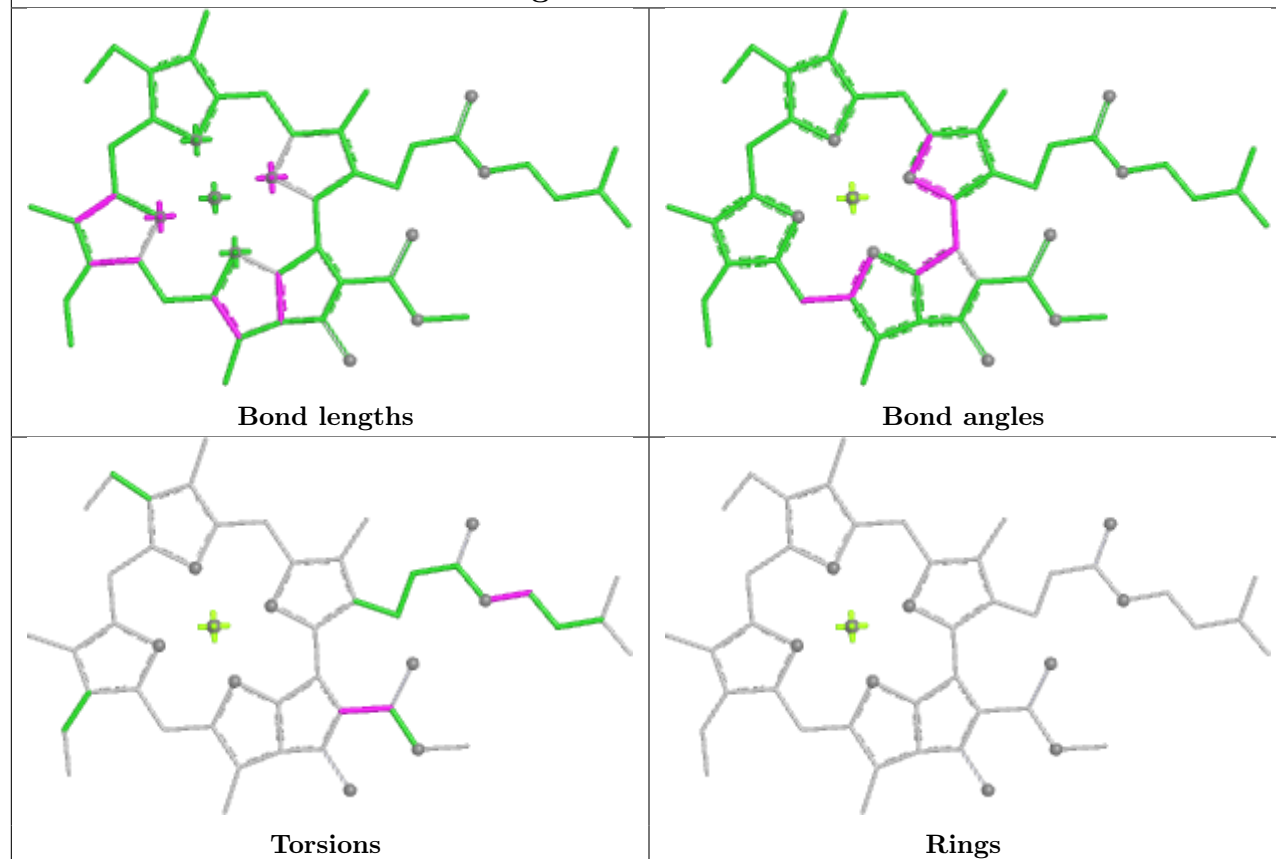


Ligand CLA B 848

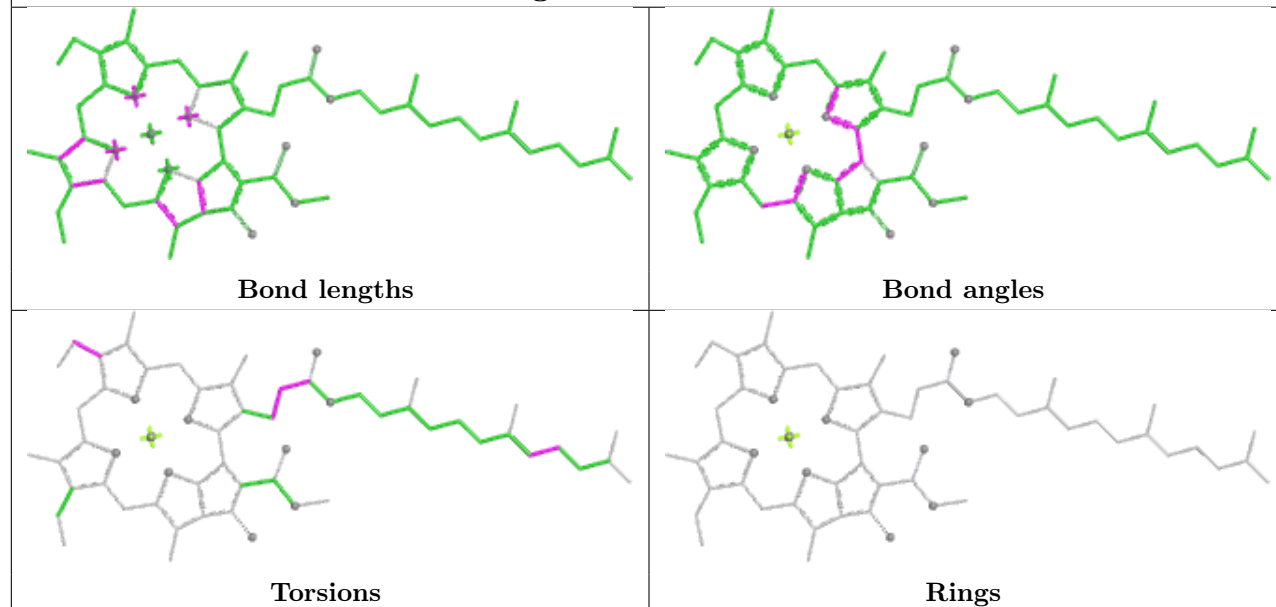


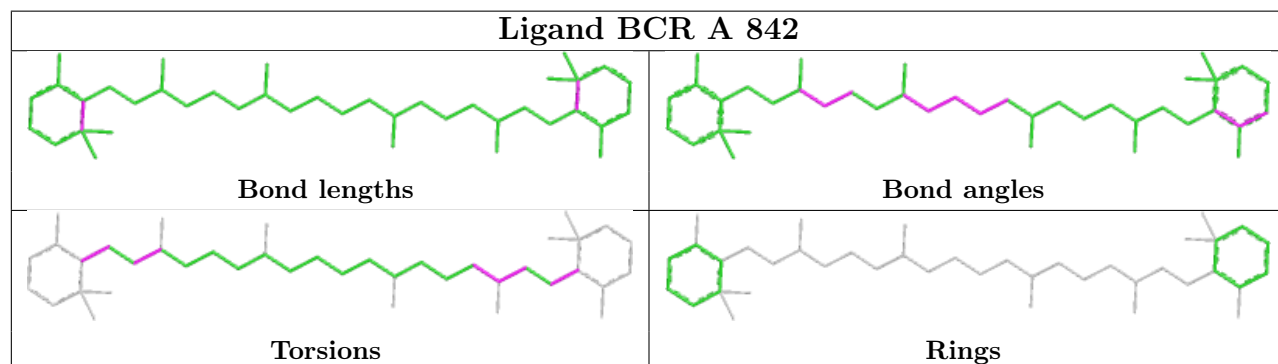
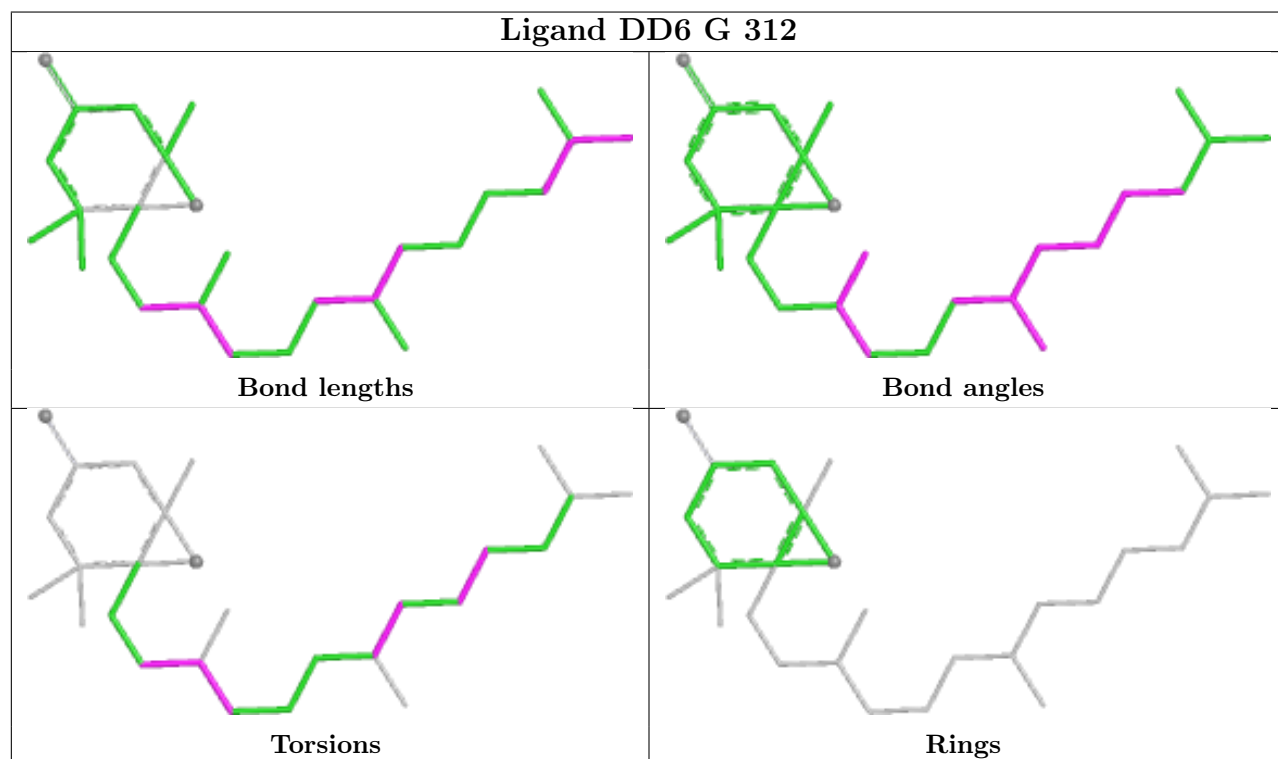
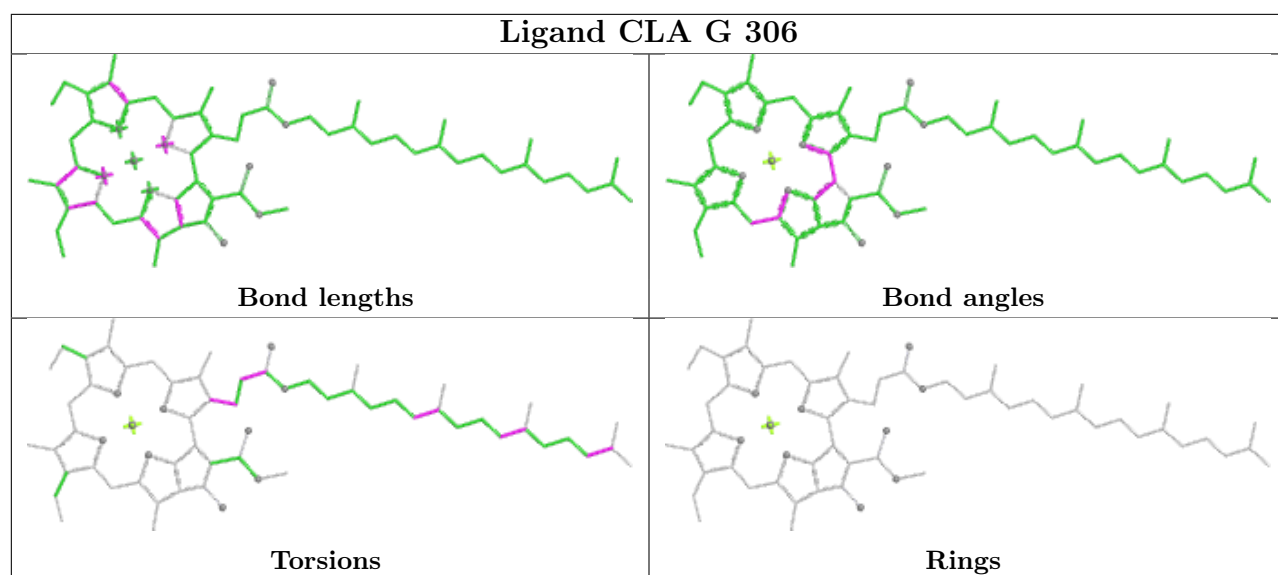


Ligand CLA A 827

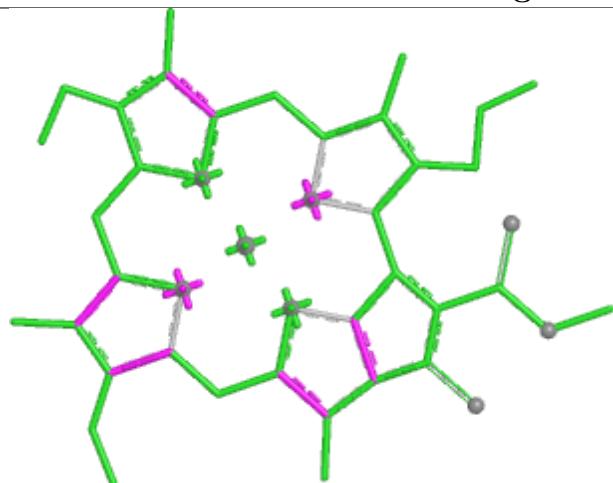


Ligand CLA A 847

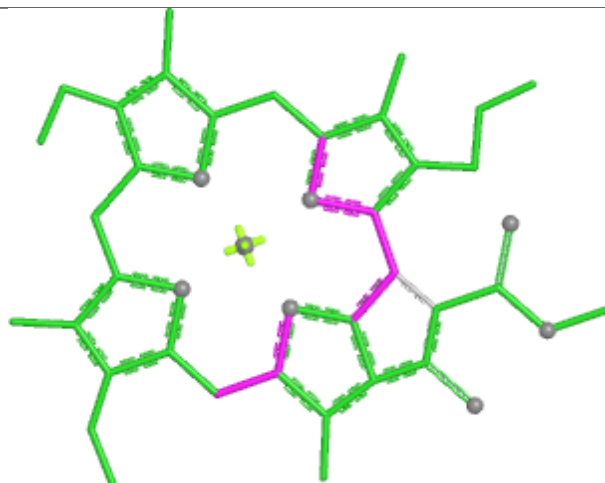




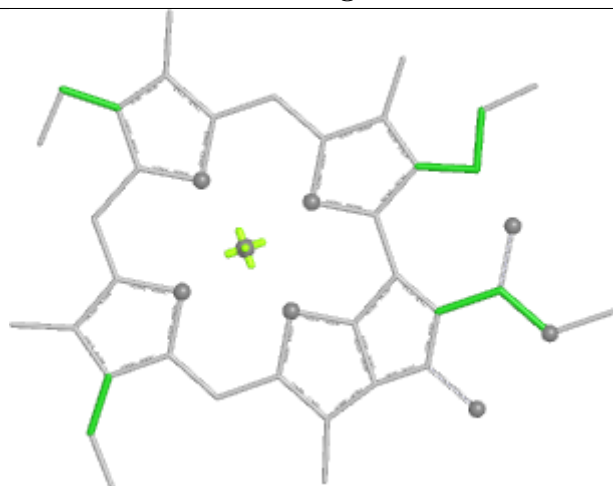
Ligand CLA A 819



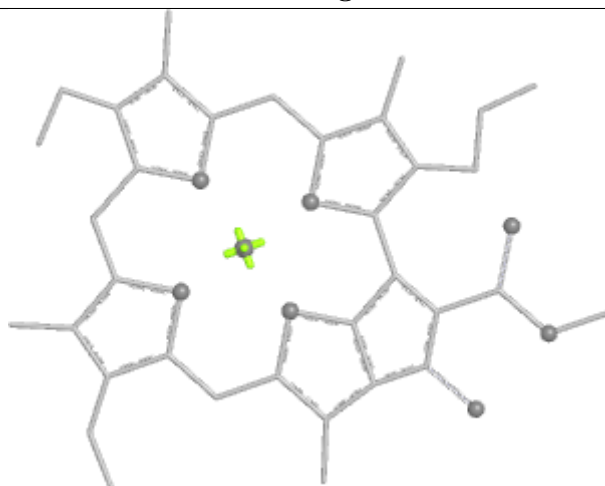
Bond lengths



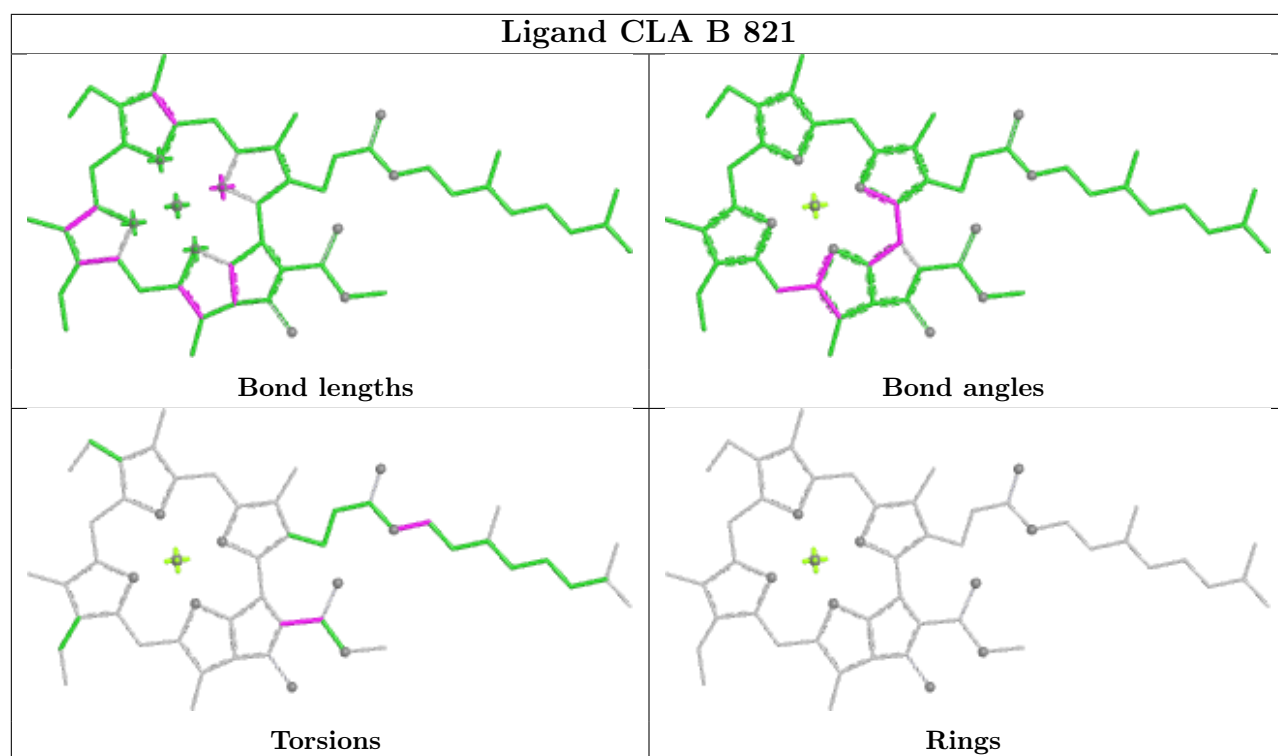
Bond angles



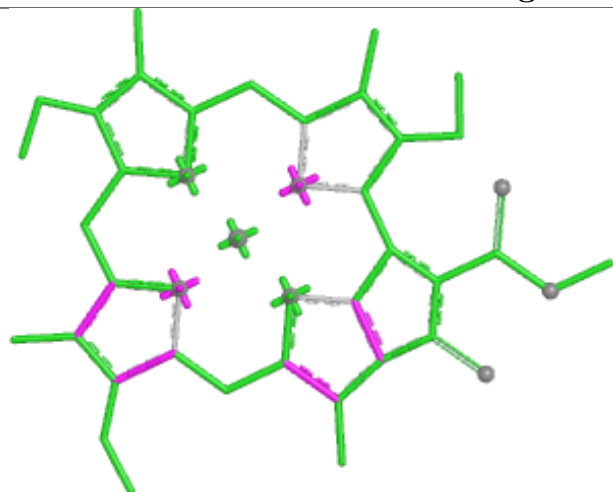
Torsions



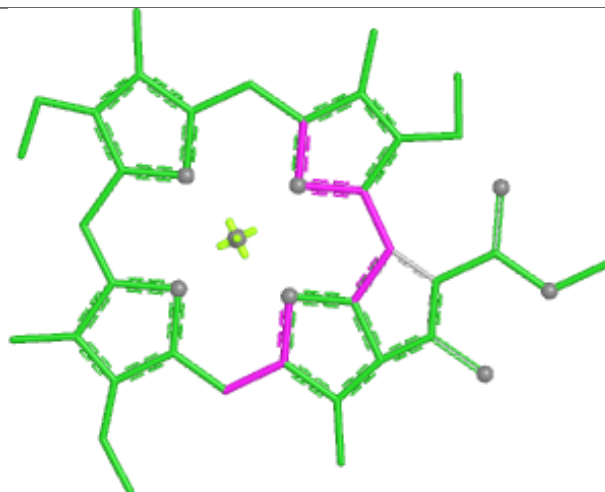
Rings



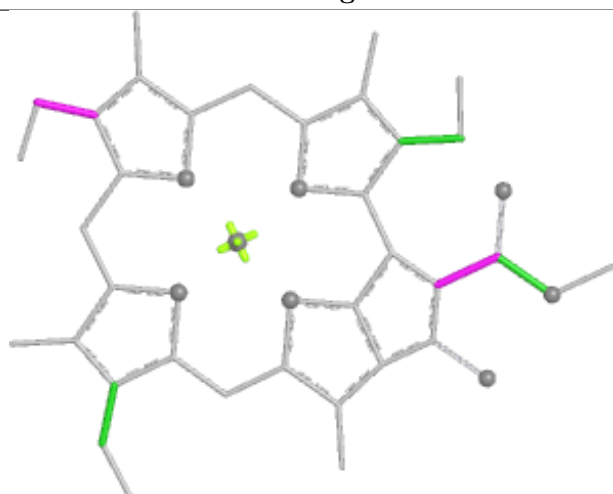
Ligand CLA J 104



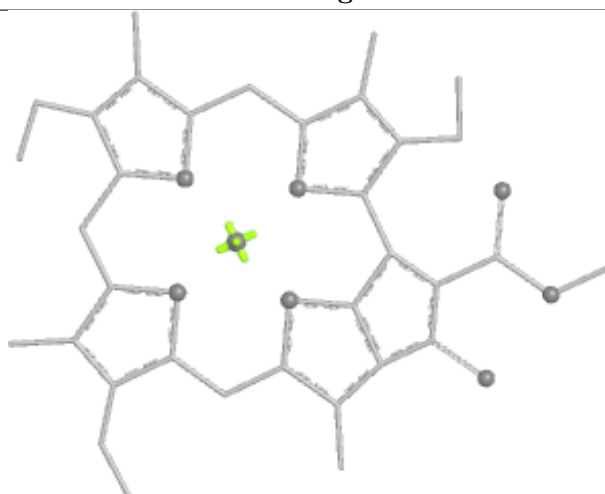
Bond lengths



Bond angles

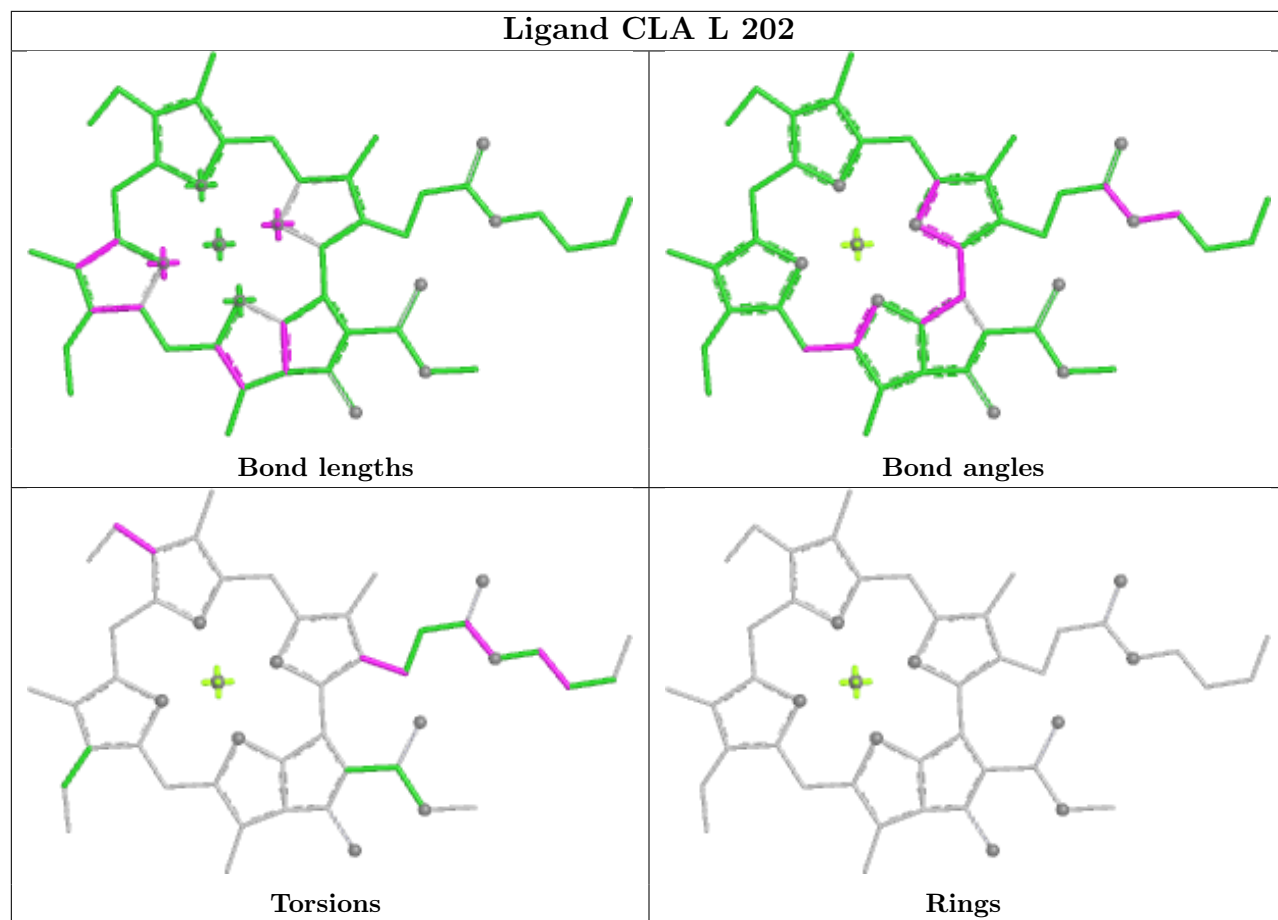


Torsions

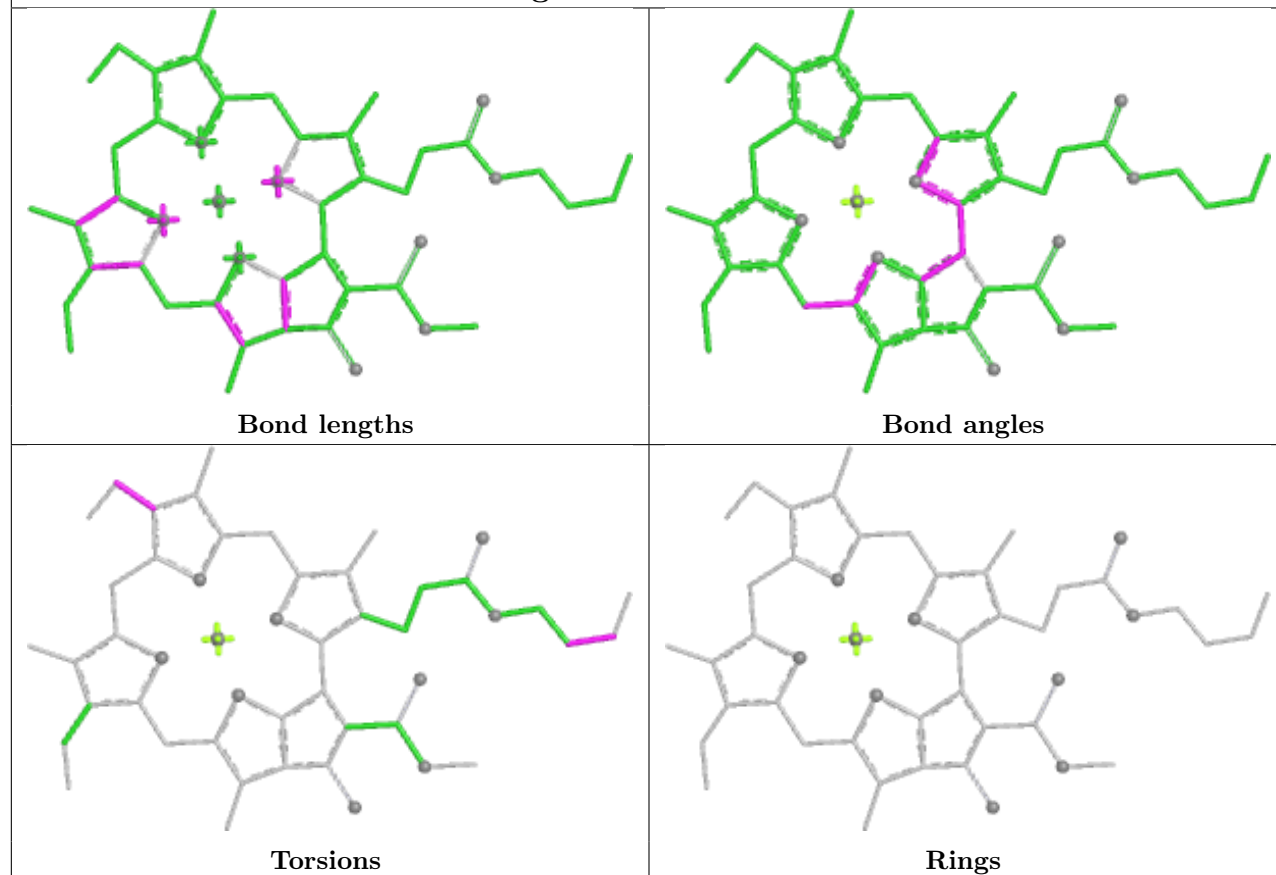


Rings

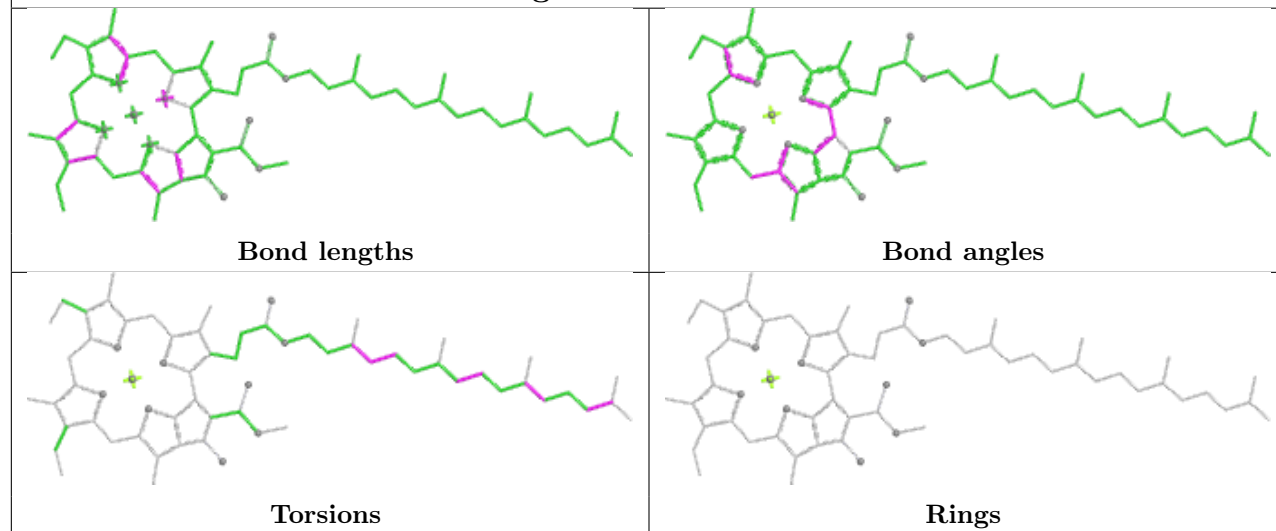
Ligand CLA L 202

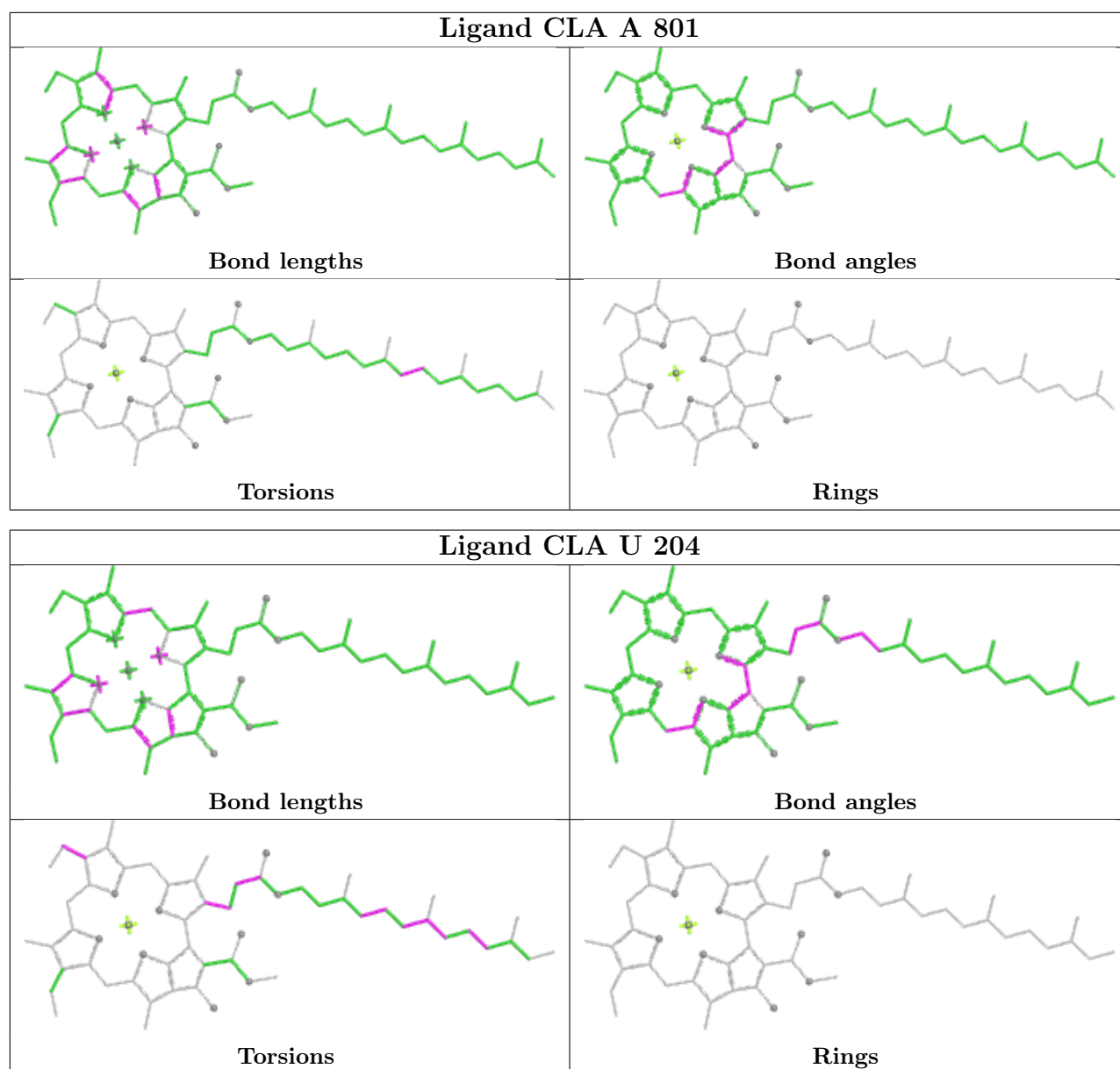


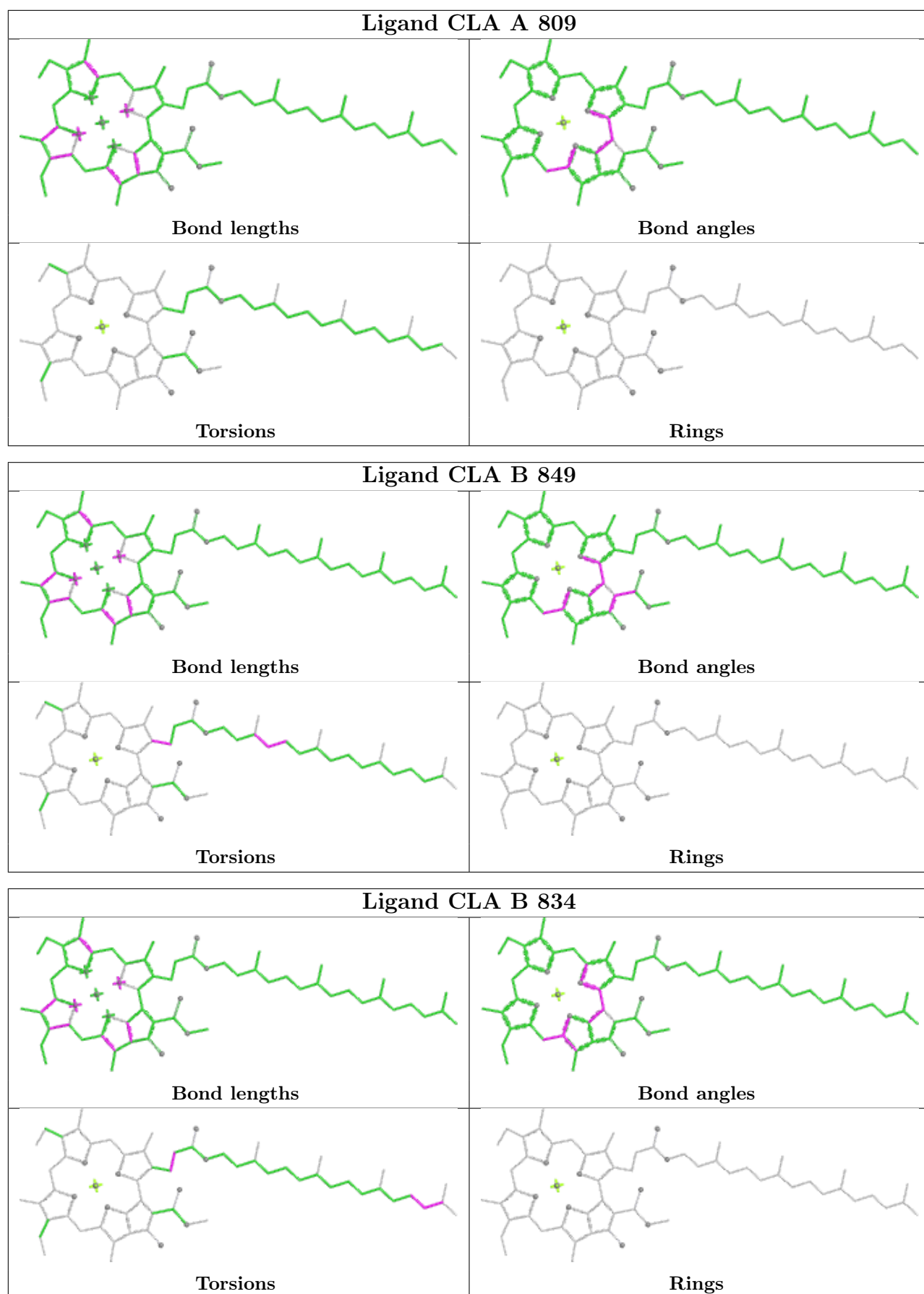
Ligand CLA A 805

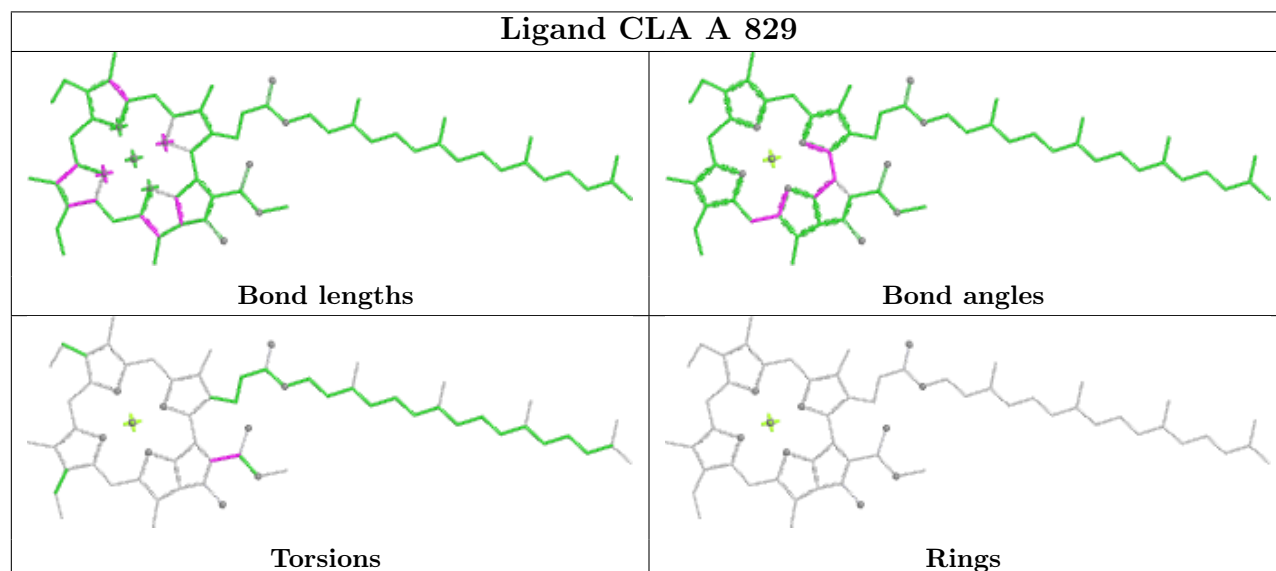
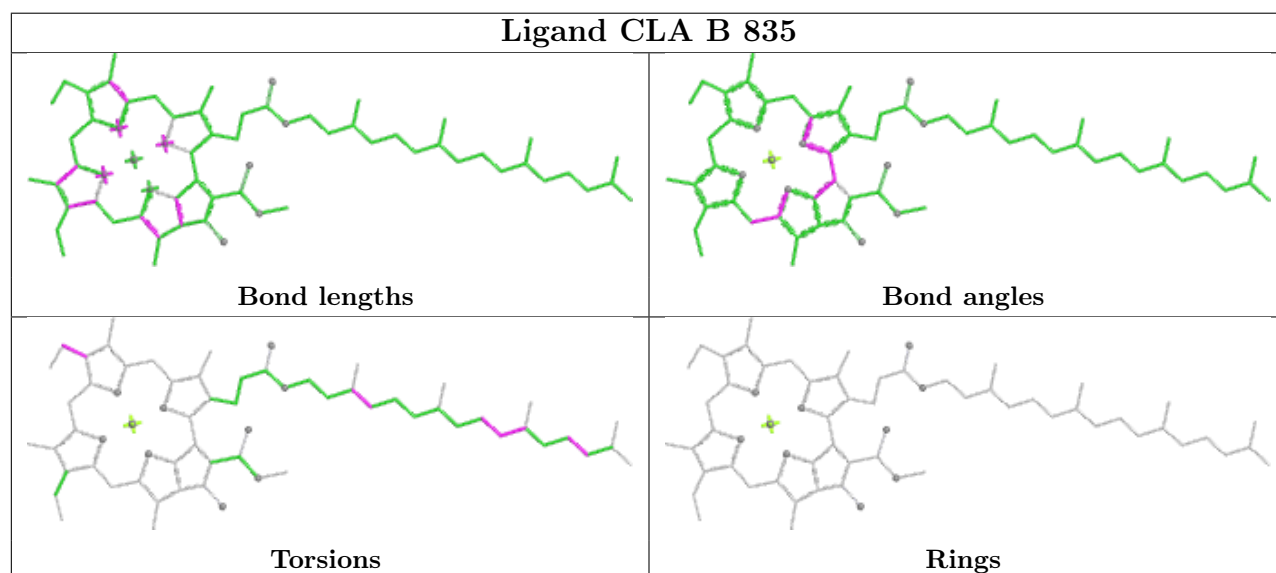
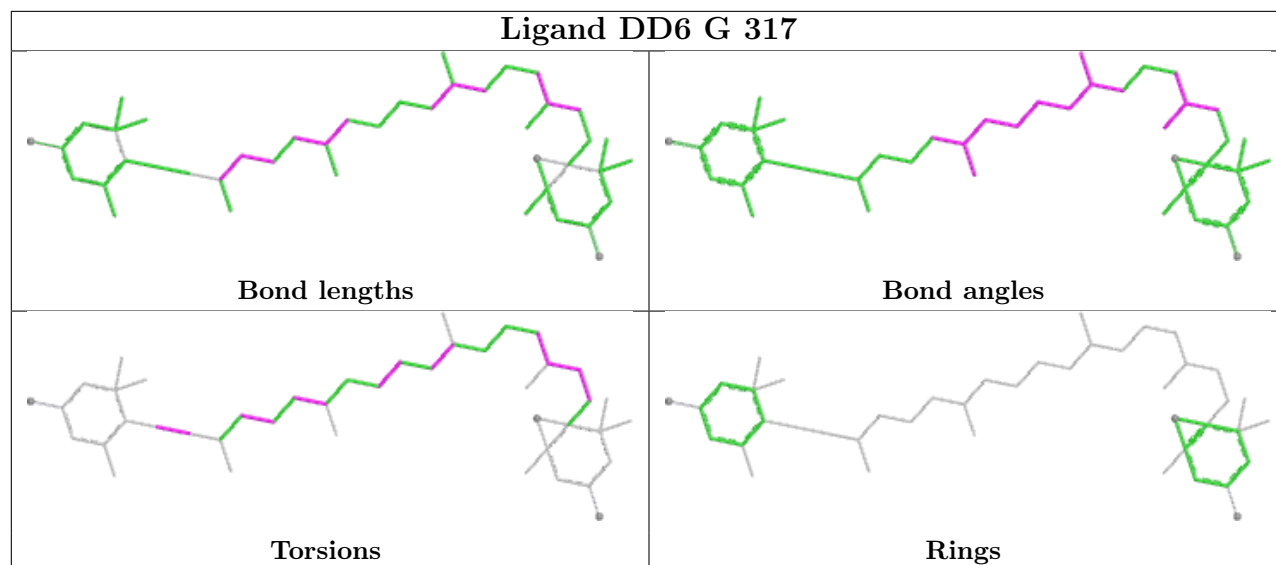


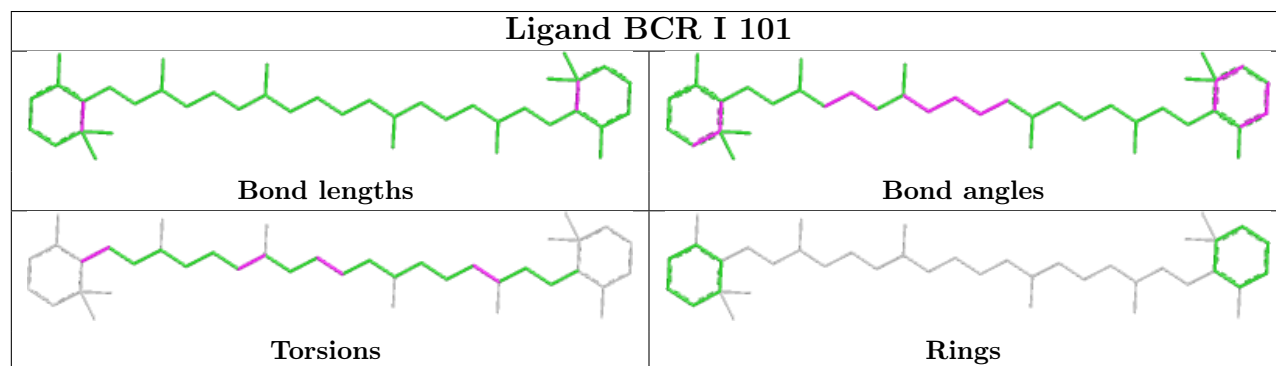
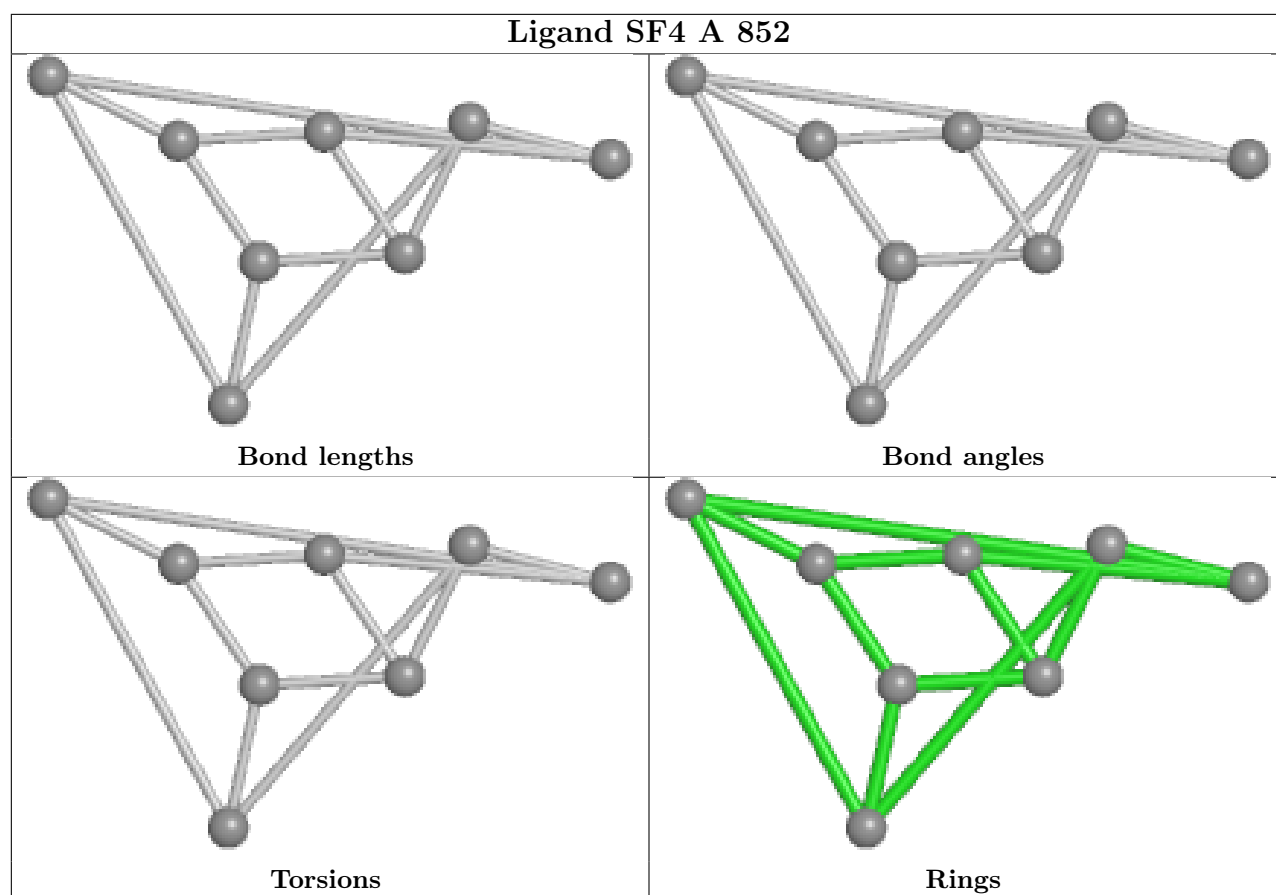
Ligand CLA B 817

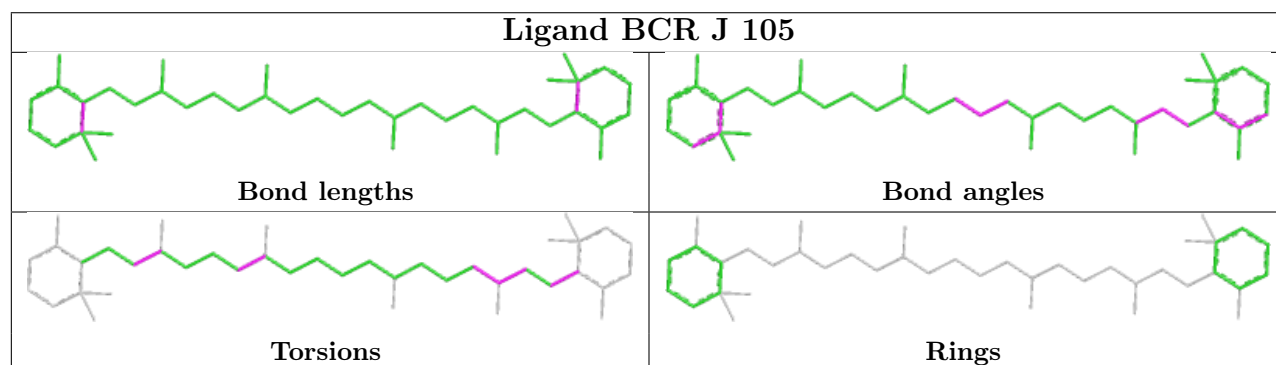
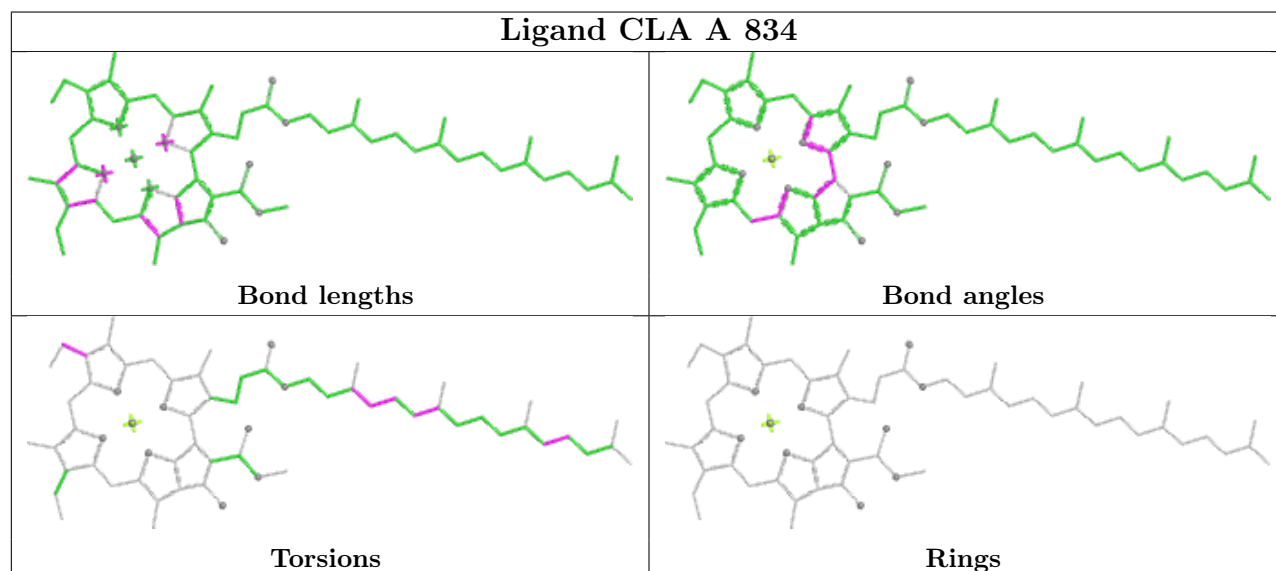
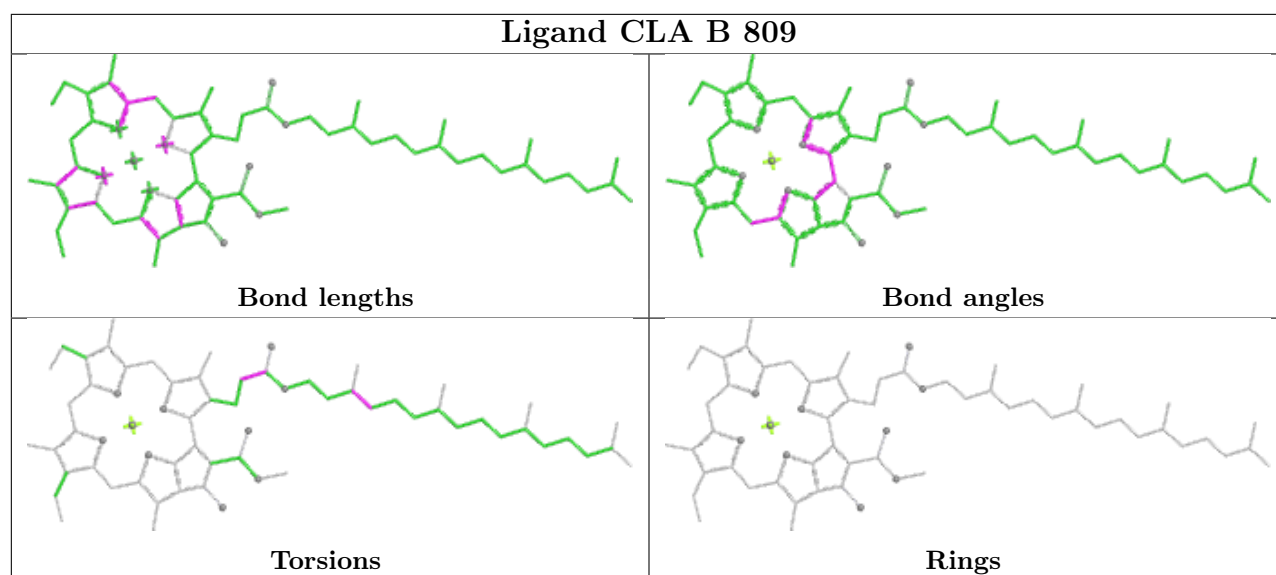


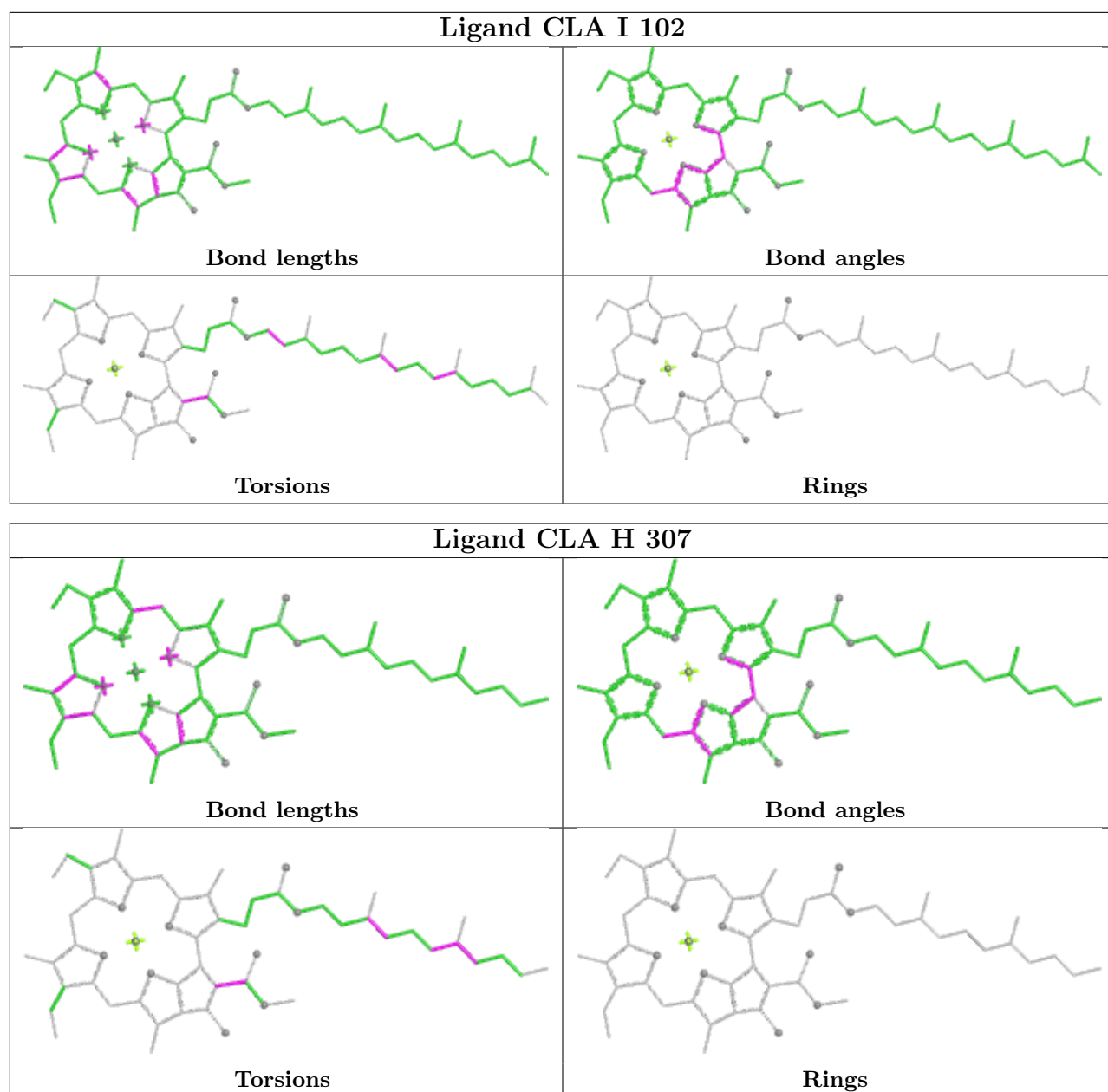


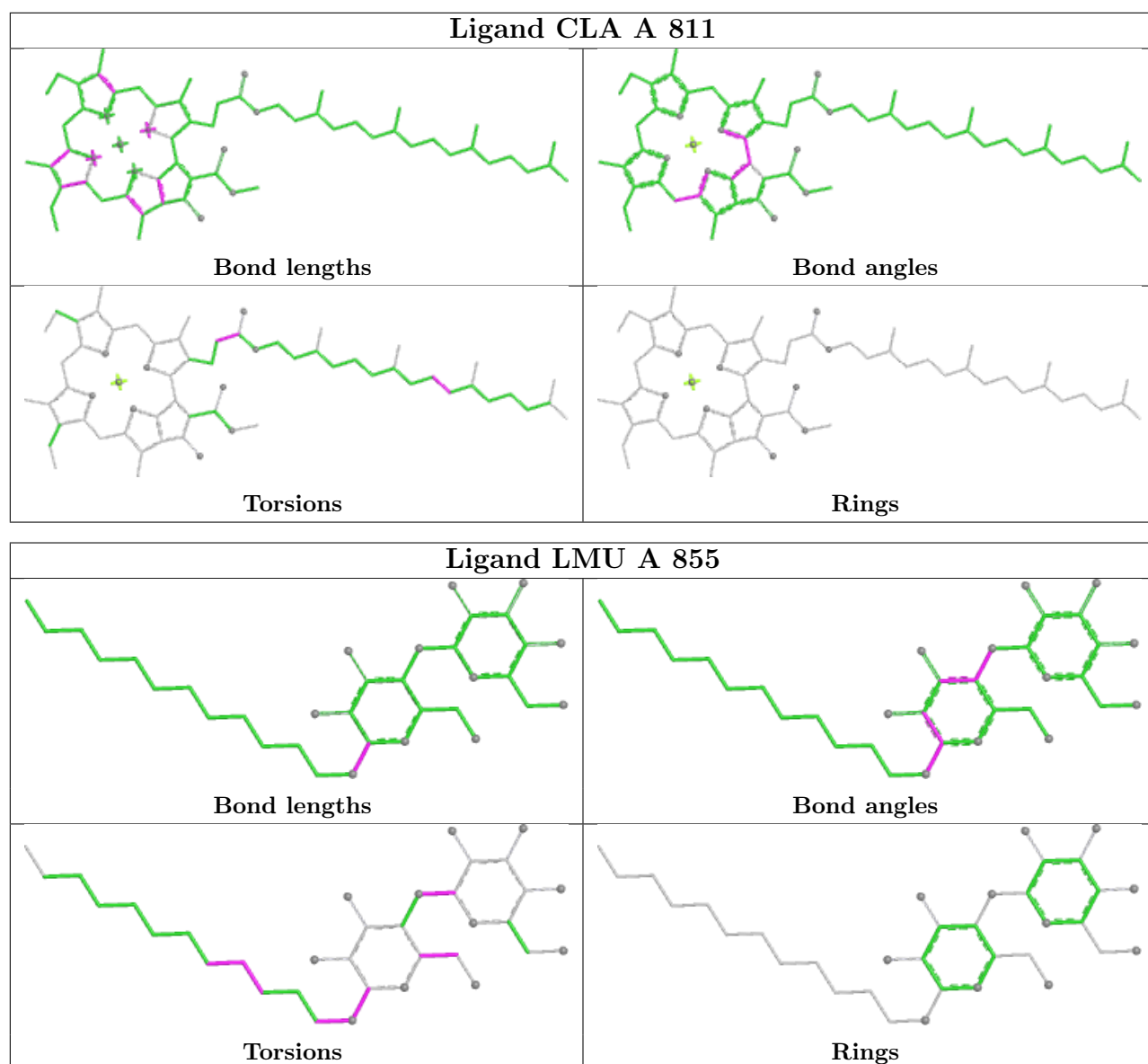




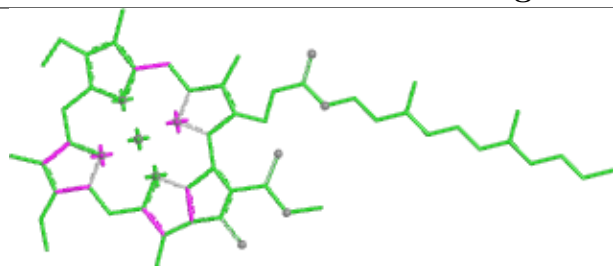




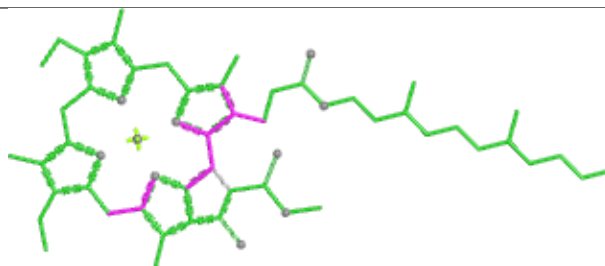




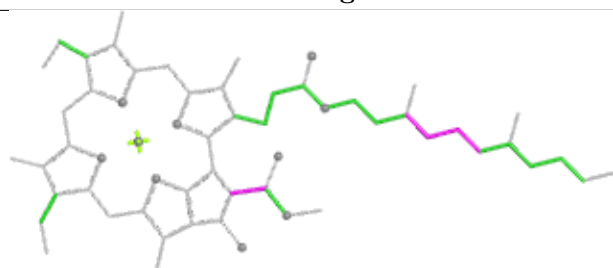
Ligand CLA B 828



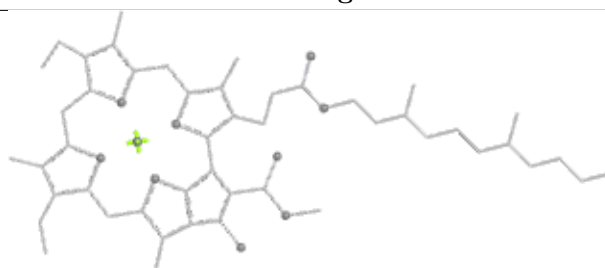
Bond lengths



Bond angles

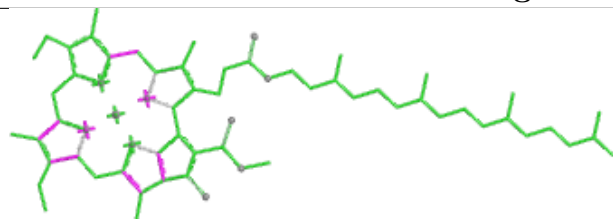


Torsions

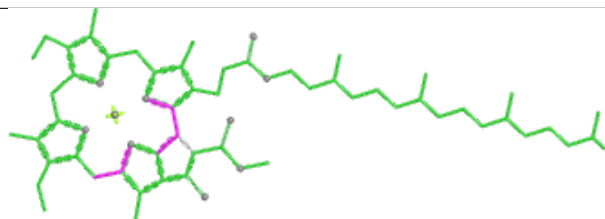


Rings

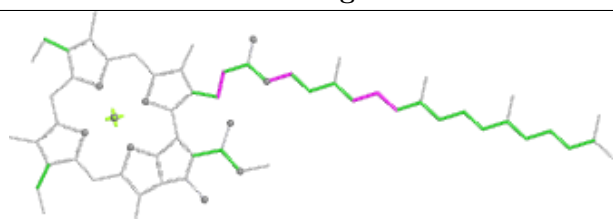
Ligand CLA A 836



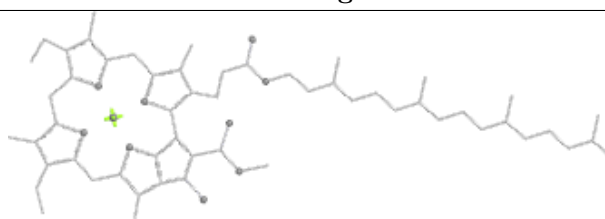
Bond lengths



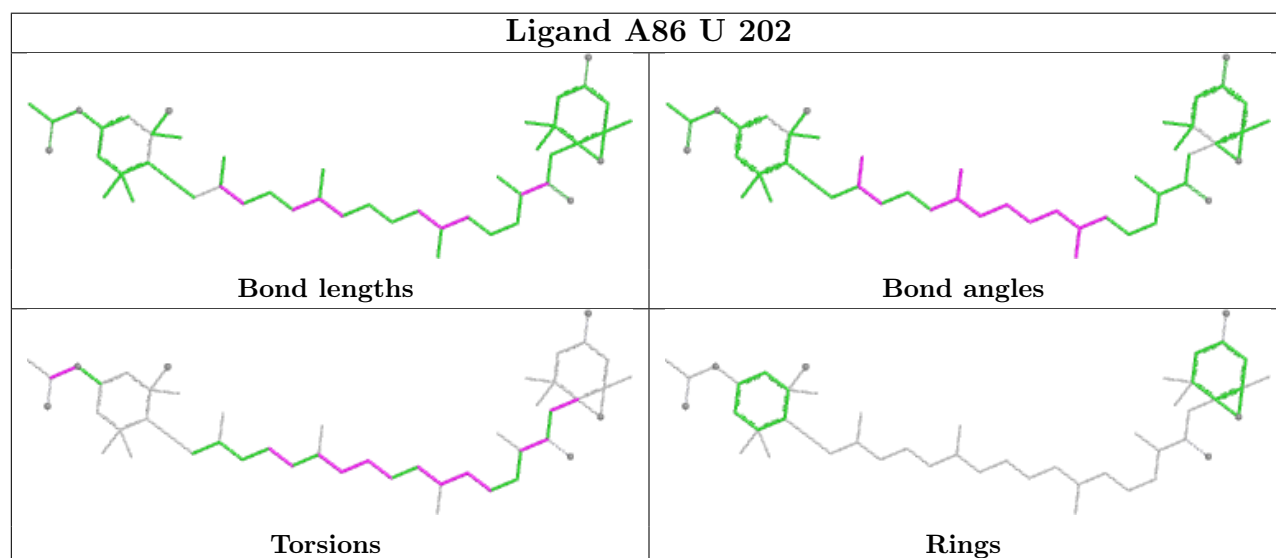
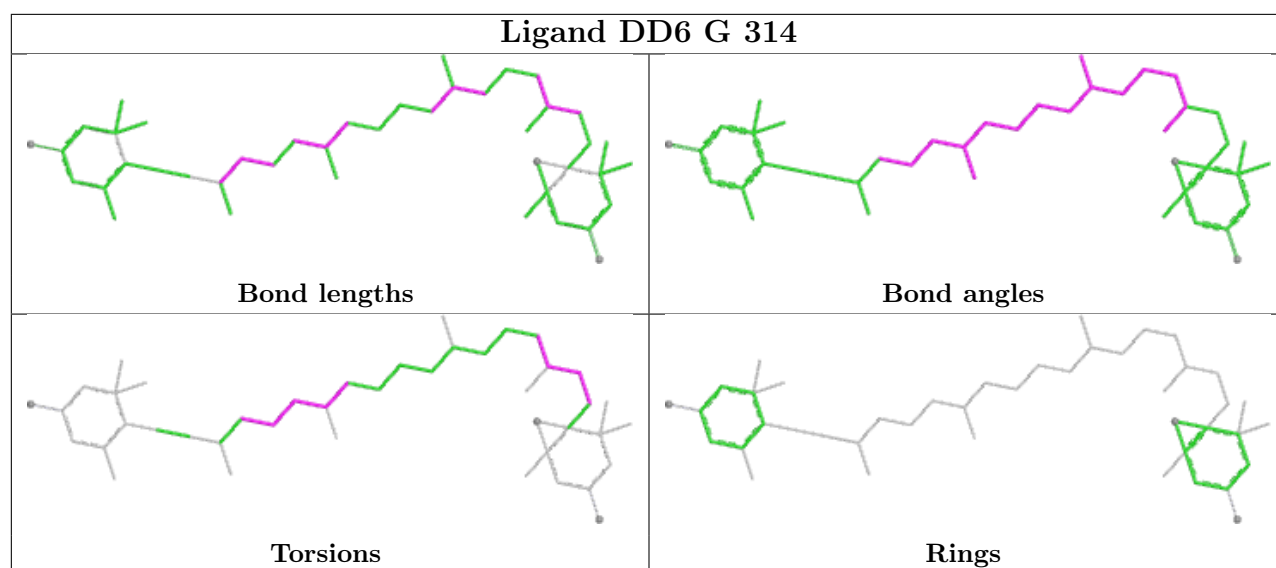
Bond angles



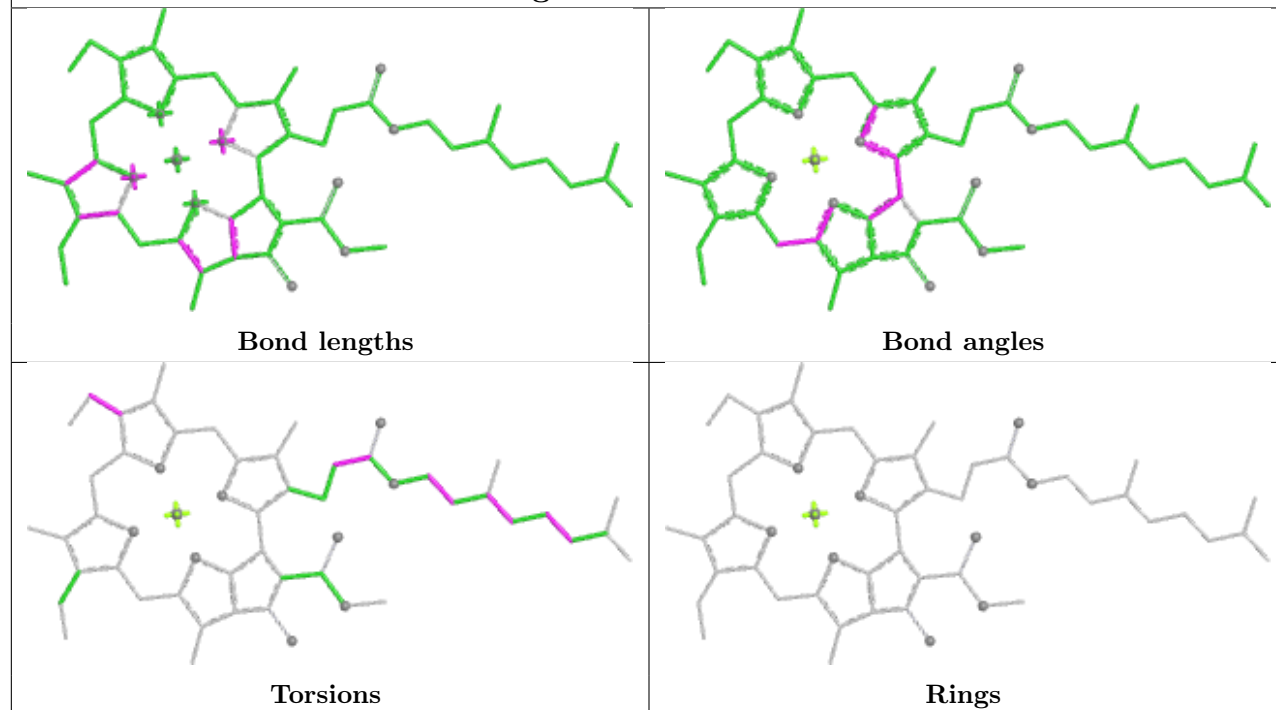
Torsions



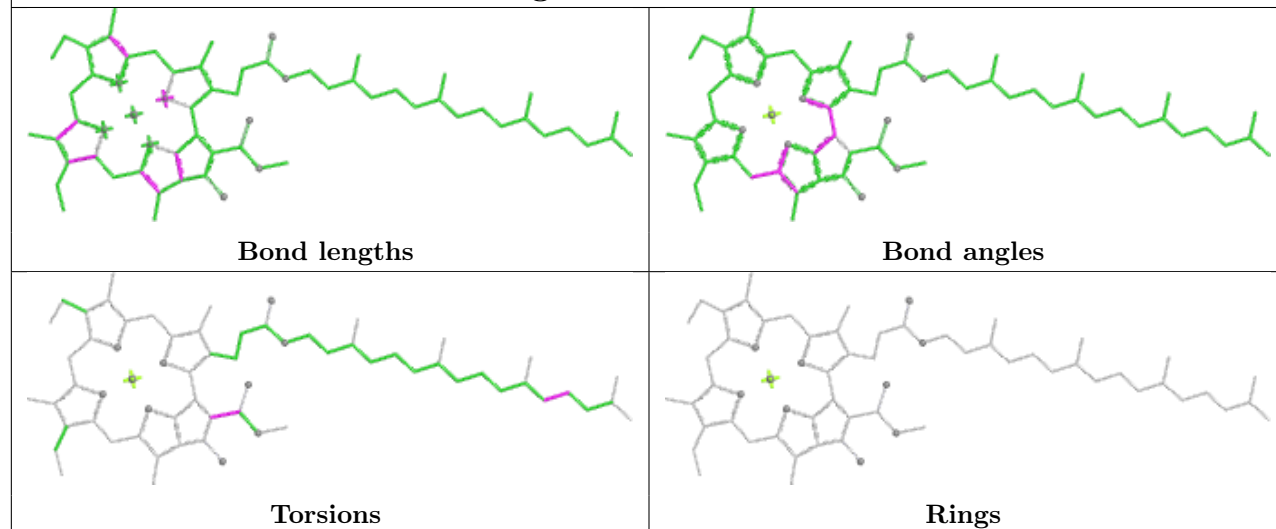
Rings



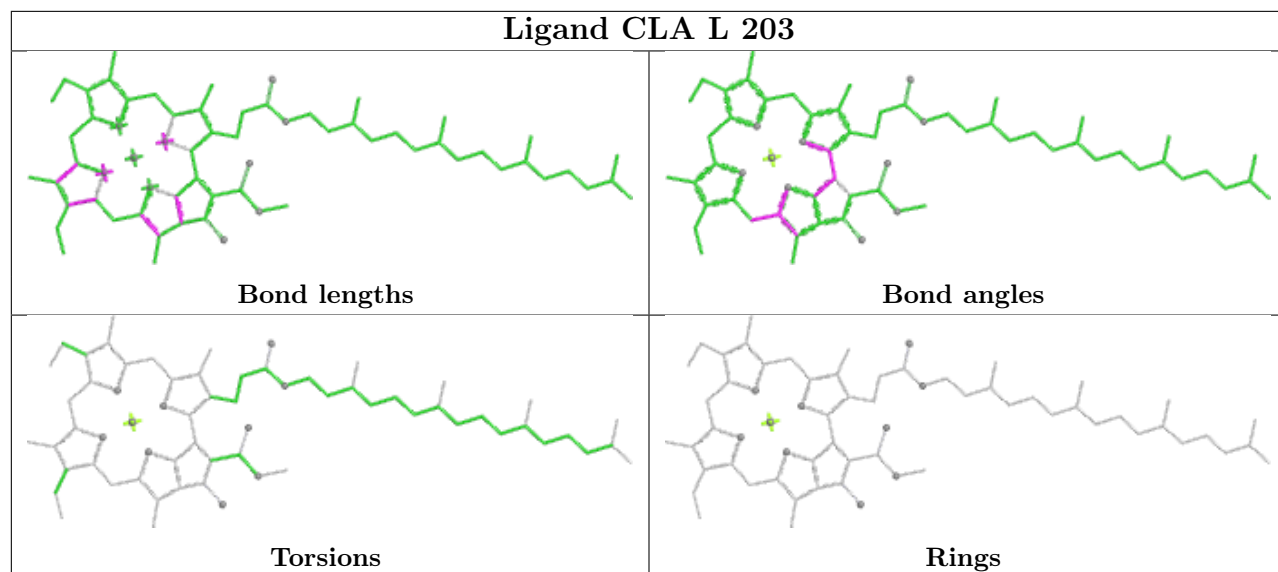
Ligand CLA B 811



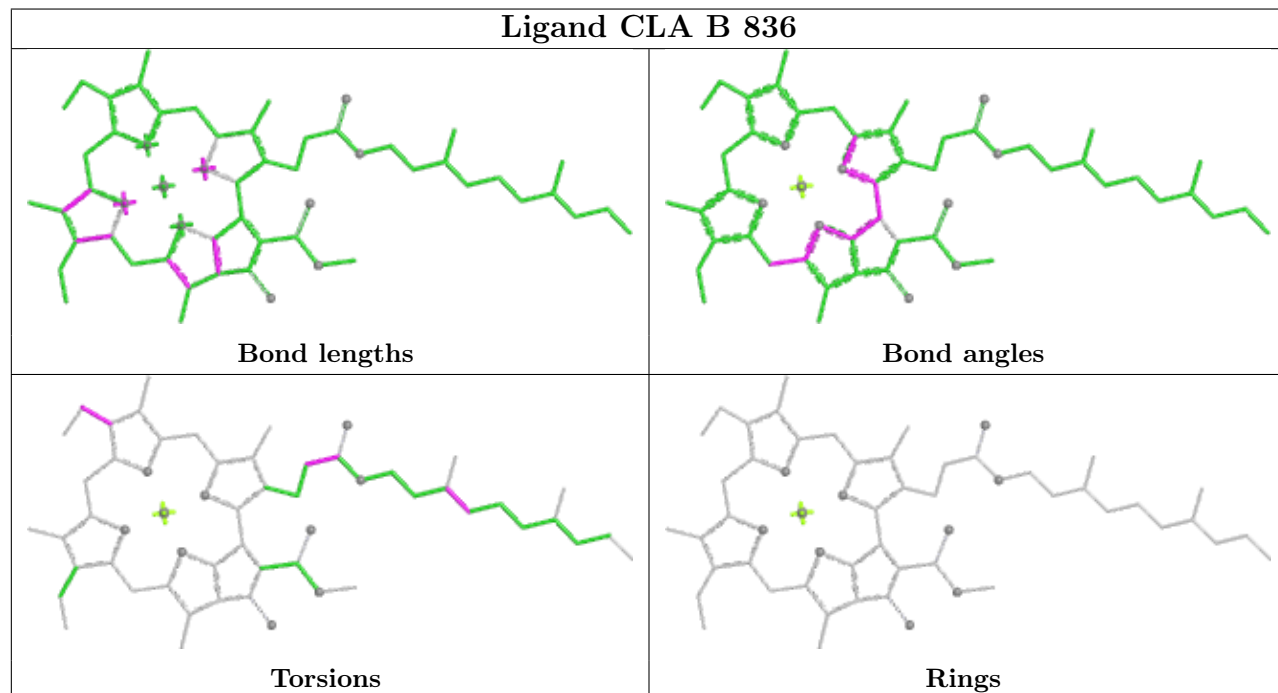
Ligand CLA A 822

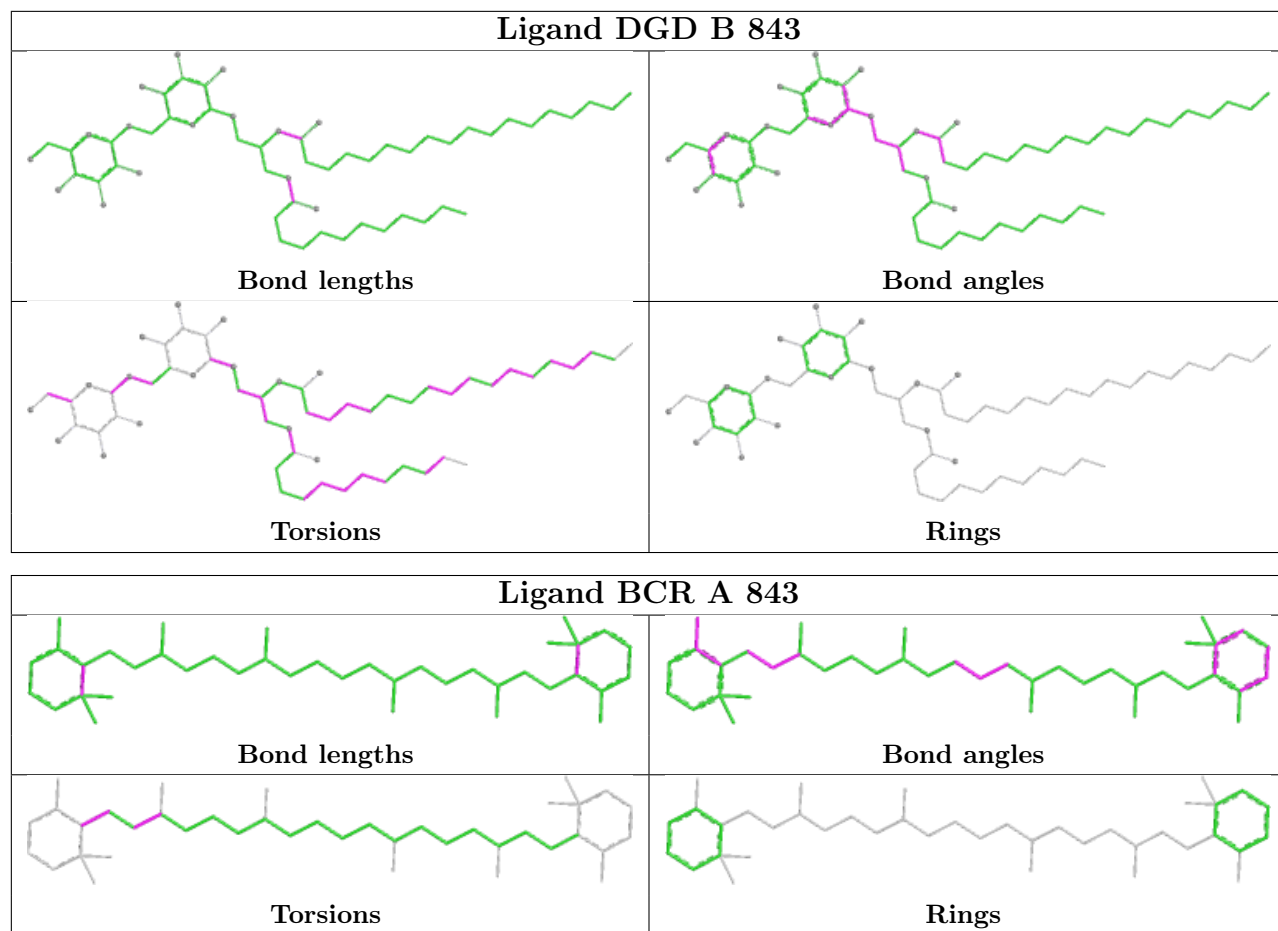


Ligand CLA L 203

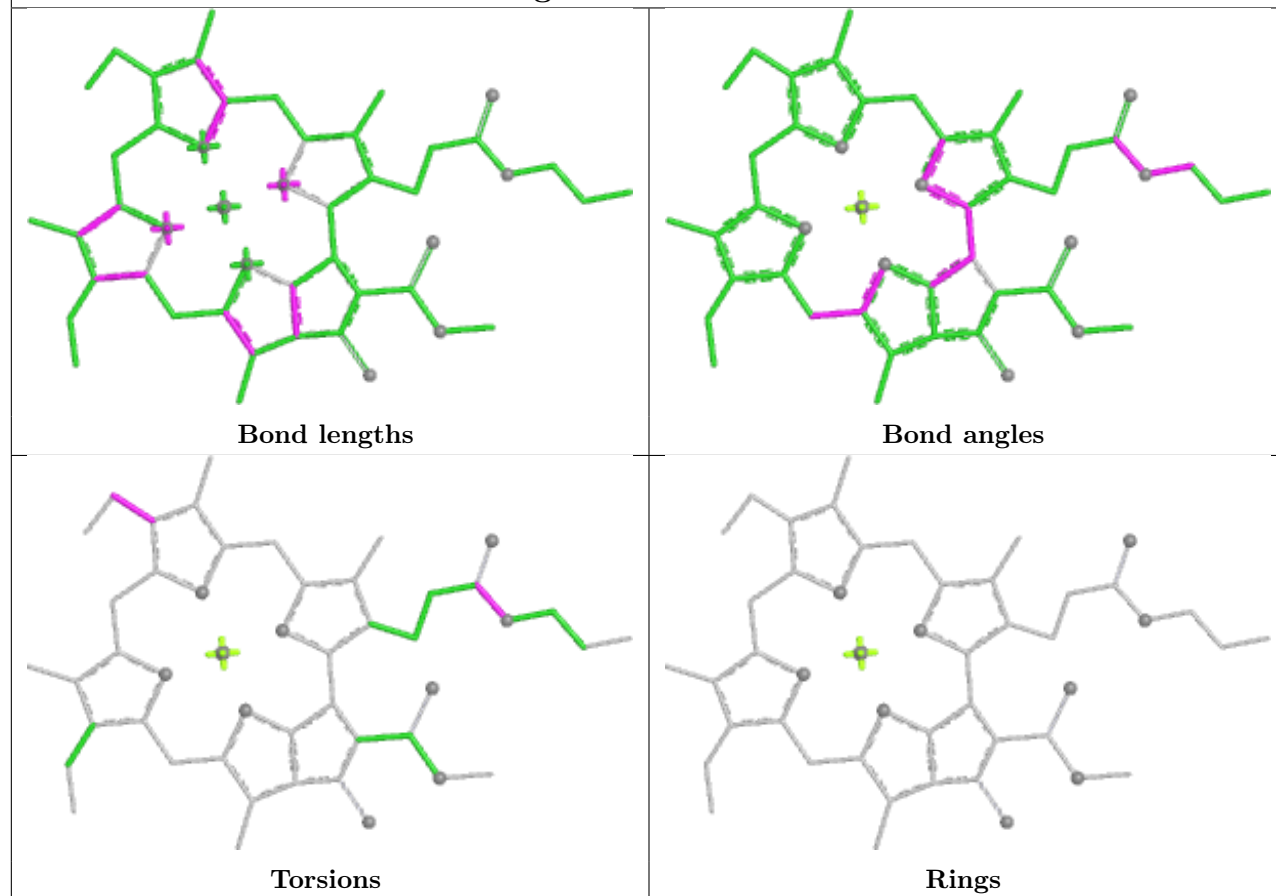


Ligand CLA B 836

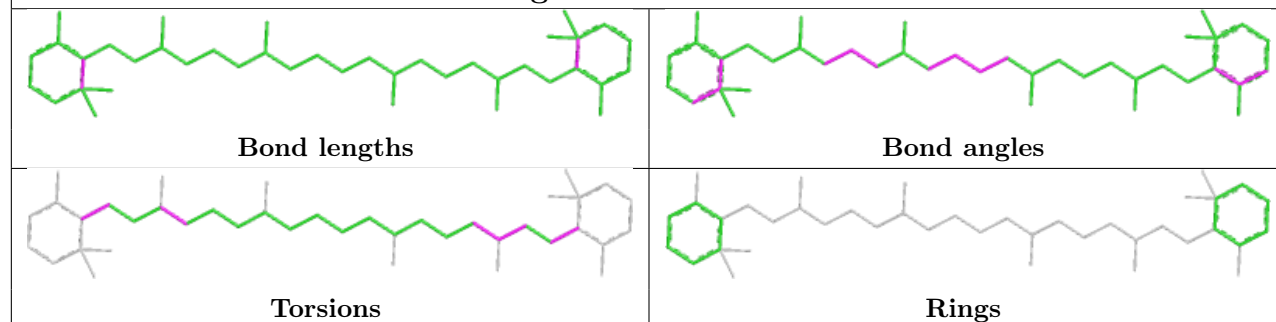




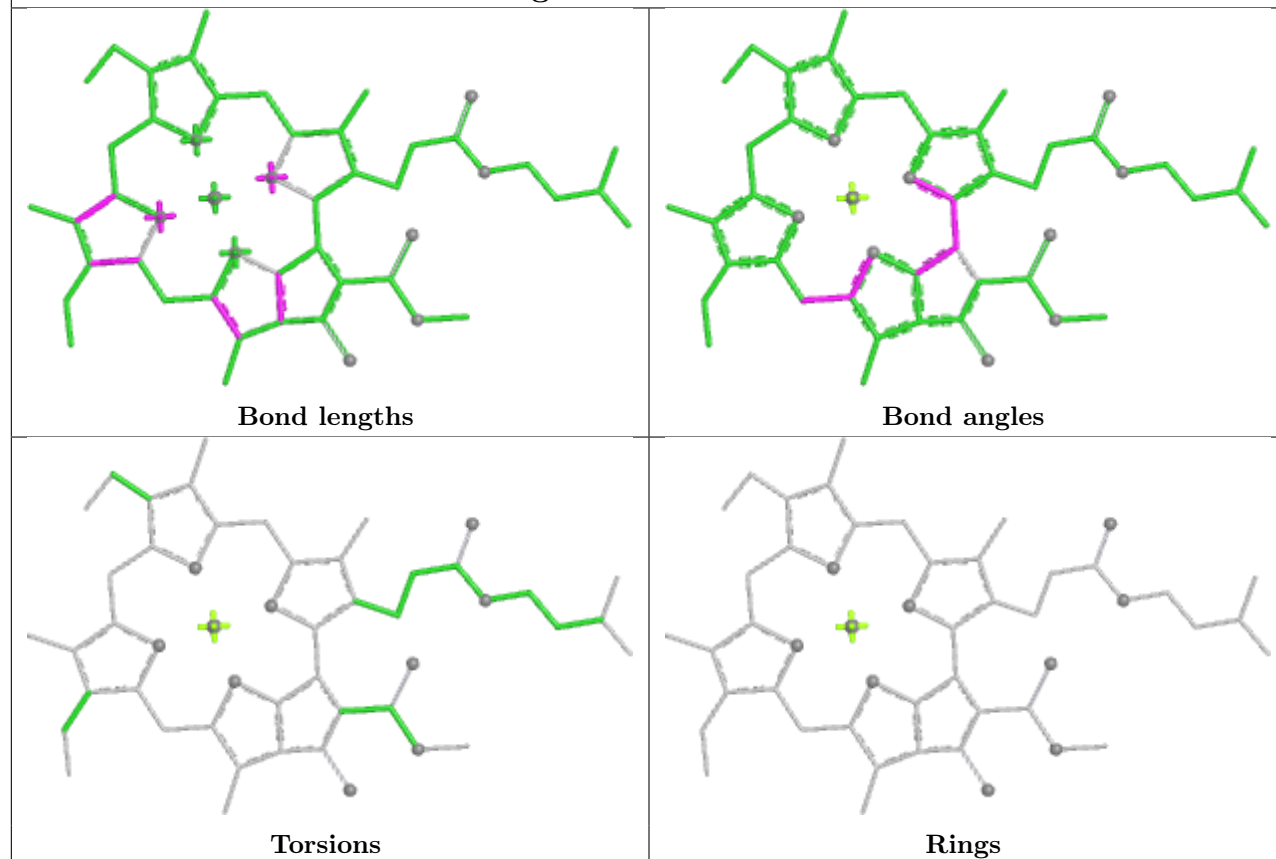
Ligand CLA F 803



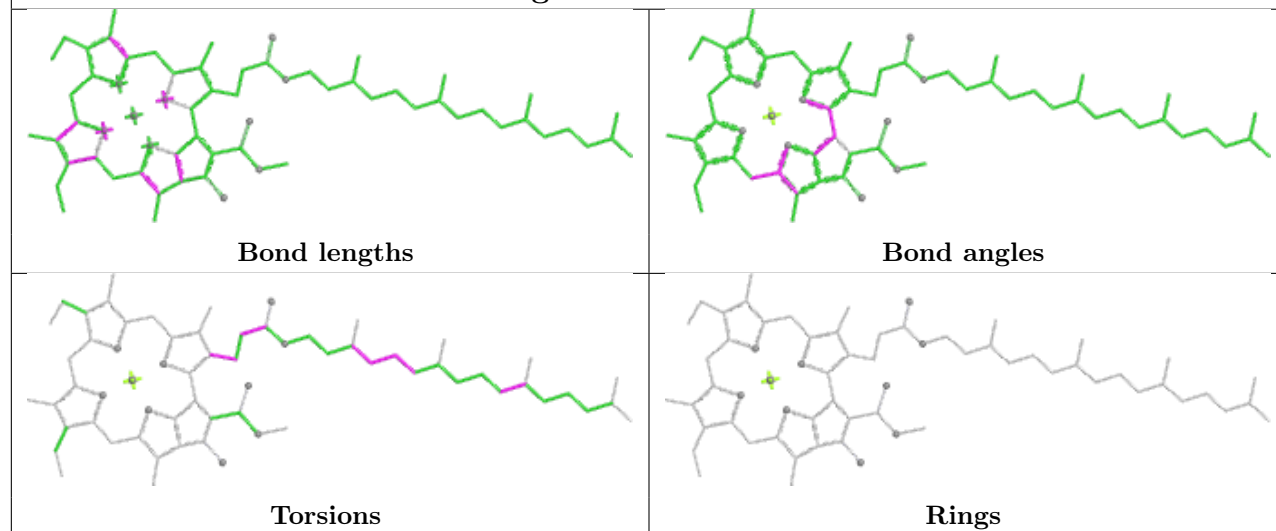
Ligand BCR B 842

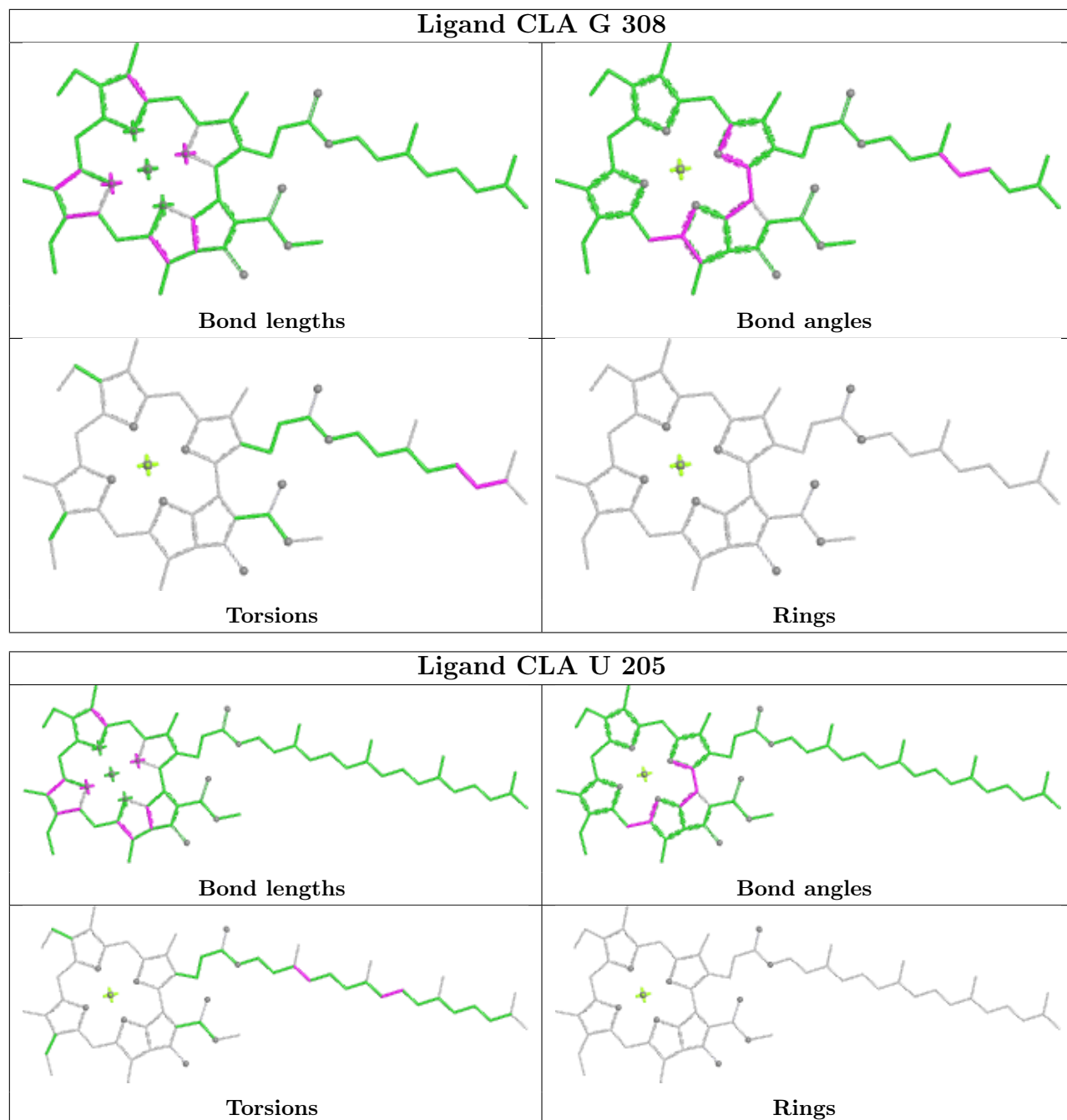


Ligand CLA A 830

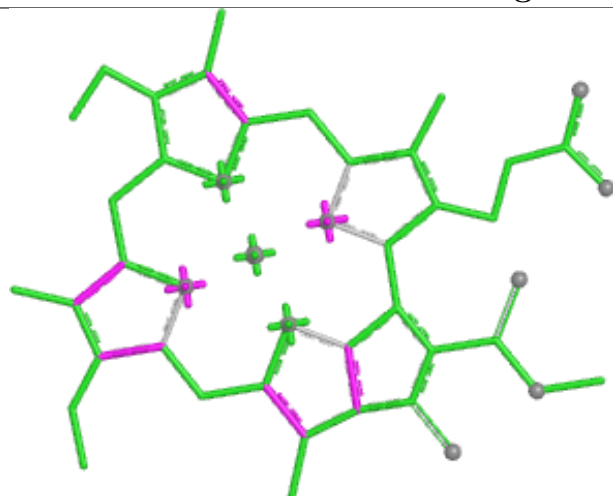


Ligand CLA A 804

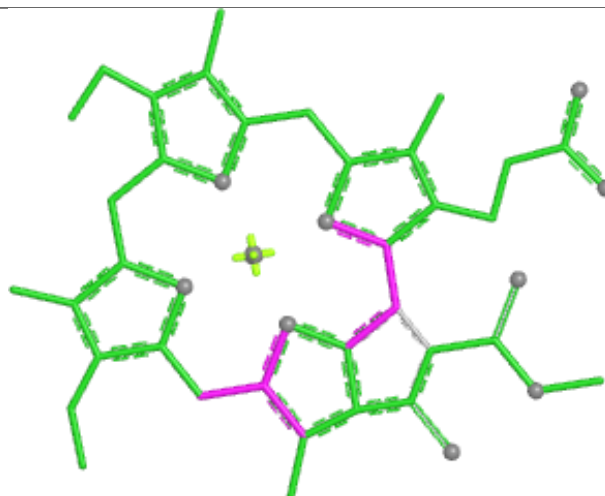




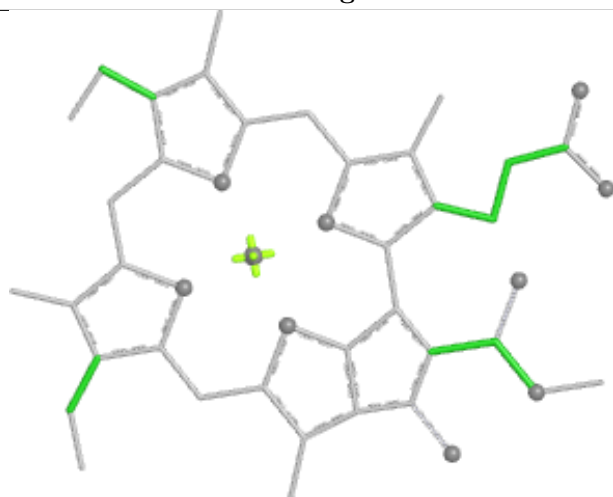
Ligand CLA B 830



Bond lengths



Bond angles

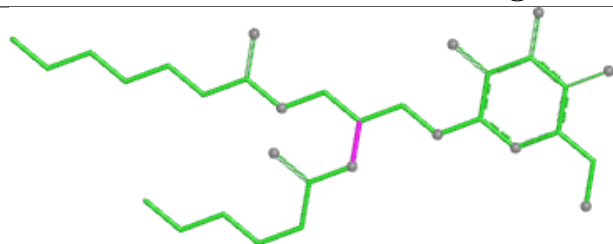


Torsions

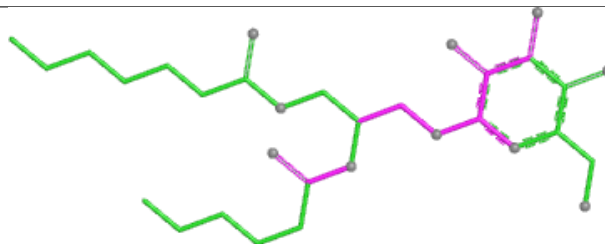


Rings

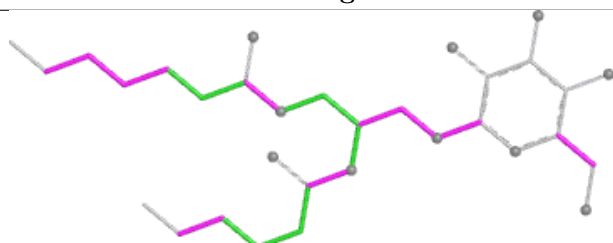
Ligand LMG U 201



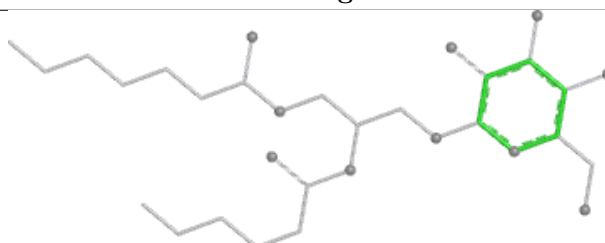
Bond lengths



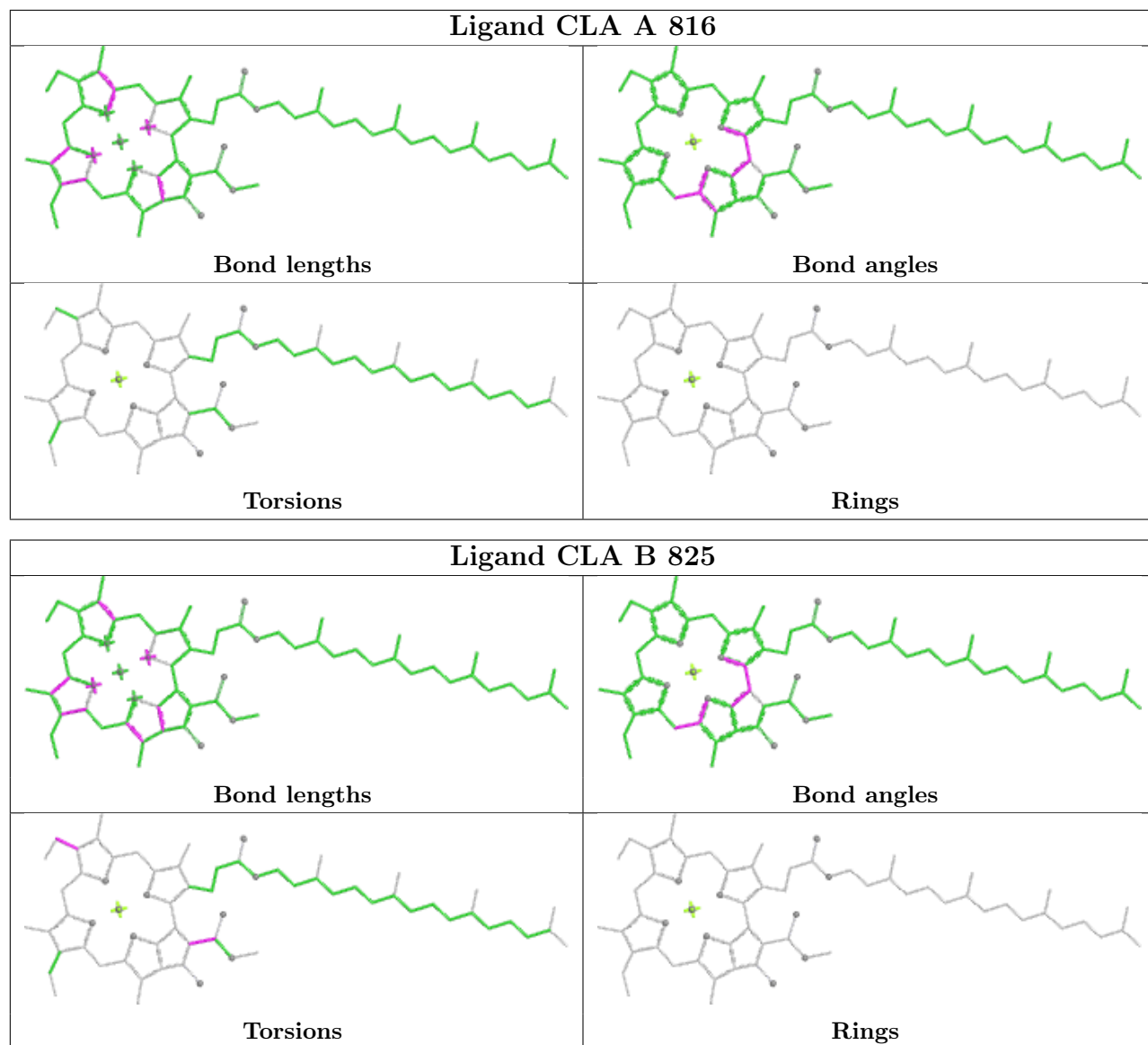
Bond angles

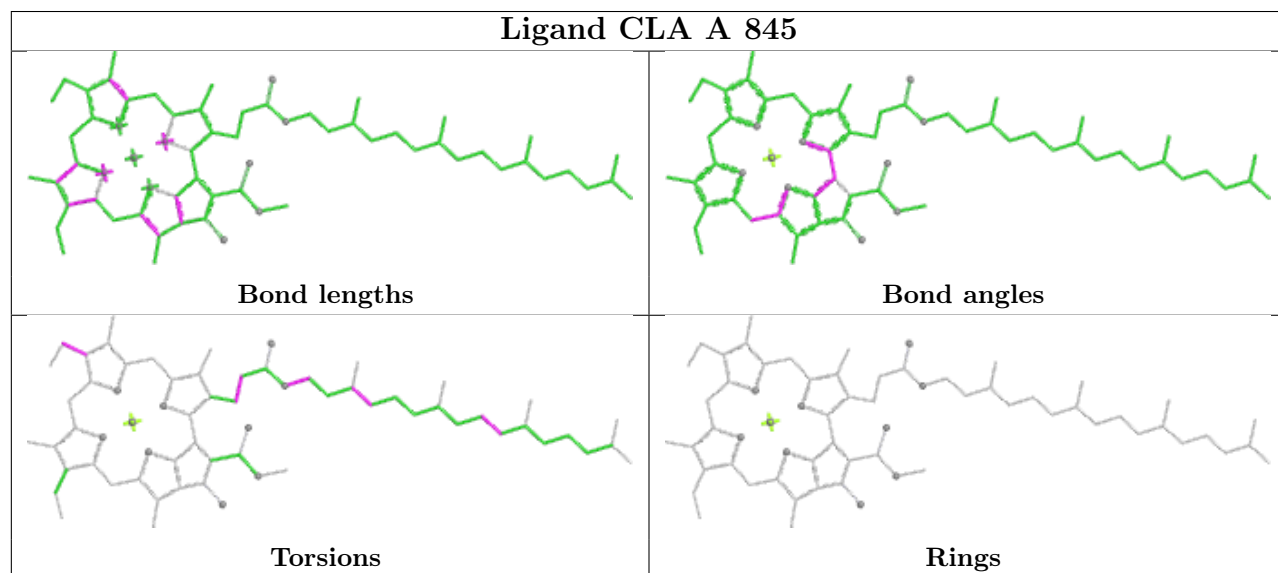
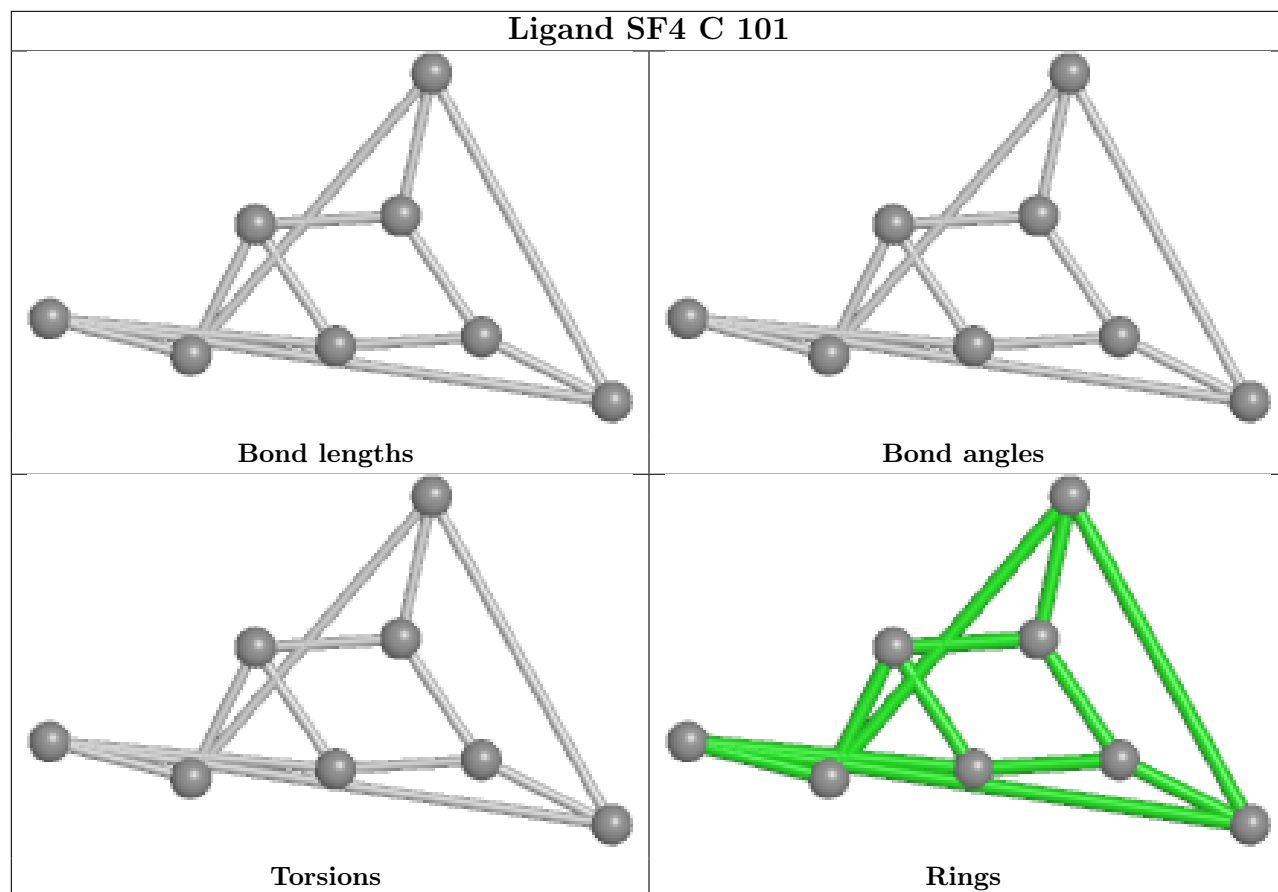


Torsions

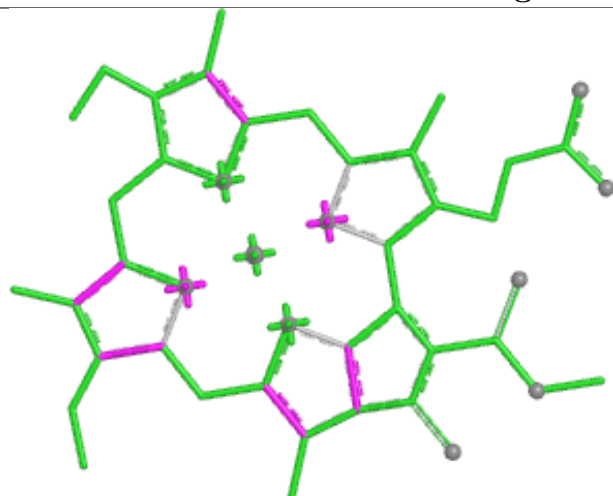


Rings

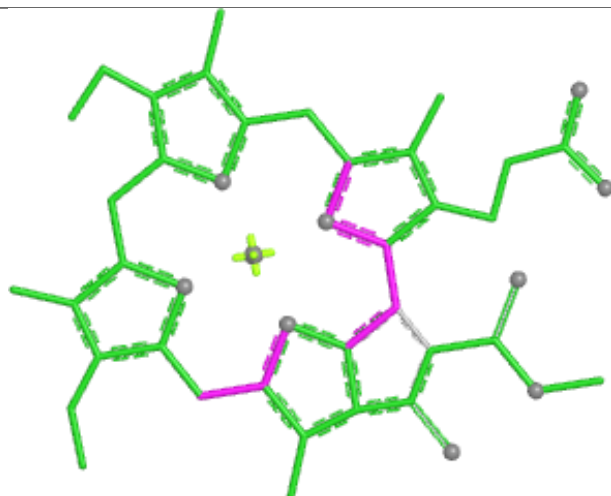




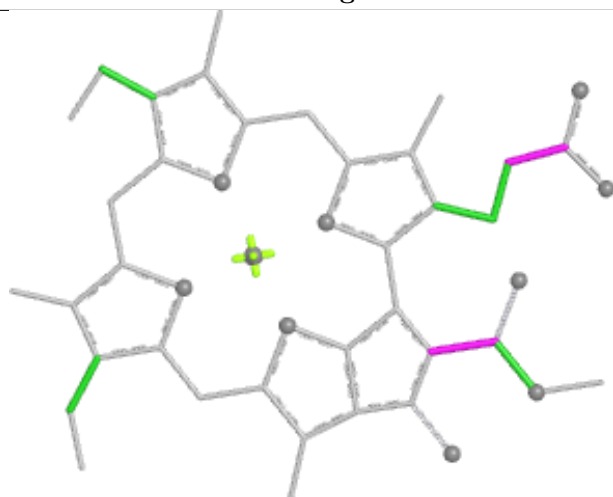
Ligand CLA B 804



Bond lengths



Bond angles

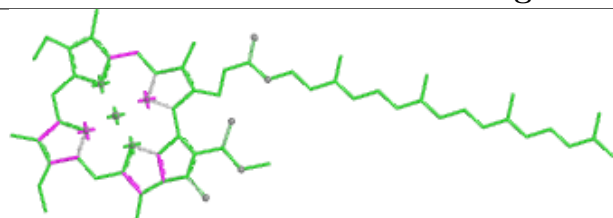


Torsions

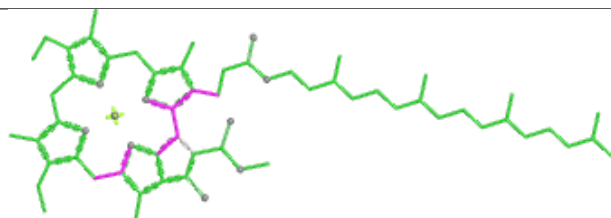


Rings

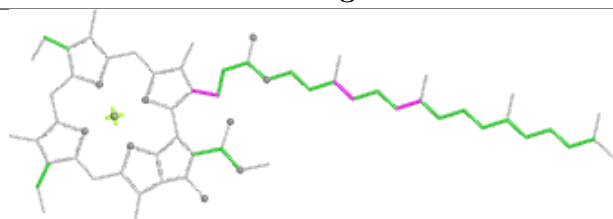
Ligand CLA B 823



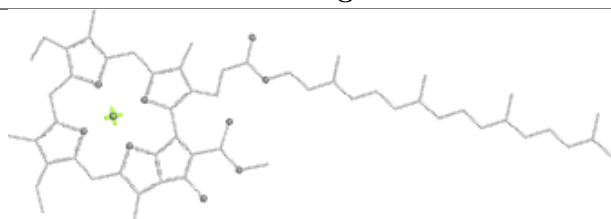
Bond lengths



Bond angles

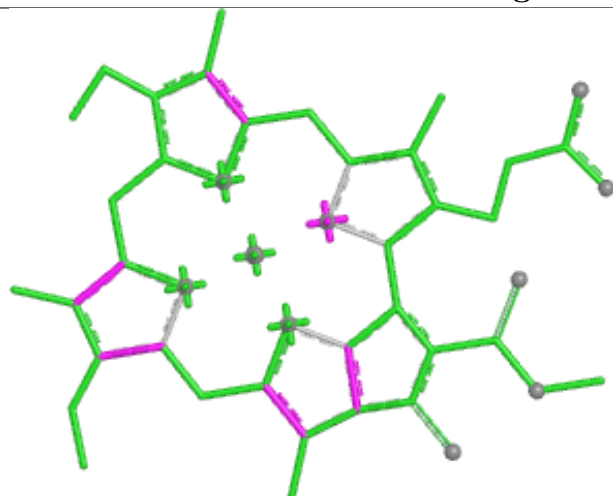


Torsions

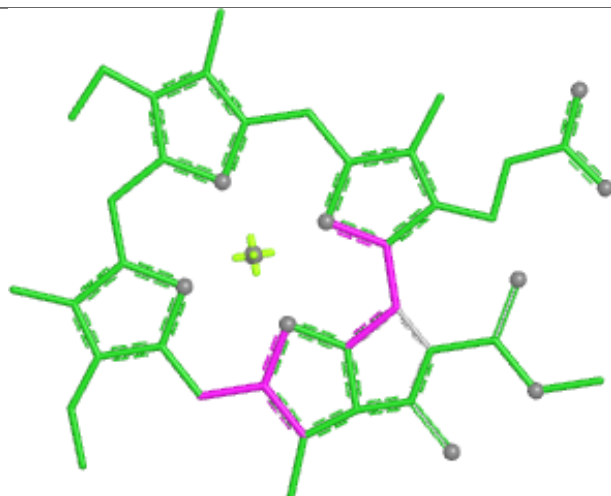


Rings

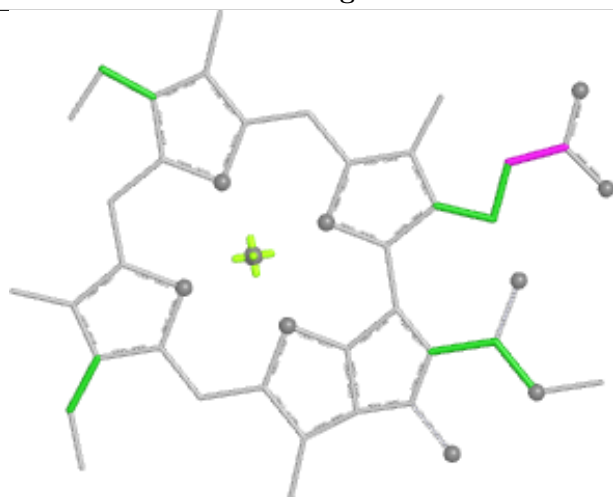
Ligand CLA G 301



Bond lengths



Bond angles

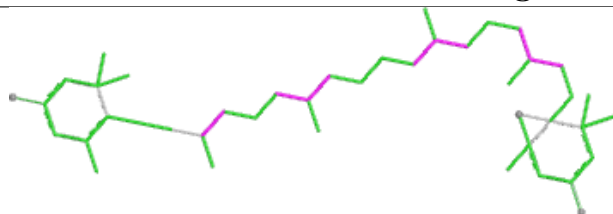


Torsions

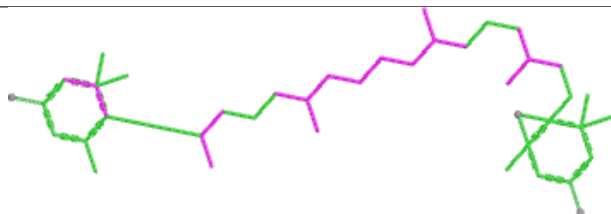


Rings

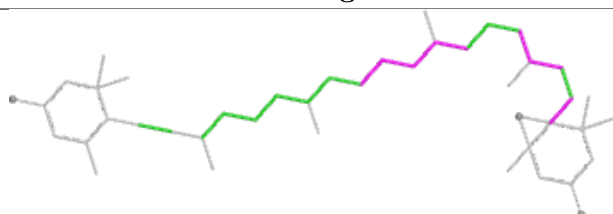
Ligand DD6 H 311



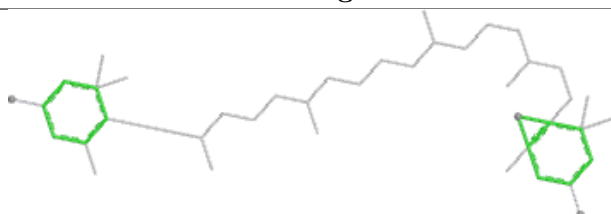
Bond lengths



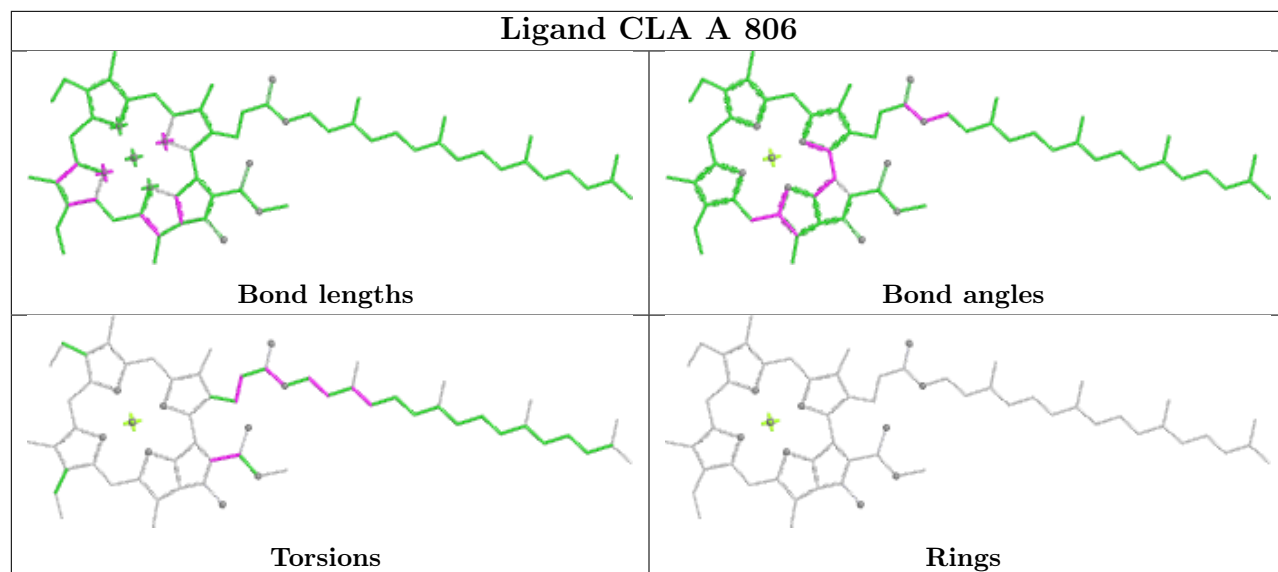
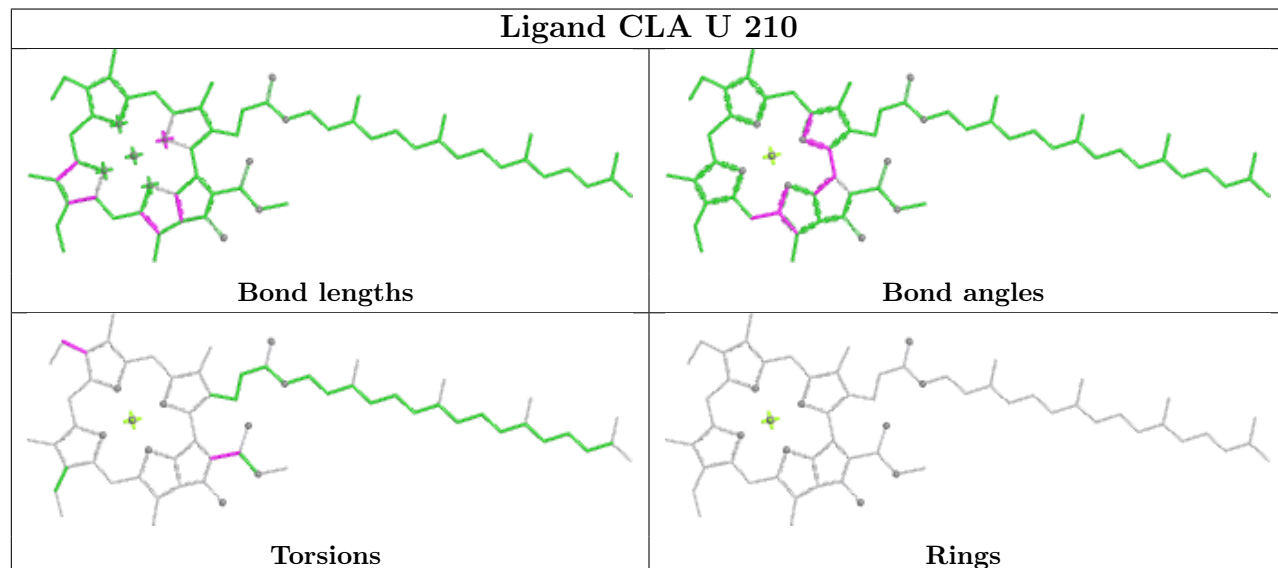
Bond angles

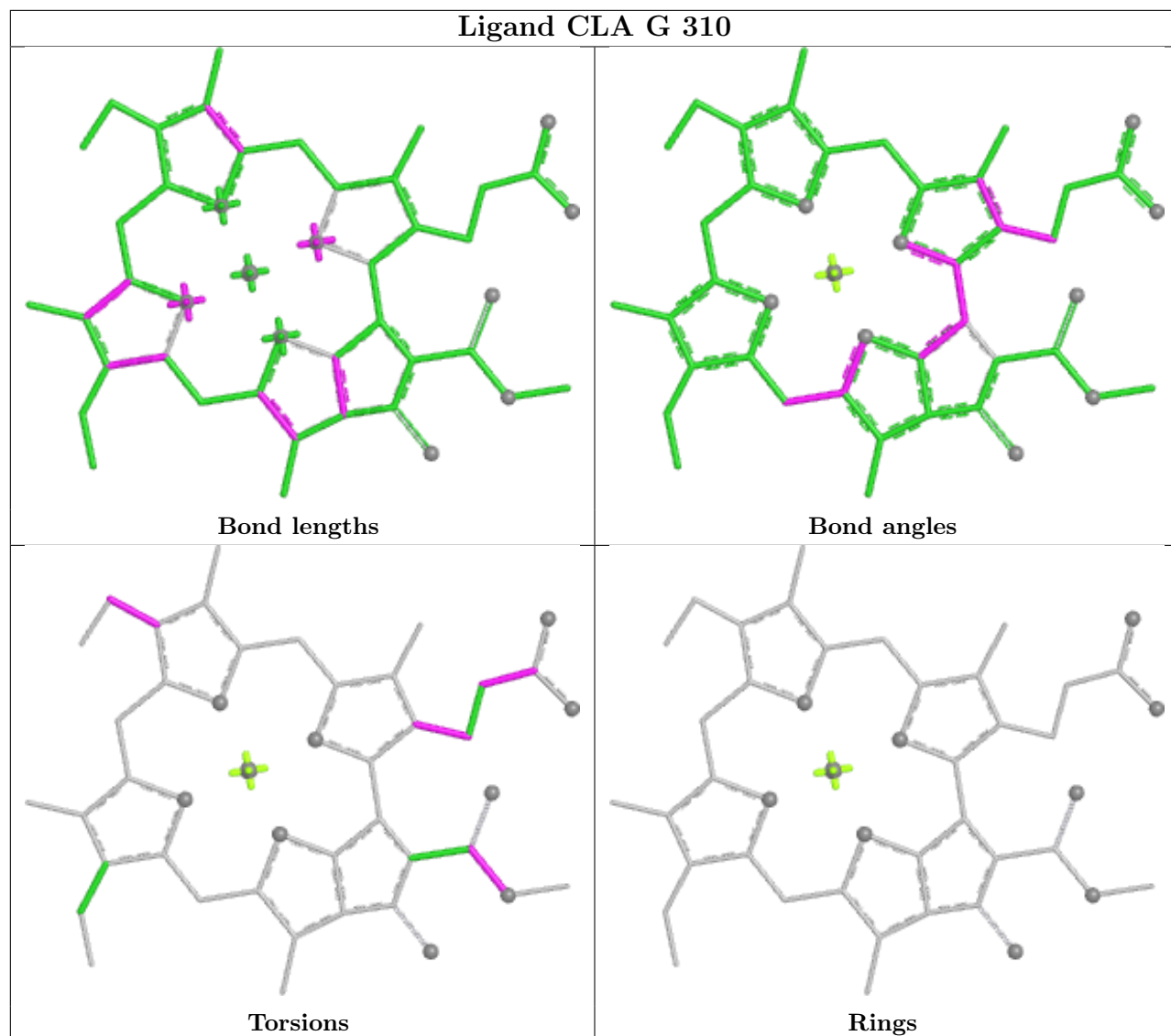


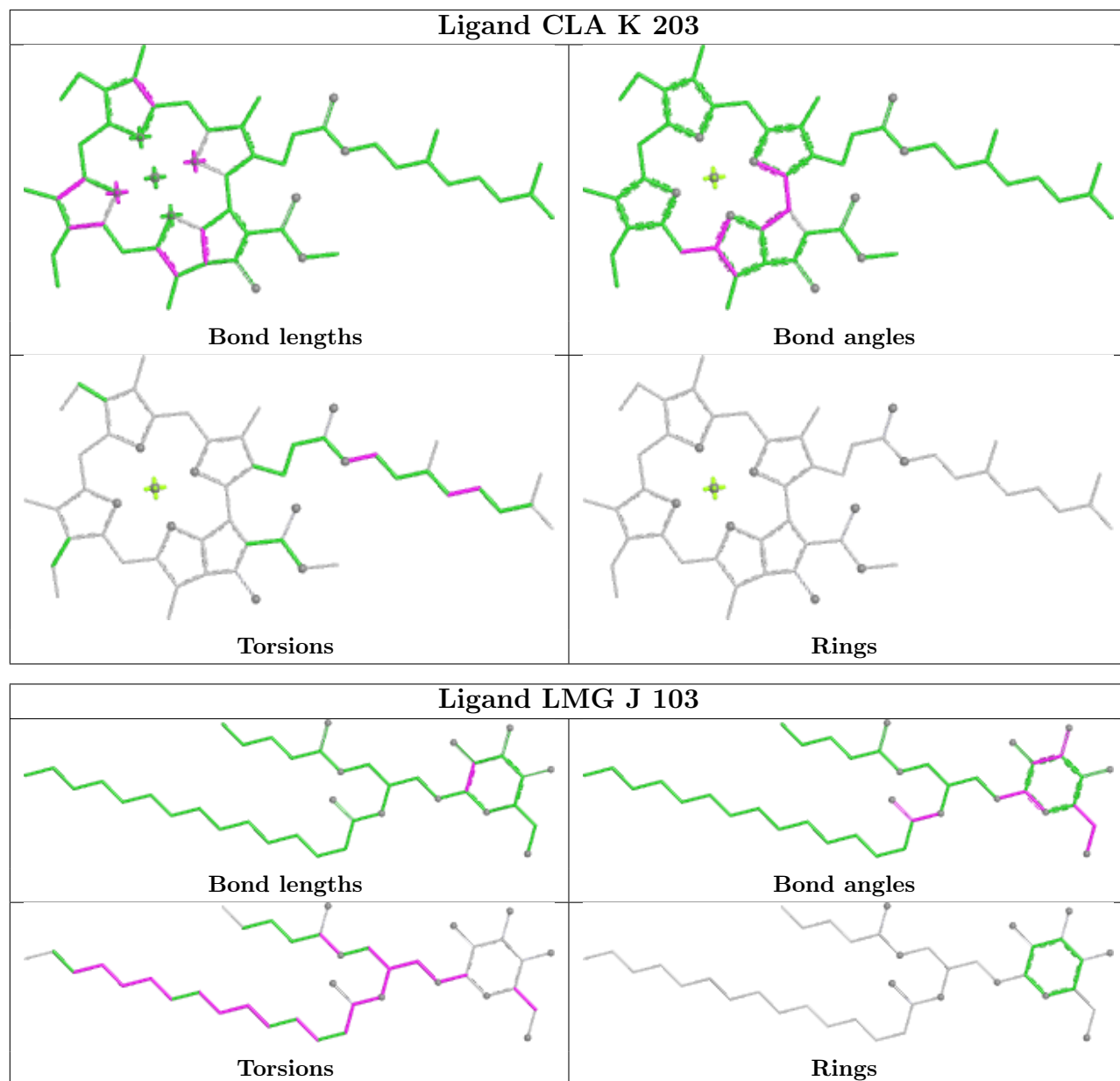
Torsions

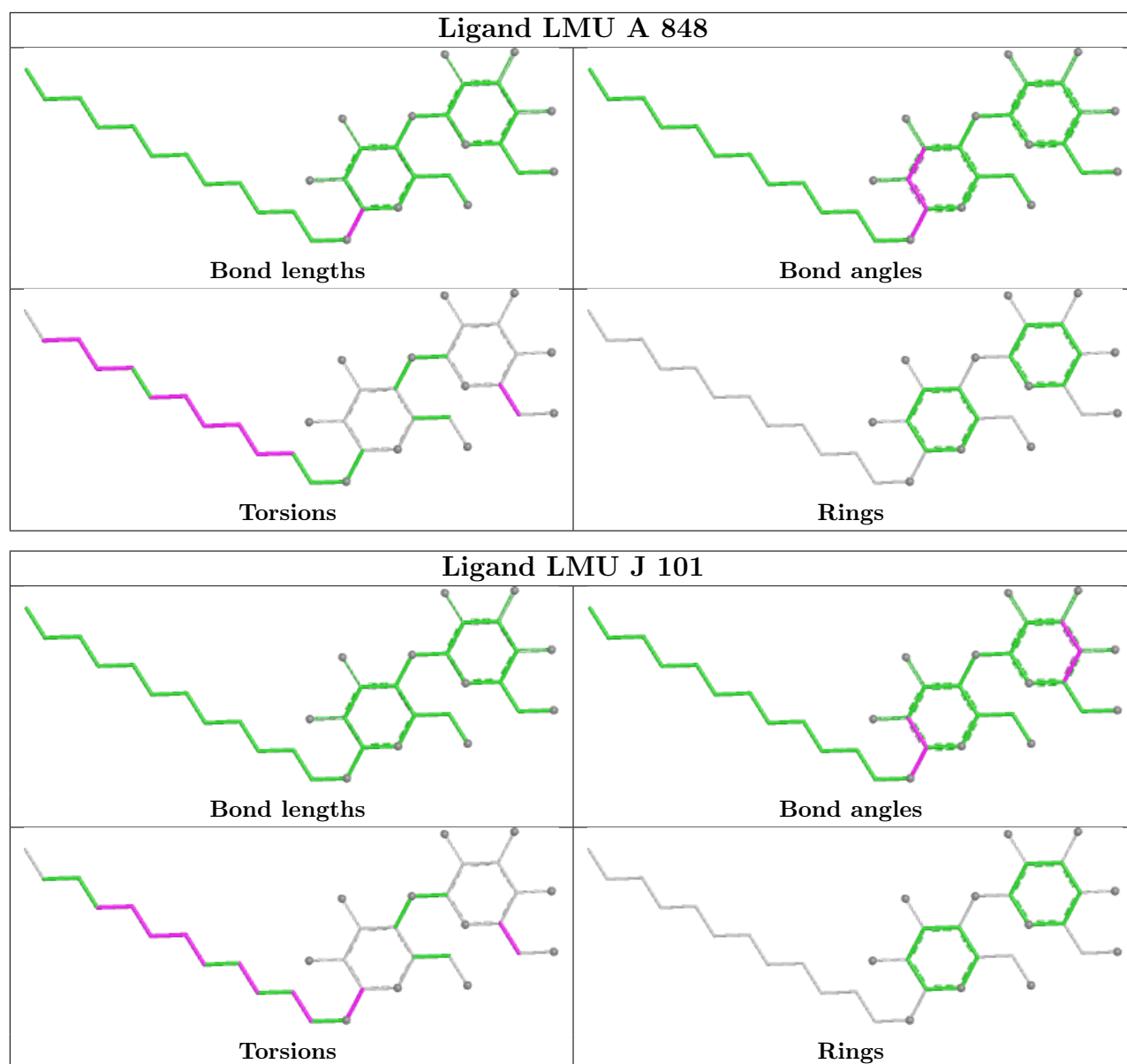


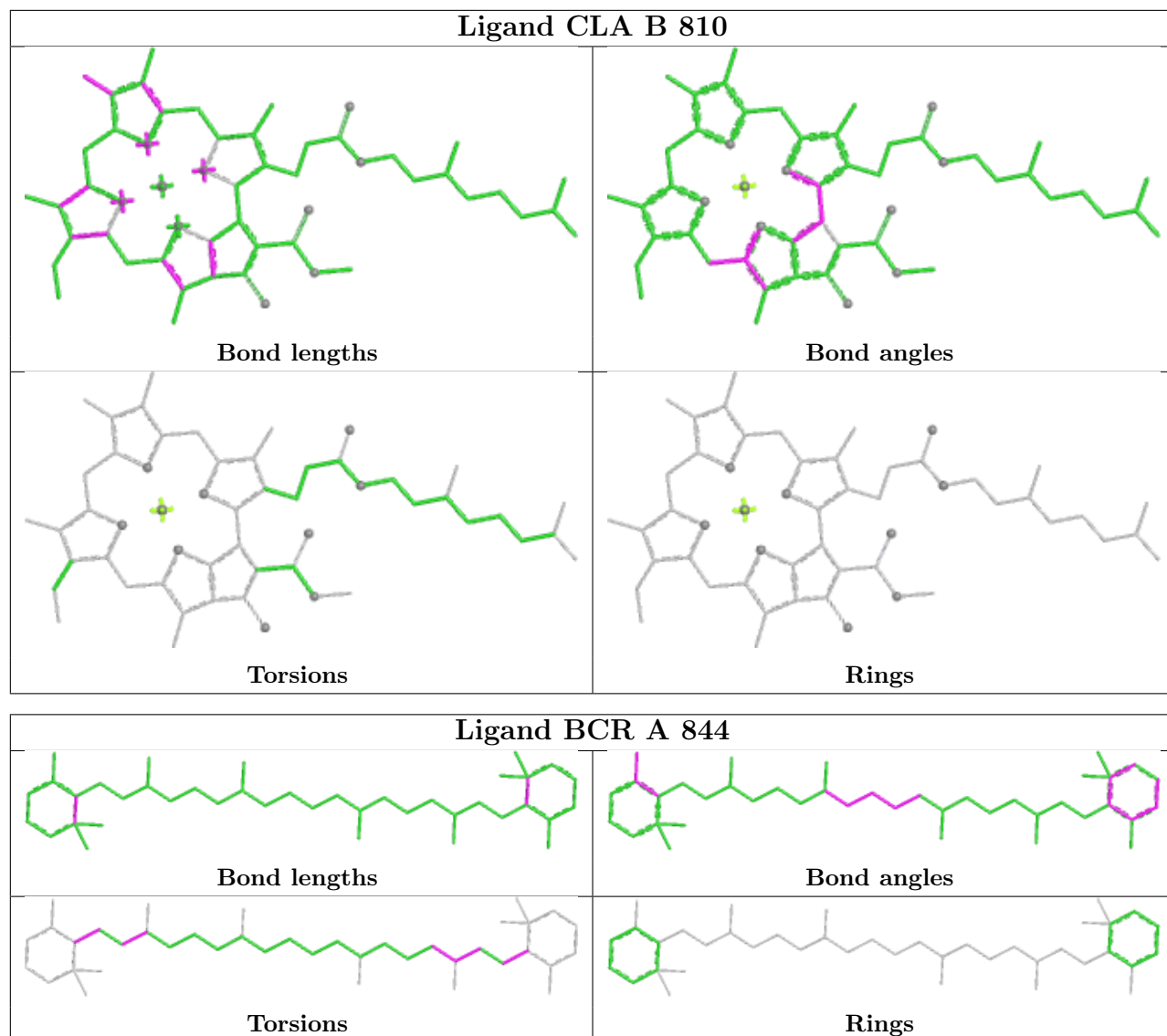
Rings

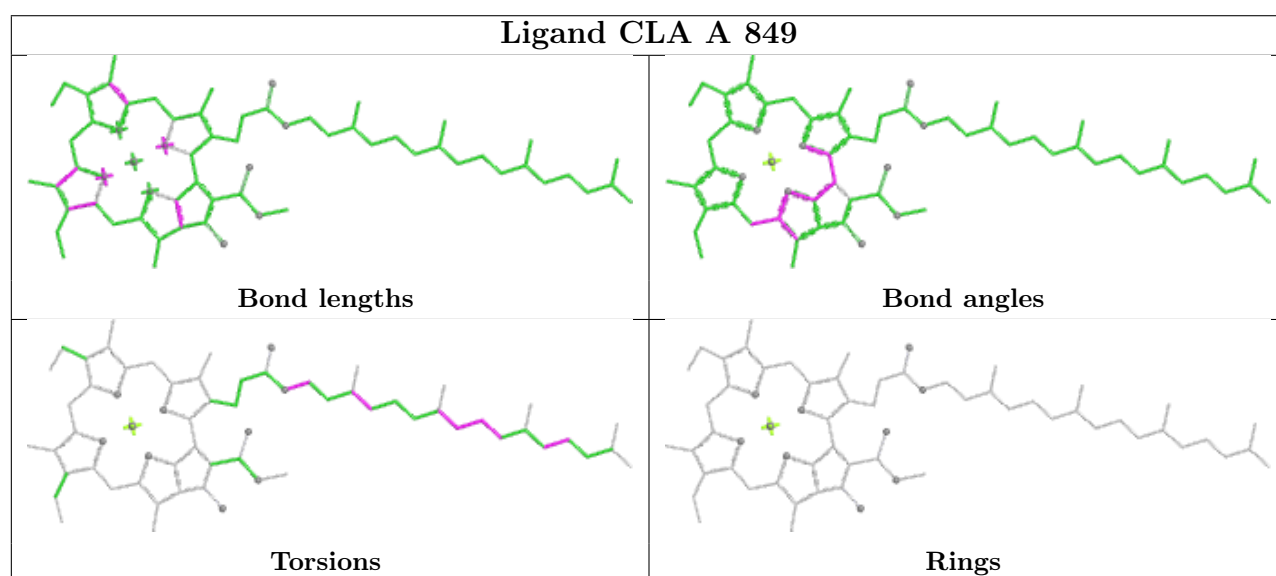
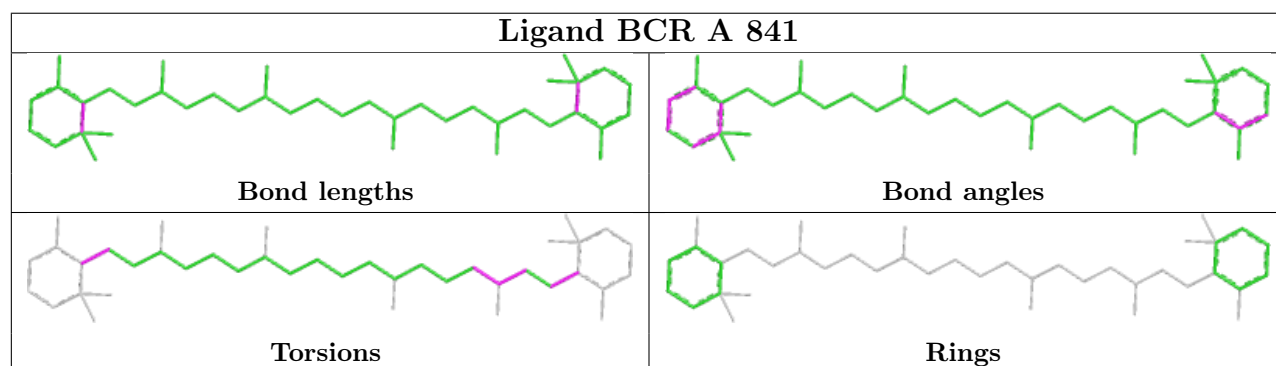
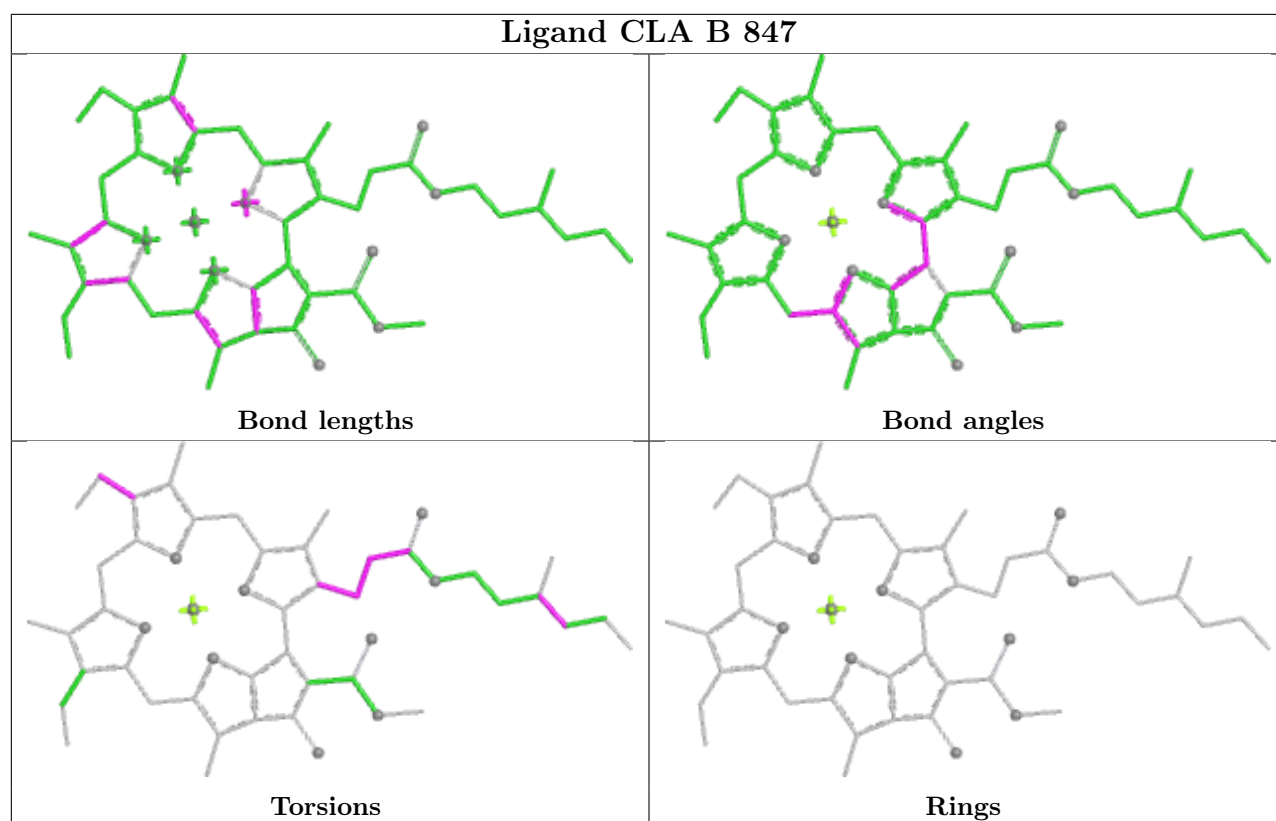
Ligand CLA A 806**Ligand CLA U 210**

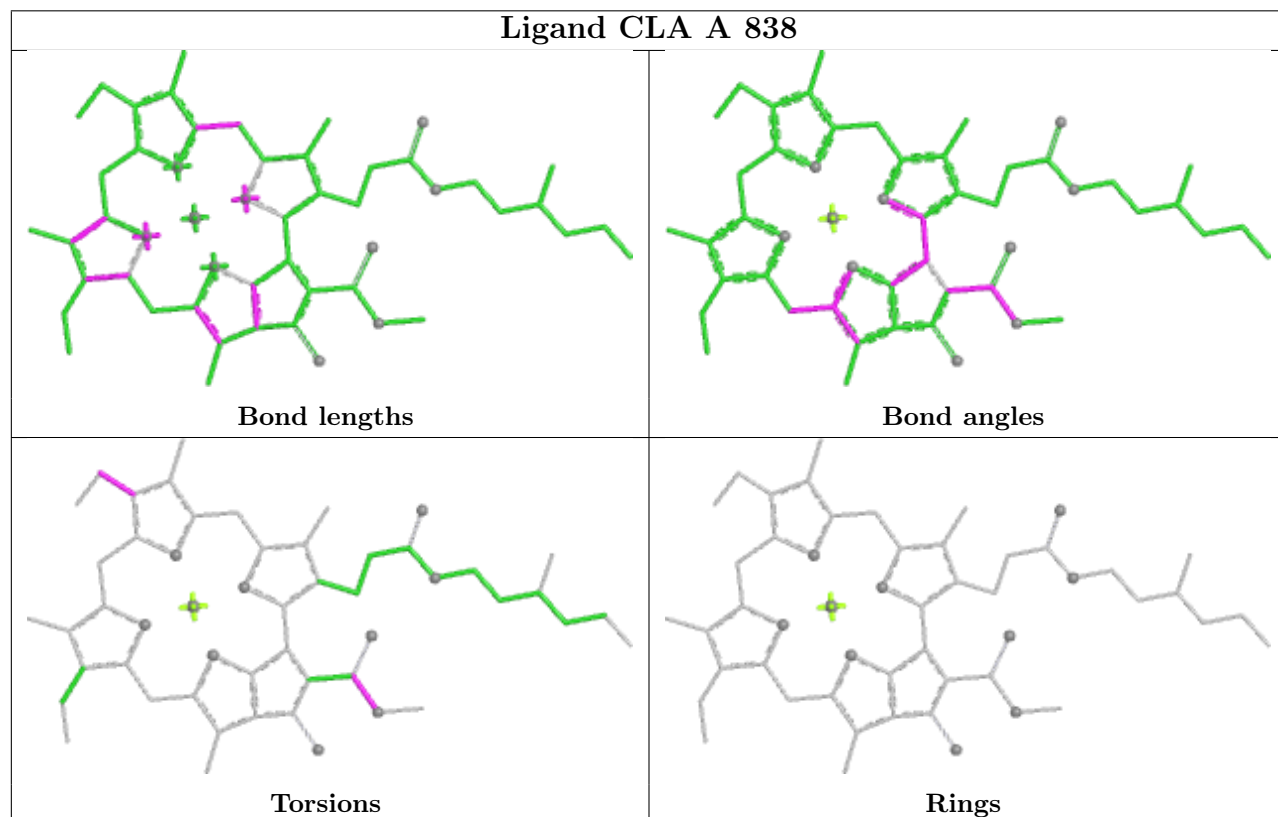
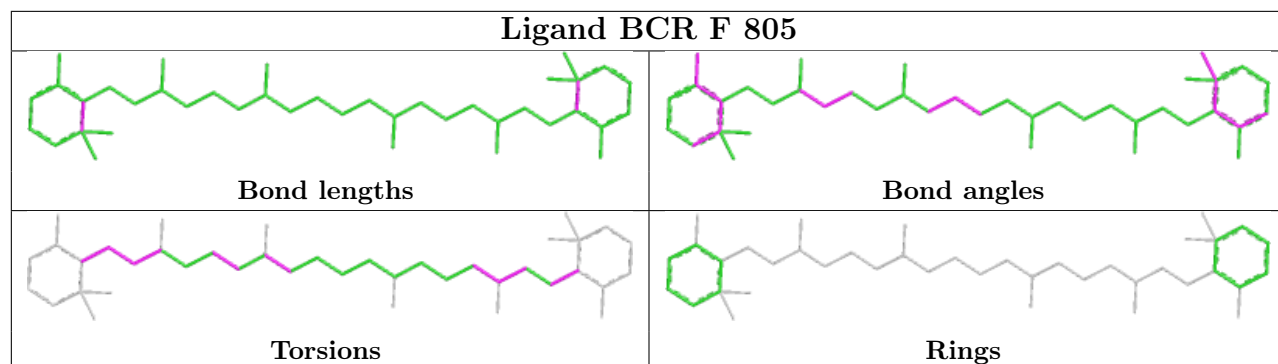


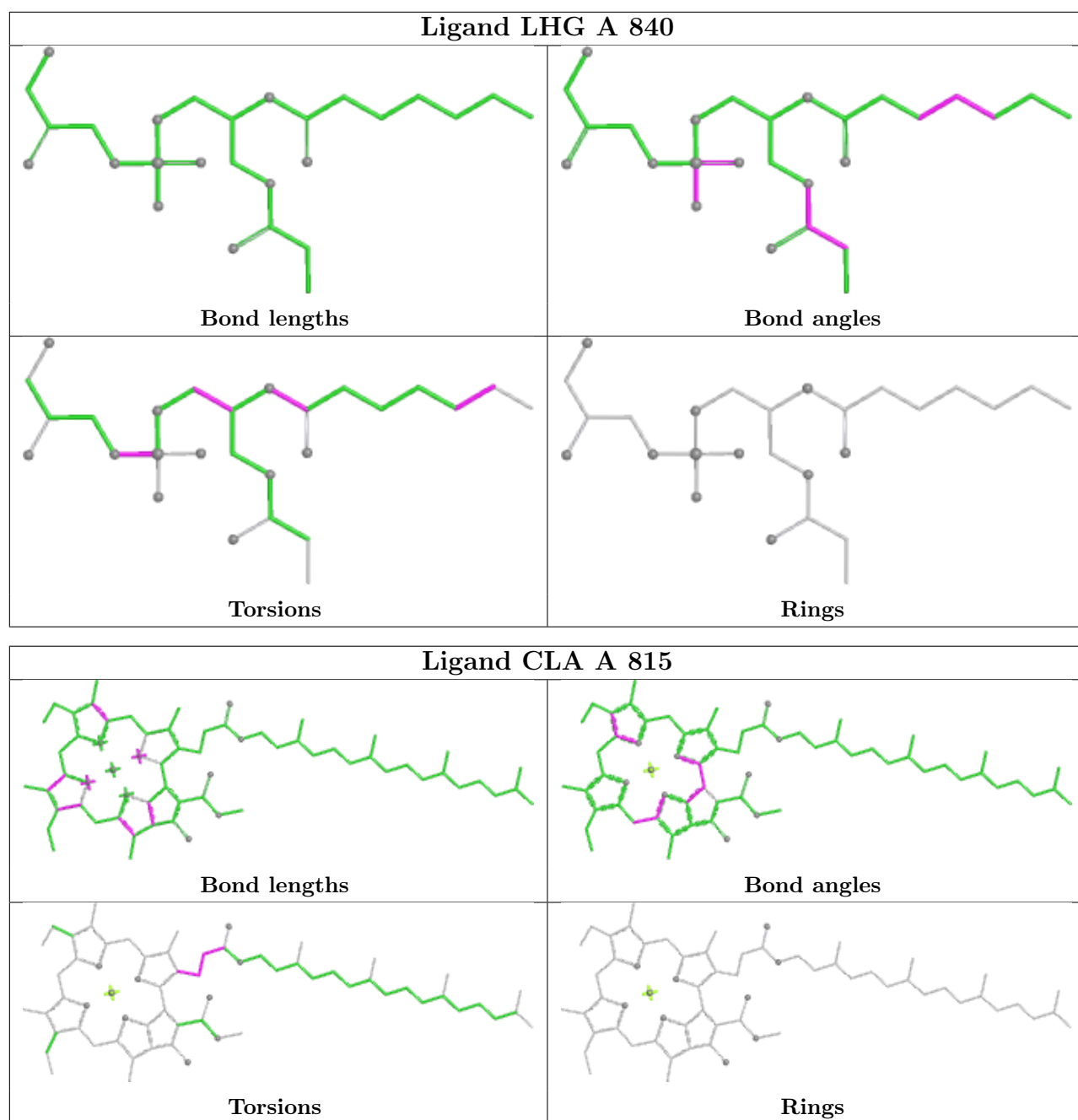


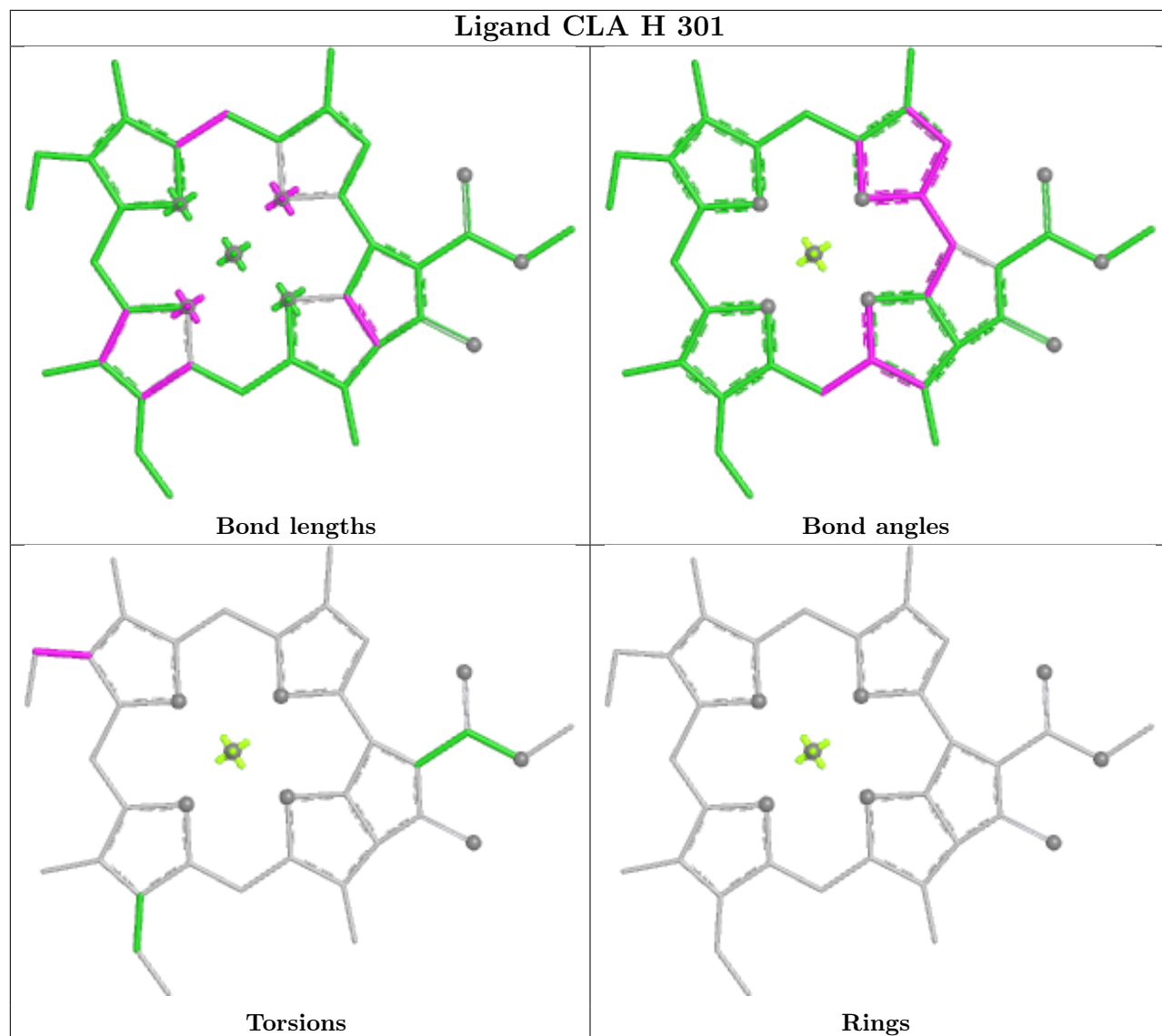




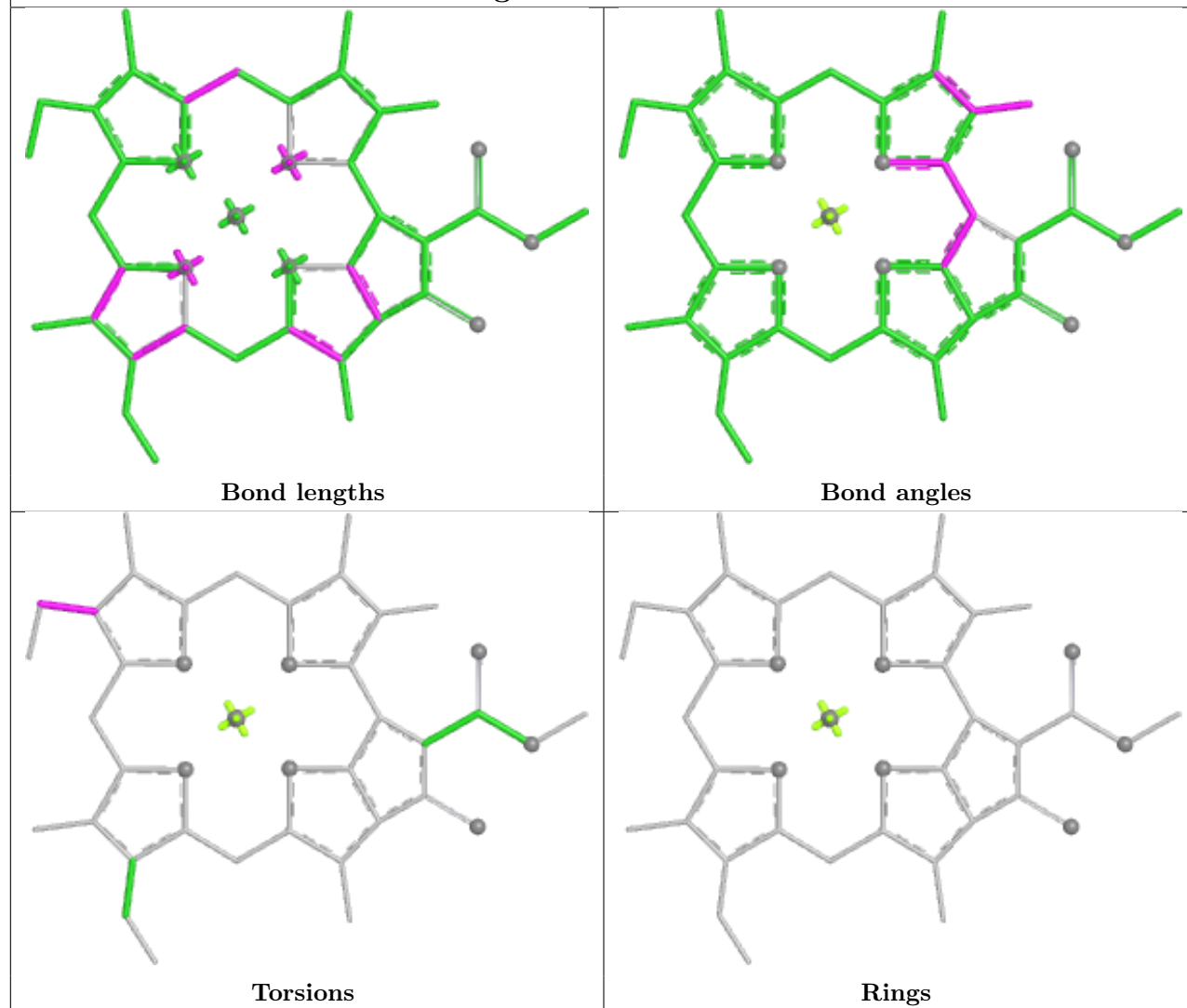




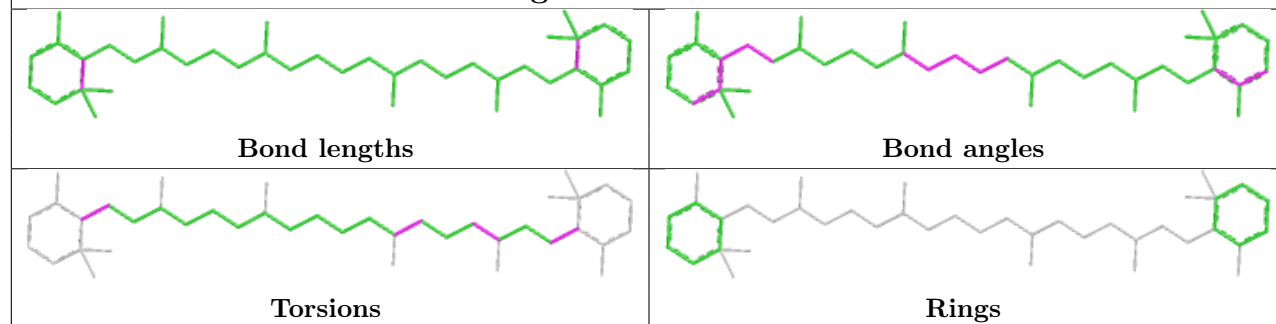


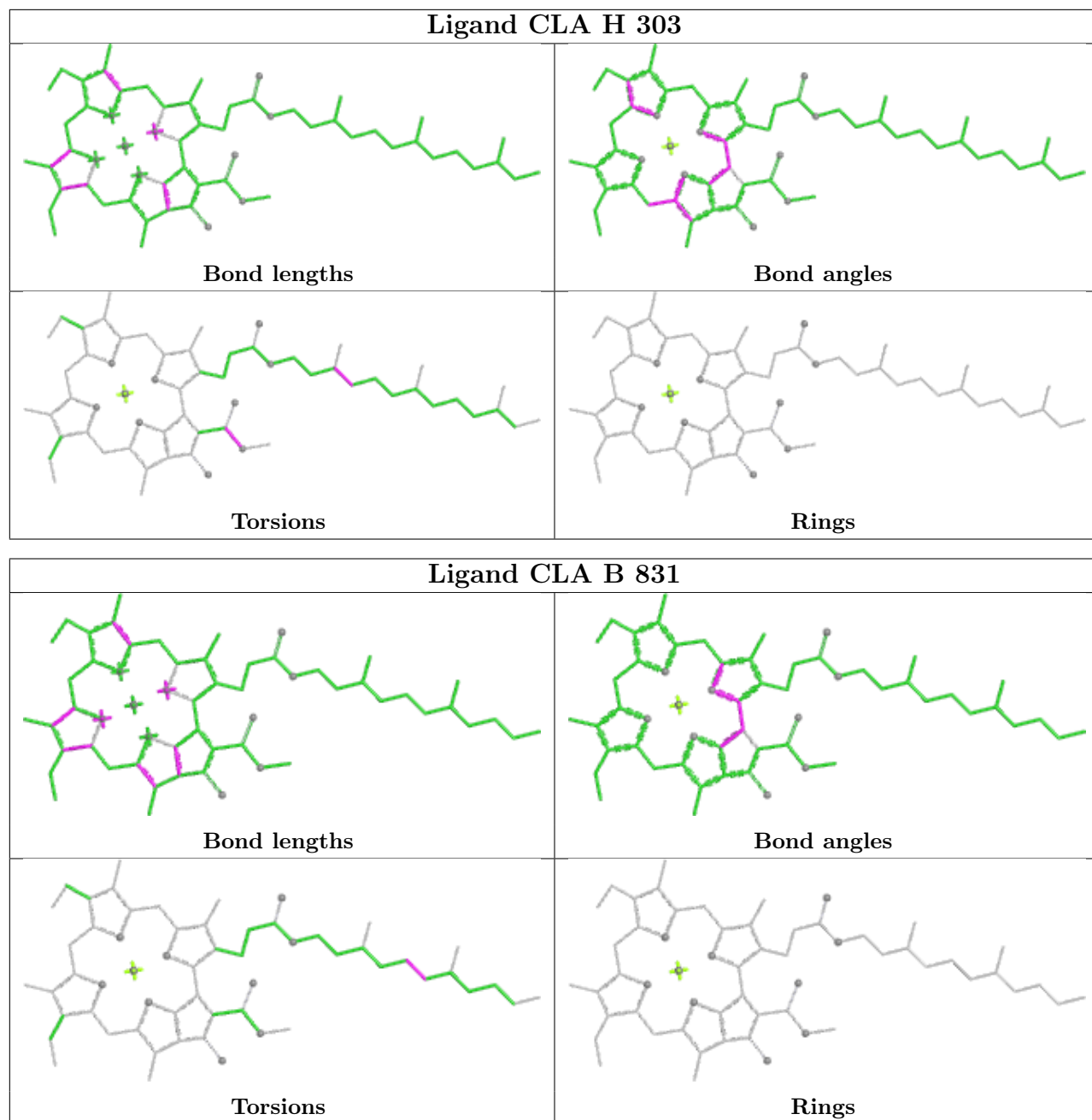


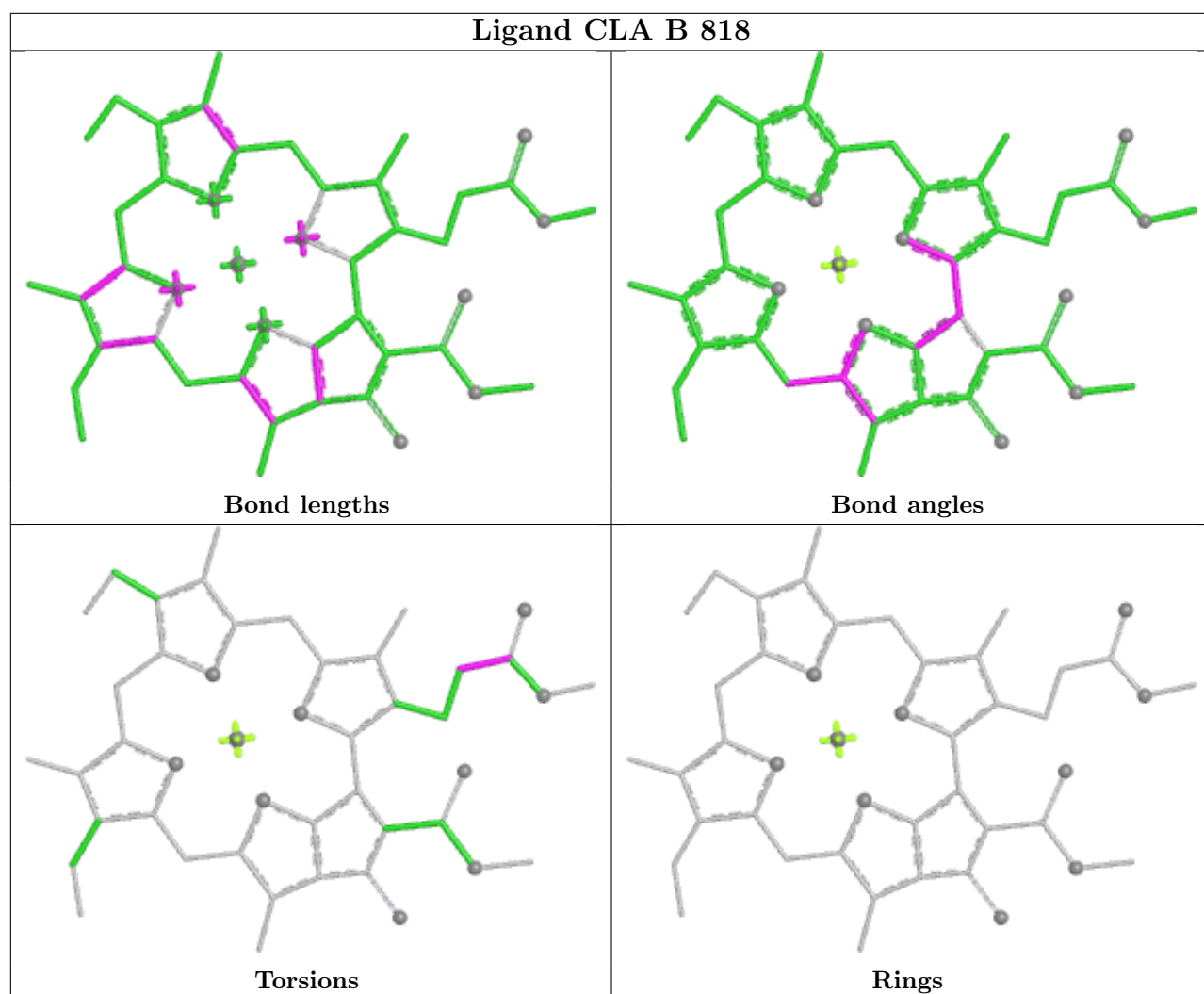
Ligand CLA G 302



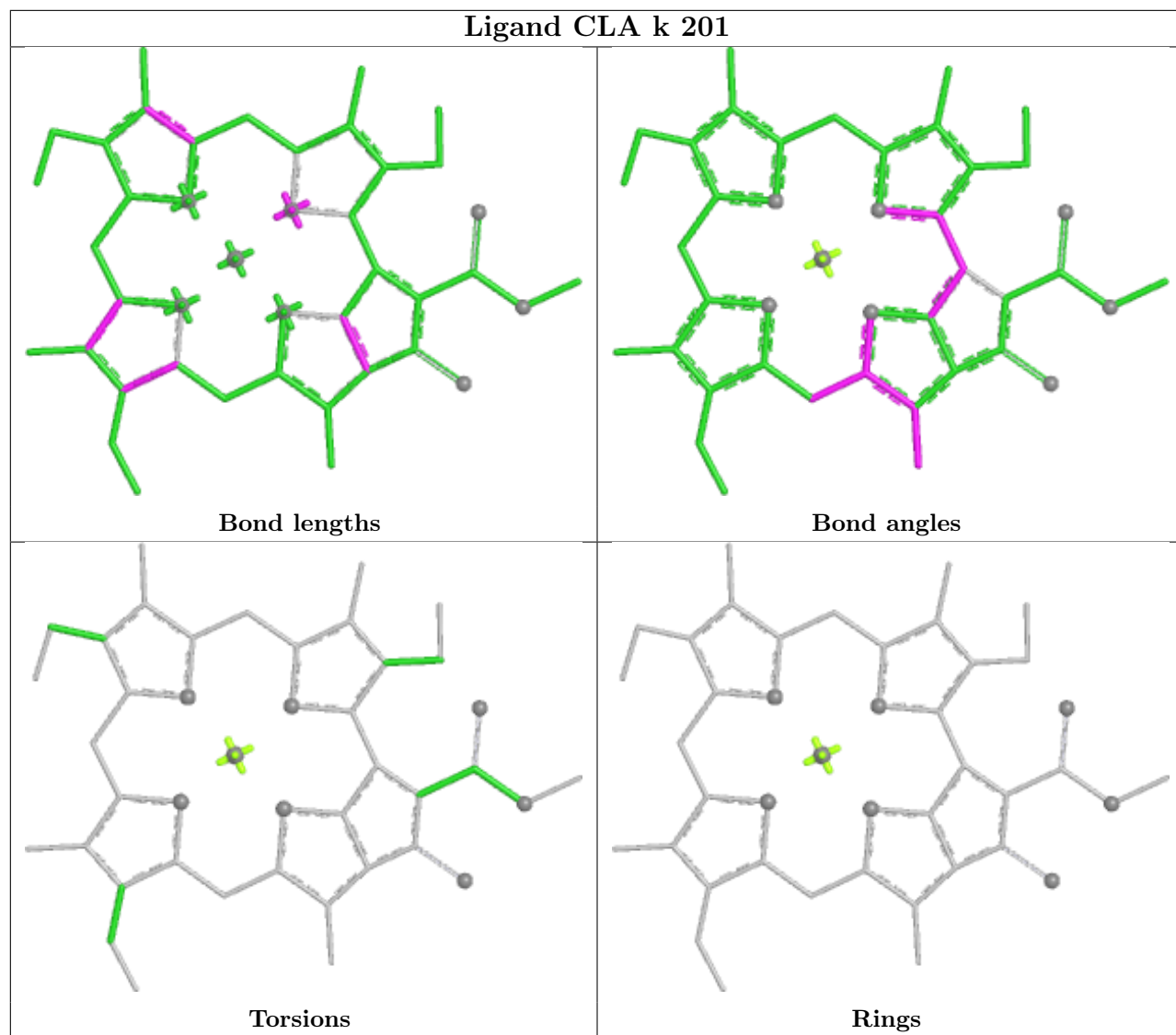
Ligand BCR B 841



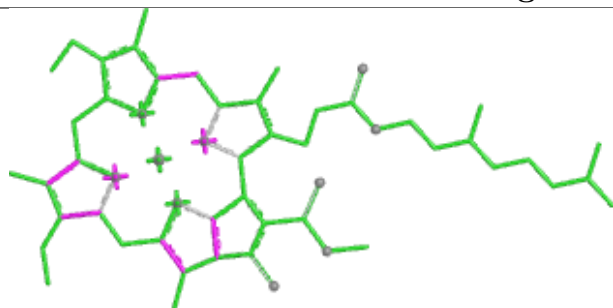




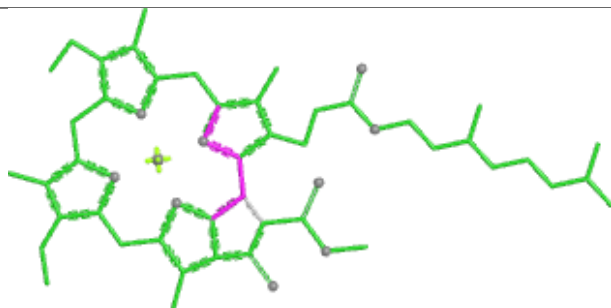
Ligand CLA k 201



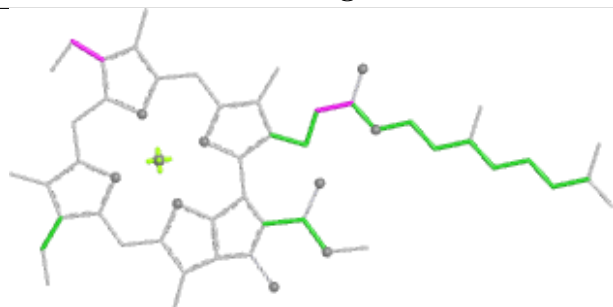
Ligand CLA k 202



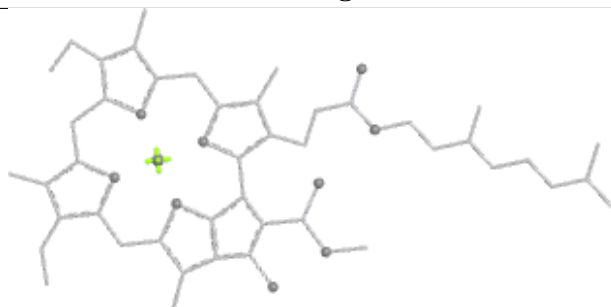
Bond lengths



Bond angles

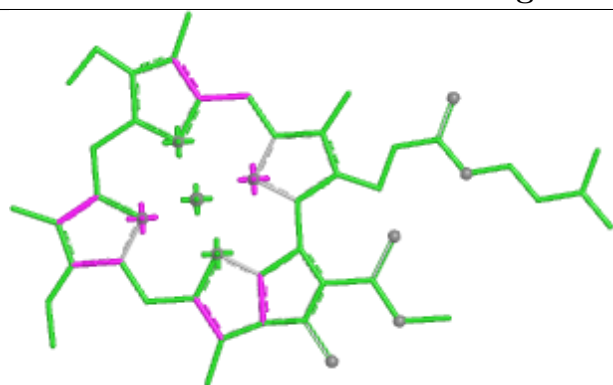


Torsions

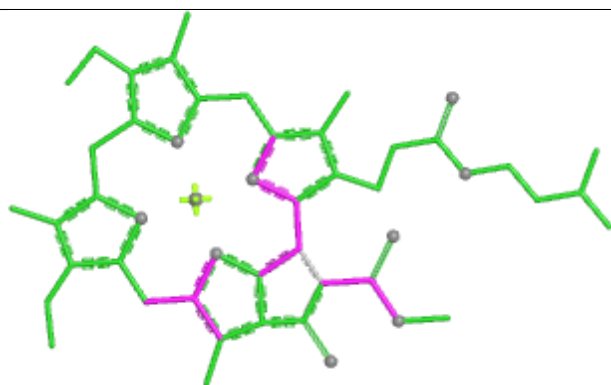


Rings

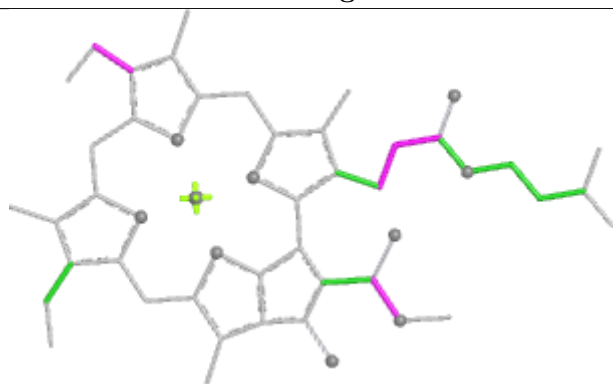
Ligand CLA L 204



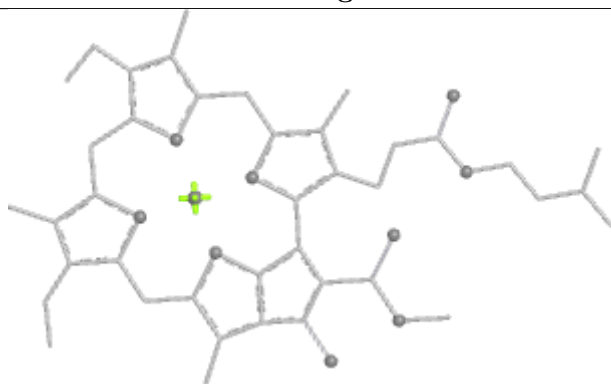
Bond lengths



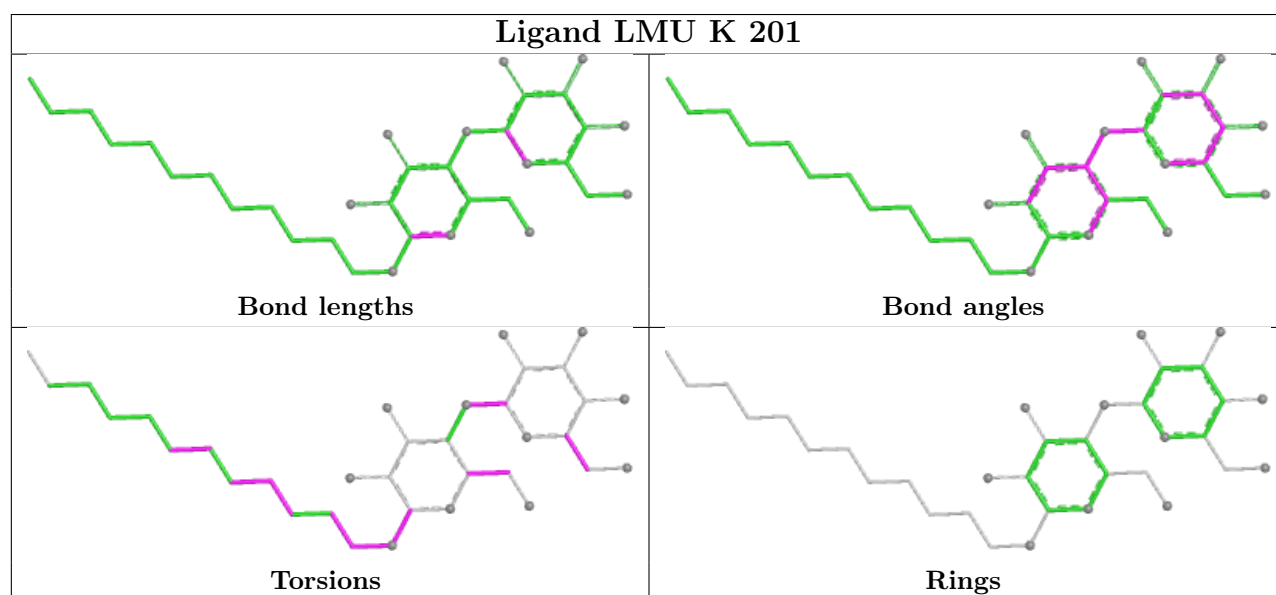
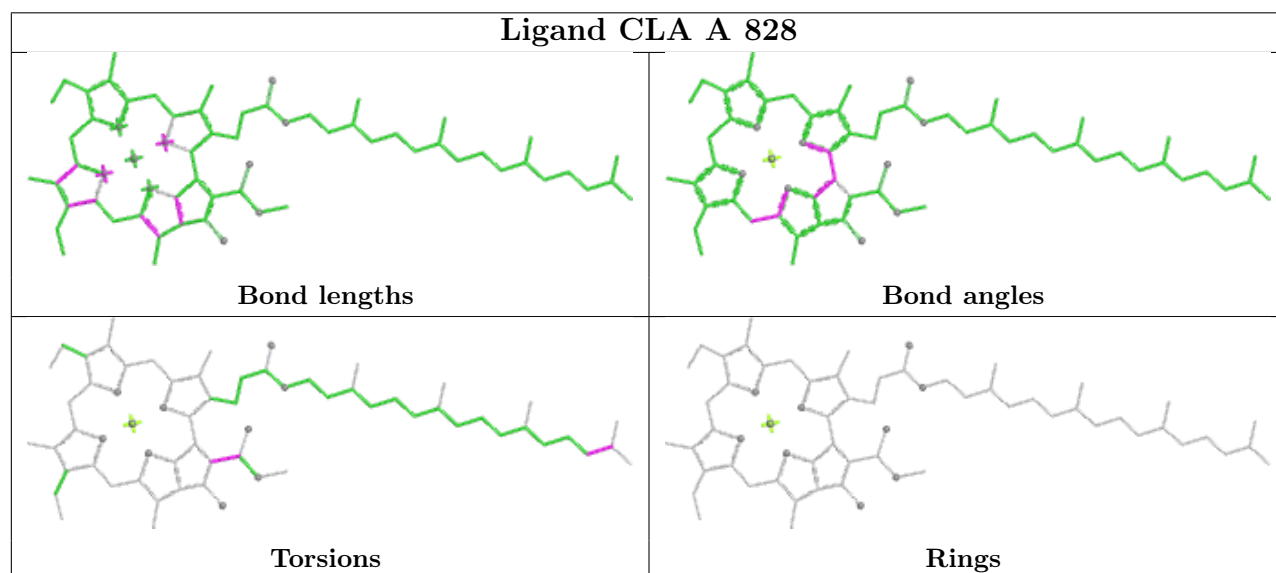
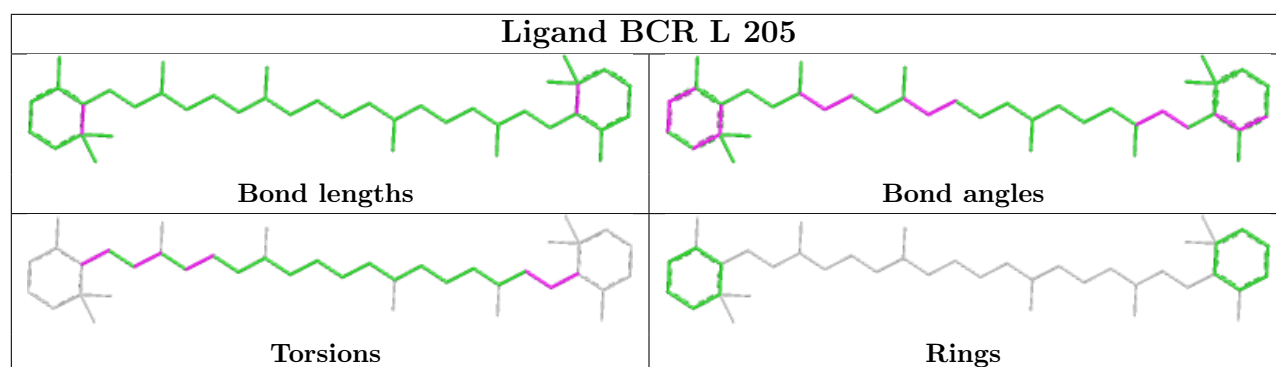
Bond angles

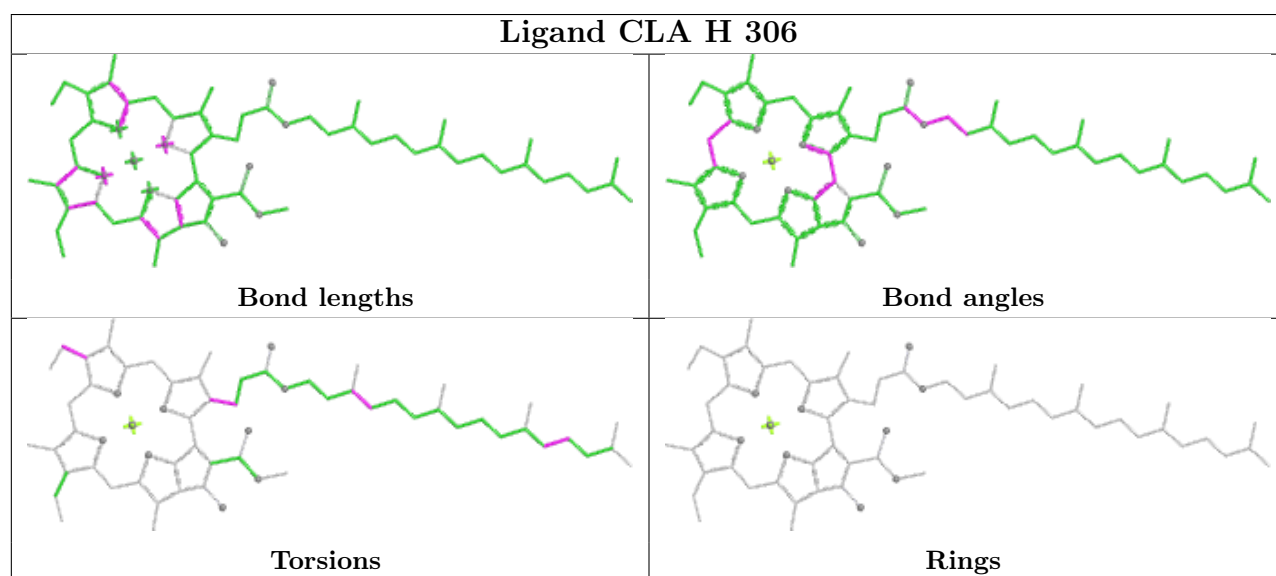
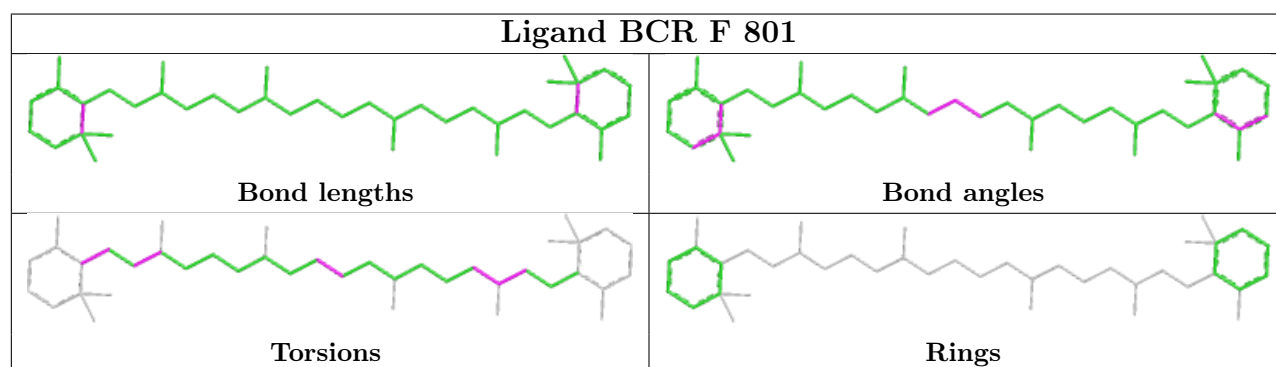
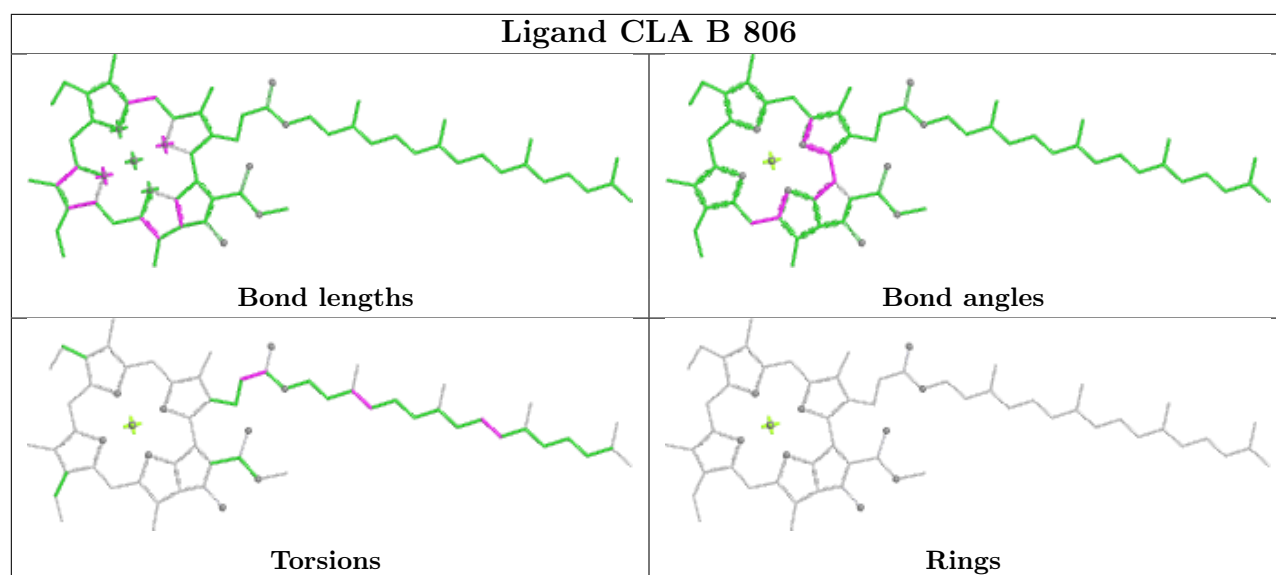


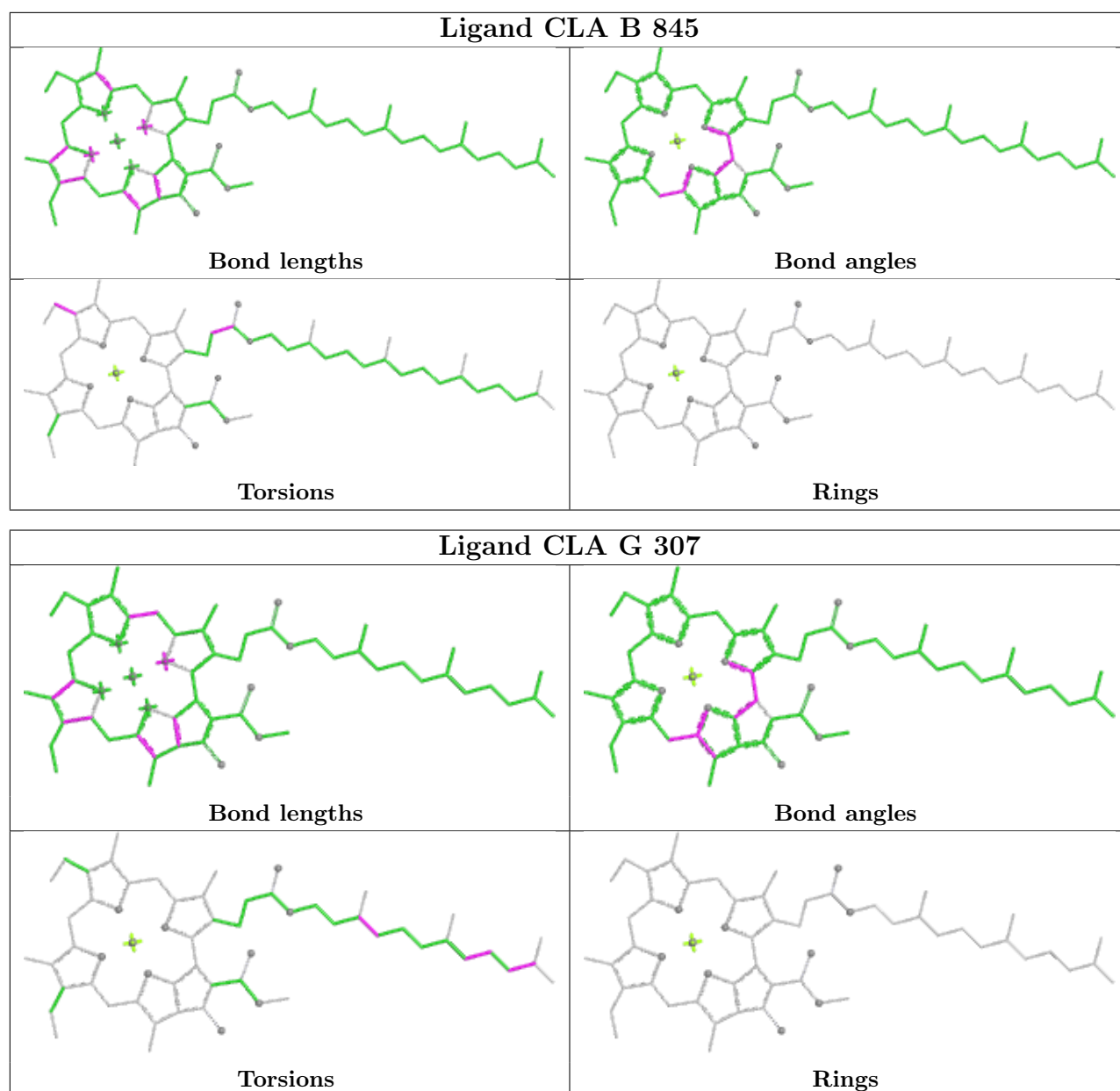
Torsions

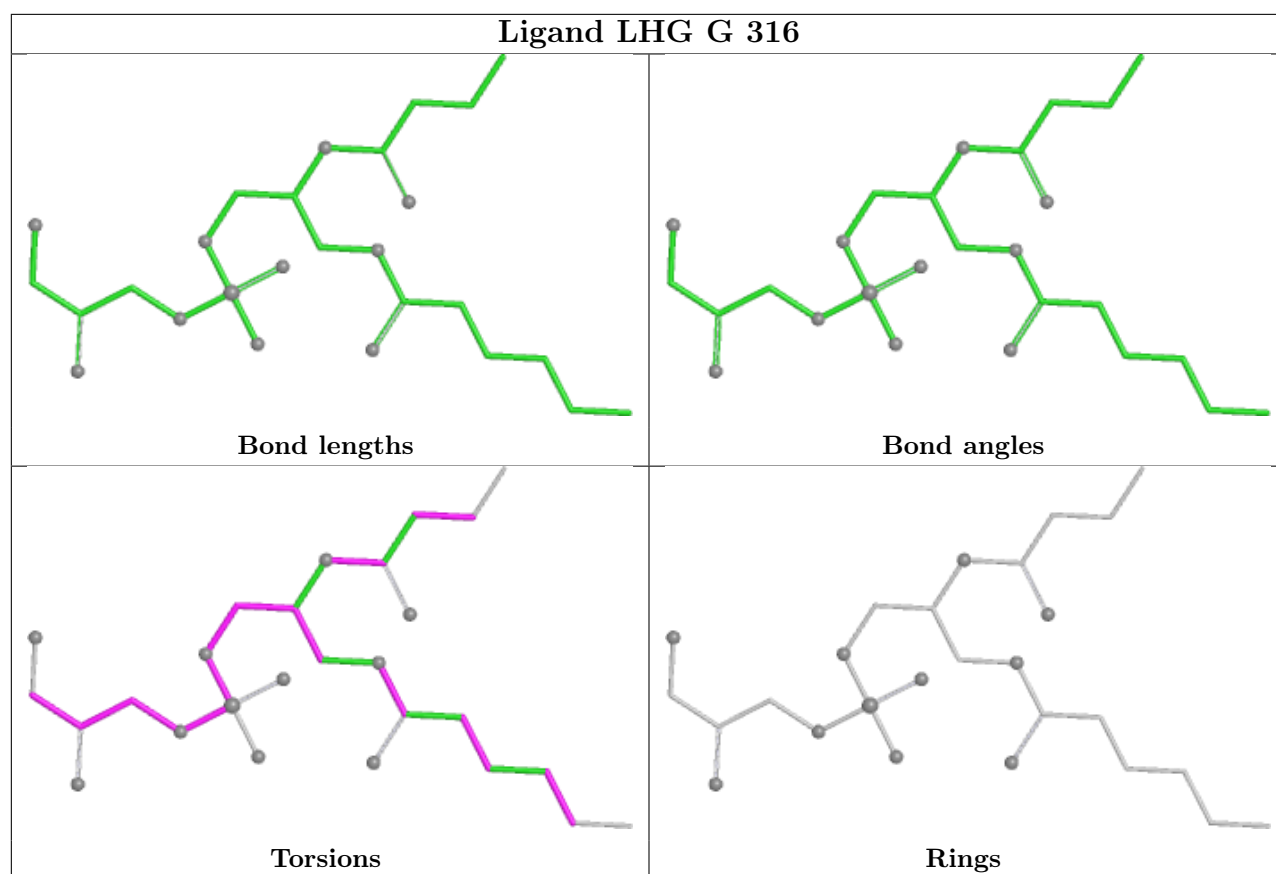


Rings









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.

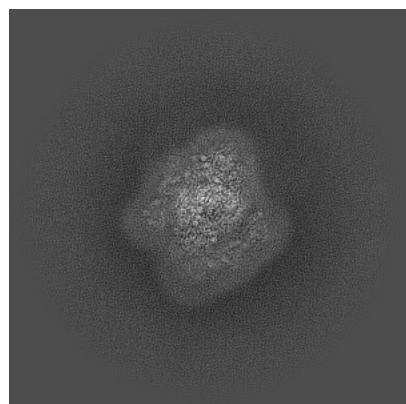
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-64154. These allow visual inspection of the internal detail of the map and identification of artifacts.

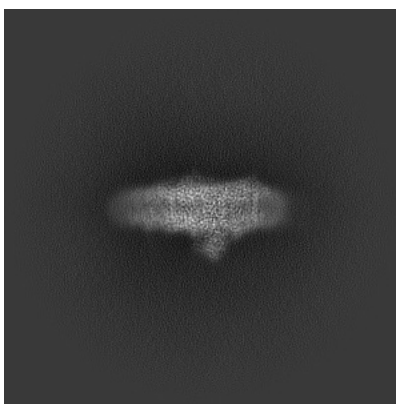
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

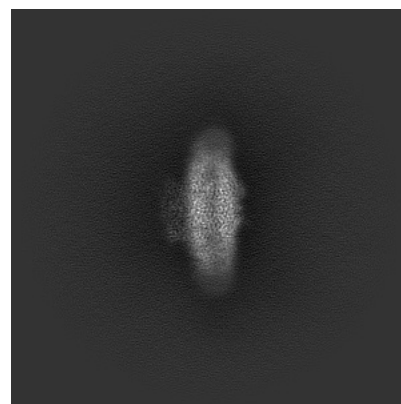
6.1.1 Primary map



X

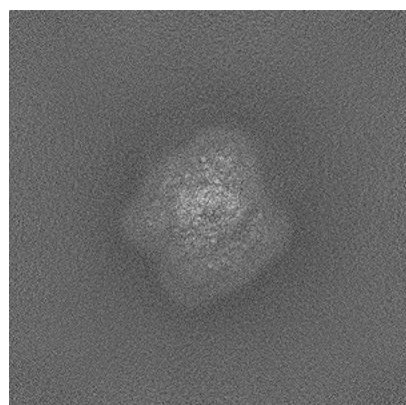


Y

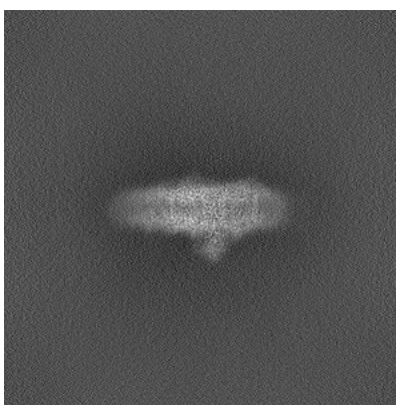


Z

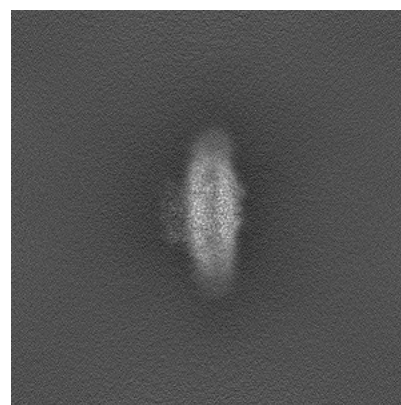
6.1.2 Raw map



X



Y

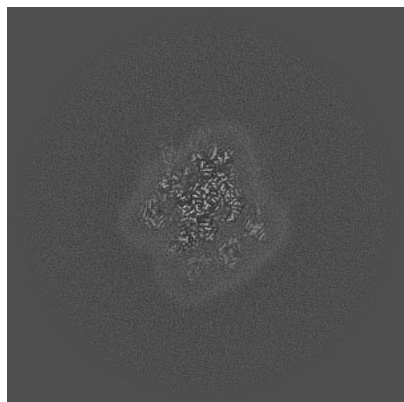


Z

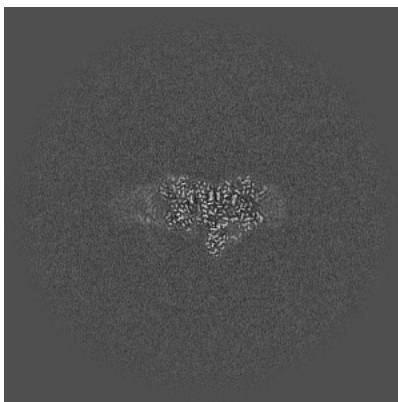
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

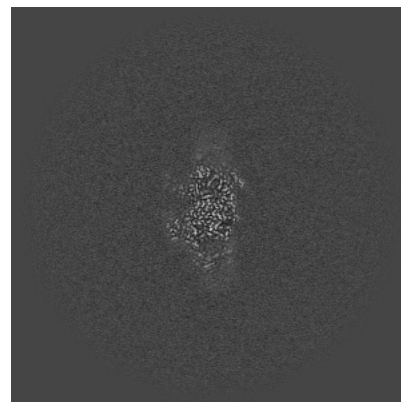
6.2.1 Primary map



X Index: 300

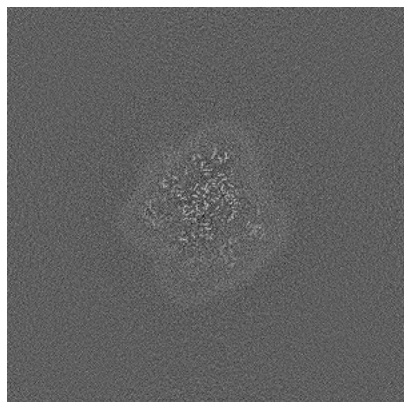


Y Index: 300

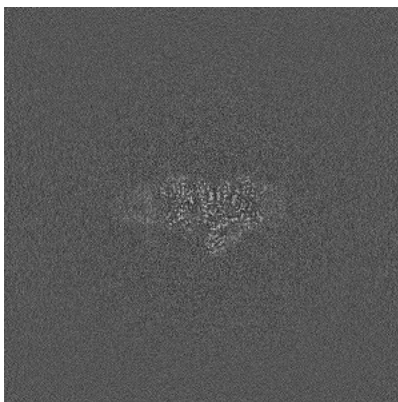


Z Index: 300

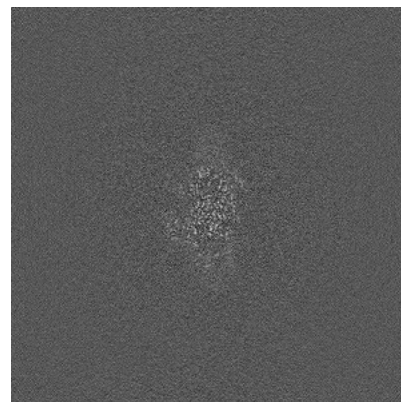
6.2.2 Raw map



X Index: 300



Y Index: 300

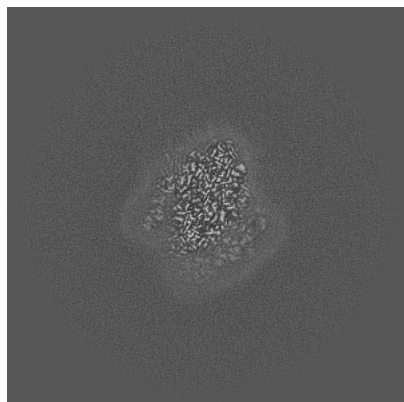


Z Index: 300

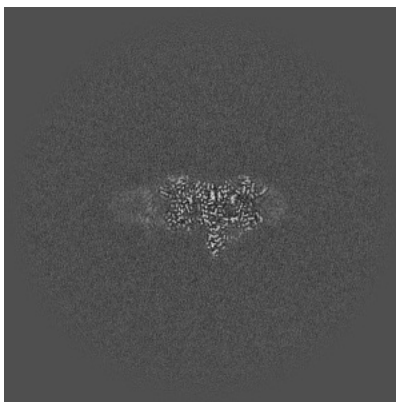
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

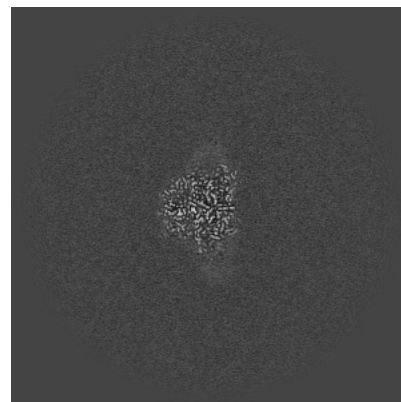
6.3.1 Primary map



X Index: 316

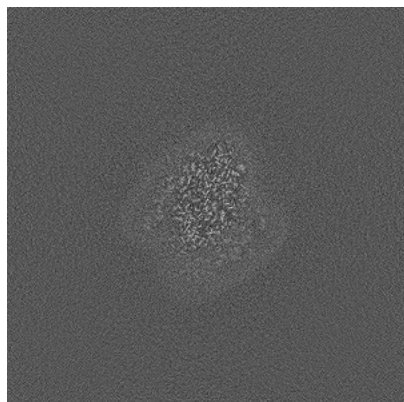


Y Index: 301

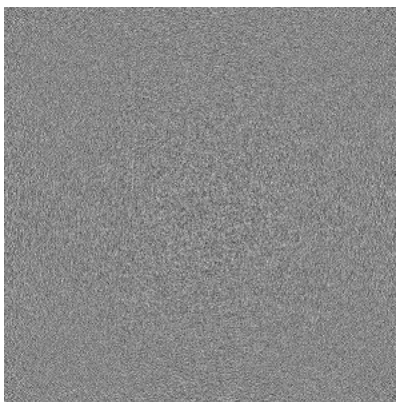


Z Index: 316

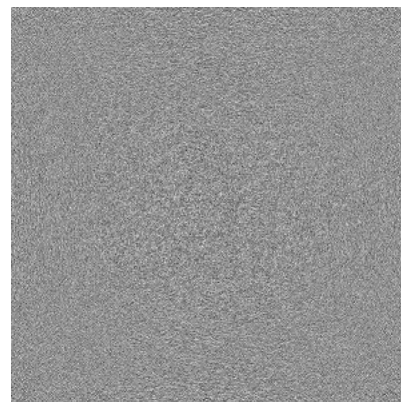
6.3.2 Raw map



X Index: 316



Y Index: 0

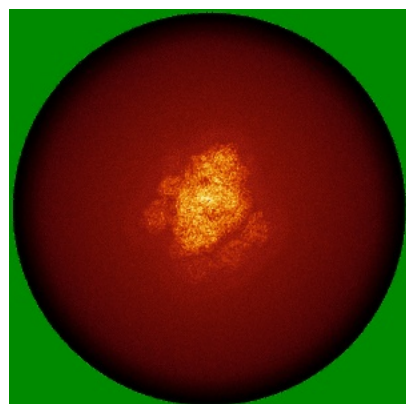


Z Index: 599

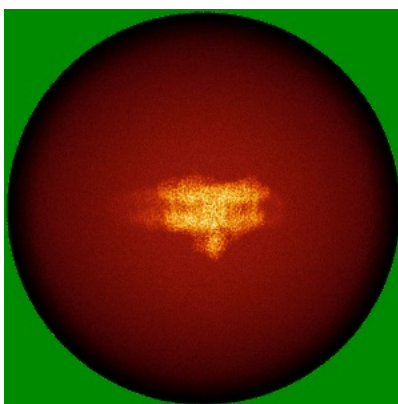
The images above show the largest variance slices of the map in three orthogonal directions.

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

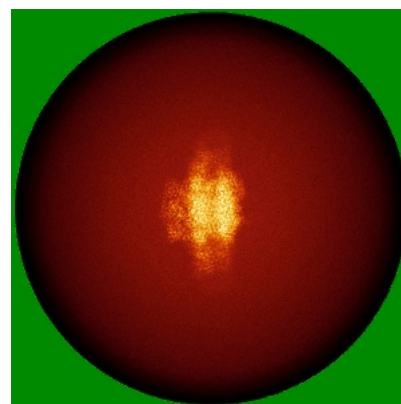
6.4.1 Primary map



X

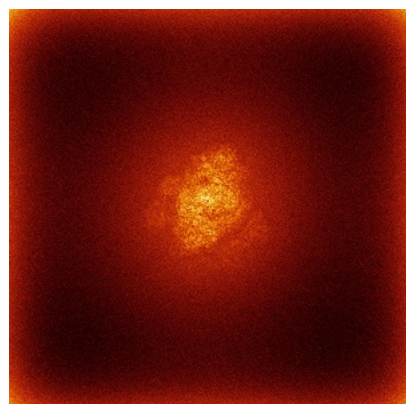


Y

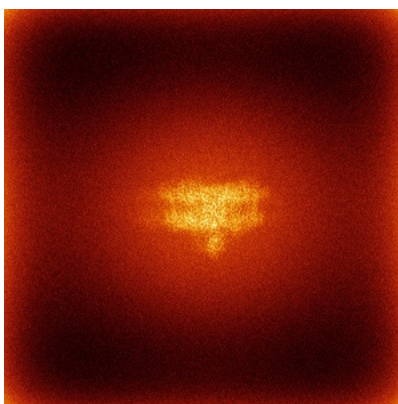


Z

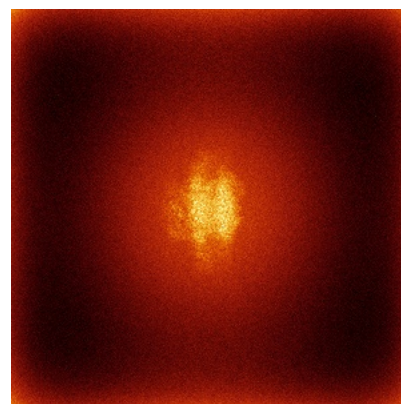
6.4.2 Raw map



X



Y

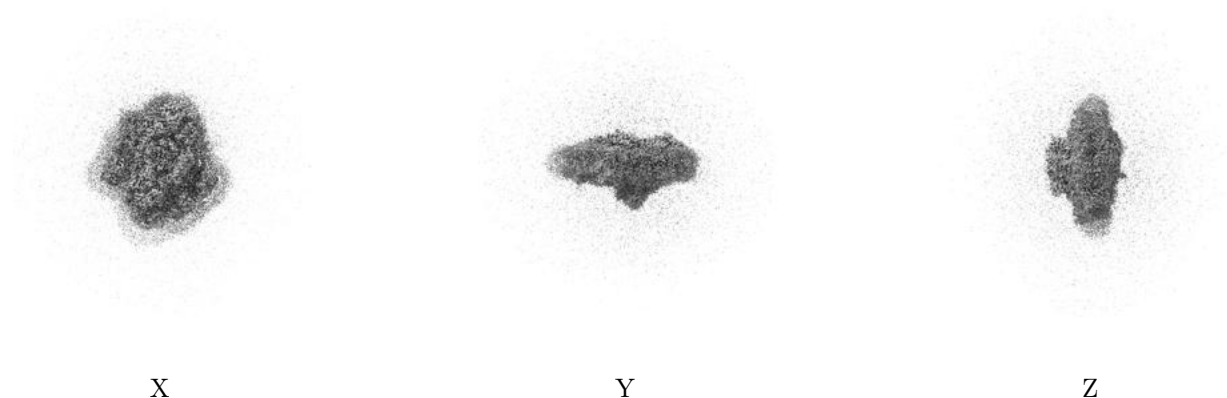


Z

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

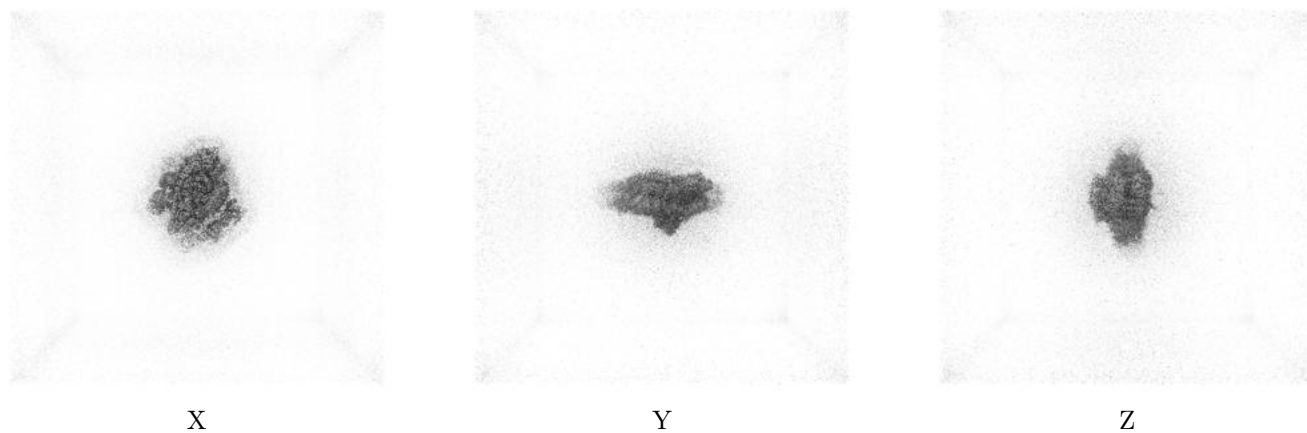
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.065. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

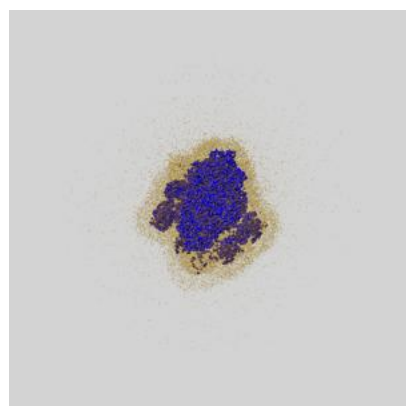
6.6 Mask visualisation [i](#)

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

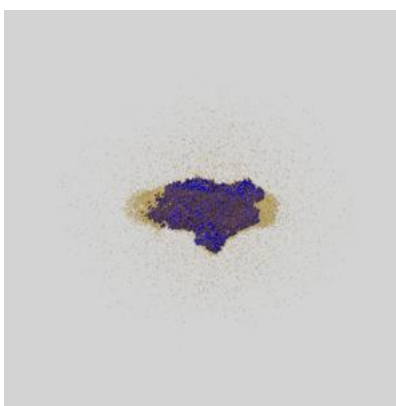
A mask typically either:

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

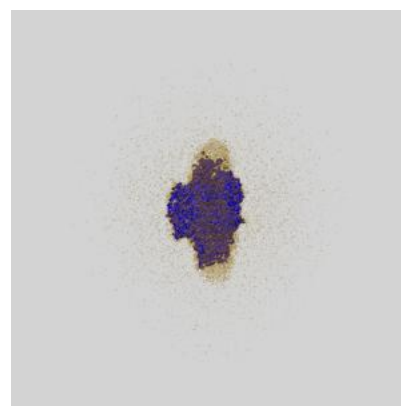
6.6.1 emd_64154_msk_1.map [i](#)



X



Y

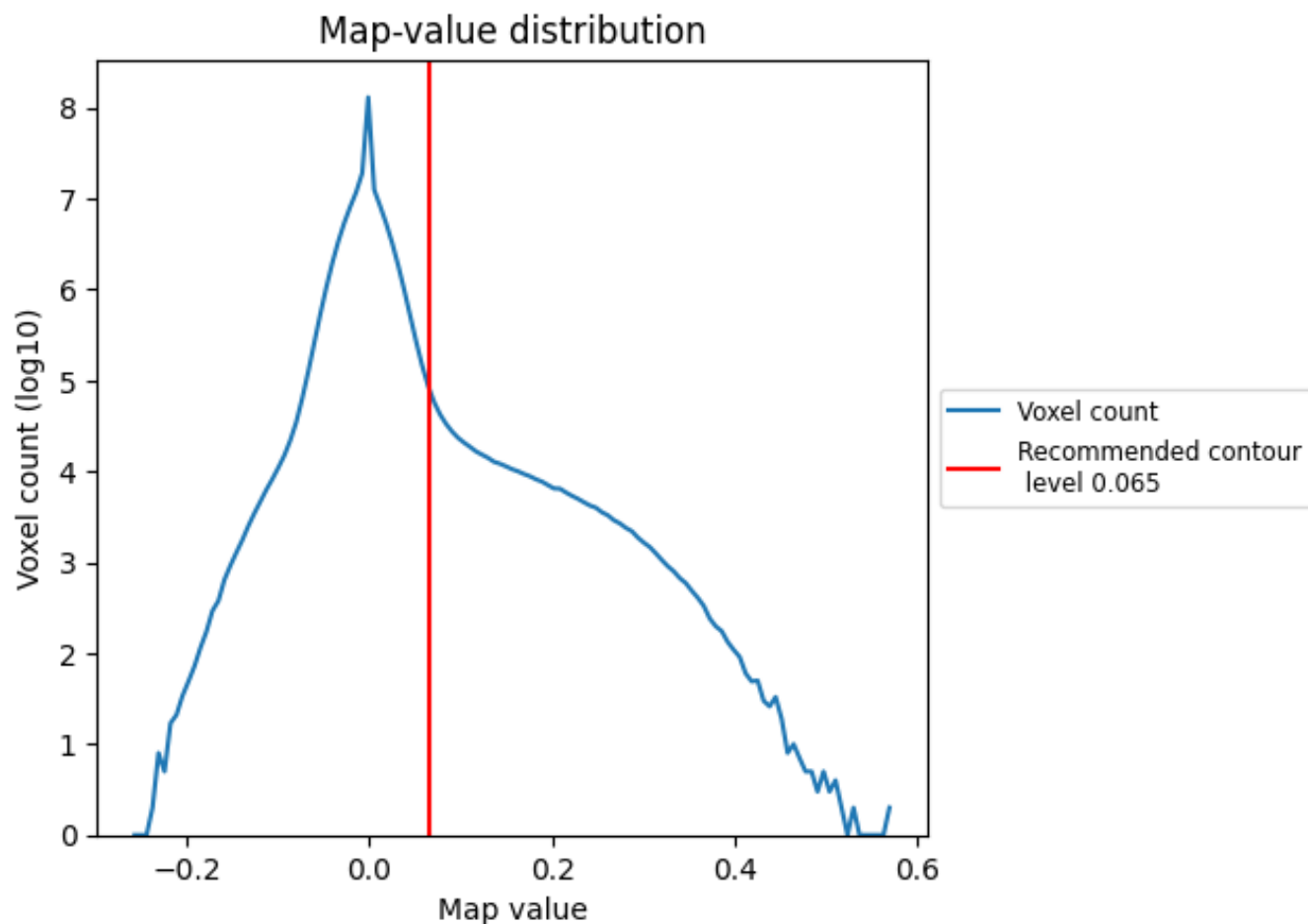


Z

7 Map analysis [i](#)

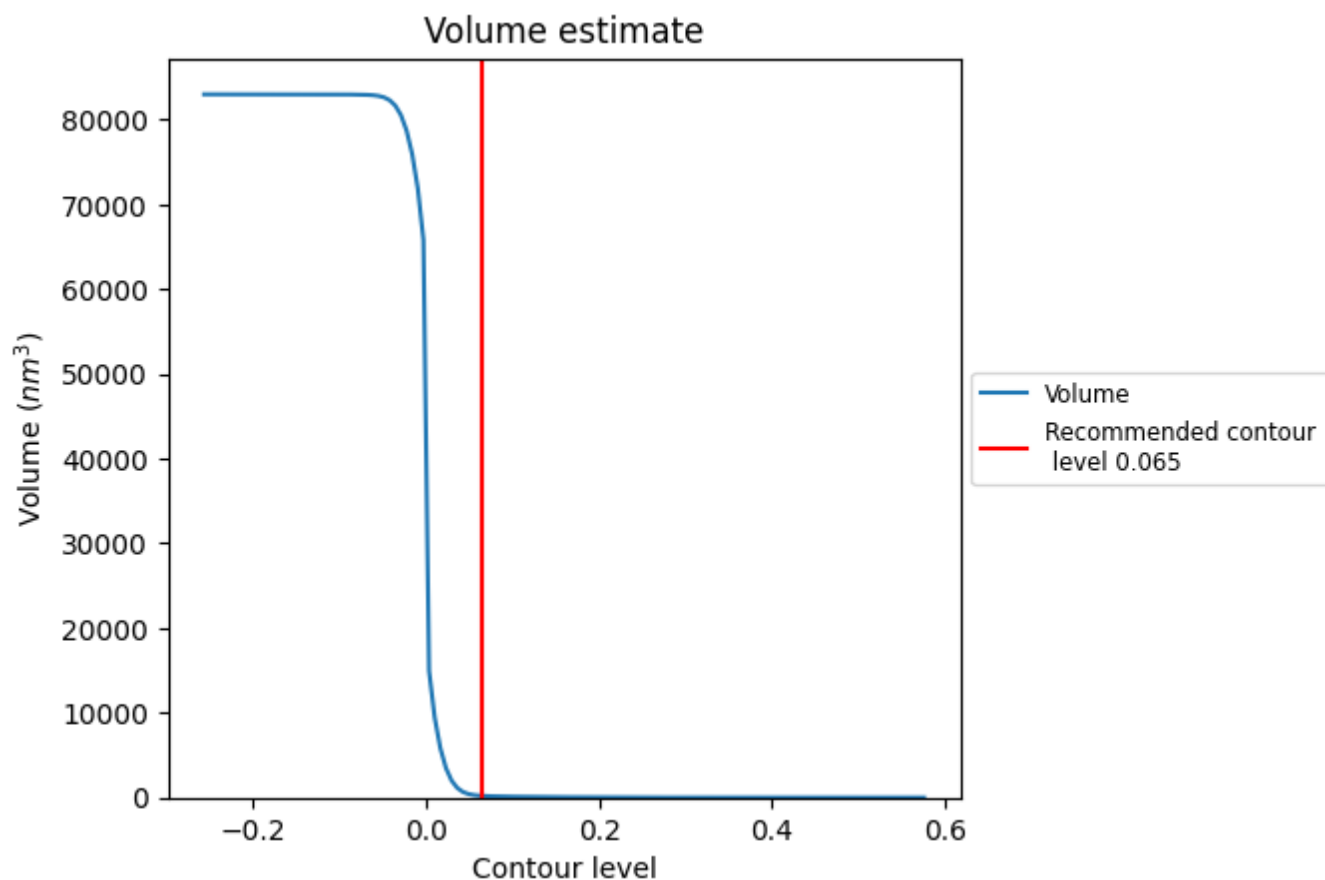
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

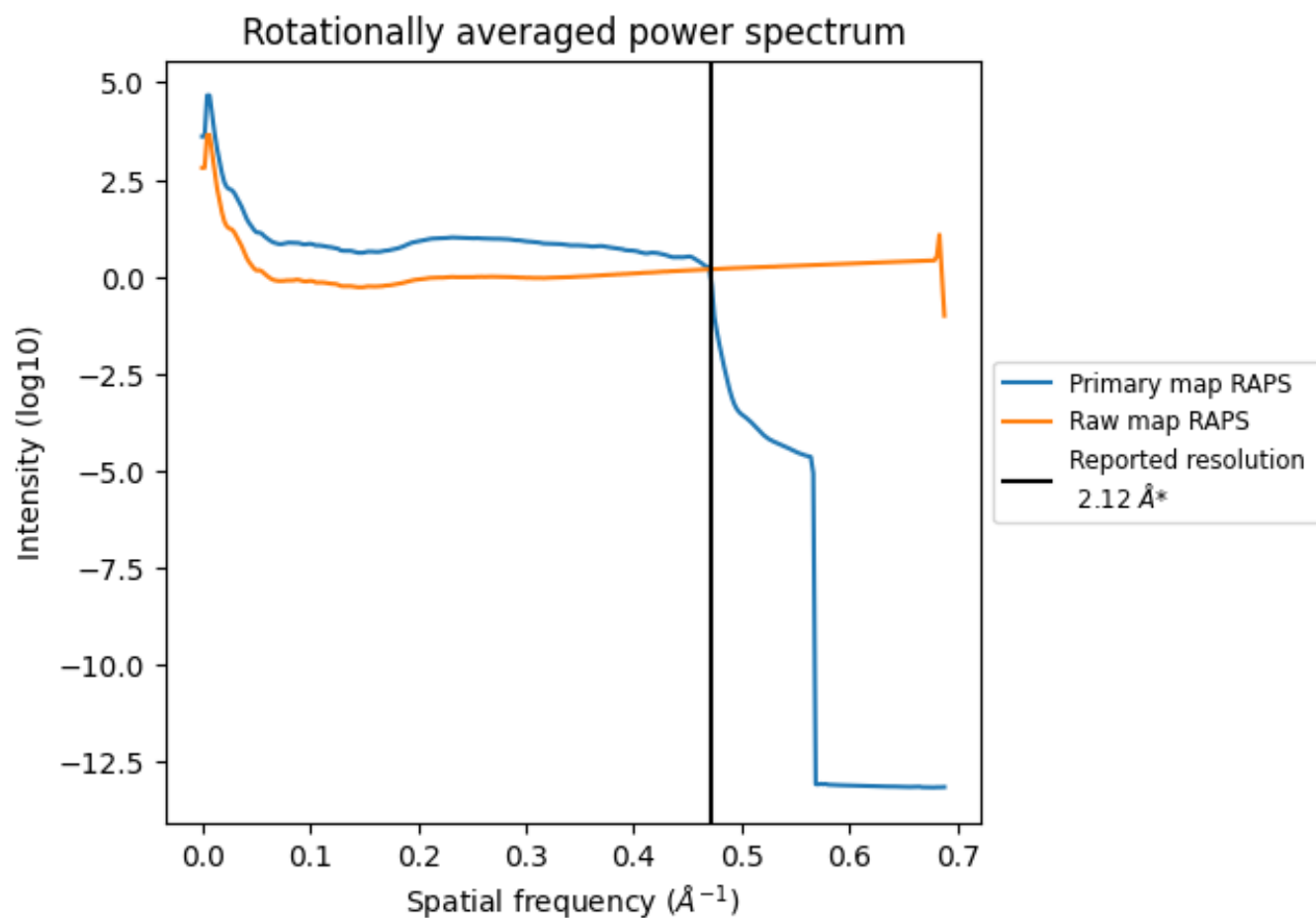
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 203 nm³; this corresponds to an approximate mass of 183 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 ⓘ

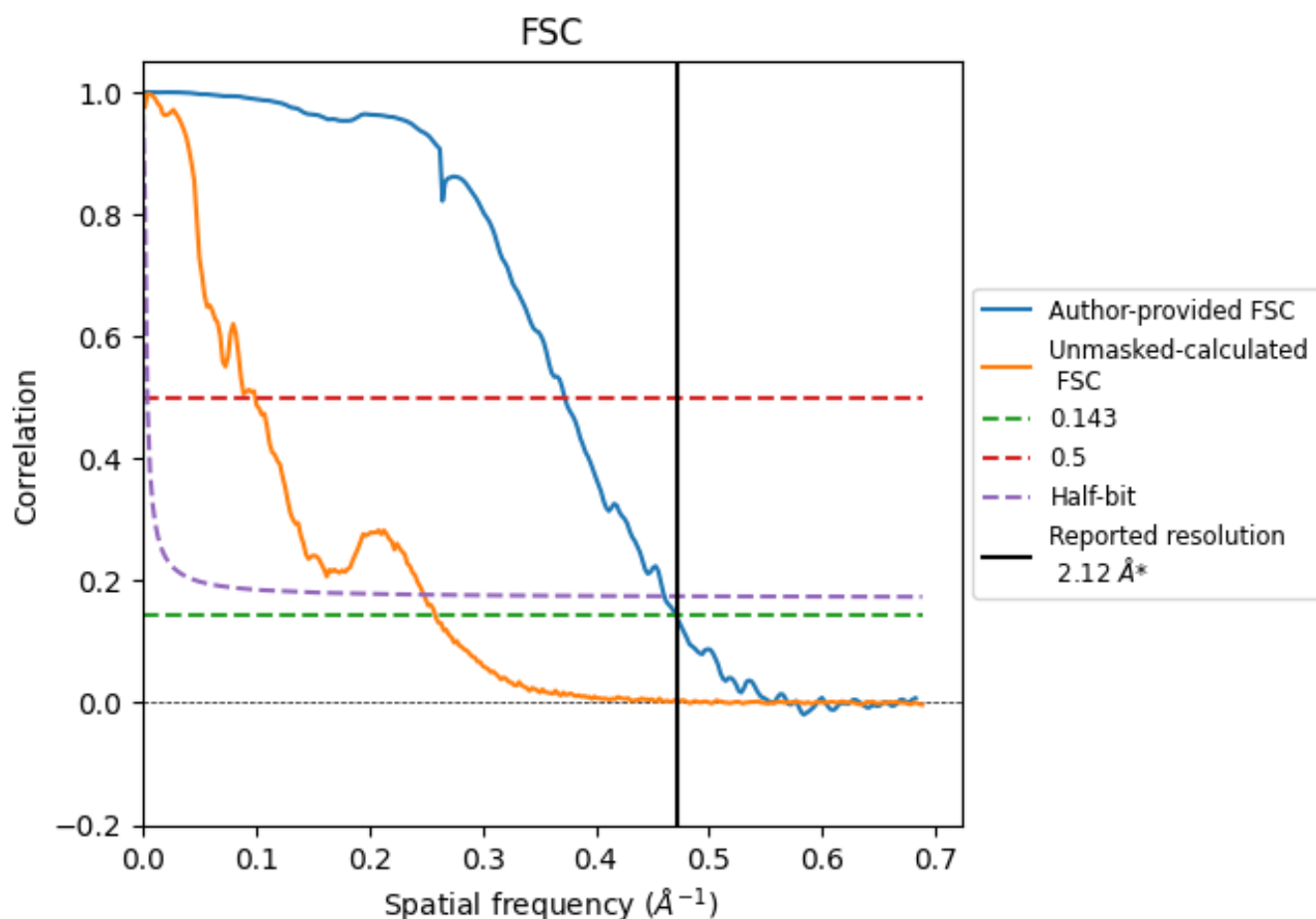


*Reported resolution corresponds to spatial frequency of 0.472 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.472 \AA^{-1}

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.12	-	-
Author-provided FSC curve	2.12	2.68	2.17
Unmasked-calculated*	3.87	10.04	4.03

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.87 differs from the reported value 2.12 by more than 10 %

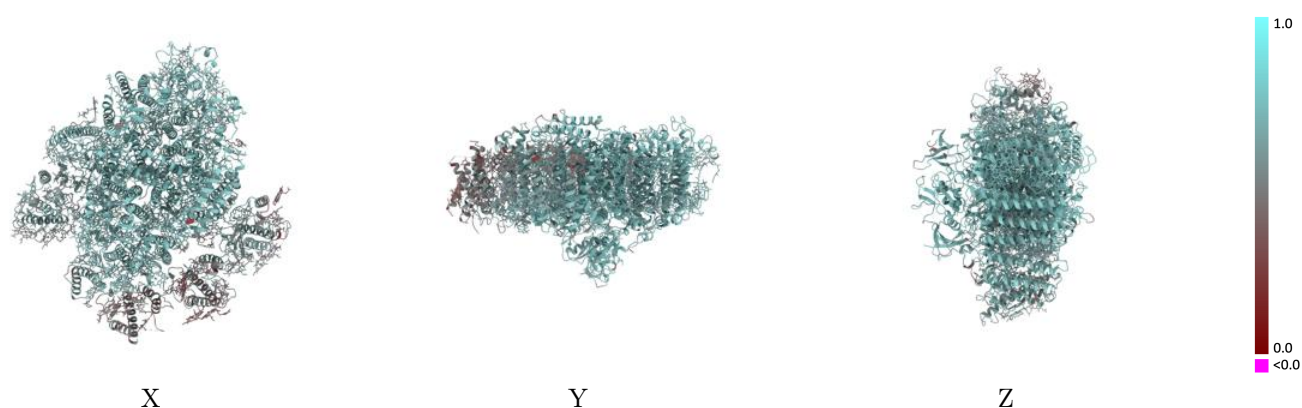
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-64154 and PDB model 9UH4. Per-residue inclusion information can be found in section 3 on page 25.

9.1 Map-model overlay [i](#)

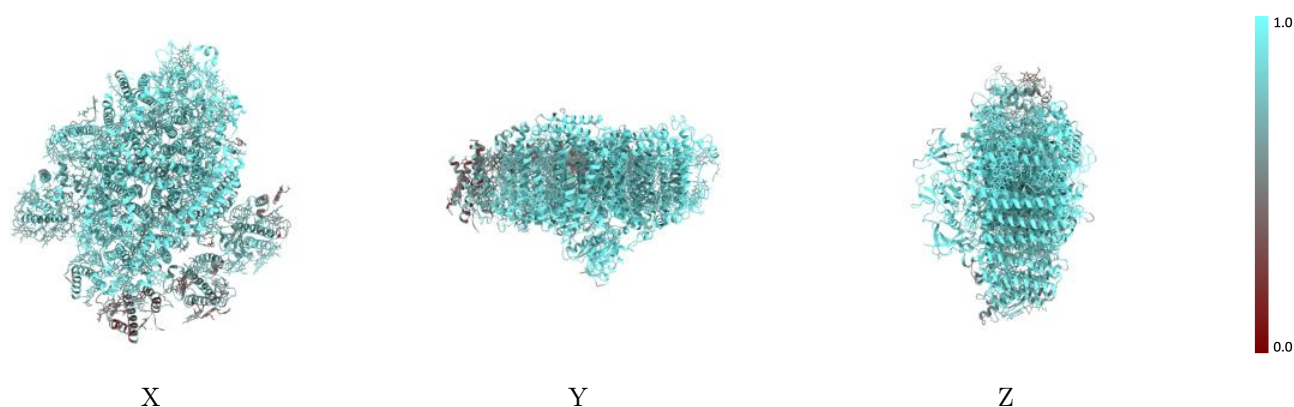
This section was not generated.

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



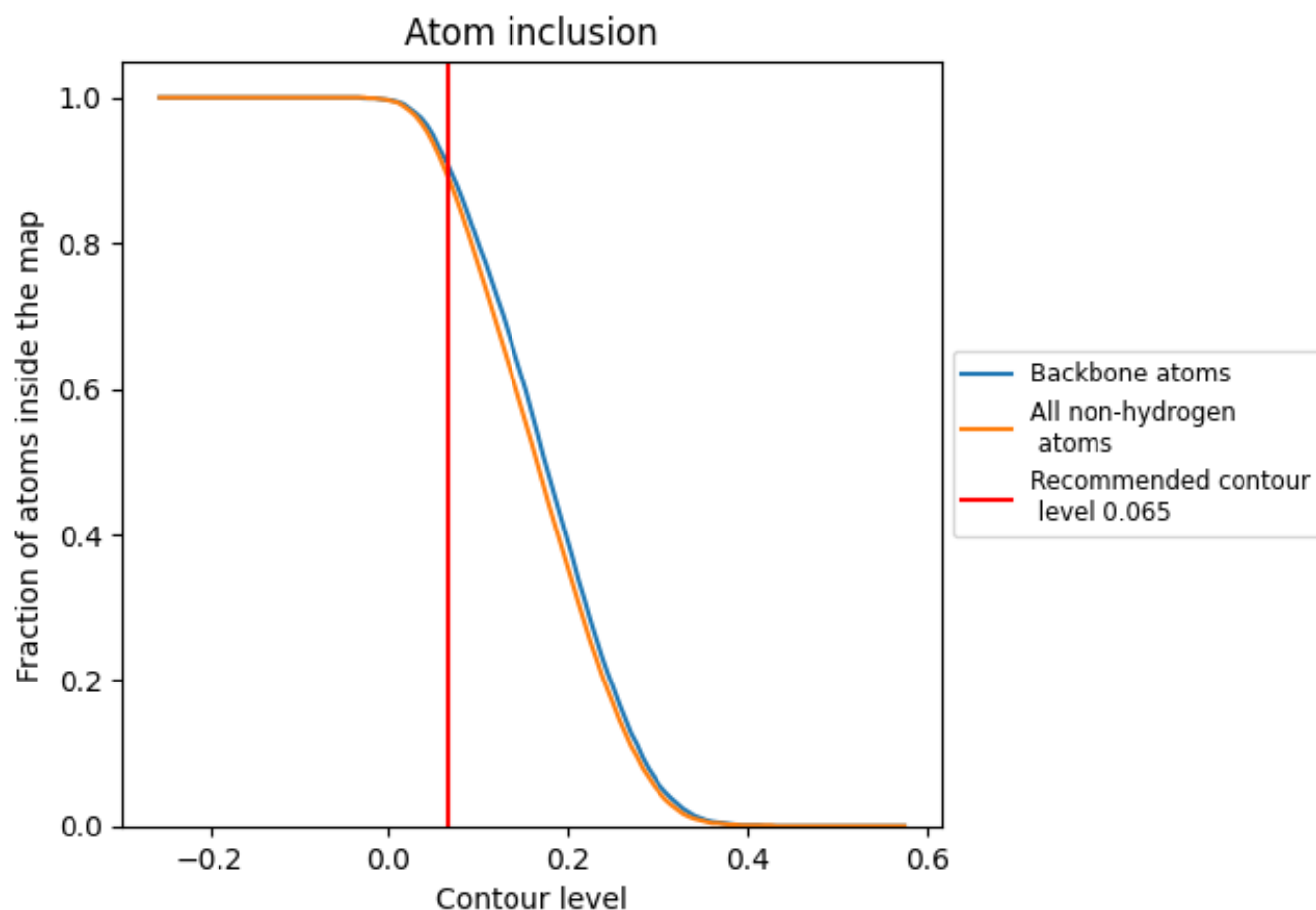
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.065).

9.4 Atom inclusion [i](#)



At the recommended contour level, 91% of all backbone atoms, 89% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.065) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.8940	<div></div> 0.6550
A	<div></div> 0.9570	<div></div> 0.7000
B	<div></div> 0.9570	<div></div> 0.7010
C	<div></div> 0.9900	<div></div> 0.7210
D	<div></div> 0.9360	<div></div> 0.6750
E	<div></div> 0.9000	<div></div> 0.6590
F	<div></div> 0.9220	<div></div> 0.6710
G	<div></div> 0.7640	<div></div> 0.5610
H	<div></div> 0.6770	<div></div> 0.4970
I	<div></div> 0.8820	<div></div> 0.6410
J	<div></div> 0.9190	<div></div> 0.6580
K	<div></div> 0.4990	<div></div> 0.4400
L	<div></div> 0.9070	<div></div> 0.6540
M	<div></div> 0.9130	<div></div> 0.6530
U	<div></div> 0.7940	<div></div> 0.5820
k	<div></div> 0.7610	<div></div> 0.5750

1.0

0.0

<0.0