



Full wwPDB EM Validation Report ⓘ

Apr 6, 2026 – 03:57 AM UTC

PDB ID : 9UNU / pdb_00009unu
EMDB ID : EMD-64362
Title : PSI-1 FCPI supercomplex from haptophyte *Chrysotila roscoffensis*
Authors : La Rocca, R.; Tsai, P.-C.; Kato, K.; Nakajima, Y.; Akita, F.; Shen, J.-R.
Deposited on : 2025-04-24
Resolution : 2.18 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:

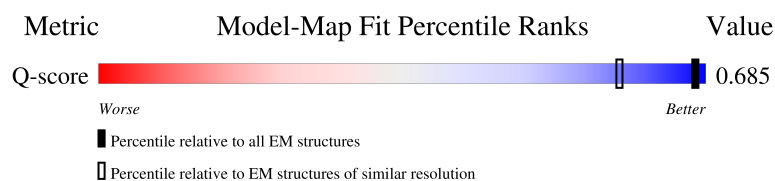
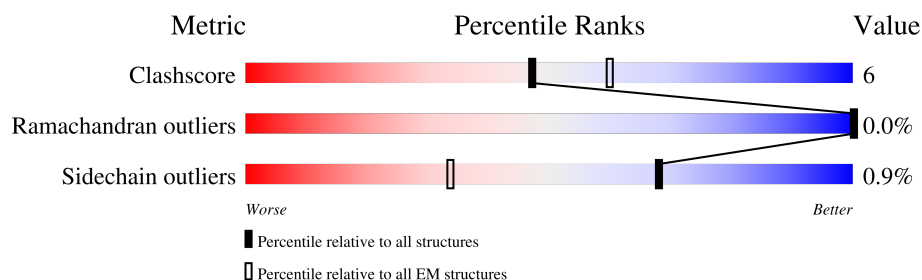
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 2.18 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	2701 (1.70 - 2.68)

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	 89% 9% .
2	B	734	 90% 9%
3	C	81	 90% 9% .
4	D	142	 9% 89% 8% . .

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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	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
12	CLA	A	802	X	-	-	-
12	CLA	A	803	X	-	-	-
12	CLA	A	804	X	-	-	-
12	CLA	A	805	X	-	-	-
12	CLA	A	808	X	-	-	-
12	CLA	A	810	X	-	-	-
12	CLA	A	811	X	-	-	-
12	CLA	A	812	X	-	-	-
12	CLA	A	815	X	-	-	-
12	CLA	A	816	X	-	-	-
12	CLA	A	817	X	-	-	-
12	CLA	A	818	X	-	-	-
12	CLA	A	820	X	-	-	-
12	CLA	A	821	X	-	-	-
12	CLA	A	822	X	-	-	-
12	CLA	A	823	X	-	-	-
12	CLA	A	824	X	-	-	-
12	CLA	A	828	X	-	-	-
12	CLA	A	829	X	-	-	-
12	CLA	A	831	X	-	-	-
12	CLA	A	832	X	-	-	-
12	CLA	A	833	X	-	-	-
12	CLA	A	834	X	-	-	-
12	CLA	A	835	X	-	-	-
12	CLA	A	836	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
12	CLA	A	844	X	-	-	-
12	CLA	A	850	X	-	-	-
12	CLA	A	852	X	-	-	-
12	CLA	B	801	X	-	-	-
12	CLA	B	802	X	-	-	-
12	CLA	B	803	X	-	-	-
12	CLA	B	804	X	-	-	-
12	CLA	B	805	X	-	-	-
12	CLA	B	806	X	-	-	-
12	CLA	B	807	X	-	-	-
12	CLA	B	808	X	-	-	-
12	CLA	B	809	X	-	-	-
12	CLA	B	811	X	-	-	-
12	CLA	B	815	X	-	-	-
12	CLA	B	816	X	-	-	-
12	CLA	B	817	X	-	-	-
12	CLA	B	820	X	-	-	-
12	CLA	B	821	X	-	-	-
12	CLA	B	822	X	-	-	-
12	CLA	B	823	X	-	-	-
12	CLA	B	827	X	-	-	-
12	CLA	B	829	X	-	-	-
12	CLA	B	830	X	-	-	-
12	CLA	B	831	X	-	-	-
12	CLA	B	832	X	-	-	-
12	CLA	B	833	X	-	-	-
12	CLA	B	835	X	-	-	-
12	CLA	B	843	X	-	-	-
12	CLA	B	844	X	-	-	-
12	CLA	B	845	X	-	-	-
12	CLA	B	846	X	-	-	-
12	CLA	B	848	X	-	-	-
12	CLA	F	802	X	-	-	-
12	CLA	F	803	X	-	-	-
12	CLA	J	103	X	-	-	-
12	CLA	L	202	X	-	-	-
12	CLA	L	204	X	-	-	-
12	CLA	U	201	X	-	-	-
12	CLA	U	205	X	-	-	-
12	CLA	U	206	X	-	-	-
12	CLA	U	207	X	-	-	-
12	CLA	U	209	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
12	CLA	U	210	X	-	-	-
12	CLA	U	212	X	-	-	-
16	CL0	A	847	X	-	-	-

2 Entry composition [i](#)

There are 23 unique types of molecules in this entry. The entry contains 25464 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		

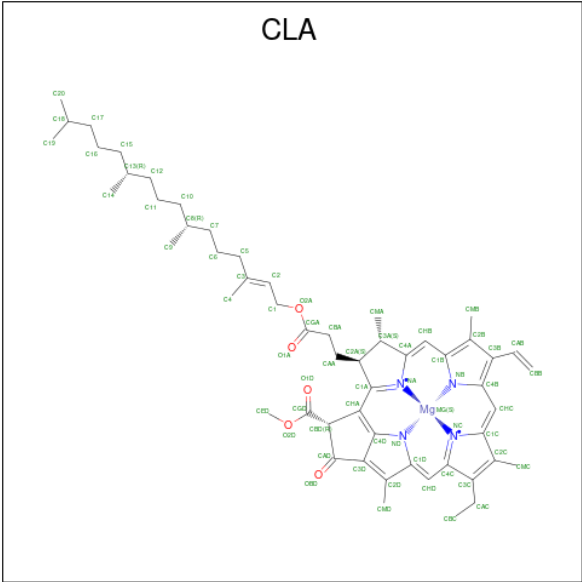
- Molecule 10 is a protein called Photosystem I reaction center subunit XII (psaM).

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



Mol	Chain	Residues	Atoms					AltConf
12	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
12	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	A	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
12	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	A	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
12	A	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
12	A	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
12	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
12	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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

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Mol	Chain	Residues	Atoms					AltConf
12	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	A	1	Total 60	C 50	Mg 1	N 4	O 5	0
12	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
12	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	B	1	Total 54	C 44	Mg 1	N 4	O 5	0
12	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
12	B	1	Total 54	C 44	Mg 1	N 4	O 5	0
12	B	1	Total 59	C 49	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
12	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
12	B	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
12	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
12	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	B	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
12	B	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
12	B	1	Total	C	Mg	N	O	0
			63	53	1	4	5	
12	B	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
12	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
12	B	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
12	B	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
12	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	B	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
12	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	B	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
12	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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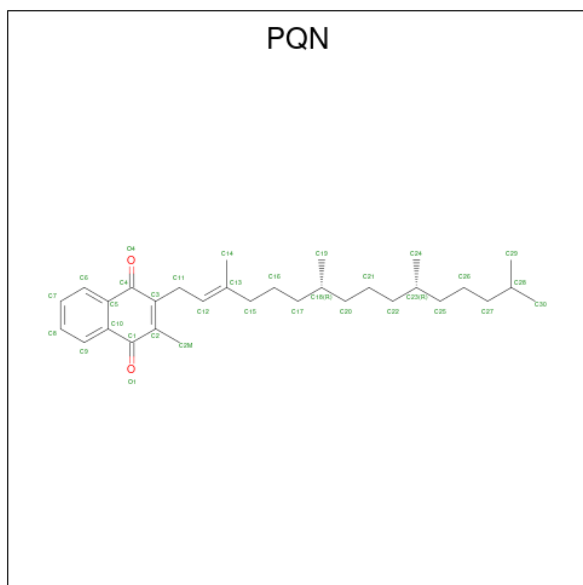
Mol	Chain	Residues	Atoms					AltConf
12	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	B	1	Total 50	C 40	Mg 1	N 4	O 5	0
12	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
12	F	1	Total 48	C 38	Mg 1	N 4	O 5	0
12	F	1	Total 46	C 36	Mg 1	N 4	O 5	0
12	J	1	Total 42	C 34	Mg 1	N 4	O 3	0
12	L	1	Total 49	C 39	Mg 1	N 4	O 5	0
12	L	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	L	1	Total 50	C 40	Mg 1	N 4	O 5	0
12	U	1	Total 52	C 42	Mg 1	N 4	O 5	0
12	U	1	Total 61	C 51	Mg 1	N 4	O 5	0
12	U	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	U	1	Total 45	C 35	Mg 1	N 4	O 5	0
12	U	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	U	1	Total 46	C 36	Mg 1	N 4	O 5	0
12	U	1	Total 42	C 34	Mg 1	N 4	O 3	0
12	U	1	Total 65	C 55	Mg 1	N 4	O 5	0

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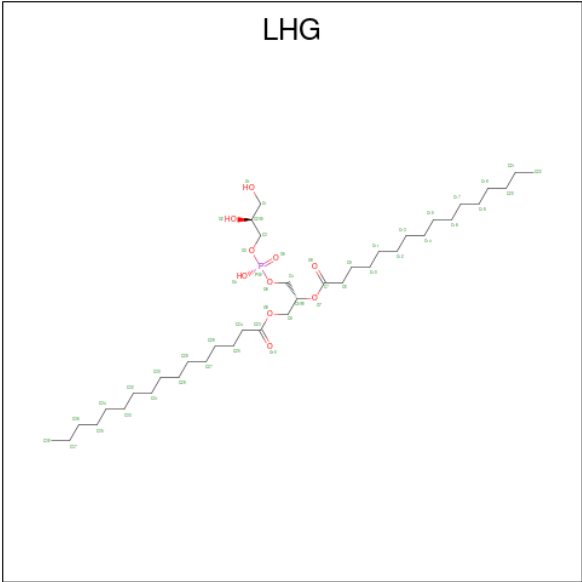
Mol	Chain	Residues	Atoms					AltConf
12	U	1	Total	C	Mg	N	O	0
			52	42	1	4	5	

- Molecule 13 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$) (labeled as "Ligand of Interest" by depositor).



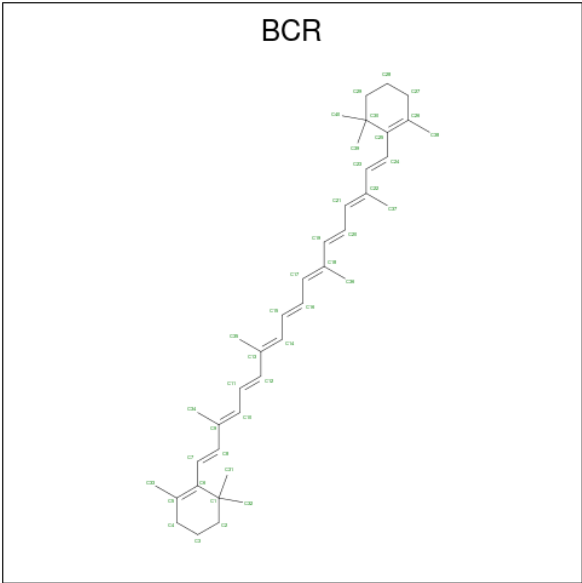
Mol	Chain	Residues	Atoms			AltConf
13	A	1	Total	C	O	0
			33	31	2	
13	B	1	Total	C	O	0
			33	31	2	

- Molecule 14 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
14	A	1	Total	C	O	P	0
			48	37	10	1	
14	A	1	Total	C	O	P	0
			27	16	10	1	

- Molecule 15 is BETA-CAROTENE (CCD ID: BCR) (formula: C₄₀H₅₆).



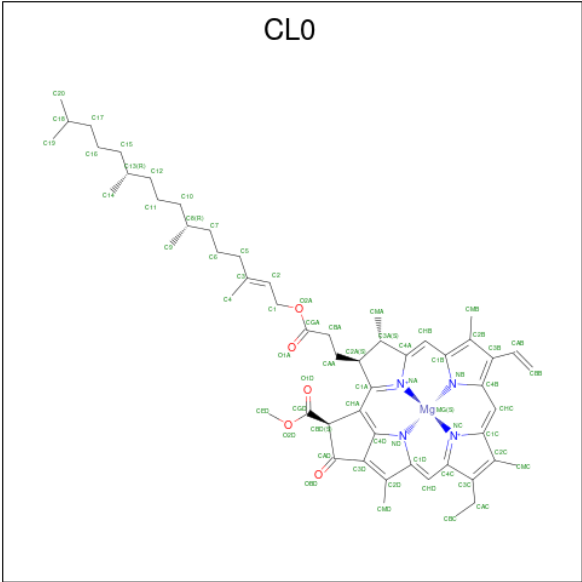
Mol	Chain	Residues	Atoms		AltConf
15	A	1	Total	C	0
			40	40	
15	A	1	Total	C	0
			40	40	

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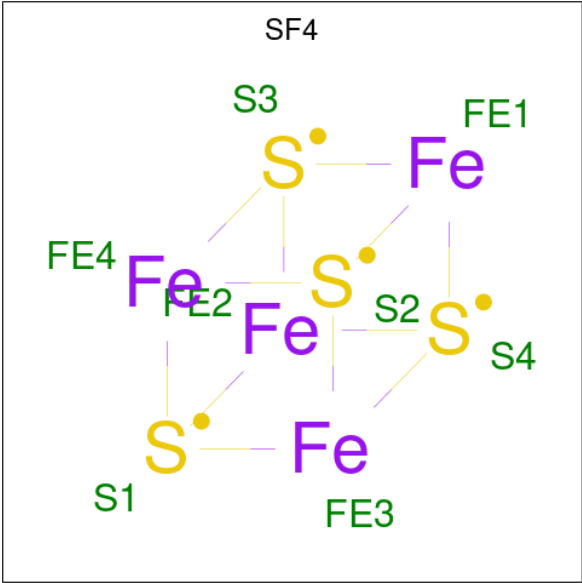
Mol	Chain	Residues	Atoms	AltConf
15	A	1	Total C 40 40	0
15	A	1	Total C 40 40	0
15	B	1	Total C 40 40	0
15	B	1	Total C 40 40	0
15	B	1	Total C 40 40	0
15	B	1	Total C 40 40	0
15	B	1	Total C 40 40	0
15	F	1	Total C 40 40	0
15	F	1	Total C 40 40	0
15	I	1	Total C 40 40	0
15	I	1	Total C 40 40	0
15	J	1	Total C 40 40	0
15	L	1	Total C 40 40	0
15	L	1	Total C 40 40	0
15	M	1	Total C 40 40	0

- Molecule 16 is CHLOROPHYLL A ISOMER (CCD ID: CL0) (formula: $C_{55}H_{72}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 17 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄) (labeled as "Ligand of Interest" by depositor).



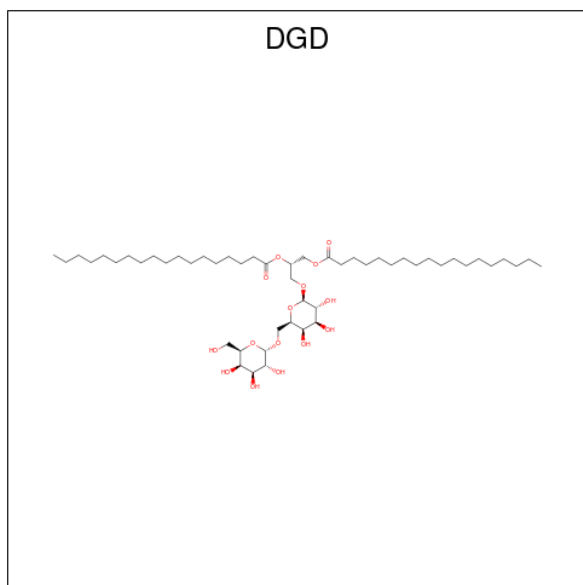
Mol	Chain	Residues	Atoms			AltConf
17	A	1	Total	Fe	S	0
			8	4	4	
17	C	1	Total	Fe	S	0
			8	4	4	

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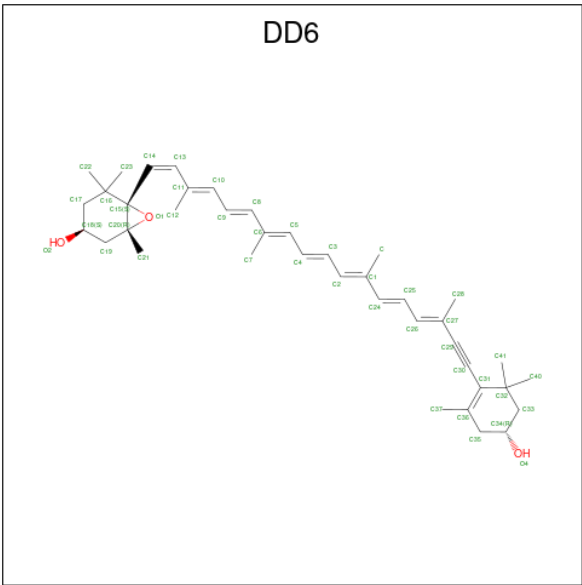
Mol	Chain	Residues	Atoms			AltConf
17	C	1	Total	Fe	S	0
			8	4	4	

- Molecule 18 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$) (labeled as "Ligand of Interest" by depositor).



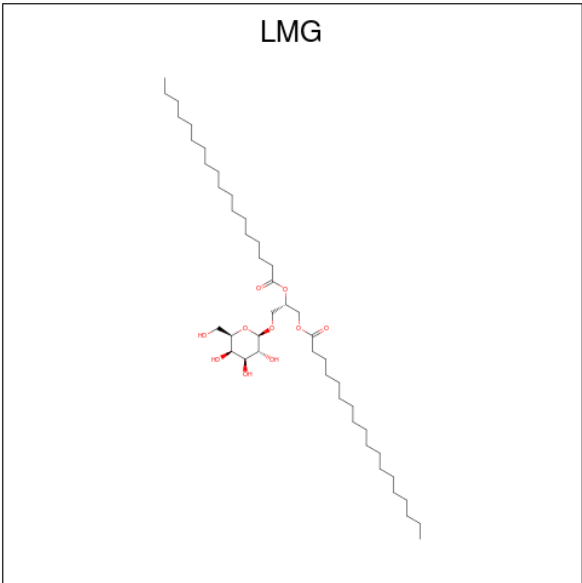
Mol	Chain	Residues	Atoms			AltConf
18	B	1	Total	C	O	0
			60	45	15	

- Molecule 19 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).



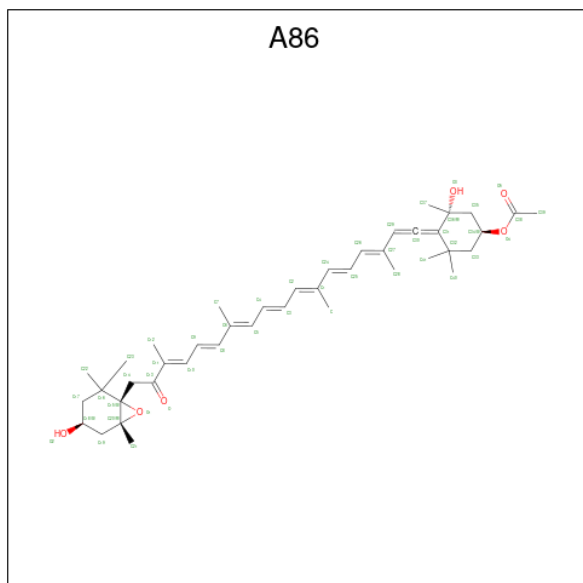
Mol	Chain	Residues	Atoms			AltConf
19	J	1	Total	C	O	0
			43	40	3	
19	U	1	Total	C	O	0
			43	40	3	
19	U	1	Total	C	O	0
			43	40	3	
19	U	1	Total	C	O	0
			26	25	1	

- Molecule 20 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: C₄₅H₈₆O₁₀) (labeled as "Ligand of Interest" by depositor).



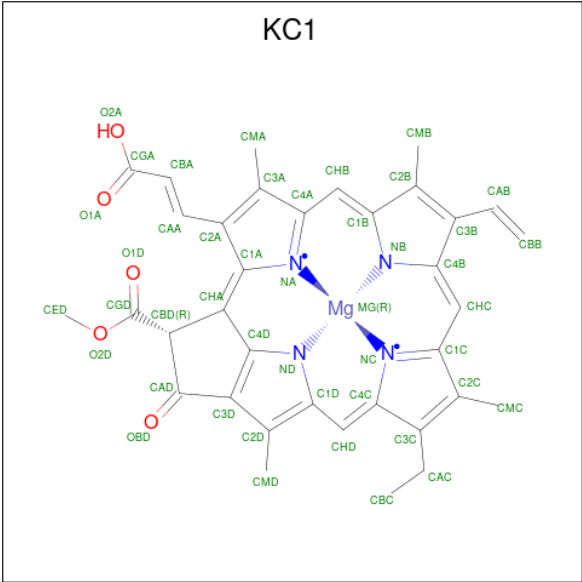
Mol	Chain	Residues	Atoms			AltConf
20	J	1	Total	C	O	0
			39	29	10	
20	U	1	Total	C	O	0
			32	22	10	

- Molecule 21 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: $C_{42}H_{58}O_6$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 22 is Chlorophyll c1 (CCD ID: KC1) (formula: $C_{35}H_{30}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



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

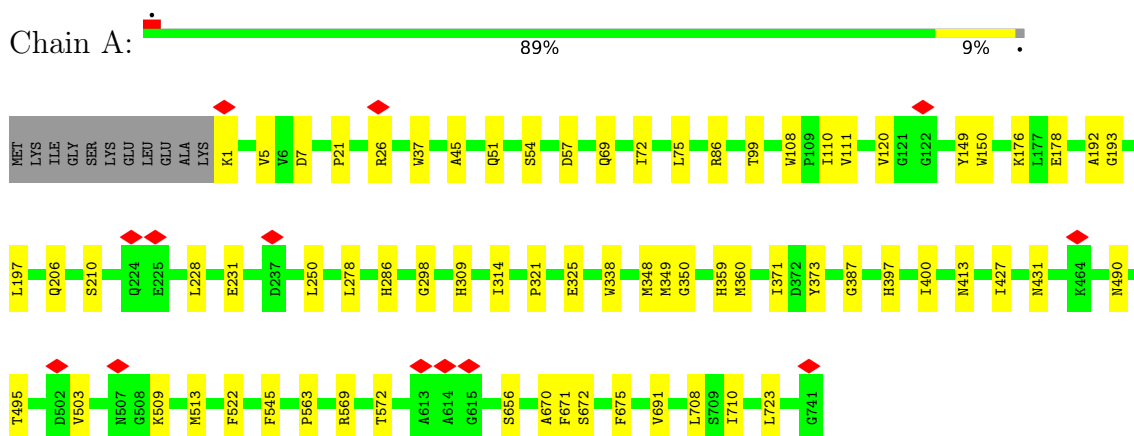
- Molecule 23 is water.

Mol	Chain	Residues	Atoms		AltConf
23	A	110	Total	O	0
			110	110	
23	B	179	Total	O	0
			179	179	
23	C	33	Total	O	0
			33	33	
23	D	19	Total	O	0
			19	19	
23	E	10	Total	O	0
			10	10	
23	F	15	Total	O	0
			15	15	
23	J	2	Total	O	0
			2	2	
23	L	18	Total	O	0
			18	18	
23	M	2	Total	O	0
			2	2	
23	U	3	Total	O	0
			3	3	

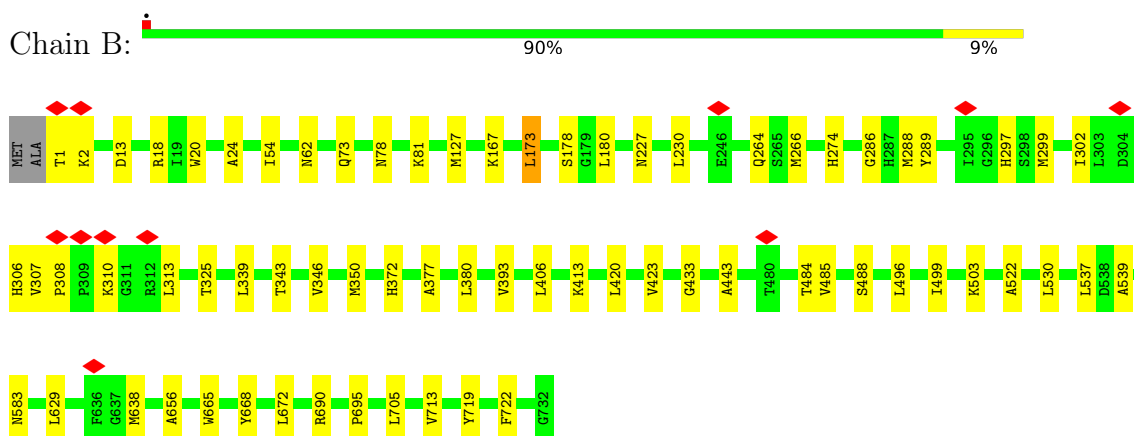
3 Residue-property plots

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

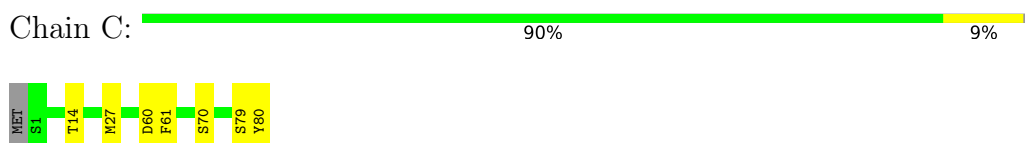
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1 (psaA)



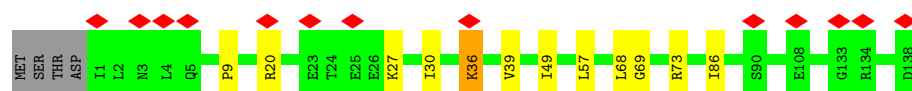
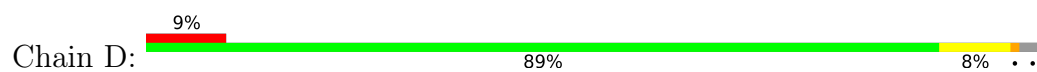
- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2 (psaB)



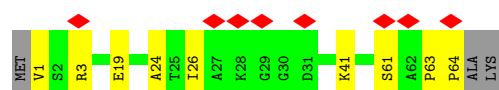
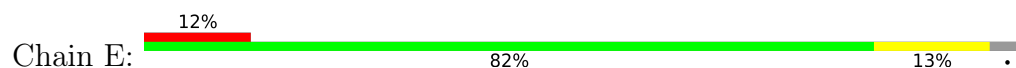
- Molecule 3: Photosystem I iron-sulfur center (psaC)



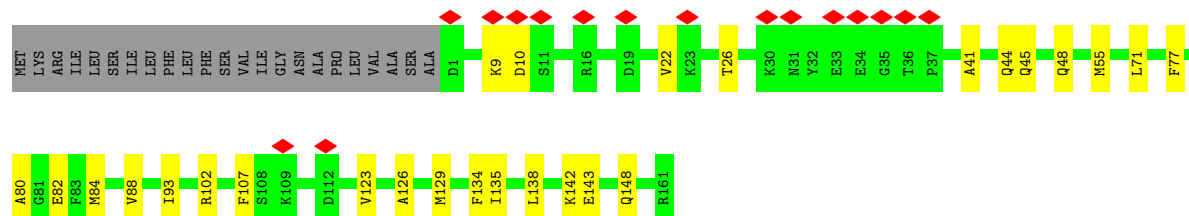
- Molecule 4: Photosystem I reaction center subunit II (psaD)



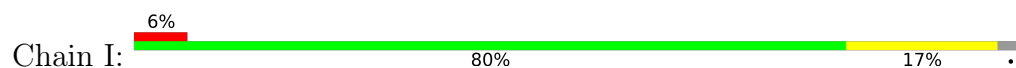
- Molecule 5: Photosystem I reaction center subunit IV (psaE)



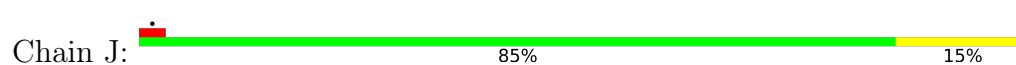
- Molecule 6: Photosystem I reaction center subunit III (psaF)



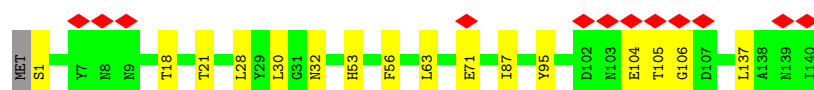
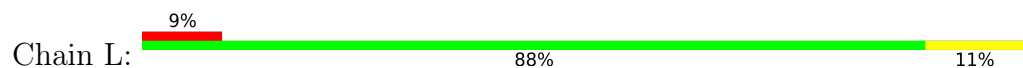
- Molecule 7: Photosystem I reaction center subunit VIII (psaI)



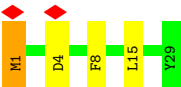
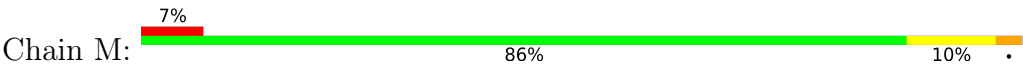
- Molecule 8: Photosystem I reaction center subunit IX (psaJ)



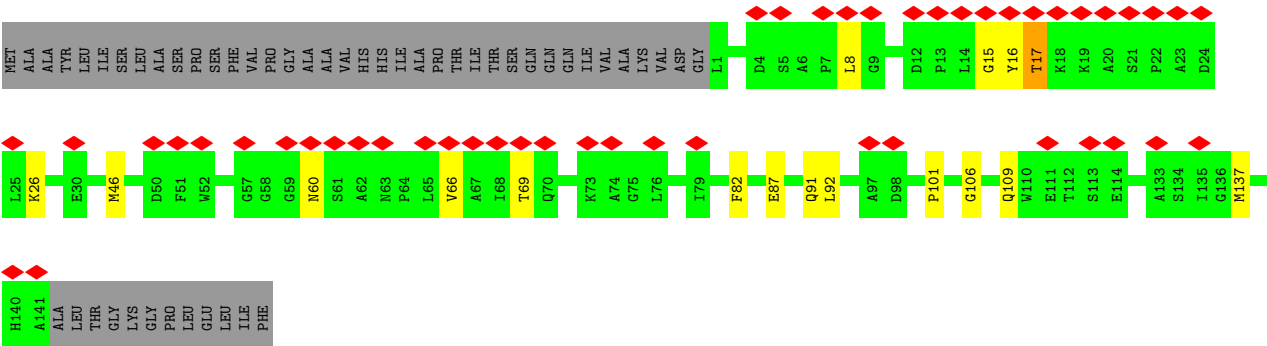
- Molecule 9: Photosystem I reaction center subunit XI (psaL)



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



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



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	18827	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	0.531	Depositor
Minimum map value	-0.210	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.014	Depositor
Recommended contour level	0.11	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: DD6, CLA, A86, CL0, LMG, BCR, PQN, KC1, SF4, LHG, DGD

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	0.20	0/6007	0.43	2/8185 (0.0%)
2	B	0.19	0/6015	0.42	0/8205
3	C	0.15	0/609	0.45	0/826
4	D	0.15	0/1116	0.43	0/1503
5	E	0.14	0/505	0.34	0/689
6	F	0.24	0/1275	0.45	0/1728
7	I	0.24	0/273	0.56	0/373
8	J	0.19	0/313	0.47	0/427
9	L	0.17	0/1081	0.41	0/1470
10	M	0.18	0/218	0.33	0/295
11	U	0.20	0/1109	0.49	0/1499
All	All	0.19	0/18521	0.43	2/25200 (0.0%)

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

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

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	250	LEU	CA-C-N	6.66	124.43	120.24
1	A	250	LEU	C-N-CA	6.66	124.43	120.24

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	665	TRP	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5813	0	5698	51	0
2	B	5805	0	5634	55	0
3	C	599	0	577	4	0
4	D	1092	0	1096	8	0
5	E	494	0	488	4	0
6	F	1246	0	1256	20	0
7	I	266	0	278	6	0
8	J	305	0	310	7	0
9	L	1056	0	1068	13	0
10	M	216	0	234	2	0
11	U	1082	0	1058	19	0
12	A	2563	0	2608	65	0
12	B	2454	0	2490	69	0
12	F	94	0	69	3	0
12	J	42	0	31	0	0
12	L	164	0	150	6	0
12	U	493	0	460	17	0
13	A	33	0	46	5	0
13	B	33	0	46	0	0
14	A	75	0	93	1	0
15	A	160	0	224	6	0
15	B	200	0	280	10	0
15	F	80	0	112	2	0
15	I	80	0	112	4	0
15	J	40	0	56	1	0
15	L	80	0	112	1	0
15	M	40	0	56	3	0
16	A	65	0	72	1	0
17	A	8	0	0	0	0
17	C	16	0	0	0	0
18	B	60	0	81	3	0
19	J	43	0	0	0	0
19	U	112	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	J	39	0	48	1	0
20	U	32	0	34	1	0
21	U	48	0	0	0	0
22	U	45	0	0	0	0
23	A	110	0	0	1	0
23	B	179	0	0	1	0
23	C	33	0	0	0	0
23	D	19	0	0	0	0
23	E	10	0	0	0	0
23	F	15	0	0	0	0
23	J	2	0	0	0	0
23	L	18	0	0	0	0
23	M	2	0	0	0	0
23	U	3	0	0	0	0
All	All	25464	0	24877	299	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 (299) 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)
11:U:46:MET:HE2	11:U:137:MET:CE	1.56	1.35
11:U:46:MET:HE2	11:U:137:MET:HE2	1.25	1.14
11:U:46:MET:CE	11:U:137:MET:CE	2.27	1.12
11:U:46:MET:CE	11:U:137:MET:HE3	1.89	1.03
11:U:46:MET:CE	11:U:137:MET:HE2	1.93	0.95
11:U:46:MET:HE3	11:U:137:MET:HE3	1.57	0.87
6:F:44:GLN:HG2	6:F:48:GLN:HE22	1.40	0.86
8:J:20:MET:HA	8:J:20:MET:HE2	1.62	0.81
1:A:193:GLY:O	1:A:197:LEU:HB2	1.80	0.80
2:B:78:ASN:ND2	2:B:81:LYS:HB2	1.99	0.78
1:A:86:ARG:HG2	1:A:149:TYR:OH	1.84	0.77
1:A:7:ASP:CG	1:A:176:LYS:NZ	2.46	0.74
6:F:107:PHE:HB2	6:F:129:MET:HE1	1.70	0.73
12:A:818:CLA:H52	12:A:846:CLA:H2	1.70	0.73
12:A:803:CLA:H72	15:A:841:BCR:HC8	1.71	0.73
12:B:818:CLA:HMD2	15:B:837:BCR:HC7	1.71	0.73
12:B:846:CLA:C3B	7:I:16:LEU:HD13	2.19	0.72
11:U:46:MET:HE2	11:U:137:MET:HE3	1.53	0.72
2:B:288:MET:HE1	12:B:817:CLA:HMD1	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:44:GLN:HG2	6:F:48:GLN:NE2	2.08	0.69
1:A:373:TYR:CE2	1:A:509:LYS:HE2	2.29	0.68
12:U:206:CLA:H92	12:U:207:CLA:HMA1	1.76	0.67
11:U:106:GLY:O	11:U:109:GLN:HG2	1.95	0.67
12:B:801:CLA:H122	15:B:841:BCR:H12C	1.76	0.67
1:A:7:ASP:CG	1:A:176:LYS:HZ3	2.03	0.65
2:B:227:ASN:ND2	2:B:230:LEU:HG	2.11	0.65
2:B:484:THR:O	2:B:488:SER:HB3	1.98	0.63
2:B:690:ARG:HE	4:D:20:ARG:NE	1.96	0.62
9:L:32:ASN:HB3	12:L:202:CLA:HAC1	1.79	0.62
1:A:348:MET:HA	1:A:348:MET:HE2	1.81	0.62
6:F:93:ILE:HG23	12:F:802:CLA:HAA1	1.82	0.62
12:A:808:CLA:HBB2	12:A:811:CLA:HMA3	1.82	0.62
1:A:522:PHE:HA	12:A:833:CLA:HED1	1.83	0.60
11:U:26:LYS:HD3	11:U:101:PRO:HD3	1.83	0.60
1:A:7:ASP:OD2	1:A:176:LYS:NZ	2.34	0.60
2:B:719:TYR:HB2	12:B:802:CLA:HED2	1.83	0.59
1:A:321:PRO:HB3	9:L:1:SER:HB2	1.83	0.59
12:B:818:CLA:HHB	12:B:844:CLA:H2	1.85	0.59
12:A:816:CLA:HBB2	12:A:816:CLA:H151	1.84	0.59
2:B:13:ASP:HB3	2:B:18:ARG:HB2	1.84	0.58
8:J:16:LEU:O	8:J:20:MET:HG2	2.02	0.58
5:E:19:GLU:OE1	5:E:41:LYS:NZ	2.37	0.56
6:F:9:LYS:HG3	6:F:10:ASP:OD1	2.05	0.56
6:F:71:LEU:HD22	6:F:82:GLU:HG2	1.88	0.56
4:D:69:GLY:O	4:D:73:ARG:HG3	2.06	0.55
6:F:123:VAL:HB	20:J:102:LMG:HC72	1.88	0.55
2:B:690:ARG:HE	4:D:20:ARG:HE	1.52	0.55
20:U:202:LMG:H302	12:U:212:CLA:H11	1.88	0.55
2:B:308:PRO:HG2	2:B:313:LEU:HG	1.89	0.55
12:A:822:CLA:H91	15:A:843:BCR:H23C	1.89	0.55
1:A:228:LEU:HB2	1:A:231:GLU:HG3	1.89	0.55
9:L:18:THR:H	9:L:21:THR:HG1	1.53	0.54
1:A:72:ILE:HG12	12:A:807:CLA:H171	1.90	0.54
12:A:851:CLA:H12	9:L:30:LEU:HD11	1.88	0.54
12:A:824:CLA:H142	12:A:826:CLA:H162	1.90	0.54
2:B:393:VAL:HG13	2:B:539:ALA:HB1	1.89	0.54
1:A:490:ASN:HB2	12:A:831:CLA:HED2	1.90	0.54
12:B:833:CLA:H203	15:I:102:BCR:H391	1.90	0.54
12:A:835:CLA:H101	8:J:17:THR:HG23	1.90	0.53
12:A:821:CLA:HBA1	12:A:825:CLA:H193	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:668:TYR:OH	12:B:803:CLA:OBD	2.22	0.53
5:E:3:ARG:HG3	5:E:24:ALA:O	2.08	0.53
12:B:808:CLA:HHC	12:B:808:CLA:HBB1	1.91	0.53
8:J:20:MET:HE2	8:J:20:MET:CA	2.36	0.53
12:U:201:CLA:HED1	12:U:211:CLA:HAA2	1.91	0.53
2:B:227:ASN:HD21	2:B:230:LEU:HG	1.73	0.53
2:B:713:VAL:HG22	18:B:842:DGD:HBV1	1.91	0.53
12:U:205:CLA:HHC	12:U:205:CLA:HBB1	1.91	0.53
12:A:852:CLA:H171	8:J:22:ILE:HD11	1.90	0.52
1:A:338:TRP:HB3	12:A:803:CLA:HAC1	1.91	0.52
2:B:1:THR:N	7:I:32:GLN:O	2.42	0.52
12:B:827:CLA:HBC3	15:F:804:BCR:H362	1.91	0.52
2:B:306:HIS:HE1	12:B:844:CLA:ND	2.07	0.52
2:B:522:ALA:HB2	12:B:831:CLA:HMA1	1.89	0.52
12:F:803:CLA:HHC	12:F:803:CLA:HBB1	1.92	0.52
13:A:837:PQN:H141	12:A:852:CLA:HBB2	1.92	0.52
1:A:7:ASP:CG	1:A:176:LYS:HZ1	2.14	0.52
2:B:297:HIS:HB3	2:B:302:ILE:HD11	1.91	0.51
11:U:60:ASN:HB3	12:U:208:CLA:HED3	1.92	0.51
2:B:288:MET:HE1	12:B:817:CLA:CMD	2.37	0.51
12:U:201:CLA:H2	12:U:211:CLA:HBA2	1.92	0.51
12:L:204:CLA:HBA2	12:U:209:CLA:H3A	1.91	0.51
2:B:339:LEU:HB3	2:B:380:LEU:HD13	1.91	0.51
12:A:846:CLA:HBB1	12:A:846:CLA:HHC	1.92	0.51
12:B:824:CLA:H11	15:B:838:BCR:H393	1.93	0.51
12:A:828:CLA:H151	12:B:834:CLA:HBA2	1.93	0.51
12:A:815:CLA:HHC	12:A:815:CLA:HBB1	1.93	0.51
12:A:817:CLA:HHC	12:A:817:CLA:HBB1	1.91	0.51
12:U:210:CLA:HHC	12:U:210:CLA:HBB1	1.91	0.51
12:B:815:CLA:HHC	12:B:815:CLA:HBB1	1.92	0.50
6:F:138:LEU:HD22	6:F:142:LYS:HD2	1.92	0.50
12:A:836:CLA:HHC	12:A:836:CLA:HBB1	1.93	0.50
12:A:844:CLA:HHC	12:B:802:CLA:H202	1.94	0.50
12:B:846:CLA:HHC	12:B:846:CLA:HBB1	1.93	0.50
12:U:209:CLA:HHC	12:U:209:CLA:HBB1	1.93	0.50
1:A:54:SER:HB3	1:A:57:ASP:HB2	1.93	0.50
12:A:844:CLA:HBC2	2:B:583:ASN:HB2	1.94	0.50
10:M:8:PHE:HB3	15:M:101:BCR:H271	1.94	0.50
1:A:569:ARG:NH1	23:A:910:HOH:O	2.43	0.50
12:B:847:CLA:HHC	12:B:847:CLA:HBB1	1.94	0.50
12:B:835:CLA:HHC	12:B:835:CLA:HBB1	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:A:810:CLA:HHC	12:A:810:CLA:HBB1	1.94	0.50
12:B:822:CLA:HBB1	12:B:822:CLA:HHC	1.93	0.50
12:A:806:CLA:H12	12:A:824:CLA:H42	1.93	0.50
6:F:138:LEU:CD2	6:F:142:LYS:HD2	2.42	0.50
12:A:820:CLA:HHC	12:A:820:CLA:HBB1	1.93	0.49
12:A:852:CLA:HHC	12:A:852:CLA:HBB1	1.94	0.49
12:B:833:CLA:HHC	12:B:833:CLA:HBB1	1.94	0.49
12:B:834:CLA:H172	9:L:87:ILE:HD13	1.95	0.49
12:U:212:CLA:HHC	12:U:212:CLA:HBB1	1.94	0.49
12:A:836:CLA:H161	12:B:834:CLA:H122	1.95	0.49
13:A:837:PQN:H271	12:A:850:CLA:H13	1.95	0.49
12:A:828:CLA:H42	12:A:836:CLA:H2	1.94	0.49
12:B:820:CLA:H62	12:B:820:CLA:H41	1.60	0.49
9:L:28:LEU:HD22	11:U:92:LEU:HB3	1.95	0.49
12:B:822:CLA:H152	15:B:840:BCR:H17C	1.95	0.49
12:B:829:CLA:HHC	12:B:829:CLA:HBB1	1.94	0.49
12:A:831:CLA:HHC	12:A:831:CLA:HBB1	1.94	0.49
12:B:819:CLA:H3A	12:B:835:CLA:HED3	1.94	0.49
1:A:503:VAL:HG13	1:A:513:MET:HB3	1.94	0.48
12:A:835:CLA:HHC	12:A:835:CLA:HBB1	1.94	0.48
12:A:814:CLA:HHC	12:A:814:CLA:HBB1	1.95	0.48
2:B:413:LYS:HB2	2:B:537:LEU:HD13	1.95	0.48
12:B:834:CLA:HHC	12:B:834:CLA:HBB1	1.94	0.48
1:A:397:HIS:HA	1:A:400:ILE:HD12	1.96	0.48
3:C:14:THR:HG22	3:C:27:MET:HE2	1.94	0.48
1:A:5:VAL:HG21	1:A:178:GLU:CG	2.44	0.48
12:B:806:CLA:H2	12:B:806:CLA:HED3	1.95	0.48
6:F:143:GLU:HG2	6:F:148:GLN:HB3	1.95	0.48
1:A:21:PRO:HB2	1:A:37:TRP:HH2	1.78	0.48
1:A:206:GLN:HA	1:A:210:SER:HB2	1.95	0.48
1:A:360:MET:HE1	12:A:825:CLA:O1D	2.13	0.48
1:A:325:GLU:HG2	1:A:413:ASN:O	2.14	0.48
2:B:78:ASN:HD21	2:B:81:LYS:CG	2.27	0.48
12:B:818:CLA:HBB1	12:B:818:CLA:HHC	1.96	0.48
12:B:819:CLA:HBB2	12:B:835:CLA:H52	1.96	0.48
12:B:844:CLA:H12	12:B:844:CLA:HBA1	1.51	0.47
2:B:24:ALA:HB2	18:B:842:DGD:HA32	1.96	0.47
1:A:371:ILE:HG23	1:A:509:LYS:HG2	1.97	0.47
1:A:45:ALA:O	1:A:51:GLN:NE2	2.45	0.47
12:A:834:CLA:HHC	12:A:834:CLA:HBB1	1.95	0.47
13:A:837:PQN:H222	13:A:837:PQN:H18	1.68	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:431:ASN:HD22	2:B:672:LEU:HD11	1.78	0.47
12:A:833:CLA:HHC	12:A:833:CLA:HBB1	1.95	0.47
2:B:705:LEU:HD22	18:B:842:DGD:HB22	1.95	0.47
2:B:289:TYR:CE1	2:B:299:MET:HE3	2.50	0.47
1:A:110:ILE:HG13	1:A:111:VAL:HG13	1.96	0.47
1:A:495:THR:HG23	12:A:830:CLA:HED3	1.96	0.47
12:A:833:CLA:H141	12:A:833:CLA:H161	1.77	0.47
2:B:127:MET:HE2	12:B:812:CLA:HMA2	1.97	0.47
12:B:846:CLA:H41	12:B:846:CLA:H61	1.60	0.47
1:A:5:VAL:HG21	1:A:178:GLU:CD	2.40	0.47
15:I:102:BCR:H361	9:L:95:TYR:HB2	1.97	0.47
12:A:851:CLA:H72	12:L:203:CLA:H12	1.95	0.47
1:A:26:ARG:HG3	1:A:26:ARG:HH11	1.81	0.46
12:A:824:CLA:H91	12:A:826:CLA:H192	1.97	0.46
1:A:656:SER:HB2	2:B:443:ALA:HB1	1.97	0.46
12:A:833:CLA:H12	12:A:833:CLA:HBA2	1.73	0.46
2:B:629:LEU:HD22	2:B:722:PHE:HA	1.96	0.46
12:A:848:CLA:H191	6:F:126:ALA:HB1	1.98	0.46
12:B:807:CLA:HBB1	12:B:808:CLA:H202	1.98	0.46
4:D:9:PRO:HG2	4:D:57:LEU:HD23	1.98	0.46
1:A:723:LEU:HD22	12:A:835:CLA:HMA1	1.97	0.46
2:B:73:GLN:HE22	10:M:1:MET:CE	2.29	0.46
11:U:46:MET:HB2	11:U:137:MET:CE	2.46	0.46
2:B:372:HIS:HE1	12:B:823:CLA:ND	2.13	0.46
1:A:192:ALA:HB2	1:A:298:GLY:HA3	1.97	0.46
2:B:496:LEU:HA	2:B:499:ILE:HG22	1.98	0.46
12:B:824:CLA:H2	12:B:843:CLA:H193	1.98	0.46
12:B:846:CLA:CAB	7:I:16:LEU:HD13	2.46	0.45
12:A:824:CLA:H102	12:A:824:CLA:H61	1.82	0.45
6:F:102:ARG:NH1	6:F:143:GLU:OE1	2.49	0.45
12:B:818:CLA:CHB	12:B:844:CLA:H2	2.47	0.45
3:C:14:THR:HG22	3:C:27:MET:HG3	1.99	0.45
12:B:830:CLA:H52	12:F:803:CLA:HBB2	1.98	0.45
9:L:71:GLU:OE1	9:L:71:GLU:O	2.35	0.45
12:B:848:CLA:HHC	12:B:848:CLA:HBB1	1.98	0.45
1:A:309:HIS:HB3	1:A:314:ILE:HD11	1.98	0.45
12:B:845:CLA:HBB1	12:B:845:CLA:HHC	1.99	0.45
12:U:206:CLA:H71	12:U:207:CLA:HHB	1.99	0.45
12:B:824:CLA:HBA2	12:B:824:CLA:H12	1.65	0.45
11:U:82:PHE:HZ	12:U:208:CLA:H161	1.82	0.45
11:U:46:MET:HB2	11:U:137:MET:HE1	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:62:ASN:ND2	23:B:904:HOH:O	2.49	0.44
12:B:848:CLA:H3A	12:B:848:CLA:HBA2	1.83	0.44
2:B:266:MET:HE1	12:B:815:CLA:HED3	1.99	0.44
12:B:847:CLA:H3A	12:B:847:CLA:HBA2	1.70	0.44
8:J:1:MET:HE2	8:J:1:MET:HB2	1.93	0.44
2:B:310:LYS:HA	2:B:310:LYS:HD2	1.84	0.44
12:B:810:CLA:H61	12:B:810:CLA:H41	1.78	0.44
11:U:15:GLY:O	11:U:17:THR:N	2.47	0.44
12:A:835:CLA:H18	15:J:104:BCR:H372	2.00	0.44
2:B:346:VAL:O	2:B:350:MET:HG3	2.18	0.44
4:D:30:ILE:HG21	4:D:68:LEU:HD23	1.99	0.44
1:A:671:PHE:HZ	12:A:835:CLA:HBC2	1.83	0.44
12:A:815:CLA:H3A	12:A:815:CLA:HBA2	1.79	0.44
2:B:78:ASN:HD21	2:B:81:LYS:HG2	1.83	0.44
11:U:46:MET:CE	11:U:137:MET:HB3	2.48	0.44
1:A:359:HIS:ND1	12:A:815:CLA:OBD	2.49	0.44
12:A:828:CLA:H172	2:B:20:TRP:HH2	1.83	0.44
2:B:423:VAL:HG23	12:B:831:CLA:HBB1	1.98	0.44
9:L:105:THR:O	9:L:105:THR:OG1	2.36	0.44
14:A:838:LHG:H312	14:A:838:LHG:H282	1.85	0.44
2:B:54:ILE:HD11	15:M:101:BCR:HC8	2.00	0.44
1:A:108:TRP:CD2	12:A:807:CLA:HED3	2.54	0.43
1:A:670:ALA:HB3	12:A:801:CLA:HBB2	2.00	0.43
12:U:206:CLA:H8	12:U:206:CLA:H51	1.80	0.43
2:B:420:LEU:HD13	2:B:530:LEU:HA	1.99	0.43
2:B:433:GLY:HA3	12:B:828:CLA:HAB	2.00	0.43
6:F:55:MET:HE2	6:F:55:MET:HB3	1.84	0.43
12:A:806:CLA:H12	12:A:806:CLA:HBA2	1.61	0.43
1:A:150:TRP:CD1	12:A:814:CLA:HAA2	2.54	0.43
12:B:806:CLA:HED1	12:B:825:CLA:H2	2.00	0.43
6:F:22:VAL:O	6:F:26:THR:OG1	2.31	0.43
7:I:5:PHE:HD2	7:I:9:ILE:HD12	1.84	0.43
9:L:137:LEU:HG	12:L:204:CLA:HED3	1.99	0.43
2:B:167:LYS:HD3	2:B:325:THR:HG22	2.00	0.43
6:F:77:PHE:HA	6:F:80:ALA:HB2	2.01	0.43
15:F:804:BCR:H20C	15:F:804:BCR:H361	1.80	0.43
1:A:350:GLY:HA2	1:A:387:GLY:HA2	2.00	0.43
1:A:427:ILE:HG13	1:A:545:PHE:HE1	1.84	0.43
12:A:828:CLA:HBB1	12:A:829:CLA:HBA1	1.99	0.43
15:B:840:BCR:H371	15:B:840:BCR:H24C	1.82	0.43
6:F:134:PHE:CE2	6:F:135:ILE:HG23	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:286:HIS:HB2	12:A:815:CLA:C1B	2.49	0.43
4:D:36:LYS:HB2	4:D:36:LYS:HE2	1.63	0.43
1:A:278:LEU:HD13	12:A:815:CLA:HMA2	2.00	0.43
12:B:843:CLA:H162	12:B:843:CLA:H141	1.82	0.43
9:L:104:GLU:CD	9:L:106:GLY:H	2.27	0.43
15:B:840:BCR:H15C	15:B:840:BCR:H351	1.83	0.43
1:A:708:LEU:HD21	13:A:837:PQN:H151	2.00	0.43
12:A:828:CLA:H142	15:B:841:BCR:H17C	2.01	0.43
3:C:60:ASP:HA	3:C:61:PHE:HA	1.86	0.43
6:F:41:ALA:O	6:F:45:GLN:HG3	2.19	0.43
2:B:339:LEU:HD11	12:B:805:CLA:H51	2.01	0.42
12:B:807:CLA:HBB	12:B:808:CLA:HMB3	2.00	0.42
15:M:101:BCR:H11C	15:M:101:BCR:H341	1.92	0.42
12:B:834:CLA:H91	12:B:834:CLA:H112	1.81	0.42
1:A:69:GLN:HG2	12:A:803:CLA:H3A	2.02	0.42
12:A:852:CLA:H161	12:A:852:CLA:H141	1.85	0.42
2:B:343:THR:HB	2:B:377:ALA:HB2	2.01	0.42
5:E:63:PRO:HA	5:E:64:PRO:HD3	1.90	0.42
2:B:656:ALA:HB3	12:B:803:CLA:HBB2	2.01	0.42
11:U:87:GLU:O	11:U:91:GLN:HG3	2.20	0.42
1:A:569:ARG:HH11	1:A:572:THR:HG21	1.84	0.42
12:B:817:CLA:H61	12:B:822:CLA:H11	2.01	0.42
15:L:205:BCR:H15C	15:L:205:BCR:H351	1.87	0.42
11:U:87:GLU:HG3	12:U:210:CLA:NB	2.35	0.42
12:A:824:CLA:H143	12:A:824:CLA:H111	1.84	0.41
15:A:842:BCR:H20C	15:A:842:BCR:H361	1.82	0.41
2:B:2:LYS:HD3	7:I:34:GLU:HB3	2.01	0.41
5:E:1:VAL:HG23	5:E:26:ILE:HD11	2.01	0.41
15:A:841:BCR:H15C	15:A:841:BCR:H351	1.90	0.41
12:A:851:CLA:C4C	12:L:203:CLA:H111	2.50	0.41
2:B:289:TYR:CZ	2:B:299:MET:HE3	2.55	0.41
15:B:837:BCR:H15C	15:B:837:BCR:H351	1.89	0.41
7:I:6:LEU:HD23	7:I:6:LEU:HA	1.88	0.41
15:I:102:BCR:H11C	15:I:102:BCR:H341	1.90	0.41
1:A:675:PHE:HA	13:A:837:PQN:H9	2.01	0.41
15:A:843:BCR:H11C	15:A:843:BCR:H341	1.93	0.41
12:U:211:CLA:H93	12:U:211:CLA:H61	1.88	0.41
2:B:173:LEU:HD23	2:B:173:LEU:HA	1.79	0.41
12:B:830:CLA:H11	12:B:830:CLA:H51	1.89	0.41
12:U:212:CLA:H12	12:U:212:CLA:HED3	2.02	0.41
12:B:813:CLA:H12	12:B:813:CLA:HBA2	1.74	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:I:102:BCR:H15C	15:I:102:BCR:H351	1.82	0.41
9:L:53:HIS:HA	9:L:56:PHE:CD2	2.55	0.41
12:A:848:CLA:HAA2	12:B:827:CLA:HMB2	2.02	0.41
11:U:66:VAL:O	11:U:69:THR:OG1	2.36	0.41
1:A:1:LYS:HE3	1:A:1:LYS:HB3	1.70	0.41
1:A:349:MET:HE1	12:A:825:CLA:H202	2.03	0.41
1:A:563:PRO:HB3	1:A:710:ILE:HB	2.01	0.41
2:B:178:SER:HB3	2:B:286:GLY:HA3	2.03	0.41
2:B:638:MET:HE2	2:B:638:MET:HB2	1.93	0.41
15:B:838:BCR:H20C	15:B:838:BCR:H361	1.86	0.41
6:F:44:GLN:CG	6:F:48:GLN:NE2	2.81	0.41
12:U:208:CLA:H161	12:U:208:CLA:H203	1.93	0.41
12:A:815:CLA:H18	12:A:815:CLA:H152	1.84	0.41
2:B:180:LEU:HD13	12:B:843:CLA:HHB	2.03	0.41
6:F:84:MET:O	6:F:88:VAL:HG23	2.21	0.41
15:A:843:BCR:H20C	15:A:843:BCR:H361	1.91	0.40
16:A:847:CL0:H39	16:A:847:CL0:H33	1.91	0.40
2:B:264:GLN:HG3	2:B:503:LYS:NZ	2.37	0.40
12:B:812:CLA:H41	12:B:812:CLA:H62	1.91	0.40
12:B:823:CLA:H141	12:B:825:CLA:H151	2.03	0.40
12:B:845:CLA:H112	12:B:845:CLA:H152	1.97	0.40
2:B:695:PRO:O	3:C:80:TYR:OH	2.35	0.40
12:A:823:CLA:H152	12:A:834:CLA:H191	2.03	0.40
2:B:274:HIS:HB2	12:B:815:CLA:C1B	2.52	0.40
12:B:808:CLA:H8	12:B:809:CLA:H52	2.03	0.40
6:F:123:VAL:HG22	8:J:15:LEU:HD11	2.03	0.40
1:A:75:LEU:HD22	12:A:807:CLA:H172	2.04	0.40
12:B:805:CLA:H93	12:B:843:CLA:H2	2.03	0.40
9:L:63:LEU:HD12	12:L:204:CLA:HHB	2.03	0.40
12:B:805:CLA:HBC2	12:B:825:CLA:HMA1	2.04	0.40
12:B:835:CLA:H143	12:B:835:CLA:H161	1.93	0.40
15:B:839:BCR:H24C	15:B:839:BCR:H371	1.88	0.40
4:D:27:LYS:HG3	4:D:86:ILE:HB	2.04	0.40
4:D:39:VAL:HG22	4:D:49:ILE:HG12	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	739/752 (98%)	719 (97%)	20 (3%)	0	100	100
2	B	730/734 (100%)	716 (98%)	14 (2%)	0	100	100
3	C	78/81 (96%)	76 (97%)	2 (3%)	0	100	100
4	D	136/142 (96%)	129 (95%)	7 (5%)	0	100	100
5	E	62/67 (92%)	60 (97%)	2 (3%)	0	100	100
6	F	159/184 (86%)	155 (98%)	4 (2%)	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%)	137 (99%)	1 (1%)	0	100	100
10	M	27/29 (93%)	27 (100%)	0	0	100	100
11	U	139/191 (73%)	132 (95%)	6 (4%)	1 (1%)	18	17
All	All	2277/2395 (95%)	2218 (97%)	58 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
11	U	16	TYR

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%)	599 (99%)	4 (1%)	76	86

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	590/591 (100%)	586 (99%)	4 (1%)	76	86
3	C	68/69 (99%)	66 (97%)	2 (3%)	37	47
4	D	118/122 (97%)	117 (99%)	1 (1%)	73	83
5	E	53/55 (96%)	52 (98%)	1 (2%)	50	63
6	F	133/152 (88%)	133 (100%)	0	100	100
7	I	31/32 (97%)	31 (100%)	0	100	100
8	J	32/32 (100%)	32 (100%)	0	100	100
9	L	111/112 (99%)	111 (100%)	0	100	100
10	M	21/21 (100%)	18 (86%)	3 (14%)	3	2
11	U	110/148 (74%)	108 (98%)	2 (2%)	51	65
All	All	1870/1946 (96%)	1853 (99%)	17 (1%)	68	81

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	99	THR
1	A	120	VAL
1	A	672	SER
1	A	691	VAL
2	B	173	LEU
2	B	307	VAL
2	B	406	LEU
2	B	485	VAL
3	C	70	SER
3	C	79	SER
4	D	36	LYS
5	E	61	SER
10	M	1	MET
10	M	4	ASP
10	M	15	LEU
11	U	8	LEU
11	U	17	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	HIS

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Mol	Chain	Res	Type
1	A	214	ASN
1	A	376	GLN
1	A	431	ASN
1	A	548	ASN
2	B	73	GLN
2	B	78	ASN
2	B	112	ASN
2	B	227	ASN
2	B	631	ASN
2	B	634	ASN
2	B	641	GLN
3	C	37	GLN
6	F	15	ASN
6	F	31	ASN
6	F	48	GLN
8	J	4	ASN
11	U	120	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

133 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	CLA	U	210	11	46,50,73	1.41	7 (15%)	53,85,113	1.13	4 (7%)
12	CLA	B	831	2	69,73,73	1.18	7 (10%)	82,113,113	0.90	4 (4%)
14	LHG	A	839	12	26,26,48	0.81	0	29,32,54	1.34	3 (10%)
12	CLA	B	803	-	69,73,73	1.14	7 (10%)	82,113,113	0.93	4 (4%)
12	CLA	A	803	1	69,73,73	1.17	7 (10%)	82,113,113	0.89	4 (4%)
19	DD6	U	215	-	24,26,45	1.53	5 (20%)	29,35,67	1.58	5 (17%)
12	CLA	U	212	11	56,60,73	1.33	7 (12%)	65,97,113	1.09	4 (6%)
12	CLA	B	804	2	49,53,73	1.44	8 (16%)	58,89,113	1.01	3 (5%)
12	CLA	B	833	23	69,73,73	1.18	7 (10%)	82,113,113	0.96	6 (7%)
12	CLA	B	812	2	58,62,73	1.28	7 (12%)	68,99,113	0.97	4 (5%)
12	CLA	B	806	2	69,73,73	1.19	6 (8%)	82,113,113	0.91	5 (6%)
12	CLA	B	811	2	59,63,73	1.22	6 (10%)	70,101,113	1.07	5 (7%)
12	CLA	B	827	2	53,57,73	1.37	7 (13%)	61,93,113	0.98	3 (4%)
12	CLA	B	848	-	49,53,73	1.43	8 (16%)	58,89,113	1.23	7 (12%)
13	PQN	A	837	-	34,34,34	0.39	0	43,45,45	0.57	1 (2%)
12	CLA	B	807	2	69,73,73	1.18	7 (10%)	82,113,113	0.90	3 (3%)
12	CLA	A	848	1	69,73,73	1.21	7 (10%)	82,113,113	0.88	3 (3%)
12	CLA	A	808	1	60,64,73	1.30	7 (11%)	71,102,113	0.90	3 (4%)
12	CLA	A	827	1	54,58,73	1.38	7 (12%)	64,95,113	0.95	3 (4%)
12	CLA	L	202	9	53,57,73	1.34	8 (15%)	61,93,113	1.14	6 (9%)
12	CLA	A	812	1	49,53,73	1.44	7 (14%)	58,89,113	1.14	5 (8%)
12	CLA	A	846	1	69,73,73	1.21	8 (11%)	82,113,113	0.98	4 (4%)
12	CLA	A	850	1	69,73,73	1.16	7 (10%)	82,113,113	0.90	3 (3%)
12	CLA	B	844	2	69,73,73	1.17	7 (10%)	82,113,113	1.04	6 (7%)
19	DD6	U	204	-	40,45,45	1.29	7 (17%)	51,67,67	1.67	11 (21%)
17	SF4	A	849	2,1	0,12,12	-	-	-	-	-
12	CLA	B	819	2	57,61,73	1.26	7 (12%)	67,98,113	0.96	5 (7%)
12	CLA	F	803	6	50,54,73	1.36	7 (14%)	59,90,113	1.07	4 (6%)
13	PQN	B	836	-	34,34,34	0.41	0	43,45,45	0.56	1 (2%)
12	CLA	U	206	11	69,73,73	1.17	6 (8%)	82,113,113	0.91	4 (4%)
12	CLA	A	814	23	49,53,73	1.39	7 (14%)	58,89,113	1.10	5 (8%)
12	CLA	U	201	14	56,60,73	1.29	8 (14%)	65,97,113	1.08	4 (6%)
15	BCR	L	205	-	41,41,41	1.09	2 (4%)	56,56,56	1.37	7 (12%)
12	CLA	B	820	23	67,71,73	1.21	8 (11%)	79,110,113	1.02	5 (6%)
12	CLA	B	813	2	63,67,73	1.26	7 (11%)	74,105,113	0.94	4 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	BCR	A	841	-	41,41,41	1.09	2 (4%)	56,56,56	1.17	4 (7%)
12	CLA	B	808	2	69,73,73	1.20	7 (10%)	82,113,113	0.90	3 (3%)
19	DD6	J	101	-	40,45,45	1.26	7 (17%)	51,67,67	1.57	9 (17%)
12	CLA	A	811	1	69,73,73	1.20	7 (10%)	82,113,113	0.90	3 (3%)
12	CLA	A	821	23	69,73,73	1.20	7 (10%)	82,113,113	0.96	6 (7%)
12	CLA	A	805	1	53,57,73	1.36	7 (13%)	61,93,113	1.05	5 (8%)
12	CLA	A	816	1	69,73,73	1.17	7 (10%)	82,113,113	0.94	4 (4%)
12	CLA	B	809	2	69,73,73	1.20	8 (11%)	82,113,113	0.91	4 (4%)
12	CLA	J	103	8	46,50,73	1.38	6 (13%)	53,85,113	1.09	4 (7%)
15	BCR	B	838	-	41,41,41	1.01	2 (4%)	56,56,56	1.27	6 (10%)
12	CLA	B	817	23	69,73,73	1.17	6 (8%)	82,113,113	0.97	5 (6%)
20	LMG	J	102	-	39,39,55	0.84	1 (2%)	47,47,63	1.21	4 (8%)
12	CLA	A	815	1	69,73,73	1.20	7 (10%)	82,113,113	0.96	4 (4%)
15	BCR	A	842	-	41,41,41	1.07	2 (4%)	56,56,56	1.35	7 (12%)
12	CLA	B	832	2	51,55,73	1.39	6 (11%)	60,91,113	1.05	5 (8%)
12	CLA	B	801	23	69,73,73	1.18	7 (10%)	82,113,113	0.92	4 (4%)
12	CLA	F	802	23	52,56,73	1.36	6 (11%)	61,92,113	1.06	4 (6%)
15	BCR	F	804	-	41,41,41	1.05	2 (4%)	56,56,56	1.25	6 (10%)
15	BCR	A	843	-	41,41,41	1.09	2 (4%)	56,56,56	1.27	6 (10%)
12	CLA	A	828	1	69,73,73	1.24	7 (10%)	82,113,113	0.88	3 (3%)
12	CLA	A	836	23	69,73,73	1.18	7 (10%)	82,113,113	0.95	3 (3%)
12	CLA	B	835	-	69,73,73	1.17	8 (11%)	82,113,113	0.96	4 (4%)
22	KC1	U	214	11	49,53,53	1.63	9 (18%)	61,89,89	1.05	3 (4%)
12	CLA	A	806	1	69,73,73	1.15	7 (10%)	82,113,113	0.96	5 (6%)
12	CLA	B	816	2	64,68,73	1.22	7 (10%)	76,107,113	0.91	4 (5%)
12	CLA	A	852	23	69,73,73	1.18	7 (10%)	82,113,113	0.97	4 (4%)
12	CLA	B	846	2	69,73,73	1.17	7 (10%)	82,113,113	1.12	6 (7%)
12	CLA	A	807	1	69,73,73	1.17	7 (10%)	82,113,113	1.00	5 (6%)
17	SF4	C	102	3	0,12,12	-	-	-	-	-
12	CLA	A	817	1	49,53,73	1.41	7 (14%)	58,89,113	1.12	4 (6%)
12	CLA	A	831	1	49,53,73	1.37	6 (12%)	58,89,113	1.14	5 (8%)
18	DGD	B	842	-	61,61,67	0.90	2 (3%)	75,75,81	1.33	8 (10%)
15	BCR	F	801	-	41,41,41	1.08	2 (4%)	56,56,56	1.31	6 (10%)
17	SF4	C	101	3	0,12,12	-	-	-	-	-
12	CLA	U	211	11	69,73,73	1.14	5 (7%)	82,113,113	0.96	5 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	CLA	A	826	1	69,73,73	1.27	9 (13%)	82,113,113	0.84	2 (2%)
12	CLA	B	814	2	59,63,73	1.31	7 (11%)	70,101,113	0.93	3 (4%)
12	CLA	U	208	23	69,73,73	1.13	5 (7%)	82,113,113	1.07	8 (9%)
12	CLA	B	845	2	69,73,73	1.28	8 (11%)	82,113,113	0.97	4 (4%)
15	BCR	B	840	-	41,41,41	1.09	2 (4%)	56,56,56	1.23	4 (7%)
12	CLA	A	829	1	69,73,73	1.20	6 (8%)	82,113,113	0.90	4 (4%)
15	BCR	M	101	-	41,41,41	1.07	2 (4%)	56,56,56	1.36	8 (14%)
12	CLA	A	835	1	69,73,73	1.24	7 (10%)	82,113,113	0.90	3 (3%)
20	LMG	U	202	-	32,32,55	0.96	1 (3%)	40,40,63	1.20	5 (12%)
15	BCR	I	101	-	41,41,41	1.05	2 (4%)	56,56,56	1.27	7 (12%)
12	CLA	A	804	1	69,73,73	1.17	8 (11%)	82,113,113	0.89	4 (4%)
12	CLA	B	810	2	58,62,73	1.40	8 (13%)	71,100,113	0.94	4 (5%)
12	CLA	A	813	1	54,58,73	1.38	6 (11%)	64,95,113	1.00	5 (7%)
12	CLA	A	810	1	58,62,73	1.30	7 (12%)	68,99,113	1.04	4 (5%)
12	CLA	B	821	23	68,72,73	1.15	6 (8%)	80,111,113	0.92	4 (5%)
12	CLA	A	820	1	55,59,73	1.32	7 (12%)	64,96,113	1.09	4 (6%)
15	BCR	J	104	-	41,41,41	1.08	2 (4%)	56,56,56	1.20	5 (8%)
12	CLA	A	819	1	47,51,73	1.40	6 (12%)	55,86,113	1.07	5 (9%)
12	CLA	U	205	23	65,69,73	1.21	8 (12%)	77,108,113	0.95	3 (3%)
12	CLA	A	809	1	66,70,73	1.23	6 (9%)	78,109,113	0.85	3 (3%)
12	CLA	B	828	2	62,66,73	1.30	7 (11%)	73,104,113	1.01	5 (6%)
15	BCR	B	839	-	41,41,41	1.04	2 (4%)	56,56,56	1.25	5 (8%)
12	CLA	B	824	2	69,73,73	1.21	7 (10%)	82,113,113	0.93	5 (6%)
12	CLA	B	822	2	69,73,73	1.26	7 (10%)	82,113,113	0.97	4 (4%)
12	CLA	A	832	1	55,59,73	1.36	8 (14%)	64,96,113	1.05	4 (6%)
12	CLA	A	801	-	69,73,73	1.15	7 (10%)	82,113,113	0.90	5 (6%)
12	CLA	A	822	23	69,73,73	1.14	7 (10%)	82,113,113	0.92	4 (4%)
12	CLA	B	805	2	69,73,73	1.18	7 (10%)	82,113,113	0.87	4 (4%)
12	CLA	B	847	2	54,58,73	1.34	7 (12%)	64,95,113	1.07	5 (7%)
12	CLA	A	845	1	64,68,73	1.32	6 (9%)	76,107,113	0.96	4 (5%)
21	A86	U	203	-	47,50,50	1.38	4 (8%)	51,76,76	1.65	10 (19%)
12	CLA	A	833	1	69,73,73	1.20	7 (10%)	82,113,113	1.00	5 (6%)
12	CLA	A	851	1	69,73,73	1.18	7 (10%)	82,113,113	0.88	4 (4%)
15	BCR	B	837	-	41,41,41	1.10	3 (7%)	56,56,56	1.28	8 (14%)
12	CLA	B	825	2	69,73,73	1.19	7 (10%)	82,113,113	0.93	5 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	CLA	A	844	23	69,73,73	1.15	7 (10%)	82,113,113	0.90	3 (3%)
12	CLA	B	826	2	54,58,73	1.33	6 (11%)	64,95,113	0.99	4 (6%)
12	CLA	A	802	1	59,63,73	1.25	6 (10%)	70,101,113	1.04	6 (8%)
19	DD6	U	213	-	40,45,45	1.25	6 (15%)	51,67,67	1.76	13 (25%)
12	CLA	B	829	23	69,73,73	1.15	6 (8%)	82,113,113	0.95	4 (4%)
12	CLA	B	818	2	50,54,73	1.35	6 (12%)	59,90,113	1.08	4 (6%)
15	BCR	B	841	-	41,41,41	1.12	2 (4%)	56,56,56	1.15	3 (5%)
12	CLA	U	207	11	49,53,73	1.44	6 (12%)	58,89,113	1.00	3 (5%)
12	CLA	U	209	11	50,54,73	1.34	5 (10%)	59,90,113	1.15	5 (8%)
12	CLA	B	802	2	69,73,73	1.24	7 (10%)	82,113,113	0.80	3 (3%)
15	BCR	L	201	-	41,41,41	1.12	2 (4%)	56,56,56	1.20	5 (8%)
16	CL0	A	847	1	58,73,73	0.89	4 (6%)	60,113,113	1.73	8 (13%)
12	CLA	B	823	2	69,73,73	1.21	7 (10%)	82,113,113	0.95	3 (3%)
12	CLA	A	818	23	69,73,73	1.16	8 (11%)	82,113,113	0.95	4 (4%)
12	CLA	A	825	1	69,73,73	1.22	7 (10%)	82,113,113	0.90	3 (3%)
12	CLA	B	843	2	69,73,73	1.21	7 (10%)	82,113,113	0.90	4 (4%)
12	CLA	B	830	2	62,66,73	1.31	7 (11%)	73,104,113	0.99	3 (4%)
15	BCR	I	102	-	41,41,41	1.11	2 (4%)	56,56,56	1.29	6 (10%)
12	CLA	B	834	2	69,73,73	1.25	8 (11%)	82,113,113	0.94	4 (4%)
15	BCR	A	840	-	41,41,41	1.02	2 (4%)	56,56,56	1.31	7 (12%)
14	LHG	A	838	-	47,47,48	0.64	1 (2%)	50,53,54	1.26	6 (12%)
12	CLA	A	823	1	69,73,73	1.24	7 (10%)	82,113,113	0.89	4 (4%)
12	CLA	A	824	1	66,70,73	1.23	7 (10%)	78,109,113	0.99	5 (6%)
12	CLA	A	830	1	54,58,73	1.31	6 (11%)	64,95,113	0.97	4 (6%)
12	CLA	A	834	1	69,73,73	1.29	8 (11%)	82,113,113	0.97	4 (4%)
12	CLA	B	815	2	63,67,73	1.22	6 (9%)	74,105,113	0.98	5 (6%)
12	CLA	L	203	9	69,73,73	1.17	6 (8%)	82,113,113	0.86	3 (3%)
12	CLA	L	204	23	54,58,73	1.30	7 (12%)	64,95,113	1.03	4 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	CLA	U	210	11	1/1/10/20	1/12/88/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	CLA	B	831	2	1/1/15/20	6/39/115/115	-
14	LHG	A	839	12	-	7/31/31/53	-
12	CLA	B	803	-	1/1/15/20	4/39/115/115	-
12	CLA	A	803	1	1/1/15/20	3/39/115/115	-
19	DD6	U	215	-	-	8/14/37/80	0/1/1/3
12	CLA	U	212	11	1/1/12/20	2/24/100/115	-
12	CLA	B	804	2	1/1/11/20	5/15/91/115	-
12	CLA	B	833	23	1/1/15/20	5/39/115/115	-
12	CLA	B	812	2	-	3/26/102/115	-
12	CLA	B	806	2	1/1/15/20	2/39/115/115	-
12	CLA	B	811	2	1/1/13/20	5/27/103/115	-
12	CLA	B	827	2	1/1/11/20	4/20/96/115	-
12	CLA	B	848	-	1/1/11/20	2/15/91/115	-
13	PQN	A	837	-	-	2/23/43/43	0/2/2/2
12	CLA	B	807	2	1/1/15/20	4/39/115/115	-
12	CLA	A	848	1	-	7/39/115/115	-
12	CLA	A	808	1	1/1/13/20	3/29/105/115	-
12	CLA	A	827	1	-	2/21/97/115	-
12	CLA	L	202	9	1/1/11/20	4/20/96/115	-
12	CLA	A	812	1	1/1/11/20	0/15/91/115	-
12	CLA	A	850	1	1/1/15/20	10/39/115/115	-
12	CLA	A	846	1	-	3/39/115/115	-
12	CLA	B	844	2	1/1/15/20	8/39/115/115	-
19	DD6	U	204	-	-	5/26/80/80	0/3/3/3
17	SF4	A	849	2,1	-	-	0/6/5/5
12	CLA	B	819	2	-	1/25/101/115	-
12	CLA	F	803	6	1/1/11/20	3/17/93/115	-
13	PQN	B	836	-	-	1/23/43/43	0/2/2/2
12	CLA	U	206	11	1/1/15/20	4/39/115/115	-
12	CLA	A	814	23	-	1/15/91/115	-
12	CLA	U	201	14	1/1/12/20	5/24/100/115	-
15	BCR	L	205	-	-	8/29/63/63	0/2/2/2
12	CLA	B	820	23	1/1/14/20	8/37/113/115	-
12	CLA	B	813	2	-	7/32/108/115	-
15	BCR	A	841	-	-	8/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	CLA	B	808	2	1/1/15/20	5/39/115/115	-
19	DD6	J	101	-	-	6/26/80/80	0/3/3/3
12	CLA	A	811	1	1/1/15/20	2/39/115/115	-
12	CLA	A	821	23	1/1/15/20	9/39/115/115	-
12	CLA	A	805	1	1/1/11/20	2/20/96/115	-
12	CLA	A	816	1	1/1/15/20	0/39/115/115	-
12	CLA	B	809	2	1/1/15/20	4/39/115/115	-
12	CLA	J	103	8	1/1/10/20	3/12/88/115	-
15	BCR	B	838	-	-	10/29/63/63	0/2/2/2
12	CLA	B	817	23	1/1/15/20	4/39/115/115	-
20	LMG	J	102	-	-	17/34/54/70	0/1/1/1
12	CLA	A	815	1	1/1/15/20	5/39/115/115	-
15	BCR	A	842	-	-	2/29/63/63	0/2/2/2
12	CLA	B	832	2	1/1/11/20	0/18/94/115	-
12	CLA	B	801	23	1/1/15/20	3/39/115/115	-
12	CLA	F	802	23	1/1/11/20	2/19/95/115	-
15	BCR	F	804	-	-	8/29/63/63	0/2/2/2
15	BCR	A	843	-	-	11/29/63/63	0/2/2/2
12	CLA	A	828	1	1/1/15/20	5/39/115/115	-
12	CLA	A	836	23	1/1/15/20	5/39/115/115	-
12	CLA	B	835	-	1/1/15/20	8/39/115/115	-
22	KC1	U	214	11	-	0/15/71/71	-
12	CLA	B	816	2	1/1/14/20	3/33/109/115	-
12	CLA	A	806	1	-	6/39/115/115	-
12	CLA	A	852	23	1/1/15/20	2/39/115/115	-
12	CLA	B	846	2	1/1/15/20	8/39/115/115	-
12	CLA	A	807	1	-	5/39/115/115	-
17	SF4	C	102	3	-	-	0/6/5/5
12	CLA	A	817	1	1/1/11/20	2/15/91/115	-
12	CLA	A	831	1	1/1/11/20	0/15/91/115	-
18	DGD	B	842	-	-	24/49/89/95	0/2/2/2
15	BCR	F	801	-	-	7/29/63/63	0/2/2/2
17	SF4	C	101	3	-	-	0/6/5/5
12	CLA	U	211	11	-	8/39/115/115	-
12	CLA	A	826	1	-	2/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	CLA	B	814	2	-	0/27/103/115	-
12	CLA	U	208	23	-	3/39/115/115	-
12	CLA	B	845	2	1/1/15/20	2/39/115/115	-
15	BCR	B	840	-	-	8/29/63/63	0/2/2/2
12	CLA	A	829	1	1/1/15/20	3/39/115/115	-
15	BCR	M	101	-	-	13/29/63/63	0/2/2/2
12	CLA	A	835	1	1/1/15/20	0/39/115/115	-
20	LMG	U	202	-	-	12/27/47/70	0/1/1/1
15	BCR	I	101	-	-	5/29/63/63	0/2/2/2
12	CLA	A	804	1	1/1/15/20	10/39/115/115	-
12	CLA	B	810	2	-	2/25/101/115	-
12	CLA	A	813	1	-	1/21/97/115	-
12	CLA	A	810	1	1/1/12/20	0/26/102/115	-
12	CLA	B	821	23	1/1/14/20	5/38/114/115	-
12	CLA	A	820	1	1/1/12/20	1/23/99/115	-
15	BCR	J	104	-	-	8/29/63/63	0/2/2/2
12	CLA	U	205	23	1/1/14/20	1/35/111/115	-
12	CLA	A	819	1	-	2/13/89/115	-
12	CLA	A	809	1	-	6/36/112/115	-
12	CLA	B	828	2	-	6/31/107/115	-
15	BCR	B	839	-	-	6/29/63/63	0/2/2/2
12	CLA	B	824	2	-	3/39/115/115	-
12	CLA	B	822	2	1/1/15/20	0/39/115/115	-
12	CLA	A	832	1	1/1/12/20	1/23/99/115	-
12	CLA	A	801	-	-	1/39/115/115	-
12	CLA	A	822	23	1/1/15/20	5/39/115/115	-
12	CLA	B	805	2	1/1/15/20	6/39/115/115	-
12	CLA	B	847	2	-	4/21/97/115	-
12	CLA	A	845	1	-	12/33/109/115	-
21	A86	U	203	-	-	21/34/90/90	0/3/3/3
12	CLA	A	833	1	1/1/15/20	9/39/115/115	-
12	CLA	A	851	1	-	6/39/115/115	-
15	BCR	B	837	-	-	11/29/63/63	0/2/2/2
12	CLA	B	825	2	-	5/39/115/115	-
12	CLA	A	844	23	1/1/15/20	6/39/115/115	-
12	CLA	B	826	2	-	2/21/97/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	CLA	A	802	1	1/1/13/20	5/27/103/115	-
19	DD6	U	213	-	-	13/26/80/80	0/3/3/3
12	CLA	B	829	23	1/1/15/20	8/39/115/115	-
12	CLA	B	818	2	-	1/17/93/115	-
15	BCR	B	841	-	-	7/29/63/63	0/2/2/2
12	CLA	U	207	11	1/1/11/20	3/15/91/115	-
12	CLA	U	209	11	1/1/11/20	4/17/93/115	-
12	CLA	B	802	2	1/1/15/20	2/39/115/115	-
15	BCR	L	201	-	-	9/29/63/63	0/2/2/2
16	CL0	A	847	1	1/1/20/25	3/37/135/135	-
12	CLA	B	823	2	1/1/15/20	9/39/115/115	-
12	CLA	A	818	23	1/1/15/20	2/39/115/115	-
12	CLA	A	825	1	-	6/39/115/115	-
12	CLA	B	843	2	1/1/15/20	5/39/115/115	-
12	CLA	B	830	2	1/1/13/20	0/31/107/115	-
15	BCR	I	102	-	-	10/29/63/63	0/2/2/2
12	CLA	B	834	2	-	4/39/115/115	-
15	BCR	A	840	-	-	10/29/63/63	0/2/2/2
14	LHG	A	838	-	-	21/52/52/53	-
12	CLA	A	823	1	1/1/15/20	4/39/115/115	-
12	CLA	A	824	1	1/1/14/20	3/36/112/115	-
12	CLA	A	830	1	-	0/21/97/115	-
12	CLA	A	834	1	1/1/15/20	5/39/115/115	-
12	CLA	B	815	2	1/1/13/20	6/32/108/115	-
12	CLA	L	203	9	-	0/39/115/115	-
12	CLA	L	204	23	1/1/12/20	2/21/97/115	-

All (765) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	U	203	A86	C13-C11	-6.36	1.37	1.49
12	B	845	CLA	MG-NA	5.09	2.18	2.06
12	B	822	CLA	MG-NA	4.91	2.17	2.06
12	A	826	CLA	MG-NA	4.91	2.17	2.06
12	B	830	CLA	MG-NA	4.84	2.17	2.06
12	A	834	CLA	MG-NA	4.83	2.17	2.06
12	A	845	CLA	MG-NA	4.72	2.17	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	B	810	CLA	MG-NA	4.70	2.17	2.06
12	A	823	CLA	MG-NA	4.68	2.17	2.06
12	A	823	CLA	C4C-C3C	-4.64	1.37	1.45
12	B	802	CLA	C4C-C3C	-4.59	1.37	1.45
12	B	822	CLA	C4C-C3C	-4.59	1.37	1.45
12	A	815	CLA	C4C-C3C	-4.58	1.37	1.45
12	A	828	CLA	MG-NA	4.57	2.17	2.06
12	B	804	CLA	C4C-C3C	-4.56	1.37	1.45
12	A	832	CLA	MG-NA	4.56	2.17	2.06
12	A	813	CLA	MG-NA	4.56	2.17	2.06
12	A	833	CLA	C4C-C3C	-4.55	1.37	1.45
12	B	843	CLA	MG-NA	4.55	2.17	2.06
12	B	813	CLA	C4C-C3C	-4.55	1.37	1.45
12	A	819	CLA	C4C-C3C	-4.54	1.37	1.45
12	A	845	CLA	C4C-C3C	-4.54	1.37	1.45
12	B	816	CLA	C4C-C3C	-4.54	1.37	1.45
12	A	808	CLA	C4C-C3C	-4.53	1.37	1.45
12	B	828	CLA	MG-NA	4.53	2.17	2.06
12	A	827	CLA	C4C-C3C	-4.52	1.37	1.45
12	A	817	CLA	C4C-C3C	-4.52	1.37	1.45
12	B	815	CLA	C4C-C3C	-4.52	1.37	1.45
12	A	825	CLA	MG-NA	4.52	2.17	2.06
12	B	808	CLA	C4C-C3C	-4.52	1.37	1.45
12	A	824	CLA	C4C-C3C	-4.51	1.37	1.45
12	B	834	CLA	C4C-C3C	-4.51	1.37	1.45
12	L	202	CLA	C4C-C3C	-4.51	1.37	1.45
12	B	817	CLA	C4C-C3C	-4.51	1.37	1.45
12	A	825	CLA	C4C-C3C	-4.50	1.37	1.45
12	B	812	CLA	C4C-C3C	-4.50	1.37	1.45
12	A	812	CLA	MG-NA	4.50	2.17	2.06
12	U	206	CLA	C4C-C3C	-4.50	1.37	1.45
12	A	822	CLA	C4C-C3C	-4.50	1.37	1.45
12	A	828	CLA	C4C-C3C	-4.50	1.37	1.45
12	A	809	CLA	C4C-C3C	-4.49	1.37	1.45
12	A	851	CLA	C4C-C3C	-4.49	1.37	1.45
12	A	814	CLA	C4C-C3C	-4.49	1.37	1.45
12	B	828	CLA	C4C-C3C	-4.49	1.37	1.45
12	B	818	CLA	C4C-C3C	-4.49	1.37	1.45
12	A	834	CLA	C4C-C3C	-4.48	1.37	1.45
12	B	805	CLA	C4C-C3C	-4.48	1.37	1.45
12	A	802	CLA	C4C-C3C	-4.48	1.37	1.45
12	A	807	CLA	C4C-C3C	-4.48	1.37	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	A	805	CLA	C4C-C3C	-4.47	1.37	1.45
12	A	832	CLA	C4C-C3C	-4.47	1.37	1.45
12	A	850	CLA	C4C-C3C	-4.47	1.37	1.45
12	A	806	CLA	C4C-C3C	-4.47	1.37	1.45
12	A	804	CLA	C4C-C3C	-4.47	1.37	1.45
12	A	848	CLA	C4C-C3C	-4.47	1.37	1.45
12	B	846	CLA	C4C-C3C	-4.47	1.37	1.45
12	U	205	CLA	C4C-C3C	-4.47	1.37	1.45
12	B	823	CLA	C4C-C3C	-4.47	1.37	1.45
12	B	806	CLA	C4C-C3C	-4.47	1.37	1.45
12	B	847	CLA	C4C-C3C	-4.47	1.37	1.45
12	B	832	CLA	C4C-C3C	-4.47	1.37	1.45
12	A	844	CLA	C4C-C3C	-4.46	1.37	1.45
12	B	844	CLA	C4C-C3C	-4.46	1.37	1.45
12	B	833	CLA	C4C-C3C	-4.46	1.37	1.45
12	U	212	CLA	C4C-C3C	-4.46	1.37	1.45
12	A	801	CLA	C4C-C3C	-4.46	1.37	1.45
12	U	201	CLA	C4C-C3C	-4.46	1.37	1.45
12	B	803	CLA	C4C-C3C	-4.46	1.37	1.45
12	B	814	CLA	C4C-C3C	-4.45	1.37	1.45
12	A	810	CLA	C4C-C3C	-4.45	1.37	1.45
12	B	820	CLA	C4C-C3C	-4.45	1.37	1.45
12	A	826	CLA	C4C-C3C	-4.45	1.37	1.45
12	U	207	CLA	C4C-C3C	-4.45	1.37	1.45
12	A	829	CLA	C4C-C3C	-4.44	1.37	1.45
12	A	831	CLA	C4C-C3C	-4.44	1.37	1.45
12	B	827	CLA	C4C-C3C	-4.44	1.37	1.45
12	A	813	CLA	C4C-C3C	-4.43	1.37	1.45
12	J	103	CLA	C4C-C3C	-4.43	1.37	1.45
12	B	807	CLA	C4C-C3C	-4.43	1.37	1.45
12	B	824	CLA	C4C-C3C	-4.43	1.37	1.45
12	L	203	CLA	C4C-C3C	-4.43	1.37	1.45
12	A	852	CLA	C4C-C3C	-4.43	1.37	1.45
12	B	825	CLA	C4C-C3C	-4.42	1.37	1.45
12	A	820	CLA	C4C-C3C	-4.42	1.37	1.45
12	B	801	CLA	C4C-C3C	-4.42	1.37	1.45
12	U	207	CLA	MG-NA	4.42	2.16	2.06
12	A	836	CLA	C4C-C3C	-4.42	1.37	1.45
12	B	804	CLA	MG-NA	4.41	2.16	2.06
12	B	831	CLA	C4C-C3C	-4.41	1.37	1.45
12	U	208	CLA	C4C-C3C	-4.41	1.37	1.45
12	B	819	CLA	C4C-C3C	-4.41	1.37	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	L	204	CLA	C4C-C3C	-4.41	1.37	1.45
12	U	211	CLA	C4C-C3C	-4.41	1.37	1.45
12	B	821	CLA	C4C-C3C	-4.40	1.37	1.45
12	A	835	CLA	C4C-C3C	-4.40	1.37	1.45
12	U	209	CLA	C4C-C3C	-4.39	1.37	1.45
12	B	835	CLA	C4C-C3C	-4.39	1.37	1.45
12	A	803	CLA	C4C-C3C	-4.38	1.37	1.45
12	B	830	CLA	C4C-C3C	-4.38	1.37	1.45
12	B	810	CLA	C4C-C3C	-4.38	1.37	1.45
12	F	803	CLA	C4C-C3C	-4.38	1.37	1.45
12	B	811	CLA	C4C-C3C	-4.37	1.37	1.45
22	U	214	KC1	C4C-C3C	-4.36	1.37	1.45
12	A	830	CLA	C4C-C3C	-4.36	1.37	1.45
12	A	821	CLA	MG-NA	4.36	2.16	2.06
12	A	821	CLA	C4C-C3C	-4.36	1.37	1.45
12	F	802	CLA	C4C-C3C	-4.36	1.37	1.45
12	A	816	CLA	C4C-C3C	-4.35	1.37	1.45
12	A	811	CLA	C4C-C3C	-4.35	1.37	1.45
12	B	809	CLA	C4C-C3C	-4.34	1.37	1.45
12	B	848	CLA	C4C-C3C	-4.34	1.37	1.45
12	U	210	CLA	C4C-C3C	-4.34	1.37	1.45
12	B	845	CLA	C4C-C3C	-4.34	1.37	1.45
12	A	835	CLA	MG-NA	4.33	2.16	2.06
12	B	848	CLA	MG-NA	4.33	2.16	2.06
12	B	827	CLA	MG-NA	4.33	2.16	2.06
12	B	826	CLA	C4C-C3C	-4.33	1.37	1.45
12	B	814	CLA	MG-NA	4.31	2.16	2.06
12	A	818	CLA	C4C-C3C	-4.31	1.37	1.45
12	A	846	CLA	C4C-C3C	-4.31	1.37	1.45
12	B	829	CLA	C4C-C3C	-4.31	1.37	1.45
12	B	803	CLA	C1C-C2C	-4.27	1.35	1.44
12	B	824	CLA	MG-NA	4.26	2.16	2.06
12	A	805	CLA	MG-NA	4.26	2.16	2.06
12	B	809	CLA	C1C-C2C	-4.26	1.35	1.44
12	U	212	CLA	MG-NA	4.24	2.16	2.06
12	A	812	CLA	C4C-C3C	-4.24	1.37	1.45
12	B	808	CLA	C1C-C2C	-4.23	1.35	1.44
12	A	829	CLA	C1C-C2C	-4.23	1.35	1.44
12	A	808	CLA	MG-NA	4.23	2.16	2.06
12	B	843	CLA	C4C-C3C	-4.22	1.37	1.45
12	A	809	CLA	MG-NA	4.22	2.16	2.06
12	B	813	CLA	MG-NA	4.21	2.16	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	B	825	CLA	MG-NA	4.19	2.16	2.06
12	B	820	CLA	C1C-C2C	-4.18	1.36	1.44
12	A	811	CLA	MG-NA	4.17	2.16	2.06
12	A	812	CLA	C1C-C2C	-4.17	1.36	1.44
12	A	823	CLA	C1C-C2C	-4.17	1.36	1.44
12	B	834	CLA	C1C-C2C	-4.17	1.36	1.44
12	B	834	CLA	MG-NA	4.16	2.16	2.06
12	F	802	CLA	MG-NA	4.16	2.16	2.06
12	U	211	CLA	C1C-C2C	-4.16	1.36	1.44
12	A	830	CLA	C1C-C2C	-4.15	1.36	1.44
12	A	827	CLA	C1C-C2C	-4.15	1.36	1.44
12	A	820	CLA	C1C-C2C	-4.15	1.36	1.44
12	A	848	CLA	MG-NA	4.15	2.16	2.06
12	B	832	CLA	MG-NA	4.14	2.16	2.06
12	A	815	CLA	MG-NA	4.14	2.16	2.06
12	B	823	CLA	MG-NA	4.14	2.16	2.06
12	A	803	CLA	C1C-C2C	-4.14	1.36	1.44
12	A	818	CLA	C1C-C2C	-4.14	1.36	1.44
12	A	828	CLA	C1C-C2C	-4.14	1.36	1.44
12	A	827	CLA	MG-NA	4.13	2.16	2.06
12	B	816	CLA	C1C-C2C	-4.12	1.36	1.44
12	B	806	CLA	MG-NA	4.12	2.16	2.06
12	A	846	CLA	C1C-C2C	-4.12	1.36	1.44
12	A	829	CLA	MG-NA	4.12	2.16	2.06
12	A	836	CLA	C1C-C2C	-4.12	1.36	1.44
12	B	822	CLA	C1C-C2C	-4.11	1.36	1.44
12	A	826	CLA	C1C-C2C	-4.11	1.36	1.44
12	A	807	CLA	C1C-C2C	-4.11	1.36	1.44
12	B	818	CLA	C1C-C2C	-4.11	1.36	1.44
12	B	811	CLA	C1C-C2C	-4.11	1.36	1.44
22	U	214	KC1	C3B-C4B	-4.11	1.38	1.46
12	A	810	CLA	MG-NA	4.10	2.16	2.06
12	A	824	CLA	MG-NA	4.10	2.16	2.06
12	B	828	CLA	C1C-C2C	-4.10	1.36	1.44
12	B	819	CLA	C1C-C2C	-4.10	1.36	1.44
12	A	848	CLA	C1C-C2C	-4.10	1.36	1.44
12	B	829	CLA	C1C-C2C	-4.10	1.36	1.44
12	B	809	CLA	MG-NA	4.09	2.16	2.06
12	A	811	CLA	C1C-C2C	-4.09	1.36	1.44
12	A	825	CLA	C1C-C2C	-4.09	1.36	1.44
12	U	201	CLA	C1C-C2C	-4.09	1.36	1.44
12	A	846	CLA	MG-NA	4.08	2.16	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	B	843	CLA	C1C-C2C	-4.08	1.36	1.44
12	B	802	CLA	C1C-C2C	-4.08	1.36	1.44
12	A	816	CLA	C1C-C2C	-4.07	1.36	1.44
12	L	202	CLA	C1C-C2C	-4.07	1.36	1.44
12	B	824	CLA	C1C-C2C	-4.07	1.36	1.44
12	B	846	CLA	C1C-C2C	-4.07	1.36	1.44
12	L	203	CLA	C1C-C2C	-4.06	1.36	1.44
12	B	825	CLA	C1C-C2C	-4.06	1.36	1.44
12	A	819	CLA	C1C-C2C	-4.06	1.36	1.44
12	B	823	CLA	C1C-C2C	-4.06	1.36	1.44
12	A	831	CLA	C1C-C2C	-4.06	1.36	1.44
12	U	212	CLA	C1C-C2C	-4.05	1.36	1.44
12	A	813	CLA	C1C-C2C	-4.05	1.36	1.44
12	B	801	CLA	C1C-C2C	-4.05	1.36	1.44
12	B	810	CLA	C1C-C2C	-4.05	1.36	1.44
12	U	207	CLA	C1C-C2C	-4.05	1.36	1.44
12	A	804	CLA	C1C-C2C	-4.05	1.36	1.44
12	B	832	CLA	C1C-C2C	-4.04	1.36	1.44
12	B	827	CLA	C1C-C2C	-4.04	1.36	1.44
12	A	832	CLA	C1C-C2C	-4.04	1.36	1.44
12	A	850	CLA	C1C-C2C	-4.04	1.36	1.44
12	U	208	CLA	C1C-C2C	-4.04	1.36	1.44
12	B	820	CLA	MG-NA	4.04	2.15	2.06
12	B	812	CLA	C1C-C2C	-4.04	1.36	1.44
12	B	805	CLA	C1C-C2C	-4.03	1.36	1.44
12	A	801	CLA	C1C-C2C	-4.03	1.36	1.44
12	A	821	CLA	C1C-C2C	-4.03	1.36	1.44
12	J	103	CLA	C1C-C2C	-4.03	1.36	1.44
12	B	826	CLA	C1C-C2C	-4.03	1.36	1.44
12	A	809	CLA	C1C-C2C	-4.03	1.36	1.44
12	A	833	CLA	MG-NA	4.03	2.15	2.06
12	B	847	CLA	MG-NA	4.03	2.15	2.06
12	F	803	CLA	C1C-C2C	-4.02	1.36	1.44
12	B	807	CLA	C1C-C2C	-4.02	1.36	1.44
12	B	806	CLA	C1C-C2C	-4.02	1.36	1.44
12	A	808	CLA	C1C-C2C	-4.02	1.36	1.44
12	F	802	CLA	C1C-C2C	-4.02	1.36	1.44
12	A	814	CLA	C1C-C2C	-4.02	1.36	1.44
12	A	806	CLA	C1C-C2C	-4.01	1.36	1.44
12	A	845	CLA	C1C-C2C	-4.01	1.36	1.44
12	U	209	CLA	C1C-C2C	-4.01	1.36	1.44
12	A	817	CLA	C1C-C2C	-4.01	1.36	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	B	831	CLA	C1C-C2C	-4.01	1.36	1.44
12	L	204	CLA	C1C-C2C	-4.01	1.36	1.44
12	B	826	CLA	MG-NA	4.00	2.15	2.06
12	A	835	CLA	C1C-C2C	-4.00	1.36	1.44
12	A	844	CLA	C1C-C2C	-4.00	1.36	1.44
12	B	848	CLA	C1C-C2C	-4.00	1.36	1.44
12	U	205	CLA	C1C-C2C	-4.00	1.36	1.44
12	A	805	CLA	C1C-C2C	-4.00	1.36	1.44
12	A	815	CLA	C1C-C2C	-4.00	1.36	1.44
12	B	801	CLA	MG-NA	4.00	2.15	2.06
12	A	851	CLA	C1C-C2C	-3.99	1.36	1.44
12	A	822	CLA	C1C-C2C	-3.99	1.36	1.44
12	B	847	CLA	C1C-C2C	-3.99	1.36	1.44
12	U	206	CLA	C1C-C2C	-3.99	1.36	1.44
12	B	845	CLA	C1C-C2C	-3.99	1.36	1.44
12	A	833	CLA	C1C-C2C	-3.99	1.36	1.44
22	U	214	KC1	C1C-C2C	-3.99	1.36	1.44
12	B	815	CLA	C1C-C2C	-3.99	1.36	1.44
12	B	821	CLA	C1C-C2C	-3.98	1.36	1.44
12	A	817	CLA	MG-NA	3.98	2.15	2.06
12	A	851	CLA	MG-NA	3.98	2.15	2.06
12	B	835	CLA	C1C-C2C	-3.98	1.36	1.44
12	A	807	CLA	MG-NA	3.98	2.15	2.06
12	B	835	CLA	MG-NA	3.97	2.15	2.06
12	B	814	CLA	C1C-C2C	-3.97	1.36	1.44
12	B	804	CLA	C1C-C2C	-3.97	1.36	1.44
12	A	802	CLA	C1C-C2C	-3.97	1.36	1.44
12	B	833	CLA	C1C-C2C	-3.97	1.36	1.44
12	A	834	CLA	C1C-C2C	-3.97	1.36	1.44
12	A	852	CLA	C1C-C2C	-3.96	1.36	1.44
12	A	852	CLA	MG-NA	3.96	2.15	2.06
12	B	844	CLA	C1C-C2C	-3.96	1.36	1.44
12	B	813	CLA	C1C-C2C	-3.96	1.36	1.44
12	A	810	CLA	C1C-C2C	-3.96	1.36	1.44
12	B	817	CLA	C1C-C2C	-3.96	1.36	1.44
12	B	807	CLA	MG-NA	3.96	2.15	2.06
12	A	824	CLA	C1C-C2C	-3.95	1.36	1.44
12	L	202	CLA	MG-NA	3.95	2.15	2.06
12	B	831	CLA	MG-NA	3.94	2.15	2.06
12	B	830	CLA	C1C-C2C	-3.94	1.36	1.44
12	B	808	CLA	MG-NA	3.94	2.15	2.06
12	B	833	CLA	MG-NA	3.93	2.15	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	B	816	CLA	MG-NA	3.92	2.15	2.06
12	A	816	CLA	MG-NA	3.89	2.15	2.06
12	B	802	CLA	MG-NA	3.86	2.15	2.06
22	U	214	KC1	MG-NA	3.86	2.15	2.06
12	U	206	CLA	MG-NA	3.84	2.15	2.06
12	U	205	CLA	MG-NA	3.83	2.15	2.06
12	B	844	CLA	MG-NA	3.83	2.15	2.06
12	U	201	CLA	MG-NA	3.83	2.15	2.06
12	U	210	CLA	C1C-C2C	-3.83	1.36	1.44
12	A	814	CLA	MG-NA	3.82	2.15	2.06
12	F	803	CLA	MG-NA	3.81	2.15	2.06
12	B	805	CLA	MG-NA	3.81	2.15	2.06
12	L	204	CLA	MG-NA	3.79	2.15	2.06
12	A	819	CLA	MG-NA	3.77	2.15	2.06
12	A	804	CLA	MG-NA	3.77	2.15	2.06
12	B	812	CLA	MG-NA	3.76	2.15	2.06
12	A	836	CLA	MG-NA	3.72	2.15	2.06
12	L	203	CLA	MG-NA	3.69	2.15	2.06
12	A	820	CLA	MG-NA	3.69	2.15	2.06
12	B	817	CLA	MG-NA	3.67	2.15	2.06
12	A	850	CLA	MG-NA	3.65	2.14	2.06
22	U	214	KC1	C4A-C3A	-3.64	1.37	1.44
12	A	830	CLA	MG-NA	3.63	2.14	2.06
12	A	844	CLA	MG-NA	3.63	2.14	2.06
12	B	818	CLA	MG-NA	3.63	2.14	2.06
12	A	818	CLA	MG-NA	3.62	2.14	2.06
12	A	834	CLA	MG-NC	3.60	2.14	2.06
12	A	802	CLA	MG-NA	3.59	2.14	2.06
12	B	815	CLA	MG-NA	3.58	2.14	2.06
12	B	802	CLA	MG-NC	3.57	2.14	2.06
12	A	803	CLA	MG-NA	3.57	2.14	2.06
12	A	806	CLA	MG-NA	3.56	2.14	2.06
12	U	211	CLA	MG-NA	3.55	2.14	2.06
12	B	846	CLA	MG-NA	3.55	2.14	2.06
12	B	829	CLA	MG-NA	3.55	2.14	2.06
15	B	837	BCR	C1-C6	-3.53	1.49	1.53
12	A	845	CLA	MG-NC	3.51	2.14	2.06
12	A	831	CLA	MG-NA	3.50	2.14	2.06
12	B	821	CLA	MG-NA	3.49	2.14	2.06
12	B	819	CLA	MG-NA	3.49	2.14	2.06
19	U	215	DD6	C8-C6	-3.42	1.41	1.50
12	A	801	CLA	MG-NA	3.42	2.14	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	J	104	BCR	C30-C25	-3.41	1.49	1.53
19	U	215	DD6	C26-C27	3.41	1.44	1.37
12	U	209	CLA	MG-NA	3.39	2.14	2.06
22	U	214	KC1	C1B-C2B	-3.37	1.38	1.45
12	J	103	CLA	MG-NA	3.37	2.14	2.06
12	A	822	CLA	MG-NA	3.36	2.14	2.06
15	A	843	BCR	C1-C6	-3.34	1.49	1.53
12	B	803	CLA	MG-NA	3.34	2.14	2.06
15	L	205	BCR	C30-C25	-3.29	1.49	1.53
15	B	840	BCR	C1-C6	-3.29	1.49	1.53
15	L	201	BCR	C1-C6	-3.28	1.49	1.53
12	B	811	CLA	MG-NA	3.28	2.14	2.06
15	B	841	BCR	C30-C25	-3.28	1.49	1.53
15	A	841	BCR	C1-C6	-3.26	1.49	1.53
15	I	102	BCR	C30-C25	-3.23	1.49	1.53
15	I	102	BCR	C1-C6	-3.22	1.49	1.53
15	L	201	BCR	C30-C25	-3.22	1.49	1.53
19	U	204	DD6	C26-C27	3.20	1.43	1.37
22	U	214	KC1	MG-NC	3.19	2.13	2.06
12	U	210	CLA	MG-NC	3.18	2.13	2.06
12	A	828	CLA	MG-NC	3.13	2.13	2.06
12	B	834	CLA	MG-NC	3.11	2.13	2.06
12	B	830	CLA	MG-NC	3.10	2.13	2.06
15	B	841	BCR	C1-C6	-3.09	1.49	1.53
12	A	826	CLA	MG-NC	3.09	2.13	2.06
15	F	804	BCR	C1-C6	-3.09	1.49	1.53
15	A	841	BCR	C30-C25	-3.07	1.49	1.53
12	A	835	CLA	MG-NC	3.07	2.13	2.06
12	B	810	CLA	MG-NC	3.07	2.13	2.06
12	U	208	CLA	MG-NA	3.03	2.13	2.06
16	A	847	CL0	CHB-C1B	3.01	1.44	1.39
15	M	101	BCR	C30-C25	-3.01	1.49	1.53
12	B	814	CLA	MG-NC	2.99	2.13	2.06
12	A	812	CLA	MG-NC	2.98	2.13	2.06
12	A	848	CLA	MG-NC	2.98	2.13	2.06
15	B	840	BCR	C30-C25	-2.96	1.50	1.53
12	A	827	CLA	MG-NC	2.96	2.13	2.06
15	F	801	BCR	C1-C6	-2.94	1.50	1.53
12	B	845	CLA	MG-NC	2.91	2.13	2.06
12	A	808	CLA	MG-NC	2.89	2.13	2.06
12	B	843	CLA	MG-NC	2.89	2.13	2.06
12	B	823	CLA	MG-NC	2.88	2.13	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	J	101	DD6	C26-C27	2.88	1.43	1.37
15	F	801	BCR	C30-C25	-2.87	1.50	1.53
12	U	210	CLA	MG-NA	2.87	2.13	2.06
15	I	101	BCR	C1-C6	-2.87	1.50	1.53
16	A	847	CL0	C3B-C4B	-2.86	1.38	1.41
15	M	101	BCR	C1-C6	-2.82	1.50	1.53
12	A	805	CLA	MG-NC	2.80	2.12	2.06
12	B	828	CLA	MG-NC	2.79	2.12	2.06
15	J	104	BCR	C1-C6	-2.79	1.50	1.53
15	B	839	BCR	C1-C6	-2.78	1.50	1.53
19	U	213	DD6	C26-C27	2.77	1.42	1.37
15	A	842	BCR	C1-C6	-2.76	1.50	1.53
12	B	826	CLA	MG-NC	2.75	2.12	2.06
12	A	821	CLA	MG-NC	2.72	2.12	2.06
12	B	807	CLA	MG-NC	2.71	2.12	2.06
15	A	842	BCR	C30-C25	-2.71	1.50	1.53
12	B	832	CLA	MG-NC	2.71	2.12	2.06
12	A	813	CLA	MG-NC	2.71	2.12	2.06
15	L	205	BCR	C1-C6	-2.69	1.50	1.53
12	A	811	CLA	MG-NC	2.67	2.12	2.06
12	A	824	CLA	MG-NC	2.67	2.12	2.06
15	B	839	BCR	C30-C25	-2.65	1.50	1.53
15	A	840	BCR	C1-C6	-2.64	1.50	1.53
15	B	837	BCR	C30-C25	-2.64	1.50	1.53
12	B	804	CLA	MG-NC	2.63	2.12	2.06
12	B	805	CLA	MG-NC	2.63	2.12	2.06
12	U	207	CLA	MG-NC	2.63	2.12	2.06
15	A	843	BCR	C30-C25	-2.61	1.50	1.53
12	B	817	CLA	C1B-C2B	-2.61	1.37	1.43
12	B	802	CLA	C1D-C2D	-2.61	1.40	1.45
12	B	846	CLA	C3D-C4D	-2.59	1.38	1.44
12	A	827	CLA	C3D-C4D	-2.59	1.38	1.44
12	B	819	CLA	C3D-C4D	-2.59	1.38	1.44
12	A	832	CLA	MG-NC	2.59	2.12	2.06
12	B	813	CLA	MG-NC	2.58	2.12	2.06
12	B	827	CLA	MG-NC	2.58	2.12	2.06
12	B	824	CLA	MG-NC	2.57	2.12	2.06
15	A	840	BCR	C30-C25	-2.57	1.50	1.53
12	A	846	CLA	MG-NC	2.56	2.12	2.06
12	B	817	CLA	C3D-C4D	-2.56	1.38	1.44
12	B	807	CLA	C3D-C4D	-2.55	1.38	1.44
12	F	802	CLA	MG-NC	2.55	2.12	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	A	830	CLA	MG-NC	2.55	2.12	2.06
12	A	809	CLA	MG-NC	2.55	2.12	2.06
12	A	822	CLA	C3D-C4D	-2.54	1.38	1.44
12	B	825	CLA	C3D-C4D	-2.54	1.38	1.44
12	B	801	CLA	MG-NC	2.54	2.12	2.06
12	A	803	CLA	C3D-C4D	-2.54	1.38	1.44
12	A	825	CLA	MG-NC	2.54	2.12	2.06
12	A	827	CLA	C1D-C2D	-2.54	1.40	1.45
12	B	815	CLA	C3D-C4D	-2.54	1.38	1.44
12	B	812	CLA	C3D-C4D	-2.53	1.38	1.44
12	B	821	CLA	C3D-C4D	-2.53	1.38	1.44
12	A	851	CLA	MG-NC	2.53	2.12	2.06
12	U	209	CLA	C3D-C4D	-2.52	1.38	1.44
12	B	830	CLA	C3D-C4D	-2.52	1.38	1.44
12	B	834	CLA	C3D-C4D	-2.52	1.38	1.44
12	B	826	CLA	C3D-C4D	-2.52	1.38	1.44
12	B	833	CLA	C3D-C4D	-2.52	1.38	1.44
12	U	208	CLA	C3D-C4D	-2.51	1.38	1.44
12	A	829	CLA	C3D-C4D	-2.51	1.38	1.44
12	B	831	CLA	MG-NC	2.51	2.12	2.06
15	F	804	BCR	C30-C25	-2.51	1.50	1.53
12	B	844	CLA	C3D-C4D	-2.50	1.38	1.44
12	B	806	CLA	C3D-C4D	-2.50	1.38	1.44
19	U	213	DD6	C10-C11	2.49	1.41	1.35
12	B	806	CLA	MG-NC	2.49	2.12	2.06
12	B	805	CLA	C3D-C4D	-2.49	1.38	1.44
12	B	824	CLA	C3D-C4D	-2.48	1.38	1.44
12	A	806	CLA	C3D-C4D	-2.48	1.38	1.44
12	A	818	CLA	C3D-C4D	-2.48	1.38	1.44
12	B	808	CLA	C3D-C4D	-2.48	1.38	1.44
12	A	823	CLA	C1D-C2D	-2.48	1.40	1.45
12	B	848	CLA	C1B-C2B	-2.48	1.37	1.43
12	B	810	CLA	C3D-C4D	-2.47	1.38	1.44
12	U	205	CLA	C3D-C4D	-2.47	1.38	1.44
12	A	819	CLA	C3D-C4D	-2.47	1.38	1.44
12	L	203	CLA	C3D-C4D	-2.47	1.38	1.44
12	A	811	CLA	C3D-C4D	-2.47	1.38	1.44
12	B	812	CLA	MG-NC	2.47	2.12	2.06
12	B	831	CLA	C3D-C4D	-2.46	1.38	1.44
12	A	835	CLA	C3D-C4D	-2.46	1.38	1.44
12	A	850	CLA	C3D-C4D	-2.46	1.38	1.44
12	A	845	CLA	C3D-C4D	-2.46	1.38	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	A	816	CLA	C3D-C4D	-2.46	1.38	1.44
12	A	831	CLA	C3D-C4D	-2.45	1.38	1.44
12	A	836	CLA	C3D-C4D	-2.45	1.38	1.44
12	B	814	CLA	C3D-C4D	-2.45	1.38	1.44
12	B	845	CLA	MG-NB	2.45	2.10	2.05
12	A	817	CLA	C3D-C4D	-2.45	1.38	1.44
15	B	838	BCR	C1-C6	-2.45	1.50	1.53
12	B	822	CLA	C3D-C4D	-2.45	1.38	1.44
12	A	820	CLA	C3D-C4D	-2.45	1.38	1.44
21	U	203	A86	C2-C1	2.45	1.41	1.35
12	B	827	CLA	C3D-C4D	-2.45	1.38	1.44
12	B	825	CLA	MG-NC	2.45	2.12	2.06
12	A	852	CLA	C3D-C4D	-2.45	1.38	1.44
22	U	214	KC1	C1A-CHA	2.44	1.46	1.40
12	B	829	CLA	C3D-C4D	-2.44	1.38	1.44
12	B	822	CLA	C1D-C2D	-2.44	1.40	1.45
12	A	829	CLA	MG-NC	2.44	2.12	2.06
12	A	802	CLA	C3D-C4D	-2.44	1.38	1.44
12	A	848	CLA	C3D-C4D	-2.44	1.38	1.44
19	U	215	DD6	C2-C1	2.44	1.41	1.35
19	U	204	DD6	C10-C11	2.44	1.41	1.35
12	A	825	CLA	C3D-C4D	-2.44	1.38	1.44
12	A	851	CLA	C3D-C4D	-2.44	1.38	1.44
19	U	204	DD6	C2-C1	2.43	1.41	1.35
12	A	809	CLA	C3D-C4D	-2.43	1.38	1.44
12	B	848	CLA	MG-NC	2.43	2.12	2.06
12	A	833	CLA	C3D-C4D	-2.43	1.38	1.44
12	A	823	CLA	C3D-C4D	-2.43	1.38	1.44
12	A	804	CLA	C3D-C4D	-2.43	1.38	1.44
12	B	823	CLA	C3D-C4D	-2.43	1.38	1.44
12	A	830	CLA	C3D-C4D	-2.43	1.38	1.44
21	U	203	A86	C5-C6	2.42	1.41	1.35
12	A	828	CLA	C3D-C4D	-2.42	1.38	1.44
12	B	848	CLA	C3D-C4D	-2.42	1.38	1.44
12	B	822	CLA	MG-NC	2.42	2.12	2.06
12	A	846	CLA	C3D-C4D	-2.42	1.38	1.44
12	B	832	CLA	C3D-C4D	-2.41	1.38	1.44
19	U	213	DD6	C5-C6	2.41	1.41	1.35
12	A	801	CLA	C3D-C4D	-2.41	1.38	1.44
12	A	815	CLA	C3D-C4D	-2.41	1.38	1.44
12	B	845	CLA	C3D-C4D	-2.41	1.38	1.44
12	A	814	CLA	C3D-C4D	-2.41	1.38	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	F	803	CLA	C3D-C4D	-2.41	1.38	1.44
12	A	823	CLA	MG-NC	2.41	2.12	2.06
12	A	805	CLA	C3D-C4D	-2.41	1.38	1.44
12	B	820	CLA	C3D-C4D	-2.41	1.38	1.44
12	B	802	CLA	C3D-C4D	-2.40	1.38	1.44
12	A	810	CLA	C3D-C4D	-2.40	1.38	1.44
12	B	843	CLA	C3D-C4D	-2.40	1.38	1.44
12	U	201	CLA	C3D-C4D	-2.40	1.38	1.44
12	A	824	CLA	C3D-C4D	-2.40	1.38	1.44
12	A	826	CLA	C1D-C2D	-2.40	1.40	1.45
12	A	808	CLA	C3D-C4D	-2.40	1.38	1.44
12	U	206	CLA	C3D-C4D	-2.40	1.38	1.44
19	J	101	DD6	C2-C1	2.39	1.41	1.35
12	L	204	CLA	C3D-C4D	-2.39	1.38	1.44
12	B	809	CLA	C1D-C2D	-2.39	1.40	1.45
12	B	847	CLA	C3D-C4D	-2.39	1.38	1.44
12	U	207	CLA	C3D-C4D	-2.39	1.38	1.44
12	B	833	CLA	C1B-C2B	-2.39	1.37	1.43
12	A	813	CLA	C3D-C4D	-2.39	1.38	1.44
19	U	204	DD6	C5-C6	2.39	1.41	1.35
12	B	808	CLA	C1D-C2D	-2.39	1.40	1.45
12	B	818	CLA	C3D-C4D	-2.38	1.38	1.44
12	B	811	CLA	C3D-C4D	-2.38	1.38	1.44
12	B	816	CLA	C3D-C4D	-2.38	1.38	1.44
12	L	202	CLA	C3D-C4D	-2.38	1.38	1.44
19	U	215	DD6	C5-C6	2.38	1.41	1.34
15	B	838	BCR	C30-C25	-2.38	1.50	1.53
12	F	802	CLA	C3D-C4D	-2.38	1.38	1.44
12	J	103	CLA	C3D-C4D	-2.38	1.38	1.44
12	A	850	CLA	MG-NC	2.38	2.11	2.06
19	U	213	DD6	C2-C1	2.38	1.41	1.35
12	B	809	CLA	MG-NC	2.37	2.11	2.06
12	A	825	CLA	C1D-C2D	-2.37	1.40	1.45
12	B	809	CLA	C3D-C4D	-2.37	1.38	1.44
12	B	808	CLA	MG-NC	2.37	2.11	2.06
12	A	816	CLA	C1B-C2B	-2.37	1.37	1.43
12	A	807	CLA	C3D-C4D	-2.37	1.38	1.44
12	A	810	CLA	MG-NC	2.36	2.11	2.06
12	B	804	CLA	C3D-C4D	-2.36	1.38	1.44
12	B	813	CLA	C3D-C4D	-2.36	1.38	1.44
12	A	832	CLA	C3D-C4D	-2.35	1.38	1.44
12	A	817	CLA	C1D-C2D	-2.35	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	A	834	CLA	C3D-C4D	-2.35	1.38	1.44
19	J	101	DD6	C13-C11	-2.35	1.40	1.46
12	B	815	CLA	C1B-C2B	-2.35	1.37	1.43
12	B	820	CLA	MG-NC	2.35	2.11	2.06
12	B	807	CLA	C1D-C2D	-2.35	1.40	1.45
12	U	211	CLA	C3D-C4D	-2.34	1.38	1.44
12	A	815	CLA	MG-NC	2.34	2.11	2.06
12	B	835	CLA	C3D-C4D	-2.34	1.38	1.44
12	A	821	CLA	C3D-C4D	-2.34	1.38	1.44
12	A	812	CLA	C3D-C4D	-2.34	1.38	1.44
12	U	206	CLA	MG-NC	2.33	2.11	2.06
12	A	828	CLA	C1D-C2D	-2.33	1.40	1.45
12	A	844	CLA	C3D-C4D	-2.33	1.38	1.44
12	B	845	CLA	C1D-C2D	-2.33	1.40	1.45
12	B	803	CLA	C1D-C2D	-2.33	1.40	1.45
12	A	807	CLA	C1D-C2D	-2.33	1.40	1.45
12	A	826	CLA	C3D-C4D	-2.33	1.38	1.44
12	B	830	CLA	C1D-C2D	-2.33	1.40	1.45
12	B	835	CLA	MG-NC	2.33	2.11	2.06
12	U	212	CLA	C3D-C4D	-2.32	1.39	1.44
12	A	852	CLA	C1B-C2B	-2.32	1.37	1.43
12	B	833	CLA	C1D-C2D	-2.32	1.40	1.45
19	J	101	DD6	C5-C6	2.32	1.41	1.35
12	L	202	CLA	MG-NC	2.32	2.11	2.06
12	A	801	CLA	C1B-C2B	-2.31	1.37	1.43
12	A	845	CLA	C1D-C2D	-2.31	1.40	1.45
12	B	823	CLA	C1D-C2D	-2.31	1.40	1.45
12	U	212	CLA	MG-NC	2.31	2.11	2.06
12	A	810	CLA	C1D-C2D	-2.31	1.40	1.45
12	A	803	CLA	MG-NC	2.31	2.11	2.06
12	B	845	CLA	C1B-C2B	-2.31	1.37	1.43
12	A	836	CLA	C1B-C2B	-2.31	1.37	1.43
12	A	834	CLA	C1B-C2B	-2.31	1.37	1.43
12	A	833	CLA	C1B-C2B	-2.30	1.37	1.43
12	A	810	CLA	C1B-C2B	-2.30	1.37	1.43
12	A	814	CLA	C1B-C2B	-2.30	1.37	1.43
15	I	101	BCR	C30-C25	-2.30	1.50	1.53
19	J	101	DD6	C10-C11	2.30	1.41	1.35
12	A	852	CLA	MG-NC	2.30	2.11	2.06
12	B	810	CLA	CAB-C3B	-2.30	1.46	1.50
12	B	828	CLA	C3D-C4D	-2.30	1.39	1.44
12	A	835	CLA	C1B-C2B	-2.30	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	B	813	CLA	C1D-C2D	-2.29	1.40	1.45
12	B	844	CLA	MG-NC	2.29	2.11	2.06
12	U	206	CLA	C1D-C2D	-2.29	1.40	1.45
12	B	816	CLA	MG-NC	2.29	2.11	2.06
12	B	828	CLA	C1D-C2D	-2.29	1.40	1.45
12	B	820	CLA	C1D-C2D	-2.28	1.40	1.45
12	B	803	CLA	C3D-C4D	-2.28	1.39	1.44
12	B	829	CLA	C1B-C2B	-2.28	1.37	1.43
12	B	801	CLA	C3D-C4D	-2.28	1.39	1.44
12	A	817	CLA	C1B-C2B	-2.28	1.37	1.43
12	A	801	CLA	C1D-C2D	-2.27	1.40	1.45
12	U	210	CLA	C3D-C4D	-2.27	1.39	1.44
12	B	808	CLA	C1B-C2B	-2.27	1.37	1.43
12	B	830	CLA	C1B-C2B	-2.27	1.37	1.43
12	A	846	CLA	C1B-C2B	-2.27	1.37	1.43
12	A	831	CLA	C1B-C2B	-2.27	1.37	1.43
12	A	836	CLA	C1D-C2D	-2.27	1.40	1.45
12	A	804	CLA	MG-NC	2.26	2.11	2.06
12	A	818	CLA	C1B-C2B	-2.26	1.37	1.43
12	U	205	CLA	C1D-C2D	-2.26	1.40	1.45
12	A	816	CLA	MG-NC	2.26	2.11	2.06
12	B	817	CLA	C1D-C2D	-2.26	1.40	1.45
12	B	819	CLA	C1D-C2D	-2.26	1.40	1.45
12	B	822	CLA	C1B-C2B	-2.26	1.37	1.43
12	A	832	CLA	C1B-C2B	-2.26	1.37	1.43
12	A	815	CLA	C1B-C2B	-2.25	1.37	1.43
12	A	852	CLA	C1D-C2D	-2.25	1.40	1.45
12	B	806	CLA	C1D-C2D	-2.25	1.40	1.45
12	A	835	CLA	C1D-C2D	-2.25	1.40	1.45
12	B	825	CLA	C1D-C2D	-2.25	1.40	1.45
12	L	203	CLA	MG-NC	2.24	2.11	2.06
12	A	817	CLA	MG-NC	2.24	2.11	2.06
12	B	804	CLA	C1D-C2D	-2.24	1.40	1.45
19	J	101	DD6	C24-C1	-2.24	1.41	1.46
12	B	802	CLA	CHB-C1B	2.23	1.44	1.39
19	U	204	DD6	C13-C11	-2.23	1.41	1.46
12	A	824	CLA	C1D-C2D	-2.23	1.40	1.45
12	F	803	CLA	C1B-C2B	-2.23	1.37	1.43
12	A	820	CLA	C1B-C2B	-2.23	1.37	1.43
12	A	821	CLA	C1D-C2D	-2.23	1.40	1.45
12	U	212	CLA	C1B-C2B	-2.23	1.37	1.43
12	A	834	CLA	MG-NB	2.23	2.10	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	U	209	CLA	C1B-C2B	-2.22	1.37	1.43
12	B	847	CLA	MG-NC	2.22	2.11	2.06
12	A	815	CLA	C1D-C2D	-2.22	1.40	1.45
12	B	835	CLA	C1B-C2B	-2.22	1.37	1.43
12	A	836	CLA	MG-NC	2.22	2.11	2.06
12	L	203	CLA	C1D-C2D	-2.22	1.40	1.45
19	U	213	DD6	C8-C6	-2.21	1.41	1.46
12	B	846	CLA	C1B-C2B	-2.21	1.37	1.43
12	A	820	CLA	MG-NC	2.21	2.11	2.06
12	A	808	CLA	C1D-C2D	-2.21	1.41	1.45
12	A	807	CLA	MG-NC	2.21	2.11	2.06
12	B	803	CLA	C1B-C2B	-2.21	1.38	1.43
12	B	847	CLA	C1B-C2B	-2.21	1.38	1.43
12	B	827	CLA	C1D-C2D	-2.20	1.41	1.45
12	A	806	CLA	C1D-C2D	-2.20	1.41	1.45
12	A	844	CLA	MG-NC	2.20	2.11	2.06
12	A	813	CLA	C1D-C2D	-2.20	1.41	1.45
12	A	832	CLA	C1D-C2D	-2.20	1.41	1.45
12	A	803	CLA	C1D-C2D	-2.19	1.41	1.45
12	A	811	CLA	C1D-C2D	-2.19	1.41	1.45
12	B	801	CLA	C1B-C2B	-2.19	1.38	1.43
12	B	834	CLA	C1B-C2B	-2.19	1.38	1.43
20	U	202	LMG	O7-C8	-2.19	1.41	1.46
12	U	205	CLA	C1B-C2B	-2.19	1.38	1.43
12	A	818	CLA	C1D-C2D	-2.19	1.41	1.45
12	B	826	CLA	C1D-C2D	-2.19	1.41	1.45
22	U	214	KC1	C3B-C2B	2.19	1.41	1.37
18	B	842	DGD	O2G-C2G	-2.19	1.41	1.46
12	U	201	CLA	MG-NC	2.19	2.11	2.06
12	A	802	CLA	C1B-C2B	-2.18	1.38	1.43
12	A	809	CLA	C1D-C2D	-2.18	1.41	1.45
12	A	834	CLA	C1D-C2D	-2.18	1.41	1.45
12	B	809	CLA	C1B-NB	-2.18	1.35	1.37
12	B	834	CLA	MG-NB	2.18	2.10	2.05
19	U	215	DD6	C24-C1	-2.17	1.41	1.46
12	F	803	CLA	C1D-C2D	-2.17	1.41	1.45
12	B	811	CLA	C1D-C2D	-2.17	1.41	1.45
12	A	804	CLA	C1D-C2D	-2.17	1.41	1.45
16	A	847	CL0	MG-ND	-2.17	2.01	2.05
12	B	824	CLA	C1D-C2D	-2.17	1.41	1.45
12	B	834	CLA	C1D-C2D	-2.17	1.41	1.45
12	U	207	CLA	C1D-C2D	-2.17	1.41	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	A	830	CLA	C1D-C2D	-2.16	1.41	1.45
12	U	201	CLA	C1D-C2D	-2.16	1.41	1.45
12	B	818	CLA	C1B-C2B	-2.16	1.38	1.43
12	F	802	CLA	C1D-C2D	-2.16	1.41	1.45
12	F	803	CLA	MG-NC	2.16	2.11	2.06
19	U	204	DD6	C8-C6	-2.16	1.41	1.46
12	B	821	CLA	C1D-C2D	-2.15	1.41	1.45
12	B	809	CLA	C1B-C2B	-2.15	1.38	1.43
12	A	848	CLA	C1D-C2D	-2.15	1.41	1.45
12	B	816	CLA	C1D-C2D	-2.15	1.41	1.45
12	A	814	CLA	C1D-C2D	-2.15	1.41	1.45
12	A	803	CLA	C1B-C2B	-2.15	1.38	1.43
16	A	847	CL0	MG-NB	-2.15	2.01	2.05
12	B	848	CLA	C1D-C2D	-2.14	1.41	1.45
12	A	851	CLA	C1D-C2D	-2.14	1.41	1.45
12	B	847	CLA	C1D-C2D	-2.14	1.41	1.45
12	A	844	CLA	C1B-C2B	-2.14	1.38	1.43
12	A	807	CLA	C1B-NB	-2.14	1.35	1.37
19	J	101	DD6	C8-C6	-2.14	1.41	1.46
12	L	204	CLA	MG-NC	2.14	2.11	2.06
12	A	819	CLA	C1D-C2D	-2.14	1.41	1.45
12	A	832	CLA	C1B-NB	-2.14	1.35	1.37
21	U	203	A86	C26-C27	2.13	1.40	1.35
12	L	204	CLA	C1D-C2D	-2.13	1.41	1.45
12	B	843	CLA	C1D-C2D	-2.13	1.41	1.45
12	B	814	CLA	C1D-C2D	-2.13	1.41	1.45
12	A	846	CLA	MG-NB	2.13	2.10	2.05
12	A	850	CLA	C1D-C2D	-2.13	1.41	1.45
12	A	844	CLA	C1D-C2D	-2.12	1.41	1.45
12	A	812	CLA	C1D-C2D	-2.12	1.41	1.45
12	L	202	CLA	C1D-C2D	-2.12	1.41	1.45
12	B	827	CLA	C1B-C2B	-2.12	1.38	1.43
12	B	824	CLA	C1B-C2B	-2.12	1.38	1.43
12	U	205	CLA	MG-NC	2.12	2.11	2.06
12	A	833	CLA	C1D-C2D	-2.12	1.41	1.45
12	B	831	CLA	C1D-C2D	-2.12	1.41	1.45
12	A	833	CLA	MG-NC	2.12	2.11	2.06
12	A	814	CLA	MG-NC	2.12	2.11	2.06
12	B	825	CLA	C1B-C2B	-2.12	1.38	1.43
12	B	805	CLA	C1D-C2D	-2.12	1.41	1.45
12	U	210	CLA	C1D-C2D	-2.11	1.41	1.45
12	B	804	CLA	C1B-C2B	-2.11	1.38	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	B	812	CLA	C1D-C2D	-2.11	1.41	1.45
12	B	828	CLA	C1B-NB	-2.11	1.35	1.37
12	A	822	CLA	C1B-C2B	-2.11	1.38	1.43
12	U	201	CLA	CHB-C1B	2.10	1.44	1.39
12	B	846	CLA	MG-NC	2.10	2.11	2.06
12	B	832	CLA	C1D-C2D	-2.10	1.41	1.45
12	B	820	CLA	C1B-NB	-2.10	1.35	1.37
12	A	846	CLA	C1D-C2D	-2.10	1.41	1.45
12	A	802	CLA	MG-NC	2.10	2.11	2.06
12	B	805	CLA	C1B-C2B	-2.10	1.38	1.43
12	B	823	CLA	CHB-C1B	2.10	1.44	1.39
12	B	844	CLA	CHB-C1B	2.09	1.44	1.39
12	B	846	CLA	C1D-C2D	-2.09	1.41	1.45
12	A	801	CLA	C1B-NB	-2.09	1.35	1.37
12	A	826	CLA	C1B-NB	-2.09	1.35	1.37
12	B	815	CLA	C1D-C2D	-2.09	1.41	1.45
12	B	814	CLA	C1B-C2B	-2.09	1.38	1.43
12	B	821	CLA	C1B-C2B	-2.08	1.38	1.43
18	B	842	DGD	O1G-C1G	-2.08	1.40	1.45
12	A	804	CLA	C1B-C2B	-2.08	1.38	1.43
12	U	208	CLA	C1B-C2B	-2.08	1.38	1.43
12	B	819	CLA	MG-NC	2.08	2.11	2.06
12	A	826	CLA	C1B-C2B	-2.08	1.38	1.43
12	A	822	CLA	C1D-C2D	-2.07	1.41	1.45
12	A	818	CLA	MG-NC	2.07	2.11	2.06
12	U	210	CLA	C1B-C2B	-2.07	1.38	1.43
12	B	810	CLA	C1D-C2D	-2.07	1.41	1.45
12	A	805	CLA	C1D-C2D	-2.07	1.41	1.45
12	A	818	CLA	C1B-NB	-2.07	1.35	1.37
12	B	810	CLA	C1B-C2B	-2.07	1.38	1.43
12	U	212	CLA	C1D-C2D	-2.07	1.41	1.45
12	A	820	CLA	C1D-C2D	-2.06	1.41	1.45
12	A	825	CLA	C1B-C2B	-2.06	1.38	1.43
12	A	816	CLA	C1B-NB	-2.06	1.35	1.37
20	J	102	LMG	C4-C5	2.06	1.57	1.53
12	B	819	CLA	C1B-C2B	-2.06	1.38	1.43
14	A	838	LHG	P-O6	2.06	1.67	1.59
12	U	211	CLA	C1D-C2D	-2.06	1.41	1.45
12	A	806	CLA	MG-NC	2.06	2.11	2.06
12	L	204	CLA	C1B-C2B	-2.06	1.38	1.43
12	A	829	CLA	C1B-C2B	-2.06	1.38	1.43
15	B	837	BCR	C33-C5	-2.06	1.47	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	B	812	CLA	CHB-C1B	2.06	1.44	1.39
12	B	816	CLA	C1B-C2B	-2.05	1.38	1.43
19	U	213	DD6	C24-C1	-2.05	1.41	1.46
12	A	819	CLA	C1B-C2B	-2.05	1.38	1.43
12	J	103	CLA	CHB-C1B	2.05	1.44	1.39
12	A	808	CLA	C1B-C2B	-2.05	1.38	1.43
12	B	831	CLA	C1B-C2B	-2.05	1.38	1.43
12	B	813	CLA	C1B-C2B	-2.05	1.38	1.43
12	B	835	CLA	CHB-C1B	2.05	1.44	1.39
12	A	831	CLA	C1D-C2D	-2.04	1.41	1.45
12	B	801	CLA	C1D-C2D	-2.04	1.41	1.45
12	B	820	CLA	C1B-C2B	-2.04	1.38	1.43
12	J	103	CLA	C1B-C2B	-2.04	1.38	1.43
12	U	205	CLA	CHB-C1B	2.04	1.44	1.39
12	B	844	CLA	C1D-C2D	-2.04	1.41	1.45
12	U	201	CLA	C1B-C2B	-2.03	1.38	1.43
12	A	811	CLA	C1B-C2B	-2.03	1.38	1.43
12	A	848	CLA	C1B-C2B	-2.03	1.38	1.43
12	A	812	CLA	CHB-C1B	2.03	1.44	1.39
12	A	850	CLA	C1B-C2B	-2.03	1.38	1.43
12	B	811	CLA	C1B-C2B	-2.03	1.38	1.43
12	A	822	CLA	MG-NC	2.03	2.11	2.06
12	A	821	CLA	CHB-C1B	2.03	1.44	1.39
12	B	848	CLA	C1B-NB	-2.03	1.35	1.37
12	B	843	CLA	C1B-C2B	-2.03	1.38	1.43
12	A	828	CLA	C1B-C2B	-2.02	1.38	1.43
12	A	806	CLA	C1B-C2B	-2.02	1.38	1.43
12	A	827	CLA	C1B-C2B	-2.02	1.38	1.43
19	U	204	DD6	C24-C1	-2.02	1.41	1.46
12	L	202	CLA	C1B-NB	-2.02	1.35	1.37
12	L	202	CLA	C1B-C2B	-2.02	1.38	1.43
12	A	805	CLA	C1B-C2B	-2.02	1.38	1.43
12	B	835	CLA	C1D-C2D	-2.02	1.41	1.45
12	B	804	CLA	C1B-NB	-2.02	1.35	1.37
12	A	826	CLA	CHB-C1B	2.01	1.43	1.39
12	B	829	CLA	C1D-C2D	-2.01	1.41	1.45
12	A	851	CLA	C1B-C2B	-2.01	1.38	1.43
12	B	803	CLA	C1B-NB	-2.01	1.35	1.37
12	B	818	CLA	C1D-C2D	-2.01	1.41	1.45
12	A	823	CLA	C1B-NB	-2.01	1.35	1.37
12	B	833	CLA	MG-NC	2.01	2.11	2.06
12	A	804	CLA	C1B-NB	-2.00	1.35	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	A	824	CLA	C1B-C2B	-2.00	1.38	1.43
12	B	807	CLA	C1B-C2B	-2.00	1.38	1.43

All (602) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	A	847	CL0	C1B-CHB-C4A	9.64	127.52	121.32
19	U	213	DD6	C3-C4-C5	5.16	134.07	123.52
21	U	203	A86	C3-C4-C5	4.95	133.65	123.52
19	U	213	DD6	C14-C13-C11	4.56	132.61	125.53
14	A	839	LHG	O4-P-O5	4.40	132.91	112.44
14	A	838	LHG	O4-P-O5	4.38	132.80	112.44
19	U	215	DD6	C4-C3-C2	4.04	131.78	123.52
21	U	203	A86	C33-C32-C31	4.02	113.12	109.21
12	B	846	CLA	C1-O2A-CGA	4.02	126.37	116.65
12	U	201	CLA	C4D-CHA-C1A	3.98	126.00	121.24
15	F	801	BCR	C2-C1-C6	3.97	116.20	110.44
19	J	101	DD6	C3-C4-C5	3.97	131.63	123.52
15	A	842	BCR	C2-C1-C6	3.95	116.17	110.44
12	B	832	CLA	C4D-CHA-C1A	3.94	125.94	121.24
12	B	801	CLA	C4D-CHA-C1A	3.92	125.92	121.24
12	B	830	CLA	C4D-CHA-C1A	3.88	125.88	121.24
12	A	822	CLA	C4D-CHA-C1A	3.83	125.82	121.24
19	U	215	DD6	C3-C4-C5	3.81	131.32	123.52
12	L	203	CLA	C4D-CHA-C1A	3.81	125.79	121.24
15	J	104	BCR	C2-C1-C6	3.81	115.97	110.44
15	M	101	BCR	C2-C1-C6	3.78	115.93	110.44
12	B	835	CLA	C4D-CHA-C1A	3.77	125.74	121.24
12	A	831	CLA	C4D-CHA-C1A	3.76	125.73	121.24
12	F	803	CLA	C4D-CHA-C1A	3.74	125.71	121.24
12	L	204	CLA	C4D-CHA-C1A	3.72	125.69	121.24
19	U	204	DD6	C3-C4-C5	3.72	131.13	123.52
15	A	840	BCR	C2-C1-C6	3.72	115.84	110.44
12	F	802	CLA	C4D-CHA-C1A	3.71	125.66	121.24
12	A	829	CLA	C4D-CHA-C1A	3.70	125.66	121.24
12	B	807	CLA	C4D-CHA-C1A	3.69	125.65	121.24
19	U	204	DD6	C12-C11-C10	-3.69	116.84	122.82
12	A	812	CLA	C4D-CHA-C1A	3.67	125.63	121.24
12	U	207	CLA	C4D-CHA-C1A	3.67	125.62	121.24
12	A	852	CLA	C4D-CHA-C1A	3.67	125.62	121.24
12	A	816	CLA	C4D-CHA-C1A	3.65	125.59	121.24
19	J	101	DD6	C4-C3-C2	3.64	130.96	123.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	B	843	CLA	C4D-CHA-C1A	3.63	125.57	121.24
12	B	816	CLA	C4D-CHA-C1A	3.61	125.56	121.24
19	U	204	DD6	C4-C3-C2	3.61	130.91	123.52
19	J	101	DD6	C12-C11-C10	-3.61	116.97	122.82
12	A	817	CLA	C4D-CHA-C1A	3.60	125.54	121.24
12	U	209	CLA	C4D-CHA-C1A	3.58	125.52	121.24
12	B	826	CLA	C4D-CHA-C1A	3.58	125.51	121.24
12	A	811	CLA	C4D-CHA-C1A	3.58	125.51	121.24
12	A	805	CLA	C4D-CHA-C1A	3.58	125.51	121.24
15	B	840	BCR	C15-C16-C17	-3.57	116.22	123.52
12	B	814	CLA	C4D-CHA-C1A	3.56	125.49	121.24
12	A	810	CLA	C4D-CHA-C1A	3.54	125.47	121.24
12	A	851	CLA	C4D-CHA-C1A	3.54	125.47	121.24
12	B	812	CLA	C4D-CHA-C1A	3.54	125.46	121.24
15	L	205	BCR	C2-C1-C6	3.53	115.57	110.44
12	A	819	CLA	C4D-CHA-C1A	3.53	125.45	121.24
12	B	831	CLA	C4D-CHA-C1A	3.52	125.44	121.24
12	A	815	CLA	C4D-CHA-C1A	3.51	125.44	121.24
12	A	803	CLA	C4D-CHA-C1A	3.51	125.44	121.24
19	U	213	DD6	C12-C11-C10	-3.51	117.13	122.82
12	B	810	CLA	C4D-CHA-C1A	3.50	125.42	121.24
12	A	820	CLA	C4D-CHA-C1A	3.49	125.41	121.24
16	A	847	CL0	C1C-CHC-C4B	3.49	128.57	116.07
12	A	814	CLA	C4D-CHA-C1A	3.48	125.40	121.24
12	B	845	CLA	C4D-CHA-C1A	3.48	125.39	121.24
19	J	101	DD6	C8-C6-C5	3.47	124.47	119.01
12	A	845	CLA	C4D-CHA-C1A	3.47	125.38	121.24
12	A	846	CLA	C4D-CHA-C1A	3.46	125.37	121.24
15	M	101	BCR	C15-C16-C17	-3.46	116.44	123.52
12	B	833	CLA	C4D-CHA-C1A	3.45	125.36	121.24
12	B	811	CLA	C4D-CHA-C1A	3.45	125.36	121.24
12	B	834	CLA	C4D-CHA-C1A	3.45	125.36	121.24
12	A	818	CLA	C4D-CHA-C1A	3.45	125.36	121.24
12	U	205	CLA	C4D-CHA-C1A	3.45	125.36	121.24
12	A	835	CLA	C4D-CHA-C1A	3.44	125.35	121.24
12	B	847	CLA	C4D-CHA-C1A	3.44	125.35	121.24
12	A	808	CLA	C4D-CHA-C1A	3.43	125.33	121.24
12	B	818	CLA	C4D-CHA-C1A	3.42	125.33	121.24
12	B	822	CLA	C4D-CHA-C1A	3.41	125.32	121.24
12	U	212	CLA	C4D-CHA-C1A	3.41	125.31	121.24
12	A	844	CLA	C4D-CHA-C1A	3.40	125.29	121.24
12	A	828	CLA	C4D-CHA-C1A	3.39	125.29	121.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	B	815	CLA	C4D-CHA-C1A	3.39	125.29	121.24
12	U	206	CLA	C4D-CHA-C1A	3.39	125.28	121.24
16	A	847	CL0	C3D-C4D-CHA	3.38	113.68	108.54
12	A	807	CLA	C4D-CHA-C1A	3.38	125.28	121.24
12	A	833	CLA	C4D-CHA-C1A	3.37	125.26	121.24
12	A	834	CLA	C4D-CHA-C1A	3.35	125.25	121.24
12	A	832	CLA	C4D-CHA-C1A	3.35	125.24	121.24
12	A	813	CLA	C4D-CHA-C1A	3.35	125.24	121.24
12	U	211	CLA	C4D-CHA-C1A	3.35	125.23	121.24
12	B	805	CLA	C4D-CHA-C1A	3.34	125.23	121.24
15	L	205	BCR	C3-C4-C5	-3.34	108.09	114.06
12	A	848	CLA	C4D-CHA-C1A	3.34	125.23	121.24
12	A	830	CLA	C4D-CHA-C1A	3.33	125.22	121.24
12	A	836	CLA	C4D-CHA-C1A	3.33	125.22	121.24
12	B	824	CLA	C4D-CHA-C1A	3.33	125.22	121.24
21	U	203	A86	C4-C3-C2	3.31	130.30	123.52
19	U	204	DD6	C8-C6-C5	3.31	124.21	119.01
12	A	825	CLA	C4D-CHA-C1A	3.30	125.19	121.24
12	B	846	CLA	C4D-CHA-C1A	3.30	125.19	121.24
12	B	844	CLA	C4D-CHA-C1A	3.28	125.15	121.24
12	U	208	CLA	CHD-C1D-ND	-3.27	120.20	124.80
12	U	208	CLA	C4D-CHA-C1A	3.27	125.14	121.24
12	A	827	CLA	C4D-CHA-C1A	3.26	125.14	121.24
12	B	844	CLA	C1-O2A-CGA	3.26	124.55	116.65
12	A	850	CLA	C4D-CHA-C1A	3.26	125.13	121.24
12	B	827	CLA	C4D-CHA-C1A	3.25	125.12	121.24
12	B	829	CLA	C4D-CHA-C1A	3.24	125.11	121.24
12	B	817	CLA	C4D-CHA-C1A	3.24	125.11	121.24
19	U	204	DD6	C13-C11-C10	3.24	124.10	119.01
12	L	202	CLA	C4D-CHA-C1A	3.21	125.08	121.24
12	A	806	CLA	C4D-CHA-C1A	3.21	125.08	121.24
12	A	807	CLA	C4A-NA-C1A	3.21	108.14	106.68
19	U	213	DD6	C8-C6-C5	3.21	124.06	119.01
15	L	205	BCR	C11-C10-C9	-3.21	122.78	127.28
12	A	809	CLA	C4D-CHA-C1A	3.20	125.06	121.24
12	A	824	CLA	C4D-CHA-C1A	3.19	125.05	121.24
12	B	823	CLA	C4D-CHA-C1A	3.18	125.04	121.24
15	I	102	BCR	C27-C26-C25	3.18	127.00	122.70
12	B	806	CLA	C4D-CHA-C1A	3.17	125.03	121.24
12	L	202	CLA	C1-O2A-CGA	3.17	124.32	116.65
12	B	813	CLA	C4D-CHA-C1A	3.16	125.01	121.24
21	U	203	A86	C8-C6-C5	3.16	123.98	119.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	B	828	CLA	C4D-CHA-C1A	3.16	125.01	121.24
12	A	804	CLA	C4D-CHA-C1A	3.16	125.01	121.24
19	J	101	DD6	C13-C11-C10	3.15	123.97	119.01
21	U	203	A86	C36-C31-C32	3.14	122.81	119.70
12	B	809	CLA	C4D-CHA-C1A	3.11	124.96	121.24
12	B	828	CLA	C4A-NA-C1A	3.10	108.09	106.68
15	A	842	BCR	C28-C27-C26	-3.10	108.53	114.06
16	A	847	CL0	C1A-CHA-C4D	3.09	124.14	118.98
12	A	821	CLA	CHA-C1A-NA	-3.09	119.39	126.39
19	J	101	DD6	C7-C6-C5	-3.09	117.82	122.82
14	A	839	LHG	O8-C23-C24	3.08	120.51	111.15
22	U	214	KC1	CAA-C2A-C1A	3.08	138.13	124.64
12	U	210	CLA	C4D-CHA-C1A	3.07	124.91	121.24
12	U	208	CLA	CAA-C2A-C3A	-3.07	104.70	113.00
12	B	820	CLA	CHA-C1A-NA	-3.07	119.45	126.39
19	U	204	DD6	C7-C6-C5	-3.06	117.86	122.82
15	M	101	BCR	C15-C14-C13	-3.06	122.99	127.28
15	L	201	BCR	C27-C26-C25	3.06	126.83	122.70
12	J	103	CLA	C4D-CHA-C1A	3.05	124.88	121.24
12	B	848	CLA	C4D-CHA-C1A	3.00	124.83	121.24
19	U	213	DD6	C7-C6-C5	-3.00	117.96	122.82
19	U	215	DD6	C24-C1-C2	2.99	123.72	119.01
21	U	203	A86	C7-C6-C5	-2.99	117.97	122.82
12	B	824	CLA	C1-O2A-CGA	2.99	123.89	116.65
12	B	821	CLA	C4D-CHA-C1A	2.98	124.80	121.24
12	A	821	CLA	C4D-CHA-C1A	2.98	124.80	121.24
12	B	828	CLA	CHA-C1A-NA	-2.97	119.66	126.39
12	B	848	CLA	CHA-C1A-NA	-2.97	119.67	126.39
12	A	834	CLA	CHA-C1A-NA	-2.96	119.68	126.39
12	A	802	CLA	C4D-CHA-C1A	2.96	124.77	121.24
12	A	823	CLA	C4D-CHA-C1A	2.96	124.77	121.24
12	A	807	CLA	CHA-C1A-NA	-2.94	119.74	126.39
12	B	818	CLA	CHD-C1D-ND	-2.92	120.69	124.80
12	B	802	CLA	CHA-C1A-NA	-2.92	119.78	126.39
15	I	102	BCR	C15-C14-C13	-2.91	123.20	127.28
12	A	826	CLA	C4D-CHA-C1A	2.91	124.71	121.24
15	A	840	BCR	C27-C26-C25	2.90	126.62	122.70
12	B	809	CLA	CHA-C1A-NA	-2.90	119.83	126.39
19	U	215	DD6	C-C1-C2	-2.90	118.12	122.82
21	U	203	A86	C-C1-C2	-2.89	118.14	122.82
12	B	823	CLA	CHA-C1A-NA	-2.89	119.85	126.39
22	U	214	KC1	C2A-C3A-C4A	2.89	108.58	106.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	A	825	CLA	CHA-C1A-NA	-2.87	119.89	126.39
12	A	822	CLA	CHD-C1D-ND	-2.87	120.77	124.80
12	A	812	CLA	CHA-C1A-NA	-2.86	119.91	126.39
12	A	832	CLA	CHA-C1A-NA	-2.86	119.92	126.39
12	A	802	CLA	CHD-C1D-ND	-2.86	120.78	124.80
12	B	845	CLA	CHA-C1A-NA	-2.85	119.93	126.39
12	A	816	CLA	CHD-C1D-ND	-2.85	120.79	124.80
12	A	828	CLA	CHA-C1A-NA	-2.85	119.93	126.39
12	A	829	CLA	CHD-C1D-ND	-2.85	120.79	124.80
12	A	817	CLA	CHA-C1A-NA	-2.85	119.94	126.39
12	B	808	CLA	C4D-CHA-C1A	2.85	124.64	121.24
15	L	205	BCR	C27-C26-C25	2.85	126.55	122.70
12	B	822	CLA	CHA-C1A-NA	-2.85	119.95	126.39
12	B	815	CLA	CHD-C1D-ND	-2.84	120.80	124.80
15	B	840	BCR	C15-C14-C13	-2.84	123.29	127.28
12	B	801	CLA	CHA-C1A-NA	-2.84	119.96	126.39
12	U	209	CLA	CHD-C1D-ND	-2.84	120.81	124.80
21	U	203	A86	C24-C1-C2	2.84	123.47	119.01
12	A	831	CLA	CHD-C1D-ND	-2.84	120.81	124.80
12	A	823	CLA	CHA-C1A-NA	-2.83	119.98	126.39
12	L	202	CLA	C4A-NA-C1A	2.83	107.97	106.68
12	B	803	CLA	C4D-CHA-C1A	2.83	124.62	121.24
12	B	844	CLA	CHD-C1D-ND	-2.83	120.82	124.80
12	A	813	CLA	CHA-C1A-NA	-2.82	120.00	126.39
12	A	815	CLA	CHA-C1A-NA	-2.82	120.00	126.39
12	A	810	CLA	CHA-C1A-NA	-2.82	120.00	126.39
19	U	213	DD6	C-C1-C2	-2.82	118.25	122.82
19	U	204	DD6	C-C1-C2	-2.82	118.25	122.82
12	A	844	CLA	CHA-C1A-NA	-2.81	120.02	126.39
12	B	848	CLA	C4A-NA-C1A	2.81	107.96	106.68
12	B	830	CLA	CHA-C1A-NA	-2.81	120.03	126.39
12	L	202	CLA	CHA-C1A-NA	-2.81	120.04	126.39
15	B	841	BCR	C27-C26-C25	2.80	126.49	122.70
12	B	803	CLA	CHA-C1A-NA	-2.80	120.06	126.39
21	U	203	A86	C28-C27-C26	-2.80	118.28	122.82
12	B	819	CLA	CHA-C1A-NA	-2.80	120.06	126.39
12	U	211	CLA	CHD-C1D-ND	-2.79	120.88	124.80
12	A	846	CLA	CHD-C1D-ND	-2.79	120.88	124.80
20	J	102	LMG	O6-C1-O1	-2.78	103.47	110.04
12	B	827	CLA	CHA-C1A-NA	-2.78	120.09	126.39
18	B	842	DGD	O6D-C1D-O3G	-2.78	103.47	110.04
12	F	802	CLA	CHA-C1A-NA	-2.78	120.09	126.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	A	845	CLA	CHA-C1A-NA	-2.78	120.09	126.39
12	B	804	CLA	C4D-CHA-C1A	2.78	124.56	121.24
12	U	212	CLA	CHA-C1A-NA	-2.77	120.12	126.39
12	B	806	CLA	CHA-C1A-NA	-2.77	120.12	126.39
12	A	826	CLA	CHA-C1A-NA	-2.77	120.13	126.39
12	A	846	CLA	CHA-C1A-NA	-2.77	120.13	126.39
12	B	847	CLA	CHA-C1A-NA	-2.77	120.13	126.39
12	A	852	CLA	CHA-C1A-NA	-2.76	120.13	126.39
12	J	103	CLA	CHD-C1D-ND	-2.76	120.92	124.80
15	I	102	BCR	C15-C16-C17	-2.76	117.87	123.52
12	A	824	CLA	CHA-C1A-NA	-2.76	120.14	126.39
12	A	812	CLA	C4A-NA-C1A	2.75	107.94	106.68
15	B	839	BCR	C27-C26-C25	2.75	126.42	122.70
12	B	804	CLA	CHA-C1A-NA	-2.75	120.17	126.39
18	B	842	DGD	O5D-C6D-C5D	-2.75	103.23	109.42
12	B	832	CLA	CHA-C1A-NA	-2.75	120.17	126.39
15	B	840	BCR	C27-C26-C25	2.74	126.41	122.70
12	U	210	CLA	CHA-C1A-NA	-2.74	120.18	126.39
12	A	835	CLA	CHA-C1A-NA	-2.74	120.19	126.39
12	A	827	CLA	CHA-C1A-NA	-2.74	120.19	126.39
18	B	842	DGD	CDB-CCB-CBB	-2.74	100.52	114.37
18	B	842	DGD	O3G-C3G-C2G	-2.73	104.17	110.82
12	F	802	CLA	C4A-NA-C1A	2.73	107.93	106.68
12	A	848	CLA	CHA-C1A-NA	-2.73	120.20	126.39
12	B	833	CLA	CHA-C1A-NA	-2.73	120.20	126.39
12	B	843	CLA	CHA-C1A-NA	-2.73	120.20	126.39
15	B	838	BCR	C2-C1-C6	2.73	114.41	110.44
12	B	825	CLA	CHA-C1A-NA	-2.73	120.21	126.39
12	L	203	CLA	CHD-C1D-ND	-2.73	120.96	124.80
14	A	838	LHG	O8-C23-C24	2.73	120.16	111.83
12	B	834	CLA	CHA-C1A-NA	-2.72	120.22	126.39
12	A	801	CLA	C4D-CHA-C1A	2.72	124.49	121.24
12	A	811	CLA	CHA-C1A-NA	-2.72	120.23	126.39
12	A	851	CLA	CHA-C1A-NA	-2.72	120.23	126.39
12	A	819	CLA	CHD-C1D-ND	-2.72	120.97	124.80
12	B	807	CLA	CHA-C1A-NA	-2.72	120.23	126.39
15	L	205	BCR	C24-C23-C22	-2.72	122.21	126.23
12	U	201	CLA	CHA-C1A-NA	-2.72	120.23	126.39
12	A	836	CLA	CHA-C1A-NA	-2.72	120.23	126.39
19	U	213	DD6	C24-C1-C2	2.72	123.28	119.01
12	B	805	CLA	CHA-C1A-NA	-2.71	120.25	126.39
12	A	819	CLA	CHA-C1A-NA	-2.71	120.26	126.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	B	810	CLA	CHA-C1A-NA	-2.71	120.26	126.39
12	A	801	CLA	CHA-C1A-NA	-2.71	120.26	126.39
12	B	835	CLA	CHA-C1A-NA	-2.71	120.26	126.39
12	F	803	CLA	CHA-C1A-NA	-2.71	120.26	126.39
12	A	808	CLA	CHA-C1A-NA	-2.71	120.26	126.39
15	B	837	BCR	C7-C8-C9	-2.71	122.23	126.23
12	B	813	CLA	C1-O2A-CGA	2.70	123.19	116.65
19	U	213	DD6	C12-C11-C13	2.70	122.22	118.09
12	A	814	CLA	CHA-C1A-NA	-2.70	120.27	126.39
12	A	833	CLA	CHD-C1D-ND	-2.70	121.00	124.80
15	J	104	BCR	C27-C26-C25	2.70	126.35	122.70
12	A	805	CLA	CHA-C1A-NA	-2.70	120.28	126.39
12	A	824	CLA	CHD-C1D-ND	-2.70	121.00	124.80
12	U	211	CLA	CHA-C1A-NA	-2.70	120.28	126.39
12	U	205	CLA	CHA-C1A-NA	-2.70	120.28	126.39
12	B	813	CLA	CHA-C1A-NA	-2.70	120.28	126.39
12	U	201	CLA	CHD-C1D-ND	-2.70	121.01	124.80
12	A	803	CLA	CHD-C1D-ND	-2.69	121.01	124.80
12	U	206	CLA	CHA-C1A-NA	-2.69	120.29	126.39
12	B	818	CLA	CHA-C1A-NA	-2.69	120.29	126.39
12	A	820	CLA	CHA-C1A-NA	-2.69	120.30	126.39
12	B	817	CLA	CHA-C1A-NA	-2.69	120.30	126.39
12	B	825	CLA	C4D-CHA-C1A	2.69	124.45	121.24
12	B	825	CLA	CHD-C1D-ND	-2.69	121.02	124.80
15	L	201	BCR	C15-C16-C17	-2.69	118.02	123.52
12	A	804	CLA	CHA-C1A-NA	-2.68	120.31	126.39
12	B	820	CLA	C4D-CHA-C1A	2.68	124.44	121.24
12	A	820	CLA	CHD-C1D-ND	-2.68	121.03	124.80
12	B	812	CLA	CHA-C1A-NA	-2.67	120.33	126.39
12	B	832	CLA	CHD-C1D-ND	-2.67	121.04	124.80
19	J	101	DD6	C10-C9-C8	2.67	130.94	123.20
12	B	829	CLA	CHA-C1A-NA	-2.67	120.35	126.39
12	A	830	CLA	CHA-C1A-NA	-2.67	120.35	126.39
12	L	204	CLA	CHA-C1A-NA	-2.67	120.35	126.39
12	B	847	CLA	CHD-C1D-ND	-2.66	121.05	124.80
12	B	819	CLA	C4D-CHA-C1A	2.66	124.42	121.24
12	A	818	CLA	CHA-C1A-NA	-2.66	120.36	126.39
12	A	805	CLA	CHD-C1D-ND	-2.66	121.06	124.80
12	B	829	CLA	CHD-C1D-ND	-2.66	121.06	124.80
19	U	213	DD6	C4-C3-C2	2.65	128.95	123.52
12	B	816	CLA	CHD-C1D-ND	-2.65	121.07	124.80
12	U	212	CLA	C4A-NA-C1A	2.65	107.89	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	U	204	DD6	C33-C32-C31	2.65	114.71	109.49
12	B	817	CLA	CHD-C1D-ND	-2.65	121.07	124.80
12	A	815	CLA	CHD-C1D-ND	-2.65	121.08	124.80
19	J	101	DD6	C-C1-C2	-2.64	118.53	122.82
19	J	101	DD6	C24-C1-C2	2.64	123.17	119.01
12	B	801	CLA	CHD-C1D-ND	-2.64	121.08	124.80
12	U	207	CLA	CHA-C1A-NA	-2.64	120.41	126.39
12	A	831	CLA	CHA-C1A-NA	-2.64	120.42	126.39
15	F	801	BCR	C3-C4-C5	-2.63	109.36	114.06
12	L	204	CLA	CHD-C1D-ND	-2.63	121.10	124.80
12	B	824	CLA	CHA-C1A-NA	-2.63	120.43	126.39
12	B	816	CLA	CHA-C1A-NA	-2.63	120.43	126.39
15	A	843	BCR	C15-C16-C17	-2.63	118.13	123.52
12	A	806	CLA	CHD-C1D-ND	-2.63	121.10	124.80
12	B	826	CLA	CHA-C1A-NA	-2.63	120.44	126.39
12	A	801	CLA	CHD-C1D-ND	-2.63	121.11	124.80
12	A	813	CLA	CHD-C1D-ND	-2.62	121.11	124.80
12	A	818	CLA	CHD-C1D-ND	-2.62	121.12	124.80
12	A	816	CLA	CHA-C1A-NA	-2.62	120.46	126.39
12	B	824	CLA	CHD-C1D-ND	-2.62	121.12	124.80
12	B	831	CLA	CHA-C1A-NA	-2.62	120.47	126.39
12	A	806	CLA	CHA-C1A-NA	-2.61	120.47	126.39
12	B	846	CLA	CHD-C1D-ND	-2.61	121.12	124.80
12	B	814	CLA	CHA-C1A-NA	-2.61	120.47	126.39
12	A	802	CLA	CHA-C1A-NA	-2.61	120.48	126.39
12	A	834	CLA	C4A-NA-C1A	2.61	107.87	106.68
12	B	821	CLA	CHA-C1A-NA	-2.60	120.49	126.39
12	J	103	CLA	CHA-C1A-NA	-2.60	120.50	126.39
12	B	811	CLA	CHA-C1A-NA	-2.60	120.50	126.39
15	A	841	BCR	C27-C26-C25	2.60	126.22	122.70
15	B	837	BCR	C33-C5-C6	-2.60	121.65	124.48
12	B	811	CLA	CHD-C1D-ND	-2.59	121.15	124.80
15	A	842	BCR	C3-C4-C5	-2.59	109.43	114.06
15	M	101	BCR	C27-C26-C25	2.59	126.20	122.70
12	B	844	CLA	CHA-C1A-NA	-2.59	120.53	126.39
12	B	814	CLA	CHD-C1D-ND	-2.59	121.16	124.80
12	A	809	CLA	CHA-C1A-NA	-2.59	120.53	126.39
12	A	814	CLA	CHD-C1D-ND	-2.59	121.16	124.80
12	B	826	CLA	CHD-C1D-ND	-2.59	121.16	124.80
13	A	837	PQN	C11-C3-C2	-2.58	120.46	124.89
12	A	821	CLA	C4A-NA-C1A	2.58	107.86	106.68
15	F	801	BCR	C27-C26-C25	2.58	126.19	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	B	821	CLA	CHD-C1D-ND	-2.58	121.17	124.80
12	B	846	CLA	CHA-C1A-NA	-2.57	120.57	126.39
12	B	822	CLA	C4A-NA-C1A	2.57	107.85	106.68
15	B	838	BCR	C28-C27-C26	-2.57	109.48	114.06
12	A	829	CLA	CHA-C1A-NA	-2.56	120.59	126.39
12	A	850	CLA	CHA-C1A-NA	-2.56	120.59	126.39
12	A	833	CLA	C1-O2A-CGA	2.56	122.84	116.65
12	A	833	CLA	CHA-C1A-NA	-2.56	120.60	126.39
13	B	836	PQN	C11-C3-C2	-2.56	120.50	124.89
12	A	804	CLA	CHD-C1D-ND	-2.56	121.20	124.80
12	B	815	CLA	CHA-C1A-NA	-2.55	120.62	126.39
12	A	803	CLA	CHA-C1A-NA	-2.54	120.63	126.39
12	L	203	CLA	CHA-C1A-NA	-2.54	120.63	126.39
12	B	812	CLA	CHD-C1D-ND	-2.54	121.23	124.80
16	A	847	CL0	CHA-C1A-C2A	-2.54	127.34	133.31
15	B	838	BCR	C3-C4-C5	-2.54	109.53	114.06
19	U	204	DD6	C24-C1-C2	2.54	123.00	119.01
12	B	808	CLA	CHA-C1A-NA	-2.54	120.65	126.39
12	U	211	CLA	C4A-NA-C1A	2.53	107.83	106.68
12	F	803	CLA	CHD-C1D-ND	-2.53	121.24	124.80
12	A	806	CLA	C1-O2A-CGA	2.53	122.78	116.65
12	A	832	CLA	C4A-NA-C1A	2.53	107.83	106.68
12	B	831	CLA	CHD-C1D-ND	-2.53	121.24	124.80
12	U	209	CLA	CHA-C1A-NA	-2.52	120.68	126.39
12	B	803	CLA	CHD-C1D-ND	-2.52	121.25	124.80
15	A	840	BCR	C40-C30-C25	2.52	114.19	110.24
12	B	844	CLA	CAA-C2A-C3A	-2.52	106.19	113.00
15	A	841	BCR	C24-C23-C22	-2.51	122.52	126.23
12	A	830	CLA	CHD-C1D-ND	-2.51	121.27	124.80
20	U	202	LMG	O6-C1-O1	-2.51	104.11	110.04
12	L	202	CLA	CHD-C1D-ND	-2.51	121.27	124.80
12	U	212	CLA	CHD-C1D-ND	-2.51	121.27	124.80
12	A	822	CLA	CHA-C1A-NA	-2.51	120.72	126.39
15	F	804	BCR	C11-C10-C9	-2.50	123.77	127.28
12	B	810	CLA	CHD-C1D-ND	-2.50	121.28	124.80
12	U	208	CLA	CHD-C1D-C2D	2.50	130.69	125.49
12	B	820	CLA	C4A-NA-C1A	2.50	107.82	106.68
12	A	850	CLA	CHD-C1D-ND	-2.50	121.29	124.80
12	A	852	CLA	CHD-C1D-ND	-2.50	121.29	124.80
12	B	835	CLA	CHD-C1D-ND	-2.50	121.29	124.80
15	A	843	BCR	C28-C27-C26	-2.50	109.60	114.06
12	B	813	CLA	CHD-C1D-ND	-2.49	121.30	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	B	833	CLA	CHD-C1D-ND	-2.49	121.30	124.80
15	F	804	BCR	C27-C26-C25	2.49	126.07	122.70
12	U	207	CLA	CHD-C1D-ND	-2.48	121.31	124.80
15	B	838	BCR	C15-C16-C17	-2.48	118.44	123.52
12	A	844	CLA	CHD-C1D-ND	-2.48	121.31	124.80
12	A	851	CLA	CHD-C1D-ND	-2.48	121.31	124.80
12	B	834	CLA	CHD-C1D-ND	-2.48	121.31	124.80
15	B	839	BCR	C15-C16-C17	-2.48	118.45	123.52
12	B	805	CLA	CHD-C1D-ND	-2.47	121.33	124.80
15	B	837	BCR	C29-C30-C25	2.47	114.02	110.44
15	L	201	BCR	C15-C14-C13	-2.47	123.82	127.28
14	A	839	LHG	C11-C10-C9	-2.46	101.92	114.37
15	M	101	BCR	C3-C4-C5	-2.46	109.67	114.06
12	B	811	CLA	O2A-C1-C2	2.45	117.55	108.11
12	B	819	CLA	CHD-C1D-ND	-2.45	121.35	124.80
12	B	802	CLA	C4D-CHA-C1A	2.45	124.16	121.24
12	U	205	CLA	CHD-C1D-ND	-2.45	121.36	124.80
12	A	810	CLA	CHD-C1D-ND	-2.44	121.37	124.80
15	B	839	BCR	C2-C1-C6	2.44	113.98	110.44
12	A	813	CLA	C4A-NA-C1A	2.43	107.79	106.68
12	A	823	CLA	C4A-NA-C1A	2.43	107.79	106.68
12	B	807	CLA	CHD-C1D-ND	-2.43	121.39	124.80
15	I	102	BCR	C11-C10-C9	-2.42	123.88	127.28
12	A	825	CLA	CHD-C1D-ND	-2.42	121.39	124.80
12	B	806	CLA	CHD-C1D-ND	-2.42	121.39	124.80
12	A	809	CLA	CHD-C1D-ND	-2.42	121.39	124.80
12	A	811	CLA	CHD-C1D-ND	-2.42	121.40	124.80
12	A	845	CLA	C4A-NA-C1A	2.41	107.78	106.68
15	B	837	BCR	C11-C10-C9	-2.41	123.90	127.28
15	A	843	BCR	C15-C14-C13	-2.41	123.90	127.28
15	A	841	BCR	C15-C16-C17	-2.40	118.60	123.52
12	B	846	CLA	O2A-C1-C2	-2.40	98.87	108.11
12	B	827	CLA	CHD-C1D-ND	-2.40	121.43	124.80
12	A	817	CLA	C4A-NA-C1A	2.39	107.77	106.68
12	B	845	CLA	C4A-NA-C1A	2.39	107.77	106.68
15	M	101	BCR	C24-C23-C22	-2.39	122.70	126.23
14	A	838	LHG	C11-C10-C9	-2.39	102.31	114.37
19	U	204	DD6	C10-C9-C8	2.38	130.11	123.20
15	I	101	BCR	C15-C16-C17	-2.38	118.64	123.52
12	B	809	CLA	C4A-NA-C1A	2.38	107.77	106.68
12	U	209	CLA	O2D-CGD-CBD	2.38	115.39	111.23
15	B	838	BCR	C29-C30-C25	2.38	113.90	110.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	B	841	BCR	C15-C16-C17	-2.38	118.65	123.52
12	B	848	CLA	CHD-C1D-ND	-2.38	121.45	124.80
12	U	206	CLA	CHD-C1D-ND	-2.38	121.45	124.80
12	A	810	CLA	C4A-NA-C1A	2.38	107.76	106.68
15	M	101	BCR	C11-C10-C9	-2.37	123.95	127.28
15	F	801	BCR	C16-C15-C14	-2.36	118.68	123.52
12	A	808	CLA	CHD-C1D-ND	-2.36	121.47	124.80
12	B	845	CLA	CHD-C1D-ND	-2.36	121.47	124.80
12	F	802	CLA	CHD-C1D-ND	-2.36	121.48	124.80
12	A	832	CLA	CHD-C1D-ND	-2.36	121.48	124.80
12	A	848	CLA	CHD-C1D-ND	-2.36	121.48	124.80
12	B	833	CLA	C4A-NA-C1A	2.36	107.75	106.68
15	F	804	BCR	C16-C15-C14	-2.35	118.71	123.52
12	U	208	CLA	CHA-C1A-NA	-2.35	121.07	126.39
19	U	213	DD6	C15-C14-C13	2.34	130.95	125.99
12	A	807	CLA	CHD-C1D-ND	-2.34	121.51	124.80
15	B	841	BCR	C10-C11-C12	-2.34	116.42	123.20
14	A	838	LHG	O8-C6-C5	-2.33	101.67	108.40
15	A	843	BCR	C33-C5-C6	-2.33	121.94	124.48
12	A	819	CLA	C4A-NA-C1A	2.33	107.74	106.68
12	A	829	CLA	CHD-C1D-C2D	2.32	130.32	125.49
12	A	835	CLA	CHD-C1D-ND	-2.32	121.54	124.80
15	A	843	BCR	C29-C30-C25	2.32	113.80	110.44
12	A	846	CLA	CHD-C1D-C2D	2.31	130.28	125.49
12	A	816	CLA	CHD-C1D-C2D	2.30	130.28	125.49
16	A	847	CL0	C4D-CHA-CBD	-2.30	106.65	108.97
12	A	831	CLA	CHD-C1D-C2D	2.30	130.27	125.49
15	B	837	BCR	C15-C16-C17	-2.30	118.82	123.52
12	A	817	CLA	CHD-C1D-ND	-2.29	121.57	124.80
15	A	841	BCR	C15-C14-C13	-2.29	124.07	127.28
19	U	204	DD6	O1-C15-C14	-2.29	110.32	116.88
12	U	209	CLA	CHD-C1D-C2D	2.28	130.24	125.49
12	B	804	CLA	CHD-C1D-ND	-2.28	121.59	124.80
12	U	208	CLA	C3A-C2A-C1A	-2.28	97.93	101.34
12	B	818	CLA	CHD-C1D-C2D	2.28	130.22	125.49
18	B	842	DGD	CFB-CEB-CDB	-2.28	102.87	114.37
12	A	812	CLA	CHD-C1D-ND	-2.27	121.61	124.80
12	B	844	CLA	CHD-C1D-C2D	2.27	130.21	125.49
14	A	838	LHG	C27-C26-C25	-2.27	102.91	114.37
12	U	211	CLA	CHD-C1D-C2D	2.27	130.20	125.49
12	B	828	CLA	CHD-C1D-ND	-2.27	121.61	124.80
12	A	845	CLA	CHD-C1D-ND	-2.26	121.62	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	A	812	CLA	C1D-ND-C4D	2.26	107.90	106.31
12	A	802	CLA	O2A-C1-C2	2.26	116.81	108.11
16	A	847	CL0	C4C-CHD-C1D	2.26	124.16	116.07
16	A	847	CL0	C3C-C4C-NC	-2.26	109.13	114.65
12	J	103	CLA	CHD-C1D-C2D	2.26	130.18	125.49
12	B	815	CLA	CHD-C1D-C2D	2.26	130.18	125.49
15	A	842	BCR	C24-C23-C22	-2.25	122.90	126.23
12	A	802	CLA	CAA-CBA-CGA	-2.25	106.81	113.21
15	F	804	BCR	C2-C1-C6	2.25	113.71	110.44
15	A	842	BCR	C29-C30-C25	2.25	113.70	110.44
12	B	817	CLA	C3B-C4B-NB	-2.25	108.52	110.53
12	A	834	CLA	CHD-C1D-ND	-2.25	121.64	124.80
15	A	840	BCR	C11-C10-C9	-2.25	124.13	127.28
12	U	208	CLA	O2A-C1-C2	2.25	116.75	108.11
12	A	836	CLA	CHD-C1D-ND	-2.25	121.64	124.80
12	B	834	CLA	C4A-NA-C1A	2.24	107.70	106.68
20	J	102	LMG	C1-C2-C3	-2.24	105.29	110.01
15	I	101	BCR	C2-C1-C6	2.24	113.69	110.44
15	B	838	BCR	C15-C14-C13	-2.24	124.14	127.28
15	B	839	BCR	C31-C1-C6	2.24	113.75	110.24
12	A	822	CLA	CHD-C1D-C2D	2.23	130.13	125.49
15	F	804	BCR	C33-C5-C6	-2.23	122.05	124.48
12	B	825	CLA	CHD-C1D-C2D	2.23	130.12	125.49
15	L	201	BCR	C33-C5-C6	-2.23	122.05	124.48
15	J	104	BCR	C3-C4-C5	-2.23	110.08	114.06
12	A	802	CLA	CHD-C1D-C2D	2.22	130.11	125.49
12	B	843	CLA	CHD-C1D-ND	-2.22	121.68	124.80
12	B	825	CLA	CAA-C2A-C3A	-2.22	107.00	113.00
19	U	213	DD6	C9-C10-C11	2.22	130.39	127.28
12	U	208	CLA	C2A-C3A-C4A	-2.22	98.29	101.87
12	A	824	CLA	O2A-C1-C2	2.21	116.63	108.11
12	U	210	CLA	CHD-C1D-ND	-2.21	121.69	124.80
15	J	104	BCR	C24-C23-C22	-2.21	122.96	126.23
15	B	839	BCR	C24-C23-C22	-2.21	122.96	126.23
12	A	818	CLA	CHD-C1D-C2D	2.20	130.07	125.49
12	B	819	CLA	C2A-C1A-CHA	2.20	127.68	123.87
12	B	823	CLA	CHD-C1D-ND	-2.20	121.71	124.80
12	B	815	CLA	C3B-C4B-NB	-2.19	108.57	110.53
15	B	837	BCR	C15-C14-C13	-2.19	124.20	127.28
19	U	215	DD6	C33-C32-C31	2.19	113.81	109.49
12	A	803	CLA	CHD-C1D-C2D	2.19	130.04	125.49
12	A	814	CLA	C4A-NA-C1A	2.19	107.68	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	U	213	DD6	C28-C27-C26	-2.19	119.93	124.18
12	A	828	CLA	CHD-C1D-ND	-2.18	121.73	124.80
12	A	820	CLA	CHD-C1D-C2D	2.18	130.03	125.49
12	B	817	CLA	CHD-C1D-C2D	2.18	130.03	125.49
15	B	837	BCR	C28-C27-C26	-2.18	110.17	114.06
15	A	842	BCR	C15-C16-C17	-2.18	119.06	123.52
15	I	101	BCR	C15-C14-C13	-2.18	124.22	127.28
15	J	104	BCR	C15-C16-C17	-2.17	119.08	123.52
12	B	829	CLA	CHD-C1D-C2D	2.17	130.00	125.49
12	B	821	CLA	CHD-C1D-C2D	2.17	130.00	125.49
12	B	802	CLA	C2A-C1A-CHA	2.17	127.63	123.87
15	F	801	BCR	C11-C10-C9	-2.16	124.24	127.28
15	I	102	BCR	C38-C26-C25	-2.16	122.12	124.48
12	A	852	CLA	C4A-NA-C1A	2.16	107.67	106.68
14	A	838	LHG	C18-C17-C16	-2.16	103.43	114.37
12	A	819	CLA	CHD-C1D-C2D	2.16	129.97	125.49
18	B	842	DGD	CBB-CAB-C9B	-2.15	103.49	114.37
12	A	851	CLA	C4A-NA-C1A	2.15	107.66	106.68
21	U	203	A86	C26-C25-C24	2.15	129.43	123.20
18	B	842	DGD	C1D-C2D-C3D	-2.15	105.49	110.01
15	L	205	BCR	C15-C14-C13	-2.14	124.27	127.28
15	A	840	BCR	C16-C15-C14	-2.14	119.14	123.52
12	L	204	CLA	CHD-C1D-C2D	2.14	129.94	125.49
12	A	827	CLA	CHD-C1D-ND	-2.14	121.79	124.80
12	B	830	CLA	CHD-C1D-ND	-2.14	121.79	124.80
12	B	848	CLA	C3B-C4B-NB	-2.14	108.62	110.53
15	I	102	BCR	C24-C23-C22	-2.14	123.07	126.23
12	B	833	CLA	C3B-C4B-NB	-2.14	108.62	110.53
20	U	202	LMG	O2-C2-C1	-2.13	104.99	110.08
12	B	809	CLA	CHD-C1D-ND	-2.13	121.80	124.80
12	A	807	CLA	C1D-ND-C4D	2.13	107.81	106.31
19	U	213	DD6	C33-C32-C31	2.13	113.68	109.49
15	A	840	BCR	C30-C25-C26	-2.13	119.73	122.64
20	J	102	LMG	O7-C10-O9	-2.12	118.74	123.70
12	B	819	CLA	CHD-C1D-C2D	2.12	129.91	125.49
15	I	101	BCR	C16-C15-C14	-2.12	119.17	123.52
20	U	202	LMG	O3-C3-C2	-2.12	105.38	110.38
12	A	814	CLA	CHD-C1D-C2D	2.12	129.89	125.49
12	A	805	CLA	CHD-C1D-C2D	2.11	129.88	125.49
12	U	201	CLA	CHD-C1D-C2D	2.11	129.88	125.49
12	B	832	CLA	C4A-NA-C1A	2.11	107.64	106.68
12	B	820	CLA	CHD-C1D-ND	-2.11	121.83	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	A	842	BCR	C16-C15-C14	-2.11	119.20	123.52
12	B	824	CLA	CHD-C1D-C2D	2.11	129.88	125.49
12	B	832	CLA	CHD-C1D-C2D	2.11	129.87	125.49
12	B	822	CLA	CHD-C1D-ND	-2.11	121.83	124.80
12	U	210	CLA	C4B-CHC-C1C	2.11	131.20	126.25
12	B	847	CLA	CHD-C1D-C2D	2.11	129.87	125.49
15	I	101	BCR	C10-C11-C12	-2.11	117.10	123.20
12	A	824	CLA	CHD-C1D-C2D	2.11	129.87	125.49
20	U	202	LMG	C1-C2-C3	-2.11	105.58	110.01
12	A	806	CLA	CHD-C1D-C2D	2.11	129.87	125.49
15	I	101	BCR	C28-C27-C26	-2.11	110.30	114.06
12	B	801	CLA	CHD-C1D-C2D	2.11	129.87	125.49
15	I	101	BCR	C31-C1-C6	2.10	113.54	110.24
12	B	811	CLA	CHD-C1D-C2D	2.10	129.87	125.49
12	A	821	CLA	C1D-ND-C4D	2.10	107.79	106.31
12	B	826	CLA	CHD-C1D-C2D	2.10	129.85	125.49
20	U	202	LMG	O1-C7-C8	-2.10	105.72	110.82
12	B	846	CLA	CHD-C1D-C2D	2.09	129.84	125.49
12	A	804	CLA	CHD-C1D-C2D	2.09	129.83	125.49
12	A	823	CLA	CHD-C1D-ND	-2.09	121.87	124.80
20	J	102	LMG	O3-C3-C2	-2.08	105.47	110.38
12	B	812	CLA	CHD-C1D-C2D	2.08	129.81	125.49
15	L	201	BCR	C2-C1-C6	2.08	113.46	110.44
15	A	843	BCR	C11-C10-C9	-2.08	124.37	127.28
12	B	833	CLA	CHD-C1D-C2D	2.07	129.80	125.49
12	B	847	CLA	C4A-NA-C1A	2.07	107.62	106.68
22	U	214	KC1	CBA-CAA-C2A	2.07	133.77	125.45
12	A	821	CLA	CHD-C1D-ND	-2.07	121.89	124.80
15	L	205	BCR	C15-C16-C17	-2.07	119.28	123.52
15	F	804	BCR	C24-C23-C22	-2.07	123.17	126.23
12	B	835	CLA	CHD-C1D-C2D	2.07	129.79	125.49
12	A	821	CLA	C2A-C1A-CHA	2.06	127.44	123.87
12	A	813	CLA	CHD-C1D-C2D	2.06	129.78	125.49
18	B	842	DGD	O2D-C2D-C1D	-2.06	105.16	110.08
12	B	816	CLA	CHD-C1D-C2D	2.06	129.77	125.49
12	A	833	CLA	CHD-C1D-C2D	2.06	129.77	125.49
15	M	101	BCR	C7-C8-C9	-2.06	123.19	126.23
12	B	803	CLA	C2A-C1A-CHA	2.05	127.43	123.87
15	A	840	BCR	C3-C4-C5	-2.05	110.40	114.06
12	B	848	CLA	CAA-C2A-C1A	2.05	118.69	111.97
12	L	202	CLA	CHD-C1D-C2D	2.05	129.75	125.49
12	A	830	CLA	CHD-C1D-C2D	2.05	129.75	125.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	B	831	CLA	CHD-C1D-C2D	2.05	129.75	125.49
12	B	820	CLA	CAA-C2A-C1A	2.04	118.68	111.97
12	B	810	CLA	CHD-C1D-C2D	2.04	129.72	125.49
12	B	843	CLA	C4A-NA-C1A	2.03	107.61	106.68
12	B	848	CLA	CGD-CBD-CAD	-2.03	104.27	110.85
12	B	806	CLA	C4A-NA-C1A	2.03	107.61	106.68
12	A	801	CLA	C2A-C1A-CHA	2.03	127.39	123.87
15	B	837	BCR	C27-C26-C25	2.03	125.44	122.70
12	F	803	CLA	CHD-C1D-C2D	2.03	129.70	125.49
15	B	840	BCR	C33-C5-C6	-2.03	122.27	124.48
12	A	815	CLA	CHD-C1D-C2D	2.02	129.69	125.49
12	A	801	CLA	CHD-C1D-C2D	2.02	129.69	125.49
12	B	805	CLA	CHD-C1D-C2D	2.02	129.69	125.49
12	B	828	CLA	C2A-C1A-CHA	2.02	127.37	123.87
12	A	805	CLA	C4A-NA-C1A	2.01	107.60	106.68
12	B	806	CLA	CHD-C1D-C2D	2.01	129.68	125.49
15	F	801	BCR	C24-C23-C22	-2.01	123.26	126.23
12	U	206	CLA	C4A-NA-C1A	2.01	107.60	106.68
12	A	831	CLA	C4A-NA-C1A	2.01	107.59	106.68
12	B	808	CLA	CHD-C1D-ND	-2.01	121.98	124.80

All (70) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
12	A	802	CLA	ND
12	A	803	CLA	ND
12	A	804	CLA	ND
12	A	805	CLA	ND
12	A	808	CLA	ND
12	A	810	CLA	ND
12	A	811	CLA	ND
12	A	812	CLA	ND
12	A	815	CLA	ND
12	A	816	CLA	ND
12	A	817	CLA	ND
12	A	818	CLA	ND
12	A	820	CLA	ND
12	A	821	CLA	ND
12	A	822	CLA	ND
12	A	823	CLA	ND
12	A	824	CLA	ND
12	A	828	CLA	ND

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Mol	Chain	Res	Type	Atom
12	A	829	CLA	ND
12	A	831	CLA	ND
12	A	832	CLA	ND
12	A	833	CLA	ND
12	A	834	CLA	ND
12	A	835	CLA	ND
12	A	836	CLA	ND
12	A	844	CLA	ND
12	A	850	CLA	ND
12	A	852	CLA	ND
12	B	801	CLA	ND
12	B	802	CLA	ND
12	B	803	CLA	ND
12	B	804	CLA	ND
12	B	805	CLA	ND
12	B	806	CLA	ND
12	B	807	CLA	ND
12	B	808	CLA	ND
12	B	809	CLA	ND
12	B	811	CLA	ND
12	B	815	CLA	ND
12	B	816	CLA	ND
12	B	817	CLA	ND
12	B	820	CLA	ND
12	B	821	CLA	ND
12	B	822	CLA	ND
12	B	823	CLA	ND
12	B	827	CLA	ND
12	B	829	CLA	ND
12	B	830	CLA	ND
12	B	831	CLA	ND
12	B	832	CLA	ND
12	B	833	CLA	ND
12	B	835	CLA	ND
12	B	843	CLA	ND
12	B	844	CLA	ND
12	B	845	CLA	ND
12	B	846	CLA	ND
12	B	848	CLA	ND
12	F	802	CLA	ND
12	F	803	CLA	ND
12	J	103	CLA	ND

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Mol	Chain	Res	Type	Atom
12	L	202	CLA	ND
12	L	204	CLA	ND
12	U	201	CLA	ND
12	U	205	CLA	ND
12	U	206	CLA	ND
12	U	207	CLA	ND
12	U	209	CLA	ND
12	U	210	CLA	ND
12	U	212	CLA	ND
16	A	847	CL0	NC

All (657) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	A	804	CLA	C1A-C2A-CAA-CBA
12	A	804	CLA	C3A-C2A-CAA-CBA
12	A	806	CLA	CBA-CGA-O2A-C1
12	A	806	CLA	O1A-CGA-O2A-C1
12	A	806	CLA	CHA-CBD-CGD-O1D
12	A	806	CLA	CHA-CBD-CGD-O2D
12	A	815	CLA	C3A-C2A-CAA-CBA
12	A	820	CLA	C4-C3-C5-C6
12	A	826	CLA	CHA-CBD-CGD-O1D
12	A	826	CLA	CHA-CBD-CGD-O2D
12	A	827	CLA	CHA-CBD-CGD-O1D
12	A	827	CLA	CHA-CBD-CGD-O2D
12	A	829	CLA	CHA-CBD-CGD-O1D
12	A	829	CLA	CHA-CBD-CGD-O2D
12	A	833	CLA	CBA-CGA-O2A-C1
12	A	833	CLA	O1A-CGA-O2A-C1
12	A	845	CLA	C6-C7-C8-C9
12	A	850	CLA	CHA-CBD-CGD-O1D
12	A	850	CLA	CHA-CBD-CGD-O2D
12	B	804	CLA	CHA-CBD-CGD-O1D
12	B	804	CLA	CHA-CBD-CGD-O2D
12	B	808	CLA	CHA-CBD-CGD-O1D
12	B	808	CLA	CHA-CBD-CGD-O2D
12	B	813	CLA	CBA-CGA-O2A-C1
12	B	813	CLA	O1A-CGA-O2A-C1
12	B	813	CLA	CHA-CBD-CGD-O2D
12	B	820	CLA	CHA-CBD-CGD-O1D
12	B	820	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
12	B	821	CLA	CHA-CBD-CGD-O1D
12	B	821	CLA	CHA-CBD-CGD-O2D
12	B	824	CLA	CBA-CGA-O2A-C1
12	B	824	CLA	O1A-CGA-O2A-C1
12	B	825	CLA	CHA-CBD-CGD-O1D
12	B	825	CLA	CHA-CBD-CGD-O2D
12	B	844	CLA	CBA-CGA-O2A-C1
12	B	844	CLA	O1A-CGA-O2A-C1
12	B	846	CLA	C1A-C2A-CAA-CBA
12	B	847	CLA	C1A-C2A-CAA-CBA
12	B	847	CLA	C3A-C2A-CAA-CBA
12	J	103	CLA	CAD-CBD-CGD-O1D
12	J	103	CLA	CAD-CBD-CGD-O2D
12	L	202	CLA	CBA-CGA-O2A-C1
12	L	202	CLA	O1A-CGA-O2A-C1
12	U	201	CLA	CBD-CGD-O2D-CED
12	U	201	CLA	O1D-CGD-O2D-CED
12	U	209	CLA	CBD-CGD-O2D-CED
12	U	209	CLA	O1D-CGD-O2D-CED
12	U	211	CLA	CHA-CBD-CGD-O1D
12	U	211	CLA	CHA-CBD-CGD-O2D
14	A	838	LHG	C3-O3-P-O5
14	A	839	LHG	C4-O6-P-O3
15	A	840	BCR	C20-C21-C22-C37
15	A	840	BCR	C21-C22-C23-C24
15	A	841	BCR	C7-C8-C9-C10
15	A	841	BCR	C20-C21-C22-C37
15	A	841	BCR	C21-C22-C23-C24
15	A	843	BCR	C20-C21-C22-C23
15	A	843	BCR	C20-C21-C22-C37
15	A	843	BCR	C21-C22-C23-C24
15	B	837	BCR	C7-C8-C9-C34
15	B	837	BCR	C21-C22-C23-C24
15	B	837	BCR	C37-C22-C23-C24
15	B	838	BCR	C6-C7-C8-C9
15	B	838	BCR	C7-C8-C9-C10
15	B	838	BCR	C7-C8-C9-C34
15	B	838	BCR	C37-C22-C23-C24
15	B	839	BCR	C7-C8-C9-C10
15	B	839	BCR	C7-C8-C9-C34
15	F	801	BCR	C7-C8-C9-C10
15	F	801	BCR	C37-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
15	I	102	BCR	C7-C8-C9-C34
15	I	102	BCR	C20-C21-C22-C23
15	I	102	BCR	C20-C21-C22-C37
15	J	104	BCR	C7-C8-C9-C34
15	J	104	BCR	C21-C22-C23-C24
15	M	101	BCR	C7-C8-C9-C10
15	M	101	BCR	C7-C8-C9-C34
15	M	101	BCR	C20-C21-C22-C37
15	M	101	BCR	C22-C23-C24-C25
19	U	213	DD6	C9-C10-C11-C12
19	U	213	DD6	C11-C13-C14-C15
19	U	213	DD6	C5-C6-C8-C9
19	U	213	DD6	C7-C6-C8-C9
19	U	215	DD6	C2-C3-C4-C5
19	U	215	DD6	C3-C4-C5-C6
19	U	215	DD6	C4-C5-C6-C7
19	U	215	DD6	C4-C5-C6-C8
20	J	102	LMG	O6-C1-O1-C7
20	J	102	LMG	O9-C10-O7-C8
20	U	202	LMG	C11-C10-O7-C8
21	U	203	A86	C9-C10-C11-C12
21	U	203	A86	C9-C10-C11-C13
21	U	203	A86	C10-C11-C13-O
21	U	203	A86	C12-C11-C13-O
21	U	203	A86	C1-C24-C25-C26
21	U	203	A86	C2-C3-C4-C5
21	U	203	A86	C39-C38-O4-C34
21	U	203	A86	C4-C5-C6-C7
21	U	203	A86	C4-C5-C6-C8
21	U	203	A86	C6-C8-C9-C10
21	U	203	A86	O5-C38-O4-C34
20	U	202	LMG	O9-C10-O7-C8
12	A	836	CLA	C3-C5-C6-C7
12	B	834	CLA	C3-C5-C6-C7
12	B	846	CLA	C3-C5-C6-C7
12	U	211	CLA	C3-C5-C6-C7
12	A	844	CLA	C4-C3-C5-C6
12	B	810	CLA	C4-C3-C5-C6
12	B	846	CLA	C4-C3-C5-C6
12	A	844	CLA	C2-C3-C5-C6
12	B	810	CLA	C2-C3-C5-C6
12	B	846	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
12	A	825	CLA	C2A-CAA-CBA-CGA
12	A	808	CLA	C3-C5-C6-C7
12	B	815	CLA	C3-C5-C6-C7
12	B	817	CLA	C3-C5-C6-C7
19	U	215	DD6	C1-C2-C3-C4
12	B	829	CLA	C3-C5-C6-C7
12	U	205	CLA	C3-C5-C6-C7
12	B	811	CLA	C3-C5-C6-C7
18	B	842	DGD	O6E-C5E-C6E-O5E
20	U	202	LMG	O6-C1-O1-C7
19	U	213	DD6	C24-C25-C26-C27
12	B	835	CLA	C14-C13-C15-C16
20	J	102	LMG	C2-C1-O1-C7
15	A	841	BCR	C7-C8-C9-C34
15	A	842	BCR	C7-C8-C9-C34
15	A	843	BCR	C11-C12-C13-C35
15	A	843	BCR	C37-C22-C23-C24
15	F	801	BCR	C7-C8-C9-C34
15	F	804	BCR	C37-C22-C23-C24
15	I	101	BCR	C37-C22-C23-C24
15	J	104	BCR	C11-C12-C13-C35
15	L	201	BCR	C37-C22-C23-C24
19	J	101	DD6	C12-C11-C13-C14
19	U	213	DD6	C-C1-C24-C25
21	U	203	A86	C-C1-C24-C25
15	B	838	BCR	C21-C22-C23-C24
19	J	101	DD6	C10-C11-C13-C14
19	U	213	DD6	C2-C1-C24-C25
21	U	203	A86	C2-C1-C24-C25
12	B	833	CLA	C2A-CAA-CBA-CGA
20	J	102	LMG	O10-C28-O8-C9
12	B	829	CLA	C5-C6-C7-C8
12	A	823	CLA	C12-C13-C15-C16
12	A	833	CLA	C11-C10-C8-C7
14	A	838	LHG	C28-C29-C30-C31
12	A	848	CLA	C8-C10-C11-C12
12	B	844	CLA	C10-C11-C12-C13
14	A	838	LHG	C7-C8-C9-C10
14	A	839	LHG	C7-C8-C9-C10
12	A	809	CLA	C8-C10-C11-C12
12	A	824	CLA	C10-C11-C12-C13
12	B	807	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
12	B	813	CLA	C2A-CAA-CBA-CGA
12	B	820	CLA	C2A-CAA-CBA-CGA
12	B	844	CLA	C2A-CAA-CBA-CGA
15	B	837	BCR	C10-C11-C12-C13
12	A	851	CLA	C15-C16-C17-C18
12	A	852	CLA	C15-C16-C17-C18
12	B	805	CLA	C10-C11-C12-C13
12	B	807	CLA	C8-C10-C11-C12
15	M	101	BCR	C6-C7-C8-C9
12	A	850	CLA	C8-C10-C11-C12
12	B	821	CLA	C13-C15-C16-C17
12	B	817	CLA	C8-C10-C11-C12
12	A	834	CLA	C3-C5-C6-C7
12	A	844	CLA	C15-C16-C17-C18
12	B	820	CLA	C4-C3-C5-C6
12	A	807	CLA	C8-C10-C11-C12
18	B	842	DGD	C4E-C5E-C6E-O5E
12	B	845	CLA	C15-C16-C17-C18
12	A	836	CLA	C5-C6-C7-C8
12	A	846	CLA	C13-C15-C16-C17
12	B	845	CLA	C13-C15-C16-C17
20	U	202	LMG	O6-C5-C6-O5
20	J	102	LMG	C11-C10-O7-C8
18	B	842	DGD	O1B-C1B-O2G-C2G
20	U	202	LMG	C2-C1-O1-C7
12	B	843	CLA	C10-C11-C12-C13
20	U	202	LMG	C4-C5-C6-O5
15	B	840	BCR	C20-C21-C22-C37
15	B	841	BCR	C20-C21-C22-C37
15	J	104	BCR	C20-C21-C22-C37
15	L	201	BCR	C16-C17-C18-C36
15	F	804	BCR	C7-C8-C9-C34
15	I	102	BCR	C37-C22-C23-C24
15	J	104	BCR	C37-C22-C23-C24
15	B	837	BCR	C7-C8-C9-C10
15	I	102	BCR	C21-C22-C23-C24
15	L	205	BCR	C7-C8-C9-C10
12	A	807	CLA	C2A-CAA-CBA-CGA
12	B	823	CLA	C16-C17-C18-C19
12	A	829	CLA	C15-C16-C17-C18
15	I	101	BCR	C20-C21-C22-C23
15	L	201	BCR	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
15	L	205	BCR	C11-C10-C9-C8
19	U	213	DD6	C9-C10-C11-C13
13	B	836	PQN	C23-C25-C26-C27
12	F	802	CLA	O2A-C1-C2-C3
14	A	838	LHG	C24-C25-C26-C27
19	U	215	DD6	C27-C29-C30-C31
12	B	823	CLA	C16-C17-C18-C20
12	A	833	CLA	C13-C15-C16-C17
14	A	838	LHG	C27-C28-C29-C30
12	B	846	CLA	C3A-C2A-CAA-CBA
12	F	803	CLA	C3A-C2A-CAA-CBA
12	U	209	CLA	C3A-C2A-CAA-CBA
12	B	811	CLA	C5-C6-C7-C8
20	J	102	LMG	C29-C28-O8-C9
18	B	842	DGD	C9B-CAB-CBB-CCB
18	B	842	DGD	CBB-CCB-CDB-CEB
18	B	842	DGD	CEB-CFB-CGB-CHB
12	B	831	CLA	C16-C17-C18-C19
15	A	843	BCR	C23-C24-C25-C30
15	I	102	BCR	C23-C24-C25-C26
15	I	102	BCR	C23-C24-C25-C30
15	L	205	BCR	C23-C24-C25-C30
14	A	838	LHG	C34-C35-C36-C37
18	B	842	DGD	C2B-C1B-O2G-C2G
12	A	844	CLA	C2A-CAA-CBA-CGA
18	B	842	DGD	C3A-C4A-C5A-C6A
18	B	842	DGD	C3B-C4B-C5B-C6B
15	I	101	BCR	C10-C11-C12-C13
15	M	101	BCR	C18-C19-C20-C21
19	J	101	DD6	C1-C24-C25-C26
12	B	820	CLA	C2-C3-C5-C6
12	A	845	CLA	C11-C12-C13-C15
14	A	838	LHG	C10-C11-C12-C13
15	I	102	BCR	C22-C23-C24-C25
18	B	842	DGD	C4A-C5A-C6A-C7A
14	A	839	LHG	C8-C7-O7-C5
20	J	102	LMG	C20-C21-C22-C23
12	B	835	CLA	C13-C15-C16-C17
15	A	843	BCR	C7-C8-C9-C34
15	I	101	BCR	C7-C8-C9-C34
18	B	842	DGD	C1B-C2B-C3B-C4B
12	B	820	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
20	U	202	LMG	C29-C28-O8-C9
12	U	201	CLA	C4-C3-C5-C6
12	B	808	CLA	C3-C5-C6-C7
12	A	845	CLA	C5-C6-C7-C8
12	U	208	CLA	C15-C16-C17-C18
20	U	202	LMG	C30-C31-C32-C33
12	B	831	CLA	C16-C17-C18-C20
12	A	833	CLA	C3-C5-C6-C7
12	U	201	CLA	C2-C3-C5-C6
14	A	838	LHG	C30-C31-C32-C33
12	B	847	CLA	C2A-CAA-CBA-CGA
12	B	831	CLA	C13-C15-C16-C17
12	A	845	CLA	C3-C5-C6-C7
12	A	815	CLA	C1A-C2A-CAA-CBA
12	B	812	CLA	C1A-C2A-CAA-CBA
12	U	209	CLA	C1A-C2A-CAA-CBA
18	B	842	DGD	C5A-C6A-C7A-C8A
12	B	828	CLA	C6-C7-C8-C10
12	A	852	CLA	C13-C15-C16-C17
12	B	843	CLA	C8-C10-C11-C12
12	A	809	CLA	C4-C3-C5-C6
18	B	842	DGD	C2A-C3A-C4A-C5A
12	A	833	CLA	C11-C10-C8-C9
18	B	842	DGD	O1G-C1G-C2G-C3G
15	A	840	BCR	C16-C17-C18-C36
15	B	838	BCR	C20-C21-C22-C37
15	M	101	BCR	C16-C17-C18-C36
12	A	809	CLA	C2-C3-C5-C6
15	L	205	BCR	C7-C8-C9-C34
19	U	204	DD6	C12-C11-C13-C14
18	B	842	DGD	C4B-C5B-C6B-C7B
12	A	833	CLA	O2A-C1-C2-C3
15	B	837	BCR	C18-C19-C20-C21
19	U	213	DD6	C1-C24-C25-C26
12	A	834	CLA	C13-C15-C16-C17
15	A	840	BCR	C16-C17-C18-C19
15	A	840	BCR	C20-C21-C22-C23
14	A	838	LHG	C32-C33-C34-C35
20	U	202	LMG	C29-C30-C31-C32
12	A	824	CLA	C5-C6-C7-C8
15	M	101	BCR	C14-C15-C16-C17
12	A	850	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
12	A	823	CLA	C4-C3-C5-C6
12	A	851	CLA	C4-C3-C5-C6
12	B	829	CLA	C4-C3-C5-C6
14	A	838	LHG	O9-C7-O7-C5
12	B	828	CLA	C6-C7-C8-C9
12	B	829	CLA	C11-C10-C8-C9
12	A	845	CLA	C11-C12-C13-C14
14	A	838	LHG	C25-C26-C27-C28
12	A	822	CLA	C12-C13-C15-C16
12	A	845	CLA	C6-C7-C8-C10
12	B	829	CLA	C11-C10-C8-C7
12	A	825	CLA	C4-C3-C5-C6
12	B	807	CLA	C4-C3-C5-C6
12	B	829	CLA	C10-C11-C12-C13
18	B	842	DGD	O1A-C1A-O1G-C1G
19	J	101	DD6	C24-C25-C26-C27
19	U	204	DD6	C24-C25-C26-C27
15	B	840	BCR	C7-C8-C9-C34
19	U	204	DD6	C10-C11-C13-C14
14	A	838	LHG	C1-C2-C3-O3
18	B	842	DGD	CAB-CBB-CCB-CDB
12	B	831	CLA	C4-C3-C5-C6
12	A	823	CLA	C2-C3-C5-C6
12	A	825	CLA	C2-C3-C5-C6
12	B	829	CLA	C2-C3-C5-C6
12	A	807	CLA	C13-C15-C16-C17
15	A	843	BCR	C1-C6-C7-C8
15	B	837	BCR	C1-C6-C7-C8
15	B	837	BCR	C23-C24-C25-C30
15	B	840	BCR	C1-C6-C7-C8
15	B	840	BCR	C23-C24-C25-C30
15	B	841	BCR	C1-C6-C7-C8
15	F	804	BCR	C1-C6-C7-C8
15	L	201	BCR	C1-C6-C7-C8
15	L	201	BCR	C23-C24-C25-C30
15	M	101	BCR	C23-C24-C25-C30
12	U	211	CLA	C5-C6-C7-C8
12	A	806	CLA	C2A-CAA-CBA-CGA
18	B	842	DGD	O2G-C2G-C3G-O3G
12	A	822	CLA	C14-C13-C15-C16
15	B	837	BCR	C22-C23-C24-C25
19	J	101	DD6	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
20	J	102	LMG	C29-C30-C31-C32
12	A	805	CLA	O2A-C1-C2-C3
12	B	815	CLA	C4-C3-C5-C6
12	B	807	CLA	C2-C3-C5-C6
15	B	838	BCR	C16-C17-C18-C36
19	U	213	DD6	C4-C5-C6-C7
19	U	215	DD6	C-C1-C24-C25
12	A	809	CLA	C11-C12-C13-C15
12	A	825	CLA	C12-C13-C15-C16
12	A	828	CLA	C12-C13-C15-C16
12	B	823	CLA	C11-C10-C8-C7
12	B	834	CLA	C11-C12-C13-C15
20	J	102	LMG	C10-C11-C12-C13
15	F	801	BCR	C21-C22-C23-C24
15	J	104	BCR	C7-C8-C9-C10
12	A	850	CLA	C2-C3-C5-C6
12	A	851	CLA	C2-C3-C5-C6
12	B	811	CLA	O2A-C1-C2-C3
20	J	102	LMG	C7-C8-O7-C10
15	B	838	BCR	C11-C10-C9-C8
12	B	820	CLA	C5-C6-C7-C8
12	A	850	CLA	C4-C3-C5-C6
21	U	203	A86	C28-C27-C29-C30
18	B	842	DGD	O1G-C1G-C2G-O2G
12	A	825	CLA	C14-C13-C15-C16
12	A	848	CLA	C11-C10-C8-C9
12	A	851	CLA	C11-C10-C8-C9
14	A	838	LHG	C9-C10-C11-C12
20	J	102	LMG	C11-C12-C13-C14
12	B	846	CLA	C8-C10-C11-C12
21	U	203	A86	C13-C14-C15-O1
12	B	833	CLA	C16-C17-C18-C19
12	B	831	CLA	C2-C3-C5-C6
14	A	838	LHG	O2-C2-C3-O3
12	A	833	CLA	C1A-C2A-CAA-CBA
12	B	823	CLA	C1A-C2A-CAA-CBA
12	F	803	CLA	C1A-C2A-CAA-CBA
14	A	838	LHG	C24-C23-O8-C6
14	A	838	LHG	C12-C13-C14-C15
12	A	818	CLA	C4-C3-C5-C6
12	A	821	CLA	C4-C3-C5-C6
12	B	808	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
15	I	102	BCR	C7-C8-C9-C10
12	A	815	CLA	C2A-CAA-CBA-CGA
13	A	837	PQN	C17-C18-C20-C21
12	B	817	CLA	C16-C17-C18-C19
20	J	102	LMG	C16-C17-C18-C19
12	A	834	CLA	C4-C3-C5-C6
12	B	823	CLA	C4-C3-C5-C6
14	A	838	LHG	O6-C4-C5-O7
12	B	823	CLA	C11-C10-C8-C9
12	A	801	CLA	C10-C11-C12-C13
19	U	213	DD6	C3-C4-C5-C6
12	B	844	CLA	C13-C15-C16-C17
12	B	827	CLA	C1-C2-C3-C4
21	U	203	A86	C26-C27-C29-C30
12	A	828	CLA	C15-C16-C17-C18
20	J	102	LMG	C28-C29-C30-C31
12	A	803	CLA	CAD-CBD-CGD-O2D
12	B	801	CLA	C2A-CAA-CBA-CGA
12	A	821	CLA	C15-C16-C17-C18
12	A	802	CLA	CHA-CBD-CGD-O1D
12	A	802	CLA	CHA-CBD-CGD-O2D
12	A	803	CLA	CAD-CBD-CGD-O1D
12	A	819	CLA	CHA-CBD-CGD-O1D
12	A	819	CLA	CHA-CBD-CGD-O2D
12	A	821	CLA	CHA-CBD-CGD-O1D
12	B	812	CLA	CHA-CBD-CGD-O1D
12	B	813	CLA	CHA-CBD-CGD-O1D
14	A	839	LHG	C3-O3-P-O5
14	A	839	LHG	C4-O6-P-O5
19	U	213	DD6	C1-C2-C3-C4
15	A	843	BCR	C23-C24-C25-C26
15	L	205	BCR	C1-C6-C7-C8
12	B	823	CLA	C2-C3-C5-C6
21	U	203	A86	C7-C6-C8-C9
12	B	827	CLA	C2A-CAA-CBA-CGA
12	B	833	CLA	C16-C17-C18-C20
12	B	825	CLA	C10-C11-C12-C13
14	A	838	LHG	O6-C4-C5-C6
12	A	850	CLA	C10-C11-C12-C13
12	A	809	CLA	C11-C12-C13-C14
12	B	834	CLA	C11-C12-C13-C14
12	B	843	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
15	B	840	BCR	C11-C10-C9-C8
15	I	101	BCR	C16-C17-C18-C19
15	M	101	BCR	C20-C21-C22-C23
18	B	842	DGD	C7B-C8B-C9B-CAB
12	B	823	CLA	C10-C11-C12-C13
12	B	821	CLA	C16-C17-C18-C19
14	A	838	LHG	C11-C10-C9-C8
12	A	848	CLA	C4-C3-C5-C6
12	B	835	CLA	C15-C16-C17-C18
20	J	102	LMG	O1-C7-C8-C9
12	A	815	CLA	C16-C17-C18-C20
12	U	211	CLA	C4-C3-C5-C6
12	B	808	CLA	C2-C3-C5-C6
16	A	847	CL0	CAA-CBA-CGA-O2A
12	A	845	CLA	C11-C10-C8-C9
18	B	842	DGD	C8A-C9A-CAA-CBA
20	J	102	LMG	C19-C20-C21-C22
12	A	834	CLA	C6-C7-C8-C10
12	B	835	CLA	C12-C13-C15-C16
12	B	843	CLA	C11-C10-C8-C7
12	B	826	CLA	C3A-C2A-CAA-CBA
12	B	828	CLA	C4-C3-C5-C6
12	B	844	CLA	C3A-C2A-CAA-CBA
15	B	839	BCR	C20-C21-C22-C37
15	F	804	BCR	C35-C13-C14-C15
21	U	203	A86	C25-C26-C27-C28
12	A	807	CLA	C2-C1-O2A-CGA
12	B	802	CLA	C2-C1-O2A-CGA
12	B	846	CLA	C5-C6-C7-C8
12	A	823	CLA	C13-C15-C16-C17
15	L	205	BCR	C11-C12-C13-C14
12	B	801	CLA	C4-C3-C5-C6
12	B	809	CLA	C4-C3-C5-C6
12	A	834	CLA	C2-C3-C5-C6
12	A	848	CLA	C2-C3-C5-C6
12	B	827	CLA	O2A-C1-C2-C3
12	B	846	CLA	C11-C12-C13-C14
12	U	206	CLA	C14-C13-C15-C16
14	A	839	LHG	C9-C10-C11-C12
12	A	815	CLA	CAA-CBA-CGA-O2A
12	B	828	CLA	C2-C3-C5-C6
12	B	804	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
12	L	204	CLA	C2A-CAA-CBA-CGA
12	B	805	CLA	C1A-C2A-CAA-CBA
12	B	813	CLA	C1A-C2A-CAA-CBA
12	B	819	CLA	C1A-C2A-CAA-CBA
12	B	828	CLA	C1A-C2A-CAA-CBA
15	B	839	BCR	C20-C21-C22-C23
21	U	203	A86	C25-C26-C27-C29
15	A	840	BCR	C23-C24-C25-C30
15	A	841	BCR	C1-C6-C7-C8
15	A	841	BCR	C23-C24-C25-C30
15	A	842	BCR	C23-C24-C25-C30
15	A	843	BCR	C5-C6-C7-C8
15	B	837	BCR	C5-C6-C7-C8
15	B	837	BCR	C23-C24-C25-C26
15	B	838	BCR	C1-C6-C7-C8
15	B	840	BCR	C5-C6-C7-C8
15	B	840	BCR	C23-C24-C25-C26
15	B	841	BCR	C5-C6-C7-C8
15	B	841	BCR	C23-C24-C25-C30
15	F	801	BCR	C1-C6-C7-C8
15	F	804	BCR	C5-C6-C7-C8
15	I	102	BCR	C1-C6-C7-C8
15	J	104	BCR	C23-C24-C25-C30
15	L	201	BCR	C5-C6-C7-C8
15	L	201	BCR	C23-C24-C25-C26
15	L	205	BCR	C5-C6-C7-C8
15	L	205	BCR	C23-C24-C25-C26
15	M	101	BCR	C1-C6-C7-C8
12	A	808	CLA	C4-C3-C5-C6
12	A	818	CLA	C2-C3-C5-C6
12	A	821	CLA	C2-C3-C5-C6
12	B	801	CLA	C2-C3-C5-C6
12	U	211	CLA	C2-C3-C5-C6
12	L	202	CLA	O2A-C1-C2-C3
12	B	804	CLA	CAA-CBA-CGA-O1A
12	A	804	CLA	C11-C10-C8-C7
12	A	848	CLA	C11-C10-C8-C7
12	B	823	CLA	C11-C12-C13-C15
12	B	829	CLA	C11-C12-C13-C15
12	A	845	CLA	C2A-CAA-CBA-CGA
12	A	828	CLA	C13-C15-C16-C17
12	U	207	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
12	B	804	CLA	CAA-CBA-CGA-O2A
12	B	816	CLA	C4-C3-C5-C6
12	B	817	CLA	C4-C3-C5-C6
12	B	809	CLA	C2-C3-C5-C6
15	L	201	BCR	C21-C22-C23-C24
12	A	844	CLA	C14-C13-C15-C16
12	A	804	CLA	C4-C3-C5-C6
12	B	835	CLA	C4-C3-C5-C6
12	A	804	CLA	C8-C10-C11-C12
20	U	202	LMG	C7-C8-C9-O8
12	B	803	CLA	C2A-CAA-CBA-CGA
12	U	206	CLA	C2A-CAA-CBA-CGA
19	J	101	DD6	C27-C29-C30-C31
19	U	204	DD6	C27-C29-C30-C31
12	A	806	CLA	C4-C3-C5-C6
12	B	835	CLA	C2-C3-C5-C6
12	A	817	CLA	CAA-CBA-CGA-O2A
15	B	841	BCR	C11-C10-C9-C34
15	L	201	BCR	C11-C10-C9-C34
16	A	847	CL0	CHA-CBD-CGD-O1D
16	A	847	CL0	CHA-CBD-CGD-O2D
20	J	102	LMG	O1-C7-C8-O7
12	A	821	CLA	C11-C10-C8-C7
19	U	215	DD6	C2-C1-C24-C25
12	B	831	CLA	C14-C13-C15-C16
12	U	206	CLA	C6-C7-C8-C9
20	J	102	LMG	C8-C7-O1-C1
12	A	836	CLA	C2-C1-O2A-CGA
12	B	821	CLA	C2-C1-O2A-CGA
12	B	833	CLA	C5-C6-C7-C8
12	B	805	CLA	C3A-C2A-CAA-CBA
12	U	208	CLA	C3A-C2A-CAA-CBA
12	U	207	CLA	CAA-CBA-CGA-O1A
12	A	817	CLA	CAA-CBA-CGA-O1A
12	B	848	CLA	CAA-CBA-CGA-O2A
12	B	815	CLA	CAA-CBA-CGA-O2A
13	A	837	PQN	C18-C20-C21-C22
15	F	804	BCR	C12-C13-C14-C15
19	U	213	DD6	C4-C5-C6-C8
12	B	848	CLA	CAA-CBA-CGA-O1A
18	B	842	DGD	C1G-C2G-C3G-O3G
20	U	202	LMG	O1-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
20	U	202	LMG	O7-C8-C9-O8
12	A	821	CLA	C14-C13-C15-C16
12	A	824	CLA	C11-C12-C13-C14
12	B	805	CLA	C14-C13-C15-C16
12	B	844	CLA	C11-C12-C13-C14
12	A	845	CLA	C11-C10-C8-C7
12	B	805	CLA	C11-C12-C13-C15
12	B	835	CLA	C11-C12-C13-C15
12	A	805	CLA	C2B-C3B-CAB-CBB
12	A	809	CLA	C2B-C3B-CAB-CBB
12	A	813	CLA	C2B-C3B-CAB-CBB
12	A	822	CLA	C2B-C3B-CAB-CBB
12	A	825	CLA	C2B-C3B-CAB-CBB
12	A	832	CLA	C2B-C3B-CAB-CBB
12	A	844	CLA	C2B-C3B-CAB-CBB
12	A	845	CLA	C2B-C3B-CAB-CBB
12	A	848	CLA	C2B-C3B-CAB-CBB
12	A	850	CLA	C2B-C3B-CAB-CBB
12	A	851	CLA	C2B-C3B-CAB-CBB
12	B	805	CLA	C2B-C3B-CAB-CBB
12	B	806	CLA	C2B-C3B-CAB-CBB
12	B	811	CLA	C2B-C3B-CAB-CBB
12	B	816	CLA	C2B-C3B-CAB-CBB
12	B	820	CLA	C2B-C3B-CAB-CBB
12	B	824	CLA	C2B-C3B-CAB-CBB
12	B	825	CLA	C2B-C3B-CAB-CBB
12	B	827	CLA	C2B-C3B-CAB-CBB
12	B	844	CLA	C2B-C3B-CAB-CBB
12	F	802	CLA	C2B-C3B-CAB-CBB
12	J	103	CLA	C2B-C3B-CAB-CBB
12	L	202	CLA	C2B-C3B-CAB-CBB
12	U	201	CLA	C2B-C3B-CAB-CBB
12	U	206	CLA	C2B-C3B-CAB-CBB
12	U	207	CLA	C2B-C3B-CAB-CBB
15	A	840	BCR	C1-C6-C7-C8
15	A	840	BCR	C5-C6-C7-C8
15	A	840	BCR	C23-C24-C25-C26
15	A	841	BCR	C5-C6-C7-C8
15	A	841	BCR	C23-C24-C25-C26
15	B	838	BCR	C5-C6-C7-C8
15	B	839	BCR	C5-C6-C7-C8
15	B	839	BCR	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
15	B	841	BCR	C23-C24-C25-C26
15	F	801	BCR	C5-C6-C7-C8
15	F	801	BCR	C23-C24-C25-C26
15	F	804	BCR	C23-C24-C25-C26
15	F	804	BCR	C23-C24-C25-C30
15	J	104	BCR	C23-C24-C25-C26
15	M	101	BCR	C5-C6-C7-C8
15	M	101	BCR	C23-C24-C25-C26
12	A	845	CLA	CAA-CBA-CGA-O2A
12	A	848	CLA	C2-C1-O2A-CGA
19	U	204	DD6	C11-C13-C14-C15
12	B	811	CLA	C2A-CAA-CBA-CGA
12	B	803	CLA	C8-C10-C11-C12
12	A	811	CLA	CAA-CBA-CGA-O2A
12	B	803	CLA	CAA-CBA-CGA-O2A
12	B	809	CLA	CAA-CBA-CGA-O2A
18	B	842	DGD	C2A-C1A-O1G-C1G
12	U	212	CLA	CAA-CBA-CGA-O2A
12	A	836	CLA	C2A-CAA-CBA-CGA
12	B	815	CLA	C5-C6-C7-C8
12	A	836	CLA	C6-C7-C8-C9
12	B	835	CLA	C11-C10-C8-C9
12	A	802	CLA	CAA-CBA-CGA-O2A
12	U	211	CLA	CAA-CBA-CGA-O2A
12	A	814	CLA	C4B-C3B-CAB-CBB
12	A	846	CLA	C4B-C3B-CAB-CBB
12	A	850	CLA	C1A-C2A-CAA-CBA
12	B	826	CLA	C1A-C2A-CAA-CBA
12	B	843	CLA	C1A-C2A-CAA-CBA
15	A	840	BCR	C6-C7-C8-C9
12	A	804	CLA	C2-C3-C5-C6
12	B	815	CLA	C2-C3-C5-C6
14	A	838	LHG	C16-C17-C18-C19
15	B	841	BCR	C21-C22-C23-C24
21	U	203	A86	C5-C6-C8-C9
12	A	821	CLA	CAA-CBA-CGA-O2A
14	A	838	LHG	C33-C34-C35-C36
12	A	804	CLA	CAA-CBA-CGA-O2A
12	A	804	CLA	C11-C12-C13-C15
12	B	815	CLA	C6-C7-C8-C10
12	B	834	CLA	C13-C15-C16-C17
12	A	822	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
12	B	806	CLA	C16-C17-C18-C19
12	L	204	CLA	O2A-C1-C2-C3
12	A	833	CLA	C2A-CAA-CBA-CGA
14	A	839	LHG	O8-C23-C24-C25
12	A	850	CLA	C3A-C2A-CAA-CBA
12	A	822	CLA	C13-C15-C16-C17
18	B	842	DGD	C2G-C1G-O1G-C1A
12	A	803	CLA	CAA-CBA-CGA-O2A
12	B	809	CLA	CAA-CBA-CGA-O1A
12	A	804	CLA	C11-C10-C8-C9
12	A	828	CLA	C14-C13-C15-C16
12	A	811	CLA	CAA-CBA-CGA-O1A
12	A	851	CLA	C5-C6-C7-C8
12	A	845	CLA	CAA-CBA-CGA-O1A
12	B	803	CLA	CAA-CBA-CGA-O1A
12	A	808	CLA	C2-C3-C5-C6
12	A	821	CLA	C13-C15-C16-C17
12	B	802	CLA	CAA-CBA-CGA-O2A
12	A	807	CLA	C16-C17-C18-C20
15	A	843	BCR	C18-C19-C20-C21
12	A	846	CLA	C8-C10-C11-C12
12	U	212	CLA	CAA-CBA-CGA-O1A
12	B	825	CLA	C4-C3-C5-C6
12	A	802	CLA	C5-C6-C7-C8
12	B	816	CLA	C2-C3-C5-C6
21	U	203	A86	C1-C2-C3-C4
12	A	821	CLA	CAA-CBA-CGA-O1A
12	A	828	CLA	CAD-CBD-CGD-O2D
12	B	818	CLA	CAD-CBD-CGD-O2D
12	B	828	CLA	CAD-CBD-CGD-O2D
12	B	833	CLA	CAD-CBD-CGD-O2D
12	U	208	CLA	CAD-CBD-CGD-O2D
12	U	210	CLA	CAD-CBD-CGD-O2D
12	B	813	CLA	CAA-CBA-CGA-O2A
12	B	847	CLA	CAA-CBA-CGA-O2A
15	B	840	BCR	C6-C7-C8-C9
12	A	804	CLA	CAA-CBA-CGA-O1A
12	U	211	CLA	CAA-CBA-CGA-O1A
12	B	812	CLA	CAA-CBA-CGA-O2A
12	F	803	CLA	CAA-CBA-CGA-O2A
12	A	802	CLA	CAA-CBA-CGA-O1A

There are no ring outliers.

100 monomers are involved in 178 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	U	210	CLA	2	0
12	B	831	CLA	2	0
12	B	803	CLA	2	0
12	A	803	CLA	3	0
12	U	212	CLA	3	0
12	B	833	CLA	2	0
12	B	812	CLA	2	0
12	B	806	CLA	2	0
12	B	827	CLA	2	0
12	B	848	CLA	2	0
13	A	837	PQN	5	0
12	B	807	CLA	2	0
12	A	848	CLA	2	0
12	A	808	CLA	1	0
12	L	202	CLA	1	0
12	A	846	CLA	2	0
12	A	850	CLA	1	0
12	B	844	CLA	4	0
12	B	819	CLA	2	0
12	F	803	CLA	2	0
12	U	206	CLA	3	0
12	A	814	CLA	2	0
12	U	201	CLA	2	0
15	L	205	BCR	1	0
12	B	820	CLA	1	0
12	B	813	CLA	1	0
15	A	841	BCR	2	0
12	B	808	CLA	4	0
12	A	811	CLA	1	0
12	A	821	CLA	1	0
12	A	816	CLA	1	0
12	B	809	CLA	1	0
15	B	838	BCR	2	0
12	B	817	CLA	3	0
20	J	102	LMG	1	0
12	A	815	CLA	6	0
15	A	842	BCR	1	0
12	B	801	CLA	1	0
12	F	802	CLA	1	0
15	F	804	BCR	2	0
15	A	843	BCR	3	0
12	A	828	CLA	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	A	836	CLA	3	0
12	B	835	CLA	4	0
12	A	806	CLA	2	0
12	A	852	CLA	4	0
12	B	846	CLA	4	0
12	A	807	CLA	3	0
12	A	817	CLA	1	0
12	A	831	CLA	2	0
18	B	842	DGD	3	0
12	U	211	CLA	3	0
12	A	826	CLA	2	0
12	U	208	CLA	3	0
12	B	845	CLA	2	0
15	B	840	BCR	3	0
12	A	829	CLA	1	0
15	M	101	BCR	3	0
12	A	835	CLA	5	0
20	U	202	LMG	1	0
12	B	810	CLA	1	0
12	A	810	CLA	1	0
12	A	820	CLA	1	0
15	J	104	BCR	1	0
12	U	205	CLA	1	0
12	B	828	CLA	1	0
15	B	839	BCR	1	0
12	B	824	CLA	3	0
12	B	822	CLA	3	0
12	A	801	CLA	1	0
12	A	822	CLA	1	0
12	B	805	CLA	3	0
12	B	847	CLA	2	0
12	A	833	CLA	4	0
12	A	851	CLA	3	0
15	B	837	BCR	2	0
12	B	825	CLA	3	0
12	A	844	CLA	2	0
12	B	829	CLA	1	0
12	B	818	CLA	4	0
15	B	841	BCR	2	0
12	U	207	CLA	2	0
12	U	209	CLA	2	0
12	B	802	CLA	2	0

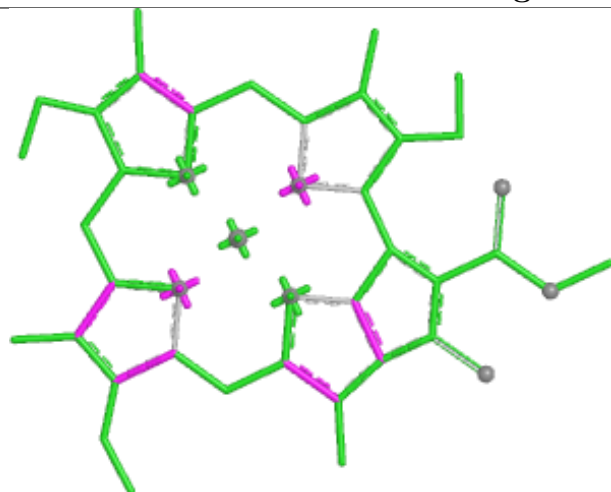
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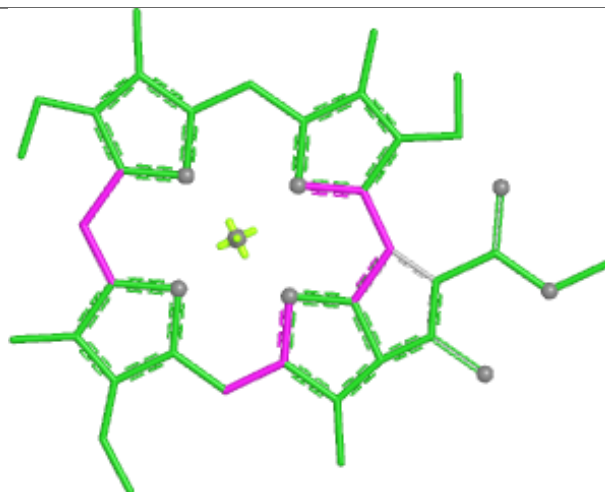
Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	A	847	CL0	1	0
12	B	823	CLA	2	0
12	A	818	CLA	1	0
12	A	825	CLA	3	0
12	B	843	CLA	4	0
12	B	830	CLA	2	0
15	I	102	BCR	4	0
12	B	834	CLA	5	0
14	A	838	LHG	1	0
12	A	823	CLA	1	0
12	A	824	CLA	5	0
12	A	830	CLA	1	0
12	A	834	CLA	2	0
12	B	815	CLA	3	0
12	L	203	CLA	2	0
12	L	204	CLA	3	0

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

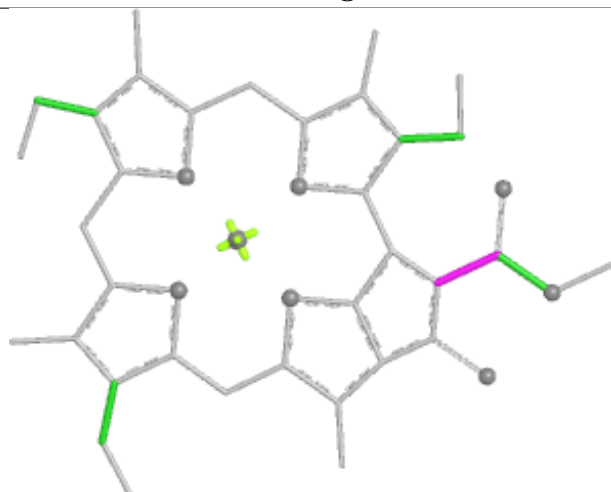
Ligand CLA U 210



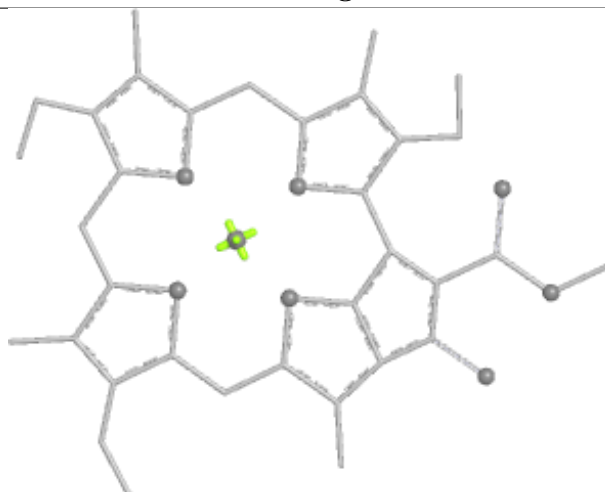
Bond lengths



Bond angles

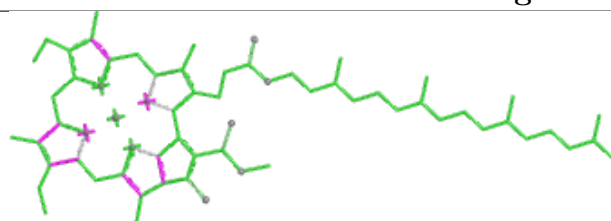


Torsions

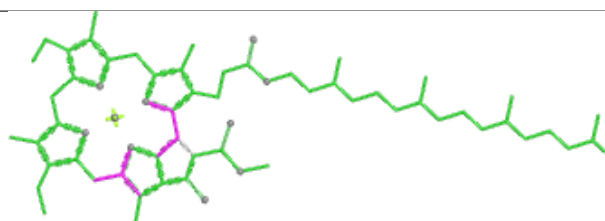


Rings

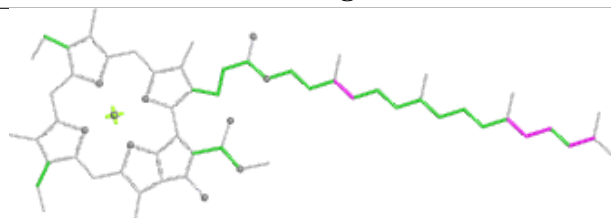
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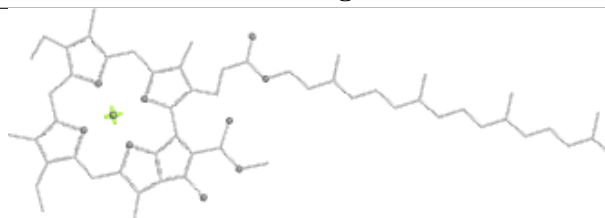
Bond lengths



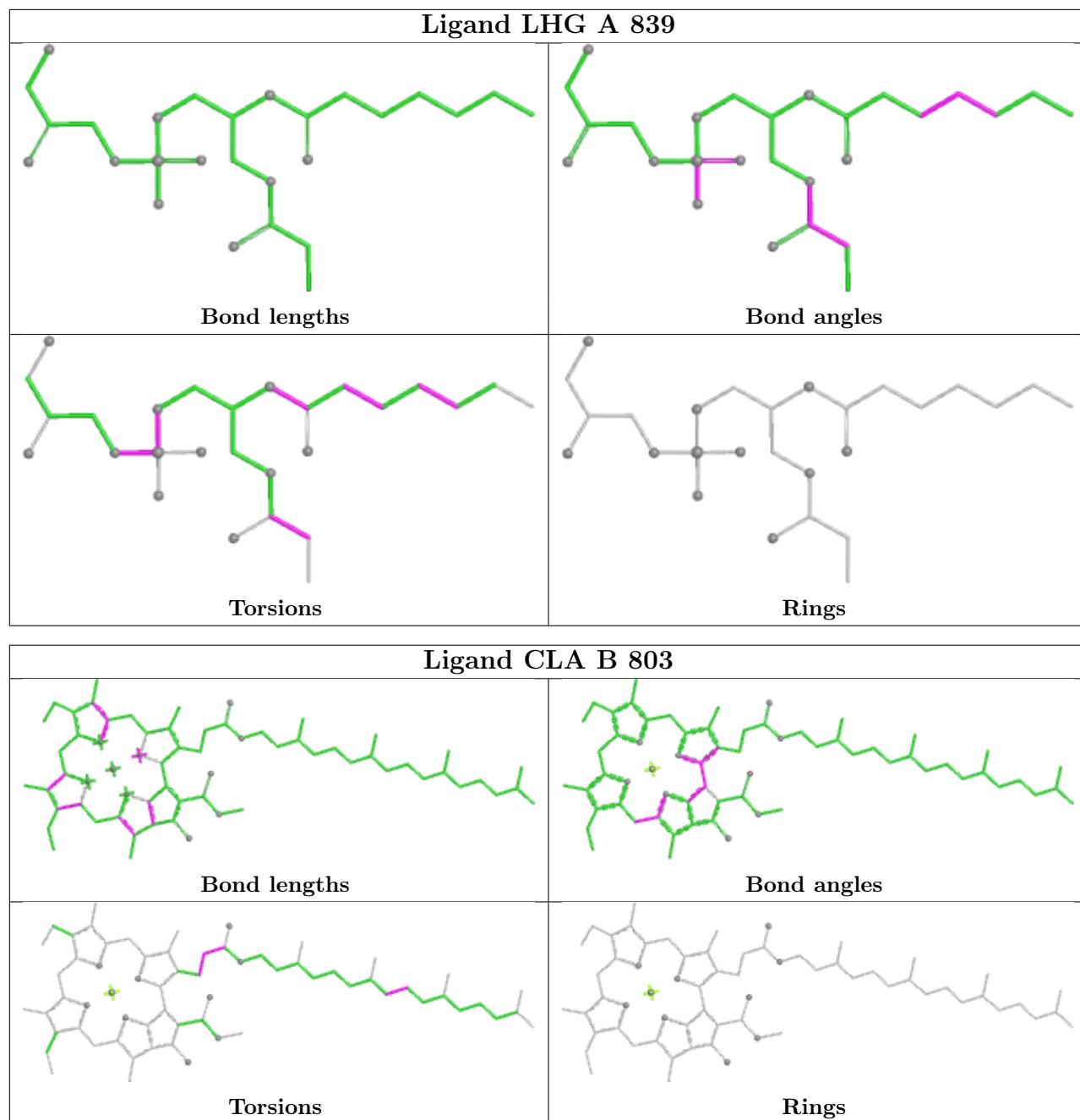
Bond angles

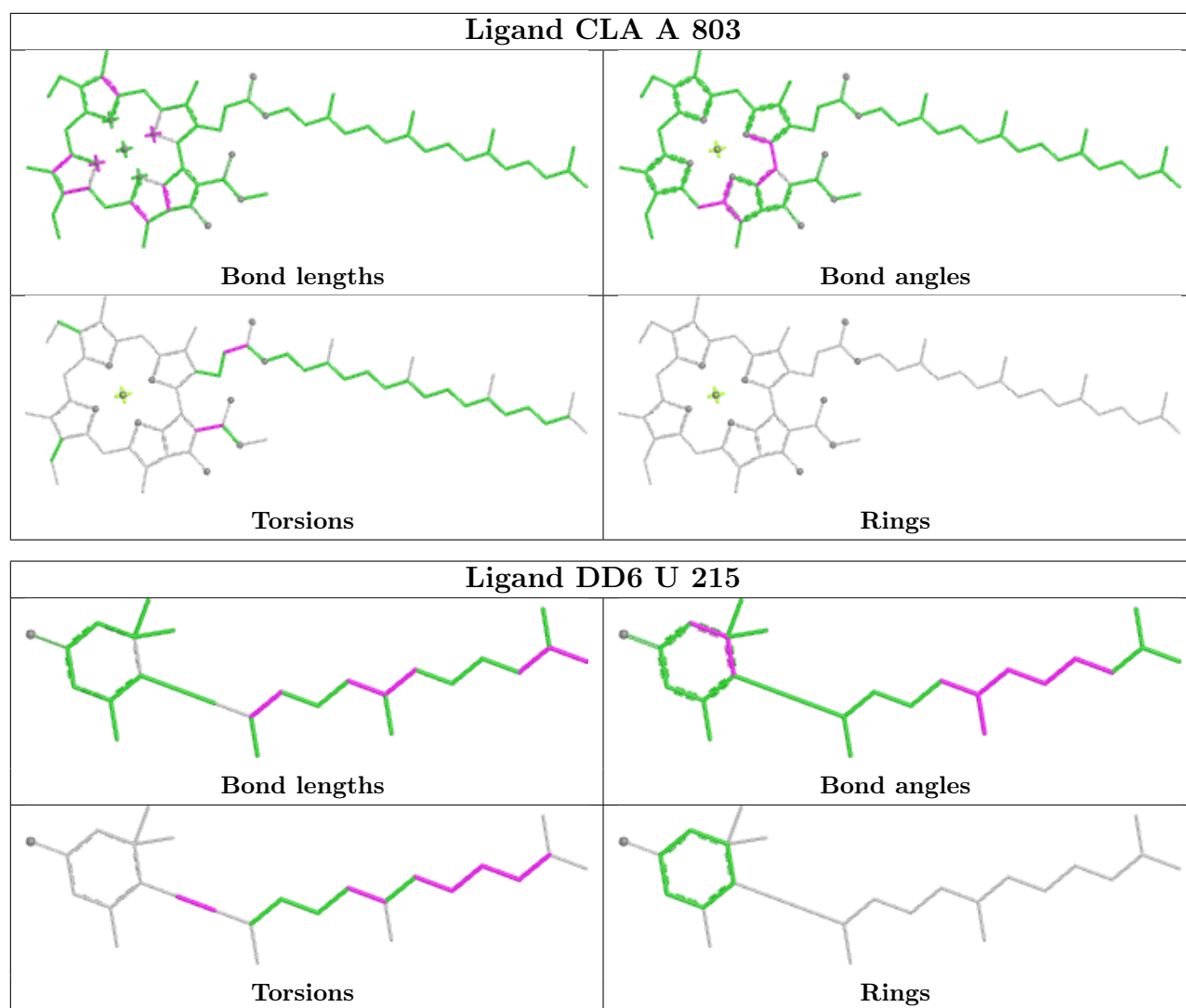


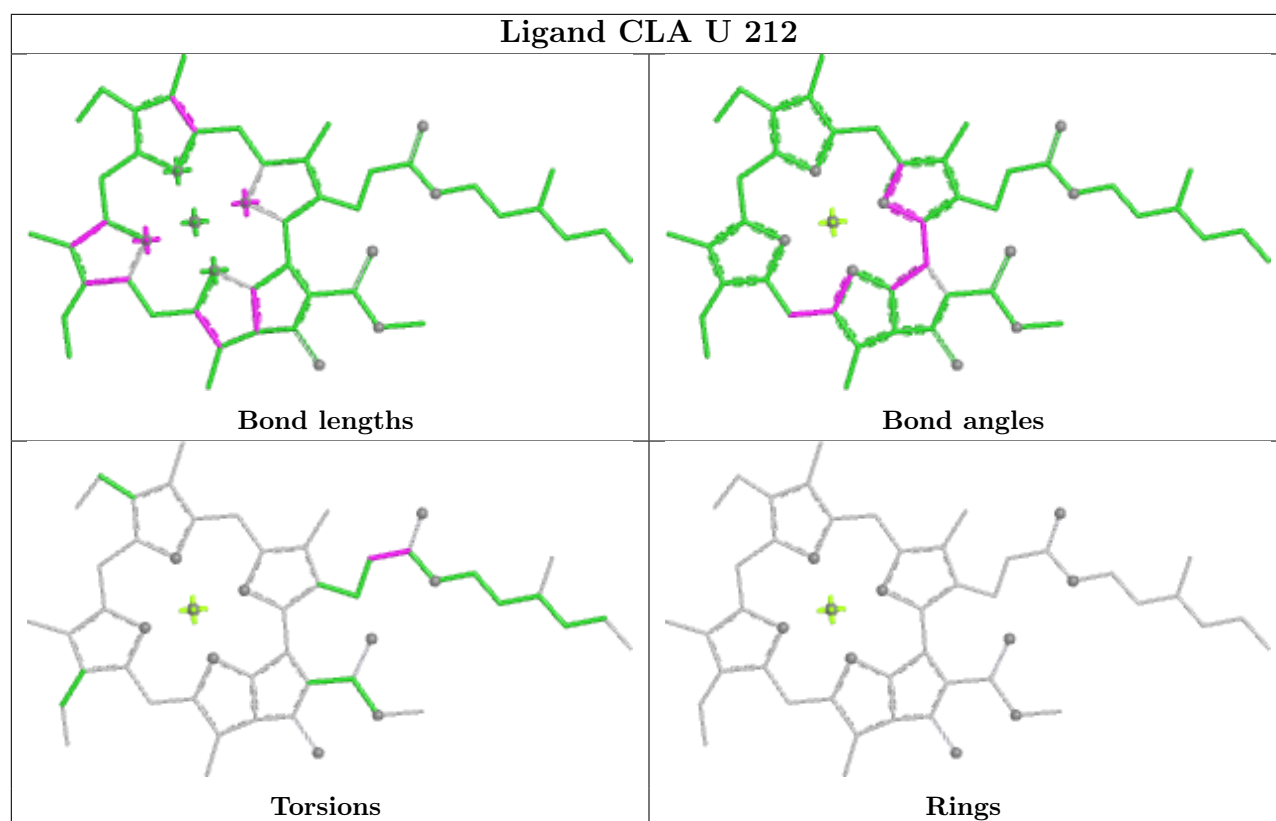
Torsions



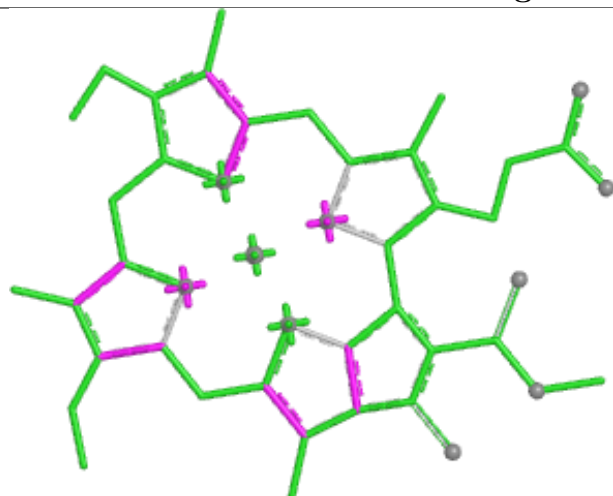
Rings



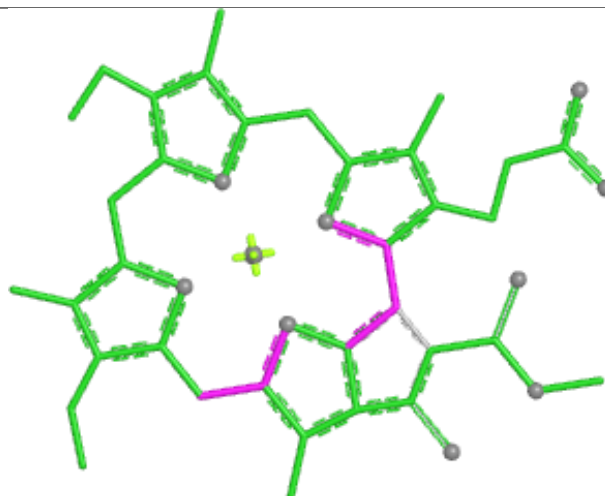




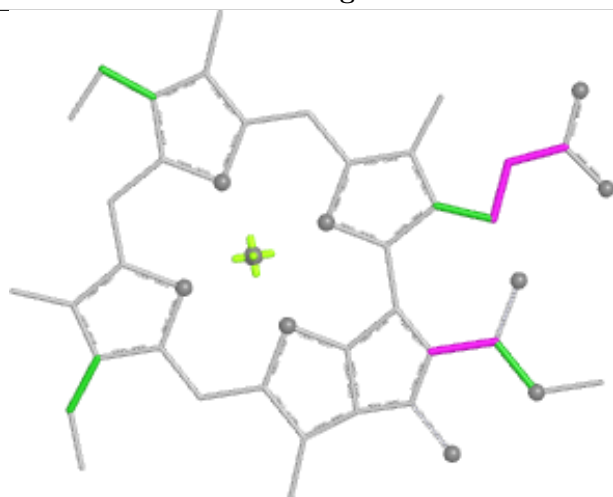
Ligand CLA B 804



Bond lengths



Bond angles

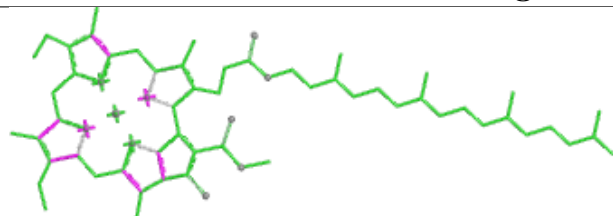


Torsions

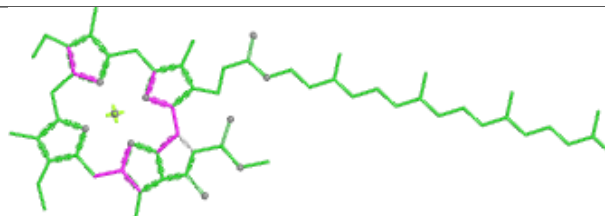


Rings

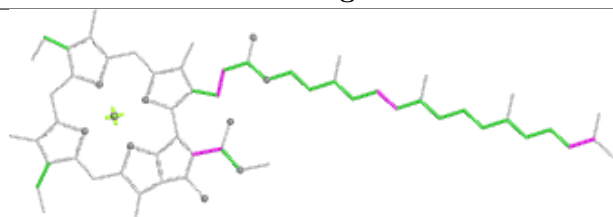
Ligand CLA B 833



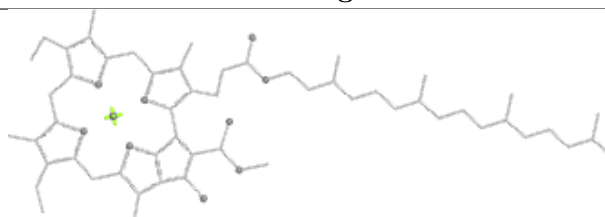
Bond lengths



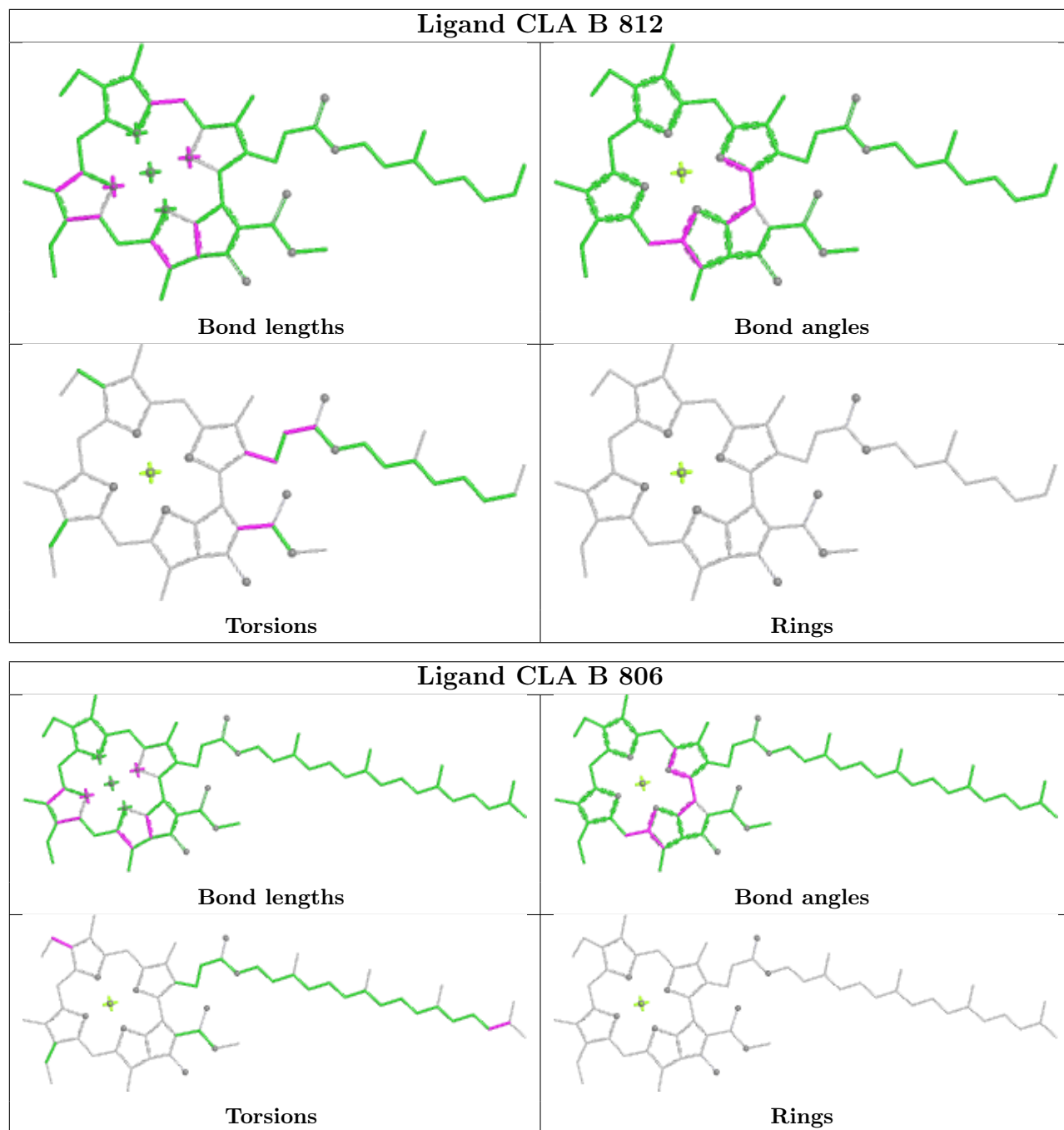
Bond angles



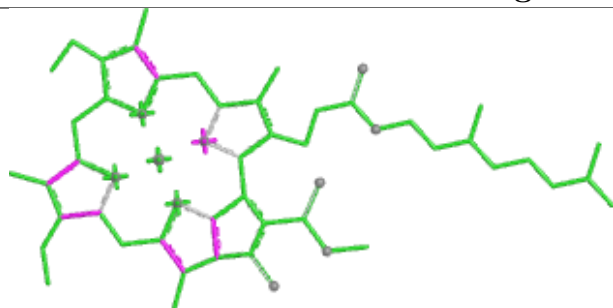
Torsions



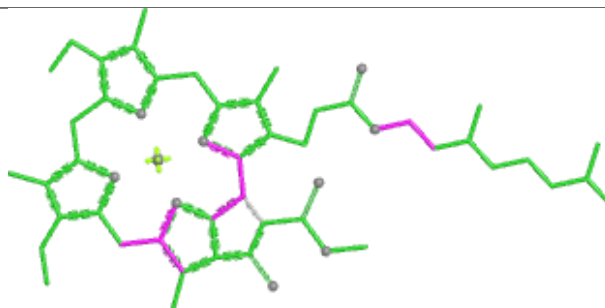
Rings



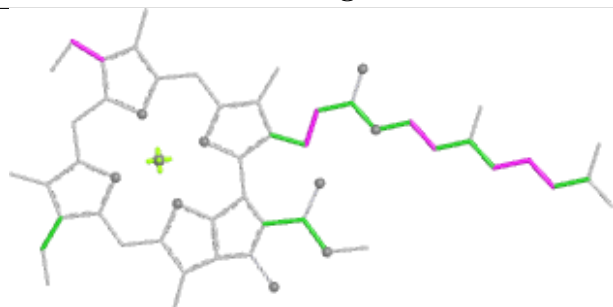
Ligand CLA B 811



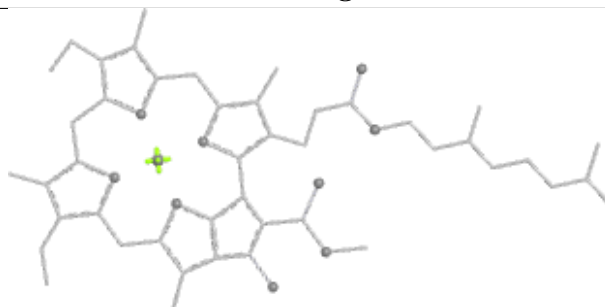
Bond lengths



Bond angles

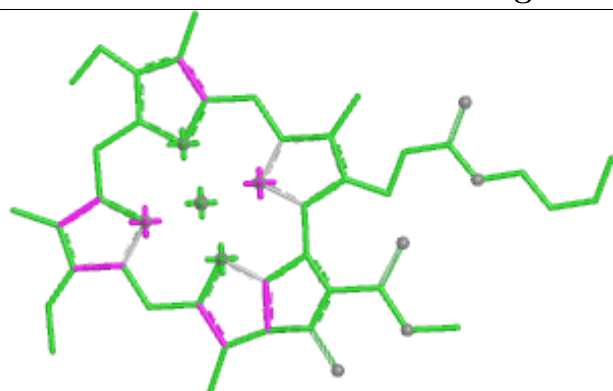


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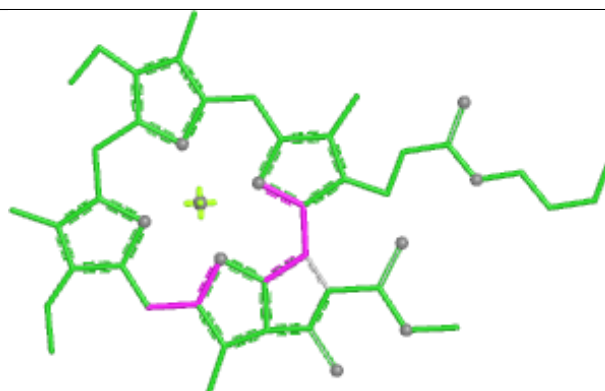


Rings

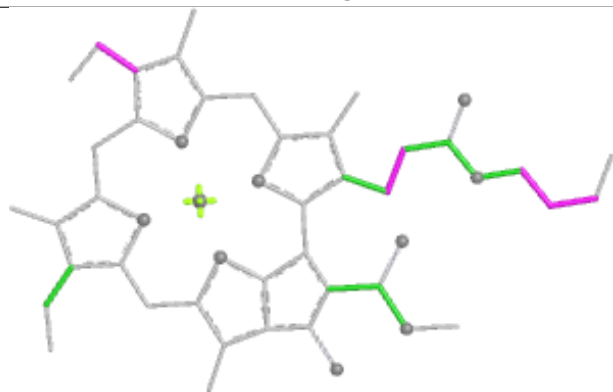
Ligand CLA B 827



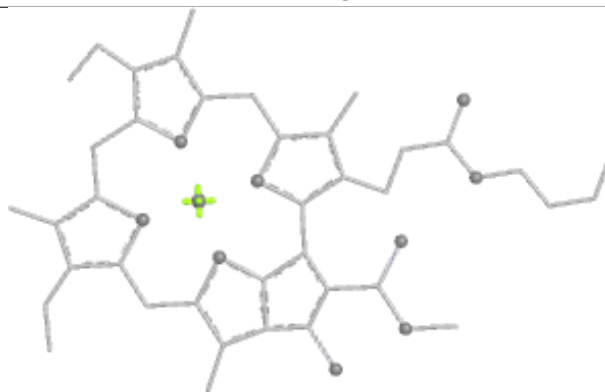
Bond lengths



Bond angles

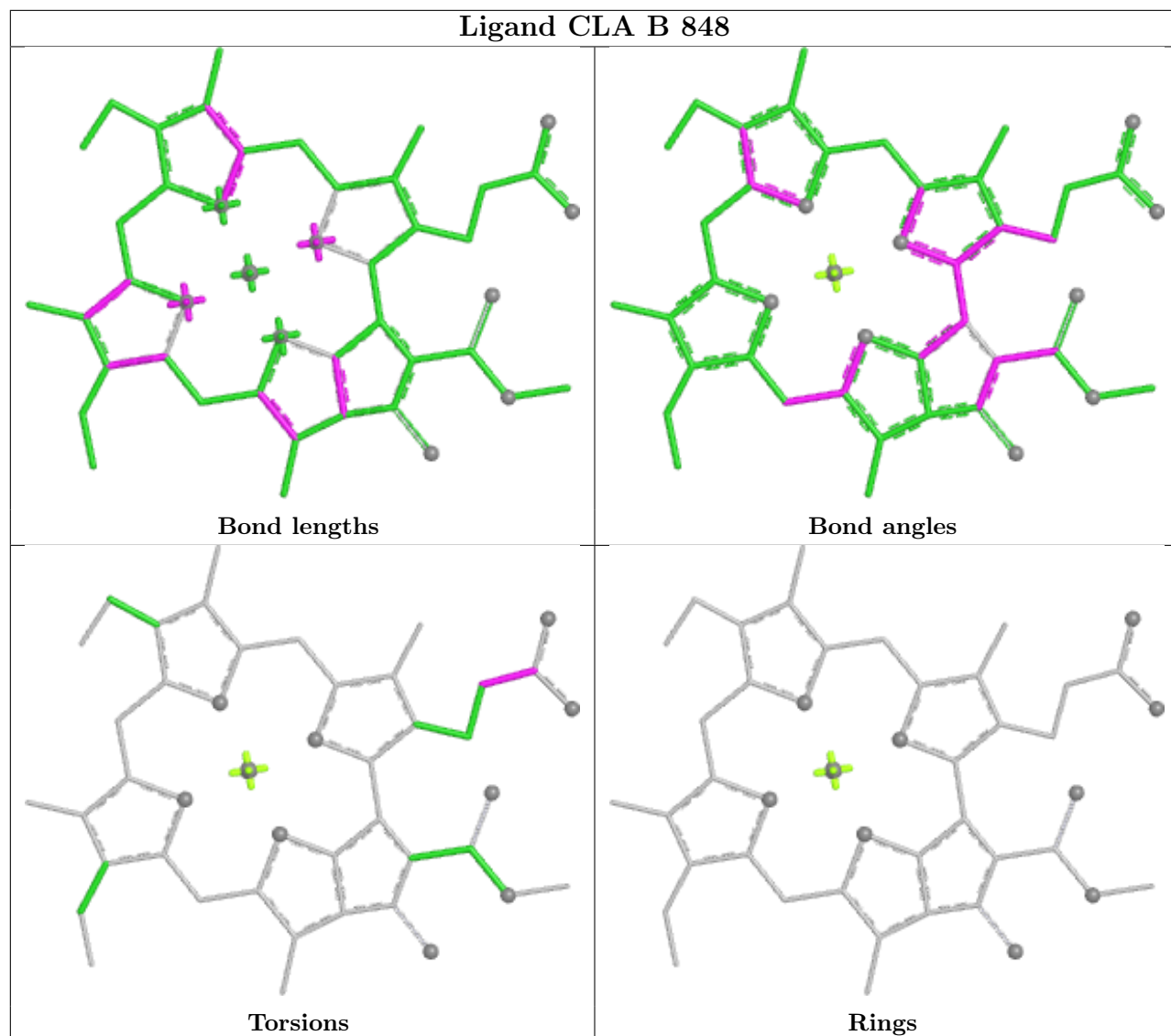


Torsions

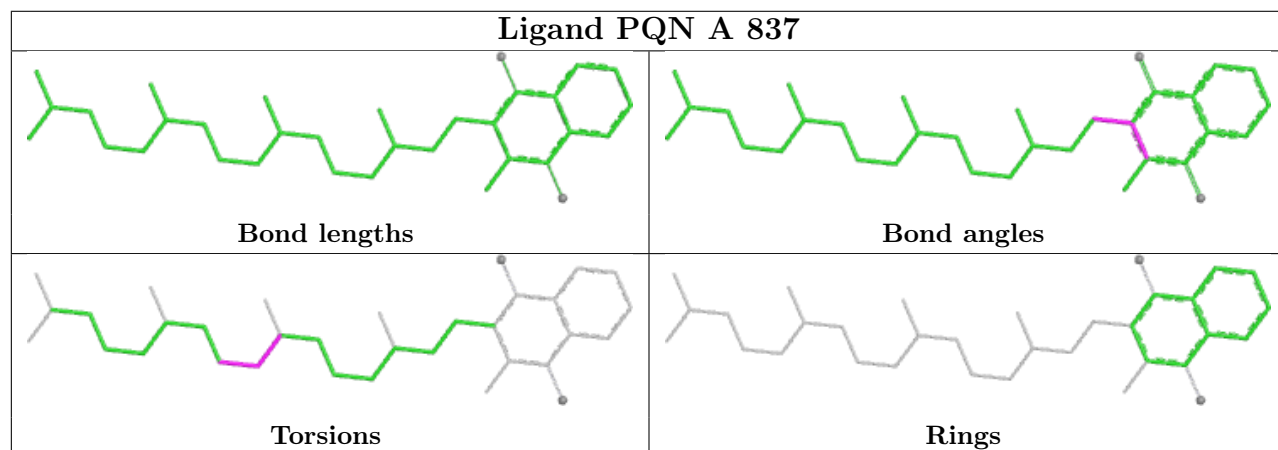


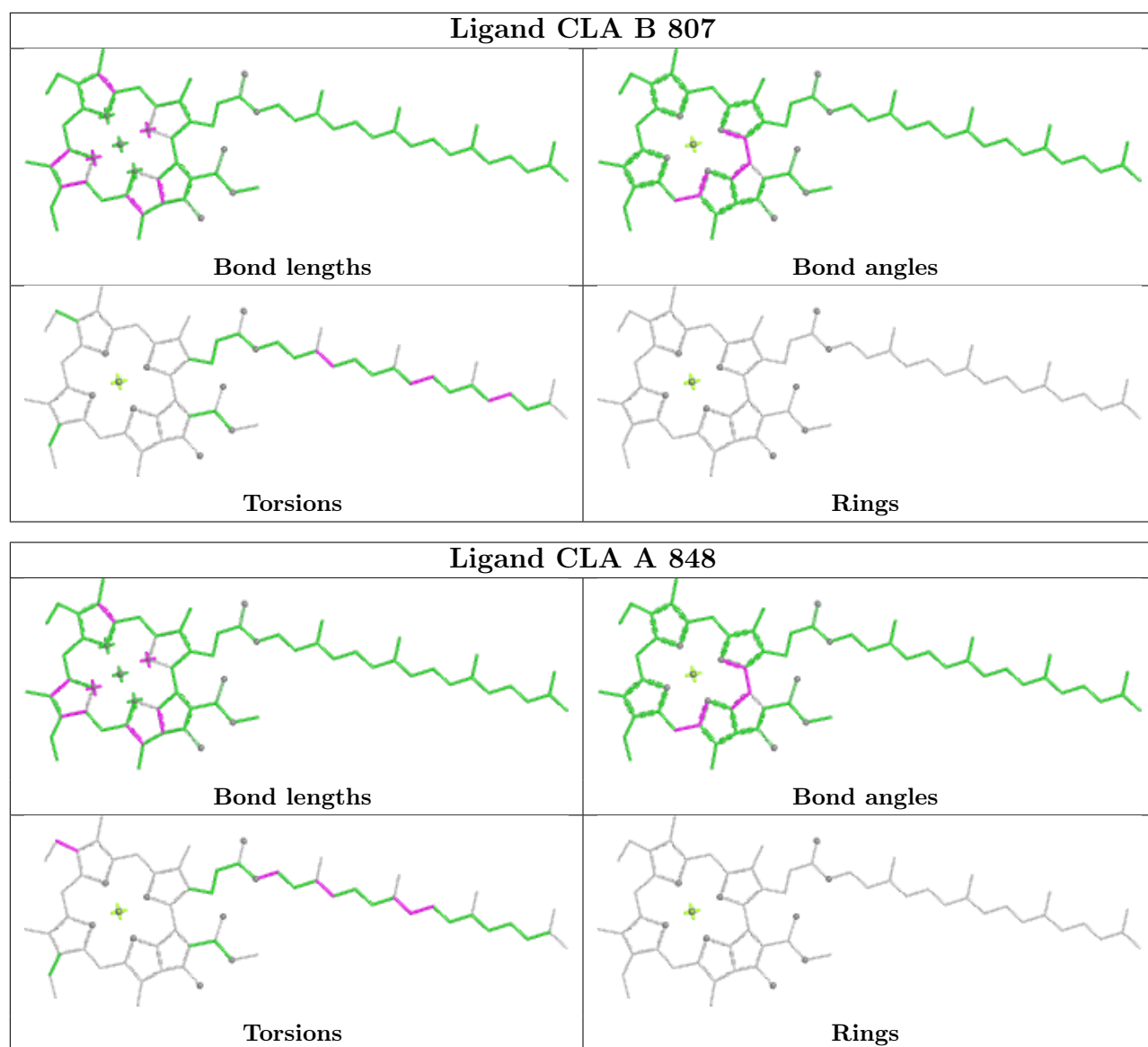
Rings

Ligand CLA B 848

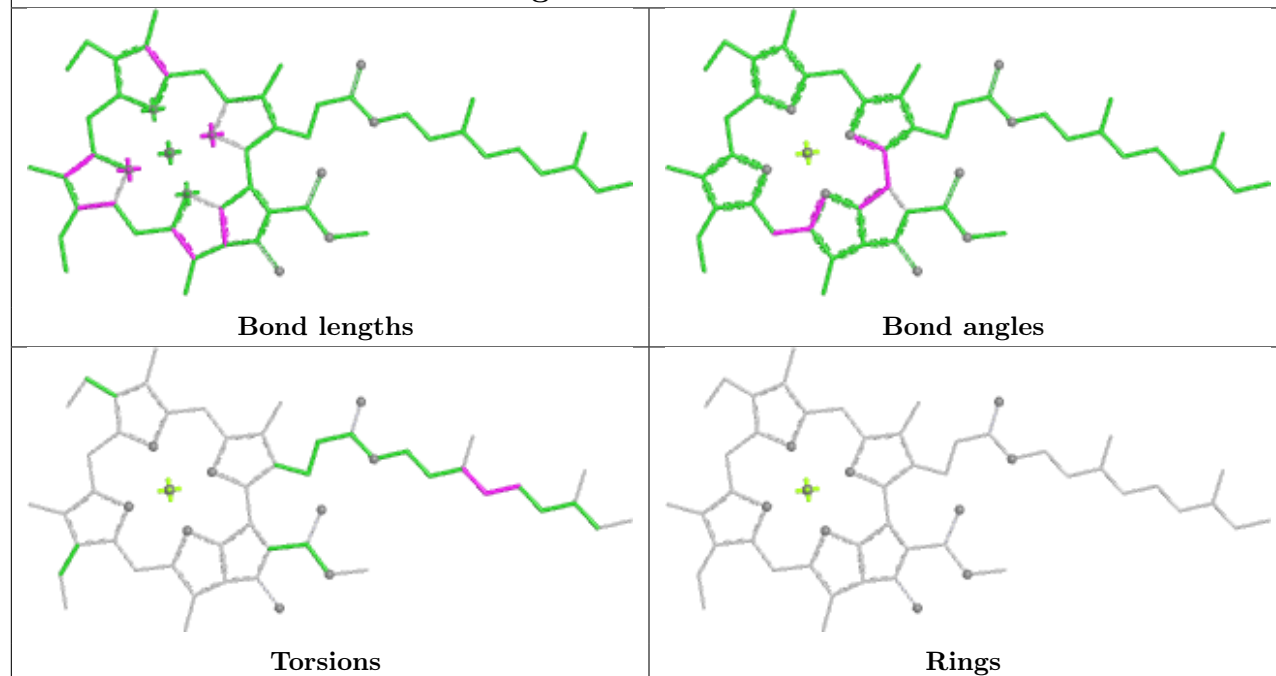


Ligand PQN A 837

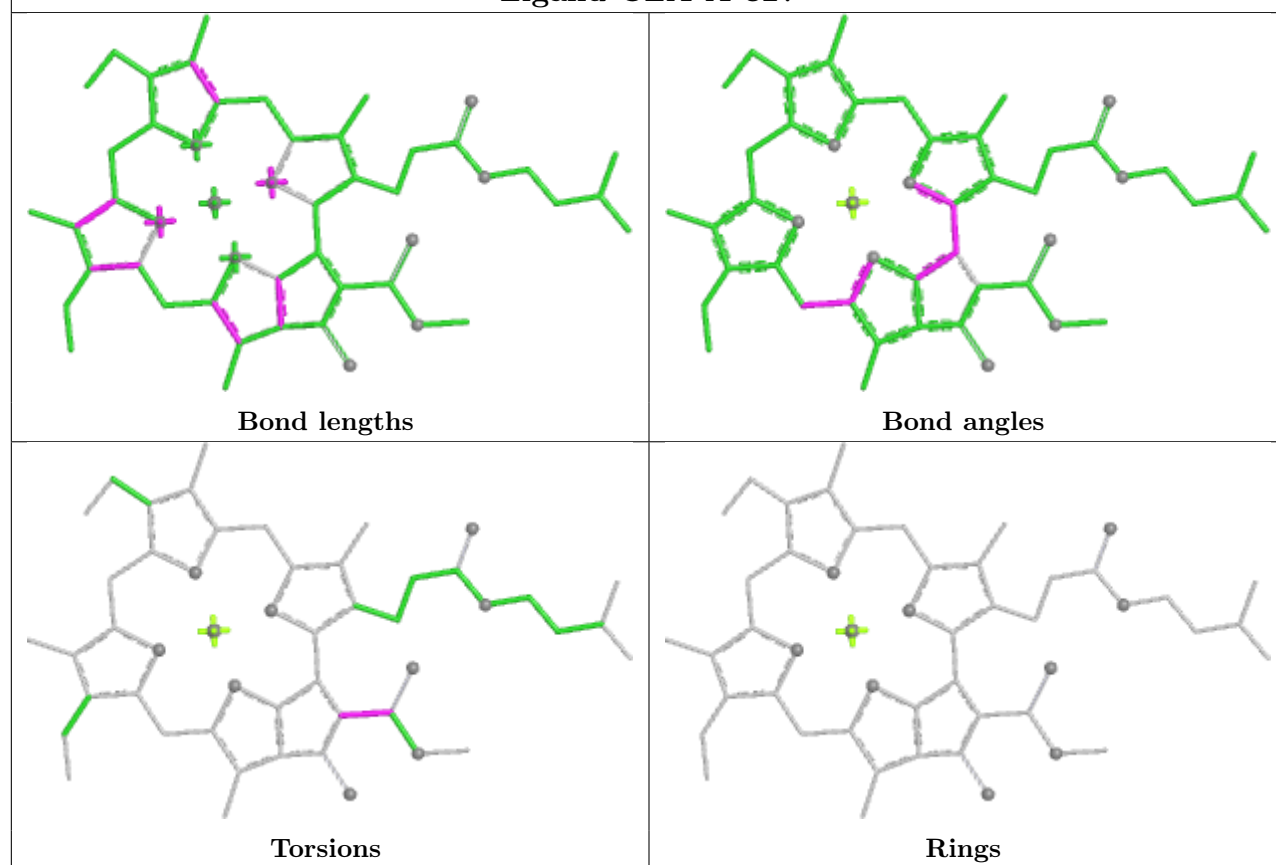




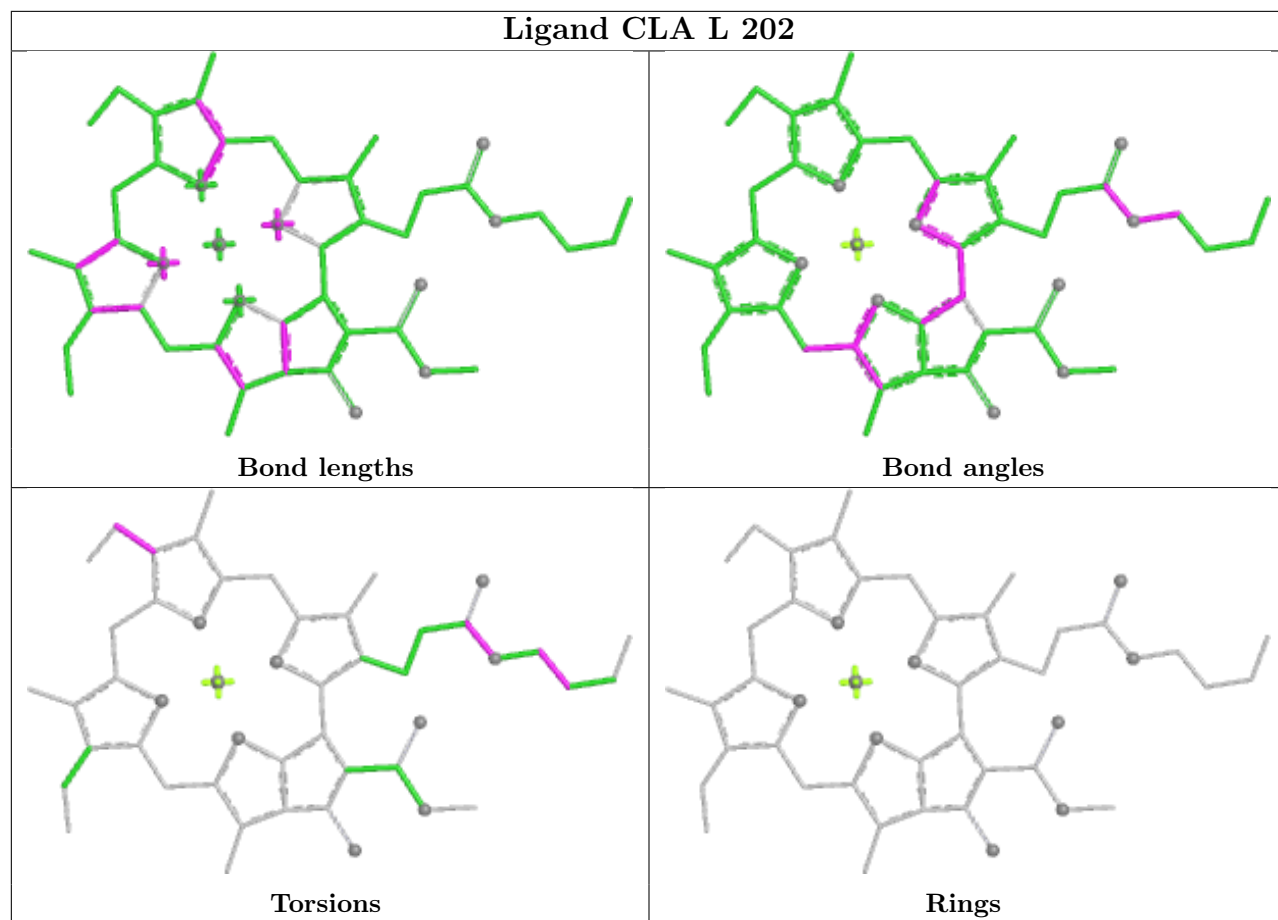
Ligand CLA A 808



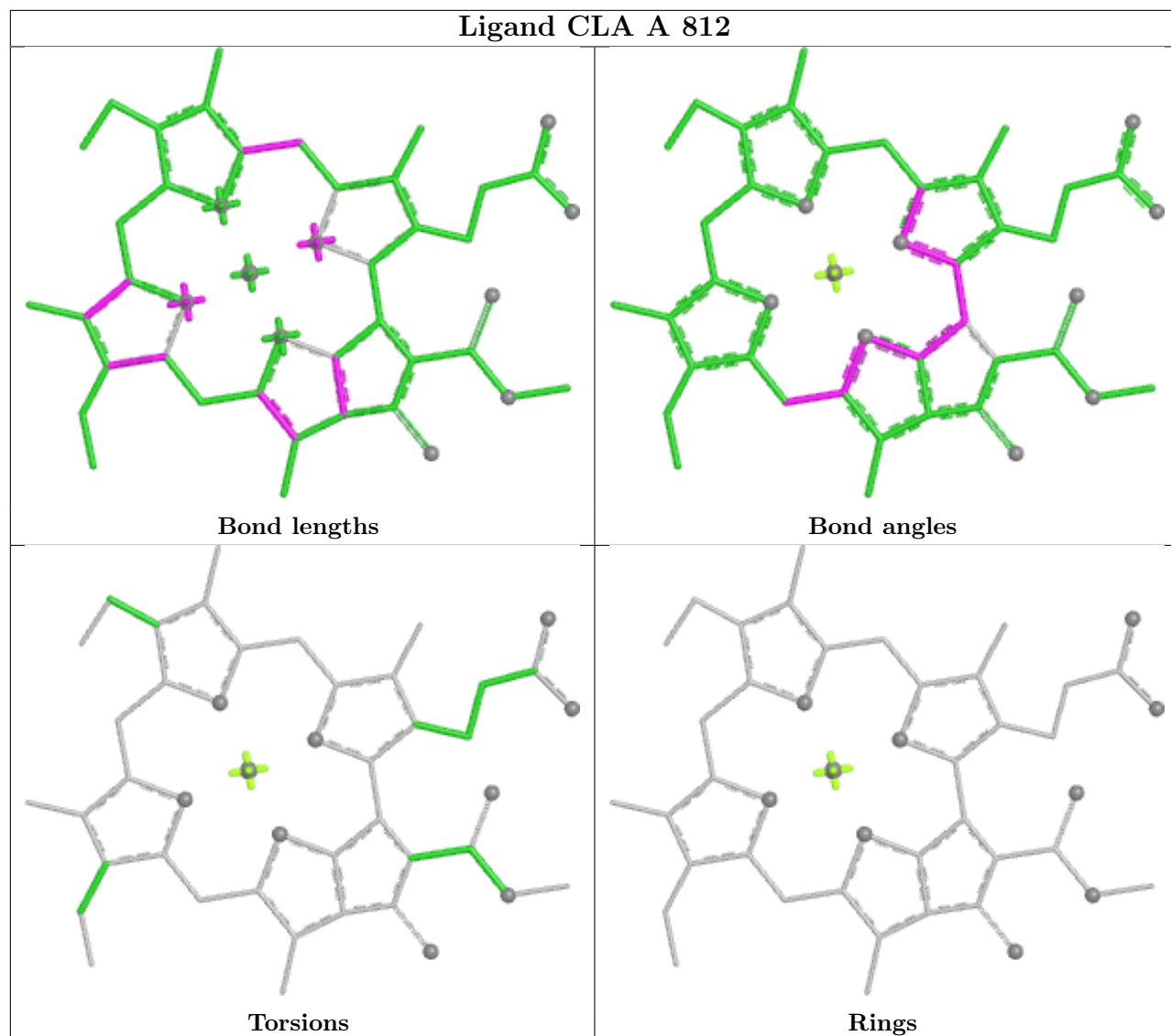
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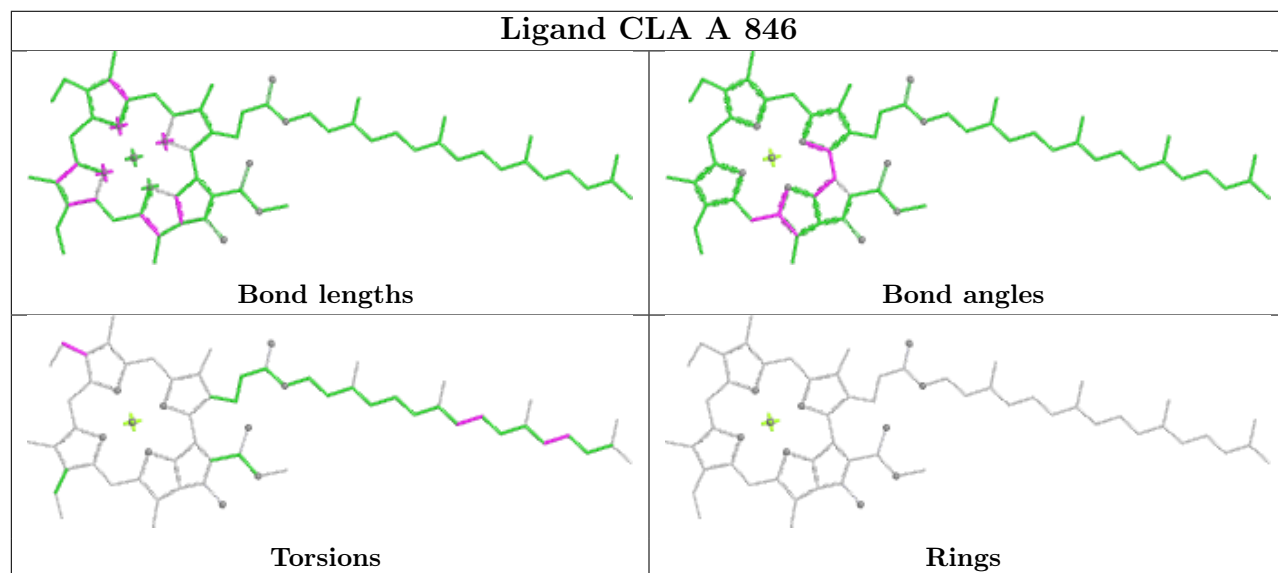
Ligand CLA L 202

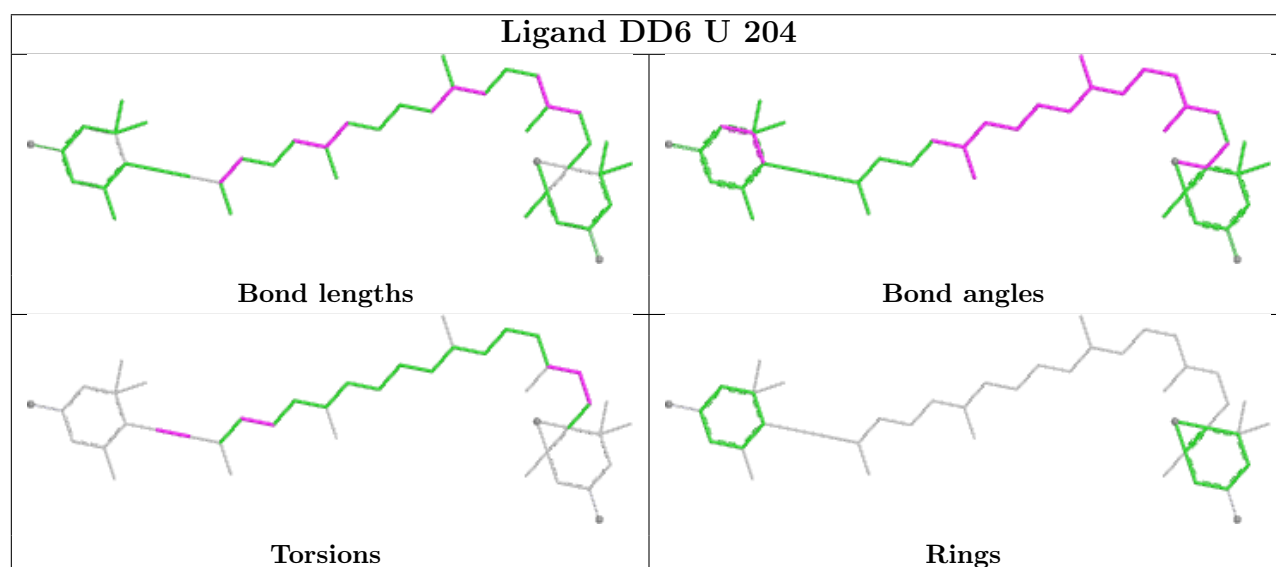
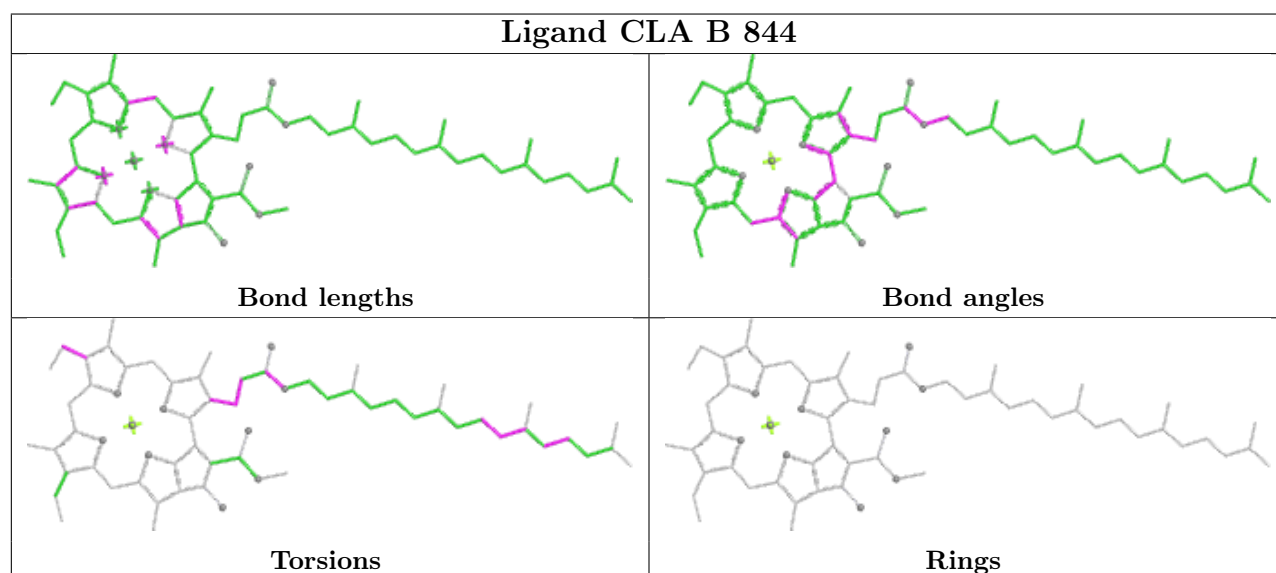
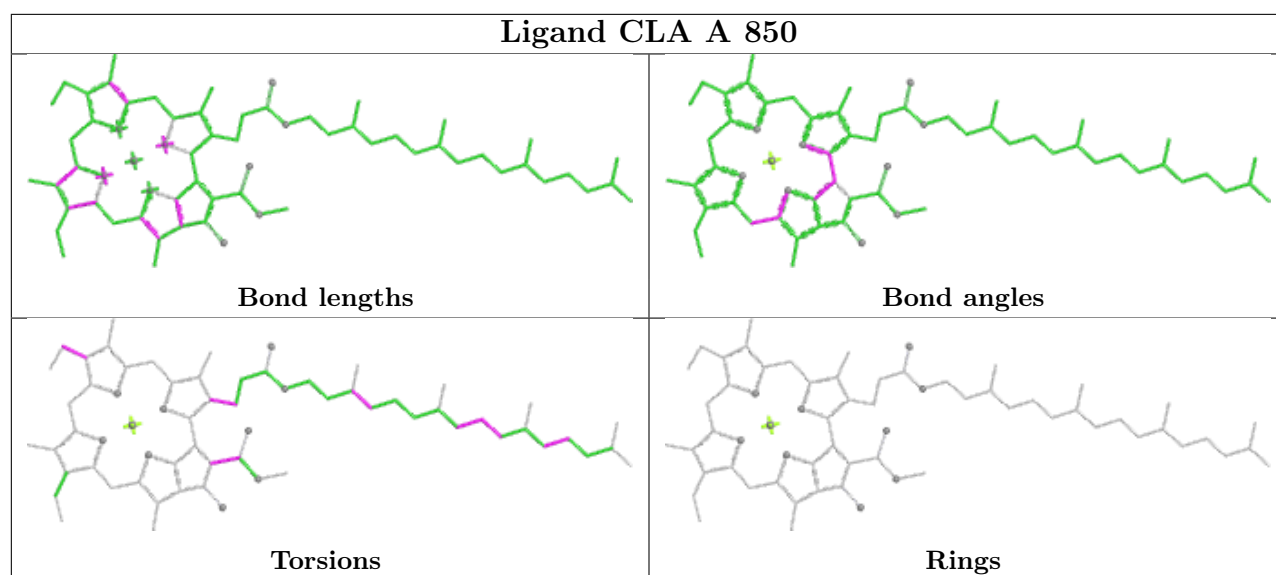


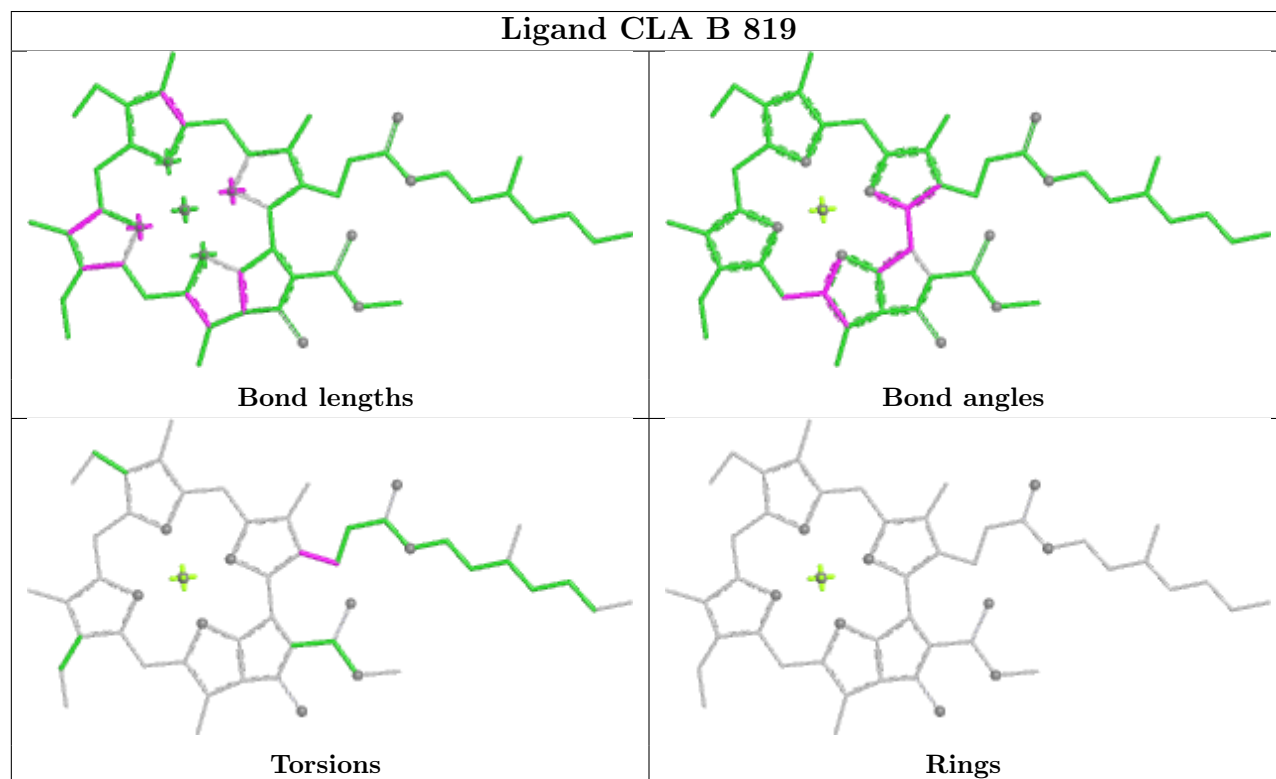
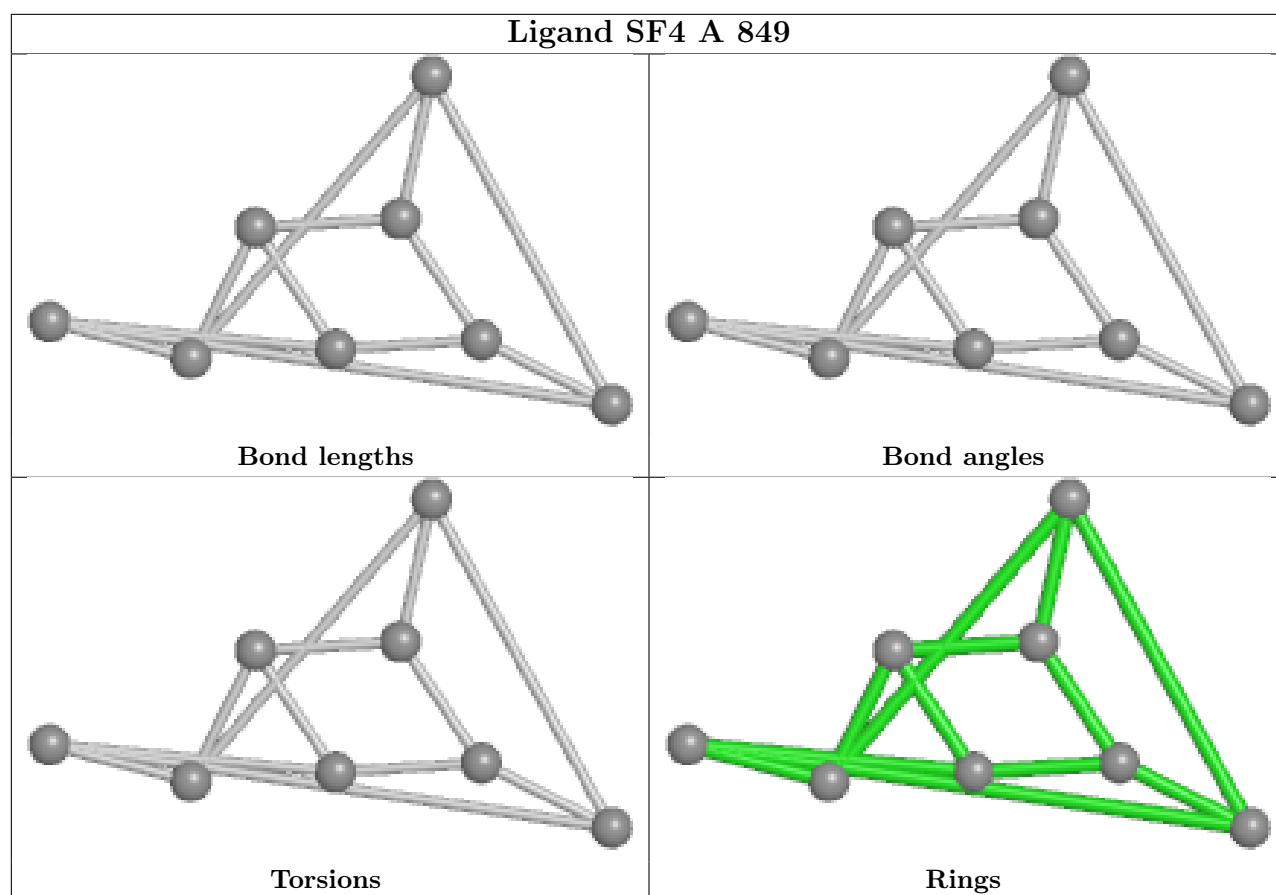
Ligand CLA A 812



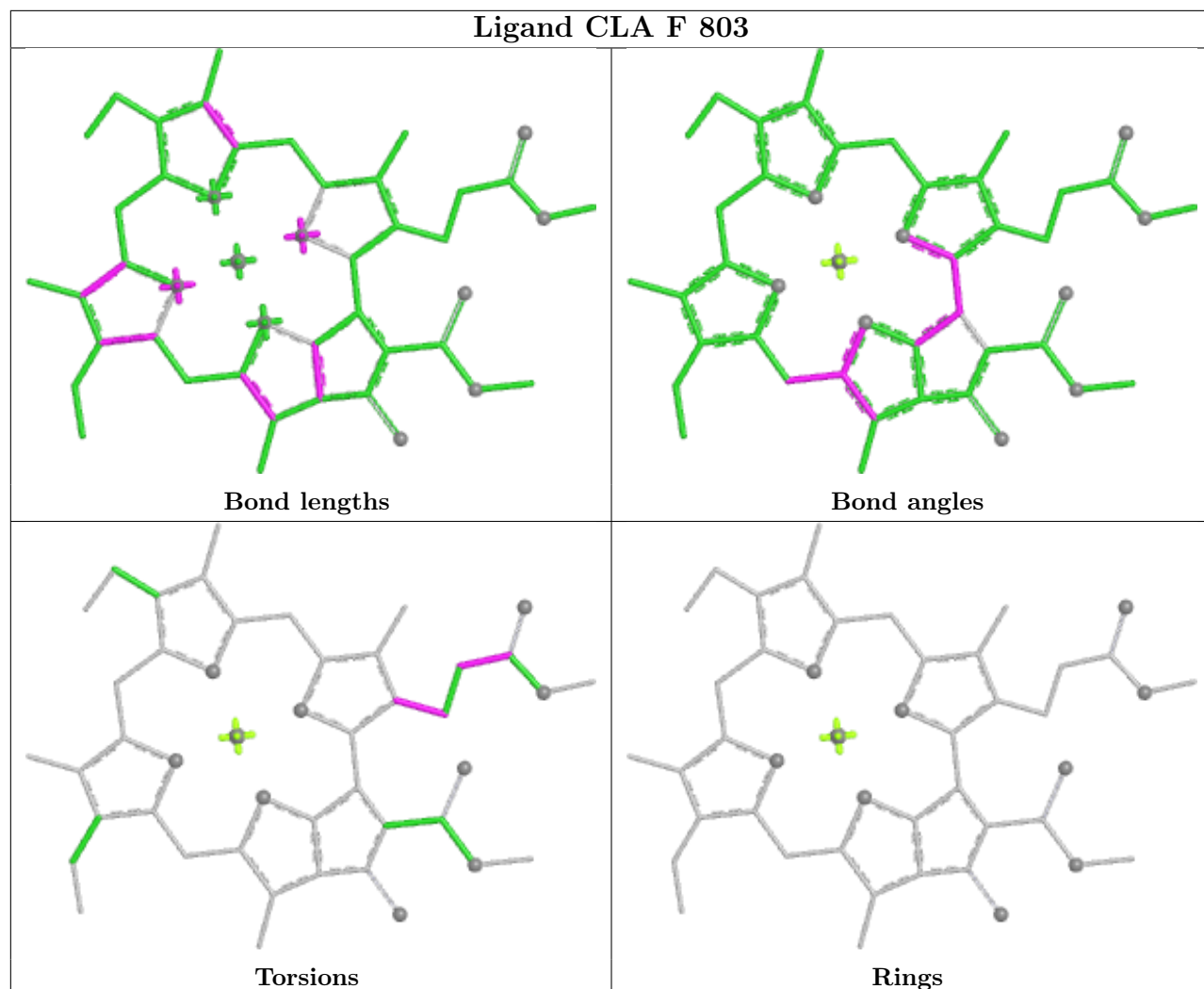
Ligand CLA A 846



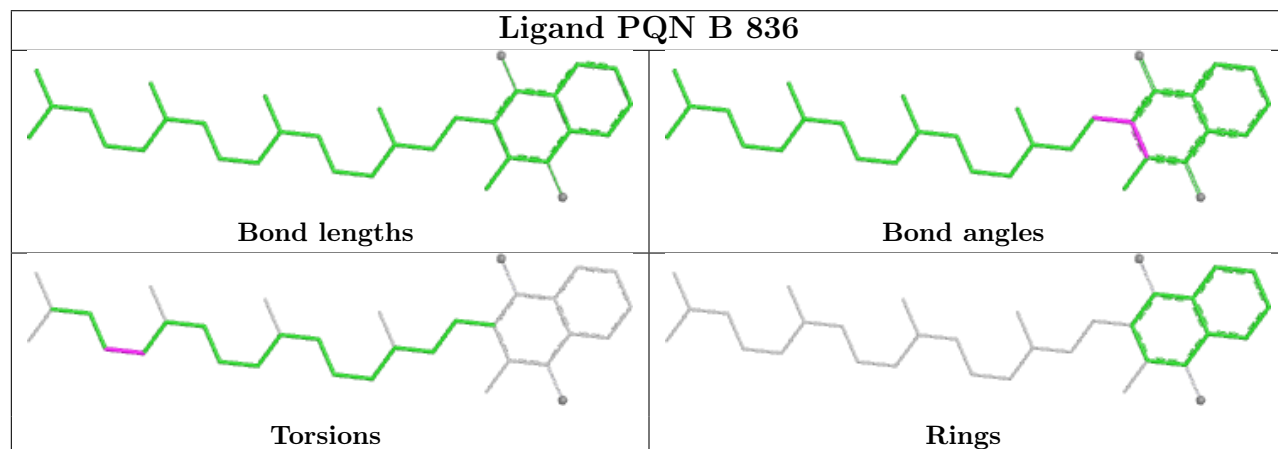


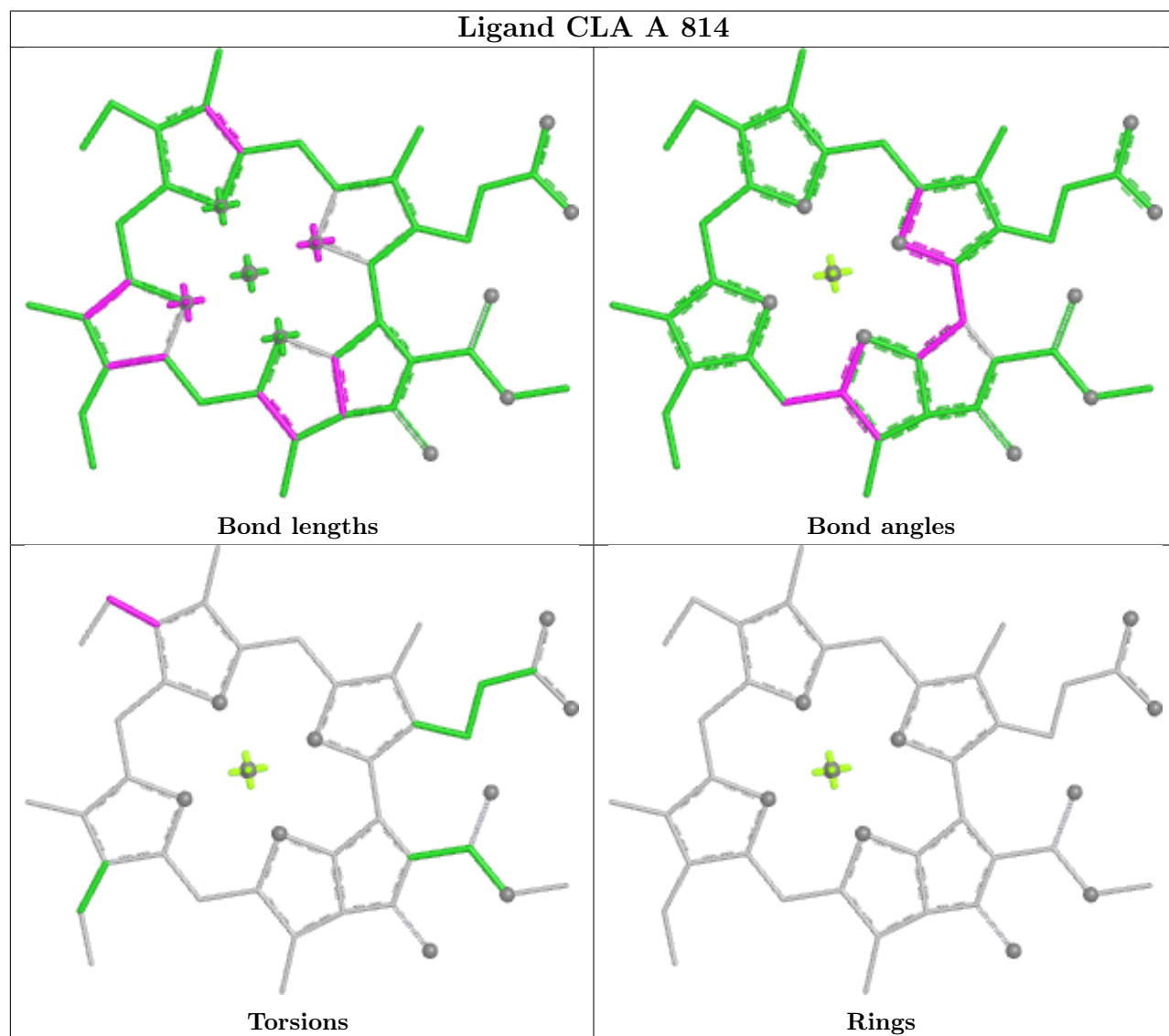
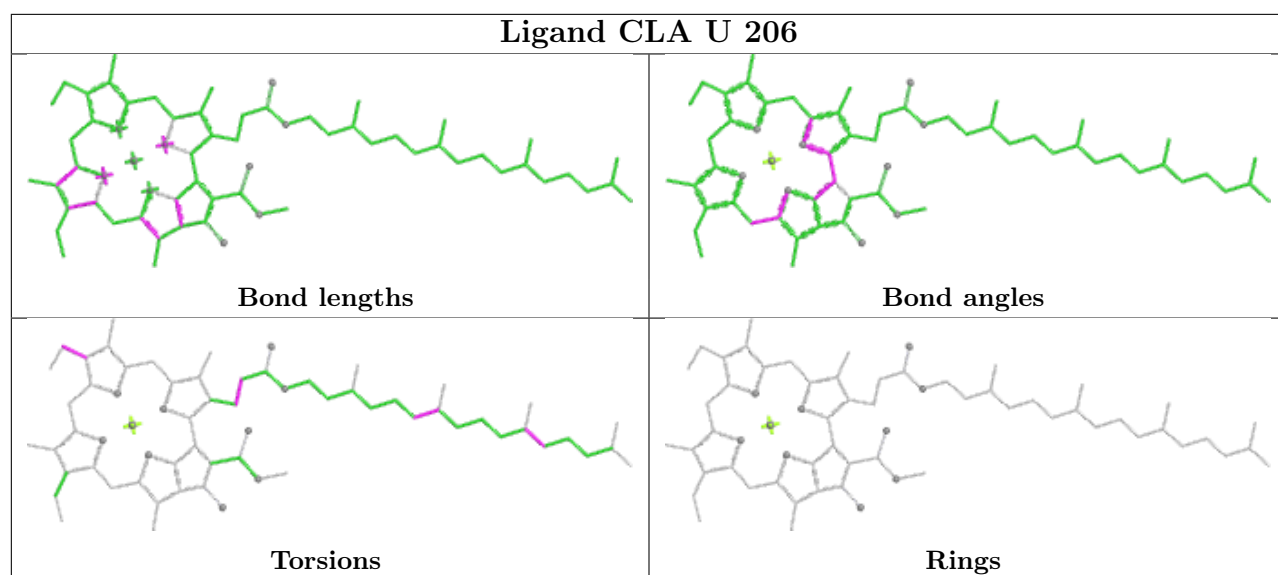


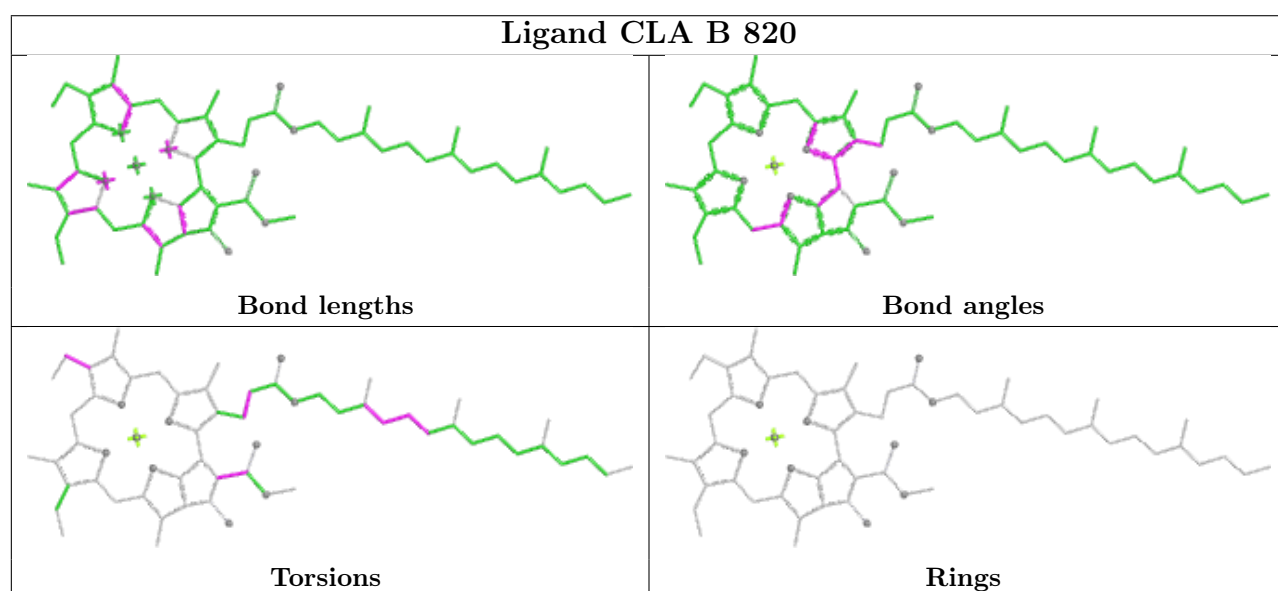
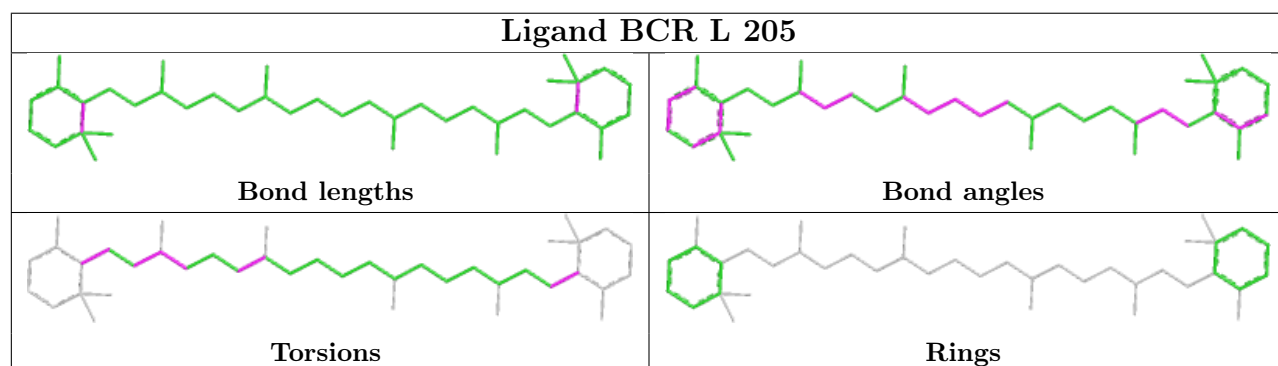
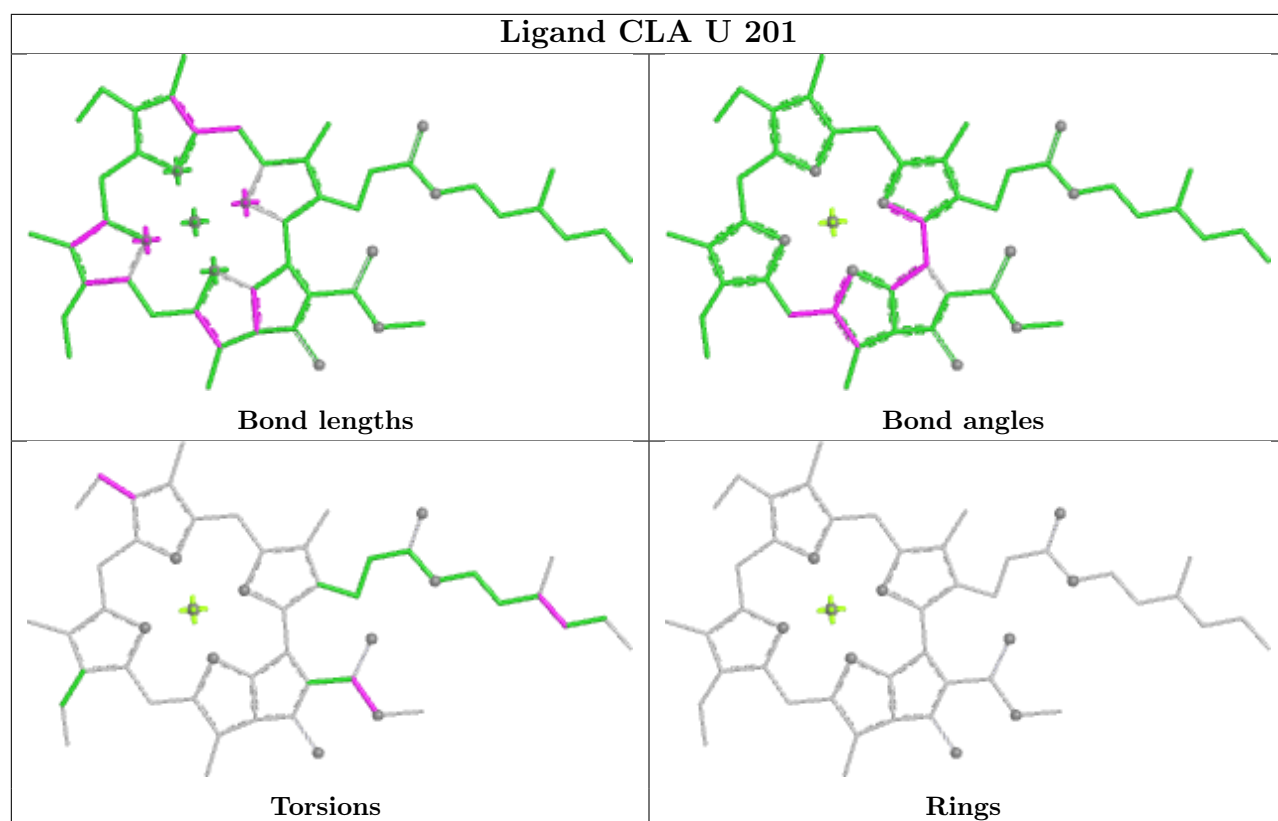
Ligand CLA F 803



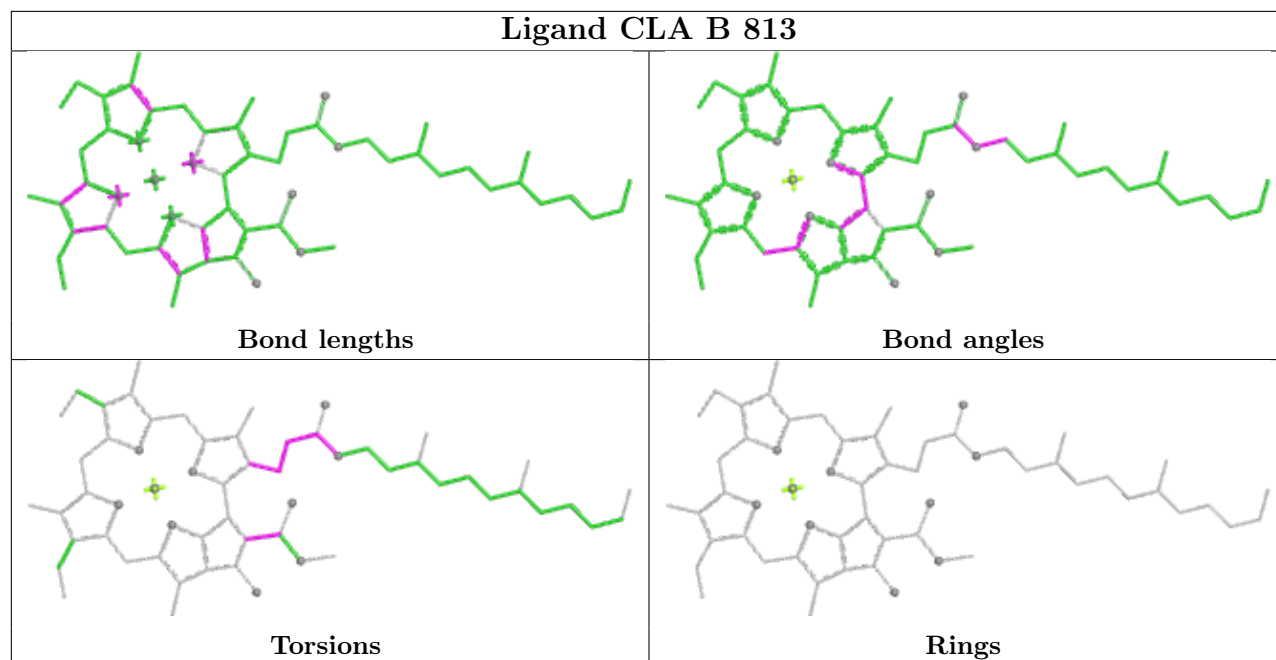
Ligand PQN B 836



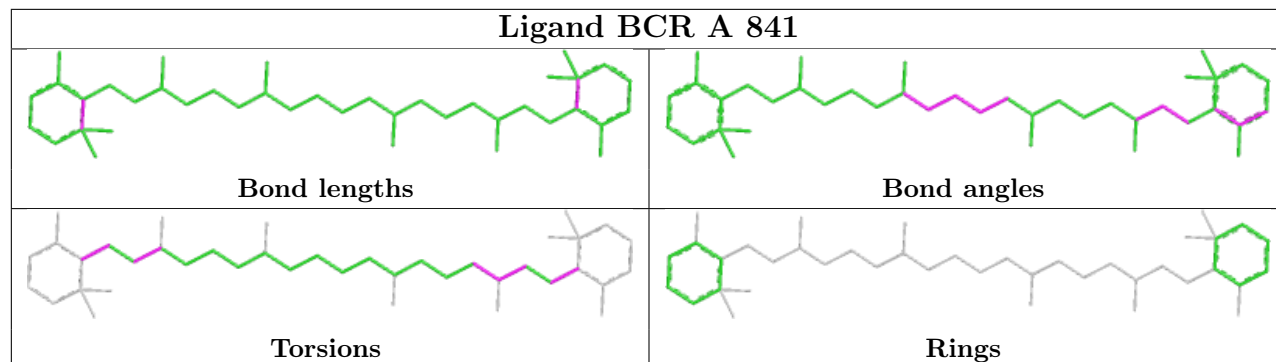




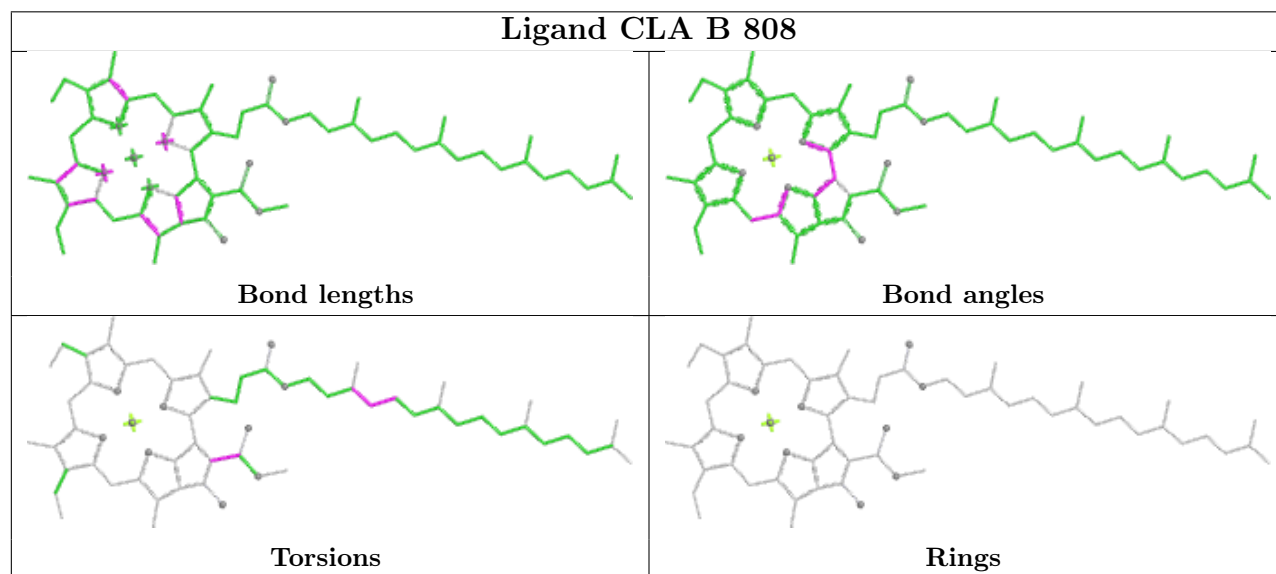
Ligand CLA B 813

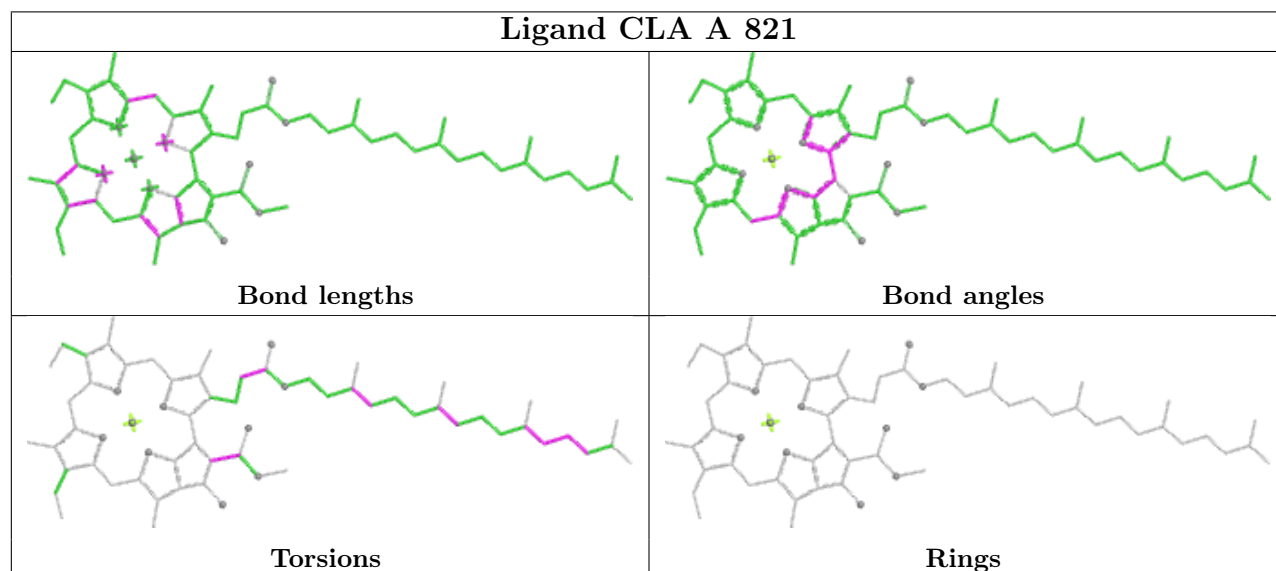
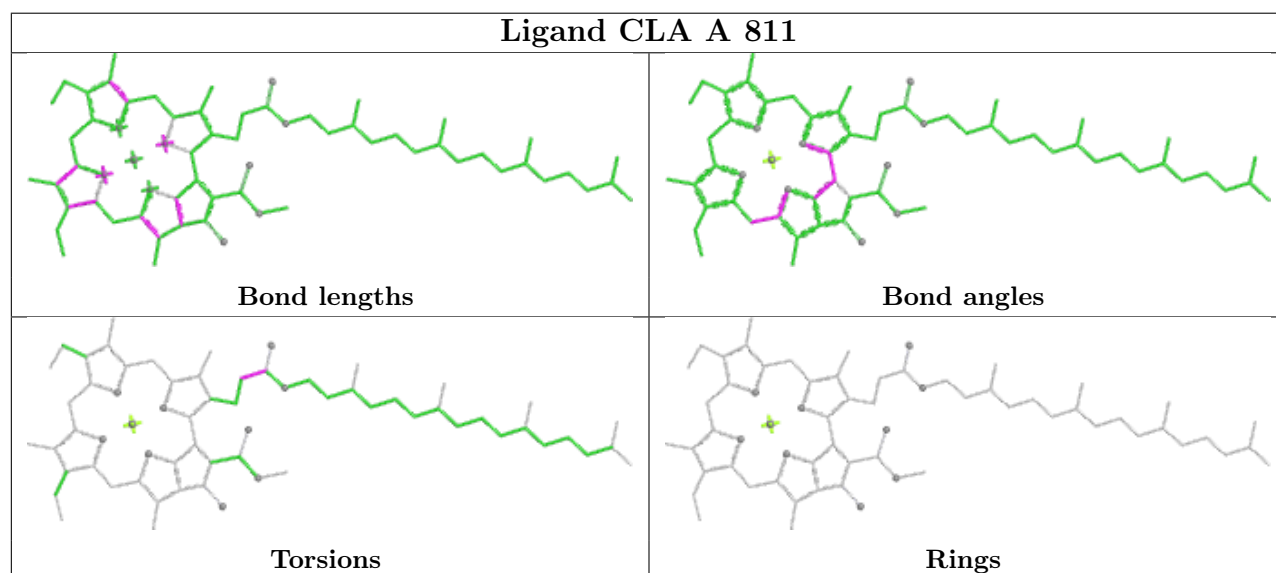
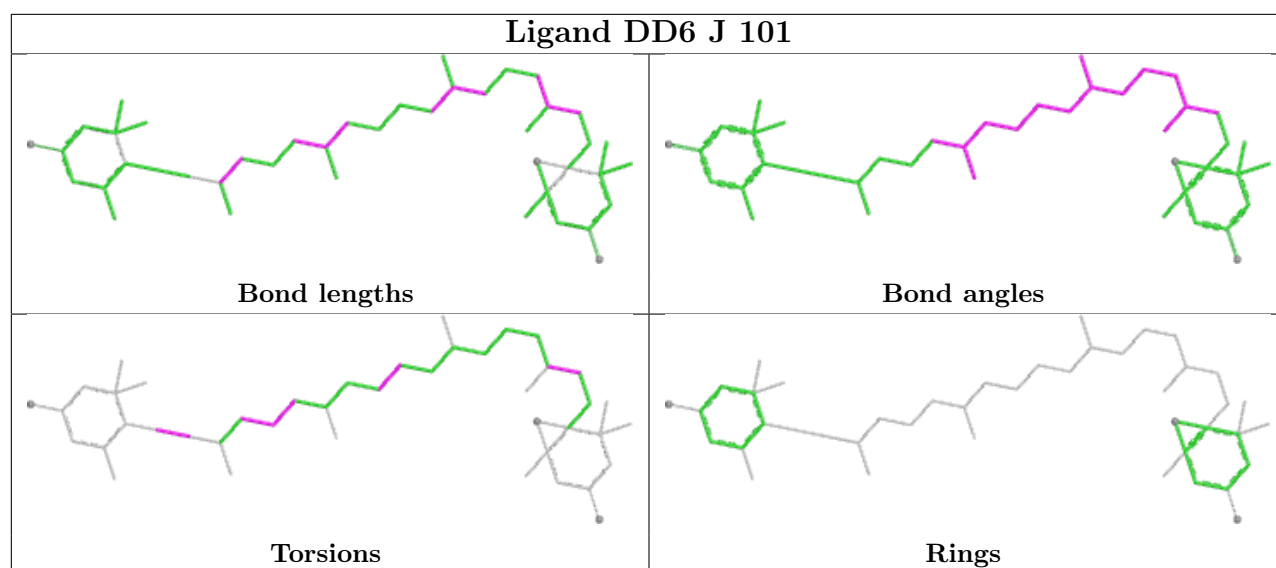


Ligand BCR A 841

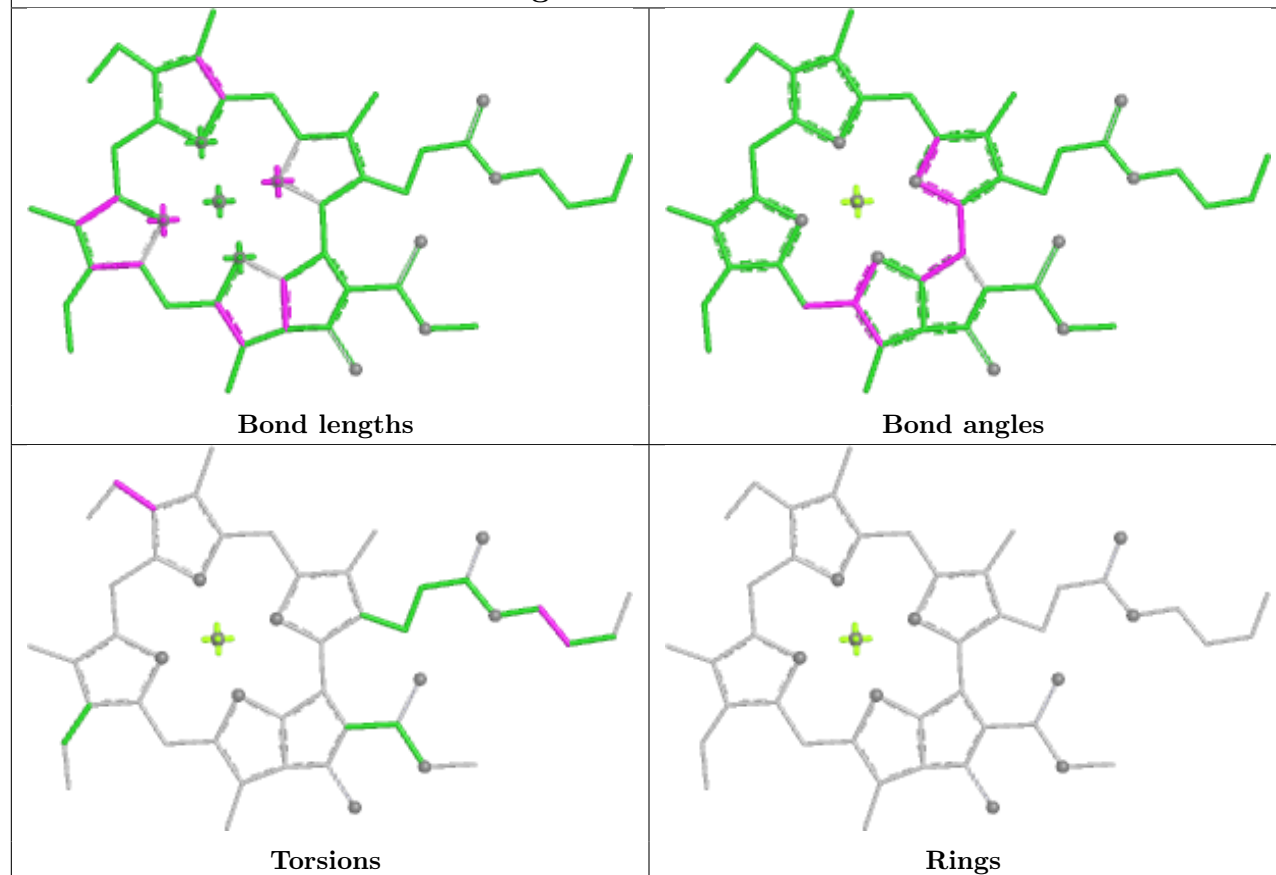


Ligand CLA B 808

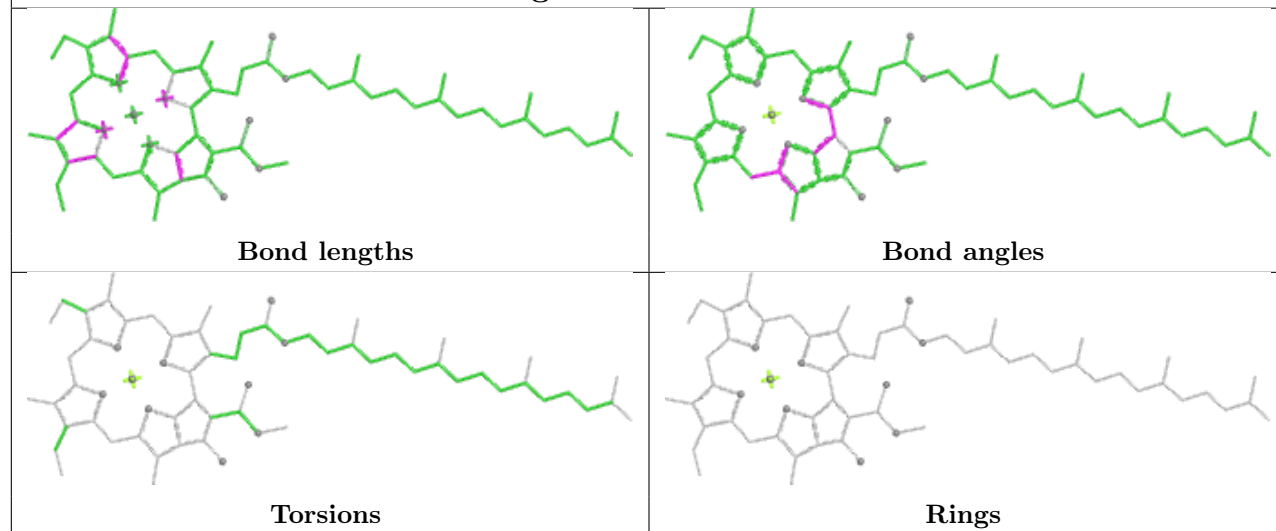




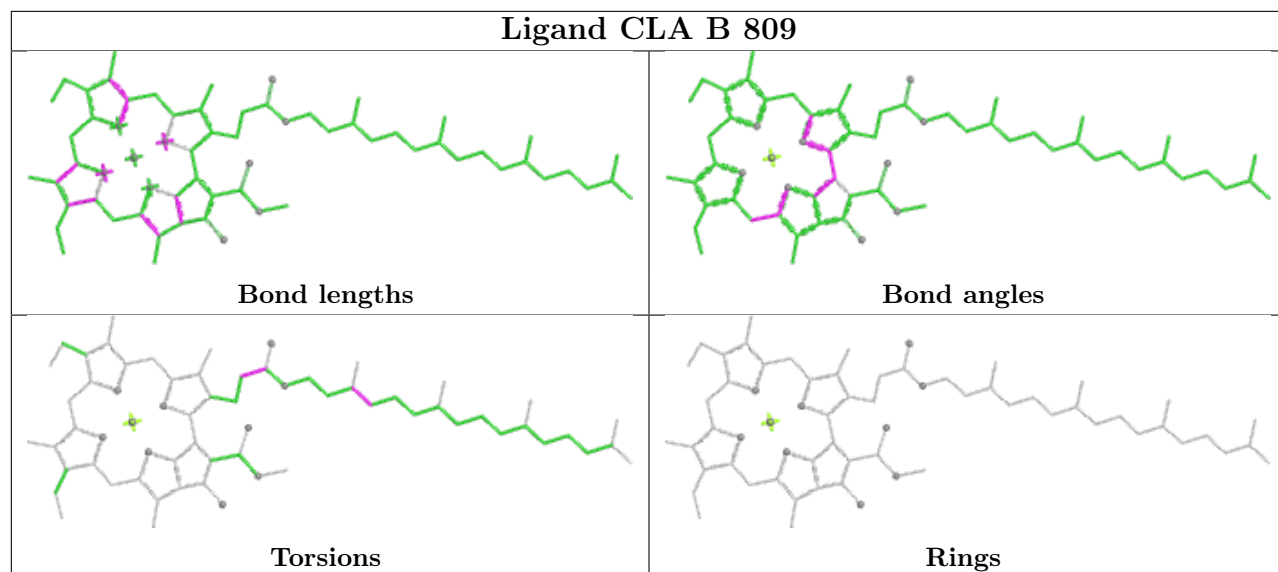
Ligand CLA A 805



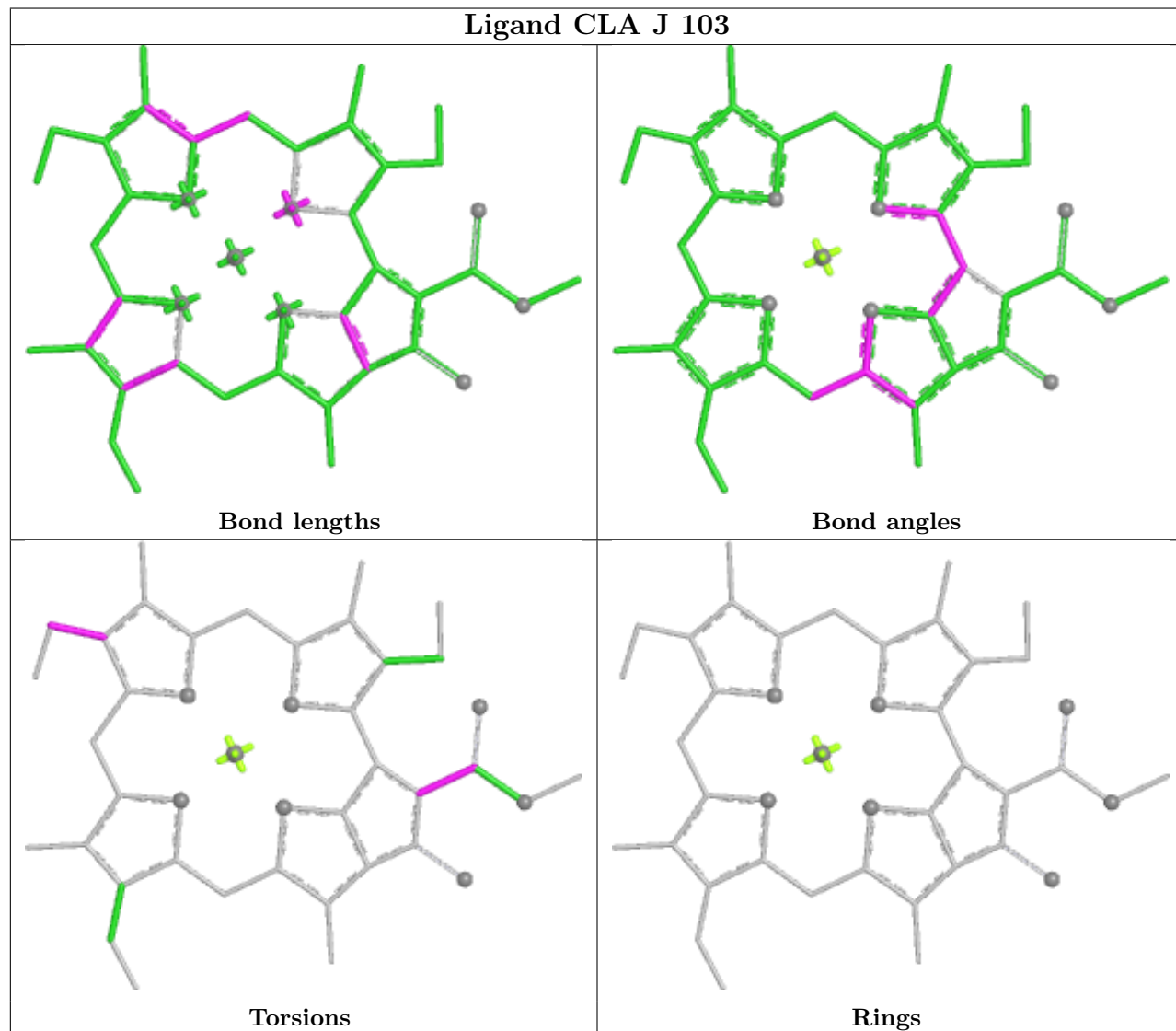
Ligand CLA A 816

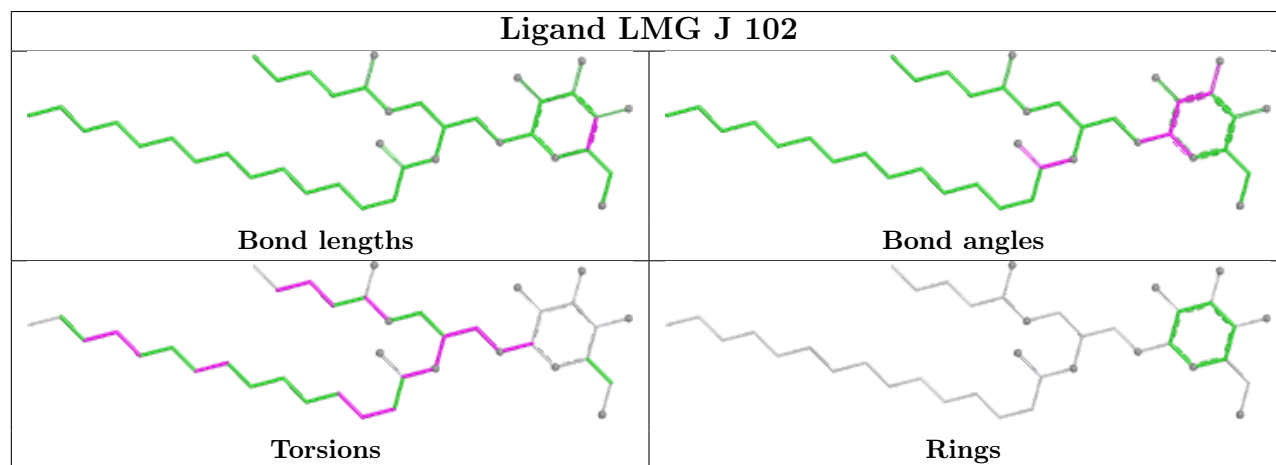
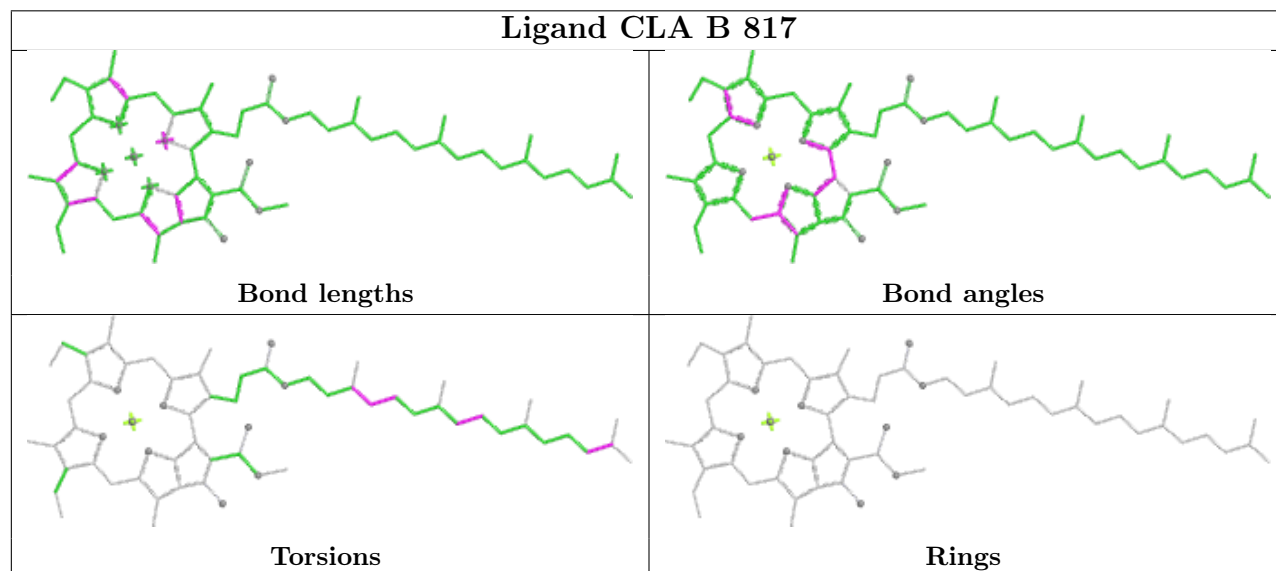
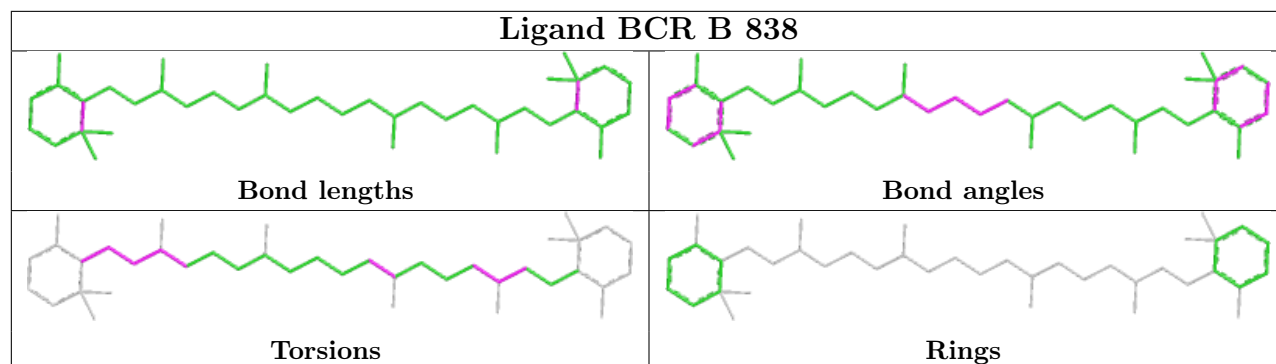


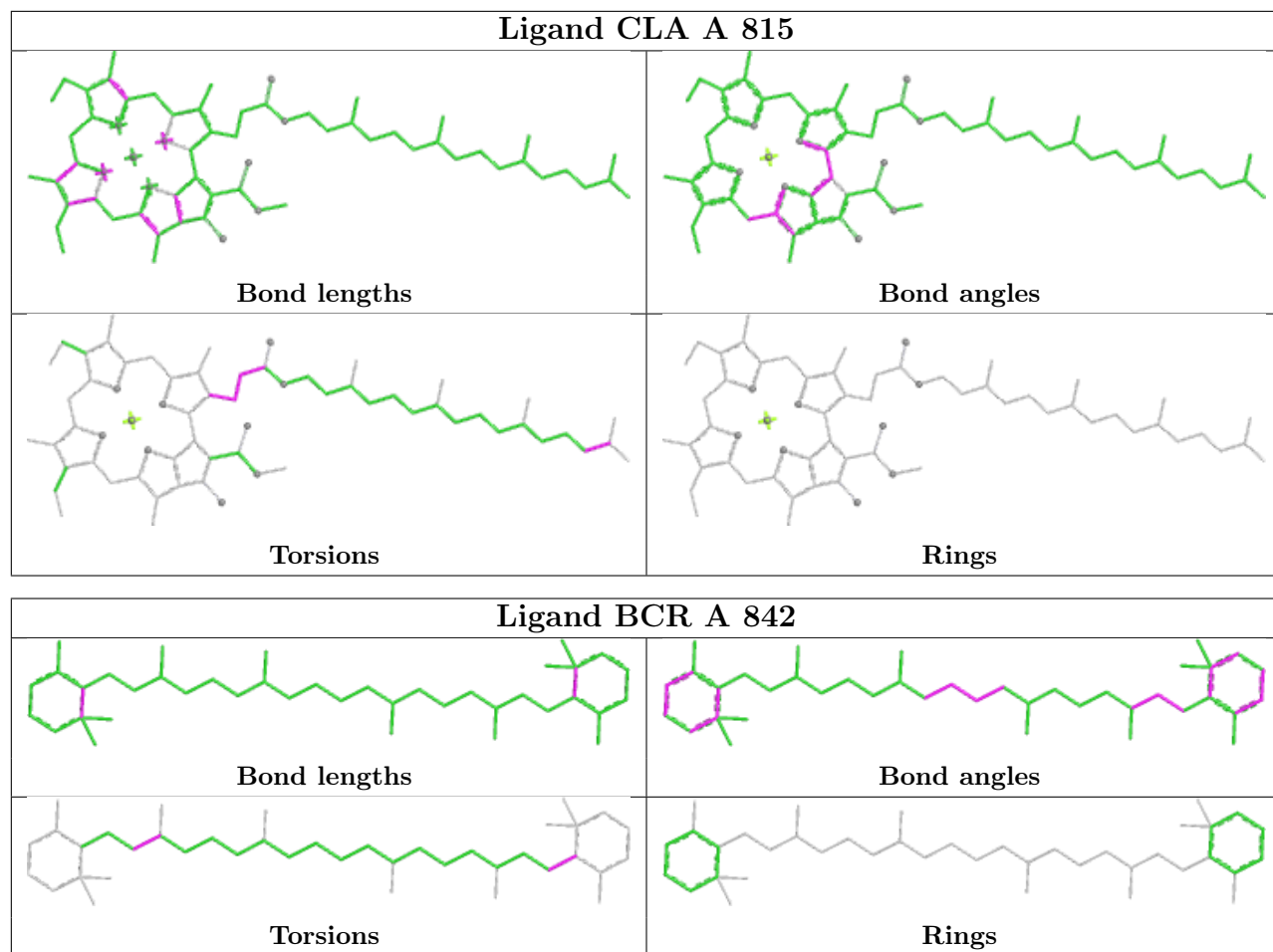
Ligand CLA B 809



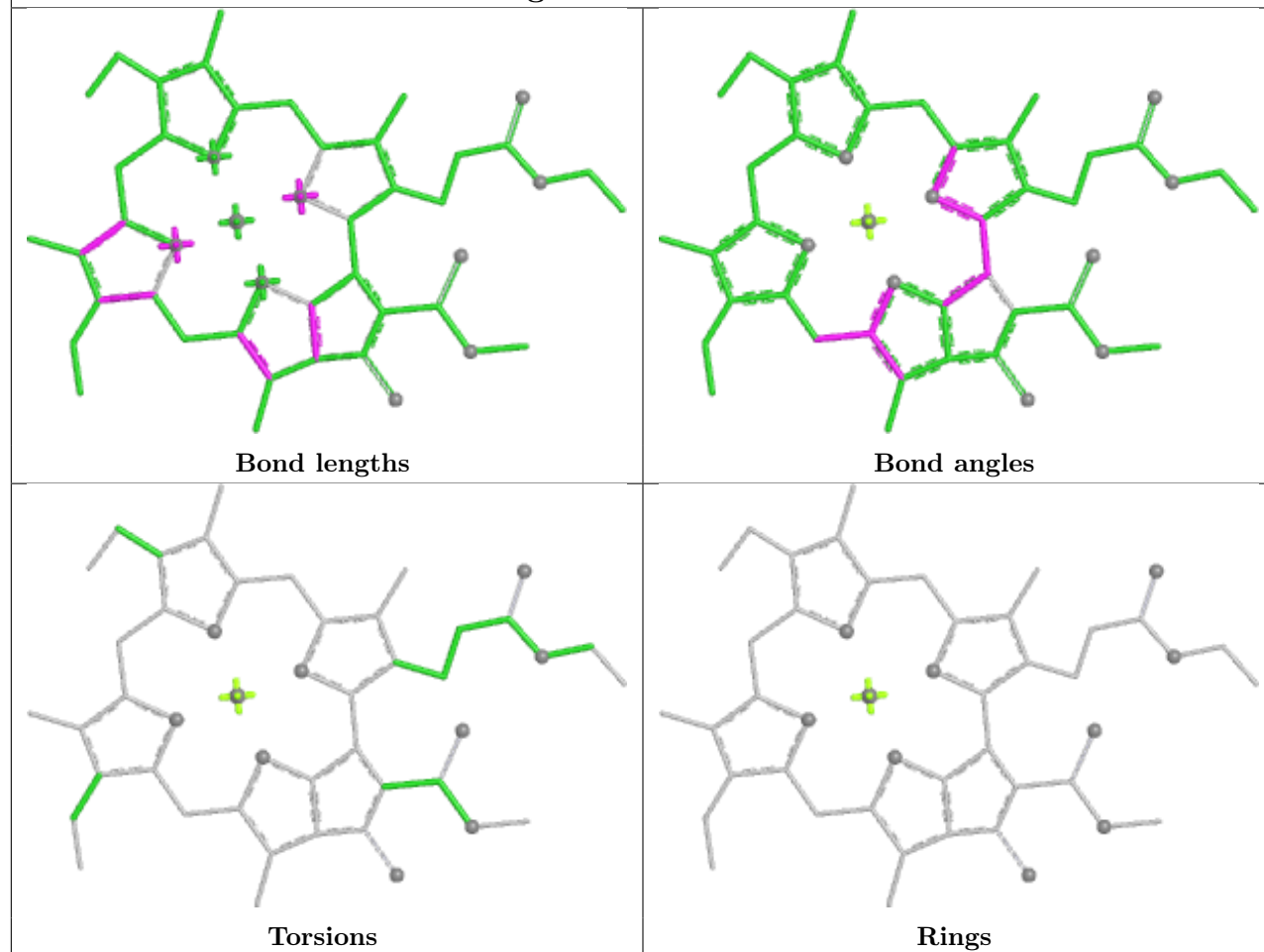
Ligand CLA J 103



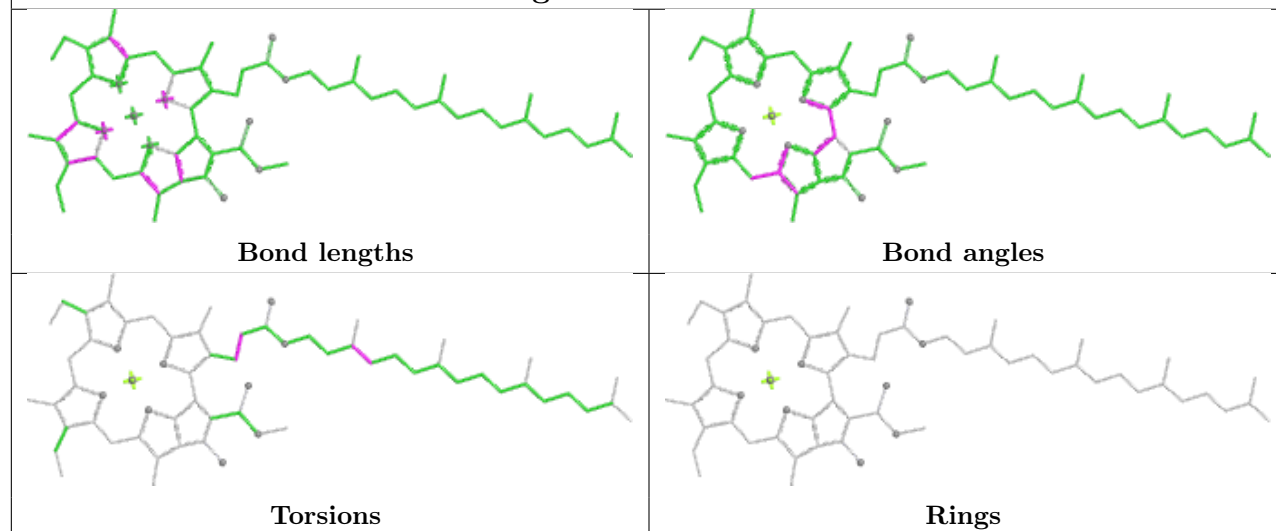




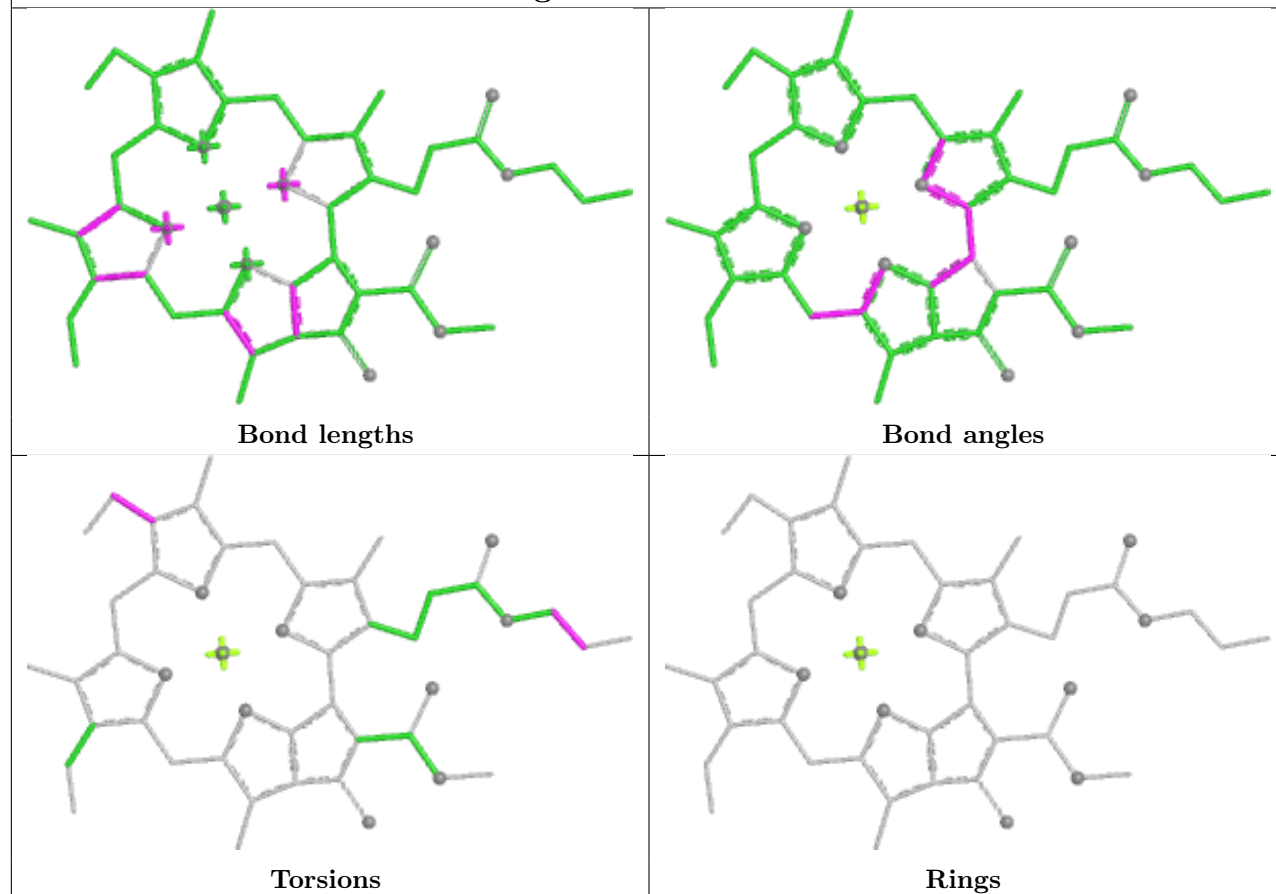
Ligand CLA B 832



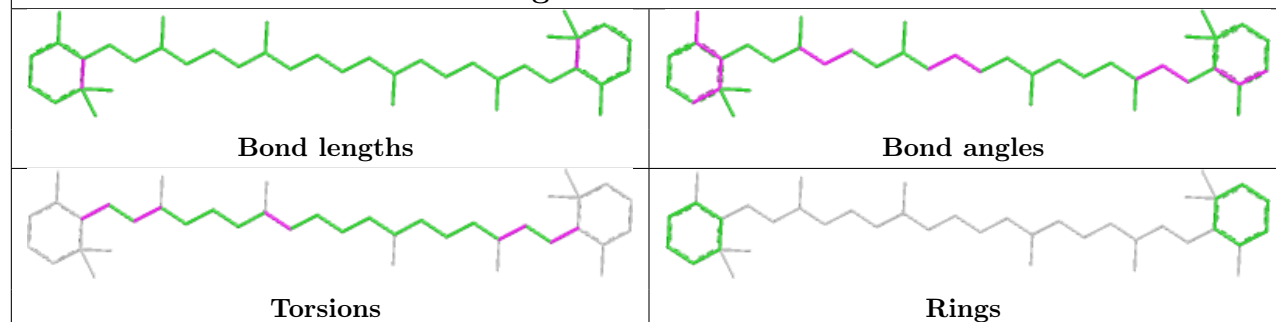
Ligand CLA B 801



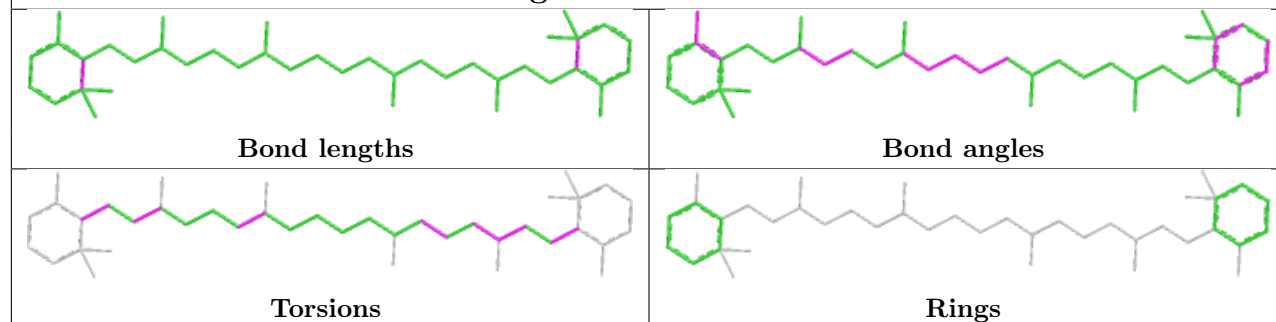
Ligand CLA F 802

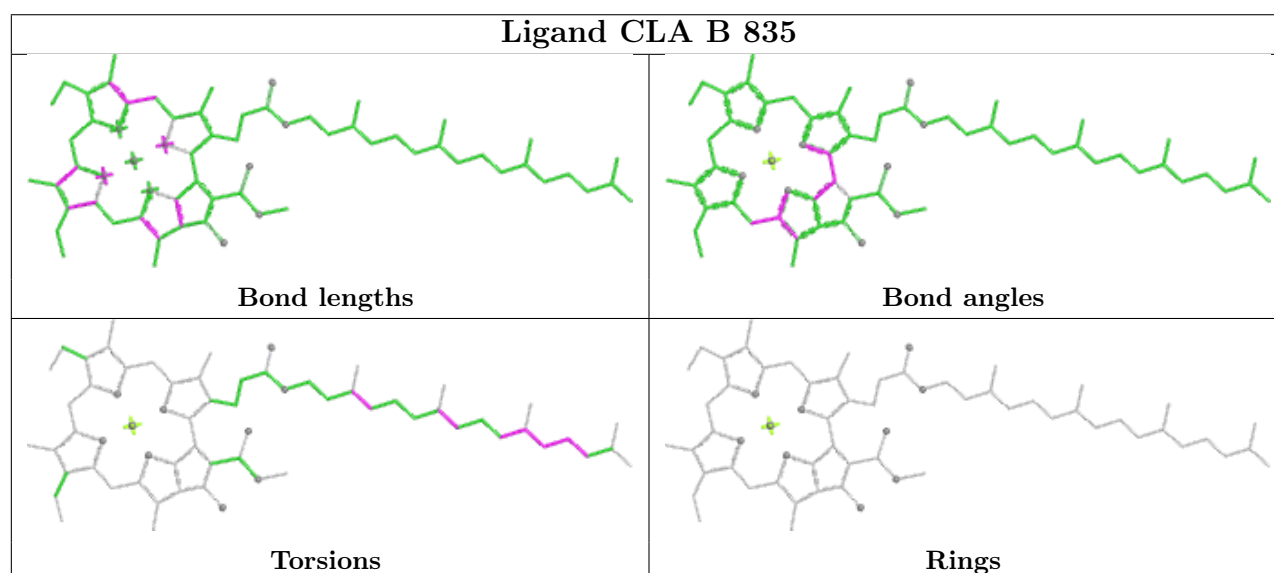
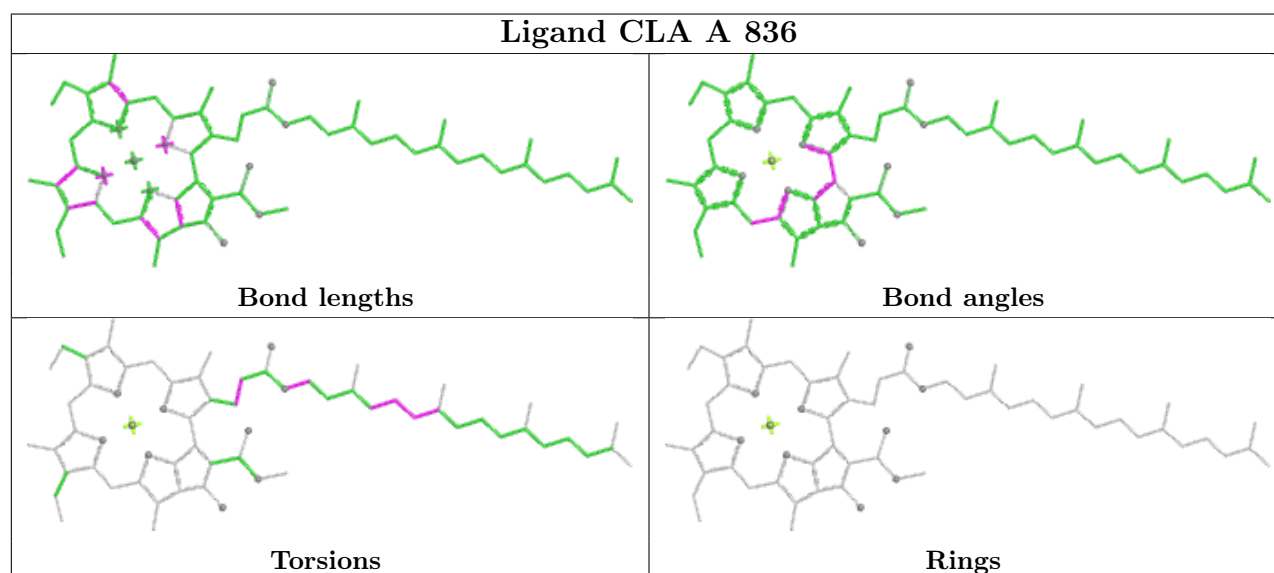
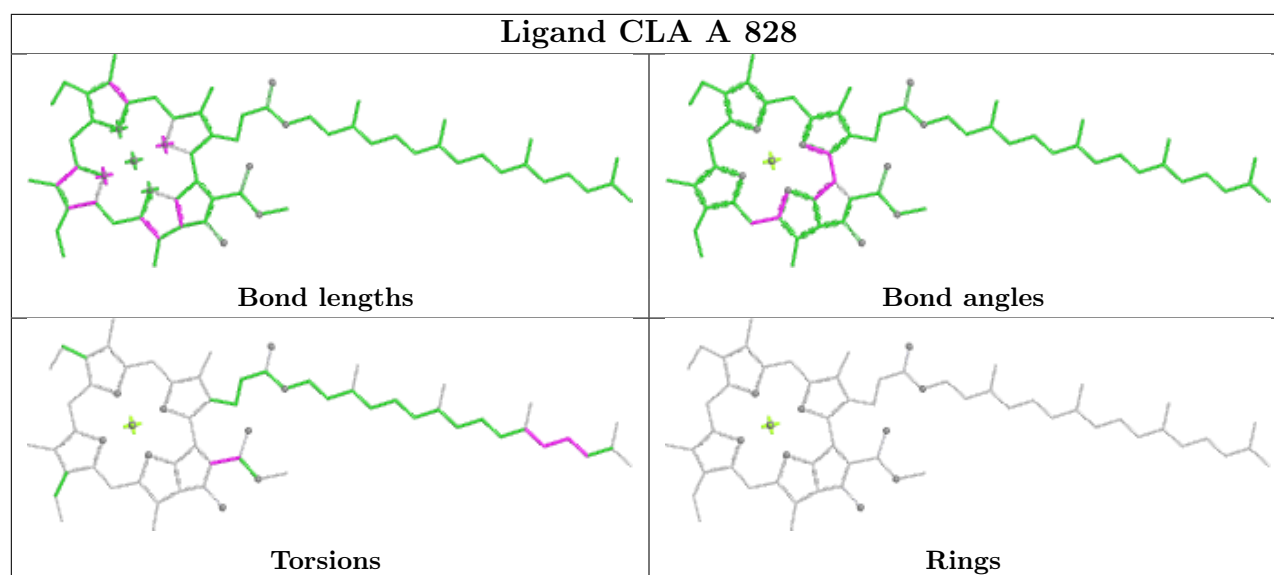


Ligand BCR F 804

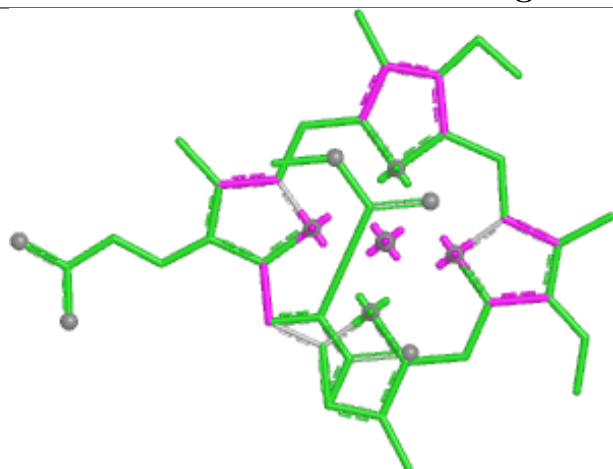


Ligand BCR A 843

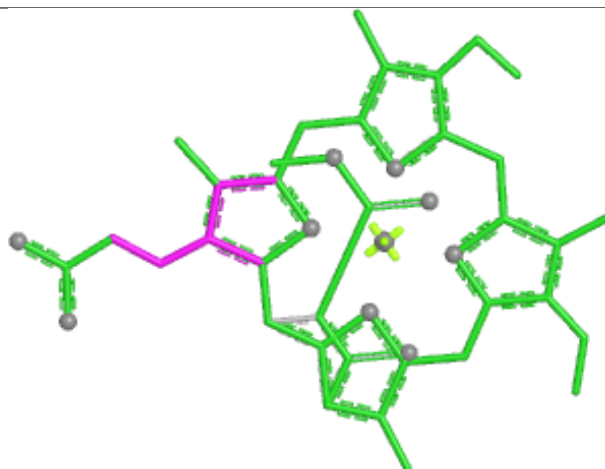




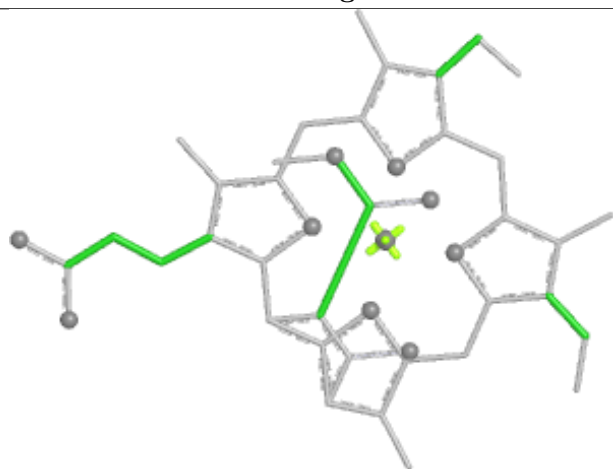
Ligand KC1 U 214



Bond lengths



Bond angles

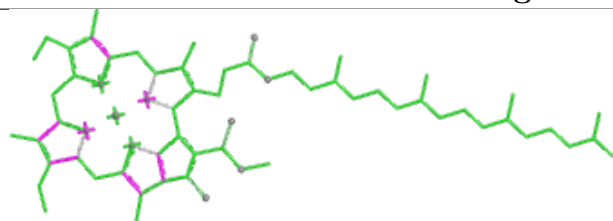


Torsions

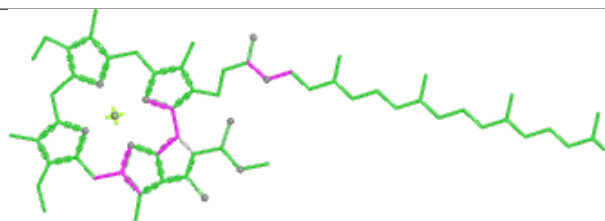


Rings

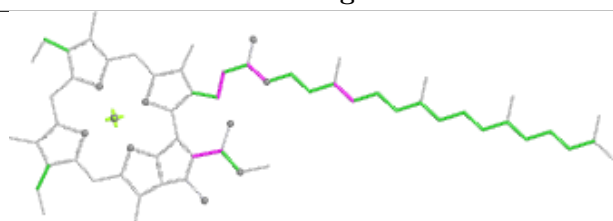
Ligand CLA A 806



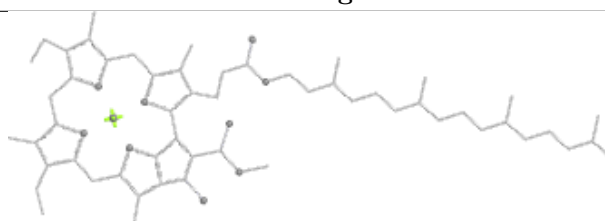
Bond lengths



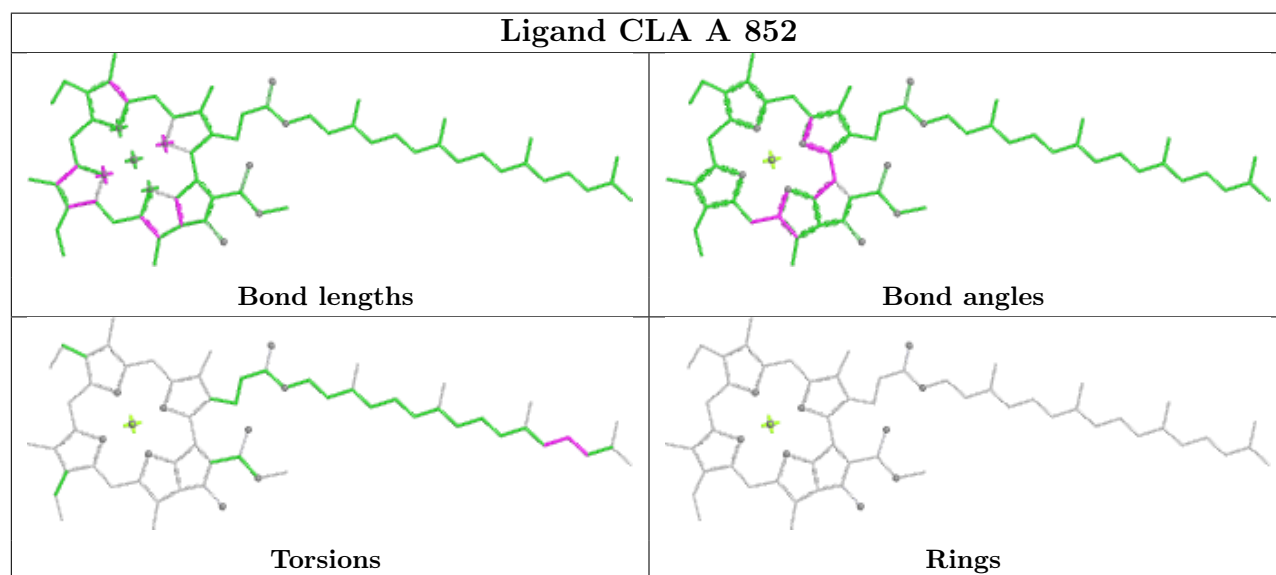
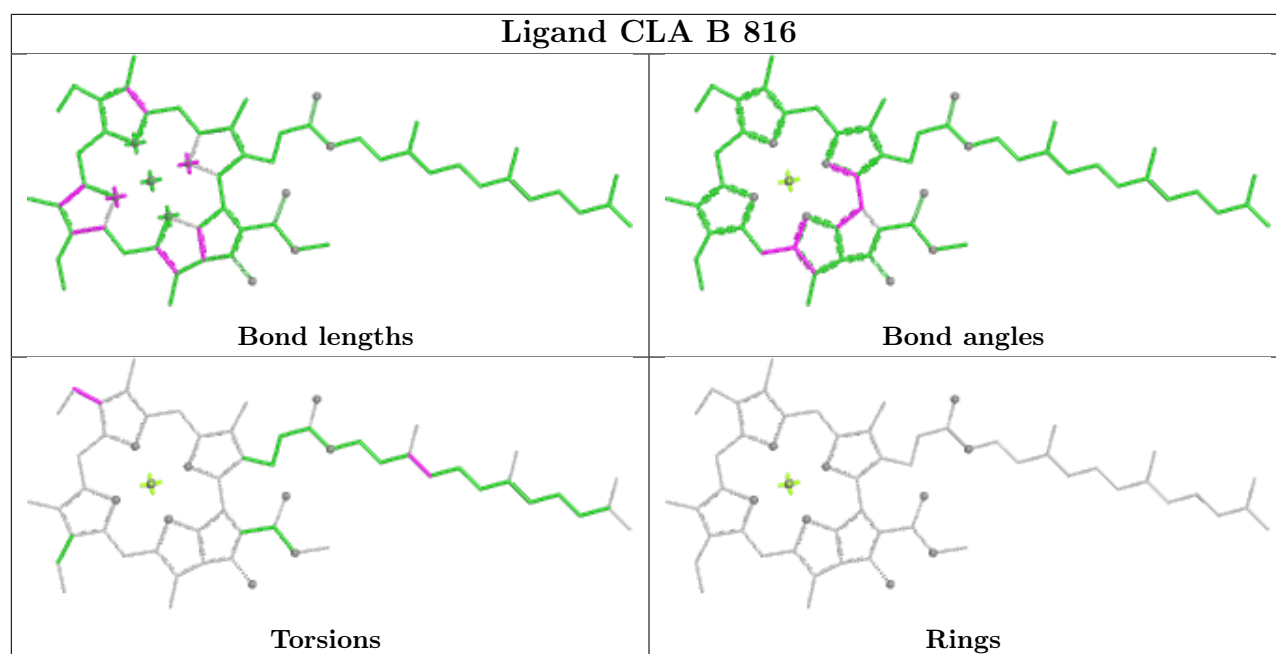
Bond angles

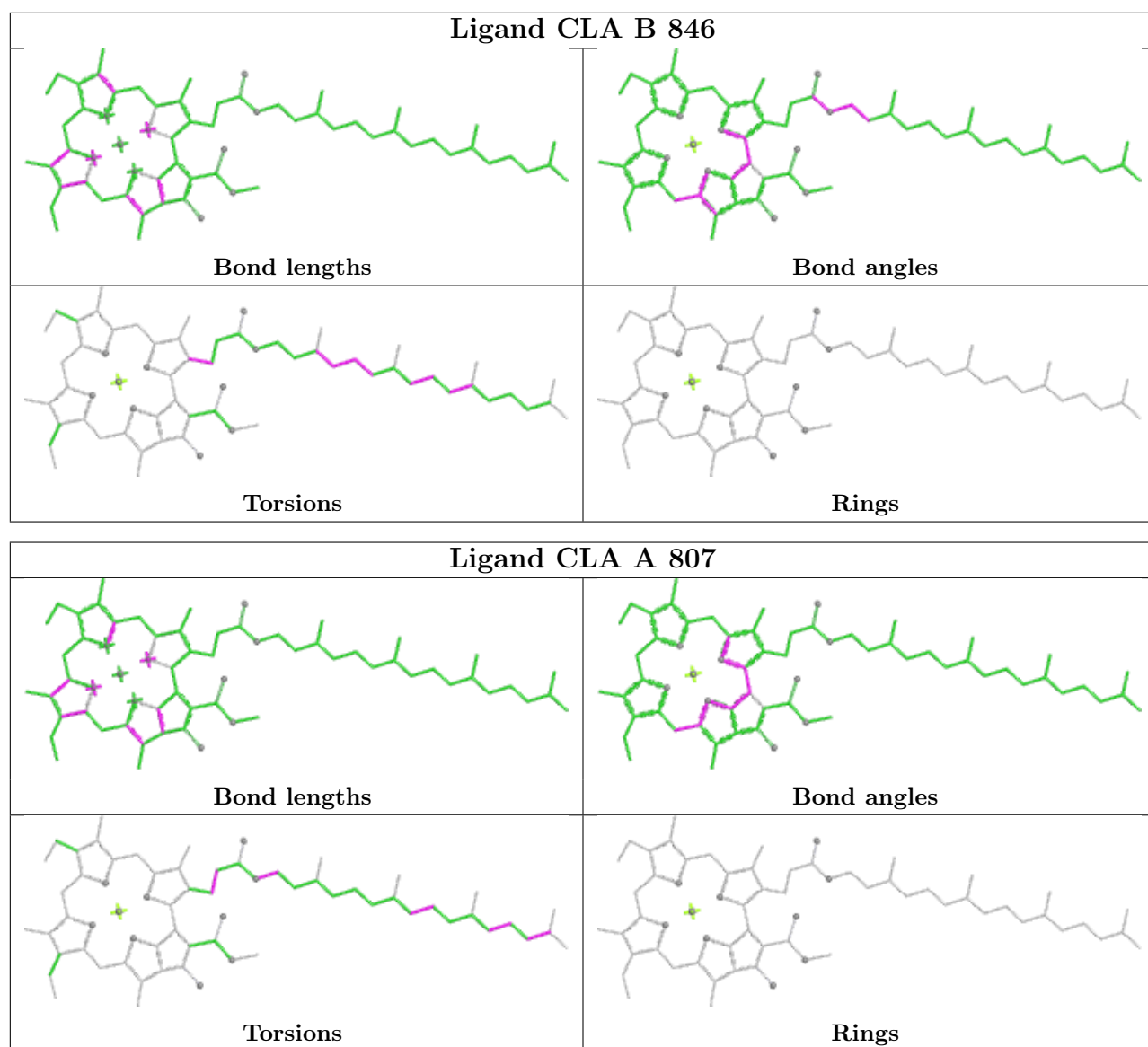


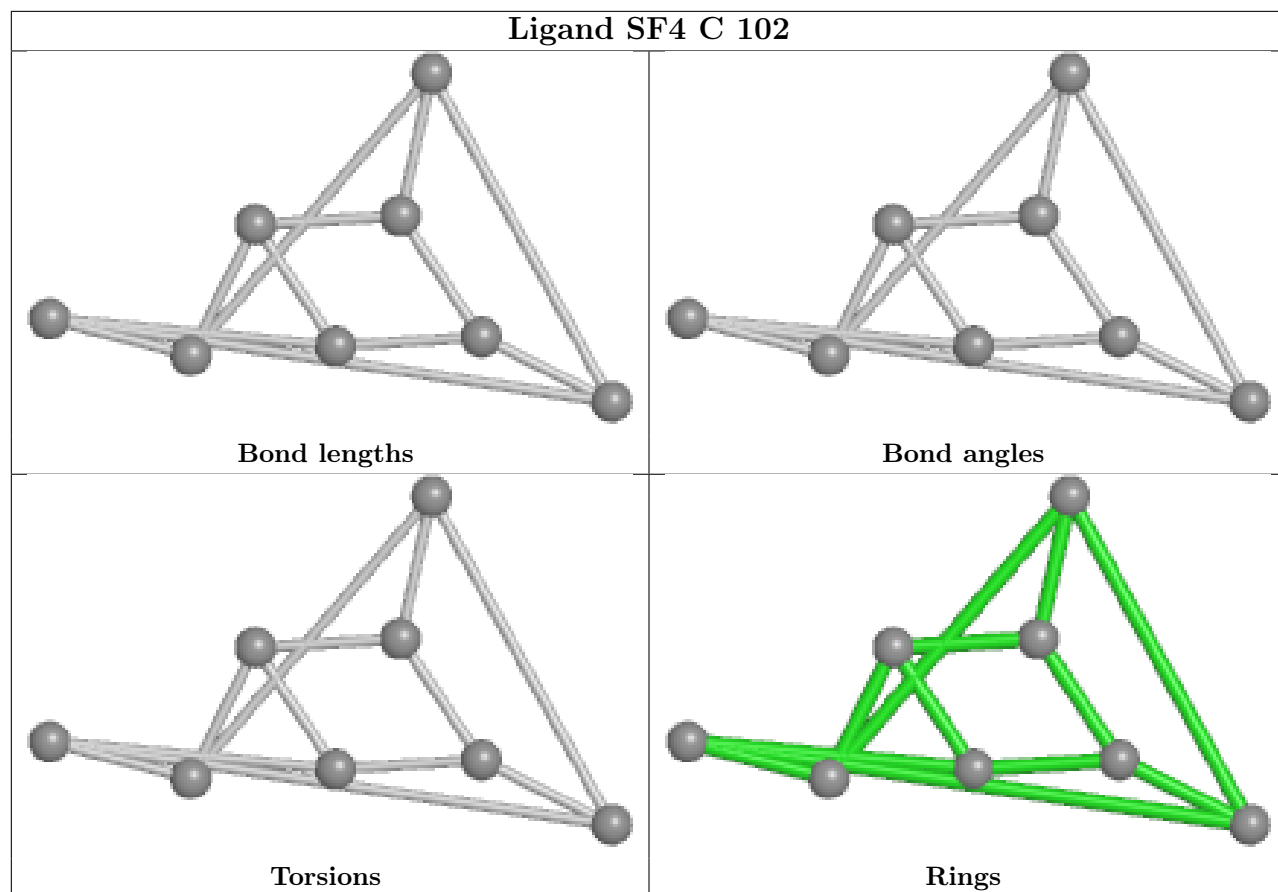
Torsions

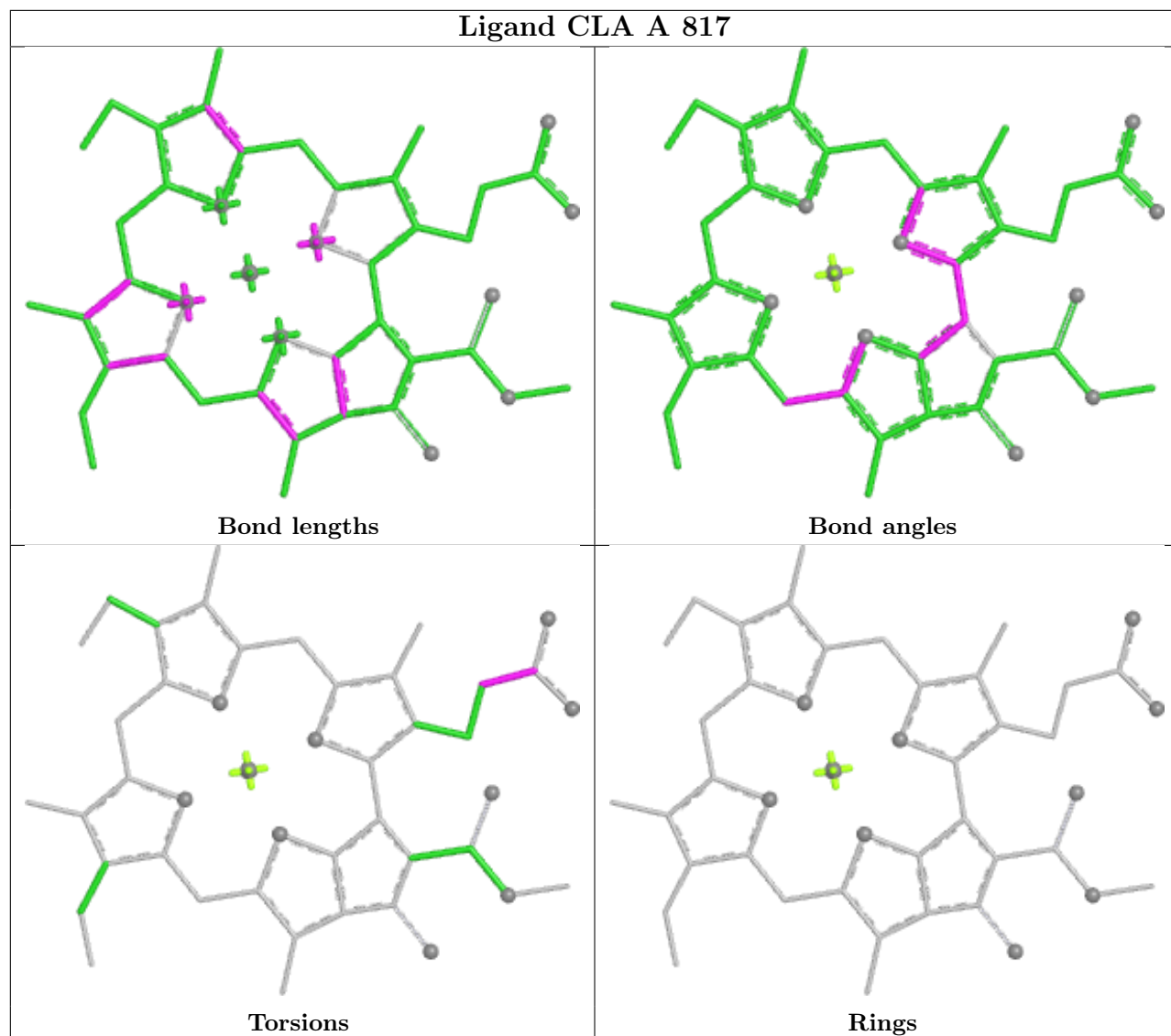


Rings

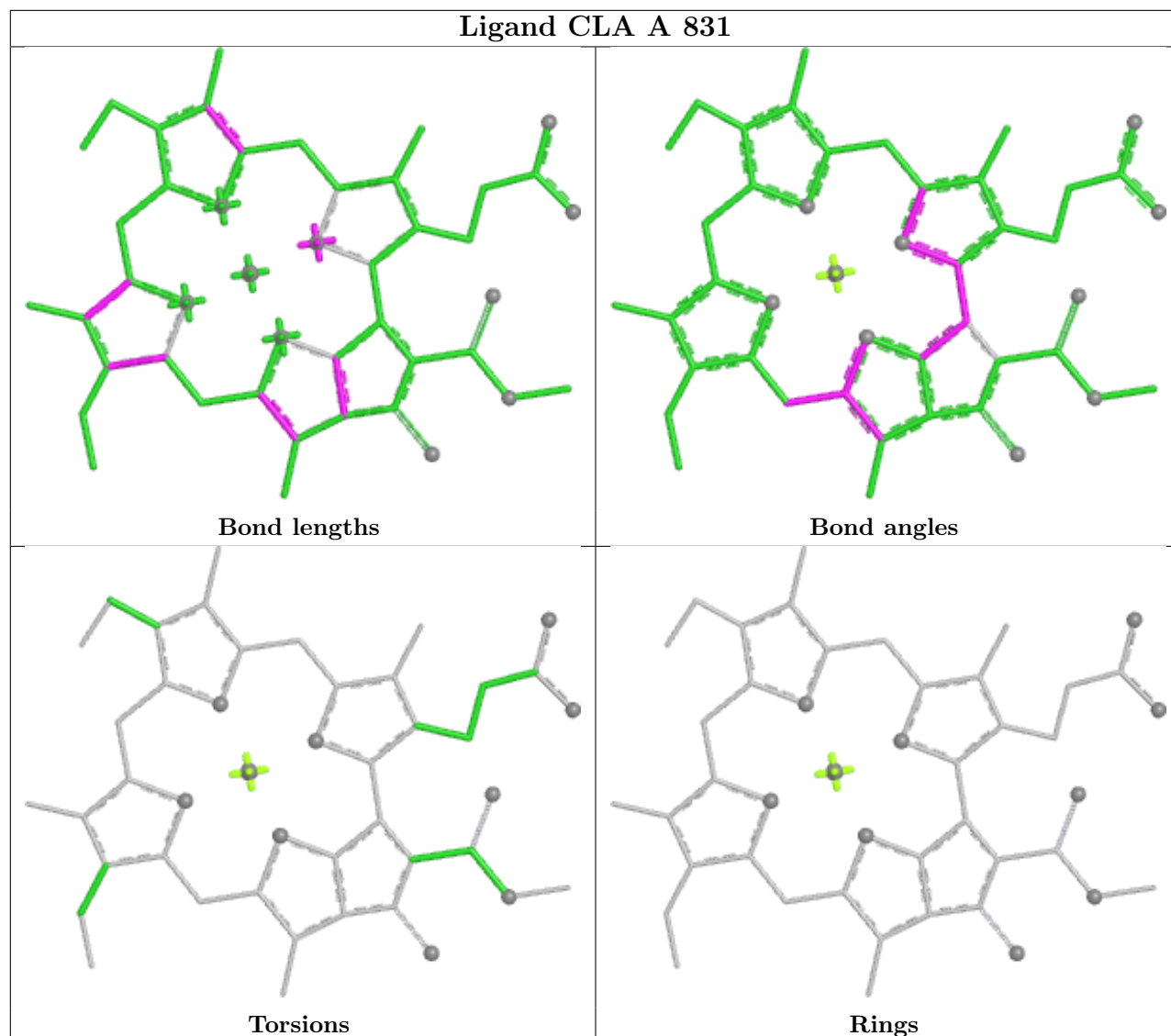




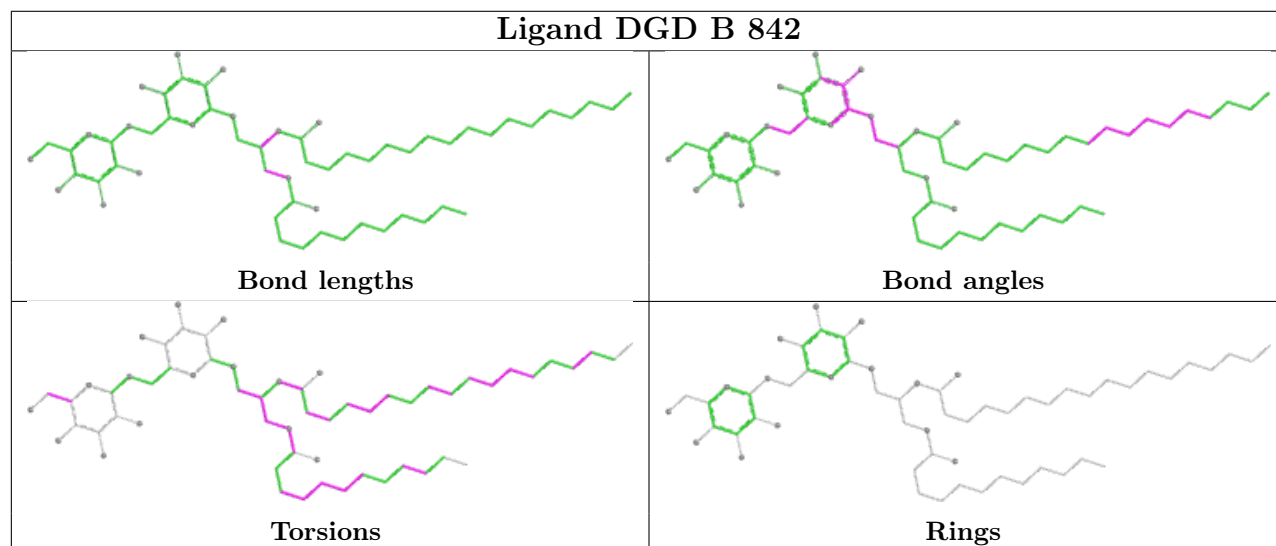


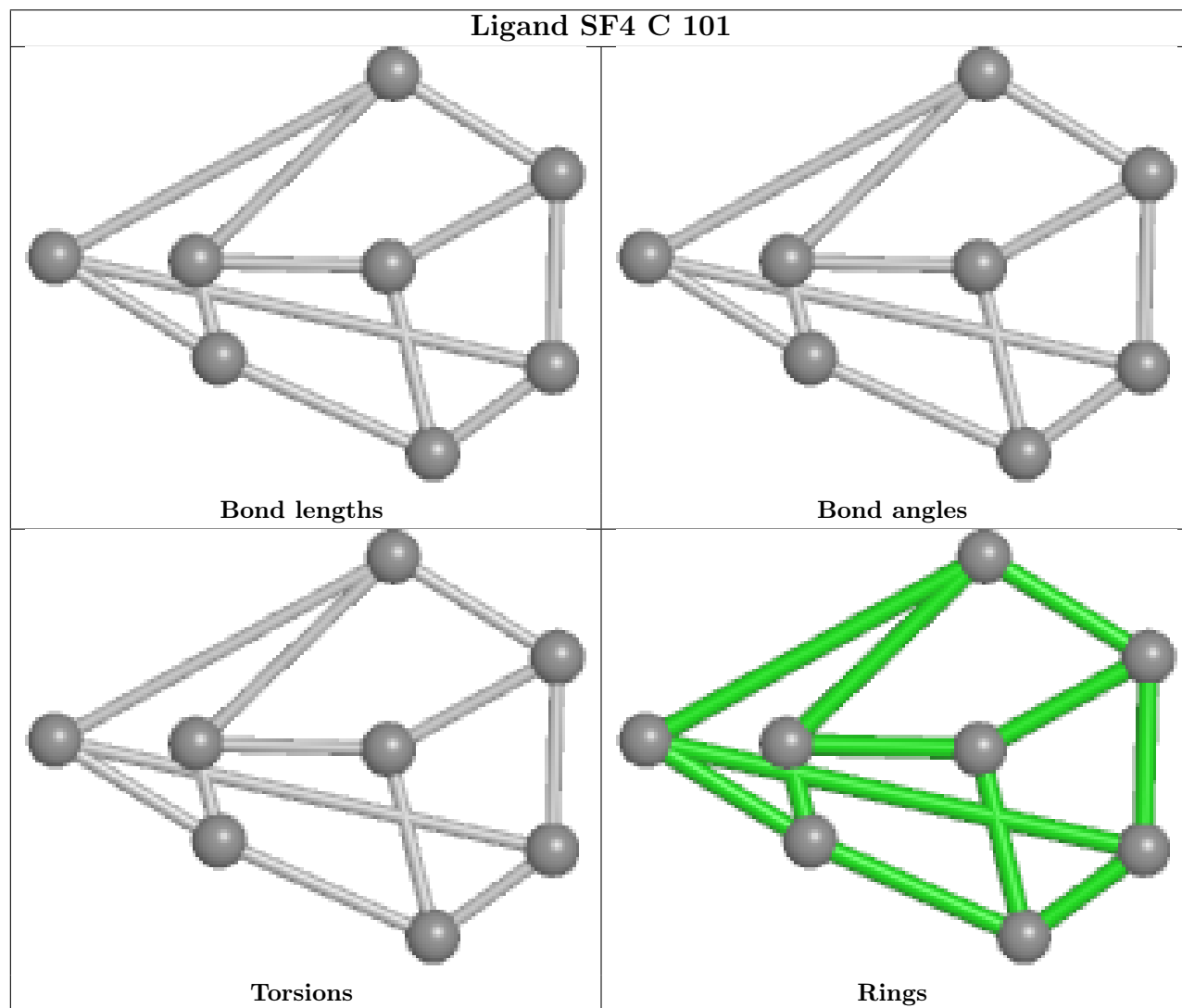
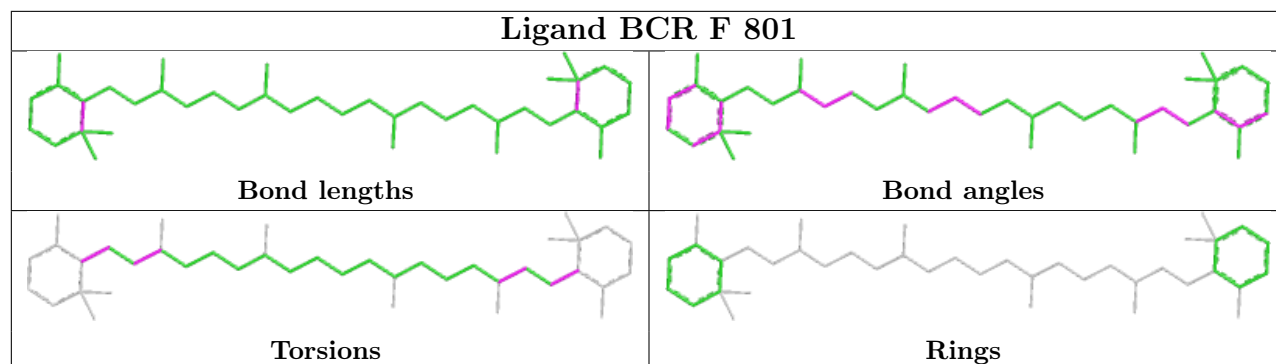


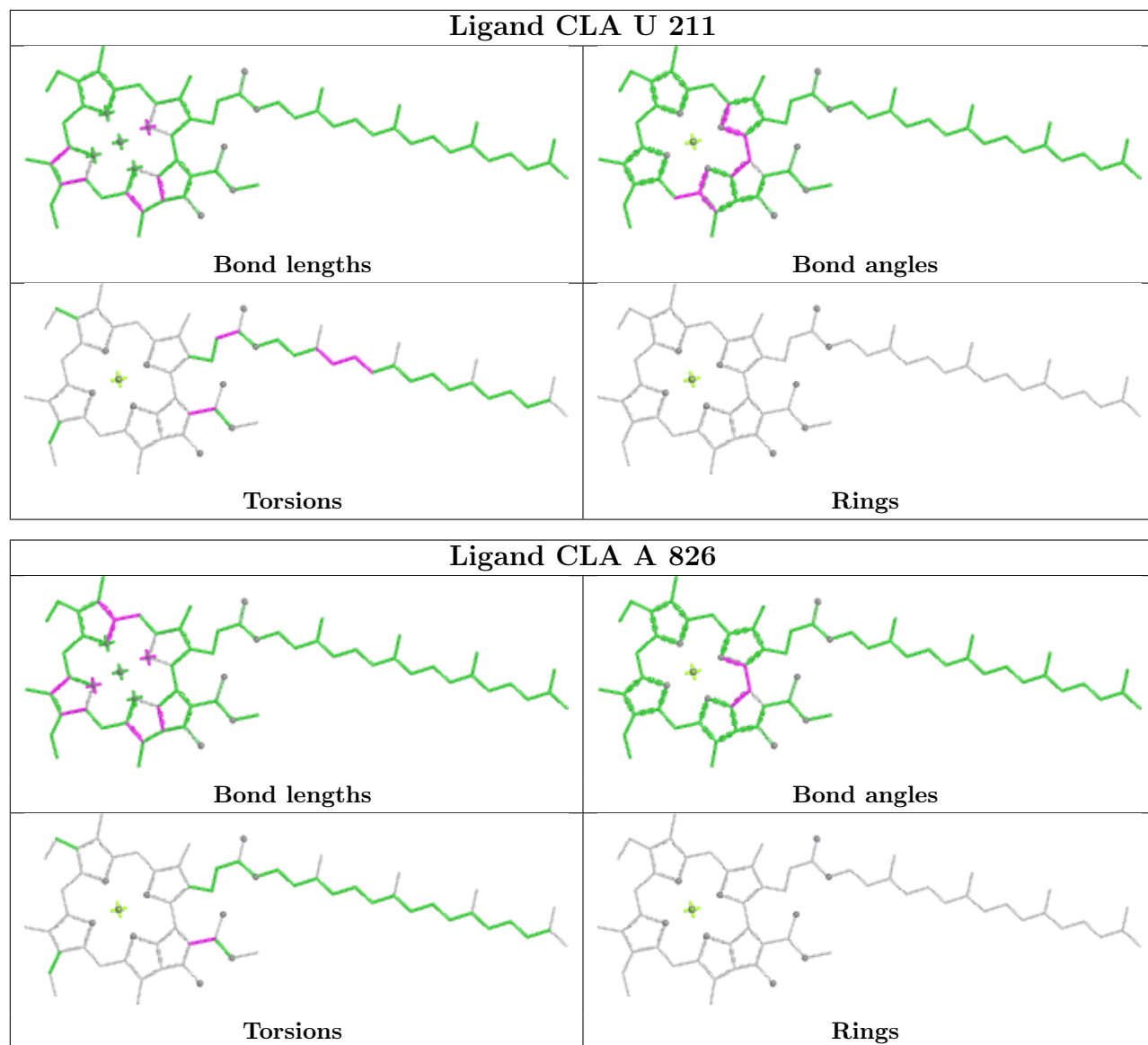
Ligand CLA A 831



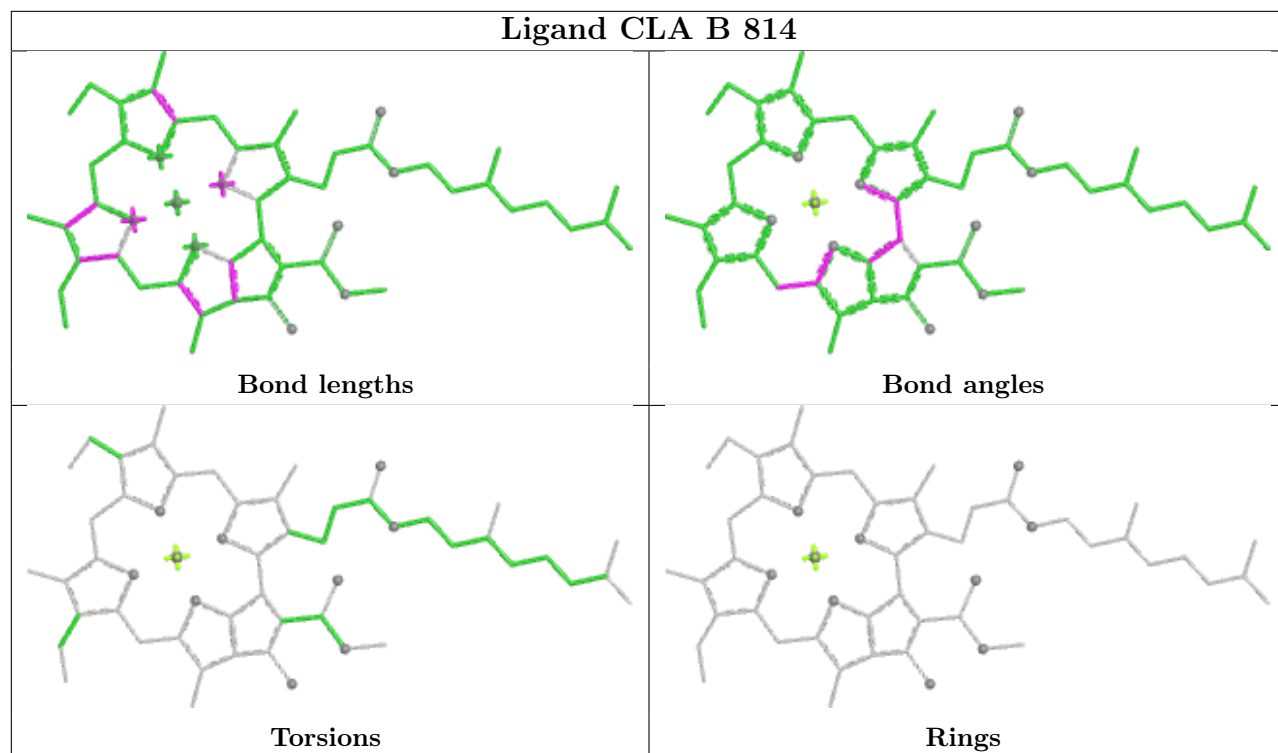
Ligand DGD B 842



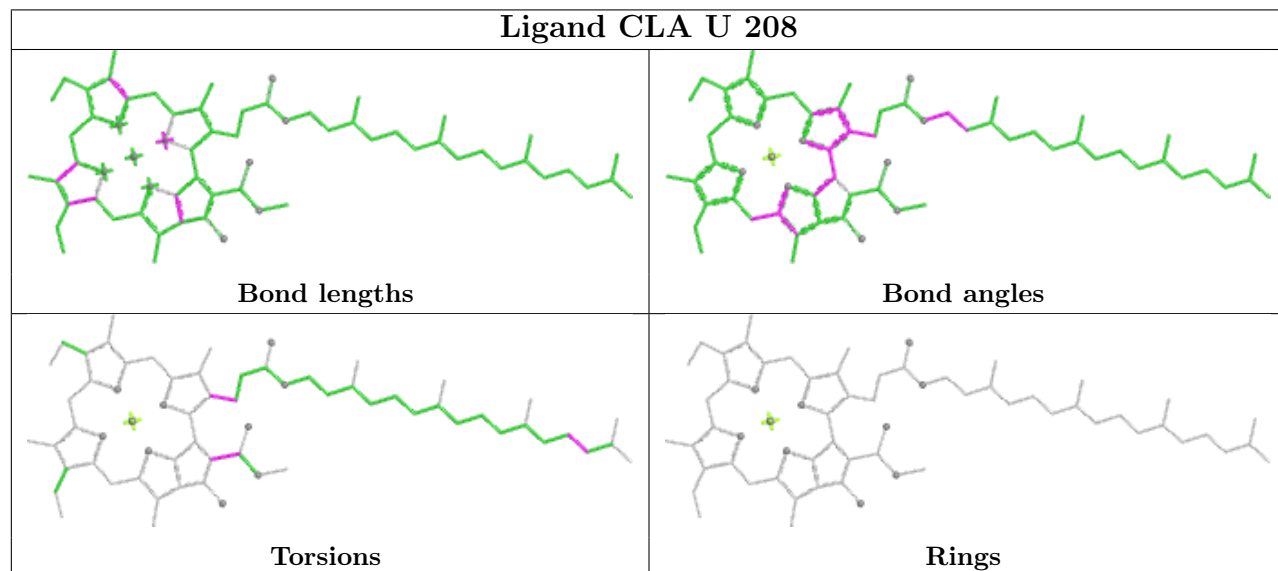


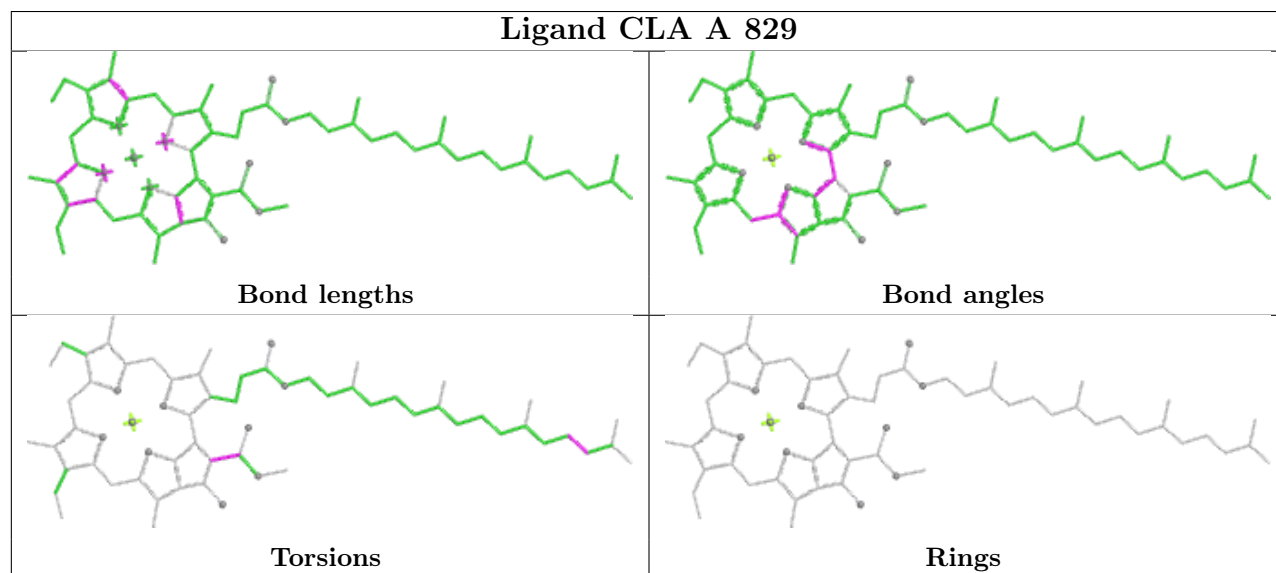
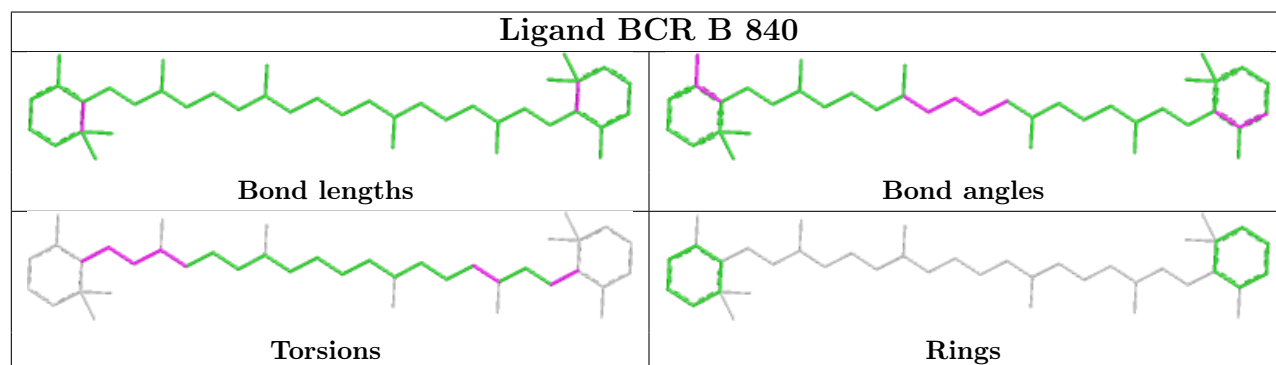
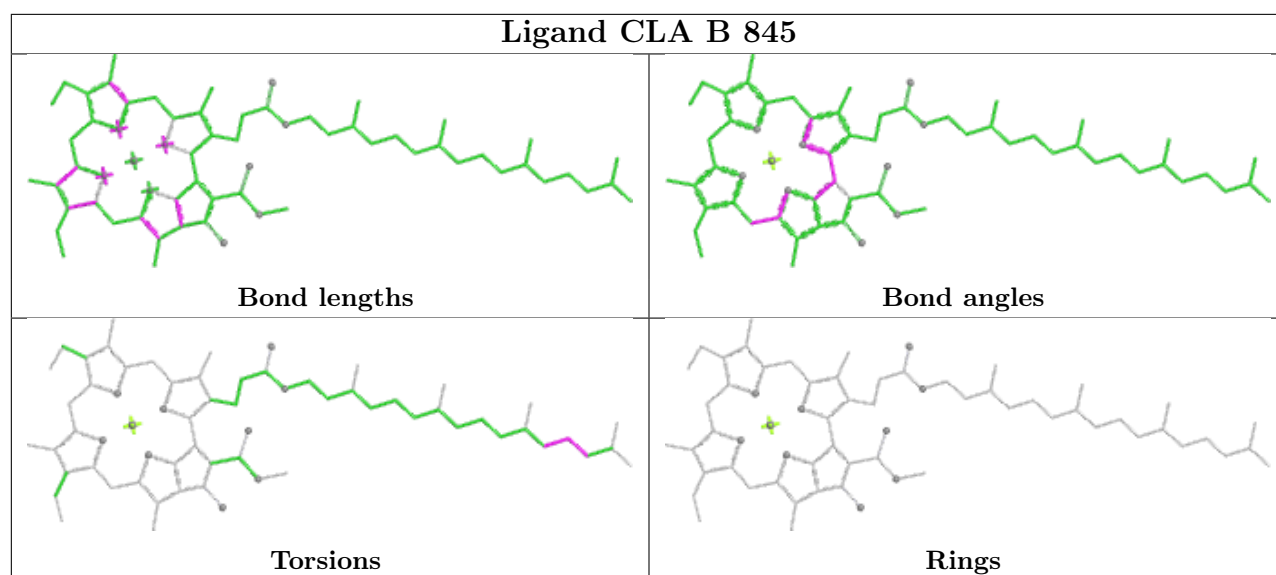


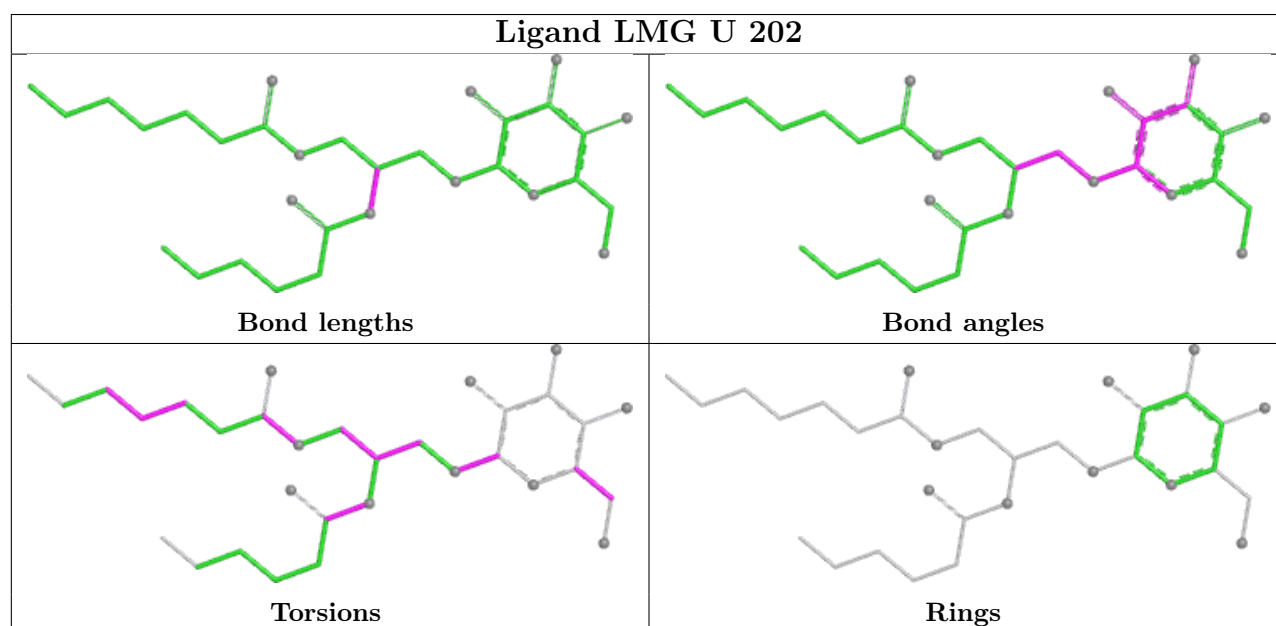
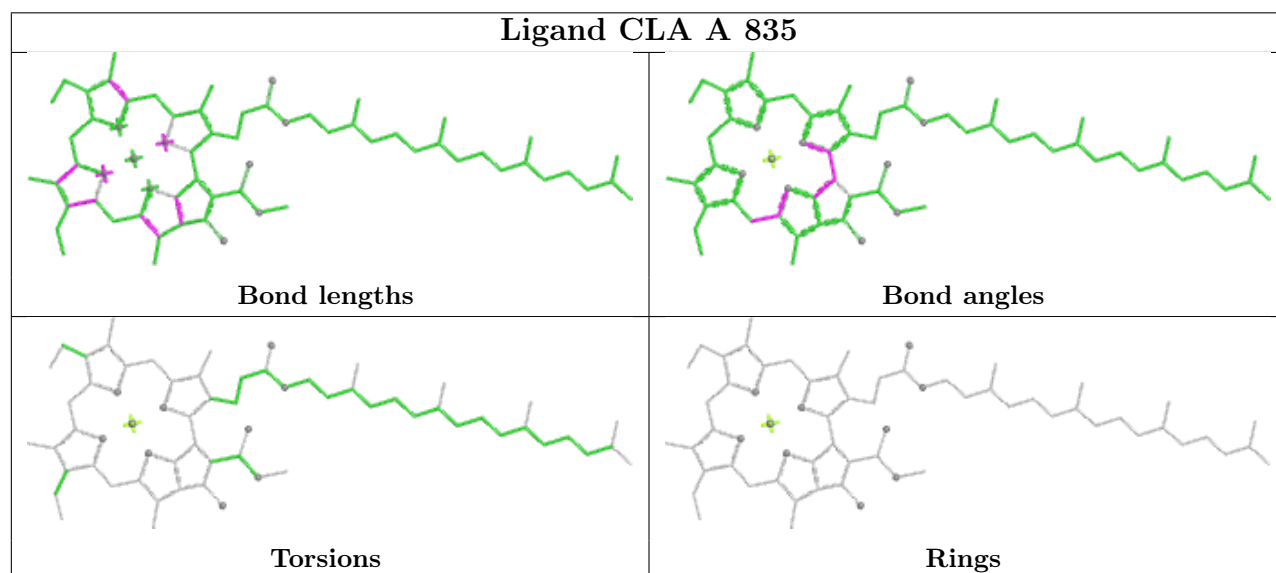
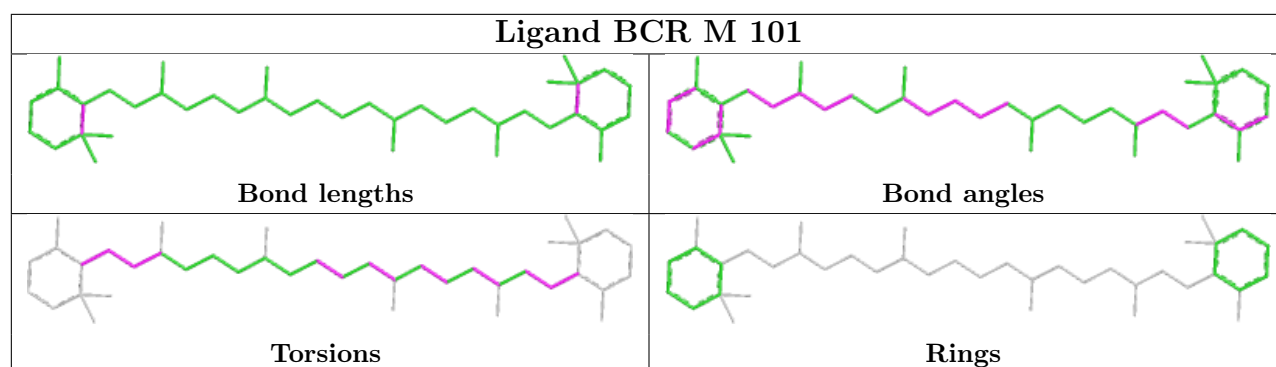
Ligand CLA B 814

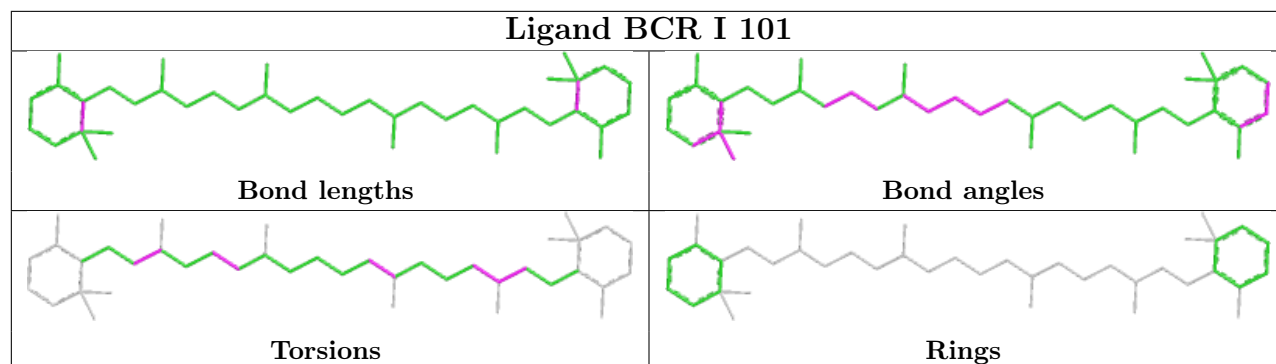
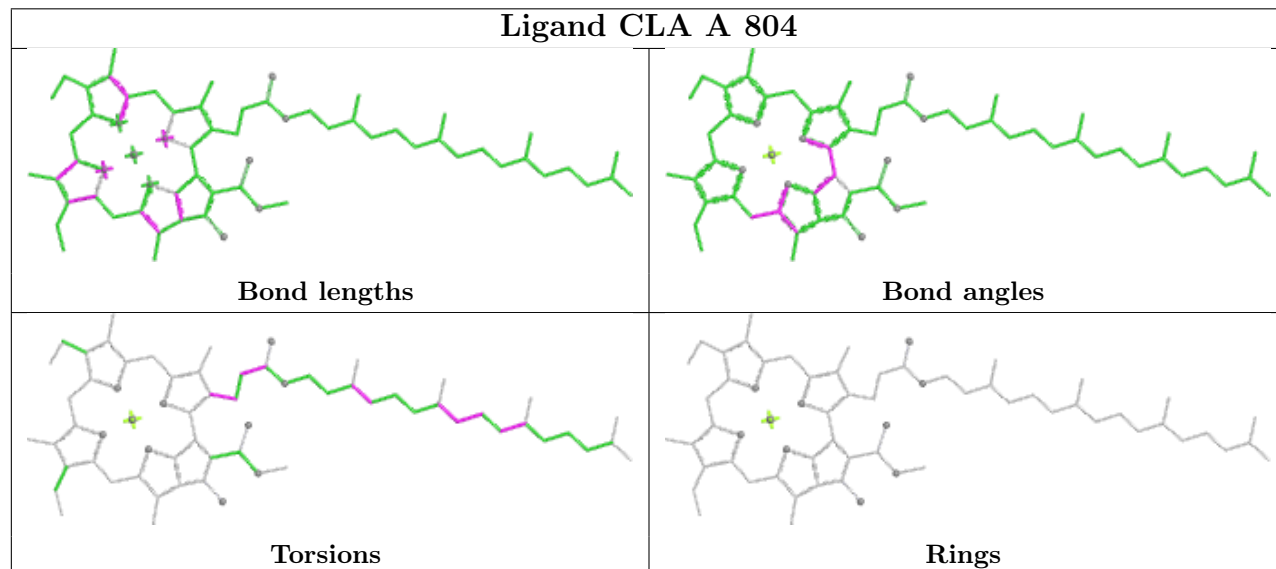
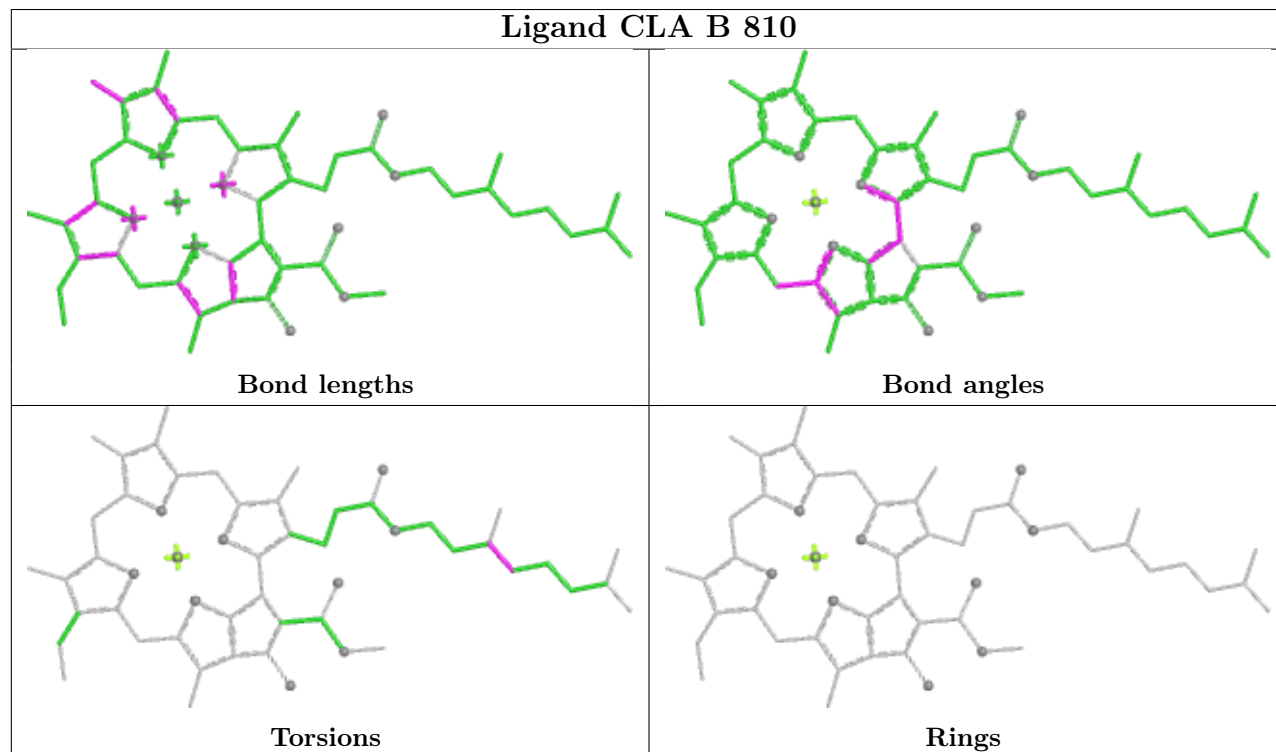


Ligand CLA U 208

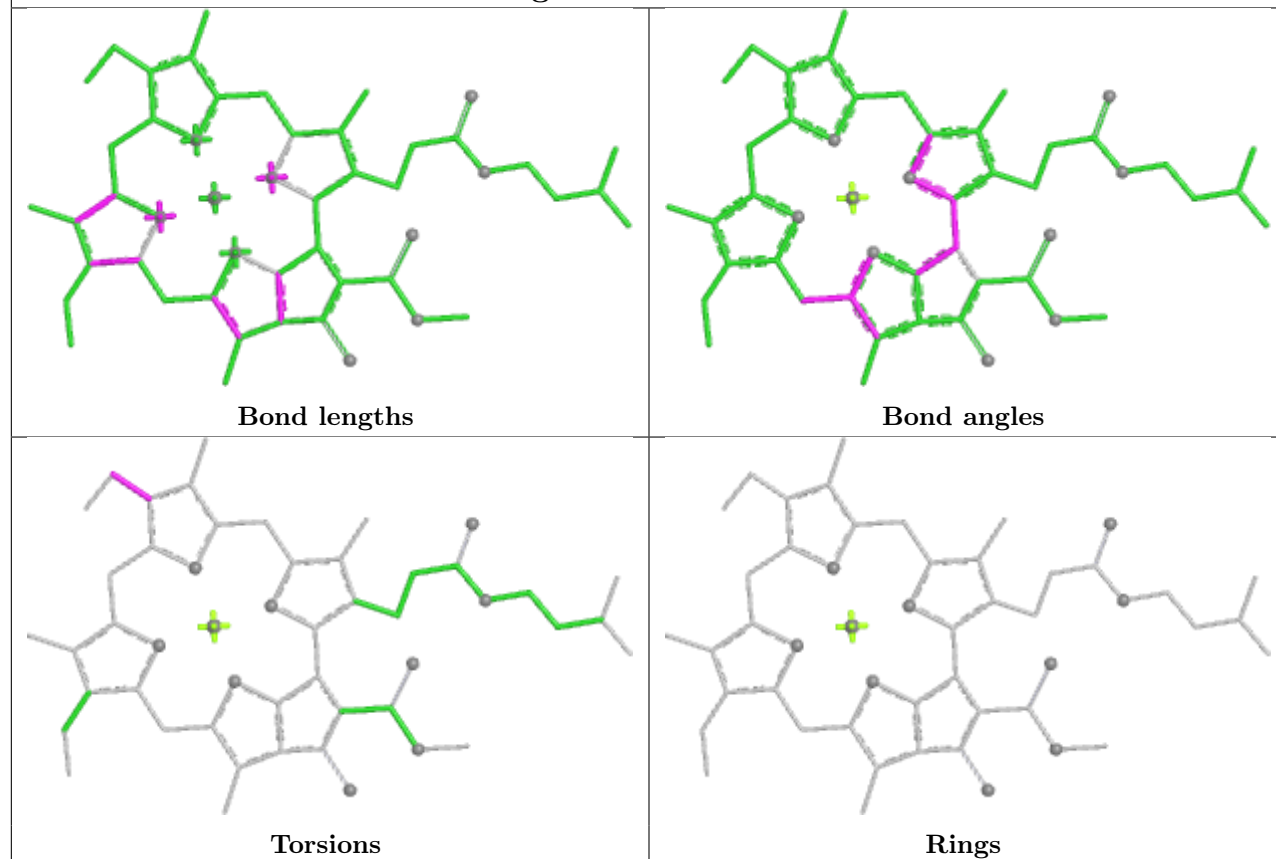




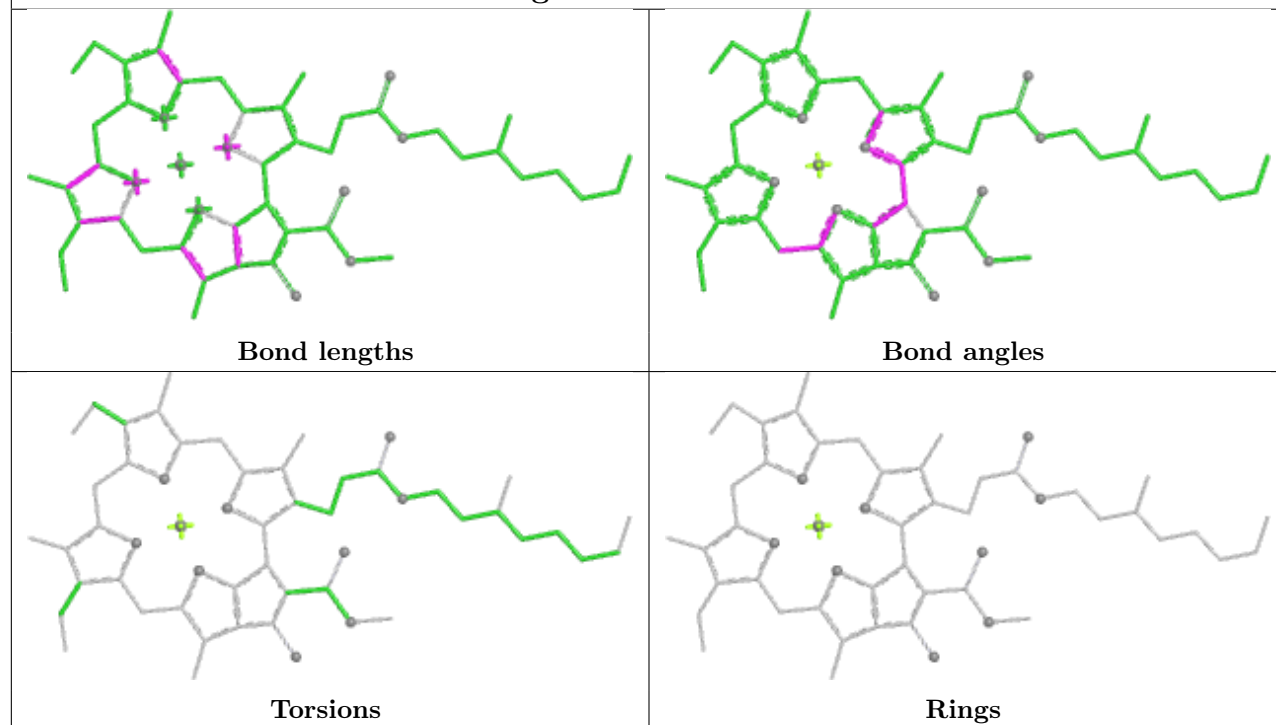


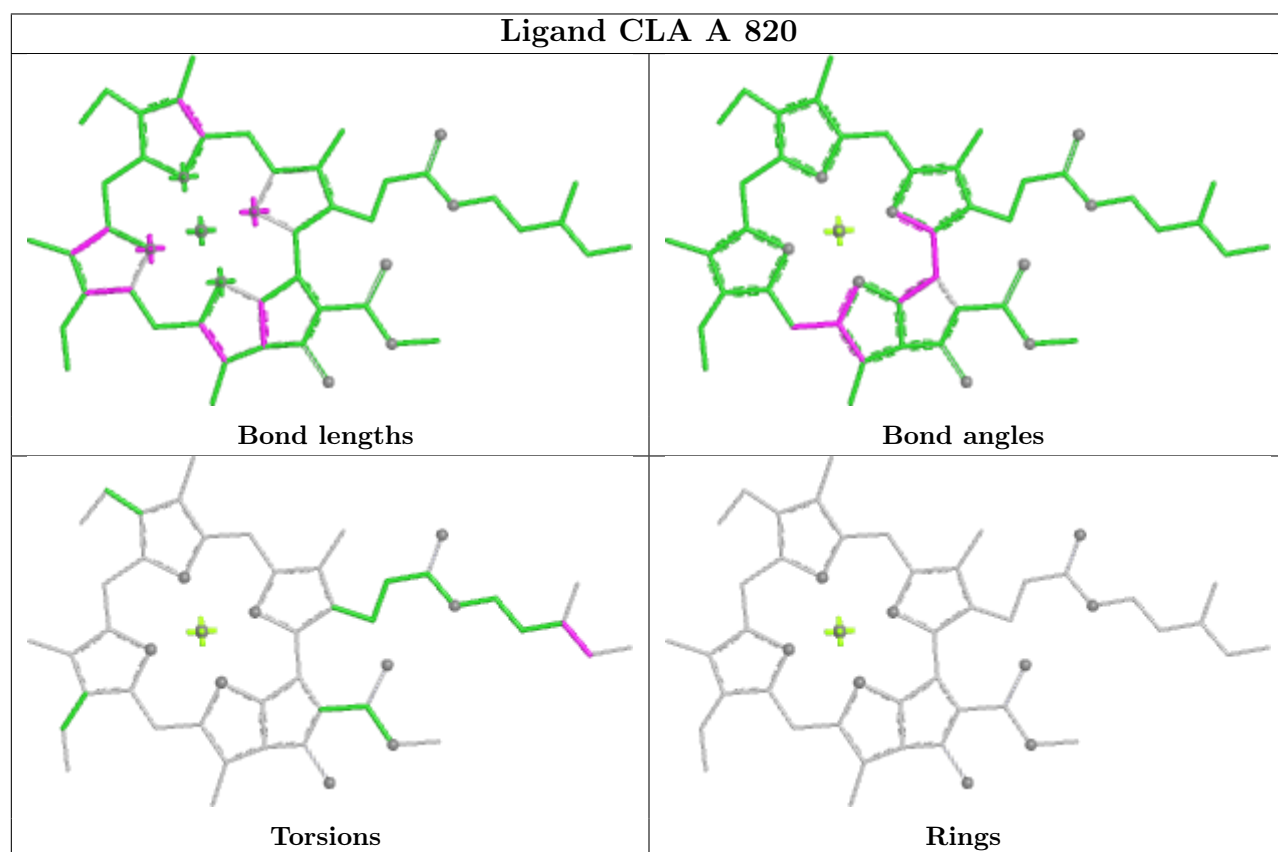
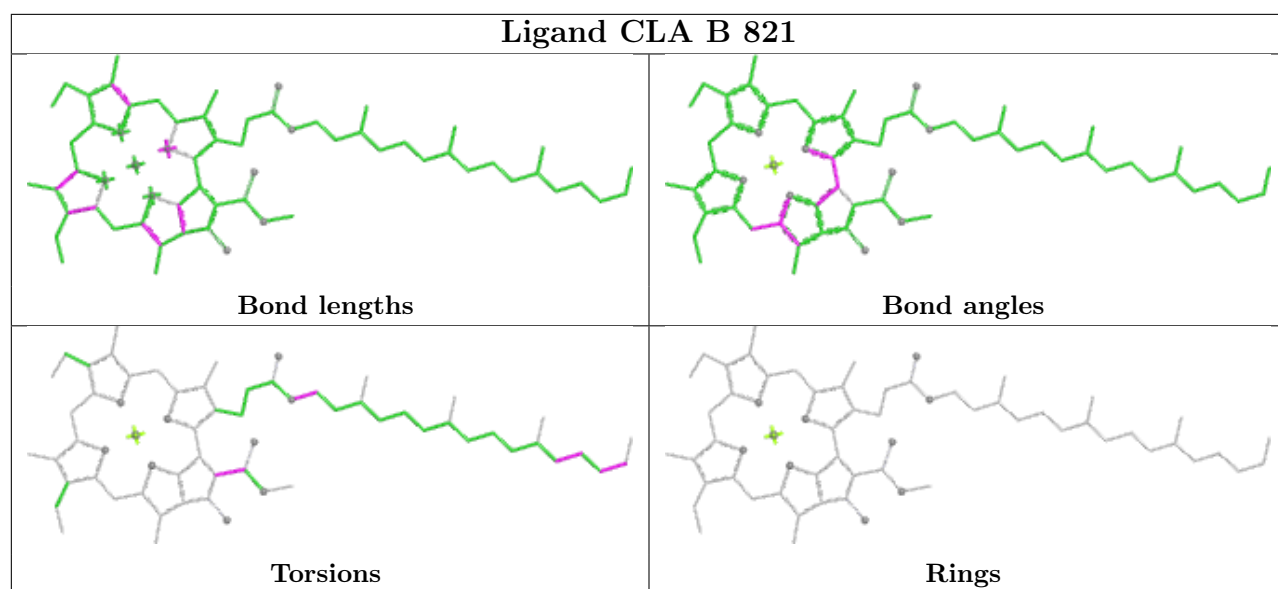
Ligand BCR I 101**Ligand CLA A 804****Ligand CLA B 810**

Ligand CLA A 813

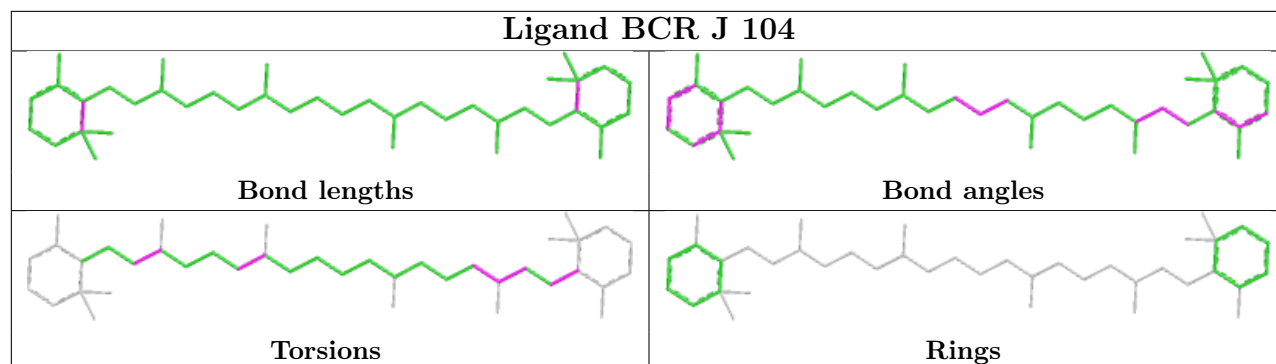


Ligand CLA A 810

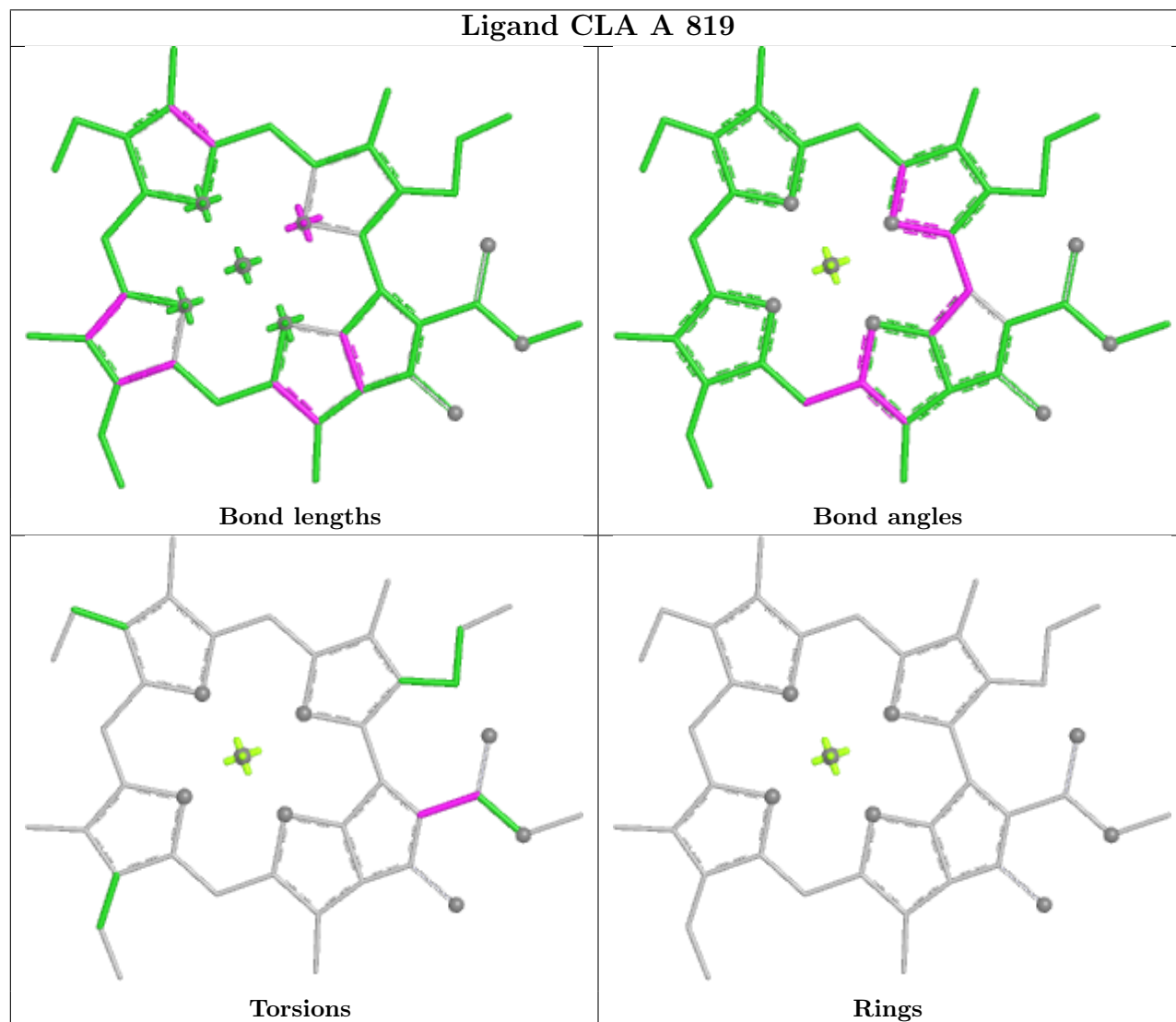


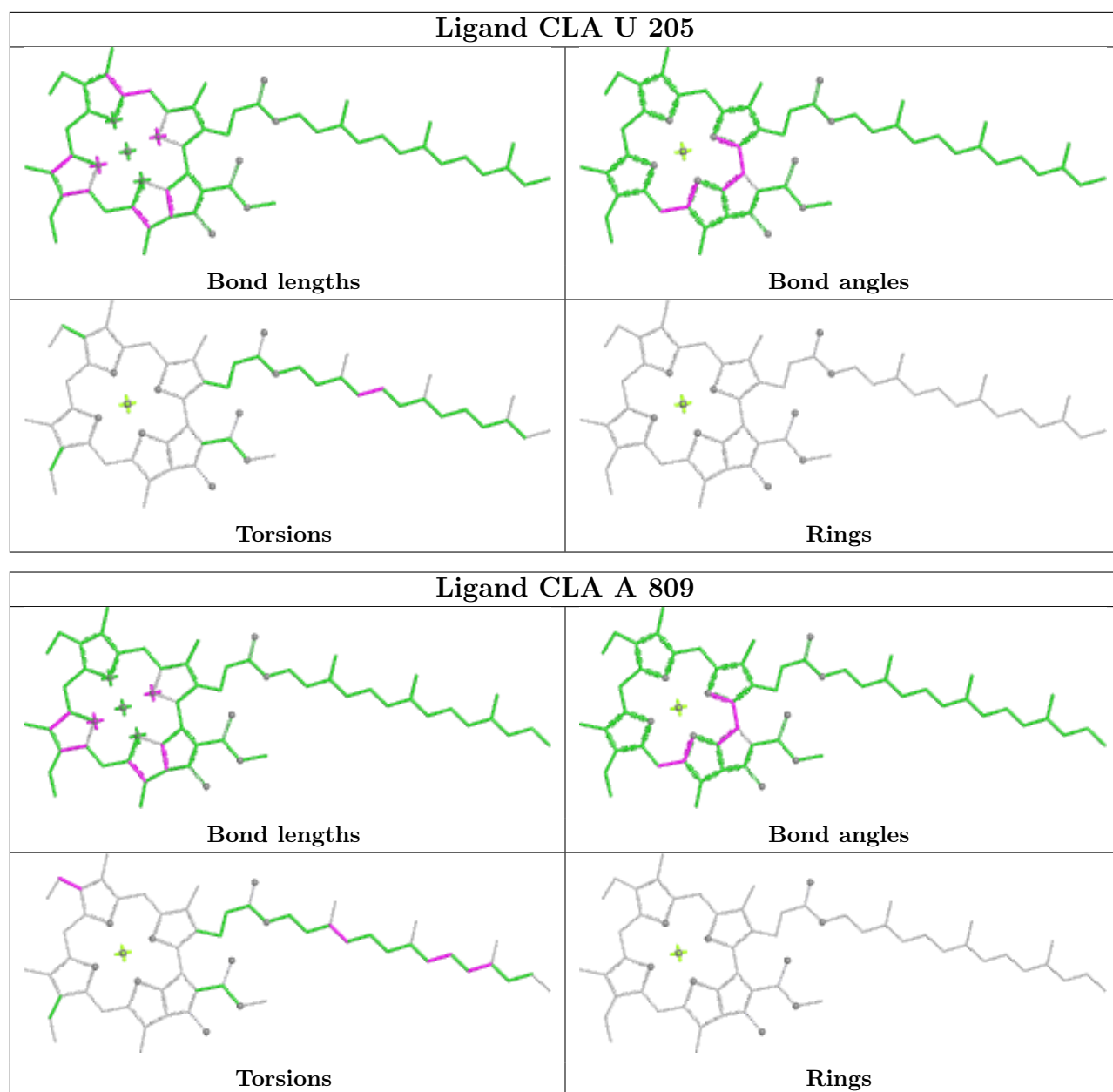


Ligand BCR J 104

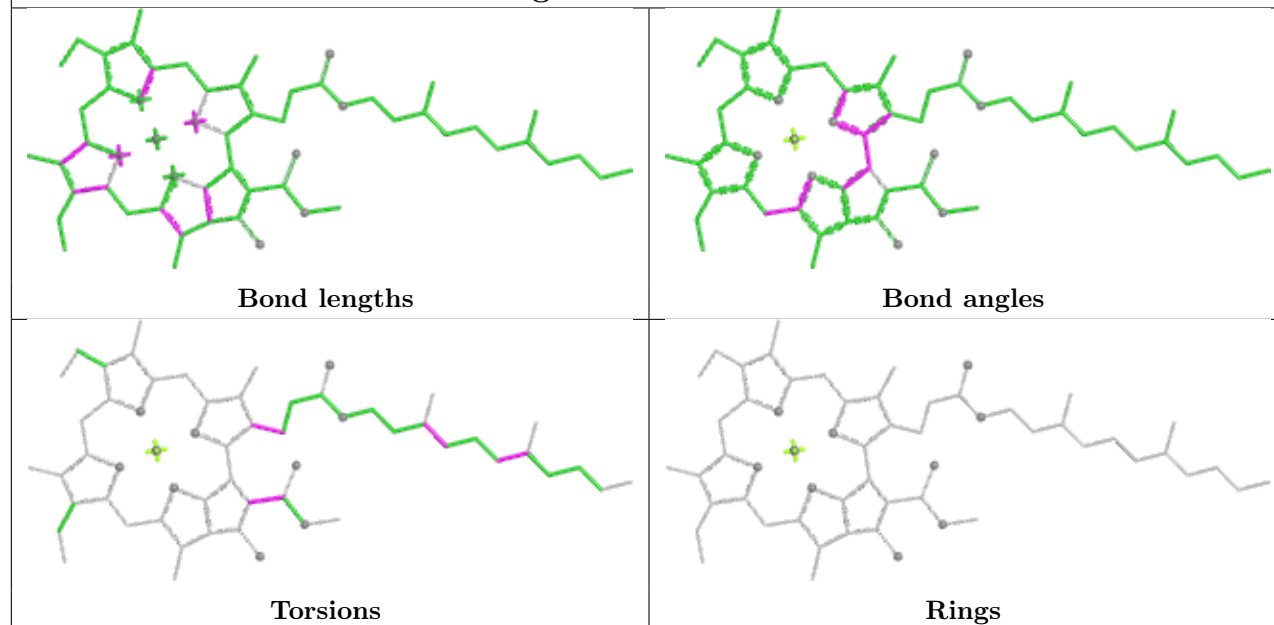


Ligand CLA A 819

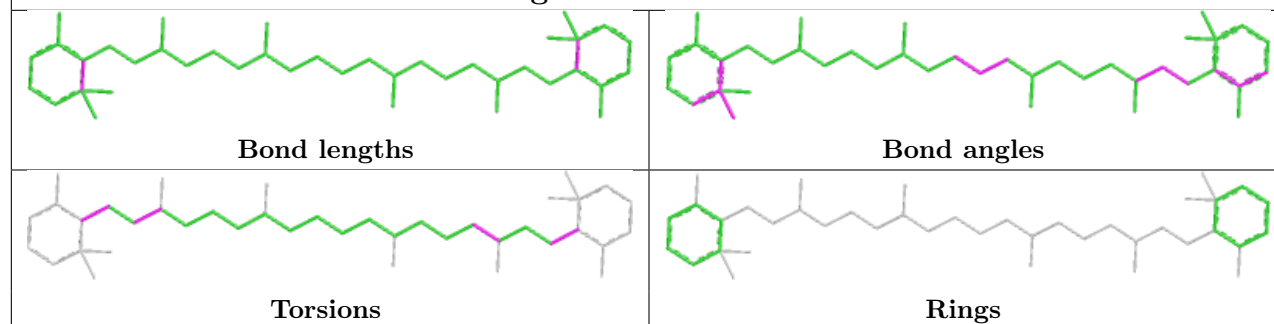




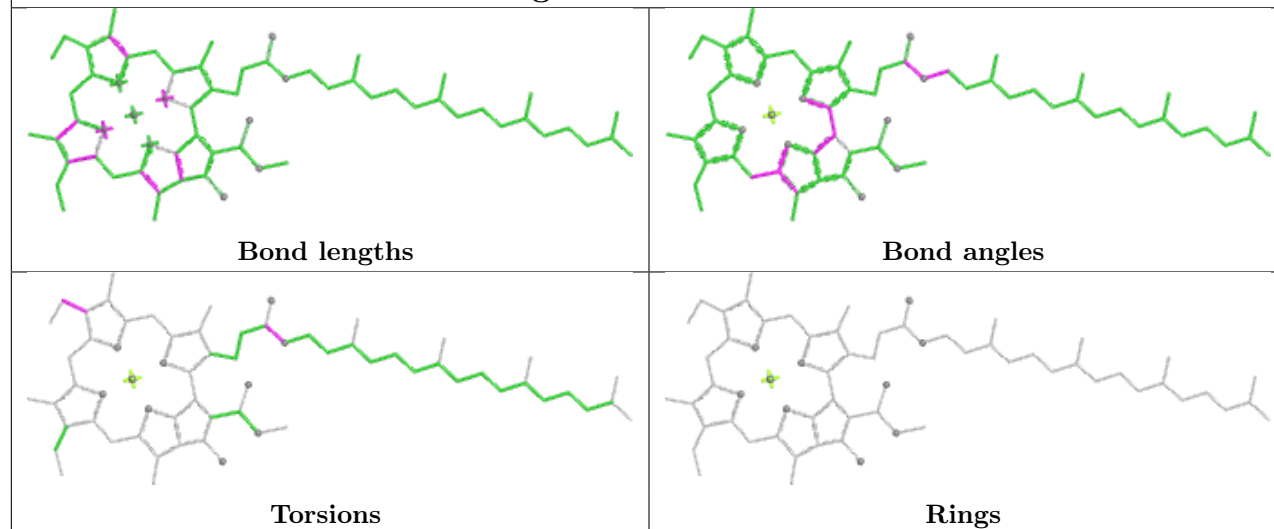
Ligand CLA B 828

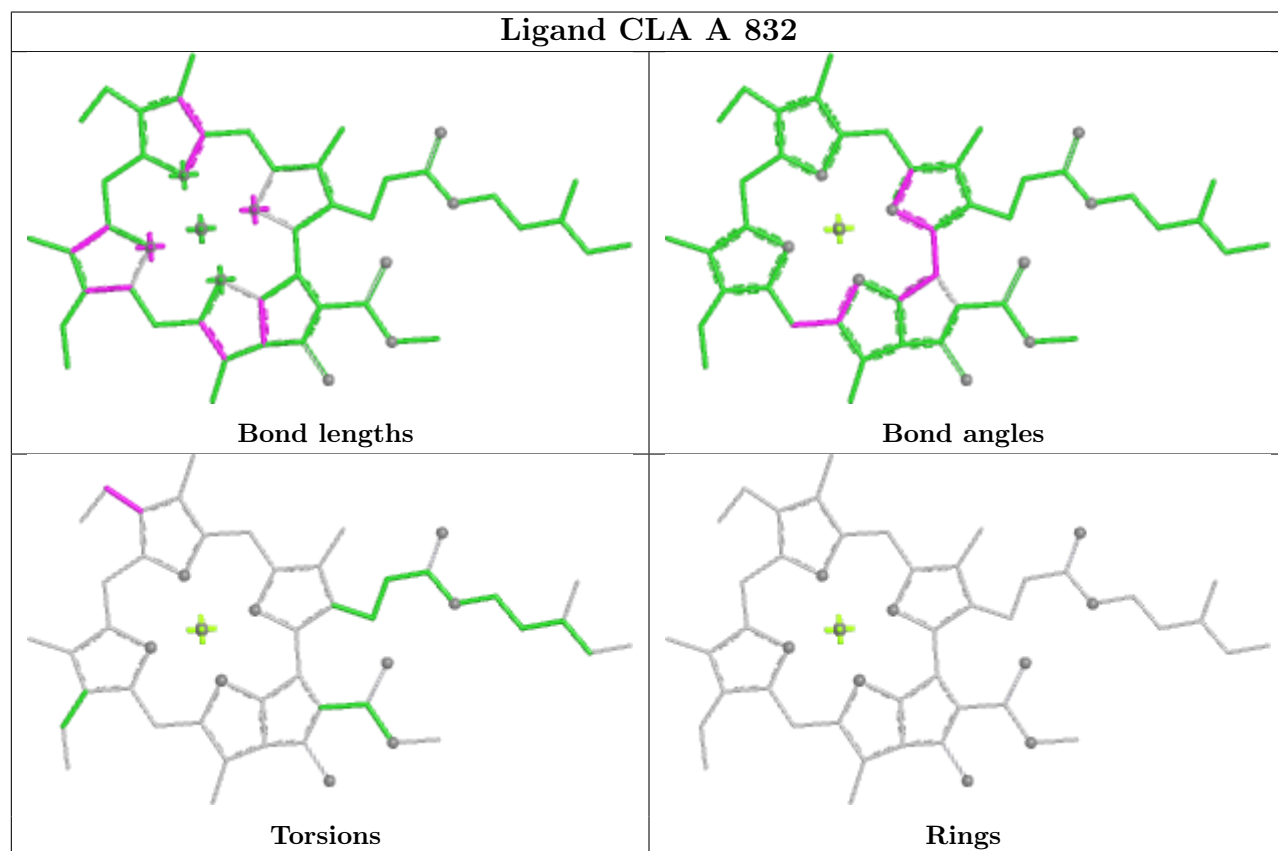
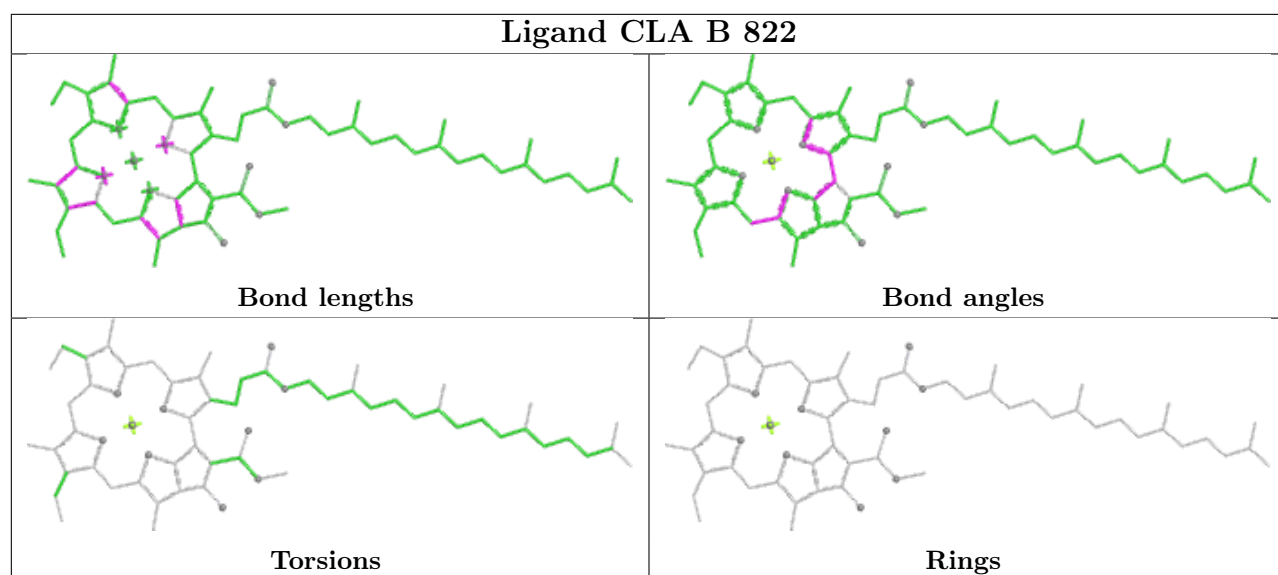


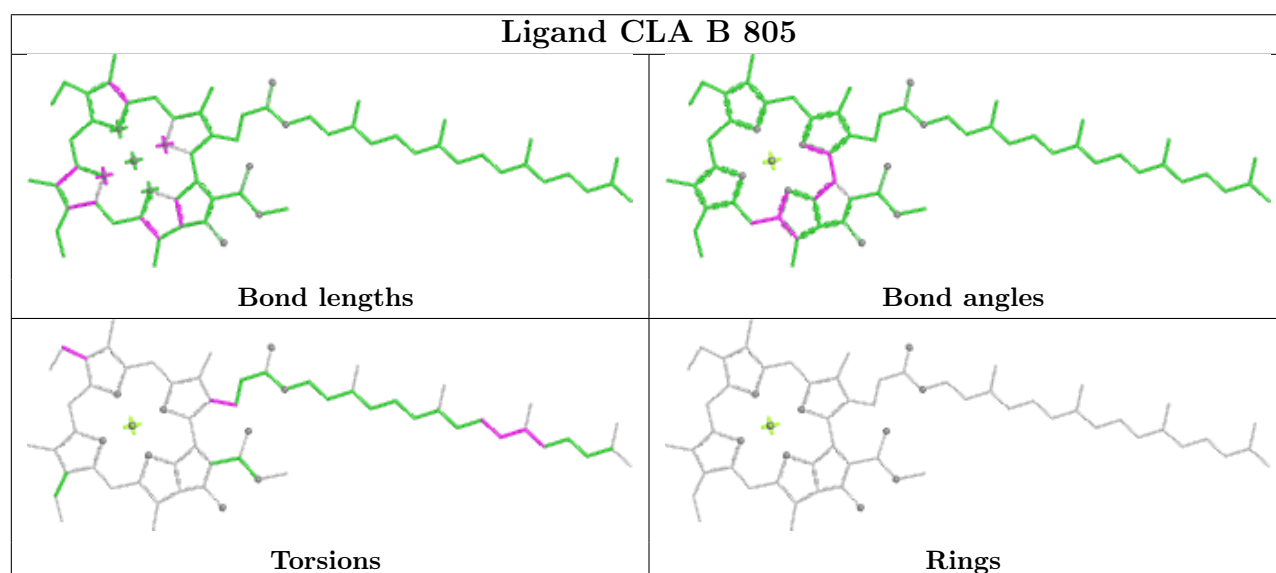
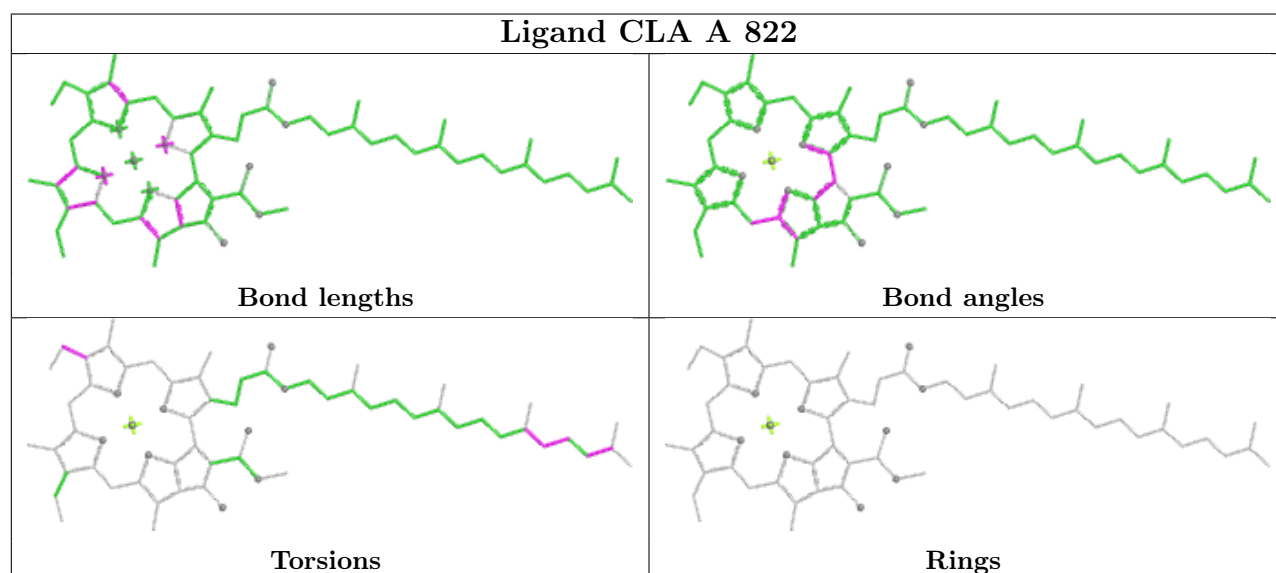
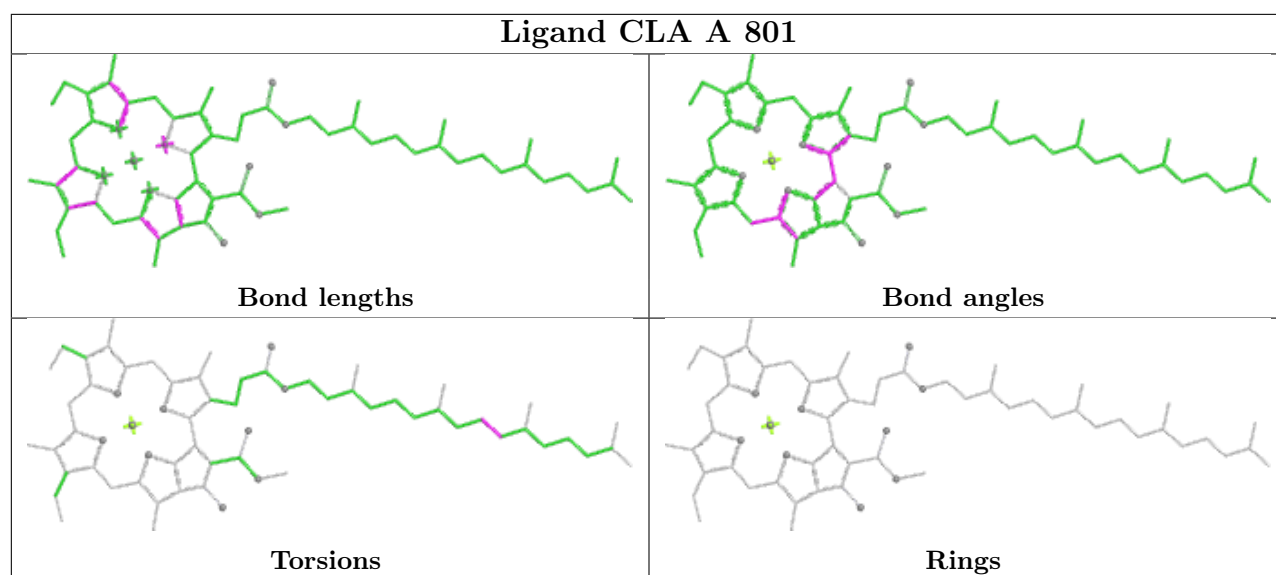
Ligand BCR B 839



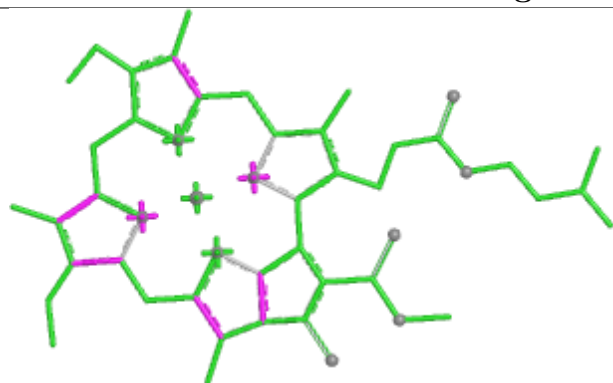
Ligand CLA B 824



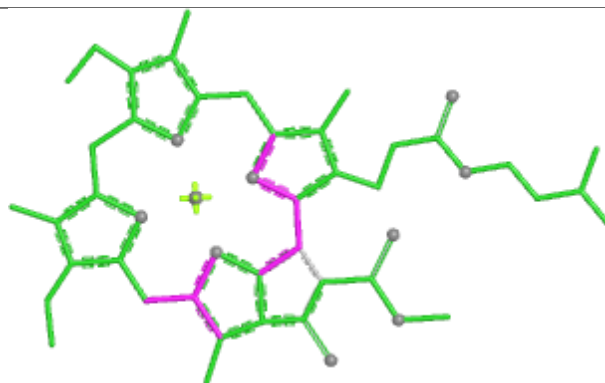




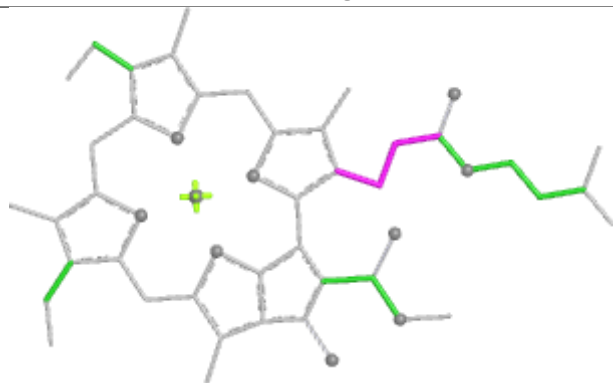
Ligand CLA B 847



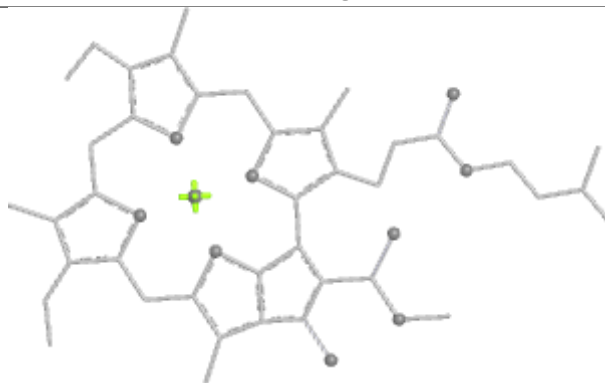
Bond lengths



Bond angles

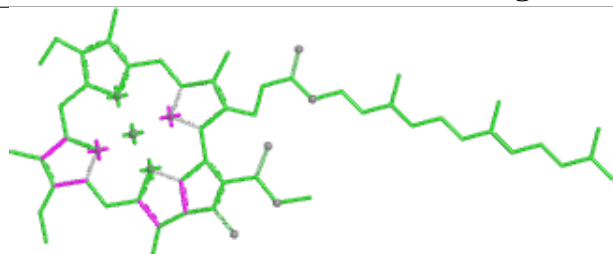


Torsions

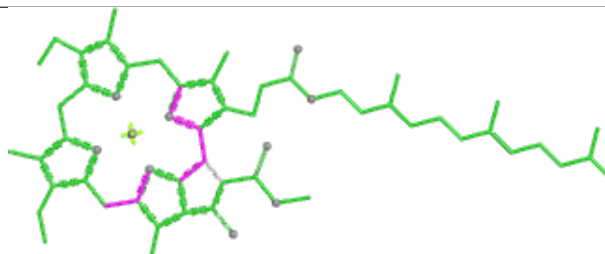


Rings

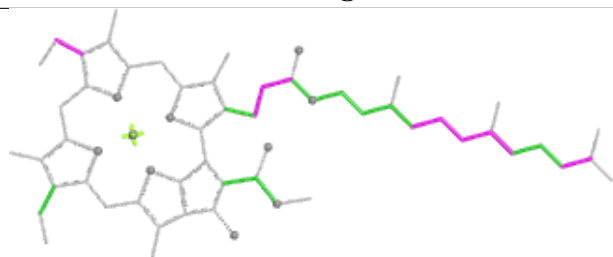
Ligand CLA A 845



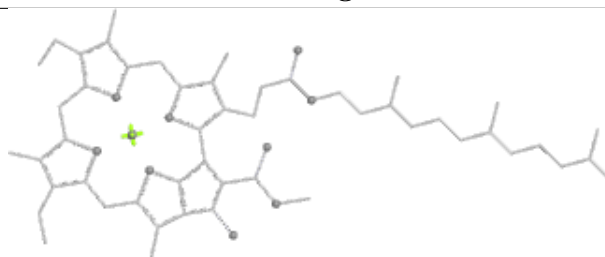
Bond lengths



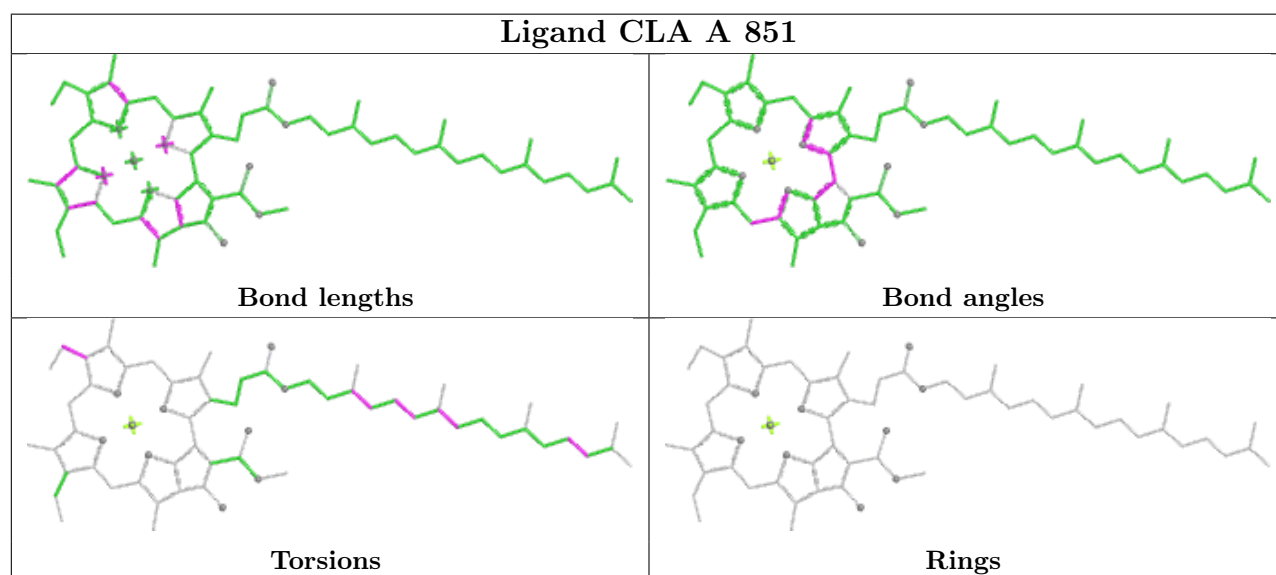
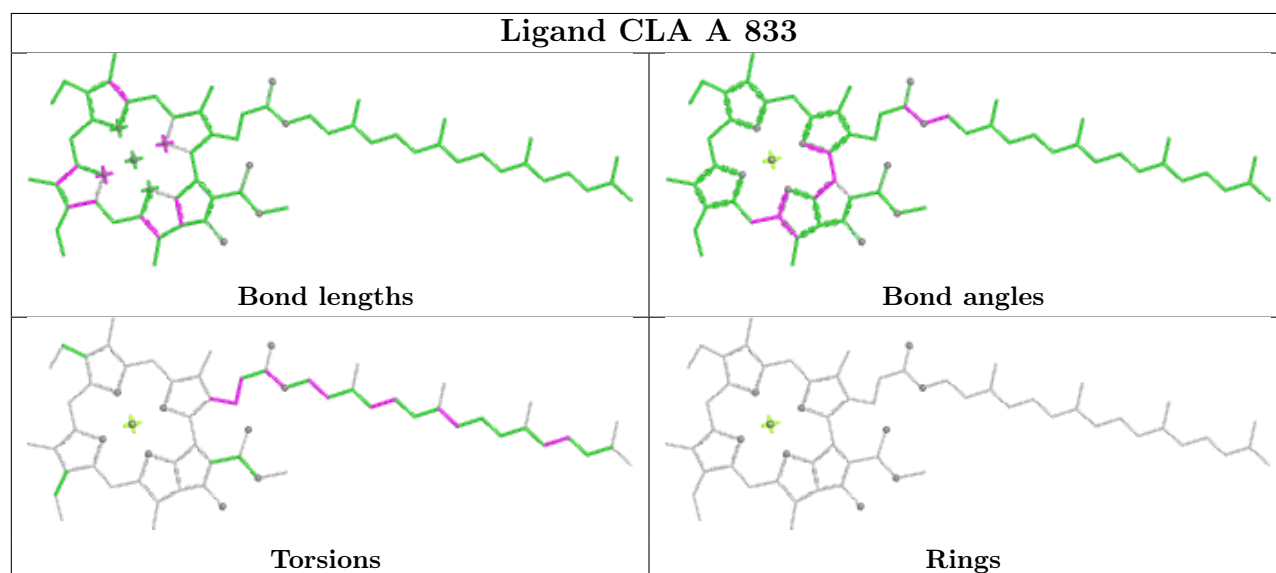
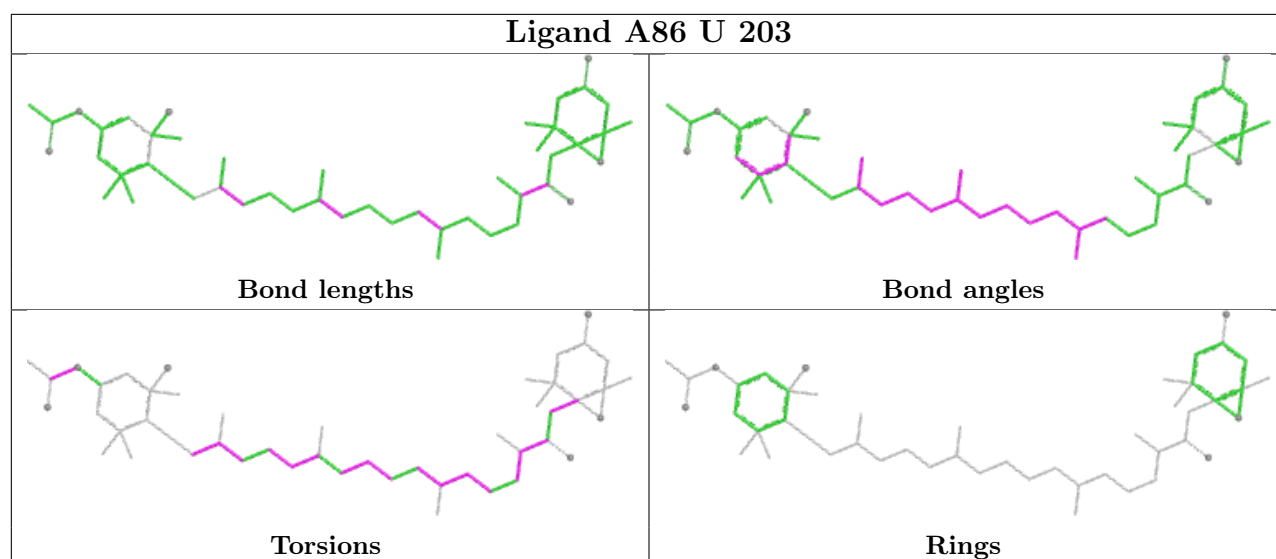
Bond angles

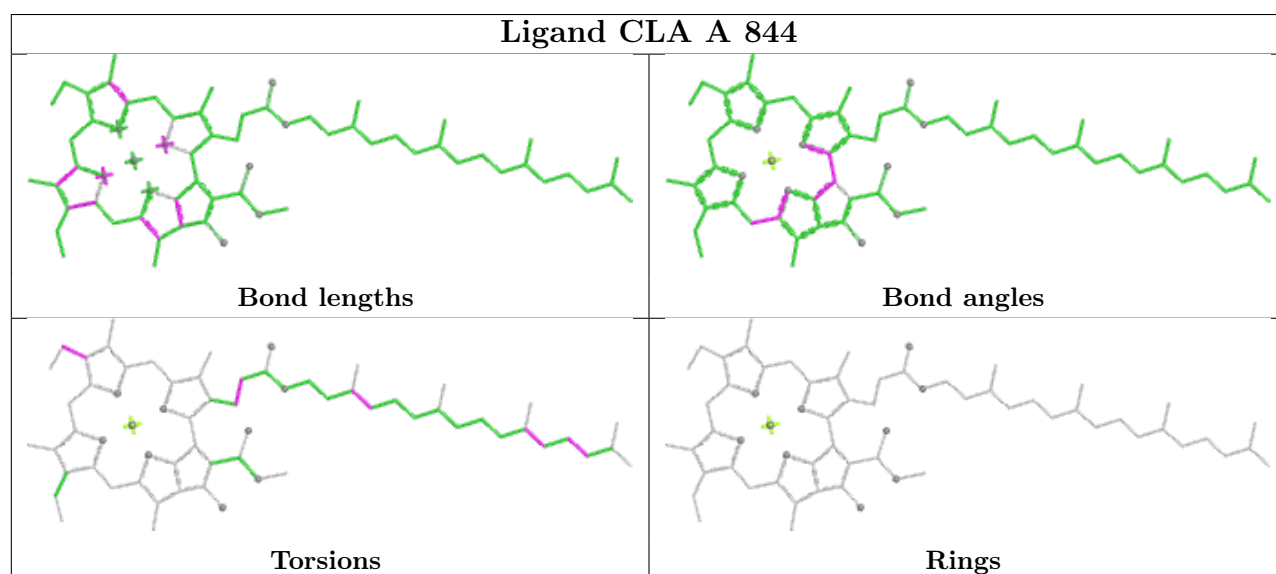
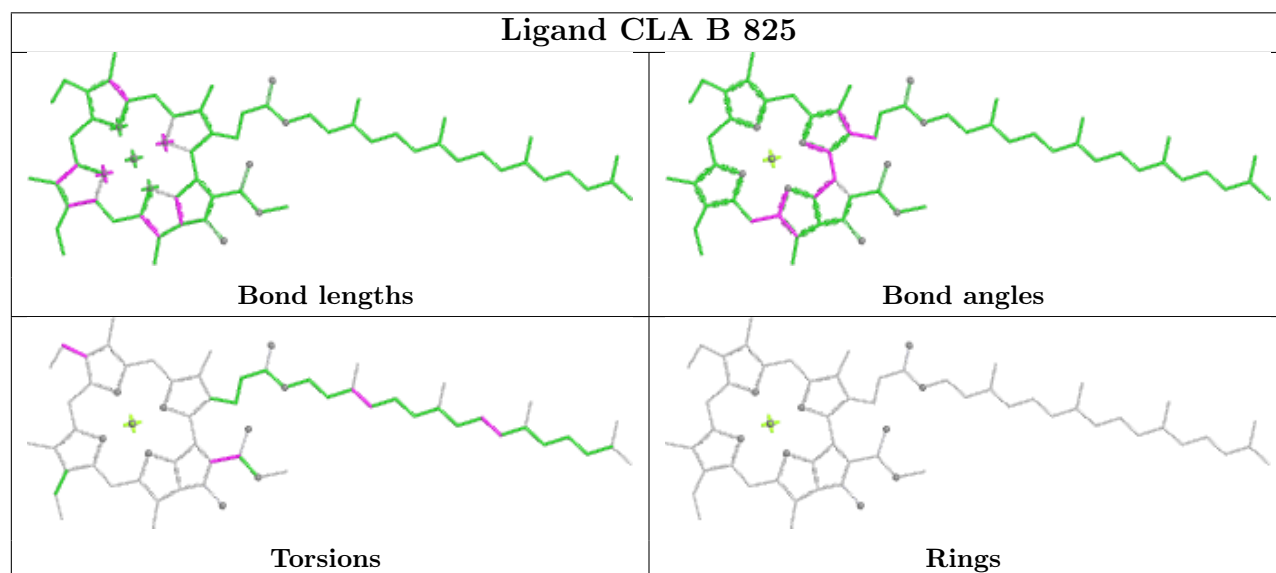
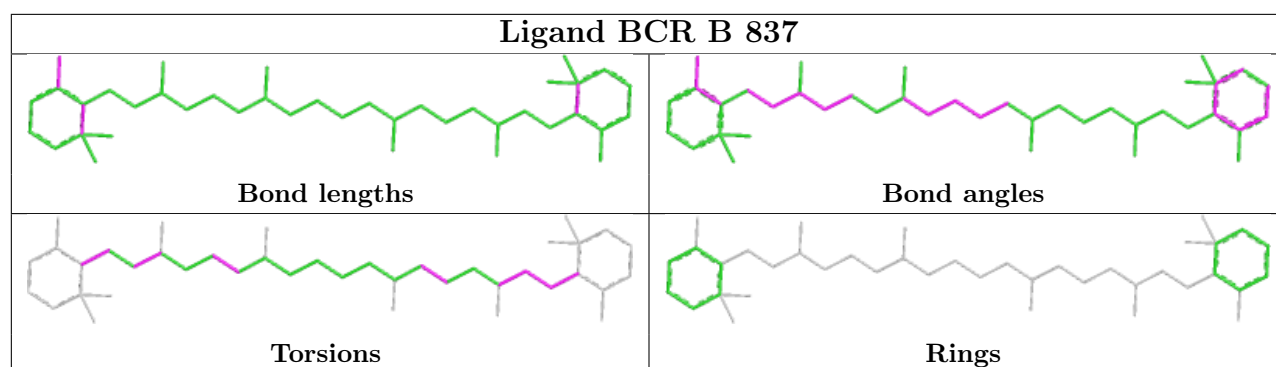


Torsions

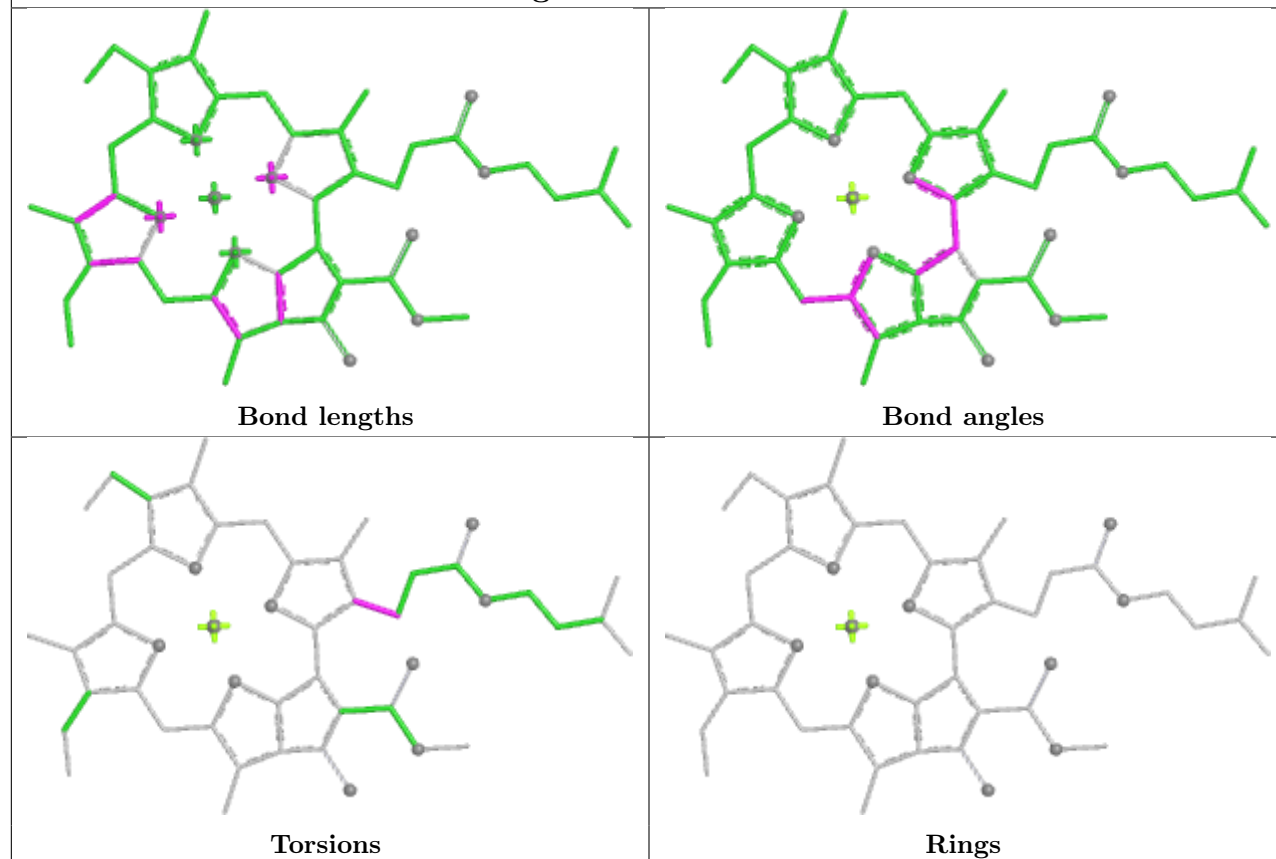


Rings

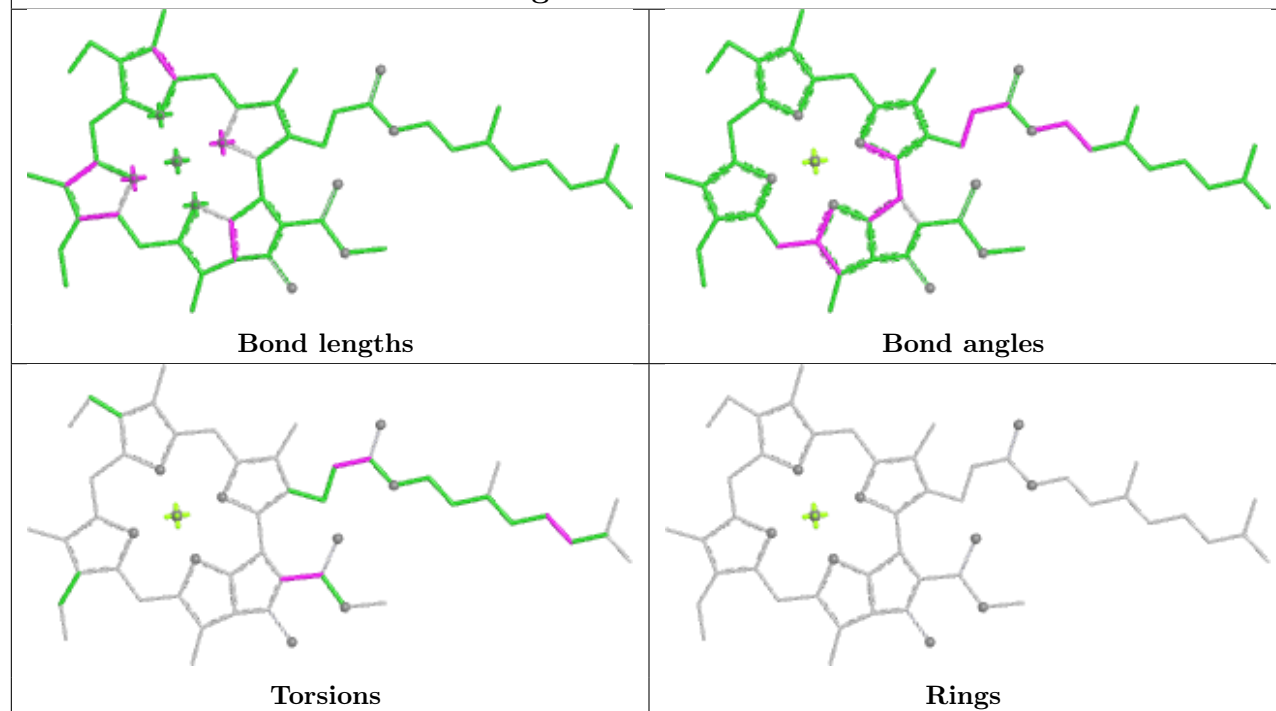


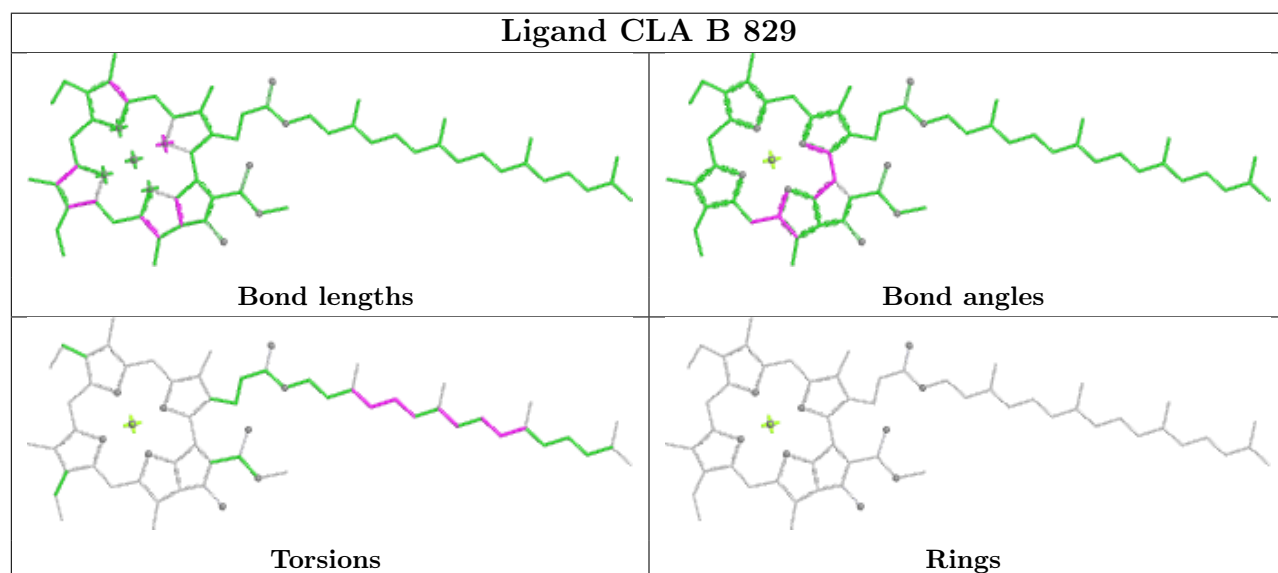
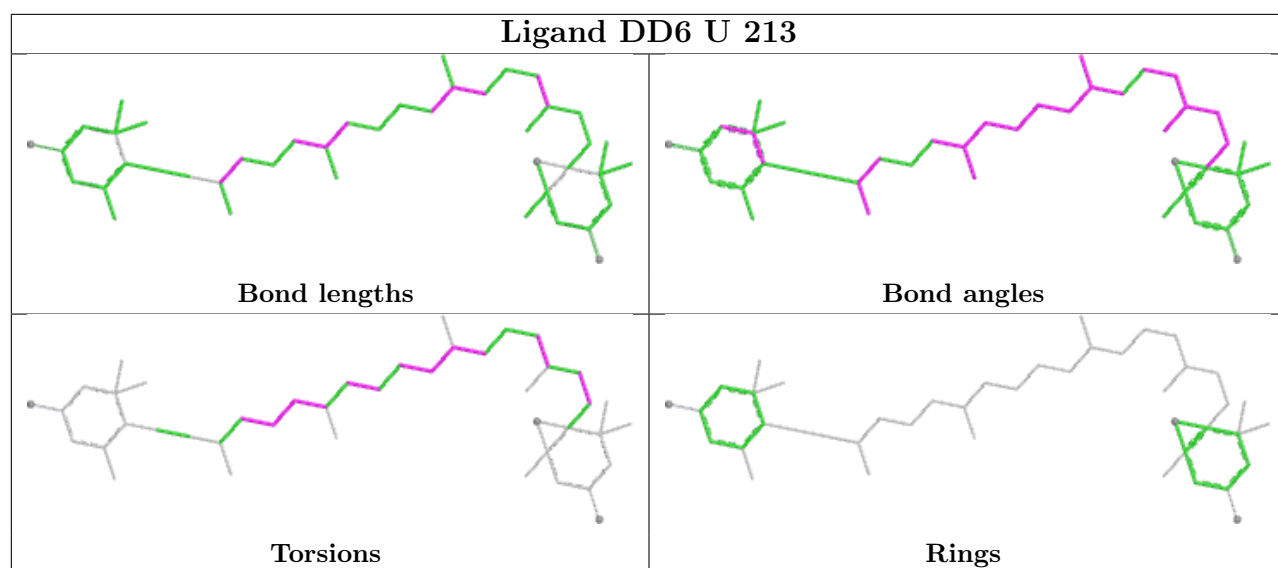


Ligand CLA B 826

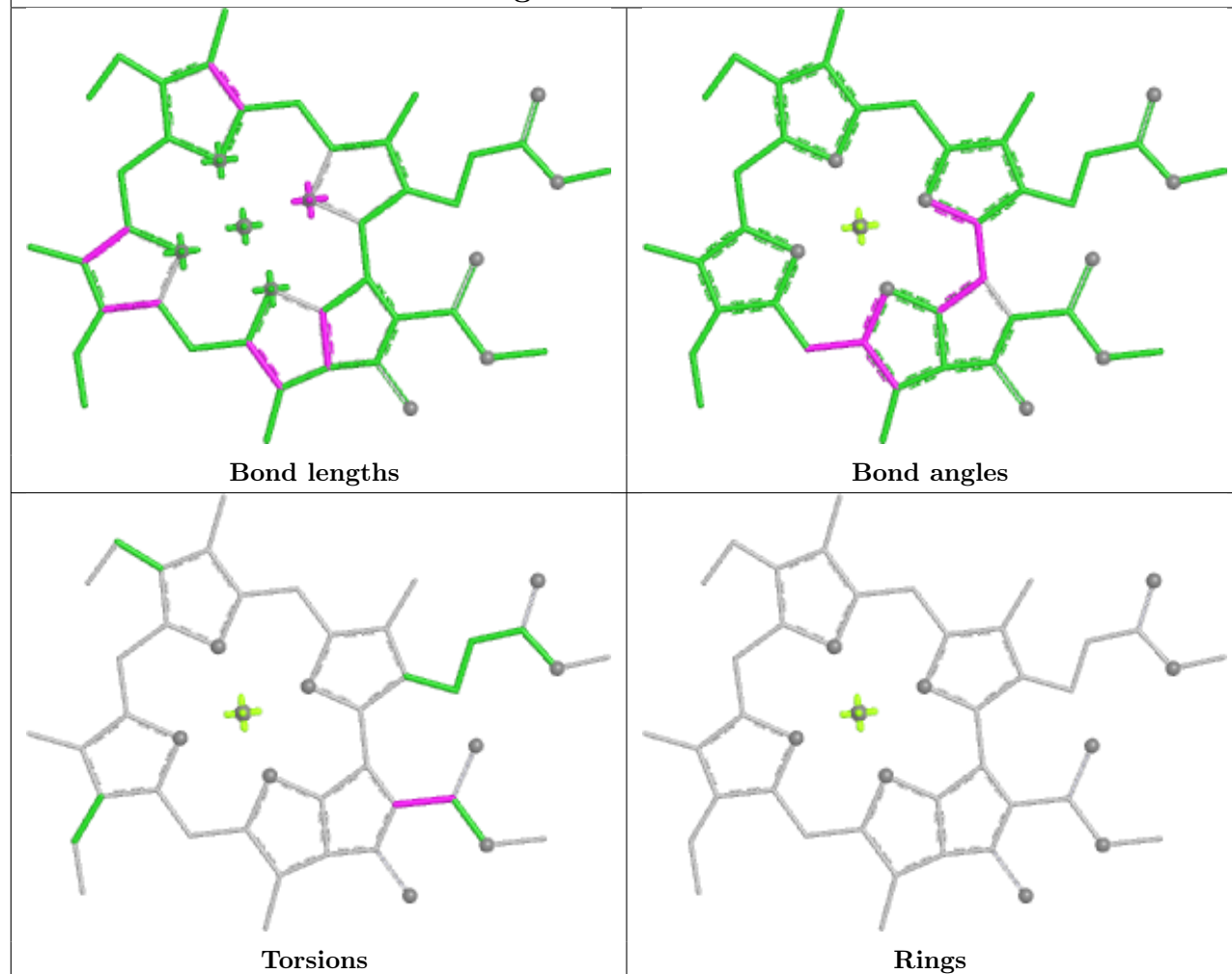


Ligand CLA A 802

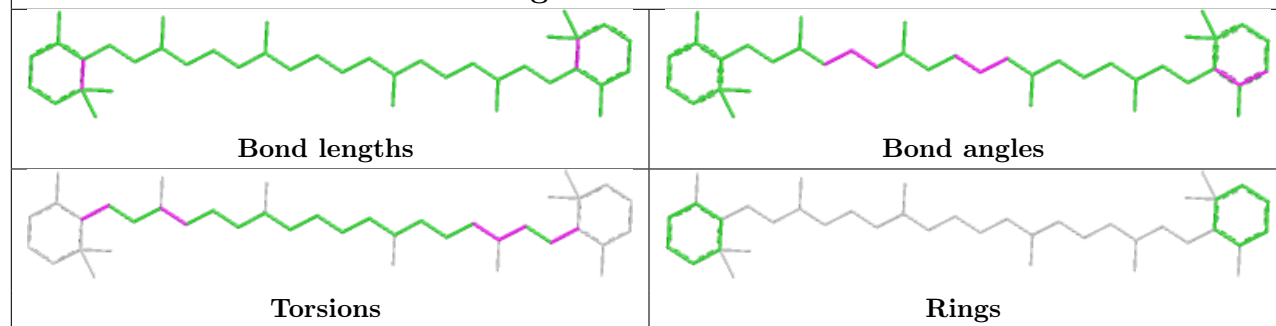


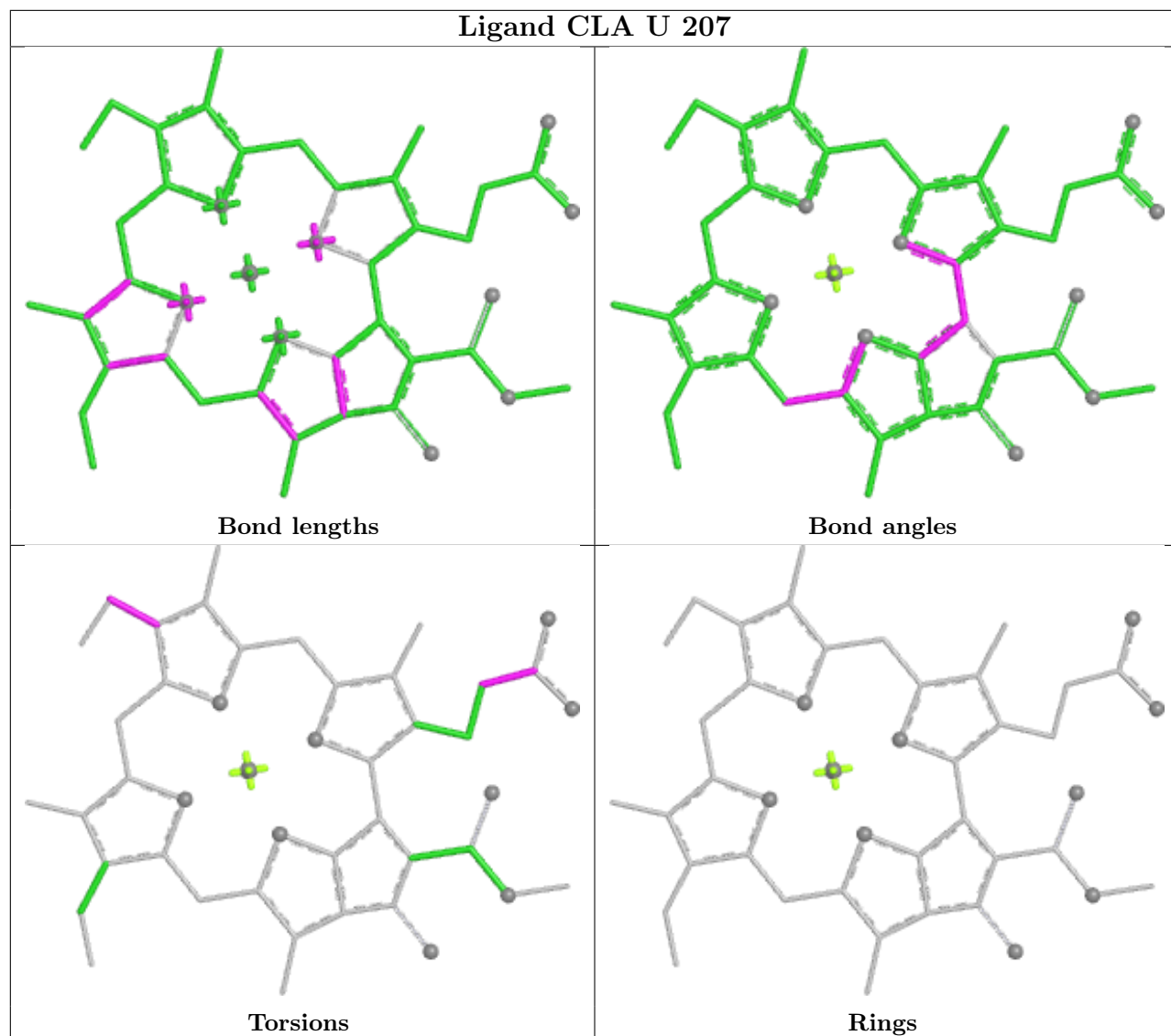


Ligand CLA B 818

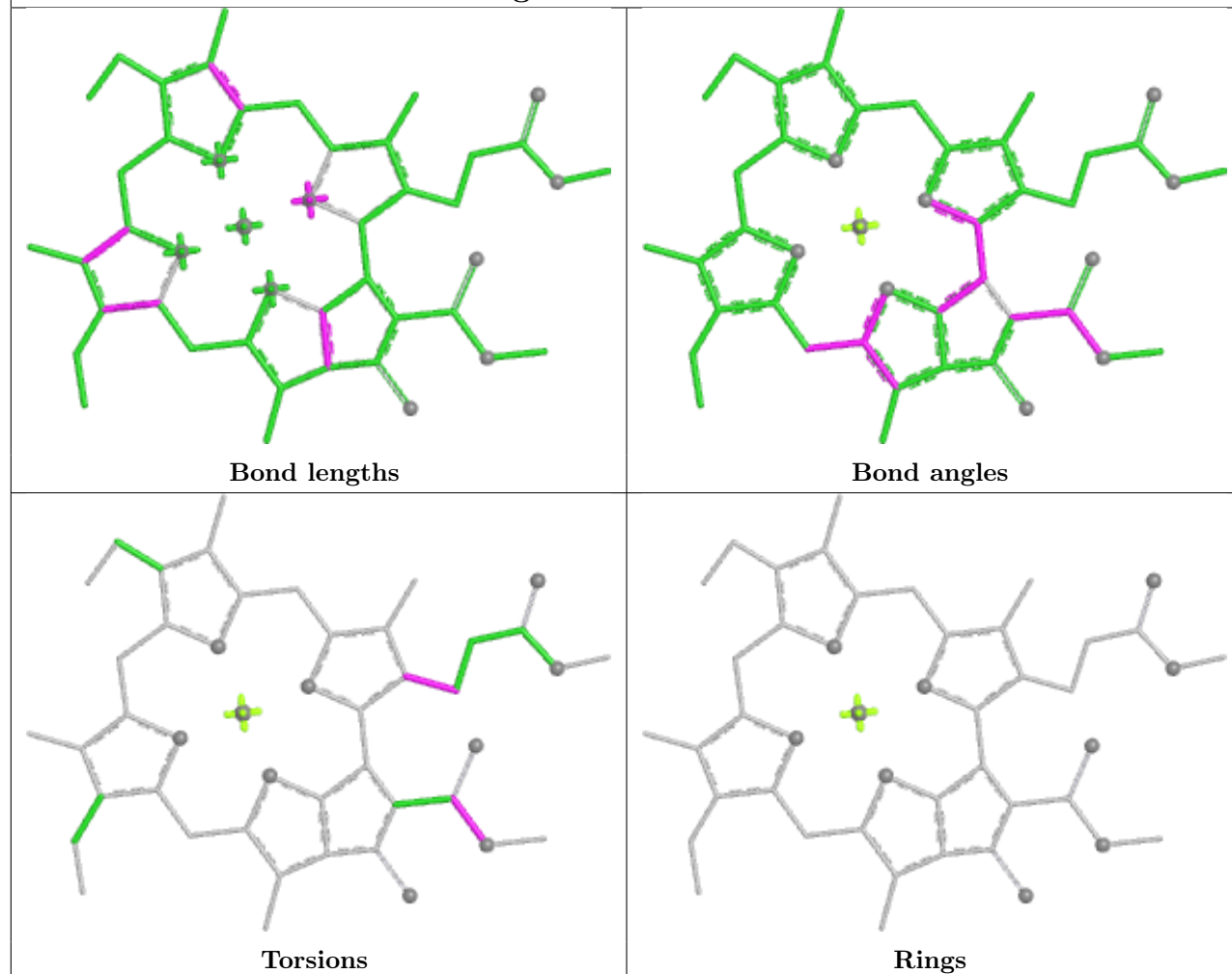


Ligand BCR B 841

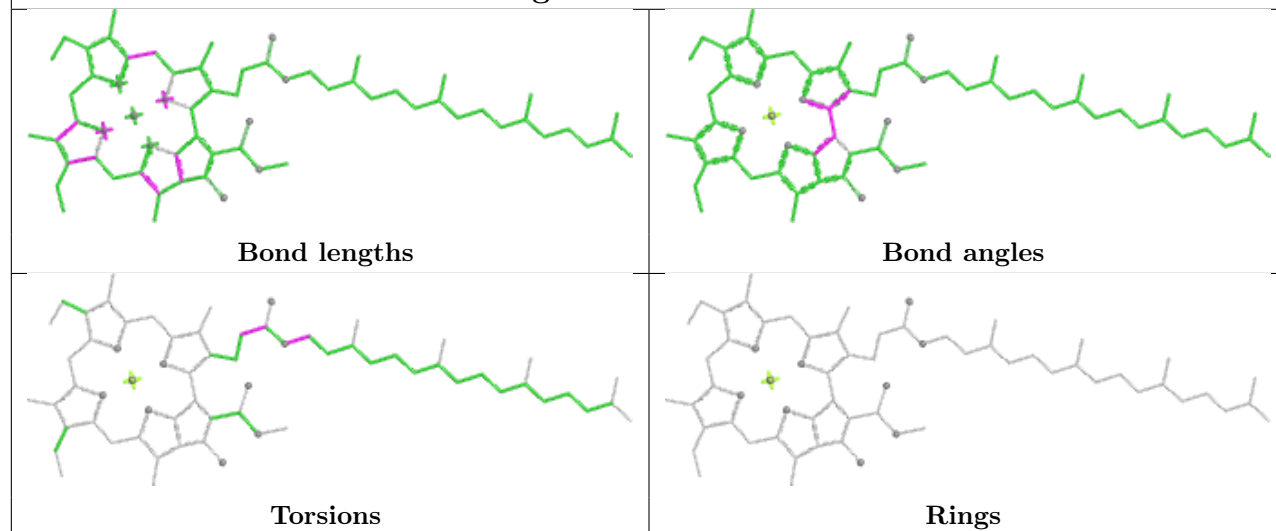


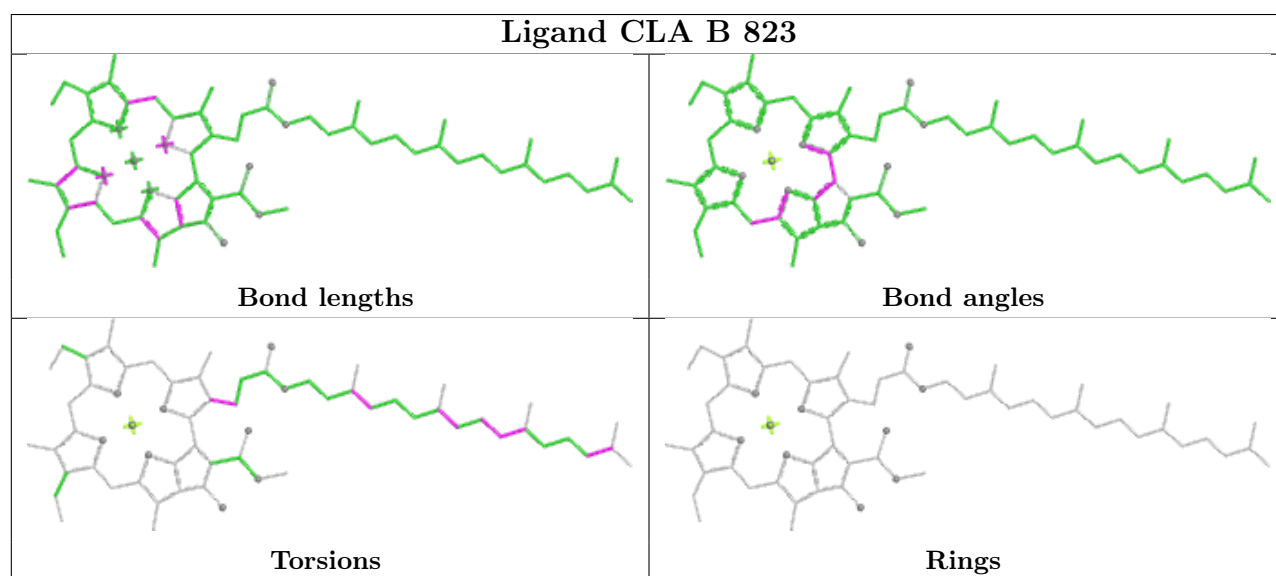
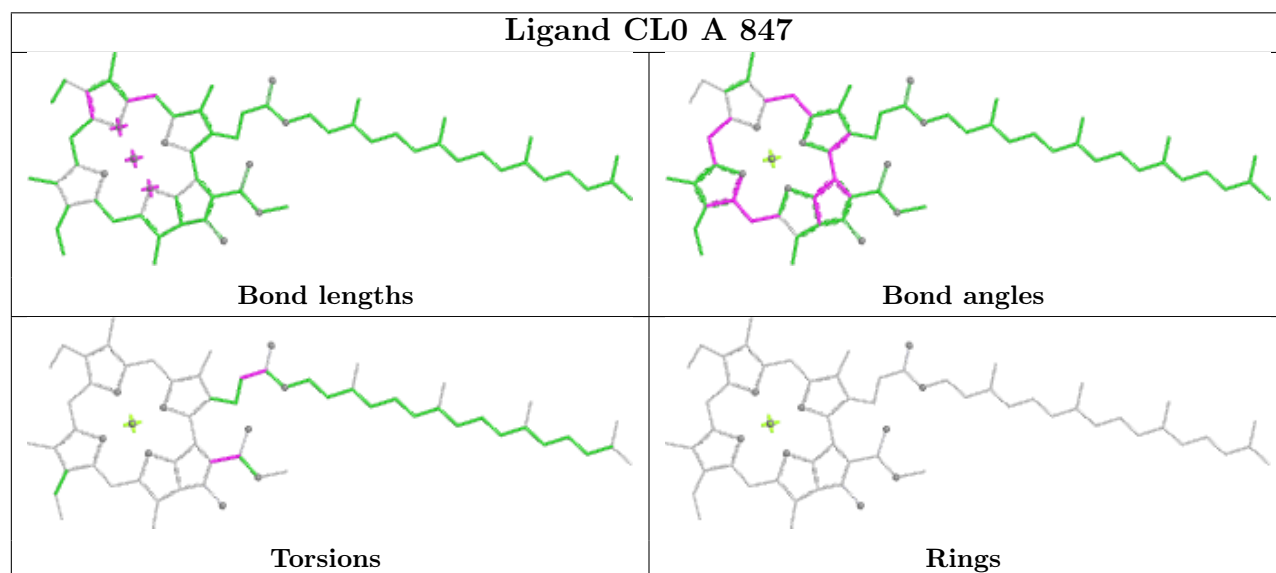
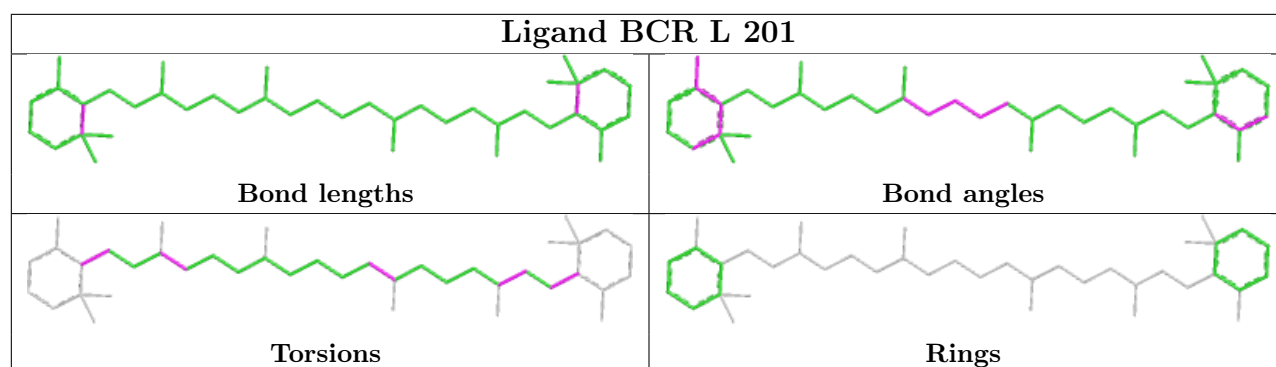


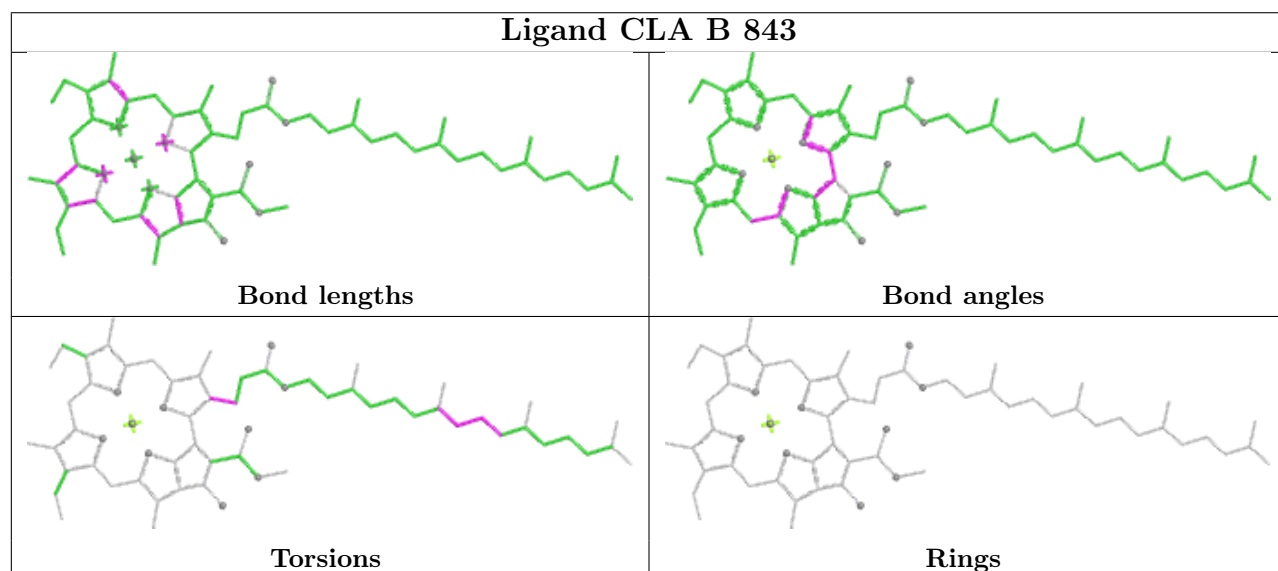
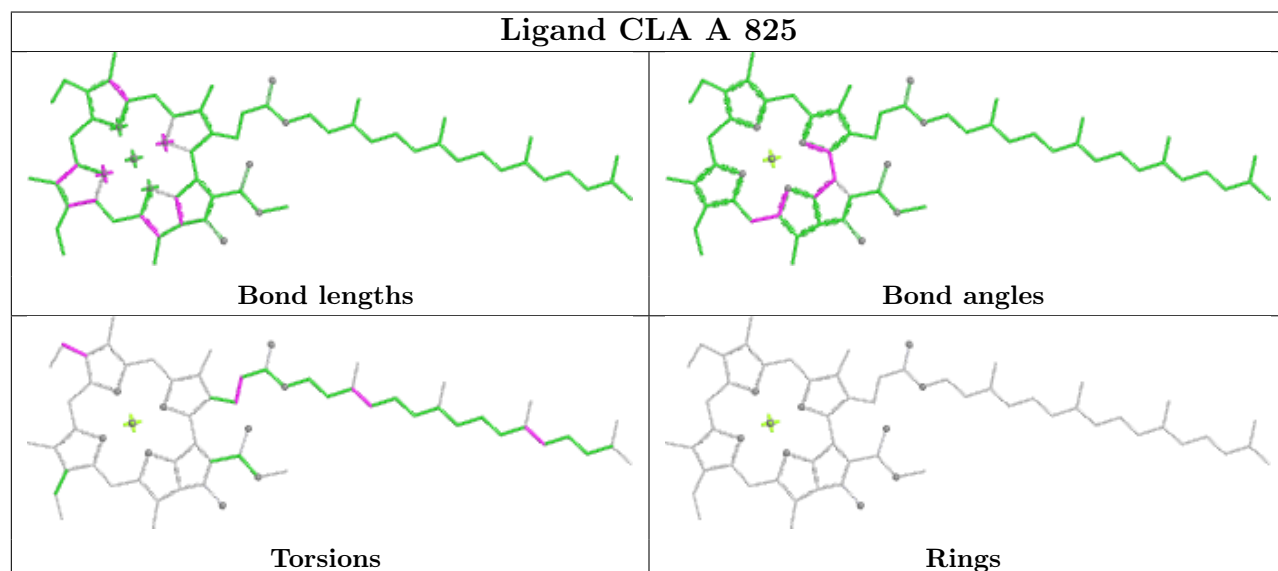
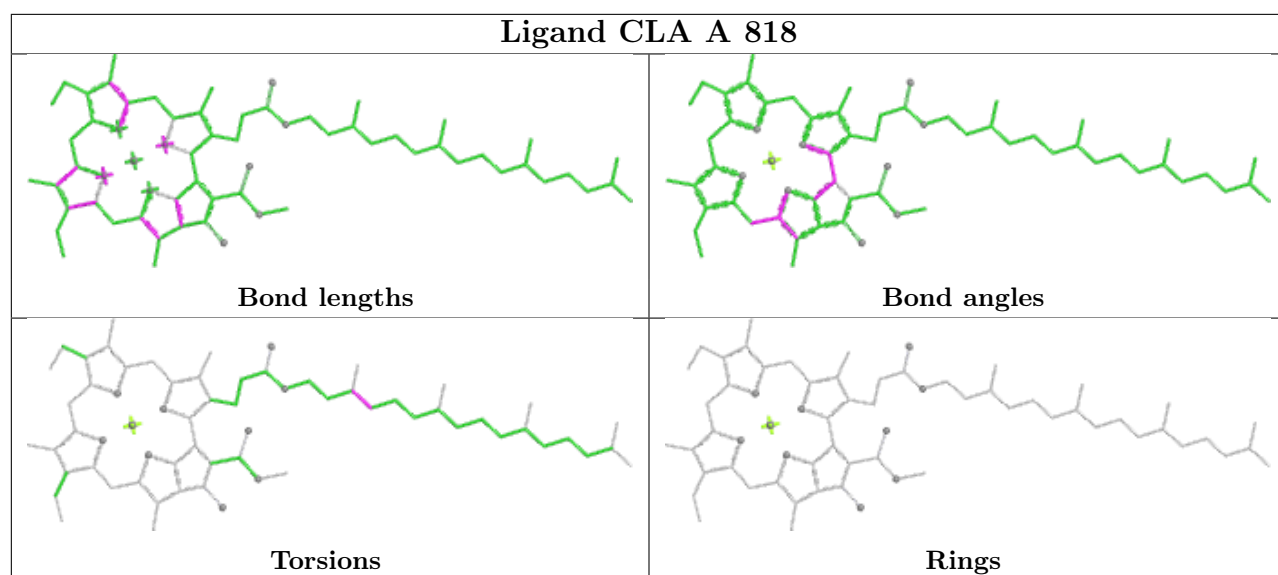
Ligand CLA U 209



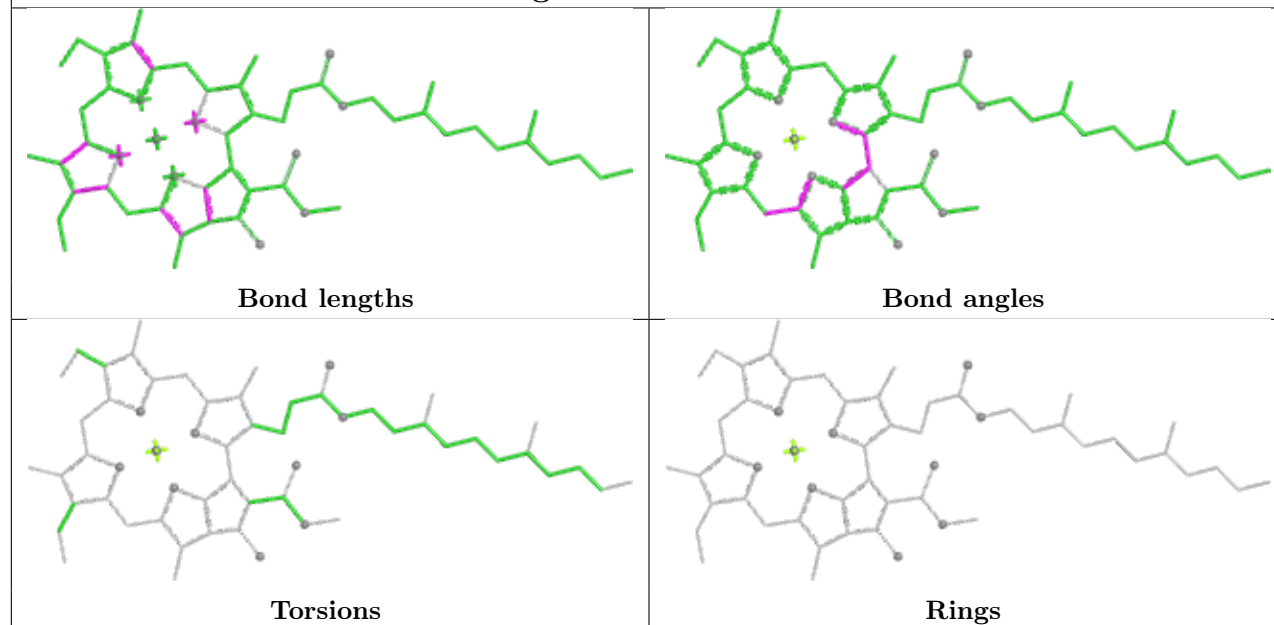
Ligand CLA B 802



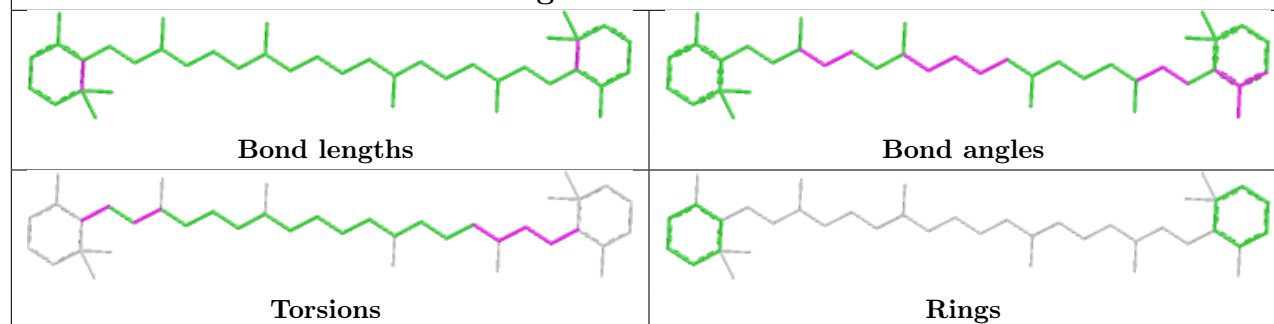




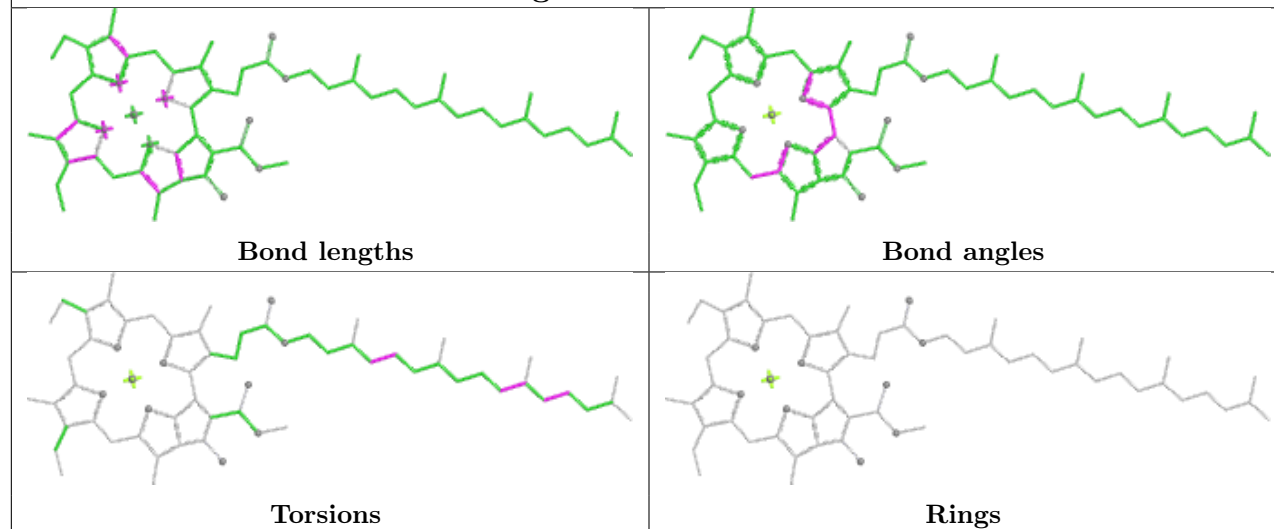
Ligand CLA B 830

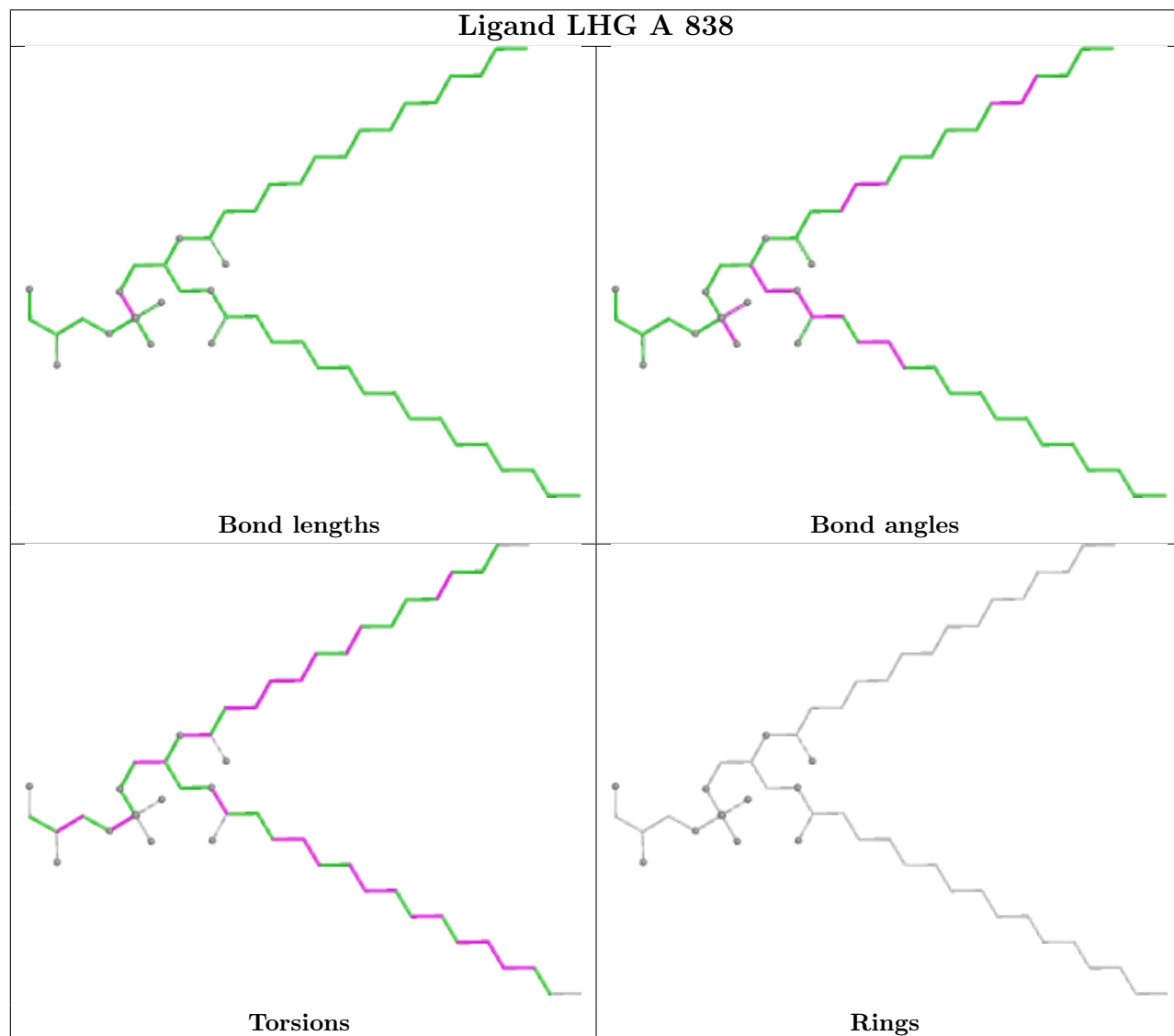
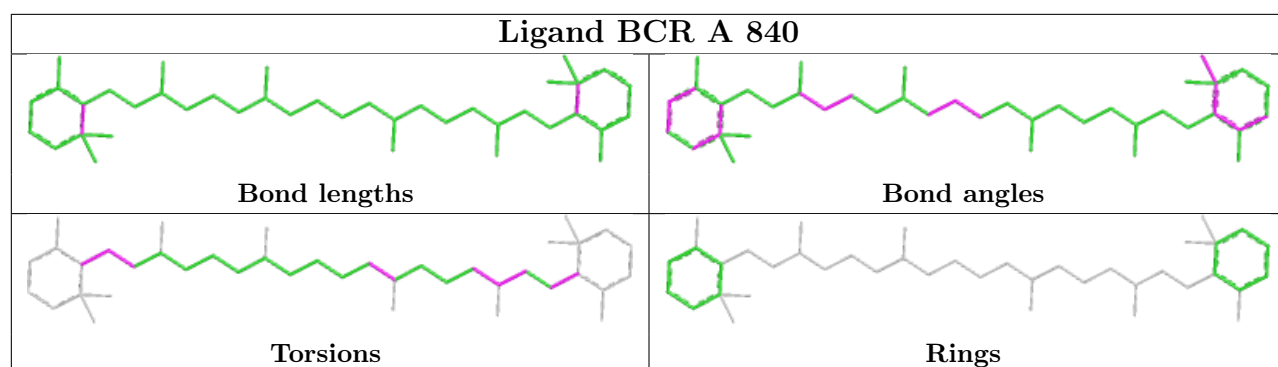


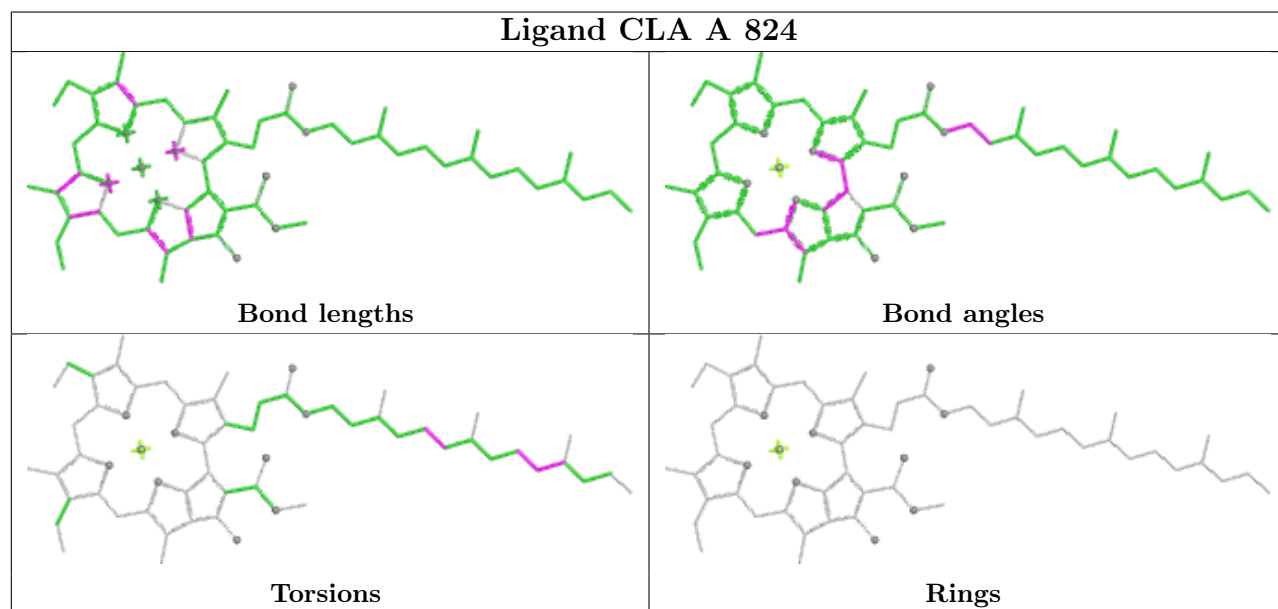
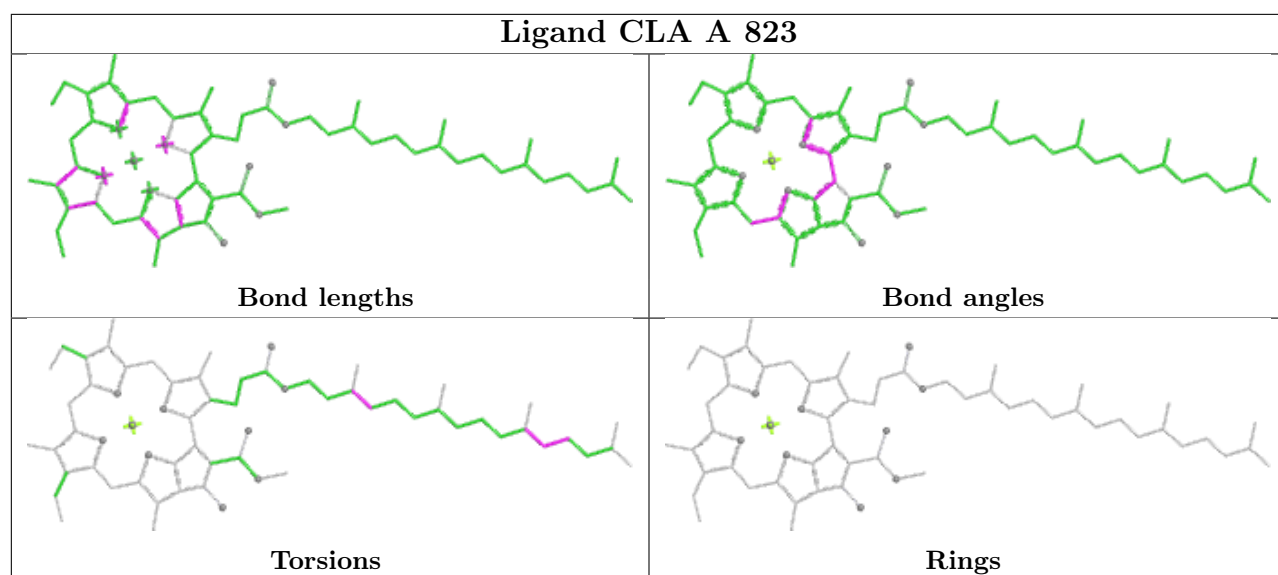
Ligand BCR I 102

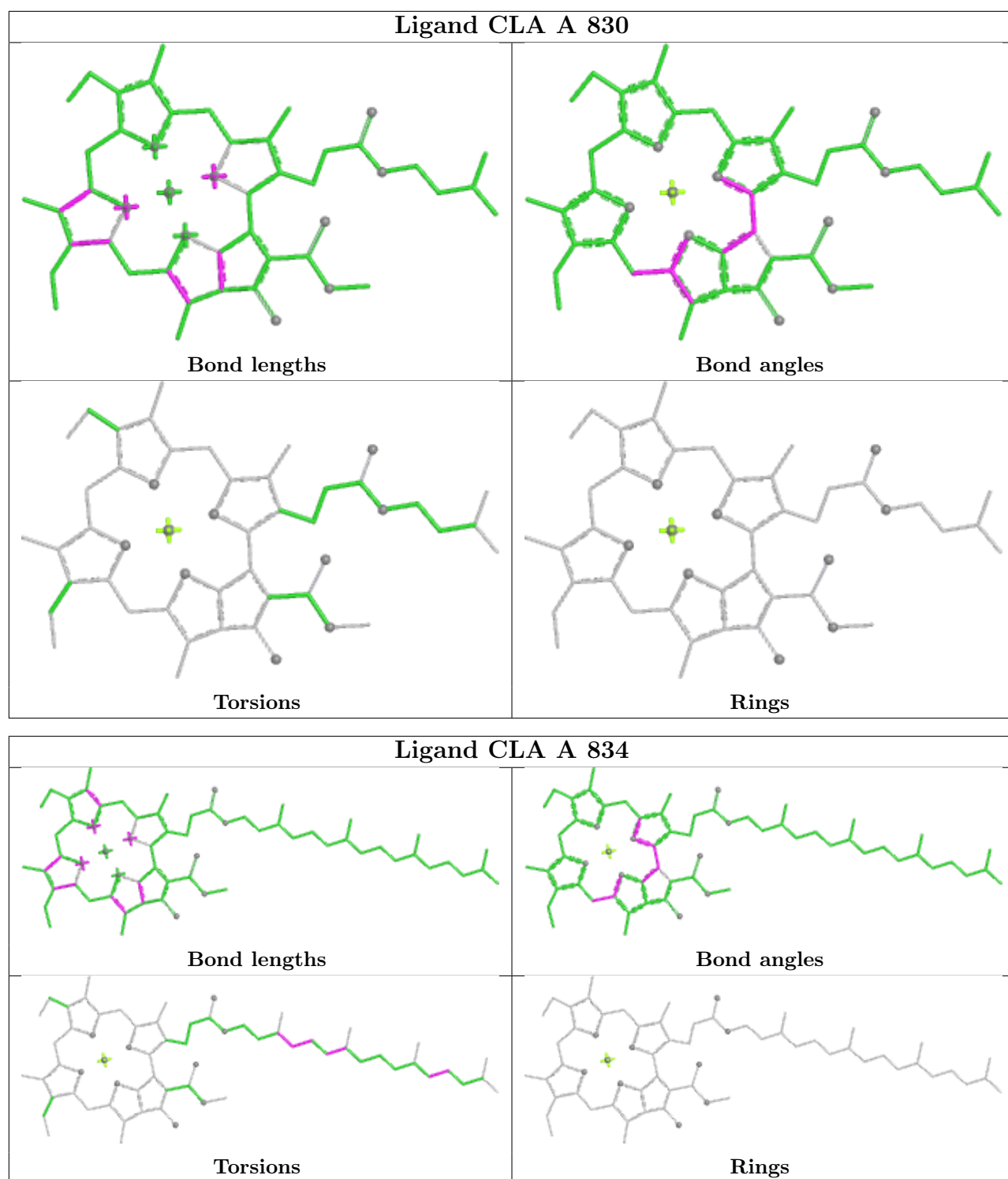


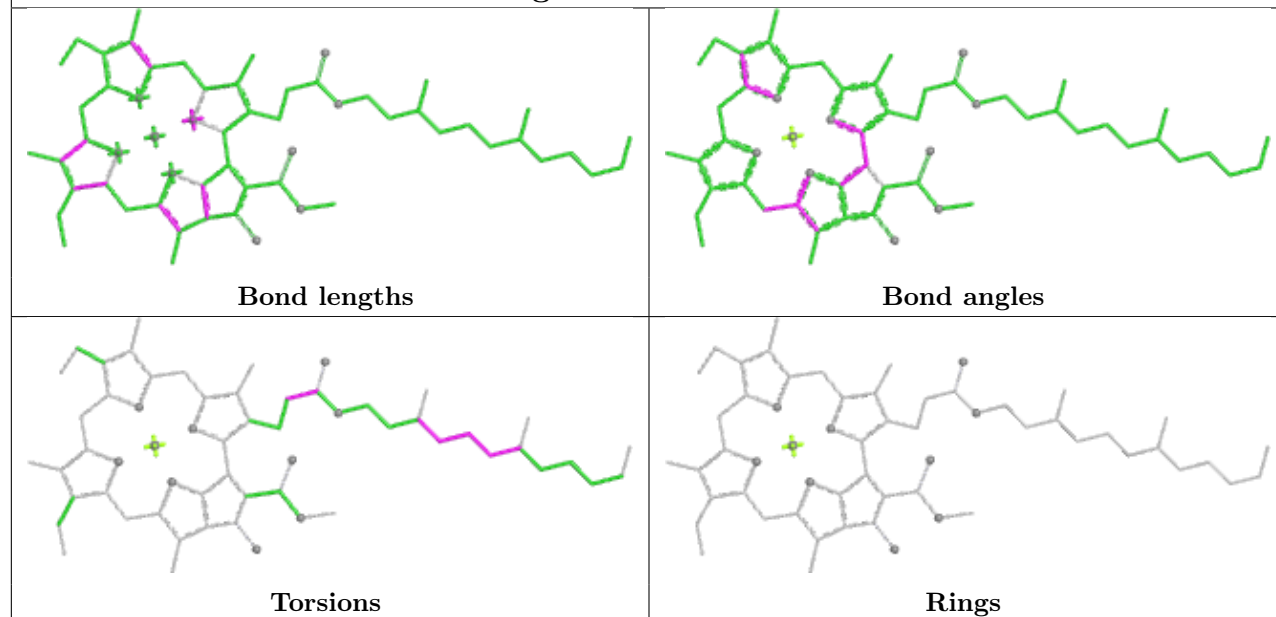
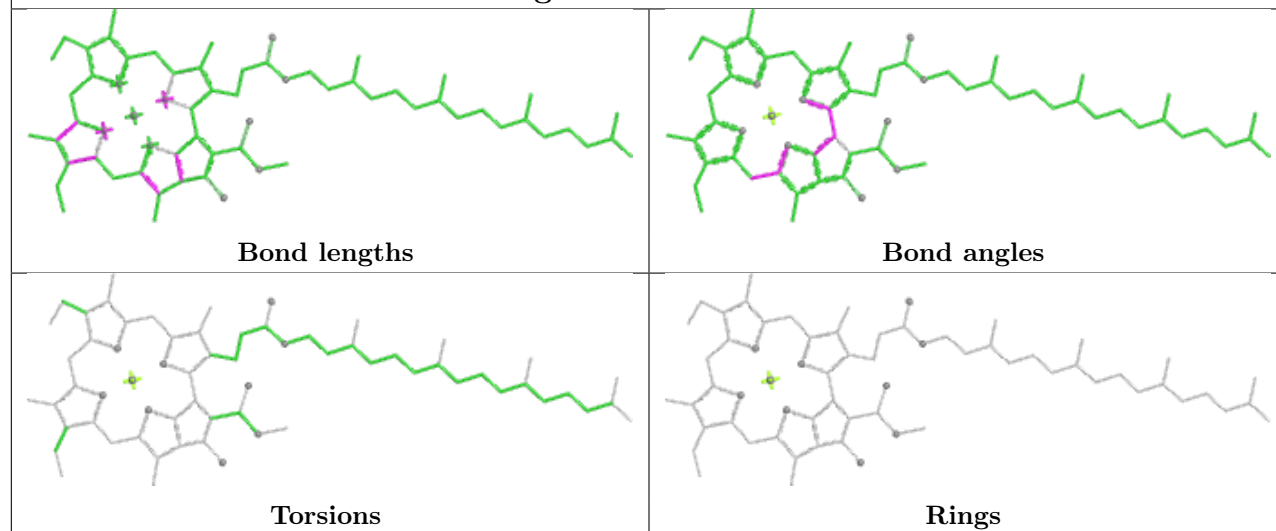
Ligand CLA B 834

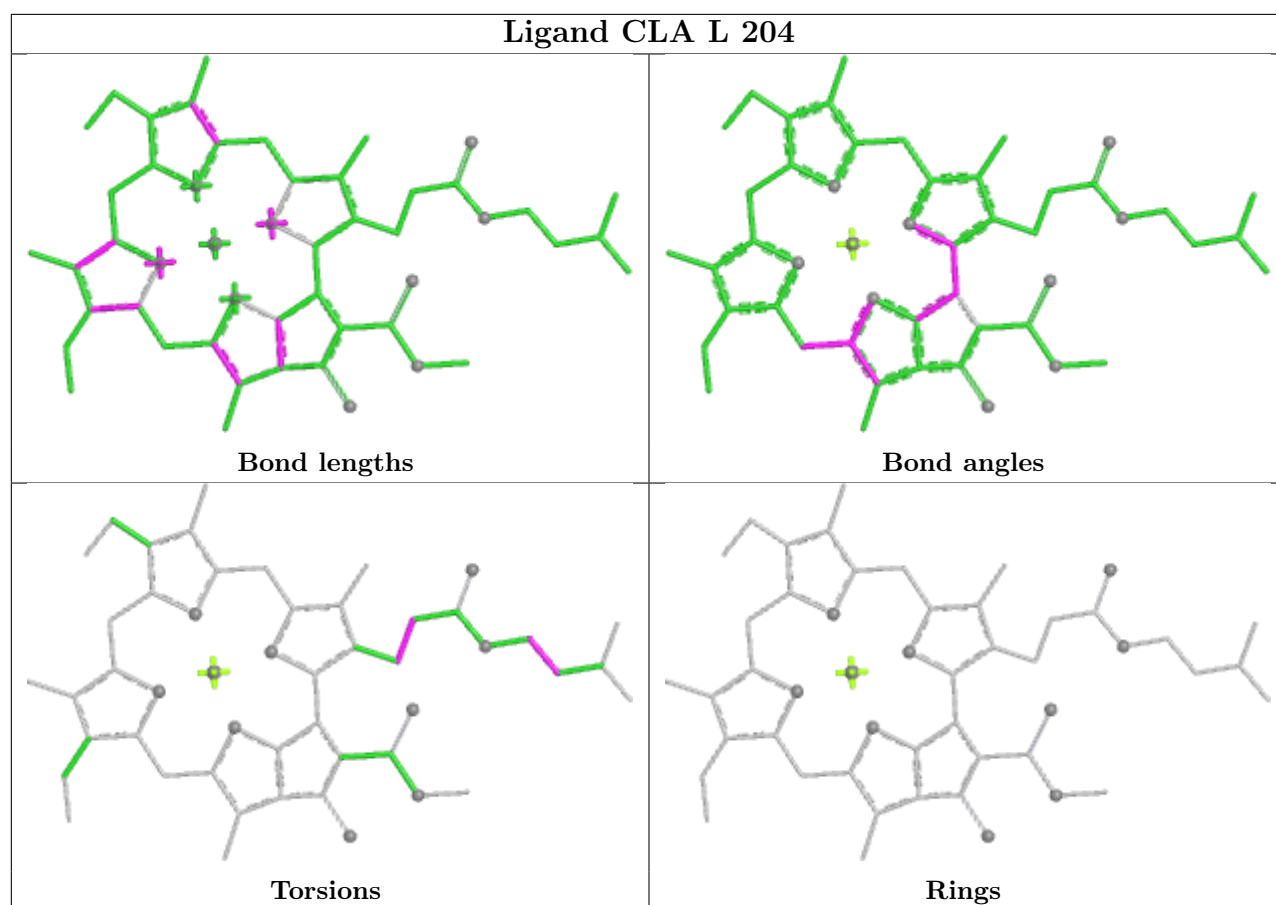








Ligand CLA B 815**Ligand CLA L 203**



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.

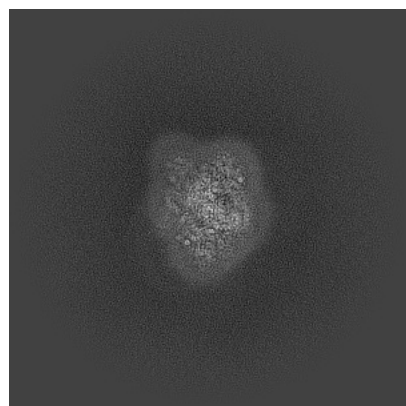
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-64362. These allow visual inspection of the internal detail of the map and identification of artifacts.

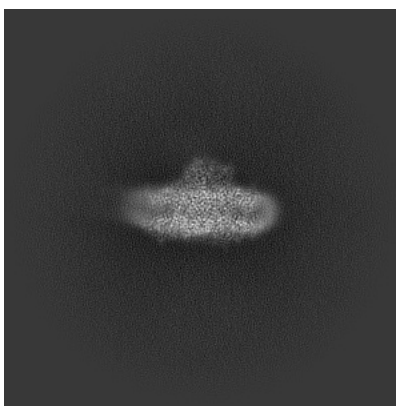
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

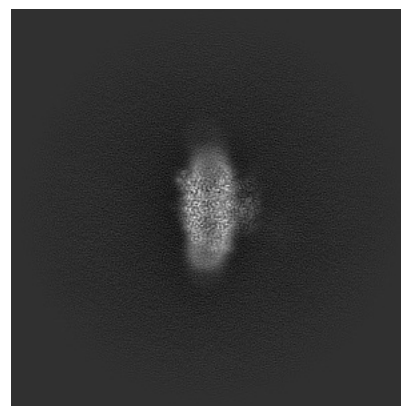
6.1.1 Primary map



X

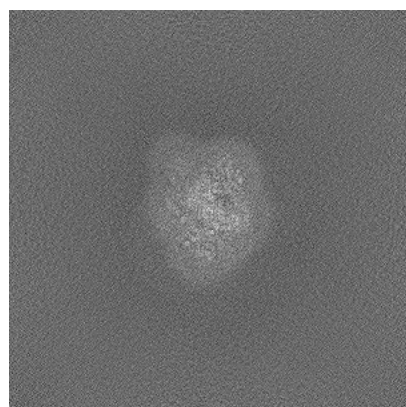


Y

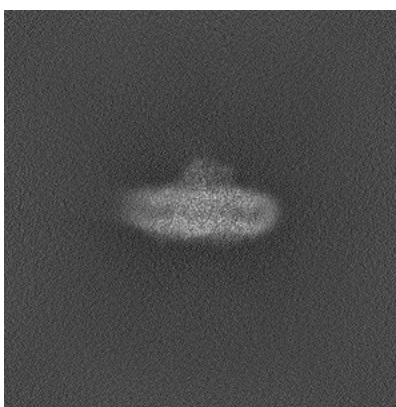


Z

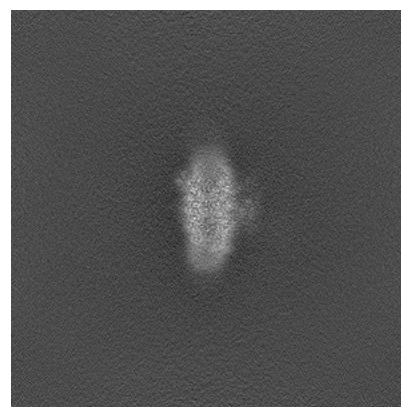
6.1.2 Raw map



X



Y

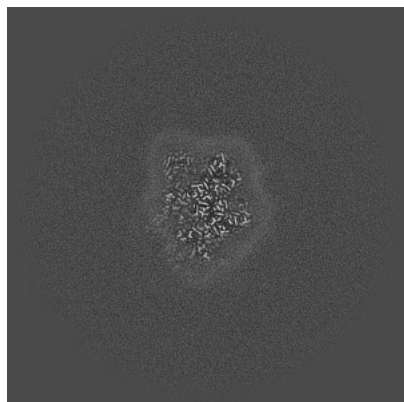


Z

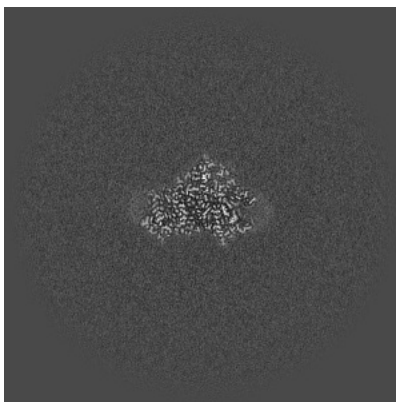
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

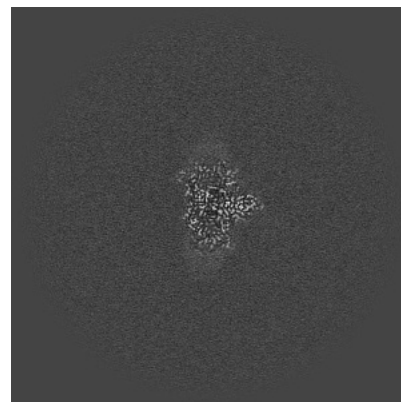
6.2.1 Primary map



X Index: 300

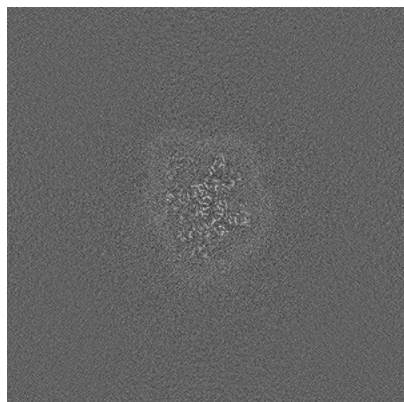


Y Index: 300

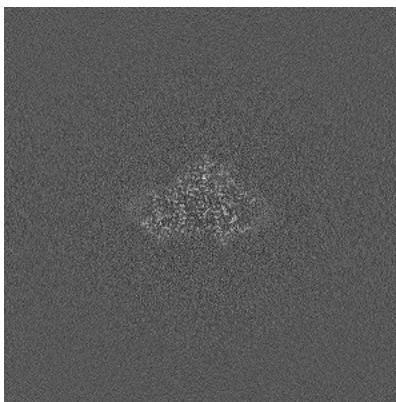


Z Index: 300

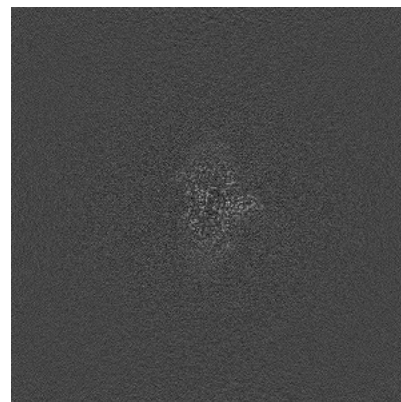
6.2.2 Raw map



X Index: 300



Y Index: 300

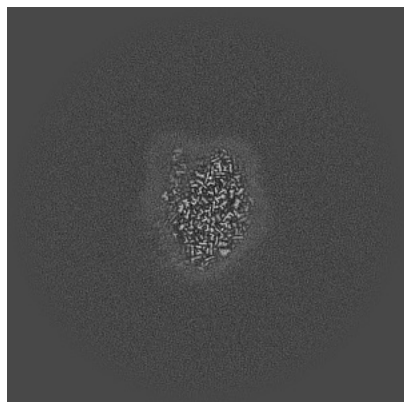


Z Index: 300

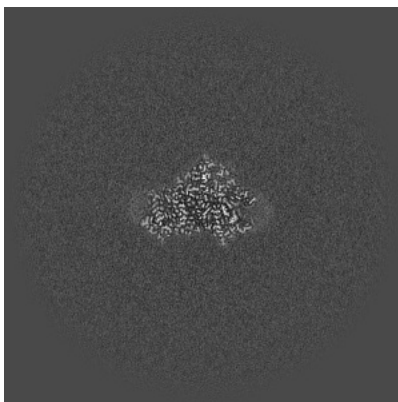
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

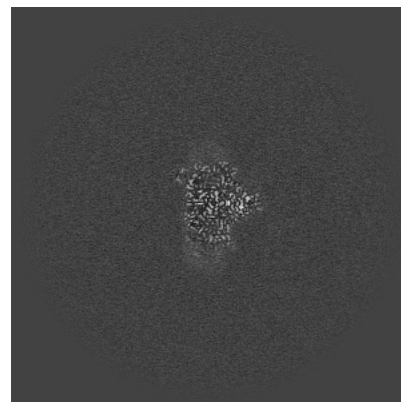
6.3.1 Primary map



X Index: 282

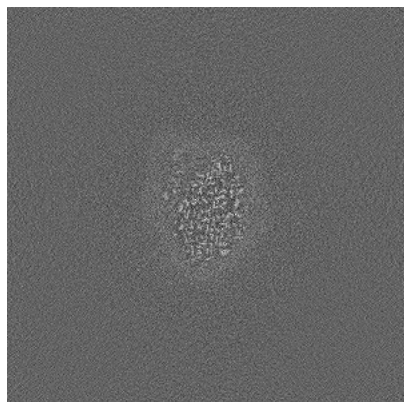


Y Index: 300

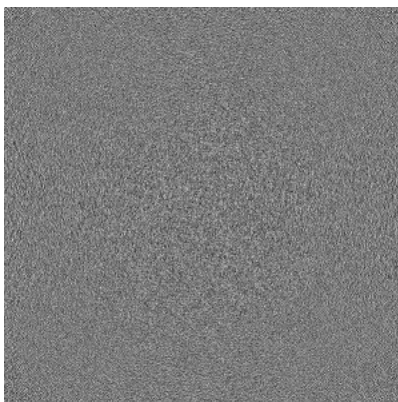


Z Index: 298

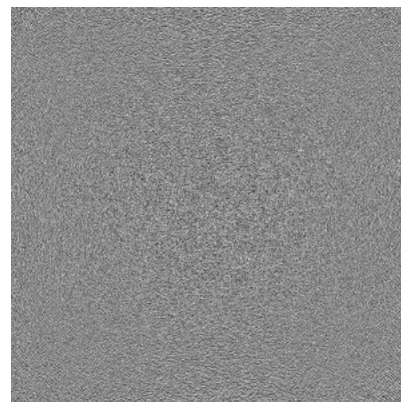
6.3.2 Raw map



X Index: 282



Y Index: 0

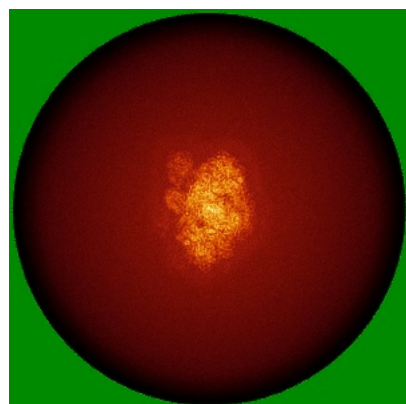


Z Index: 599

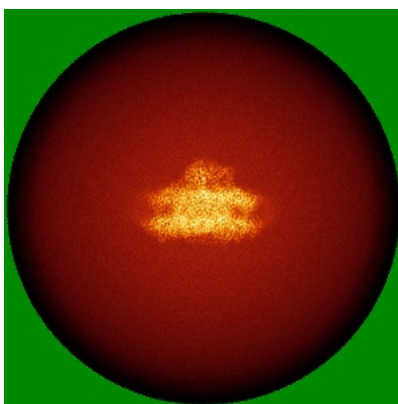
The images above show the largest variance slices of the map in three orthogonal directions.

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

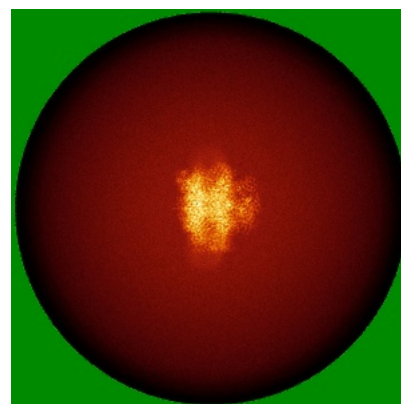
6.4.1 Primary map



X

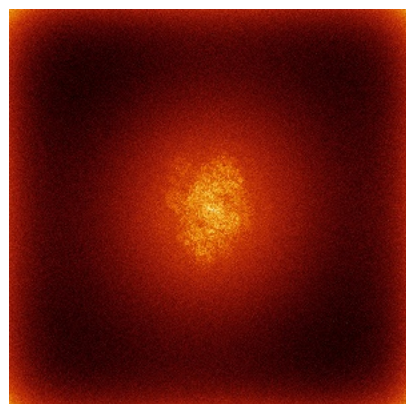


Y

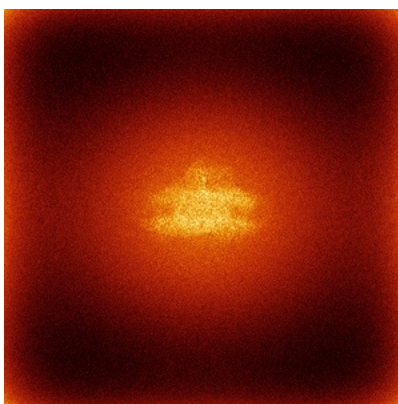


Z

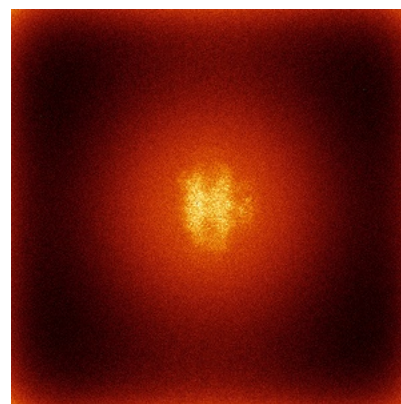
6.4.2 Raw map



X



Y



Z

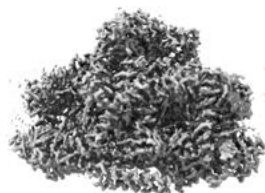
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

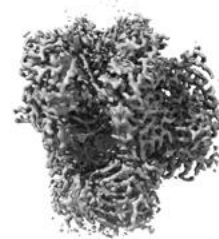
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.11. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

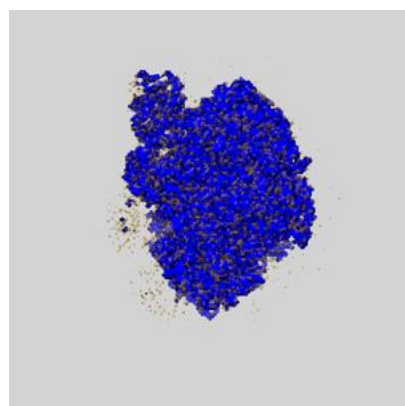
6.6 Mask visualisation [i](#)

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

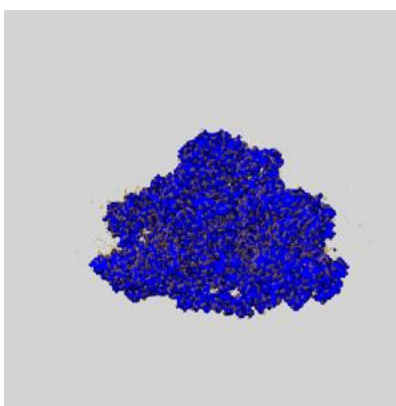
A mask typically either:

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

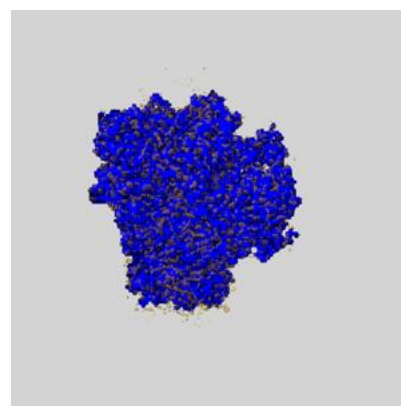
6.6.1 emd_64362_msk_1.map [i](#)



X



Y

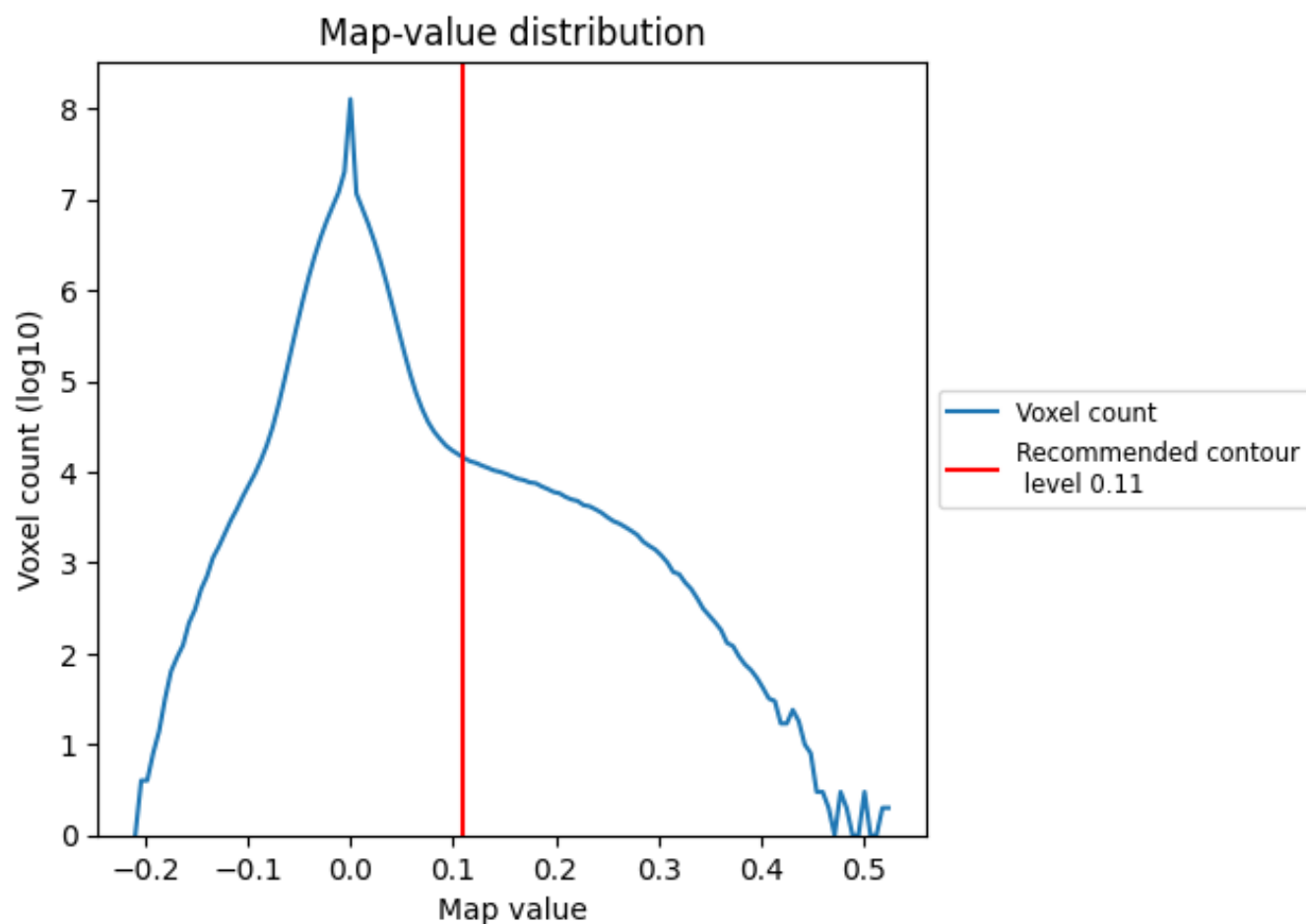


Z

7 Map analysis [i](#)

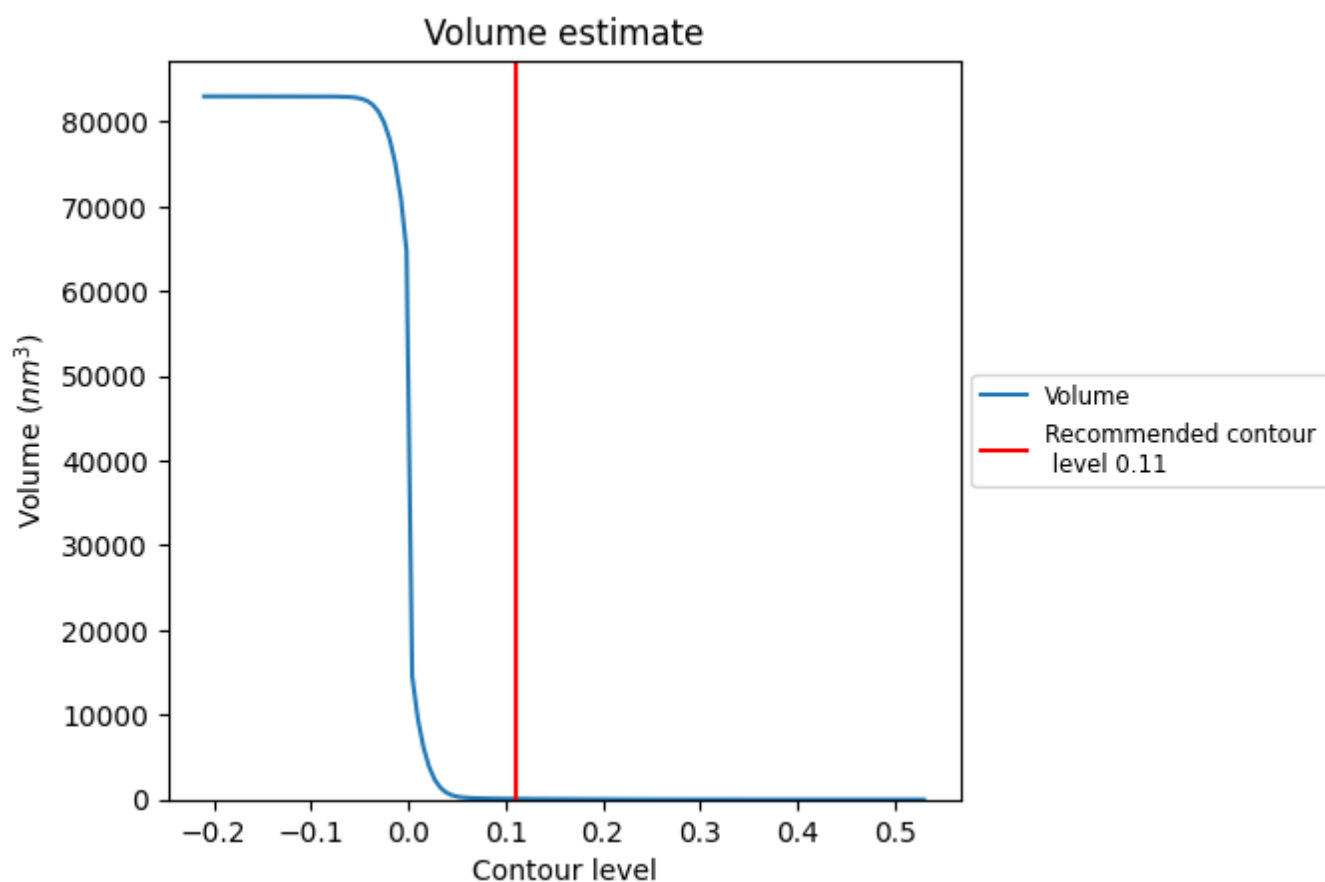
This section contains the results of statistical analysis of the map.

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.

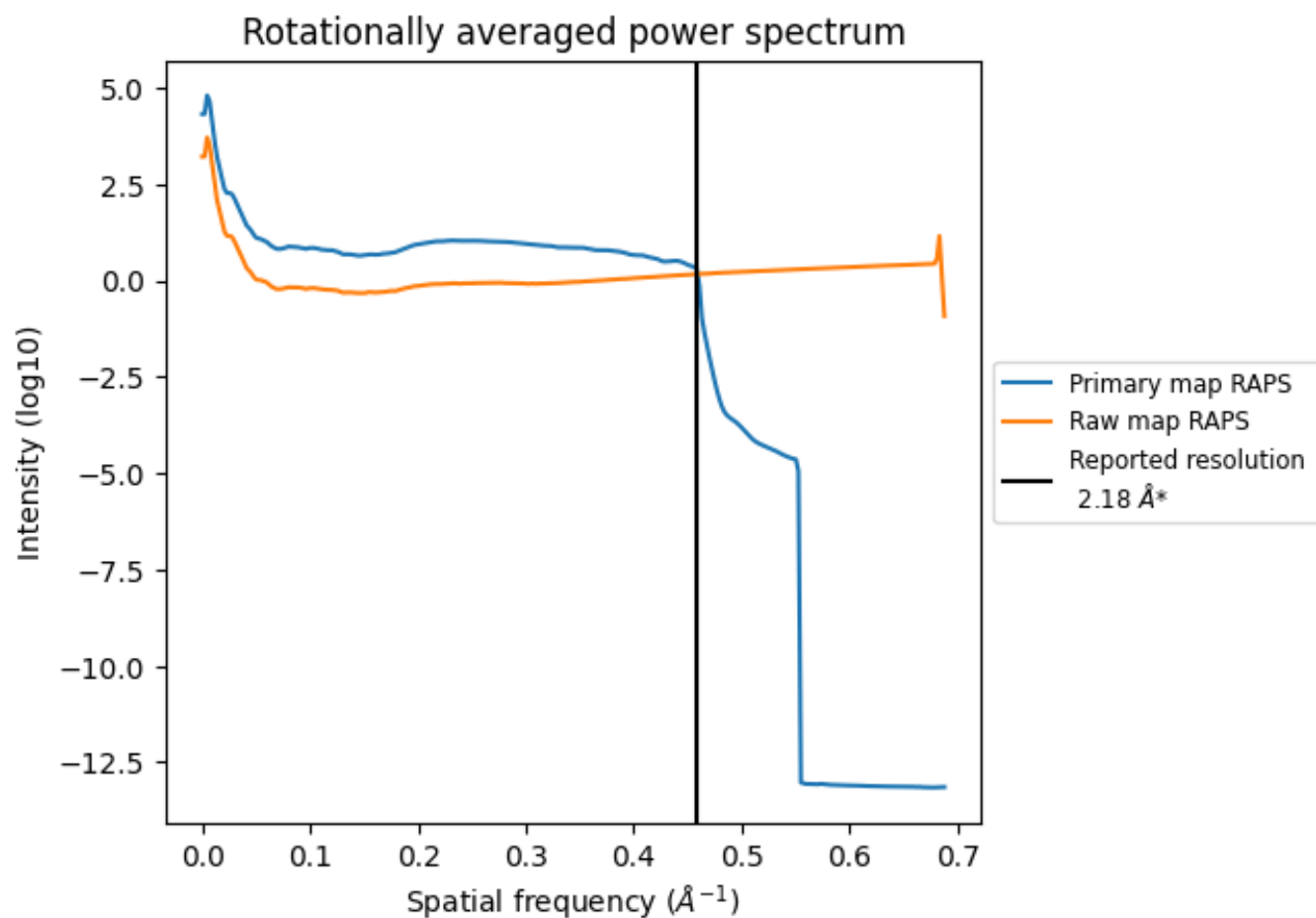
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 84 nm³; this corresponds to an approximate mass of 76 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 ⓘ

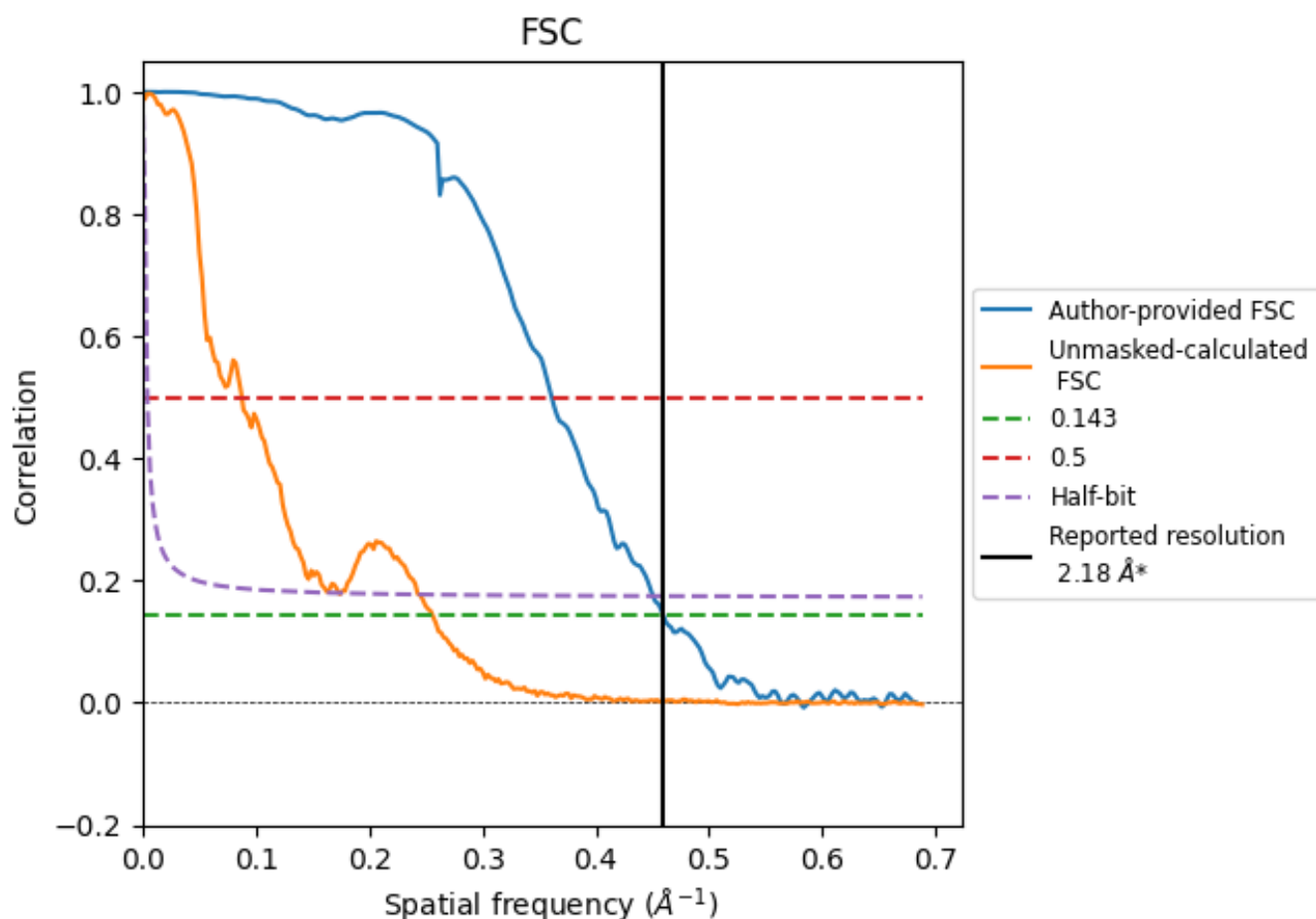


*Reported resolution corresponds to spatial frequency of 0.459 \AA^{-1}

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 0.459 \AA^{-1}

8.2 Resolution estimates [i](#)

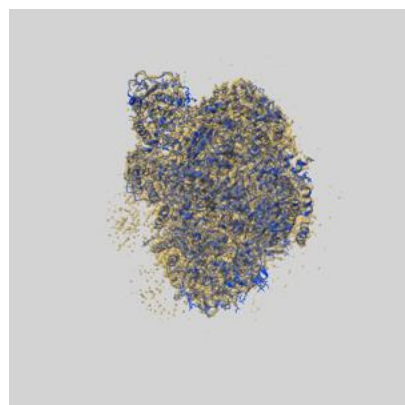
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.18	-	-
Author-provided FSC curve	2.18	2.77	2.22
Unmasked-calculated*	3.91	11.39	5.76

*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 3.91 differs from the reported value 2.18 by more than 10 %

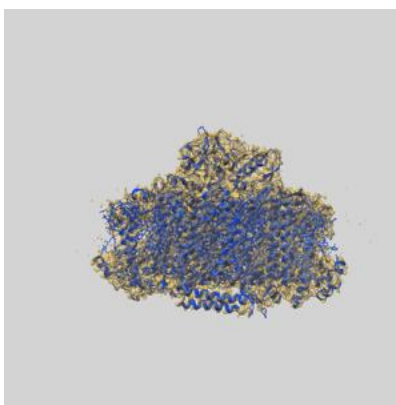
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-64362 and PDB model 9UNU. Per-residue inclusion information can be found in section [3](#) on page [21](#).

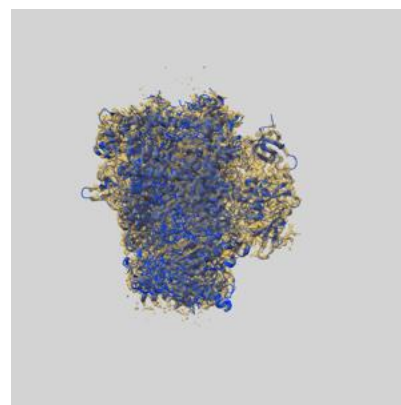
9.1 Map-model overlay [i](#)



X



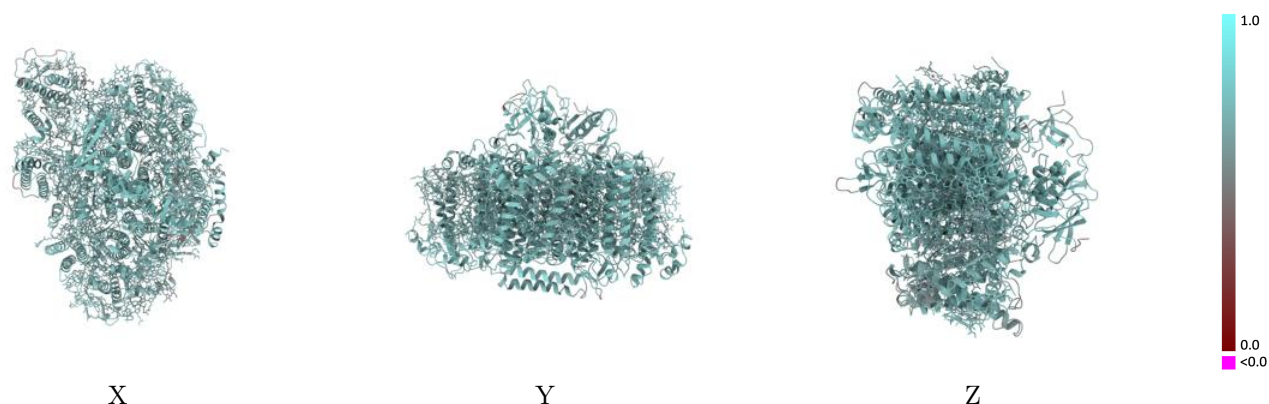
Y



Z

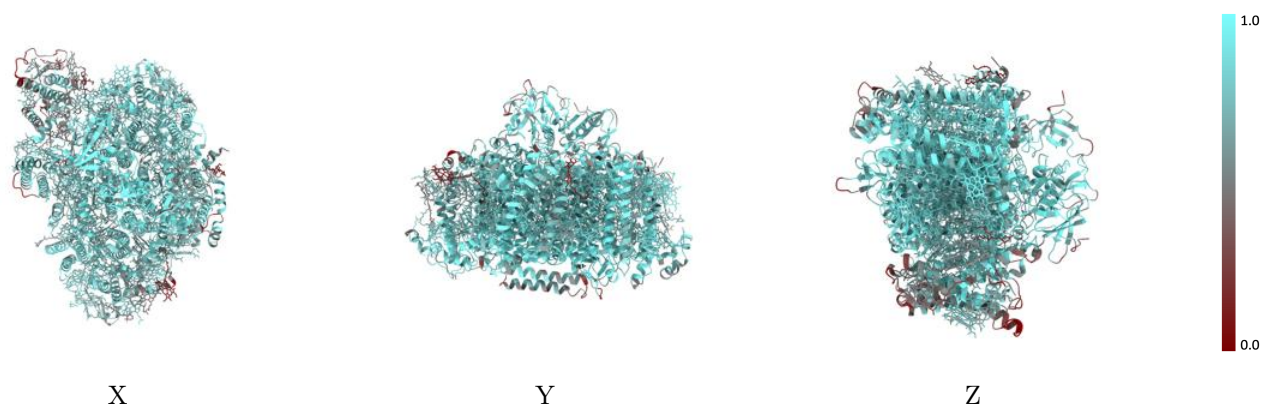
The images above show the 3D surface view of the map at the recommended contour level 0.11 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



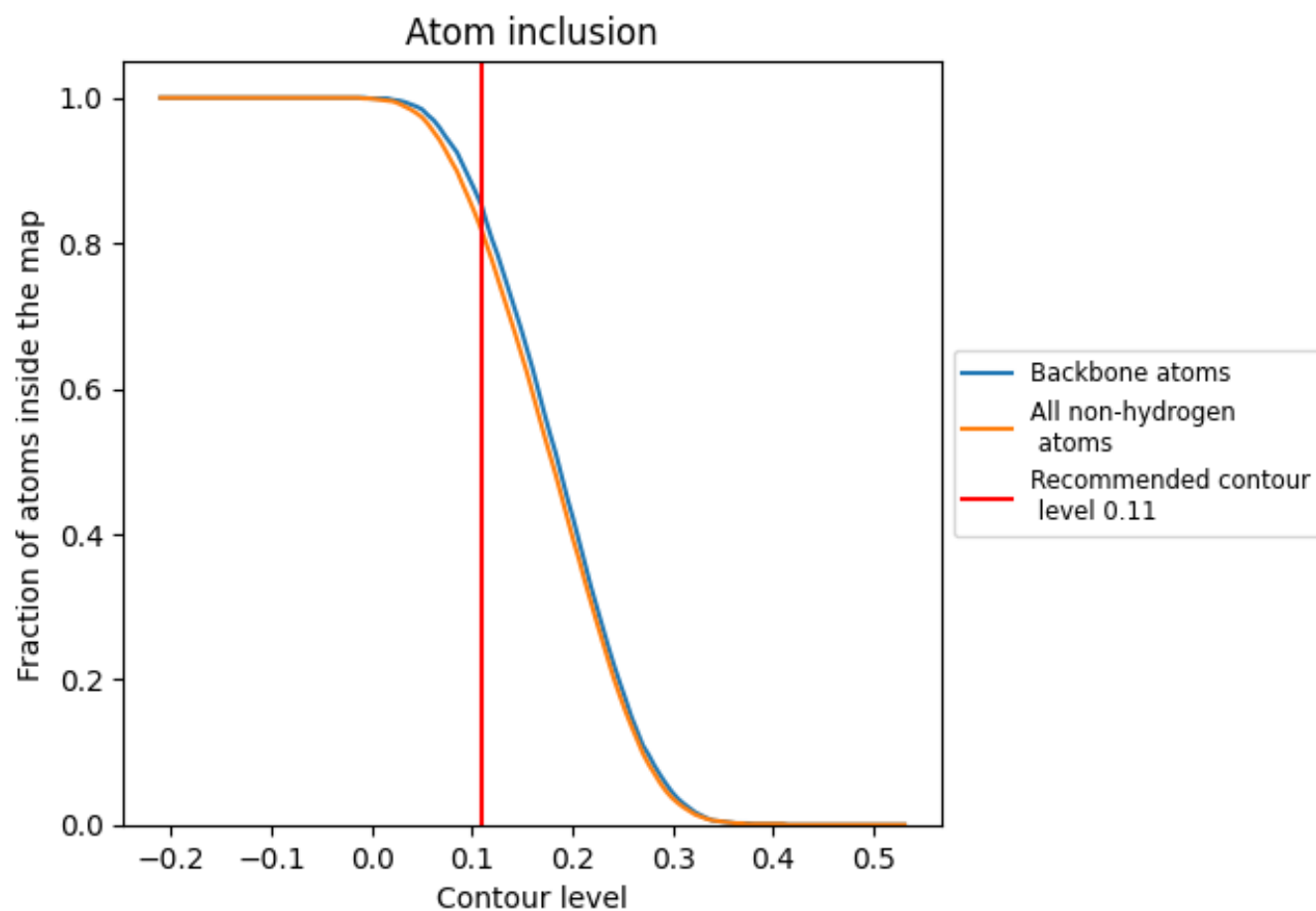
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.11).

9.4 Atom inclusion [i](#)



At the recommended contour level, 85% of all backbone atoms, 82% 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 (0.11) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.8160	<div></div> 0.6850
A	<div></div> 0.8700	<div></div> 0.6970
B	<div></div> 0.8510	<div></div> 0.6940
C	<div></div> 0.9180	<div></div> 0.7110
D	<div></div> 0.7640	<div></div> 0.6730
E	<div></div> 0.7560	<div></div> 0.6610
F	<div></div> 0.7180	<div></div> 0.6660
I	<div></div> 0.7800	<div></div> 0.6710
J	<div></div> 0.6750	<div></div> 0.6620
L	<div></div> 0.7720	<div></div> 0.6720
M	<div></div> 0.7550	<div></div> 0.6740
U	<div></div> 0.5340	<div></div> 0.6190

1.0

0.0

<0.0