



## Full wwPDB EM Validation Report ⓘ

Apr 6, 2026 – 04:01 AM UTC

PDB ID : 9UOV / pdb\_00009uov  
EMDB ID : EMD-64383  
Title : PSI-8 FCPI supercomplex from haptophyte *Chrysotila roscoffensis*  
Authors : La Rocca, R.; Tsai, P.-C.; Kato, K.; Nakajima, Y.; Akita, F.; Shen, J.-R.  
Deposited on : 2025-04-26  
Resolution : 2.33 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](mailto: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>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

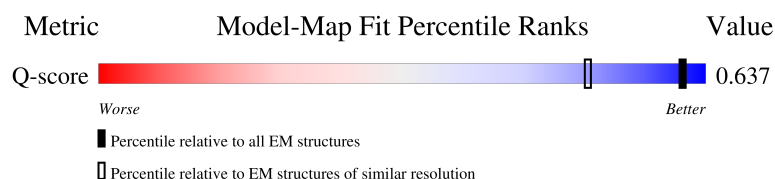
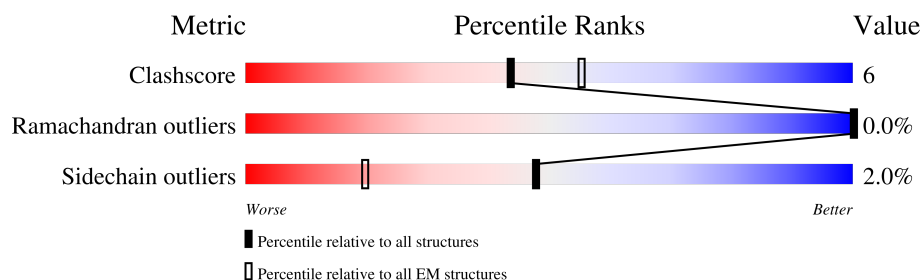
EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (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 2.33 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	4434 ( 1.83 - 2.83 )

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	752	
2	B	734	
3	C	81	
4	D	142	

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Mol	Chain	Length	Quality of chain
5	E	67	
6	F	184	
7	I	35	
8	J	39	
9	L	141	
10	M	29	
11	O	201	
12	P	231	
13	Q	197	
14	R	90	
15	S	215	
16	U	191	
17	G	209	
18	H	169	
19	T	202	

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
20	CLA	A	802	X	-	-	-
20	CLA	A	803	X	-	-	-
20	CLA	A	804	X	-	-	-
20	CLA	A	805	X	-	-	-
20	CLA	A	806	X	-	-	-
20	CLA	A	808	X	-	-	-
20	CLA	A	810	X	-	-	-
20	CLA	A	811	X	-	-	-
20	CLA	A	812	X	-	-	-
20	CLA	A	814	X	-	-	-
20	CLA	A	815	X	-	-	-
20	CLA	A	816	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
20	CLA	A	817	X	-	-	-
20	CLA	A	818	X	-	-	-
20	CLA	A	820	X	-	-	-
20	CLA	A	821	X	-	-	-
20	CLA	A	822	X	-	-	-
20	CLA	A	823	X	-	-	-
20	CLA	A	824	X	-	-	-
20	CLA	A	825	X	-	-	-
20	CLA	A	828	X	-	-	-
20	CLA	A	829	X	-	-	-
20	CLA	A	831	X	-	-	-
20	CLA	A	832	X	-	-	-
20	CLA	A	833	X	-	-	-
20	CLA	A	834	X	-	-	-
20	CLA	A	835	X	-	-	-
20	CLA	A	836	X	-	-	-
20	CLA	A	838	X	-	-	-
20	CLA	A	845	X	-	-	-
20	CLA	A	849	X	-	-	-
20	CLA	A	851	X	-	-	-
20	CLA	A	852	X	-	-	-
20	CLA	A	853	X	-	-	-
20	CLA	A	854	X	-	-	-
20	CLA	B	801	X	-	-	-
20	CLA	B	802	X	-	-	-
20	CLA	B	803	X	-	-	-
20	CLA	B	804	X	-	-	-
20	CLA	B	805	X	-	-	-
20	CLA	B	806	X	-	-	-
20	CLA	B	807	X	-	-	-
20	CLA	B	808	X	-	-	-
20	CLA	B	809	X	-	-	-
20	CLA	B	812	X	-	-	-
20	CLA	B	815	X	-	-	-
20	CLA	B	816	X	-	-	-
20	CLA	B	817	X	-	-	-
20	CLA	B	820	X	-	-	-
20	CLA	B	821	X	-	-	-
20	CLA	B	822	X	-	-	-
20	CLA	B	823	X	-	-	-
20	CLA	B	827	X	-	-	-
20	CLA	B	829	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
20	CLA	B	830	X	-	-	-
20	CLA	B	831	X	-	-	-
20	CLA	B	832	X	-	-	-
20	CLA	B	833	X	-	-	-
20	CLA	B	834	X	-	-	-
20	CLA	B	835	X	-	-	-
20	CLA	B	843	X	-	-	-
20	CLA	B	844	X	-	-	-
20	CLA	B	845	X	-	-	-
20	CLA	B	846	X	-	-	-
20	CLA	B	848	X	-	-	-
20	CLA	F	802	X	-	-	-
20	CLA	F	803	X	-	-	-
20	CLA	G	202	X	-	-	-
20	CLA	G	203	X	-	-	-
20	CLA	G	205	X	-	-	-
20	CLA	G	206	X	-	-	-
20	CLA	G	207	X	-	-	-
20	CLA	G	208	X	-	-	-
20	CLA	G	210	X	-	-	-
20	CLA	G	215	X	-	-	-
20	CLA	H	201	X	-	-	-
20	CLA	H	202	X	-	-	-
20	CLA	H	203	X	-	-	-
20	CLA	H	204	X	-	-	-
20	CLA	H	205	X	-	-	-
20	CLA	H	206	X	-	-	-
20	CLA	H	207	X	-	-	-
20	CLA	H	208	X	-	-	-
20	CLA	H	209	X	-	-	-
20	CLA	J	103	X	-	-	-
20	CLA	L	202	X	-	-	-
20	CLA	O	203	X	-	-	-
20	CLA	O	204	X	-	-	-
20	CLA	O	205	X	-	-	-
20	CLA	O	206	X	-	-	-
20	CLA	O	207	X	-	-	-
20	CLA	O	208	X	-	-	-
20	CLA	P	207	X	-	-	-
20	CLA	P	208	X	-	-	-
20	CLA	P	209	X	-	-	-
20	CLA	P	213	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
20	CLA	P	214	X	-	-	-
20	CLA	P	216	X	-	-	-
20	CLA	Q	204	X	-	-	-
20	CLA	Q	205	X	-	-	-
20	CLA	Q	206	X	-	-	-
20	CLA	Q	207	X	-	-	-
20	CLA	Q	208	X	-	-	-
20	CLA	Q	211	X	-	-	-
20	CLA	Q	213	X	-	-	-
20	CLA	R	101	X	-	-	-
20	CLA	S	205	X	-	-	-
20	CLA	S	206	X	-	-	-
20	CLA	S	207	X	-	-	-
20	CLA	S	214	X	-	-	-
20	CLA	S	215	X	-	-	-
20	CLA	T	201	X	-	-	-
20	CLA	T	202	X	-	-	-
20	CLA	T	203	X	-	-	-
20	CLA	T	205	X	-	-	-
20	CLA	T	206	X	-	-	-
20	CLA	T	211	X	-	-	-
20	CLA	U	204	X	-	-	-
20	CLA	U	206	X	-	-	-
20	CLA	U	208	X	-	-	-
20	CLA	U	209	X	-	-	-
20	CLA	U	211	X	-	-	-

## 2 Entry composition [i](#)

There are 32 unique types of molecules in this entry. The entry contains 39964 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 III (FCPI-3).

Mol	Chain	Residues	Atoms					AltConf	Trace
11	O	176	Total	C	N	O	S	0	0
			1341	872	217	244	8		

- Molecule 12 is a protein called Fucoxanthin chlorophyll a/c binding protein VI (FCPI-6).

Mol	Chain	Residues	Atoms					AltConf	Trace
12	P	193	Total	C	N	O	S	0	0
			1441	927	239	264	11		

- Molecule 13 is a protein called Fucoxanthin chlorophyll a/c binding protein IV (FCPI-4).

Mol	Chain	Residues	Atoms					AltConf	Trace
13	Q	167	Total	C	N	O	S	0	0
			1257	809	202	234	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	R	88	Total	C	N	O	S	0	0
			664	434	106	123	1		

- Molecule 15 is a protein called Fucoxanthin chlorophyll a/c binding protein II (FCPI-2).

Mol	Chain	Residues	Atoms					AltConf	Trace
15	S	165	Total	C	N	O	S	0	0
			1238	802	204	226	6		

- Molecule 16 is a protein called Fucoxanthin chlorophyll a/c binding protein I (FCPI-1).

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

- Molecule 17 is a protein called Fucoxanthin chlorophyll a/c binding protein VII (FCPI-7).

Mol	Chain	Residues	Atoms					AltConf	Trace
17	G	155	Total	C	N	O	S	0	0
			1179	756	190	224	9		

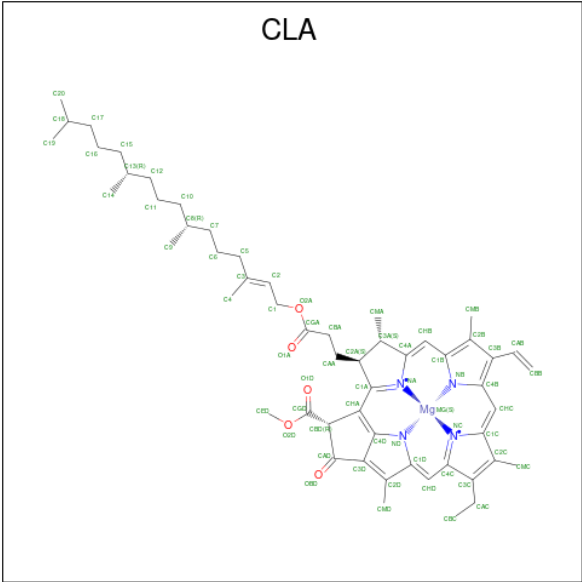
- Molecule 18 is a protein called Fucoxanthin chlorophyll a/c binding protein VIII (FCPI-8).

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

- Molecule 19 is a protein called Fucoxanthin chlorophyll a/c binding protein V (FCPI-5).

Mol	Chain	Residues	Atoms					AltConf	Trace
19	T	99	Total	C	N	O	S	0	0
			731	471	122	130	8		

- Molecule 20 is CHLOROPHYLL A (CCD ID: CLA) (formula: C<sub>55</sub>H<sub>72</sub>MgN<sub>4</sub>O<sub>5</sub>) (labeled as "Ligand of Interest" by depositor).



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

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

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Mol	Chain	Residues	Atoms					AltConf
20	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	A	1	Total 52	C 42	Mg 1	N 4	O 5	0
20	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	A	1	Total 60	C 50	Mg 1	N 4	O 5	0
20	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	B	1	Total 54	C 44	Mg 1	N 4	O 5	0
20	B	1	Total 55	C 45	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
20	B	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			63	53	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			47	37	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	B	1	Total 50	C 40	Mg 1	N 4	O 5	0
20	F	1	Total 48	C 38	Mg 1	N 4	O 5	0
20	F	1	Total 46	C 36	Mg 1	N 4	O 5	0
20	J	1	Total 42	C 34	Mg 1	N 4	O 3	0
20	L	1	Total 49	C 39	Mg 1	N 4	O 5	0
20	L	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	L	1	Total 50	C 40	Mg 1	N 4	O 5	0
20	O	1	Total 43	C 35	Mg 1	N 4	O 3	0
20	O	1	Total 45	C 35	Mg 1	N 4	O 5	0
20	O	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	O	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	O	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	O	1	Total 46	C 36	Mg 1	N 4	O 5	0
20	O	1	Total 60	C 50	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
20	O	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	O	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
20	P	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	P	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
20	P	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
20	P	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
20	P	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
20	P	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
20	P	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
20	P	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
20	Q	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
20	Q	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
20	Q	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
20	Q	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
20	Q	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
20	Q	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
20	Q	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	Q	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
20	Q	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	Q	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
20	Q	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
20	R	1	Total 45	C 35	Mg 1	N 4	O 5	0
20	R	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	S	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	S	1	Total 46	C 36	Mg 1	N 4	O 5	0
20	S	1	Total 46	C 36	Mg 1	N 4	O 5	0
20	S	1	Total 45	C 35	Mg 1	N 4	O 5	0
20	S	1	Total 52	C 42	Mg 1	N 4	O 5	0
20	S	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	S	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	U	1	Total 61	C 51	Mg 1	N 4	O 5	0
20	U	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	U	1	Total 45	C 35	Mg 1	N 4	O 5	0
20	U	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	U	1	Total 46	C 36	Mg 1	N 4	O 5	0
20	U	1	Total 42	C 34	Mg 1	N 4	O 3	0
20	U	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	U	1	Total 52	C 42	Mg 1	N 4	O 5	0
20	G	1	Total 45	C 35	Mg 1	N 4	O 5	0
20	G	1	Total 41	C 33	Mg 1	N 4	O 3	0
20	G	1	Total 45	C 35	Mg 1	N 4	O 5	0
20	G	1	Total 43	C 35	Mg 1	N 4	O 3	0

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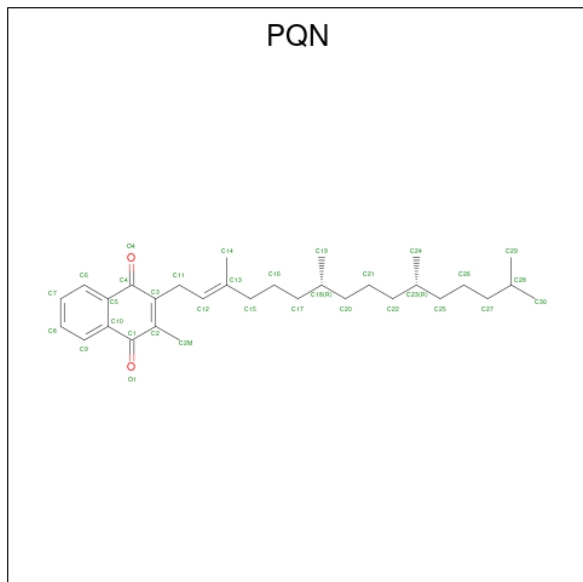
Mol	Chain	Residues	Atoms					AltConf
20	G	1	Total 61	C 51	Mg 1	N 4	O 5	0
20	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	G	1	Total 60	C 50	Mg 1	N 4	O 5	0
20	G	1	Total 55	C 45	Mg 1	N 4	O 5	0
20	G	1	Total 56	C 46	Mg 1	N 4	O 5	0
20	G	1	Total 45	C 35	Mg 1	N 4	O 5	0
20	G	1	Total 45	C 35	Mg 1	N 4	O 5	0
20	H	1	Total 40	C 32	Mg 1	N 4	O 3	0
20	H	1	Total 60	C 50	Mg 1	N 4	O 5	0
20	H	1	Total 61	C 51	Mg 1	N 4	O 5	0
20	H	1	Total 44	C 35	Mg 1	N 4	O 4	0
20	H	1	Total 45	C 35	Mg 1	N 4	O 5	0
20	H	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	H	1	Total 58	C 48	Mg 1	N 4	O 5	0
20	H	1	Total 41	C 33	Mg 1	N 4	O 3	0
20	H	1	Total 45	C 35	Mg 1	N 4	O 5	0
20	T	1	Total 42	C 34	Mg 1	N 4	O 3	0
20	T	1	Total 41	C 33	Mg 1	N 4	O 3	0
20	T	1	Total 46	C 36	Mg 1	N 4	O 5	0
20	T	1	Total 57	C 47	Mg 1	N 4	O 5	0
20	T	1	Total 46	C 36	Mg 1	N 4	O 5	0

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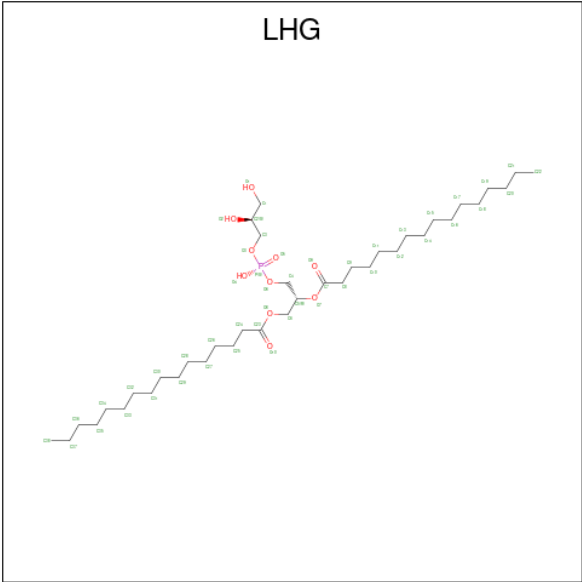
Mol	Chain	Residues	Atoms					AltConf
20	T	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
20	T	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	T	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
20	T	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
20	T	1	Total	C	Mg	N	O	0
			47	37	1	4	5	

- Molecule 21 is PHYLLOQUINONE (CCD ID: PQN) (formula:  $C_{31}H_{46}O_2$ ) (labeled as "Ligand of Interest" by depositor).



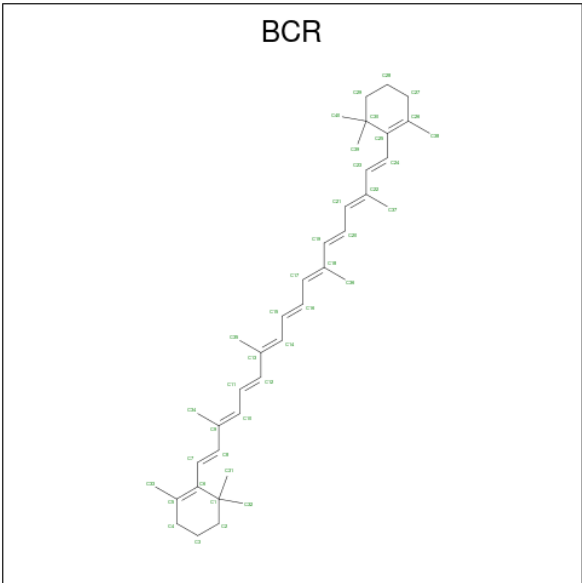
Mol	Chain	Residues	Atoms			AltConf
21	A	1	Total	C	O	0
			33	31	2	
21	B	1	Total	C	O	0
			33	31	2	

- Molecule 22 is 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
22	A	1	Total	C	O	P	0
			48	37	10	1	
22	A	1	Total	C	O	P	0
			27	16	10	1	
22	P	1	Total	C	O	P	0
			49	38	10	1	
22	G	1	Total	C	O	P	0
			27	16	10	1	

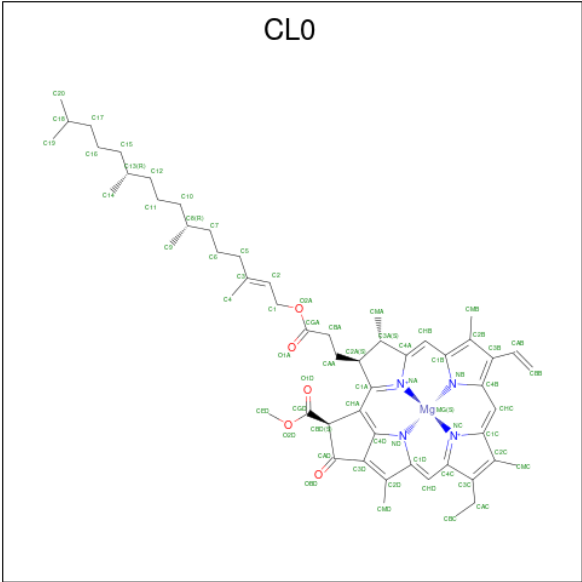
- Molecule 23 is BETA-CAROTENE (CCD ID: BCR) (formula: C<sub>40</sub>H<sub>56</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms		AltConf
23	A	1	Total 40	C 40	0
23	A	1	Total 40	C 40	0
23	A	1	Total 40	C 40	0
23	A	1	Total 40	C 40	0
23	B	1	Total 40	C 40	0
23	B	1	Total 40	C 40	0
23	B	1	Total 40	C 40	0
23	B	1	Total 40	C 40	0
23	B	1	Total 40	C 40	0
23	F	1	Total 40	C 40	0
23	F	1	Total 40	C 40	0
23	I	1	Total 40	C 40	0
23	I	1	Total 40	C 40	0
23	J	1	Total 40	C 40	0
23	L	1	Total 40	C 40	0
23	L	1	Total 40	C 40	0
23	M	1	Total 40	C 40	0
23	R	1	Total 39	C 39	0

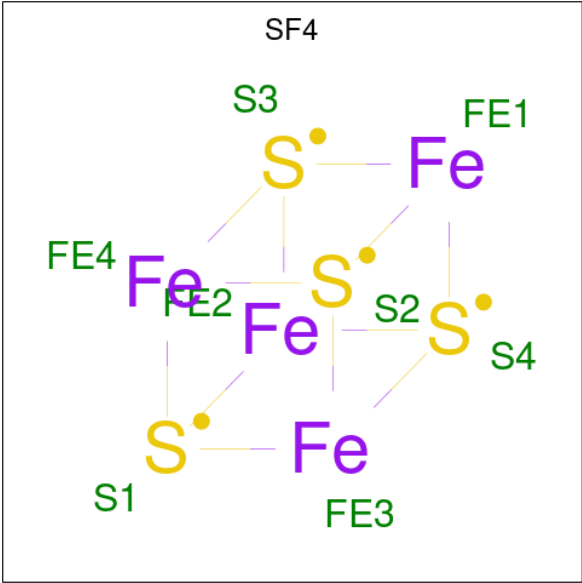
- Molecule 24 is CHLOROPHYLL A ISOMER (CCD ID: CL0) (formula:  $C_{55}H_{72}MgN_4O_5$ ) (labeled as "Ligand of Interest" by depositor).





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

- Molecule 25 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>) (labeled as "Ligand of Interest" by depositor).



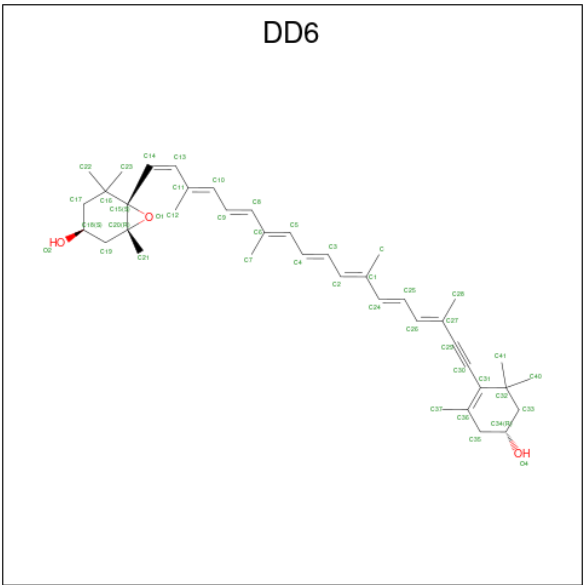
Mol	Chain	Residues	Atoms			AltConf
25	A	1	Total	Fe	S	0
			8	4	4	
25	C	1	Total	Fe	S	0
			8	4	4	

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

- Molecule 26 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<sub>40</sub>H<sub>54</sub>O<sub>3</sub>) (labeled as "Ligand of Interest" by depositor).



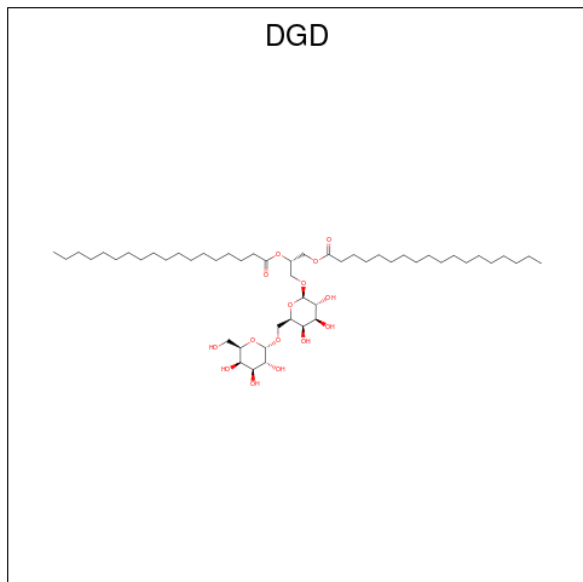
Mol	Chain	Residues	Atoms			AltConf
26	A	1	Total	C	O	0
			43	40	3	
26	J	1	Total	C	O	0
			43	40	3	
26	O	1	Total	C	O	0
			43	40	3	
26	O	1	Total	C	O	0
			43	40	3	
26	O	1	Total	C	O	0
			43	40	3	
26	O	1	Total	C	O	0
			43	40	3	
26	P	1	Total	C	O	0
			43	40	3	
26	P	1	Total	C	O	0
			43	40	3	

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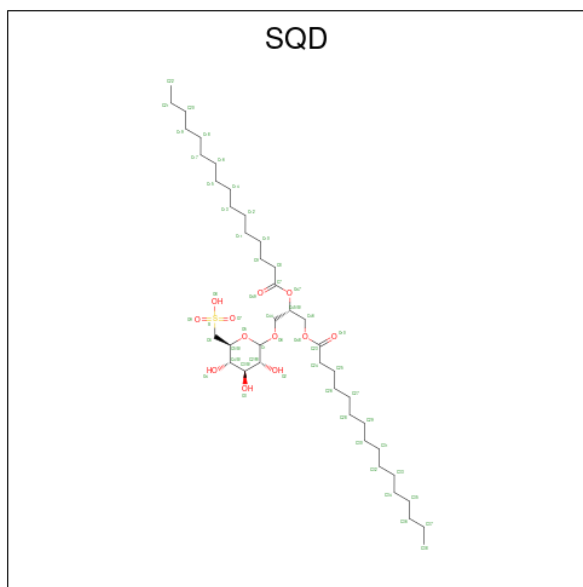
Mol	Chain	Residues	Atoms			AltConf
26	P	1	Total 43	C 40	O 3	0
26	P	1	Total 43	C 40	O 3	0
26	Q	1	Total 43	C 40	O 3	0
26	Q	1	Total 43	C 40	O 3	0
26	S	1	Total 43	C 40	O 3	0
26	S	1	Total 43	C 40	O 3	0
26	S	1	Total 43	C 40	O 3	0
26	S	1	Total 43	C 40	O 3	0
26	S	1	Total 43	C 40	O 3	0
26	U	1	Total 43	C 40	O 3	0
26	U	1	Total 43	C 40	O 3	0
26	U	1	Total 26	C 25	O 1	0
26	G	1	Total 43	C 40	O 3	0
26	G	1	Total 43	C 40	O 3	0
26	G	1	Total 43	C 40	O 3	0
26	G	1	Total 43	C 40	O 3	0
26	G	1	Total 43	C 40	O 3	0
26	H	1	Total 43	C 40	O 3	0
26	H	1	Total 43	C 40	O 3	0
26	T	1	Total 43	C 40	O 3	0
26	T	1	Total 43	C 40	O 3	0

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



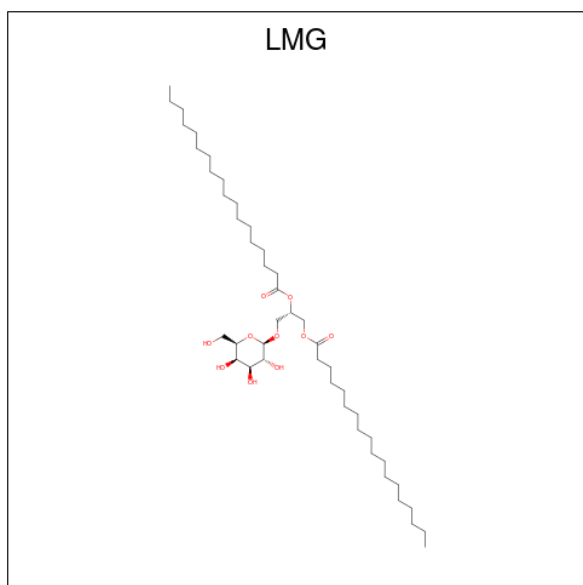
Mol	Chain	Residues	Atoms			AltConf
27	B	1	Total	C	O	0
			60	45	15	

- Molecule 28 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula:  $C_{41}H_{78}O_{12}S$ ) (labeled as "Ligand of Interest" by depositor).



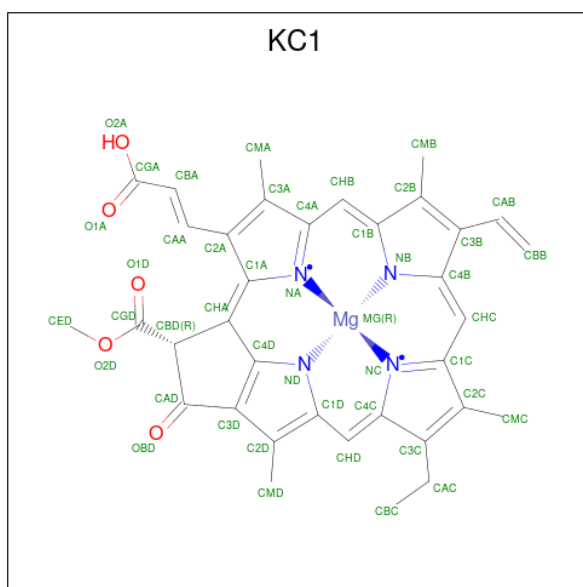
Mol	Chain	Residues	Atoms				AltConf
28	B	1	Total	C	O	S	0
			50	37	12	1	
28	S	1	Total	C	O	S	0
			46	33	12	1	

- Molecule 29 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula:  $C_{45}H_{86}O_{10}$ ) (labeled as "Ligand of Interest" by depositor).



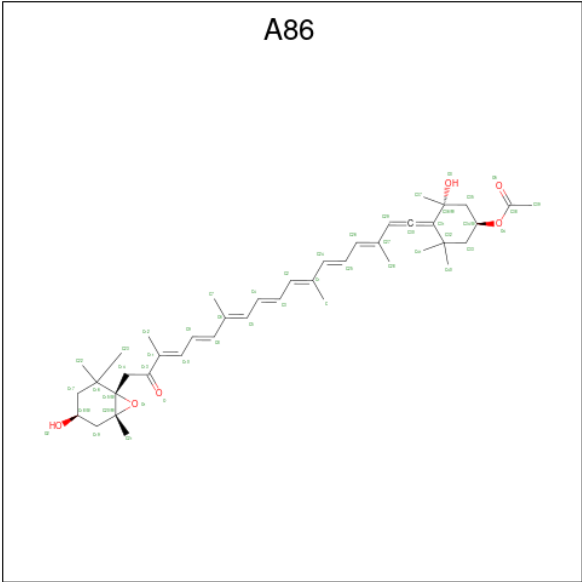
Mol	Chain	Residues	Atoms			AltConf
29	I	1	Total	C	O	0
			49	39	10	
29	J	1	Total	C	O	0
			39	29	10	
29	P	1	Total	C	O	0
			34	24	10	
29	P	1	Total	C	O	0
			25	15	10	
29	Q	1	Total	C	O	0
			55	45	10	
29	U	1	Total	C	O	0
			32	22	10	

- Molecule 30 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
30	O	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	P	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	P	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	P	1	Total 44	C 35	Mg 1	N 4	O 4	0
30	P	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	Q	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	S	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	S	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	U	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	T	1	Total 45	C 35	Mg 1	N 4	O 5	0

- Molecule 31 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<sub>42</sub>H<sub>58</sub>O<sub>6</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
31	P	1	Total	C	O	0
			48	42	6	
31	Q	1	Total	C	O	0
			48	42	6	
31	Q	1	Total	C	O	0
			48	42	6	
31	Q	1	Total	C	O	0
			48	42	6	
31	R	1	Total	C	O	0
			44	40	4	
31	R	1	Total	C	O	0
			48	42	6	
31	U	1	Total	C	O	0
			48	42	6	

- Molecule 32 is water.

Mol	Chain	Residues	Atoms		AltConf
32	A	55	Total	O	0
			55	55	
32	B	91	Total	O	0
			91	91	
32	C	9	Total	O	0
			9	9	
32	D	8	Total	O	0
			8	8	
32	E	5	Total	O	0
			5	5	

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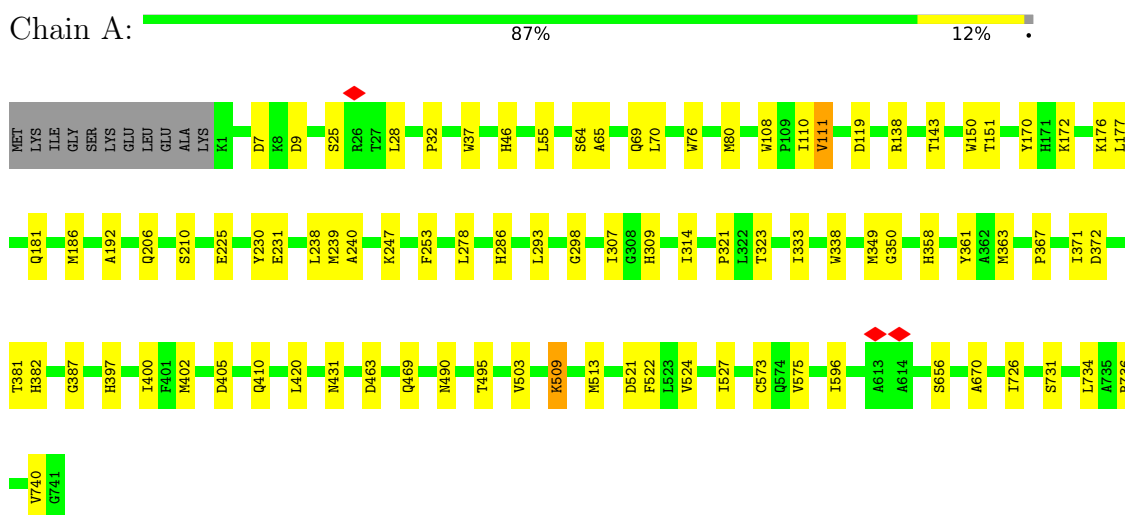
Mol	Chain	Residues	Atoms		AltConf
32	F	9	Total 9	O 9	0
32	I	1	Total 1	O 1	0
32	J	4	Total 4	O 4	0
32	L	5	Total 5	O 5	0
32	M	1	Total 1	O 1	0
32	O	7	Total 7	O 7	0
32	P	8	Total 8	O 8	0
32	Q	3	Total 3	O 3	0
32	R	4	Total 4	O 4	0
32	S	5	Total 5	O 5	0
32	U	4	Total 4	O 4	0
32	G	6	Total 6	O 6	0
32	H	2	Total 2	O 2	0
32	T	2	Total 2	O 2	0



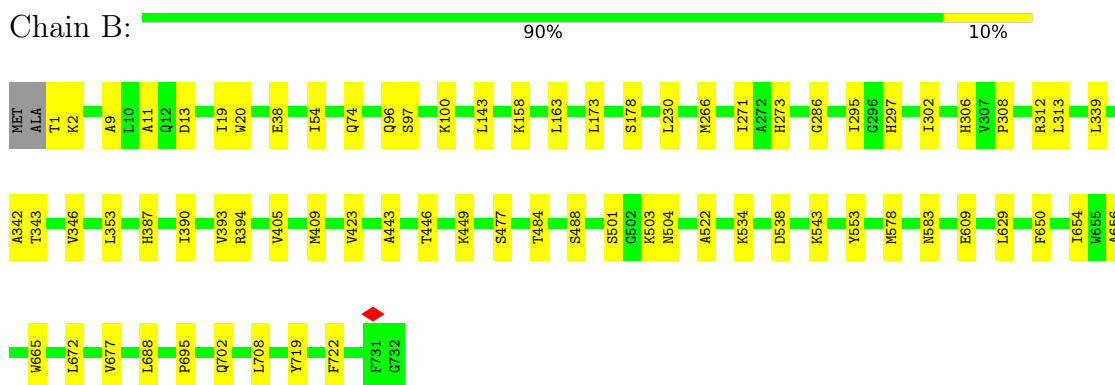
### 3 Residue-property plots

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

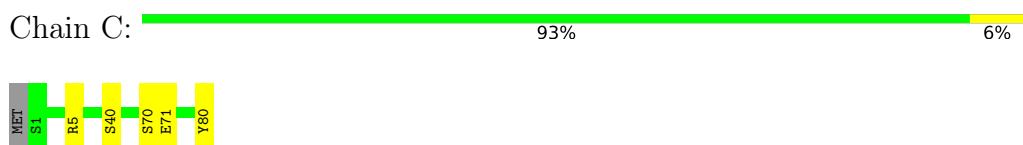
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1 (psaA)




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



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




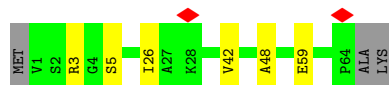
- Molecule 4: Photosystem I reaction center subunit II (psaD)

Chain D:  91% 6% ..




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

Chain E:  87% 9% .



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

Chain F:  78% 9% 12%




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

Chain I:  69% 26% ..



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

Chain J:  82% 18%



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

Chain L:  87% 11% ..




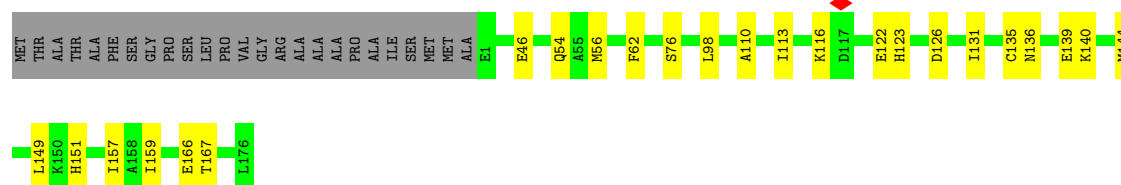
- Molecule 10: Photosystem I reaction center subunit XII (psaM)

Chain M:  97% .




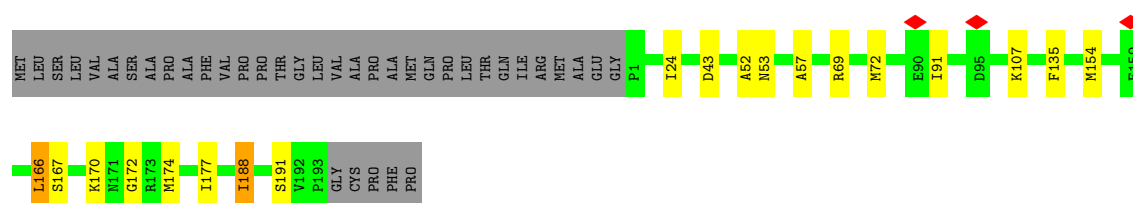
- Molecule 11: Fucoxanthin chlorophyll a/c binding protein III (FCPI-3)

Chain O:  76% 12% 12%




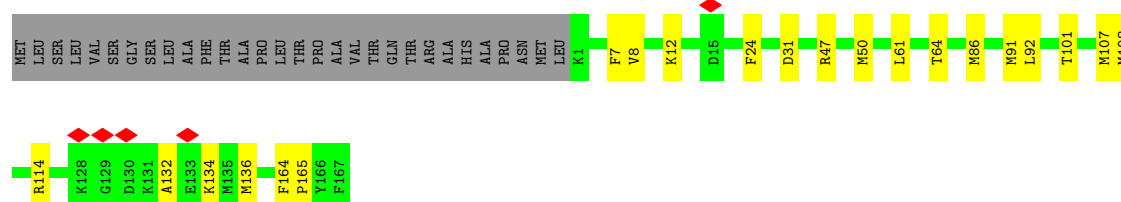
- Molecule 12: Fucoxanthin chlorophyll a/c binding protein VI (FCPI-6)

Chain P:  75% 7% 16%




- Molecule 13: Fucoxanthin chlorophyll a/c binding protein IV (FCPI-4)

Chain Q:  74% 11% 15%



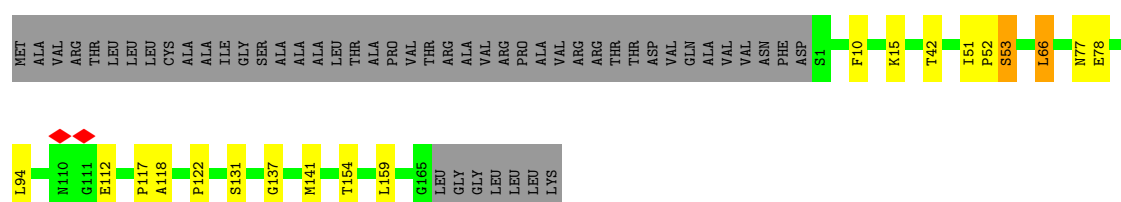
- Molecule 14: Photosystem I reaction center subunit psaR

Chain R:  89% 9% 2%



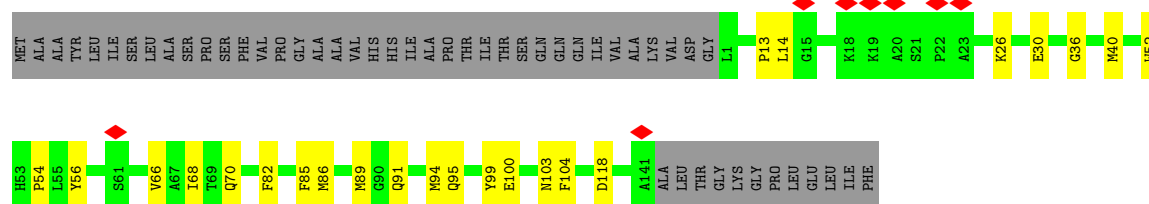
- Molecule 15: Fucoxanthin chlorophyll a/c binding protein II (FCPI-2)

Chain S:  68% 8% 23%



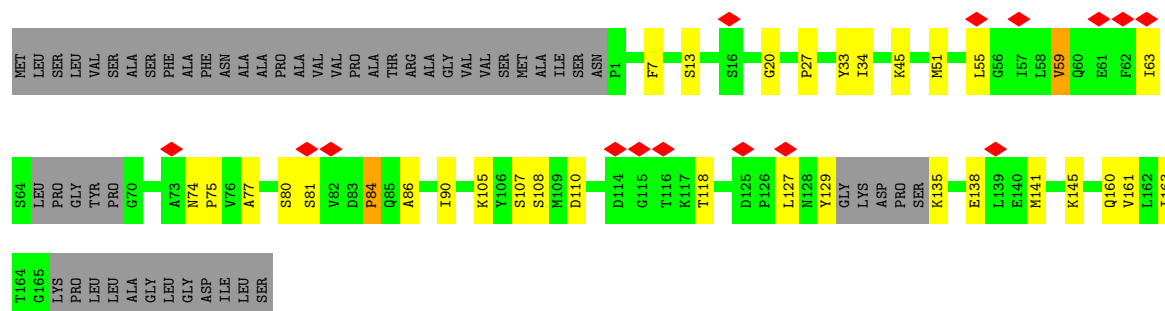
- Molecule 16: Fucoxanthin chlorophyll a/c binding protein I (FCPI-1)

Chain U: 



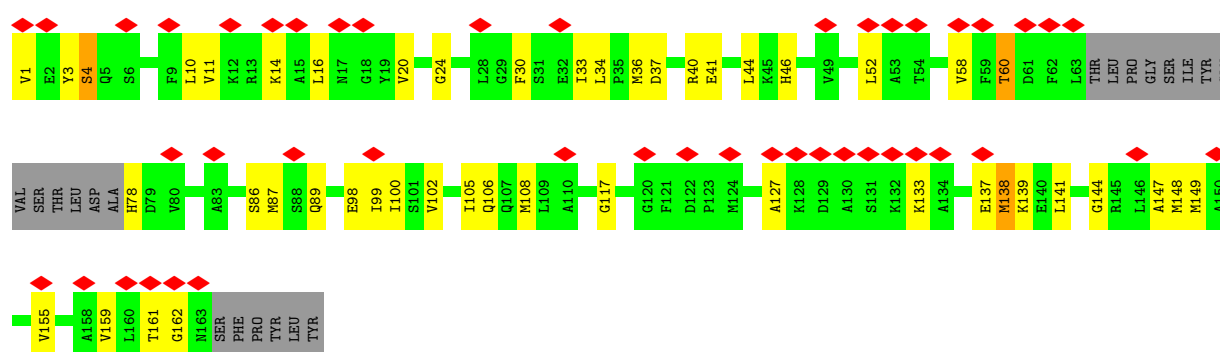
- Molecule 17: Fucoxanthin chlorophyll a/c binding protein VII (FCPI-7)

Chain G: 




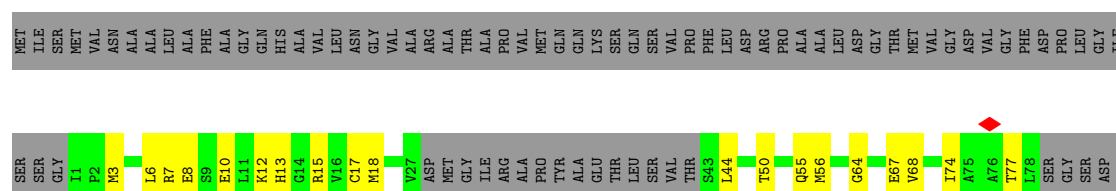
- Molecule 18: Fucoxanthin chlorophyll a/c binding protein VIII (FCPI-8)

Chain H: 



- Molecule 19: Fucoxanthin chlorophyll a/c binding protein V (FCPI-5)

Chain T: 





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	17450	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	0.480	Depositor
Minimum map value	-0.232	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.014	Depositor
Recommended contour level	0.07	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: CLA, DGD, LHG, SF4, BCR, CL0, LMG, DD6, A86, SQD, KC1, PQN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.24	0/6007	0.45	0/8185
2	B	0.23	0/6015	0.46	0/8205
3	C	0.20	0/609	0.44	0/826
4	D	0.24	0/1116	0.51	0/1503
5	E	0.21	0/505	0.38	0/689
6	F	0.22	0/1275	0.44	0/1728
7	I	0.25	0/273	0.53	0/373
8	J	0.23	0/313	0.53	0/427
9	L	0.29	0/1081	0.56	0/1470
10	M	0.19	0/218	0.30	0/295
11	O	0.29	0/1376	0.57	0/1865
12	P	0.25	0/1480	0.47	0/2010
13	Q	0.36	0/1285	0.65	1/1736 (0.1%)
14	R	0.23	0/681	0.40	0/930
15	S	0.23	0/1272	0.46	0/1732
16	U	0.26	0/1109	0.57	0/1499
17	G	1.35	1/1204 (0.1%)	0.80	2/1624 (0.1%)
18	H	0.44	0/1149	0.83	2/1546 (0.1%)
19	T	0.32	0/741	0.57	0/999
All	All	0.38	1/27709 (0.0%)	0.52	5/37642 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
13	Q	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	G	84	PRO	N-CD	45.36	2.11	1.47

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	G	84	PRO	N-CD-CG	-18.97	74.75	103.20
13	Q	165	PRO	CB-CA-C	-10.53	97.53	111.12
17	G	84	PRO	CA-N-CD	-9.21	99.11	112.00
18	H	159	VAL	N-CA-C	-8.01	105.39	112.12
18	H	155	VAL	N-CA-C	-6.60	106.40	111.62

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
13	Q	164	PHE	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	60	0
2	B	5805	0	5634	52	0
3	C	599	0	577	4	0
4	D	1092	0	1096	6	0
5	E	494	0	488	3	0
6	F	1246	0	1256	11	0
7	I	266	0	278	9	0
8	J	305	0	310	6	0
9	L	1056	0	1068	17	0
10	M	216	0	234	1	0
11	O	1341	0	1347	21	0
12	P	1441	0	1421	14	0
13	Q	1257	0	1260	15	0
14	R	664	0	668	4	0
15	S	1238	0	1217	13	0
16	U	1082	0	1058	16	0
17	G	1179	0	1166	25	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	H	1128	0	1134	34	0
19	T	731	0	749	23	0
20	A	2669	0	2699	70	0
20	B	2409	0	2457	61	0
20	F	94	0	69	4	0
20	G	561	0	486	17	0
20	H	459	0	403	15	0
20	J	42	0	31	1	0
20	L	164	0	150	2	0
20	O	495	0	475	11	0
20	P	403	0	337	9	0
20	Q	609	0	566	12	0
20	R	110	0	105	3	0
20	S	384	0	358	12	0
20	T	473	0	379	17	0
20	U	441	0	417	11	0
21	A	33	0	46	4	0
21	B	33	0	46	4	0
22	A	75	0	93	1	0
22	G	27	0	24	1	0
22	P	49	0	74	1	0
23	A	160	0	224	9	0
23	B	200	0	280	14	0
23	F	80	0	112	2	0
23	I	80	0	112	3	0
23	J	40	0	56	1	0
23	L	80	0	112	5	0
23	M	40	0	56	4	0
23	R	39	0	53	1	0
24	A	65	0	72	2	0
25	A	8	0	0	0	0
25	C	16	0	0	0	0
26	A	43	0	0	0	0
26	G	215	0	0	1	0
26	H	86	0	0	0	0
26	J	43	0	0	0	0
26	O	215	0	0	0	0
26	P	172	0	0	0	0
26	Q	86	0	0	0	0
26	S	215	0	0	0	0
26	T	86	0	0	0	0
26	U	112	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
27	B	60	0	81	0	0
28	B	50	0	67	0	0
28	S	46	0	56	5	0
29	I	49	0	68	2	0
29	J	39	0	48	1	0
29	P	59	0	57	5	0
29	Q	55	0	86	3	0
29	U	32	0	34	1	0
30	O	45	0	0	0	0
30	P	179	0	0	1	0
30	Q	45	0	0	0	0
30	S	90	0	0	0	0
30	T	45	0	0	0	0
30	U	45	0	0	0	0
31	P	48	0	0	0	0
31	Q	144	0	0	0	0
31	R	92	0	0	0	0
31	U	48	0	0	0	0
32	A	55	0	0	1	0
32	B	91	0	0	1	0
32	C	9	0	0	0	0
32	D	8	0	0	0	0
32	E	5	0	0	0	0
32	F	9	0	0	0	0
32	G	6	0	0	0	0
32	H	2	0	0	0	0
32	I	1	0	0	0	0
32	J	4	0	0	0	0
32	L	5	0	0	0	0
32	M	1	0	0	0	0
32	O	7	0	0	0	0
32	P	8	0	0	0	0
32	Q	3	0	0	0	0
32	R	4	0	0	0	0
32	S	5	0	0	0	0
32	T	2	0	0	0	0
32	U	4	0	0	0	0
All	All	39964	0	37448	499	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 (499) 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)
17:G:84:PRO:N	17:G:84:PRO:CD	2.11	1.02
18:H:161:THR:HG22	18:H:162:GLY:H	1.29	0.95
18:H:161:THR:HG22	18:H:162:GLY:N	1.83	0.92
9:L:47:LEU:HG	9:L:51:MET:HE2	1.58	0.85
18:H:161:THR:CG2	18:H:162:GLY:H	1.93	0.82
4:D:2:LEU:HD22	4:D:4:LEU:HD23	1.62	0.82
8:J:1:MET:HE2	18:H:106:GLN:HG3	1.64	0.80
20:A:822:CLA:H91	23:A:844:BCR:H23C	1.62	0.79
16:U:85:PHE:CE1	16:U:89:MET:HE3	2.15	0.79
18:H:41:GLU:OE2	18:H:105:ILE:HG12	1.83	0.79
17:G:20:GLY:HA2	17:G:141:MET:HE1	1.66	0.78
12:P:174:MET:HE3	12:P:177:ILE:HB	1.69	0.73
18:H:41:GLU:CD	18:H:105:ILE:HG12	2.13	0.72
20:U:205:CLA:H92	20:U:206:CLA:HMA1	1.72	0.72
20:A:804:CLA:H152	20:A:825:CLA:HBB2	1.72	0.71
20:A:803:CLA:H203	23:A:841:BCR:H10C	1.72	0.71
19:T:55:GLN:NE2	20:T:205:CLA:O1D	2.24	0.71
17:G:55:LEU:O	17:G:59:VAL:HB	1.90	0.70
17:G:34:ILE:HD13	20:G:206:CLA:H11	1.73	0.70
18:H:44:LEU:HD12	18:H:117:GLY:HA3	1.73	0.69
2:B:609:GLU:OE1	6:F:17:ARG:NH2	2.26	0.68
16:U:26:LYS:NZ	16:U:99:TYR:CD2	2.62	0.67
20:A:808:CLA:HBB2	20:A:811:CLA:HMA3	1.76	0.67
19:T:102:MET:HE2	20:T:207:CLA:HMA2	1.76	0.67
18:H:60:THR:HG23	20:H:207:CLA:HED2	1.77	0.67
13:Q:132:ALA:O	13:Q:136:MET:HG3	1.94	0.67
1:A:321:PRO:HB3	9:L:1:SER:HB2	1.76	0.66
23:A:843:BCR:H23C	20:A:847:CLA:HBC2	1.78	0.65
20:B:828:CLA:H111	6:F:93:ILE:HD11	1.78	0.65
20:Q:208:CLA:HBA1	29:Q:217:LMG:H342	1.78	0.64
1:A:206:GLN:HA	1:A:210:SER:HB2	1.80	0.64
19:T:56:MET:HG3	20:T:210:CLA:HBC3	1.80	0.64
9:L:47:LEU:O	9:L:51:MET:HG3	1.98	0.64
1:A:110:ILE:HG13	1:A:111:VAL:HG13	1.80	0.63
20:B:833:CLA:H161	23:L:201:BCR:H15C	1.82	0.62
18:H:16:LEU:HA	18:H:36:MET:HE2	1.81	0.62
1:A:490:ASN:HB2	20:A:831:CLA:HED2	1.81	0.62
20:A:845:CLA:HBC2	2:B:583:ASN:HB2	1.81	0.62
20:A:835:CLA:H101	8:J:17:THR:HG23	1.81	0.62
23:B:837:BCR:H322	29:Q:217:LMG:H151	1.82	0.62
2:B:158:LYS:HD2	11:O:116:LYS:NZ	2.15	0.62
16:U:82:PHE:O	16:U:86:MET:HG2	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:T:102:MET:CE	20:T:207:CLA:HMA2	2.31	0.61
23:B:839:BCR:HC22	11:O:167:THR:HB	1.82	0.61
20:B:846:CLA:H43	9:L:76:ILE:HD12	1.82	0.61
19:T:7:ARG:NH1	19:T:10:GLU:OE1	2.33	0.61
20:A:818:CLA:H101	23:A:844:BCR:H10C	1.84	0.60
19:T:119:ALA:O	19:T:123:ILE:HG13	2.01	0.60
15:S:42:THR:HG22	15:S:159:LEU:HD11	1.83	0.60
20:B:818:CLA:HMD2	23:B:837:BCR:HC7	1.83	0.59
6:F:113:LYS:HD2	6:F:116:GLU:HG3	1.84	0.59
2:B:9:ALA:HB1	3:C:70:SER:HB3	1.84	0.59
2:B:393:VAL:HG23	2:B:394:ARG:HG3	1.83	0.59
16:U:100:GLU:OE2	16:U:103:ASN:HB2	2.02	0.59
17:G:27:PRO:HB2	18:H:100:ILE:CD1	2.32	0.59
2:B:719:TYR:HB2	20:B:802:CLA:HED2	1.85	0.59
1:A:230:TYR:CE1	1:A:231:GLU:HG3	2.38	0.58
20:A:838:CLA:HED1	20:U:210:CLA:HAA2	1.85	0.58
23:B:838:BCR:H16C	20:O:205:CLA:H172	1.85	0.58
12:P:91:ILE:HG22	12:P:107:LYS:HD3	1.84	0.58
17:G:74:ASN:HD21	17:G:77:ALA:HB3	1.69	0.58
6:F:107:PHE:HB2	6:F:129:MET:HE1	1.86	0.57
18:H:37:ASP:HB3	18:H:108:MET:HE3	1.85	0.57
19:T:107:LEU:HD11	19:T:111:LYS:HE3	1.87	0.57
20:B:824:CLA:H11	23:B:838:BCR:H393	1.87	0.56
29:I:103:LMG:H352	20:S:214:CLA:H93	1.87	0.56
20:A:821:CLA:HBA1	20:A:825:CLA:H193	1.86	0.56
18:H:4:SER:HB2	18:H:24:GLY:HA3	1.85	0.56
19:T:18:MET:HE3	19:T:113:GLY:HA2	1.86	0.56
20:B:819:CLA:H3A	20:B:835:CLA:HED3	1.88	0.56
12:P:52:ALA:HB3	29:P:217:LMG:HC62	1.86	0.56
8:J:22:ILE:HG23	20:J:103:CLA:HBB2	1.86	0.56
12:P:53:ASN:HA	29:P:217:LMG:HC71	1.88	0.55
14:R:25:VAL:O	14:R:83:GLN:NE2	2.39	0.55
20:A:803:CLA:H72	23:A:842:BCR:HC8	1.88	0.55
4:D:85:ARG:HB2	4:D:95:LEU:HD11	1.87	0.55
18:H:41:GLU:OE1	18:H:105:ILE:HG12	2.06	0.55
19:T:112:ASN:OD1	20:T:201:CLA:HMD1	2.07	0.55
20:A:828:CLA:H142	23:B:841:BCR:H15C	1.88	0.54
1:A:338:TRP:HB3	20:A:803:CLA:HAC1	1.89	0.54
15:S:118:ALA:HB1	15:S:122:PRO:HB3	1.87	0.54
15:S:117:PRO:HB2	20:S:215:CLA:HED3	1.90	0.54
1:A:656:SER:HB2	2:B:443:ALA:HB1	1.87	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:G:205:CLA:HBC3	20:G:205:CLA:HHD	1.90	0.54
20:U:205:CLA:H71	20:U:206:CLA:HBB	1.89	0.54
4:D:43:PRO:HD3	4:D:68:LEU:HD13	1.90	0.54
17:G:105:LYS:HD2	17:G:110:ASP:HB2	1.90	0.54
20:B:830:CLA:H122	23:B:840:BCR:H311	1.91	0.53
17:G:110:ASP:OD1	17:G:110:ASP:N	2.40	0.53
20:O:208:CLA:HHC	20:O:208:CLA:HBB1	1.91	0.53
1:A:509:LYS:NZ	32:A:902:HOH:O	2.41	0.53
2:B:446:THR:O	2:B:446:THR:OG1	2.25	0.53
17:G:75:PRO:HD2	17:G:161:VAL:HG11	1.91	0.53
2:B:297:HIS:HB3	2:B:302:ILE:HD11	1.91	0.53
1:A:522:PHE:HA	20:A:833:CLA:HED1	1.90	0.53
1:A:238:LEU:HD12	1:A:238:LEU:O	2.09	0.53
12:P:188:ILE:O	12:P:191:SER:OG	2.25	0.53
13:Q:107:MET:HG3	13:Q:114:ARG:O	2.09	0.53
20:S:205:CLA:HBB2	20:S:214:CLA:HAB	1.91	0.53
11:O:54:GLN:HE22	20:O:208:CLA:HHD	1.74	0.53
2:B:501:SER:HB2	2:B:503:LYS:NZ	2.24	0.52
20:U:209:CLA:HHC	20:U:209:CLA:HBB1	1.91	0.52
1:A:527:ILE:HD12	24:A:848:CL0:H63	1.91	0.52
20:B:819:CLA:HBB2	20:B:835:CLA:H52	1.91	0.52
16:U:13:PRO:HD2	26:U:203:DD6:O4	2.09	0.52
2:B:19:ILE:HG12	7:I:30:ILE:HD12	1.91	0.52
29:I:103:LMG:H401	29:I:103:LMG:H201	1.90	0.52
9:L:28:LEU:O	9:L:32:ASN:ND2	2.33	0.52
20:Q:203:CLA:HHC	20:Q:203:CLA:HBB1	1.92	0.52
20:S:206:CLA:HHC	20:S:206:CLA:HBB1	1.92	0.52
20:G:205:CLA:H72	20:G:206:CLA:H142	1.91	0.52
5:E:5:SER:OG	5:E:59:GLU:OE1	2.27	0.52
18:H:1:VAL:HG12	18:H:3:TYR:CE1	2.44	0.52
19:T:56:MET:SD	20:T:204:CLA:H3A	2.50	0.52
18:H:20:VAL:O	18:H:40:ARG:NH2	2.43	0.52
20:A:817:CLA:HHC	20:A:817:CLA:HBB1	1.92	0.52
20:F:803:CLA:HHC	20:F:803:CLA:HBB1	1.92	0.52
20:A:835:CLA:HHC	20:A:835:CLA:HBB1	1.93	0.51
20:B:848:CLA:HHC	20:B:848:CLA:HBB1	1.92	0.51
20:Q:207:CLA:HHC	20:Q:207:CLA:HBB1	1.91	0.51
20:T:211:CLA:HHC	20:T:211:CLA:HBB1	1.92	0.51
9:L:47:LEU:HG	9:L:51:MET:CE	2.35	0.51
20:B:833:CLA:HBB2	21:B:836:PQN:H141	1.90	0.51
20:T:206:CLA:HHC	20:T:206:CLA:HBB1	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:A:853:CLA:HHC	20:A:853:CLA:HBB1	1.92	0.51
2:B:273:HIS:HB3	20:B:815:CLA:HMB2	1.92	0.51
18:H:102:VAL:HG22	20:H:204:CLA:HMA1	1.91	0.51
1:A:150:TRP:CD1	20:A:814:CLA:HAA2	2.46	0.51
20:U:208:CLA:HHC	20:U:208:CLA:HBB1	1.93	0.51
20:T:201:CLA:HHC	20:T:201:CLA:HBB1	1.92	0.51
2:B:158:LYS:HD2	11:O:116:LYS:HZ1	1.74	0.51
20:A:854:CLA:H92	20:A:854:CLA:HAA1	1.92	0.51
11:O:157:ILE:HG22	20:O:211:CLA:HBB1	1.91	0.51
16:U:30:GLU:HG3	16:U:99:TYR:OH	2.11	0.51
18:H:20:VAL:HG21	18:H:137:GLU:OE1	2.11	0.51
20:O:207:CLA:HHC	20:O:207:CLA:HBB1	1.93	0.51
20:S:205:CLA:HHC	20:S:205:CLA:HBB1	1.92	0.51
1:A:25:SER:HB3	1:A:28:LEU:HB2	1.94	0.50
20:A:836:CLA:HHC	20:A:836:CLA:HBB1	1.93	0.50
2:B:96:GLN:O	2:B:100:LYS:HG2	2.11	0.50
1:A:495:THR:HG22	20:A:815:CLA:H11	1.93	0.50
20:A:845:CLA:HBB	20:B:802:CLA:H202	1.93	0.50
12:P:174:MET:CE	12:P:177:ILE:HB	2.39	0.50
20:P:210:CLA:HHC	20:P:210:CLA:HBB1	1.93	0.50
20:Q:212:CLA:H143	29:Q:217:LMG:H401	1.94	0.50
20:G:201:CLA:HHC	20:G:201:CLA:HBB1	1.92	0.50
20:A:847:CLA:HHC	20:A:847:CLA:HBB1	1.92	0.50
20:B:821:CLA:H171	20:B:827:CLA:HBC1	1.93	0.50
20:B:846:CLA:HHC	20:B:846:CLA:HBB1	1.93	0.50
11:O:131:ILE:HD11	20:O:209:CLA:HED2	1.94	0.50
12:P:135:PHE:HZ	29:P:217:LMG:HC2	1.77	0.50
20:P:214:CLA:HHC	20:P:214:CLA:HBB1	1.92	0.50
18:H:148:MET:HE1	20:H:206:CLA:HHC	1.93	0.50
15:S:52:PRO:O	15:S:77:ASN:ND2	2.45	0.50
20:H:201:CLA:HHC	20:H:201:CLA:HBB1	1.92	0.50
20:A:810:CLA:HHC	20:A:810:CLA:HBB1	1.94	0.50
20:B:829:CLA:HHC	20:B:829:CLA:HBB1	1.92	0.50
20:P:213:CLA:HHC	20:P:213:CLA:HBB1	1.93	0.50
20:Q:204:CLA:HHC	20:Q:204:CLA:HBB1	1.94	0.50
20:A:824:CLA:H121	20:A:826:CLA:H18	1.92	0.50
20:H:208:CLA:HHC	20:H:208:CLA:HBB1	1.93	0.50
20:A:833:CLA:H121	20:A:852:CLA:H193	1.94	0.50
20:G:215:CLA:HHC	20:G:215:CLA:HBB1	1.93	0.50
20:A:820:CLA:HHC	20:A:820:CLA:HBB1	1.93	0.50
9:L:32:ASN:HB3	20:L:202:CLA:HAC1	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:G:203:CLA:HHC	20:G:203:CLA:HBB1	1.93	0.50
20:B:833:CLA:HHC	20:B:833:CLA:HBB1	1.94	0.49
16:U:85:PHE:CD1	16:U:89:MET:HE3	2.47	0.49
20:G:208:CLA:HHC	20:G:208:CLA:HBB1	1.94	0.49
1:A:397:HIS:HA	1:A:400:ILE:HD12	1.93	0.49
2:B:13:ASP:OD2	3:C:71:GLU:HB2	2.11	0.49
20:B:848:CLA:HBA1	13:Q:101:THR:HG21	1.94	0.49
19:T:112:ASN:OD1	20:T:201:CLA:CMD	2.60	0.49
3:C:5:ARG:HE	4:D:138:ASP:HB3	1.76	0.49
15:S:53:SER:O	15:S:53:SER:OG	2.25	0.49
19:T:50:THR:HG21	20:T:204:CLA:H2A	1.94	0.49
20:A:838:CLA:HMD1	29:U:201:LMG:HC72	1.94	0.49
20:B:835:CLA:HBB2	20:R:104:CLA:O2A	2.12	0.49
2:B:346:VAL:HG21	20:B:824:CLA:HHD	1.94	0.49
18:H:144:GLY:HA2	18:H:147:ALA:HB3	1.94	0.49
20:R:101:CLA:HHC	20:R:101:CLA:HBB1	1.95	0.49
20:U:211:CLA:HBB1	20:U:211:CLA:HHC	1.94	0.49
19:T:17:CYS:SG	19:T:117:MET:HA	2.53	0.49
20:B:808:CLA:HHC	20:B:808:CLA:HBB1	1.94	0.49
11:O:139:GLU:OE1	11:O:139:GLU:O	2.31	0.49
12:P:24:ILE:HD13	12:P:57:ALA:HB1	1.95	0.49
15:S:154:THR:O	15:S:154:THR:OG1	2.28	0.49
20:A:815:CLA:HHC	20:A:815:CLA:HBB1	1.94	0.48
20:A:831:CLA:HHC	20:A:831:CLA:HBB1	1.95	0.48
11:O:135:CYS:HB3	11:O:144:MET:HG3	1.94	0.48
13:Q:92:LEU:HD12	20:Q:216:CLA:H41	1.94	0.48
20:H:204:CLA:HHC	20:H:204:CLA:HBB1	1.94	0.48
11:O:98:LEU:HD23	20:O:207:CLA:HBC3	1.96	0.48
12:P:72:MET:HE2	12:P:172:GLY:CA	2.43	0.48
20:A:814:CLA:HHC	20:A:814:CLA:HBB1	1.95	0.48
19:T:12:LYS:HE2	19:T:67:GLU:OE1	2.14	0.48
1:A:371:ILE:HD12	1:A:509:LYS:HB3	1.94	0.48
21:A:837:PQN:H141	20:A:853:CLA:HBB2	1.95	0.48
20:B:830:CLA:H52	20:F:803:CLA:HBB2	1.95	0.48
1:A:108:TRP:CD2	20:A:807:CLA:HED3	2.49	0.48
20:A:854:CLA:HHC	20:A:854:CLA:HBB1	1.95	0.48
2:B:629:LEU:HD22	2:B:722:PHE:HA	1.95	0.48
20:Q:205:CLA:H41	20:Q:206:CLA:H3A	1.95	0.48
1:A:350:GLY:HA2	1:A:387:GLY:HA2	1.96	0.48
20:B:822:CLA:HBB1	20:B:822:CLA:HHC	1.94	0.48
17:G:141:MET:HB3	20:G:202:CLA:HED2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:225:GLU:OE1	1:A:225:GLU:N	2.46	0.48
2:B:266:MET:HE1	20:B:815:CLA:HED3	1.96	0.48
2:B:405:VAL:O	2:B:409:MET:HG2	2.14	0.48
17:G:141:MET:O	17:G:145:LYS:HG3	2.14	0.48
1:A:253:PHE:HE1	20:A:846:CLA:HBB1	1.78	0.47
2:B:1:THR:HG22	2:B:11:ALA:O	2.14	0.47
13:Q:108:MET:HE3	13:Q:108:MET:HB3	1.73	0.47
18:H:133:LYS:O	18:H:137:GLU:HG3	2.13	0.47
10:M:8:PHE:HB3	23:M:101:BCR:H381	1.95	0.47
12:P:166:LEU:HD13	12:P:170:LYS:HD2	1.96	0.47
16:U:52:TRP:CE2	16:U:54:PRO:HG3	2.49	0.47
16:U:68:ILE:HD13	26:U:203:DD6:O2	2.15	0.47
1:A:333:ILE:HG13	1:A:410:GLN:HE22	1.80	0.47
1:A:463:ASP:OD1	1:A:469:GLN:NE2	2.48	0.47
20:B:819:CLA:HBB	20:B:835:CLA:O1D	2.15	0.47
20:O:202:CLA:HHC	20:O:202:CLA:HBB1	1.96	0.47
1:A:119:ASP:OD1	6:F:32:TYR:OH	2.30	0.47
20:A:813:CLA:HHC	20:A:813:CLA:HBB1	1.97	0.47
2:B:409:MET:HG3	23:R:102:BCR:H402	1.97	0.47
2:B:501:SER:HB2	2:B:503:LYS:HZ2	1.80	0.47
20:B:846:CLA:HBA2	9:L:66:PRO:HG3	1.96	0.47
1:A:240:ALA:CB	1:A:247:LYS:HD3	2.45	0.47
20:P:207:CLA:H61	20:P:207:CLA:H41	1.77	0.47
20:S:202:CLA:HHC	20:S:202:CLA:HBB1	1.96	0.47
1:A:382:HIS:HE1	20:A:824:CLA:ND	2.13	0.47
20:B:810:CLA:H52	20:B:811:CLA:HBC2	1.97	0.47
18:H:1:VAL:HG12	18:H:3:TYR:HE1	1.79	0.47
20:B:815:CLA:HHC	20:B:815:CLA:HBB1	1.95	0.47
9:L:53:HIS:HA	9:L:56:PHE:CE2	2.49	0.47
18:H:138:MET:HE2	18:H:138:MET:HB2	1.79	0.47
20:A:833:CLA:HHC	20:A:833:CLA:HBB1	1.96	0.46
11:O:144:MET:HE3	11:O:144:MET:HB3	1.76	0.46
1:A:9:ASP:N	1:A:172:LYS:O	2.43	0.46
1:A:358:HIS:HA	1:A:361:TYR:CD2	2.51	0.46
20:A:834:CLA:HHC	20:A:834:CLA:HBB1	1.96	0.46
2:B:143:LEU:HD13	20:B:812:CLA:H71	1.98	0.46
20:B:825:CLA:H41	20:B:825:CLA:H61	1.75	0.46
17:G:160:GLN:HA	17:G:163:ILE:HG12	1.97	0.46
2:B:342:ALA:HB2	20:B:820:CLA:H43	1.96	0.46
20:B:824:CLA:H12	20:B:824:CLA:HBA2	1.63	0.46
20:B:845:CLA:HBB1	20:B:845:CLA:HHC	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:S:137:GLY:O	15:S:141:MET:HG3	2.16	0.46
1:A:172:LYS:HB3	1:A:172:LYS:HE3	1.68	0.46
2:B:178:SER:HB3	2:B:286:GLY:HA3	1.97	0.46
20:B:809:CLA:H91	20:B:809:CLA:H112	1.72	0.46
9:L:86:LEU:HD11	15:S:94:LEU:HD22	1.97	0.46
19:T:3:MET:HE2	19:T:3:MET:HB2	1.82	0.46
20:T:210:CLA:HHC	20:T:210:CLA:HBB1	1.96	0.46
20:A:854:CLA:H152	20:H:205:CLA:HBB2	1.98	0.46
2:B:54:ILE:HD11	23:M:101:BCR:HC8	1.97	0.46
20:B:834:CLA:H41	20:B:834:CLA:H61	1.52	0.46
14:R:46:ALA:HA	14:R:50:LEU:HD12	1.98	0.46
20:B:833:CLA:H3A	21:B:836:PQN:H293	1.97	0.46
9:L:85:ILE:HG12	9:L:126:ALA:HB1	1.98	0.46
23:L:201:BCR:H15C	23:L:201:BCR:H351	1.83	0.46
2:B:534:LYS:O	2:B:538:ASP:HB2	2.15	0.46
20:B:813:CLA:H12	23:B:837:BCR:H272	1.97	0.46
18:H:30:PHE:HE2	20:H:206:CLA:H72	1.80	0.46
20:A:838:CLA:HED2	20:A:838:CLA:HBD	1.81	0.46
2:B:449:LYS:HB3	2:B:449:LYS:HE2	1.77	0.46
9:L:51:MET:HB3	23:L:205:BCR:H12C	1.97	0.46
20:P:208:CLA:H41	20:P:208:CLA:H61	1.67	0.46
18:H:149:MET:HE2	18:H:149:MET:HB2	1.89	0.46
20:G:206:CLA:HBB2	26:G:214:DD6:C5	2.46	0.46
1:A:309:HIS:HB3	1:A:314:ILE:HD11	1.97	0.45
11:O:126:ASP:OD2	11:O:131:ILE:HG13	2.17	0.45
1:A:186:MET:HB2	20:A:811:CLA:HBC2	1.99	0.45
20:B:809:CLA:H201	7:I:19:PRO:HA	1.98	0.45
11:O:56:MET:SD	11:O:151:HIS:HB3	2.57	0.45
20:B:818:CLA:HBB1	20:B:818:CLA:HHC	1.98	0.45
20:U:210:CLA:H141	20:U:210:CLA:H162	1.73	0.45
1:A:573:CYS:HB2	2:B:665:TRP:HB3	1.97	0.45
2:B:38:GLU:HA	2:B:163:LEU:HD13	1.98	0.45
9:L:24:THR:O	9:L:28:LEU:HG	2.17	0.45
13:Q:24:PHE:HE1	20:Q:203:CLA:HBC3	1.81	0.45
20:U:205:CLA:H141	20:U:205:CLA:H161	1.68	0.45
17:G:51:MET:HE1	20:G:204:CLA:CAB	2.47	0.45
18:H:41:GLU:OE2	18:H:105:ILE:CG1	2.60	0.45
2:B:656:ALA:HB3	20:B:803:CLA:HBB2	1.98	0.45
8:J:23:THR:HA	8:J:26:PHE:CE2	2.51	0.45
15:S:10:PHE:HD1	28:S:201:SQD:H111	1.81	0.45
15:S:66:LEU:HD22	20:S:202:CLA:HMA1	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:U:56:TYR:HE2	20:U:207:CLA:HBA1	1.82	0.45
17:G:33:TYR:OH	22:G:216:LHG:HC42	2.17	0.45
1:A:65:ALA:HB2	20:A:802:CLA:HMA1	1.98	0.45
16:U:66:VAL:HG12	16:U:70:GLN:NE2	2.31	0.45
19:T:74:ILE:HA	19:T:77:THR:HG22	1.98	0.45
1:A:55:LEU:HD23	1:A:177:LEU:HD21	1.98	0.45
20:A:854:CLA:H171	20:H:205:CLA:HBB2	1.99	0.45
17:G:27:PRO:HB2	18:H:100:ILE:HD12	1.98	0.45
17:G:77:ALA:O	17:G:81:SER:OG	2.25	0.45
18:H:52:LEU:HB3	20:H:207:CLA:HBB1	1.98	0.45
19:T:64:GLY:O	19:T:68:VAL:HG23	2.16	0.45
20:S:206:CLA:HAA2	20:S:206:CLA:HED2	1.99	0.45
20:A:818:CLA:HBC3	20:A:823:CLA:H172	1.99	0.45
23:A:842:BCR:H361	23:A:842:BCR:H20C	1.81	0.45
12:P:154:MET:HB2	20:P:211:CLA:HAA2	1.98	0.45
20:R:104:CLA:H41	20:R:104:CLA:H61	1.76	0.45
20:L:202:CLA:HBA2	20:L:202:CLA:H3A	1.80	0.44
16:U:91:GLN:O	16:U:95:GLN:HG3	2.16	0.44
20:H:207:CLA:HBB1	20:H:207:CLA:HHC	1.99	0.44
6:F:143:GLU:HG3	6:F:148:GLN:HB2	1.98	0.44
23:F:804:BCR:H361	23:F:804:BCR:H20C	1.73	0.44
23:L:201:BCR:H20C	23:L:201:BCR:H361	1.79	0.44
20:G:208:CLA:H61	20:G:208:CLA:H2	1.72	0.44
1:A:138:ARG:HD3	1:A:367:PRO:HB2	1.98	0.44
2:B:423:VAL:HG23	20:B:831:CLA:HBB1	1.98	0.44
15:S:15:LYS:HB3	15:S:15:LYS:HE2	1.79	0.44
17:G:13:SER:OG	20:G:207:CLA:O2D	2.34	0.44
5:E:42:VAL:HG12	5:E:48:ALA:HB2	2.00	0.44
2:B:339:LEU:O	2:B:343:THR:OG1	2.34	0.44
23:L:205:BCR:H20C	23:L:205:BCR:H361	1.78	0.44
13:Q:91:MET:HE1	20:Q:212:CLA:H191	1.98	0.44
2:B:271:ILE:HG23	20:B:816:CLA:HMA3	1.99	0.44
20:B:830:CLA:H11	20:B:830:CLA:H51	1.86	0.44
20:B:848:CLA:H3A	20:B:848:CLA:HBA2	1.80	0.44
7:I:1:MET:HG2	20:S:214:CLA:CGA	2.47	0.44
11:O:46:GLU:CD	11:O:123:HIS:HE2	2.26	0.44
20:O:205:CLA:H91	20:O:205:CLA:H112	1.72	0.44
20:A:847:CLA:H152	20:A:847:CLA:H112	1.69	0.44
20:B:844:CLA:H142	20:B:844:CLA:H112	1.77	0.44
5:E:3:ARG:HH21	5:E:26:ILE:H	1.65	0.44
17:G:86:ALA:O	17:G:90:ILE:HG13	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:130:MET:HG2	20:F:802:CLA:OBD	2.18	0.44
23:B:839:BCR:H20C	23:B:839:BCR:H361	1.87	0.43
11:O:131:ILE:HA	11:O:135:CYS:SG	2.58	0.43
20:H:206:CLA:H62	20:H:206:CLA:H41	1.80	0.43
20:B:807:CLA:HHB	20:B:808:CLA:HMB3	2.00	0.43
13:Q:61:LEU:HD23	13:Q:61:LEU:HA	1.60	0.43
13:Q:86:MET:HE2	13:Q:86:MET:HA	1.99	0.43
13:Q:134:LYS:NZ	13:Q:134:LYS:HB3	2.32	0.43
1:A:230:TYR:CD1	1:A:231:GLU:HG3	2.53	0.43
7:I:27:PHE:O	7:I:31:GLU:HG2	2.18	0.43
1:A:230:TYR:CD1	1:A:230:TYR:C	2.96	0.43
20:A:810:CLA:H62	20:A:810:CLA:H41	1.86	0.43
20:A:849:CLA:H172	6:F:101:GLY:HA2	2.00	0.43
9:L:25:ALA:HB2	16:U:104:PHE:HB3	1.99	0.43
11:O:62:PHE:CE2	11:O:166:GLU:HG3	2.53	0.43
17:G:7:PHE:HE2	18:H:100:ILE:HG22	1.83	0.43
17:G:127:LEU:HD12	17:G:129:TYR:HE1	1.83	0.43
19:T:12:LYS:NZ	20:T:206:CLA:O1D	2.48	0.43
2:B:74:GLN:NE2	32:B:908:HOH:O	2.51	0.43
20:B:809:CLA:H161	20:B:809:CLA:H141	1.83	0.43
23:M:101:BCR:H11C	23:M:101:BCR:H341	1.88	0.43
20:B:822:CLA:HED1	20:B:829:CLA:HAB	2.01	0.43
18:H:14:LYS:HA	18:H:14:LYS:HD3	1.88	0.43
1:A:46:HIS:CD2	20:A:803:CLA:HBB2	2.53	0.43
23:A:843:BCR:H20C	23:A:843:BCR:H361	1.78	0.43
6:F:71:LEU:HD22	6:F:82:GLU:HG2	1.99	0.43
13:Q:31:ASP:OD1	13:Q:31:ASP:N	2.52	0.43
20:G:209:CLA:H102	20:G:209:CLA:H61	1.87	0.43
4:D:27:LYS:HG3	4:D:86:ILE:HB	2.01	0.43
6:F:76:ARG:HG3	20:F:803:CLA:HMD3	2.01	0.43
23:I:101:BCR:H15C	23:I:101:BCR:H351	1.88	0.43
20:S:214:CLA:H122	20:S:214:CLA:H162	1.82	0.43
19:T:113:GLY:O	19:T:117:MET:HG3	2.19	0.43
2:B:393:VAL:HG21	2:B:553:TYR:HB2	1.99	0.43
2:B:688:LEU:HD11	9:L:109:LEU:HD23	1.99	0.43
20:B:816:CLA:H91	20:B:816:CLA:H111	1.86	0.43
8:J:18:ALA:HB2	29:J:102:LMG:H181	2.00	0.43
20:S:202:CLA:H151	20:S:202:CLA:H112	1.78	0.43
17:G:59:VAL:HG11	20:G:209:CLA:HBC3	2.00	0.43
19:T:118:LEU:HD11	20:T:202:CLA:HAC1	2.00	0.43
1:A:151:THR:HG22	23:A:841:BCR:HC32	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:670:ALA:HB3	20:A:801:CLA:HBB2	2.00	0.43
2:B:20:TRP:CG	2:B:702:GLN:HE22	2.36	0.43
2:B:308:PRO:HD2	2:B:313:LEU:HB2	2.00	0.43
16:U:36:GLY:O	16:U:40:MET:HG3	2.18	0.43
18:H:78:HIS:CD2	18:H:87:MET:HE1	2.53	0.43
18:H:127:ALA:HB1	18:H:133:LYS:HG3	2.01	0.43
1:A:286:HIS:HE2	20:A:816:CLA:C2B	2.31	0.42
11:O:46:GLU:OE2	11:O:113:ILE:HG22	2.18	0.42
11:O:122:GLU:OE2	11:O:122:GLU:N	2.51	0.42
21:A:837:PQN:H18	21:A:837:PQN:H222	1.82	0.42
23:A:843:BCR:H15C	23:A:843:BCR:H351	1.90	0.42
20:P:213:CLA:H2A	20:P:213:CLA:HED2	2.00	0.42
20:H:206:CLA:H93	20:H:206:CLA:H61	1.82	0.42
7:I:17:ILE:HD11	20:S:202:CLA:HBB1	2.01	0.42
1:A:64:SER:OG	1:A:170:TYR:HB2	2.20	0.42
1:A:402:MET:HE1	1:A:420:LEU:HD11	2.02	0.42
1:A:734:LEU:HD23	1:A:734:LEU:HA	1.79	0.42
2:B:312:ARG:HD2	29:P:217:LMG:HC3	2.02	0.42
23:B:838:BCR:H20C	23:B:838:BCR:H361	1.81	0.42
13:Q:47:ARG:HA	13:Q:50:MET:HE3	2.01	0.42
20:Q:216:CLA:H62	20:Q:216:CLA:H93	1.78	0.42
20:H:208:CLA:HED2	20:H:208:CLA:HBD	1.89	0.42
2:B:387:HIS:HA	2:B:390:ILE:HD12	2.01	0.42
13:Q:86:MET:HE3	20:Q:216:CLA:H3A	2.01	0.42
20:H:203:CLA:H62	20:H:203:CLA:H41	1.75	0.42
20:A:847:CLA:H91	20:A:847:CLA:H111	1.80	0.42
23:M:101:BCR:H15C	23:M:101:BCR:H351	1.82	0.42
22:P:201:LHG:H261	29:P:217:LMG:H121	2.00	0.42
17:G:107:SER:OG	17:G:108:SER:N	2.53	0.42
1:A:323:THR:HG21	22:A:840:LHG:HC11	2.01	0.42
2:B:484:THR:O	2:B:488:SER:HB3	2.20	0.42
11:O:110:ALA:HB2	20:O:208:CLA:HMA1	2.02	0.42
13:Q:7:PHE:CD2	13:Q:8:VAL:HG13	2.55	0.42
20:G:209:CLA:H2	20:G:209:CLA:H62	1.79	0.42
1:A:32:PRO:HB3	1:A:37:TRP:CE3	2.55	0.42
20:A:849:CLA:H93	20:A:849:CLA:H61	1.87	0.42
2:B:695:PRO:O	3:C:80:TYR:OH	2.36	0.42
20:B:808:CLA:H143	20:B:808:CLA:H161	1.90	0.42
1:A:521:ASP:HA	1:A:524:VAL:HG12	2.02	0.42
20:A:833:CLA:H51	20:A:833:CLA:H11	1.88	0.42
4:D:27:LYS:HB2	4:D:27:LYS:HE3	1.79	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:Q:12:LYS:HB3	13:Q:12:LYS:HE2	1.76	0.42
14:R:46:ALA:HB1	14:R:51:LEU:HD12	2.02	0.42
17:G:163:ILE:HG22	20:G:210:CLA:HED2	2.02	0.42
1:A:358:HIS:HA	1:A:361:TYR:HD2	1.85	0.41
2:B:295:ILE:HG13	20:B:848:CLA:HED3	2.02	0.41
2:B:353:LEU:HD22	20:B:815:CLA:HBA1	2.01	0.41
2:B:578:MET:HG3	2:B:708:LEU:HD21	2.02	0.41
20:B:833:CLA:CBB	21:B:836:PQN:H141	2.50	0.41
17:G:55:LEU:HB3	20:G:209:CLA:HBC2	2.01	0.41
1:A:76:TRP:O	1:A:80:MET:HG2	2.20	0.41
1:A:293:LEU:HD23	1:A:293:LEU:HA	1.89	0.41
20:A:816:CLA:HBB2	20:A:816:CLA:H151	2.01	0.41
20:B:807:CLA:H122	20:B:807:CLA:H161	1.65	0.41
20:B:835:CLA:HED1	20:B:844:CLA:HHC	2.01	0.41
19:T:13:HIS:O	19:T:17:CYS:HB2	2.20	0.41
1:A:192:ALA:HB2	1:A:298:GLY:HA3	2.02	0.41
1:A:736:ARG:O	1:A:740:VAL:HG22	2.20	0.41
23:B:838:BCR:H11C	23:B:838:BCR:H341	1.91	0.41
23:I:102:BCR:H20C	23:I:102:BCR:H361	1.87	0.41
23:J:104:BCR:H20C	23:J:104:BCR:H361	1.87	0.41
17:G:45:LYS:HE3	17:G:45:LYS:HB2	1.85	0.41
18:H:98:GLU:O	18:H:102:VAL:HG23	2.21	0.41
20:A:804:CLA:HHC	20:A:804:CLA:HAB	1.90	0.41
2:B:173:LEU:HD12	2:B:173:LEU:HA	1.88	0.41
20:A:811:CLA:H61	20:A:811:CLA:H102	1.75	0.41
21:A:837:PQN:H111	21:A:837:PQN:H2M1	1.90	0.41
7:I:29:LEU:HD11	28:S:201:SQD:H101	2.02	0.41
9:L:74:LEU:HD13	9:L:74:LEU:HA	1.96	0.41
11:O:136:ASN:HB3	11:O:140:LYS:HZ1	1.85	0.41
15:S:51:ILE:HD13	15:S:78:GLU:HG3	2.02	0.41
20:U:205:CLA:H8	20:U:205:CLA:H51	1.89	0.41
1:A:239:MET:HE3	1:A:239:MET:HB3	1.90	0.41
24:A:848:CL0:H14	24:A:848:CL0:H2	1.83	0.41
20:A:852:CLA:H41	20:A:852:CLA:H61	1.80	0.41
11:O:149:LEU:HD12	11:O:149:LEU:HA	1.94	0.41
15:S:10:PHE:HA	28:S:201:SQD:H81	2.01	0.41
20:A:811:CLA:H61	20:A:811:CLA:H41	1.87	0.41
20:A:818:CLA:H122	20:A:847:CLA:H92	2.03	0.41
20:A:829:CLA:H203	20:A:833:CLA:H193	2.02	0.41
16:U:94:MET:HA	16:U:99:TYR:CD1	2.56	0.41
1:A:70:LEU:HD22	20:A:803:CLA:H92	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:A:829:CLA:H203	20:A:829:CLA:H162	1.89	0.41
23:I:102:BCR:H351	23:I:102:BCR:H15C	1.85	0.41
20:O:211:CLA:HBB1	20:O:211:CLA:HHC	2.03	0.41
12:P:69:ARG:HA	12:P:72:MET:HE3	2.01	0.41
12:P:174:MET:HE3	12:P:174:MET:HA	2.03	0.41
20:P:208:CLA:H92	20:P:208:CLA:H62	1.93	0.41
18:H:33:ILE:HG22	18:H:34:LEU:HG	2.03	0.41
20:B:819:CLA:CBB	20:B:835:CLA:H52	2.50	0.41
11:O:136:ASN:HB3	11:O:140:LYS:NZ	2.36	0.41
12:P:170:LYS:HD3	30:P:206:KC1:C3D	2.51	0.41
20:U:205:CLA:H112	20:U:205:CLA:H151	1.95	0.41
19:T:15:ARG:HD3	20:T:207:CLA:CHD	2.51	0.41
1:A:381:THR:HG23	1:A:596:ILE:HG21	2.04	0.40
1:A:431:ASN:HD22	2:B:672:LEU:HD11	1.87	0.40
1:A:726:ILE:HG23	20:A:824:CLA:HAB	2.03	0.40
23:B:837:BCR:H361	23:B:837:BCR:H20C	1.84	0.40
7:I:25:LEU:HD21	28:S:201:SQD:H121	2.02	0.40
1:A:278:LEU:HD21	1:A:363:MET:HB3	2.02	0.40
20:A:811:CLA:HAA2	20:A:821:CLA:H52	2.04	0.40
21:A:837:PQN:H243	21:A:837:PQN:H211	1.85	0.40
2:B:2:LYS:HD2	7:I:34:GLU:HG2	2.02	0.40
20:B:814:CLA:H61	20:B:814:CLA:H41	1.88	0.40
21:B:836:PQN:H2M1	21:B:836:PQN:H111	1.90	0.40
23:B:837:BCR:H15C	23:B:837:BCR:H351	1.97	0.40
6:F:123:VAL:HG22	8:J:15:LEU:HD11	2.03	0.40
23:F:801:BCR:H11C	23:F:801:BCR:H341	1.96	0.40
14:R:8:TRP:CE2	14:R:14:PRO:HG3	2.57	0.40
1:A:503:VAL:HG22	1:A:513:MET:HB2	2.04	0.40
23:B:838:BCR:H15C	23:B:838:BCR:H351	1.83	0.40
19:T:6:LEU:HD13	20:T:202:CLA:H3A	2.03	0.40
20:T:204:CLA:HHC	20:T:204:CLA:HAB	1.94	0.40
1:A:7:ASP:OD2	1:A:176:LYS:HE3	2.21	0.40
20:A:835:CLA:H92	20:A:851:CLA:H171	2.04	0.40
20:A:835:CLA:H172	20:A:835:CLA:H13	1.85	0.40
20:B:808:CLA:H142	20:B:808:CLA:HMB2	2.04	0.40
9:L:75:LEU:HD23	9:L:75:LEU:HA	1.93	0.40
20:P:214:CLA:HBA2	20:P:214:CLA:H3A	1.83	0.40
1:A:69:GLN:HG2	20:A:803:CLA:H3A	2.02	0.40
20:A:824:CLA:H61	20:A:824:CLA:H102	1.54	0.40
2:B:306:HIS:HE1	20:B:844:CLA:ND	2.16	0.40
2:B:522:ALA:HB2	20:B:831:CLA:HMA1	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:650:PHE:O	2:B:654:ILE:HG13	2.21	0.40
20:B:826:CLA:HHC	20:B:826:CLA:HAB	1.94	0.40
7:I:29:LEU:HB3	28:S:201:SQD:H242	2.03	0.40
20:Q:213:CLA:H61	20:Q:213:CLA:H41	1.99	0.40
16:U:86:MET:HE3	16:U:86:MET:HA	2.03	0.40
18:H:46:HIS:HB3	18:H:148:MET:SD	2.61	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	739/752 (98%)	718 (97%)	20 (3%)	1 (0%)	48	57
2	B	730/734 (100%)	713 (98%)	17 (2%)	0	100	100
3	C	78/81 (96%)	77 (99%)	1 (1%)	0	100	100
4	D	136/142 (96%)	127 (93%)	9 (7%)	0	100	100
5	E	62/67 (92%)	62 (100%)	0	0	100	100
6	F	159/184 (86%)	156 (98%)	3 (2%)	0	100	100
7	I	32/35 (91%)	32 (100%)	0	0	100	100
8	J	37/39 (95%)	37 (100%)	0	0	100	100
9	L	138/141 (98%)	136 (99%)	2 (1%)	0	100	100
10	M	27/29 (93%)	27 (100%)	0	0	100	100
11	O	174/201 (87%)	172 (99%)	2 (1%)	0	100	100
12	P	191/231 (83%)	186 (97%)	5 (3%)	0	100	100
13	Q	165/197 (84%)	160 (97%)	5 (3%)	0	100	100
14	R	86/90 (96%)	85 (99%)	1 (1%)	0	100	100
15	S	163/215 (76%)	156 (96%)	7 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	U	139/191 (73%)	135 (97%)	4 (3%)	0	100	100
17	G	149/209 (71%)	144 (97%)	5 (3%)	0	100	100
18	H	145/169 (86%)	133 (92%)	12 (8%)	0	100	100
19	T	91/202 (45%)	90 (99%)	1 (1%)	0	100	100
All	All	3441/3909 (88%)	3346 (97%)	94 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	111	VAL

### 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%)	594 (98%)	9 (2%)	57	69
2	B	590/591 (100%)	584 (99%)	6 (1%)	68	79
3	C	68/69 (99%)	67 (98%)	1 (2%)	57	69
4	D	118/122 (97%)	117 (99%)	1 (1%)	73	82
5	E	53/55 (96%)	53 (100%)	0	100	100
6	F	133/152 (88%)	131 (98%)	2 (2%)	57	69
7	I	31/32 (97%)	29 (94%)	2 (6%)	15	17
8	J	32/32 (100%)	32 (100%)	0	100	100
9	L	111/112 (99%)	110 (99%)	1 (1%)	70	80
10	M	21/21 (100%)	21 (100%)	0	100	100
11	O	145/161 (90%)	143 (99%)	2 (1%)	59	71
12	P	144/173 (83%)	140 (97%)	4 (3%)	38	50
13	Q	133/157 (85%)	132 (99%)	1 (1%)	73	82
14	R	71/73 (97%)	70 (99%)	1 (1%)	59	71

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	S	125/162 (77%)	121 (97%)	4 (3%)	34	44
16	U	110/148 (74%)	108 (98%)	2 (2%)	51	64
17	G	127/167 (76%)	121 (95%)	6 (5%)	23	30
18	H	119/137 (87%)	108 (91%)	11 (9%)	8	8
19	T	73/153 (48%)	70 (96%)	3 (4%)	27	35
All	All	2807/3129 (90%)	2751 (98%)	56 (2%)	48	61

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	143	THR
1	A	181	GLN
1	A	307	ILE
1	A	349	MET
1	A	372	ASP
1	A	405	ASP
1	A	509	LYS
1	A	575	VAL
1	A	731	SER
2	B	97	SER
2	B	230	LEU
2	B	477	SER
2	B	504	ASN
2	B	543	LYS
2	B	677	VAL
3	C	40	SER
4	D	27	LYS
6	F	10	ASP
6	F	78	SER
7	I	14	VAL
7	I	34	GLU
9	L	74	LEU
11	O	76	SER
11	O	159	ILE
12	P	43	ASP
12	P	166	LEU
12	P	167	SER
12	P	188	ILE
13	Q	64	THR
14	R	31	SER

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Mol	Chain	Res	Type
15	S	53	SER
15	S	66	LEU
15	S	112	GLU
15	S	131	SER
16	U	14	LEU
16	U	118	ASP
17	G	59	VAL
17	G	63	ILE
17	G	80	SER
17	G	118	THR
17	G	135	LYS
17	G	138	GLU
18	H	4	SER
18	H	10	LEU
18	H	11	VAL
18	H	58	VAL
18	H	60	THR
18	H	86	SER
18	H	89	GLN
18	H	99	ILE
18	H	138	MET
18	H	139	LYS
18	H	141	LEU
19	T	8	GLU
19	T	44	LEU
19	T	110	ILE

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

Mol	Chain	Res	Type
1	A	3	GLN
1	A	206	GLN
1	A	431	ASN
1	A	486	ASN
2	B	12	GLN
2	B	112	ASN
2	B	641	GLN
4	D	3	ASN
4	D	128	ASN
6	F	44	GLN
9	L	69	ASN
10	M	27	GLN

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Mol	Chain	Res	Type
12	P	186	HIS
13	Q	120	GLN
14	R	52	ASN
15	S	77	ASN
16	U	70	GLN
16	U	93	ASN
16	U	120	GLN
17	G	146	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

250 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
20	CLA	G	203	17	49,53,73	1.43	8 (16%)	58,89,113	1.03	3 (5%)
20	CLA	B	824	2	69,73,73	1.21	7 (10%)	82,113,113	0.97	5 (6%)
20	CLA	T	201	-	46,50,73	1.42	8 (17%)	53,85,113	1.08	3 (5%)
20	CLA	A	830	1	54,58,73	1.31	6 (11%)	64,95,113	0.97	4 (6%)
20	CLA	A	852	1	69,73,73	1.18	8 (11%)	82,113,113	0.92	4 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
26	DD6	U	212	-	40,45,45	1.30	7 (17%)	51,67,67	1.71	13 (25%)
20	CLA	O	202	11	47,51,73	1.40	6 (12%)	55,86,113	1.10	4 (7%)
20	CLA	B	822	2	69,73,73	1.23	7 (10%)	82,113,113	0.92	3 (3%)
20	CLA	A	814	32	49,53,73	1.40	7 (14%)	58,89,113	1.15	5 (8%)
20	CLA	A	815	1	69,73,73	1.20	7 (10%)	82,113,113	0.93	4 (4%)
20	CLA	T	207	19	69,73,73	1.12	6 (8%)	82,113,113	1.01	5 (6%)
23	BCR	R	102	-	40,40,41	1.13	2 (5%)	54,54,56	1.39	9 (16%)
26	DD6	G	214	-	40,45,45	1.32	7 (17%)	51,67,67	1.68	14 (27%)
20	CLA	U	208	16	50,54,73	1.32	6 (12%)	59,90,113	1.17	5 (8%)
20	CLA	B	810	2	58,62,73	1.43	9 (15%)	71,100,113	0.91	3 (4%)
20	CLA	B	815	2	63,67,73	1.24	7 (11%)	74,105,113	1.00	5 (6%)
20	CLA	B	820	-	67,71,73	1.21	8 (11%)	79,110,113	0.98	6 (7%)
20	CLA	G	202	-	45,49,73	1.45	6 (13%)	54,84,113	1.07	4 (7%)
20	CLA	A	817	1	49,53,73	1.42	7 (14%)	58,89,113	1.11	4 (6%)
20	CLA	A	826	1	69,73,73	1.28	8 (11%)	82,113,113	0.82	2 (2%)
20	CLA	G	201	17	49,53,73	1.36	7 (14%)	58,89,113	1.10	4 (6%)
20	CLA	A	835	1	69,73,73	1.24	8 (11%)	82,113,113	1.07	5 (6%)
22	LHG	A	840	20	26,26,48	0.83	1 (3%)	29,32,54	1.35	3 (10%)
30	KC1	U	213	16	49,53,53	1.62	9 (18%)	61,89,89	1.17	5 (8%)
20	CLA	B	835	-	69,73,73	1.22	7 (10%)	82,113,113	0.95	5 (6%)
20	CLA	Q	216	-	69,73,73	1.13	7 (10%)	82,113,113	0.88	4 (4%)
23	BCR	I	101	-	41,41,41	1.06	2 (4%)	56,56,56	1.25	5 (8%)
31	A86	U	202	-	47,50,50	1.37	5 (10%)	51,76,76	1.37	7 (13%)
26	DD6	T	213	-	40,45,45	1.34	8 (20%)	51,67,67	1.66	12 (23%)
20	CLA	A	820	1	55,59,73	1.37	8 (14%)	64,96,113	1.02	3 (4%)
26	DD6	T	212	-	40,45,45	1.31	7 (17%)	51,67,67	1.76	12 (23%)
23	BCR	F	804	-	41,41,41	1.05	2 (4%)	56,56,56	1.28	4 (7%)
26	DD6	S	213	-	40,45,45	1.29	6 (15%)	51,67,67	1.81	12 (23%)
26	DD6	U	203	-	40,45,45	1.38	9 (22%)	51,67,67	2.12	15 (29%)
20	CLA	B	809	2	69,73,73	1.19	8 (11%)	82,113,113	0.92	4 (4%)
20	CLA	B	821	32	68,72,73	1.14	7 (10%)	80,111,113	0.93	4 (5%)
20	CLA	A	804	1	69,73,73	1.15	7 (10%)	82,113,113	0.90	4 (4%)
20	CLA	U	210	16	69,73,73	1.15	6 (8%)	82,113,113	0.90	5 (6%)
20	CLA	A	813	1	54,58,73	1.39	7 (12%)	64,95,113	1.07	4 (6%)
20	CLA	A	834	1	69,73,73	1.27	8 (11%)	82,113,113	0.98	4 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
20	CLA	A	819	1	47,51,73	1.39	7 (14%)	55,86,113	1.10	4 (7%)
20	CLA	Q	209	13	69,73,73	1.15	7 (10%)	82,113,113	0.90	4 (4%)
20	CLA	L	204	32	54,58,73	1.30	7 (12%)	64,95,113	1.24	7 (10%)
25	SF4	C	101	3	0,12,12	-	-	-		
30	KC1	Q	210	13	49,53,53	1.65	9 (18%)	61,89,89	1.14	7 (11%)
30	KC1	S	211	15	49,53,53	1.51	7 (14%)	61,89,89	1.12	6 (9%)
20	CLA	B	807	2	69,73,73	1.20	8 (11%)	82,113,113	0.89	3 (3%)
26	DD6	S	204	-	40,45,45	1.44	9 (22%)	51,67,67	1.68	13 (25%)
20	CLA	A	806	1	69,73,73	1.16	8 (11%)	82,113,113	0.88	4 (4%)
20	CLA	T	205	-	50,54,73	1.31	6 (12%)	59,90,113	1.20	7 (11%)
20	CLA	S	206	15	50,54,73	1.49	8 (16%)	59,90,113	1.10	4 (6%)
20	CLA	S	214	-	69,73,73	1.14	7 (10%)	82,113,113	0.93	4 (4%)
20	CLA	B	801	-	69,73,73	1.19	7 (10%)	82,113,113	0.93	4 (4%)
20	CLA	B	843	2	69,73,73	1.22	7 (10%)	82,113,113	0.92	4 (4%)
20	CLA	S	215	15	69,73,73	1.17	7 (10%)	82,113,113	0.90	3 (3%)
26	DD6	G	217	-	40,45,45	1.24	7 (17%)	51,67,67	1.48	10 (19%)
20	CLA	G	207	17	64,68,73	1.16	7 (10%)	76,107,113	1.01	4 (5%)
20	CLA	A	823	1	69,73,73	1.23	6 (8%)	82,113,113	0.92	4 (4%)
20	CLA	L	202	9	53,57,73	1.33	8 (15%)	61,93,113	1.16	6 (9%)
26	DD6	H	211	-	40,45,45	1.28	7 (17%)	51,67,67	1.54	10 (19%)
20	CLA	T	210	19	50,54,73	1.45	8 (16%)	59,90,113	1.13	5 (8%)
30	KC1	T	208	-	49,53,53	1.67	9 (18%)	61,89,89	1.12	5 (8%)
20	CLA	L	203	9	69,73,73	1.16	7 (10%)	82,113,113	0.87	4 (4%)
20	CLA	G	206	17	69,73,73	1.26	7 (10%)	82,113,113	0.88	3 (3%)
20	CLA	S	205	15	50,54,73	1.39	7 (14%)	59,90,113	1.07	4 (6%)
20	CLA	A	809	1	66,70,73	1.24	7 (10%)	78,109,113	0.89	3 (3%)
20	CLA	A	803	1	69,73,73	1.15	7 (10%)	82,113,113	0.93	4 (4%)
26	DD6	G	212	-	40,45,45	1.32	7 (17%)	51,67,67	1.58	10 (19%)
20	CLA	O	206	-	69,73,73	1.15	7 (10%)	82,113,113	0.97	5 (6%)
23	BCR	B	838	-	41,41,41	1.07	2 (4%)	56,56,56	1.24	6 (10%)
20	CLA	A	829	1	69,73,73	1.22	7 (10%)	82,113,113	0.91	4 (4%)
30	KC1	P	206	12	49,53,53	1.55	8 (16%)	61,89,89	1.02	3 (4%)
20	CLA	F	803	6	50,54,73	1.37	7 (14%)	59,90,113	1.06	4 (6%)
20	CLA	U	207	-	69,73,73	1.13	7 (10%)	82,113,113	1.08	9 (10%)
20	CLA	P	213	12	45,49,73	1.42	6 (13%)	54,84,113	1.31	7 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
20	CLA	H	205	18	49,53,73	1.52	8 (16%)	58,89,113	0.97	3 (5%)
30	KC1	O	210	11	49,53,53	1.67	11 (22%)	61,89,89	0.99	4 (6%)
20	CLA	A	851	1	69,73,73	1.18	7 (10%)	82,113,113	0.90	3 (3%)
20	CLA	B	812	2	58,62,73	1.30	6 (10%)	68,99,113	0.93	4 (5%)
28	SQD	S	201	-	44,46,54	1.02	4 (9%)	54,57,65	1.55	9 (16%)
29	LMG	Q	217	-	55,55,55	0.70	0	63,63,63	1.29	6 (9%)
26	DD6	O	214	-	40,45,45	1.25	8 (20%)	51,67,67	1.56	9 (17%)
20	CLA	G	209	17	60,64,73	1.22	7 (11%)	71,102,113	0.95	4 (5%)
20	CLA	O	211	11	45,49,73	1.45	6 (13%)	54,84,113	1.21	6 (11%)
20	CLA	G	215	17	49,53,73	1.34	7 (14%)	58,89,113	1.11	4 (6%)
20	CLA	Q	213	32	61,65,73	1.21	7 (11%)	72,103,113	1.10	6 (8%)
20	CLA	G	208	-	59,63,73	1.20	7 (11%)	70,101,113	1.04	4 (5%)
20	CLA	R	104	14	69,73,73	1.45	9 (13%)	82,113,113	0.93	4 (4%)
20	CLA	B	805	2	69,73,73	1.18	8 (11%)	82,113,113	0.89	4 (4%)
31	A86	Q	218	-	47,50,50	1.42	6 (12%)	51,76,76	1.41	9 (17%)
31	A86	R	105	-	47,50,50	1.39	5 (10%)	51,76,76	1.37	8 (15%)
20	CLA	J	103	8	46,50,73	1.39	7 (15%)	53,85,113	1.03	3 (5%)
26	DD6	S	203	-	40,45,45	1.30	8 (20%)	51,67,67	1.57	10 (19%)
26	DD6	O	212	-	40,45,45	1.30	7 (17%)	51,67,67	1.64	11 (21%)
20	CLA	A	808	1	60,64,73	1.28	7 (11%)	71,102,113	0.94	3 (4%)
26	DD6	O	213	-	40,45,45	1.29	8 (20%)	51,67,67	1.42	7 (13%)
26	DD6	P	218	-	40,45,45	1.40	8 (20%)	51,67,67	1.75	11 (21%)
23	BCR	M	101	-	41,41,41	1.11	2 (4%)	56,56,56	1.30	6 (10%)
26	DD6	G	213	-	40,45,45	1.36	8 (20%)	51,67,67	1.54	9 (17%)
20	CLA	B	831	2	69,73,73	1.19	7 (10%)	82,113,113	0.87	4 (4%)
20	CLA	A	807	1	58,62,73	1.30	8 (13%)	68,99,113	1.07	5 (7%)
25	SF4	A	850	1,2	0,12,12	-	-	-	-	-
20	CLA	Q	203	13	52,56,73	1.39	8 (15%)	61,92,113	1.19	6 (9%)
26	DD6	P	205	-	40,45,45	1.30	8 (20%)	51,67,67	1.62	9 (17%)
20	CLA	B	808	2	69,73,73	1.22	7 (10%)	82,113,113	0.88	2 (2%)
20	CLA	G	205	17	65,69,73	1.14	7 (10%)	77,108,113	1.15	8 (10%)
20	CLA	O	205	11	69,73,73	1.19	5 (7%)	82,113,113	0.90	4 (4%)
20	CLA	A	828	1	69,73,73	1.22	6 (8%)	82,113,113	0.88	3 (3%)
20	CLA	H	207	-	62,66,73	1.23	7 (11%)	73,104,113	1.19	8 (10%)
20	CLA	H	206	18	69,73,73	1.17	8 (11%)	82,113,113	1.28	9 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
23	BCR	A	844	-	41,41,41	1.12	2 (4%)	56,56,56	1.21	5 (8%)
20	CLA	B	848	2	54,58,73	1.33	8 (14%)	64,95,113	1.02	3 (4%)
20	CLA	O	209	11	69,73,73	1.15	6 (8%)	82,113,113	1.04	5 (6%)
20	CLA	B	814	2	59,63,73	1.35	8 (13%)	70,101,113	0.95	3 (4%)
20	CLA	A	825	1	69,73,73	1.23	7 (10%)	82,113,113	0.89	3 (3%)
26	DD6	O	215	-	40,45,45	1.41	9 (22%)	51,67,67	1.56	13 (25%)
20	CLA	G	204	17	47,51,73	1.38	7 (14%)	55,86,113	1.02	3 (5%)
20	CLA	A	846	1	64,68,73	1.31	6 (9%)	76,107,113	0.95	4 (5%)
20	CLA	U	204	-	65,69,73	1.21	7 (10%)	77,108,113	0.89	4 (5%)
21	PQN	A	837	-	34,34,34	0.39	0	43,45,45	0.59	1 (2%)
29	LMG	J	102	-	39,39,55	0.88	0	47,47,63	1.24	4 (8%)
30	KC1	P	219	12	49,53,53	1.53	7 (14%)	61,89,89	1.02	2 (3%)
28	SQD	B	847	-	48,50,54	1.00	5 (10%)	58,61,65	1.52	9 (15%)
26	DD6	O	201	-	40,45,45	1.31	9 (22%)	51,67,67	1.47	8 (15%)
20	CLA	A	824	1	66,70,73	1.21	7 (10%)	78,109,113	0.96	3 (3%)
23	BCR	A	841	-	41,41,41	1.05	2 (4%)	56,56,56	1.29	5 (8%)
26	DD6	P	215	-	40,45,45	1.33	8 (20%)	51,67,67	1.50	9 (17%)
31	A86	P	204	-	47,50,50	1.36	4 (8%)	51,76,76	1.70	11 (21%)
23	BCR	F	801	-	41,41,41	1.05	2 (4%)	56,56,56	1.23	4 (7%)
22	LHG	A	839	-	47,47,48	0.61	0	50,53,54	1.20	5 (10%)
20	CLA	A	812	1	49,53,73	1.44	6 (12%)	58,89,113	1.11	5 (8%)
20	CLA	T	209	19	45,49,73	1.40	5 (11%)	54,84,113	1.15	5 (9%)
20	CLA	B	818	2	50,54,73	1.39	7 (14%)	59,90,113	1.13	4 (6%)
31	A86	Q	214	-	47,50,50	1.41	5 (10%)	51,76,76	1.67	10 (19%)
20	CLA	P	209	-	56,60,73	1.27	6 (10%)	65,97,113	0.95	3 (4%)
20	CLA	P	216	12	51,55,73	1.38	7 (13%)	60,91,113	1.12	5 (8%)
20	CLA	B	811	2	59,63,73	1.24	7 (11%)	70,101,113	0.95	4 (5%)
20	CLA	H	202	18	64,68,73	1.18	7 (10%)	76,107,113	1.01	3 (3%)
20	CLA	B	845	2	69,73,73	1.26	8 (11%)	82,113,113	0.97	4 (4%)
20	CLA	Q	208	13	54,58,73	1.32	9 (16%)	64,95,113	1.00	4 (6%)
26	DD6	J	101	-	40,45,45	1.28	7 (17%)	51,67,67	1.52	9 (17%)
20	CLA	T	202	19	45,49,73	1.43	8 (17%)	54,84,113	1.16	4 (7%)
20	CLA	O	204	11	69,73,73	1.18	8 (11%)	82,113,113	0.89	3 (3%)
20	CLA	P	214	12	49,53,73	1.45	8 (16%)	58,89,113	1.09	3 (5%)
20	CLA	U	211	16	56,60,73	1.33	8 (14%)	65,97,113	1.06	4 (6%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
26	DD6	Q	215	-	40,45,45	1.29	7 (17%)	51,67,67	1.51	9 (17%)
24	CL0	A	848	1	58,73,73	0.89	4 (6%)	60,113,113	1.74	8 (13%)
31	A86	R	103	-	44,46,50	1.43	4 (9%)	49,70,76	1.63	10 (20%)
25	SF4	C	102	3	0,12,12	-	-	-		
20	CLA	A	827	1	54,58,73	1.39	7 (12%)	64,95,113	1.00	4 (6%)
20	CLA	B	819	2	57,61,73	1.30	7 (12%)	67,98,113	0.96	4 (5%)
20	CLA	A	833	1	69,73,73	1.23	7 (10%)	82,113,113	0.98	4 (4%)
20	CLA	T	203	19	50,54,73	1.43	8 (16%)	59,90,113	0.98	3 (5%)
20	CLA	B	827	2	53,57,73	1.36	8 (15%)	61,93,113	0.98	3 (4%)
20	CLA	A	849	1	69,73,73	1.20	6 (8%)	82,113,113	0.93	4 (4%)
20	CLA	H	201	-	44,48,73	1.45	6 (13%)	51,82,113	1.35	7 (13%)
26	DD6	A	855	-	40,45,45	1.29	8 (20%)	51,67,67	1.54	10 (19%)
20	CLA	A	838	22	56,60,73	1.28	6 (10%)	65,97,113	1.07	4 (6%)
20	CLA	B	828	2	62,66,73	1.27	6 (9%)	73,104,113	0.93	3 (4%)
20	CLA	Q	204	-	65,69,73	1.19	6 (9%)	77,108,113	1.02	5 (6%)
20	CLA	R	101	32	49,53,73	1.41	7 (14%)	58,89,113	1.10	4 (6%)
20	CLA	U	209	16	46,50,73	1.35	6 (13%)	53,85,113	1.15	6 (11%)
26	DD6	Q	202	-	40,45,45	1.30	7 (17%)	51,67,67	1.72	14 (27%)
26	DD6	S	212	-	40,45,45	1.32	7 (17%)	51,67,67	1.64	10 (19%)
20	CLA	P	208	12	60,64,73	1.31	8 (13%)	71,102,113	0.97	4 (5%)
20	CLA	B	825	2	69,73,73	1.22	9 (13%)	82,113,113	0.91	3 (3%)
20	CLA	F	802	-	52,56,73	1.38	8 (15%)	61,92,113	1.18	7 (11%)
23	BCR	I	102	-	41,41,41	1.11	2 (4%)	56,56,56	1.24	5 (8%)
31	A86	Q	201	-	47,50,50	1.31	5 (10%)	51,76,76	1.45	10 (19%)
20	CLA	A	836	-	69,73,73	1.19	8 (11%)	82,113,113	1.03	6 (7%)
20	CLA	U	205	16	69,73,73	1.17	7 (10%)	82,113,113	0.98	3 (3%)
20	CLA	U	206	16	49,53,73	1.45	7 (14%)	58,89,113	0.97	3 (5%)
23	BCR	B	841	-	41,41,41	1.09	2 (4%)	56,56,56	1.13	3 (5%)
20	CLA	B	816	2	64,68,73	1.24	8 (12%)	76,107,113	0.93	4 (5%)
26	DD6	G	211	-	40,45,45	1.29	6 (15%)	51,67,67	1.40	7 (13%)
20	CLA	A	818	32	69,73,73	1.17	8 (11%)	82,113,113	0.87	3 (3%)
30	KC1	S	209	15	49,53,53	1.56	7 (14%)	61,89,89	1.22	7 (11%)
20	CLA	B	802	2	69,73,73	1.24	7 (10%)	82,113,113	0.80	3 (3%)
21	PQN	B	836	-	34,34,34	0.41	0	43,45,45	0.57	1 (2%)
20	CLA	A	816	1	69,73,73	1.17	8 (11%)	82,113,113	0.95	4 (4%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
20	CLA	S	207	15	49,53,73	1.36	7 (14%)	58,89,113	1.04	5 (8%)
20	CLA	Q	206	13	54,59,73	1.41	6 (11%)	62,96,113	0.95	3 (4%)
20	CLA	A	854	-	69,73,73	1.16	5 (7%)	82,113,113	1.29	9 (10%)
20	CLA	O	207	11	50,54,73	1.36	7 (14%)	59,90,113	1.07	4 (6%)
20	CLA	Q	212	13	69,73,73	1.23	7 (10%)	82,113,113	1.01	8 (9%)
20	CLA	A	811	1	69,73,73	1.21	8 (11%)	82,113,113	0.93	3 (3%)
20	CLA	A	845	32	69,73,73	1.18	7 (10%)	82,113,113	0.96	3 (3%)
20	CLA	P	210	32	51,55,73	1.33	6 (11%)	60,91,113	1.05	4 (6%)
20	CLA	Q	211	13	45,49,73	1.48	7 (15%)	54,84,113	1.22	6 (11%)
20	CLA	B	823	2	69,73,73	1.23	7 (10%)	82,113,113	0.96	5 (6%)
23	BCR	B	837	-	41,41,41	1.16	3 (7%)	56,56,56	1.26	7 (12%)
30	KC1	P	212	12	46,52,53	1.72	10 (21%)	59,87,89	1.11	6 (10%)
20	CLA	T	206	19	46,50,73	1.41	6 (13%)	53,85,113	1.09	4 (7%)
26	DD6	P	220	-	40,45,45	1.33	8 (20%)	51,67,67	1.79	12 (23%)
20	CLA	A	822	32	69,73,73	1.14	6 (8%)	82,113,113	0.94	4 (4%)
20	CLA	B	833	32	69,73,73	1.17	7 (10%)	82,113,113	0.98	6 (7%)
20	CLA	B	830	2	62,66,73	1.29	7 (11%)	73,104,113	0.96	3 (4%)
20	CLA	B	817	32	69,73,73	1.19	7 (10%)	82,113,113	0.95	5 (6%)
20	CLA	B	829	-	69,73,73	1.17	7 (10%)	82,113,113	0.95	4 (4%)
23	BCR	L	205	-	41,41,41	1.09	2 (4%)	56,56,56	1.35	5 (8%)
20	CLA	A	810	1	58,62,73	1.30	7 (12%)	68,99,113	1.06	5 (7%)
20	CLA	P	207	12	69,73,73	1.15	7 (10%)	82,113,113	0.94	4 (4%)
26	DD6	H	210	-	40,45,45	1.33	5 (12%)	51,67,67	1.57	10 (19%)
20	CLA	A	853	32	69,73,73	1.17	7 (10%)	82,113,113	0.97	4 (4%)
20	CLA	O	208	11	64,68,73	1.18	6 (9%)	76,107,113	0.97	4 (5%)
20	CLA	T	204	-	61,65,73	1.19	5 (8%)	72,103,113	1.00	5 (6%)
23	BCR	B	839	-	41,41,41	1.09	3 (7%)	56,56,56	1.29	10 (17%)
20	CLA	P	211	12	54,58,73	1.28	6 (11%)	64,95,113	1.06	3 (4%)
20	CLA	H	209	18	49,53,73	1.40	7 (14%)	58,89,113	1.08	4 (6%)
20	CLA	A	802	1	59,63,73	1.35	7 (11%)	70,101,113	0.96	3 (4%)
29	LMG	U	201	-	32,32,55	0.97	1 (3%)	40,40,63	1.21	3 (7%)
20	CLA	H	208	18	45,49,73	1.43	7 (15%)	54,84,113	1.29	7 (12%)
23	BCR	B	840	-	41,41,41	1.07	2 (4%)	56,56,56	1.28	7 (12%)
20	CLA	H	203	18	65,69,73	1.19	5 (7%)	77,108,113	1.01	5 (6%)
23	BCR	L	201	-	41,41,41	1.11	2 (4%)	56,56,56	1.25	5 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
20	CLA	B	826	2	54,58,73	1.39	7 (12%)	64,95,113	0.96	3 (4%)
30	KC1	P	203	12	49,53,53	1.68	10 (20%)	61,89,89	1.12	7 (11%)
20	CLA	G	210	17	49,53,73	1.42	7 (14%)	58,89,113	1.01	3 (5%)
20	CLA	B	846	2	69,73,73	1.18	7 (10%)	82,113,113	1.04	5 (6%)
20	CLA	B	803	-	69,73,73	1.15	7 (10%)	82,113,113	0.99	7 (8%)
20	CLA	S	208	15	56,60,73	1.25	6 (10%)	65,97,113	1.09	4 (6%)
23	BCR	A	843	-	41,41,41	1.10	2 (4%)	56,56,56	1.22	5 (8%)
27	DGD	B	842	-	61,61,67	0.89	1 (1%)	75,75,81	1.36	9 (12%)
20	CLA	A	805	1	53,57,73	1.38	6 (11%)	61,93,113	1.04	4 (6%)
20	CLA	A	832	1	55,59,73	1.37	8 (14%)	64,96,113	1.04	5 (7%)
20	CLA	S	202	32	69,73,73	1.14	5 (7%)	82,113,113	1.06	6 (7%)
26	DD6	U	214	-	24,26,45	1.50	5 (20%)	29,35,67	1.63	7 (24%)
23	BCR	A	842	-	41,41,41	1.05	2 (4%)	56,56,56	1.16	3 (5%)
20	CLA	A	821	32	69,73,73	1.21	7 (10%)	82,113,113	1.00	6 (7%)
20	CLA	B	832	2	51,55,73	1.40	6 (11%)	60,91,113	1.03	4 (6%)
20	CLA	Q	205	13	64,68,73	1.22	8 (12%)	76,107,113	0.94	3 (3%)
20	CLA	B	806	2	69,73,73	1.21	7 (10%)	82,113,113	0.89	3 (3%)
29	LMG	P	217	-	25,25,55	1.34	5 (20%)	33,33,63	1.28	4 (12%)
20	CLA	Q	207	13	50,54,73	1.39	7 (14%)	59,90,113	1.22	6 (10%)
29	LMG	P	202	-	34,34,55	1.04	3 (8%)	42,42,63	1.23	4 (9%)
20	CLA	B	844	2	69,73,73	1.21	6 (8%)	82,113,113	0.89	4 (4%)
23	BCR	J	104	-	41,41,41	1.12	2 (4%)	56,56,56	1.29	5 (8%)
20	CLA	B	813	2	63,67,73	1.30	8 (12%)	74,105,113	1.09	7 (9%)
20	CLA	B	834	2	69,73,73	1.12	6 (8%)	82,113,113	0.90	4 (4%)
29	LMG	I	103	-	49,49,55	0.79	1 (2%)	57,57,63	1.24	6 (10%)
20	CLA	T	211	-	51,55,73	1.35	7 (13%)	60,91,113	1.18	4 (6%)
20	CLA	B	804	2	49,53,73	1.45	8 (16%)	58,89,113	1.05	4 (6%)
20	CLA	A	801	-	69,73,73	1.17	8 (11%)	82,113,113	0.86	4 (4%)
20	CLA	O	203	-	49,53,73	1.39	7 (14%)	58,89,113	1.07	4 (6%)
22	LHG	G	216	-	26,26,48	0.85	1 (3%)	29,32,54	1.26	2 (6%)
20	CLA	H	204	18	47,52,73	1.40	7 (14%)	55,87,113	1.07	3 (5%)
26	DD6	S	210	-	40,45,45	1.31	7 (17%)	51,67,67	1.46	10 (19%)
22	LHG	P	201	-	48,48,48	0.63	1 (2%)	51,54,54	1.23	6 (11%)
20	CLA	A	831	1	49,53,73	1.37	6 (12%)	58,89,113	1.10	4 (6%)
20	CLA	A	847	1	69,73,73	1.23	8 (11%)	82,113,113	1.06	6 (7%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	G	203	17	1/1/11/20	7/15/91/115	-
20	CLA	B	824	2	-	3/39/115/115	-
20	CLA	T	201	-	1/1/10/20	0/12/88/115	-
20	CLA	A	830	1	-	1/21/97/115	-
20	CLA	A	852	1	1/1/15/20	7/39/115/115	-
26	DD6	U	212	-	-	10/26/80/80	0/3/3/3
20	CLA	O	202	11	-	2/13/89/115	-
20	CLA	B	822	2	1/1/15/20	0/39/115/115	-
20	CLA	A	814	32	1/1/11/20	4/15/91/115	-
20	CLA	A	815	1	1/1/15/20	10/39/115/115	-
20	CLA	T	207	19	-	5/39/115/115	-
23	BCR	R	102	-	-	9/27/61/63	0/2/2/2
26	DD6	G	214	-	-	12/26/80/80	0/3/3/3
20	CLA	U	208	16	1/1/11/20	2/17/93/115	-
20	CLA	B	815	2	1/1/13/20	8/32/108/115	-
20	CLA	B	810	2	-	2/25/101/115	-
20	CLA	B	820	-	1/1/14/20	4/37/113/115	-
20	CLA	G	202	-	1/1/10/20	0/10/86/115	-
20	CLA	A	817	1	1/1/11/20	0/15/91/115	-
20	CLA	A	826	1	-	3/39/115/115	-
20	CLA	G	201	17	-	2/15/91/115	-
20	CLA	A	835	1	1/1/15/20	11/39/115/115	-
22	LHG	A	840	20	-	8/31/31/53	-
30	KC1	U	213	16	-	2/15/71/71	-
20	CLA	B	835	-	1/1/15/20	0/39/115/115	-
20	CLA	Q	216	-	-	11/39/115/115	-
23	BCR	I	101	-	-	8/29/63/63	0/2/2/2
31	A86	U	202	-	-	15/34/90/90	0/3/3/3
26	DD6	T	213	-	-	19/26/80/80	0/3/3/3
20	CLA	A	820	1	1/1/12/20	0/23/99/115	-
26	DD6	T	212	-	-	14/26/80/80	0/3/3/3
23	BCR	F	804	-	-	10/29/63/63	0/2/2/2
26	DD6	S	213	-	-	16/26/80/80	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	DD6	U	203	-	-	16/26/80/80	0/3/3/3
20	CLA	B	809	2	1/1/15/20	8/39/115/115	-
20	CLA	B	821	32	1/1/14/20	6/38/114/115	-
20	CLA	A	804	1	1/1/15/20	5/39/115/115	-
20	CLA	U	210	16	-	8/39/115/115	-
20	CLA	A	813	1	-	0/21/97/115	-
20	CLA	A	834	1	1/1/15/20	5/39/115/115	-
20	CLA	A	819	1	-	0/13/89/115	-
20	CLA	Q	209	13	-	10/39/115/115	-
20	CLA	L	204	32	-	6/21/97/115	-
30	KC1	Q	210	13	-	2/15/71/71	-
25	SF4	C	101	3	-	-	0/6/5/5
30	KC1	S	211	15	-	6/15/71/71	-
20	CLA	B	807	2	1/1/15/20	3/39/115/115	-
26	DD6	S	204	-	-	13/26/80/80	0/3/3/3
20	CLA	A	806	1	1/1/15/20	3/39/115/115	-
20	CLA	T	205	-	1/1/11/20	5/17/93/115	-
20	CLA	S	206	15	1/1/11/20	2/17/93/115	-
20	CLA	S	214	-	1/1/15/20	7/39/115/115	-
20	CLA	B	801	-	1/1/15/20	3/39/115/115	-
20	CLA	B	843	2	1/1/15/20	6/39/115/115	-
20	CLA	S	215	15	1/1/15/20	6/39/115/115	-
26	DD6	G	217	-	-	12/26/80/80	0/3/3/3
20	CLA	G	207	17	1/1/14/20	5/33/109/115	-
20	CLA	A	823	1	1/1/15/20	6/39/115/115	-
20	CLA	L	202	9	1/1/11/20	6/20/96/115	-
26	DD6	H	211	-	-	11/26/80/80	0/3/3/3
20	CLA	T	210	19	-	3/17/93/115	-
30	KC1	T	208	-	-	3/15/71/71	-
20	CLA	L	203	9	-	2/39/115/115	-
20	CLA	G	206	17	1/1/15/20	11/39/115/115	-
20	CLA	S	205	15	1/1/11/20	0/17/93/115	-
20	CLA	A	809	1	-	2/36/112/115	-
20	CLA	A	803	1	1/1/15/20	5/39/115/115	-
26	DD6	G	212	-	-	13/26/80/80	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	O	206	-	1/1/15/20	7/39/115/115	-
23	BCR	B	838	-	-	7/29/63/63	0/2/2/2
20	CLA	A	829	1	1/1/15/20	3/39/115/115	-
30	KC1	P	206	12	-	3/15/71/71	-
20	CLA	F	803	6	1/1/11/20	4/17/93/115	-
20	CLA	U	207	-	-	9/39/115/115	-
20	CLA	P	213	12	1/1/10/20	2/10/86/115	-
20	CLA	H	205	18	1/1/11/20	3/15/91/115	-
30	KC1	O	210	11	-	0/15/71/71	-
20	CLA	A	851	1	1/1/15/20	11/39/115/115	-
20	CLA	B	812	2	1/1/12/20	1/26/102/115	-
28	SQD	S	201	-	-	16/41/61/69	0/1/1/1
29	LMG	Q	217	-	-	16/50/70/70	0/1/1/1
26	DD6	O	214	-	-	11/26/80/80	0/3/3/3
20	CLA	G	209	17	-	5/29/105/115	-
20	CLA	O	211	11	-	1/10/86/115	-
20	CLA	G	215	17	1/1/11/20	2/15/91/115	-
20	CLA	Q	213	32	1/1/13/20	7/30/106/115	-
20	CLA	G	208	-	1/1/13/20	6/27/103/115	-
20	CLA	R	104	14	-	12/39/115/115	-
20	CLA	B	805	2	1/1/15/20	7/39/115/115	-
31	A86	Q	218	-	-	21/34/90/90	0/3/3/3
31	A86	R	105	-	-	15/34/90/90	0/3/3/3
20	CLA	J	103	8	1/1/10/20	2/12/88/115	-
26	DD6	S	203	-	-	4/26/80/80	0/3/3/3
26	DD6	O	212	-	-	6/26/80/80	0/3/3/3
20	CLA	A	808	1	1/1/13/20	4/29/105/115	-
26	DD6	O	213	-	-	9/26/80/80	0/3/3/3
26	DD6	P	218	-	-	14/26/80/80	0/3/3/3
23	BCR	M	101	-	-	8/29/63/63	0/2/2/2
26	DD6	G	213	-	-	10/26/80/80	0/3/3/3
20	CLA	B	831	2	1/1/15/20	8/39/115/115	-
20	CLA	A	807	1	-	6/26/102/115	-
25	SF4	A	850	1,2	-	-	0/6/5/5
20	CLA	Q	203	13	-	5/19/95/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	DD6	P	205	-	-	6/26/80/80	0/3/3/3
20	CLA	B	808	2	1/1/15/20	7/39/115/115	-
20	CLA	G	205	17	1/1/14/20	10/35/111/115	-
20	CLA	O	205	11	1/1/15/20	5/39/115/115	-
20	CLA	A	828	1	1/1/15/20	3/39/115/115	-
20	CLA	H	207	-	1/1/13/20	5/31/107/115	-
20	CLA	H	206	18	1/1/15/20	16/39/115/115	-
23	BCR	A	844	-	-	9/29/63/63	0/2/2/2
20	CLA	B	848	2	1/1/12/20	3/21/97/115	-
20	CLA	O	209	11	-	7/39/115/115	-
20	CLA	B	814	2	-	2/27/103/115	-
20	CLA	A	825	1	1/1/15/20	7/39/115/115	-
26	DD6	O	215	-	-	14/26/80/80	0/3/3/3
20	CLA	G	204	17	-	3/13/89/115	-
20	CLA	A	846	1	-	3/33/109/115	-
20	CLA	U	204	-	1/1/14/20	4/35/111/115	-
21	PQN	A	837	-	-	4/23/43/43	0/2/2/2
29	LMG	J	102	-	-	14/34/54/70	0/1/1/1
30	KC1	P	219	12	-	4/15/71/71	-
28	SQD	B	847	-	-	18/45/65/69	0/1/1/1
26	DD6	O	201	-	-	8/26/80/80	0/3/3/3
20	CLA	A	824	1	1/1/14/20	9/36/112/115	-
23	BCR	A	841	-	-	7/29/63/63	0/2/2/2
26	DD6	P	215	-	-	5/26/80/80	0/3/3/3
31	A86	P	204	-	-	17/34/90/90	0/3/3/3
23	BCR	F	801	-	-	6/29/63/63	0/2/2/2
22	LHG	A	839	-	-	24/52/52/53	-
20	CLA	A	812	1	1/1/11/20	1/15/91/115	-
20	CLA	T	209	19	-	1/10/86/115	-
20	CLA	B	818	2	-	0/17/93/115	-
31	A86	Q	214	-	-	13/34/90/90	0/3/3/3
20	CLA	P	209	-	1/1/12/20	1/24/100/115	-
20	CLA	P	216	12	1/1/11/20	0/18/94/115	-
20	CLA	B	811	2	-	1/27/103/115	-
20	CLA	H	202	18	1/1/14/20	7/33/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	B	845	2	1/1/15/20	4/39/115/115	-
20	CLA	Q	208	13	1/1/12/20	2/21/97/115	-
26	DD6	J	101	-	-	6/26/80/80	0/3/3/3
20	CLA	T	202	19	1/1/10/20	0/10/86/115	-
20	CLA	O	204	11	1/1/15/20	2/39/115/115	-
20	CLA	P	214	12	1/1/11/20	5/15/91/115	-
20	CLA	U	211	16	1/1/12/20	3/24/100/115	-
26	DD6	Q	215	-	-	12/26/80/80	0/3/3/3
24	CL0	A	848	1	-	3/37/135/135	-
31	A86	R	103	-	-	12/30/84/90	0/3/3/3
25	SF4	C	102	3	-	-	0/6/5/5
20	CLA	A	827	1	-	3/21/97/115	-
20	CLA	B	819	2	-	1/25/101/115	-
20	CLA	A	833	1	1/1/15/20	7/39/115/115	-
20	CLA	T	203	19	1/1/11/20	3/17/93/115	-
20	CLA	B	827	2	1/1/11/20	3/20/96/115	-
20	CLA	A	849	1	1/1/15/20	4/39/115/115	-
20	CLA	H	201	-	1/1/9/20	0/10/82/115	-
26	DD6	A	855	-	-	14/26/80/80	0/3/3/3
20	CLA	A	838	22	1/1/12/20	5/24/100/115	-
20	CLA	Q	204	-	1/1/14/20	0/35/111/115	-
20	CLA	B	828	2	-	7/31/107/115	-
20	CLA	R	101	32	1/1/11/20	2/15/91/115	-
20	CLA	U	209	16	1/1/10/20	0/12/88/115	-
26	DD6	Q	202	-	-	6/26/80/80	0/3/3/3
26	DD6	S	212	-	-	13/26/80/80	0/3/3/3
20	CLA	P	208	12	1/1/13/20	6/29/105/115	-
20	CLA	B	825	2	-	8/39/115/115	-
20	CLA	F	802	-	1/1/11/20	3/19/95/115	-
23	BCR	I	102	-	-	8/29/63/63	0/2/2/2
31	A86	Q	201	-	-	16/34/90/90	0/3/3/3
20	CLA	A	836	-	1/1/15/20	3/39/115/115	-
20	CLA	U	206	16	1/1/11/20	3/15/91/115	-
20	CLA	U	205	16	-	3/39/115/115	-
23	BCR	B	841	-	-	7/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	B	816	2	1/1/14/20	3/33/109/115	-
26	DD6	G	211	-	-	6/26/80/80	0/3/3/3
20	CLA	A	818	32	1/1/15/20	6/39/115/115	-
30	KC1	S	209	15	-	1/15/71/71	-
20	CLA	B	802	2	1/1/15/20	2/39/115/115	-
21	PQN	B	836	-	-	4/23/43/43	0/2/2/2
20	CLA	A	816	1	1/1/15/20	0/39/115/115	-
20	CLA	S	207	15	1/1/11/20	2/15/91/115	-
20	CLA	Q	206	13	1/1/12/20	3/22/98/115	-
20	CLA	A	854	-	1/1/15/20	9/39/115/115	-
20	CLA	O	207	11	1/1/11/20	0/17/93/115	-
20	CLA	Q	212	13	-	3/39/115/115	-
20	CLA	A	811	1	1/1/15/20	8/39/115/115	-
20	CLA	A	845	32	1/1/15/20	8/39/115/115	-
20	CLA	P	210	32	-	4/18/94/115	-
20	CLA	Q	211	13	1/1/10/20	3/10/86/115	-
20	CLA	B	823	2	1/1/15/20	9/39/115/115	-
23	BCR	B	837	-	-	9/29/63/63	0/2/2/2
30	KC1	P	212	12	-	4/12/68/71	-
20	CLA	T	206	19	1/1/10/20	1/12/88/115	-
26	DD6	P	220	-	-	15/26/80/80	0/3/3/3
20	CLA	A	822	32	1/1/15/20	6/39/115/115	-
20	CLA	B	833	32	1/1/15/20	2/39/115/115	-
20	CLA	B	830	2	1/1/13/20	1/31/107/115	-
20	CLA	B	817	32	1/1/15/20	4/39/115/115	-
20	CLA	B	829	-	1/1/15/20	1/39/115/115	-
23	BCR	L	205	-	-	7/29/63/63	0/2/2/2
20	CLA	A	810	1	1/1/12/20	3/26/102/115	-
20	CLA	P	207	12	1/1/15/20	7/39/115/115	-
26	DD6	H	210	-	-	14/26/80/80	0/3/3/3
20	CLA	A	853	32	1/1/15/20	2/39/115/115	-
20	CLA	O	208	11	1/1/14/20	2/33/109/115	-
20	CLA	T	204	-	-	9/30/106/115	-
23	BCR	B	839	-	-	2/29/63/63	0/2/2/2
20	CLA	H	209	18	1/1/11/20	4/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	P	211	12	-	2/21/97/115	-
20	CLA	A	802	1	1/1/13/20	1/27/103/115	-
29	LMG	U	201	-	-	14/27/47/70	0/1/1/1
20	CLA	H	208	18	1/1/10/20	2/10/86/115	-
23	BCR	B	840	-	-	5/29/63/63	0/2/2/2
20	CLA	H	203	18	1/1/14/20	6/35/111/115	-
23	BCR	L	201	-	-	11/29/63/63	0/2/2/2
20	CLA	B	826	2	-	0/21/97/115	-
30	KC1	P	203	12	-	1/15/71/71	-
20	CLA	G	210	17	1/1/11/20	4/15/91/115	-
20	CLA	B	846	2	1/1/15/20	5/39/115/115	-
20	CLA	B	803	-	1/1/15/20	5/39/115/115	-
20	CLA	S	208	15	-	5/24/100/115	-
23	BCR	A	843	-	-	4/29/63/63	0/2/2/2
27	DGD	B	842	-	-	19/49/89/95	0/2/2/2
20	CLA	A	805	1	1/1/11/20	1/20/96/115	-
20	CLA	A	832	1	1/1/12/20	0/23/99/115	-
20	CLA	S	202	32	-	3/39/115/115	-
26	DD6	U	214	-	-	10/14/37/80	0/1/1/3
23	BCR	A	842	-	-	7/29/63/63	0/2/2/2
20	CLA	A	821	32	1/1/15/20	5/39/115/115	-
20	CLA	B	832	2	1/1/11/20	1/18/94/115	-
20	CLA	Q	205	13	1/1/14/20	5/33/109/115	-
20	CLA	B	806	2	1/1/15/20	9/39/115/115	-
29	LMG	P	217	-	-	8/19/39/70	0/1/1/1
20	CLA	Q	207	13	1/1/11/20	4/17/93/115	-
29	LMG	P	202	-	-	15/29/49/70	0/1/1/1
20	CLA	B	844	2	1/1/15/20	5/39/115/115	-
23	BCR	J	104	-	-	13/29/63/63	0/2/2/2
20	CLA	B	813	2	-	13/32/108/115	-
20	CLA	B	834	2	1/1/15/20	20/39/115/115	-
29	LMG	I	103	-	-	16/44/64/70	0/1/1/1
20	CLA	T	211	-	1/1/11/20	6/18/94/115	-
20	CLA	B	804	2	1/1/11/20	5/15/91/115	-
20	CLA	O	203	-	1/1/11/20	0/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	A	801	-	-	4/39/115/115	-
22	LHG	G	216	-	-	20/31/31/53	-
20	CLA	H	204	18	1/1/10/20	0/14/90/115	-
26	DD6	S	210	-	-	7/26/80/80	0/3/3/3
22	LHG	P	201	-	-	25/53/53/53	-
20	CLA	A	831	1	1/1/11/20	4/15/91/115	-
20	CLA	A	847	1	-	6/39/115/115	-

All (1573) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	Q	214	A86	C13-C11	-6.76	1.36	1.49
31	Q	218	A86	C13-C11	-6.75	1.36	1.49
31	R	105	A86	C13-C11	-6.62	1.37	1.49
31	U	202	A86	C13-C11	-6.44	1.37	1.49
31	P	204	A86	C13-C11	-6.37	1.37	1.49
31	R	103	A86	C13-C11	-6.34	1.37	1.49
31	Q	201	A86	C13-C11	-5.83	1.38	1.49
20	R	104	CLA	MG-NA	5.76	2.20	2.06
20	A	826	CLA	MG-NA	5.02	2.18	2.06
20	H	205	CLA	MG-NA	5.01	2.18	2.06
20	B	845	CLA	MG-NA	4.98	2.18	2.06
20	S	206	CLA	MG-NA	4.95	2.18	2.06
20	G	206	CLA	MG-NA	4.87	2.17	2.06
20	A	823	CLA	C4C-C3C	-4.72	1.37	1.45
20	B	808	CLA	C4C-C3C	-4.71	1.37	1.45
20	B	848	CLA	C4C-C3C	-4.70	1.37	1.45
20	B	834	CLA	C4C-C3C	-4.67	1.37	1.45
20	A	802	CLA	MG-NA	4.66	2.17	2.06
20	R	104	CLA	MG-NC	4.64	2.17	2.06
20	B	810	CLA	MG-NA	4.64	2.17	2.06
20	O	209	CLA	C4C-C3C	-4.63	1.37	1.45
20	B	816	CLA	C4C-C3C	-4.63	1.37	1.45
20	U	205	CLA	C4C-C3C	-4.63	1.37	1.45
20	A	846	CLA	MG-NA	4.63	2.17	2.06
20	H	207	CLA	C4C-C3C	-4.63	1.37	1.45
30	P	206	KC1	C4C-C3C	-4.62	1.37	1.45
20	Q	212	CLA	MG-NA	4.62	2.17	2.06
20	O	204	CLA	C4C-C3C	-4.62	1.37	1.45
20	U	210	CLA	C4C-C3C	-4.62	1.37	1.45
20	P	211	CLA	C4C-C3C	-4.62	1.37	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	Q	206	CLA	MG-NA	4.62	2.17	2.06
20	B	802	CLA	C4C-C3C	-4.61	1.37	1.45
20	T	207	CLA	C4C-C3C	-4.61	1.37	1.45
20	A	809	CLA	C4C-C3C	-4.60	1.37	1.45
20	H	206	CLA	C4C-C3C	-4.60	1.37	1.45
20	B	831	CLA	C4C-C3C	-4.60	1.37	1.45
20	A	834	CLA	MG-NA	4.59	2.17	2.06
20	A	825	CLA	C4C-C3C	-4.59	1.37	1.45
20	B	807	CLA	C4C-C3C	-4.59	1.37	1.45
20	Q	204	CLA	C4C-C3C	-4.58	1.37	1.45
20	S	206	CLA	C4C-C3C	-4.58	1.37	1.45
30	Q	210	KC1	C4C-C3C	-4.58	1.37	1.45
20	A	836	CLA	C4C-C3C	-4.58	1.37	1.45
20	A	846	CLA	C4C-C3C	-4.57	1.37	1.45
20	A	838	CLA	C4C-C3C	-4.57	1.37	1.45
20	A	804	CLA	C4C-C3C	-4.57	1.37	1.45
30	P	219	KC1	C4C-C3C	-4.57	1.37	1.45
20	B	822	CLA	C4C-C3C	-4.57	1.37	1.45
20	B	804	CLA	C4C-C3C	-4.57	1.37	1.45
20	G	203	CLA	C4C-C3C	-4.56	1.37	1.45
20	A	801	CLA	C4C-C3C	-4.56	1.37	1.45
20	G	206	CLA	C4C-C3C	-4.56	1.37	1.45
20	A	832	CLA	MG-NA	4.56	2.17	2.06
20	B	821	CLA	C4C-C3C	-4.56	1.37	1.45
20	A	824	CLA	C4C-C3C	-4.56	1.37	1.45
20	U	206	CLA	C4C-C3C	-4.56	1.37	1.45
20	A	808	CLA	C4C-C3C	-4.55	1.37	1.45
20	B	812	CLA	C4C-C3C	-4.53	1.37	1.45
20	B	823	CLA	C4C-C3C	-4.53	1.37	1.45
20	T	202	CLA	C4C-C3C	-4.53	1.37	1.45
20	A	810	CLA	C4C-C3C	-4.53	1.37	1.45
20	A	817	CLA	C4C-C3C	-4.53	1.37	1.45
20	A	805	CLA	C4C-C3C	-4.53	1.37	1.45
20	A	834	CLA	C4C-C3C	-4.53	1.37	1.45
20	B	811	CLA	C4C-C3C	-4.53	1.37	1.45
20	Q	209	CLA	C4C-C3C	-4.53	1.37	1.45
20	B	806	CLA	C4C-C3C	-4.52	1.37	1.45
20	P	214	CLA	C4C-C3C	-4.52	1.37	1.45
20	T	205	CLA	C4C-C3C	-4.52	1.37	1.45
20	P	207	CLA	C4C-C3C	-4.52	1.37	1.45
20	B	828	CLA	C4C-C3C	-4.52	1.37	1.45
20	A	813	CLA	C4C-C3C	-4.52	1.37	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B	832	CLA	C4C-C3C	-4.52	1.37	1.45
20	A	827	CLA	C4C-C3C	-4.52	1.37	1.45
20	U	206	CLA	MG-NA	4.52	2.17	2.06
20	O	203	CLA	C4C-C3C	-4.51	1.37	1.45
20	A	806	CLA	C4C-C3C	-4.51	1.37	1.45
20	B	813	CLA	C4C-C3C	-4.51	1.37	1.45
20	U	211	CLA	C4C-C3C	-4.51	1.37	1.45
20	L	203	CLA	C4C-C3C	-4.51	1.37	1.45
20	P	209	CLA	C4C-C3C	-4.51	1.37	1.45
20	B	820	CLA	C4C-C3C	-4.51	1.37	1.45
20	A	832	CLA	C4C-C3C	-4.50	1.37	1.45
20	T	211	CLA	C4C-C3C	-4.50	1.37	1.45
20	A	833	CLA	C4C-C3C	-4.50	1.37	1.45
20	B	814	CLA	C4C-C3C	-4.50	1.37	1.45
20	R	101	CLA	C4C-C3C	-4.50	1.37	1.45
20	A	819	CLA	C4C-C3C	-4.50	1.37	1.45
20	T	210	CLA	MG-NA	4.50	2.17	2.06
20	A	818	CLA	C4C-C3C	-4.50	1.37	1.45
20	B	801	CLA	C4C-C3C	-4.50	1.37	1.45
20	A	802	CLA	C4C-C3C	-4.49	1.37	1.45
20	T	203	CLA	C4C-C3C	-4.49	1.37	1.45
20	A	852	CLA	C4C-C3C	-4.49	1.37	1.45
20	B	819	CLA	C4C-C3C	-4.49	1.37	1.45
20	Q	206	CLA	C4C-C3C	-4.49	1.37	1.45
20	A	831	CLA	C4C-C3C	-4.49	1.37	1.45
20	A	812	CLA	MG-NA	4.49	2.16	2.06
20	A	815	CLA	C4C-C3C	-4.49	1.37	1.45
20	O	211	CLA	C4C-C3C	-4.49	1.37	1.45
20	S	205	CLA	C4C-C3C	-4.48	1.37	1.45
20	A	828	CLA	C4C-C3C	-4.48	1.37	1.45
20	B	846	CLA	C4C-C3C	-4.48	1.37	1.45
20	B	833	CLA	C4C-C3C	-4.48	1.37	1.45
20	A	814	CLA	C4C-C3C	-4.48	1.37	1.45
20	F	803	CLA	C4C-C3C	-4.48	1.37	1.45
20	A	851	CLA	C4C-C3C	-4.48	1.37	1.45
20	T	206	CLA	C4C-C3C	-4.48	1.37	1.45
20	L	202	CLA	C4C-C3C	-4.48	1.37	1.45
20	P	208	CLA	C4C-C3C	-4.48	1.37	1.45
20	A	830	CLA	C4C-C3C	-4.47	1.37	1.45
20	A	829	CLA	C4C-C3C	-4.47	1.37	1.45
20	B	815	CLA	C4C-C3C	-4.47	1.37	1.45
20	G	207	CLA	C4C-C3C	-4.47	1.37	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	P	213	CLA	C4C-C3C	-4.47	1.37	1.45
20	T	201	CLA	C4C-C3C	-4.47	1.37	1.45
20	A	803	CLA	C4C-C3C	-4.47	1.37	1.45
20	A	816	CLA	C4C-C3C	-4.47	1.37	1.45
30	U	213	KC1	C4C-C3C	-4.47	1.37	1.45
20	B	843	CLA	MG-NA	4.47	2.16	2.06
20	A	807	CLA	C4C-C3C	-4.46	1.37	1.45
20	B	826	CLA	C4C-C3C	-4.46	1.37	1.45
20	B	804	CLA	MG-NA	4.46	2.16	2.06
20	B	827	CLA	C4C-C3C	-4.46	1.37	1.45
20	Q	216	CLA	C4C-C3C	-4.46	1.37	1.45
20	U	204	CLA	C4C-C3C	-4.46	1.37	1.45
20	G	204	CLA	C4C-C3C	-4.46	1.37	1.45
20	B	805	CLA	C4C-C3C	-4.46	1.37	1.45
20	L	204	CLA	C4C-C3C	-4.46	1.37	1.45
20	S	207	CLA	C4C-C3C	-4.46	1.37	1.45
20	B	810	CLA	C4C-C3C	-4.46	1.37	1.45
20	G	210	CLA	C4C-C3C	-4.46	1.37	1.45
20	Q	205	CLA	C4C-C3C	-4.46	1.37	1.45
20	A	822	CLA	C4C-C3C	-4.46	1.37	1.45
20	P	216	CLA	C4C-C3C	-4.45	1.37	1.45
20	U	207	CLA	C4C-C3C	-4.45	1.37	1.45
20	B	830	CLA	C4C-C3C	-4.45	1.37	1.45
20	B	824	CLA	C4C-C3C	-4.45	1.37	1.45
20	B	817	CLA	C4C-C3C	-4.45	1.37	1.45
20	B	835	CLA	C4C-C3C	-4.45	1.37	1.45
20	A	823	CLA	C1C-C2C	-4.45	1.35	1.44
20	U	209	CLA	C4C-C3C	-4.45	1.37	1.45
20	P	208	CLA	MG-NA	4.44	2.16	2.06
20	O	202	CLA	C4C-C3C	-4.44	1.37	1.45
20	A	820	CLA	C4C-C3C	-4.44	1.37	1.45
20	T	204	CLA	C4C-C3C	-4.44	1.37	1.45
20	T	209	CLA	C4C-C3C	-4.44	1.37	1.45
20	A	853	CLA	C4C-C3C	-4.44	1.37	1.45
20	R	104	CLA	C4C-C3C	-4.44	1.37	1.45
30	S	209	KC1	C4C-C3C	-4.43	1.37	1.45
20	H	203	CLA	C4C-C3C	-4.43	1.37	1.45
20	A	826	CLA	C4C-C3C	-4.43	1.37	1.45
20	F	802	CLA	C4C-C3C	-4.42	1.37	1.45
20	B	813	CLA	MG-NA	4.42	2.16	2.06
20	O	206	CLA	C4C-C3C	-4.42	1.37	1.45
20	P	210	CLA	C4C-C3C	-4.42	1.37	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	G	209	CLA	C4C-C3C	-4.42	1.37	1.45
20	O	205	CLA	C4C-C3C	-4.41	1.37	1.45
20	H	202	CLA	C4C-C3C	-4.41	1.37	1.45
20	A	849	CLA	C4C-C3C	-4.41	1.37	1.45
20	B	845	CLA	C4C-C3C	-4.41	1.37	1.45
20	A	825	CLA	MG-NA	4.41	2.16	2.06
20	G	201	CLA	C4C-C3C	-4.41	1.37	1.45
20	B	825	CLA	C4C-C3C	-4.41	1.37	1.45
20	B	803	CLA	C4C-C3C	-4.41	1.37	1.45
20	B	818	CLA	C4C-C3C	-4.40	1.37	1.45
20	H	205	CLA	C4C-C3C	-4.40	1.37	1.45
20	J	103	CLA	C4C-C3C	-4.40	1.37	1.45
20	A	813	CLA	MG-NA	4.40	2.16	2.06
20	Q	213	CLA	C4C-C3C	-4.40	1.37	1.45
20	B	823	CLA	MG-NA	4.40	2.16	2.06
20	B	809	CLA	C4C-C3C	-4.39	1.37	1.45
20	G	202	CLA	C4C-C3C	-4.39	1.37	1.45
20	A	835	CLA	C4C-C3C	-4.39	1.37	1.45
20	G	215	CLA	C4C-C3C	-4.39	1.37	1.45
20	H	201	CLA	C4C-C3C	-4.39	1.37	1.45
20	A	811	CLA	C4C-C3C	-4.38	1.37	1.45
20	B	844	CLA	C4C-C3C	-4.38	1.37	1.45
20	U	208	CLA	C4C-C3C	-4.38	1.37	1.45
20	B	830	CLA	MG-NA	4.38	2.16	2.06
20	S	215	CLA	C4C-C3C	-4.38	1.37	1.45
20	A	828	CLA	MG-NA	4.38	2.16	2.06
20	A	829	CLA	MG-NA	4.37	2.16	2.06
20	S	202	CLA	C4C-C3C	-4.37	1.37	1.45
20	Q	203	CLA	C4C-C3C	-4.37	1.37	1.45
20	H	204	CLA	C4C-C3C	-4.37	1.37	1.45
20	A	827	CLA	MG-NA	4.37	2.16	2.06
30	Q	210	KC1	MG-NA	4.37	2.16	2.06
20	A	811	CLA	MG-NA	4.37	2.16	2.06
20	H	205	CLA	C1C-C2C	-4.36	1.35	1.44
20	A	854	CLA	C4C-C3C	-4.36	1.37	1.45
20	F	802	CLA	MG-NA	4.36	2.16	2.06
20	B	829	CLA	C4C-C3C	-4.35	1.37	1.45
20	B	803	CLA	C1C-C2C	-4.34	1.35	1.44
20	B	835	CLA	MG-NA	4.34	2.16	2.06
20	A	820	CLA	MG-NA	4.34	2.16	2.06
20	Q	207	CLA	C4C-C3C	-4.34	1.37	1.45
20	A	821	CLA	MG-NA	4.34	2.16	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	A	845	CLA	C4C-C3C	-4.34	1.37	1.45
20	T	203	CLA	MG-NA	4.34	2.16	2.06
20	A	835	CLA	MG-NA	4.32	2.16	2.06
20	B	806	CLA	MG-NA	4.32	2.16	2.06
30	O	210	KC1	C4C-C3C	-4.32	1.37	1.45
30	T	208	KC1	MG-NA	4.32	2.16	2.06
20	A	833	CLA	MG-NA	4.31	2.16	2.06
20	B	814	CLA	MG-NA	4.31	2.16	2.06
20	Q	212	CLA	C4C-C3C	-4.31	1.37	1.45
20	B	822	CLA	MG-NA	4.30	2.16	2.06
20	H	208	CLA	C4C-C3C	-4.29	1.37	1.45
20	O	207	CLA	C4C-C3C	-4.29	1.37	1.45
20	S	208	CLA	C4C-C3C	-4.29	1.37	1.45
20	G	208	CLA	C4C-C3C	-4.29	1.37	1.45
20	Q	208	CLA	C4C-C3C	-4.28	1.37	1.45
20	H	209	CLA	C4C-C3C	-4.28	1.37	1.45
20	B	809	CLA	C1C-C2C	-4.28	1.35	1.44
20	A	812	CLA	C4C-C3C	-4.28	1.37	1.45
20	S	214	CLA	C4C-C3C	-4.28	1.37	1.45
20	T	210	CLA	C4C-C3C	-4.27	1.37	1.45
20	B	844	CLA	MG-NA	4.27	2.16	2.06
30	T	208	KC1	C4C-C3C	-4.27	1.37	1.45
20	A	849	CLA	C1C-C2C	-4.27	1.35	1.44
20	Q	212	CLA	C1C-C2C	-4.26	1.35	1.44
20	B	843	CLA	C4C-C3C	-4.26	1.37	1.45
20	O	208	CLA	C4C-C3C	-4.26	1.37	1.45
20	A	805	CLA	MG-NA	4.26	2.16	2.06
20	A	847	CLA	C1C-C2C	-4.25	1.35	1.44
20	B	808	CLA	C1C-C2C	-4.25	1.35	1.44
20	Q	211	CLA	C4C-C3C	-4.25	1.37	1.45
20	B	825	CLA	MG-NA	4.24	2.16	2.06
20	A	821	CLA	C4C-C3C	-4.24	1.37	1.45
20	B	827	CLA	MG-NA	4.23	2.16	2.06
20	B	811	CLA	C1C-C2C	-4.23	1.35	1.44
20	T	210	CLA	C1C-C2C	-4.23	1.35	1.44
20	A	803	CLA	C1C-C2C	-4.23	1.35	1.44
30	S	211	KC1	C4C-C3C	-4.23	1.37	1.45
20	B	826	CLA	MG-NA	4.21	2.16	2.06
20	B	835	CLA	C1C-C2C	-4.21	1.36	1.44
30	O	210	KC1	C1C-C2C	-4.21	1.36	1.44
30	P	212	KC1	MG-NA	4.21	2.16	2.06
20	B	816	CLA	C1C-C2C	-4.20	1.36	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	Q	203	CLA	MG-NA	4.20	2.16	2.06
20	A	823	CLA	MG-NA	4.20	2.16	2.06
20	Q	206	CLA	C1C-C2C	-4.20	1.36	1.44
30	P	203	KC1	C4C-C3C	-4.19	1.37	1.45
20	Q	207	CLA	MG-NA	4.19	2.16	2.06
20	A	847	CLA	C4C-C3C	-4.19	1.37	1.45
30	P	203	KC1	C1C-C2C	-4.19	1.36	1.44
20	A	815	CLA	MG-NA	4.19	2.16	2.06
20	A	804	CLA	C1C-C2C	-4.18	1.36	1.44
20	A	812	CLA	C1C-C2C	-4.18	1.36	1.44
20	B	822	CLA	C1C-C2C	-4.18	1.36	1.44
20	G	206	CLA	C1C-C2C	-4.18	1.36	1.44
20	B	834	CLA	C1C-C2C	-4.18	1.36	1.44
20	A	829	CLA	C1C-C2C	-4.18	1.36	1.44
20	A	847	CLA	MG-NA	4.17	2.16	2.06
20	A	830	CLA	C1C-C2C	-4.17	1.36	1.44
20	A	826	CLA	C1C-C2C	-4.17	1.36	1.44
20	B	824	CLA	MG-NA	4.17	2.16	2.06
20	B	820	CLA	C1C-C2C	-4.17	1.36	1.44
20	A	809	CLA	MG-NA	4.17	2.16	2.06
20	A	807	CLA	MG-NA	4.17	2.16	2.06
20	R	104	CLA	C1C-C2C	-4.17	1.36	1.44
20	O	208	CLA	C1C-C2C	-4.17	1.36	1.44
20	A	828	CLA	C1C-C2C	-4.16	1.36	1.44
20	B	819	CLA	C1C-C2C	-4.16	1.36	1.44
20	B	826	CLA	C1C-C2C	-4.15	1.36	1.44
30	P	212	KC1	C4C-C3C	-4.15	1.38	1.45
20	P	214	CLA	C1C-C2C	-4.14	1.36	1.44
20	B	843	CLA	C1C-C2C	-4.14	1.36	1.44
20	B	812	CLA	C1C-C2C	-4.14	1.36	1.44
20	A	821	CLA	C1C-C2C	-4.13	1.36	1.44
20	A	838	CLA	C1C-C2C	-4.13	1.36	1.44
20	A	809	CLA	C1C-C2C	-4.13	1.36	1.44
20	P	216	CLA	MG-NA	4.13	2.16	2.06
30	T	208	KC1	C1C-C2C	-4.13	1.36	1.44
20	A	816	CLA	C1C-C2C	-4.13	1.36	1.44
30	Q	210	KC1	C1C-C2C	-4.13	1.36	1.44
20	H	201	CLA	C1C-C2C	-4.12	1.36	1.44
20	T	203	CLA	C1C-C2C	-4.12	1.36	1.44
20	B	844	CLA	C1C-C2C	-4.12	1.36	1.44
20	P	208	CLA	C1C-C2C	-4.12	1.36	1.44
30	U	213	KC1	C1B-C2B	-4.12	1.37	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	T	206	CLA	C1C-C2C	-4.12	1.36	1.44
20	A	832	CLA	C1C-C2C	-4.12	1.36	1.44
20	P	209	CLA	C1C-C2C	-4.12	1.36	1.44
20	B	802	CLA	C1C-C2C	-4.12	1.36	1.44
20	S	215	CLA	C1C-C2C	-4.12	1.36	1.44
30	P	212	KC1	C1C-C2C	-4.11	1.36	1.44
20	A	818	CLA	C1C-C2C	-4.11	1.36	1.44
20	B	828	CLA	C1C-C2C	-4.11	1.36	1.44
20	O	206	CLA	C1C-C2C	-4.11	1.36	1.44
20	A	836	CLA	C1C-C2C	-4.11	1.36	1.44
20	B	805	CLA	C1C-C2C	-4.11	1.36	1.44
20	L	202	CLA	C1C-C2C	-4.11	1.36	1.44
20	O	205	CLA	C1C-C2C	-4.11	1.36	1.44
20	Q	207	CLA	C1C-C2C	-4.10	1.36	1.44
20	S	206	CLA	C1C-C2C	-4.10	1.36	1.44
20	G	210	CLA	C1C-C2C	-4.10	1.36	1.44
20	B	820	CLA	MG-NA	4.09	2.16	2.06
20	G	203	CLA	MG-NA	4.09	2.16	2.06
20	H	209	CLA	MG-NA	4.09	2.16	2.06
20	A	811	CLA	C1C-C2C	-4.09	1.36	1.44
20	A	819	CLA	C1C-C2C	-4.09	1.36	1.44
20	S	214	CLA	C1C-C2C	-4.09	1.36	1.44
20	A	827	CLA	C1C-C2C	-4.09	1.36	1.44
20	A	825	CLA	C1C-C2C	-4.09	1.36	1.44
20	O	205	CLA	MG-NA	4.09	2.16	2.06
20	B	831	CLA	C1C-C2C	-4.09	1.36	1.44
20	U	210	CLA	C1C-C2C	-4.09	1.36	1.44
20	G	215	CLA	C1C-C2C	-4.09	1.36	1.44
30	P	206	KC1	C1C-C2C	-4.09	1.36	1.44
20	B	810	CLA	C1C-C2C	-4.09	1.36	1.44
20	B	812	CLA	MG-NA	4.08	2.16	2.06
20	A	807	CLA	C1C-C2C	-4.08	1.36	1.44
20	F	802	CLA	C1C-C2C	-4.08	1.36	1.44
20	A	820	CLA	C1C-C2C	-4.08	1.36	1.44
20	B	832	CLA	MG-NA	4.08	2.16	2.06
20	B	829	CLA	C1C-C2C	-4.08	1.36	1.44
30	P	219	KC1	C1C-C2C	-4.08	1.36	1.44
20	U	211	CLA	C1C-C2C	-4.08	1.36	1.44
20	A	854	CLA	C1C-C2C	-4.08	1.36	1.44
20	G	201	CLA	C1C-C2C	-4.08	1.36	1.44
30	S	211	KC1	C1C-C2C	-4.08	1.36	1.44
20	B	828	CLA	MG-NA	4.08	2.16	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	H	208	CLA	C1C-C2C	-4.08	1.36	1.44
20	Q	209	CLA	C1C-C2C	-4.07	1.36	1.44
20	U	206	CLA	C1C-C2C	-4.07	1.36	1.44
20	A	810	CLA	C1C-C2C	-4.07	1.36	1.44
20	B	815	CLA	C1C-C2C	-4.07	1.36	1.44
20	A	808	CLA	C1C-C2C	-4.07	1.36	1.44
20	B	848	CLA	C1C-C2C	-4.07	1.36	1.44
20	F	803	CLA	C1C-C2C	-4.07	1.36	1.44
20	B	833	CLA	C1C-C2C	-4.07	1.36	1.44
20	Q	203	CLA	C1C-C2C	-4.07	1.36	1.44
20	T	209	CLA	C1C-C2C	-4.07	1.36	1.44
20	U	211	CLA	MG-NA	4.07	2.15	2.06
20	Q	216	CLA	C1C-C2C	-4.06	1.36	1.44
20	A	810	CLA	MG-NA	4.06	2.15	2.06
20	A	833	CLA	C1C-C2C	-4.06	1.36	1.44
20	O	203	CLA	C1C-C2C	-4.06	1.36	1.44
20	Q	204	CLA	C1C-C2C	-4.06	1.36	1.44
30	S	209	KC1	C1C-C2C	-4.05	1.36	1.44
20	A	851	CLA	MG-NA	4.05	2.15	2.06
20	B	846	CLA	C1C-C2C	-4.05	1.36	1.44
20	L	204	CLA	C1C-C2C	-4.05	1.36	1.44
20	B	824	CLA	C1C-C2C	-4.05	1.36	1.44
20	Q	211	CLA	C1C-C2C	-4.05	1.36	1.44
20	B	827	CLA	C1C-C2C	-4.05	1.36	1.44
20	A	802	CLA	C1C-C2C	-4.05	1.36	1.44
20	B	806	CLA	C1C-C2C	-4.04	1.36	1.44
20	A	806	CLA	C1C-C2C	-4.04	1.36	1.44
20	T	204	CLA	C1C-C2C	-4.04	1.36	1.44
20	G	209	CLA	C1C-C2C	-4.04	1.36	1.44
20	A	852	CLA	C1C-C2C	-4.04	1.36	1.44
20	A	835	CLA	C1C-C2C	-4.04	1.36	1.44
20	B	821	CLA	C1C-C2C	-4.03	1.36	1.44
20	O	211	CLA	C1C-C2C	-4.03	1.36	1.44
20	B	817	CLA	C1C-C2C	-4.03	1.36	1.44
20	B	825	CLA	C1C-C2C	-4.03	1.36	1.44
20	P	213	CLA	C1C-C2C	-4.03	1.36	1.44
20	J	103	CLA	C1C-C2C	-4.03	1.36	1.44
20	R	101	CLA	C1C-C2C	-4.03	1.36	1.44
20	S	207	CLA	C1C-C2C	-4.03	1.36	1.44
20	A	817	CLA	MG-NA	4.03	2.15	2.06
20	A	822	CLA	C1C-C2C	-4.03	1.36	1.44
20	B	801	CLA	MG-NA	4.03	2.15	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	A	817	CLA	C1C-C2C	-4.03	1.36	1.44
20	B	832	CLA	C1C-C2C	-4.03	1.36	1.44
20	B	813	CLA	C1C-C2C	-4.03	1.36	1.44
20	O	202	CLA	C1C-C2C	-4.03	1.36	1.44
20	G	205	CLA	C1C-C2C	-4.03	1.36	1.44
20	U	204	CLA	C1C-C2C	-4.03	1.36	1.44
20	S	202	CLA	C1C-C2C	-4.02	1.36	1.44
20	O	203	CLA	MG-NA	4.02	2.15	2.06
20	A	845	CLA	C1C-C2C	-4.02	1.36	1.44
20	P	216	CLA	C1C-C2C	-4.02	1.36	1.44
20	G	202	CLA	C1C-C2C	-4.02	1.36	1.44
20	A	846	CLA	C1C-C2C	-4.02	1.36	1.44
20	O	207	CLA	C1C-C2C	-4.02	1.36	1.44
20	H	209	CLA	C1C-C2C	-4.02	1.36	1.44
20	Q	213	CLA	C1C-C2C	-4.02	1.36	1.44
20	P	210	CLA	C1C-C2C	-4.02	1.36	1.44
20	S	208	CLA	C1C-C2C	-4.02	1.36	1.44
20	T	202	CLA	C1C-C2C	-4.01	1.36	1.44
20	O	204	CLA	C1C-C2C	-4.01	1.36	1.44
20	B	823	CLA	C1C-C2C	-4.01	1.36	1.44
20	U	207	CLA	C1C-C2C	-4.01	1.36	1.44
20	U	208	CLA	C1C-C2C	-4.01	1.36	1.44
20	G	203	CLA	C1C-C2C	-4.01	1.36	1.44
20	A	851	CLA	C1C-C2C	-4.01	1.36	1.44
20	A	814	CLA	C1C-C2C	-4.00	1.36	1.44
20	G	207	CLA	C1C-C2C	-4.00	1.36	1.44
20	A	801	CLA	C1C-C2C	-4.00	1.36	1.44
20	A	853	CLA	C1C-C2C	-4.00	1.36	1.44
20	Q	208	CLA	C1C-C2C	-4.00	1.36	1.44
20	B	814	CLA	C1C-C2C	-4.00	1.36	1.44
20	A	805	CLA	C1C-C2C	-4.00	1.36	1.44
20	A	824	CLA	C1C-C2C	-4.00	1.36	1.44
20	A	808	CLA	MG-NA	3.99	2.15	2.06
20	Q	205	CLA	C1C-C2C	-3.99	1.36	1.44
20	T	201	CLA	C1C-C2C	-3.99	1.36	1.44
30	P	203	KC1	MG-NA	3.99	2.15	2.06
30	S	209	KC1	C4A-C3A	-3.99	1.36	1.44
20	B	830	CLA	C1C-C2C	-3.99	1.36	1.44
20	T	205	CLA	C1C-C2C	-3.99	1.36	1.44
20	A	815	CLA	C1C-C2C	-3.98	1.36	1.44
20	T	211	CLA	C1C-C2C	-3.98	1.36	1.44
20	Q	205	CLA	MG-NA	3.98	2.15	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B	818	CLA	C1C-C2C	-3.98	1.36	1.44
20	B	818	CLA	MG-NA	3.98	2.15	2.06
30	O	210	KC1	C3B-C4B	-3.98	1.39	1.46
20	S	205	CLA	C1C-C2C	-3.98	1.36	1.44
20	B	801	CLA	C1C-C2C	-3.98	1.36	1.44
20	B	845	CLA	C1C-C2C	-3.98	1.36	1.44
20	A	813	CLA	C1C-C2C	-3.97	1.36	1.44
20	L	203	CLA	C1C-C2C	-3.97	1.36	1.44
20	P	207	CLA	C1C-C2C	-3.97	1.36	1.44
20	T	207	CLA	C1C-C2C	-3.96	1.36	1.44
20	U	205	CLA	C1C-C2C	-3.96	1.36	1.44
20	B	802	CLA	MG-NA	3.96	2.15	2.06
20	B	807	CLA	C1C-C2C	-3.95	1.36	1.44
20	G	208	CLA	C1C-C2C	-3.95	1.36	1.44
20	A	831	CLA	C1C-C2C	-3.95	1.36	1.44
20	S	205	CLA	MG-NA	3.95	2.15	2.06
20	Q	208	CLA	MG-NA	3.95	2.15	2.06
20	B	804	CLA	C1C-C2C	-3.94	1.36	1.44
20	P	211	CLA	C1C-C2C	-3.94	1.36	1.44
20	A	834	CLA	C1C-C2C	-3.94	1.36	1.44
30	O	210	KC1	C4A-C3A	-3.93	1.36	1.44
20	H	207	CLA	MG-NA	3.93	2.15	2.06
30	P	203	KC1	C4A-C3A	-3.92	1.36	1.44
20	H	204	CLA	C1C-C2C	-3.92	1.36	1.44
20	A	849	CLA	MG-NA	3.92	2.15	2.06
20	G	204	CLA	C1C-C2C	-3.92	1.36	1.44
20	H	201	CLA	MG-NA	3.92	2.15	2.06
20	A	836	CLA	MG-NA	3.91	2.15	2.06
20	B	807	CLA	MG-NA	3.91	2.15	2.06
20	U	209	CLA	C1C-C2C	-3.91	1.36	1.44
30	S	209	KC1	C1B-C2B	-3.91	1.37	1.45
20	T	211	CLA	MG-NA	3.91	2.15	2.06
20	H	202	CLA	C1C-C2C	-3.90	1.36	1.44
30	U	213	KC1	C1C-C2C	-3.90	1.36	1.44
20	B	831	CLA	MG-NA	3.89	2.15	2.06
20	Q	211	CLA	MG-NA	3.89	2.15	2.06
20	A	824	CLA	MG-NA	3.89	2.15	2.06
20	F	803	CLA	MG-NA	3.87	2.15	2.06
30	T	208	KC1	C1B-C2B	-3.87	1.37	1.45
20	A	845	CLA	MG-NA	3.87	2.15	2.06
20	A	854	CLA	MG-NA	3.87	2.15	2.06
20	H	203	CLA	C1C-C2C	-3.86	1.36	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	T	208	KC1	C4A-C3A	-3.86	1.36	1.44
20	U	204	CLA	MG-NA	3.86	2.15	2.06
30	P	203	KC1	C1B-C2B	-3.86	1.37	1.45
26	P	218	DD6	C26-C27	3.83	1.45	1.37
20	G	210	CLA	MG-NA	3.83	2.15	2.06
20	A	852	CLA	MG-NA	3.83	2.15	2.06
30	P	206	KC1	C1B-C2B	-3.83	1.37	1.45
20	H	207	CLA	C1C-C2C	-3.82	1.36	1.44
20	P	214	CLA	MG-NA	3.82	2.15	2.06
20	H	203	CLA	MG-NA	3.82	2.15	2.06
30	Q	210	KC1	C3B-C4B	-3.82	1.39	1.46
30	S	211	KC1	C1B-C2B	-3.82	1.37	1.45
20	B	809	CLA	MG-NA	3.82	2.15	2.06
30	P	219	KC1	C3B-C4B	-3.81	1.39	1.46
20	L	202	CLA	MG-NA	3.81	2.15	2.06
20	G	202	CLA	MG-NA	3.81	2.15	2.06
20	B	816	CLA	MG-NA	3.81	2.15	2.06
20	A	830	CLA	MG-NA	3.80	2.15	2.06
30	P	203	KC1	C3B-C4B	-3.80	1.39	1.46
30	P	212	KC1	C3B-C4B	-3.79	1.39	1.46
20	O	204	CLA	MG-NA	3.79	2.15	2.06
20	B	802	CLA	MG-NC	3.79	2.15	2.06
20	O	207	CLA	MG-NA	3.79	2.15	2.06
30	T	208	KC1	C3B-C4B	-3.79	1.39	1.46
20	B	808	CLA	MG-NA	3.79	2.15	2.06
30	P	206	KC1	C3B-C4B	-3.78	1.39	1.46
20	B	815	CLA	MG-NA	3.78	2.15	2.06
26	O	215	DD6	C28-C27	-3.77	1.48	1.50
20	A	814	CLA	MG-NA	3.77	2.15	2.06
20	B	819	CLA	MG-NA	3.77	2.15	2.06
20	H	202	CLA	MG-NA	3.77	2.15	2.06
20	O	202	CLA	MG-NA	3.76	2.15	2.06
20	B	829	CLA	MG-NA	3.75	2.15	2.06
30	S	209	KC1	C3B-C4B	-3.75	1.39	1.46
30	P	212	KC1	C1B-C2B	-3.75	1.37	1.45
30	U	213	KC1	C4A-C3A	-3.75	1.36	1.44
30	O	210	KC1	MG-NA	3.74	2.15	2.06
20	U	205	CLA	MG-NA	3.73	2.15	2.06
20	A	853	CLA	MG-NA	3.73	2.15	2.06
30	P	219	KC1	C1B-C2B	-3.72	1.38	1.45
20	B	833	CLA	MG-NA	3.72	2.15	2.06
20	R	101	CLA	MG-NA	3.72	2.15	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	H	206	CLA	MG-NA	3.72	2.15	2.06
30	P	206	KC1	C4A-C3A	-3.71	1.37	1.44
20	T	202	CLA	MG-NA	3.71	2.15	2.06
23	B	837	BCR	C1-C6	-3.71	1.49	1.53
30	S	211	KC1	C3B-C4B	-3.71	1.39	1.46
20	O	209	CLA	C1C-C2C	-3.71	1.37	1.44
20	G	204	CLA	MG-NA	3.70	2.15	2.06
20	H	208	CLA	MG-NA	3.69	2.15	2.06
30	S	211	KC1	C4A-C3A	-3.69	1.37	1.44
20	A	816	CLA	MG-NA	3.68	2.15	2.06
20	S	215	CLA	MG-NA	3.68	2.15	2.06
20	J	103	CLA	MG-NA	3.68	2.15	2.06
30	P	212	KC1	C4A-C3A	-3.67	1.37	1.44
30	U	213	KC1	C3B-C4B	-3.66	1.39	1.46
20	Q	204	CLA	MG-NA	3.66	2.15	2.06
20	B	846	CLA	MG-NA	3.65	2.15	2.06
20	G	205	CLA	C4C-C3C	-3.65	1.38	1.45
20	G	209	CLA	MG-NA	3.65	2.14	2.06
20	H	206	CLA	C1C-C2C	-3.65	1.37	1.44
20	B	805	CLA	MG-NA	3.65	2.14	2.06
30	Q	210	KC1	C1B-C2B	-3.64	1.38	1.45
20	B	848	CLA	MG-NA	3.64	2.14	2.06
23	J	104	BCR	C30-C25	-3.64	1.49	1.53
20	A	819	CLA	MG-NA	3.64	2.14	2.06
30	O	210	KC1	C1B-C2B	-3.63	1.38	1.45
20	S	202	CLA	MG-NA	3.62	2.14	2.06
20	P	207	CLA	MG-NA	3.61	2.14	2.06
23	A	843	BCR	C1-C6	-3.60	1.49	1.53
30	U	213	KC1	MG-NA	3.60	2.14	2.06
20	A	838	CLA	MG-NA	3.59	2.14	2.06
20	B	817	CLA	MG-NA	3.59	2.14	2.06
20	A	818	CLA	MG-NA	3.59	2.14	2.06
20	O	206	CLA	MG-NA	3.58	2.14	2.06
20	A	801	CLA	MG-NA	3.58	2.14	2.06
20	T	201	CLA	MG-NA	3.57	2.14	2.06
20	O	211	CLA	MG-NA	3.56	2.14	2.06
26	G	213	DD6	C26-C27	3.55	1.44	1.37
20	T	206	CLA	MG-NA	3.55	2.14	2.06
20	A	831	CLA	MG-NA	3.55	2.14	2.06
20	P	210	CLA	MG-NA	3.55	2.14	2.06
20	Q	209	CLA	MG-NA	3.55	2.14	2.06
26	S	204	DD6	C26-C27	3.53	1.44	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	H	204	CLA	MG-NA	3.52	2.14	2.06
30	P	219	KC1	C4A-C3A	-3.52	1.37	1.44
20	A	846	CLA	MG-NC	3.51	2.14	2.06
20	L	204	CLA	MG-NA	3.50	2.14	2.06
26	U	214	DD6	C8-C6	-3.49	1.41	1.50
20	S	207	CLA	MG-NA	3.47	2.14	2.06
26	O	212	DD6	C26-C27	3.46	1.44	1.37
20	A	806	CLA	MG-NA	3.46	2.14	2.06
20	A	804	CLA	MG-NA	3.46	2.14	2.06
26	S	204	DD6	C28-C27	-3.45	1.48	1.50
20	L	203	CLA	MG-NA	3.45	2.14	2.06
20	Q	213	CLA	MG-NA	3.44	2.14	2.06
20	S	208	CLA	MG-NA	3.44	2.14	2.06
20	A	834	CLA	MG-NC	3.42	2.14	2.06
20	S	214	CLA	MG-NA	3.42	2.14	2.06
26	H	210	DD6	C26-C27	3.42	1.44	1.37
23	L	205	BCR	C30-C25	-3.42	1.49	1.53
23	A	844	BCR	C1-C6	-3.40	1.49	1.53
20	G	201	CLA	MG-NA	3.40	2.14	2.06
20	U	210	CLA	MG-NA	3.38	2.14	2.06
20	T	204	CLA	MG-NA	3.38	2.14	2.06
23	B	838	BCR	C1-C6	-3.37	1.49	1.53
20	P	213	CLA	MG-NA	3.36	2.14	2.06
30	Q	210	KC1	C4A-C3A	-3.35	1.37	1.44
20	B	826	CLA	MG-NC	3.33	2.14	2.06
20	T	209	CLA	MG-NA	3.32	2.14	2.06
26	G	214	DD6	C26-C27	3.32	1.44	1.37
20	B	810	CLA	MG-NC	3.31	2.14	2.06
20	O	209	CLA	MG-NA	3.30	2.14	2.06
20	P	209	CLA	MG-NA	3.28	2.14	2.06
20	A	822	CLA	MG-NA	3.28	2.14	2.06
20	G	208	CLA	MG-NA	3.25	2.14	2.06
23	I	102	BCR	C1-C6	-3.24	1.49	1.53
20	O	208	CLA	MG-NA	3.24	2.14	2.06
23	B	839	BCR	C1-C6	-3.23	1.49	1.53
20	B	814	CLA	MG-NC	3.23	2.13	2.06
20	A	835	CLA	MG-NC	3.22	2.13	2.06
26	S	213	DD6	C26-C27	3.22	1.43	1.37
26	S	212	DD6	C26-C27	3.21	1.43	1.37
23	R	102	BCR	C1-C6	-3.20	1.49	1.53
20	A	803	CLA	MG-NA	3.20	2.13	2.06
20	G	215	CLA	MG-NA	3.20	2.13	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	U	203	DD6	C26-C27	3.19	1.43	1.37
23	L	201	BCR	C30-C25	-3.18	1.49	1.53
20	R	104	CLA	MG-NB	3.18	2.12	2.05
23	I	102	BCR	C30-C25	-3.18	1.49	1.53
20	U	207	CLA	MG-NA	3.18	2.13	2.06
20	U	208	CLA	MG-NA	3.18	2.13	2.06
20	G	205	CLA	MG-NA	3.17	2.13	2.06
20	P	211	CLA	MG-NA	3.16	2.13	2.06
23	L	201	BCR	C1-C6	-3.15	1.49	1.53
30	P	203	KC1	C2A-C3A	3.14	1.43	1.37
23	B	841	BCR	C30-C25	-3.14	1.49	1.53
26	T	212	DD6	C26-C27	3.13	1.43	1.37
20	A	826	CLA	MG-NC	3.13	2.13	2.06
26	U	214	DD6	C26-C27	3.12	1.43	1.37
20	Q	216	CLA	MG-NA	3.12	2.13	2.06
20	T	205	CLA	MG-NA	3.11	2.13	2.06
20	A	827	CLA	MG-NC	3.11	2.13	2.06
20	B	811	CLA	MG-NA	3.11	2.13	2.06
26	H	211	DD6	C26-C27	3.11	1.43	1.37
20	A	802	CLA	MG-NC	3.10	2.13	2.06
26	P	215	DD6	C26-C27	3.10	1.43	1.37
23	M	101	BCR	C30-C25	-3.10	1.49	1.53
28	S	201	SQD	O48-C23	3.09	1.42	1.33
23	R	102	BCR	C30-C25	-3.09	1.49	1.53
23	M	101	BCR	C1-C6	-3.08	1.49	1.53
20	B	803	CLA	MG-NA	3.08	2.13	2.06
26	T	213	DD6	C26-C27	3.08	1.43	1.37
26	U	212	DD6	C26-C27	3.07	1.43	1.37
26	Q	202	DD6	C26-C27	3.04	1.43	1.37
26	J	101	DD6	C26-C27	3.04	1.43	1.37
30	O	210	KC1	C2A-C3A	3.03	1.43	1.37
20	B	823	CLA	MG-NC	3.03	2.13	2.06
20	A	828	CLA	MG-NC	3.03	2.13	2.06
20	B	832	CLA	MG-NC	3.01	2.13	2.06
20	U	209	CLA	MG-NA	3.01	2.13	2.06
26	O	213	DD6	C26-C27	3.01	1.43	1.37
20	B	821	CLA	MG-NA	3.01	2.13	2.06
30	S	209	KC1	MG-NA	3.00	2.13	2.06
24	A	848	CL0	CHB-C1B	3.00	1.44	1.39
26	O	201	DD6	C26-C27	2.99	1.43	1.37
23	B	841	BCR	C1-C6	-2.99	1.50	1.53
26	S	203	DD6	C26-C27	2.98	1.43	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B	813	CLA	MG-NC	2.98	2.13	2.06
23	A	842	BCR	C1-C6	-2.98	1.50	1.53
20	G	206	CLA	MG-NC	2.98	2.13	2.06
20	H	205	CLA	MG-NC	2.98	2.13	2.06
30	S	211	KC1	MG-NA	2.97	2.13	2.06
24	A	848	CL0	C3B-C4B	-2.97	1.38	1.41
20	A	821	CLA	MG-NC	2.97	2.13	2.06
20	T	207	CLA	MG-NA	2.95	2.13	2.06
28	B	847	SQD	O48-C23	2.95	1.41	1.33
26	G	212	DD6	C26-C27	2.93	1.43	1.37
26	P	205	DD6	C26-C27	2.92	1.43	1.37
26	Q	215	DD6	C26-C27	2.91	1.43	1.37
23	B	840	BCR	C1-C6	-2.91	1.50	1.53
20	B	843	CLA	MG-NC	2.91	2.13	2.06
26	P	220	DD6	C26-C27	2.90	1.43	1.37
23	B	837	BCR	C30-C25	-2.89	1.50	1.53
26	S	212	DD6	C10-C11	2.88	1.42	1.35
26	P	218	DD6	C28-C27	-2.87	1.49	1.50
23	J	104	BCR	C1-C6	-2.87	1.50	1.53
30	P	219	KC1	MG-NA	2.87	2.13	2.06
20	Q	212	CLA	MG-NC	2.86	2.13	2.06
26	A	855	DD6	C26-C27	2.86	1.43	1.37
26	G	211	DD6	C24-C1	-2.85	1.39	1.46
23	I	101	BCR	C1-C6	-2.84	1.50	1.53
26	S	210	DD6	C26-C27	2.84	1.43	1.37
23	L	205	BCR	C1-C6	-2.84	1.50	1.53
20	G	207	CLA	MG-NA	2.83	2.13	2.06
20	B	845	CLA	MG-NC	2.83	2.13	2.06
20	H	209	CLA	MG-NC	2.82	2.13	2.06
23	F	804	BCR	C1-C6	-2.81	1.50	1.53
20	A	849	CLA	MG-NC	2.81	2.12	2.06
30	T	208	KC1	MG-NC	2.80	2.12	2.06
26	O	215	DD6	C26-C27	2.80	1.42	1.37
20	B	844	CLA	C3D-C4D	-2.80	1.37	1.44
20	R	104	CLA	MG-ND	2.80	2.11	2.05
20	B	830	CLA	MG-NC	2.79	2.12	2.06
20	B	835	CLA	MG-NC	2.79	2.12	2.06
23	A	844	BCR	C30-C25	-2.79	1.50	1.53
20	B	817	CLA	C1B-C2B	-2.79	1.36	1.43
20	P	208	CLA	MG-NC	2.78	2.12	2.06
28	S	201	SQD	O47-C7	2.78	1.42	1.34
26	P	220	DD6	C28-C27	-2.78	1.49	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	F	801	BCR	C1-C6	-2.77	1.50	1.53
20	B	844	CLA	MG-NC	2.77	2.12	2.06
20	P	214	CLA	MG-NC	2.76	2.12	2.06
26	G	211	DD6	C26-C27	2.76	1.42	1.37
29	P	217	LMG	C4-C5	2.75	1.58	1.53
30	Q	210	KC1	MG-NC	2.75	2.12	2.06
23	A	841	BCR	C1-C6	-2.75	1.50	1.53
20	P	214	CLA	MG-NB	2.74	2.11	2.05
30	P	212	KC1	MG-NC	2.74	2.12	2.06
20	Q	206	CLA	MG-NC	2.73	2.12	2.06
23	A	841	BCR	C30-C25	-2.73	1.50	1.53
26	H	210	DD6	C24-C1	-2.73	1.40	1.46
20	G	210	CLA	MG-NC	2.73	2.12	2.06
20	B	825	CLA	MG-NC	2.73	2.12	2.06
20	A	820	CLA	MG-NC	2.72	2.12	2.06
20	A	812	CLA	MG-NC	2.72	2.12	2.06
20	B	825	CLA	C3D-C4D	-2.72	1.38	1.44
20	B	807	CLA	MG-NC	2.72	2.12	2.06
20	B	806	CLA	MG-NC	2.71	2.12	2.06
20	O	209	CLA	C1D-C2D	-2.71	1.40	1.45
26	G	217	DD6	C26-C27	2.71	1.42	1.37
28	B	847	SQD	O47-C7	2.70	1.41	1.34
20	A	805	CLA	MG-NC	2.70	2.12	2.06
20	U	206	CLA	MG-NC	2.70	2.12	2.06
20	A	811	CLA	MG-NC	2.70	2.12	2.06
20	O	209	CLA	C3D-C4D	-2.70	1.38	1.44
26	G	212	DD6	C8-C6	-2.69	1.40	1.46
20	B	817	CLA	C3D-C4D	-2.68	1.38	1.44
20	A	802	CLA	C1D-C2D	-2.68	1.40	1.45
20	B	824	CLA	C3D-C4D	-2.68	1.38	1.44
20	A	825	CLA	MG-NC	2.67	2.12	2.06
26	G	212	DD6	C24-C1	-2.67	1.40	1.46
26	S	210	DD6	C24-C1	-2.67	1.40	1.46
20	B	807	CLA	C3D-C4D	-2.66	1.38	1.44
23	B	840	BCR	C30-C25	-2.66	1.50	1.53
30	P	206	KC1	MG-NA	2.66	2.12	2.06
20	B	821	CLA	C3D-C4D	-2.66	1.38	1.44
26	G	213	DD6	C28-C27	-2.66	1.49	1.50
20	A	847	CLA	MG-NC	2.65	2.12	2.06
20	B	801	CLA	MG-NC	2.65	2.12	2.06
20	B	834	CLA	MG-NA	2.64	2.12	2.06
20	B	846	CLA	C3D-C4D	-2.64	1.38	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B	828	CLA	MG-NC	2.64	2.12	2.06
20	U	208	CLA	C3D-C4D	-2.64	1.38	1.44
20	B	804	CLA	MG-NC	2.63	2.12	2.06
20	B	830	CLA	C3D-C4D	-2.63	1.38	1.44
23	B	839	BCR	C30-C25	-2.62	1.50	1.53
20	A	832	CLA	MG-NC	2.62	2.12	2.06
20	B	819	CLA	C3D-C4D	-2.62	1.38	1.44
26	S	210	DD6	C13-C11	-2.62	1.40	1.46
20	B	822	CLA	C3D-C4D	-2.62	1.38	1.44
20	Q	211	CLA	MG-NC	2.62	2.12	2.06
20	A	827	CLA	C3D-C4D	-2.61	1.38	1.44
20	B	810	CLA	C3D-C4D	-2.61	1.38	1.44
26	O	215	DD6	C24-C1	-2.61	1.40	1.46
20	B	805	CLA	C3D-C4D	-2.61	1.38	1.44
26	A	855	DD6	C24-C1	-2.61	1.40	1.46
20	B	834	CLA	C3D-C4D	-2.60	1.38	1.44
20	A	813	CLA	MG-NC	2.60	2.12	2.06
20	P	216	CLA	MG-NC	2.60	2.12	2.06
20	R	101	CLA	C1B-C2B	-2.60	1.37	1.43
20	T	203	CLA	MG-NC	2.60	2.12	2.06
20	A	820	CLA	C3D-C4D	-2.60	1.38	1.44
26	P	220	DD6	C24-C1	-2.59	1.40	1.46
31	R	103	A86	C5-C6	2.59	1.41	1.35
20	A	809	CLA	MG-NC	2.59	2.12	2.06
26	H	210	DD6	C8-C6	-2.59	1.40	1.46
30	U	213	KC1	C1A-CHA	2.59	1.47	1.40
26	S	210	DD6	C8-C6	-2.59	1.40	1.46
20	Q	211	CLA	C3D-C4D	-2.59	1.38	1.44
20	A	845	CLA	MG-NC	2.59	2.12	2.06
31	R	103	A86	C2-C1	2.58	1.41	1.35
23	F	801	BCR	C30-C25	-2.58	1.50	1.53
20	G	207	CLA	C3D-C4D	-2.58	1.38	1.44
20	B	833	CLA	C3D-C4D	-2.58	1.38	1.44
20	B	802	CLA	C1D-C2D	-2.58	1.40	1.45
20	A	803	CLA	C3D-C4D	-2.58	1.38	1.44
20	B	815	CLA	C3D-C4D	-2.58	1.38	1.44
26	G	212	DD6	C13-C11	-2.58	1.40	1.46
20	S	208	CLA	C3D-C4D	-2.57	1.38	1.44
20	A	805	CLA	C3D-C4D	-2.57	1.38	1.44
26	U	203	DD6	C10-C11	2.57	1.41	1.35
20	B	815	CLA	C1B-C2B	-2.57	1.37	1.43
20	H	204	CLA	MG-NC	2.57	2.12	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	O	214	DD6	C24-C1	-2.56	1.40	1.46
30	P	212	KC1	C1A-CHA	2.56	1.46	1.40
20	Q	213	CLA	C3D-C4D	-2.56	1.38	1.44
20	A	835	CLA	C3D-C4D	-2.55	1.38	1.44
20	A	833	CLA	MG-NC	2.55	2.12	2.06
20	B	811	CLA	C3D-C4D	-2.55	1.38	1.44
20	A	806	CLA	C3D-C4D	-2.55	1.38	1.44
20	B	808	CLA	C1D-C2D	-2.55	1.40	1.45
29	P	217	LMG	O4-C4	-2.55	1.36	1.43
26	H	210	DD6	C13-C11	-2.55	1.40	1.46
29	P	217	LMG	C4-C3	2.55	1.59	1.52
26	U	212	DD6	C10-C11	2.55	1.41	1.35
20	L	203	CLA	C3D-C4D	-2.55	1.38	1.44
20	A	829	CLA	MG-NC	2.55	2.12	2.06
26	S	212	DD6	C2-C1	2.55	1.41	1.35
20	R	101	CLA	C3D-C4D	-2.54	1.38	1.44
20	B	829	CLA	C3D-C4D	-2.54	1.38	1.44
20	A	816	CLA	C3D-C4D	-2.54	1.38	1.44
20	Q	206	CLA	C3D-C4D	-2.54	1.38	1.44
20	O	211	CLA	C3D-C4D	-2.54	1.38	1.44
20	B	806	CLA	C3D-C4D	-2.53	1.38	1.44
20	G	202	CLA	C3D-C4D	-2.53	1.38	1.44
20	B	835	CLA	C1D-C2D	-2.53	1.40	1.45
20	A	822	CLA	C3D-C4D	-2.53	1.38	1.44
20	P	207	CLA	C3D-C4D	-2.53	1.38	1.44
20	B	831	CLA	MG-NC	2.53	2.12	2.06
20	A	804	CLA	C3D-C4D	-2.53	1.38	1.44
31	P	204	A86	C2-C1	2.53	1.41	1.35
20	S	214	CLA	C3D-C4D	-2.53	1.38	1.44
30	P	203	KC1	C1A-CHA	2.53	1.46	1.40
20	Q	216	CLA	C3D-C4D	-2.53	1.38	1.44
20	A	853	CLA	C3D-C4D	-2.53	1.38	1.44
20	A	849	CLA	C3D-C4D	-2.52	1.38	1.44
20	B	824	CLA	MG-NC	2.52	2.12	2.06
20	S	207	CLA	C3D-C4D	-2.52	1.38	1.44
20	B	816	CLA	C3D-C4D	-2.52	1.38	1.44
20	G	205	CLA	C1D-C2D	-2.52	1.40	1.45
26	P	205	DD6	C24-C1	-2.52	1.40	1.46
20	A	831	CLA	C3D-C4D	-2.52	1.38	1.44
31	P	204	A86	C5-C6	2.52	1.41	1.35
20	B	812	CLA	C3D-C4D	-2.52	1.38	1.44
29	P	202	LMG	C4-C5	2.52	1.58	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	T	213	DD6	C13-C11	-2.52	1.40	1.46
20	A	808	CLA	MG-NC	2.52	2.12	2.06
20	B	819	CLA	C1D-C2D	-2.52	1.40	1.45
26	O	215	DD6	C8-C6	-2.52	1.40	1.46
20	S	205	CLA	C3D-C4D	-2.52	1.38	1.44
26	T	213	DD6	C8-C6	-2.51	1.40	1.46
20	T	201	CLA	C1D-C2D	-2.51	1.40	1.45
20	G	206	CLA	C3D-C4D	-2.51	1.38	1.44
20	H	206	CLA	C3D-C4D	-2.51	1.38	1.44
26	P	218	DD6	C2-C1	2.51	1.41	1.35
20	U	207	CLA	C3D-C4D	-2.51	1.38	1.44
20	T	207	CLA	C3D-C4D	-2.51	1.38	1.44
20	O	208	CLA	C3D-C4D	-2.51	1.38	1.44
20	A	851	CLA	C3D-C4D	-2.51	1.38	1.44
26	O	213	DD6	C24-C1	-2.50	1.40	1.46
20	A	802	CLA	C3D-C4D	-2.50	1.38	1.44
20	P	209	CLA	C3D-C4D	-2.50	1.38	1.44
20	A	823	CLA	C1D-C2D	-2.50	1.40	1.45
30	P	203	KC1	MG-NC	2.50	2.12	2.06
31	Q	218	A86	C8-C6	-2.50	1.40	1.46
30	P	219	KC1	C1A-CHA	2.50	1.46	1.40
20	A	818	CLA	C3D-C4D	-2.50	1.38	1.44
20	A	808	CLA	C3D-C4D	-2.50	1.38	1.44
20	A	829	CLA	C3D-C4D	-2.50	1.38	1.44
20	B	823	CLA	C1D-C2D	-2.50	1.40	1.45
20	G	205	CLA	C3D-C4D	-2.50	1.38	1.44
26	P	218	DD6	C5-C6	2.49	1.41	1.35
20	S	202	CLA	C3D-C4D	-2.49	1.38	1.44
23	A	842	BCR	C30-C25	-2.49	1.50	1.53
26	S	204	DD6	C24-C1	-2.49	1.40	1.46
20	G	203	CLA	MG-NC	2.49	2.12	2.06
26	G	214	DD6	C2-C1	2.49	1.41	1.35
20	B	831	CLA	C3D-C4D	-2.49	1.38	1.44
31	U	202	A86	C2-C1	2.49	1.41	1.35
20	B	848	CLA	C3D-C4D	-2.49	1.38	1.44
26	A	855	DD6	C8-C6	-2.49	1.40	1.46
20	A	830	CLA	C3D-C4D	-2.48	1.38	1.44
20	H	206	CLA	MG-NC	2.48	2.12	2.06
20	A	852	CLA	C3D-C4D	-2.48	1.38	1.44
20	L	204	CLA	C3D-C4D	-2.48	1.38	1.44
20	P	211	CLA	C3D-C4D	-2.48	1.38	1.44
26	P	218	DD6	C10-C11	2.48	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	A	815	CLA	C3D-C4D	-2.48	1.38	1.44
20	O	205	CLA	C3D-C4D	-2.48	1.38	1.44
26	P	215	DD6	C28-C27	-2.48	1.49	1.50
26	G	211	DD6	C8-C6	-2.48	1.40	1.46
20	A	826	CLA	C1D-C2D	-2.48	1.40	1.45
26	P	205	DD6	C13-C11	-2.47	1.40	1.46
26	S	203	DD6	C13-C11	-2.47	1.40	1.46
20	F	803	CLA	C3D-C4D	-2.47	1.38	1.44
20	B	808	CLA	C3D-C4D	-2.47	1.38	1.44
20	B	825	CLA	C1D-C2D	-2.47	1.40	1.45
20	B	826	CLA	C3D-C4D	-2.47	1.38	1.44
20	H	203	CLA	C1B-C2B	-2.47	1.37	1.43
30	O	210	KC1	C1A-CHA	2.47	1.46	1.40
20	A	811	CLA	C3D-C4D	-2.47	1.38	1.44
20	G	204	CLA	C3D-C4D	-2.47	1.38	1.44
20	B	814	CLA	C3D-C4D	-2.47	1.38	1.44
23	F	804	BCR	C30-C25	-2.47	1.50	1.53
23	I	101	BCR	C30-C25	-2.47	1.50	1.53
20	B	818	CLA	C3D-C4D	-2.47	1.38	1.44
30	T	208	KC1	C1A-CHA	2.47	1.46	1.40
20	A	817	CLA	C3D-C4D	-2.47	1.38	1.44
20	O	211	CLA	C1B-C2B	-2.47	1.37	1.43
20	A	807	CLA	MG-NC	2.47	2.12	2.06
20	B	832	CLA	C3D-C4D	-2.47	1.38	1.44
20	B	835	CLA	C3D-C4D	-2.47	1.38	1.44
20	H	208	CLA	C3D-C4D	-2.47	1.38	1.44
26	A	855	DD6	C13-C11	-2.47	1.40	1.46
20	J	103	CLA	C3D-C4D	-2.47	1.38	1.44
20	R	101	CLA	C1D-C2D	-2.47	1.40	1.45
20	A	836	CLA	C3D-C4D	-2.46	1.38	1.44
20	A	809	CLA	C3D-C4D	-2.46	1.38	1.44
20	O	202	CLA	C3D-C4D	-2.46	1.38	1.44
20	B	827	CLA	C3D-C4D	-2.46	1.38	1.44
20	T	204	CLA	C3D-C4D	-2.46	1.38	1.44
20	B	828	CLA	C3D-C4D	-2.46	1.38	1.44
20	O	206	CLA	C3D-C4D	-2.46	1.38	1.44
30	U	213	KC1	C2A-C3A	2.46	1.42	1.37
20	S	206	CLA	MG-NC	2.46	2.12	2.06
20	A	824	CLA	MG-NC	2.46	2.12	2.06
20	A	847	CLA	C3D-C4D	-2.46	1.38	1.44
26	S	213	DD6	C2-C1	2.46	1.41	1.35
20	A	823	CLA	C3D-C4D	-2.46	1.38	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	G	217	DD6	C24-C1	-2.46	1.40	1.46
26	S	204	DD6	C8-C6	-2.45	1.40	1.46
20	A	801	CLA	C1D-C2D	-2.45	1.40	1.45
20	G	210	CLA	MG-NB	2.45	2.10	2.05
20	A	833	CLA	C3D-C4D	-2.45	1.38	1.44
30	P	212	KC1	C2A-C3A	2.45	1.42	1.37
20	A	801	CLA	C1B-C2B	-2.45	1.37	1.43
26	G	214	DD6	C10-C11	2.45	1.41	1.35
20	A	824	CLA	C3D-C4D	-2.45	1.38	1.44
30	Q	210	KC1	C1A-CHA	2.45	1.46	1.40
20	P	208	CLA	C3D-C4D	-2.45	1.38	1.44
20	B	812	CLA	MG-NC	2.45	2.12	2.06
20	B	817	CLA	C1D-C2D	-2.45	1.40	1.45
30	P	206	KC1	C1A-CHA	2.44	1.46	1.40
20	T	203	CLA	C3D-C4D	-2.44	1.38	1.44
20	T	210	CLA	C3D-C4D	-2.44	1.38	1.44
20	A	828	CLA	C3D-C4D	-2.44	1.38	1.44
20	Q	212	CLA	C3D-C4D	-2.44	1.38	1.44
20	G	206	CLA	C1D-C2D	-2.44	1.40	1.45
20	A	810	CLA	C3D-C4D	-2.44	1.38	1.44
30	O	210	KC1	C1B-NB	-2.44	1.34	1.37
20	Q	203	CLA	MG-NC	2.44	2.12	2.06
20	B	833	CLA	C1B-C2B	-2.44	1.37	1.43
26	S	204	DD6	C13-C11	-2.44	1.40	1.46
20	F	802	CLA	MG-NC	2.44	2.12	2.06
20	S	205	CLA	MG-NC	2.44	2.12	2.06
20	Q	208	CLA	C3D-C4D	-2.44	1.38	1.44
20	B	807	CLA	C1D-C2D	-2.44	1.40	1.45
20	U	205	CLA	C3D-C4D	-2.44	1.38	1.44
20	G	201	CLA	C3D-C4D	-2.44	1.38	1.44
20	H	205	CLA	C3D-C4D	-2.44	1.38	1.44
20	A	825	CLA	C3D-C4D	-2.44	1.38	1.44
30	S	209	KC1	C1A-CHA	2.44	1.46	1.40
26	G	213	DD6	C10-C11	2.44	1.41	1.35
20	A	813	CLA	C3D-C4D	-2.43	1.38	1.44
20	A	838	CLA	C3D-C4D	-2.43	1.38	1.44
20	Q	203	CLA	C3D-C4D	-2.43	1.38	1.44
20	B	809	CLA	C3D-C4D	-2.43	1.38	1.44
20	B	843	CLA	C3D-C4D	-2.43	1.38	1.44
20	B	845	CLA	C3D-C4D	-2.43	1.38	1.44
20	U	211	CLA	C3D-C4D	-2.43	1.38	1.44
20	B	820	CLA	C3D-C4D	-2.43	1.38	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	O	207	CLA	C3D-C4D	-2.43	1.38	1.44
20	O	204	CLA	C3D-C4D	-2.43	1.38	1.44
20	Q	208	CLA	C1D-C2D	-2.43	1.40	1.45
20	T	209	CLA	C3D-C4D	-2.43	1.38	1.44
20	G	215	CLA	C3D-C4D	-2.43	1.38	1.44
20	A	826	CLA	C3D-C4D	-2.43	1.38	1.44
20	A	807	CLA	C3D-C4D	-2.43	1.38	1.44
26	P	215	DD6	C13-C11	-2.43	1.40	1.46
20	A	827	CLA	C1D-C2D	-2.43	1.40	1.45
20	S	215	CLA	C1D-C2D	-2.42	1.40	1.45
20	Q	206	CLA	C1D-C2D	-2.42	1.40	1.45
20	U	204	CLA	C3D-C4D	-2.42	1.38	1.44
20	G	209	CLA	C3D-C4D	-2.42	1.38	1.44
20	G	208	CLA	C3D-C4D	-2.42	1.38	1.44
26	P	220	DD6	C2-C1	2.42	1.41	1.35
20	B	827	CLA	MG-NC	2.42	2.12	2.06
20	T	210	CLA	MG-NC	2.42	2.12	2.06
26	S	203	DD6	C24-C1	-2.42	1.40	1.46
20	B	819	CLA	MG-NC	2.42	2.12	2.06
20	A	813	CLA	C1B-C2B	-2.42	1.37	1.43
20	B	803	CLA	C1D-C2D	-2.42	1.40	1.45
20	B	845	CLA	C1D-C2D	-2.42	1.40	1.45
20	A	819	CLA	C3D-C4D	-2.42	1.38	1.44
20	A	846	CLA	C3D-C4D	-2.42	1.38	1.44
20	O	204	CLA	C1D-C2D	-2.42	1.40	1.45
26	S	203	DD6	C8-C6	-2.42	1.40	1.46
31	Q	214	A86	C24-C1	-2.42	1.40	1.46
23	A	843	BCR	C30-C25	-2.42	1.50	1.53
26	S	213	DD6	C10-C11	2.42	1.41	1.35
20	Q	205	CLA	C3D-C4D	-2.41	1.38	1.44
20	H	207	CLA	C1B-C2B	-2.41	1.37	1.43
20	P	210	CLA	C3D-C4D	-2.41	1.38	1.44
20	S	206	CLA	C3D-C4D	-2.41	1.38	1.44
20	A	817	CLA	C1D-C2D	-2.41	1.40	1.45
26	S	213	DD6	C5-C6	2.41	1.41	1.35
20	B	844	CLA	C1D-C2D	-2.41	1.40	1.45
20	U	210	CLA	C3D-C4D	-2.41	1.38	1.44
20	B	822	CLA	C1D-C2D	-2.41	1.40	1.45
20	Q	212	CLA	C1D-C2D	-2.41	1.40	1.45
20	Q	209	CLA	C3D-C4D	-2.41	1.38	1.44
20	O	203	CLA	C3D-C4D	-2.41	1.38	1.44
26	O	213	DD6	C8-C6	-2.40	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	A	815	CLA	MG-NC	2.40	2.12	2.06
20	U	206	CLA	C3D-C4D	-2.40	1.38	1.44
31	Q	201	A86	C2-C1	2.40	1.41	1.35
26	O	214	DD6	C26-C27	2.40	1.42	1.37
20	A	814	CLA	C3D-C4D	-2.40	1.38	1.44
31	Q	214	A86	C8-C6	-2.40	1.40	1.46
20	A	832	CLA	C3D-C4D	-2.40	1.38	1.44
20	B	802	CLA	C3D-C4D	-2.40	1.38	1.44
20	T	202	CLA	C3D-C4D	-2.40	1.38	1.44
26	O	213	DD6	C13-C11	-2.40	1.40	1.46
30	T	208	KC1	C2A-C3A	2.40	1.42	1.37
20	A	825	CLA	C1D-C2D	-2.40	1.40	1.45
20	H	203	CLA	C3D-C4D	-2.40	1.38	1.44
20	A	845	CLA	C3D-C4D	-2.40	1.38	1.44
20	P	211	CLA	C1D-C2D	-2.40	1.40	1.45
20	B	813	CLA	C3D-C4D	-2.40	1.38	1.44
20	A	846	CLA	C1D-C2D	-2.39	1.40	1.45
20	R	104	CLA	C3D-C4D	-2.39	1.38	1.44
20	A	808	CLA	C1D-C2D	-2.39	1.40	1.45
26	O	201	DD6	C24-C1	-2.39	1.40	1.46
20	H	204	CLA	C3D-C4D	-2.39	1.38	1.44
20	A	838	CLA	C1D-C2D	-2.39	1.40	1.45
20	A	810	CLA	C1D-C2D	-2.39	1.40	1.45
20	A	816	CLA	C1B-C2B	-2.39	1.37	1.43
20	S	206	CLA	MG-NB	2.39	2.10	2.05
20	P	216	CLA	C3D-C4D	-2.39	1.38	1.44
20	P	213	CLA	C3D-C4D	-2.39	1.38	1.44
26	T	212	DD6	C5-C6	2.39	1.41	1.35
20	A	851	CLA	MG-NC	2.39	2.11	2.06
20	S	215	CLA	C3D-C4D	-2.38	1.38	1.44
20	B	804	CLA	C1D-C2D	-2.38	1.40	1.45
20	B	823	CLA	C3D-C4D	-2.38	1.38	1.44
26	Q	202	DD6	C2-C1	2.38	1.41	1.35
20	Q	211	CLA	C1D-C2D	-2.38	1.40	1.45
20	A	831	CLA	C1B-C2B	-2.38	1.37	1.43
20	A	801	CLA	C3D-C4D	-2.38	1.38	1.44
20	A	824	CLA	C1D-C2D	-2.38	1.40	1.45
20	G	204	CLA	C1D-C2D	-2.38	1.40	1.45
20	B	806	CLA	C1D-C2D	-2.38	1.40	1.45
20	T	206	CLA	C3D-C4D	-2.38	1.38	1.44
20	Q	207	CLA	C3D-C4D	-2.38	1.38	1.44
20	B	805	CLA	MG-NC	2.37	2.11	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	A	852	CLA	C1B-C2B	-2.37	1.37	1.43
30	P	203	KC1	C1B-NB	-2.37	1.34	1.37
20	B	804	CLA	C3D-C4D	-2.37	1.38	1.44
20	H	209	CLA	C3D-C4D	-2.37	1.38	1.44
20	B	830	CLA	C1D-C2D	-2.37	1.40	1.45
20	G	210	CLA	C3D-C4D	-2.37	1.38	1.44
20	T	201	CLA	C3D-C4D	-2.37	1.38	1.44
20	A	821	CLA	C3D-C4D	-2.37	1.38	1.44
26	O	212	DD6	C13-C11	-2.37	1.40	1.46
20	A	834	CLA	C3D-C4D	-2.37	1.38	1.44
26	G	213	DD6	C2-C1	2.36	1.41	1.35
26	U	203	DD6	C2-C1	2.36	1.41	1.35
26	P	215	DD6	C24-C1	-2.36	1.40	1.46
20	T	205	CLA	C3D-C4D	-2.36	1.38	1.44
20	Q	205	CLA	MG-NC	2.36	2.11	2.06
26	U	203	DD6	C13-C11	-2.36	1.40	1.46
20	A	812	CLA	C3D-C4D	-2.36	1.38	1.44
20	L	202	CLA	C3D-C4D	-2.36	1.38	1.44
20	B	822	CLA	C1B-C2B	-2.36	1.37	1.43
20	B	813	CLA	C1D-C2D	-2.36	1.40	1.45
20	Q	203	CLA	C1D-C2D	-2.36	1.40	1.45
26	H	210	DD6	C2-C1	2.36	1.41	1.35
20	Q	204	CLA	C3D-C4D	-2.36	1.38	1.44
20	H	201	CLA	C3D-C4D	-2.35	1.38	1.44
26	G	211	DD6	C13-C11	-2.35	1.40	1.46
31	R	105	A86	C8-C6	-2.35	1.40	1.46
26	J	101	DD6	C24-C1	-2.35	1.40	1.46
26	P	205	DD6	C8-C6	-2.35	1.40	1.46
31	U	202	A86	C5-C6	2.35	1.41	1.35
20	B	803	CLA	C3D-C4D	-2.35	1.38	1.44
26	G	211	DD6	C25-C26	-2.35	1.35	1.43
30	O	210	KC1	MG-NC	2.35	2.11	2.06
20	A	832	CLA	C1B-C2B	-2.35	1.37	1.43
30	S	211	KC1	C1A-CHA	2.35	1.46	1.40
20	A	814	CLA	C1B-C2B	-2.35	1.37	1.43
20	U	205	CLA	C1D-C2D	-2.35	1.40	1.45
20	B	820	CLA	MG-NC	2.35	2.11	2.06
26	H	211	DD6	C13-C11	-2.34	1.40	1.46
26	U	212	DD6	C2-C1	2.34	1.41	1.35
26	O	214	DD6	C8-C6	-2.34	1.40	1.46
20	G	203	CLA	C3D-C4D	-2.34	1.38	1.44
20	B	845	CLA	C1B-C2B	-2.34	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	T	213	DD6	C10-C11	2.34	1.41	1.35
20	B	826	CLA	C1D-C2D	-2.34	1.40	1.45
20	B	809	CLA	C1B-NB	-2.34	1.34	1.37
20	H	202	CLA	C3D-C4D	-2.34	1.38	1.44
20	O	202	CLA	C1B-C2B	-2.34	1.37	1.43
26	H	211	DD6	C5-C6	2.34	1.41	1.35
20	A	818	CLA	C1D-C2D	-2.34	1.40	1.45
26	T	212	DD6	C2-C1	2.34	1.41	1.35
20	A	815	CLA	C1B-C2B	-2.34	1.37	1.43
26	G	213	DD6	C5-C6	2.34	1.41	1.35
20	A	815	CLA	C1D-C2D	-2.33	1.40	1.45
20	A	820	CLA	C1D-C2D	-2.33	1.40	1.45
20	B	810	CLA	CAB-C3B	-2.33	1.46	1.50
22	A	840	LHG	O7-C5	-2.33	1.41	1.46
26	S	213	DD6	C13-C11	-2.33	1.41	1.46
20	A	806	CLA	C1D-C2D	-2.33	1.40	1.45
26	G	214	DD6	C5-C6	2.33	1.41	1.35
20	A	813	CLA	C1D-C2D	-2.33	1.40	1.45
20	B	810	CLA	C1D-C2D	-2.33	1.40	1.45
26	Q	202	DD6	C5-C6	2.33	1.41	1.35
20	A	845	CLA	C1D-C2D	-2.33	1.40	1.45
20	B	803	CLA	C1B-C2B	-2.33	1.37	1.43
26	G	217	DD6	C13-C11	-2.33	1.41	1.46
26	Q	215	DD6	C8-C6	-2.33	1.41	1.46
20	A	834	CLA	C1B-C2B	-2.33	1.37	1.43
20	Q	208	CLA	MG-NC	2.33	2.11	2.06
20	B	848	CLA	C1D-C2D	-2.33	1.40	1.45
26	J	101	DD6	C10-C11	2.33	1.41	1.35
20	F	802	CLA	C3D-C4D	-2.32	1.39	1.44
23	B	838	BCR	C30-C25	-2.32	1.50	1.53
20	F	803	CLA	C1B-C2B	-2.32	1.37	1.43
20	B	834	CLA	C1D-C2D	-2.32	1.40	1.45
26	O	212	DD6	C8-C6	-2.32	1.41	1.46
20	A	836	CLA	C1D-C2D	-2.32	1.40	1.45
26	O	201	DD6	C8-C6	-2.32	1.41	1.46
26	Q	215	DD6	C24-C1	-2.32	1.41	1.46
20	A	817	CLA	MG-NC	2.31	2.11	2.06
20	O	205	CLA	MG-NC	2.31	2.11	2.06
26	H	211	DD6	C2-C1	2.31	1.41	1.35
26	S	213	DD6	C8-C6	-2.31	1.41	1.46
26	Q	215	DD6	C5-C6	2.31	1.41	1.35
20	L	203	CLA	C1D-C2D	-2.31	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B	808	CLA	C1B-C2B	-2.31	1.37	1.43
20	Q	203	CLA	C1B-C2B	-2.31	1.37	1.43
26	P	215	DD6	C8-C6	-2.31	1.41	1.46
20	A	809	CLA	C1D-C2D	-2.30	1.40	1.45
20	B	828	CLA	C1D-C2D	-2.30	1.40	1.45
26	P	215	DD6	C10-C11	2.30	1.41	1.35
26	U	203	DD6	C5-C6	2.30	1.41	1.35
31	R	105	A86	C2-C1	2.30	1.41	1.35
20	B	832	CLA	C1D-C2D	-2.30	1.40	1.45
20	A	849	CLA	C1D-C2D	-2.30	1.40	1.45
20	S	205	CLA	C1B-C2B	-2.30	1.37	1.43
26	G	214	DD6	C8-C6	-2.30	1.41	1.46
20	B	830	CLA	C1B-C2B	-2.30	1.37	1.43
20	T	210	CLA	C1B-C2B	-2.30	1.37	1.43
31	Q	218	A86	C2-C1	2.29	1.41	1.35
20	O	207	CLA	C1B-C2B	-2.29	1.37	1.43
20	A	821	CLA	C1D-C2D	-2.29	1.40	1.45
26	T	213	DD6	C24-C1	-2.29	1.41	1.46
20	B	801	CLA	C1B-C2B	-2.29	1.37	1.43
20	B	809	CLA	C1D-C2D	-2.29	1.40	1.45
20	A	847	CLA	MG-NB	2.29	2.10	2.05
26	S	212	DD6	C5-C6	2.29	1.41	1.35
20	S	202	CLA	C1B-C2B	-2.29	1.37	1.43
26	T	213	DD6	C5-C6	2.29	1.41	1.35
20	O	203	CLA	MG-NC	2.29	2.11	2.06
20	B	813	CLA	MG-NB	2.29	2.10	2.05
20	B	846	CLA	C1B-C2B	-2.29	1.37	1.43
20	B	801	CLA	C3D-C4D	-2.29	1.39	1.44
20	O	207	CLA	MG-NC	2.29	2.11	2.06
26	U	212	DD6	C5-C6	2.29	1.41	1.35
20	B	805	CLA	C1B-C2B	-2.29	1.37	1.43
26	Q	215	DD6	C13-C11	-2.29	1.41	1.46
20	H	206	CLA	C1D-C2D	-2.29	1.40	1.45
26	O	201	DD6	C13-C11	-2.29	1.41	1.46
20	O	204	CLA	C1B-C2B	-2.29	1.37	1.43
20	A	807	CLA	C1D-C2D	-2.29	1.40	1.45
20	A	847	CLA	C1B-C2B	-2.29	1.37	1.43
20	B	818	CLA	C1B-C2B	-2.29	1.37	1.43
20	T	206	CLA	C1D-C2D	-2.28	1.40	1.45
26	U	214	DD6	C5-C6	2.28	1.40	1.34
20	P	214	CLA	C3D-C4D	-2.28	1.39	1.44
31	Q	201	A86	C8-C6	-2.28	1.41	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B	811	CLA	C1D-C2D	-2.28	1.40	1.45
20	T	211	CLA	C3D-C4D	-2.28	1.39	1.44
20	P	216	CLA	C1D-C2D	-2.28	1.40	1.45
20	A	852	CLA	MG-NC	2.28	2.11	2.06
20	A	828	CLA	C1D-C2D	-2.28	1.40	1.45
20	A	853	CLA	C1D-C2D	-2.28	1.40	1.45
26	G	217	DD6	C8-C6	-2.28	1.41	1.46
26	T	212	DD6	C10-C11	2.28	1.41	1.35
26	O	215	DD6	C13-C11	-2.28	1.41	1.46
20	F	802	CLA	C1D-C2D	-2.28	1.40	1.45
20	S	205	CLA	C1D-C2D	-2.28	1.40	1.45
26	J	101	DD6	C13-C11	-2.28	1.41	1.46
20	A	803	CLA	C1B-C2B	-2.28	1.37	1.43
20	B	808	CLA	MG-NC	2.27	2.11	2.06
20	Q	207	CLA	MG-NC	2.27	2.11	2.06
26	U	214	DD6	C24-C1	-2.27	1.41	1.46
31	Q	218	A86	C24-C1	-2.27	1.41	1.46
20	B	827	CLA	C1D-C2D	-2.27	1.40	1.45
26	T	212	DD6	C8-C6	-2.27	1.41	1.46
20	G	203	CLA	C1D-C2D	-2.27	1.40	1.45
20	P	209	CLA	C1D-C2D	-2.27	1.40	1.45
22	G	216	LHG	P-O6	2.27	1.68	1.59
20	A	833	CLA	C1B-C2B	-2.27	1.37	1.43
20	H	202	CLA	C1B-C2B	-2.27	1.37	1.43
20	U	204	CLA	MG-NC	2.27	2.11	2.06
20	B	816	CLA	MG-NC	2.26	2.11	2.06
20	B	843	CLA	C1D-C2D	-2.26	1.40	1.45
26	Q	202	DD6	C10-C11	2.26	1.41	1.35
20	A	810	CLA	C1B-C2B	-2.26	1.37	1.43
26	G	213	DD6	C13-C11	-2.26	1.41	1.46
20	A	814	CLA	MG-NC	2.26	2.11	2.06
20	A	812	CLA	C1D-C2D	-2.26	1.40	1.45
20	B	846	CLA	C1D-C2D	-2.26	1.40	1.45
20	U	209	CLA	C3D-C4D	-2.26	1.39	1.44
20	B	803	CLA	C1B-NB	-2.26	1.34	1.37
20	U	209	CLA	C1B-C2B	-2.26	1.37	1.43
20	Q	205	CLA	C1D-C2D	-2.26	1.40	1.45
26	P	215	DD6	C2-C1	2.26	1.41	1.35
20	A	835	CLA	C1D-C2D	-2.25	1.40	1.45
20	G	206	CLA	C1B-C2B	-2.25	1.37	1.43
20	G	202	CLA	MG-NC	2.25	2.11	2.06
20	P	208	CLA	C1D-C2D	-2.25	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	T	213	DD6	C28-C27	-2.25	1.49	1.50
26	P	220	DD6	C10-C11	2.25	1.41	1.35
31	Q	201	A86	C24-C1	-2.25	1.41	1.46
20	H	205	CLA	MG-NB	2.25	2.10	2.05
20	T	203	CLA	C1D-C2D	-2.25	1.40	1.45
20	A	852	CLA	C1D-C2D	-2.25	1.40	1.45
20	L	202	CLA	MG-NC	2.24	2.11	2.06
20	A	830	CLA	C1D-C2D	-2.24	1.40	1.45
20	A	832	CLA	C1B-NB	-2.24	1.34	1.37
26	J	101	DD6	C5-C6	2.24	1.41	1.35
26	J	101	DD6	C2-C1	2.24	1.41	1.35
31	Q	201	A86	C5-C6	2.24	1.41	1.35
20	B	809	CLA	C1B-C2B	-2.24	1.37	1.43
26	Q	202	DD6	C24-C1	-2.24	1.41	1.46
20	U	205	CLA	C1B-C2B	-2.24	1.37	1.43
20	G	204	CLA	C1B-C2B	-2.24	1.37	1.43
20	A	833	CLA	C1D-C2D	-2.24	1.40	1.45
20	B	819	CLA	C1B-C2B	-2.24	1.37	1.43
26	Q	202	DD6	C13-C11	-2.24	1.41	1.46
26	G	214	DD6	C13-C11	-2.24	1.41	1.46
26	Q	215	DD6	C10-C11	2.24	1.41	1.35
26	H	211	DD6	C24-C1	-2.24	1.41	1.46
31	R	105	A86	C24-C1	-2.24	1.41	1.46
20	H	205	CLA	C1D-C2D	-2.23	1.40	1.45
20	B	831	CLA	C1D-C2D	-2.23	1.40	1.45
26	U	203	DD6	C28-C27	-2.23	1.49	1.50
26	O	215	DD6	C25-C26	-2.23	1.36	1.43
20	H	204	CLA	C1B-C2B	-2.23	1.37	1.43
20	O	208	CLA	C1B-C2B	-2.23	1.37	1.43
29	P	217	LMG	O7-C8	-2.23	1.41	1.46
20	B	814	CLA	C1D-C2D	-2.23	1.40	1.45
20	A	817	CLA	C1B-C2B	-2.23	1.37	1.43
29	P	217	LMG	O1-C7	-2.23	1.39	1.43
20	Q	209	CLA	C1D-C2D	-2.23	1.40	1.45
20	A	832	CLA	C1D-C2D	-2.23	1.40	1.45
20	B	816	CLA	C1D-C2D	-2.23	1.40	1.45
20	S	206	CLA	C1B-C2B	-2.23	1.37	1.43
24	A	848	CL0	MG-ND	-2.23	2.01	2.05
20	O	204	CLA	C1B-NB	-2.22	1.34	1.37
20	P	210	CLA	C1B-C2B	-2.22	1.37	1.43
26	O	212	DD6	C2-C1	2.22	1.40	1.35
20	A	811	CLA	C1D-C2D	-2.22	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	A	854	CLA	C3D-C4D	-2.22	1.39	1.44
26	O	201	DD6	C5-C6	2.22	1.40	1.35
20	S	206	CLA	C1D-C2D	-2.22	1.40	1.45
20	U	211	CLA	C1B-C2B	-2.22	1.37	1.43
20	R	104	CLA	C1D-C2D	-2.22	1.40	1.45
20	A	854	CLA	C1B-C2B	-2.22	1.37	1.43
26	O	212	DD6	C10-C11	2.22	1.40	1.35
26	H	211	DD6	C8-C6	-2.21	1.41	1.46
20	A	853	CLA	C1B-C2B	-2.21	1.37	1.43
20	B	829	CLA	MG-NC	2.21	2.11	2.06
26	O	214	DD6	C13-C11	-2.21	1.41	1.46
20	A	836	CLA	C1B-C2B	-2.21	1.37	1.43
20	T	206	CLA	C1B-C2B	-2.21	1.37	1.43
20	T	211	CLA	MG-NC	2.21	2.11	2.06
31	U	202	A86	C8-C6	-2.21	1.41	1.46
26	U	214	DD6	C2-C1	2.21	1.40	1.35
20	B	829	CLA	C1D-C2D	-2.21	1.41	1.45
20	A	835	CLA	C1B-C2B	-2.21	1.38	1.43
20	A	804	CLA	C1D-C2D	-2.21	1.41	1.45
20	S	214	CLA	C1B-C2B	-2.21	1.38	1.43
26	O	201	DD6	C10-C11	2.20	1.40	1.35
20	A	818	CLA	C1B-C2B	-2.20	1.38	1.43
20	G	201	CLA	C1B-C2B	-2.20	1.38	1.43
20	A	820	CLA	C1B-C2B	-2.20	1.38	1.43
20	A	851	CLA	C1B-C2B	-2.20	1.38	1.43
26	G	213	DD6	C24-C1	-2.20	1.41	1.46
28	B	847	SQD	O3-C3	-2.20	1.37	1.43
31	Q	218	A86	C5-C6	2.20	1.40	1.35
20	A	851	CLA	C1D-C2D	-2.20	1.41	1.45
20	U	211	CLA	C1D-C2D	-2.20	1.41	1.45
26	S	204	DD6	C10-C11	2.20	1.40	1.35
26	P	205	DD6	C10-C11	2.20	1.40	1.35
26	U	212	DD6	C13-C11	-2.20	1.41	1.46
20	F	803	CLA	C1D-C2D	-2.19	1.41	1.45
20	A	834	CLA	C1D-C2D	-2.19	1.41	1.45
20	G	208	CLA	C1B-C2B	-2.19	1.38	1.43
20	H	207	CLA	C3D-C4D	-2.19	1.39	1.44
26	G	217	DD6	C10-C11	2.19	1.40	1.35
20	B	824	CLA	C1D-C2D	-2.19	1.41	1.45
29	P	202	LMG	C4-C3	2.19	1.58	1.52
20	L	202	CLA	C1D-C2D	-2.19	1.41	1.45
20	B	846	CLA	MG-NC	2.19	2.11	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	S	204	DD6	C5-C6	2.19	1.40	1.35
20	Q	213	CLA	C1D-C2D	-2.19	1.41	1.45
20	B	820	CLA	C1B-NB	-2.19	1.35	1.37
26	O	213	DD6	C2-C1	2.19	1.40	1.35
20	B	805	CLA	C1D-C2D	-2.19	1.41	1.45
26	Q	215	DD6	C2-C1	2.19	1.40	1.35
20	Q	207	CLA	C1B-C2B	-2.19	1.38	1.43
20	A	827	CLA	C1B-C2B	-2.19	1.38	1.43
20	T	204	CLA	C1D-C2D	-2.19	1.41	1.45
26	J	101	DD6	C8-C6	-2.19	1.41	1.46
31	P	204	A86	C25-C24	2.18	1.40	1.34
20	G	202	CLA	C1D-C2D	-2.18	1.41	1.45
20	A	830	CLA	MG-NC	2.18	2.11	2.06
20	B	848	CLA	C1B-C2B	-2.18	1.38	1.43
20	O	206	CLA	MG-NC	2.18	2.11	2.06
20	B	820	CLA	C1D-C2D	-2.18	1.41	1.45
20	B	833	CLA	C1D-C2D	-2.18	1.41	1.45
20	T	207	CLA	C1B-C2B	-2.18	1.38	1.43
20	A	845	CLA	C1B-C2B	-2.18	1.38	1.43
20	U	211	CLA	MG-NC	2.18	2.11	2.06
26	A	855	DD6	C25-C26	-2.18	1.36	1.43
20	B	829	CLA	C1B-C2B	-2.18	1.38	1.43
20	U	204	CLA	C1D-C2D	-2.18	1.41	1.45
31	R	105	A86	C5-C6	2.18	1.40	1.35
20	A	814	CLA	C1D-C2D	-2.18	1.41	1.45
20	Q	213	CLA	MG-NC	2.18	2.11	2.06
31	Q	214	A86	C2-C1	2.18	1.40	1.35
20	B	821	CLA	C1D-C2D	-2.18	1.41	1.45
20	H	204	CLA	C1D-C2D	-2.18	1.41	1.45
20	A	823	CLA	C1B-NB	-2.18	1.35	1.37
20	T	211	CLA	C1B-C2B	-2.18	1.38	1.43
20	U	206	CLA	C1D-C2D	-2.17	1.41	1.45
26	O	214	DD6	C2-C1	2.17	1.40	1.35
26	S	203	DD6	C2-C1	2.17	1.40	1.35
20	A	834	CLA	MG-NB	2.17	2.10	2.05
20	G	210	CLA	C1D-C2D	-2.17	1.41	1.45
26	U	212	DD6	C8-C6	-2.17	1.41	1.46
20	B	816	CLA	C1B-C2B	-2.17	1.38	1.43
26	G	217	DD6	C2-C1	2.17	1.40	1.35
20	Q	204	CLA	C1B-C2B	-2.17	1.38	1.43
26	S	212	DD6	C13-C11	-2.17	1.41	1.46
20	H	208	CLA	MG-NC	2.17	2.11	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	A	822	CLA	C1B-C2B	-2.17	1.38	1.43
20	A	818	CLA	MG-NC	2.17	2.11	2.06
20	U	208	CLA	C1B-C2B	-2.17	1.38	1.43
20	H	201	CLA	C1B-C2B	-2.17	1.38	1.43
20	T	207	CLA	C1D-C2D	-2.17	1.41	1.45
26	T	212	DD6	C24-C1	-2.17	1.41	1.46
20	P	214	CLA	C1B-C2B	-2.17	1.38	1.43
20	B	825	CLA	C1B-C2B	-2.16	1.38	1.43
20	T	210	CLA	MG-NB	2.16	2.10	2.05
20	P	214	CLA	C1D-C2D	-2.16	1.41	1.45
20	G	205	CLA	C1B-C2B	-2.16	1.38	1.43
26	G	212	DD6	C25-C26	-2.16	1.36	1.43
26	Q	202	DD6	C8-C6	-2.16	1.41	1.46
20	U	208	CLA	CHB-C1B	2.16	1.44	1.39
20	P	213	CLA	C1B-C2B	-2.16	1.38	1.43
26	P	215	DD6	C5-C6	2.16	1.40	1.35
20	O	202	CLA	C1D-C2D	-2.16	1.41	1.45
20	A	807	CLA	C1B-NB	-2.16	1.35	1.37
26	P	220	DD6	C5-C6	2.16	1.40	1.35
26	S	203	DD6	C5-C6	2.16	1.40	1.35
26	S	204	DD6	C2-C1	2.15	1.40	1.35
20	H	207	CLA	MG-NC	2.15	2.11	2.06
20	B	809	CLA	MG-NC	2.15	2.11	2.06
26	P	205	DD6	C25-C26	-2.15	1.36	1.43
20	G	215	CLA	C1B-C2B	-2.15	1.38	1.43
20	T	201	CLA	MG-NC	2.15	2.11	2.06
20	U	207	CLA	C1D-C2D	-2.15	1.41	1.45
20	A	829	CLA	C1B-C2B	-2.15	1.38	1.43
29	P	202	LMG	O7-C8	-2.15	1.41	1.46
20	G	207	CLA	CHB-C1B	2.15	1.44	1.39
20	B	848	CLA	MG-NC	2.14	2.11	2.06
26	S	210	DD6	C25-C26	-2.14	1.36	1.43
26	P	218	DD6	C24-C1	-2.14	1.41	1.46
20	H	202	CLA	MG-NC	2.14	2.11	2.06
26	O	213	DD6	C5-C6	2.14	1.40	1.35
20	A	804	CLA	MG-NC	2.14	2.11	2.06
20	Q	207	CLA	C1D-C2D	-2.14	1.41	1.45
20	A	819	CLA	C1B-C2B	-2.14	1.38	1.43
26	G	217	DD6	C5-C6	2.14	1.40	1.35
31	R	103	A86	C26-C27	2.14	1.40	1.35
20	G	203	CLA	C1B-C2B	-2.14	1.38	1.43
20	B	815	CLA	C1D-C2D	-2.14	1.41	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	J	103	CLA	C1D-C2D	-2.14	1.41	1.45
20	B	827	CLA	C1B-C2B	-2.14	1.38	1.43
26	O	215	DD6	C5-C6	2.14	1.40	1.35
20	L	204	CLA	C1D-C2D	-2.14	1.41	1.45
20	G	208	CLA	C1D-C2D	-2.13	1.41	1.45
20	B	811	CLA	C1B-C2B	-2.13	1.38	1.43
20	Q	216	CLA	C1D-C2D	-2.13	1.41	1.45
26	O	213	DD6	C10-C11	2.13	1.40	1.35
20	P	207	CLA	C1B-C2B	-2.13	1.38	1.43
26	S	204	DD6	C25-C26	-2.13	1.36	1.43
20	P	208	CLA	C1B-NB	-2.13	1.35	1.37
20	B	812	CLA	C1D-C2D	-2.13	1.41	1.45
26	O	215	DD6	C2-C1	2.13	1.40	1.35
20	A	847	CLA	C1D-C2D	-2.13	1.41	1.45
20	G	207	CLA	C1D-C2D	-2.13	1.41	1.45
20	G	201	CLA	C1D-C2D	-2.13	1.41	1.45
26	S	203	DD6	C10-C11	2.13	1.40	1.35
20	A	835	CLA	CHB-C1B	2.13	1.44	1.39
22	P	201	LHG	P-O6	2.13	1.67	1.59
20	A	826	CLA	C1B-NB	-2.12	1.35	1.37
20	O	207	CLA	C1D-C2D	-2.12	1.41	1.45
20	B	833	CLA	MG-NC	2.12	2.11	2.06
20	P	207	CLA	C1D-C2D	-2.12	1.41	1.45
20	A	821	CLA	C1B-NB	-2.12	1.35	1.37
20	G	205	CLA	MG-NC	2.12	2.11	2.06
20	O	203	CLA	C1D-C2D	-2.12	1.41	1.45
20	A	831	CLA	C1D-C2D	-2.12	1.41	1.45
20	A	803	CLA	C1B-NB	-2.12	1.35	1.37
26	O	201	DD6	C2-C1	2.12	1.40	1.35
20	B	807	CLA	C1B-C2B	-2.12	1.38	1.43
20	A	801	CLA	C1B-NB	-2.12	1.35	1.37
20	B	843	CLA	C1B-C2B	-2.12	1.38	1.43
23	B	837	BCR	C33-C5	-2.12	1.47	1.50
20	A	829	CLA	C1D-C2D	-2.12	1.41	1.45
20	L	204	CLA	C1B-C2B	-2.12	1.38	1.43
20	T	201	CLA	C1B-C2B	-2.12	1.38	1.43
20	H	208	CLA	C1B-C2B	-2.12	1.38	1.43
30	P	212	KC1	C1B-NB	-2.12	1.35	1.37
20	A	806	CLA	MG-NC	2.11	2.11	2.06
26	O	212	DD6	C5-C6	2.11	1.40	1.35
20	B	818	CLA	MG-NC	2.11	2.11	2.06
26	P	218	DD6	C13-C11	-2.11	1.41	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	A	836	CLA	MG-NC	2.11	2.11	2.06
20	B	801	CLA	C1D-C2D	-2.11	1.41	1.45
26	G	214	DD6	C25-C24	2.11	1.40	1.34
20	A	824	CLA	C1B-C2B	-2.11	1.38	1.43
20	P	210	CLA	C1D-C2D	-2.11	1.41	1.45
26	O	213	DD6	C25-C26	-2.11	1.36	1.43
20	T	205	CLA	C1D-C2D	-2.11	1.41	1.45
20	B	814	CLA	C1B-C2B	-2.11	1.38	1.43
20	A	816	CLA	MG-NC	2.11	2.11	2.06
26	O	214	DD6	C10-C11	2.11	1.40	1.35
20	B	835	CLA	C1B-C2B	-2.11	1.38	1.43
20	L	203	CLA	C1B-C2B	-2.11	1.38	1.43
20	A	811	CLA	C1B-C2B	-2.11	1.38	1.43
26	S	212	DD6	C24-C1	-2.10	1.41	1.46
20	B	806	CLA	C1B-C2B	-2.10	1.38	1.43
26	O	201	DD6	C28-C27	-2.10	1.49	1.50
30	Q	210	KC1	C2A-C3A	2.10	1.41	1.37
31	Q	214	A86	C5-C6	2.10	1.40	1.35
20	B	802	CLA	CHB-C1B	2.10	1.44	1.39
20	B	848	CLA	CHB-C1B	2.10	1.44	1.39
20	S	215	CLA	MG-NC	2.10	2.11	2.06
20	B	804	CLA	C1B-C2B	-2.10	1.38	1.43
20	L	202	CLA	C1B-NB	-2.10	1.35	1.37
20	G	215	CLA	C1D-C2D	-2.10	1.41	1.45
20	U	210	CLA	C1D-C2D	-2.10	1.41	1.45
20	A	836	CLA	CHB-C1B	2.10	1.44	1.39
20	T	209	CLA	CHB-C1B	2.10	1.44	1.39
20	Q	209	CLA	C1B-C2B	-2.10	1.38	1.43
26	H	211	DD6	C10-C11	2.10	1.40	1.35
20	R	101	CLA	MG-NC	2.10	2.11	2.06
20	A	822	CLA	C1D-C2D	-2.10	1.41	1.45
20	B	824	CLA	C1B-C2B	-2.09	1.38	1.43
26	G	213	DD6	C8-C6	-2.09	1.41	1.46
20	A	853	CLA	MG-NC	2.09	2.11	2.06
20	F	802	CLA	C1B-C2B	-2.09	1.38	1.43
20	B	804	CLA	C1B-NB	-2.09	1.35	1.37
20	T	211	CLA	C1D-C2D	-2.09	1.41	1.45
29	I	103	LMG	O7-C8	-2.09	1.41	1.46
24	A	848	CL0	MG-NB	-2.09	2.01	2.05
29	U	201	LMG	O7-C8	-2.09	1.41	1.46
26	O	214	DD6	C5-C6	2.09	1.40	1.35
20	H	202	CLA	C1D-C2D	-2.09	1.41	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	Q	216	CLA	C1B-NB	-2.09	1.35	1.37
20	T	202	CLA	C1D-C2D	-2.09	1.41	1.45
20	A	852	CLA	C1B-NB	-2.09	1.35	1.37
20	P	207	CLA	MG-NC	2.09	2.11	2.06
26	P	205	DD6	C2-C1	2.09	1.40	1.35
20	B	811	CLA	C1B-NB	-2.09	1.35	1.37
20	B	821	CLA	C1B-C2B	-2.09	1.38	1.43
20	T	202	CLA	C1B-C2B	-2.09	1.38	1.43
26	S	212	DD6	C8-C6	-2.09	1.41	1.46
20	B	814	CLA	MG-NB	2.09	2.09	2.05
20	G	209	CLA	MG-NC	2.09	2.11	2.06
20	A	825	CLA	C1B-C2B	-2.09	1.38	1.43
31	U	202	A86	C26-C27	2.09	1.40	1.35
20	B	813	CLA	C1B-C2B	-2.09	1.38	1.43
20	B	834	CLA	C1B-C2B	-2.09	1.38	1.43
20	B	845	CLA	MG-NB	2.09	2.09	2.05
20	B	810	CLA	C1B-C2B	-2.09	1.38	1.43
20	Q	216	CLA	C1B-C2B	-2.09	1.38	1.43
20	A	802	CLA	C1B-C2B	-2.08	1.38	1.43
20	G	204	CLA	MG-NC	2.08	2.11	2.06
20	R	104	CLA	C1B-C2B	-2.08	1.38	1.43
20	S	215	CLA	C1B-NB	-2.08	1.35	1.37
20	P	211	CLA	C1B-C2B	-2.08	1.38	1.43
20	B	817	CLA	C1B-NB	-2.08	1.35	1.37
20	A	816	CLA	C1D-C2D	-2.08	1.41	1.45
20	O	208	CLA	C1D-C2D	-2.08	1.41	1.45
20	A	826	CLA	C1B-C2B	-2.08	1.38	1.43
20	A	806	CLA	C1B-NB	-2.08	1.35	1.37
20	A	808	CLA	C1B-C2B	-2.08	1.38	1.43
20	B	827	CLA	C1B-NB	-2.08	1.35	1.37
20	H	209	CLA	C1D-C2D	-2.08	1.41	1.45
20	B	820	CLA	C1B-C2B	-2.08	1.38	1.43
20	B	831	CLA	C1B-C2B	-2.08	1.38	1.43
20	L	202	CLA	C1B-C2B	-2.08	1.38	1.43
20	S	207	CLA	C1D-C2D	-2.08	1.41	1.45
20	B	822	CLA	MG-NC	2.08	2.11	2.06
26	A	855	DD6	C10-C11	2.08	1.40	1.35
26	P	218	DD6	C8-C6	-2.08	1.41	1.46
20	O	206	CLA	C1D-C2D	-2.08	1.41	1.45
30	O	210	KC1	C3B-C2B	2.08	1.41	1.37
20	B	805	CLA	C1B-NB	-2.07	1.35	1.37
20	H	206	CLA	C1B-C2B	-2.07	1.38	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	T	213	DD6	C2-C1	2.07	1.40	1.35
20	B	810	CLA	MG-NB	2.07	2.09	2.05
26	P	220	DD6	C25-C26	-2.07	1.36	1.43
26	S	210	DD6	C10-C11	2.07	1.40	1.35
20	L	203	CLA	MG-NC	2.07	2.11	2.06
26	U	203	DD6	C25-C24	2.07	1.40	1.34
20	B	823	CLA	C1B-C2B	-2.07	1.38	1.43
26	U	212	DD6	C24-C1	-2.07	1.41	1.46
20	O	211	CLA	C1D-C2D	-2.07	1.41	1.45
30	P	206	KC1	C1B-NB	-2.07	1.35	1.37
20	A	807	CLA	C1B-C2B	-2.07	1.38	1.43
20	B	816	CLA	C1B-NB	-2.06	1.35	1.37
28	B	847	SQD	O2-C2	-2.06	1.37	1.43
20	F	802	CLA	C1B-NB	-2.06	1.35	1.37
20	Q	213	CLA	C1B-C2B	-2.06	1.38	1.43
20	H	201	CLA	C1D-C2D	-2.06	1.41	1.45
20	A	809	CLA	C1B-C2B	-2.06	1.38	1.43
20	A	803	CLA	C1D-C2D	-2.06	1.41	1.45
20	A	819	CLA	MG-NC	2.06	2.11	2.06
20	A	805	CLA	C1D-C2D	-2.06	1.41	1.45
20	T	203	CLA	C1B-C2B	-2.06	1.38	1.43
20	T	205	CLA	C1B-C2B	-2.06	1.38	1.43
20	H	206	CLA	CHB-C1B	2.06	1.44	1.39
20	B	826	CLA	C1B-C2B	-2.06	1.38	1.43
20	H	205	CLA	C1B-C2B	-2.06	1.38	1.43
20	P	208	CLA	C1B-C2B	-2.06	1.38	1.43
20	G	209	CLA	C1D-C2D	-2.06	1.41	1.45
20	S	214	CLA	MG-NC	2.05	2.11	2.06
20	T	203	CLA	MG-NB	2.05	2.09	2.05
20	A	818	CLA	C1B-NB	-2.05	1.35	1.37
20	F	803	CLA	MG-NC	2.05	2.11	2.06
20	U	205	CLA	MG-NC	2.05	2.11	2.06
26	P	220	DD6	C13-C11	-2.05	1.41	1.46
20	A	838	CLA	C1B-C2B	-2.05	1.38	1.43
20	Q	205	CLA	CHB-C1B	2.05	1.44	1.39
20	T	201	CLA	CHB-C1B	2.05	1.44	1.39
31	Q	218	A86	C26-C27	2.05	1.40	1.35
20	B	825	CLA	C1B-NB	-2.05	1.35	1.37
20	O	203	CLA	C1B-C2B	-2.05	1.38	1.43
27	B	842	DGD	C3G-C2G	2.05	1.57	1.50
26	O	212	DD6	C24-C1	-2.05	1.41	1.46
26	S	203	DD6	C25-C26	-2.05	1.36	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	U	213	KC1	MG-NC	2.05	2.11	2.06
20	G	208	CLA	CHB-C1B	2.05	1.44	1.39
20	Q	203	CLA	CHB-C1B	2.05	1.44	1.39
20	G	203	CLA	CHB-C1B	2.05	1.44	1.39
20	H	207	CLA	C1D-C2D	-2.05	1.41	1.45
20	S	214	CLA	C1D-C2D	-2.05	1.41	1.45
28	S	201	SQD	O4-C4	-2.05	1.37	1.43
20	A	819	CLA	C1D-C2D	-2.04	1.41	1.45
20	A	801	CLA	MG-NC	2.04	2.11	2.06
20	A	804	CLA	C1B-C2B	-2.04	1.38	1.43
26	O	215	DD6	C10-C11	2.04	1.40	1.35
20	O	209	CLA	C1B-C2B	-2.04	1.38	1.43
20	U	210	CLA	C1B-NB	-2.04	1.35	1.37
20	Q	209	CLA	MG-NC	2.04	2.11	2.06
20	H	209	CLA	CHB-C1B	2.04	1.44	1.39
20	J	103	CLA	MG-NC	2.04	2.11	2.06
20	A	811	CLA	C1B-NB	-2.04	1.35	1.37
20	B	807	CLA	C1B-NB	-2.04	1.35	1.37
23	B	839	BCR	C33-C5	-2.04	1.47	1.50
20	L	204	CLA	MG-NC	2.03	2.11	2.06
20	P	213	CLA	C1D-C2D	-2.03	1.41	1.45
20	O	204	CLA	MG-NC	2.03	2.11	2.06
26	G	212	DD6	C28-C27	-2.03	1.49	1.50
20	B	821	CLA	C1B-NB	-2.03	1.35	1.37
20	Q	208	CLA	C1B-C2B	-2.03	1.38	1.43
20	U	209	CLA	C1D-C2D	-2.03	1.41	1.45
26	U	203	DD6	C24-C1	-2.03	1.41	1.46
26	A	855	DD6	C5-C6	2.03	1.40	1.35
28	S	201	SQD	O2-C2	-2.03	1.37	1.43
20	A	816	CLA	C1B-NB	-2.03	1.35	1.37
20	J	103	CLA	C1B-C2B	-2.03	1.38	1.43
20	S	207	CLA	MG-NC	2.03	2.11	2.06
20	G	215	CLA	CHB-C1B	2.03	1.44	1.39
26	T	212	DD6	C13-C11	-2.03	1.41	1.46
20	S	208	CLA	C1B-C2B	-2.03	1.38	1.43
20	P	209	CLA	MG-NC	2.03	2.11	2.06
20	A	806	CLA	C1B-C2B	-2.03	1.38	1.43
20	Q	205	CLA	C1B-C2B	-2.03	1.38	1.43
20	U	204	CLA	CHB-C1B	2.02	1.44	1.39
20	S	207	CLA	C1B-C2B	-2.02	1.38	1.43
26	O	201	DD6	C25-C26	-2.02	1.36	1.43
20	Q	212	CLA	C1B-C2B	-2.02	1.38	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	G	212	DD6	C5-C6	2.02	1.40	1.35
20	H	208	CLA	CHB-C1B	2.02	1.44	1.39
20	B	818	CLA	CHB-C1B	2.02	1.43	1.39
20	U	207	CLA	CHB-C1B	2.02	1.43	1.39
20	U	211	CLA	MG-NB	2.02	2.09	2.05
20	Q	211	CLA	CHB-C1B	2.02	1.43	1.39
26	S	210	DD6	C28-C27	-2.02	1.49	1.50
26	G	211	DD6	C10-C11	2.02	1.40	1.35
20	G	201	CLA	CHB-C1B	2.02	1.43	1.39
20	G	209	CLA	C1B-C2B	-2.02	1.38	1.43
20	A	810	CLA	MG-NC	2.01	2.11	2.06
26	P	205	DD6	C5-C6	2.01	1.40	1.35
28	B	847	SQD	O47-C45	-2.01	1.41	1.46
20	G	207	CLA	C1B-C2B	-2.01	1.38	1.43
20	Q	208	CLA	C1B-NB	-2.01	1.35	1.37
20	Q	208	CLA	CHB-C1B	2.01	1.43	1.39
20	B	825	CLA	CHB-C1B	2.01	1.43	1.39
20	O	206	CLA	CHB-C1B	2.01	1.43	1.39
20	U	206	CLA	CHB-C1B	2.01	1.43	1.39
20	T	210	CLA	C1D-C2D	-2.01	1.41	1.45
20	Q	204	CLA	C1D-C2D	-2.01	1.41	1.45
26	O	214	DD6	C25-C26	-2.00	1.37	1.43
20	S	208	CLA	CHB-C1B	2.00	1.43	1.39
20	B	815	CLA	MG-NC	2.00	2.11	2.06
20	T	202	CLA	MG-NC	2.00	2.11	2.06
20	A	820	CLA	CHB-C1B	2.00	1.43	1.39
20	P	216	CLA	CHB-C1B	2.00	1.43	1.39
20	U	207	CLA	C1B-C2B	-2.00	1.38	1.43
26	U	203	DD6	C8-C6	-2.00	1.41	1.46
26	A	855	DD6	C2-C1	2.00	1.40	1.35
20	T	202	CLA	CHB-C1B	2.00	1.43	1.39

All (1330) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	848	CL0	C1B-CHB-C4A	9.49	127.43	121.32
31	Q	214	A86	C29-C30-C31	-5.98	170.60	177.66
31	P	204	A86	C26-C25-C24	5.79	139.97	123.20
26	U	203	DD6	C4-C3-C2	5.70	135.18	123.52
26	P	220	DD6	C10-C9-C8	5.46	139.01	123.20
20	A	854	CLA	C1-O2A-CGA	5.42	129.78	116.65
20	H	206	CLA	O2A-C1-C2	5.41	128.93	108.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	S	213	DD6	C4-C3-C2	5.28	134.31	123.52
26	T	213	DD6	C4-C3-C2	5.21	134.19	123.52
26	P	220	DD6	C4-C3-C2	5.06	133.87	123.52
26	P	218	DD6	C4-C3-C2	4.90	133.54	123.52
26	S	212	DD6	C3-C4-C5	4.85	133.44	123.52
26	P	218	DD6	C3-C4-C5	4.79	133.32	123.52
26	U	212	DD6	C3-C4-C5	4.75	133.23	123.52
26	U	203	DD6	O1-C15-C14	-4.64	103.59	116.88
26	Q	215	DD6	C4-C3-C2	4.59	132.92	123.52
31	Q	201	A86	C3-C4-C5	4.57	132.88	123.52
26	T	212	DD6	C13-C11-C10	4.51	126.11	119.01
26	O	212	DD6	C4-C3-C2	4.49	132.72	123.52
26	U	214	DD6	C4-C3-C2	4.46	132.65	123.52
26	G	217	DD6	C4-C3-C2	4.46	132.65	123.52
26	Q	202	DD6	C3-C4-C5	4.45	132.63	123.52
31	Q	218	A86	C4-C3-C2	4.43	132.59	123.52
26	O	213	DD6	C4-C3-C2	4.41	132.54	123.52
22	A	840	LHG	O4-P-O5	4.39	132.86	112.44
31	P	204	A86	C3-C4-C5	4.38	132.48	123.52
22	A	839	LHG	O4-P-O5	4.36	132.74	112.44
22	P	201	LHG	O4-P-O5	4.33	132.61	112.44
20	Q	207	CLA	C4D-CHA-C1A	4.33	126.41	121.24
26	G	212	DD6	C3-C4-C5	4.32	132.37	123.52
20	H	202	CLA	C4D-CHA-C1A	4.31	126.39	121.24
22	G	216	LHG	O4-P-O5	4.31	132.48	112.44
26	G	211	DD6	C4-C3-C2	4.25	132.22	123.52
26	T	212	DD6	C12-C11-C10	-4.24	115.94	122.82
20	Q	213	CLA	C1-O2A-CGA	4.23	126.88	116.65
26	U	203	DD6	C24-C1-C2	4.22	125.64	119.01
26	T	212	DD6	C4-C3-C2	4.21	132.12	123.52
26	H	210	DD6	C4-C3-C2	4.19	132.09	123.52
20	A	838	CLA	C4D-CHA-C1A	4.16	126.21	121.24
20	T	205	CLA	C4D-CHA-C1A	4.16	126.20	121.24
26	J	101	DD6	C3-C4-C5	4.16	132.02	123.52
28	S	201	SQD	O9-S-O7	-4.15	100.32	113.82
26	T	212	DD6	C3-C4-C5	4.12	131.94	123.52
26	O	214	DD6	C3-C4-C5	4.10	131.91	123.52
20	H	201	CLA	C3A-C2A-C1A	-4.07	102.14	106.30
31	Q	214	A86	C3-C4-C5	4.06	131.82	123.52
31	R	103	A86	C4-C3-C2	4.04	131.78	123.52
28	B	847	SQD	O9-S-O7	-4.03	100.70	113.82
31	U	202	A86	C4-C3-C2	4.03	131.77	123.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	S	201	SQD	O47-C7-C8	4.03	120.19	111.48
26	O	214	DD6	C12-C11-C10	-4.02	116.30	122.82
26	A	855	DD6	C4-C3-C2	4.02	131.75	123.52
31	R	103	A86	C3-C4-C5	4.02	131.75	123.52
23	F	801	BCR	C2-C1-C6	4.01	116.26	110.44
26	G	214	DD6	C3-C4-C5	3.97	131.64	123.52
23	M	101	BCR	C2-C1-C6	3.97	116.20	110.44
26	S	212	DD6	C8-C6-C5	3.96	125.24	119.01
28	S	201	SQD	O9-S-C6	3.95	112.65	106.76
20	H	206	CLA	C4D-CHA-C1A	3.94	125.95	121.24
20	A	835	CLA	O2A-C1-C2	3.93	123.24	108.11
20	T	202	CLA	C4D-CHA-C1A	3.93	125.93	121.24
26	S	203	DD6	C4-C3-C2	3.92	131.55	123.52
20	G	207	CLA	C4D-CHA-C1A	3.92	125.92	121.24
26	H	211	DD6	C3-C4-C5	3.92	131.54	123.52
20	A	819	CLA	C4D-CHA-C1A	3.92	125.92	121.24
23	A	841	BCR	C2-C1-C6	3.92	116.13	110.44
26	G	213	DD6	C3-C4-C5	3.91	131.52	123.52
26	O	212	DD6	C3-C4-C5	3.90	131.50	123.52
26	S	213	DD6	C3-C4-C5	3.89	131.47	123.52
26	S	203	DD6	C3-C4-C5	3.88	131.47	123.52
26	S	204	DD6	C3-C4-C5	3.88	131.45	123.52
20	P	207	CLA	C4D-CHA-C1A	3.84	125.82	121.24
20	B	801	CLA	C4D-CHA-C1A	3.84	125.82	121.24
20	A	847	CLA	C4D-CHA-C1A	3.83	125.82	121.24
26	U	203	DD6	C3-C4-C5	3.79	131.27	123.52
31	U	202	A86	C3-C4-C5	3.79	131.27	123.52
28	B	847	SQD	O47-C7-C8	3.78	119.67	111.48
20	B	818	CLA	C4D-CHA-C1A	3.78	125.76	121.24
20	G	209	CLA	C4D-CHA-C1A	3.78	125.75	121.24
26	P	205	DD6	C12-C11-C10	-3.78	116.70	122.82
20	A	822	CLA	C4D-CHA-C1A	3.77	125.74	121.24
20	A	829	CLA	C4D-CHA-C1A	3.77	125.74	121.24
20	Q	204	CLA	C4D-CHA-C1A	3.76	125.73	121.24
20	F	803	CLA	C4D-CHA-C1A	3.76	125.73	121.24
20	B	830	CLA	C4D-CHA-C1A	3.75	125.72	121.24
23	L	205	BCR	C2-C1-C6	3.74	115.87	110.44
20	A	814	CLA	C4D-CHA-C1A	3.74	125.70	121.24
26	H	211	DD6	C4-C3-C2	3.74	131.16	123.52
31	R	105	A86	C3-C4-C5	3.73	131.16	123.52
20	B	843	CLA	C4D-CHA-C1A	3.73	125.70	121.24
20	F	802	CLA	C4D-CHA-C1A	3.73	125.70	121.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	J	104	BCR	C2-C1-C6	3.72	115.84	110.44
26	P	205	DD6	C4-C3-C2	3.72	131.13	123.52
20	B	807	CLA	C4D-CHA-C1A	3.72	125.68	121.24
20	B	814	CLA	C4D-CHA-C1A	3.72	125.68	121.24
20	S	205	CLA	C4D-CHA-C1A	3.71	125.67	121.24
20	O	206	CLA	C4D-CHA-C1A	3.71	125.66	121.24
26	P	215	DD6	C4-C3-C2	3.70	131.08	123.52
20	G	215	CLA	C4D-CHA-C1A	3.69	125.64	121.24
20	G	205	CLA	CAC-C3C-C4C	3.68	129.57	124.79
20	A	811	CLA	C4D-CHA-C1A	3.67	125.63	121.24
26	H	210	DD6	C3-C4-C5	3.67	131.03	123.52
26	J	101	DD6	C12-C11-C10	-3.66	116.89	122.82
26	H	210	DD6	C12-C11-C10	-3.66	116.89	122.82
20	T	209	CLA	C4D-CHA-C1A	3.65	125.60	121.24
20	B	816	CLA	C4D-CHA-C1A	3.65	125.60	121.24
26	O	215	DD6	C4-C3-C2	3.65	130.99	123.52
26	S	213	DD6	C8-C6-C5	3.64	124.74	119.01
26	S	213	DD6	C12-C11-C10	-3.64	116.91	122.82
26	Q	202	DD6	C12-C11-C10	-3.64	116.92	122.82
26	G	213	DD6	C4-C3-C2	3.64	130.96	123.52
26	P	215	DD6	C12-C11-C10	-3.64	116.93	122.82
26	G	212	DD6	C12-C11-C10	-3.64	116.93	122.82
20	H	201	CLA	C4D-CHA-C1A	3.64	125.58	121.24
20	L	203	CLA	C4D-CHA-C1A	3.63	125.58	121.24
20	O	211	CLA	C4D-CHA-C1A	3.63	125.57	121.24
26	S	210	DD6	C12-C11-C10	-3.61	116.96	122.82
26	P	218	DD6	C12-C11-C10	-3.61	116.96	122.82
20	A	831	CLA	C4D-CHA-C1A	3.61	125.54	121.24
26	T	213	DD6	C24-C1-C2	3.60	124.67	119.01
20	A	816	CLA	C4D-CHA-C1A	3.60	125.53	121.24
26	P	205	DD6	C10-C9-C8	3.59	133.62	123.20
26	U	203	DD6	C-C1-C2	-3.59	117.01	122.82
20	Q	205	CLA	C4D-CHA-C1A	3.58	125.52	121.24
26	U	212	DD6	C10-C9-C8	3.58	133.59	123.20
20	G	203	CLA	C4D-CHA-C1A	3.58	125.52	121.24
26	O	212	DD6	C12-C11-C10	-3.58	117.02	122.82
26	P	220	DD6	C12-C11-C10	-3.58	117.02	122.82
20	B	832	CLA	C4D-CHA-C1A	3.58	125.51	121.24
26	P	215	DD6	C3-C4-C5	3.57	130.82	123.52
20	B	833	CLA	C4D-CHA-C1A	3.57	125.50	121.24
20	A	803	CLA	C4D-CHA-C1A	3.57	125.50	121.24
26	U	203	DD6	C13-C11-C10	3.56	124.61	119.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	U	203	DD6	C26-C25-C24	3.56	133.52	123.20
26	S	204	DD6	C12-C11-C10	-3.56	117.05	122.82
20	B	826	CLA	C4D-CHA-C1A	3.56	125.49	121.24
20	S	202	CLA	C4D-CHA-C1A	3.55	125.48	121.24
26	U	203	DD6	O1-C20-C19	-3.55	110.16	113.49
26	Q	215	DD6	C12-C11-C10	-3.55	117.06	122.82
26	S	210	DD6	C3-C4-C5	3.54	130.77	123.52
20	P	209	CLA	C4D-CHA-C1A	3.54	125.47	121.24
26	O	212	DD6	C24-C1-C2	3.54	124.58	119.01
20	U	211	CLA	C4D-CHA-C1A	3.53	125.46	121.24
20	Q	213	CLA	C4D-CHA-C1A	3.53	125.46	121.24
26	S	203	DD6	C12-C11-C10	-3.53	117.10	122.82
26	O	201	DD6	C4-C3-C2	3.53	130.73	123.52
20	P	214	CLA	C4D-CHA-C1A	3.52	125.45	121.24
20	U	208	CLA	C4D-CHA-C1A	3.52	125.45	121.24
26	O	201	DD6	C3-C4-C5	3.52	130.73	123.52
26	A	855	DD6	C12-C11-C10	-3.52	117.12	122.82
26	A	855	DD6	C24-C1-C2	3.52	124.54	119.01
26	A	855	DD6	C26-C25-C24	3.52	133.39	123.20
20	A	854	CLA	C4D-CHA-C1A	3.52	125.44	121.24
26	O	215	DD6	C12-C11-C10	-3.52	117.12	122.82
20	H	206	CLA	C1-O2A-CGA	-3.52	108.14	116.65
20	A	812	CLA	C4D-CHA-C1A	3.51	125.43	121.24
20	H	207	CLA	C4D-CHA-C1A	3.50	125.42	121.24
20	U	207	CLA	CAA-C2A-C3A	-3.50	103.54	113.00
23	B	840	BCR	C15-C16-C17	-3.50	116.36	123.52
20	A	853	CLA	C4D-CHA-C1A	3.50	125.41	121.24
20	B	815	CLA	C4D-CHA-C1A	3.49	125.41	121.24
20	B	811	CLA	C4D-CHA-C1A	3.49	125.41	121.24
26	G	217	DD6	C12-C11-C10	-3.49	117.16	122.82
26	G	214	DD6	C12-C11-C10	-3.49	117.16	122.82
20	U	205	CLA	C4D-CHA-C1A	3.48	125.40	121.24
20	A	828	CLA	C4D-CHA-C1A	3.48	125.40	121.24
20	B	831	CLA	C4D-CHA-C1A	3.48	125.40	121.24
20	O	203	CLA	C4D-CHA-C1A	3.48	125.40	121.24
20	B	812	CLA	C4D-CHA-C1A	3.48	125.39	121.24
20	B	828	CLA	C4D-CHA-C1A	3.48	125.39	121.24
20	U	204	CLA	C4D-CHA-C1A	3.48	125.39	121.24
26	G	214	DD6	C26-C25-C24	3.47	133.26	123.20
26	G	211	DD6	C12-C11-C10	-3.47	117.20	122.82
23	L	205	BCR	C3-C4-C5	-3.47	107.87	114.06
26	G	214	DD6	C8-C6-C5	3.47	124.46	119.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	O	201	DD6	C12-C11-C10	-3.47	117.20	122.82
20	L	204	CLA	C4D-CHA-C1A	3.46	125.37	121.24
20	A	846	CLA	C4D-CHA-C1A	3.46	125.37	121.24
20	P	211	CLA	C4D-CHA-C1A	3.46	125.37	121.24
26	Q	202	DD6	C4-C3-C2	3.46	130.59	123.52
28	B	847	SQD	C44-O6-C1	3.45	121.20	113.80
26	G	213	DD6	C12-C11-C10	-3.45	117.22	122.82
20	Q	203	CLA	C4D-CHA-C1A	3.45	125.36	121.24
20	S	206	CLA	C4D-CHA-C1A	3.45	125.36	121.24
26	P	205	DD6	C3-C4-C5	3.45	130.57	123.52
20	A	849	CLA	C4D-CHA-C1A	3.44	125.35	121.24
20	A	830	CLA	C4D-CHA-C1A	3.44	125.35	121.24
31	R	105	A86	C4-C3-C2	3.44	130.56	123.52
20	H	203	CLA	C4D-CHA-C1A	3.44	125.35	121.24
20	A	808	CLA	C4D-CHA-C1A	3.44	125.34	121.24
20	O	207	CLA	C4D-CHA-C1A	3.44	125.34	121.24
20	A	852	CLA	C4D-CHA-C1A	3.44	125.34	121.24
20	B	845	CLA	C4D-CHA-C1A	3.44	125.34	121.24
20	R	101	CLA	C4D-CHA-C1A	3.43	125.34	121.24
26	U	203	DD6	C15-C14-C13	3.43	133.25	125.99
20	B	824	CLA	C4D-CHA-C1A	3.43	125.34	121.24
20	A	815	CLA	C4D-CHA-C1A	3.43	125.34	121.24
30	S	209	KC1	CAA-C2A-C1A	3.43	139.68	124.64
26	O	212	DD6	C-C1-C2	-3.43	117.26	122.82
20	P	213	CLA	C4D-CHA-C1A	3.43	125.33	121.24
24	A	848	CL0	C3D-C4D-CHA	3.42	113.74	108.54
20	G	204	CLA	C4D-CHA-C1A	3.42	125.33	121.24
26	U	203	DD6	C12-C11-C10	-3.42	117.28	122.82
20	O	204	CLA	C4D-CHA-C1A	3.42	125.32	121.24
24	A	848	CL0	C1C-CHC-C4B	3.42	128.29	116.07
20	A	810	CLA	C4D-CHA-C1A	3.41	125.31	121.24
20	A	836	CLA	C4D-CHA-C1A	3.41	125.31	121.24
20	A	835	CLA	CAA-CBA-CGA	3.40	122.87	113.21
20	A	805	CLA	C4D-CHA-C1A	3.39	125.29	121.24
20	S	214	CLA	C4D-CHA-C1A	3.39	125.29	121.24
31	P	204	A86	C4-C3-C2	3.39	130.45	123.52
20	B	829	CLA	C4D-CHA-C1A	3.39	125.28	121.24
29	P	202	LMG	C1-C2-C3	-3.38	102.90	110.01
26	S	203	DD6	C24-C1-C2	3.38	124.33	119.01
20	T	201	CLA	C4D-CHA-C1A	3.38	125.28	121.24
26	T	213	DD6	C-C1-C2	-3.38	117.34	122.82
20	B	846	CLA	C4D-CHA-C1A	3.38	125.27	121.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	833	CLA	C4D-CHA-C1A	3.37	125.27	121.24
20	A	835	CLA	C4D-CHA-C1A	3.37	125.27	121.24
26	P	205	DD6	C13-C11-C10	3.37	124.31	119.01
20	P	216	CLA	C4D-CHA-C1A	3.36	125.26	121.24
26	G	212	DD6	C24-C1-C2	3.36	124.30	119.01
20	A	824	CLA	C4D-CHA-C1A	3.36	125.25	121.24
31	Q	201	A86	C8-C6-C5	3.36	124.29	119.01
26	O	214	DD6	C4-C3-C2	3.36	130.39	123.52
26	O	213	DD6	C12-C11-C10	-3.36	117.38	122.82
20	A	827	CLA	C4D-CHA-C1A	3.35	125.24	121.24
20	B	835	CLA	C4D-CHA-C1A	3.35	125.24	121.24
20	A	845	CLA	C4D-CHA-C1A	3.34	125.22	121.24
26	S	212	DD6	C7-C6-C5	-3.34	117.41	122.82
26	O	215	DD6	C3-C4-C5	3.33	130.34	123.52
26	S	204	DD6	C22-C16-C17	-3.33	103.11	108.97
20	T	211	CLA	C4D-CHA-C1A	3.33	125.22	121.24
20	H	208	CLA	C4D-CHA-C1A	3.33	125.22	121.24
20	H	209	CLA	C4D-CHA-C1A	3.33	125.21	121.24
26	S	204	DD6	C4-C3-C2	3.33	130.33	123.52
20	A	817	CLA	C4D-CHA-C1A	3.33	125.21	121.24
30	U	213	KC1	CAB-C3B-C4B	3.33	132.76	124.82
26	S	213	DD6	C13-C11-C10	3.32	124.24	119.01
20	A	834	CLA	C4D-CHA-C1A	3.32	125.21	121.24
20	O	208	CLA	C4D-CHA-C1A	3.32	125.20	121.24
20	B	848	CLA	C4D-CHA-C1A	3.32	125.20	121.24
26	Q	202	DD6	C8-C6-C5	3.32	124.23	119.01
20	L	202	CLA	C4D-CHA-C1A	3.31	125.19	121.24
26	U	212	DD6	C8-C6-C5	3.31	124.21	119.01
26	T	212	DD6	C8-C6-C5	3.31	124.21	119.01
20	A	813	CLA	C4D-CHA-C1A	3.31	125.19	121.24
20	T	210	CLA	C4D-CHA-C1A	3.31	125.19	121.24
20	S	202	CLA	CHD-C1D-ND	-3.31	120.15	124.80
20	P	210	CLA	C4D-CHA-C1A	3.30	125.18	121.24
20	A	825	CLA	C4D-CHA-C1A	3.29	125.17	121.24
20	P	216	CLA	C4A-NA-C1A	3.29	108.18	106.68
30	Q	210	KC1	CBA-CAA-C2A	3.28	138.63	125.45
26	H	211	DD6	C12-C11-C10	-3.28	117.50	122.82
26	T	213	DD6	C12-C11-C10	-3.28	117.50	122.82
26	S	204	DD6	C8-C6-C5	3.28	124.17	119.01
20	G	208	CLA	C4D-CHA-C1A	3.28	125.15	121.24
23	L	205	BCR	C24-C23-C22	-3.28	121.39	126.23
20	B	813	CLA	O2A-C1-C2	3.28	120.72	108.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	P	220	DD6	C3-C4-C5	3.28	130.22	123.52
20	H	209	CLA	CAA-C2A-C3A	-3.28	104.15	113.00
20	A	818	CLA	C4D-CHA-C1A	3.27	125.15	121.24
20	B	834	CLA	C4D-CHA-C1A	3.27	125.14	121.24
26	T	213	DD6	C3-C4-C5	3.27	130.20	123.52
23	I	102	BCR	C27-C26-C25	3.26	127.11	122.70
26	J	101	DD6	C13-C11-C10	3.26	124.14	119.01
20	A	804	CLA	C4D-CHA-C1A	3.25	125.12	121.24
20	L	204	CLA	O2A-C1-C2	3.25	120.62	108.11
20	G	206	CLA	C4D-CHA-C1A	3.25	125.12	121.24
26	P	205	DD6	C8-C6-C5	3.25	124.11	119.01
20	B	822	CLA	C4D-CHA-C1A	3.25	125.11	121.24
20	T	204	CLA	C4D-CHA-C1A	3.24	125.11	121.24
26	O	214	DD6	C8-C6-C5	3.24	124.11	119.01
20	A	807	CLA	C4A-NA-C1A	3.24	108.16	106.68
26	S	213	DD6	C10-C9-C8	3.23	132.57	123.20
28	B	847	SQD	O7-S-C6	3.23	111.58	106.76
26	G	212	DD6	C14-C13-C11	-3.23	120.52	125.53
26	H	211	DD6	C24-C1-C2	3.23	124.08	119.01
20	G	201	CLA	C4D-CHA-C1A	3.22	125.09	121.24
20	G	202	CLA	C4D-CHA-C1A	3.22	125.09	121.24
26	Q	215	DD6	C24-C1-C2	3.21	124.06	119.01
20	U	209	CLA	C4D-CHA-C1A	3.21	125.07	121.24
26	U	214	DD6	C26-C25-C24	3.21	132.50	123.20
20	A	854	CLA	CHA-C1A-NA	-3.21	119.13	126.39
20	A	807	CLA	C4D-CHA-C1A	3.21	125.07	121.24
20	A	832	CLA	C4D-CHA-C1A	3.21	125.07	121.24
26	P	218	DD6	C8-C6-C5	3.20	124.05	119.01
26	G	212	DD6	C-C1-C2	-3.20	117.64	122.82
20	A	809	CLA	C4D-CHA-C1A	3.19	125.05	121.24
20	G	205	CLA	C4D-CHA-C1A	3.19	125.05	121.24
20	S	208	CLA	C4D-CHA-C1A	3.19	125.05	121.24
20	B	820	CLA	CHA-C1A-NA	-3.18	119.18	126.39
20	R	104	CLA	C4D-CHA-C1A	3.17	125.03	121.24
23	A	841	BCR	C27-C26-C25	3.17	126.99	122.70
20	Q	209	CLA	C4D-CHA-C1A	3.17	125.02	121.24
28	B	847	SQD	O9-S-C6	3.17	111.48	106.76
26	G	213	DD6	C8-C6-C5	3.16	123.99	119.01
20	B	810	CLA	C4D-CHA-C1A	3.16	125.02	121.24
31	P	204	A86	C8-C6-C5	3.16	123.98	119.01
20	A	851	CLA	C4D-CHA-C1A	3.16	125.01	121.24
26	P	215	DD6	C8-C6-C5	3.16	123.97	119.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	806	CLA	C4D-CHA-C1A	3.15	125.00	121.24
26	G	212	DD6	C4-C3-C2	3.15	129.97	123.52
31	R	103	A86	C8-C6-C5	3.15	123.96	119.01
20	H	204	CLA	C4D-CHA-C1A	3.15	125.00	121.24
20	Q	208	CLA	C4D-CHA-C1A	3.15	125.00	121.24
26	U	203	DD6	C33-C32-C31	3.14	115.68	109.49
31	Q	201	A86	C7-C6-C5	-3.14	117.73	122.82
20	B	806	CLA	C4D-CHA-C1A	3.13	124.98	121.24
20	T	207	CLA	C4D-CHA-C1A	3.13	124.98	121.24
26	U	212	DD6	C12-C11-C10	-3.13	117.74	122.82
20	B	805	CLA	C4D-CHA-C1A	3.13	124.98	121.24
20	B	827	CLA	C4D-CHA-C1A	3.13	124.98	121.24
26	O	201	DD6	C24-C1-C2	3.13	123.93	119.01
26	J	101	DD6	C8-C6-C5	3.12	123.92	119.01
26	G	214	DD6	C4-C3-C2	3.12	129.90	123.52
20	Q	203	CLA	O2A-C1-C2	3.12	119.87	109.44
20	B	817	CLA	C4D-CHA-C1A	3.11	124.96	121.24
26	O	212	DD6	C8-C6-C5	3.11	123.91	119.01
20	A	821	CLA	CHA-C1A-NA	-3.11	119.35	126.39
20	Q	212	CLA	CHA-C1A-NA	-3.11	119.35	126.39
26	U	212	DD6	C7-C6-C5	-3.11	117.78	122.82
20	B	813	CLA	C4D-CHA-C1A	3.11	124.95	121.24
24	A	848	CL0	C1A-CHA-C4D	3.10	124.16	118.98
26	P	215	DD6	C13-C11-C10	3.10	123.89	119.01
20	U	210	CLA	C4D-CHA-C1A	3.10	124.94	121.24
31	Q	214	A86	C35-C34-C33	3.09	115.44	109.89
20	U	206	CLA	C4D-CHA-C1A	3.09	124.93	121.24
26	S	212	DD6	C12-C11-C10	-3.09	117.81	122.82
26	J	101	DD6	C4-C3-C2	3.09	129.83	123.52
20	B	823	CLA	C4D-CHA-C1A	3.08	124.92	121.24
20	O	202	CLA	C4D-CHA-C1A	3.08	124.91	121.24
31	R	103	A86	C24-C1-C2	3.07	123.84	119.01
26	Q	202	DD6	C24-C1-C2	3.07	123.84	119.01
30	T	208	KC1	CGD-CBD-CAD	-3.07	100.91	110.85
20	J	103	CLA	C4D-CHA-C1A	3.06	124.90	121.24
20	U	207	CLA	C4D-CHA-C1A	3.06	124.89	121.24
20	T	203	CLA	C4D-CHA-C1A	3.06	124.89	121.24
26	A	855	DD6	C-C1-C2	-3.06	117.86	122.82
26	Q	202	DD6	C7-C6-C5	-3.06	117.86	122.82
26	P	205	DD6	C7-C6-C5	-3.05	117.87	122.82
23	J	104	BCR	C24-C23-C22	-3.05	121.72	126.23
26	G	211	DD6	C24-C1-C2	3.05	123.80	119.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	G	217	DD6	C13-C11-C10	3.04	123.79	119.01
20	B	821	CLA	C4D-CHA-C1A	3.04	124.87	121.24
20	B	818	CLA	CHD-C1D-ND	-3.03	120.53	124.80
26	P	220	DD6	C24-C1-C2	3.03	123.78	119.01
20	T	206	CLA	C4D-CHA-C1A	3.03	124.86	121.24
20	H	207	CLA	O2A-C1-C2	3.03	119.75	108.11
20	G	210	CLA	C4D-CHA-C1A	3.03	124.85	121.24
20	G	205	CLA	CAA-C2A-C3A	-3.02	104.83	113.00
31	Q	218	A86	C3-C4-C5	3.02	129.71	123.52
20	A	820	CLA	C4D-CHA-C1A	3.02	124.85	121.24
23	B	837	BCR	C24-C23-C22	-3.02	121.76	126.23
26	S	213	DD6	C7-C6-C5	-3.02	117.92	122.82
26	P	205	DD6	C24-C1-C2	3.02	123.76	119.01
26	G	213	DD6	C7-C6-C5	-3.02	117.93	122.82
23	B	840	BCR	C15-C14-C13	-3.02	123.05	127.28
20	A	803	CLA	CHD-C1D-ND	-3.02	120.56	124.80
26	S	203	DD6	C8-C6-C5	3.01	123.75	119.01
26	G	214	DD6	C7-C6-C5	-3.01	117.94	122.82
26	S	213	DD6	C24-C1-C2	3.01	123.75	119.01
20	Q	206	CLA	C4D-CHA-C1A	3.01	124.83	121.24
20	B	824	CLA	C1-O2A-CGA	3.01	123.94	116.65
26	Q	215	DD6	C-C1-C2	-3.01	117.94	122.82
26	U	212	DD6	C24-C1-C2	3.01	123.74	119.01
20	F	802	CLA	CHA-C1A-NA	-3.00	119.59	126.39
20	O	209	CLA	C4D-CHA-C1A	3.00	124.82	121.24
26	U	203	DD6	C8-C6-C5	3.00	123.72	119.01
26	H	210	DD6	C8-C6-C5	3.00	123.72	119.01
20	O	205	CLA	C4D-CHA-C1A	2.99	124.82	121.24
26	H	211	DD6	C8-C6-C5	2.99	123.72	119.01
20	A	823	CLA	C4D-CHA-C1A	2.99	124.81	121.24
26	J	101	DD6	C7-C6-C5	-2.99	117.97	122.82
20	A	822	CLA	CHD-C1D-ND	-2.99	120.59	124.80
26	P	215	DD6	C7-C6-C5	-2.99	117.97	122.82
26	S	203	DD6	C-C1-C2	-2.98	117.98	122.82
20	S	208	CLA	CHD-C1D-ND	-2.98	120.61	124.80
26	U	212	DD6	C4-C3-C2	2.98	129.62	123.52
26	U	214	DD6	C3-C4-C5	2.98	129.62	123.52
26	H	211	DD6	C-C1-C2	-2.98	117.99	122.82
20	T	205	CLA	CHD-C1D-ND	-2.98	120.61	124.80
26	U	214	DD6	C-C1-C2	-2.98	117.99	122.82
22	A	840	LHG	O8-C23-C24	2.97	120.17	111.15
20	B	809	CLA	C4D-CHA-C1A	2.97	124.79	121.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	802	CLA	CHA-C1A-NA	-2.97	119.67	126.39
26	G	212	DD6	C13-C11-C10	2.97	123.68	119.01
26	O	214	DD6	C7-C6-C5	-2.97	118.01	122.82
20	A	834	CLA	CHA-C1A-NA	-2.97	119.67	126.39
20	A	845	CLA	CHA-C1A-NA	-2.96	119.68	126.39
23	F	804	BCR	C2-C1-C6	2.96	114.74	110.44
26	O	201	DD6	C-C1-C2	-2.96	118.02	122.82
31	P	204	A86	C7-C6-C5	-2.96	118.02	122.82
26	T	212	DD6	C7-C6-C5	-2.96	118.02	122.82
31	R	103	A86	C23-C16-C17	-2.96	103.77	108.97
20	A	812	CLA	CHA-C1A-NA	-2.96	119.70	126.39
26	U	212	DD6	C-C1-C2	-2.96	118.03	122.82
20	A	854	CLA	C4A-NA-C1A	2.95	108.03	106.68
20	B	803	CLA	C4D-CHA-C1A	2.95	124.76	121.24
30	U	213	KC1	CHC-C4B-C3B	2.95	130.18	125.21
20	B	823	CLA	CHA-C1A-NA	-2.95	119.71	126.39
26	U	203	DD6	C7-C6-C5	-2.95	118.04	122.82
20	P	208	CLA	C4D-CHA-C1A	2.95	124.76	121.24
31	R	105	A86	C24-C1-C2	2.95	123.64	119.01
26	P	218	DD6	C24-C1-C2	2.95	123.64	119.01
23	M	101	BCR	C11-C10-C9	-2.94	123.15	127.28
31	U	202	A86	C8-C6-C5	2.94	123.64	119.01
31	Q	214	A86	C8-C6-C5	2.94	123.64	119.01
26	P	218	DD6	C7-C6-C5	-2.94	118.05	122.82
31	R	103	A86	C7-C6-C5	-2.94	118.05	122.82
26	P	218	DD6	C22-C16-C17	-2.94	103.81	108.97
22	A	839	LHG	O8-C23-C24	2.94	120.79	111.83
26	S	204	DD6	C7-C6-C5	-2.94	118.06	122.82
26	P	215	DD6	C24-C1-C2	2.94	123.63	119.01
31	Q	214	A86	C4-C3-C2	2.93	129.52	123.52
20	B	802	CLA	CHA-C1A-NA	-2.93	119.75	126.39
20	B	845	CLA	CHA-C1A-NA	-2.93	119.76	126.39
20	P	216	CLA	CHA-C1A-NA	-2.93	119.76	126.39
20	A	805	CLA	CHD-C1D-ND	-2.93	120.68	124.80
26	U	214	DD6	C24-C1-C2	2.93	123.61	119.01
26	G	214	DD6	C-C1-C2	-2.92	118.08	122.82
31	R	103	A86	C-C1-C2	-2.92	118.08	122.82
26	O	212	DD6	C7-C6-C5	-2.92	118.08	122.82
26	G	213	DD6	C24-C1-C2	2.92	123.60	119.01
26	S	212	DD6	C4-C3-C2	2.92	129.49	123.52
26	S	213	DD6	C-C1-C2	-2.92	118.09	122.82
22	G	216	LHG	O8-C23-C24	2.92	120.73	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	L	202	CLA	CHA-C1A-NA	-2.91	119.79	126.39
26	P	205	DD6	C-C1-C2	-2.91	118.10	122.82
23	L	205	BCR	C11-C10-C9	-2.91	123.20	127.28
26	Q	202	DD6	C-C1-C2	-2.91	118.10	122.82
20	S	215	CLA	C4D-CHA-C1A	2.91	124.71	121.24
20	A	847	CLA	CHD-C1D-ND	-2.91	120.71	124.80
23	I	102	BCR	C15-C16-C17	-2.91	117.57	123.52
30	S	209	KC1	C2A-C3A-C4A	2.91	108.59	106.41
26	Q	202	DD6	O1-C15-C14	-2.91	108.55	116.88
26	T	213	DD6	C8-C6-C5	2.90	123.57	119.01
26	H	211	DD6	C7-C6-C5	-2.90	118.12	122.82
31	R	103	A86	C28-C27-C26	-2.90	118.12	122.82
26	S	212	DD6	C13-C11-C10	2.90	123.56	119.01
26	S	212	DD6	C10-C9-C8	2.89	131.59	123.20
20	A	807	CLA	CHA-C1A-NA	-2.89	119.84	126.39
31	Q	214	A86	C7-C6-C5	-2.89	118.13	122.82
31	Q	218	A86	C-C1-C2	-2.89	118.13	122.82
20	T	211	CLA	CHA-C1A-NA	-2.89	119.84	126.39
26	O	213	DD6	C24-C1-C2	2.89	123.55	119.01
20	B	844	CLA	C4D-CHA-C1A	2.88	124.68	121.24
20	L	204	CLA	CHD-C1D-ND	-2.88	120.75	124.80
20	A	819	CLA	CHD-C1D-ND	-2.88	120.75	124.80
23	R	102	BCR	C19-C18-C17	-2.88	118.06	124.72
20	H	205	CLA	C4D-CHA-C1A	2.88	124.67	121.24
26	G	213	DD6	C-C1-C2	-2.88	118.16	122.82
26	A	855	DD6	C3-C4-C5	2.87	129.40	123.52
20	T	211	CLA	C4A-NA-C1A	2.87	107.99	106.68
26	T	212	DD6	C-C1-C2	-2.87	118.16	122.82
20	A	832	CLA	CHA-C1A-NA	-2.87	119.89	126.39
20	B	806	CLA	CHA-C1A-NA	-2.87	119.89	126.39
20	A	816	CLA	CHD-C1D-ND	-2.87	120.76	124.80
20	B	835	CLA	CHA-C1A-NA	-2.87	119.89	126.39
20	A	810	CLA	CHA-C1A-NA	-2.87	119.90	126.39
20	A	813	CLA	CHA-C1A-NA	-2.86	119.90	126.39
20	B	834	CLA	CHA-C1A-NA	-2.86	119.90	126.39
26	H	210	DD6	C26-C25-C24	2.86	131.50	123.20
26	S	204	DD6	C24-C1-C2	2.86	123.51	119.01
20	Q	208	CLA	CHA-C1A-NA	-2.86	119.91	126.39
20	B	804	CLA	CHA-C1A-NA	-2.86	119.91	126.39
20	B	821	CLA	CHD-C1D-ND	-2.86	120.78	124.80
20	B	827	CLA	CHA-C1A-NA	-2.86	119.92	126.39
20	P	213	CLA	CHD-C1D-ND	-2.86	120.78	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	U	202	A86	C-C1-C2	-2.86	118.19	122.82
31	Q	218	A86	C24-C1-C2	2.86	123.50	119.01
31	R	105	A86	C7-C6-C5	-2.85	118.19	122.82
20	T	202	CLA	CHD-C1D-ND	-2.85	120.78	124.80
20	B	808	CLA	C4D-CHA-C1A	2.85	124.65	121.24
26	A	855	DD6	C8-C6-C5	2.85	123.50	119.01
26	S	203	DD6	C7-C6-C5	-2.85	118.20	122.82
31	P	204	A86	C-C1-C2	-2.85	118.20	122.82
20	Q	207	CLA	CHA-C1A-NA	-2.85	119.94	126.39
20	O	211	CLA	CHD-C1D-ND	-2.85	120.79	124.80
23	M	101	BCR	C15-C14-C13	-2.85	123.28	127.28
20	A	825	CLA	CHA-C1A-NA	-2.85	119.94	126.39
20	U	207	CLA	O2A-C1-C2	2.84	119.06	108.11
20	A	815	CLA	CHA-C1A-NA	-2.84	119.95	126.39
20	B	819	CLA	C4D-CHA-C1A	2.84	124.63	121.24
23	A	841	BCR	C30-C25-C26	-2.84	118.75	122.64
27	B	842	DGD	O5D-C6D-C5D	-2.84	103.02	109.42
20	Q	204	CLA	CHD-C1D-ND	-2.84	120.81	124.80
20	G	206	CLA	CHA-C1A-NA	-2.84	119.96	126.39
20	Q	212	CLA	CAA-C2A-C1A	2.84	121.28	111.97
26	O	213	DD6	C-C1-C2	-2.84	118.22	122.82
31	U	202	A86	C7-C6-C5	-2.84	118.22	122.82
20	A	817	CLA	CHA-C1A-NA	-2.84	119.97	126.39
20	G	205	CLA	CHD-C1D-ND	-2.84	120.81	124.80
20	H	203	CLA	CHD-C1D-ND	-2.84	120.81	124.80
20	Q	204	CLA	CHA-C1A-NA	-2.84	119.97	126.39
26	P	215	DD6	C-C1-C2	-2.84	118.22	122.82
20	B	848	CLA	CHA-C1A-NA	-2.84	119.97	126.39
20	O	205	CLA	CHD-C1D-ND	-2.83	120.81	124.80
20	R	101	CLA	CHA-C1A-NA	-2.83	119.97	126.39
20	Q	212	CLA	C4A-NA-C1A	2.83	107.97	106.68
26	H	210	DD6	C7-C6-C5	-2.83	118.23	122.82
26	U	212	DD6	C28-C27-C26	-2.83	118.68	124.18
20	G	208	CLA	CHD-C1D-ND	-2.83	120.82	124.80
31	R	105	A86	C8-C6-C5	2.83	123.46	119.01
20	S	215	CLA	CHA-C1A-NA	-2.83	119.98	126.39
20	T	209	CLA	CHD-C1D-ND	-2.83	120.82	124.80
20	A	828	CLA	CHA-C1A-NA	-2.83	119.99	126.39
26	O	215	DD6	C24-C1-C2	2.83	123.46	119.01
20	A	827	CLA	CHA-C1A-NA	-2.82	120.00	126.39
26	S	210	DD6	C7-C6-C5	-2.82	118.24	122.82
20	B	804	CLA	C4D-CHA-C1A	2.82	124.61	121.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	T	208	KC1	CAB-C3B-C4B	2.82	131.56	124.82
20	P	208	CLA	CHA-C1A-NA	-2.82	120.00	126.39
20	B	832	CLA	CHA-C1A-NA	-2.82	120.01	126.39
20	G	207	CLA	CHD-C1D-ND	-2.82	120.84	124.80
20	T	201	CLA	CHA-C1A-NA	-2.82	120.01	126.39
26	S	204	DD6	C-C1-C2	-2.82	118.25	122.82
20	Q	203	CLA	CHA-C1A-NA	-2.81	120.02	126.39
20	U	208	CLA	CHD-C1D-ND	-2.81	120.84	124.80
20	L	203	CLA	CHD-C1D-ND	-2.81	120.84	124.80
20	Q	204	CLA	C4A-NA-C1A	2.81	107.96	106.68
20	A	846	CLA	CHA-C1A-NA	-2.81	120.03	126.39
20	B	809	CLA	CHA-C1A-NA	-2.81	120.03	126.39
20	O	204	CLA	CHA-C1A-NA	-2.81	120.03	126.39
20	Q	216	CLA	C4D-CHA-C1A	2.81	124.59	121.24
20	B	801	CLA	CHA-C1A-NA	-2.80	120.04	126.39
20	A	835	CLA	CHA-C1A-NA	-2.80	120.04	126.39
26	T	212	DD6	C24-C1-C2	2.80	123.42	119.01
20	R	104	CLA	CHA-C1A-NA	-2.80	120.05	126.39
26	S	210	DD6	C8-C6-C5	2.80	123.42	119.01
28	S	201	SQD	C4-C3-C2	2.80	115.75	110.83
20	T	210	CLA	CHA-C1A-NA	-2.80	120.05	126.39
20	B	803	CLA	CHA-C1A-NA	-2.80	120.06	126.39
26	G	212	DD6	C7-C6-C5	-2.80	118.28	122.82
20	G	215	CLA	CHD-C1D-ND	-2.80	120.87	124.80
31	R	105	A86	C-C1-C2	-2.79	118.29	122.82
31	Q	201	A86	C4-C3-C2	2.79	129.24	123.52
20	U	207	CLA	CHD-C1D-ND	-2.79	120.87	124.80
20	A	811	CLA	CHA-C1A-NA	-2.79	120.07	126.39
23	L	205	BCR	C27-C26-C25	2.79	126.48	122.70
26	O	214	DD6	C13-C11-C10	2.79	123.40	119.01
26	G	211	DD6	C-C1-C2	-2.79	118.30	122.82
20	B	846	CLA	C1-O2A-CGA	2.79	123.40	116.65
26	P	218	DD6	C-C1-C2	-2.79	118.30	122.82
26	A	855	DD6	C7-C6-C5	-2.78	118.31	122.82
20	H	204	CLA	CHA-C1A-NA	-2.78	120.09	126.39
27	B	842	DGD	CDB-CCB-CBB	-2.78	100.31	114.37
20	A	821	CLA	C4D-CHA-C1A	2.78	124.56	121.24
20	L	202	CLA	C4A-NA-C1A	2.78	107.95	106.68
20	A	852	CLA	CHA-C1A-NA	-2.78	120.10	126.39
20	O	203	CLA	CHA-C1A-NA	-2.78	120.10	126.39
23	B	839	BCR	C27-C26-C25	2.78	126.45	122.70
20	A	831	CLA	CHD-C1D-ND	-2.78	120.90	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	T	207	CLA	CHD-C1D-ND	-2.78	120.90	124.80
20	A	820	CLA	CHA-C1A-NA	-2.77	120.11	126.39
20	U	209	CLA	CHA-C1A-NA	-2.77	120.11	126.39
20	Q	211	CLA	C4D-CHA-C1A	2.77	124.55	121.24
20	B	819	CLA	CHA-C1A-NA	-2.77	120.11	126.39
20	Q	207	CLA	CHD-C1D-ND	-2.77	120.90	124.80
26	O	214	DD6	C10-C9-C8	2.77	131.23	123.20
20	O	206	CLA	CHD-C1D-ND	-2.77	120.90	124.80
20	Q	211	CLA	CHA-C1A-NA	-2.77	120.12	126.39
23	A	844	BCR	C28-C27-C26	-2.77	109.12	114.06
20	A	824	CLA	CHA-C1A-NA	-2.77	120.12	126.39
20	S	202	CLA	CHA-C1A-NA	-2.77	120.12	126.39
20	Q	206	CLA	CHA-C1A-NA	-2.77	120.13	126.39
20	A	823	CLA	CHA-C1A-NA	-2.77	120.13	126.39
23	F	804	BCR	C16-C15-C14	-2.76	117.86	123.52
20	B	815	CLA	CHD-C1D-ND	-2.76	120.92	124.80
30	Q	210	KC1	C1A-C2A-C3A	-2.76	104.74	107.28
20	H	205	CLA	CHA-C1A-NA	-2.76	120.14	126.39
20	U	209	CLA	CHD-C1D-ND	-2.76	120.92	124.80
20	A	838	CLA	CHD-C1D-ND	-2.76	120.92	124.80
20	A	826	CLA	CHA-C1A-NA	-2.76	120.14	126.39
20	A	817	CLA	C4A-NA-C1A	2.76	107.94	106.68
31	U	202	A86	C24-C1-C2	2.76	123.35	119.01
26	O	201	DD6	C7-C6-C5	-2.76	118.35	122.82
20	A	801	CLA	CHA-C1A-NA	-2.76	120.15	126.39
26	S	213	DD6	C28-C27-C26	-2.75	118.83	124.18
20	Q	212	CLA	C4D-CHA-C1A	2.75	124.53	121.24
20	A	853	CLA	CHA-C1A-NA	-2.75	120.17	126.39
20	A	814	CLA	CHA-C1A-NA	-2.75	120.17	126.39
20	B	829	CLA	CHA-C1A-NA	-2.75	120.17	126.39
26	P	220	DD6	C7-C6-C5	-2.75	118.36	122.82
20	B	824	CLA	CHD-C1D-ND	-2.75	120.94	124.80
20	H	208	CLA	CHD-C1D-ND	-2.75	120.94	124.80
26	P	220	DD6	C9-C8-C6	2.75	133.89	126.36
23	B	837	BCR	C33-C5-C6	-2.75	121.49	124.48
20	B	830	CLA	CHA-C1A-NA	-2.74	120.18	126.39
20	A	854	CLA	CHD-C1D-ND	-2.74	120.94	124.80
20	U	210	CLA	CHD-C1D-ND	-2.74	120.94	124.80
23	L	201	BCR	C15-C14-C13	-2.74	123.43	127.28
26	S	210	DD6	C4-C3-C2	2.74	129.13	123.52
22	P	201	LHG	O8-C23-C24	2.74	120.19	111.83
20	S	214	CLA	CHD-C1D-ND	-2.74	120.95	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	T	212	DD6	C9-C10-C11	2.74	131.12	127.28
26	Q	215	DD6	C3-C4-C5	2.74	129.12	123.52
26	T	213	DD6	C7-C6-C5	-2.74	118.38	122.82
20	B	813	CLA	CHA-C1A-NA	-2.74	120.20	126.39
20	H	207	CLA	CHA-C1A-NA	-2.73	120.20	126.39
20	G	210	CLA	CHA-C1A-NA	-2.73	120.20	126.39
20	A	814	CLA	C4A-NA-C1A	2.73	107.93	106.68
20	H	202	CLA	CHD-C1D-ND	-2.73	120.96	124.80
23	B	841	BCR	C27-C26-C25	2.73	126.39	122.70
20	F	802	CLA	C4A-NA-C1A	2.73	107.92	106.68
20	B	822	CLA	CHA-C1A-NA	-2.73	120.21	126.39
20	G	203	CLA	CHA-C1A-NA	-2.73	120.21	126.39
20	T	205	CLA	CHA-C1A-NA	-2.73	120.21	126.39
26	G	217	DD6	C-C1-C2	-2.73	118.40	122.82
30	P	206	KC1	CAB-C3B-C4B	2.73	131.33	124.82
20	A	849	CLA	CHA-C1A-NA	-2.73	120.22	126.39
20	S	207	CLA	C4D-CHA-C1A	2.73	124.50	121.24
20	O	202	CLA	CHA-C1A-NA	-2.73	120.22	126.39
26	Q	202	DD6	C15-C14-C13	2.73	131.75	125.99
20	A	847	CLA	CHA-C1A-NA	-2.73	120.22	126.39
20	H	206	CLA	CHD-C1D-ND	-2.72	120.97	124.80
26	P	215	DD6	C10-C9-C8	2.72	131.09	123.20
31	P	204	A86	C25-C24-C1	2.72	133.83	126.36
20	H	206	CLA	CHA-C1A-NA	-2.72	120.23	126.39
20	B	820	CLA	C4D-CHA-C1A	2.72	124.49	121.24
20	A	838	CLA	CHA-C1A-NA	-2.72	120.24	126.39
20	H	209	CLA	CHA-C1A-NA	-2.72	120.24	126.39
20	B	805	CLA	CHA-C1A-NA	-2.72	120.24	126.39
20	A	833	CLA	O2A-C1-C2	2.72	118.56	108.11
23	B	839	BCR	C24-C23-C22	-2.72	122.22	126.23
23	J	104	BCR	C27-C26-C25	2.72	126.37	122.70
20	O	203	CLA	C4A-NA-C1A	2.71	107.92	106.68
26	Q	202	DD6	C23-C16-C17	-2.71	104.20	108.97
23	M	101	BCR	C3-C4-C5	-2.71	109.22	114.06
20	B	825	CLA	CHA-C1A-NA	-2.71	120.25	126.39
20	A	836	CLA	CHA-C1A-NA	-2.71	120.25	126.39
20	U	211	CLA	CHA-C1A-NA	-2.71	120.25	126.39
20	A	812	CLA	C4A-NA-C1A	2.71	107.92	106.68
20	H	203	CLA	CHA-C1A-NA	-2.71	120.25	126.39
20	P	214	CLA	CHA-C1A-NA	-2.71	120.25	126.39
23	L	201	BCR	C27-C26-C25	2.71	126.36	122.70
20	B	833	CLA	CHA-C1A-NA	-2.71	120.26	126.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	T	206	CLA	CHA-C1A-NA	-2.70	120.27	126.39
20	Q	216	CLA	CHA-C1A-NA	-2.70	120.27	126.39
20	B	843	CLA	CHA-C1A-NA	-2.70	120.27	126.39
20	A	808	CLA	CHA-C1A-NA	-2.70	120.27	126.39
23	B	838	BCR	C15-C14-C13	-2.70	123.49	127.28
20	H	202	CLA	CHA-C1A-NA	-2.70	120.27	126.39
20	A	831	CLA	CHA-C1A-NA	-2.70	120.27	126.39
20	B	816	CLA	CHA-C1A-NA	-2.70	120.27	126.39
20	F	802	CLA	C1-O2A-CGA	2.70	123.19	116.65
20	P	213	CLA	CHA-C1A-NA	-2.70	120.27	126.39
20	T	210	CLA	CHD-C1D-ND	-2.70	121.00	124.80
20	S	205	CLA	CHA-C1A-NA	-2.70	120.28	126.39
20	G	202	CLA	CHA-C1A-NA	-2.70	120.28	126.39
20	B	813	CLA	C1-C2-C3	2.70	130.62	126.20
20	Q	211	CLA	CAA-C2A-C3A	-2.70	110.05	116.23
20	P	207	CLA	CHD-C1D-ND	-2.70	121.01	124.80
20	U	206	CLA	CHA-C1A-NA	-2.69	120.29	126.39
20	H	208	CLA	CHA-C1A-NA	-2.69	120.30	126.39
20	T	203	CLA	CHA-C1A-NA	-2.69	120.30	126.39
20	B	807	CLA	CHA-C1A-NA	-2.69	120.30	126.39
29	U	201	LMG	O6-C1-O1	-2.69	103.69	110.04
30	P	203	KC1	CAB-C3B-C4B	2.69	131.24	124.82
20	S	207	CLA	CHD-C1D-ND	-2.69	121.02	124.80
20	Q	205	CLA	CHA-C1A-NA	-2.69	120.31	126.39
26	J	101	DD6	C-C1-C2	-2.69	118.46	122.82
20	B	810	CLA	CHA-C1A-NA	-2.69	120.31	126.39
20	B	828	CLA	CHA-C1A-NA	-2.69	120.31	126.39
20	A	809	CLA	CHA-C1A-NA	-2.68	120.31	126.39
20	A	830	CLA	CHA-C1A-NA	-2.68	120.31	126.39
20	B	812	CLA	CHA-C1A-NA	-2.68	120.31	126.39
20	B	805	CLA	CHD-C1D-ND	-2.68	121.03	124.80
20	B	817	CLA	CHA-C1A-NA	-2.68	120.32	126.39
26	H	210	DD6	C10-C9-C8	2.68	130.97	123.20
20	G	209	CLA	CHD-C1D-ND	-2.68	121.03	124.80
20	T	204	CLA	CHA-C1A-NA	-2.68	120.32	126.39
20	A	833	CLA	CHA-C1A-NA	-2.68	120.33	126.39
20	A	806	CLA	CHA-C1A-NA	-2.68	120.33	126.39
20	A	819	CLA	CHA-C1A-NA	-2.68	120.33	126.39
20	U	205	CLA	CHA-C1A-NA	-2.67	120.33	126.39
20	B	811	CLA	CHA-C1A-NA	-2.67	120.33	126.39
26	O	215	DD6	C7-C6-C5	-2.67	118.48	122.82
20	A	810	CLA	C4A-NA-C1A	2.67	107.90	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	R	102	BCR	C29-C30-C25	2.67	114.32	110.44
20	S	208	CLA	CHA-C1A-NA	-2.67	120.34	126.39
26	O	215	DD6	C-C1-C2	-2.67	118.49	122.82
20	U	210	CLA	C4A-NA-C1A	2.67	107.90	106.68
26	Q	202	DD6	C13-C11-C10	2.67	123.21	119.01
20	P	210	CLA	CHD-C1D-ND	-2.67	121.05	124.80
20	A	829	CLA	CHD-C1D-ND	-2.67	121.05	124.80
30	P	212	KC1	CAB-C3B-C4B	2.67	131.19	124.82
21	A	837	PQN	C11-C3-C2	-2.67	120.32	124.89
20	U	210	CLA	CHA-C1A-NA	-2.67	120.36	126.39
23	R	102	BCR	C19-C20-C21	-2.66	118.07	123.52
20	B	844	CLA	CHA-C1A-NA	-2.66	120.37	126.39
23	B	838	BCR	C11-C10-C9	-2.66	123.55	127.28
20	P	207	CLA	CHA-C1A-NA	-2.66	120.37	126.39
20	O	207	CLA	CHA-C1A-NA	-2.66	120.38	126.39
31	Q	214	A86	C-C1-C2	-2.65	118.52	122.82
20	U	204	CLA	CHA-C1A-NA	-2.65	120.39	126.39
30	S	209	KC1	CAB-C3B-C4B	2.65	131.15	124.82
20	G	205	CLA	CHA-C1A-NA	-2.65	120.39	126.39
26	Q	215	DD6	C7-C6-C5	-2.65	118.52	122.82
20	A	829	CLA	CHA-C1A-NA	-2.65	120.39	126.39
20	B	833	CLA	CHD-C1D-ND	-2.65	121.07	124.80
20	A	818	CLA	CHA-C1A-NA	-2.65	120.39	126.39
20	P	210	CLA	CHA-C1A-NA	-2.65	120.39	126.39
20	A	804	CLA	CHA-C1A-NA	-2.65	120.40	126.39
20	B	826	CLA	CHA-C1A-NA	-2.65	120.40	126.39
20	B	845	CLA	C4A-NA-C1A	2.64	107.89	106.68
20	L	202	CLA	C1-O2A-CGA	2.64	123.05	116.65
26	S	212	DD6	C-C1-C2	-2.64	118.54	122.82
20	S	206	CLA	CHA-C1A-NA	-2.64	120.41	126.39
26	G	212	DD6	C8-C6-C5	2.64	123.16	119.01
20	B	816	CLA	CHD-C1D-ND	-2.64	121.09	124.80
20	B	834	CLA	CHD-C1D-ND	-2.64	121.09	124.80
31	Q	218	A86	C26-C25-C24	2.64	130.85	123.20
20	B	814	CLA	CHD-C1D-ND	-2.64	121.09	124.80
20	O	208	CLA	CHD-C1D-ND	-2.64	121.09	124.80
26	Q	215	DD6	C8-C6-C5	2.64	123.16	119.01
23	B	840	BCR	C27-C26-C25	2.64	126.27	122.70
20	B	846	CLA	CHA-C1A-NA	-2.64	120.42	126.39
26	P	220	DD6	C26-C25-C24	2.64	130.84	123.20
20	F	803	CLA	CHA-C1A-NA	-2.63	120.43	126.39
20	T	204	CLA	CHD-C1D-ND	-2.63	121.10	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	Q	218	A86	C7-C6-C5	-2.63	118.55	122.82
30	S	211	KC1	CAB-C3B-C4B	2.63	131.10	124.82
20	A	821	CLA	C4A-NA-C1A	2.63	107.88	106.68
20	G	204	CLA	CHA-C1A-NA	-2.63	120.44	126.39
23	M	101	BCR	C27-C26-C25	2.63	126.25	122.70
20	H	201	CLA	CHA-C1A-NA	-2.63	120.35	126.33
20	A	826	CLA	C4D-CHA-C1A	2.63	124.38	121.24
20	A	805	CLA	CHA-C1A-NA	-2.63	120.45	126.39
20	G	208	CLA	CHA-C1A-NA	-2.62	120.46	126.39
26	H	210	DD6	C33-C32-C31	2.62	114.65	109.49
26	O	214	DD6	C-C1-C2	-2.62	118.57	122.82
23	A	841	BCR	C40-C30-C25	2.62	114.35	110.24
20	A	854	CLA	O2A-C1-C2	2.62	118.18	108.11
26	S	210	DD6	C13-C11-C10	2.62	123.12	119.01
20	O	211	CLA	CHA-C1A-NA	-2.61	120.47	126.39
26	O	215	DD6	O1-C20-C19	-2.61	111.04	113.49
20	G	209	CLA	CHA-C1A-NA	-2.61	120.47	126.39
20	B	818	CLA	CHA-C1A-NA	-2.61	120.48	126.39
20	T	202	CLA	CHA-C1A-NA	-2.61	120.48	126.39
20	A	809	CLA	CHD-C1D-ND	-2.61	121.13	124.80
20	H	201	CLA	CHD-C1D-ND	-2.61	121.13	124.80
20	Q	209	CLA	CHA-C1A-NA	-2.61	120.48	126.39
20	U	205	CLA	CHD-C1D-ND	-2.61	121.13	124.80
26	S	212	DD6	C9-C10-C11	2.61	130.93	127.28
20	A	846	CLA	C4A-NA-C1A	2.61	107.87	106.68
20	O	202	CLA	CHD-C1D-ND	-2.61	121.14	124.80
20	O	209	CLA	CHA-C1A-NA	-2.61	120.49	126.39
20	S	207	CLA	CHA-C1A-NA	-2.61	120.49	126.39
23	J	104	BCR	C15-C16-C17	-2.60	118.19	123.52
26	G	211	DD6	C7-C6-C5	-2.60	118.60	122.82
26	S	210	DD6	C-C1-C2	-2.60	118.60	122.82
20	S	214	CLA	CHA-C1A-NA	-2.60	120.50	126.39
26	P	218	DD6	C13-C11-C10	2.60	123.10	119.01
20	Q	211	CLA	O2D-CGD-CBD	2.60	115.78	111.23
30	Q	210	KC1	CAB-C3B-C4B	2.60	131.03	124.82
26	O	201	DD6	C8-C6-C5	2.60	123.10	119.01
23	R	102	BCR	C17-C16-C15	-2.60	118.71	124.72
20	A	823	CLA	C4A-NA-C1A	2.60	107.86	106.68
31	U	202	A86	C28-C27-C26	-2.60	118.61	122.82
20	B	801	CLA	CHD-C1D-ND	-2.60	121.14	124.80
20	O	208	CLA	CHA-C1A-NA	-2.60	120.51	126.39
20	P	211	CLA	CHA-C1A-NA	-2.60	120.51	126.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	J	103	CLA	CHA-C1A-NA	-2.60	120.51	126.39
20	G	215	CLA	CHA-C1A-NA	-2.60	120.51	126.39
20	Q	213	CLA	CHD-C1D-ND	-2.59	121.15	124.80
26	S	212	DD6	C24-C1-C2	2.59	123.09	119.01
30	S	211	KC1	CAA-C2A-C1A	2.59	136.00	124.64
20	A	806	CLA	CHD-C1D-ND	-2.59	121.15	124.80
28	B	847	SQD	O48-C23-C24	2.59	119.74	111.83
20	G	201	CLA	CHA-C1A-NA	-2.59	120.52	126.39
20	A	804	CLA	CHD-C1D-ND	-2.59	121.16	124.80
20	F	803	CLA	CHD-C1D-ND	-2.59	121.16	124.80
20	A	816	CLA	CHA-C1A-NA	-2.59	120.53	126.39
31	Q	201	A86	C-C1-C2	-2.59	118.62	122.82
23	L	201	BCR	C15-C16-C17	-2.59	118.23	123.52
20	B	812	CLA	CHD-C1D-ND	-2.59	121.16	124.80
31	Q	214	A86	C24-C1-C2	2.58	123.07	119.01
23	B	838	BCR	C33-C5-C6	-2.58	121.67	124.48
20	L	203	CLA	CHA-C1A-NA	-2.58	120.55	126.39
20	B	824	CLA	CHA-C1A-NA	-2.58	120.55	126.39
30	P	219	KC1	CAB-C3B-C4B	2.58	130.97	124.82
20	O	207	CLA	CHD-C1D-ND	-2.58	121.18	124.80
26	G	217	DD6	C24-C1-C2	2.58	123.06	119.01
20	T	209	CLA	CHA-C1A-NA	-2.57	120.56	126.39
20	A	853	CLA	CHD-C1D-ND	-2.57	121.18	124.80
20	H	207	CLA	CHD-C1D-ND	-2.57	121.18	124.80
20	T	207	CLA	CHA-C1A-NA	-2.57	120.57	126.39
23	I	101	BCR	C31-C1-C6	2.57	114.27	110.24
20	Q	213	CLA	CHA-C1A-NA	-2.57	120.58	126.39
20	O	206	CLA	CHA-C1A-NA	-2.57	120.58	126.39
29	Q	217	LMG	O6-C1-O1	-2.57	103.98	110.04
28	S	201	SQD	O7-S-C6	2.56	110.58	106.76
20	L	204	CLA	CHA-C1A-NA	-2.56	120.58	126.39
20	U	208	CLA	CHA-C1A-NA	-2.56	120.59	126.39
26	J	101	DD6	C24-C1-C2	2.56	123.04	119.01
20	Q	209	CLA	CHD-C1D-ND	-2.56	121.20	124.80
20	A	834	CLA	C4A-NA-C1A	2.56	107.85	106.68
20	B	831	CLA	CHA-C1A-NA	-2.56	120.60	126.39
26	O	214	DD6	C24-C1-C2	2.56	123.03	119.01
28	S	201	SQD	C44-O6-C1	2.56	119.28	113.80
23	A	843	BCR	C28-C27-C26	-2.55	109.50	114.06
20	A	802	CLA	C4D-CHA-C1A	2.55	124.29	121.24
20	B	831	CLA	CHD-C1D-ND	-2.55	121.21	124.80
20	S	202	CLA	CHD-C1D-C2D	2.55	130.79	125.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	F	804	BCR	C27-C26-C25	2.55	126.15	122.70
23	F	801	BCR	C27-C26-C25	2.54	126.14	122.70
20	T	211	CLA	CHD-C1D-ND	-2.54	121.22	124.80
20	B	808	CLA	CHA-C1A-NA	-2.54	120.63	126.39
23	I	102	BCR	C15-C14-C13	-2.54	123.71	127.28
20	G	207	CLA	CHA-C1A-NA	-2.54	120.63	126.39
22	A	840	LHG	C11-C10-C9	-2.54	101.51	114.37
20	Q	216	CLA	CHD-C1D-ND	-2.54	121.22	124.80
20	A	851	CLA	CHA-C1A-NA	-2.54	120.63	126.39
20	B	807	CLA	CHD-C1D-ND	-2.54	121.23	124.80
20	P	209	CLA	CHA-C1A-NA	-2.54	120.64	126.39
20	A	832	CLA	C4A-NA-C1A	2.54	107.84	106.68
23	B	837	BCR	C29-C30-C25	2.54	114.12	110.44
20	O	203	CLA	CHD-C1D-ND	-2.53	121.23	124.80
20	B	848	CLA	CHD-C1D-ND	-2.53	121.24	124.80
20	B	815	CLA	CHA-C1A-NA	-2.53	120.66	126.39
28	B	847	SQD	C1-O5-C5	2.53	118.66	113.72
29	P	202	LMG	C1-O6-C5	-2.53	108.78	113.72
23	B	840	BCR	C2-C1-C6	2.53	114.11	110.44
20	B	826	CLA	CHD-C1D-ND	-2.53	121.25	124.80
21	B	836	PQN	C11-C3-C2	-2.53	120.56	124.89
20	A	803	CLA	CHA-C1A-NA	-2.53	120.67	126.39
20	A	801	CLA	CHD-C1D-ND	-2.53	121.25	124.80
26	G	217	DD6	C7-C6-C5	-2.52	118.73	122.82
20	B	821	CLA	CHA-C1A-NA	-2.52	120.68	126.39
20	A	836	CLA	CAA-C2A-C1A	2.52	120.24	111.97
31	Q	218	A86	C8-C6-C5	2.52	122.97	119.01
27	B	842	DGD	O6D-C1D-O3G	-2.52	104.09	110.04
24	A	848	CL0	CHA-C1A-C2A	-2.52	127.39	133.31
20	B	832	CLA	CHD-C1D-ND	-2.52	121.26	124.80
26	U	212	DD6	C9-C10-C11	2.52	130.81	127.28
20	B	803	CLA	CHD-C1D-ND	-2.52	121.26	124.80
26	U	203	DD6	C22-C16-C17	-2.52	104.55	108.97
20	B	835	CLA	C4A-NA-C1A	2.51	107.83	106.68
23	A	844	BCR	C29-C30-C25	2.51	114.09	110.44
20	O	209	CLA	O2A-C1-C2	2.51	117.78	108.11
20	B	814	CLA	CHA-C1A-NA	-2.51	120.70	126.39
20	A	801	CLA	C4D-CHA-C1A	2.51	124.24	121.24
20	L	202	CLA	CHD-C1D-ND	-2.51	121.27	124.80
20	H	209	CLA	CHD-C1D-ND	-2.51	121.27	124.80
20	A	852	CLA	CHD-C1D-ND	-2.51	121.27	124.80
20	G	201	CLA	CHD-C1D-ND	-2.51	121.28	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	P	209	CLA	CHD-C1D-ND	-2.50	121.28	124.80
20	A	814	CLA	CHD-C1D-ND	-2.50	121.28	124.80
20	Q	211	CLA	C4A-NA-C1A	2.50	107.82	106.68
20	A	830	CLA	CHD-C1D-ND	-2.50	121.28	124.80
20	S	208	CLA	CHD-C1D-C2D	2.50	130.69	125.49
20	A	802	CLA	C1-O2A-CGA	2.50	122.70	116.65
26	U	212	DD6	C26-C25-C24	2.50	130.44	123.20
20	O	205	CLA	CHA-C1A-NA	-2.49	120.75	126.39
26	O	215	DD6	C8-C6-C5	2.49	122.92	119.01
20	T	205	CLA	C4A-NA-C1A	2.49	107.81	106.68
20	H	206	CLA	CMC-C2C-C1C	2.49	128.92	125.03
26	O	212	DD6	C26-C25-C24	2.49	130.40	123.20
26	G	213	DD6	C13-C11-C10	2.48	122.92	119.01
20	P	213	CLA	CGD-CBD-CAD	-2.48	102.81	110.85
20	A	834	CLA	CHD-C1D-ND	-2.48	121.31	124.80
31	R	105	A86	C23-C16-C17	-2.47	104.62	108.97
20	A	822	CLA	CHA-C1A-NA	-2.47	120.79	126.39
23	A	843	BCR	C33-C5-C6	-2.46	121.80	124.48
28	B	847	SQD	O8-S-C6	2.46	110.72	105.97
20	U	207	CLA	CHA-C1A-NA	-2.46	120.82	126.39
29	J	102	LMG	O6-C1-O1	-2.46	104.23	110.04
26	G	214	DD6	C10-C9-C8	2.46	130.32	123.20
20	H	203	CLA	C3B-C4B-NB	-2.46	108.34	110.53
30	U	213	KC1	CHC-C4B-NB	-2.46	121.35	124.80
20	H	207	CLA	C3B-C4B-NB	-2.45	108.34	110.53
26	O	215	DD6	C12-C11-C13	2.45	121.83	118.09
20	B	827	CLA	CHD-C1D-ND	-2.45	121.36	124.80
20	B	846	CLA	CHD-C1D-ND	-2.45	121.36	124.80
26	O	213	DD6	C7-C6-C5	-2.45	118.85	122.82
26	T	213	DD6	C33-C32-C31	2.45	114.31	109.49
20	U	211	CLA	CHD-C1D-ND	-2.45	121.36	124.80
20	S	206	CLA	CHD-C1D-ND	-2.44	121.36	124.80
20	B	820	CLA	C4A-NA-C1A	2.44	107.79	106.68
20	A	824	CLA	CHD-C1D-ND	-2.44	121.37	124.80
20	B	829	CLA	CHD-C1D-ND	-2.44	121.37	124.80
20	B	811	CLA	CHD-C1D-ND	-2.44	121.37	124.80
23	B	837	BCR	C7-C8-C9	-2.44	122.63	126.23
20	Q	207	CLA	C1-O2A-CGA	2.43	123.86	116.07
26	S	213	DD6	C26-C25-C24	2.43	130.25	123.20
26	G	211	DD6	C8-C6-C5	2.43	122.83	119.01
20	A	847	CLA	CHD-C1D-C2D	2.43	130.54	125.49
20	T	207	CLA	O2A-C1-C2	2.43	117.45	108.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	815	CLA	CHD-C1D-ND	-2.42	121.39	124.80
26	G	214	DD6	C4-C5-C6	2.42	130.67	127.28
30	U	213	KC1	CGD-CBD-CAD	-2.42	103.02	110.85
20	H	208	CLA	CAA-C2A-C3A	-2.42	110.69	116.23
20	T	205	CLA	O2D-CGD-CBD	2.42	115.45	111.23
30	O	210	KC1	C1A-C2A-C3A	-2.42	105.06	107.28
26	S	204	DD6	C10-C9-C8	2.42	130.20	123.20
26	J	101	DD6	C10-C9-C8	2.41	130.19	123.20
20	J	103	CLA	CHD-C1D-ND	-2.41	121.41	124.80
26	P	220	DD6	C-C1-C2	-2.41	118.91	122.82
31	Q	214	A86	C28-C27-C26	-2.41	118.91	122.82
20	A	833	CLA	CHD-C1D-ND	-2.41	121.41	124.80
20	B	828	CLA	CHD-C1D-ND	-2.41	121.41	124.80
20	S	205	CLA	CHD-C1D-ND	-2.41	121.41	124.80
20	B	802	CLA	C4D-CHA-C1A	2.41	124.11	121.24
20	U	204	CLA	CHD-C1D-ND	-2.41	121.42	124.80
20	T	204	CLA	O2A-C1-C2	2.40	117.36	108.11
30	S	209	KC1	CHC-C4B-C3B	2.40	129.26	125.21
20	B	832	CLA	C4A-NA-C1A	2.40	107.78	106.68
20	B	809	CLA	CHD-C1D-ND	-2.40	121.42	124.80
31	Q	214	A86	C40-C32-C31	2.40	112.62	110.47
28	S	201	SQD	O6-C1-C2	2.40	111.92	108.27
27	B	842	DGD	CFB-CEB-CDB	-2.40	102.25	114.37
20	B	803	CLA	CAC-C3C-C4C	2.40	127.91	124.79
20	A	803	CLA	CHD-C1D-C2D	2.40	130.47	125.49
20	L	204	CLA	C1-C2-C3	2.40	130.64	126.76
26	T	213	DD6	C22-C16-C17	-2.40	104.76	108.97
20	Q	203	CLA	CAA-CBA-CGA	-2.39	106.43	113.21
20	A	851	CLA	CHD-C1D-ND	-2.39	121.44	124.80
26	S	210	DD6	C24-C1-C2	2.39	122.76	119.01
20	B	818	CLA	CHD-C1D-C2D	2.38	130.44	125.49
23	B	839	BCR	C31-C1-C6	2.38	113.98	110.24
23	M	101	BCR	C15-C16-C17	-2.38	118.64	123.52
26	G	214	DD6	C13-C11-C10	2.38	122.75	119.01
20	U	211	CLA	C4A-NA-C1A	2.38	107.76	106.68
26	S	203	DD6	C28-C27-C26	-2.37	119.57	124.18
26	S	204	DD6	C30-C29-C27	-2.37	168.16	176.23
29	P	217	LMG	O1-C1-C2	-2.37	104.67	108.27
31	Q	201	A86	C12-C11-C10	-2.37	117.91	123.67
20	A	838	CLA	C4A-NA-C1A	2.37	107.76	106.68
20	B	835	CLA	O2A-C1-C2	2.37	117.23	108.11
26	O	212	DD6	C13-C11-C10	2.37	122.74	119.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	G	204	CLA	CHD-C1D-ND	-2.37	121.47	124.80
20	P	208	CLA	CHD-C1D-ND	-2.37	121.47	124.80
30	S	211	KC1	C2A-C3A-C4A	2.36	108.19	106.41
20	A	836	CLA	CHD-C1D-ND	-2.36	121.48	124.80
20	T	203	CLA	CHD-C1D-ND	-2.36	121.48	124.80
20	O	209	CLA	O2D-CGD-CBD	2.36	115.36	111.23
23	B	838	BCR	C28-C27-C26	-2.36	109.84	114.06
20	A	836	CLA	C4A-NA-C1A	2.36	107.76	106.68
31	Q	201	A86	C24-C1-C2	2.36	122.72	119.01
20	A	825	CLA	CHD-C1D-ND	-2.36	121.48	124.80
20	A	813	CLA	CHD-C1D-ND	-2.36	121.48	124.80
26	H	211	DD6	C33-C32-C31	2.36	114.14	109.49
30	S	211	KC1	CHC-C4B-C3B	2.36	129.19	125.21
26	Q	215	DD6	C13-C11-C10	2.36	122.72	119.01
20	B	810	CLA	CHD-C1D-ND	-2.36	121.49	124.80
20	R	104	CLA	CHD-C1D-ND	-2.36	121.49	124.80
30	P	203	KC1	C1A-C2A-C3A	-2.35	105.12	107.28
20	P	211	CLA	CHD-C1D-ND	-2.35	121.49	124.80
31	Q	218	A86	C28-C27-C26	-2.35	119.00	122.82
20	T	210	CLA	C1-O2A-CGA	2.35	123.60	116.07
29	Q	217	LMG	O1-C7-C8	-2.35	105.10	110.82
26	S	204	DD6	O1-C15-C14	-2.35	110.14	116.88
29	I	103	LMG	C40-C39-C38	-2.35	102.49	114.37
30	U	213	KC1	CAB-C3B-C2B	-2.35	120.80	128.43
20	Q	205	CLA	CHD-C1D-ND	-2.34	121.50	124.80
26	G	211	DD6	C3-C4-C5	2.34	128.31	123.52
26	O	215	DD6	O1-C15-C14	-2.33	110.19	116.88
20	P	214	CLA	CHD-C1D-ND	-2.33	121.52	124.80
29	P	217	LMG	O2-C2-C1	-2.33	104.52	110.08
20	U	208	CLA	CHD-C1D-C2D	2.33	130.34	125.49
26	T	213	DD6	C26-C25-C24	2.33	129.96	123.20
31	Q	201	A86	C10-C9-C8	2.33	129.96	123.20
23	A	844	BCR	C15-C16-C17	-2.33	118.75	123.52
20	G	207	CLA	CHD-C1D-C2D	2.33	130.33	125.49
20	H	201	CLA	C4A-NA-C1A	2.33	107.74	106.68
20	B	817	CLA	CHD-C1D-ND	-2.33	121.53	124.80
26	S	204	DD6	C33-C32-C31	2.33	114.08	109.49
20	A	836	CLA	C1-O2A-CGA	2.33	122.28	116.65
20	A	828	CLA	CHD-C1D-ND	-2.33	121.53	124.80
20	B	821	CLA	CHD-C1D-C2D	2.32	130.32	125.49
29	P	217	LMG	O6-C1-O1	-2.32	104.56	110.04
20	A	807	CLA	CHD-C1D-ND	-2.32	121.54	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	808	CLA	CHD-C1D-ND	-2.32	121.54	124.80
26	H	210	DD6	C13-C11-C10	2.32	122.66	119.01
26	O	213	DD6	C3-C4-C5	2.32	128.27	123.52
20	A	822	CLA	CHD-C1D-C2D	2.32	130.31	125.49
20	O	204	CLA	CHD-C1D-ND	-2.32	121.54	124.80
20	U	209	CLA	C3B-C4B-NB	-2.32	108.46	110.53
23	B	840	BCR	C29-C30-C25	2.32	113.81	110.44
26	T	213	DD6	C10-C9-C8	2.32	129.92	123.20
23	L	201	BCR	C2-C1-C6	2.32	113.81	110.44
22	P	201	LHG	C20-C19-C18	-2.32	102.66	114.37
30	P	212	KC1	C1B-CHB-C4A	2.32	130.94	126.02
23	B	838	BCR	C29-C30-C25	2.32	113.80	110.44
20	A	832	CLA	CHD-C1D-ND	-2.32	121.54	124.80
26	T	212	DD6	C33-C32-C31	2.31	114.05	109.49
30	P	203	KC1	CHC-C4B-C3B	2.31	129.11	125.21
31	R	105	A86	C28-C27-C26	-2.31	119.07	122.82
26	O	212	DD6	C28-C27-C26	-2.31	119.69	124.18
20	F	802	CLA	CHD-C1D-ND	-2.31	121.55	124.80
20	A	849	CLA	CHD-C1D-ND	-2.31	121.55	124.80
29	P	217	LMG	O3-C3-C2	-2.31	104.94	110.38
26	G	217	DD6	C14-C13-C11	-2.31	121.95	125.53
30	Q	210	KC1	C2A-C3A-C4A	2.30	108.14	106.41
28	B	847	SQD	C4-C3-C2	2.30	114.87	110.83
24	A	848	CL0	C4D-CHA-CBD	-2.30	106.65	108.97
29	I	103	LMG	C38-C37-C36	-2.30	102.74	114.37
26	O	212	DD6	C10-C9-C8	2.30	129.85	123.20
20	H	204	CLA	CHD-C1D-ND	-2.30	121.57	124.80
20	B	844	CLA	CGD-CBD-CAD	-2.30	103.42	110.85
20	B	817	CLA	C3B-C4B-NB	-2.30	108.48	110.53
20	A	810	CLA	CHD-C1D-ND	-2.29	121.58	124.80
30	P	206	KC1	CHC-C4B-NB	-2.29	121.58	124.80
26	U	212	DD6	C13-C11-C10	2.29	122.61	119.01
22	P	201	LHG	C11-C10-C9	-2.29	102.78	114.37
23	A	844	BCR	C33-C5-C6	-2.29	121.98	124.48
20	A	818	CLA	CHD-C1D-ND	-2.29	121.58	124.80
26	H	211	DD6	C26-C25-C24	2.29	129.84	123.20
20	G	210	CLA	CHD-C1D-ND	-2.29	121.58	124.80
28	S	201	SQD	O48-C23-C24	2.29	118.81	111.83
28	S	201	SQD	O8-S-C6	2.28	110.38	105.97
31	R	103	A86	C10-C9-C8	2.28	129.82	123.20
20	A	811	CLA	CHD-C1D-ND	-2.28	121.59	124.80
29	J	102	LMG	O2-C2-C1	-2.28	104.63	110.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	H	208	CLA	CMD-C2D-C1D	2.28	128.75	124.73
20	S	214	CLA	CHD-C1D-C2D	2.28	130.23	125.49
26	S	203	DD6	C26-C25-C24	2.28	129.81	123.20
20	B	813	CLA	CHD-C1D-ND	-2.28	121.59	124.80
20	L	204	CLA	CHD-C1D-C2D	2.28	130.23	125.49
20	T	209	CLA	CHD-C1D-C2D	2.28	130.23	125.49
20	T	202	CLA	CHD-C1D-C2D	2.28	130.22	125.49
20	B	813	CLA	C4-C3-C2	2.28	129.48	123.63
20	G	208	CLA	O2A-C1-C2	2.28	116.87	108.11
20	A	853	CLA	C4A-NA-C1A	2.28	107.72	106.68
26	S	203	DD6	C13-C11-C10	2.27	122.59	119.01
30	P	203	KC1	C1B-CHB-C4A	2.27	130.85	126.02
20	P	213	CLA	CHD-C1D-C2D	2.27	130.21	125.49
20	Q	204	CLA	CHD-C1D-C2D	2.27	130.21	125.49
20	A	819	CLA	CHD-C1D-C2D	2.27	130.21	125.49
20	G	203	CLA	CHD-C1D-ND	-2.27	121.61	124.80
29	P	202	LMG	O3-C3-C2	-2.27	105.02	110.38
30	P	206	KC1	CHC-C4B-C3B	2.27	129.03	125.21
23	R	102	BCR	C24-C23-C22	-2.27	122.88	126.23
20	A	816	CLA	CHD-C1D-C2D	2.27	130.21	125.49
26	H	211	DD6	C28-C27-C26	-2.27	119.78	124.18
23	A	842	BCR	C27-C26-C25	2.26	125.76	122.70
20	B	815	CLA	C3B-C4B-NB	-2.26	108.51	110.53
20	Q	208	CLA	C4A-NA-C1A	2.26	107.71	106.68
20	A	831	CLA	CHD-C1D-C2D	2.26	130.18	125.49
20	U	207	CLA	C3A-C2A-C1A	-2.26	97.96	101.34
20	H	203	CLA	CHD-C1D-C2D	2.26	130.18	125.49
20	S	202	CLA	CMD-C2D-C1D	2.25	128.70	124.73
26	S	204	DD6	C13-C11-C10	2.25	122.55	119.01
31	R	103	A86	C26-C25-C24	2.25	129.73	123.20
20	G	215	CLA	CHD-C1D-C2D	2.25	130.17	125.49
26	G	217	DD6	C8-C6-C5	2.25	122.55	119.01
20	U	206	CLA	CHD-C1D-ND	-2.25	121.64	124.80
20	P	213	CLA	O2D-CGD-CBD	2.25	115.16	111.23
20	B	819	CLA	CHD-C1D-ND	-2.25	121.64	124.80
20	T	201	CLA	C4A-NA-C1A	2.25	107.70	106.68
26	U	212	DD6	C34-C35-C36	2.25	117.77	112.18
20	G	205	CLA	C1C-C2C-C3C	2.24	109.34	106.98
20	A	854	CLA	CHD-C1D-C2D	2.24	130.15	125.49
20	B	833	CLA	CHD-C1D-C2D	2.24	130.15	125.49
20	H	208	CLA	CHD-C1D-C2D	2.24	130.15	125.49
20	B	815	CLA	CHD-C1D-C2D	2.24	130.15	125.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	O	201	DD6	C13-C11-C10	2.24	122.53	119.01
24	A	848	CL0	C4C-CHD-C1D	2.24	124.08	116.07
24	A	848	CL0	C3C-C4C-NC	-2.24	109.18	114.65
20	Q	212	CLA	CHD-C1D-ND	-2.24	121.66	124.80
20	A	827	CLA	C4A-NA-C1A	2.24	107.70	106.68
20	B	806	CLA	CHD-C1D-ND	-2.24	121.66	124.80
30	P	203	KC1	CHC-C4B-NB	-2.24	121.66	124.80
26	U	214	DD6	C33-C32-C31	2.23	113.89	109.49
20	O	211	CLA	CHD-C1D-C2D	2.23	130.13	125.49
20	P	208	CLA	C4A-NA-C1A	2.23	107.70	106.68
20	A	805	CLA	CHD-C1D-C2D	2.23	130.13	125.49
29	Q	217	LMG	O2-C2-C1	-2.23	104.76	110.08
20	B	822	CLA	CHD-C1D-ND	-2.23	121.67	124.80
26	G	214	DD6	C25-C24-C1	2.23	132.47	126.36
20	O	211	CLA	C3B-C4B-NB	-2.22	108.54	110.53
20	O	205	CLA	CHD-C1D-C2D	2.22	130.11	125.49
20	G	205	CLA	CHD-C4C-C3C	2.22	128.01	124.77
20	B	843	CLA	CHD-C1D-ND	-2.22	121.68	124.80
20	G	202	CLA	CHD-C1D-ND	-2.22	121.68	124.80
30	S	209	KC1	CAA-CBA-CGA	-2.22	115.75	127.05
23	F	801	BCR	C3-C4-C5	-2.22	110.10	114.06
20	Q	207	CLA	C4A-NA-C1A	2.22	107.69	106.68
23	R	102	BCR	C40-C30-C25	2.22	113.72	110.24
26	U	203	DD6	C10-C9-C8	2.22	129.63	123.20
20	H	207	CLA	C4-C3-C2	-2.22	117.93	123.63
23	A	841	BCR	C3-C4-C5	-2.22	110.10	114.06
27	B	842	DGD	CBB-CAB-C9B	-2.22	103.17	114.37
20	H	201	CLA	C2A-C1A-CHA	2.22	126.15	122.71
31	Q	201	A86	C25-C26-C27	2.22	130.38	127.28
20	B	804	CLA	CHD-C1D-ND	-2.22	121.69	124.80
20	B	802	CLA	C2A-C1A-CHA	2.21	127.71	123.87
20	B	845	CLA	CHD-C1D-ND	-2.21	121.69	124.80
20	G	205	CLA	C2A-C1A-CHA	2.21	127.70	123.87
20	Q	203	CLA	C1-O2A-CGA	2.21	122.00	116.65
20	Q	213	CLA	CAA-CBA-CGA	-2.21	106.94	113.21
20	U	207	CLA	CHD-C1D-C2D	2.21	130.08	125.49
26	G	214	DD6	C24-C1-C2	2.21	122.48	119.01
20	G	206	CLA	CHD-C1D-ND	-2.20	121.70	124.80
30	O	210	KC1	CHB-C4A-C3A	-2.20	121.55	125.03
20	P	216	CLA	CHD-C1D-ND	-2.20	121.71	124.80
30	P	203	KC1	CHB-C4A-C3A	-2.20	121.56	125.03
26	P	220	DD6	C13-C11-C10	2.20	122.47	119.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	Q	217	LMG	O3-C3-C2	-2.20	105.19	110.38
20	A	827	CLA	CHD-C1D-ND	-2.20	121.71	124.80
26	Q	202	DD6	O1-C20-C19	-2.20	111.43	113.49
26	G	217	DD6	C28-C27-C26	-2.20	119.91	124.18
30	S	211	KC1	CAC-C3C-C4C	2.20	127.65	124.79
23	I	101	BCR	C15-C16-C17	-2.20	119.03	123.52
30	O	210	KC1	C1B-CHB-C4A	2.19	130.68	126.02
20	B	804	CLA	C4A-NA-C1A	2.19	107.68	106.68
20	B	823	CLA	CAA-C2A-C1A	2.19	119.16	111.97
20	A	849	CLA	C4A-NA-C1A	2.19	107.68	106.68
22	A	839	LHG	C11-C10-C9	-2.19	103.30	114.37
20	B	813	CLA	C5-C3-C2	-2.19	116.25	121.17
31	Q	201	A86	C28-C27-C26	-2.19	119.27	122.82
20	B	824	CLA	CHD-C1D-C2D	2.19	130.04	125.49
20	Q	212	CLA	CAA-C2A-C3A	-2.19	107.09	113.00
29	I	103	LMG	O6-C1-O1	-2.19	104.88	110.04
20	Q	208	CLA	CHD-C1D-ND	-2.19	121.73	124.80
23	B	837	BCR	C27-C26-C25	2.18	125.66	122.70
29	I	103	LMG	O3-C3-C2	-2.18	105.23	110.38
20	B	805	CLA	CHD-C1D-C2D	2.18	130.02	125.49
20	O	206	CLA	CHD-C1D-C2D	2.18	130.02	125.49
23	J	104	BCR	C16-C15-C14	-2.18	119.06	123.52
20	T	210	CLA	CHD-C1D-C2D	2.18	130.02	125.49
20	A	820	CLA	CHD-C1D-ND	-2.18	121.74	124.80
20	O	208	CLA	CHD-C1D-C2D	2.18	130.02	125.49
26	G	217	DD6	C3-C4-C5	2.18	127.97	123.52
26	T	213	DD6	C13-C11-C10	2.17	122.43	119.01
30	T	208	KC1	C1A-C2A-C3A	-2.17	105.28	107.28
20	O	209	CLA	C4B-CHC-C1C	2.17	131.36	126.25
27	B	842	DGD	C1E-O6E-C5E	2.17	117.96	113.72
26	G	214	DD6	C28-C27-C26	-2.17	119.97	124.18
23	A	842	BCR	C2-C1-C6	2.17	113.59	110.44
20	Q	212	CLA	C2A-C1A-CHA	2.17	127.63	123.87
23	I	102	BCR	C38-C26-C25	-2.17	122.12	124.48
22	A	839	LHG	C27-C26-C25	-2.17	103.42	114.37
26	P	220	DD6	C33-C32-C31	2.16	113.75	109.49
20	O	202	CLA	CHD-C1D-C2D	2.16	129.99	125.49
23	B	838	BCR	C15-C16-C17	-2.16	119.09	123.52
20	A	846	CLA	CHD-C1D-ND	-2.16	121.76	124.80
30	T	208	KC1	CHC-C4B-NB	-2.16	121.76	124.80
20	S	207	CLA	CHD-C1D-C2D	2.16	129.98	125.49
26	O	215	DD6	C33-C32-C31	2.16	113.74	109.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	845	CLA	CHD-C1D-ND	-2.16	121.77	124.80
20	B	820	CLA	CHD-C1D-ND	-2.16	121.77	124.80
20	T	205	CLA	C1-O2A-CGA	2.16	122.98	116.07
26	O	215	DD6	C26-C25-C24	2.16	129.45	123.20
20	U	208	CLA	O2D-CGD-CBD	2.16	115.00	111.23
20	B	843	CLA	CAC-C3C-C4C	2.16	127.59	124.79
29	J	102	LMG	C1-C2-C3	-2.16	105.48	110.01
20	A	817	CLA	CHD-C1D-ND	-2.15	121.77	124.80
20	Q	211	CLA	CHD-C1D-ND	-2.15	121.77	124.80
20	B	825	CLA	C4D-CHA-C1A	2.15	123.81	121.24
23	B	841	BCR	C15-C16-C17	-2.15	119.11	123.52
23	B	839	BCR	C16-C15-C14	-2.15	119.11	123.52
20	A	821	CLA	C1D-ND-C4D	2.15	107.82	106.31
20	G	209	CLA	CHD-C1D-C2D	2.15	129.96	125.49
20	T	205	CLA	CHD-C1D-C2D	2.15	129.96	125.49
23	I	101	BCR	C15-C14-C13	-2.15	124.26	127.28
23	B	839	BCR	C30-C25-C26	-2.15	119.70	122.64
20	B	833	CLA	C4A-NA-C1A	2.15	107.66	106.68
20	B	825	CLA	CHD-C1D-ND	-2.15	121.78	124.80
31	P	204	A86	C23-C16-C17	-2.15	105.19	108.97
26	T	212	DD6	C14-C13-C11	-2.15	122.20	125.53
20	R	101	CLA	C3B-C4B-NB	-2.15	108.61	110.53
26	P	220	DD6	C29-C30-C31	-2.15	170.48	175.48
20	P	210	CLA	CHD-C1D-C2D	2.15	129.95	125.49
20	A	823	CLA	CHD-C1D-ND	-2.15	121.78	124.80
20	Q	207	CLA	CHD-C1D-C2D	2.15	129.95	125.49
20	B	819	CLA	C2A-C1A-CHA	2.15	127.59	123.87
29	I	103	LMG	O2-C2-C1	-2.14	104.96	110.08
20	B	830	CLA	CHD-C1D-ND	-2.14	121.79	124.80
20	B	833	CLA	C3B-C4B-NB	-2.14	108.62	110.53
30	S	211	KC1	CHC-C4B-NB	-2.14	121.79	124.80
30	O	210	KC1	CHB-C4A-NA	2.14	127.55	124.23
20	Q	206	CLA	CHD-C1D-ND	-2.14	121.79	124.80
20	P	207	CLA	CHD-C1D-C2D	2.14	129.94	125.49
20	T	206	CLA	CHD-C1D-ND	-2.14	121.79	124.80
23	I	101	BCR	C27-C26-C25	2.14	125.60	122.70
20	Q	203	CLA	CHD-C1D-ND	-2.14	121.79	124.80
20	A	829	CLA	CHD-C1D-C2D	2.14	129.94	125.49
20	A	813	CLA	C4A-NA-C1A	2.14	107.66	106.68
31	Q	218	A86	C22-C16-C17	-2.14	105.21	108.97
23	B	841	BCR	C10-C11-C12	-2.14	117.01	123.20
20	Q	213	CLA	CHD-C1D-C2D	2.14	129.93	125.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	812	CLA	CHD-C1D-ND	-2.13	121.80	124.80
30	P	219	KC1	CHC-C4B-C3B	2.13	128.81	125.21
26	O	213	DD6	C8-C6-C5	2.13	122.36	119.01
20	A	821	CLA	CAC-C3C-C4C	2.13	127.56	124.79
23	B	839	BCR	C11-C10-C9	-2.13	124.29	127.28
20	U	209	CLA	CHD-C1D-C2D	2.13	129.92	125.49
20	B	803	CLA	C1C-C2C-C3C	2.13	109.22	106.98
20	B	834	CLA	CHD-C1D-C2D	2.13	129.92	125.49
30	S	209	KC1	CHC-C4B-NB	-2.13	121.81	124.80
31	P	204	A86	C28-C27-C26	-2.13	119.37	122.82
20	H	201	CLA	CHD-C1D-C2D	2.13	129.91	125.49
20	R	101	CLA	CHD-C1D-ND	-2.13	121.81	124.80
20	H	206	CLA	CAC-C3C-C4C	2.13	127.56	124.79
22	P	201	LHG	C27-C26-C25	-2.13	103.62	114.37
20	B	820	CLA	C2A-C1A-CHA	2.13	127.56	123.87
20	S	206	CLA	O2D-CGD-CBD	2.12	114.94	111.23
26	Q	202	DD6	C10-C9-C8	2.12	129.35	123.20
23	I	101	BCR	C1-C6-C5	-2.12	119.73	122.64
20	A	854	CLA	C2A-C1A-CHA	2.12	127.55	123.87
29	U	201	LMG	C1-C2-C3	-2.12	105.55	110.01
20	H	207	CLA	C1-O2A-CGA	-2.12	111.52	116.65
29	Q	217	LMG	C38-C37-C36	-2.12	103.66	114.37
26	Q	215	DD6	C33-C32-C31	2.12	113.66	109.49
20	A	835	CLA	CHD-C1D-ND	-2.12	121.83	124.80
20	A	821	CLA	C2A-C1A-CHA	2.12	127.54	123.87
23	B	839	BCR	C1-C6-C5	-2.11	119.75	122.64
20	A	804	CLA	CHD-C1D-C2D	2.11	129.88	125.49
20	H	206	CLA	CHD-C1D-C2D	2.11	129.88	125.49
20	A	806	CLA	CHD-C1D-C2D	2.11	129.88	125.49
20	A	854	CLA	C1D-ND-C4D	2.11	107.79	106.31
20	P	216	CLA	C1D-ND-C4D	2.11	107.79	106.31
20	B	809	CLA	C4A-NA-C1A	2.11	107.64	106.68
30	S	209	KC1	CBA-CAA-C2A	2.11	133.92	125.45
20	U	210	CLA	CHD-C1D-C2D	2.11	129.87	125.49
20	P	213	CLA	CAA-C2A-C3A	-2.11	111.40	116.23
20	A	832	CLA	CAA-C2A-C1A	2.11	118.88	111.97
29	J	102	LMG	O3-C3-C2	-2.11	105.41	110.38
20	A	847	CLA	C6-C5-C3	2.10	118.59	113.47
26	T	212	DD6	C22-C16-C17	-2.10	105.28	108.97
20	A	812	CLA	C1D-ND-C4D	2.10	107.79	106.31
23	A	843	BCR	C29-C30-C25	2.10	113.49	110.44
20	T	207	CLA	CHD-C1D-C2D	2.10	129.85	125.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	P	202	LMG	O2-C2-C1	-2.10	105.08	110.08
29	U	201	LMG	O3-C3-C2	-2.10	105.43	110.38
26	A	855	DD6	C13-C11-C10	2.09	122.30	119.01
27	B	842	DGD	O2D-C2D-C1D	-2.09	105.09	110.08
26	O	215	DD6	C14-C13-C11	2.09	128.78	125.53
23	F	801	BCR	C16-C15-C14	-2.09	119.24	123.52
20	B	803	CLA	C2A-C1A-CHA	2.09	127.49	123.87
27	B	842	DGD	O5E-C6E-C5E	-2.09	104.22	111.33
20	A	807	CLA	CAA-C2A-C1A	2.09	118.82	111.97
22	A	839	LHG	C18-C17-C16	-2.08	103.83	114.37
30	T	208	KC1	CHC-C4B-C3B	2.08	128.72	125.21
20	B	816	CLA	CHD-C1D-C2D	2.08	129.82	125.49
26	P	218	DD6	C26-C25-C24	2.08	129.23	123.20
30	P	212	KC1	CHC-C4B-C3B	2.08	128.72	125.21
23	A	844	BCR	C2-C1-C6	2.08	113.46	110.44
20	F	803	CLA	CHD-C1D-C2D	2.08	129.81	125.49
30	P	212	KC1	CAC-C3C-C4C	2.08	127.49	124.79
26	S	210	DD6	C10-C9-C8	2.08	129.22	123.20
20	G	201	CLA	CHD-C1D-C2D	2.08	129.81	125.49
23	B	840	BCR	C8-C7-C6	-2.08	121.45	127.00
20	B	812	CLA	CHD-C1D-C2D	2.08	129.80	125.49
20	Q	216	CLA	CHD-C1D-C2D	2.07	129.80	125.49
20	B	817	CLA	CHD-C1D-C2D	2.07	129.80	125.49
20	T	204	CLA	CHD-C1D-C2D	2.07	129.79	125.49
20	A	830	CLA	CHD-C1D-C2D	2.07	129.79	125.49
20	A	852	CLA	CHD-C1D-C2D	2.07	129.79	125.49
26	G	212	DD6	C22-C16-C17	-2.07	105.33	108.97
26	P	218	DD6	C28-C27-C26	-2.07	120.17	124.18
20	A	810	CLA	CAA-C2A-C1A	2.07	118.75	111.97
30	P	212	KC1	CBA-CAA-C2A	2.07	133.75	125.45
20	O	207	CLA	CHD-C1D-C2D	2.07	129.78	125.49
26	G	214	DD6	C3-C2-C1	2.06	130.17	127.28
20	Q	212	CLA	CAC-C3C-C4C	2.06	127.47	124.79
20	U	209	CLA	C2A-C1A-CHA	2.06	127.45	123.87
23	R	102	BCR	C16-C15-C14	-2.06	119.30	123.52
20	L	204	CLA	O2D-CGD-CBD	2.06	114.83	111.23
23	F	804	BCR	C11-C10-C9	-2.06	124.39	127.28
20	A	801	CLA	C2A-C1A-CHA	2.06	127.44	123.87
29	I	103	LMG	C1-O6-C5	-2.05	109.71	113.72
23	B	839	BCR	C40-C30-C25	2.05	113.46	110.24
20	H	207	CLA	C5-C3-C2	2.05	125.77	121.17
23	B	839	BCR	C7-C8-C9	-2.05	123.20	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B	842	DGD	CAB-C9B-C8B	-2.05	104.00	114.37
29	Q	217	LMG	C40-C39-C38	-2.05	104.00	114.37
23	A	843	BCR	C7-C8-C9	-2.05	123.20	126.23
20	A	847	CLA	C1D-ND-C4D	2.05	107.75	106.31
23	I	102	BCR	C24-C23-C22	-2.05	123.20	126.23
23	R	102	BCR	C27-C26-C25	2.05	125.47	122.70
20	H	208	CLA	O2D-CGD-CBD	2.05	114.81	111.23
20	S	202	CLA	C4A-NA-C1A	2.05	107.61	106.68
20	B	829	CLA	CHD-C1D-C2D	2.05	129.74	125.49
30	Q	210	KC1	CHC-C4B-NB	-2.05	121.92	124.80
23	A	843	BCR	C15-C16-C17	-2.04	119.34	123.52
26	Q	202	DD6	C26-C25-C24	2.04	129.12	123.20
20	A	814	CLA	CHD-C1D-C2D	2.04	129.73	125.49
20	L	203	CLA	CHD-C1D-C2D	2.04	129.72	125.49
20	B	803	CLA	C4A-NA-C1A	2.03	107.61	106.68
23	A	842	BCR	C28-C27-C26	-2.03	110.43	114.06
20	Q	209	CLA	CHD-C1D-C2D	2.03	129.71	125.49
20	H	206	CLA	CAA-C2A-C3A	2.03	118.49	113.00
20	L	202	CLA	CHD-C1D-C2D	2.03	129.71	125.49
23	L	201	BCR	C33-C5-C6	-2.03	122.27	124.48
20	A	815	CLA	C3B-C4B-NB	-2.03	108.72	110.53
20	B	823	CLA	C2A-C1A-CHA	2.03	127.38	123.87
20	U	207	CLA	C2A-C3A-C4A	-2.03	98.60	101.87
20	F	802	CLA	C1D-ND-C4D	2.03	107.73	106.31
20	B	811	CLA	CHD-C1D-C2D	2.03	129.70	125.49
30	Q	210	KC1	C1B-CHB-C4A	2.02	130.32	126.02
31	P	204	A86	C10-C9-C8	2.02	129.07	123.20
20	B	801	CLA	CHD-C1D-C2D	2.02	129.70	125.49
20	U	207	CLA	C1-O2A-CGA	-2.02	111.75	116.65
20	U	204	CLA	CHD-C1D-C2D	2.02	129.69	125.49
20	B	823	CLA	C4A-NA-C1A	2.02	107.60	106.68
26	S	210	DD6	C33-C32-C31	2.02	113.47	109.49
20	R	104	CLA	O2D-CGD-CBD	2.02	114.76	111.23
30	Q	210	KC1	CHC-C4B-C3B	2.02	128.62	125.21
26	G	213	DD6	C28-C27-C26	-2.02	120.26	124.18
20	G	202	CLA	C1D-ND-C4D	2.02	107.73	106.31
22	P	201	LHG	C18-C17-C16	-2.02	104.17	114.37
20	T	206	CLA	C1D-ND-C4D	2.02	107.73	106.31
26	H	210	DD6	C-C1-C2	-2.02	119.55	122.82
20	O	211	CLA	CAA-C2A-C3A	-2.02	111.61	116.23
20	H	205	CLA	CHD-C1D-ND	-2.02	121.97	124.80
23	B	837	BCR	C16-C15-C14	-2.02	119.40	123.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	F	802	CLA	CAA-C2A-C1A	2.01	118.58	111.97
20	O	206	CLA	C4A-NA-C1A	2.01	107.60	106.68
26	A	855	DD6	C28-C27-C26	-2.01	120.27	124.18
23	B	839	BCR	C15-C16-C17	-2.01	119.40	123.52
23	B	840	BCR	C11-C10-C9	-2.01	124.46	127.28
20	S	215	CLA	C2A-C1A-CHA	2.01	127.36	123.87
20	T	209	CLA	CAA-C2A-C3A	-2.01	111.62	116.23
20	B	846	CLA	CHD-C1D-C2D	2.01	129.67	125.49
20	B	835	CLA	C1D-ND-C4D	2.01	107.72	106.31
30	P	203	KC1	CHB-C4A-NA	2.01	127.35	124.23
20	S	207	CLA	C2A-C1A-CHA	2.01	127.36	123.87
26	S	213	DD6	C29-C30-C31	-2.01	170.80	175.48
20	B	831	CLA	CHD-C1D-C2D	2.01	129.67	125.49
20	S	205	CLA	CHD-C1D-C2D	2.01	129.66	125.49
23	R	102	BCR	C33-C5-C6	-2.01	122.29	124.48
26	U	214	DD6	C28-C27-C26	-2.01	120.28	124.18
20	B	844	CLA	CHD-C1D-ND	-2.01	121.98	124.80
20	B	820	CLA	C1D-ND-C4D	2.00	107.72	106.31
30	P	212	KC1	CHC-C4B-NB	-2.00	121.98	124.80
23	B	837	BCR	C10-C11-C12	-2.00	117.40	123.20
31	P	204	A86	C3-C2-C1	2.00	130.08	127.28

All (122) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
20	A	802	CLA	ND
20	A	803	CLA	ND
20	A	804	CLA	ND
20	A	805	CLA	ND
20	A	806	CLA	ND
20	A	808	CLA	ND
20	A	810	CLA	ND
20	A	811	CLA	ND
20	A	812	CLA	ND
20	A	814	CLA	ND
20	A	815	CLA	ND
20	A	816	CLA	ND
20	A	817	CLA	ND
20	A	818	CLA	ND
20	A	820	CLA	ND
20	A	821	CLA	ND
20	A	822	CLA	ND

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Mol	Chain	Res	Type	Atom
20	A	823	CLA	ND
20	A	824	CLA	ND
20	A	825	CLA	ND
20	A	828	CLA	ND
20	A	829	CLA	ND
20	A	831	CLA	ND
20	A	832	CLA	ND
20	A	833	CLA	ND
20	A	834	CLA	ND
20	A	835	CLA	ND
20	A	836	CLA	ND
20	A	838	CLA	ND
20	A	845	CLA	ND
20	A	849	CLA	ND
20	A	851	CLA	ND
20	A	852	CLA	ND
20	A	853	CLA	ND
20	A	854	CLA	ND
20	B	801	CLA	ND
20	B	802	CLA	ND
20	B	803	CLA	ND
20	B	804	CLA	ND
20	B	805	CLA	ND
20	B	806	CLA	ND
20	B	807	CLA	ND
20	B	808	CLA	ND
20	B	809	CLA	ND
20	B	812	CLA	ND
20	B	815	CLA	ND
20	B	816	CLA	ND
20	B	817	CLA	ND
20	B	820	CLA	ND
20	B	821	CLA	ND
20	B	822	CLA	ND
20	B	823	CLA	ND
20	B	827	CLA	ND
20	B	829	CLA	ND
20	B	830	CLA	ND
20	B	831	CLA	ND
20	B	832	CLA	ND
20	B	833	CLA	ND
20	B	834	CLA	ND

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Mol	Chain	Res	Type	Atom
20	B	835	CLA	ND
20	B	843	CLA	ND
20	B	844	CLA	ND
20	B	845	CLA	ND
20	B	846	CLA	ND
20	B	848	CLA	ND
20	F	802	CLA	ND
20	F	803	CLA	ND
20	J	103	CLA	ND
20	L	202	CLA	ND
20	O	203	CLA	ND
20	O	204	CLA	ND
20	O	205	CLA	ND
20	O	206	CLA	ND
20	O	207	CLA	ND
20	O	208	CLA	ND
20	P	207	CLA	ND
20	P	208	CLA	ND
20	P	209	CLA	ND
20	P	213	CLA	ND
20	P	214	CLA	ND
20	P	216	CLA	ND
20	Q	204	CLA	ND
20	Q	205	CLA	ND
20	Q	206	CLA	ND
20	Q	207	CLA	ND
20	Q	208	CLA	ND
20	Q	211	CLA	ND
20	Q	213	CLA	ND
20	R	101	CLA	ND
20	S	205	CLA	ND
20	S	206	CLA	ND
20	S	207	CLA	ND
20	S	214	CLA	ND
20	S	215	CLA	ND
20	U	204	CLA	ND
20	U	206	CLA	ND
20	U	208	CLA	ND
20	U	209	CLA	ND
20	U	211	CLA	ND
20	G	202	CLA	ND
20	G	203	CLA	ND

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Mol	Chain	Res	Type	Atom
20	G	205	CLA	ND
20	G	206	CLA	ND
20	G	207	CLA	ND
20	G	208	CLA	ND
20	G	210	CLA	ND
20	G	215	CLA	ND
20	H	201	CLA	ND
20	H	202	CLA	ND
20	H	203	CLA	ND
20	H	204	CLA	ND
20	H	205	CLA	ND
20	H	206	CLA	ND
20	H	207	CLA	ND
20	H	208	CLA	ND
20	H	209	CLA	ND
20	T	201	CLA	ND
20	T	202	CLA	ND
20	T	203	CLA	ND
20	T	205	CLA	ND
20	T	206	CLA	ND
20	T	211	CLA	ND

All (1527) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
20	A	806	CLA	CHA-CBD-CGD-O1D
20	A	806	CLA	CHA-CBD-CGD-O2D
20	A	815	CLA	C3A-C2A-CAA-CBA
20	A	826	CLA	CHA-CBD-CGD-O1D
20	A	826	CLA	CHA-CBD-CGD-O2D
20	A	827	CLA	CHA-CBD-CGD-O2D
20	A	829	CLA	CHA-CBD-CGD-O1D
20	A	829	CLA	CHA-CBD-CGD-O2D
20	A	831	CLA	C1A-C2A-CAA-CBA
20	A	835	CLA	C1A-C2A-CAA-CBA
20	A	835	CLA	C3A-C2A-CAA-CBA
20	A	838	CLA	CBD-CGD-O2D-CED
20	A	838	CLA	O1D-CGD-O2D-CED
20	A	851	CLA	CHA-CBD-CGD-O1D
20	A	851	CLA	CHA-CBD-CGD-O2D
20	A	853	CLA	C1A-C2A-CAA-CBA
20	A	854	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
20	A	854	CLA	O1A-CGA-O2A-C1
20	B	804	CLA	CHA-CBD-CGD-O2D
20	B	808	CLA	CHA-CBD-CGD-O1D
20	B	808	CLA	CHA-CBD-CGD-O2D
20	B	813	CLA	C1A-C2A-CAA-CBA
20	B	813	CLA	O2A-C1-C2-C3
20	B	820	CLA	CHA-CBD-CGD-O1D
20	B	820	CLA	CHA-CBD-CGD-O2D
20	B	821	CLA	CHA-CBD-CGD-O1D
20	B	821	CLA	CHA-CBD-CGD-O2D
20	B	824	CLA	CBA-CGA-O2A-C1
20	B	824	CLA	O1A-CGA-O2A-C1
20	B	825	CLA	CHA-CBD-CGD-O1D
20	B	825	CLA	CHA-CBD-CGD-O2D
20	B	828	CLA	C1A-C2A-CAA-CBA
20	B	834	CLA	C4B-C3B-CAB-CBB
20	B	846	CLA	C1A-C2A-CAA-CBA
20	B	848	CLA	C1A-C2A-CAA-CBA
20	B	848	CLA	C3A-C2A-CAA-CBA
20	F	802	CLA	CBA-CGA-O2A-C1
20	F	802	CLA	O1A-CGA-O2A-C1
20	J	103	CLA	CAD-CBD-CGD-O2D
20	L	202	CLA	CBA-CGA-O2A-C1
20	L	202	CLA	O1A-CGA-O2A-C1
20	L	204	CLA	CBD-CGD-O2D-CED
20	L	204	CLA	O1D-CGD-O2D-CED
20	L	204	CLA	O2A-C1-C2-C3
20	O	202	CLA	CHA-CBD-CGD-O2D
20	O	209	CLA	CBD-CGD-O2D-CED
20	O	209	CLA	O1D-CGD-O2D-CED
20	P	208	CLA	C1A-C2A-CAA-CBA
20	P	210	CLA	C1A-C2A-CAA-CBA
20	P	210	CLA	C3A-C2A-CAA-CBA
20	P	211	CLA	CBD-CGD-O2D-CED
20	P	211	CLA	O1D-CGD-O2D-CED
20	P	213	CLA	CBD-CGD-O2D-CED
20	P	213	CLA	O1D-CGD-O2D-CED
20	P	214	CLA	C1A-C2A-CAA-CBA
20	P	214	CLA	C3A-C2A-CAA-CBA
20	Q	205	CLA	C4-C3-C5-C6
20	Q	211	CLA	CBD-CGD-O2D-CED
20	Q	211	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
20	Q	212	CLA	CHA-CBD-CGD-O1D
20	Q	212	CLA	CHA-CBD-CGD-O2D
20	Q	213	CLA	CBA-CGA-O2A-C1
20	Q	213	CLA	O1A-CGA-O2A-C1
20	Q	213	CLA	C2-C3-C5-C6
20	Q	213	CLA	C4-C3-C5-C6
20	R	104	CLA	CBD-CGD-O2D-CED
20	R	104	CLA	O1D-CGD-O2D-CED
20	R	104	CLA	C11-C10-C8-C9
20	S	206	CLA	CBD-CGD-O2D-CED
20	S	206	CLA	O1D-CGD-O2D-CED
20	S	208	CLA	CHA-CBD-CGD-O1D
20	S	208	CLA	CHA-CBD-CGD-O2D
20	U	208	CLA	CBD-CGD-O2D-CED
20	U	208	CLA	O1D-CGD-O2D-CED
20	U	210	CLA	CHA-CBD-CGD-O2D
20	G	203	CLA	C1A-C2A-CAA-CBA
20	G	204	CLA	C3A-C2A-CAA-CBA
20	G	208	CLA	CHA-CBD-CGD-O1D
20	G	208	CLA	CHA-CBD-CGD-O2D
20	H	206	CLA	C3A-C2A-CAA-CBA
20	H	206	CLA	C6-C7-C8-C9
20	H	207	CLA	CAD-CBD-CGD-O1D
20	H	207	CLA	CAD-CBD-CGD-O2D
20	H	208	CLA	CBD-CGD-O2D-CED
20	H	208	CLA	O1D-CGD-O2D-CED
20	T	204	CLA	C1A-C2A-CAA-CBA
20	T	205	CLA	CBD-CGD-O2D-CED
20	T	205	CLA	O1D-CGD-O2D-CED
20	T	207	CLA	CBD-CGD-O2D-CED
20	T	207	CLA	O1D-CGD-O2D-CED
20	T	211	CLA	C1A-C2A-CAA-CBA
22	A	839	LHG	C3-O3-P-O4
22	A	839	LHG	C3-O3-P-O6
22	P	201	LHG	C3-O3-P-O5
22	P	201	LHG	C4-O6-P-O3
22	P	201	LHG	O6-C4-C5-O7
22	G	216	LHG	O1-C1-C2-C3
22	G	216	LHG	C3-O3-P-O4
22	G	216	LHG	C3-O3-P-O6
22	G	216	LHG	C4-O6-P-O3
22	G	216	LHG	C4-O6-P-O4

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Mol	Chain	Res	Type	Atoms
23	A	841	BCR	C20-C21-C22-C23
23	A	841	BCR	C21-C22-C23-C24
23	A	841	BCR	C37-C22-C23-C24
23	A	842	BCR	C7-C8-C9-C10
23	A	842	BCR	C7-C8-C9-C34
23	A	842	BCR	C20-C21-C22-C37
23	A	842	BCR	C21-C22-C23-C24
23	A	843	BCR	C7-C8-C9-C10
23	A	844	BCR	C21-C22-C23-C24
23	F	801	BCR	C7-C8-C9-C10
23	F	801	BCR	C7-C8-C9-C34
23	F	801	BCR	C37-C22-C23-C24
23	F	804	BCR	C21-C22-C23-C24
23	F	804	BCR	C37-C22-C23-C24
23	I	101	BCR	C37-C22-C23-C24
23	I	102	BCR	C7-C8-C9-C10
23	I	102	BCR	C7-C8-C9-C34
23	I	102	BCR	C23-C24-C25-C26
23	J	104	BCR	C7-C8-C9-C10
23	J	104	BCR	C7-C8-C9-C34
23	J	104	BCR	C16-C17-C18-C19
23	J	104	BCR	C16-C17-C18-C36
23	J	104	BCR	C21-C22-C23-C24
23	J	104	BCR	C37-C22-C23-C24
23	L	201	BCR	C11-C10-C9-C8
23	L	201	BCR	C11-C10-C9-C34
23	L	201	BCR	C20-C21-C22-C23
23	L	201	BCR	C20-C21-C22-C37
23	L	201	BCR	C21-C22-C23-C24
23	M	101	BCR	C7-C8-C9-C10
23	M	101	BCR	C7-C8-C9-C34
23	R	102	BCR	C22-C23-C24-C25
26	A	855	DD6	C2-C1-C24-C25
26	A	855	DD6	C9-C10-C11-C12
26	A	855	DD6	C10-C11-C13-C14
26	A	855	DD6	C12-C11-C13-C14
26	A	855	DD6	C24-C25-C26-C27
26	A	855	DD6	C5-C6-C8-C9
26	O	201	DD6	C10-C11-C13-C14
26	O	201	DD6	C12-C11-C13-C14
26	O	201	DD6	C3-C4-C5-C6
26	O	212	DD6	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
26	O	212	DD6	C4-C5-C6-C7
26	O	212	DD6	C4-C5-C6-C8
26	O	213	DD6	C9-C10-C11-C12
26	O	213	DD6	C9-C10-C11-C13
26	O	213	DD6	C10-C11-C13-C14
26	O	213	DD6	C12-C11-C13-C14
26	O	214	DD6	C10-C11-C13-C14
26	O	214	DD6	C12-C11-C13-C14
26	O	214	DD6	C11-C13-C14-C15
26	O	214	DD6	C4-C5-C6-C7
26	O	214	DD6	C4-C5-C6-C8
26	O	215	DD6	C-C1-C24-C25
26	O	215	DD6	C2-C1-C24-C25
26	O	215	DD6	C9-C10-C11-C12
26	O	215	DD6	C9-C10-C11-C13
26	O	215	DD6	C11-C13-C14-C15
26	O	215	DD6	C1-C2-C3-C4
26	O	215	DD6	C4-C5-C6-C7
26	O	215	DD6	C4-C5-C6-C8
26	O	215	DD6	C5-C6-C8-C9
26	P	205	DD6	C10-C11-C13-C14
26	P	205	DD6	C13-C14-C15-O1
26	P	215	DD6	C-C1-C24-C25
26	P	218	DD6	C9-C10-C11-C12
26	P	218	DD6	C9-C10-C11-C13
26	P	218	DD6	C11-C13-C14-C15
26	P	218	DD6	C13-C14-C15-O1
26	P	218	DD6	C2-C3-C4-C5
26	P	218	DD6	C4-C5-C6-C7
26	P	218	DD6	C4-C5-C6-C8
26	P	220	DD6	C-C1-C24-C25
26	P	220	DD6	C2-C1-C24-C25
26	P	220	DD6	C11-C13-C14-C15
26	P	220	DD6	C1-C2-C3-C4
26	P	220	DD6	C1-C24-C25-C26
26	P	220	DD6	C2-C3-C4-C5
26	Q	202	DD6	C10-C11-C13-C14
26	Q	215	DD6	C-C1-C24-C25
26	Q	215	DD6	C2-C1-C24-C25
26	Q	215	DD6	C9-C10-C11-C12
26	Q	215	DD6	C9-C10-C11-C13
26	Q	215	DD6	C10-C11-C13-C14

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Mol	Chain	Res	Type	Atoms
26	Q	215	DD6	C12-C11-C13-C14
26	Q	215	DD6	C11-C13-C14-C15
26	S	203	DD6	C11-C13-C14-C15
26	S	203	DD6	C2-C3-C4-C5
26	S	203	DD6	C4-C5-C6-C7
26	S	203	DD6	C4-C5-C6-C8
26	S	204	DD6	C-C1-C24-C25
26	S	204	DD6	C2-C1-C24-C25
26	S	204	DD6	C2-C3-C4-C5
26	S	204	DD6	C4-C5-C6-C7
26	S	204	DD6	C4-C5-C6-C8
26	S	204	DD6	C5-C6-C8-C9
26	S	204	DD6	C7-C6-C8-C9
26	S	210	DD6	C11-C13-C14-C15
26	S	210	DD6	C13-C14-C15-O1
26	S	212	DD6	C-C1-C24-C25
26	S	212	DD6	C2-C1-C24-C25
26	S	212	DD6	C9-C10-C11-C12
26	S	212	DD6	C9-C10-C11-C13
26	S	212	DD6	C11-C13-C14-C15
26	S	212	DD6	C24-C25-C26-C27
26	S	213	DD6	C2-C1-C24-C25
26	S	213	DD6	C11-C13-C14-C15
26	S	213	DD6	C1-C2-C3-C4
26	S	213	DD6	C2-C3-C4-C5
26	S	213	DD6	C4-C5-C6-C7
26	S	213	DD6	C4-C5-C6-C8
26	S	213	DD6	C5-C6-C8-C9
26	U	203	DD6	C1-C24-C25-C26
26	U	203	DD6	C25-C26-C27-C29
26	U	203	DD6	C2-C3-C4-C5
26	U	203	DD6	C5-C6-C8-C9
26	U	203	DD6	C7-C6-C8-C9
26	U	212	DD6	C9-C10-C11-C12
26	U	212	DD6	C9-C10-C11-C13
26	U	212	DD6	C11-C13-C14-C15
26	U	212	DD6	C4-C5-C6-C7
26	U	212	DD6	C4-C5-C6-C8
26	U	214	DD6	C-C1-C24-C25
26	U	214	DD6	C2-C1-C24-C25
26	U	214	DD6	C2-C3-C4-C5
26	U	214	DD6	C3-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
26	U	214	DD6	C4-C5-C6-C7
26	G	211	DD6	C9-C10-C11-C12
26	G	211	DD6	C9-C10-C11-C13
26	G	211	DD6	C11-C13-C14-C15
26	G	212	DD6	C9-C10-C11-C12
26	G	212	DD6	C9-C10-C11-C13
26	G	212	DD6	C10-C11-C13-C14
26	G	212	DD6	C4-C5-C6-C7
26	G	212	DD6	C4-C5-C6-C8
26	G	213	DD6	C5-C6-C8-C9
26	G	213	DD6	C7-C6-C8-C9
26	G	214	DD6	C-C1-C24-C25
26	G	214	DD6	C2-C1-C24-C25
26	G	214	DD6	C1-C24-C25-C26
26	G	214	DD6	C2-C3-C4-C5
26	G	214	DD6	C4-C5-C6-C7
26	G	214	DD6	C4-C5-C6-C8
26	G	217	DD6	C9-C10-C11-C12
26	G	217	DD6	C9-C10-C11-C13
26	G	217	DD6	C10-C11-C13-C14
26	G	217	DD6	C5-C6-C8-C9
26	H	210	DD6	C9-C10-C11-C12
26	H	210	DD6	C9-C10-C11-C13
26	H	210	DD6	C11-C13-C14-C15
26	H	210	DD6	C1-C2-C3-C4
26	H	210	DD6	C2-C3-C4-C5
26	H	211	DD6	C9-C10-C11-C12
26	H	211	DD6	C9-C10-C11-C13
26	H	211	DD6	C11-C13-C14-C15
26	H	211	DD6	C4-C5-C6-C7
26	H	211	DD6	C4-C5-C6-C8
26	T	212	DD6	C2-C1-C24-C25
26	T	212	DD6	C9-C10-C11-C12
26	T	212	DD6	C9-C10-C11-C13
26	T	212	DD6	C3-C4-C5-C6
26	T	212	DD6	C4-C5-C6-C7
26	T	212	DD6	C4-C5-C6-C8
26	T	213	DD6	C-C1-C24-C25
26	T	213	DD6	C2-C1-C24-C25
26	T	213	DD6	C9-C10-C11-C12
26	T	213	DD6	C9-C10-C11-C13
26	T	213	DD6	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
26	T	213	DD6	C10-C11-C13-C14
26	T	213	DD6	C12-C11-C13-C14
26	T	213	DD6	C11-C13-C14-C15
26	T	213	DD6	C1-C24-C25-C26
26	T	213	DD6	C25-C26-C27-C28
26	T	213	DD6	C25-C26-C27-C29
26	T	213	DD6	C6-C8-C9-C10
28	S	201	SQD	O5-C1-O6-C44
28	S	201	SQD	O5-C5-C6-S
29	U	201	LMG	C11-C10-O7-C8
30	P	206	KC1	C2A-CAA-CBA-CGA
30	P	212	KC1	CAD-CBD-CGD-O2D
30	P	219	KC1	C3A-C2A-CAA-CBA
30	Q	210	KC1	C2A-CAA-CBA-CGA
30	S	211	KC1	C3A-C2A-CAA-CBA
31	P	204	A86	C-C1-C2-C3
31	P	204	A86	C24-C1-C2-C3
31	P	204	A86	C2-C3-C4-C5
31	P	204	A86	C4-C5-C6-C7
31	P	204	A86	C4-C5-C6-C8
31	P	204	A86	C5-C6-C8-C9
31	P	204	A86	C7-C6-C8-C9
31	Q	201	A86	C9-C10-C11-C12
31	Q	201	A86	C10-C11-C13-O
31	Q	201	A86	C12-C11-C13-O
31	Q	201	A86	O-C13-C14-C15
31	Q	201	A86	C5-C6-C8-C9
31	Q	201	A86	C6-C8-C9-C10
31	Q	214	A86	C2-C1-C24-C25
31	Q	214	A86	C39-C38-O4-C34
31	Q	214	A86	O5-C38-O4-C34
31	Q	214	A86	C6-C8-C9-C10
31	Q	218	A86	C12-C11-C13-C14
31	Q	218	A86	O-C13-C14-C15
31	Q	218	A86	C1-C2-C3-C4
31	Q	218	A86	C1-C24-C25-C26
31	Q	218	A86	C39-C38-O4-C34
31	Q	218	A86	C6-C8-C9-C10
31	R	103	A86	C5-C6-C8-C9
31	R	103	A86	C7-C6-C8-C9
31	R	105	A86	C9-C10-C11-C12
31	R	105	A86	C9-C10-C11-C13

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Mol	Chain	Res	Type	Atoms
31	R	105	A86	C2-C3-C4-C5
31	R	105	A86	C39-C38-O4-C34
31	R	105	A86	O5-C38-O4-C34
31	R	105	A86	C4-C5-C6-C7
31	R	105	A86	C4-C5-C6-C8
31	R	105	A86	C6-C8-C9-C10
31	U	202	A86	C10-C11-C13-O
31	U	202	A86	C12-C11-C13-O
31	U	202	A86	C1-C24-C25-C26
31	U	202	A86	C2-C3-C4-C5
31	U	202	A86	C39-C38-O4-C34
31	U	202	A86	C4-C5-C6-C7
31	U	202	A86	C4-C5-C6-C8
31	U	202	A86	C6-C8-C9-C10
31	P	204	A86	C39-C38-O4-C34
31	Q	201	A86	C39-C38-O4-C34
31	Q	218	A86	O5-C38-O4-C34
31	U	202	A86	O5-C38-O4-C34
20	B	834	CLA	CBD-CGD-O2D-CED
20	Q	203	CLA	O1A-CGA-O2A-C1
31	P	204	A86	C35-C34-O4-C38
20	Q	203	CLA	CBA-CGA-O2A-C1
20	Q	207	CLA	O1A-CGA-O2A-C1
20	T	205	CLA	O1A-CGA-O2A-C1
20	T	210	CLA	O1A-CGA-O2A-C1
29	U	201	LMG	O9-C10-O7-C8
20	Q	207	CLA	CBA-CGA-O2A-C1
20	T	205	CLA	CBA-CGA-O2A-C1
20	T	210	CLA	CBA-CGA-O2A-C1
20	B	806	CLA	C3-C5-C6-C7
20	B	815	CLA	C3-C5-C6-C7
20	O	208	CLA	C3-C5-C6-C7
20	G	209	CLA	C3-C5-C6-C7
20	T	207	CLA	C3-C5-C6-C7
22	A	839	LHG	C24-C23-O8-C6
31	P	204	A86	O5-C38-O4-C34
30	T	208	KC1	CBD-CGD-O2D-CED
20	G	205	CLA	C2C-C3C-CAC-CBC
20	A	824	CLA	C4-C3-C5-C6
20	B	815	CLA	C4-C3-C5-C6
20	B	834	CLA	C4-C3-C5-C6
20	O	209	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
20	P	207	CLA	C4-C3-C5-C6
20	P	208	CLA	C4-C3-C5-C6
20	Q	209	CLA	C4-C3-C5-C6
20	H	203	CLA	C4-C3-C5-C6
20	B	834	CLA	C2-C3-C5-C6
20	O	209	CLA	C2-C3-C5-C6
20	P	207	CLA	C2-C3-C5-C6
20	P	208	CLA	C2-C3-C5-C6
20	Q	205	CLA	C2-C3-C5-C6
20	H	203	CLA	C2-C3-C5-C6
20	B	834	CLA	O1D-CGD-O2D-CED
20	A	825	CLA	C2A-CAA-CBA-CGA
20	A	807	CLA	C3-C5-C6-C7
20	B	834	CLA	C3-C5-C6-C7
20	U	210	CLA	C3-C5-C6-C7
26	O	201	DD6	C1-C2-C3-C4
26	O	215	DD6	C24-C25-C26-C27
26	P	218	DD6	C1-C2-C3-C4
26	P	218	DD6	C3-C4-C5-C6
26	Q	215	DD6	C24-C25-C26-C27
26	S	204	DD6	C24-C25-C26-C27
26	S	212	DD6	C11-C10-C9-C8
26	S	212	DD6	C1-C2-C3-C4
26	U	203	DD6	C24-C25-C26-C27
26	U	203	DD6	C3-C4-C5-C6
26	U	212	DD6	C11-C10-C9-C8
31	P	204	A86	C11-C10-C9-C8
31	R	103	A86	C11-C10-C9-C8
22	A	839	LHG	O10-C23-O8-C6
20	A	845	CLA	C3-C5-C6-C7
20	B	813	CLA	C3-C5-C6-C7
20	S	215	CLA	C3-C5-C6-C7
20	G	208	CLA	C3-C5-C6-C7
29	P	217	LMG	O6-C5-C6-O5
31	Q	201	A86	O5-C38-O4-C34
26	O	214	DD6	C2-C3-C4-C5
20	B	825	CLA	C3-C5-C6-C7
29	J	102	LMG	O6-C5-C6-O5
22	P	201	LHG	C11-C12-C13-C14
20	A	847	CLA	C4-C3-C5-C6
20	A	847	CLA	C2-C3-C5-C6
20	Q	209	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
20	G	207	CLA	C2-C3-C5-C6
29	P	217	LMG	C4-C5-C6-O5
29	Q	217	LMG	O6-C1-O1-C7
27	B	842	DGD	O6E-C5E-C6E-O5E
26	P	220	DD6	C24-C25-C26-C27
26	S	213	DD6	C24-C25-C26-C27
26	U	203	DD6	C1-C2-C3-C4
26	U	214	DD6	C24-C25-C26-C27
26	G	217	DD6	C24-C25-C26-C27
26	H	210	DD6	C24-C25-C26-C27
26	T	212	DD6	C24-C25-C26-C27
26	T	213	DD6	C3-C4-C5-C6
22	A	840	LHG	O9-C7-O7-C5
22	G	216	LHG	C1-C2-C3-O3
29	U	201	LMG	C29-C28-O8-C9
27	B	842	DGD	C4E-C5E-C6E-O5E
20	B	814	CLA	C4-C3-C5-C6
20	G	205	CLA	C4-C3-C5-C6
20	G	207	CLA	C4-C3-C5-C6
20	B	814	CLA	C2-C3-C5-C6
20	B	825	CLA	C2-C3-C5-C6
20	A	811	CLA	C11-C12-C13-C14
20	B	813	CLA	C6-C7-C8-C9
20	B	821	CLA	C11-C12-C13-C14
20	B	825	CLA	C6-C7-C8-C9
20	U	207	CLA	C11-C10-C8-C9
20	U	207	CLA	C11-C12-C13-C14
29	Q	217	LMG	C2-C1-O1-C7
23	A	843	BCR	C7-C8-C9-C34
23	A	844	BCR	C7-C8-C9-C34
23	B	838	BCR	C37-C22-C23-C24
23	I	101	BCR	C7-C8-C9-C34
23	J	104	BCR	C11-C12-C13-C35
23	M	101	BCR	C37-C22-C23-C24
23	R	102	BCR	C7-C8-C9-C34
26	A	855	DD6	C-C1-C24-C25
26	A	855	DD6	C7-C6-C8-C9
26	J	101	DD6	C12-C11-C13-C14
26	O	215	DD6	C7-C6-C8-C9
26	S	210	DD6	C12-C11-C13-C14
26	S	212	DD6	C12-C11-C13-C14
26	S	213	DD6	C-C1-C24-C25

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Mol	Chain	Res	Type	Atoms
26	S	213	DD6	C7-C6-C8-C9
26	G	212	DD6	C12-C11-C13-C14
26	G	212	DD6	C7-C6-C8-C9
26	G	217	DD6	C-C1-C24-C25
26	G	217	DD6	C12-C11-C13-C14
26	G	217	DD6	C7-C6-C8-C9
26	H	210	DD6	C-C1-C24-C25
26	H	210	DD6	C12-C11-C13-C14
26	H	211	DD6	C7-C6-C8-C9
26	T	212	DD6	C-C1-C24-C25
31	Q	201	A86	C7-C6-C8-C9
31	Q	214	A86	C-C1-C24-C25
31	Q	218	A86	C-C1-C24-C25
23	B	838	BCR	C21-C22-C23-C24
23	I	102	BCR	C21-C22-C23-C24
23	R	102	BCR	C7-C8-C9-C10
26	J	101	DD6	C10-C11-C13-C14
26	O	215	DD6	C10-C11-C13-C14
26	P	215	DD6	C2-C1-C24-C25
26	S	210	DD6	C10-C11-C13-C14
26	S	212	DD6	C10-C11-C13-C14
26	U	212	DD6	C10-C11-C13-C14
26	G	212	DD6	C5-C6-C8-C9
26	G	217	DD6	C2-C1-C24-C25
26	H	210	DD6	C10-C11-C13-C14
31	Q	218	A86	C2-C1-C24-C25
20	T	205	CLA	C2A-CAA-CBA-CGA
29	I	103	LMG	C17-C18-C19-C20
20	B	834	CLA	C10-C11-C12-C13
29	Q	217	LMG	O6-C5-C6-O5
22	G	216	LHG	O1-C1-C2-O2
20	A	823	CLA	C12-C13-C15-C16
20	S	202	CLA	C11-C12-C13-C15
20	S	214	CLA	C12-C13-C15-C16
20	B	834	CLA	CBA-CGA-O2A-C1
22	A	840	LHG	C7-C8-C9-C10
28	B	847	SQD	C7-C8-C9-C10
26	S	212	DD6	C3-C4-C5-C6
26	S	213	DD6	C3-C4-C5-C6
26	U	203	DD6	C11-C10-C9-C8
26	G	211	DD6	C24-C25-C26-C27
26	G	213	DD6	C24-C25-C26-C27

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Mol	Chain	Res	Type	Atoms
26	H	210	DD6	C3-C4-C5-C6
31	Q	201	A86	C11-C10-C9-C8
20	B	816	CLA	C10-C11-C12-C13
20	B	831	CLA	C13-C15-C16-C17
20	R	104	CLA	C13-C15-C16-C17
22	G	216	LHG	C23-C24-C25-C26
29	P	202	LMG	C10-C11-C12-C13
20	A	854	CLA	C5-C6-C7-C8
20	Q	216	CLA	C5-C6-C7-C8
20	A	807	CLA	C2A-CAA-CBA-CGA
26	G	211	DD6	C1-C24-C25-C26
26	G	212	DD6	C1-C24-C25-C26
20	A	815	CLA	C8-C10-C11-C12
20	A	829	CLA	C15-C16-C17-C18
20	B	805	CLA	C10-C11-C12-C13
20	Q	209	CLA	C13-C15-C16-C17
20	S	214	CLA	C15-C16-C17-C18
20	H	206	CLA	C5-C6-C7-C8
22	A	839	LHG	C7-C8-C9-C10
29	I	103	LMG	C28-C29-C30-C31
20	A	801	CLA	C10-C11-C12-C13
20	A	804	CLA	C8-C10-C11-C12
20	A	809	CLA	C8-C10-C11-C12
20	A	833	CLA	C15-C16-C17-C18
20	B	815	CLA	C8-C10-C11-C12
20	B	816	CLA	C8-C10-C11-C12
20	B	825	CLA	C10-C11-C12-C13
20	P	207	CLA	C13-C15-C16-C17
20	U	207	CLA	C5-C6-C7-C8
20	H	206	CLA	C10-C11-C12-C13
20	B	803	CLA	C15-C16-C17-C18
20	S	202	CLA	C5-C6-C7-C8
20	T	204	CLA	C5-C6-C7-C8
20	G	205	CLA	C4C-C3C-CAC-CBC
29	J	102	LMG	C4-C5-C6-O5
20	A	822	CLA	C13-C15-C16-C17
20	B	817	CLA	C13-C15-C16-C17
20	G	206	CLA	C13-C15-C16-C17
20	A	824	CLA	C13-C15-C16-C17
26	O	201	DD6	C24-C25-C26-C27
26	O	215	DD6	C3-C4-C5-C6
26	U	214	DD6	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
26	T	213	DD6	C1-C2-C3-C4
26	T	213	DD6	C24-C25-C26-C27
31	Q	218	A86	C3-C4-C5-C6
20	A	825	CLA	C13-C15-C16-C17
20	B	834	CLA	C13-C15-C16-C17
20	A	831	CLA	C2A-CAA-CBA-CGA
20	A	854	CLA	C2A-CAA-CBA-CGA
22	G	216	LHG	C24-C23-O8-C6
20	A	833	CLA	C8-C10-C11-C12
20	U	205	CLA	C13-C15-C16-C17
20	U	210	CLA	C5-C6-C7-C8
31	Q	218	A86	C9-C10-C11-C12
31	U	202	A86	C9-C10-C11-C12
20	A	815	CLA	C13-C15-C16-C17
20	A	828	CLA	C13-C15-C16-C17
20	B	806	CLA	C10-C11-C12-C13
20	B	830	CLA	C5-C6-C7-C8
20	H	206	CLA	C8-C10-C11-C12
20	H	206	CLA	C13-C15-C16-C17
20	A	845	CLA	C4-C3-C5-C6
20	B	834	CLA	O1A-CGA-O2A-C1
22	A	839	LHG	O9-C7-O7-C5
22	G	216	LHG	O2-C2-C3-O3
23	A	841	BCR	C20-C21-C22-C37
23	B	841	BCR	C11-C10-C9-C34
23	R	102	BCR	C20-C21-C22-C37
26	J	101	DD6	C4-C5-C6-C7
26	P	220	DD6	C4-C5-C6-C7
26	Q	215	DD6	C4-C5-C6-C7
26	S	204	DD6	C9-C10-C11-C12
26	G	213	DD6	C9-C10-C11-C12
26	G	213	DD6	C4-C5-C6-C7
26	G	217	DD6	C4-C5-C6-C7
26	T	213	DD6	C4-C5-C6-C7
31	Q	214	A86	C4-C5-C6-C7
31	R	105	A86	C-C1-C2-C3
20	G	205	CLA	C10-C11-C12-C13
23	A	844	BCR	C37-C22-C23-C24
23	B	837	BCR	C7-C8-C9-C34
23	I	102	BCR	C37-C22-C23-C24
23	L	205	BCR	C7-C8-C9-C34
26	O	215	DD6	C12-C11-C13-C14

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Mol	Chain	Res	Type	Atoms
26	Q	202	DD6	C12-C11-C13-C14
26	S	204	DD6	C12-C11-C13-C14
26	S	213	DD6	C12-C11-C13-C14
26	U	212	DD6	C12-C11-C13-C14
26	H	211	DD6	C12-C11-C13-C14
26	T	212	DD6	C7-C6-C8-C9
26	T	213	DD6	C7-C6-C8-C9
31	Q	214	A86	C7-C6-C8-C9
31	Q	218	A86	C7-C6-C8-C9
31	U	202	A86	C-C1-C24-C25
23	B	837	BCR	C7-C8-C9-C10
23	B	838	BCR	C7-C8-C9-C10
23	F	801	BCR	C21-C22-C23-C24
23	L	205	BCR	C7-C8-C9-C10
26	S	204	DD6	C10-C11-C13-C14
26	S	213	DD6	C10-C11-C13-C14
26	T	212	DD6	C5-C6-C8-C9
26	T	213	DD6	C5-C6-C8-C9
20	A	806	CLA	C2A-CAA-CBA-CGA
20	A	827	CLA	C2A-CAA-CBA-CGA
20	A	845	CLA	C2A-CAA-CBA-CGA
20	B	833	CLA	C2A-CAA-CBA-CGA
20	G	209	CLA	C5-C6-C7-C8
20	T	207	CLA	C8-C10-C11-C12
31	R	105	A86	C11-C10-C9-C8
21	B	836	PQN	C26-C27-C28-C30
20	B	808	CLA	C3-C5-C6-C7
20	B	820	CLA	C3-C5-C6-C7
20	H	207	CLA	C3-C5-C6-C7
23	A	842	BCR	C20-C21-C22-C23
23	A	844	BCR	C20-C21-C22-C23
23	B	837	BCR	C11-C10-C9-C8
23	B	839	BCR	C20-C21-C22-C23
23	I	101	BCR	C20-C21-C22-C23
26	A	855	DD6	C9-C10-C11-C13
26	J	101	DD6	C4-C5-C6-C8
26	P	220	DD6	C4-C5-C6-C8
26	Q	215	DD6	C4-C5-C6-C8
26	S	204	DD6	C9-C10-C11-C13
26	S	213	DD6	C9-C10-C11-C13
26	G	213	DD6	C9-C10-C11-C13
26	G	213	DD6	C4-C5-C6-C8

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Mol	Chain	Res	Type	Atoms
26	G	217	DD6	C4-C5-C6-C8
26	T	213	DD6	C4-C5-C6-C8
31	Q	214	A86	C4-C5-C6-C8
31	Q	218	A86	C24-C1-C2-C3
31	R	105	A86	C24-C1-C2-C3
22	A	840	LHG	C8-C7-O7-C5
20	B	815	CLA	C2-C3-C5-C6
31	P	204	A86	C9-C10-C11-C13
31	Q	214	A86	C9-C10-C11-C13
31	Q	218	A86	C9-C10-C11-C13
31	R	103	A86	C9-C10-C11-C13
31	U	202	A86	C9-C10-C11-C13
20	H	206	CLA	C16-C17-C18-C19
26	A	855	DD6	C2-C3-C4-C5
26	G	212	DD6	C2-C3-C4-C5
26	T	212	DD6	C2-C3-C4-C5
31	Q	214	A86	C2-C3-C4-C5
29	J	102	LMG	C15-C16-C17-C18
29	Q	217	LMG	C32-C33-C34-C35
29	I	103	LMG	C38-C39-C40-C41
29	Q	217	LMG	C23-C24-C25-C26
26	U	212	DD6	C27-C29-C30-C31
31	Q	201	A86	C35-C34-O4-C38
20	B	810	CLA	C6-C7-C8-C9
20	S	214	CLA	C16-C17-C18-C19
20	B	820	CLA	C2A-CAA-CBA-CGA
20	B	827	CLA	C2A-CAA-CBA-CGA
20	H	209	CLA	C2A-CAA-CBA-CGA
20	B	813	CLA	C8-C10-C11-C12
20	R	104	CLA	C8-C10-C11-C12
20	G	206	CLA	C10-C11-C12-C13
20	A	824	CLA	C6-C7-C8-C10
20	B	806	CLA	C11-C10-C8-C7
20	A	823	CLA	C13-C15-C16-C17
20	B	809	CLA	C15-C16-C17-C18
20	B	843	CLA	C10-C11-C12-C13
20	H	203	CLA	C5-C6-C7-C8
28	B	847	SQD	C13-C14-C15-C16
20	A	804	CLA	C3A-C2A-CAA-CBA
20	A	853	CLA	C3A-C2A-CAA-CBA
20	B	828	CLA	C3A-C2A-CAA-CBA
20	B	846	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
20	F	803	CLA	C3A-C2A-CAA-CBA
20	P	208	CLA	C3A-C2A-CAA-CBA
20	Q	203	CLA	C3A-C2A-CAA-CBA
20	Q	207	CLA	C3A-C2A-CAA-CBA
20	G	203	CLA	C3A-C2A-CAA-CBA
20	G	206	CLA	C3A-C2A-CAA-CBA
20	T	203	CLA	C3A-C2A-CAA-CBA
20	T	204	CLA	C3A-C2A-CAA-CBA
20	T	211	CLA	C3A-C2A-CAA-CBA
22	P	201	LHG	C33-C34-C35-C36
20	A	845	CLA	C2-C3-C5-C6
20	G	205	CLA	C2-C3-C5-C6
27	B	842	DGD	C2G-C1G-O1G-C1A
22	G	216	LHG	C7-C8-C9-C10
26	J	101	DD6	C3-C4-C5-C6
31	R	105	A86	C3-C4-C5-C6
20	B	810	CLA	C6-C7-C8-C10
28	S	201	SQD	C12-C13-C14-C15
22	P	201	LHG	C28-C29-C30-C31
22	P	201	LHG	C23-C24-C25-C26
28	S	201	SQD	C7-C8-C9-C10
22	A	839	LHG	C29-C30-C31-C32
29	J	102	LMG	C19-C20-C21-C22
22	A	839	LHG	C9-C10-C11-C12
20	H	206	CLA	C16-C17-C18-C20
22	G	216	LHG	O10-C23-O8-C6
20	B	834	CLA	C2B-C3B-CAB-CBB
23	A	844	BCR	C23-C24-C25-C30
23	B	838	BCR	C1-C6-C7-C8
23	B	838	BCR	C5-C6-C7-C8
23	I	102	BCR	C23-C24-C25-C30
29	U	201	LMG	C29-C30-C31-C32
29	I	103	LMG	C32-C33-C34-C35
20	B	813	CLA	C2A-CAA-CBA-CGA
22	A	839	LHG	C24-C25-C26-C27
22	G	216	LHG	O9-C7-O7-C5
29	J	102	LMG	C11-C12-C13-C14
23	L	201	BCR	C10-C11-C12-C13
26	S	213	DD6	C1-C24-C25-C26
26	G	213	DD6	C1-C24-C25-C26
31	R	103	A86	C1-C24-C25-C26
20	A	824	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
20	A	852	CLA	C2-C3-C5-C6
20	H	206	CLA	C2-C3-C5-C6
20	B	817	CLA	C3-C5-C6-C7
27	B	842	DGD	C4A-C5A-C6A-C7A
29	P	202	LMG	C31-C32-C33-C34
29	Q	217	LMG	C14-C15-C16-C17
26	H	211	DD6	C2-C3-C4-C5
20	Q	205	CLA	C8-C10-C11-C12
21	A	837	PQN	C23-C25-C26-C27
28	B	847	SQD	C28-C29-C30-C31
29	I	103	LMG	C39-C40-C41-C42
26	G	212	DD6	C24-C25-C26-C27
20	A	854	CLA	C16-C17-C18-C20
21	B	836	PQN	C26-C27-C28-C29
22	A	839	LHG	C8-C7-O7-C5
22	G	216	LHG	C8-C7-O7-C5
28	S	201	SQD	C8-C7-O47-C45
29	P	217	LMG	C29-C28-O8-C9
20	O	205	CLA	C8-C10-C11-C12
22	P	201	LHG	C32-C33-C34-C35
27	B	842	DGD	C9B-CAB-CBB-CCB
26	P	205	DD6	C12-C11-C13-C14
26	P	218	DD6	C12-C11-C13-C14
26	U	203	DD6	C-C1-C24-C25
26	T	212	DD6	C12-C11-C13-C14
27	B	842	DGD	C3B-C4B-C5B-C6B
22	P	201	LHG	C7-C8-C9-C10
26	H	210	DD6	C2-C1-C24-C25
26	H	211	DD6	C5-C6-C8-C9
30	S	211	KC1	CAA-CBA-CGA-O2A
20	B	825	CLA	C4-C3-C5-C6
20	B	845	CLA	C15-C16-C17-C18
22	P	201	LHG	C11-C10-C9-C8
29	Q	217	LMG	C15-C16-C17-C18
20	A	834	CLA	C3-C5-C6-C7
20	B	809	CLA	C13-C15-C16-C17
20	F	802	CLA	O2A-C1-C2-C3
22	P	201	LHG	C34-C35-C36-C37
20	B	805	CLA	C15-C16-C17-C18
21	A	837	PQN	C20-C21-C22-C23
30	P	203	KC1	C4B-C3B-CAB-CBB
30	P	219	KC1	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
30	Q	210	KC1	C4B-C3B-CAB-CBB
30	S	211	KC1	C2A-CAA-CBA-CGA
30	U	213	KC1	C4B-C3B-CAB-CBB
30	T	208	KC1	C4B-C3B-CAB-CBB
20	B	834	CLA	C16-C17-C18-C19
20	Q	212	CLA	C3-C5-C6-C7
22	A	839	LHG	C11-C10-C9-C8
29	I	103	LMG	O6-C5-C6-O5
29	I	103	LMG	C31-C32-C33-C34
20	A	823	CLA	C4-C3-C5-C6
20	A	814	CLA	C2A-CAA-CBA-CGA
20	A	815	CLA	C2A-CAA-CBA-CGA
20	B	848	CLA	C2A-CAA-CBA-CGA
29	P	202	LMG	C30-C31-C32-C33
20	A	854	CLA	C10-C11-C12-C13
26	U	203	DD6	C25-C26-C27-C28
29	J	102	LMG	C18-C19-C20-C21
27	B	842	DGD	O1A-C1A-O1G-C1G
20	A	804	CLA	C1A-C2A-CAA-CBA
20	A	815	CLA	C1A-C2A-CAA-CBA
20	B	805	CLA	C1A-C2A-CAA-CBA
20	B	812	CLA	C1A-C2A-CAA-CBA
20	B	823	CLA	C1A-C2A-CAA-CBA
20	F	803	CLA	C1A-C2A-CAA-CBA
20	Q	207	CLA	C1A-C2A-CAA-CBA
20	Q	208	CLA	C1A-C2A-CAA-CBA
20	S	215	CLA	C1A-C2A-CAA-CBA
20	G	204	CLA	C1A-C2A-CAA-CBA
20	G	206	CLA	C1A-C2A-CAA-CBA
20	H	206	CLA	C1A-C2A-CAA-CBA
20	T	203	CLA	C1A-C2A-CAA-CBA
20	G	205	CLA	C5-C6-C7-C8
20	B	817	CLA	C15-C16-C17-C18
20	G	206	CLA	C15-C16-C17-C18
31	P	204	A86	C9-C10-C11-C12
31	R	103	A86	C9-C10-C11-C12
22	A	839	LHG	O6-C4-C5-C6
29	J	102	LMG	C20-C21-C22-C23
20	A	811	CLA	C11-C12-C13-C15
20	A	815	CLA	C12-C13-C15-C16
20	A	824	CLA	C11-C10-C8-C7
20	A	836	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
20	A	852	CLA	C11-C10-C8-C7
20	B	823	CLA	C6-C7-C8-C10
20	B	825	CLA	C6-C7-C8-C10
20	B	828	CLA	C11-C10-C8-C7
20	B	831	CLA	C12-C13-C15-C16
20	O	206	CLA	C11-C12-C13-C15
20	Q	216	CLA	C11-C10-C8-C7
20	R	104	CLA	C6-C7-C8-C10
22	P	201	LHG	C29-C30-C31-C32
20	G	204	CLA	C2A-CAA-CBA-CGA
20	H	202	CLA	C8-C10-C11-C12
27	B	842	DGD	CEB-CFB-CGB-CHB
20	B	806	CLA	C6-C7-C8-C9
20	B	823	CLA	C6-C7-C8-C9
20	B	843	CLA	C11-C10-C8-C9
20	Q	205	CLA	C11-C10-C8-C9
20	Q	216	CLA	C11-C10-C8-C9
20	A	821	CLA	C8-C10-C11-C12
27	B	842	DGD	O1G-C1G-C2G-C3G
28	B	847	SQD	O6-C44-C45-C46
28	S	201	SQD	C9-C10-C11-C12
29	I	103	LMG	C30-C31-C32-C33
20	B	809	CLA	C3-C5-C6-C7
28	S	201	SQD	C32-C33-C34-C35
20	O	206	CLA	C16-C17-C18-C19
29	U	201	LMG	O6-C5-C6-O5
26	S	213	DD6	C9-C10-C11-C12
31	Q	218	A86	C-C1-C2-C3
20	U	207	CLA	C13-C15-C16-C17
20	A	835	CLA	C3-C5-C6-C7
20	A	823	CLA	C2-C3-C5-C6
20	B	815	CLA	C5-C6-C7-C8
20	P	207	CLA	C8-C10-C11-C12
23	B	838	BCR	C7-C8-C9-C34
26	P	218	DD6	C7-C6-C8-C9
26	U	203	DD6	C12-C11-C13-C14
22	P	201	LHG	C17-C18-C19-C20
29	Q	217	LMG	C17-C18-C19-C20
20	A	854	CLA	C16-C17-C18-C19
29	I	103	LMG	C16-C17-C18-C19
26	P	218	DD6	C5-C6-C8-C9
26	S	212	DD6	C5-C6-C8-C9

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Mol	Chain	Res	Type	Atoms
26	T	212	DD6	C10-C11-C13-C14
29	U	201	LMG	O10-C28-O8-C9
29	J	102	LMG	C13-C14-C15-C16
20	O	209	CLA	O2A-C1-C2-C3
29	P	202	LMG	C12-C13-C14-C15
23	I	101	BCR	C10-C11-C12-C13
26	O	212	DD6	C1-C24-C25-C26
26	O	214	DD6	C1-C24-C25-C26
26	H	210	DD6	C1-C24-C25-C26
31	R	105	A86	C1-C24-C25-C26
20	S	214	CLA	C13-C15-C16-C17
23	L	205	BCR	C9-C10-C11-C12
28	S	201	SQD	C28-C29-C30-C31
23	B	841	BCR	C11-C10-C9-C8
23	I	101	BCR	C11-C10-C9-C8
23	J	104	BCR	C20-C21-C22-C23
20	A	835	CLA	CBA-CGA-O2A-C1
27	B	842	DGD	CAB-CBB-CCB-CDB
28	S	201	SQD	C11-C12-C13-C14
29	J	102	LMG	C14-C15-C16-C17
20	A	811	CLA	C16-C17-C18-C20
29	I	103	LMG	C36-C37-C38-C39
28	S	201	SQD	O6-C44-C45-O47
29	Q	217	LMG	C24-C25-C26-C27
29	U	201	LMG	C31-C32-C33-C34
20	B	815	CLA	CAA-CBA-CGA-O2A
20	A	824	CLA	C3-C5-C6-C7
31	Q	201	A86	C9-C10-C11-C13
22	A	839	LHG	C34-C35-C36-C37
22	A	839	LHG	C11-C12-C13-C14
20	A	818	CLA	C4-C3-C5-C6
20	A	851	CLA	C4-C3-C5-C6
20	B	808	CLA	C4-C3-C5-C6
26	G	214	DD6	C27-C29-C30-C31
20	A	824	CLA	C11-C10-C8-C9
20	A	828	CLA	C11-C10-C8-C9
20	A	836	CLA	C11-C12-C13-C14
20	A	852	CLA	C11-C10-C8-C9
20	B	828	CLA	C11-C10-C8-C9
20	B	831	CLA	C14-C13-C15-C16
20	B	834	CLA	C11-C12-C13-C14
20	O	206	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
20	Q	213	CLA	C11-C10-C8-C9
20	R	104	CLA	C6-C7-C8-C9
20	U	205	CLA	C14-C13-C15-C16
29	Q	217	LMG	C33-C34-C35-C36
30	T	208	KC1	O1D-CGD-O2D-CED
20	A	801	CLA	C8-C10-C11-C12
28	B	847	SQD	C27-C28-C29-C30
20	A	847	CLA	C13-C15-C16-C17
20	S	214	CLA	C16-C17-C18-C20
20	O	209	CLA	C13-C15-C16-C17
20	A	808	CLA	C6-C7-C8-C10
20	A	828	CLA	C11-C10-C8-C7
20	A	833	CLA	C12-C13-C15-C16
20	B	834	CLA	C11-C12-C13-C15
20	Q	205	CLA	C11-C10-C8-C7
20	Q	209	CLA	C11-C12-C13-C15
20	Q	213	CLA	C11-C10-C8-C7
20	R	104	CLA	C11-C10-C8-C7
20	U	207	CLA	C11-C12-C13-C15
20	B	805	CLA	C3A-C2A-CAA-CBA
29	I	103	LMG	C35-C36-C37-C38
20	A	818	CLA	C2-C3-C5-C6
20	B	808	CLA	C2-C3-C5-C6
22	P	201	LHG	C13-C14-C15-C16
20	H	206	CLA	CBA-CGA-O2A-C1
26	O	213	DD6	C1-C2-C3-C4
26	G	217	DD6	C1-C2-C3-C4
23	L	201	BCR	C37-C22-C23-C24
29	P	202	LMG	C11-C12-C13-C14
20	A	835	CLA	O1A-CGA-O2A-C1
22	A	840	LHG	C4-C5-C6-O8
22	G	216	LHG	C4-C5-C6-O8
29	J	102	LMG	C7-C8-C9-O8
29	P	217	LMG	C7-C8-C9-O8
29	Q	217	LMG	O1-C7-C8-C9
31	Q	218	A86	C12-C11-C13-O
28	S	201	SQD	C27-C28-C29-C30
27	B	842	DGD	C3A-C4A-C5A-C6A
29	Q	217	LMG	C31-C32-C33-C34
27	B	842	DGD	CDB-CEB-CFB-CGB
20	A	851	CLA	C2-C3-C5-C6
31	Q	218	A86	C10-C11-C13-O

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Mol	Chain	Res	Type	Atoms
22	A	839	LHG	C26-C27-C28-C29
22	A	839	LHG	O6-C4-C5-O7
29	P	202	LMG	C13-C14-C15-C16
23	A	843	BCR	C1-C6-C7-C8
23	A	844	BCR	C1-C6-C7-C8
23	A	844	BCR	C23-C24-C25-C26
23	B	837	BCR	C1-C6-C7-C8
23	B	840	BCR	C23-C24-C25-C30
23	B	841	BCR	C1-C6-C7-C8
23	I	102	BCR	C1-C6-C7-C8
23	L	201	BCR	C1-C6-C7-C8
23	L	201	BCR	C23-C24-C25-C30
23	L	205	BCR	C1-C6-C7-C8
23	L	205	BCR	C23-C24-C25-C30
23	R	102	BCR	C1-C6-C7-C8
23	R	102	BCR	C23-C24-C25-C30
20	B	846	CLA	C8-C10-C11-C12
31	Q	214	A86	C9-C10-C11-C12
29	I	103	LMG	C18-C19-C20-C21
26	U	212	DD6	C24-C25-C26-C27
28	B	847	SQD	O6-C44-C45-O47
28	B	847	SQD	O47-C45-C46-O48
31	Q	201	A86	C33-C34-O4-C38
29	U	201	LMG	C10-C11-C12-C13
20	G	209	CLA	C4-C3-C5-C6
23	B	840	BCR	C10-C11-C12-C13
31	R	103	A86	C6-C8-C9-C10
20	B	845	CLA	C13-C15-C16-C17
20	A	835	CLA	C1-C2-C3-C5
20	A	845	CLA	C11-C10-C8-C9
22	P	201	LHG	C35-C36-C37-C38
27	B	842	DGD	C4B-C5B-C6B-C7B
23	B	837	BCR	C6-C7-C8-C9
29	P	217	LMG	O10-C28-O8-C9
20	B	834	CLA	C16-C17-C18-C20
20	O	206	CLA	C16-C17-C18-C20
20	P	207	CLA	C10-C11-C12-C13
26	G	214	DD6	C1-C2-C3-C4
20	G	209	CLA	C2-C3-C5-C6
20	Q	216	CLA	C8-C10-C11-C12
23	J	104	BCR	C20-C21-C22-C37
26	A	855	DD6	C4-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
26	O	214	DD6	C9-C10-C11-C12
26	Q	202	DD6	C4-C5-C6-C7
26	S	210	DD6	C9-C10-C11-C12
26	U	203	DD6	C-C1-C2-C3
26	H	210	DD6	C4-C5-C6-C7
31	R	103	A86	C4-C5-C6-C7
20	H	206	CLA	O1A-CGA-O2A-C1
20	A	824	CLA	C5-C6-C7-C8
20	B	808	CLA	C15-C16-C17-C18
20	B	844	CLA	C10-C11-C12-C13
20	L	203	CLA	C15-C16-C17-C18
22	P	201	LHG	O6-C4-C5-C6
22	G	216	LHG	O6-C4-C5-C6
20	A	811	CLA	C16-C17-C18-C19
20	B	834	CLA	C8-C10-C11-C12
23	B	841	BCR	C37-C22-C23-C24
26	O	212	DD6	C-C1-C24-C25
26	P	215	DD6	C12-C11-C13-C14
26	S	212	DD6	C7-C6-C8-C9
20	B	805	CLA	C11-C12-C13-C15
20	B	821	CLA	C11-C12-C13-C15
20	G	206	CLA	C6-C7-C8-C10
20	G	207	CLA	C6-C7-C8-C10
20	A	854	CLA	C15-C16-C17-C18
20	B	843	CLA	C13-C15-C16-C17
23	I	101	BCR	C21-C22-C23-C24
26	P	215	DD6	C10-C11-C13-C14
26	U	203	DD6	C10-C11-C13-C14
26	H	211	DD6	C10-C11-C13-C14
31	Q	214	A86	C5-C6-C8-C9
31	Q	218	A86	C5-C6-C8-C9
31	U	202	A86	C2-C1-C24-C25
26	U	214	DD6	C4-C5-C6-C8
28	S	201	SQD	C45-C44-O6-C1
20	Q	203	CLA	C2A-CAA-CBA-CGA
30	S	211	KC1	CAA-CBA-CGA-O1A
22	A	839	LHG	C31-C32-C33-C34
20	G	205	CLA	C8-C10-C11-C12
26	Q	202	DD6	C3-C4-C5-C6
29	P	202	LMG	C4-C5-C6-O5
23	F	804	BCR	C20-C21-C22-C23
22	G	216	LHG	O6-C4-C5-O7

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Mol	Chain	Res	Type	Atoms
28	B	847	SQD	C44-C45-C46-O48
29	P	202	LMG	C7-C8-C9-O8
20	U	210	CLA	C13-C15-C16-C17
20	H	207	CLA	C5-C6-C7-C8
30	P	206	KC1	C4B-C3B-CAB-CBB
30	P	212	KC1	C4B-C3B-CAB-CBB
30	P	219	KC1	C4B-C3B-CAB-CBB
30	S	209	KC1	C4B-C3B-CAB-CBB
30	S	211	KC1	C4B-C3B-CAB-CBB
28	B	847	SQD	C30-C31-C32-C33
27	B	842	DGD	C2A-C1A-O1G-C1G
20	A	801	CLA	C13-C15-C16-C17
20	B	831	CLA	C4-C3-C5-C6
22	A	840	LHG	O7-C5-C6-O8
29	P	202	LMG	O7-C8-C9-O8
20	A	823	CLA	C14-C13-C15-C16
20	A	833	CLA	C14-C13-C15-C16
20	A	834	CLA	C11-C10-C8-C9
20	B	809	CLA	C14-C13-C15-C16
20	B	846	CLA	C14-C13-C15-C16
22	A	839	LHG	C10-C11-C12-C13
27	B	842	DGD	C8B-C9B-CAB-CBB
28	B	847	SQD	C31-C32-C33-C34
29	I	103	LMG	C15-C16-C17-C18
31	Q	201	A86	C13-C14-C15-O1
31	Q	214	A86	C13-C14-C15-O1
31	R	105	A86	C13-C14-C15-O1
31	U	202	A86	C13-C14-C15-O1
26	H	211	DD6	C3-C4-C5-C6
20	A	825	CLA	C4-C3-C5-C6
20	B	813	CLA	C4-C3-C5-C6
20	R	104	CLA	C4-C3-C5-C6
27	B	842	DGD	CBB-CCB-CDB-CEB
20	A	847	CLA	C3-C5-C6-C7
28	S	201	SQD	C4-C5-C6-S
23	A	844	BCR	C18-C19-C20-C21
26	O	213	DD6	C27-C29-C30-C31
26	P	205	DD6	C27-C29-C30-C31
26	P	220	DD6	C27-C29-C30-C31
26	T	212	DD6	C27-C29-C30-C31
20	A	826	CLA	C1A-C2A-CAA-CBA
20	B	834	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
20	Q	203	CLA	C1A-C2A-CAA-CBA
20	H	207	CLA	C1A-C2A-CAA-CBA
31	R	105	A86	O-C13-C14-C15
22	P	201	LHG	C26-C27-C28-C29
20	A	810	CLA	C4-C3-C5-C6
20	A	852	CLA	C4-C3-C5-C6
20	S	215	CLA	C4-C3-C5-C6
26	U	203	DD6	C2-C1-C24-C25
26	G	214	DD6	C5-C6-C8-C9
29	P	202	LMG	C32-C33-C34-C35
20	T	204	CLA	C3-C5-C6-C7
20	B	801	CLA	C2A-CAA-CBA-CGA
29	J	102	LMG	C12-C13-C14-C15
20	A	809	CLA	C10-C11-C12-C13
20	Q	209	CLA	C10-C11-C12-C13
21	B	836	PQN	C23-C25-C26-C27
20	A	804	CLA	C11-C12-C13-C15
20	A	818	CLA	C6-C7-C8-C10
20	A	845	CLA	C11-C12-C13-C15
20	A	851	CLA	C11-C12-C13-C15
20	Q	209	CLA	C6-C7-C8-C10
20	U	207	CLA	C11-C10-C8-C7
27	B	842	DGD	C2A-C3A-C4A-C5A
20	A	821	CLA	C4-C3-C5-C6
20	A	834	CLA	C4-C3-C5-C6
20	A	838	CLA	C4-C3-C5-C6
20	A	808	CLA	C6-C7-C8-C9
20	B	806	CLA	C11-C10-C8-C9
20	G	207	CLA	C6-C7-C8-C9
26	A	855	DD6	C3-C4-C5-C6
26	J	101	DD6	C1-C2-C3-C4
26	S	210	DD6	C1-C2-C3-C4
26	G	212	DD6	C1-C2-C3-C4
26	G	214	DD6	C24-C25-C26-C27
21	B	836	PQN	C15-C16-C17-C18
20	L	202	CLA	C1-C2-C3-C4
30	P	212	KC1	C3A-C2A-CAA-CBA
30	P	212	KC1	CHA-CBD-CGD-O2D
30	P	219	KC1	C1A-C2A-CAA-CBA
31	R	103	A86	C26-C27-C29-C30
20	A	852	CLA	C3-C5-C6-C7
22	G	216	LHG	O7-C5-C6-O8

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Mol	Chain	Res	Type	Atoms
27	B	842	DGD	O1G-C1G-C2G-O2G
29	J	102	LMG	O7-C8-C9-O8
29	P	217	LMG	O7-C8-C9-O8
29	Q	217	LMG	O1-C7-C8-O7
22	A	839	LHG	C4-C5-C6-O8
28	S	201	SQD	O6-C44-C45-C46
29	U	201	LMG	C7-C8-C9-O8
22	P	201	LHG	C16-C17-C18-C19
20	A	803	CLA	CAD-CBD-CGD-O2D
20	P	210	CLA	CAD-CBD-CGD-O2D
20	Q	216	CLA	CAD-CBD-CGD-O2D
20	G	203	CLA	CAD-CBD-CGD-O2D
20	A	822	CLA	C8-C10-C11-C12
20	B	834	CLA	C5-C6-C7-C8
20	A	835	CLA	C16-C17-C18-C20
20	B	831	CLA	C16-C17-C18-C20
20	P	207	CLA	C2A-CAA-CBA-CGA
20	T	204	CLA	C2A-CAA-CBA-CGA
20	A	803	CLA	CAD-CBD-CGD-O1D
20	A	814	CLA	CHA-CBD-CGD-O2D
20	A	821	CLA	CHA-CBD-CGD-O1D
20	A	821	CLA	CHA-CBD-CGD-O2D
20	A	827	CLA	CHA-CBD-CGD-O1D
20	B	804	CLA	CHA-CBD-CGD-O1D
20	B	828	CLA	CHA-CBD-CGD-O2D
20	J	103	CLA	CAD-CBD-CGD-O1D
20	O	202	CLA	CHA-CBD-CGD-O1D
20	O	205	CLA	CHA-CBD-CGD-O1D
20	O	205	CLA	CHA-CBD-CGD-O2D
20	P	210	CLA	CAD-CBD-CGD-O1D
20	Q	209	CLA	CHA-CBD-CGD-O1D
20	Q	209	CLA	CHA-CBD-CGD-O2D
20	Q	216	CLA	CAD-CBD-CGD-O1D
20	U	210	CLA	CHA-CBD-CGD-O1D
20	G	203	CLA	CAD-CBD-CGD-O1D
20	H	202	CLA	CHA-CBD-CGD-O1D
20	H	202	CLA	CHA-CBD-CGD-O2D
20	T	204	CLA	CHA-CBD-CGD-O1D
20	T	204	CLA	CHA-CBD-CGD-O2D
22	A	840	LHG	C3-O3-P-O5
22	P	201	LHG	C3-O3-P-O6
22	P	201	LHG	C4-O6-P-O5

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Mol	Chain	Res	Type	Atoms
26	A	855	DD6	C1-C2-C3-C4
26	O	214	DD6	C3-C4-C5-C6
26	P	215	DD6	C24-C25-C26-C27
31	R	103	A86	C3-C4-C5-C6
20	A	833	CLA	C4-C3-C5-C6
20	Q	216	CLA	C4-C3-C5-C6
20	A	825	CLA	C2-C3-C5-C6
28	B	847	SQD	C34-C35-C36-C37
22	G	216	LHG	C2-C3-O3-P
29	P	202	LMG	C28-C29-C30-C31
22	A	839	LHG	C6-C5-O7-C7
26	P	220	DD6	C6-C8-C9-C10
31	P	204	A86	C1-C24-C25-C26
20	B	813	CLA	C2-C3-C5-C6
20	R	104	CLA	C2-C3-C5-C6
20	A	822	CLA	C16-C17-C18-C19
20	O	205	CLA	C16-C17-C18-C20
28	S	201	SQD	C24-C23-O48-C46
20	B	803	CLA	C6-C7-C8-C9
20	B	813	CLA	C11-C10-C8-C9
20	B	834	CLA	C14-C13-C15-C16
20	B	844	CLA	C14-C13-C15-C16
20	U	204	CLA	C11-C12-C13-C14
20	G	206	CLA	C6-C7-C8-C9
20	B	843	CLA	C11-C10-C8-C7
20	H	206	CLA	C6-C7-C8-C10
26	H	210	DD6	C4-C5-C6-C8
23	F	804	BCR	C22-C23-C24-C25
29	I	103	LMG	C37-C38-C39-C40
20	A	854	CLA	C3-C5-C6-C7
28	B	847	SQD	C35-C36-C37-C38
20	T	204	CLA	C4-C3-C5-C6
29	P	202	LMG	O1-C7-C8-C9
26	P	218	DD6	C10-C11-C13-C14
22	A	840	LHG	C10-C11-C12-C13
26	P	205	DD6	C24-C25-C26-C27
26	Q	215	DD6	C1-C2-C3-C4
28	B	847	SQD	C32-C33-C34-C35
20	A	818	CLA	C6-C7-C8-C9
20	A	824	CLA	C6-C7-C8-C9
20	A	825	CLA	C14-C13-C15-C16
20	B	805	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
29	Q	217	LMG	C36-C37-C38-C39
20	S	202	CLA	C10-C11-C12-C13
20	P	209	CLA	C2A-CAA-CBA-CGA
20	B	807	CLA	C4-C3-C5-C6
20	B	823	CLA	C4-C3-C5-C6
20	U	207	CLA	C4-C3-C5-C6
20	H	206	CLA	C4-C3-C5-C6
20	B	828	CLA	CAA-CBA-CGA-O2A
20	B	823	CLA	C2-C3-C5-C6
26	O	214	DD6	C24-C25-C26-C27
26	P	205	DD6	C3-C4-C5-C6
26	Q	202	DD6	C24-C25-C26-C27
20	B	833	CLA	C12-C13-C15-C16
20	B	834	CLA	C12-C13-C15-C16
20	A	815	CLA	C5-C6-C7-C8
20	S	208	CLA	CAA-CBA-CGA-O2A
20	A	847	CLA	C8-C10-C11-C12
20	B	823	CLA	C13-C15-C16-C17
29	U	201	LMG	O7-C8-C9-O8
20	B	813	CLA	C3A-C2A-CAA-CBA
20	L	202	CLA	C3A-C2A-CAA-CBA
20	H	209	CLA	C3A-C2A-CAA-CBA
20	B	831	CLA	C15-C16-C17-C18
20	Q	216	CLA	C2-C3-C5-C6
23	B	837	BCR	C11-C10-C9-C34
23	B	839	BCR	C20-C21-C22-C37
31	P	204	A86	C25-C26-C27-C28
31	Q	218	A86	C25-C26-C27-C28
20	B	829	CLA	C3-C5-C6-C7
20	A	849	CLA	C8-C10-C11-C12
20	A	830	CLA	C2-C1-O2A-CGA
26	G	212	DD6	C3-C4-C5-C6
26	G	214	DD6	C3-C4-C5-C6
20	A	852	CLA	C5-C6-C7-C8
20	B	808	CLA	C13-C15-C16-C17
20	U	210	CLA	C10-C11-C12-C13
26	O	212	DD6	C2-C1-C24-C25
20	A	849	CLA	C4-C3-C5-C6
20	G	206	CLA	C4-C3-C5-C6
20	A	815	CLA	CAA-CBA-CGA-O2A
20	A	834	CLA	C2-C3-C5-C6
20	B	831	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
20	S	215	CLA	C2-C3-C5-C6
20	U	207	CLA	C2-C3-C5-C6
20	A	822	CLA	C16-C17-C18-C20
20	A	831	CLA	CAA-CBA-CGA-O2A
23	J	104	BCR	C14-C15-C16-C17
20	A	815	CLA	C14-C13-C15-C16
20	Q	209	CLA	C11-C10-C8-C9
20	Q	216	CLA	C6-C7-C8-C9
20	R	101	CLA	CAA-CBA-CGA-O1A
20	A	851	CLA	C13-C15-C16-C17
20	A	849	CLA	C2-C3-C5-C6
20	B	807	CLA	C2-C3-C5-C6
28	B	847	SQD	C25-C26-C27-C28
29	Q	217	LMG	O10-C28-O8-C9
20	G	210	CLA	CAA-CBA-CGA-O2A
20	A	815	CLA	C15-C16-C17-C18
20	B	819	CLA	C1A-C2A-CAA-CBA
20	L	202	CLA	C1A-C2A-CAA-CBA
20	H	202	CLA	C1A-C2A-CAA-CBA
20	H	203	CLA	C1A-C2A-CAA-CBA
23	F	804	BCR	C12-C13-C14-C15
23	R	102	BCR	C20-C21-C22-C23
31	P	204	A86	C25-C26-C27-C29
31	Q	218	A86	C25-C26-C27-C29
20	P	214	CLA	CAA-CBA-CGA-O1A
20	R	101	CLA	CAA-CBA-CGA-O2A
20	G	201	CLA	CAA-CBA-CGA-O1A
20	G	210	CLA	CAA-CBA-CGA-O1A
23	A	841	BCR	C1-C6-C7-C8
23	A	843	BCR	C5-C6-C7-C8
23	A	844	BCR	C5-C6-C7-C8
23	B	837	BCR	C5-C6-C7-C8
23	B	840	BCR	C1-C6-C7-C8
23	B	840	BCR	C23-C24-C25-C26
23	B	841	BCR	C5-C6-C7-C8
23	B	841	BCR	C23-C24-C25-C30
23	F	804	BCR	C1-C6-C7-C8
23	F	804	BCR	C23-C24-C25-C30
23	I	102	BCR	C5-C6-C7-C8
23	J	104	BCR	C23-C24-C25-C30
23	L	201	BCR	C5-C6-C7-C8
23	L	201	BCR	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
23	L	205	BCR	C5-C6-C7-C8
23	L	205	BCR	C23-C24-C25-C26
23	M	101	BCR	C1-C6-C7-C8
23	M	101	BCR	C23-C24-C25-C30
23	R	102	BCR	C5-C6-C7-C8
23	R	102	BCR	C23-C24-C25-C26
20	B	815	CLA	CAA-CBA-CGA-O1A
20	A	831	CLA	CAA-CBA-CGA-O1A
20	S	207	CLA	CAA-CBA-CGA-O1A
20	T	204	CLA	C2-C3-C5-C6
20	B	806	CLA	C6-C7-C8-C10
20	B	813	CLA	C6-C7-C8-C10
20	B	844	CLA	C12-C13-C15-C16
20	B	845	CLA	C12-C13-C15-C16
20	U	204	CLA	C11-C12-C13-C15
20	O	205	CLA	C16-C17-C18-C19
20	B	803	CLA	C2A-CAA-CBA-CGA
20	H	203	CLA	C2A-CAA-CBA-CGA
22	A	839	LHG	O7-C5-C6-O8
22	P	201	LHG	C10-C11-C12-C13
29	U	201	LMG	C30-C31-C32-C33
20	B	809	CLA	C10-C11-C12-C13
23	B	837	BCR	C37-C22-C23-C24
26	O	213	DD6	C7-C6-C8-C9
29	I	103	LMG	C20-C21-C22-C23
20	G	201	CLA	CAA-CBA-CGA-O2A
20	U	204	CLA	C10-C11-C12-C13
20	G	206	CLA	C2-C3-C5-C6
20	B	832	CLA	C2-C1-O2A-CGA
28	B	847	SQD	C9-C10-C11-C12
20	G	210	CLA	C2A-CAA-CBA-CGA
20	P	214	CLA	CAA-CBA-CGA-O2A
20	S	207	CLA	CAA-CBA-CGA-O2A
20	O	206	CLA	C14-C13-C15-C16
22	A	839	LHG	C18-C19-C20-C21
20	A	807	CLA	C4-C3-C5-C6
20	A	811	CLA	C4-C3-C5-C6
20	B	801	CLA	C4-C3-C5-C6
20	A	838	CLA	C2-C3-C5-C6
20	B	801	CLA	C2-C3-C5-C6
29	U	201	LMG	C11-C12-C13-C14
20	G	215	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
26	U	214	DD6	C27-C29-C30-C31
26	G	213	DD6	C27-C29-C30-C31
20	U	206	CLA	CAA-CBA-CGA-O2A
20	A	835	CLA	C16-C17-C18-C19
20	B	831	CLA	C16-C17-C18-C19
23	F	804	BCR	C35-C13-C14-C15
24	A	848	CL0	CHA-CBD-CGD-O1D
24	A	848	CL0	CHA-CBD-CGD-O2D
26	P	220	DD6	C9-C10-C11-C12
31	Q	201	A86	C-C1-C2-C3
20	B	823	CLA	C15-C16-C17-C18
20	T	203	CLA	C2A-CAA-CBA-CGA
29	P	202	LMG	O1-C7-C8-O7
26	G	214	DD6	C7-C6-C8-C9
20	A	825	CLA	C12-C13-C15-C16
20	U	206	CLA	CAA-CBA-CGA-O1A
26	G	213	DD6	C1-C2-C3-C4
20	A	834	CLA	C14-C13-C15-C16
20	A	845	CLA	C6-C7-C8-C9
20	Q	209	CLA	C11-C12-C13-C14
22	P	201	LHG	C19-C20-C21-C22
28	S	201	SQD	C29-C30-C31-C32
20	B	807	CLA	C2A-CAA-CBA-CGA
20	H	206	CLA	C2A-CAA-CBA-CGA
20	L	203	CLA	C2-C1-O2A-CGA
20	H	202	CLA	C2-C1-O2A-CGA
20	O	209	CLA	C3-C5-C6-C7
20	A	851	CLA	C3A-C2A-CAA-CBA
20	H	202	CLA	C3A-C2A-CAA-CBA
20	P	208	CLA	C3-C5-C6-C7
26	Q	215	DD6	C1-C24-C25-C26
26	U	214	DD6	C1-C24-C25-C26
20	A	814	CLA	CAA-CBA-CGA-O2A
20	B	804	CLA	CAA-CBA-CGA-O2A
20	G	203	CLA	CAA-CBA-CGA-O2A
20	G	215	CLA	CAA-CBA-CGA-O1A
20	B	804	CLA	CAA-CBA-CGA-O1A
20	S	214	CLA	C4C-C3C-CAC-CBC
26	O	214	DD6	C9-C10-C11-C13
26	P	220	DD6	C9-C10-C11-C13
26	Q	202	DD6	C4-C5-C6-C8
26	S	210	DD6	C9-C10-C11-C13

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Mol	Chain	Res	Type	Atoms
26	U	203	DD6	C24-C1-C2-C3
20	A	814	CLA	CAA-CBA-CGA-O1A
20	B	827	CLA	O2A-C1-C2-C3
23	B	838	BCR	C6-C7-C8-C9
20	B	809	CLA	C4-C3-C5-C6
20	G	203	CLA	CAA-CBA-CGA-O1A
31	P	204	A86	C1-C2-C3-C4
31	Q	201	A86	C28-C27-C29-C30
31	R	103	A86	C28-C27-C29-C30
29	J	102	LMG	C21-C22-C23-C24
22	A	839	LHG	C12-C13-C14-C15
20	S	215	CLA	C5-C6-C7-C8
20	A	804	CLA	C11-C12-C13-C14
20	P	207	CLA	C11-C12-C13-C14
21	A	837	PQN	C24-C23-C25-C26
20	G	206	CLA	CAA-CBA-CGA-O2A
22	P	201	LHG	O7-C7-C8-C9
22	P	201	LHG	C24-C23-O8-C6
31	Q	218	A86	C13-C14-C15-O1
20	B	844	CLA	CAA-CBA-CGA-O2A
20	A	803	CLA	C16-C17-C18-C20
20	A	810	CLA	C2-C3-C5-C6
20	B	813	CLA	C11-C10-C8-C7
20	B	815	CLA	C11-C10-C8-C7
20	O	206	CLA	C12-C13-C15-C16
20	O	208	CLA	C6-C7-C8-C10
21	A	837	PQN	C17-C18-C20-C21
20	A	805	CLA	C2B-C3B-CAB-CBB
20	A	807	CLA	C2B-C3B-CAB-CBB
20	A	808	CLA	C2B-C3B-CAB-CBB
20	A	812	CLA	C2B-C3B-CAB-CBB
20	A	818	CLA	C2B-C3B-CAB-CBB
20	A	825	CLA	C2B-C3B-CAB-CBB
20	A	838	CLA	C2B-C3B-CAB-CBB
20	A	845	CLA	C2B-C3B-CAB-CBB
20	A	846	CLA	C2B-C3B-CAB-CBB
20	A	849	CLA	C2B-C3B-CAB-CBB
20	A	851	CLA	C2B-C3B-CAB-CBB
20	A	852	CLA	C2B-C3B-CAB-CBB
20	B	805	CLA	C2B-C3B-CAB-CBB
20	B	811	CLA	C2B-C3B-CAB-CBB
20	B	816	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
20	B	821	CLA	C2B-C3B-CAB-CBB
20	B	824	CLA	C2B-C3B-CAB-CBB
20	B	827	CLA	C2B-C3B-CAB-CBB
20	L	204	CLA	C2B-C3B-CAB-CBB
20	P	208	CLA	C2B-C3B-CAB-CBB
20	Q	208	CLA	C2B-C3B-CAB-CBB
20	Q	211	CLA	C2B-C3B-CAB-CBB
20	Q	213	CLA	C2B-C3B-CAB-CBB
20	S	208	CLA	C2B-C3B-CAB-CBB
20	S	214	CLA	C2B-C3B-CAB-CBB
20	S	215	CLA	C2B-C3B-CAB-CBB
20	U	204	CLA	C2B-C3B-CAB-CBB
20	U	205	CLA	C2B-C3B-CAB-CBB
20	U	206	CLA	C2B-C3B-CAB-CBB
20	G	205	CLA	C2B-C3B-CAB-CBB
20	G	210	CLA	C2B-C3B-CAB-CBB
20	H	205	CLA	C2B-C3B-CAB-CBB
20	T	207	CLA	C2B-C3B-CAB-CBB
20	T	209	CLA	C2B-C3B-CAB-CBB
23	A	841	BCR	C23-C24-C25-C26
23	A	841	BCR	C23-C24-C25-C30
23	A	842	BCR	C1-C6-C7-C8
23	A	842	BCR	C5-C6-C7-C8
23	B	837	BCR	C23-C24-C25-C26
23	B	840	BCR	C5-C6-C7-C8
23	B	841	BCR	C23-C24-C25-C26
23	F	801	BCR	C1-C6-C7-C8
23	F	801	BCR	C5-C6-C7-C8
23	F	804	BCR	C5-C6-C7-C8
23	F	804	BCR	C23-C24-C25-C26
23	I	101	BCR	C1-C6-C7-C8
23	I	101	BCR	C5-C6-C7-C8
23	J	104	BCR	C5-C6-C7-C8
23	J	104	BCR	C23-C24-C25-C26
23	M	101	BCR	C5-C6-C7-C8
23	M	101	BCR	C23-C24-C25-C26
24	A	848	CL0	CAA-CBA-CGA-O2A
20	A	822	CLA	C2-C1-O2A-CGA
20	A	847	CLA	C2-C1-O2A-CGA
20	B	802	CLA	C2-C1-O2A-CGA
26	O	213	DD6	C11-C13-C14-C15
26	S	204	DD6	C11-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
20	B	803	CLA	CAA-CBA-CGA-O2A
20	R	104	CLA	C5-C6-C7-C8
22	G	216	LHG	C5-C6-O8-C23
20	B	806	CLA	C5-C6-C7-C8
20	A	807	CLA	C2-C3-C5-C6
20	A	821	CLA	C2-C3-C5-C6
20	B	804	CLA	C2A-CAA-CBA-CGA
20	L	204	CLA	C2A-CAA-CBA-CGA
29	P	202	LMG	O7-C10-C11-C12
20	G	208	CLA	CAA-CBA-CGA-O2A
20	B	828	CLA	C3-C5-C6-C7
20	Q	206	CLA	C4-C3-C5-C6
20	Q	216	CLA	CAA-CBA-CGA-O2A
20	U	210	CLA	CAA-CBA-CGA-O2A
20	H	205	CLA	CAA-CBA-CGA-O1A
20	A	818	CLA	C13-C15-C16-C17
20	B	846	CLA	C13-C15-C16-C17
20	B	845	CLA	C14-C13-C15-C16
26	O	201	DD6	C7-C6-C8-C9
20	G	205	CLA	CAA-CBA-CGA-O2A
20	A	807	CLA	C1A-C2A-CAA-CBA
20	A	835	CLA	C4B-C3B-CAB-CBB
20	A	851	CLA	C1A-C2A-CAA-CBA
20	B	843	CLA	C1A-C2A-CAA-CBA
20	P	214	CLA	C4B-C3B-CAB-CBB
20	G	203	CLA	C4B-C3B-CAB-CBB
20	G	208	CLA	C4B-C3B-CAB-CBB
20	T	206	CLA	C4B-C3B-CAB-CBB
20	H	205	CLA	CAA-CBA-CGA-O2A
20	H	209	CLA	CAA-CBA-CGA-O1A
20	B	806	CLA	CAA-CBA-CGA-O2A
20	B	823	CLA	CAA-CBA-CGA-O2A
20	Q	206	CLA	CAA-CBA-CGA-O2A
23	M	101	BCR	C21-C22-C23-C24
26	O	201	DD6	C5-C6-C8-C9
26	P	220	DD6	C10-C11-C13-C14
20	H	209	CLA	CAA-CBA-CGA-O2A
20	A	810	CLA	CAA-CBA-CGA-O2A
20	A	846	CLA	CAA-CBA-CGA-O2A
20	U	211	CLA	CAA-CBA-CGA-O2A
20	A	811	CLA	CAA-CBA-CGA-O2A
20	T	211	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
29	P	217	LMG	O7-C10-C11-C12
27	B	842	DGD	C2B-C3B-C4B-C5B
28	B	847	SQD	C33-C34-C35-C36
20	A	822	CLA	C15-C16-C17-C18
20	U	211	CLA	C2-C1-O2A-CGA
20	G	207	CLA	C2-C1-O2A-CGA
20	B	817	CLA	C11-C10-C8-C7
20	A	835	CLA	C2-C3-C5-C6
20	F	803	CLA	CAA-CBA-CGA-O2A
20	R	104	CLA	C2A-CAA-CBA-CGA
20	B	809	CLA	CAA-CBA-CGA-O2A
20	B	843	CLA	C3A-C2A-CAA-CBA
20	S	208	CLA	C3A-C2A-CAA-CBA
20	U	207	CLA	C3A-C2A-CAA-CBA
20	A	851	CLA	C10-C11-C12-C13
20	O	206	CLA	C15-C16-C17-C18
20	H	206	CLA	C15-C16-C17-C18
20	A	833	CLA	C2-C3-C5-C6
26	A	855	DD6	C4-C5-C6-C8
31	R	103	A86	C4-C5-C6-C8
20	B	803	CLA	CAA-CBA-CGA-O1A
20	O	204	CLA	C13-C15-C16-C17
20	T	211	CLA	C2A-CAA-CBA-CGA
20	A	851	CLA	C11-C12-C13-C14
20	B	821	CLA	C16-C17-C18-C19
22	A	840	LHG	O2-C2-C3-O3
20	A	823	CLA	C15-C16-C17-C18
26	P	220	DD6	C12-C11-C13-C14
20	A	811	CLA	CAA-CBA-CGA-O1A
20	F	803	CLA	CAA-CBA-CGA-O1A
20	A	811	CLA	C2-C3-C5-C6
26	P	218	DD6	C13-C14-C15-C16
30	P	206	KC1	C3A-C2A-CAA-CBA
30	S	211	KC1	C1A-C2A-CAA-CBA
30	U	213	KC1	C3A-C2A-CAA-CBA
31	U	202	A86	C26-C27-C29-C30
20	B	806	CLA	CAA-CBA-CGA-O1A
20	B	844	CLA	CAA-CBA-CGA-O1A
29	U	201	LMG	O9-C10-C11-C12
26	O	201	DD6	C2-C1-C24-C25
26	O	213	DD6	C5-C6-C8-C9
26	G	211	DD6	C2-C1-C24-C25

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Mol	Chain	Res	Type	Atoms
20	B	823	CLA	CAA-CBA-CGA-O1A
20	G	208	CLA	CAA-CBA-CGA-O1A
29	I	103	LMG	C8-C7-O1-C1
29	J	102	LMG	C8-C7-O1-C1
29	Q	217	LMG	C8-C7-O1-C1
20	A	846	CLA	CAA-CBA-CGA-O1A
20	G	206	CLA	CAA-CBA-CGA-O1A
20	B	802	CLA	CAA-CBA-CGA-O2A
20	A	803	CLA	C2A-CAA-CBA-CGA
20	G	209	CLA	C2A-CAA-CBA-CGA
20	Q	206	CLA	CAA-CBA-CGA-O1A
20	U	211	CLA	CAA-CBA-CGA-O1A
20	G	205	CLA	CAA-CBA-CGA-O1A
22	P	201	LHG	O9-C7-C8-C9
29	P	202	LMG	O9-C10-C11-C12
20	L	204	CLA	CAA-CBA-CGA-O2A
20	A	808	CLA	C5-C6-C7-C8
20	Q	216	CLA	CAA-CBA-CGA-O1A
29	P	217	LMG	O9-C10-C11-C12
20	A	802	CLA	CAD-CBD-CGD-O2D
20	B	813	CLA	CAD-CBD-CGD-O2D
20	L	202	CLA	CAD-CBD-CGD-O2D
20	O	211	CLA	CAD-CBD-CGD-O2D
20	T	210	CLA	CAD-CBD-CGD-O2D
20	T	211	CLA	CAD-CBD-CGD-O2D
20	A	835	CLA	CAA-CBA-CGA-O2A
20	A	833	CLA	C13-C15-C16-C17
20	A	801	CLA	CAA-CBA-CGA-O2A
20	A	803	CLA	CAA-CBA-CGA-O2A
20	A	836	CLA	CAA-CBA-CGA-O2A
20	H	203	CLA	CAA-CBA-CGA-O2A
28	B	847	SQD	C14-C15-C16-C17
22	A	839	LHG	C35-C36-C37-C38
20	O	204	CLA	C16-C17-C18-C19
20	B	809	CLA	CAA-CBA-CGA-O1A
20	U	210	CLA	CAA-CBA-CGA-O1A
28	B	847	SQD	C11-C12-C13-C14
20	H	202	CLA	CAA-CBA-CGA-O2A
29	U	201	LMG	O7-C10-C11-C12
20	T	211	CLA	CAA-CBA-CGA-O1A

There are no ring outliers.

167 monomers are involved in 289 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	G	203	CLA	1	0
20	B	824	CLA	3	0
20	T	201	CLA	3	0
20	A	852	CLA	2	0
20	O	202	CLA	1	0
20	B	822	CLA	2	0
20	A	814	CLA	2	0
20	A	815	CLA	2	0
20	T	207	CLA	3	0
23	R	102	BCR	1	0
26	G	214	DD6	1	0
20	U	208	CLA	1	0
20	B	810	CLA	1	0
20	B	815	CLA	4	0
20	B	820	CLA	1	0
20	G	202	CLA	1	0
20	A	817	CLA	1	0
20	A	826	CLA	1	0
20	G	201	CLA	1	0
20	A	835	CLA	4	0
22	A	840	LHG	1	0
20	B	835	CLA	6	0
20	Q	216	CLA	3	0
23	I	101	BCR	1	0
20	A	820	CLA	1	0
23	F	804	BCR	1	0
26	U	203	DD6	2	0
20	B	809	CLA	3	0
20	B	821	CLA	1	0
20	A	804	CLA	2	0
20	U	210	CLA	2	0
20	A	813	CLA	1	0
20	A	834	CLA	1	0
20	B	807	CLA	2	0
20	T	205	CLA	1	0
20	S	206	CLA	2	0
20	S	214	CLA	4	0
20	S	215	CLA	1	0
20	G	207	CLA	1	0
20	A	823	CLA	1	0
20	L	202	CLA	2	0
20	T	210	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	G	206	CLA	3	0
20	S	205	CLA	2	0
20	A	803	CLA	6	0
23	B	838	BCR	5	0
20	A	829	CLA	2	0
30	P	206	KC1	1	0
20	F	803	CLA	3	0
20	U	207	CLA	1	0
20	P	213	CLA	2	0
20	H	205	CLA	2	0
20	A	851	CLA	1	0
20	B	812	CLA	1	0
28	S	201	SQD	5	0
29	Q	217	LMG	3	0
20	G	209	CLA	4	0
20	O	211	CLA	2	0
20	G	215	CLA	1	0
20	Q	213	CLA	1	0
20	G	208	CLA	2	0
20	R	104	CLA	2	0
20	J	103	CLA	1	0
20	A	808	CLA	1	0
23	M	101	BCR	4	0
20	B	831	CLA	2	0
20	A	807	CLA	1	0
20	Q	203	CLA	2	0
20	B	808	CLA	4	0
20	G	205	CLA	2	0
20	O	205	CLA	2	0
20	A	828	CLA	1	0
20	H	207	CLA	3	0
20	H	206	CLA	4	0
23	A	844	BCR	2	0
20	B	848	CLA	4	0
20	O	209	CLA	1	0
20	B	814	CLA	1	0
20	A	825	CLA	2	0
20	G	204	CLA	1	0
20	A	846	CLA	1	0
21	A	837	PQN	4	0
29	J	102	LMG	1	0
20	A	824	CLA	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	A	841	BCR	2	0
23	F	801	BCR	1	0
20	B	818	CLA	2	0
20	B	811	CLA	1	0
20	B	845	CLA	1	0
20	Q	208	CLA	1	0
20	T	202	CLA	2	0
20	P	214	CLA	2	0
20	U	211	CLA	1	0
24	A	848	CL0	2	0
20	B	819	CLA	4	0
20	A	833	CLA	5	0
20	B	827	CLA	1	0
20	A	849	CLA	2	0
20	H	201	CLA	1	0
20	A	838	CLA	3	0
20	B	828	CLA	1	0
20	Q	204	CLA	1	0
20	R	101	CLA	1	0
20	U	209	CLA	1	0
20	P	208	CLA	2	0
20	B	825	CLA	1	0
20	F	802	CLA	1	0
23	I	102	BCR	2	0
20	A	836	CLA	1	0
20	U	205	CLA	5	0
20	U	206	CLA	2	0
23	B	841	BCR	1	0
20	B	816	CLA	2	0
20	A	818	CLA	3	0
20	B	802	CLA	2	0
21	B	836	PQN	4	0
20	A	816	CLA	2	0
20	Q	206	CLA	1	0
20	A	854	CLA	4	0
20	O	207	CLA	2	0
20	Q	212	CLA	2	0
20	A	811	CLA	5	0
20	A	845	CLA	2	0
20	P	210	CLA	1	0
23	B	837	BCR	5	0
20	T	206	CLA	2	0

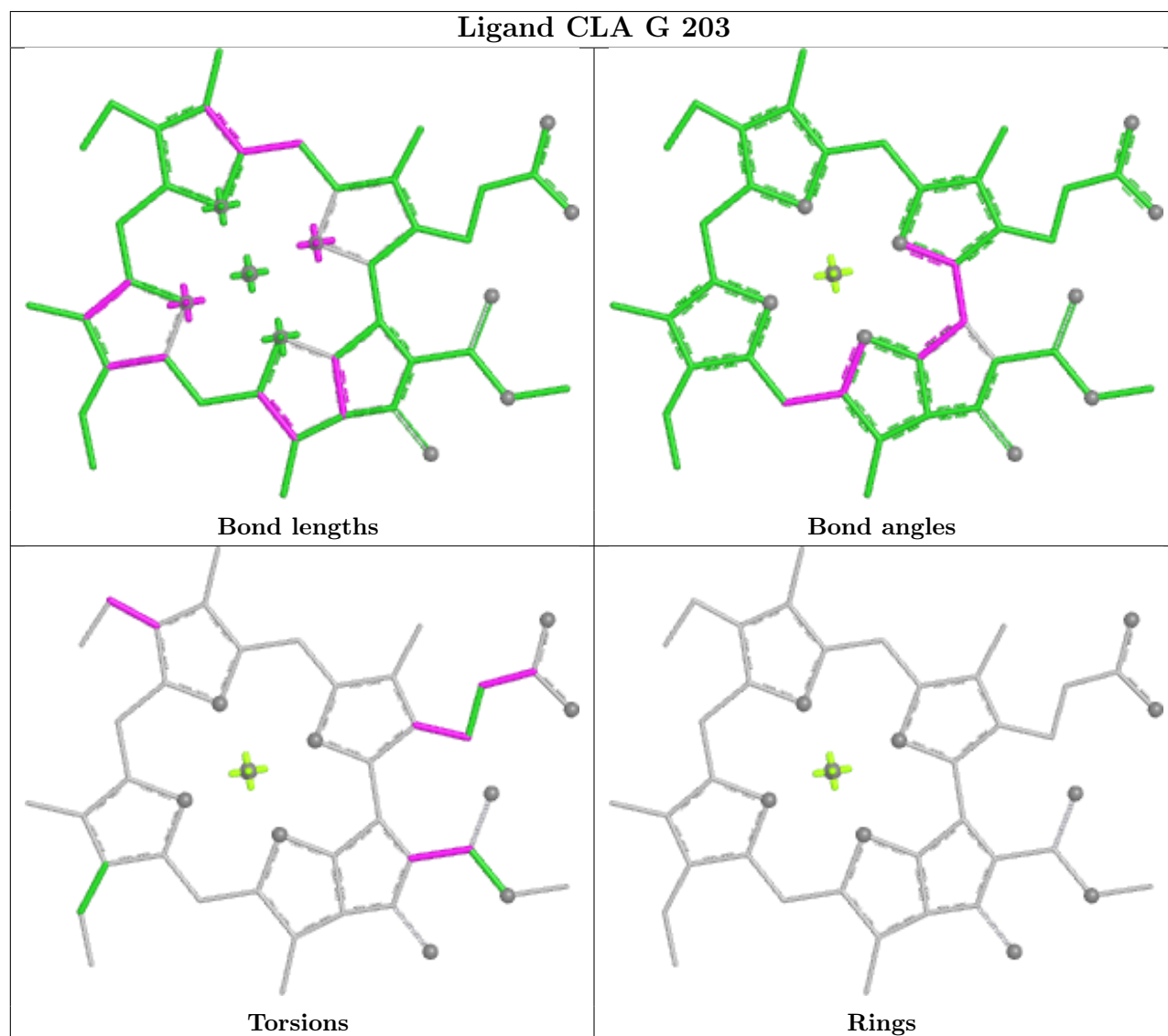
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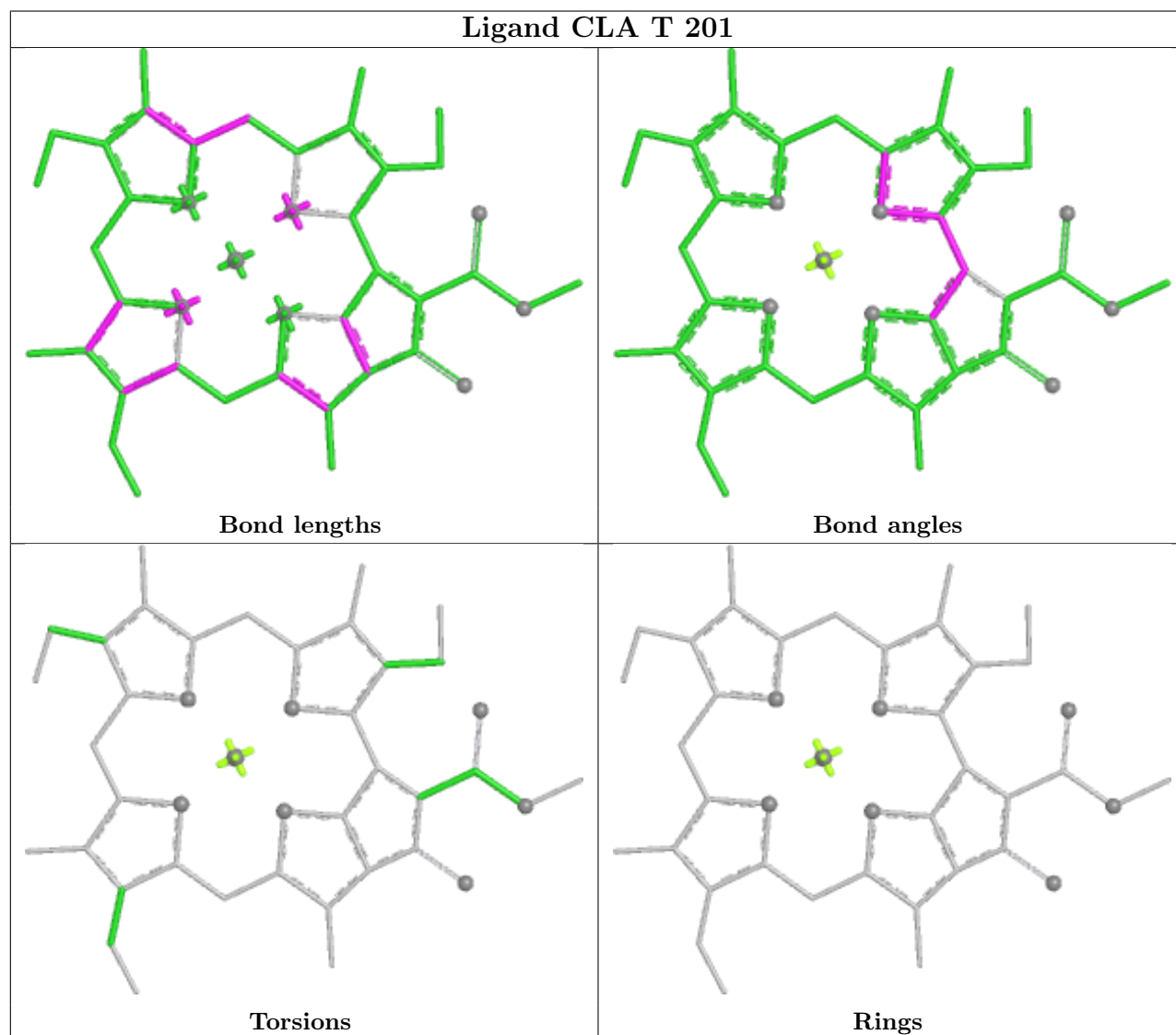
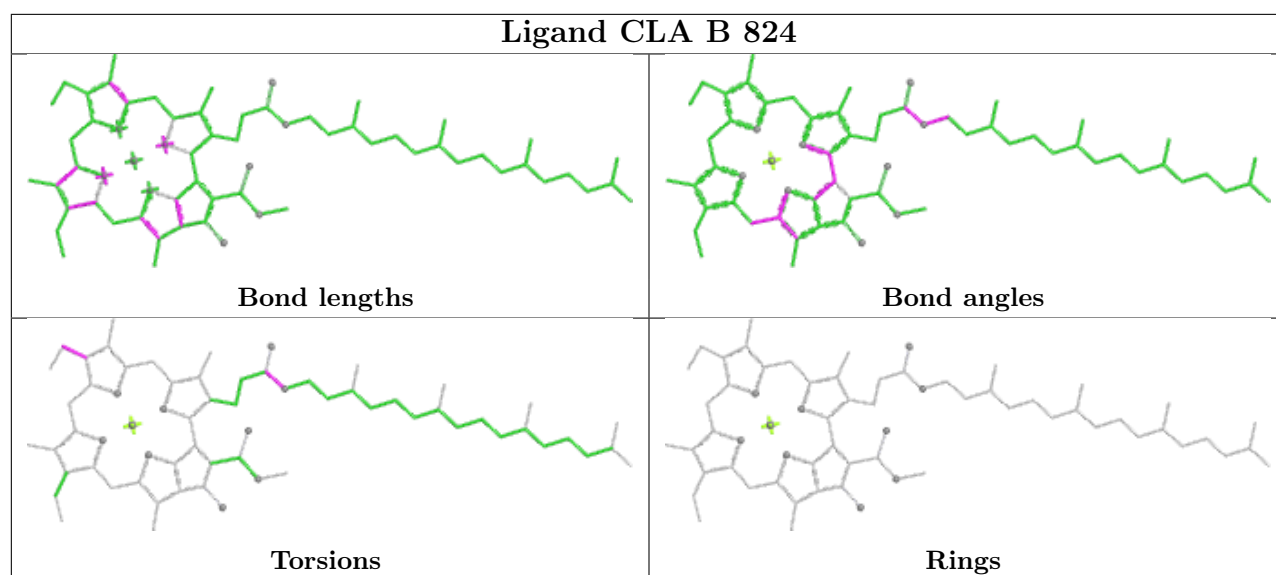
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	A	822	CLA	1	0
20	B	833	CLA	5	0
20	B	830	CLA	3	0
20	B	829	CLA	2	0
23	L	205	BCR	2	0
20	A	810	CLA	2	0
20	P	207	CLA	1	0
20	A	853	CLA	2	0
20	O	208	CLA	3	0
20	T	204	CLA	3	0
23	B	839	BCR	2	0
20	P	211	CLA	1	0
20	A	802	CLA	1	0
29	U	201	LMG	1	0
20	H	208	CLA	2	0
23	B	840	BCR	1	0
20	H	203	CLA	1	0
23	L	201	BCR	3	0
20	B	826	CLA	1	0
20	G	210	CLA	1	0
20	B	846	CLA	3	0
20	B	803	CLA	1	0
23	A	843	BCR	3	0
20	S	202	CLA	4	0
23	A	842	BCR	2	0
20	A	821	CLA	2	0
20	Q	205	CLA	1	0
29	P	217	LMG	5	0
20	Q	207	CLA	1	0
20	B	844	CLA	3	0
23	J	104	BCR	1	0
20	B	813	CLA	1	0
20	B	834	CLA	1	0
29	I	103	LMG	2	0
20	T	211	CLA	1	0
20	A	801	CLA	1	0
22	G	216	LHG	1	0
20	H	204	CLA	2	0
22	P	201	LHG	1	0
20	A	831	CLA	2	0
20	A	847	CLA	5	0

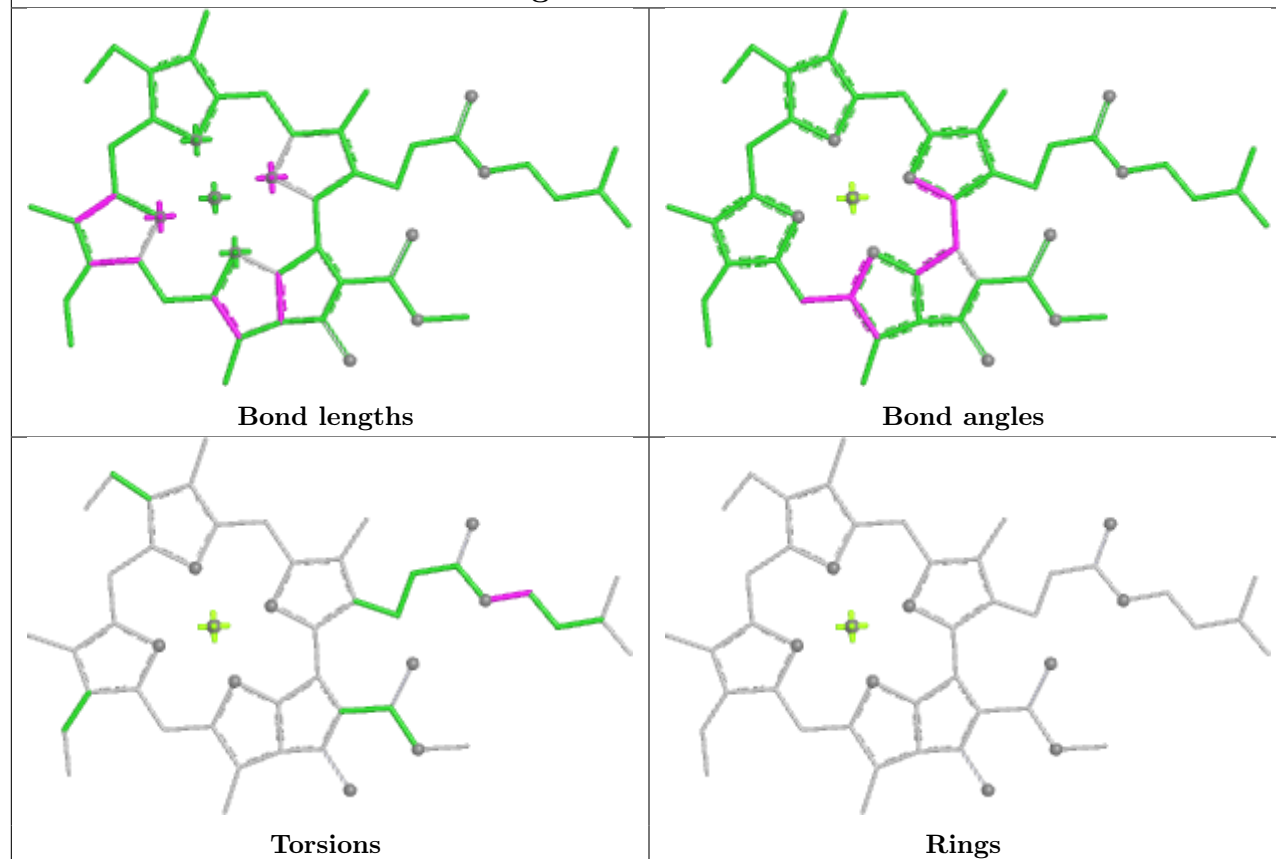
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

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

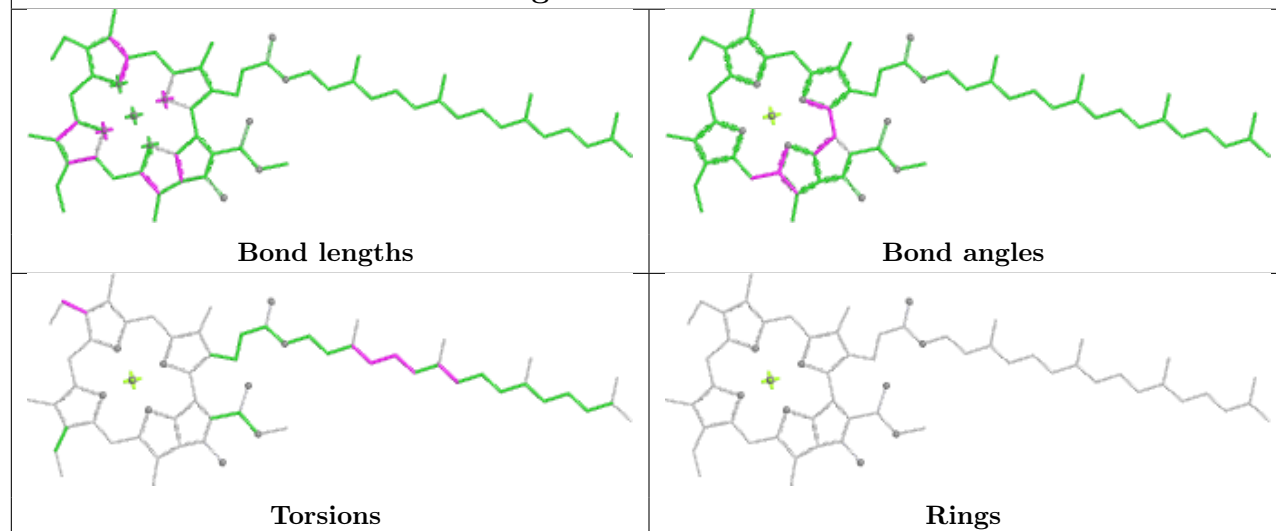


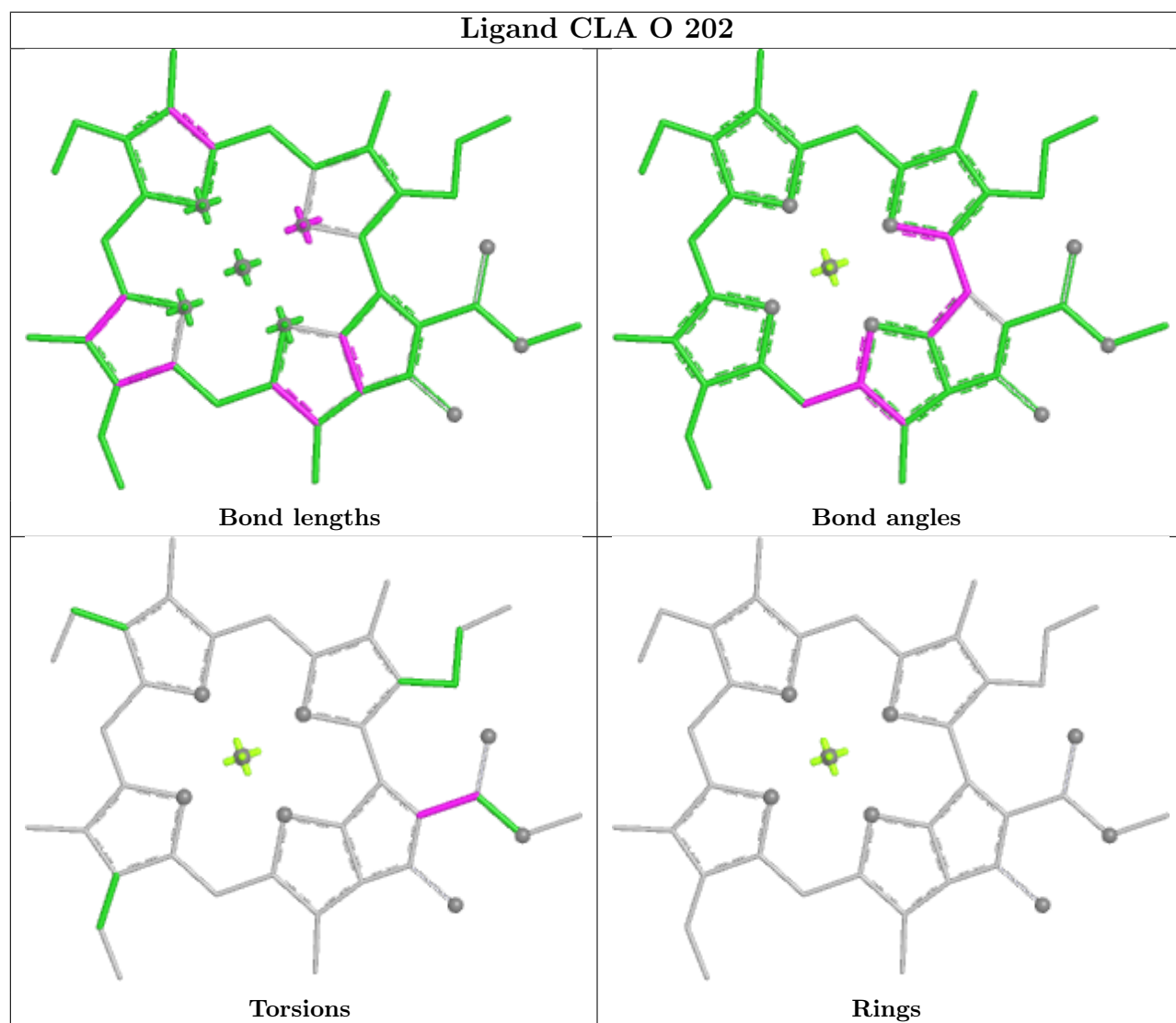
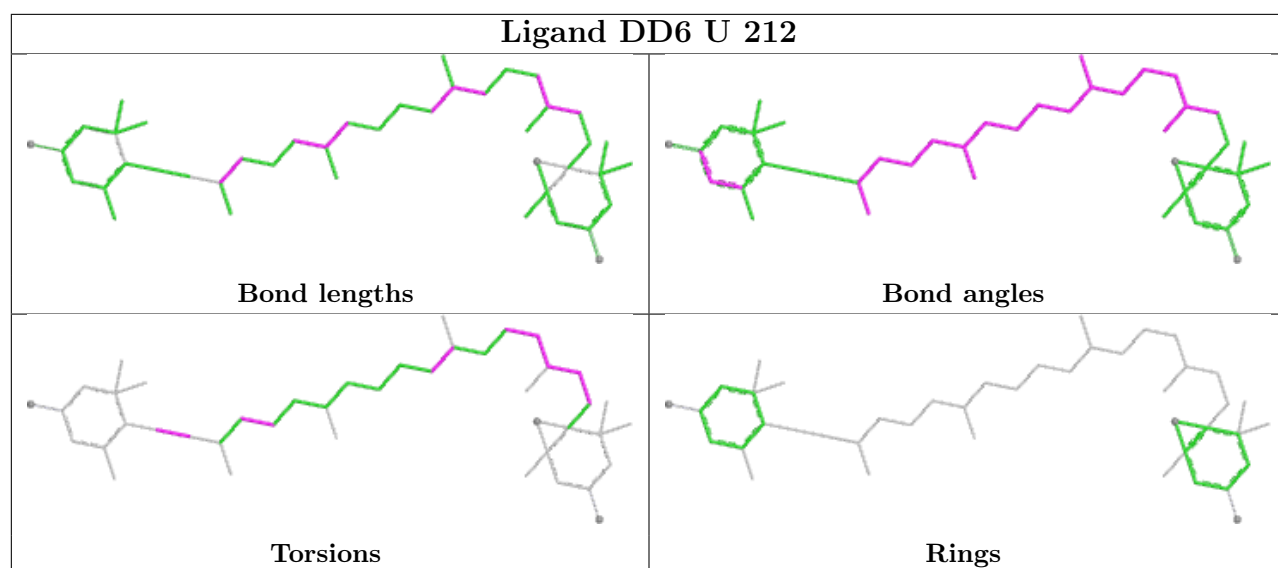


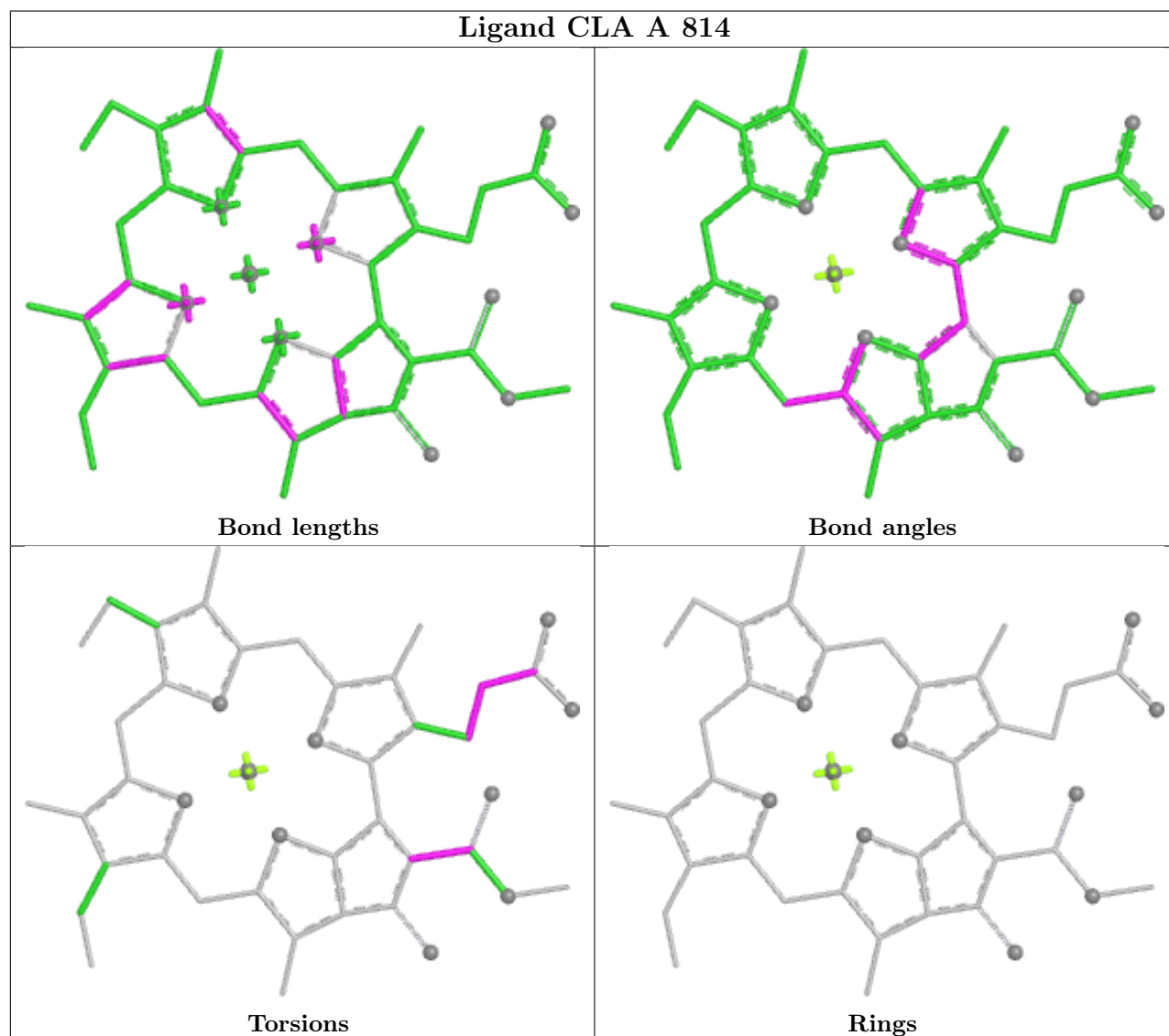
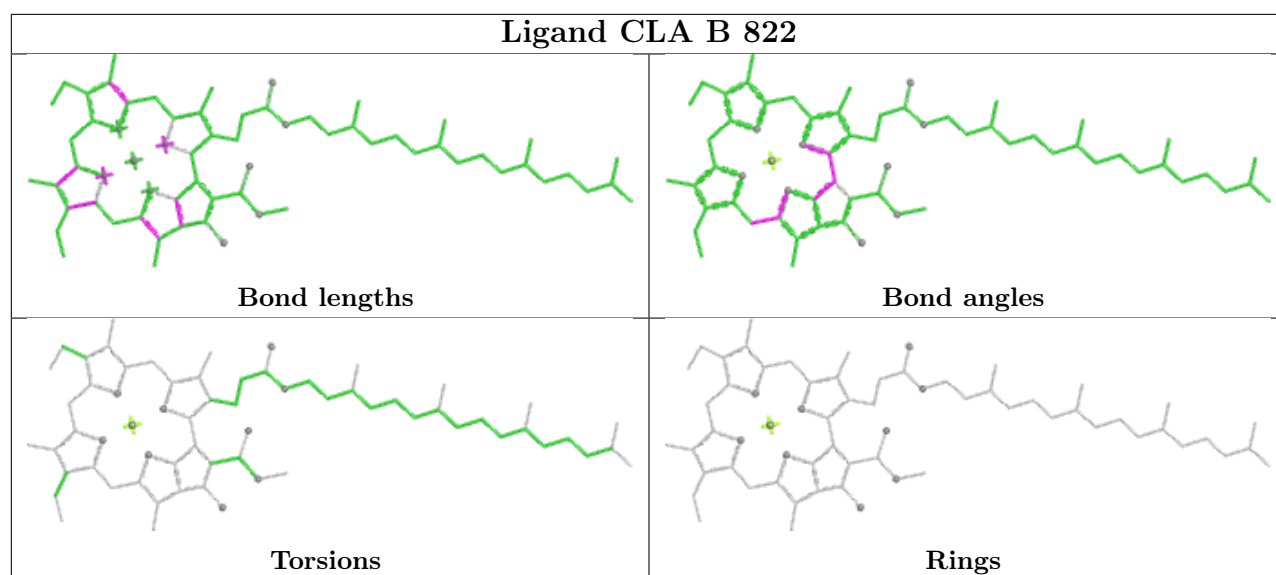
## Ligand CLA A 830

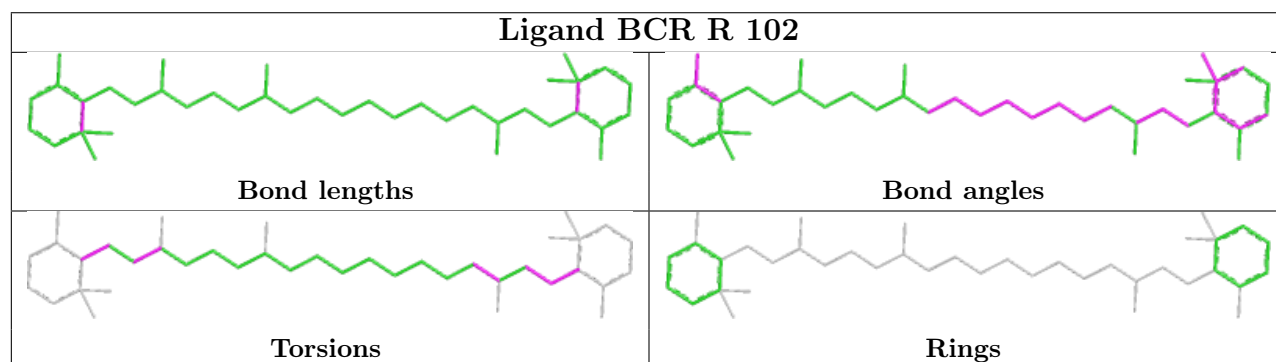
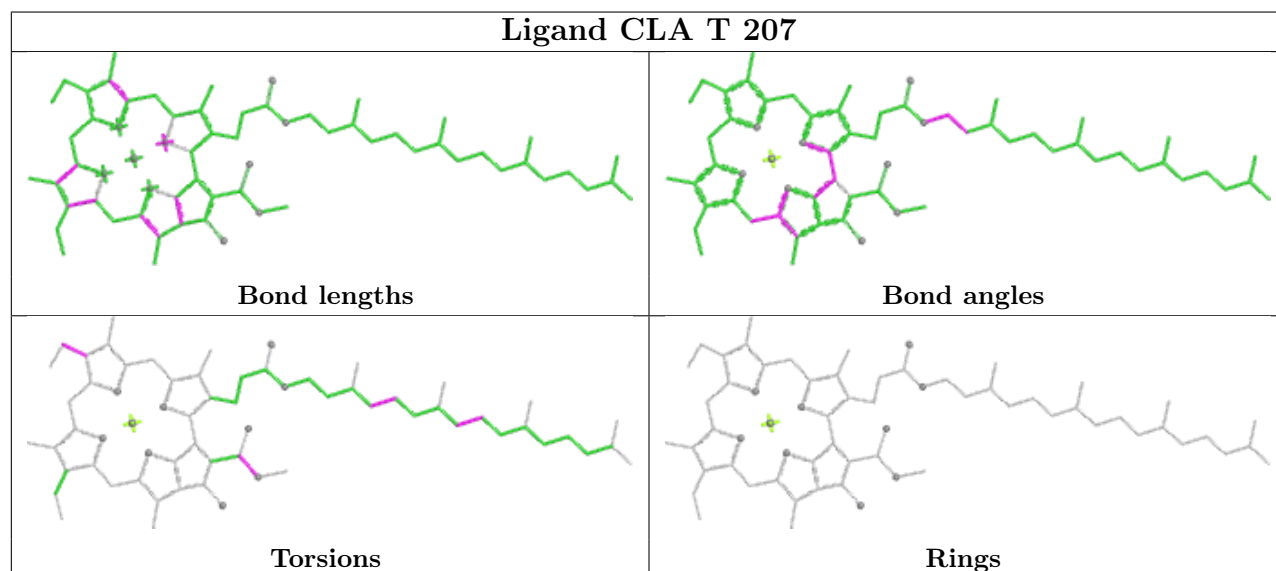
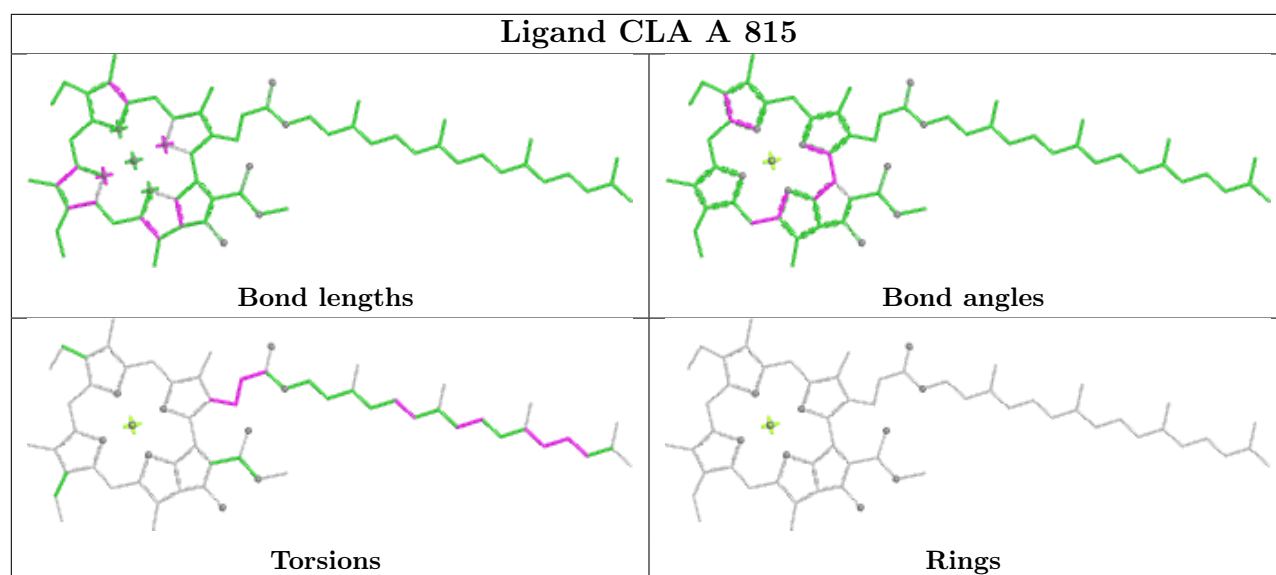


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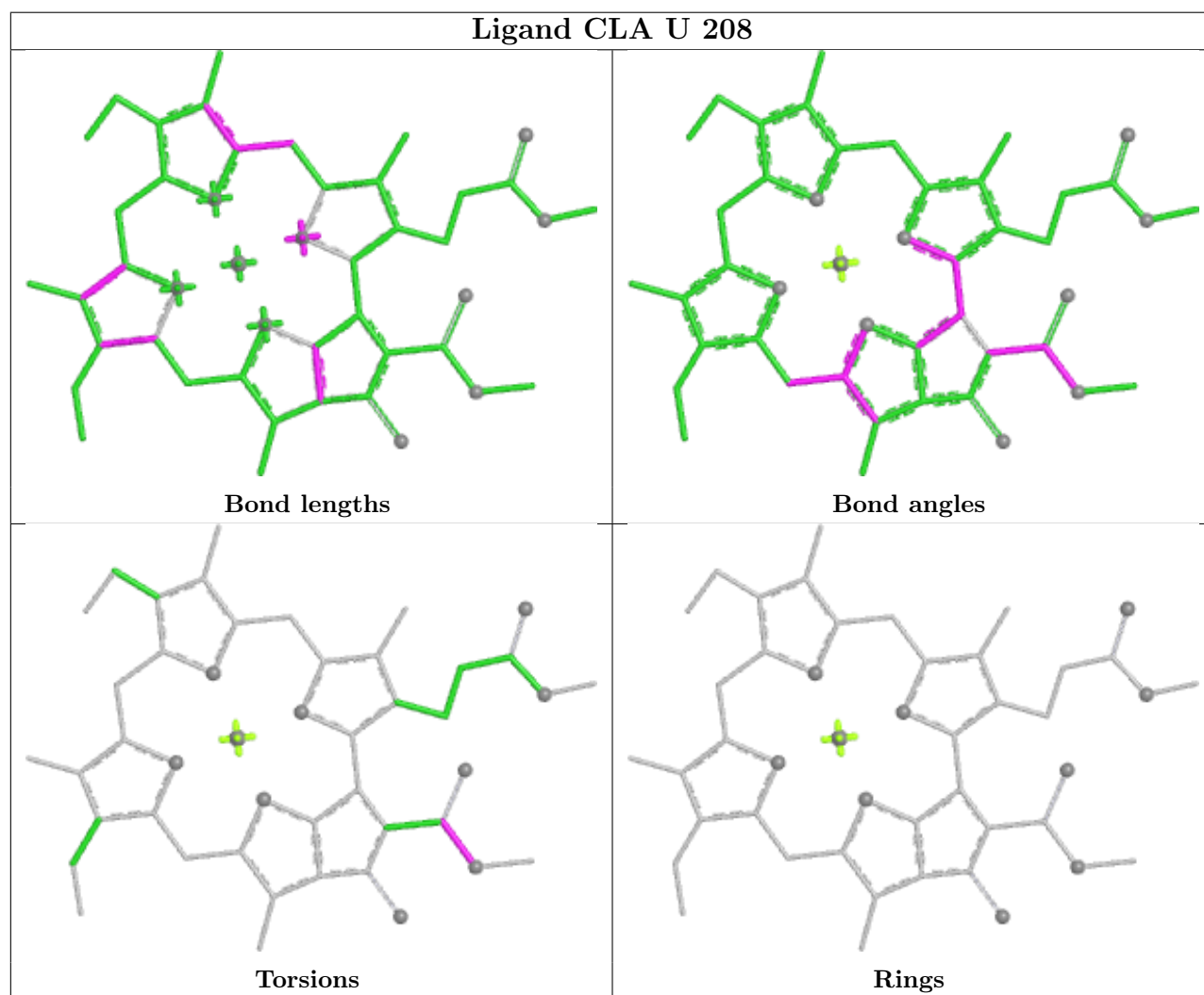
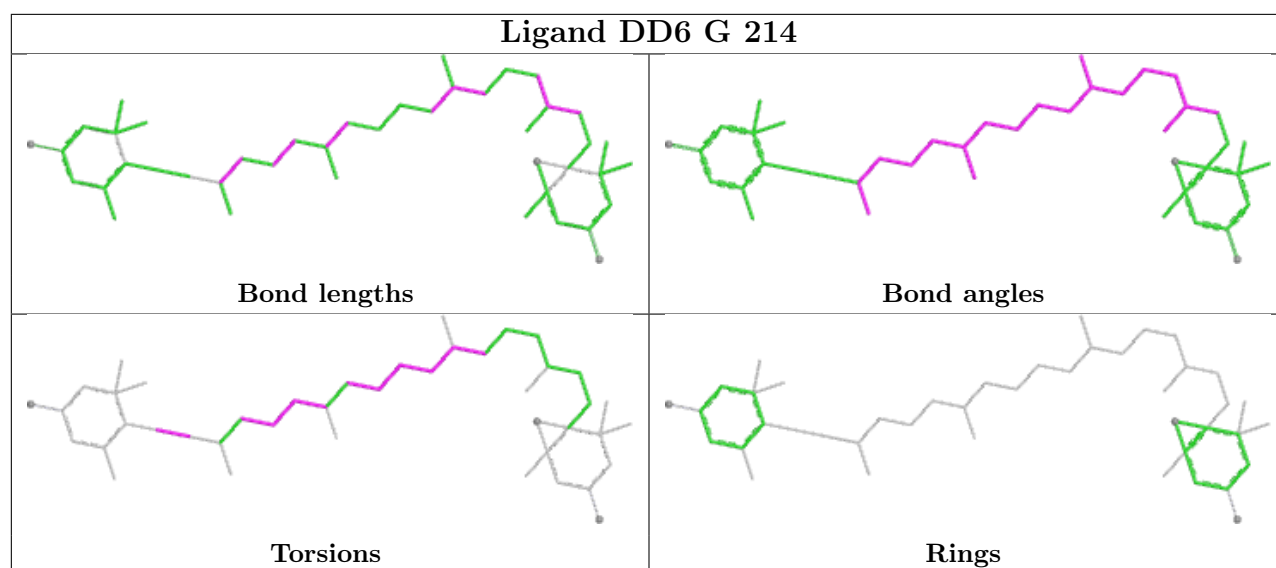


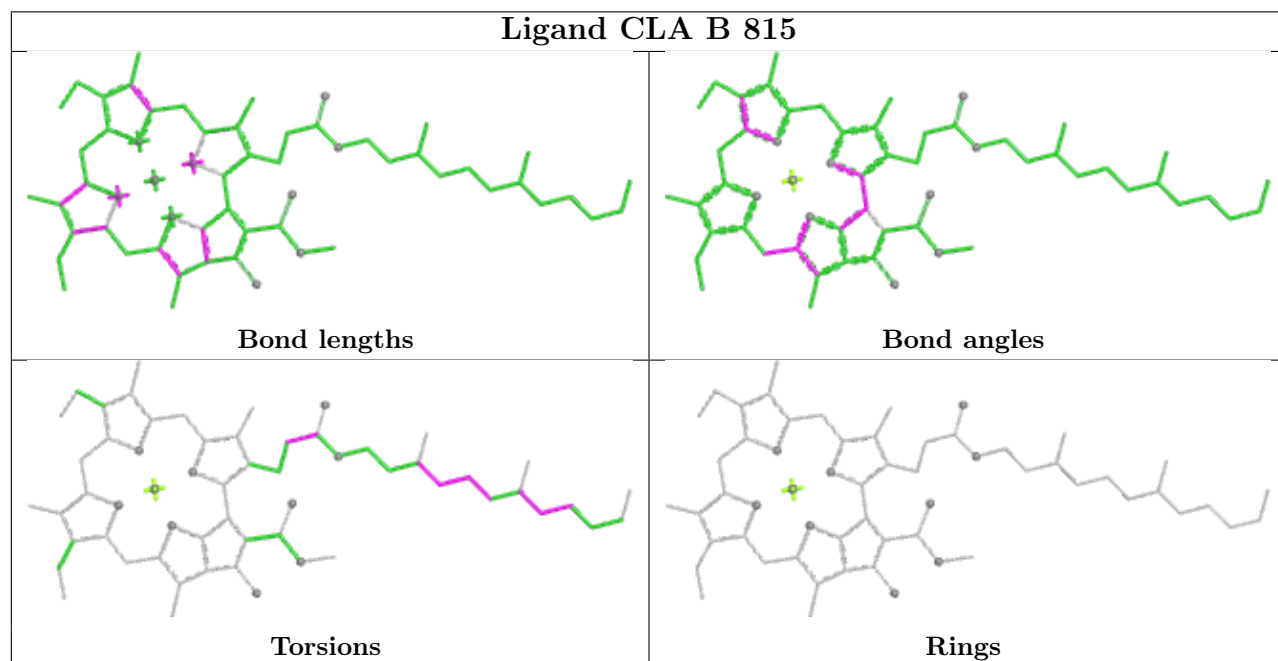
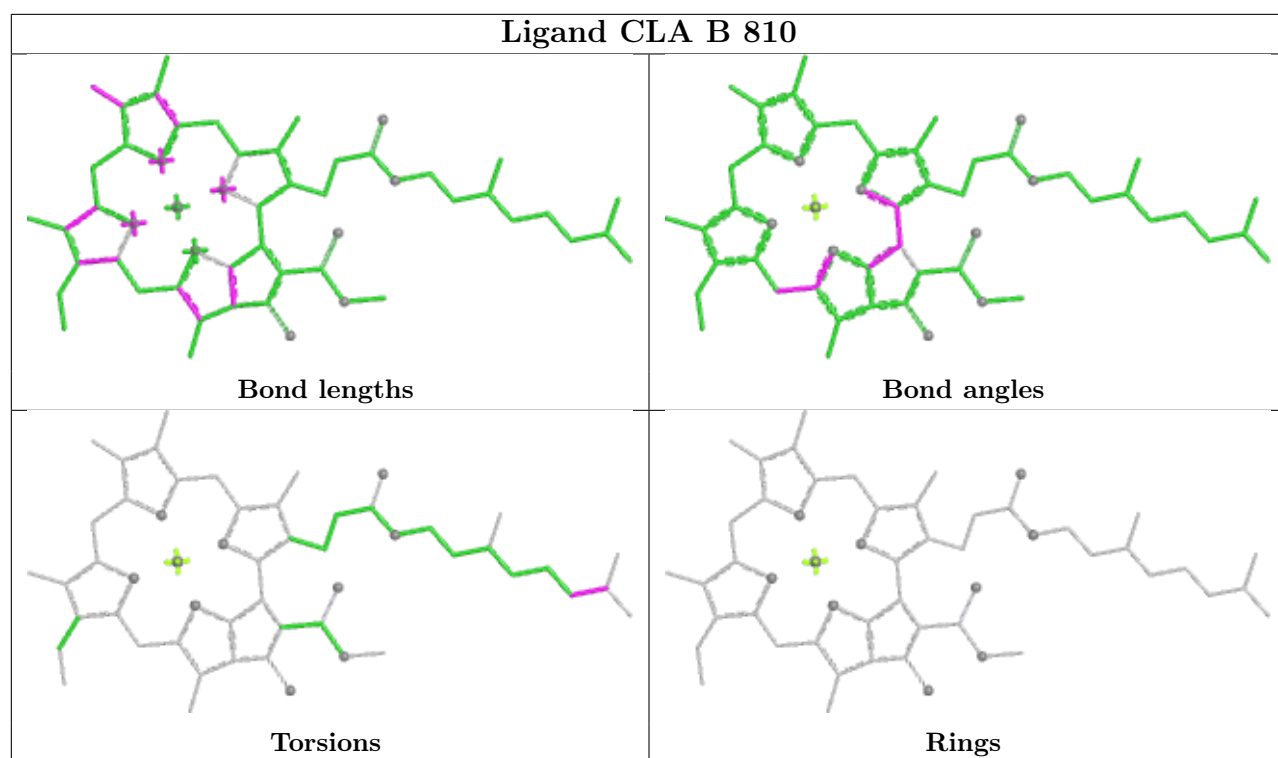




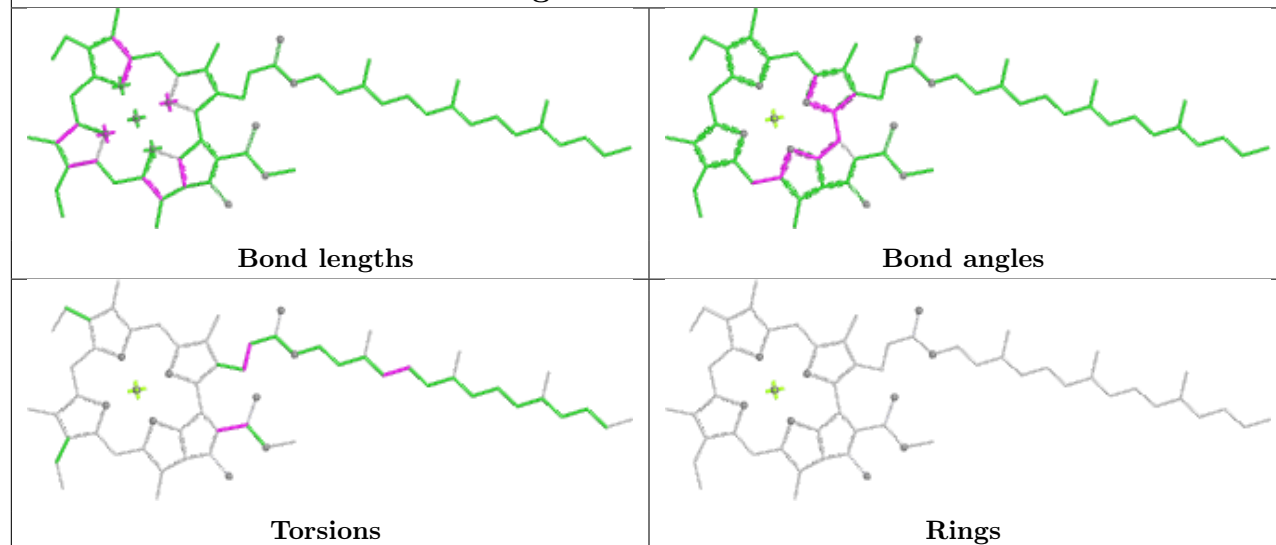




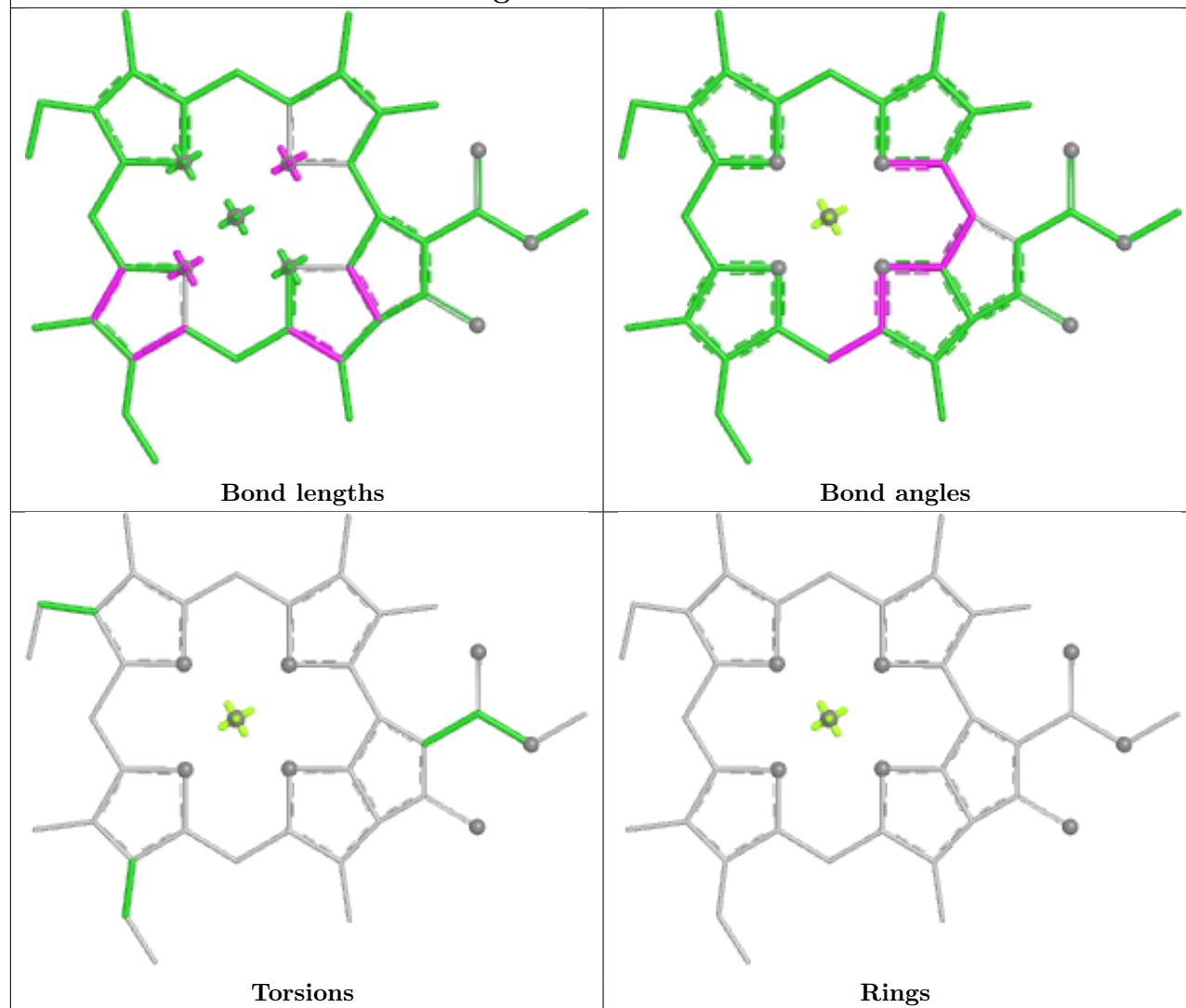




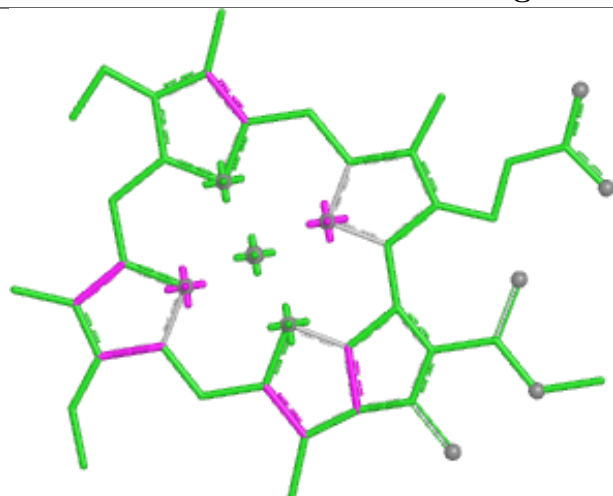
## Ligand CLA B 820



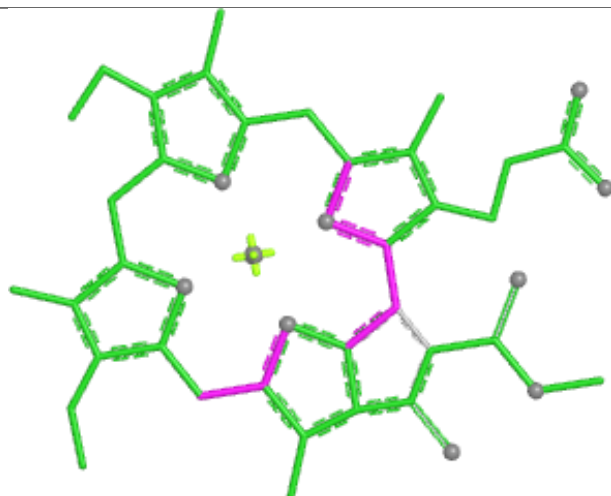
## Ligand CLA G 202



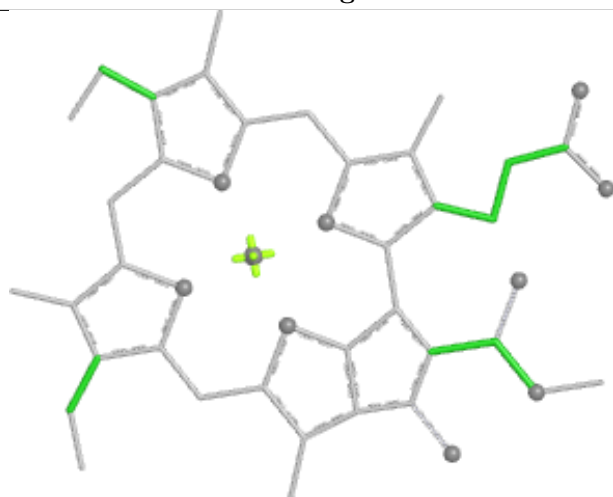
## Ligand CLA A 817



Bond lengths



Bond angles

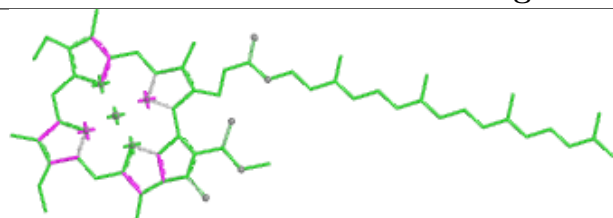


Torsions

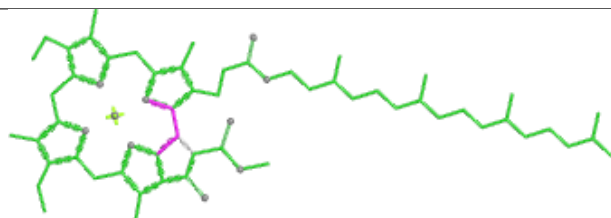


Rings

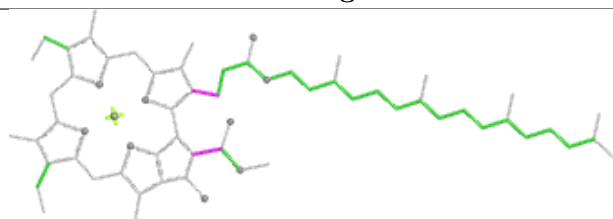
## Ligand CLA A 826



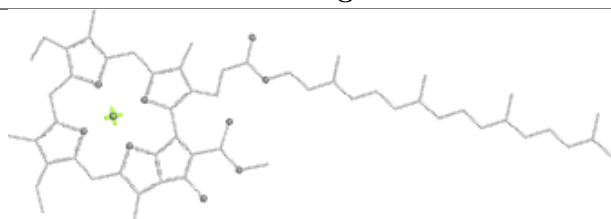
Bond lengths



Bond angles

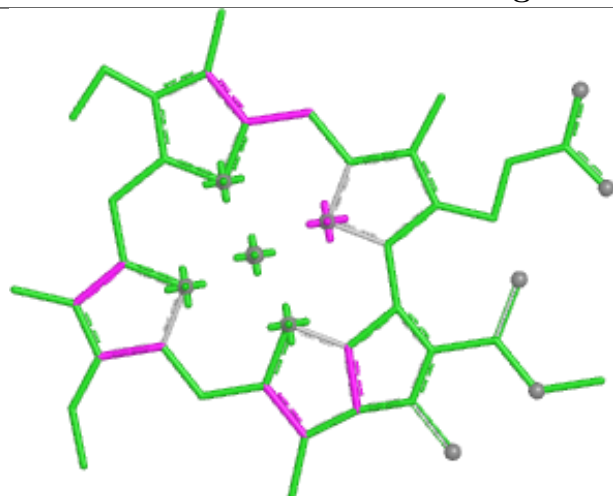


Torsions

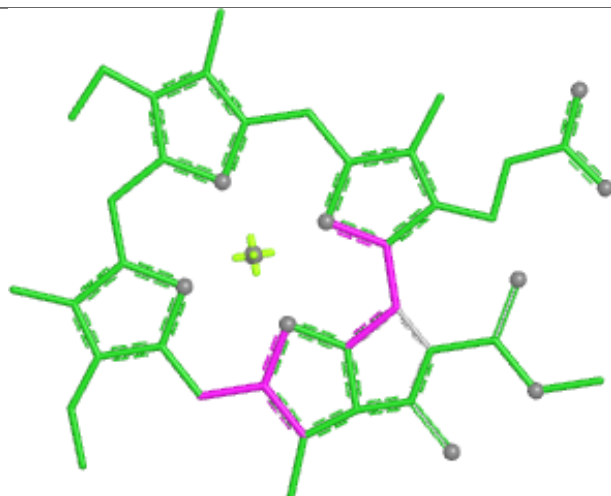


Rings

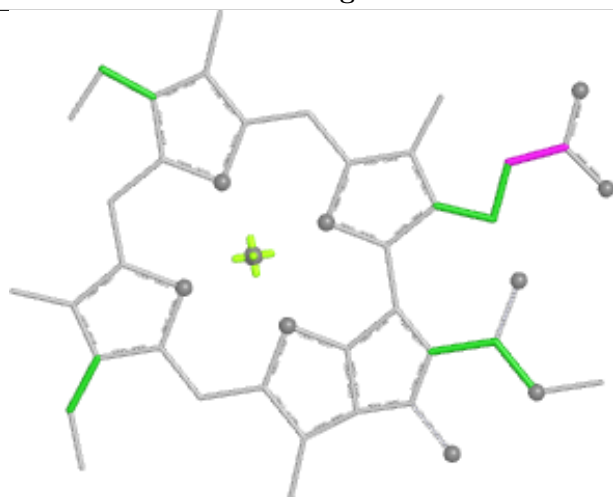
## Ligand CLA G 201



Bond lengths



Bond angles

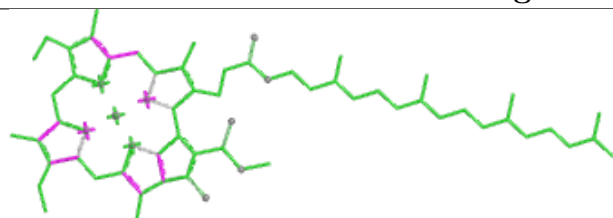


Torsions

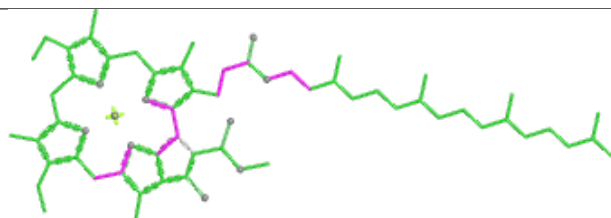


Rings

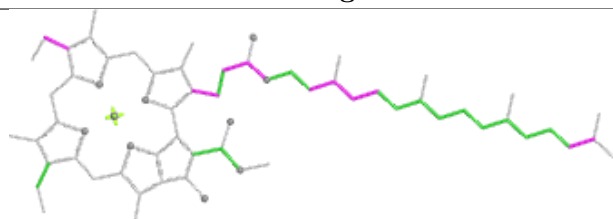
## Ligand CLA A 835



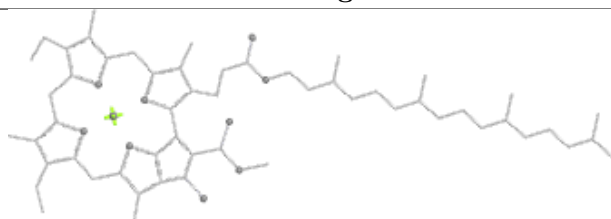
Bond lengths



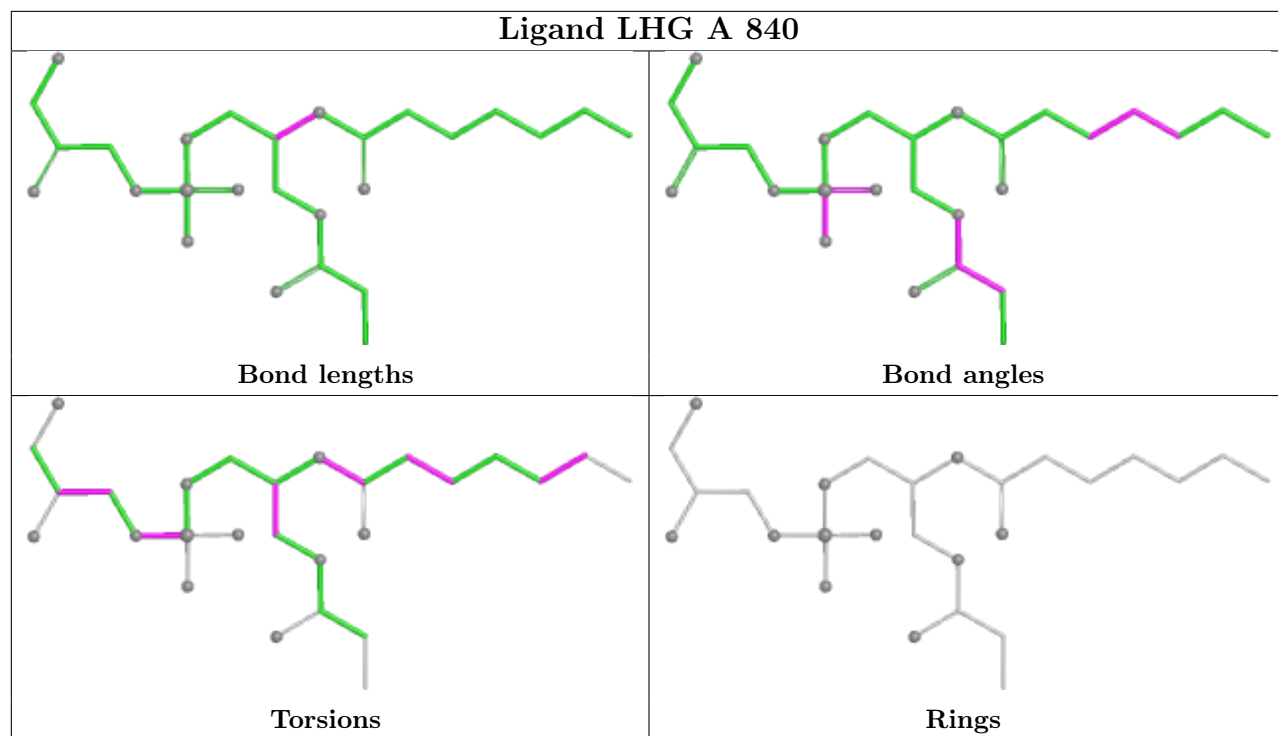
Bond angles



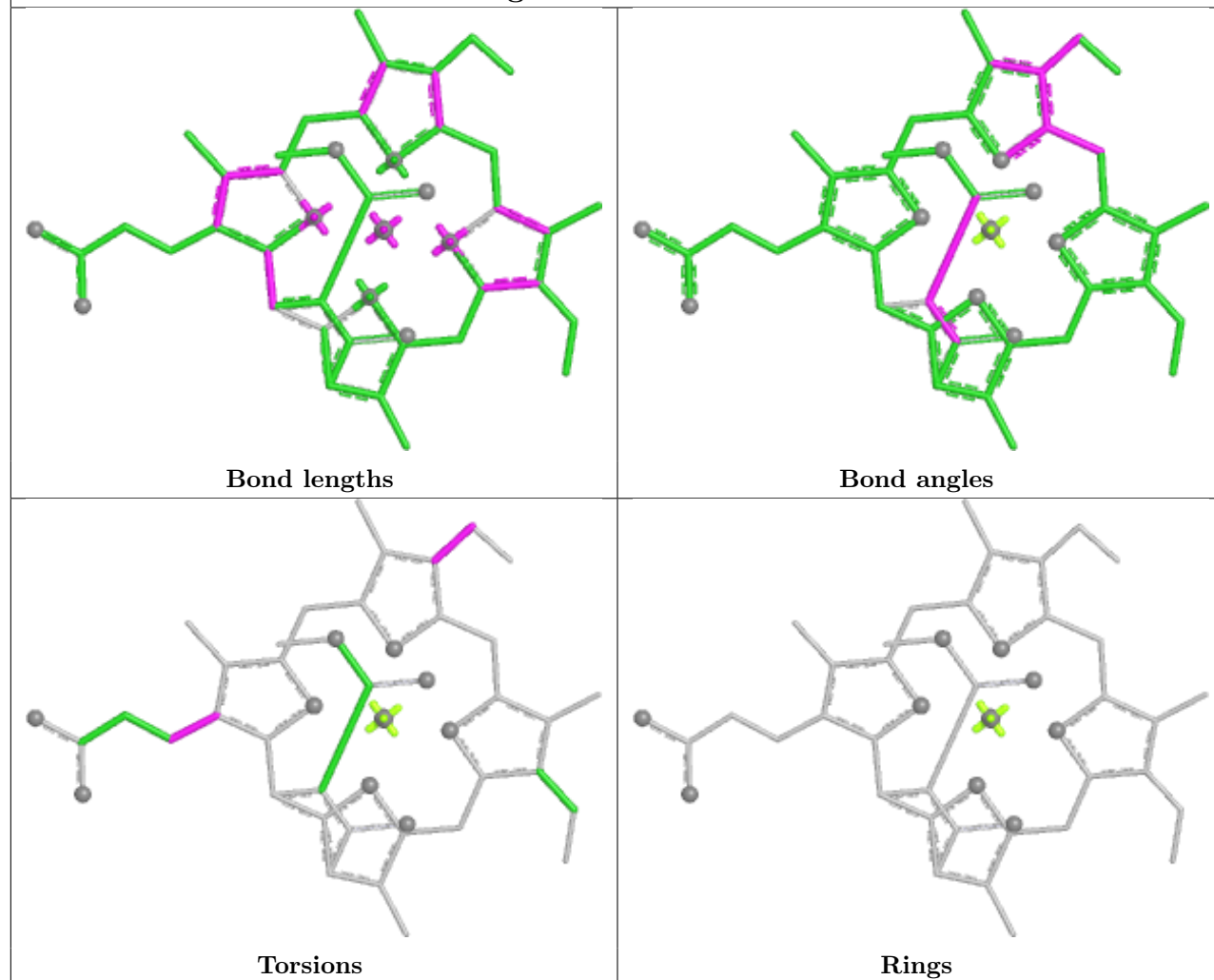
Torsions



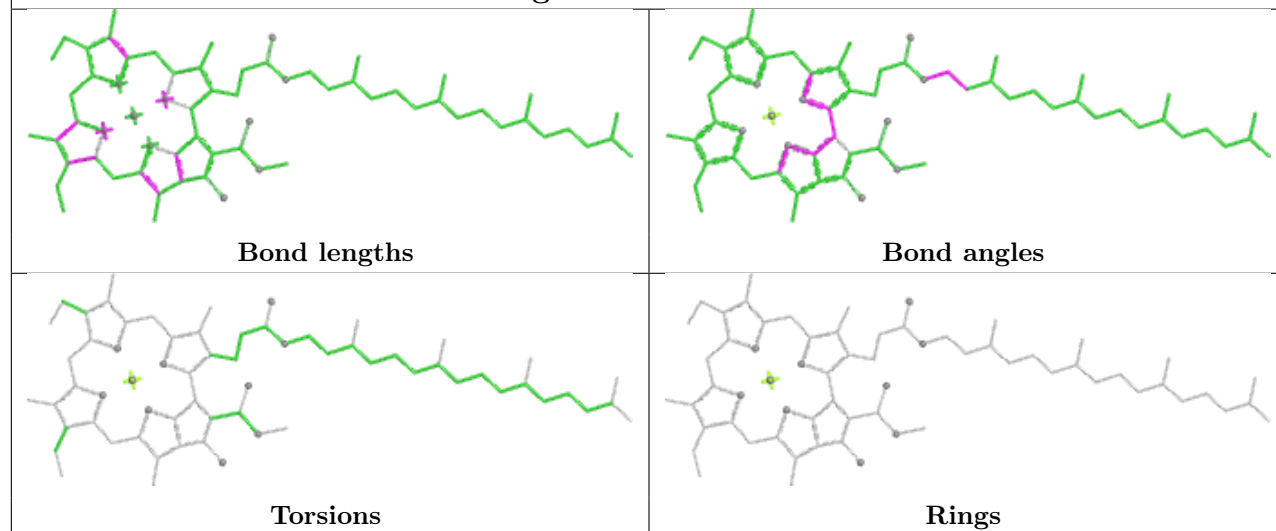
Rings

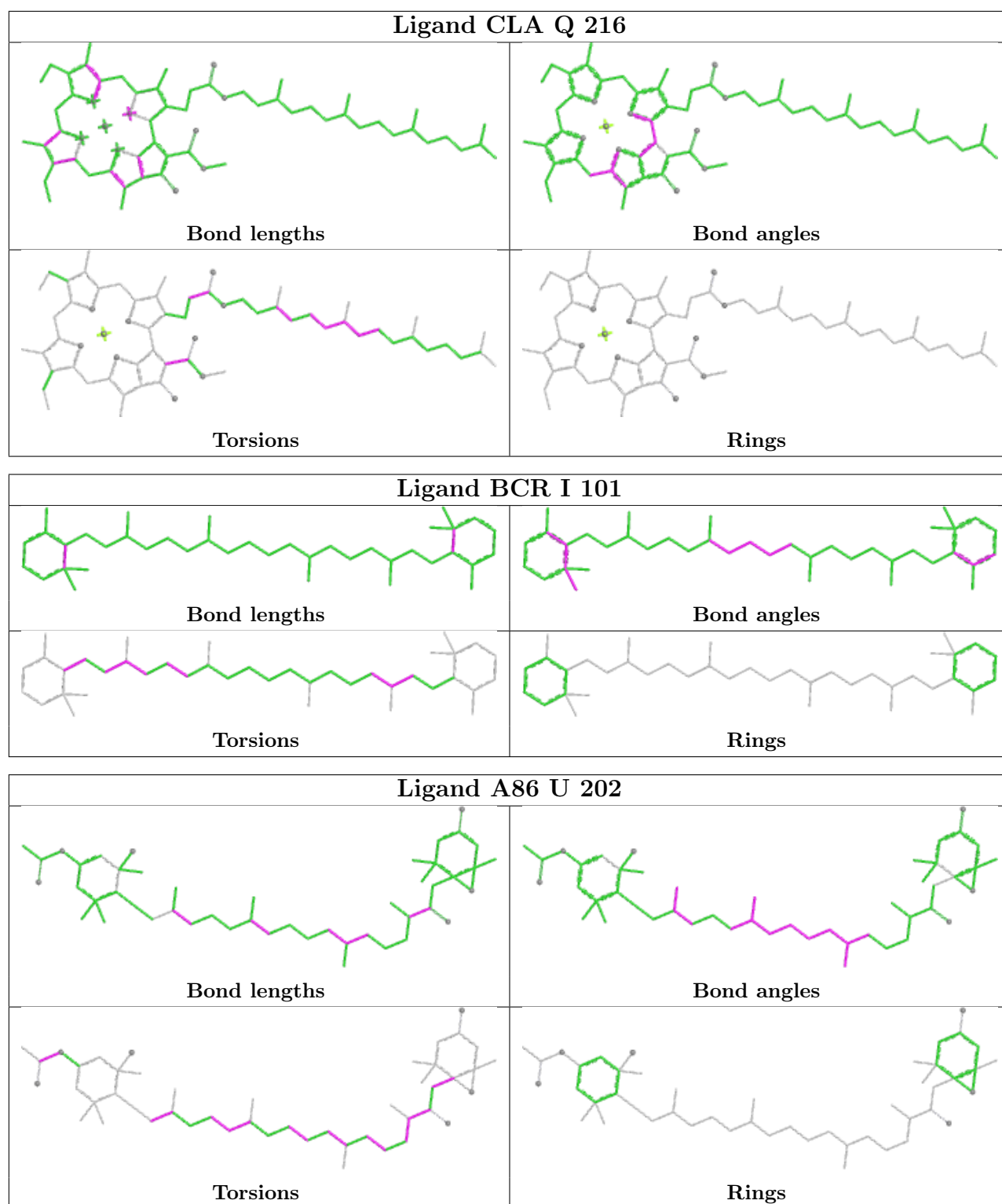


## Ligand KC1 U 213



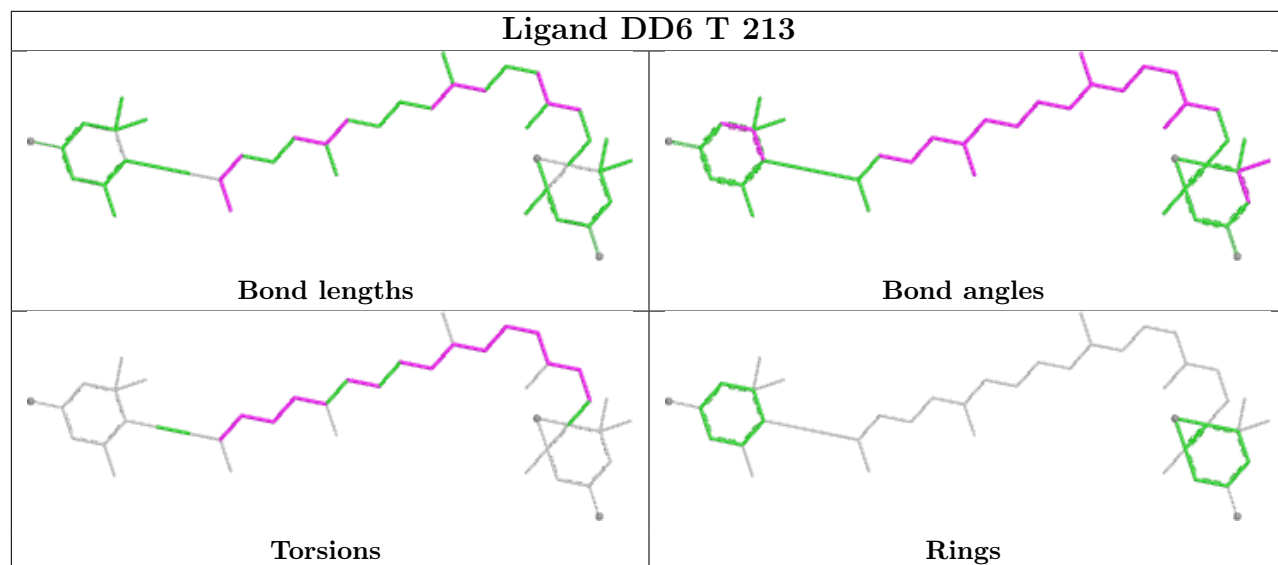
## Ligand CLA B 835



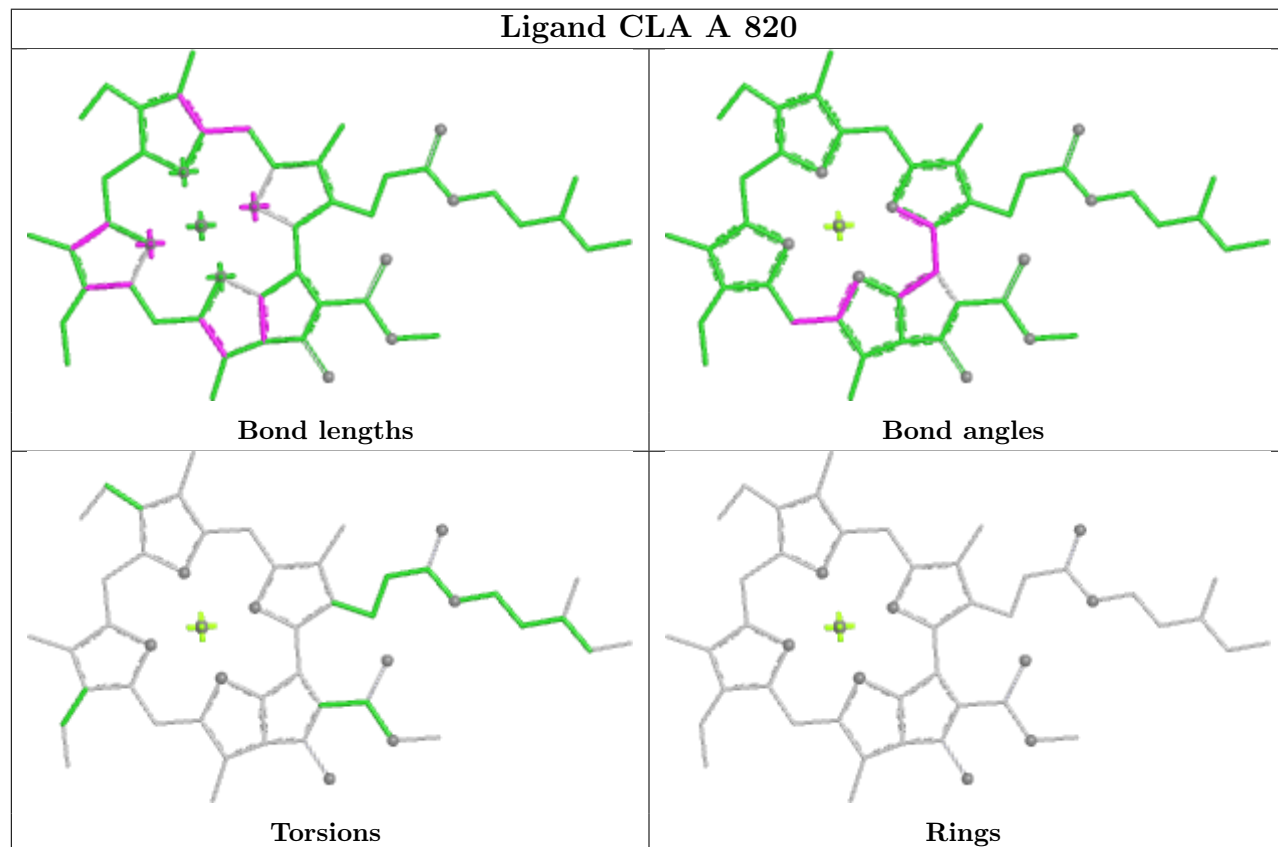




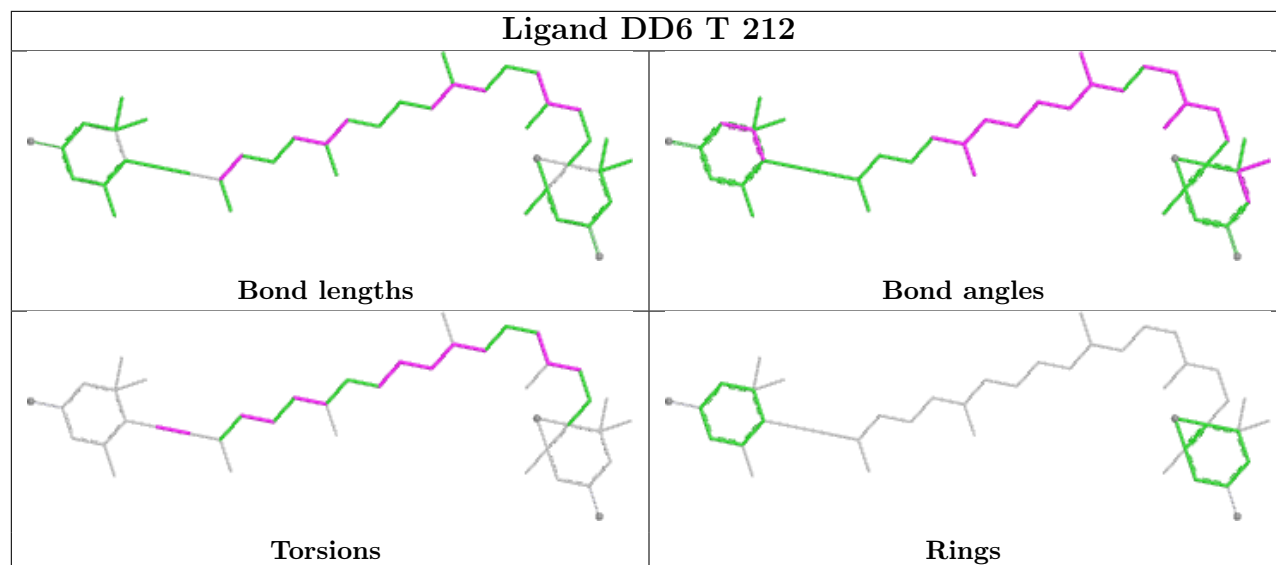
## Ligand DD6 T 213



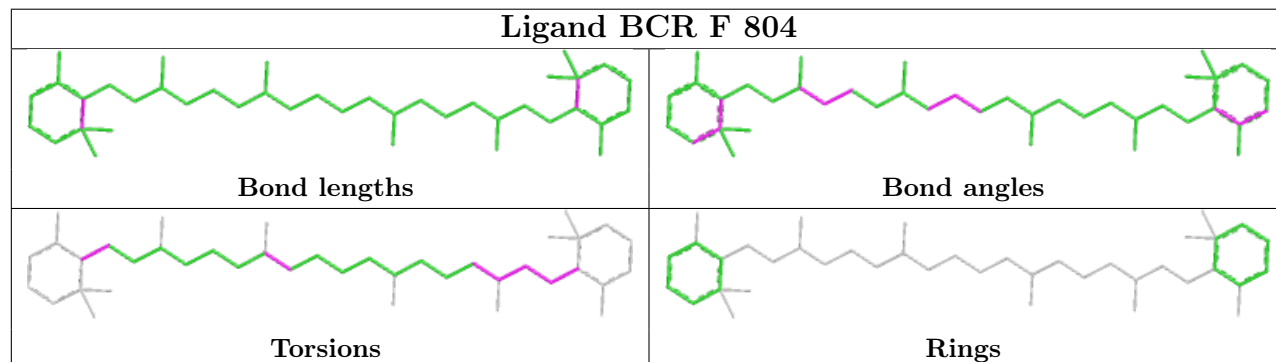
## Ligand CLA A 820



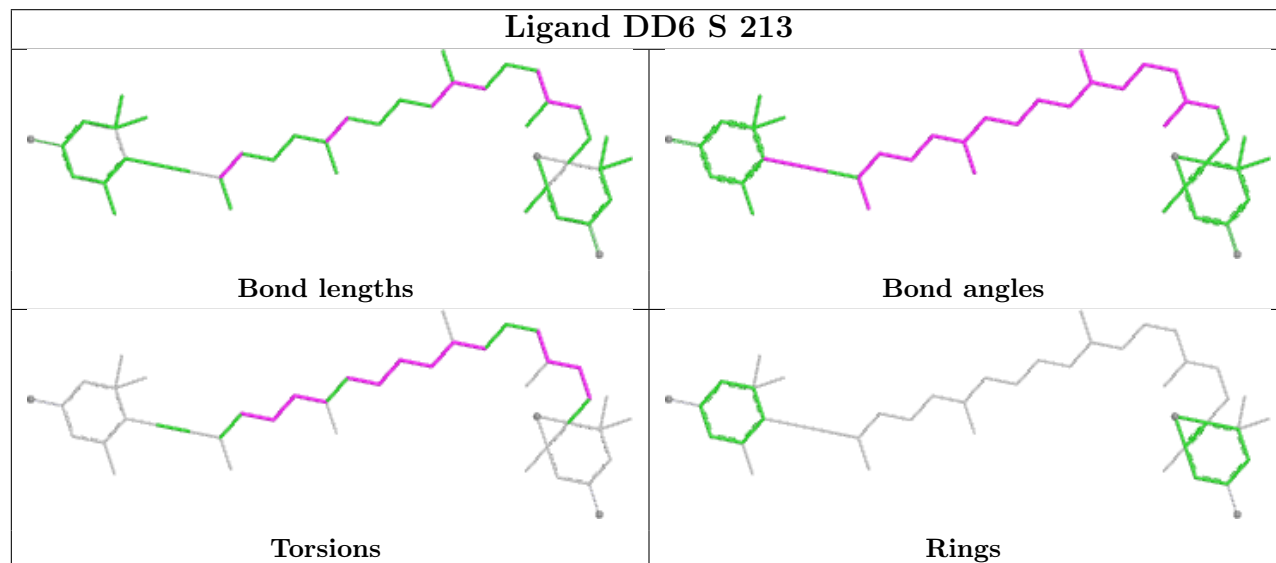
## Ligand DD6 T 212

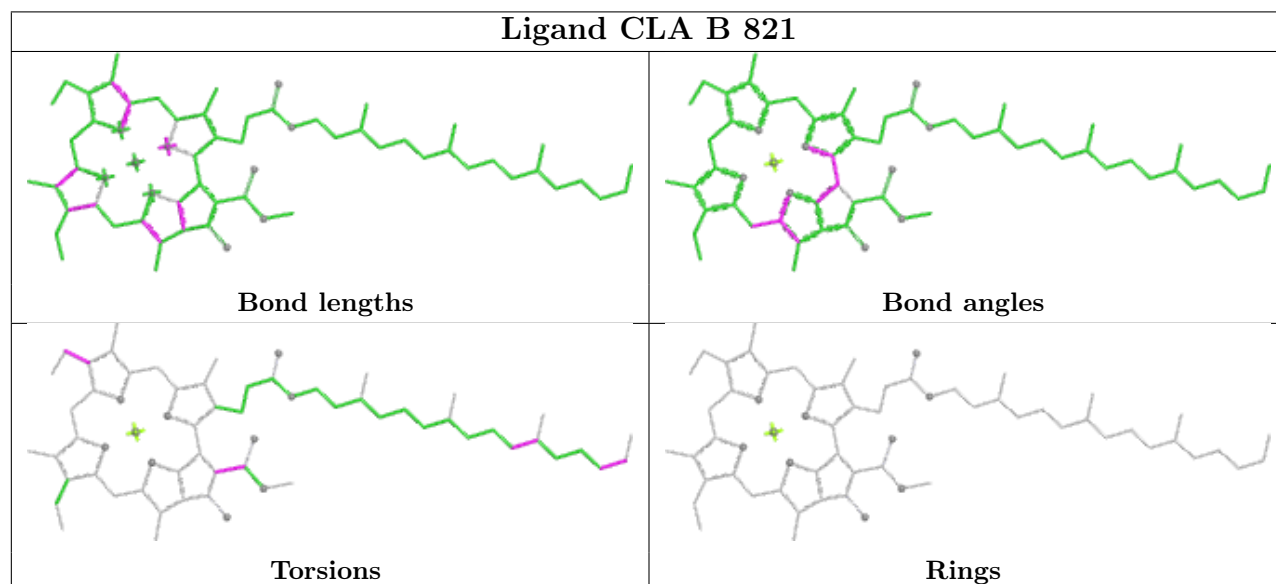
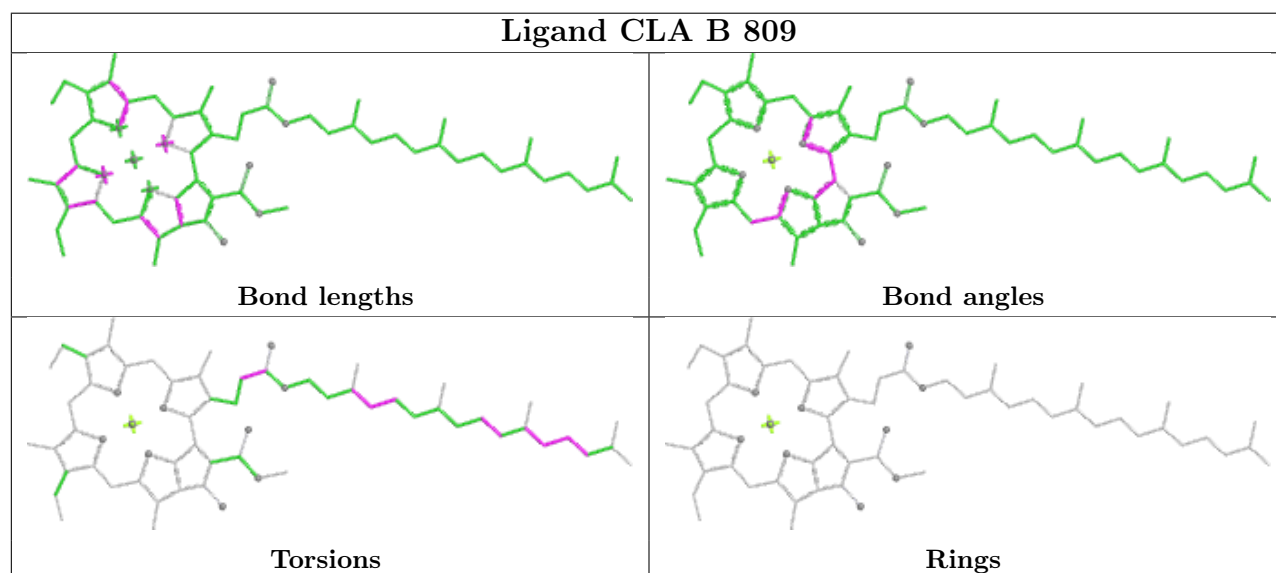
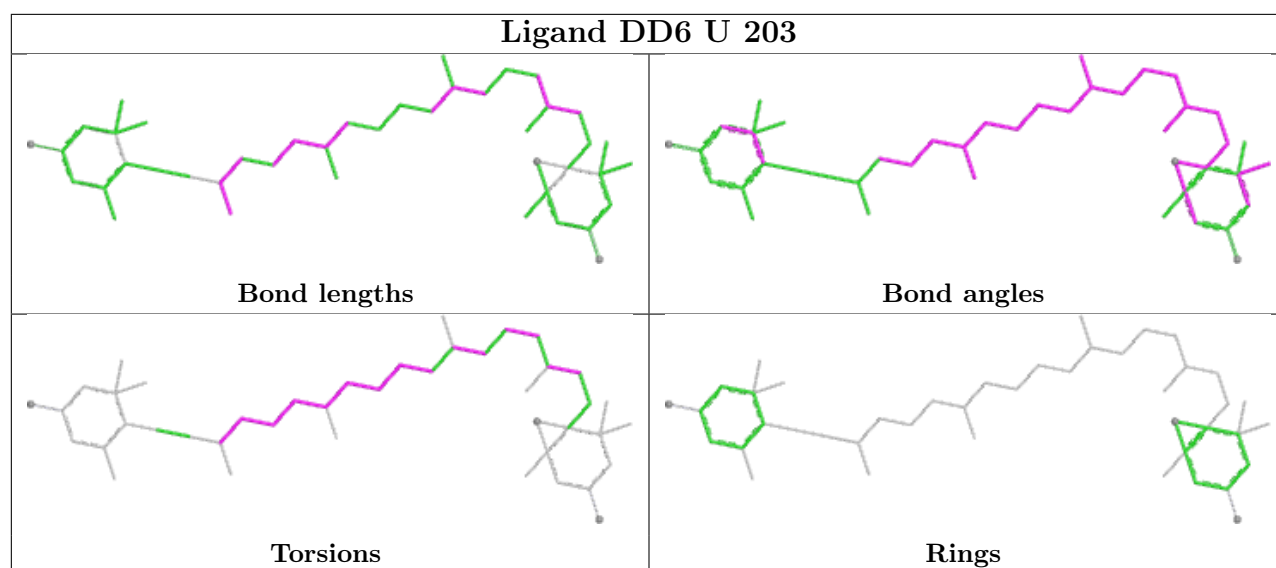


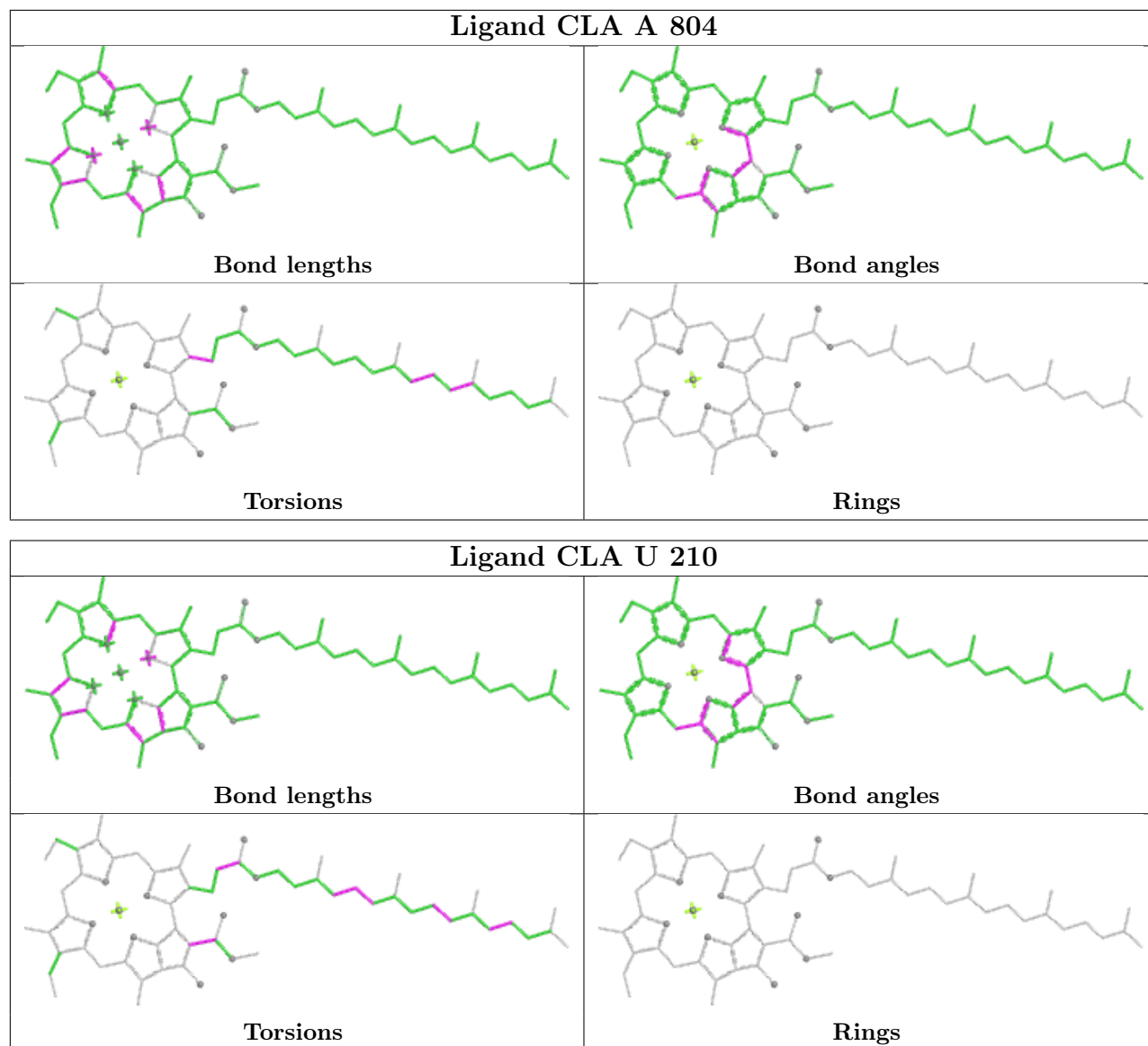
## Ligand BCR F 804



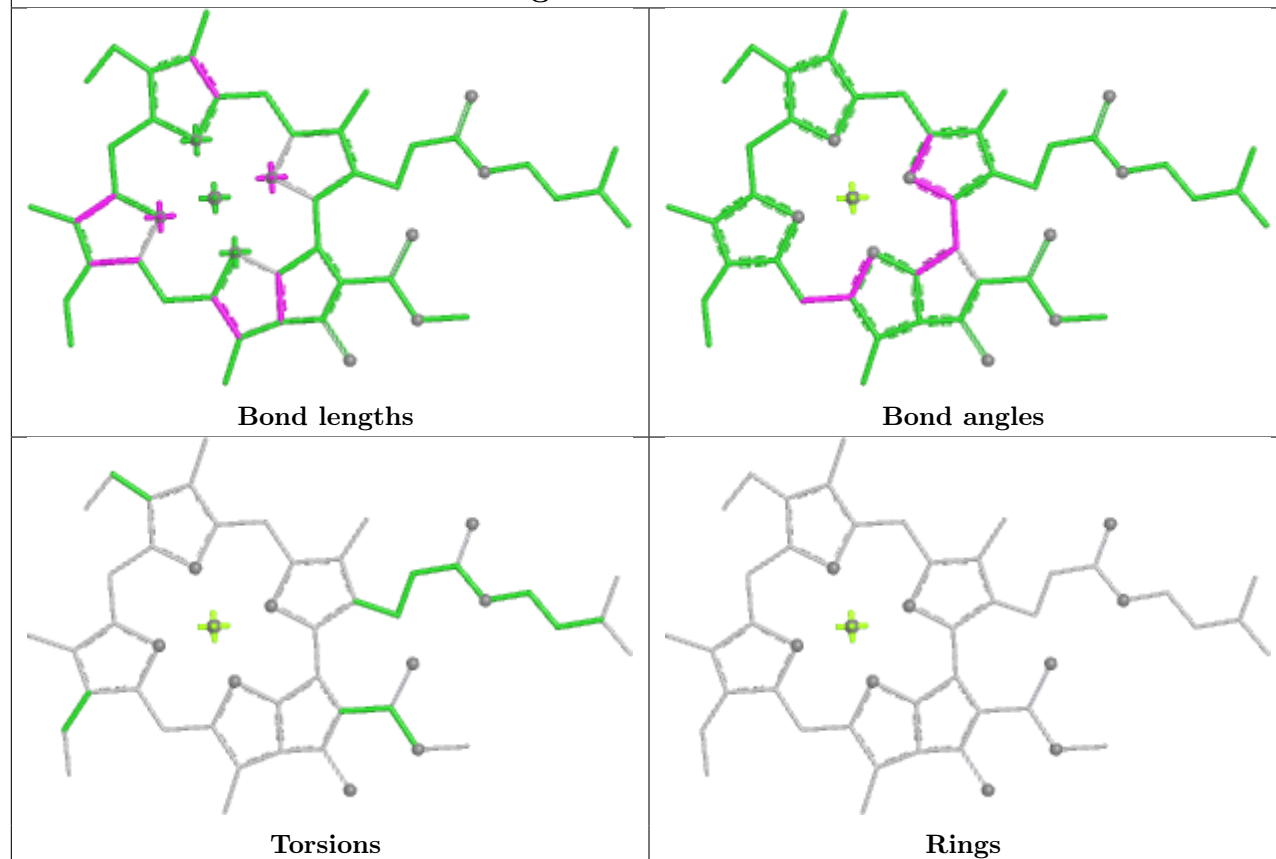
## Ligand DD6 S 213



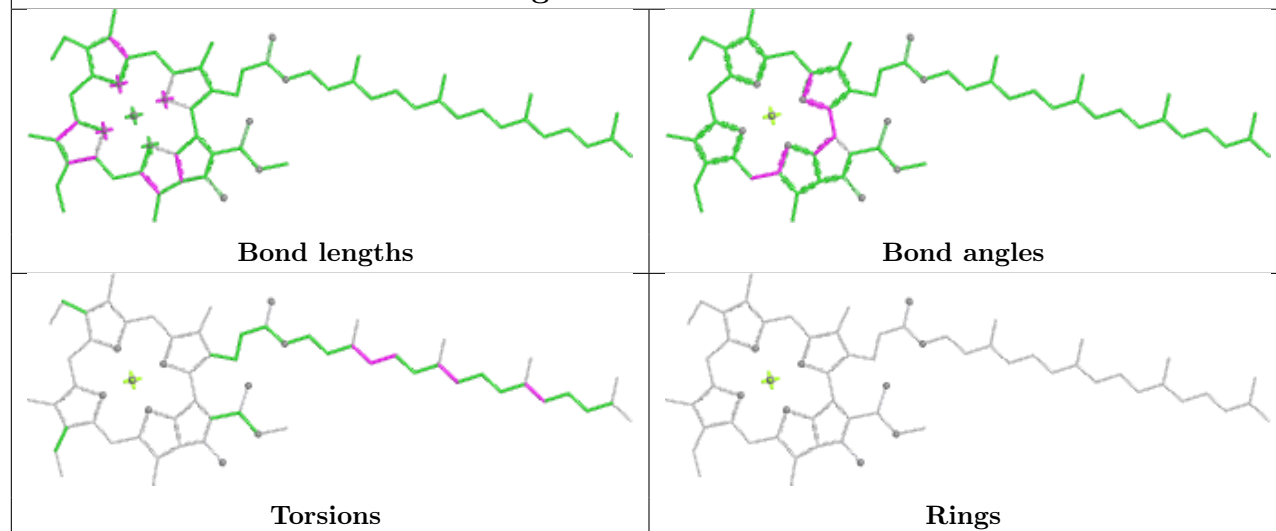




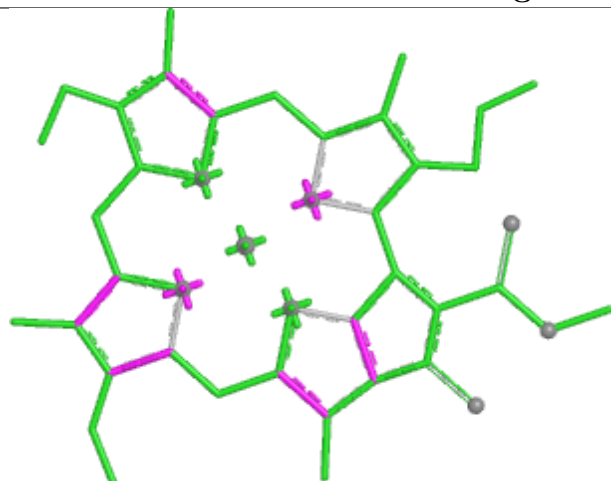
## Ligand CLA A 813



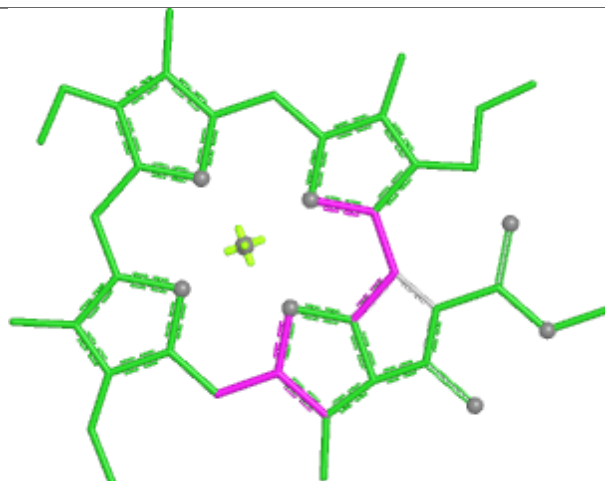
## Ligand CLA A 834



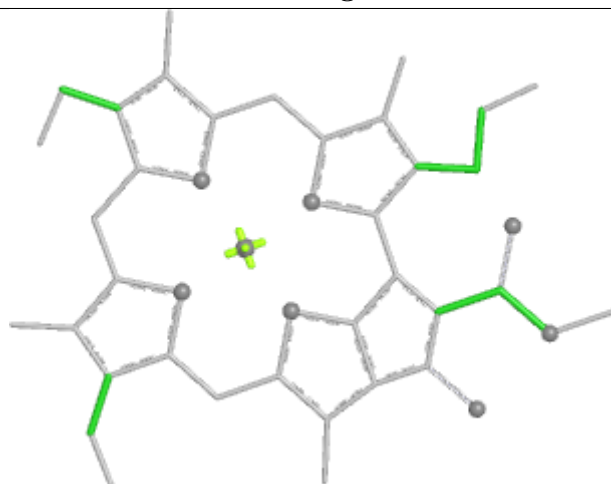
## Ligand CLA A 819



Bond lengths



Bond angles

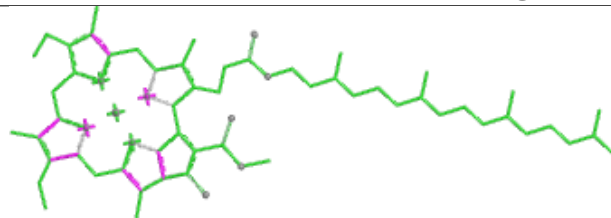


Torsions

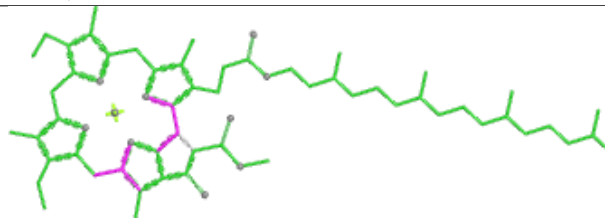


Rings

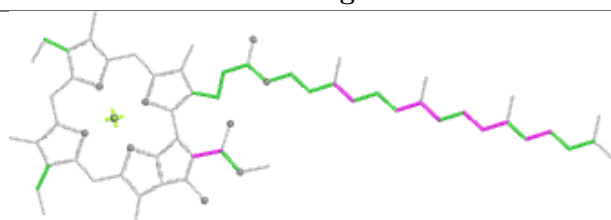
## Ligand CLA Q 209



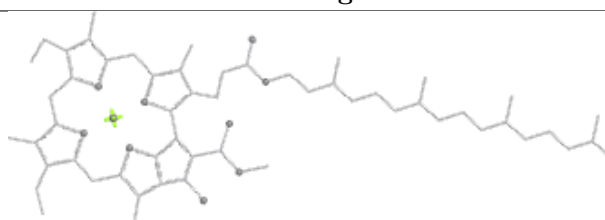
Bond lengths



Bond angles

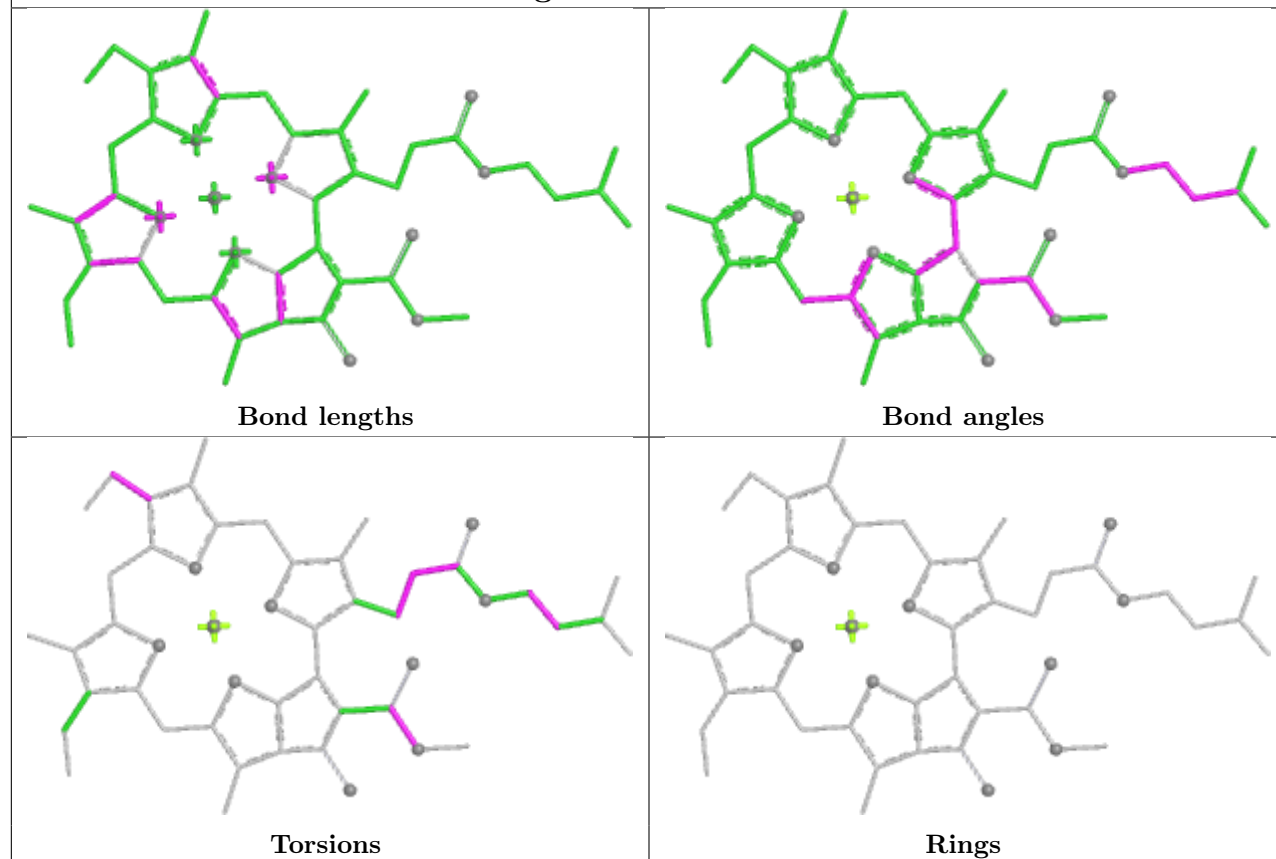


Torsions

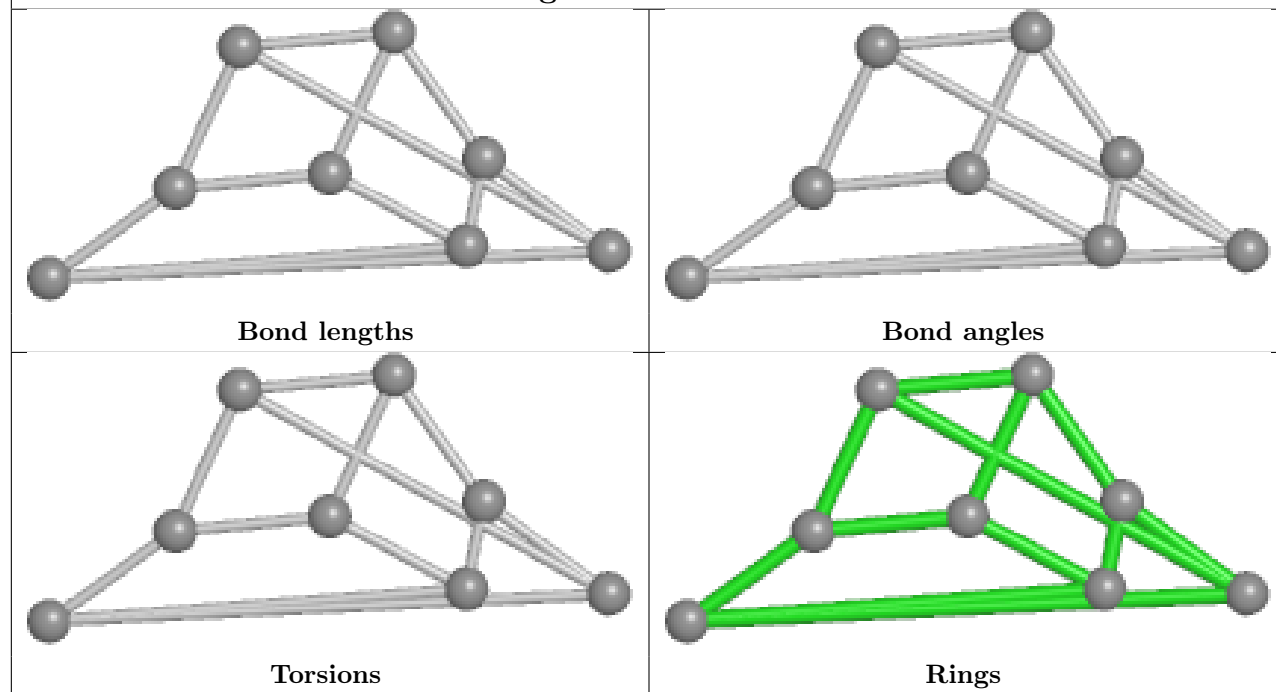


Rings

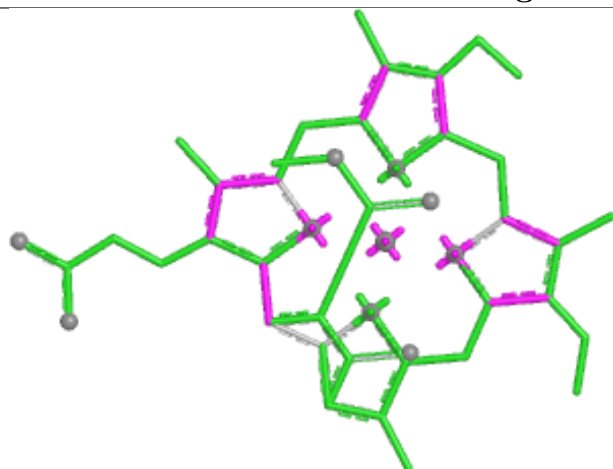
## Ligand CLA L 204



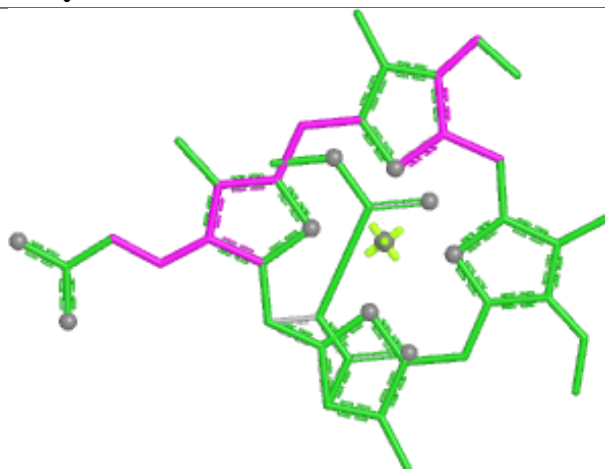
## Ligand SF4 C 101



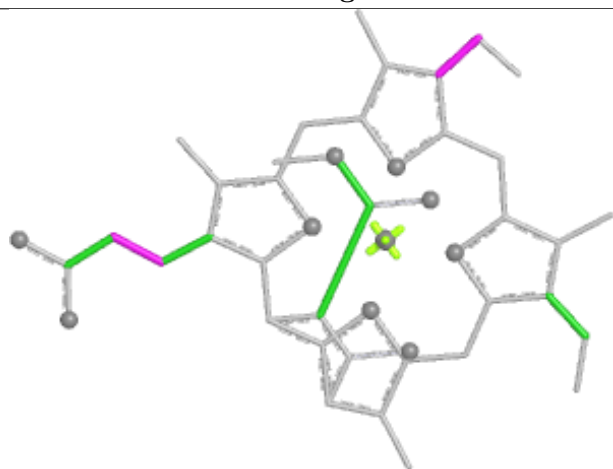
## Ligand KC1 Q 210



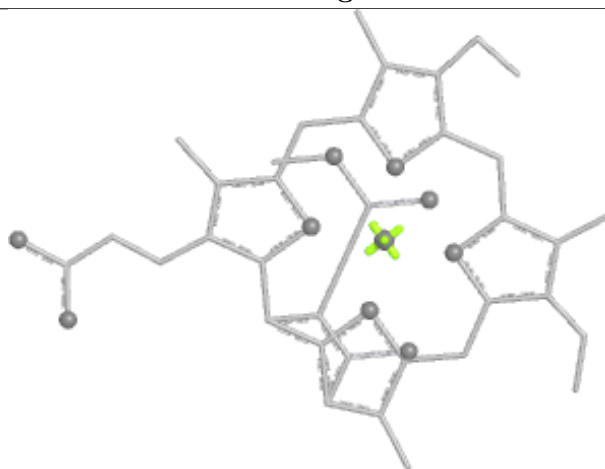
Bond lengths



Bond angles



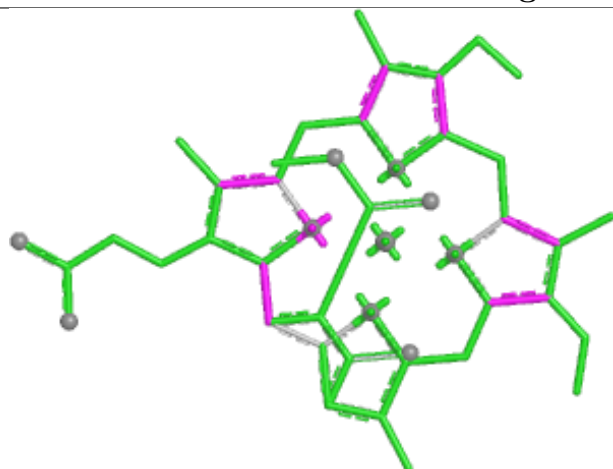
Torsions



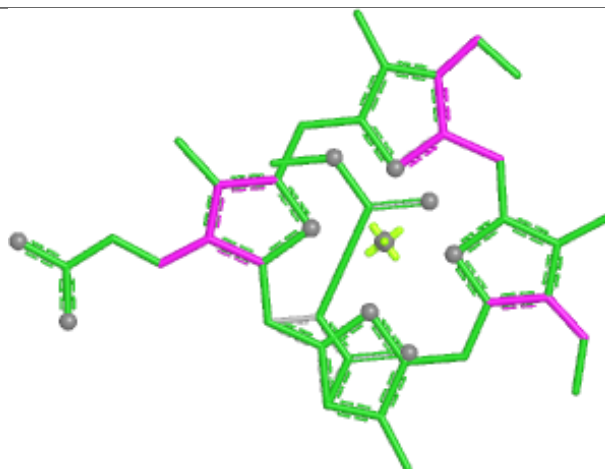
Rings



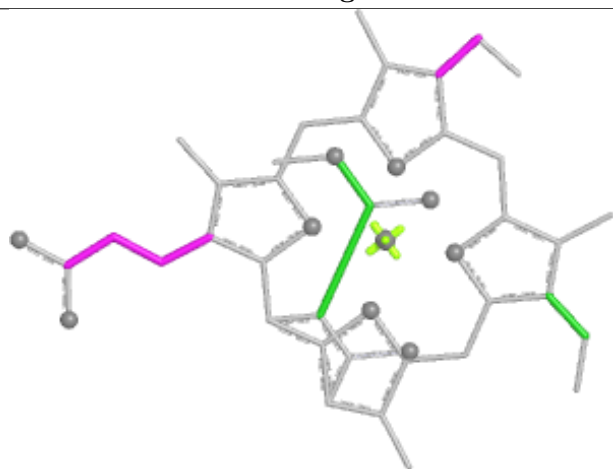
## Ligand KC1 S 211



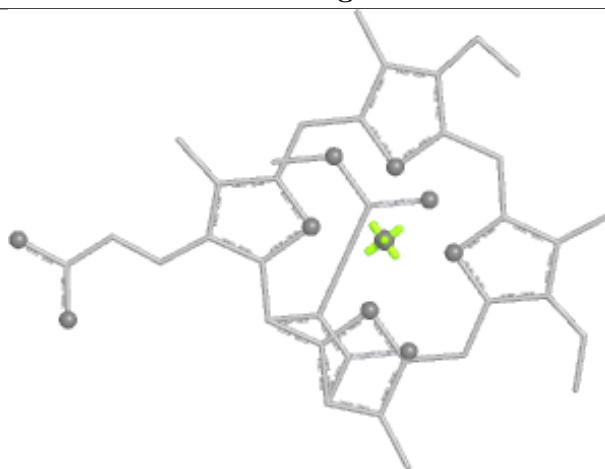
Bond lengths



Bond angles

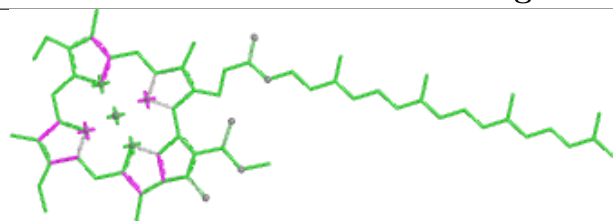


Torsions

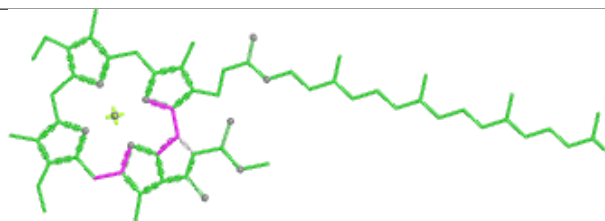


Rings

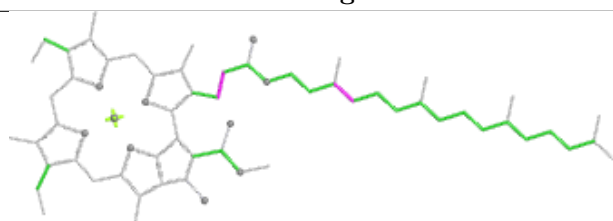
## Ligand CLA B 807



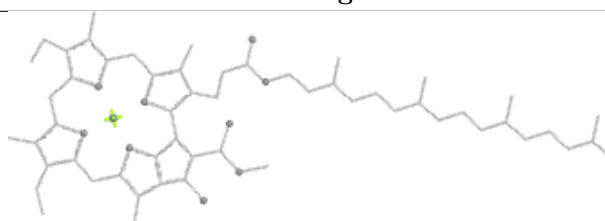
Bond lengths



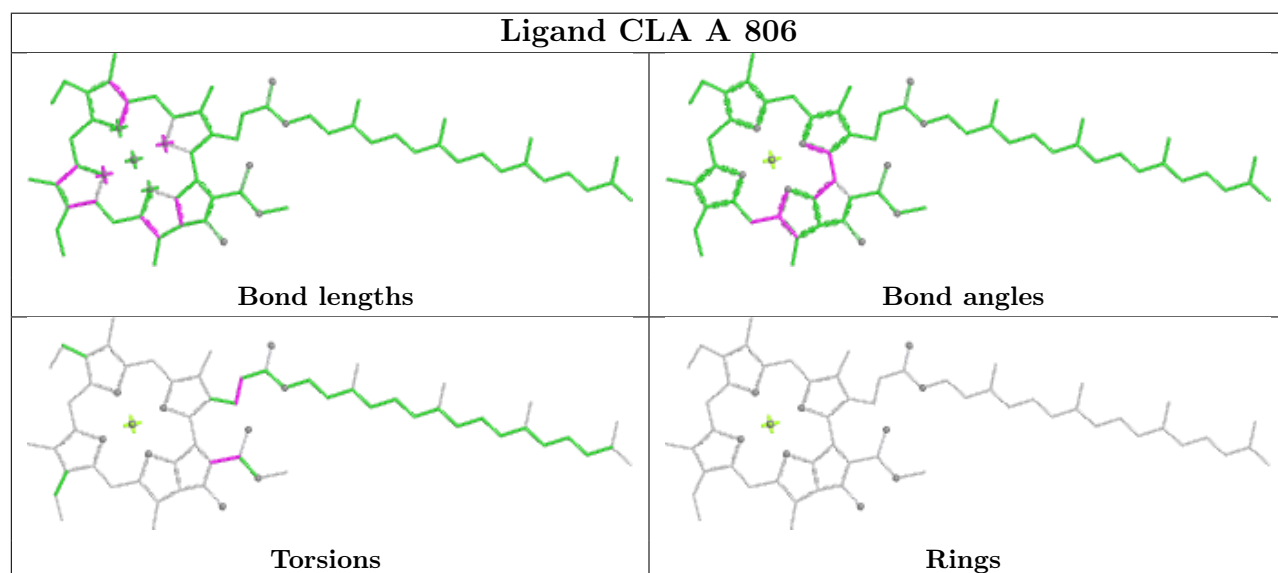
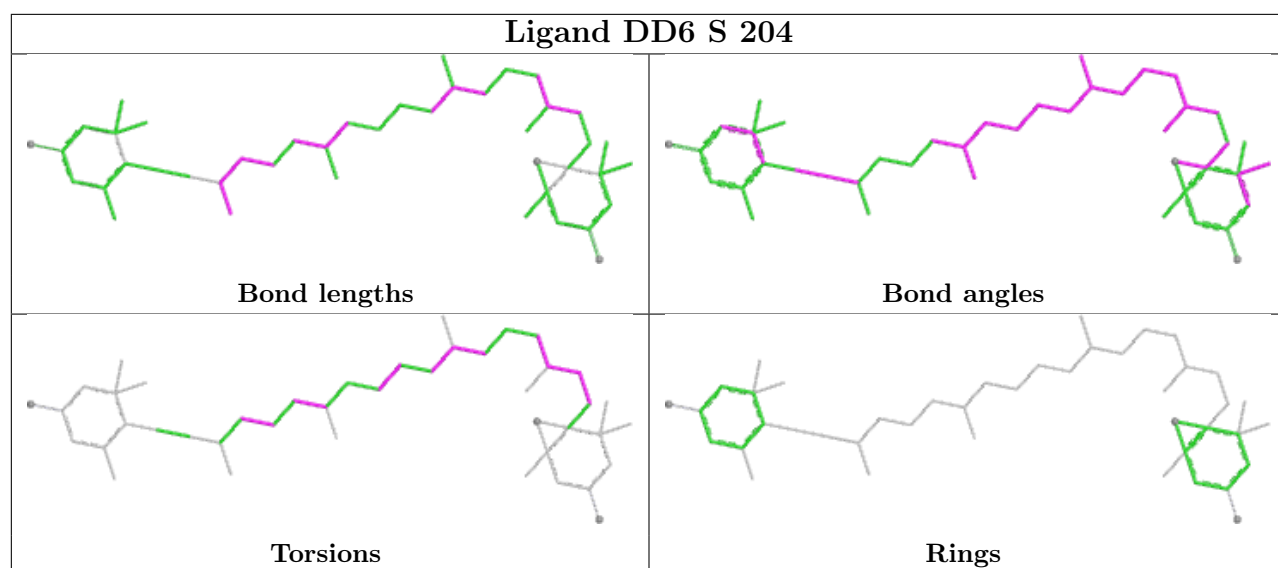
Bond angles

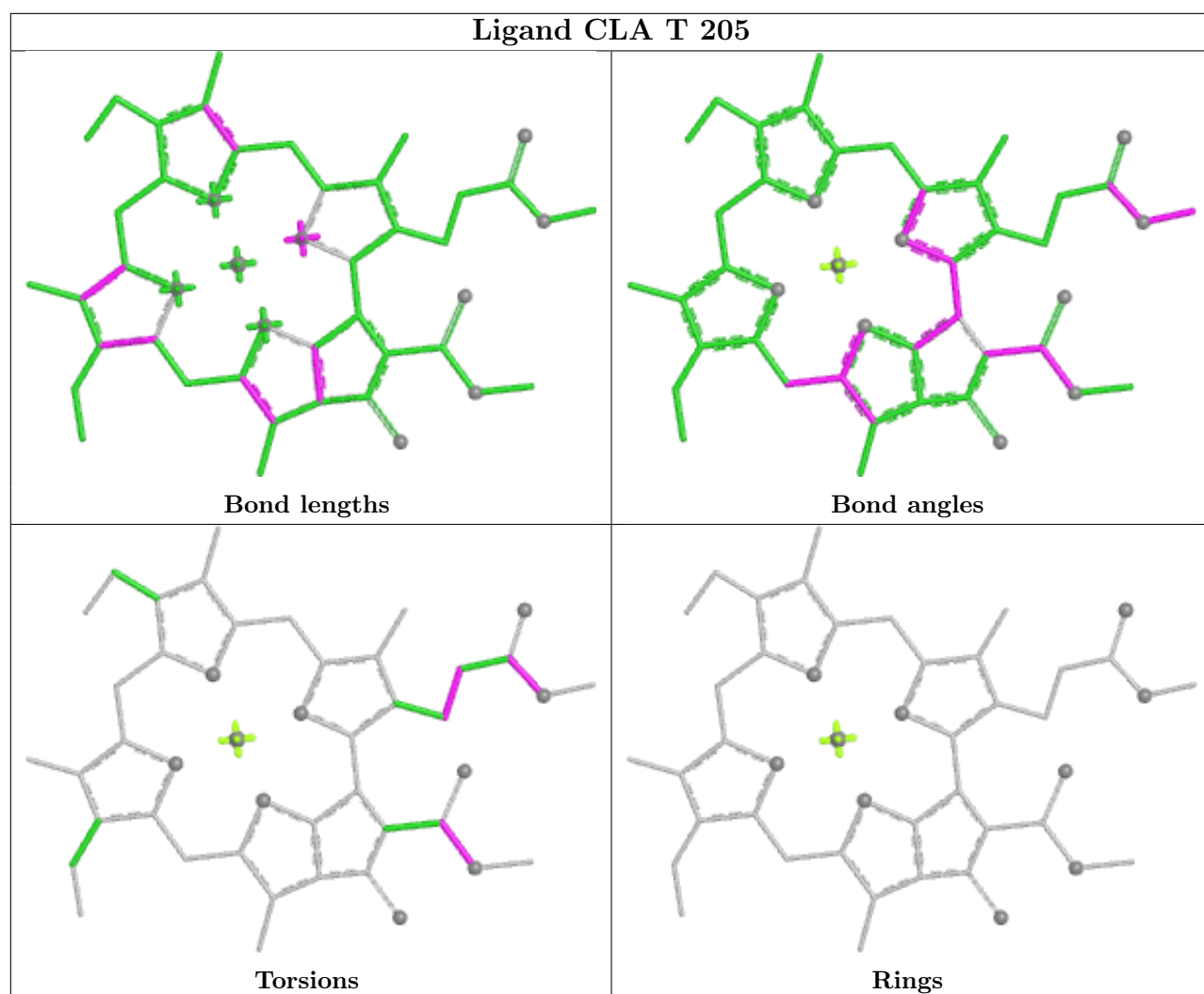


Torsions

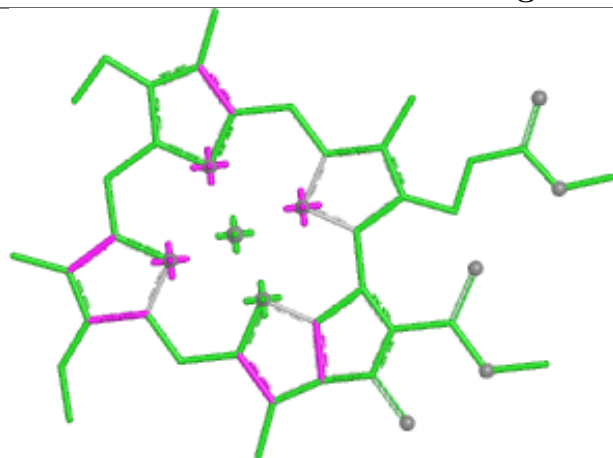


Rings

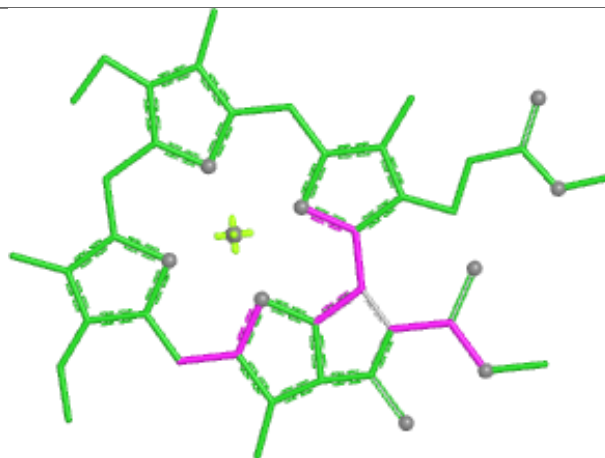




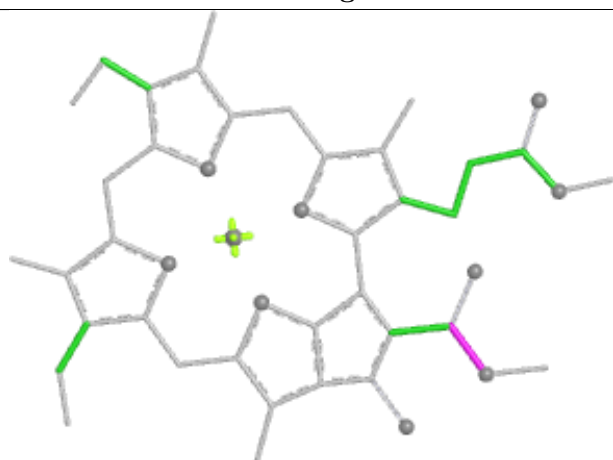
## Ligand CLA S 206



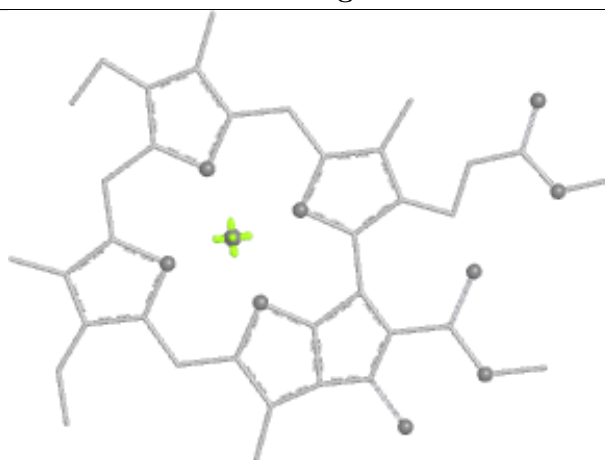
Bond lengths



Bond angles

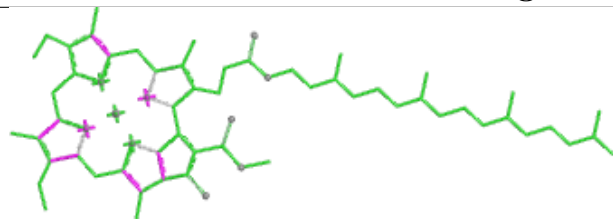


Torsions

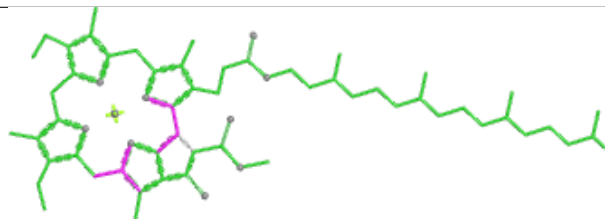


Rings

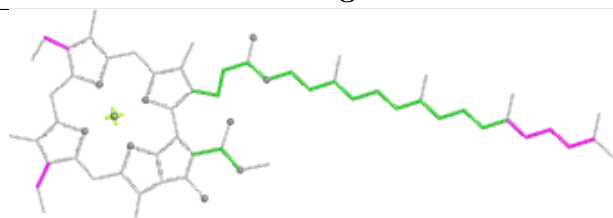
## Ligand CLA S 214



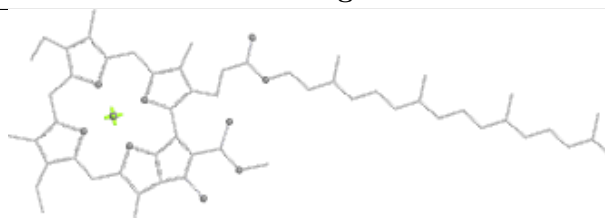
Bond lengths



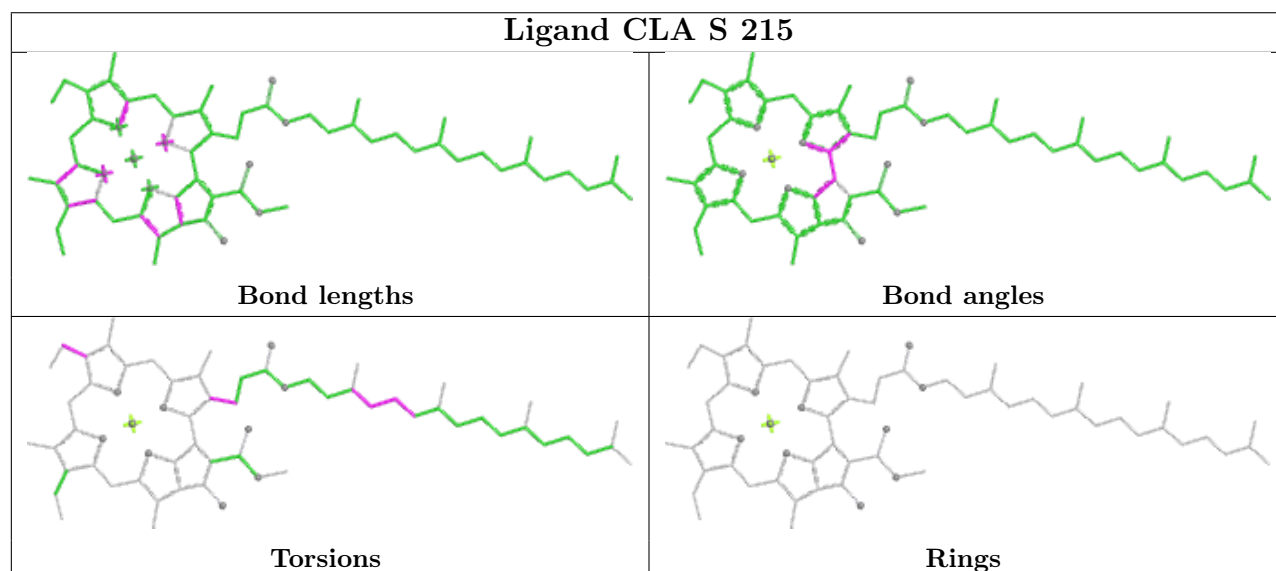
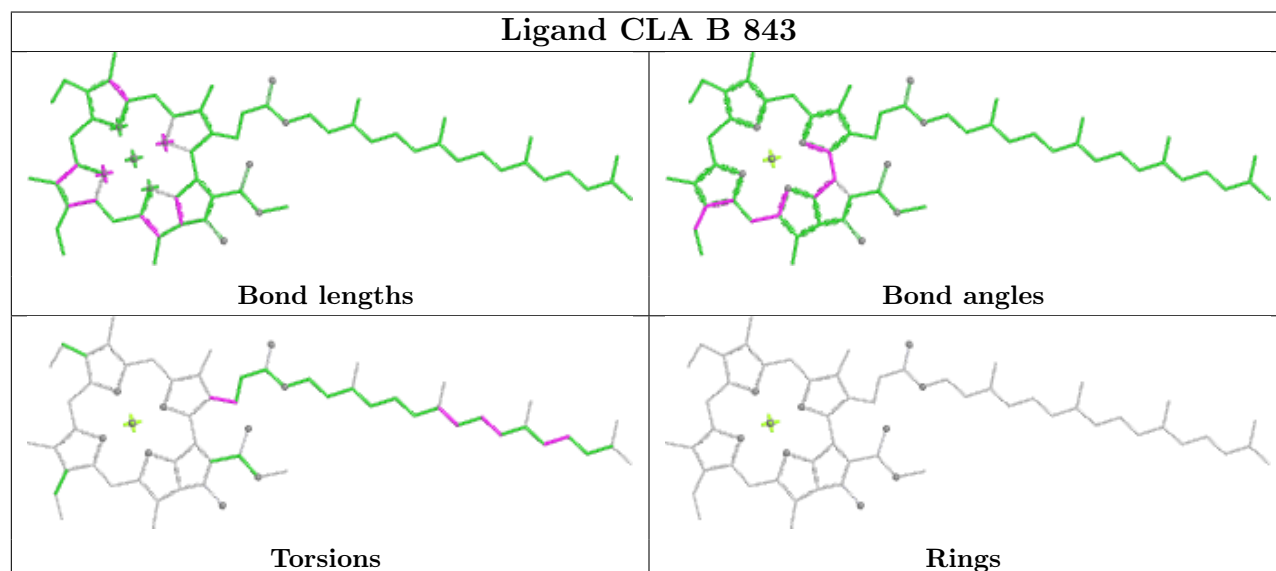
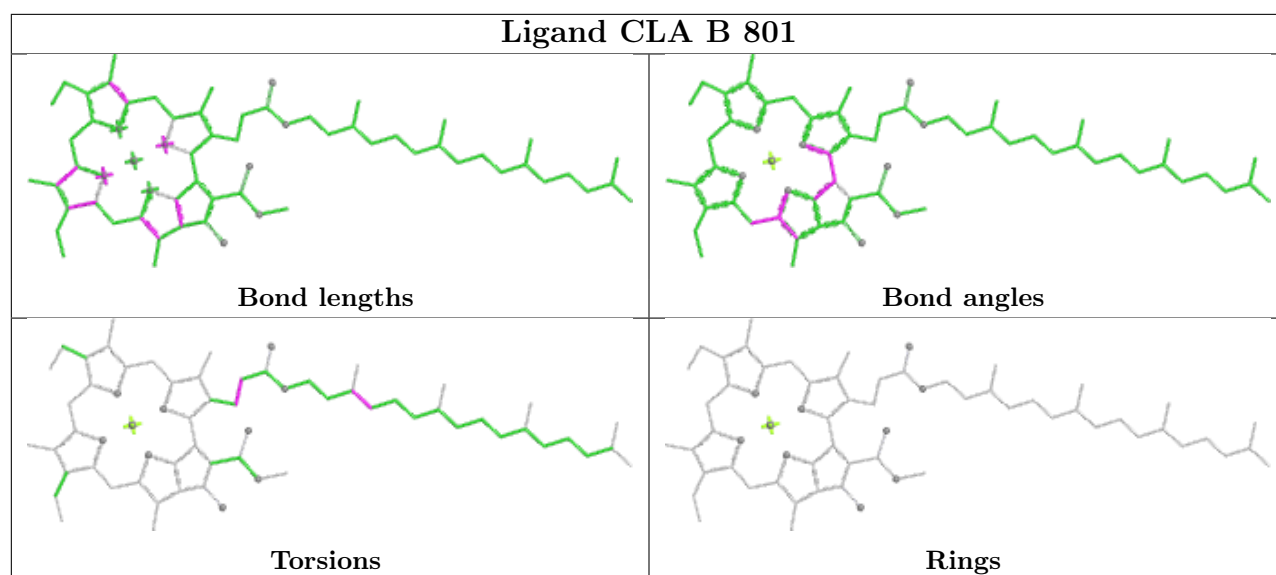
Bond angles

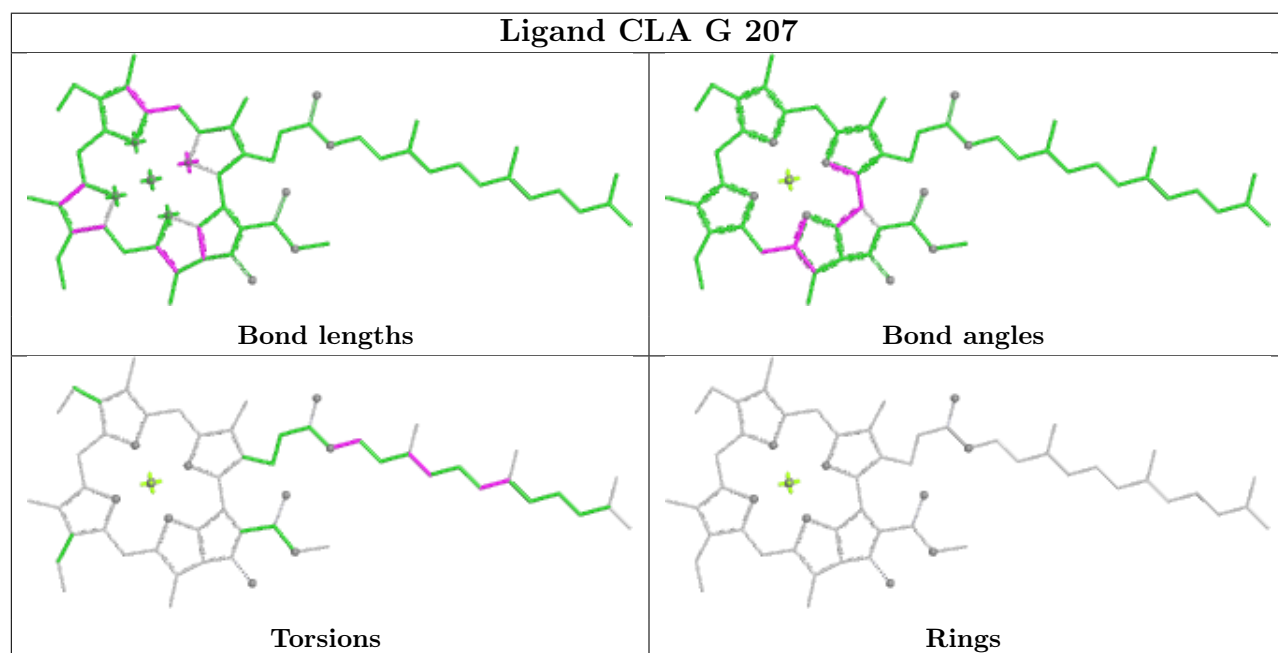
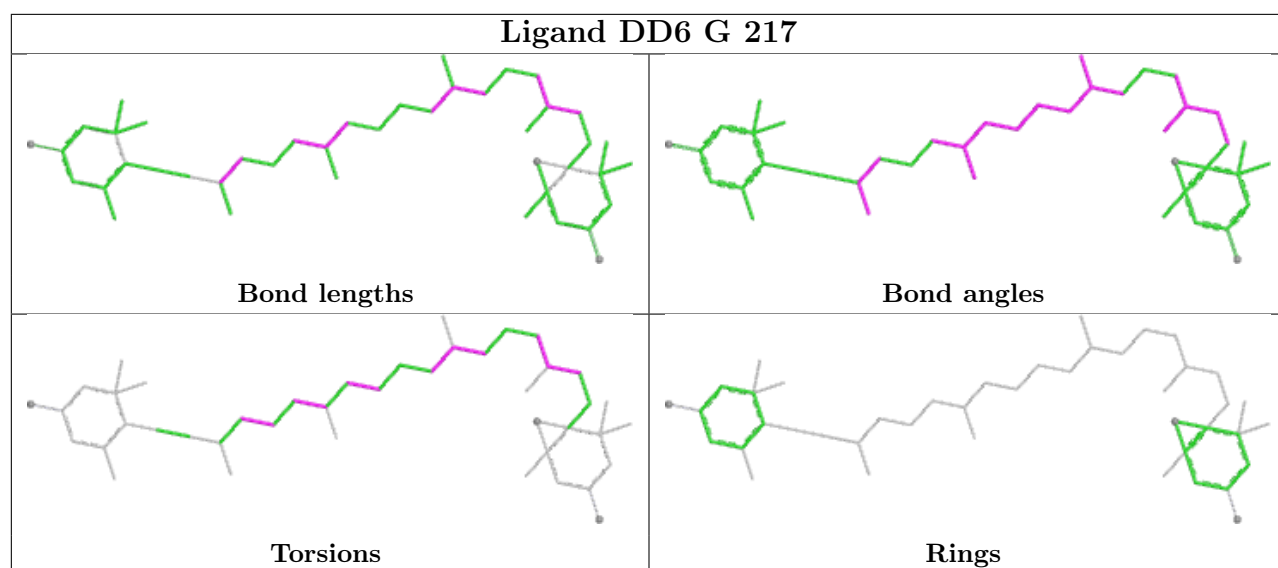


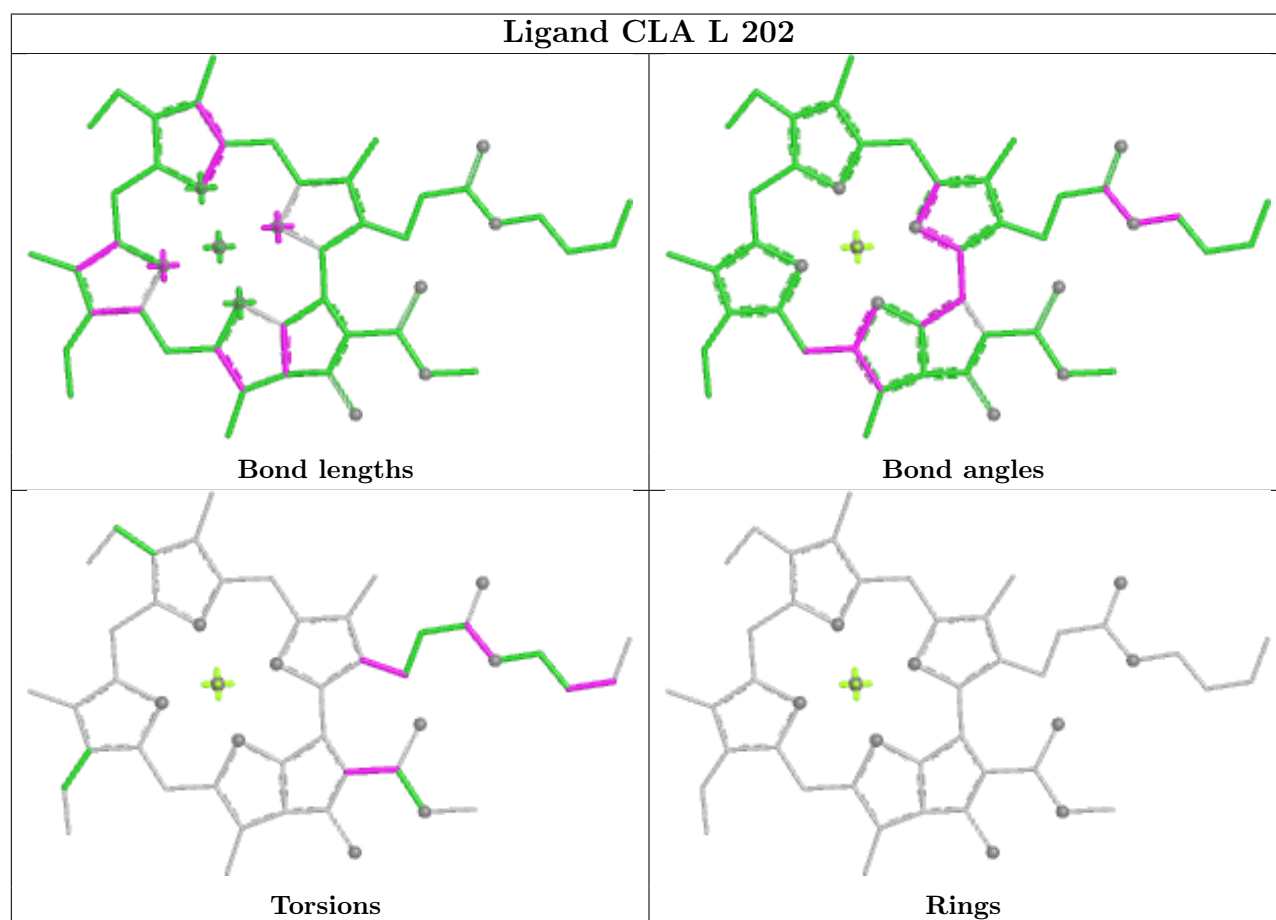
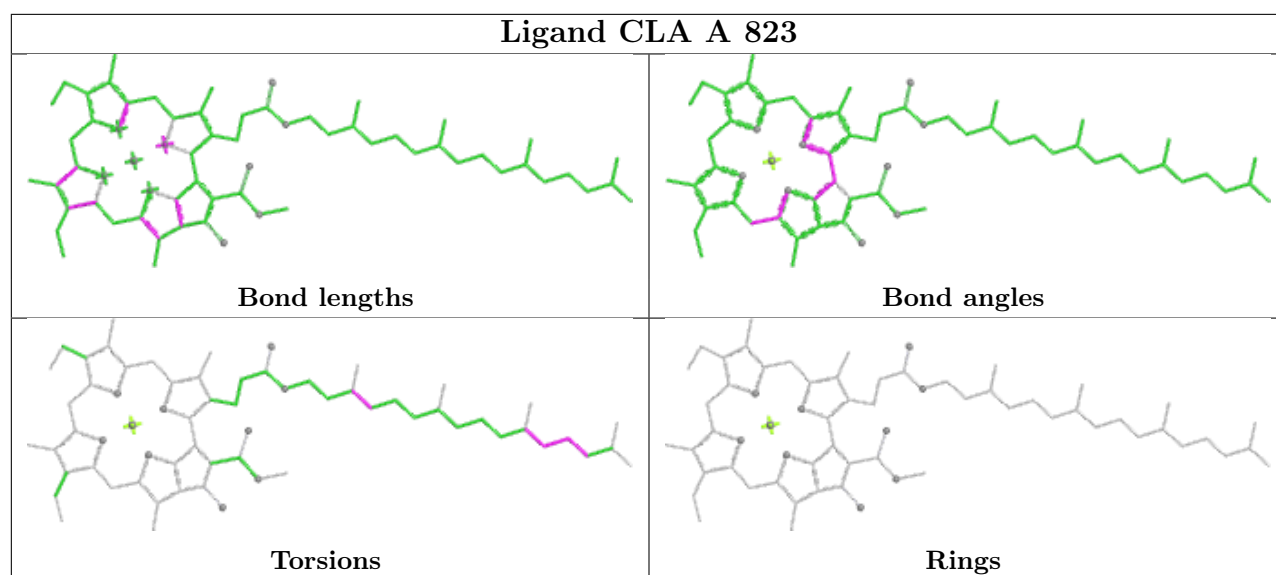
Torsions

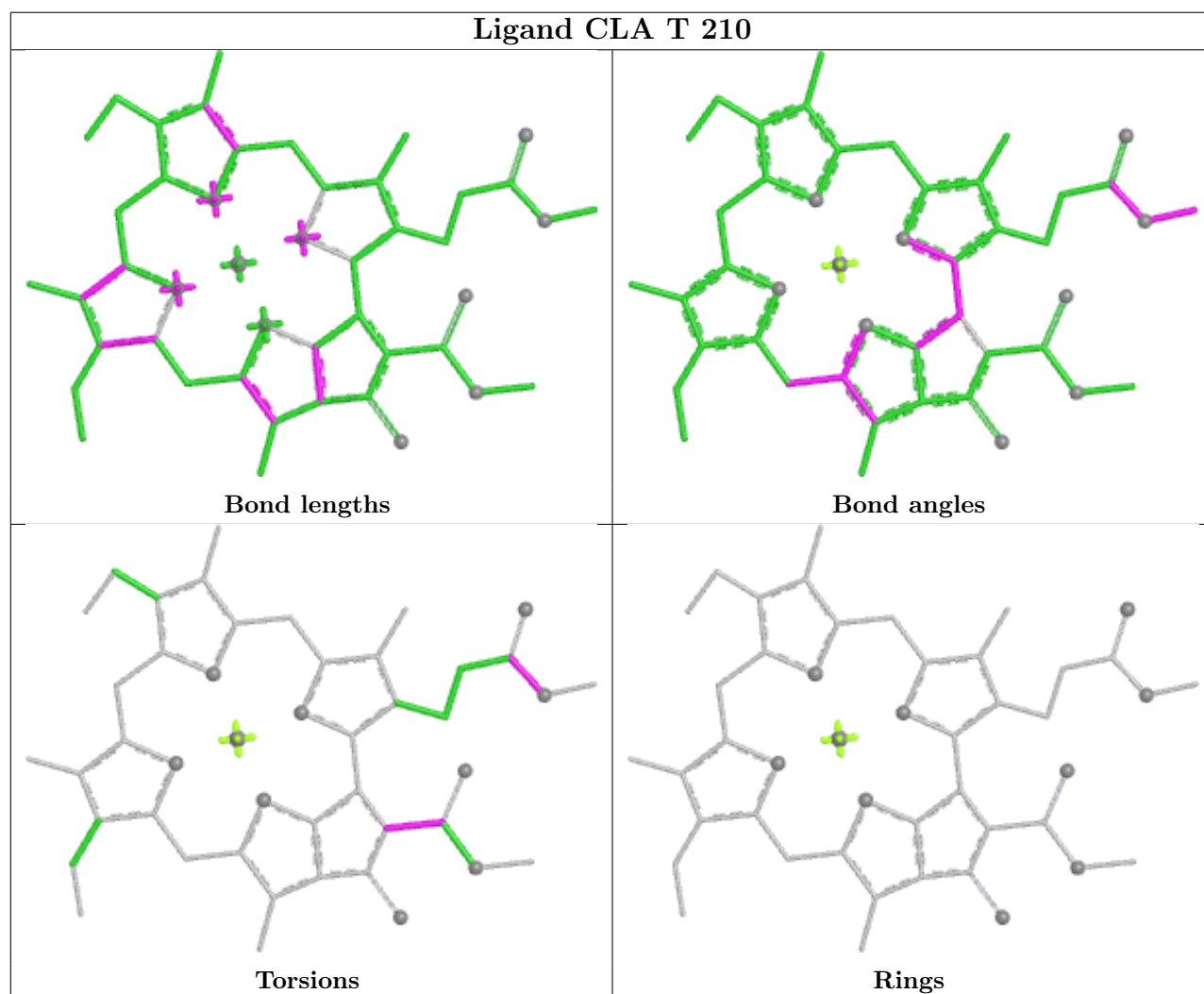
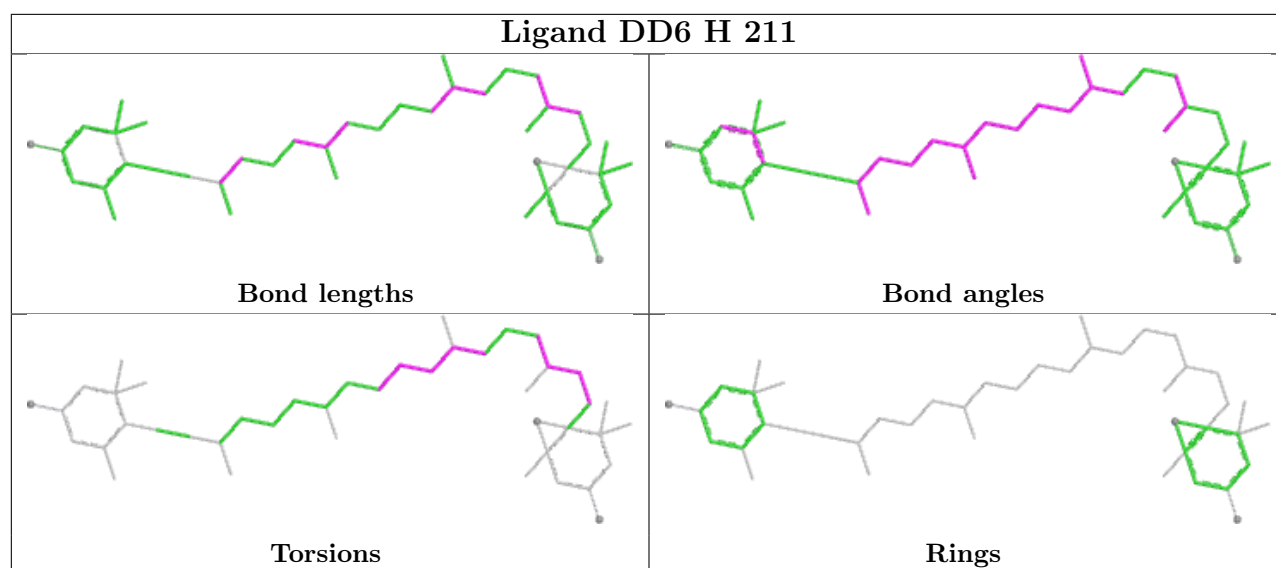


Rings



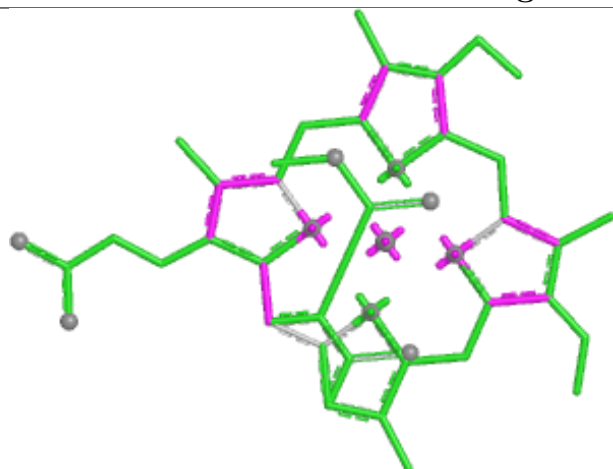




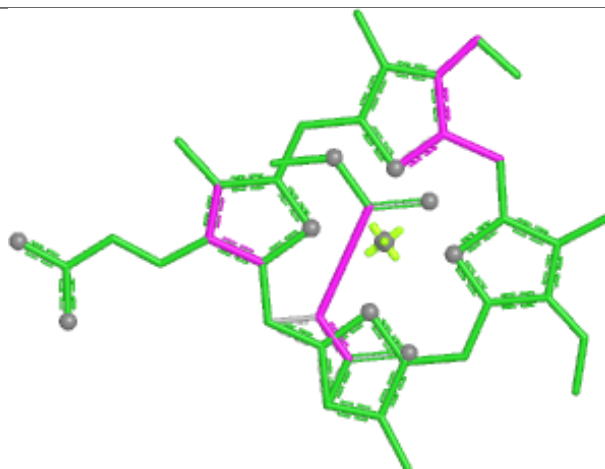




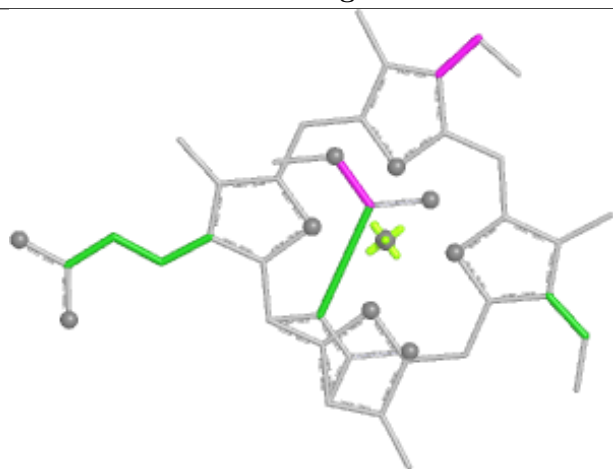
## Ligand KC1 T 208



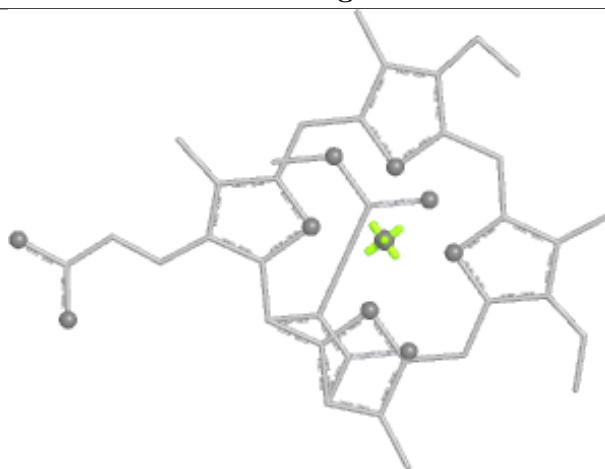
Bond lengths



Bond angles

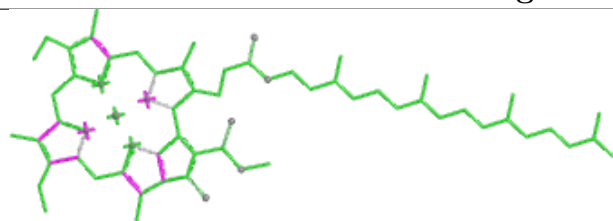


Torsions

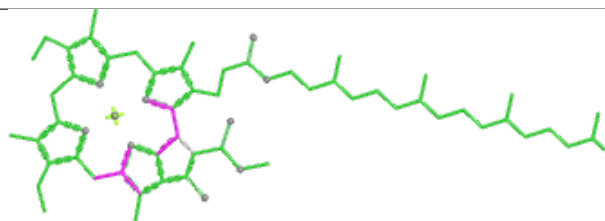


Rings

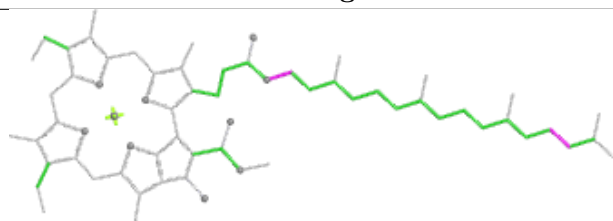
## Ligand CLA L 203



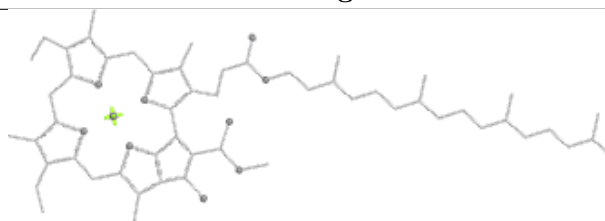
Bond lengths



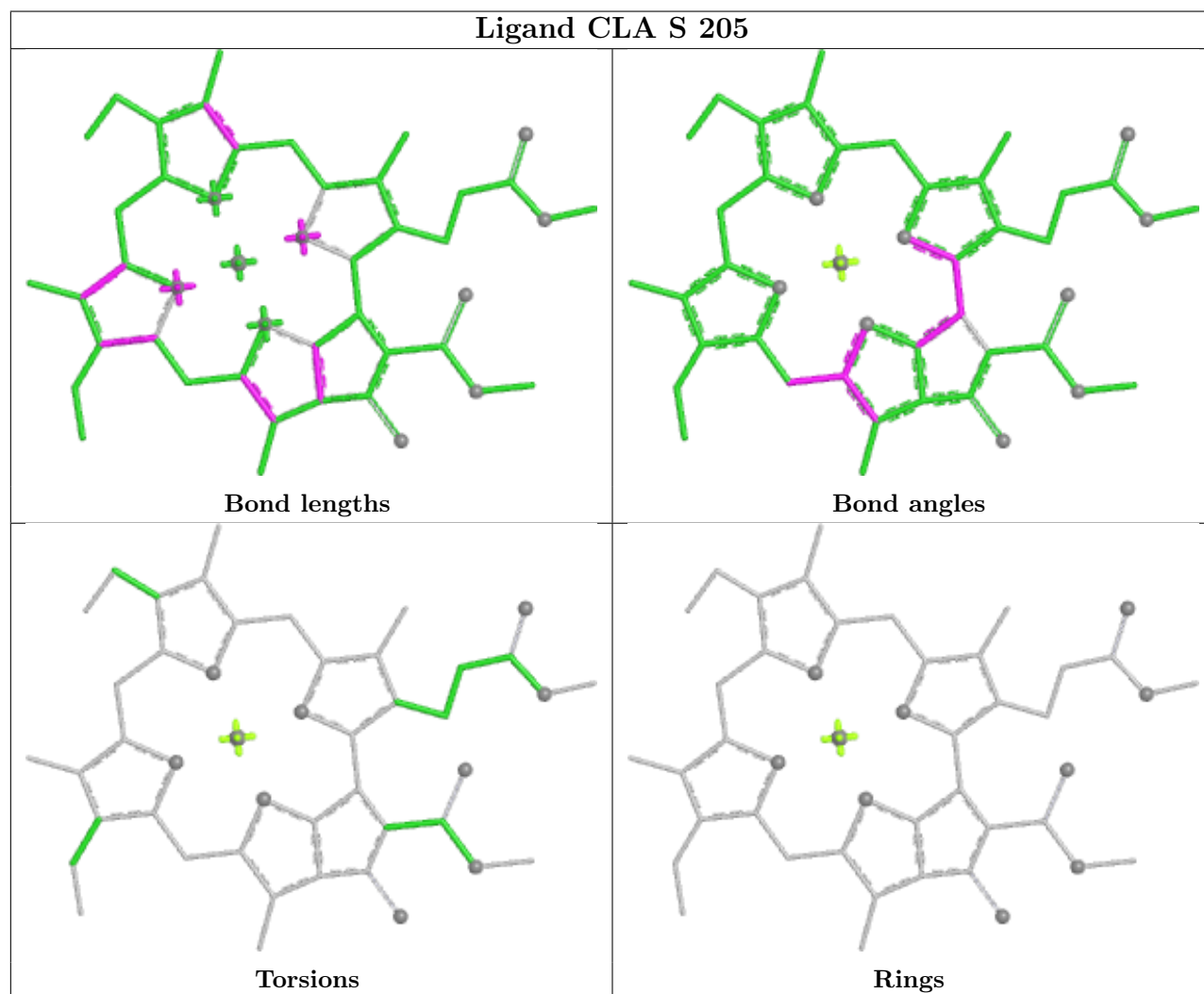
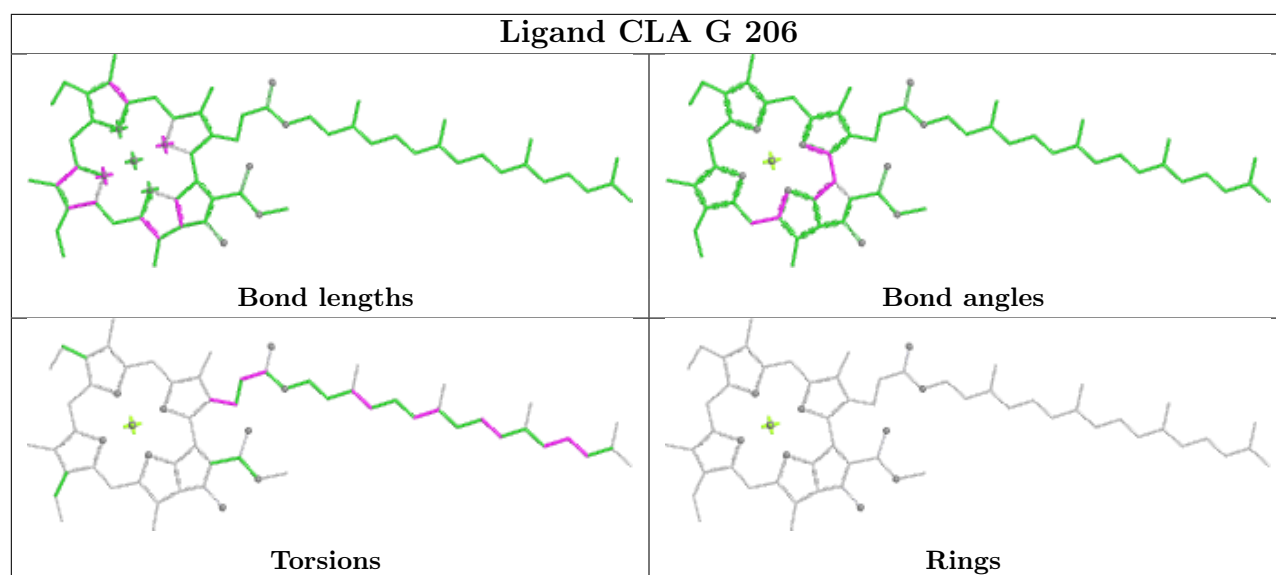
Bond angles

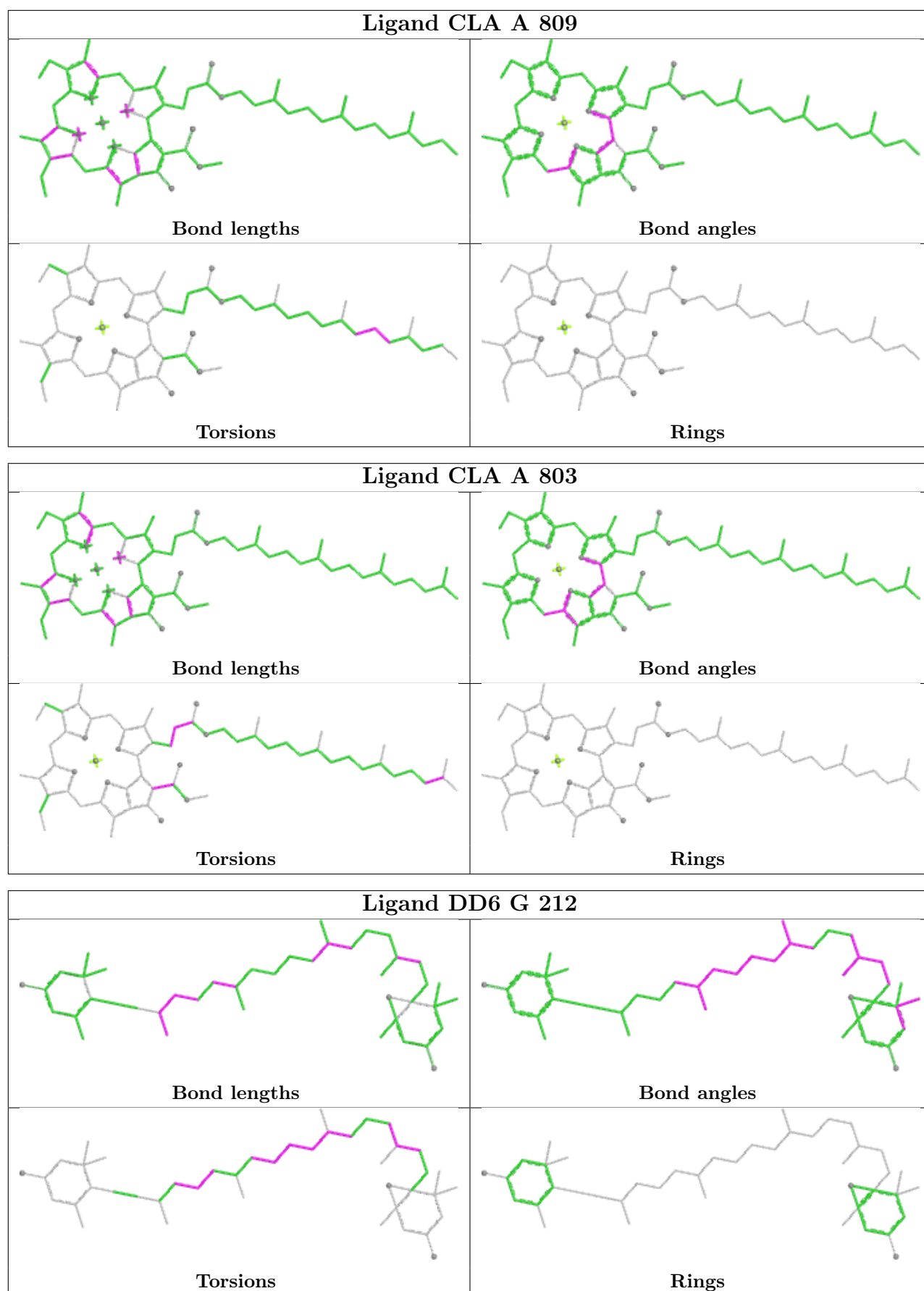


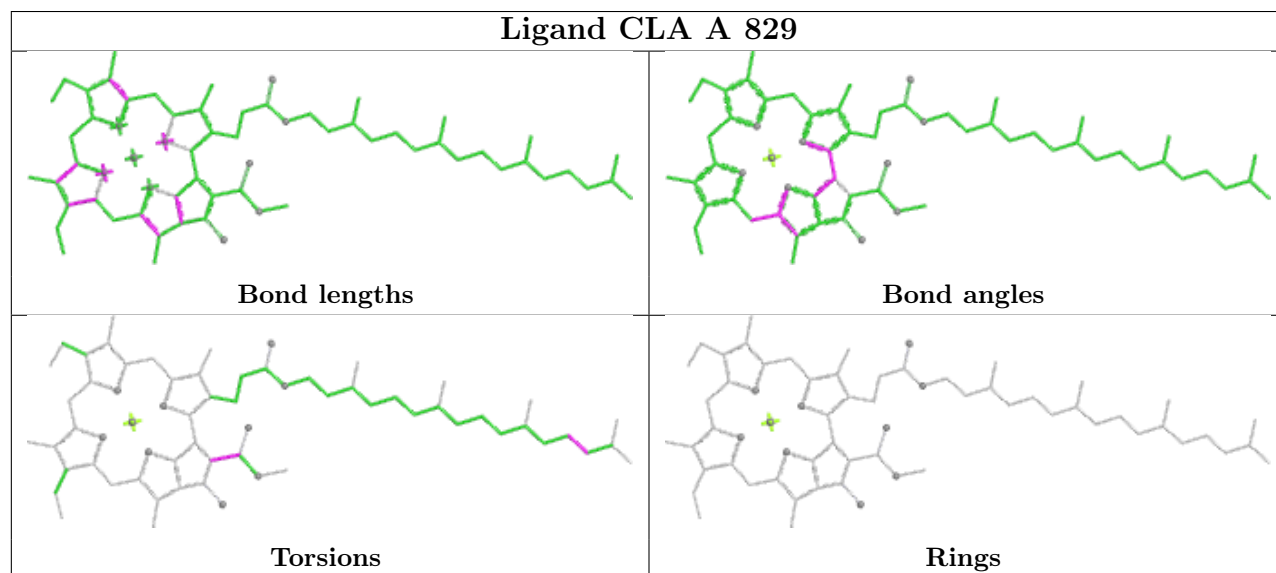
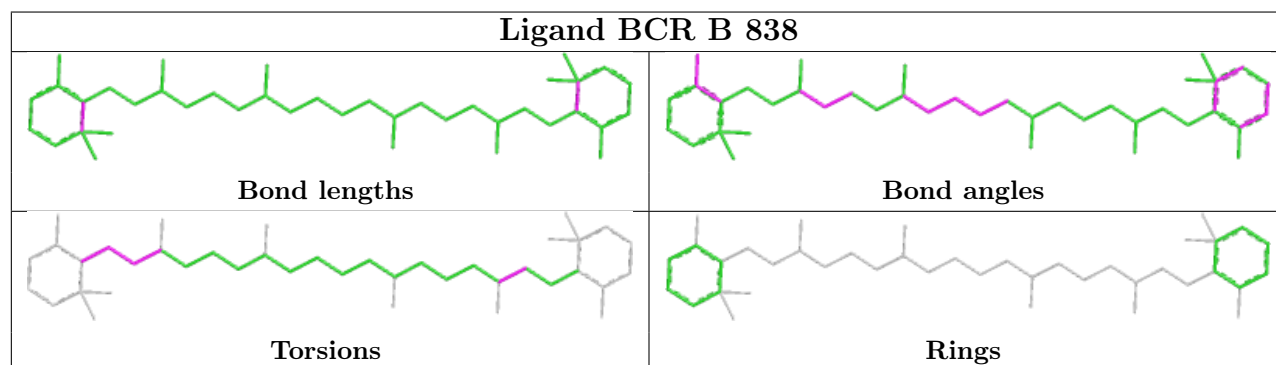
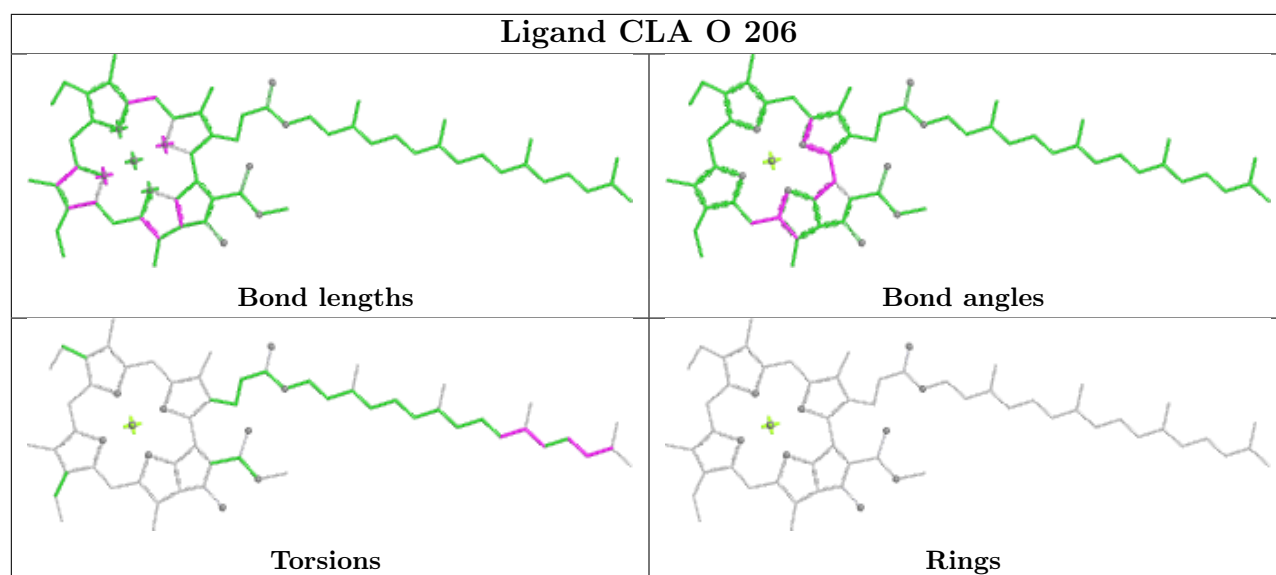
Torsions



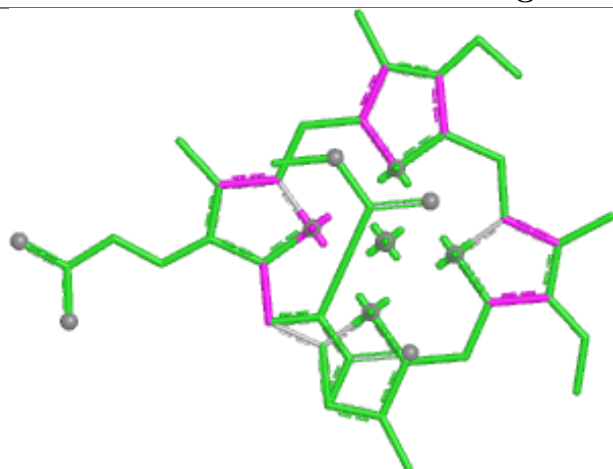
Rings



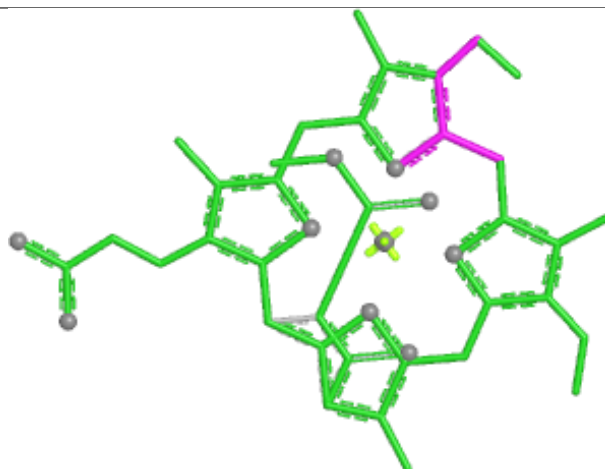




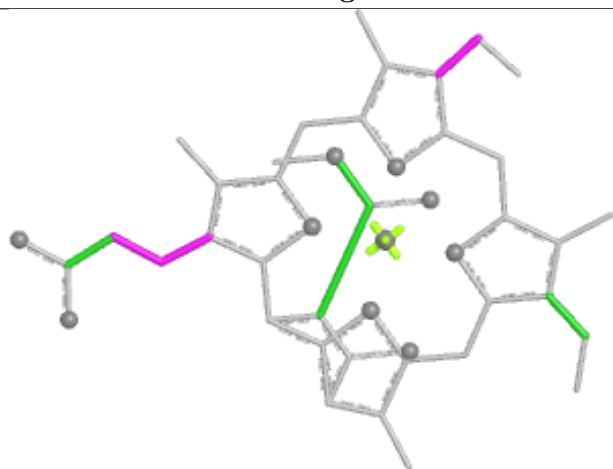
## Ligand KC1 P 206



Bond lengths



Bond angles

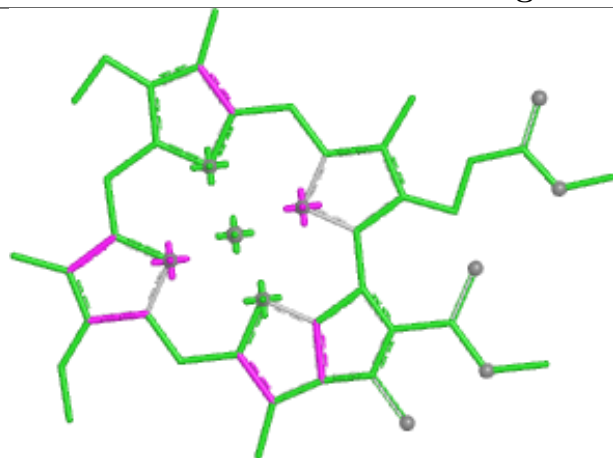


Torsions

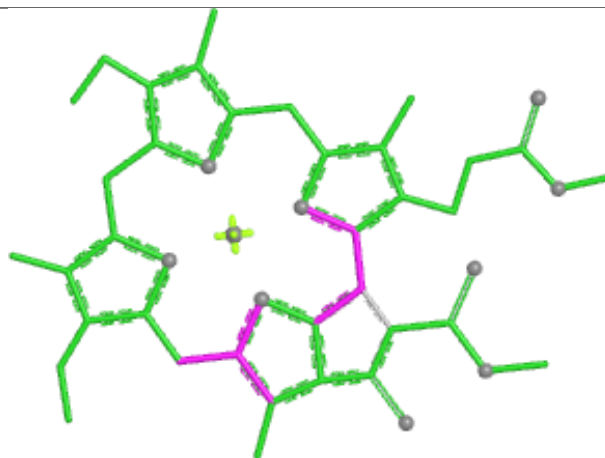


Rings

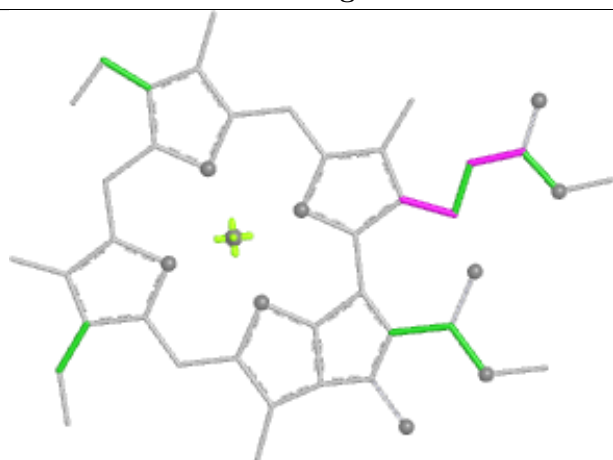
## Ligand CLA F 803



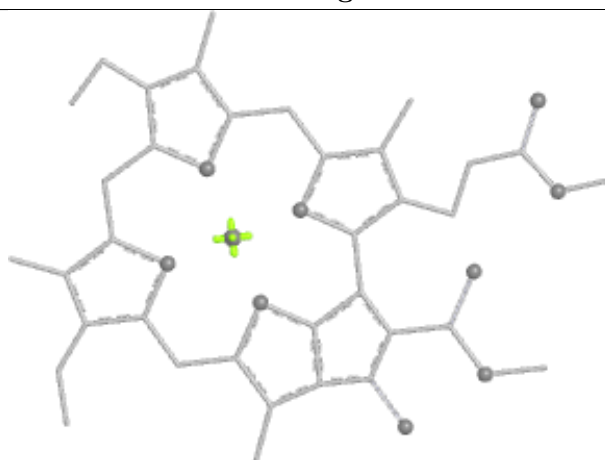
Bond lengths



Bond angles

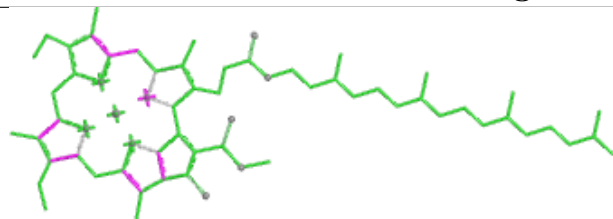


Torsions

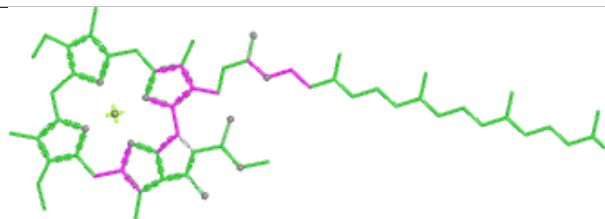


Rings

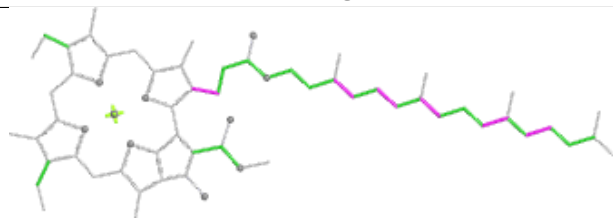
## Ligand CLA U 207



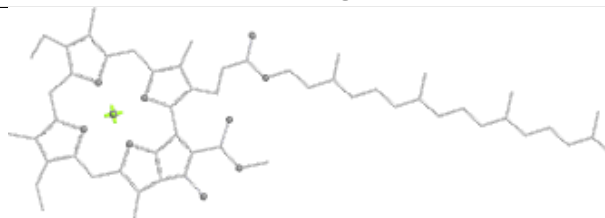
Bond lengths



Bond angles

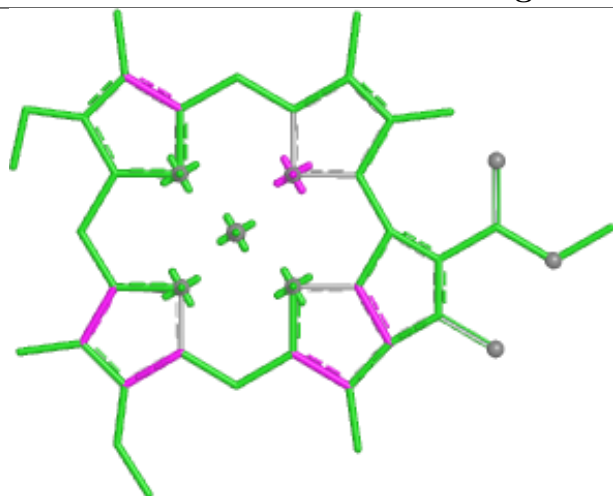


Torsions

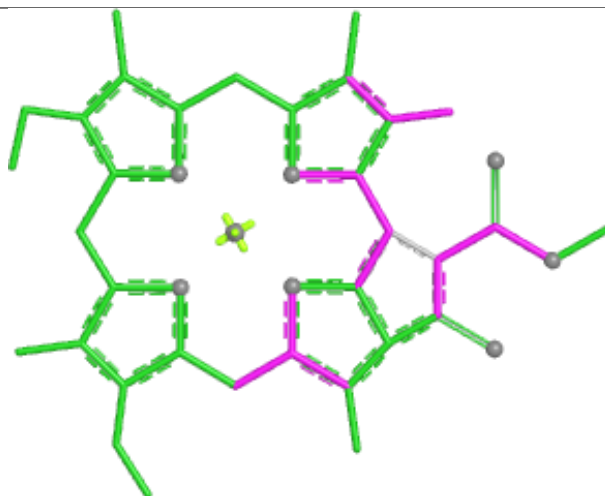


Rings

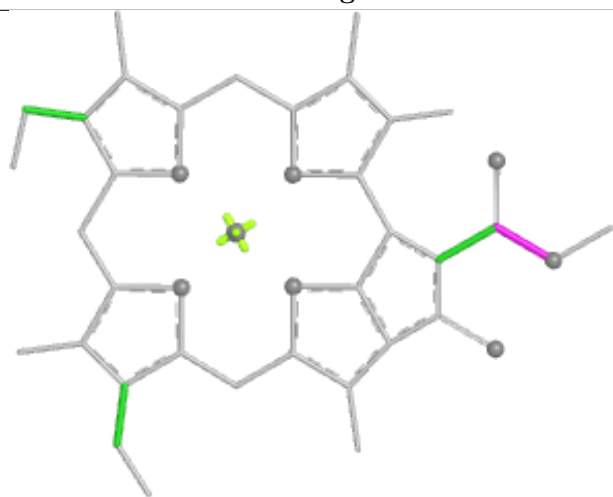
## Ligand CLA P 213



Bond lengths



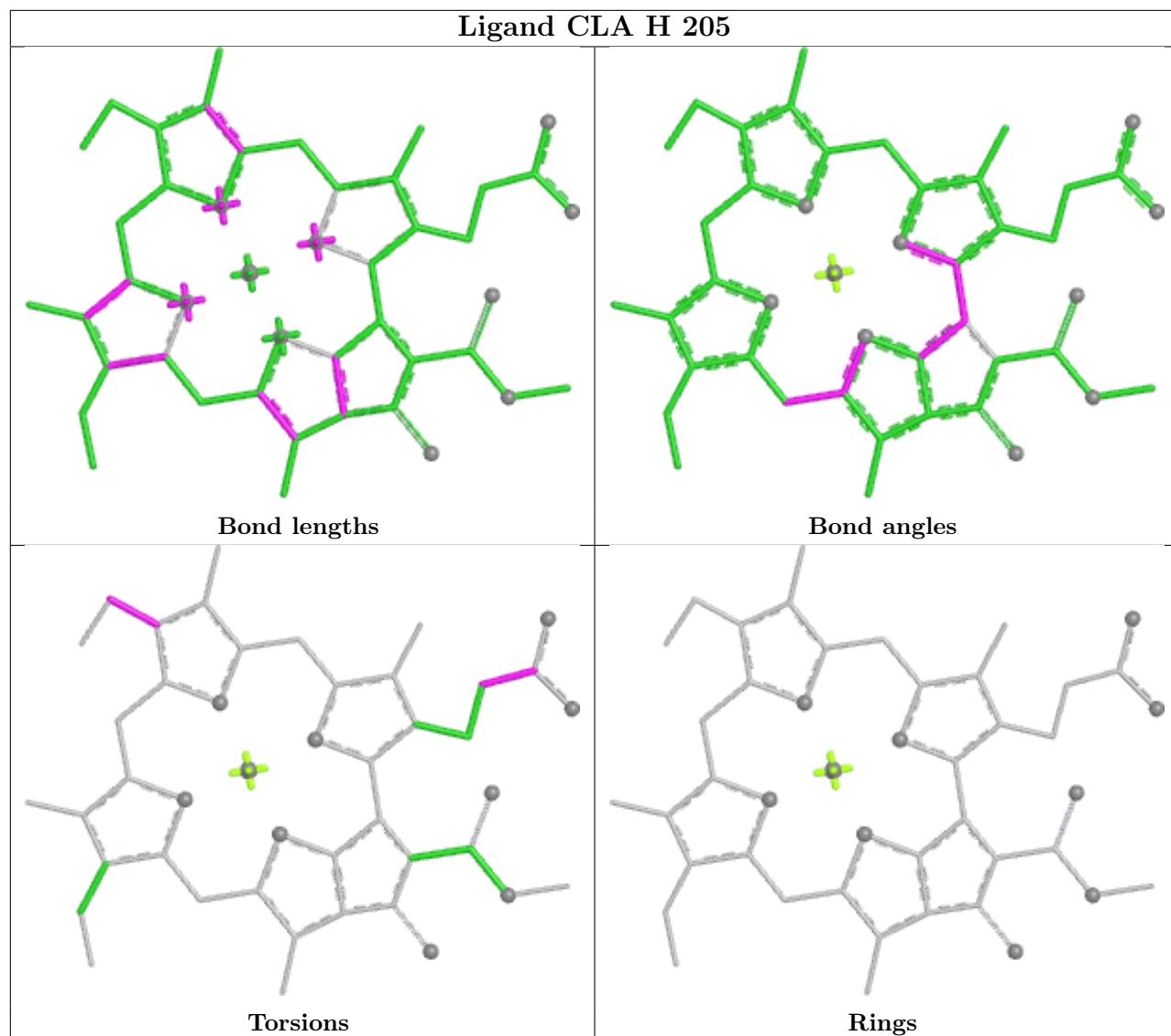
Bond angles



Torsions

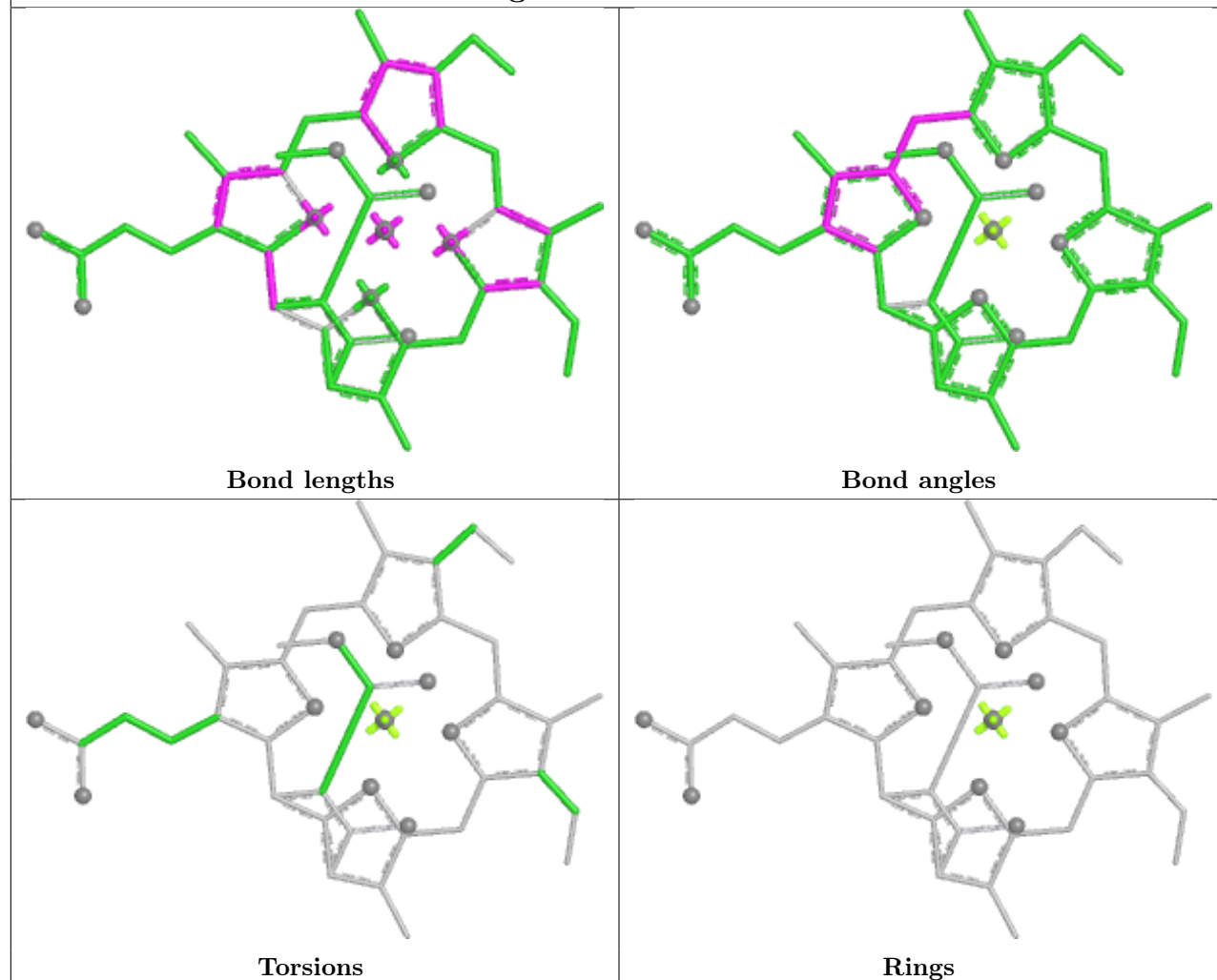


Rings

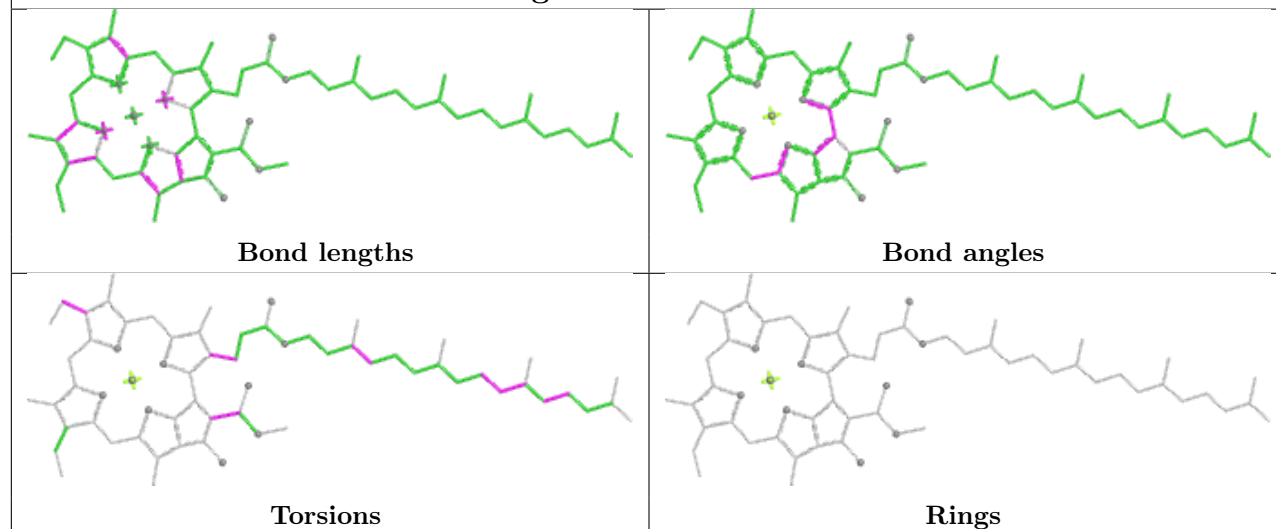


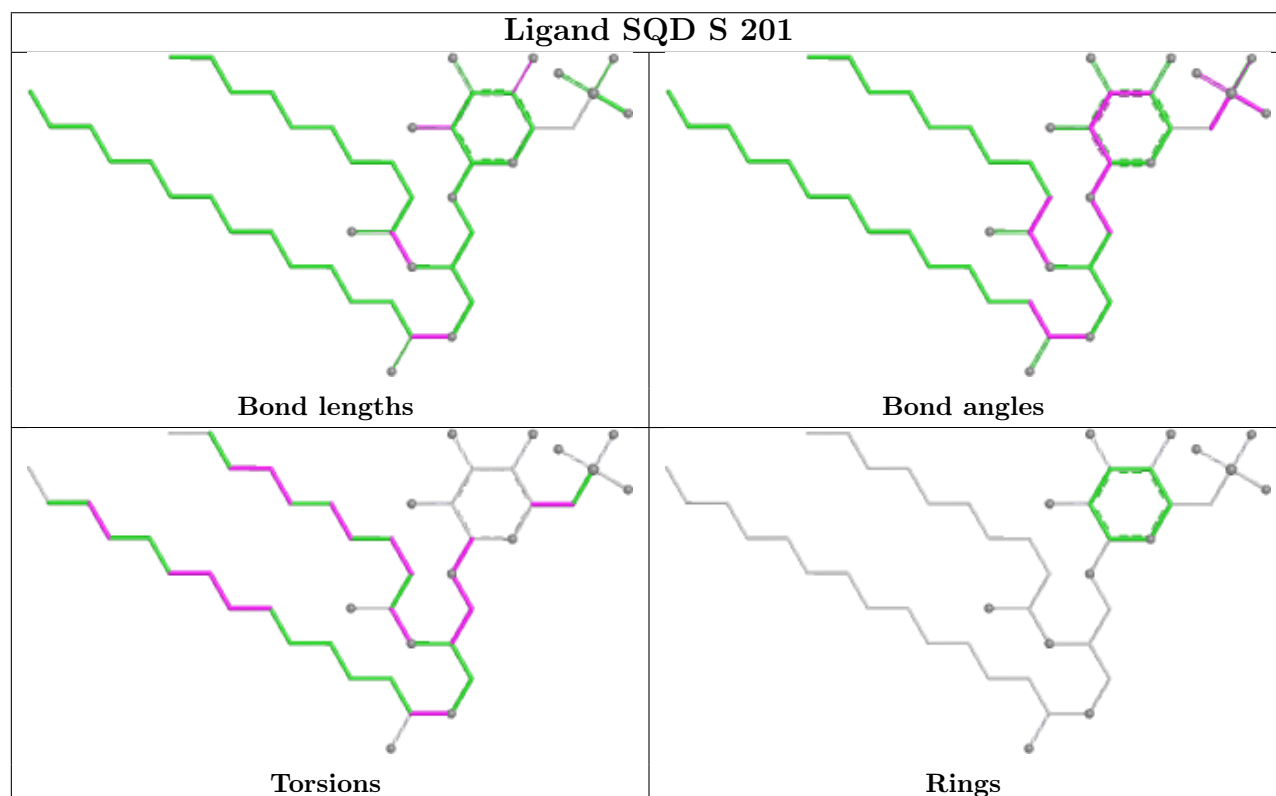
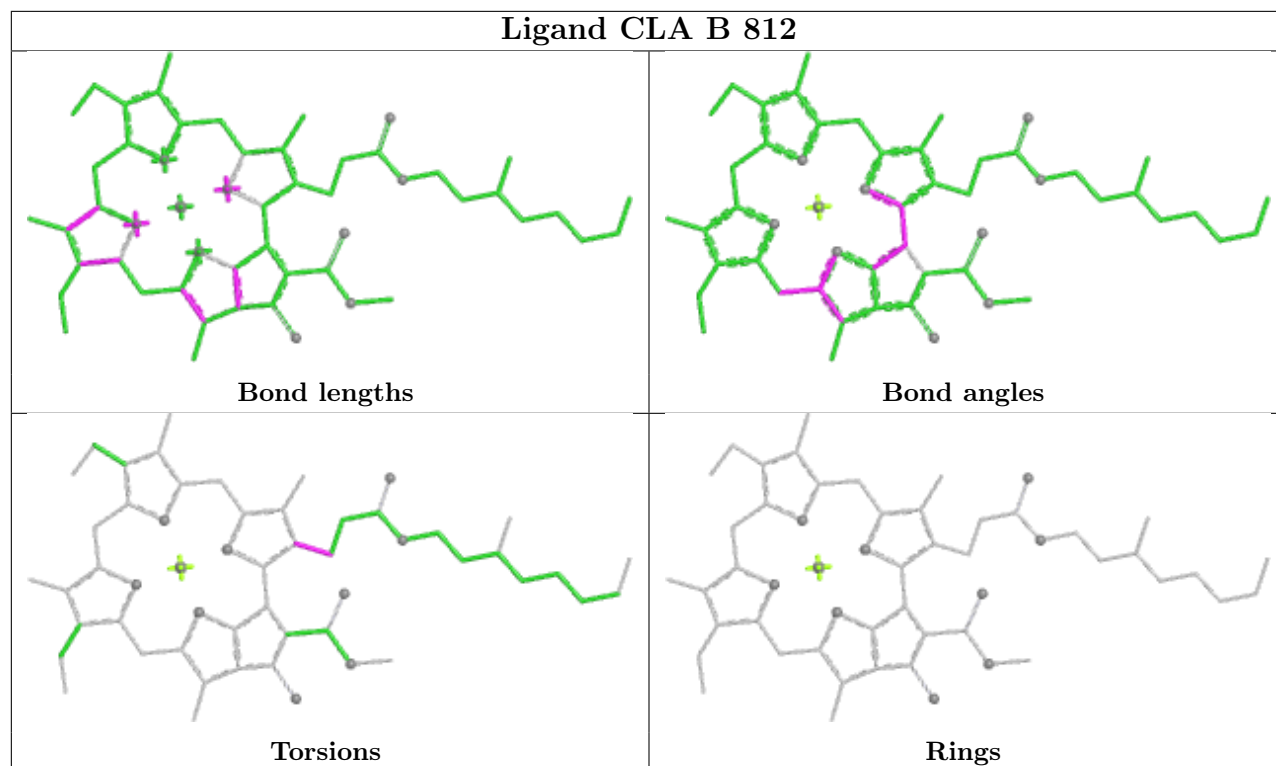


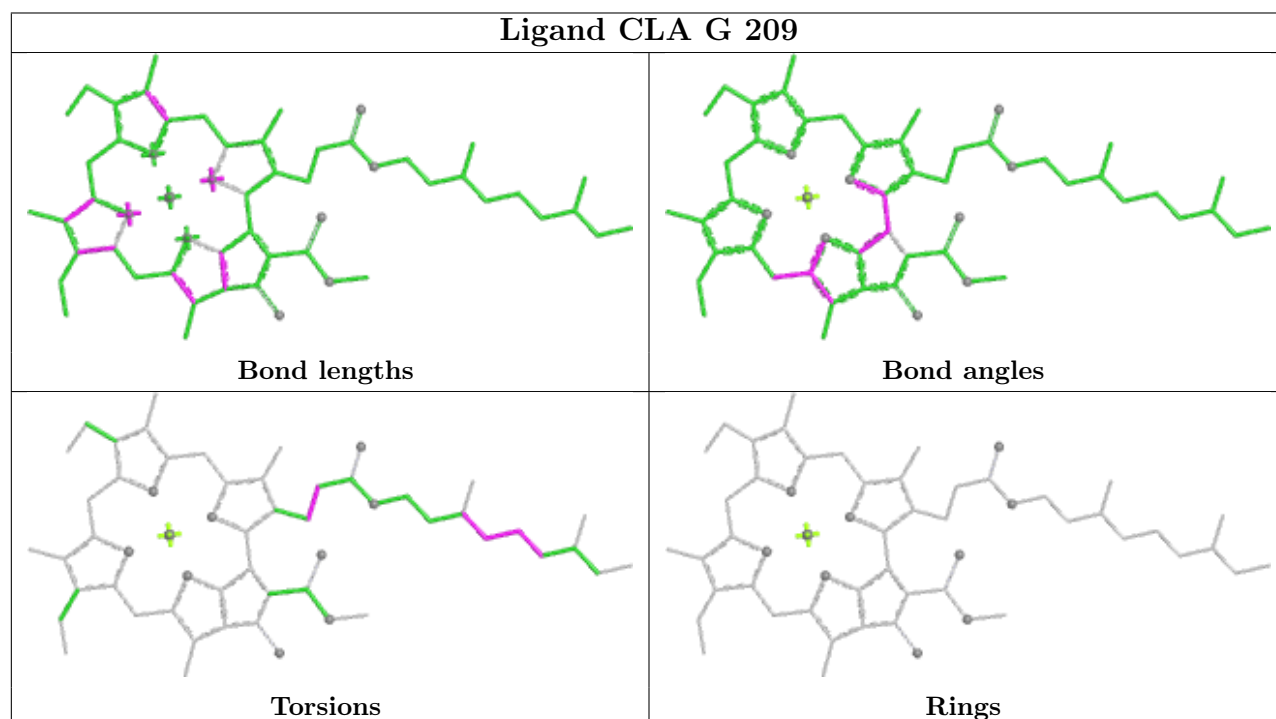
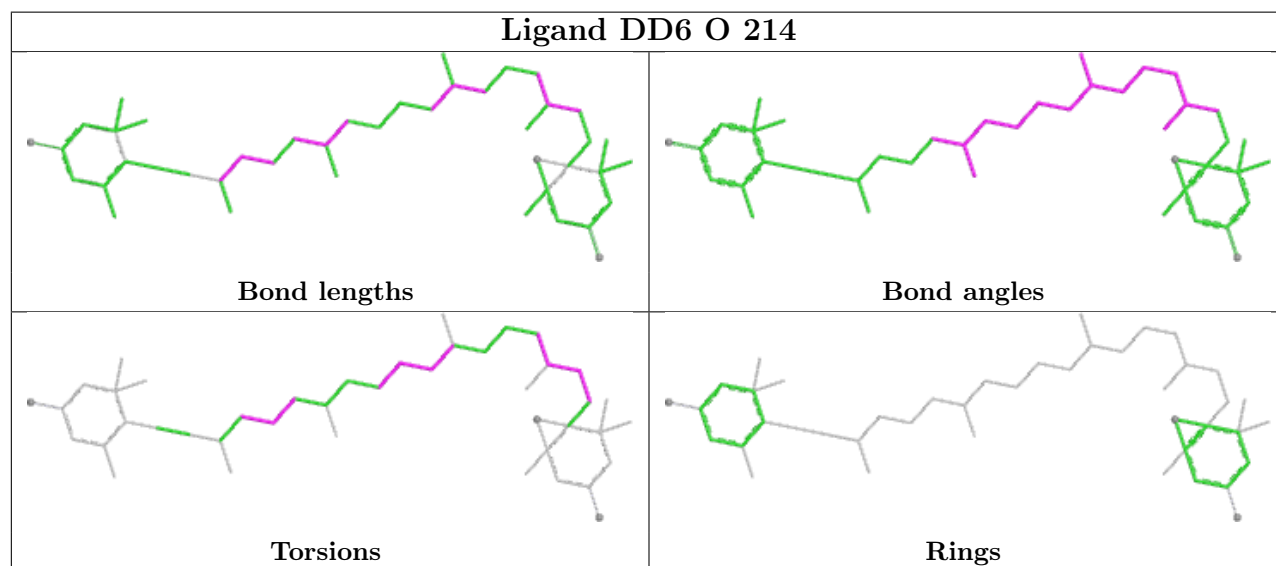
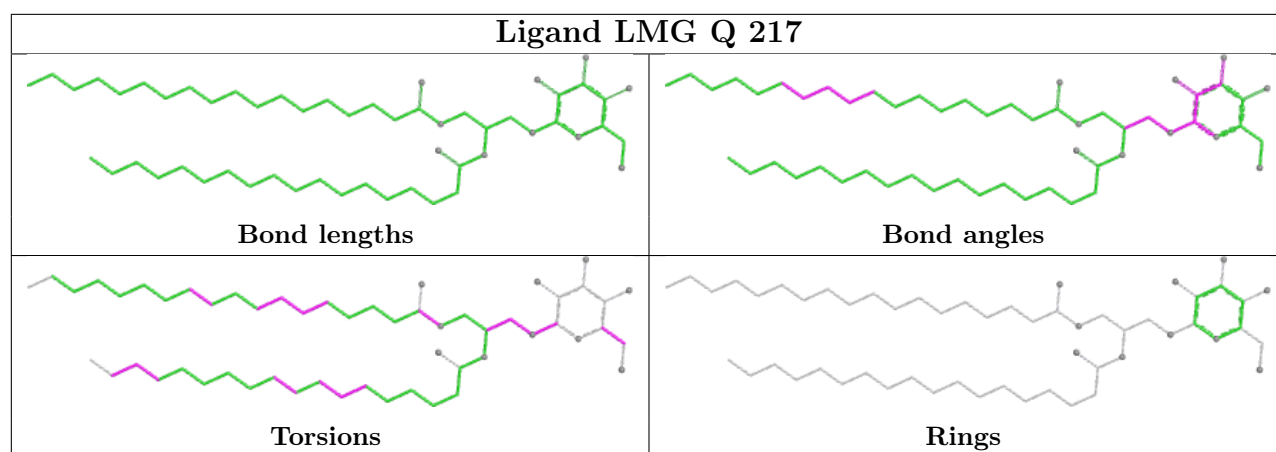
## Ligand KC1 O 210



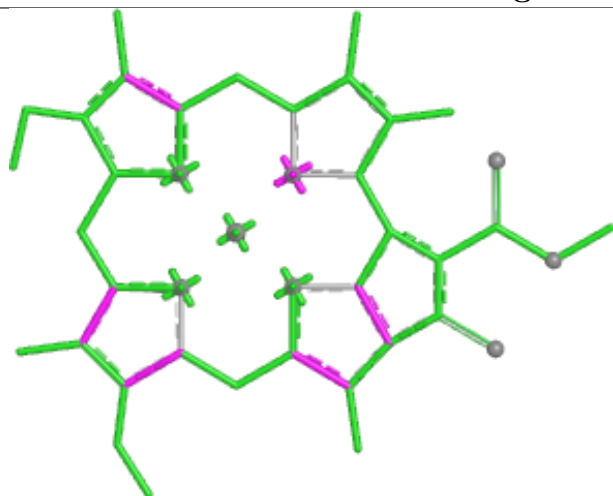
## Ligand CLA A 851



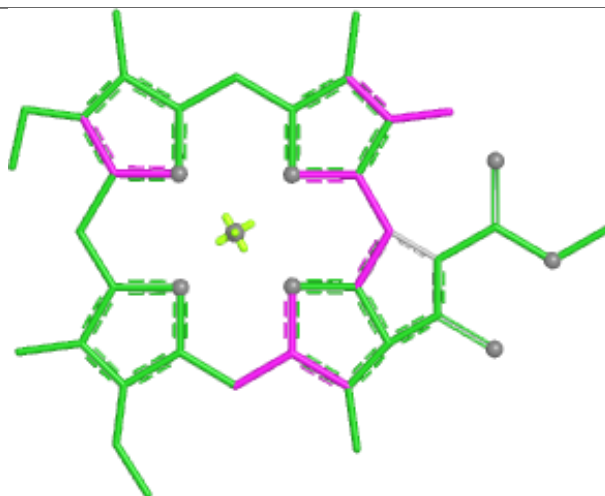




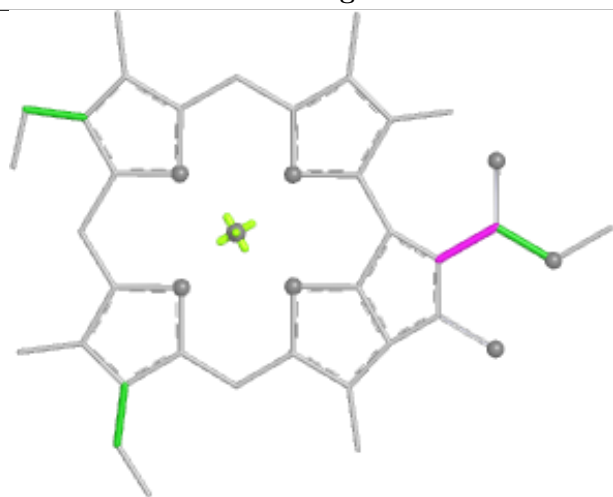
## Ligand CLA O 211



Bond lengths



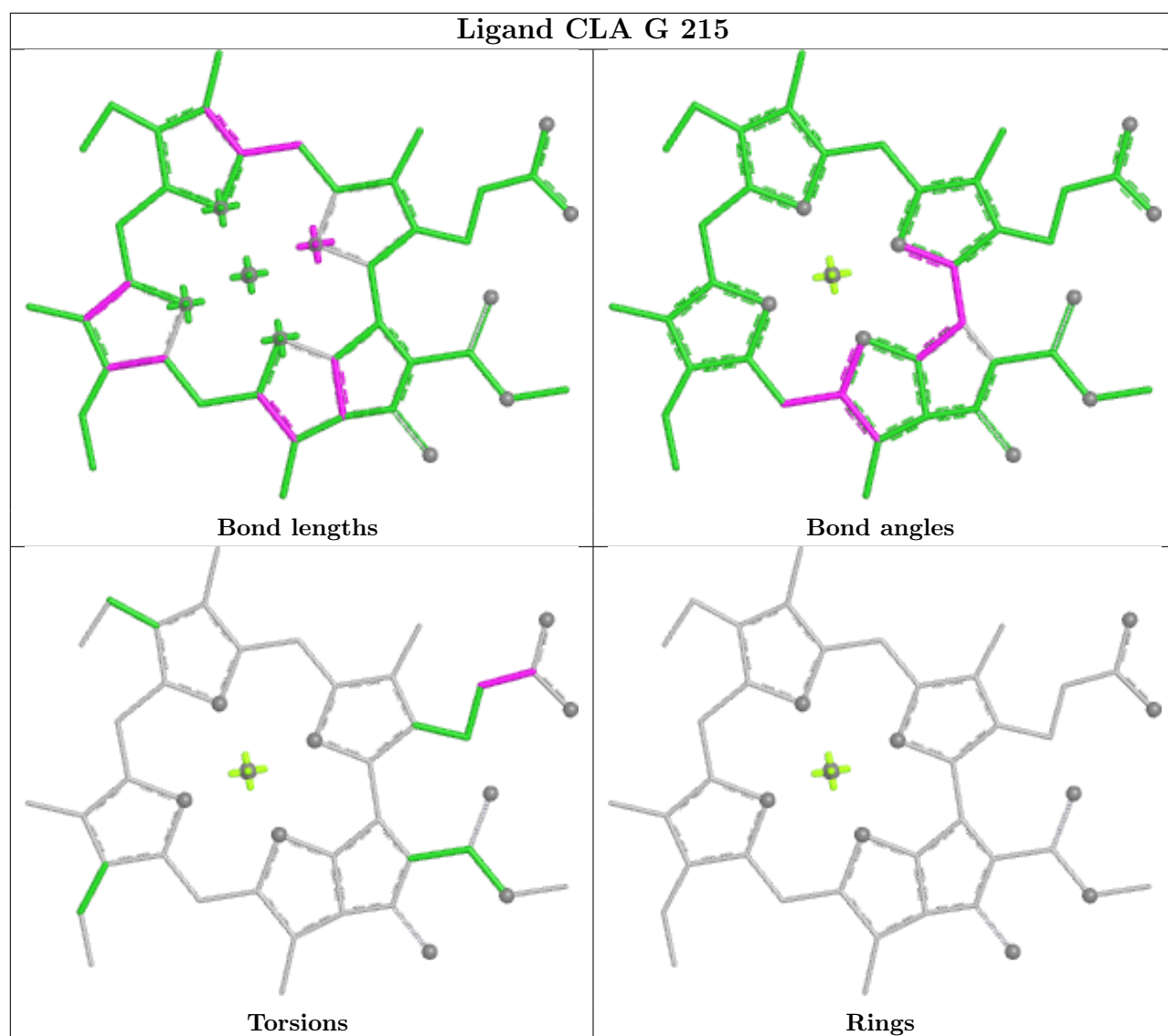
Bond angles

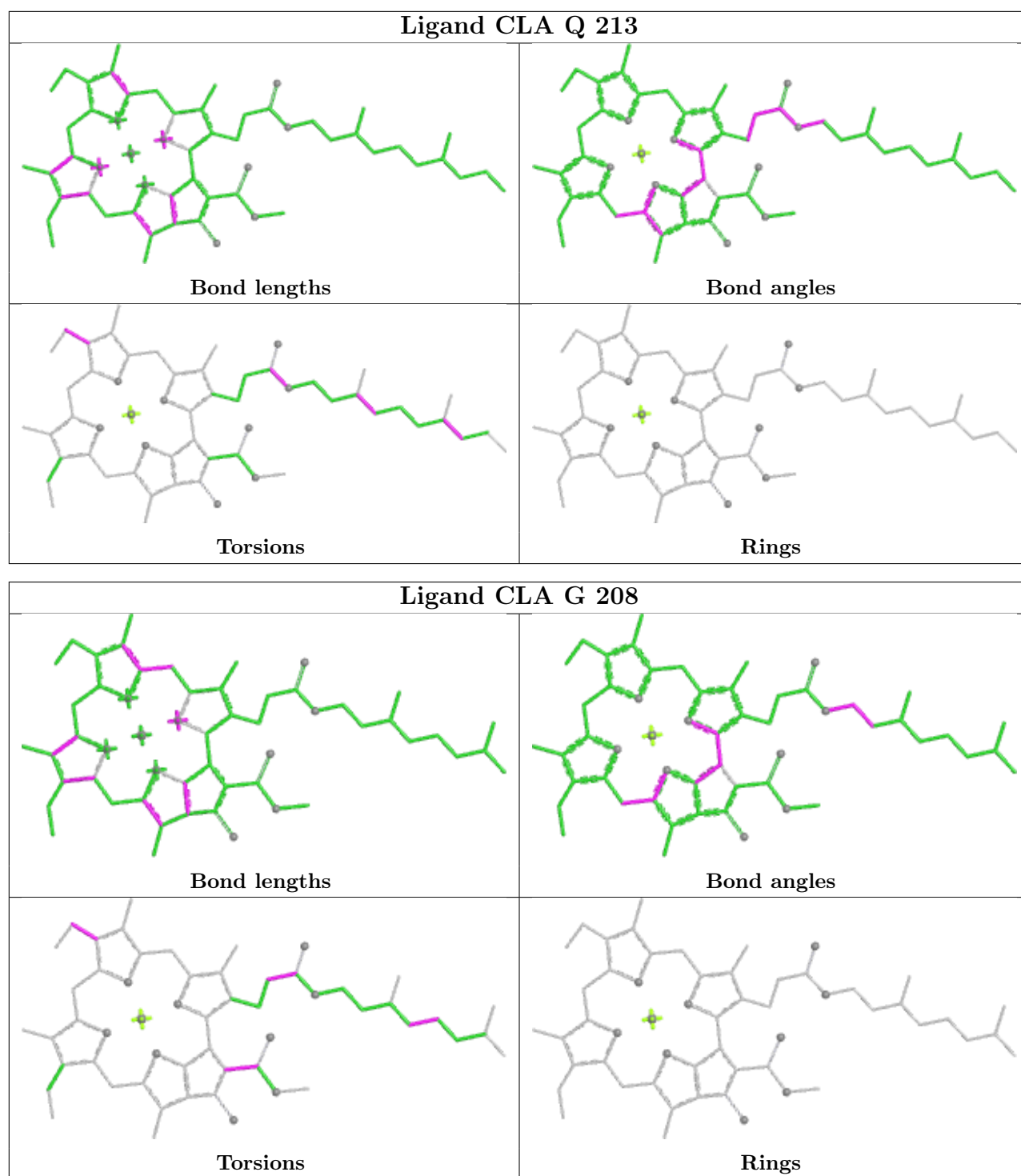


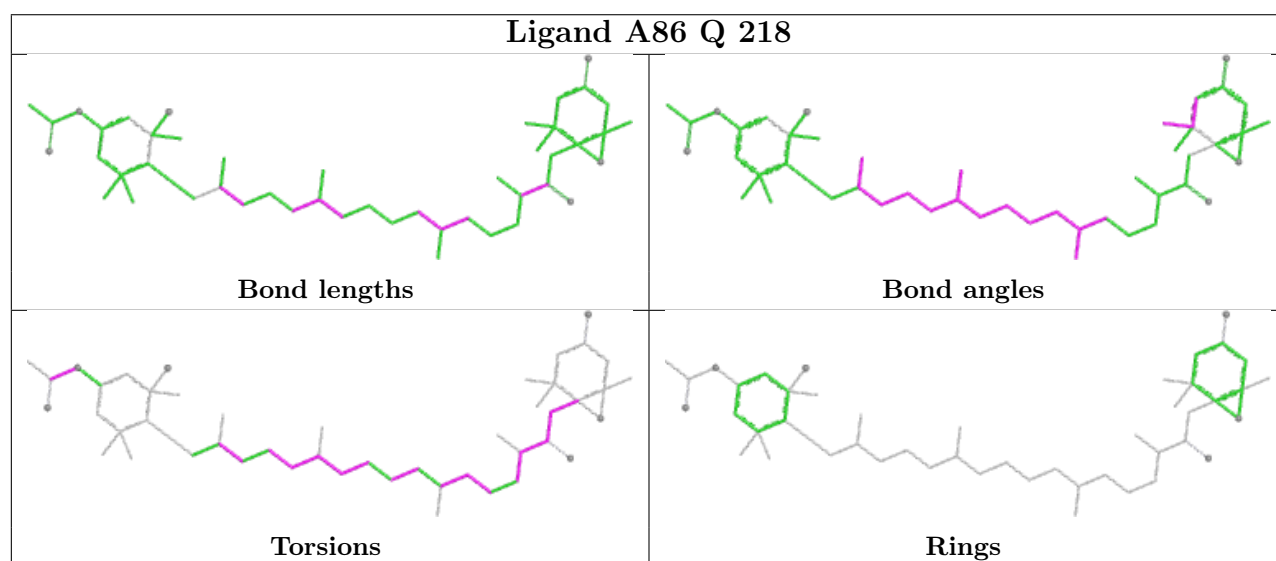
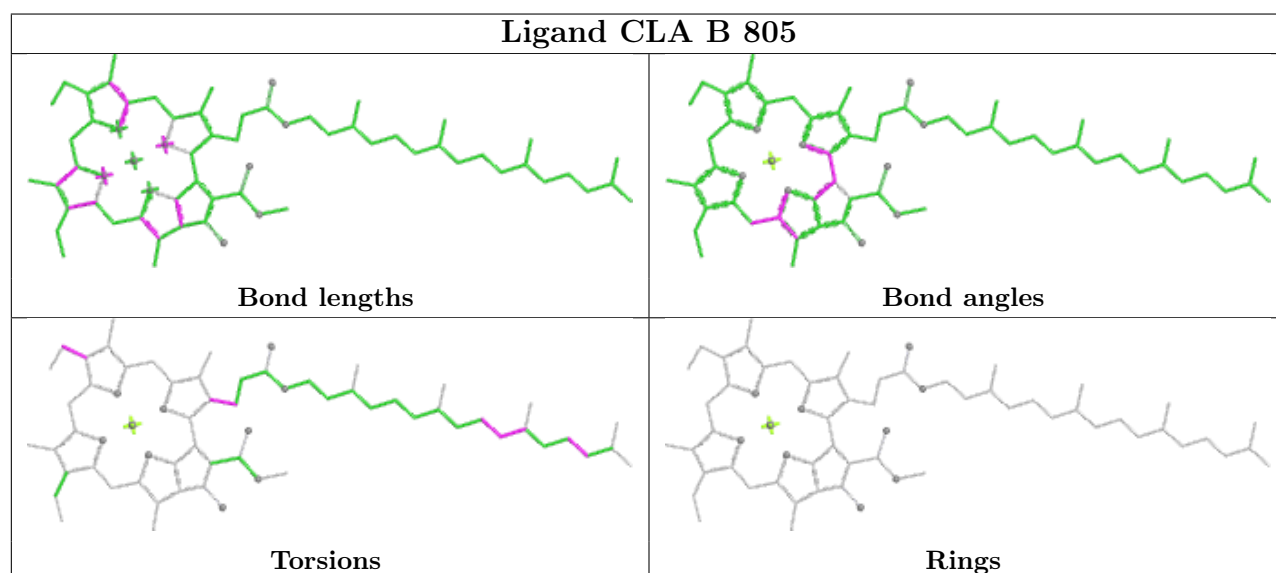
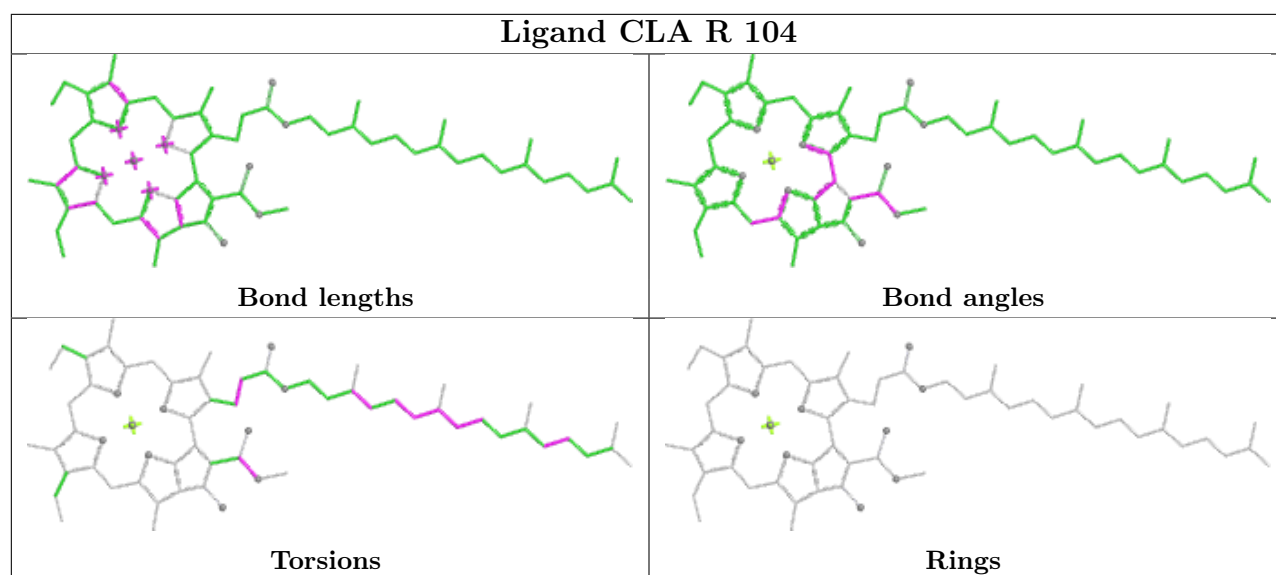
Torsions

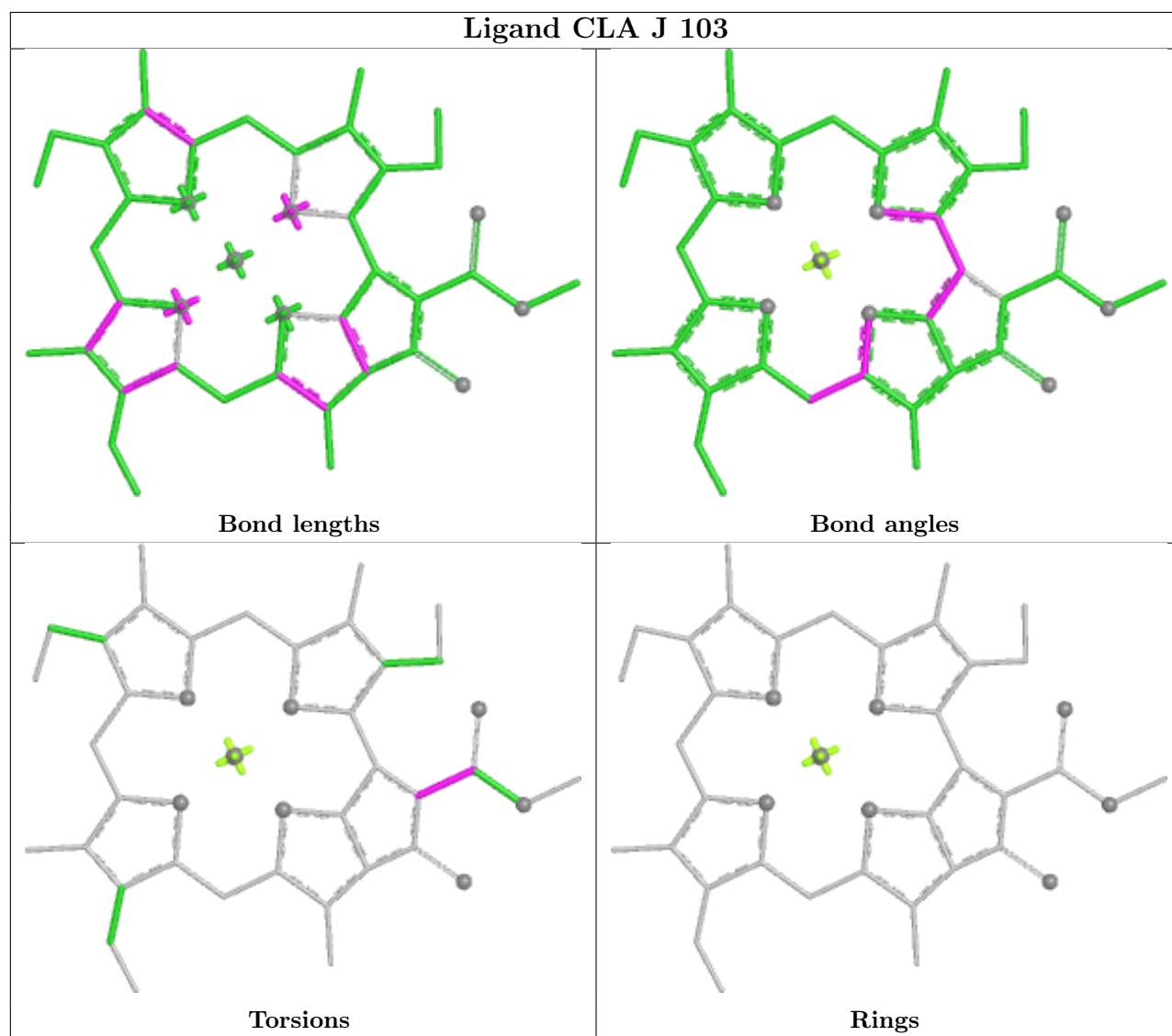
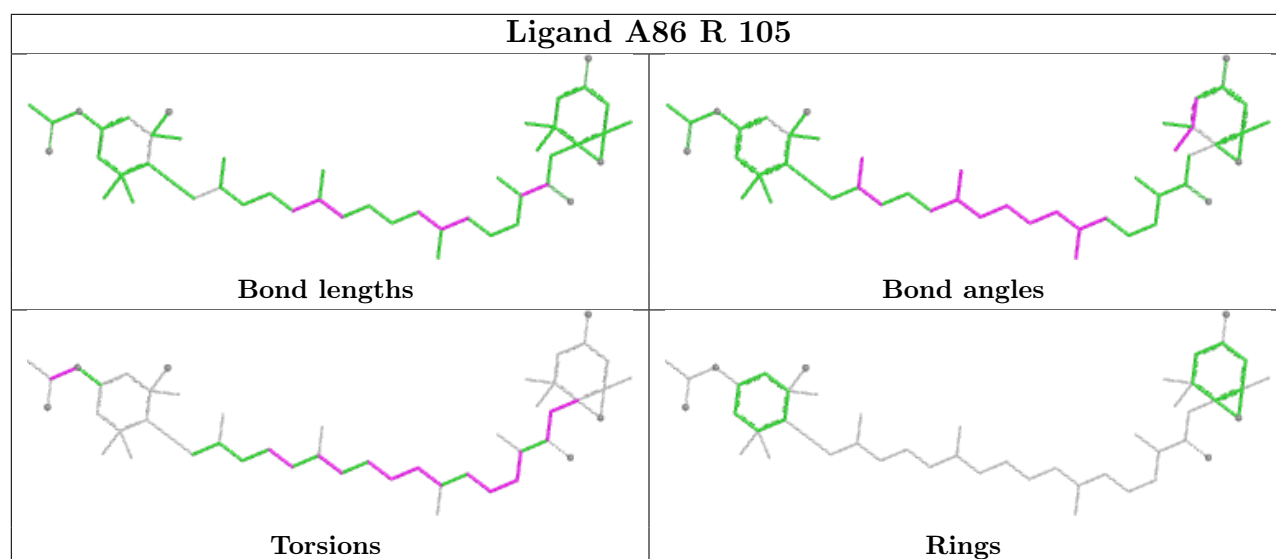


Rings

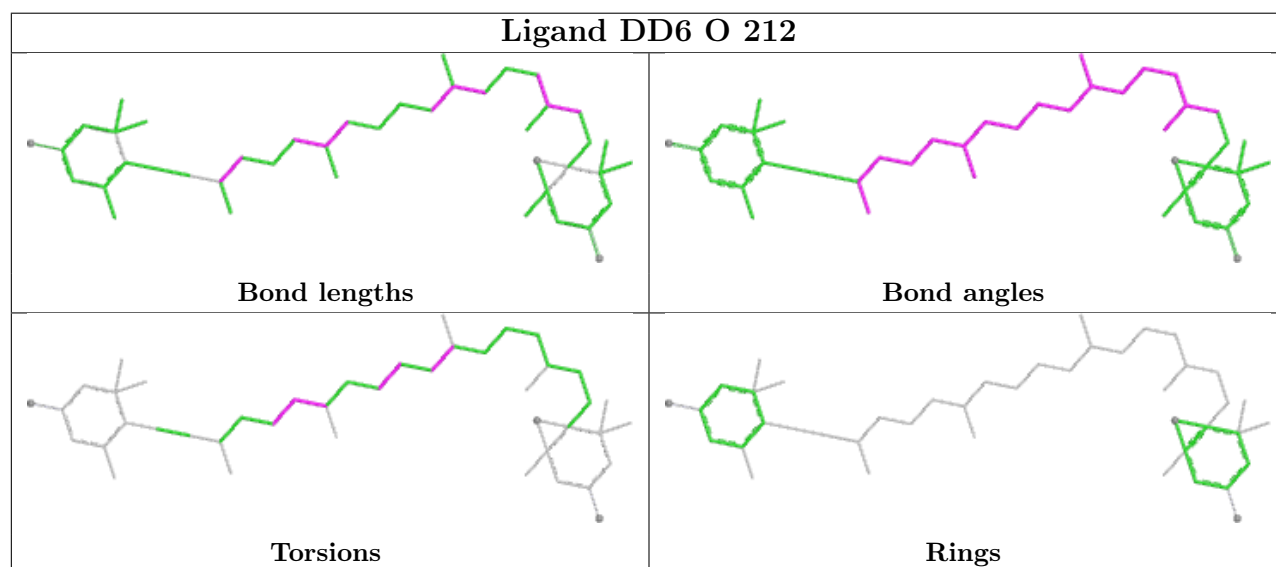
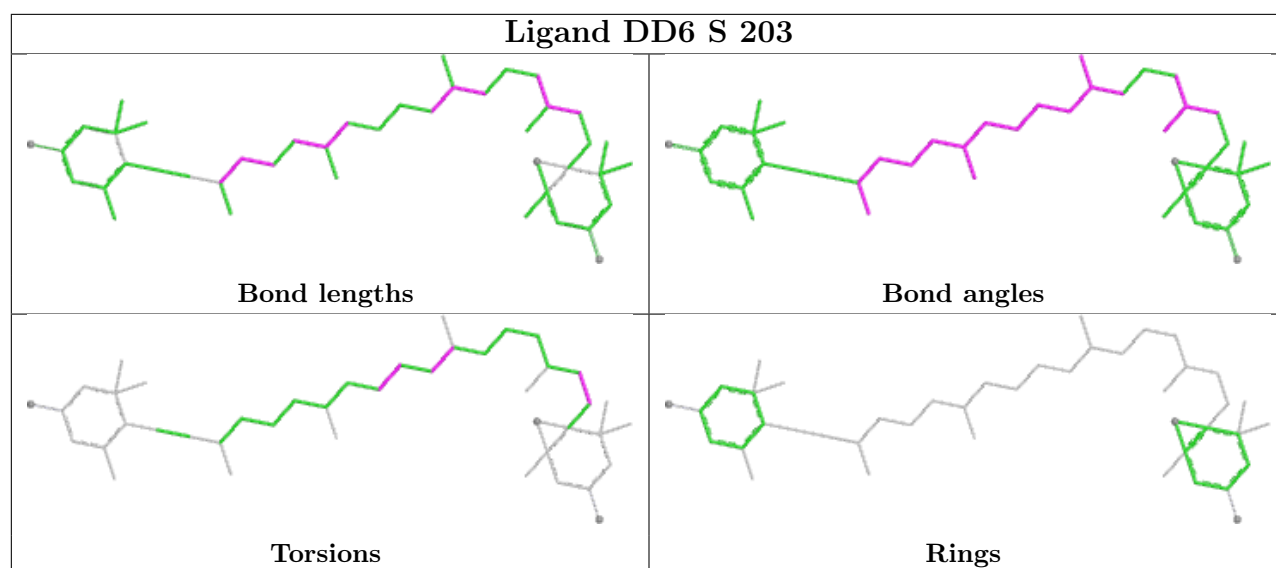


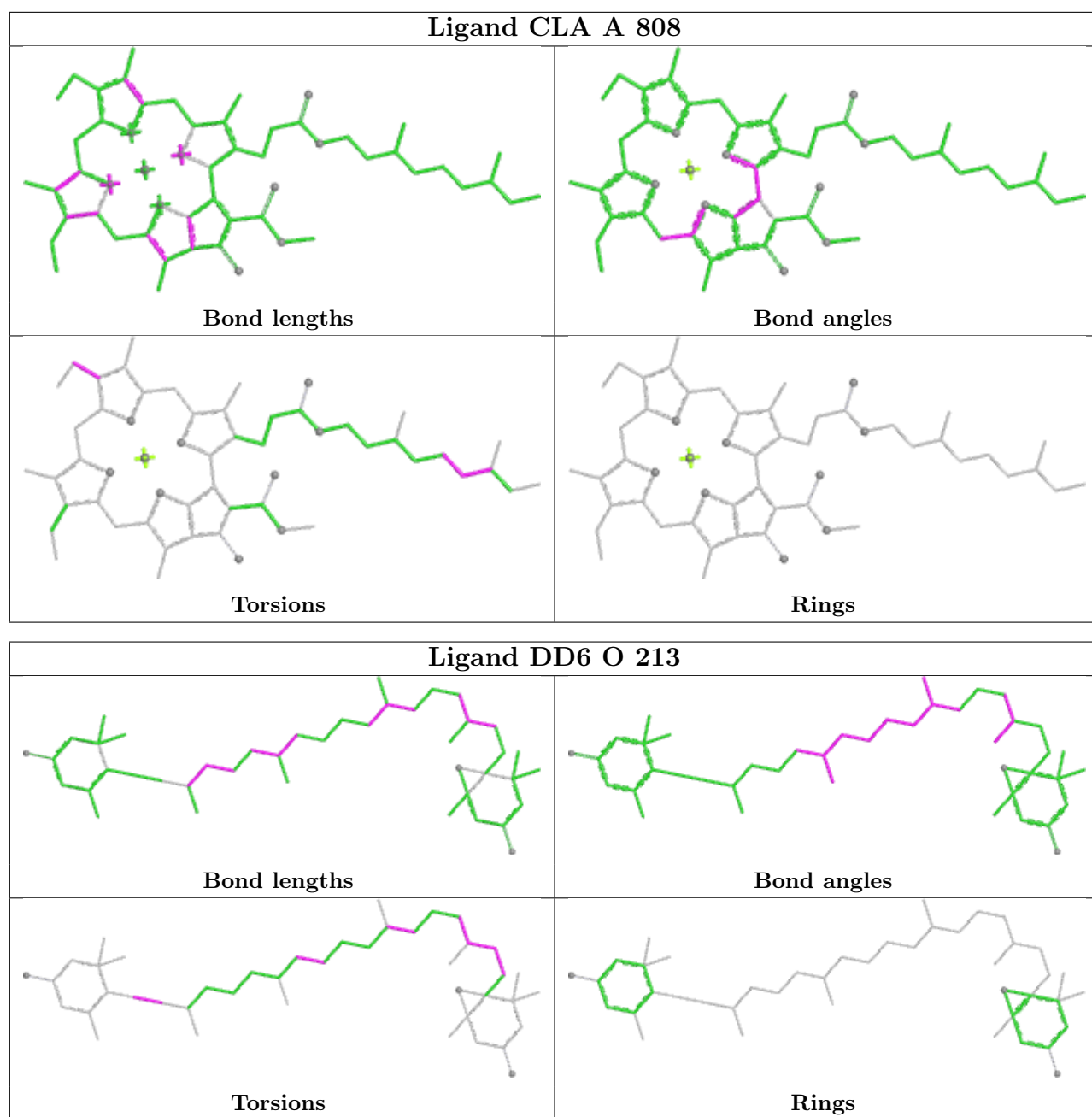




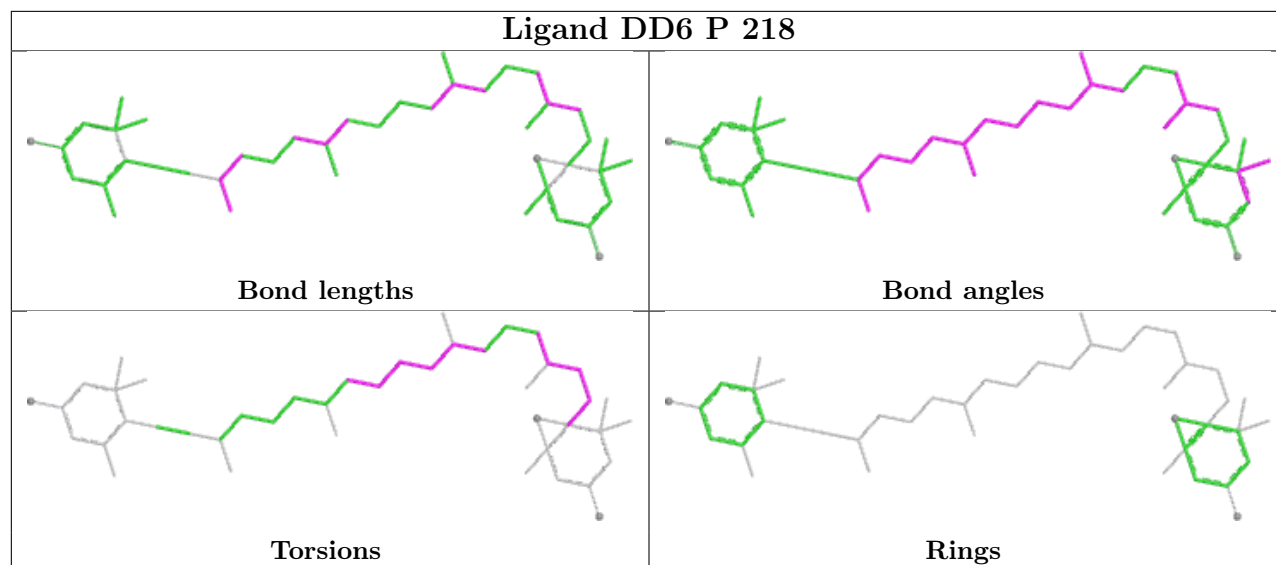




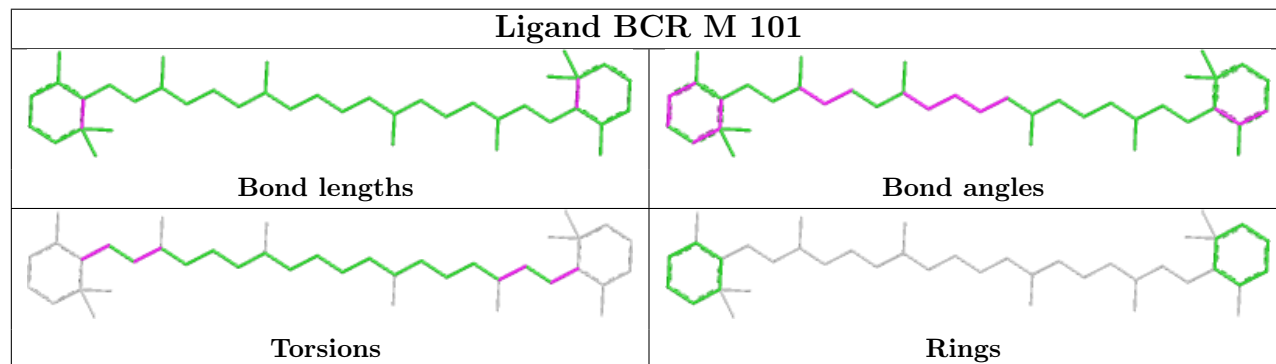




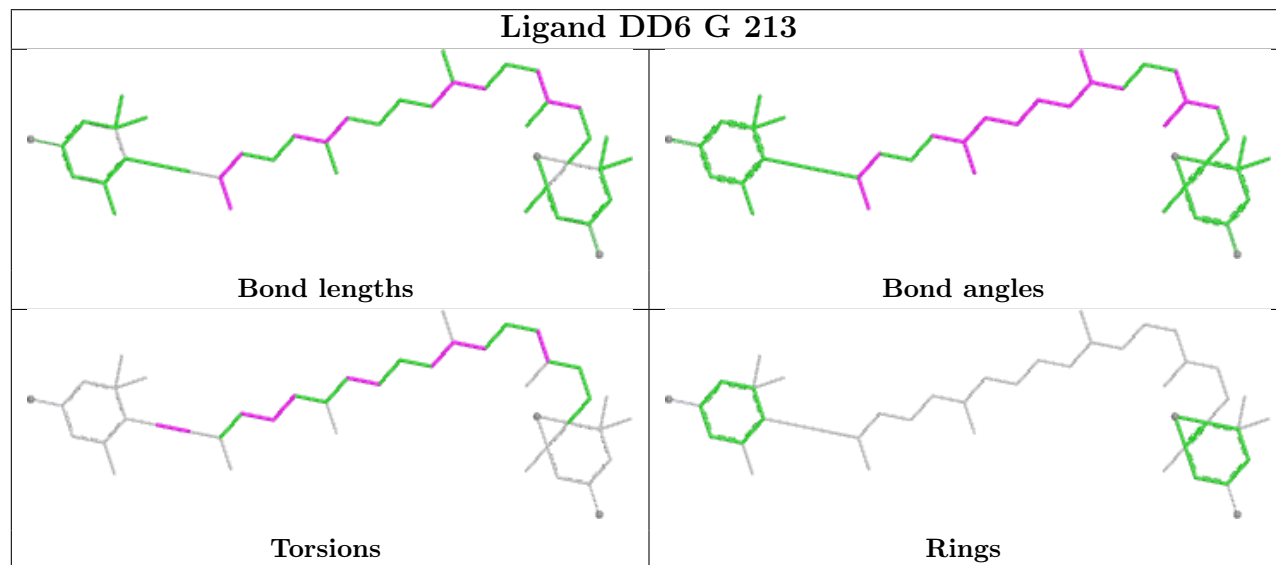
## Ligand DD6 P 218

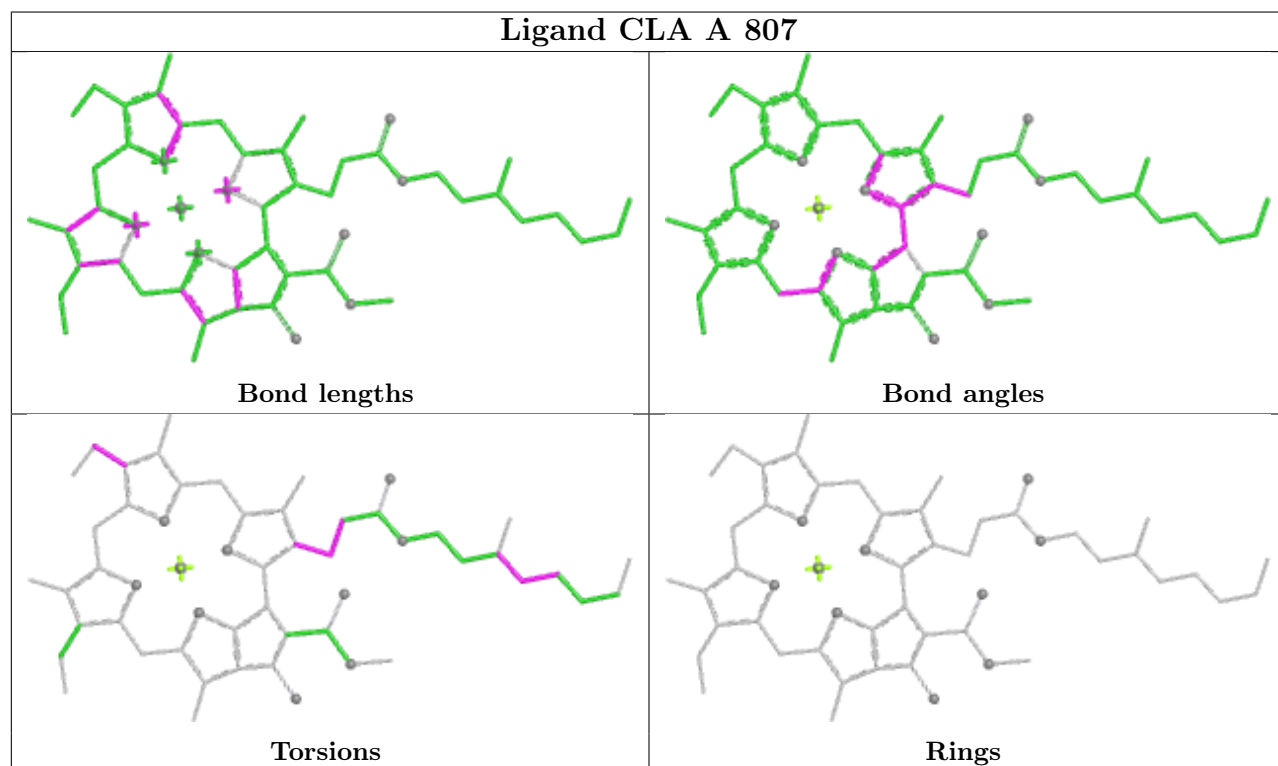
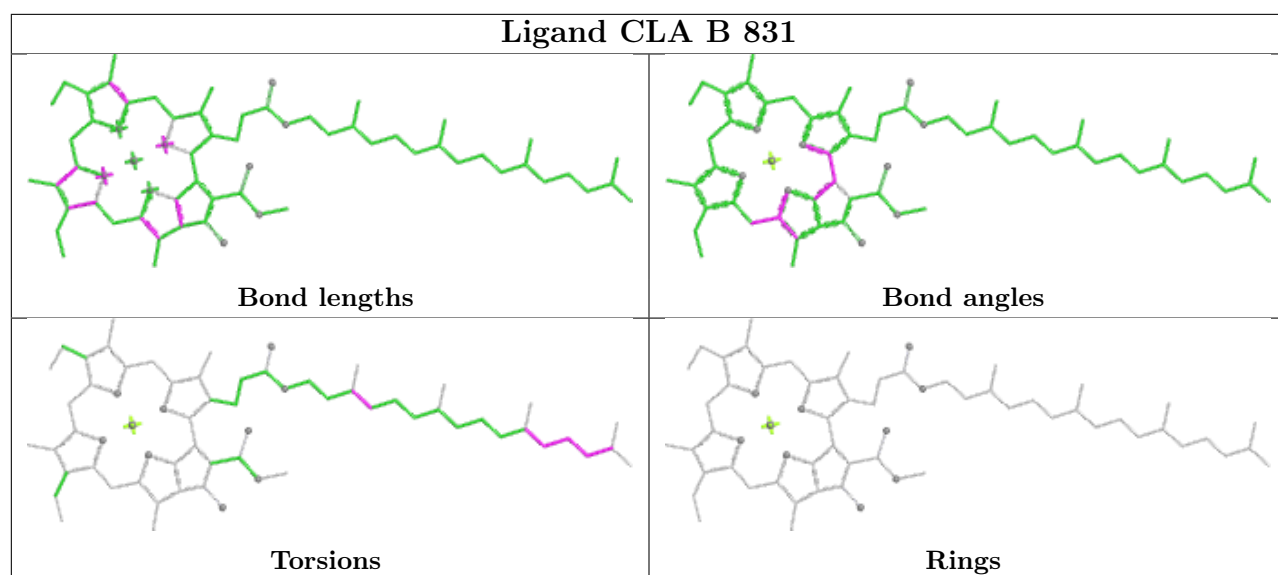


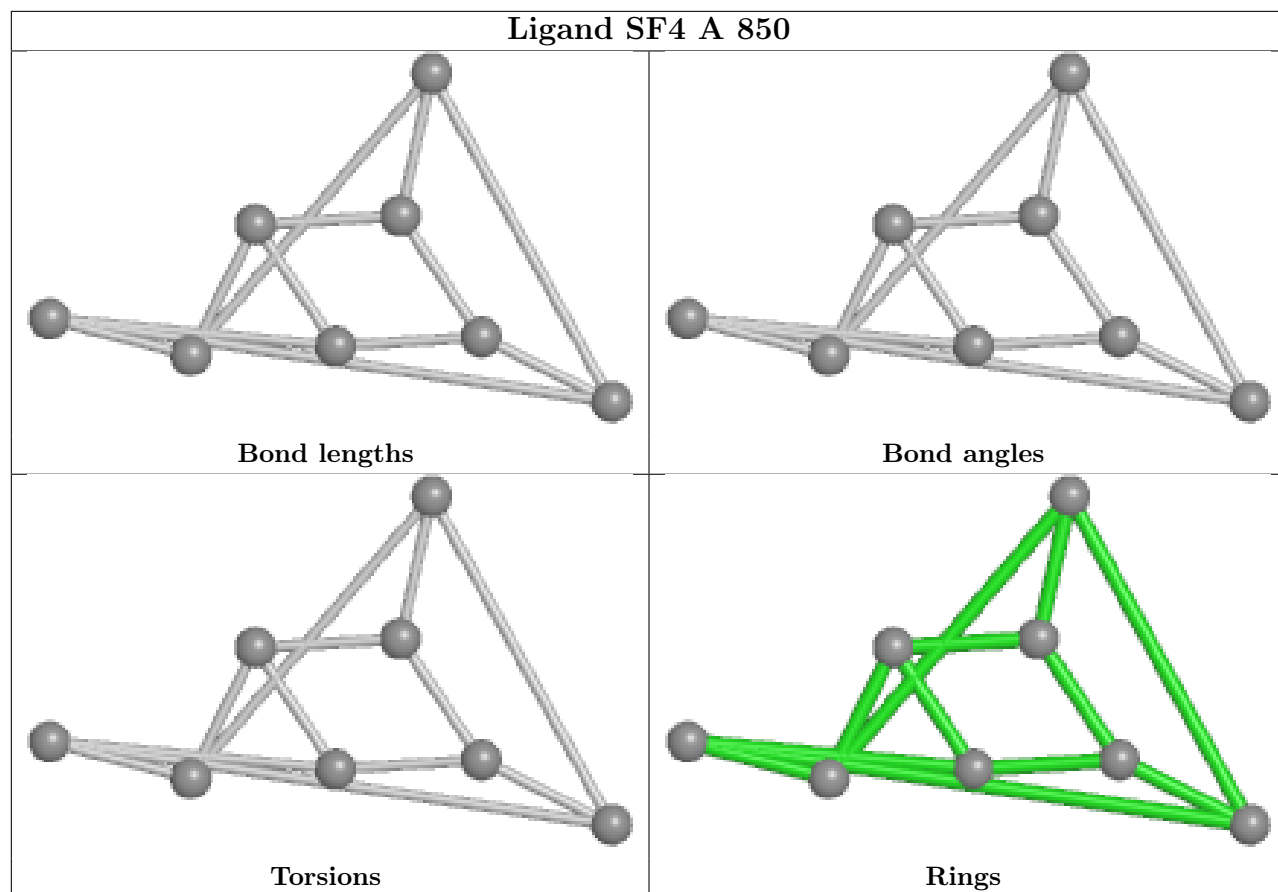
## Ligand BCR M 101

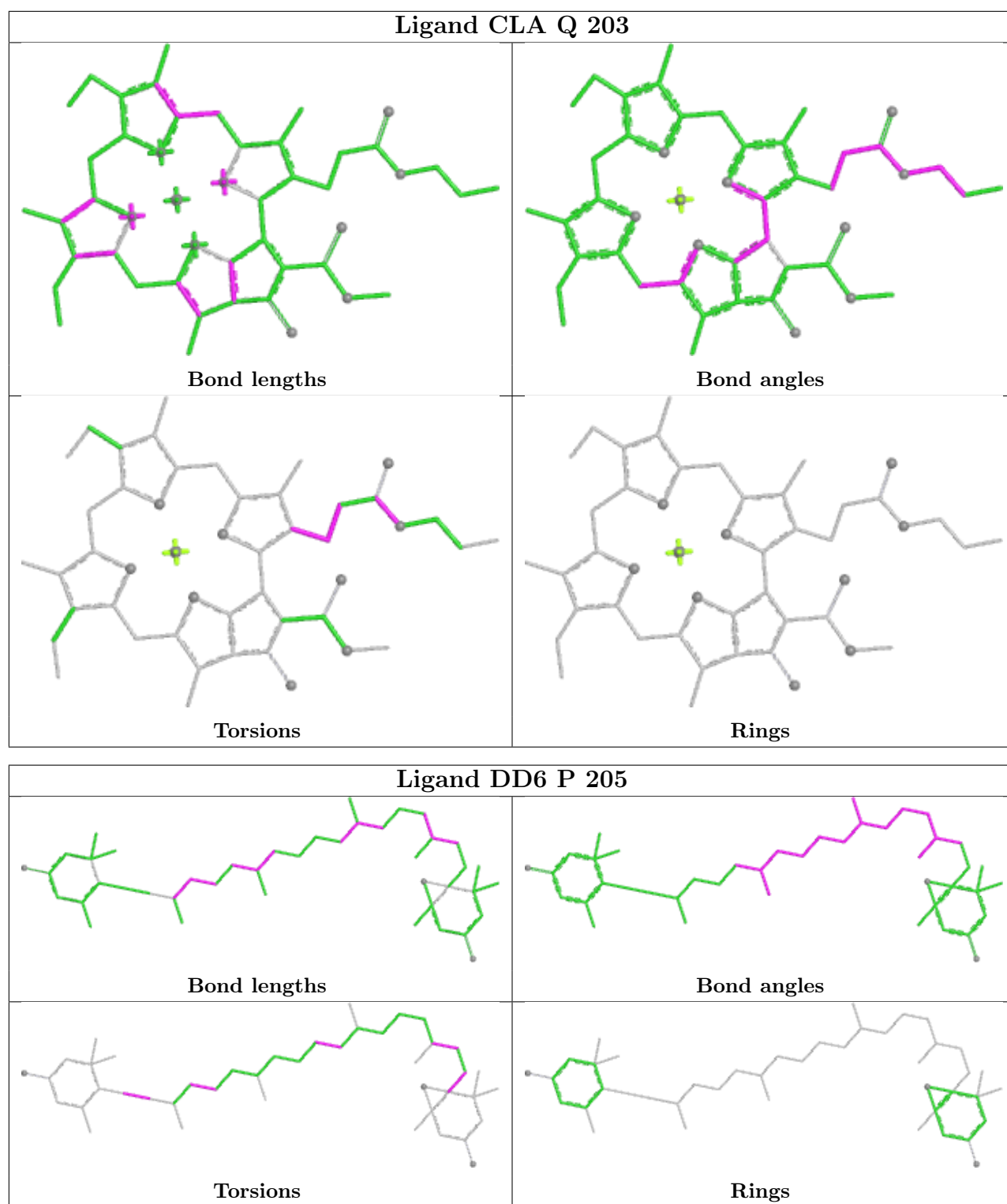


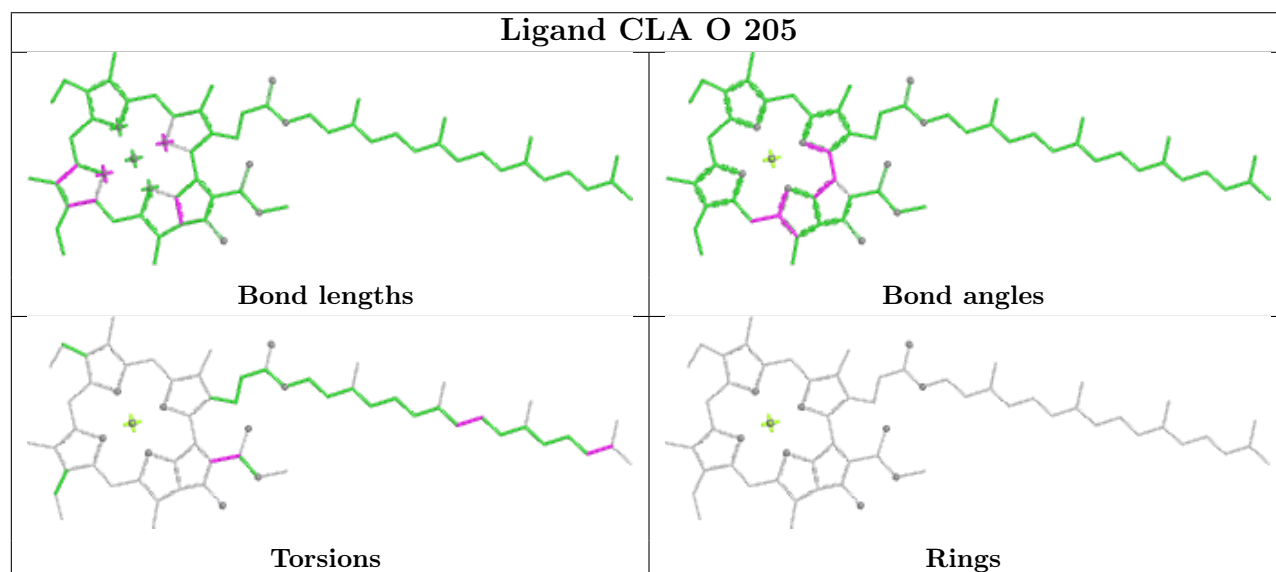
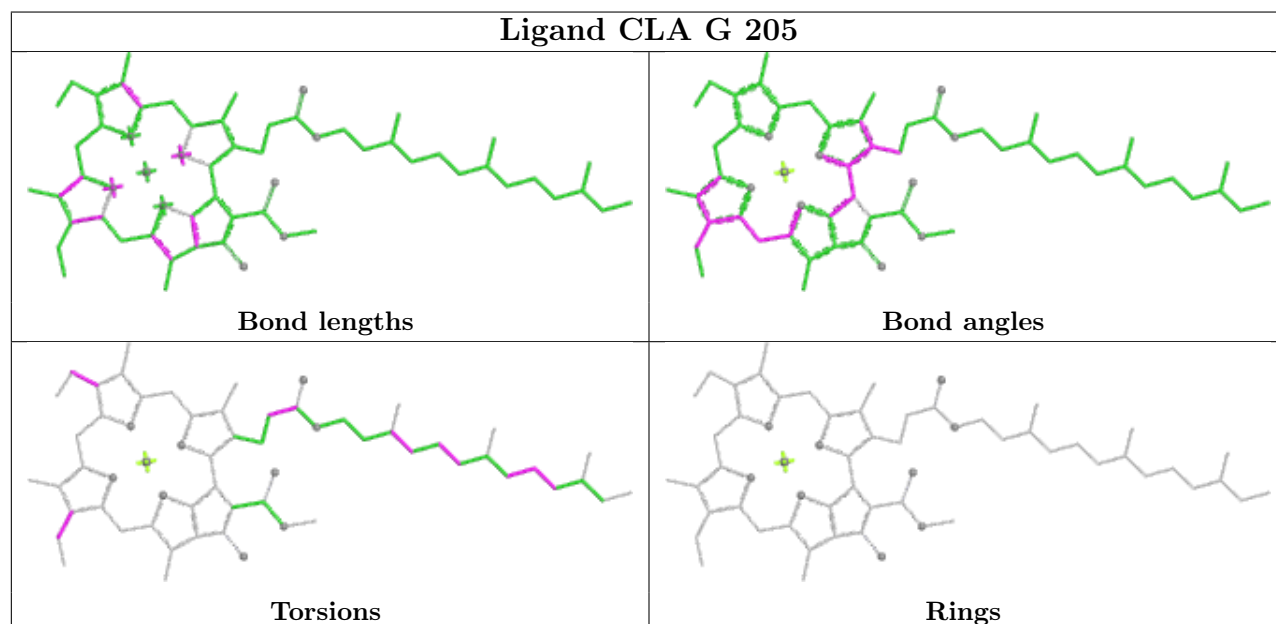
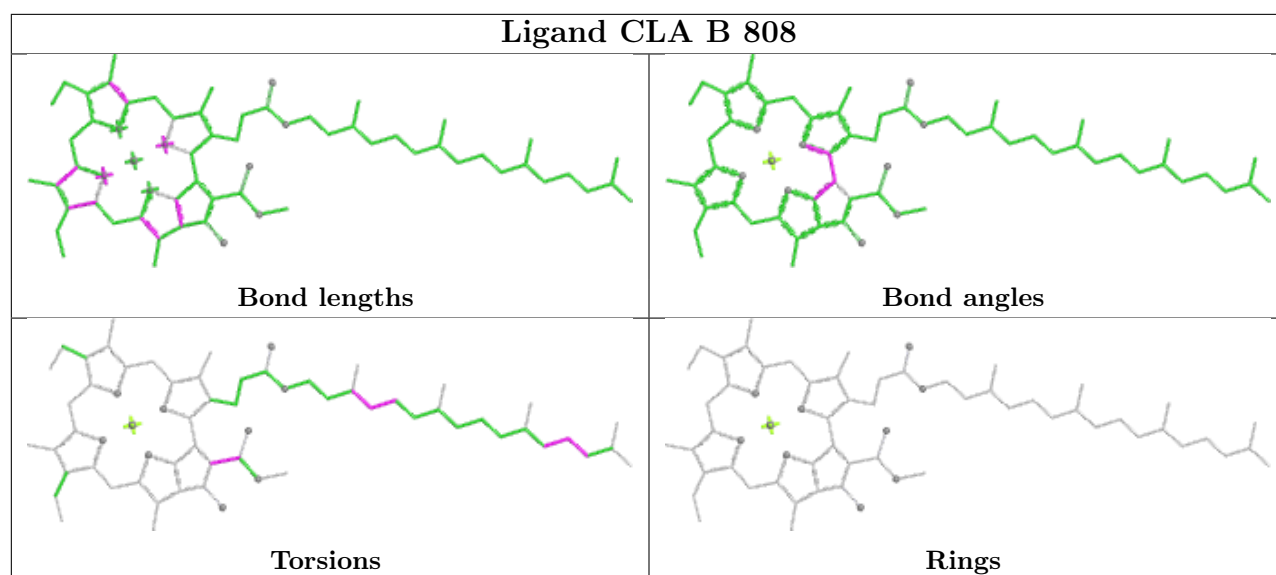
## Ligand DD6 G 213

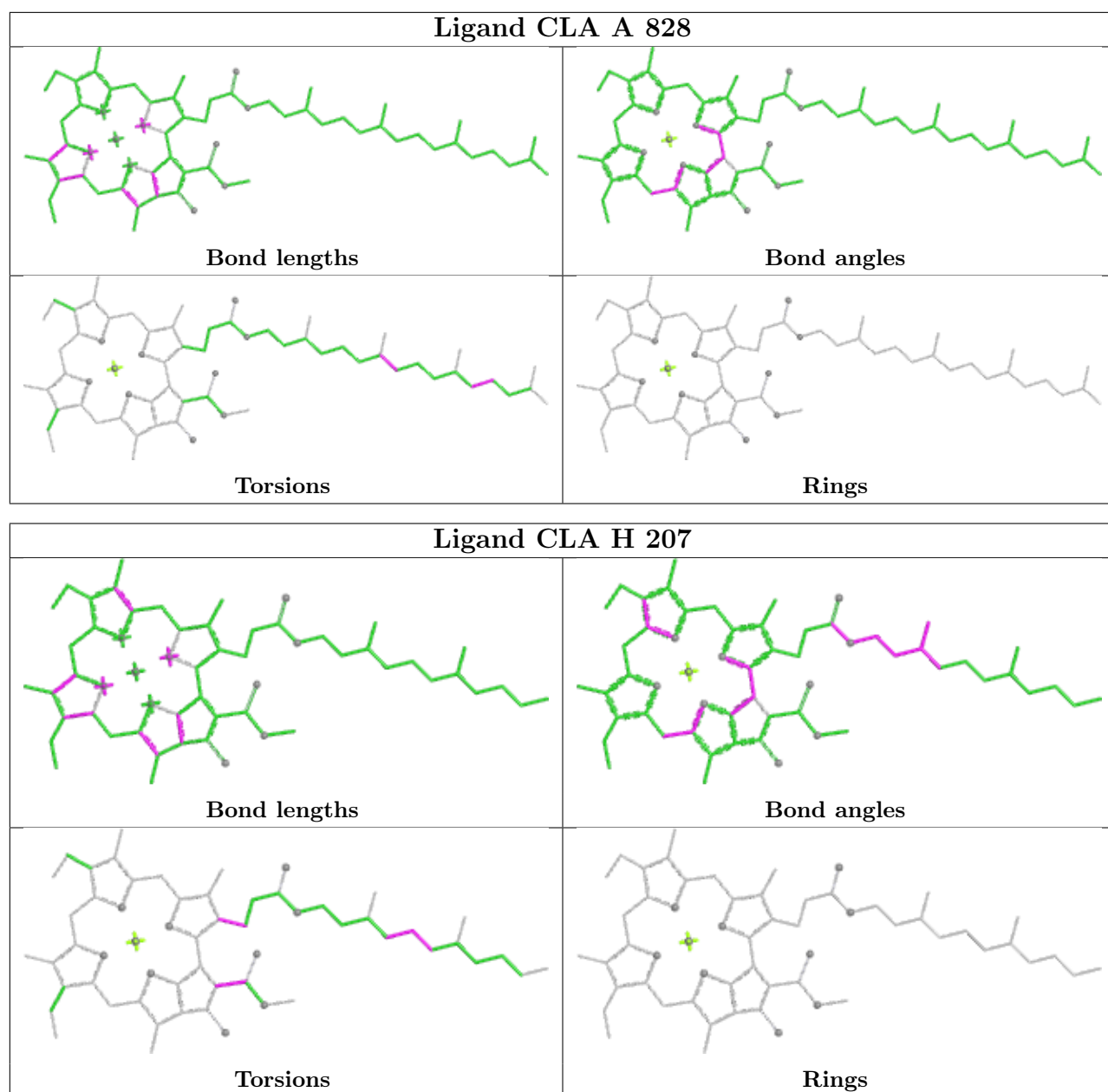




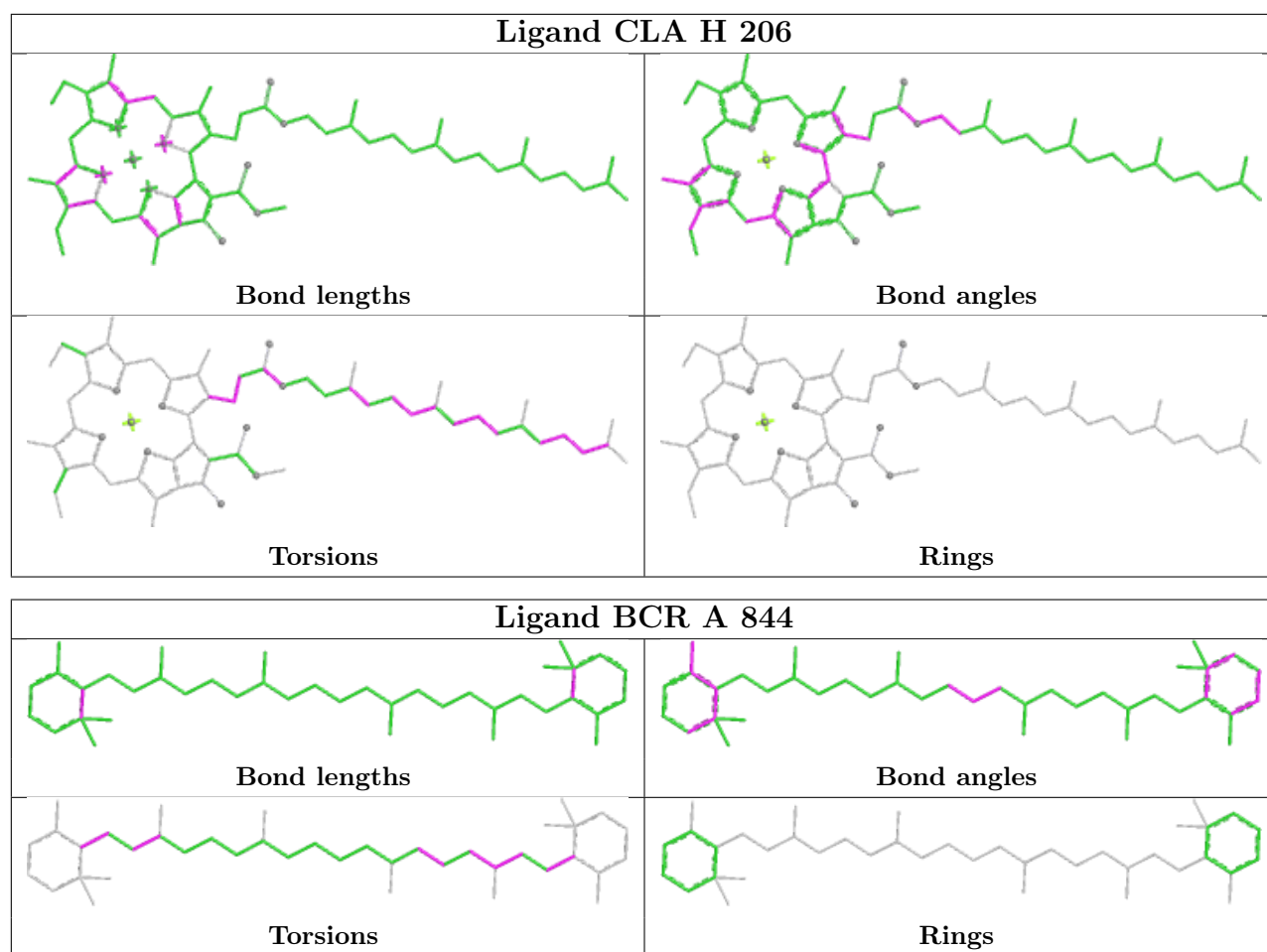




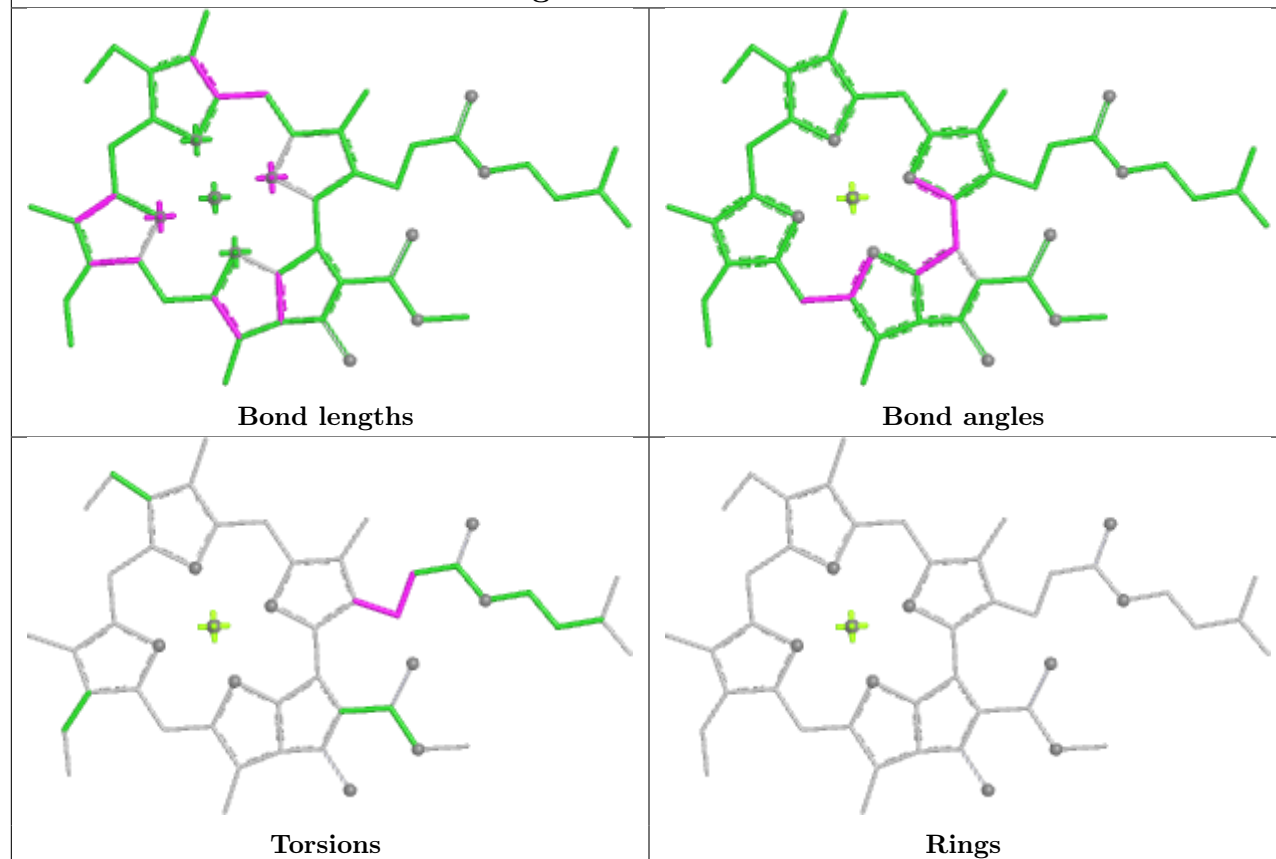




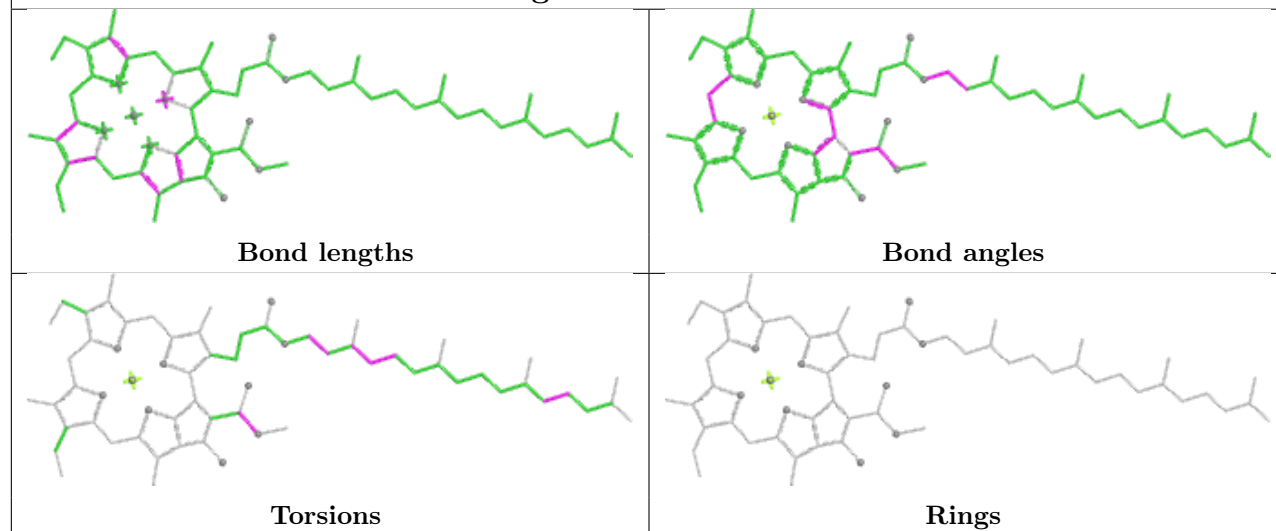


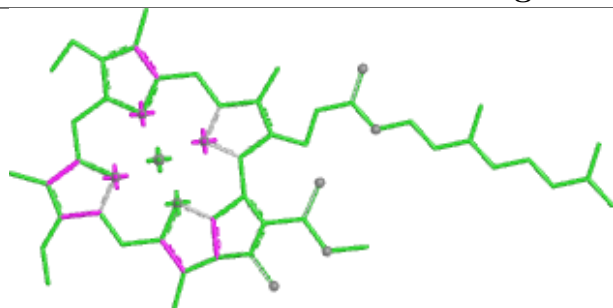


## Ligand CLA B 848

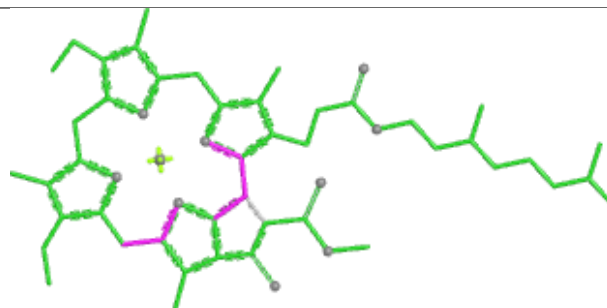


## Ligand CLA O 209

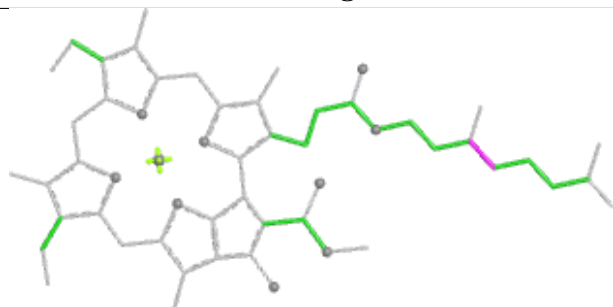


**Ligand CLA B 814**

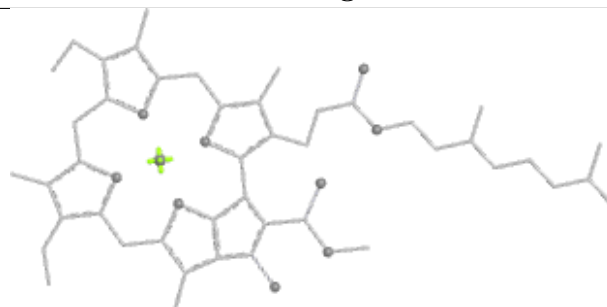
Bond lengths



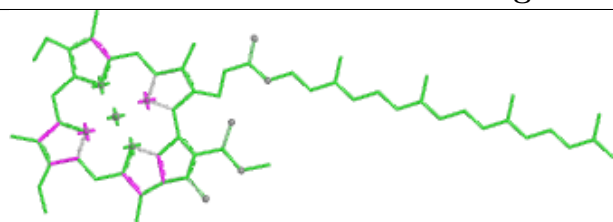
Bond angles



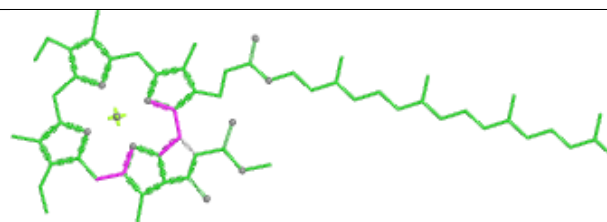
Torsions



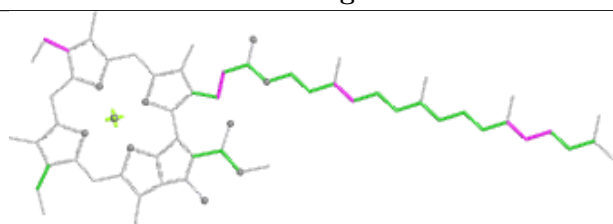
Rings

**Ligand CLA A 825**

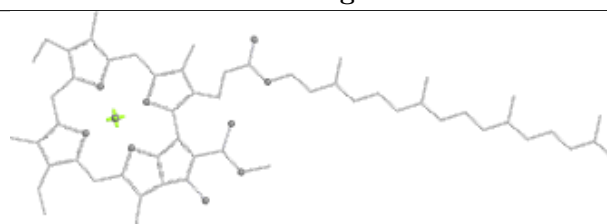
Bond lengths



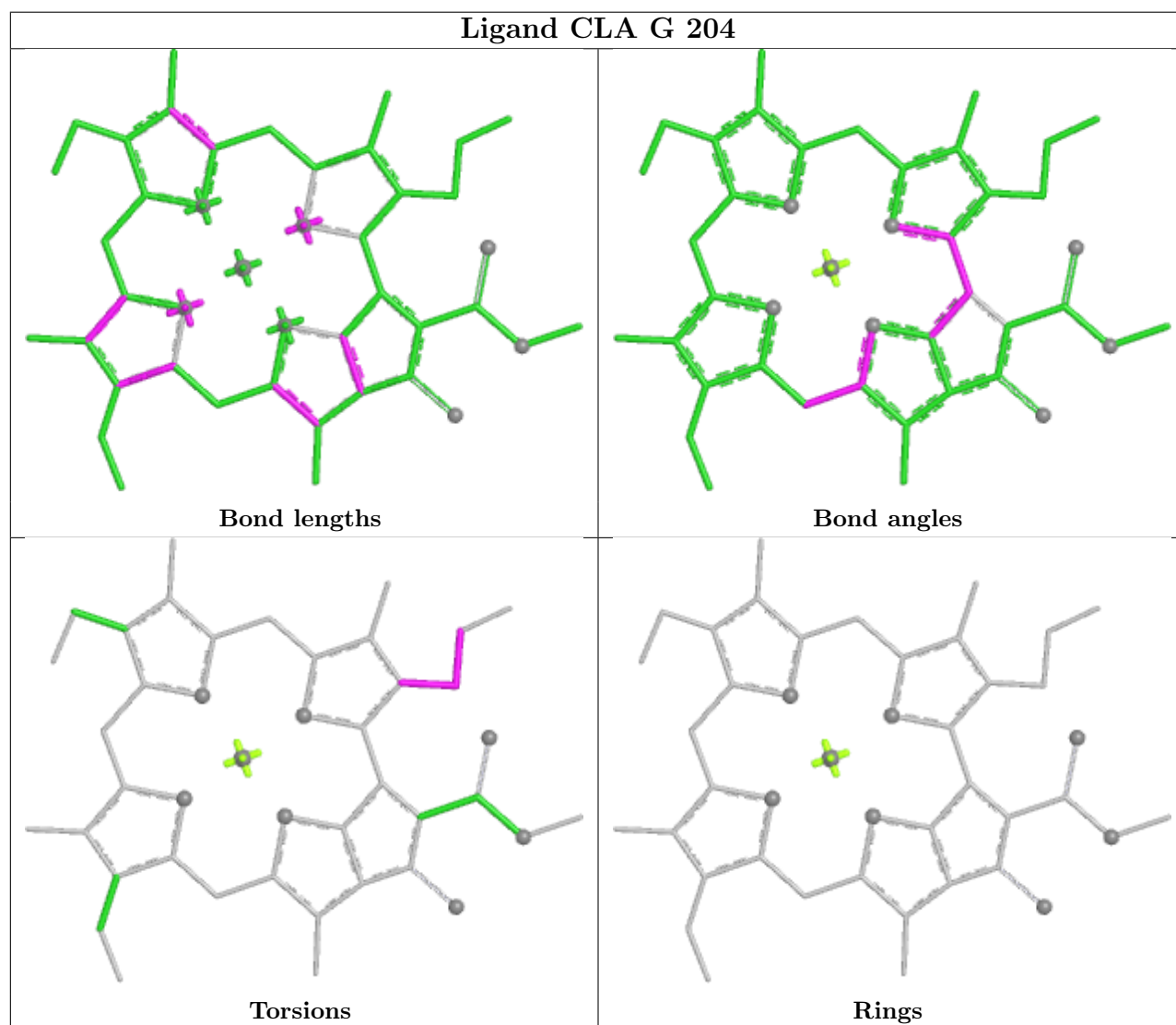
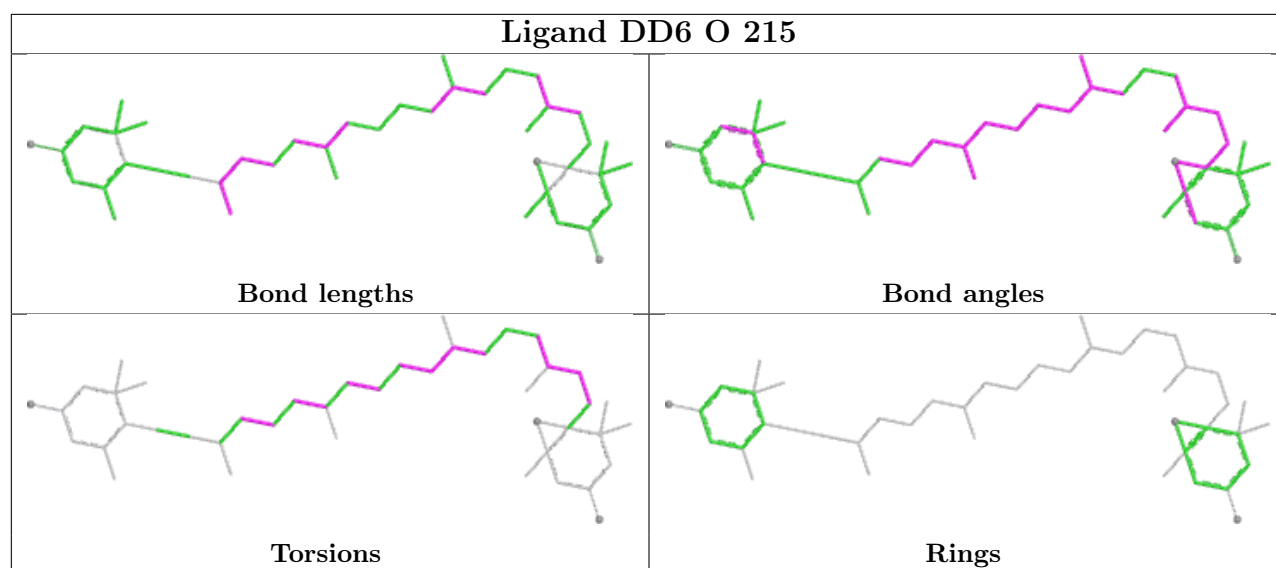
Bond angles

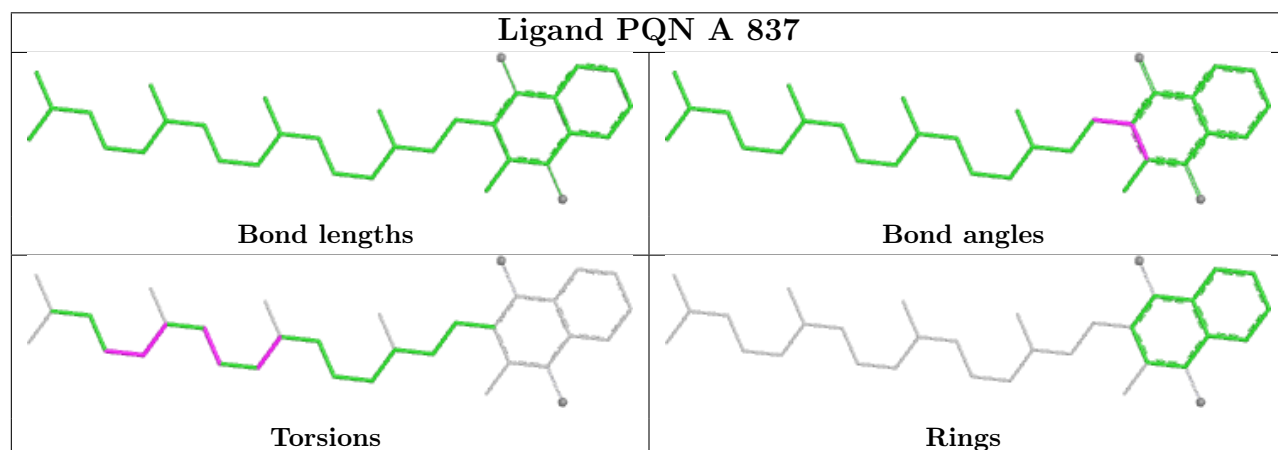
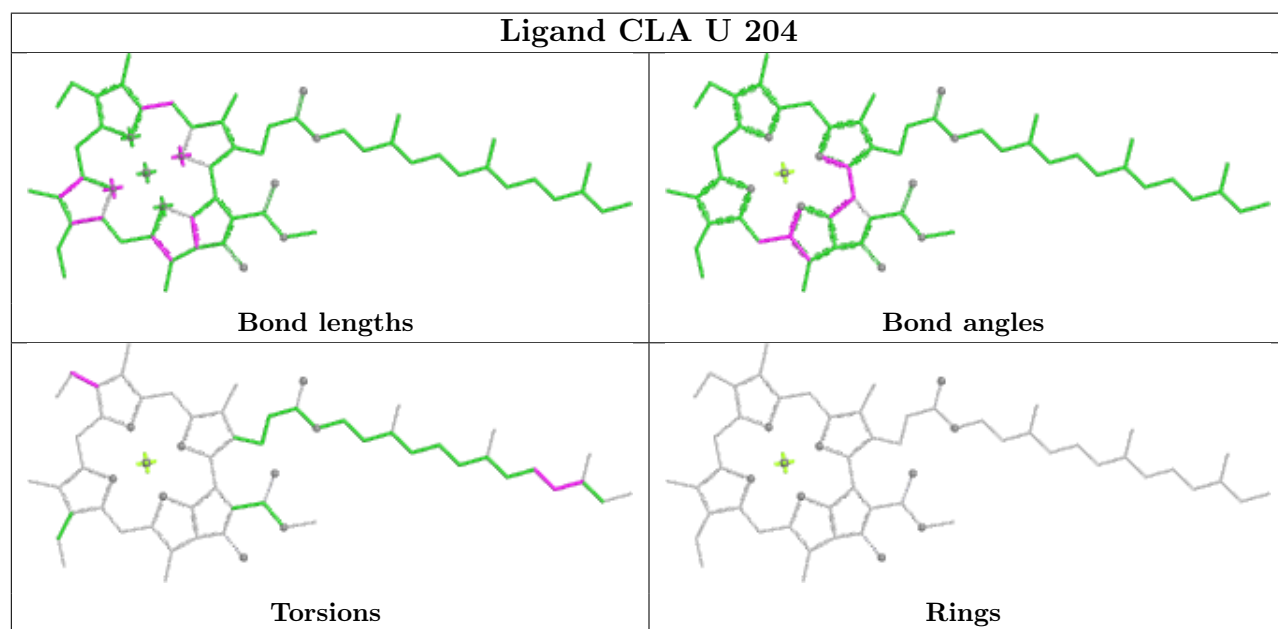
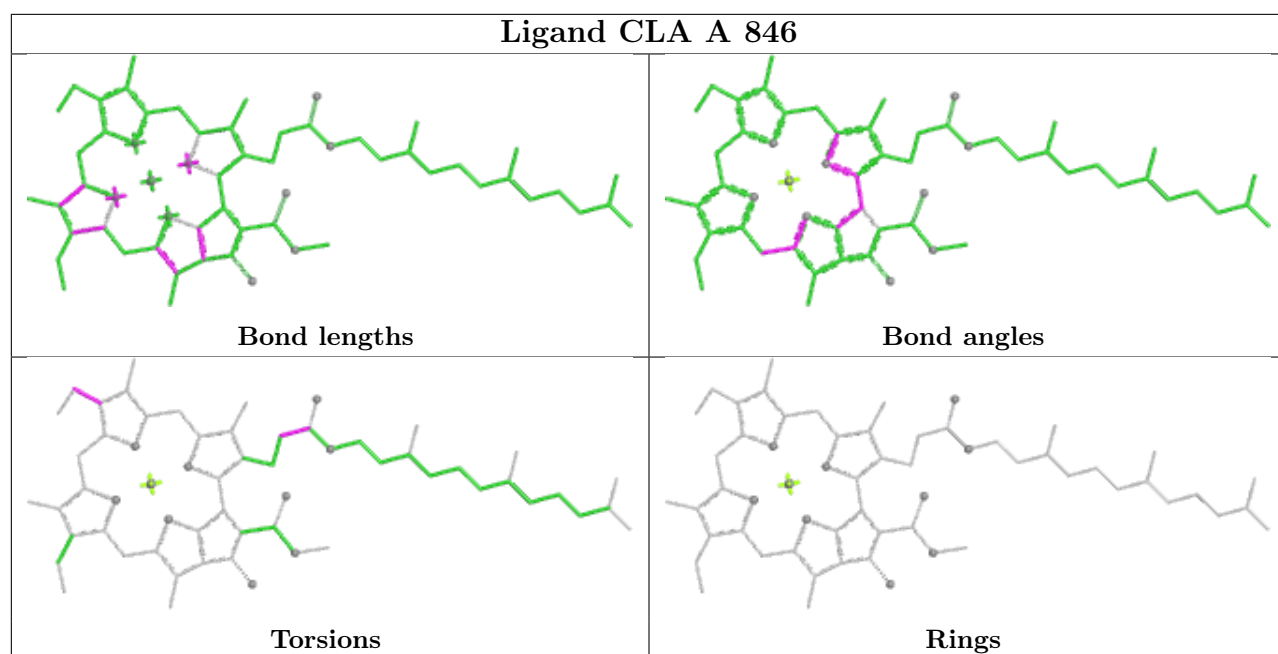


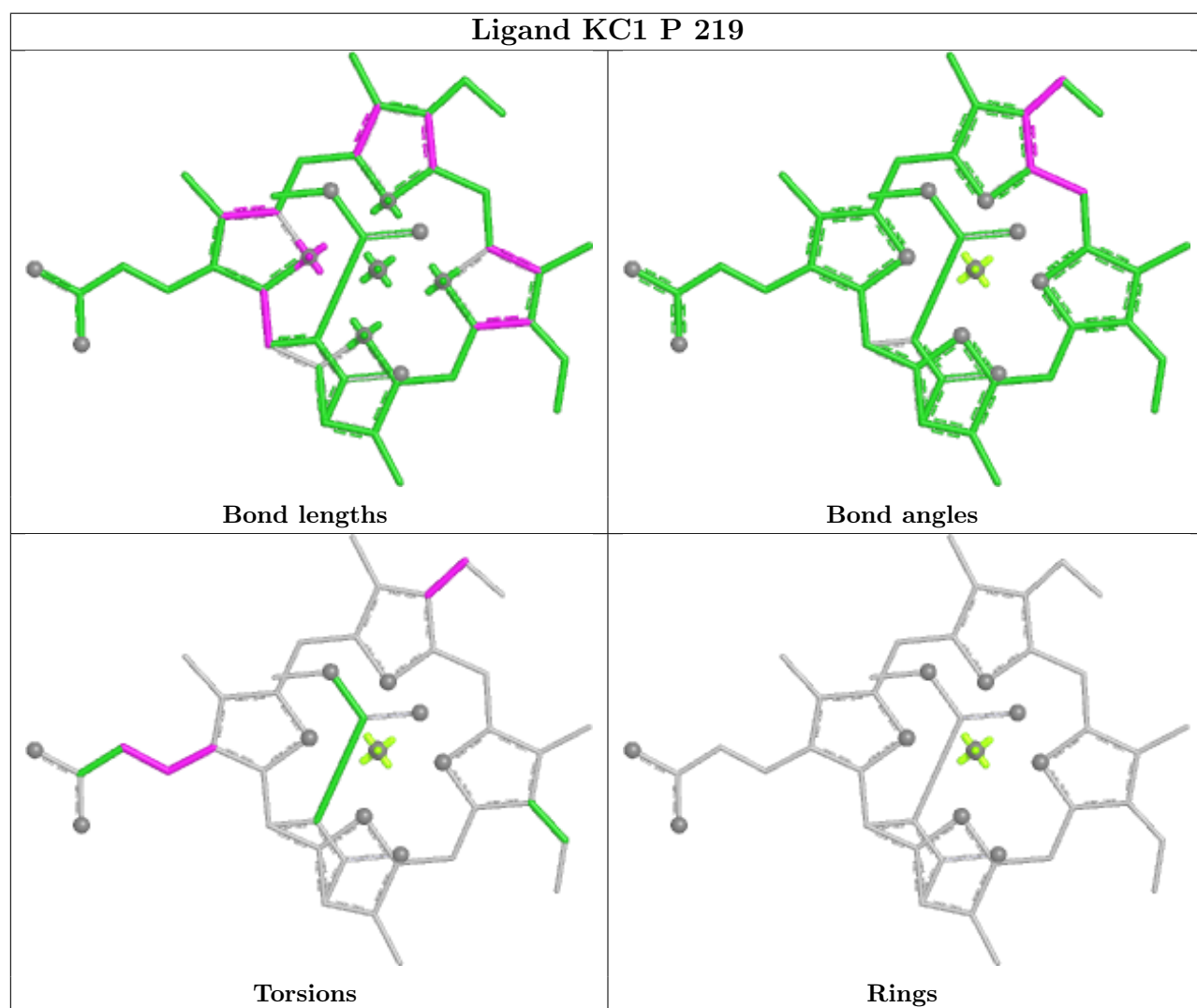
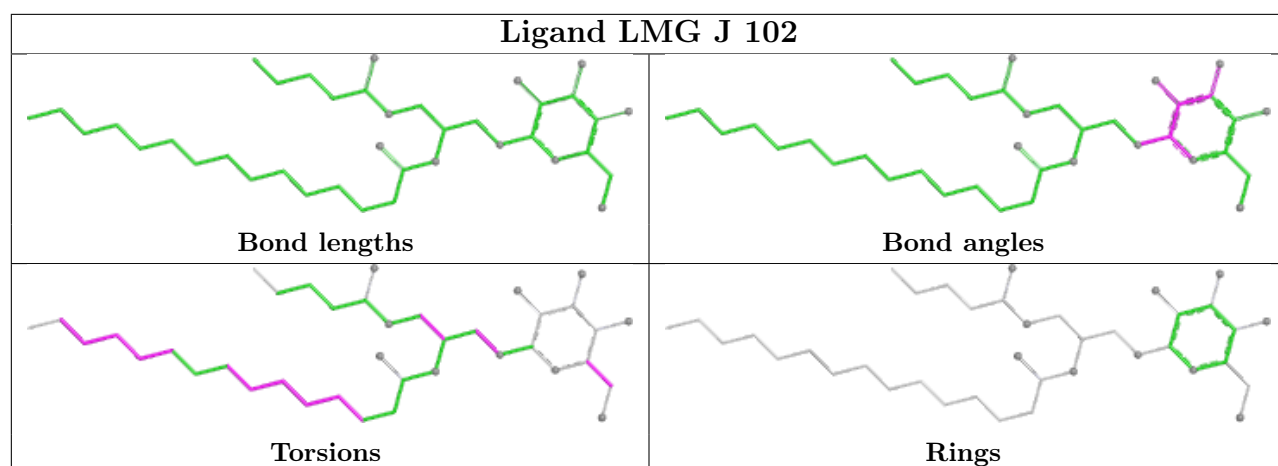
Torsions

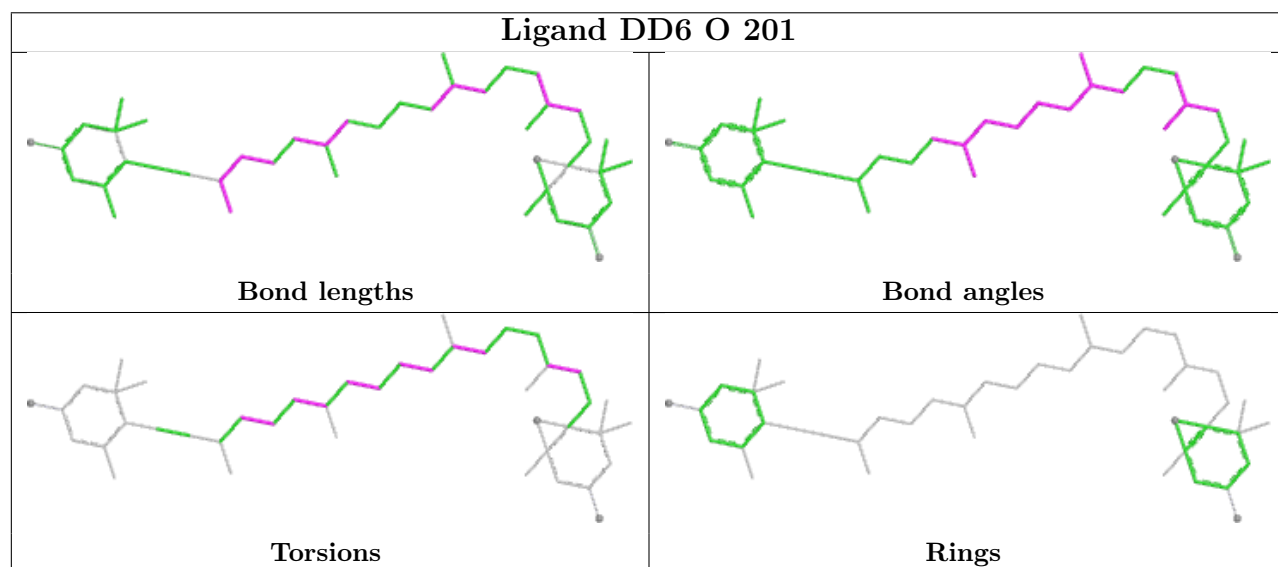
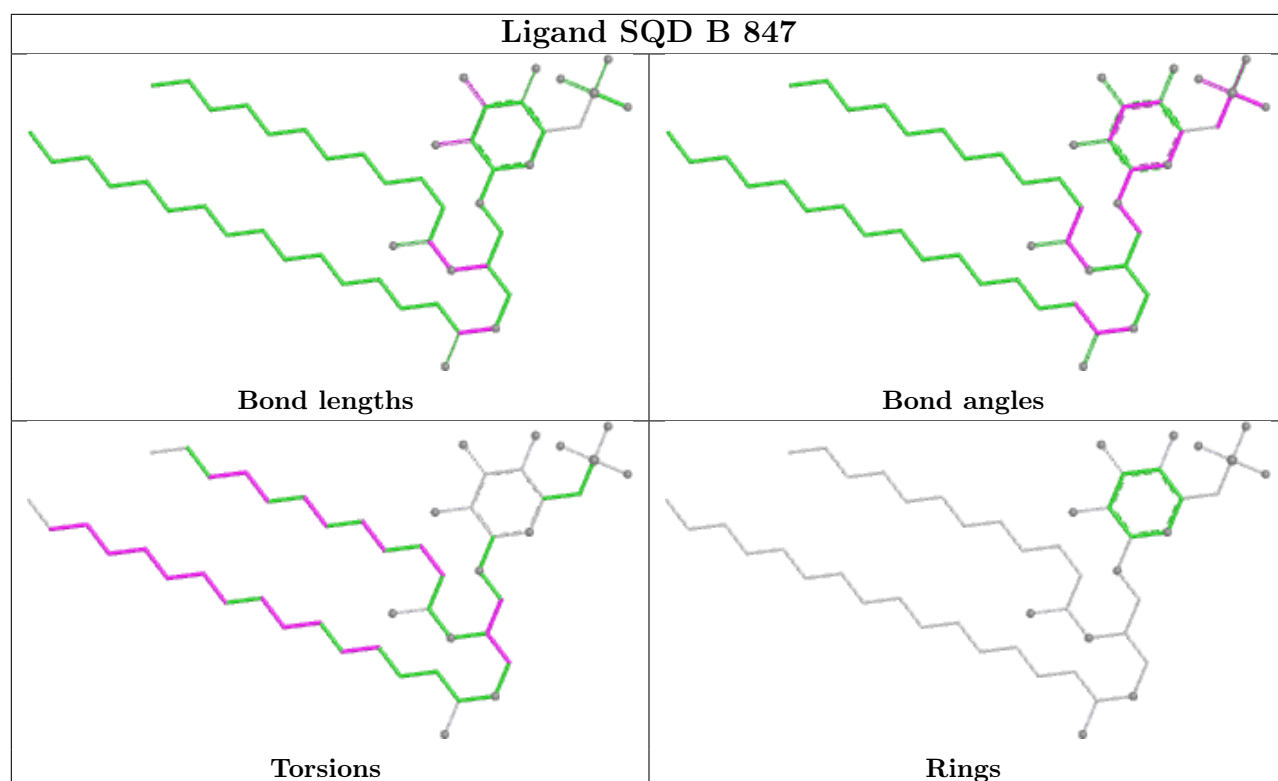


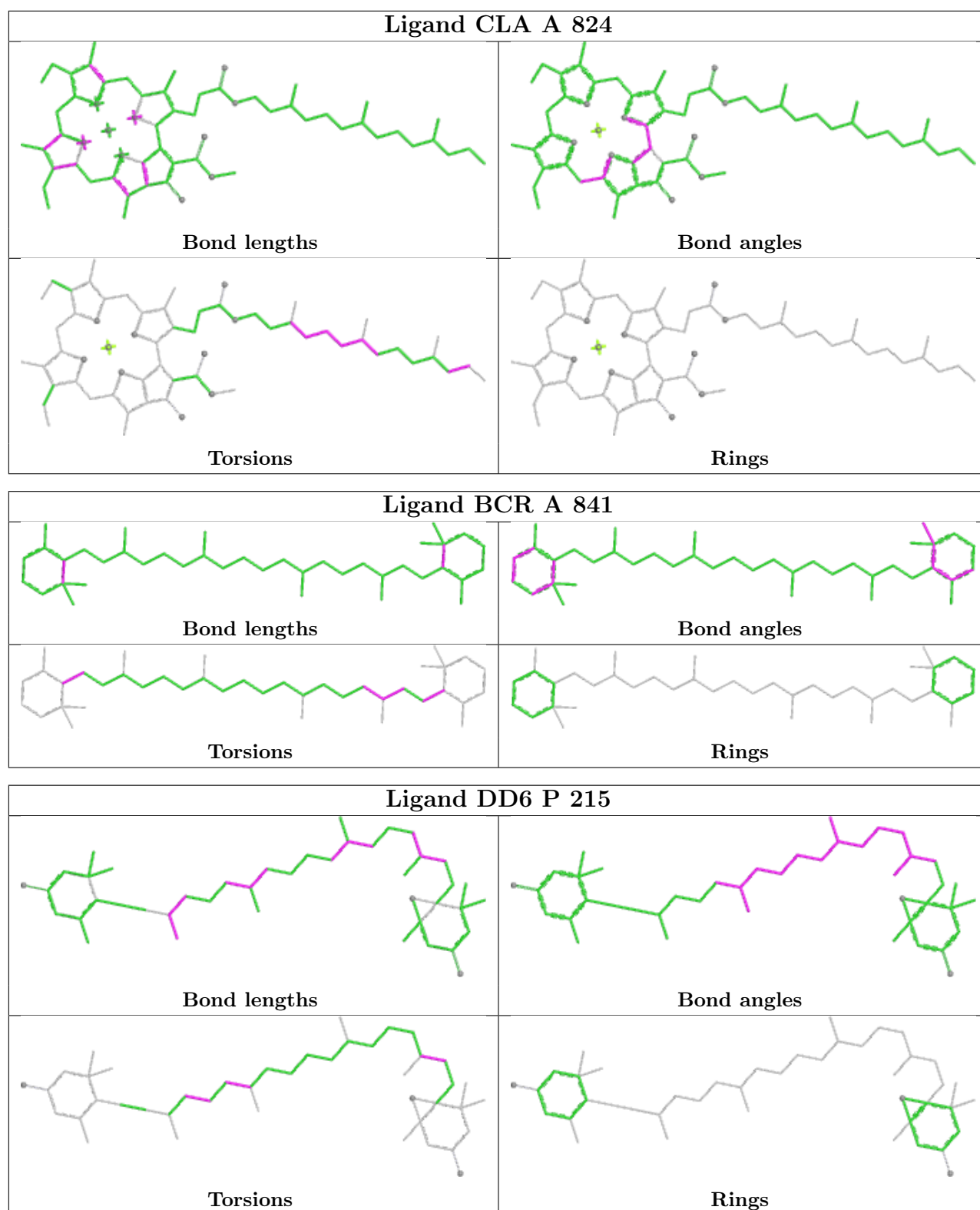
Rings



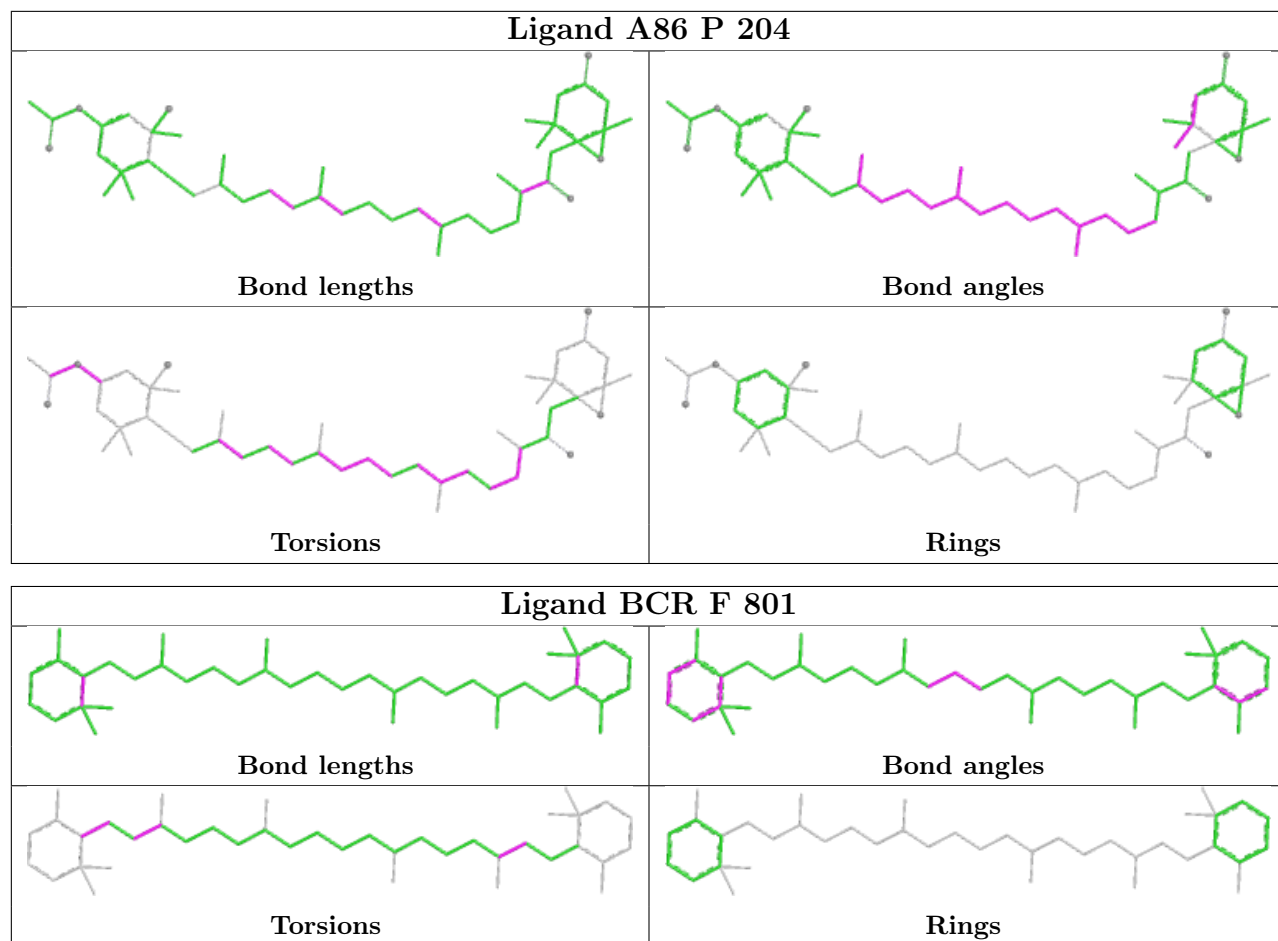


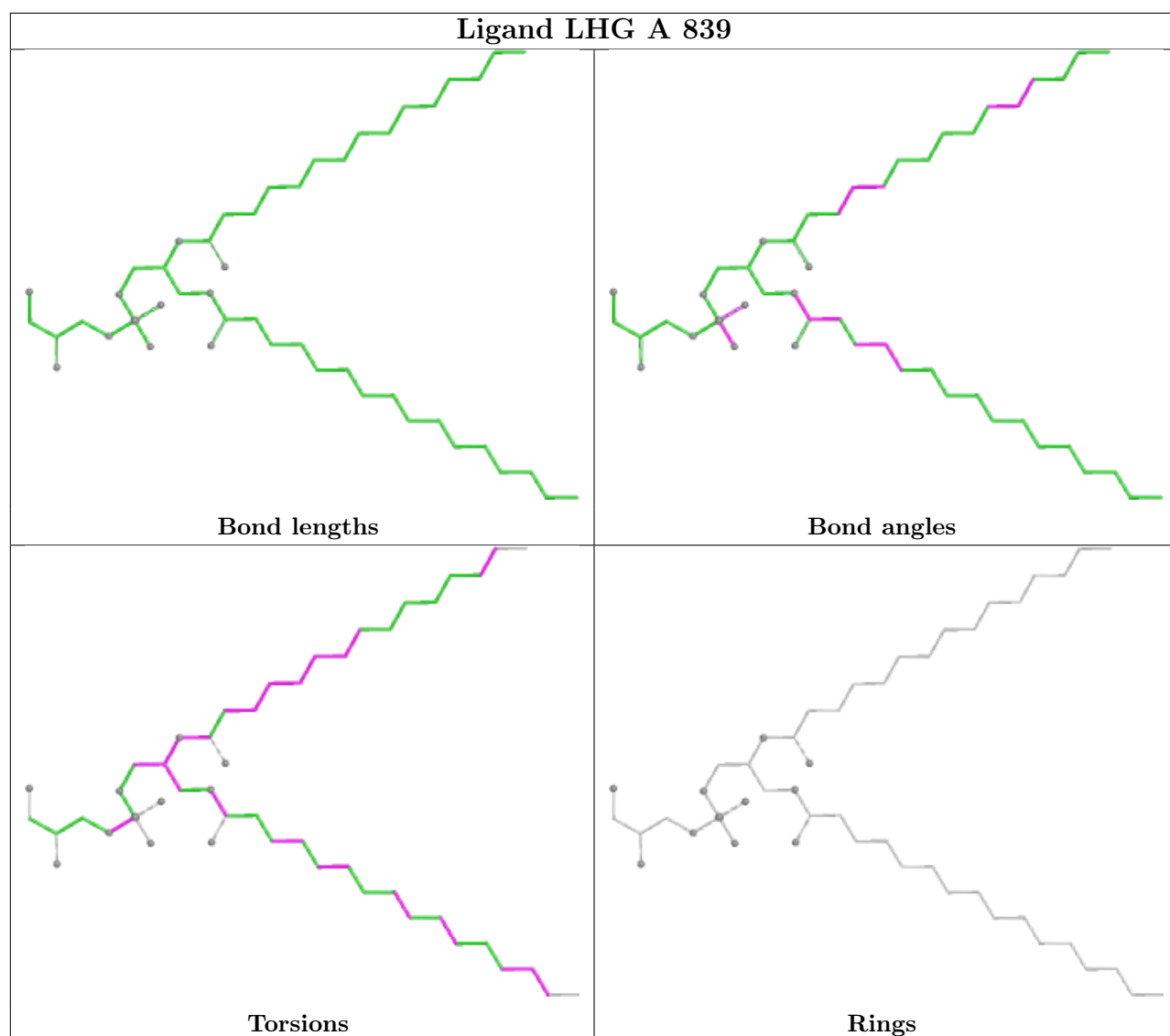


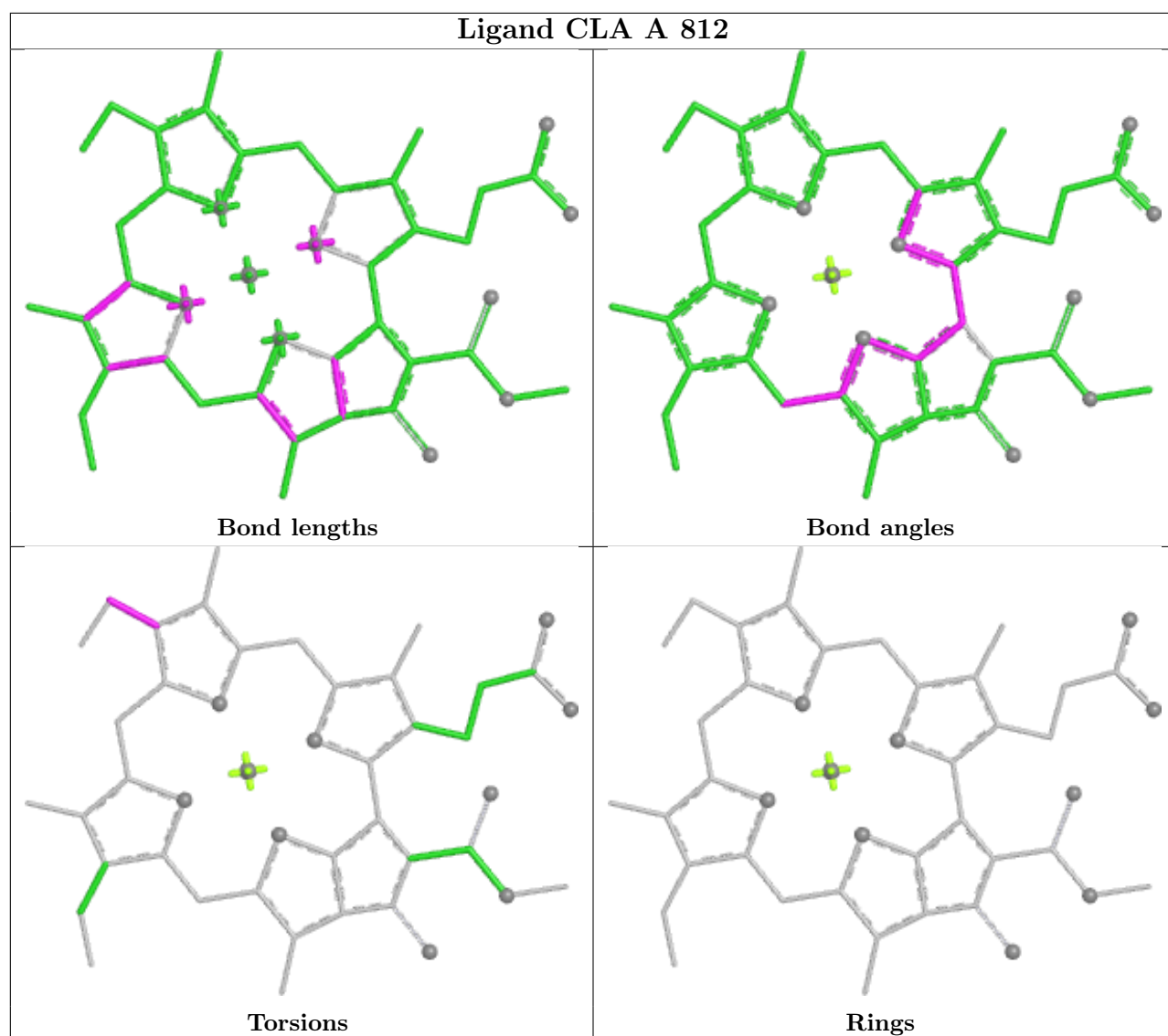




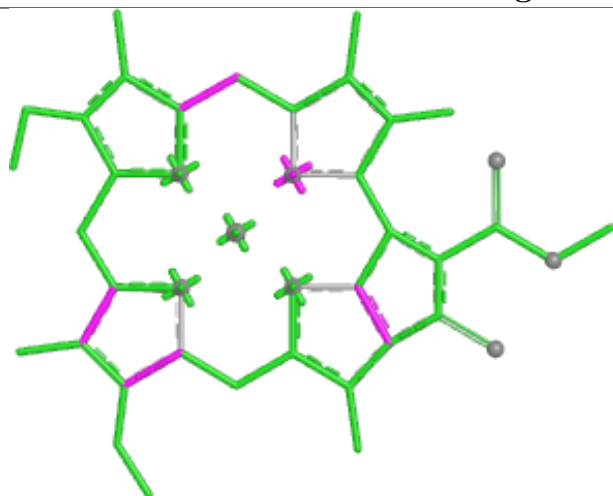




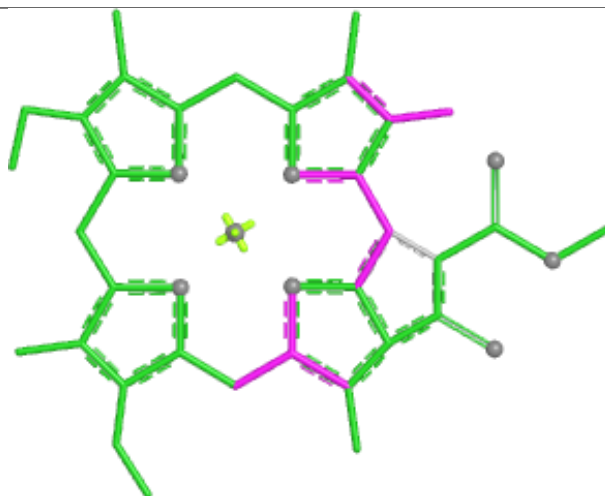




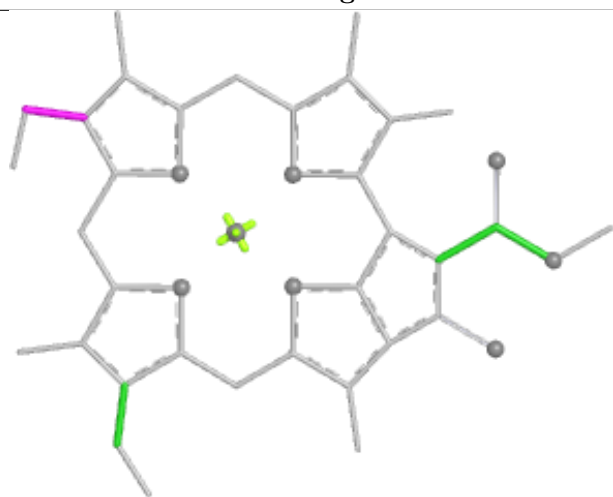
## Ligand CLA T 209



Bond lengths



Bond angles

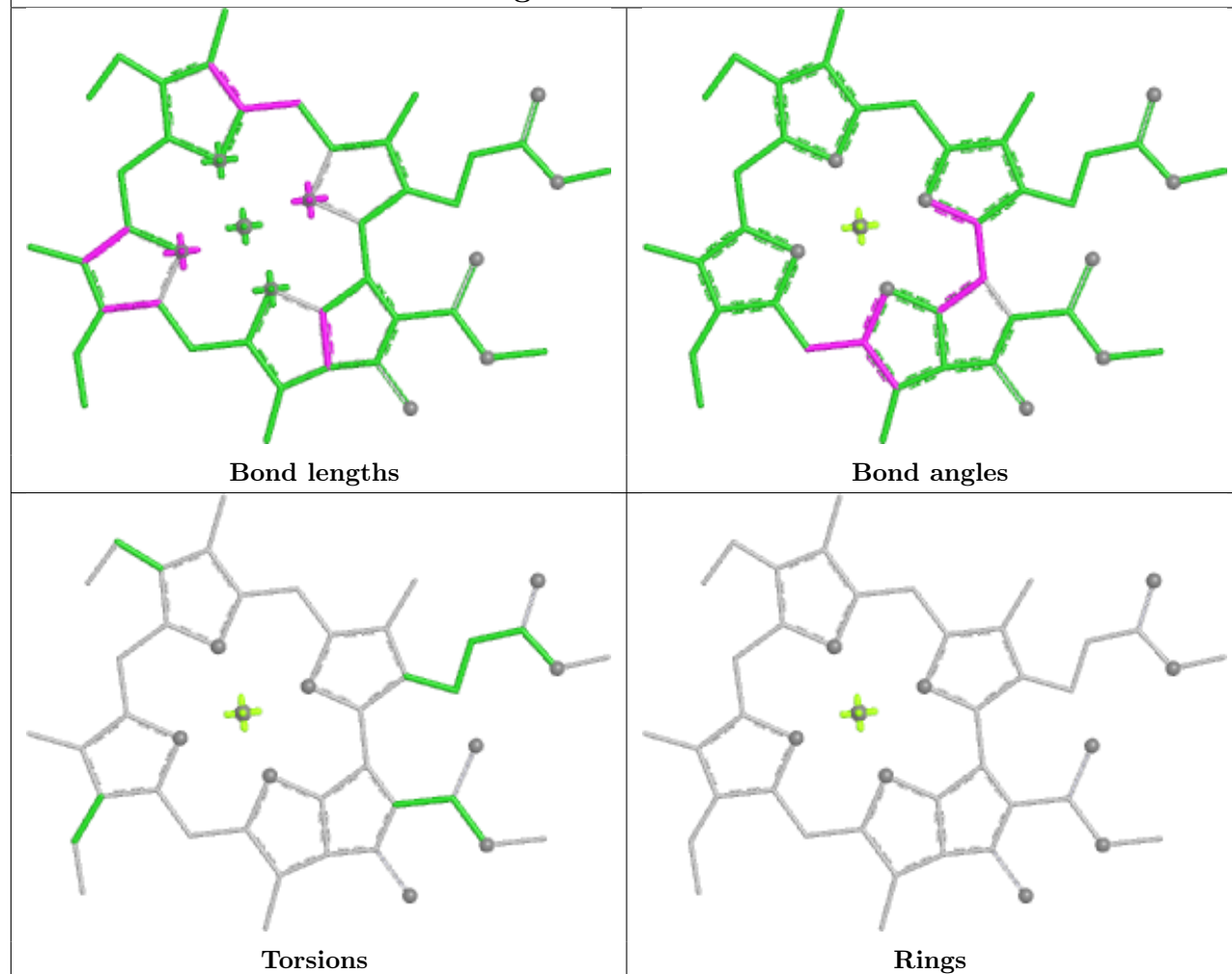


Torsions

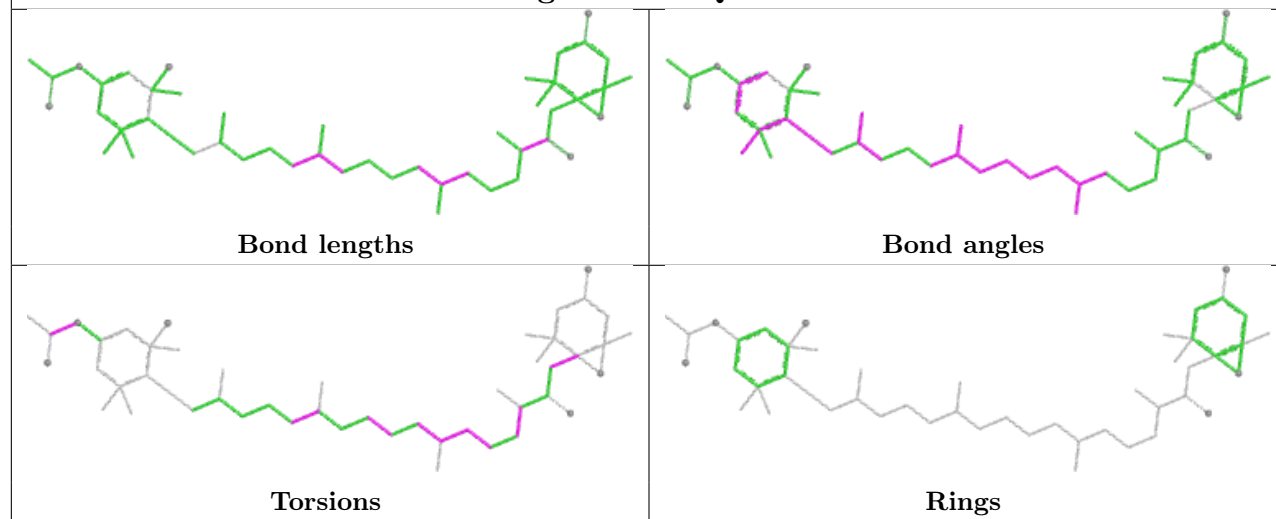


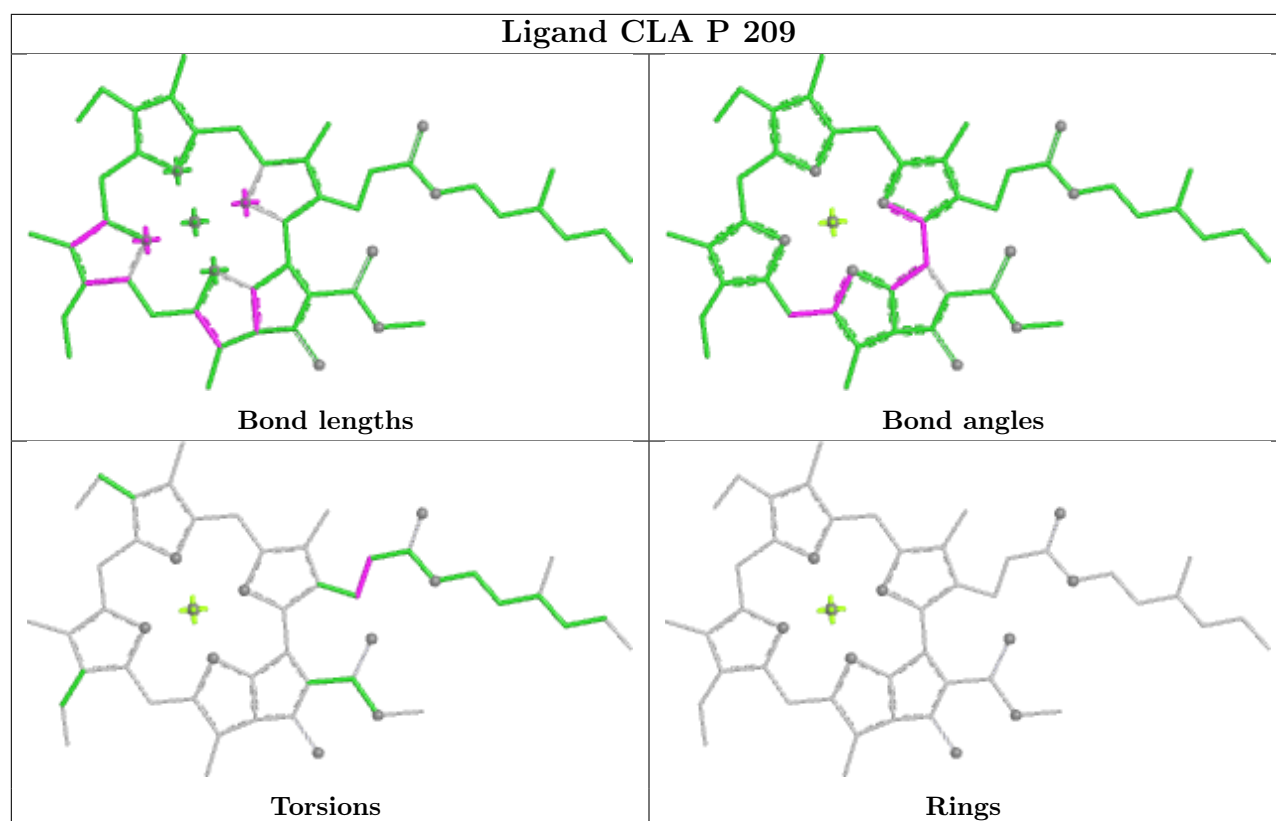
Rings

## Ligand CLA B 818

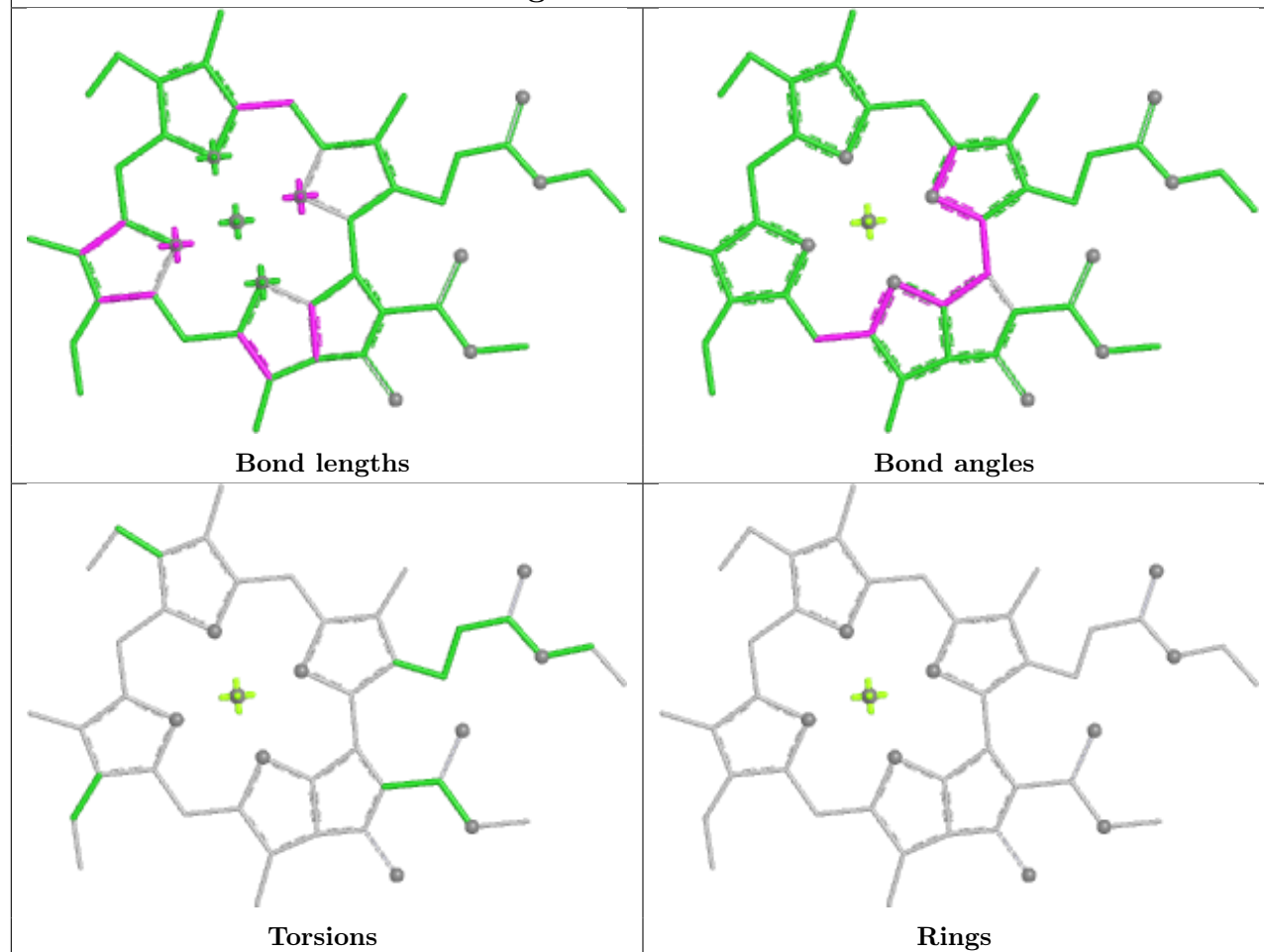


## Ligand A86 Q 214

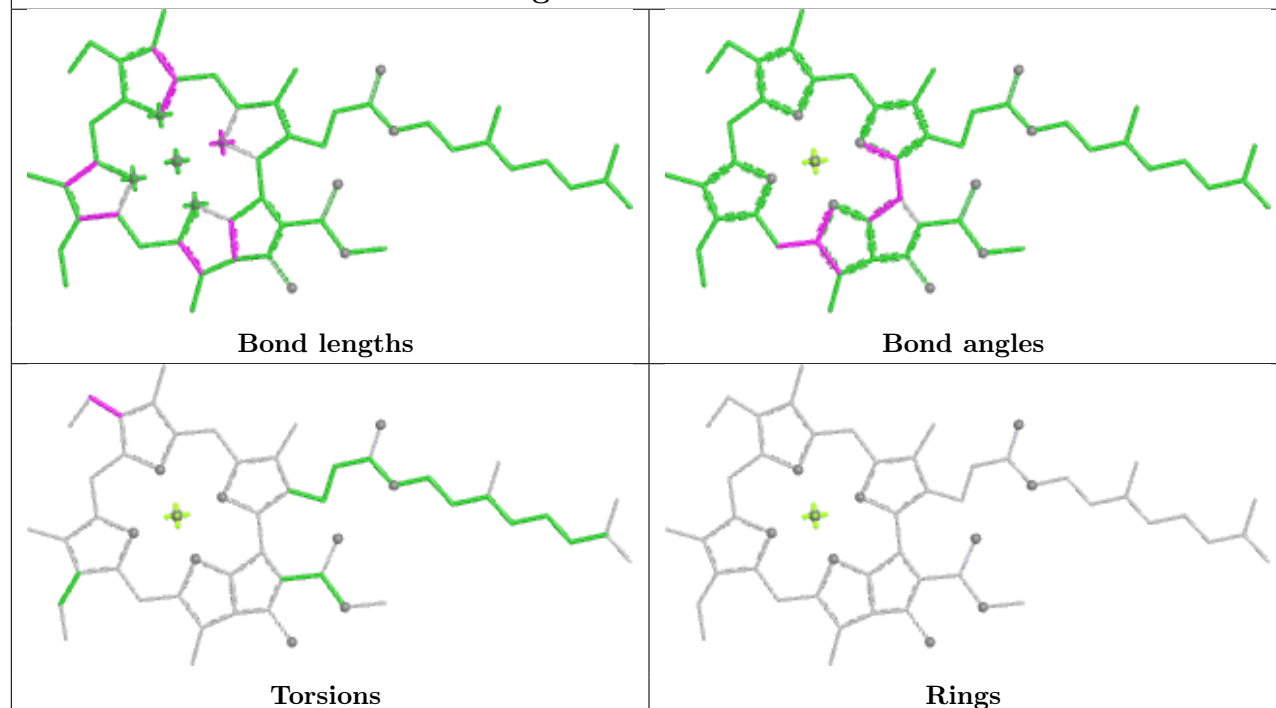


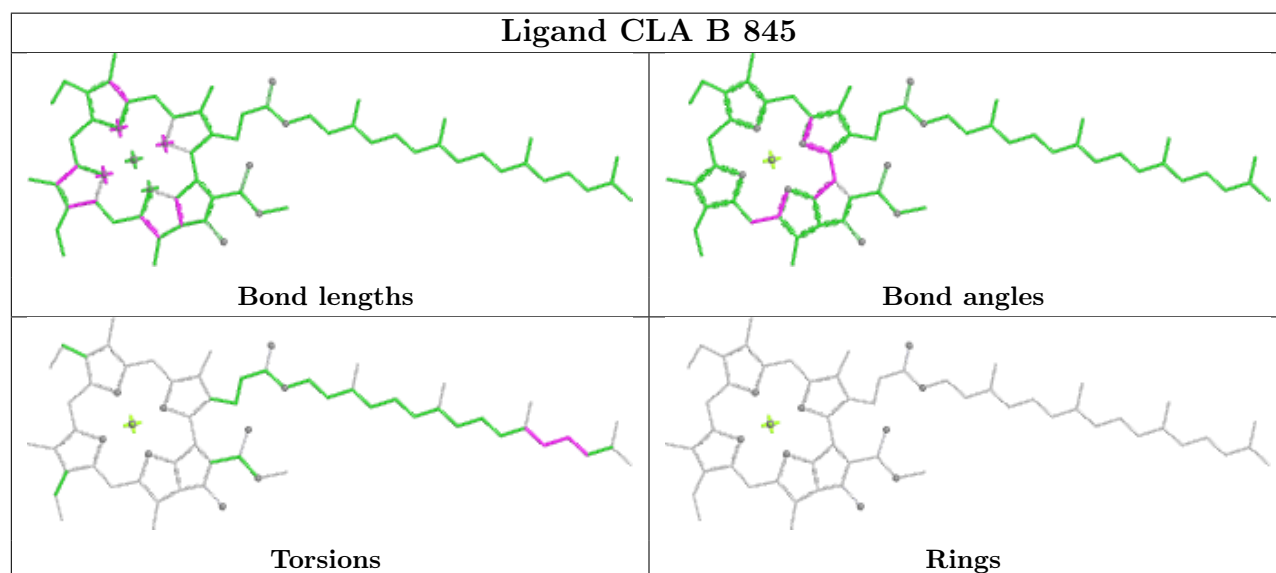
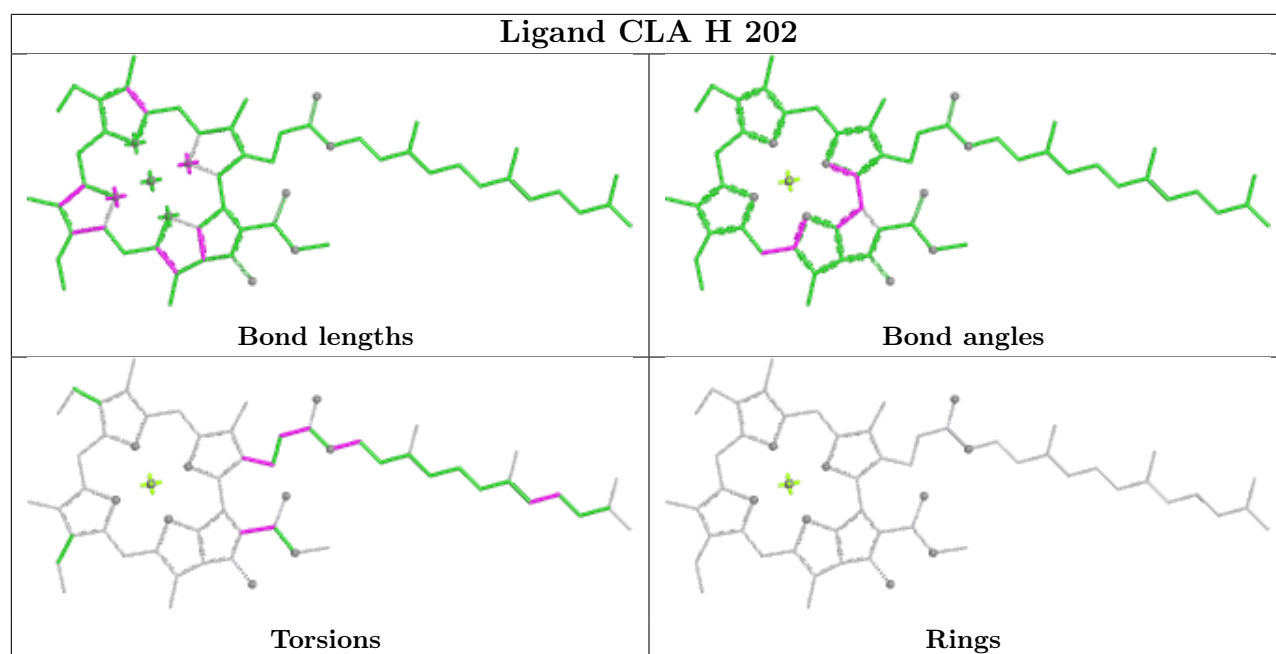


## Ligand CLA P 216



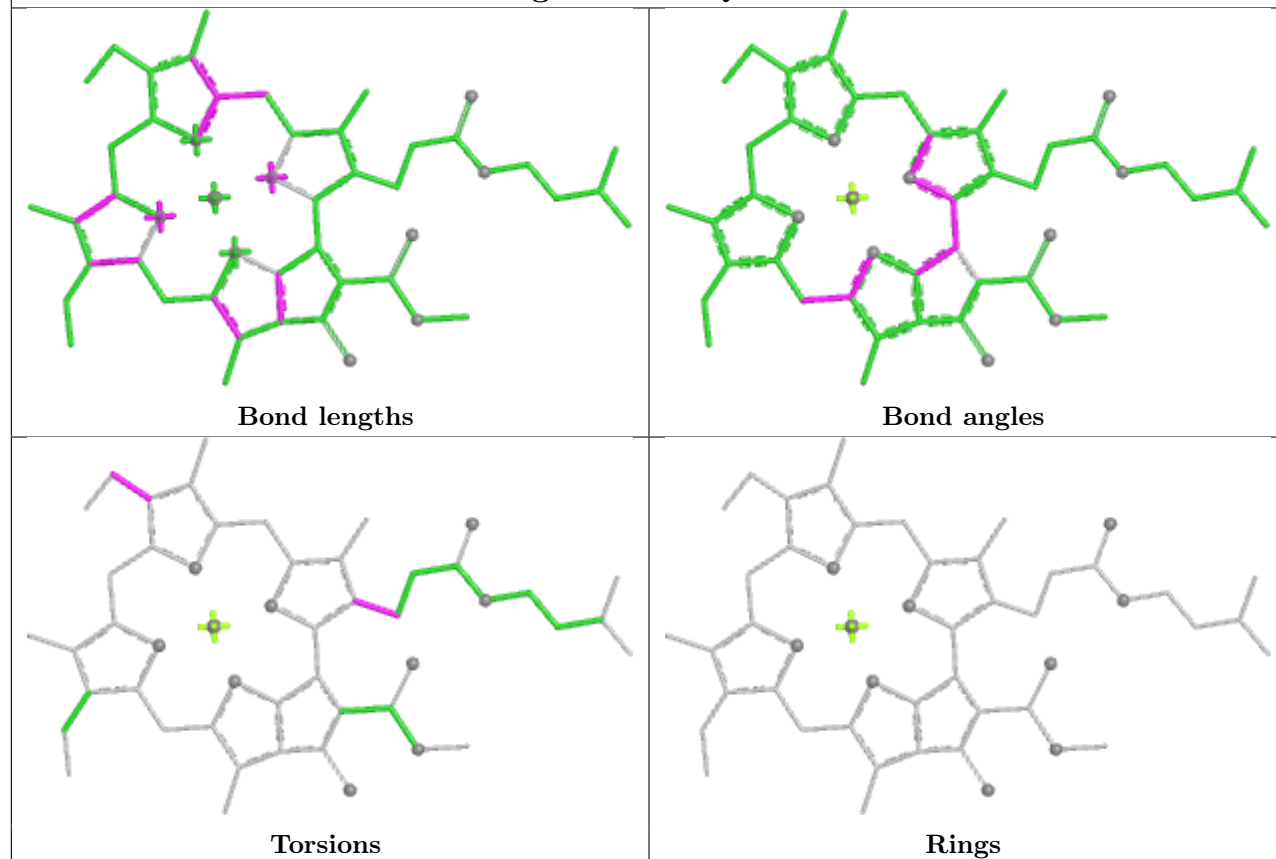
## Ligand CLA B 811



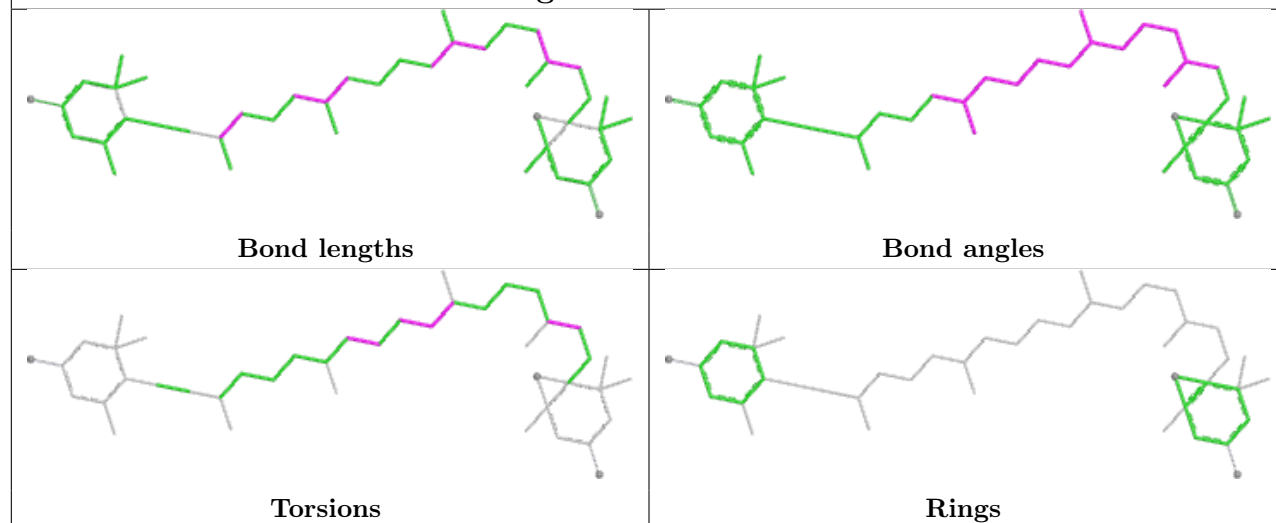




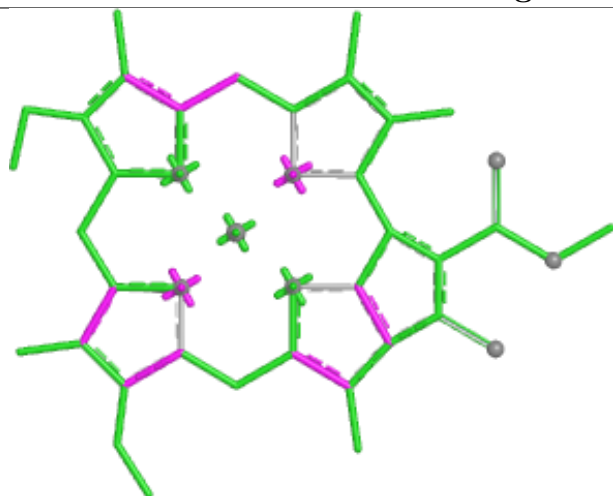
## Ligand CLA Q 208



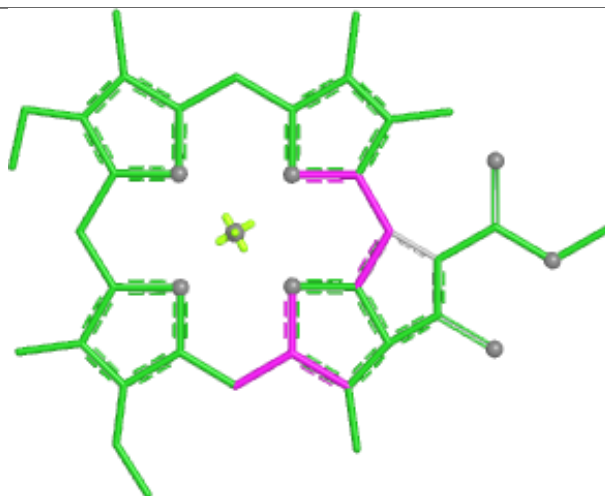
## Ligand DD6 J 101



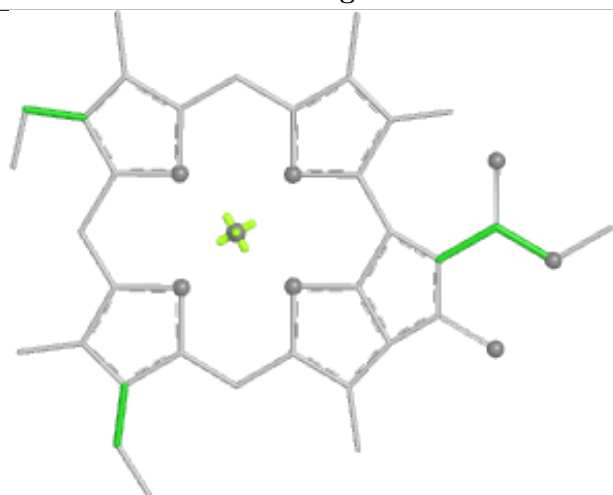
## Ligand CLA T 202



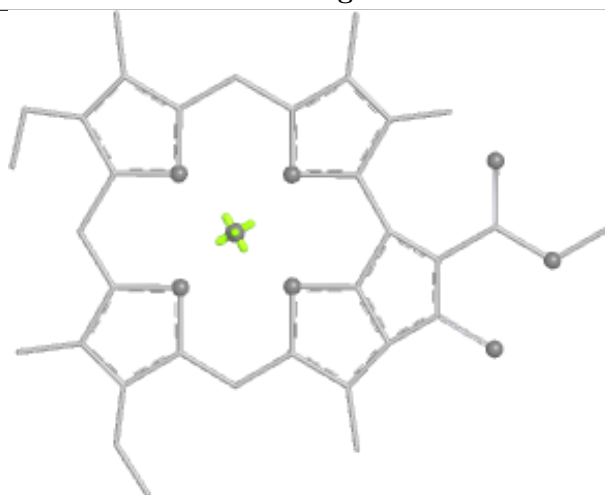
Bond lengths



Bond angles

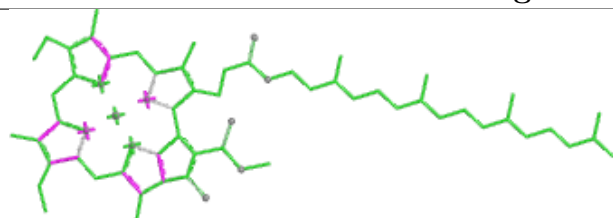


Torsions

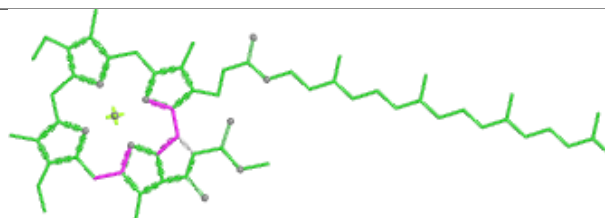


Rings

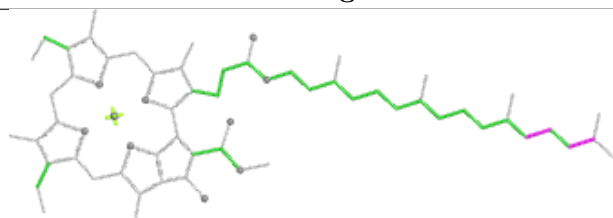
## Ligand CLA O 204



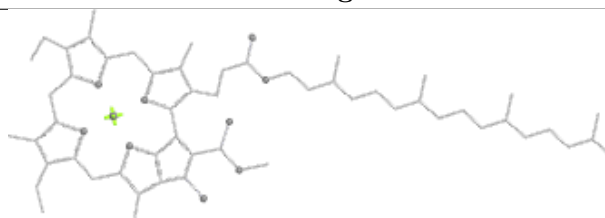
Bond lengths



Bond angles

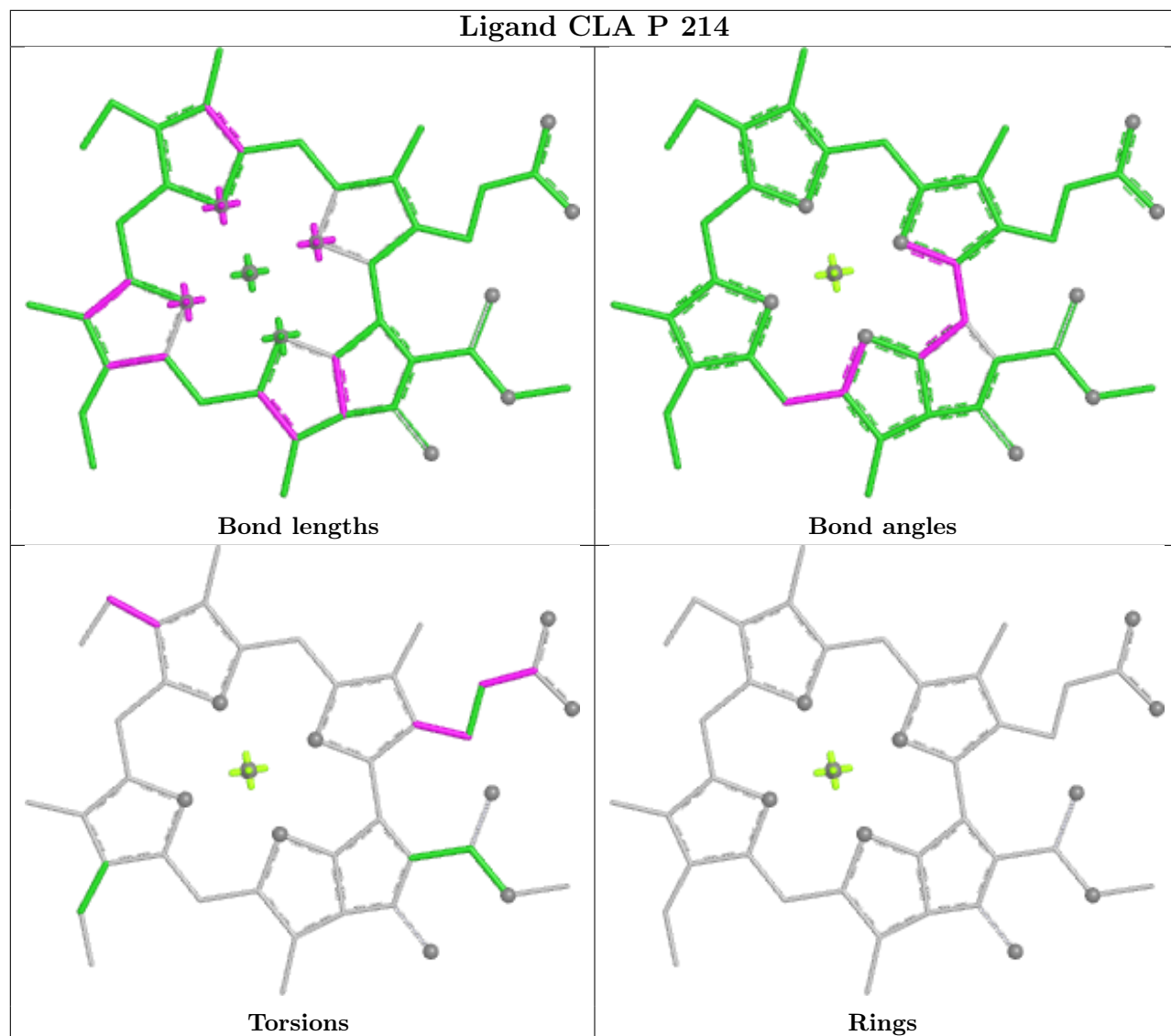


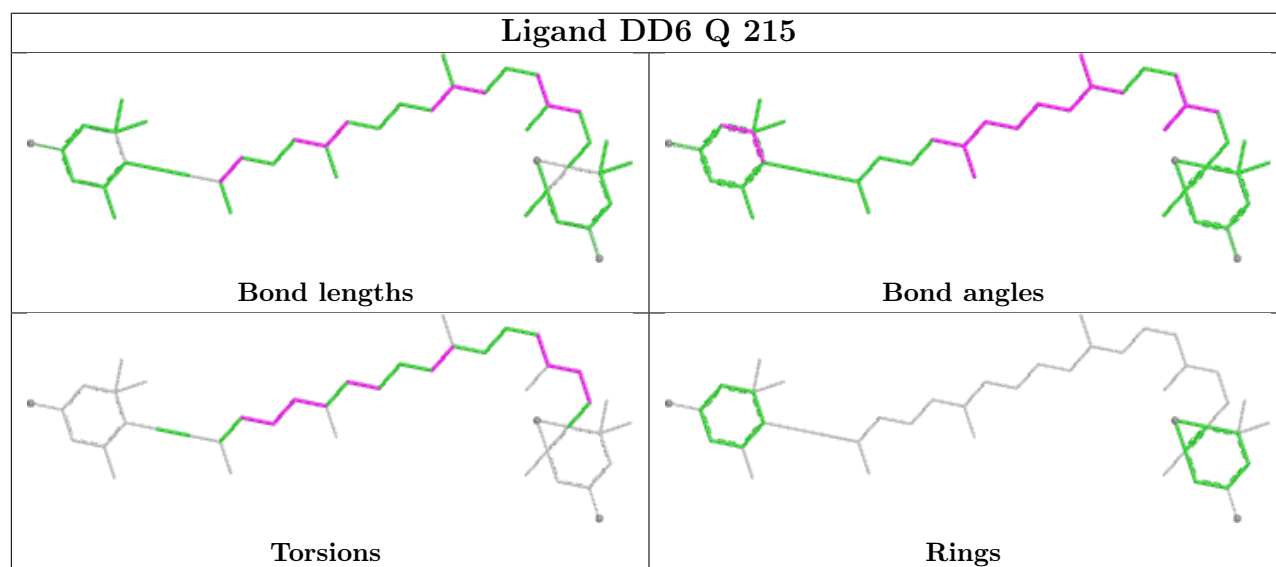
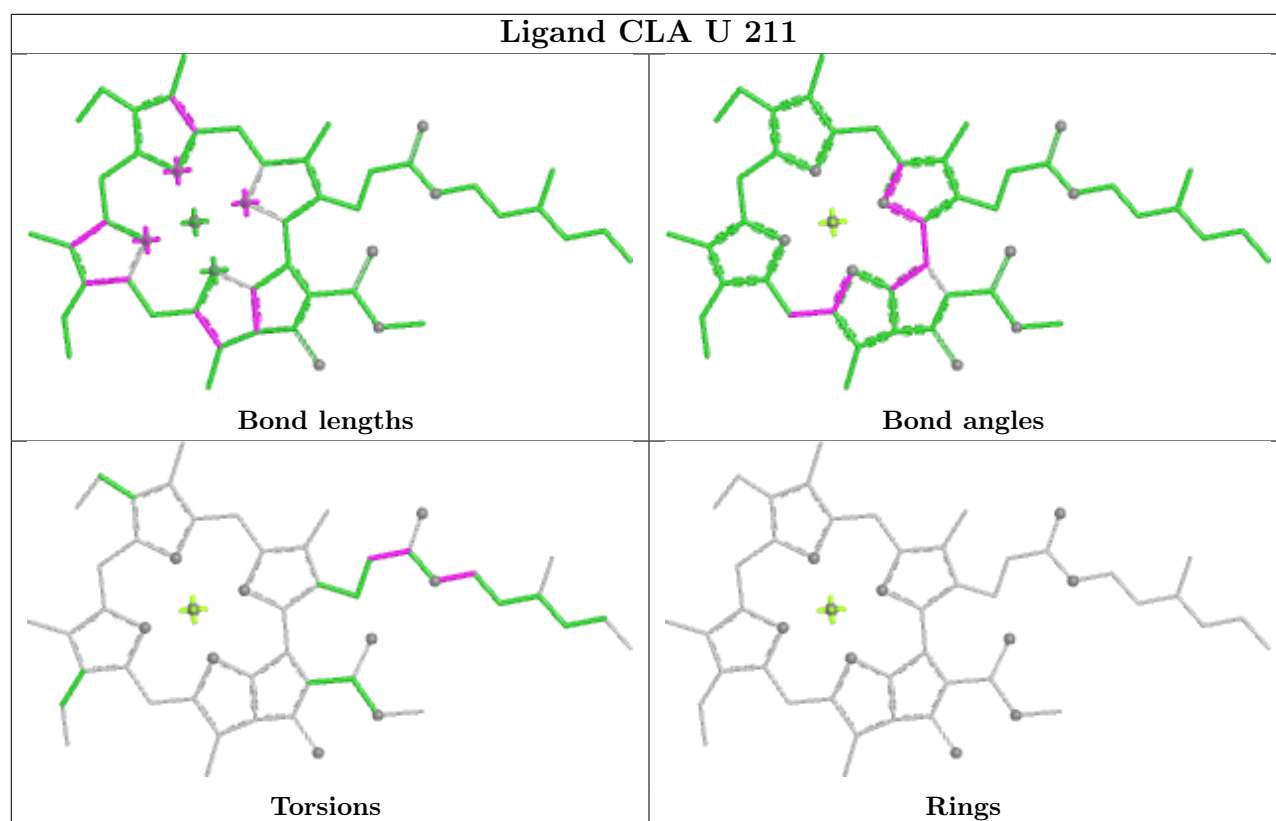
Torsions

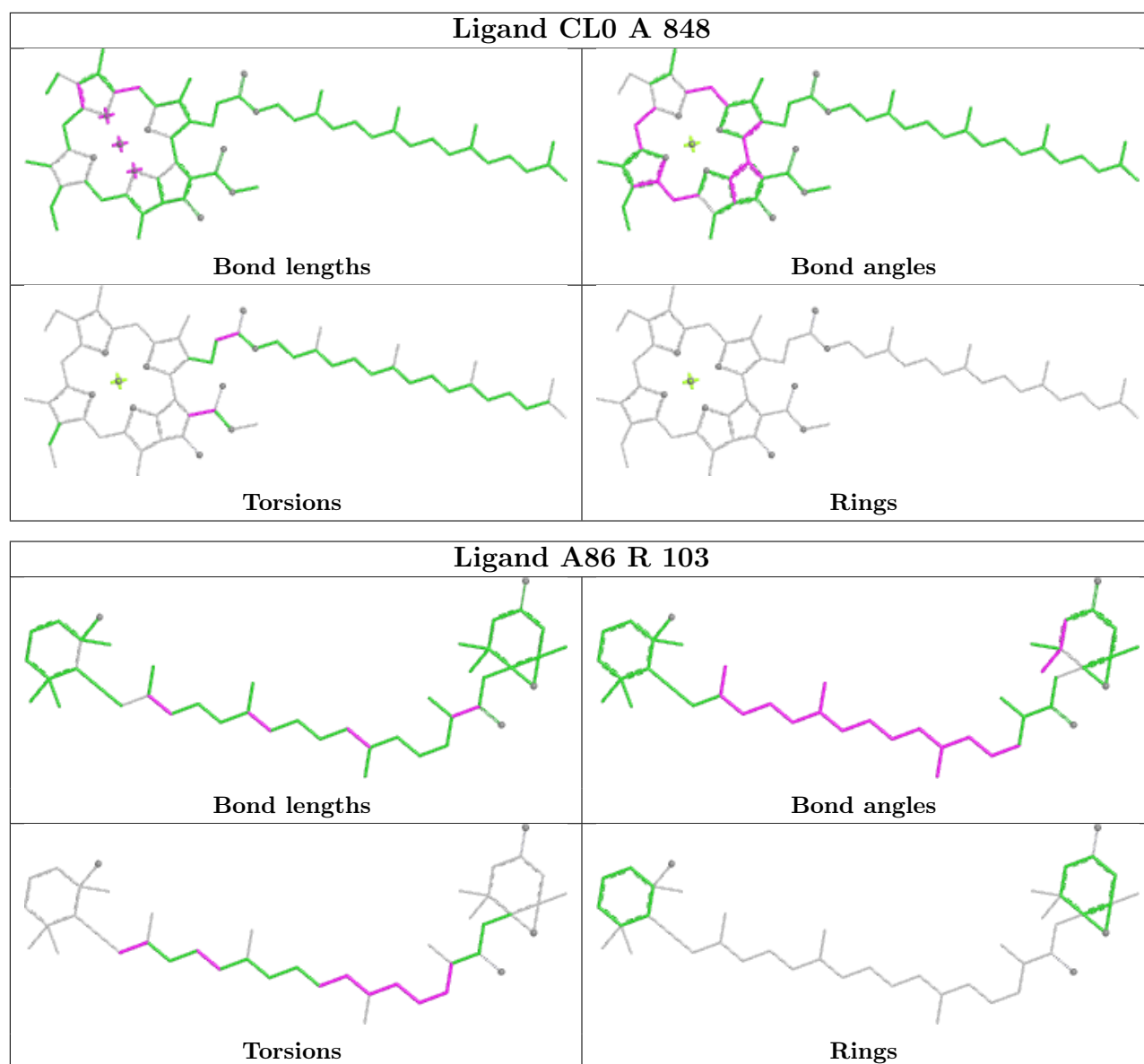


Rings

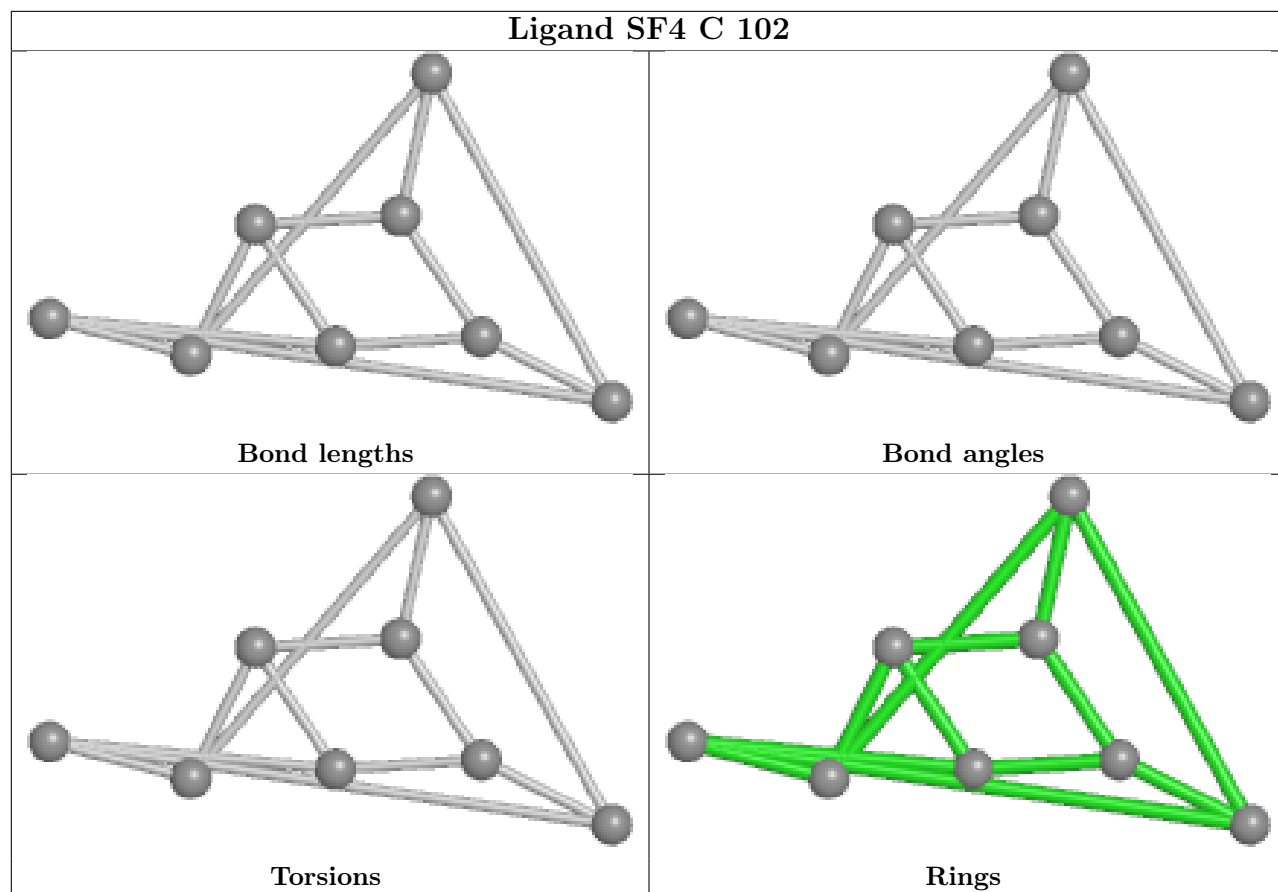
## Ligand CLA P 214



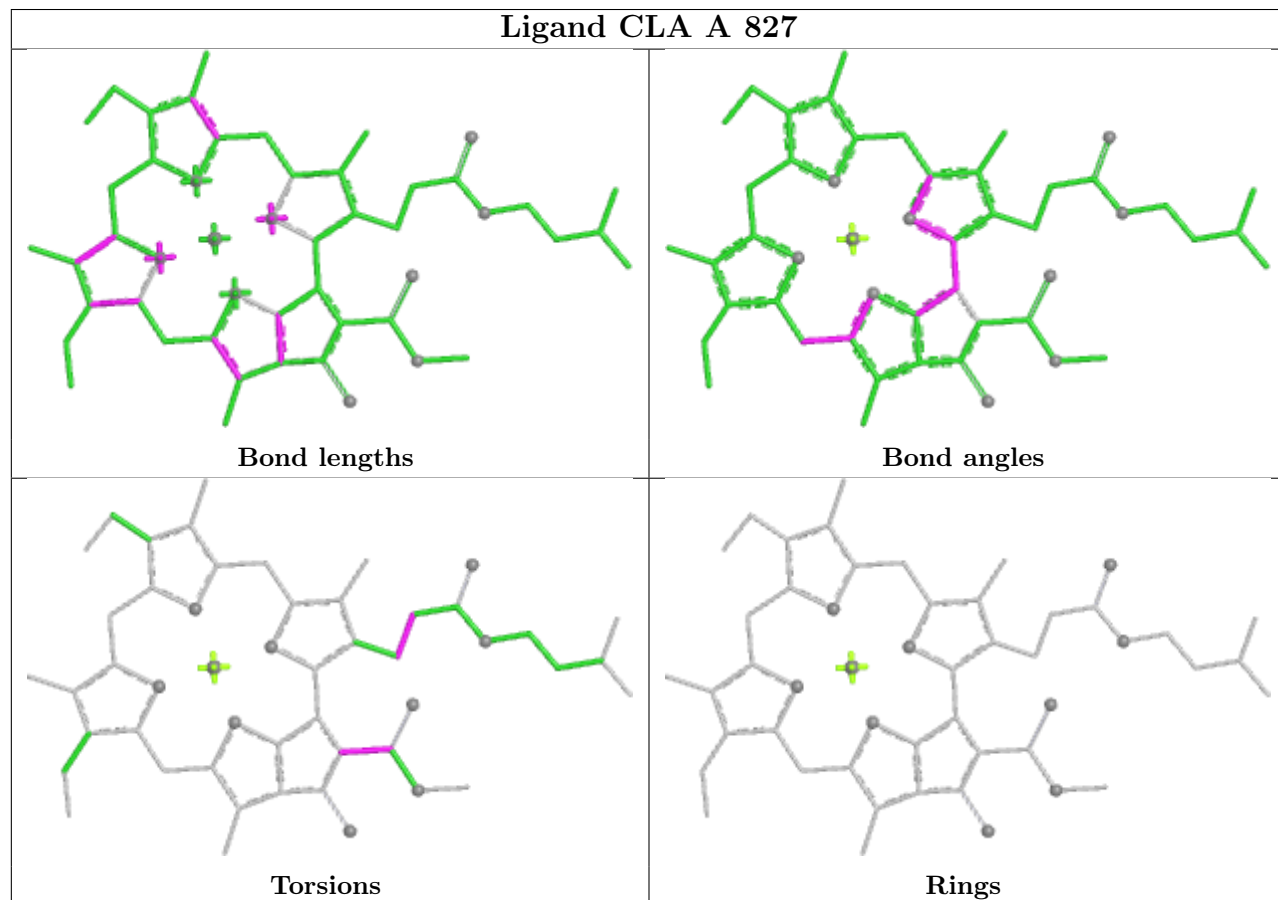


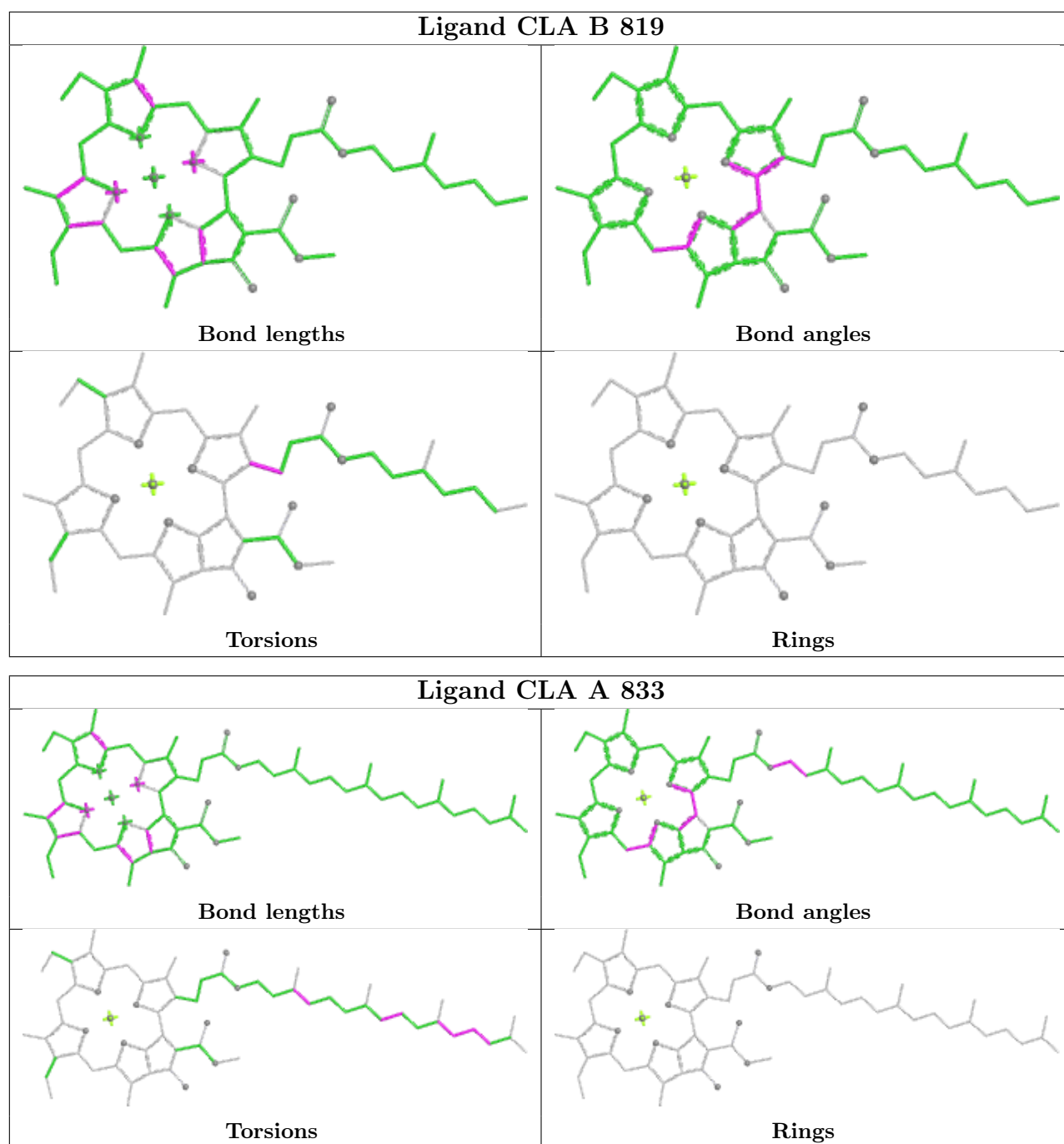


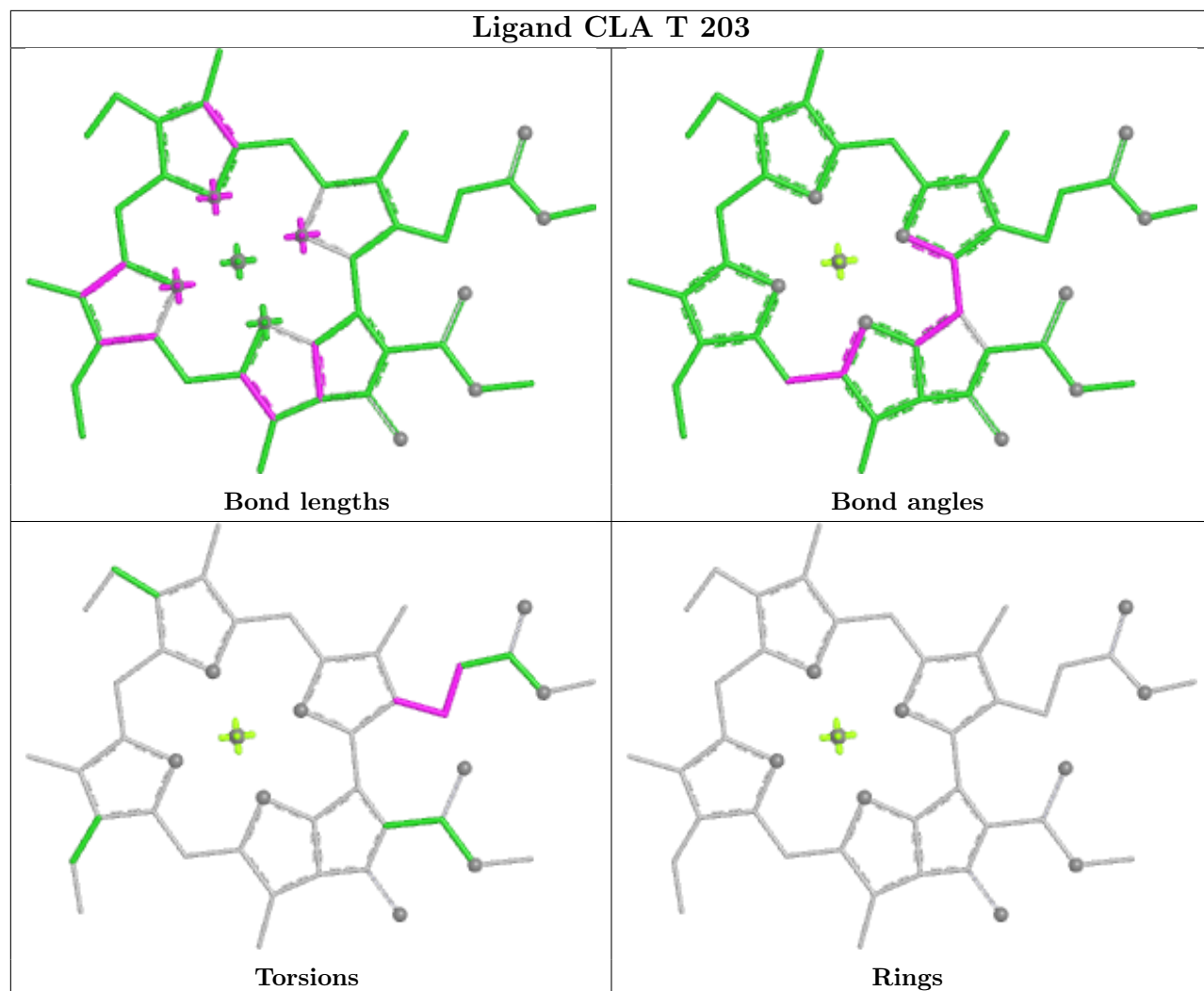
## Ligand SF4 C 102



## Ligand CLA A 827

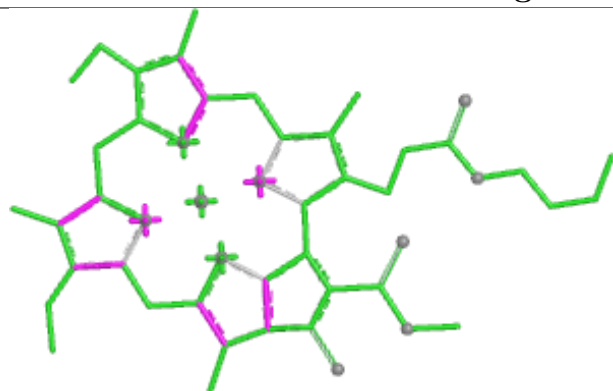




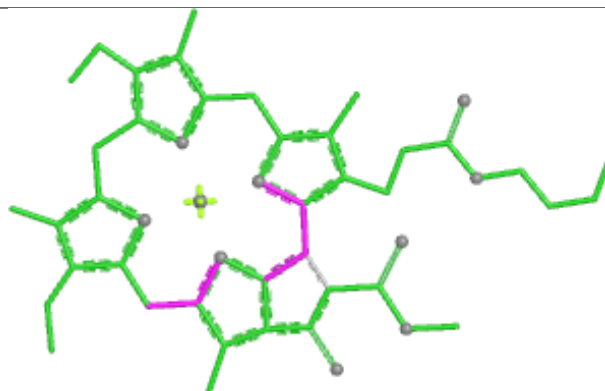




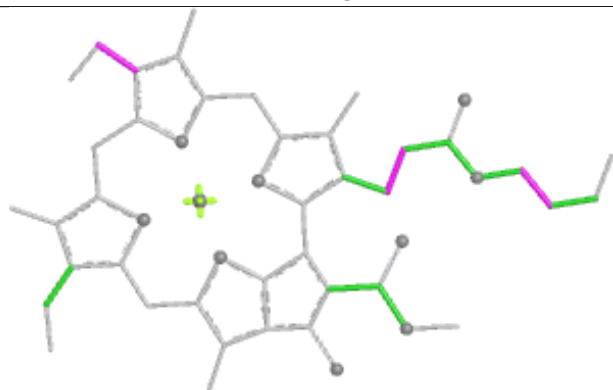
## Ligand CLA B 827



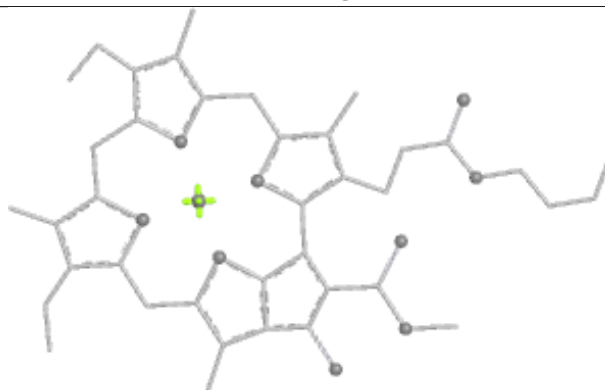
Bond lengths



Bond angles

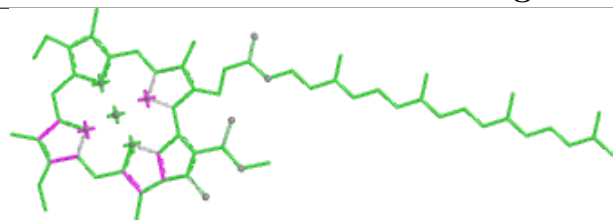


Torsions

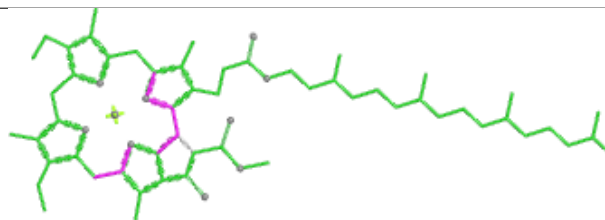


Rings

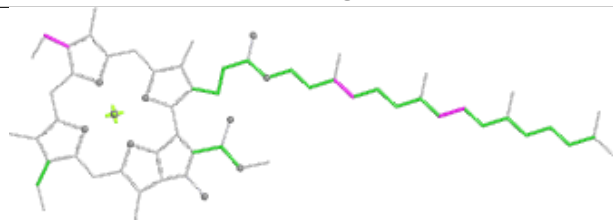
## Ligand CLA A 849



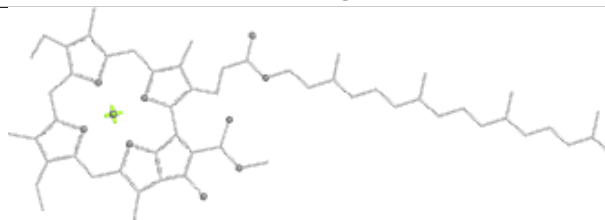
Bond lengths



Bond angles

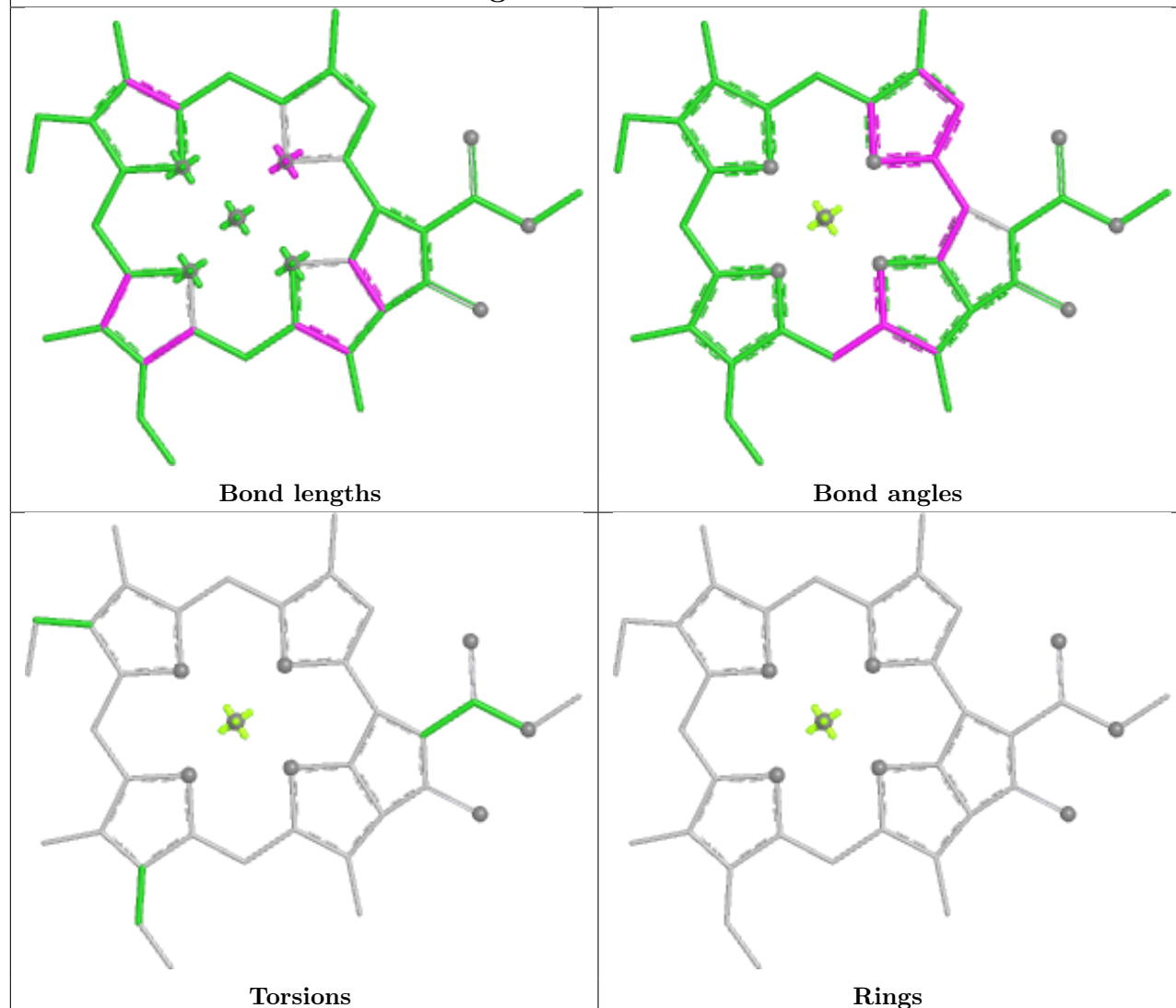


Torsions

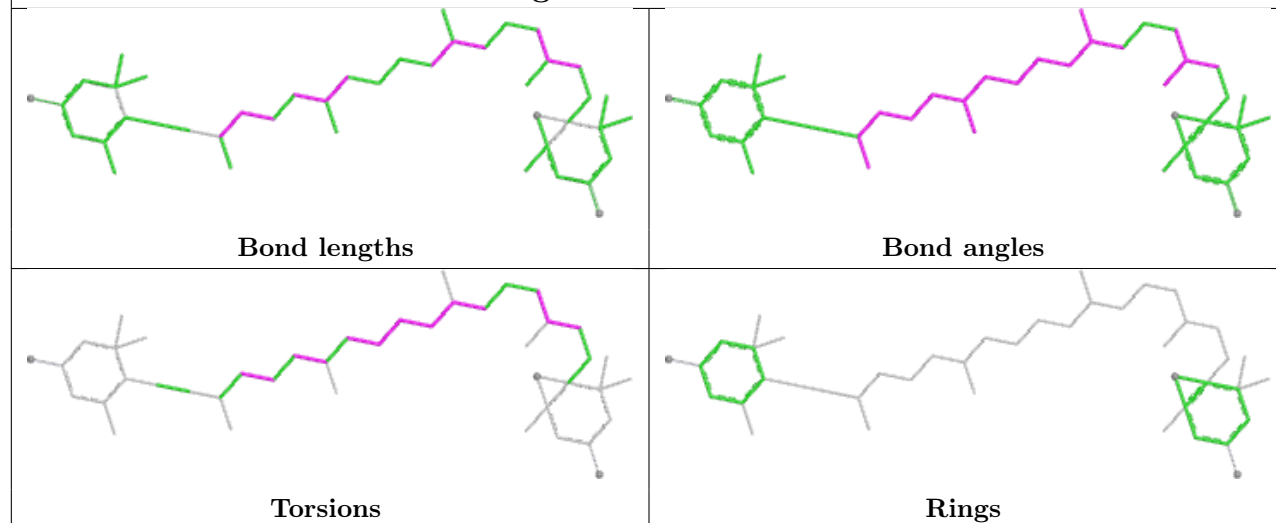


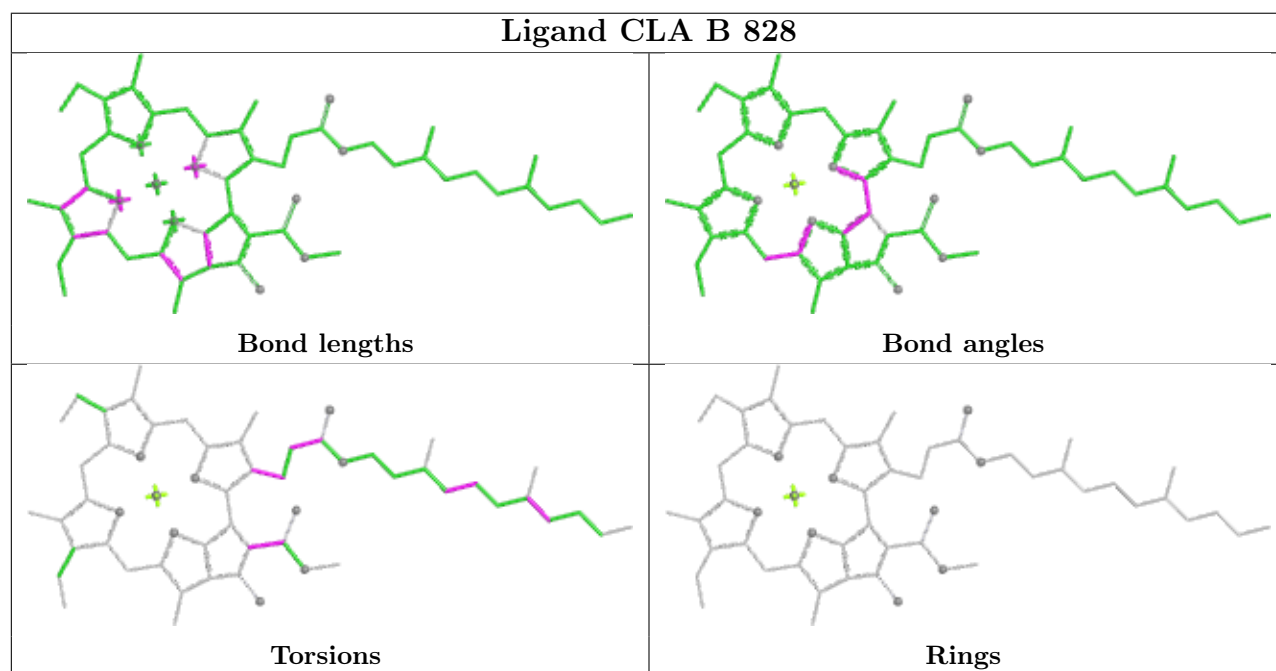
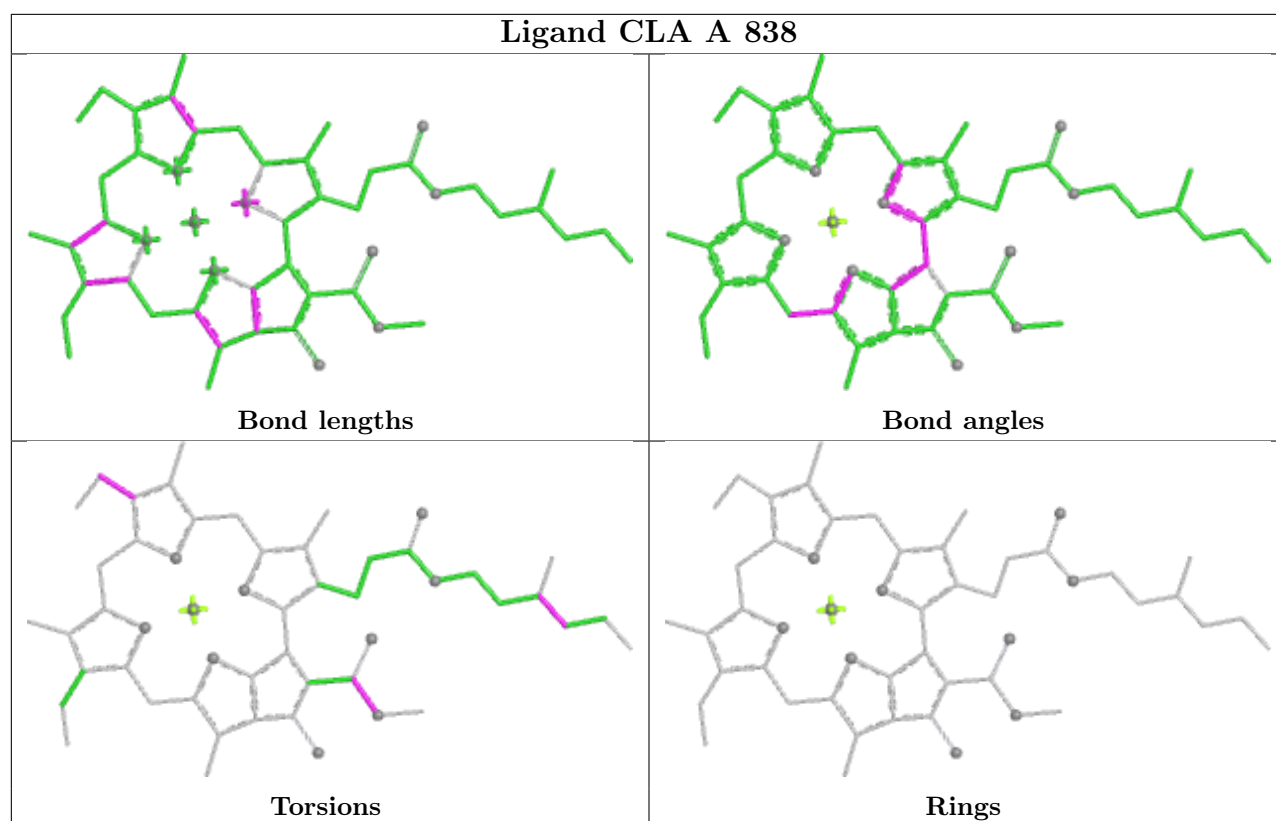
Rings

## Ligand CLA H 201

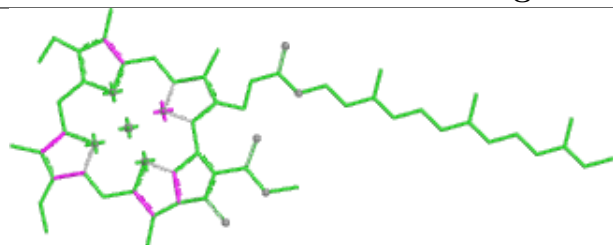


## Ligand DD6 A 855

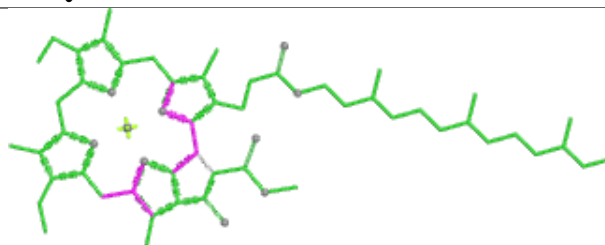




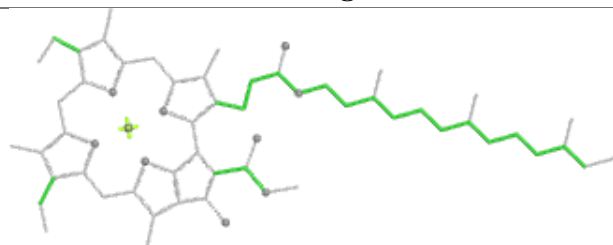
## Ligand CLA Q 204



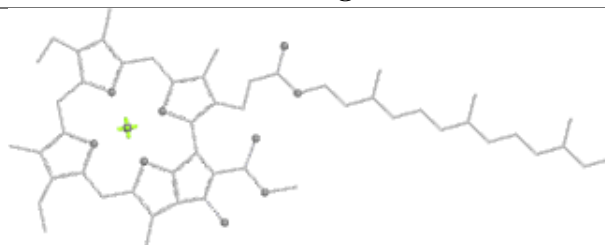
Bond lengths



Bond angles

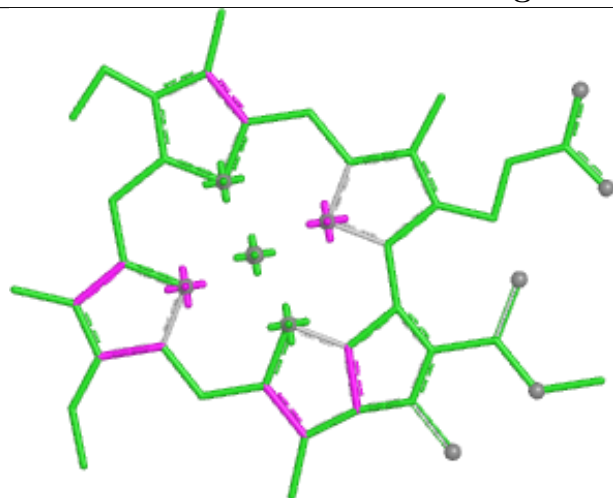


Torsions

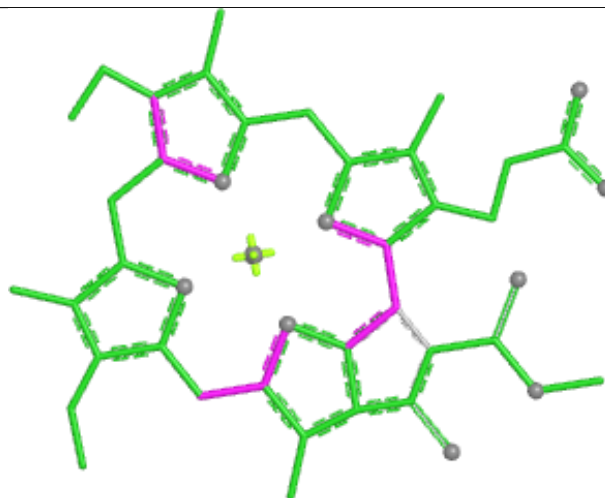


Rings

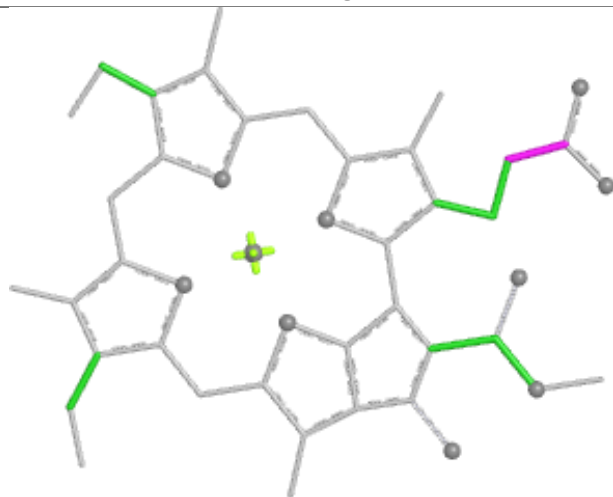
## Ligand CLA R 101



Bond lengths



Bond angles

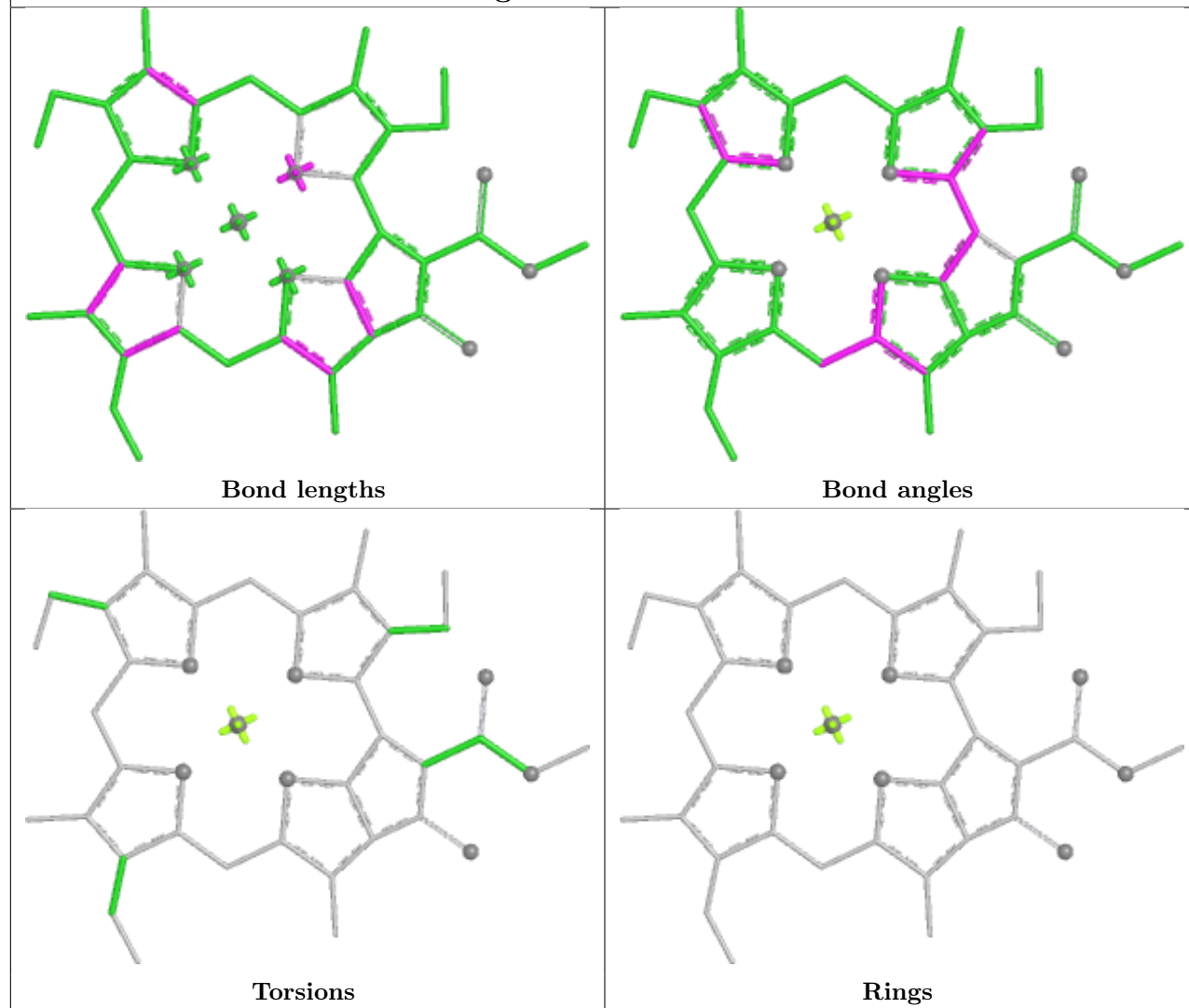


Torsions

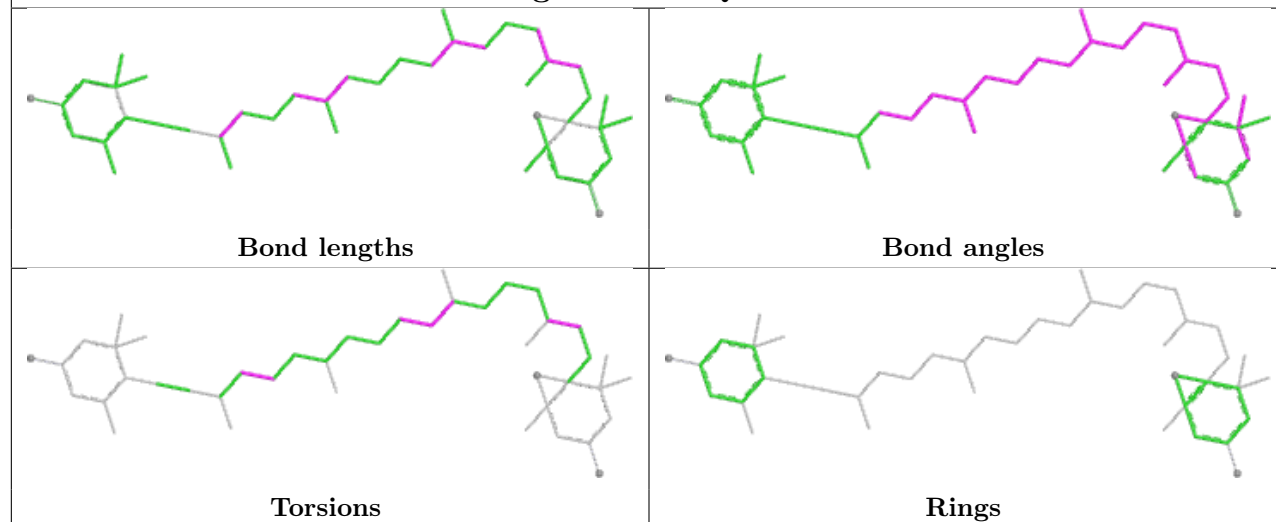


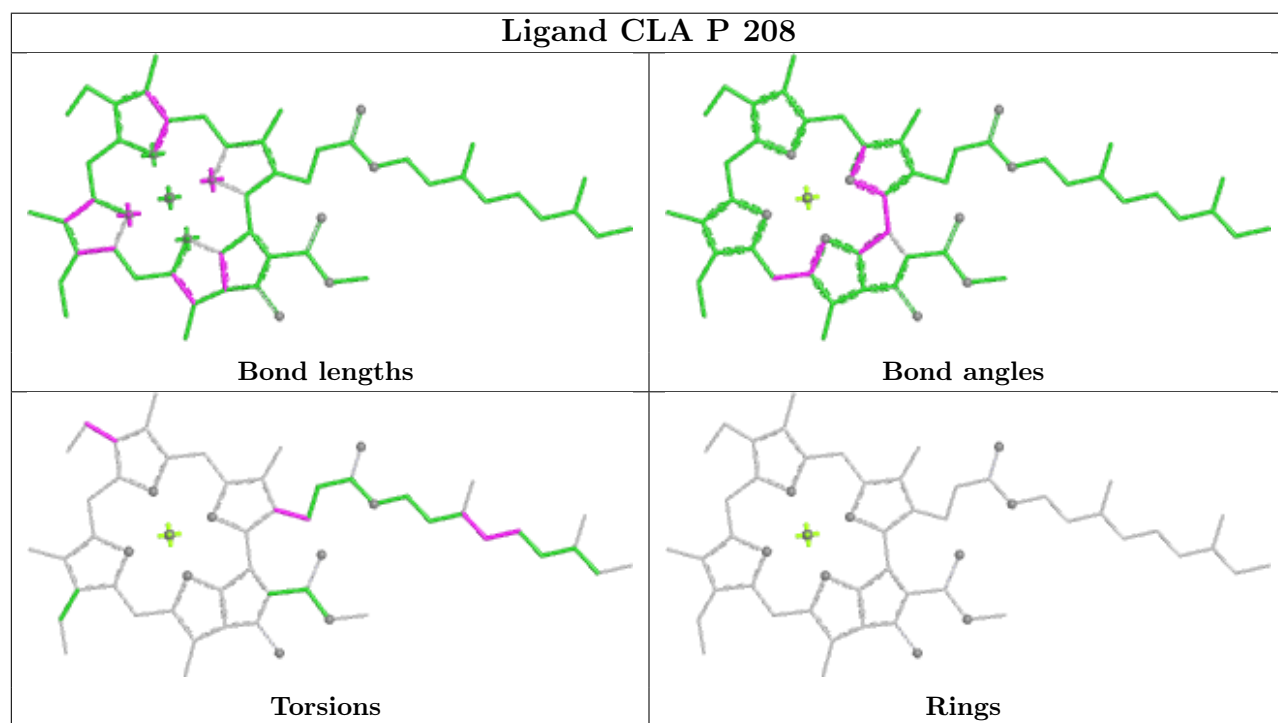
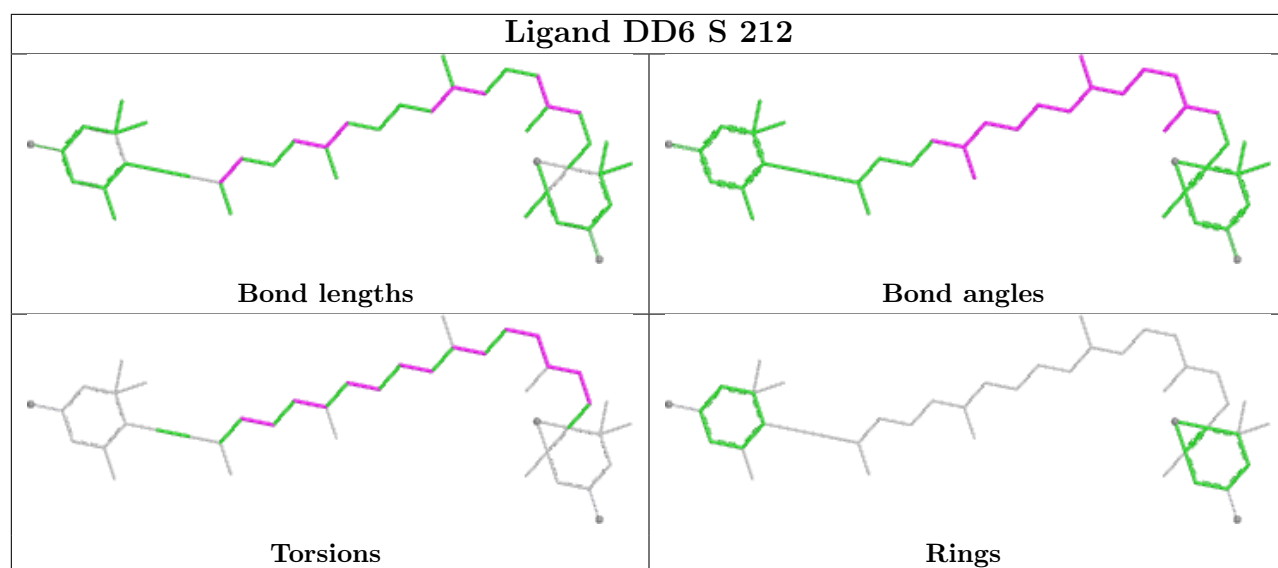
Rings

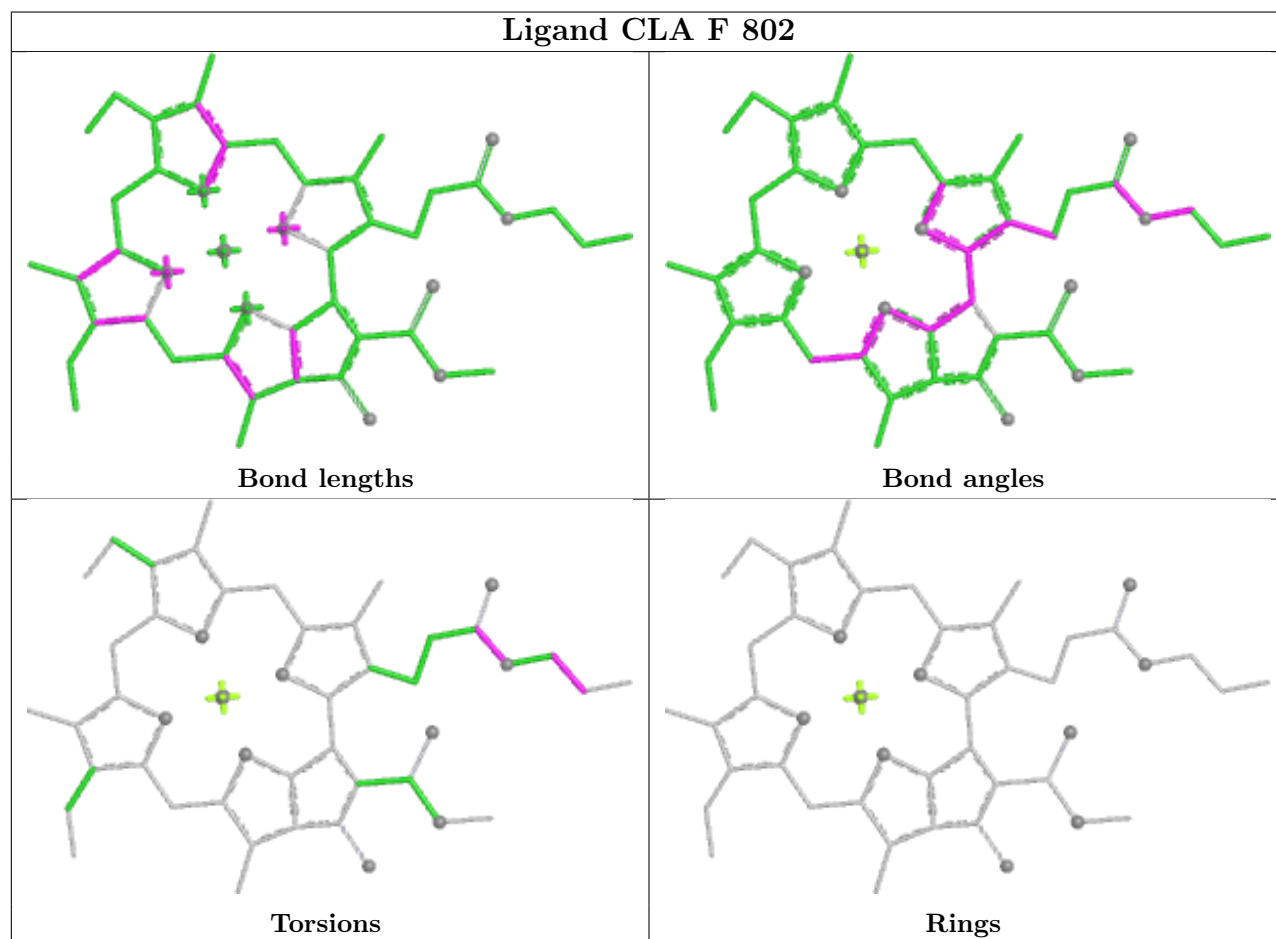
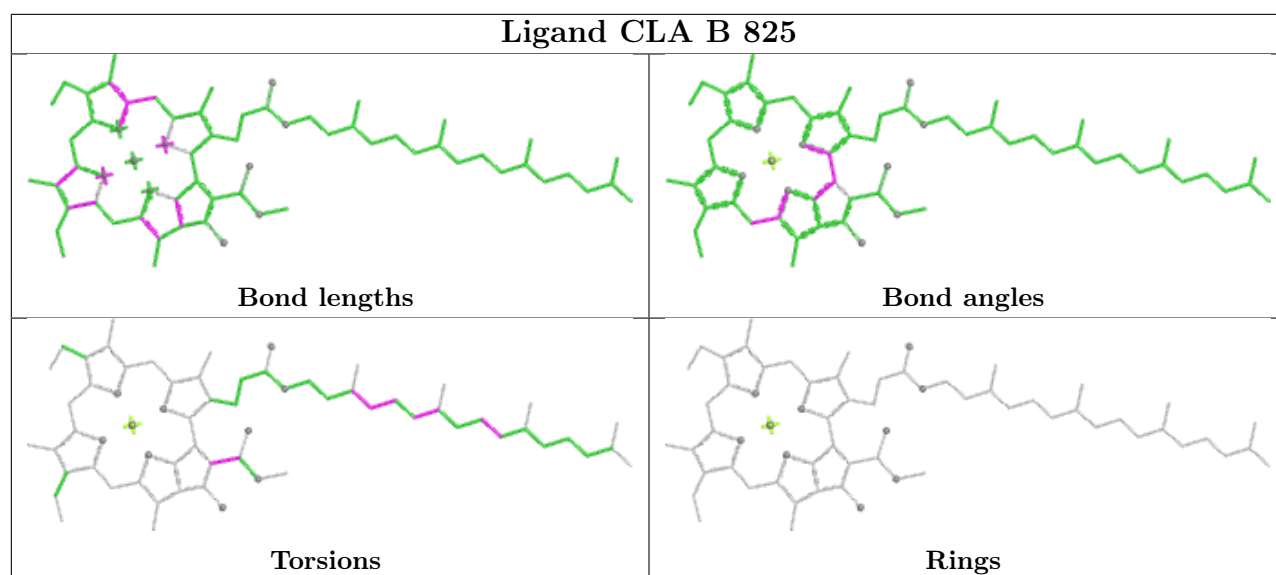
## Ligand CLA U 209

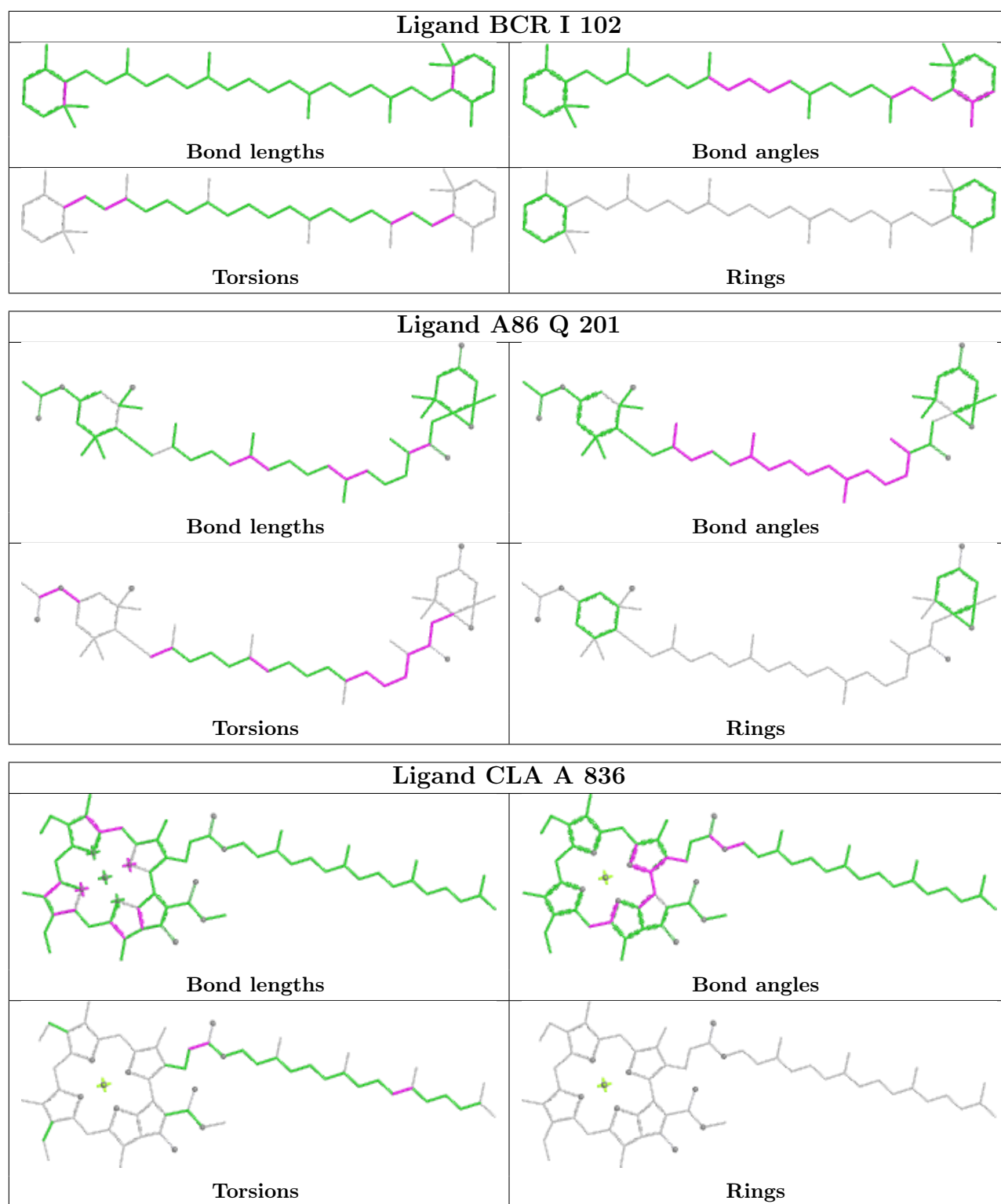


## Ligand DD6 Q 202

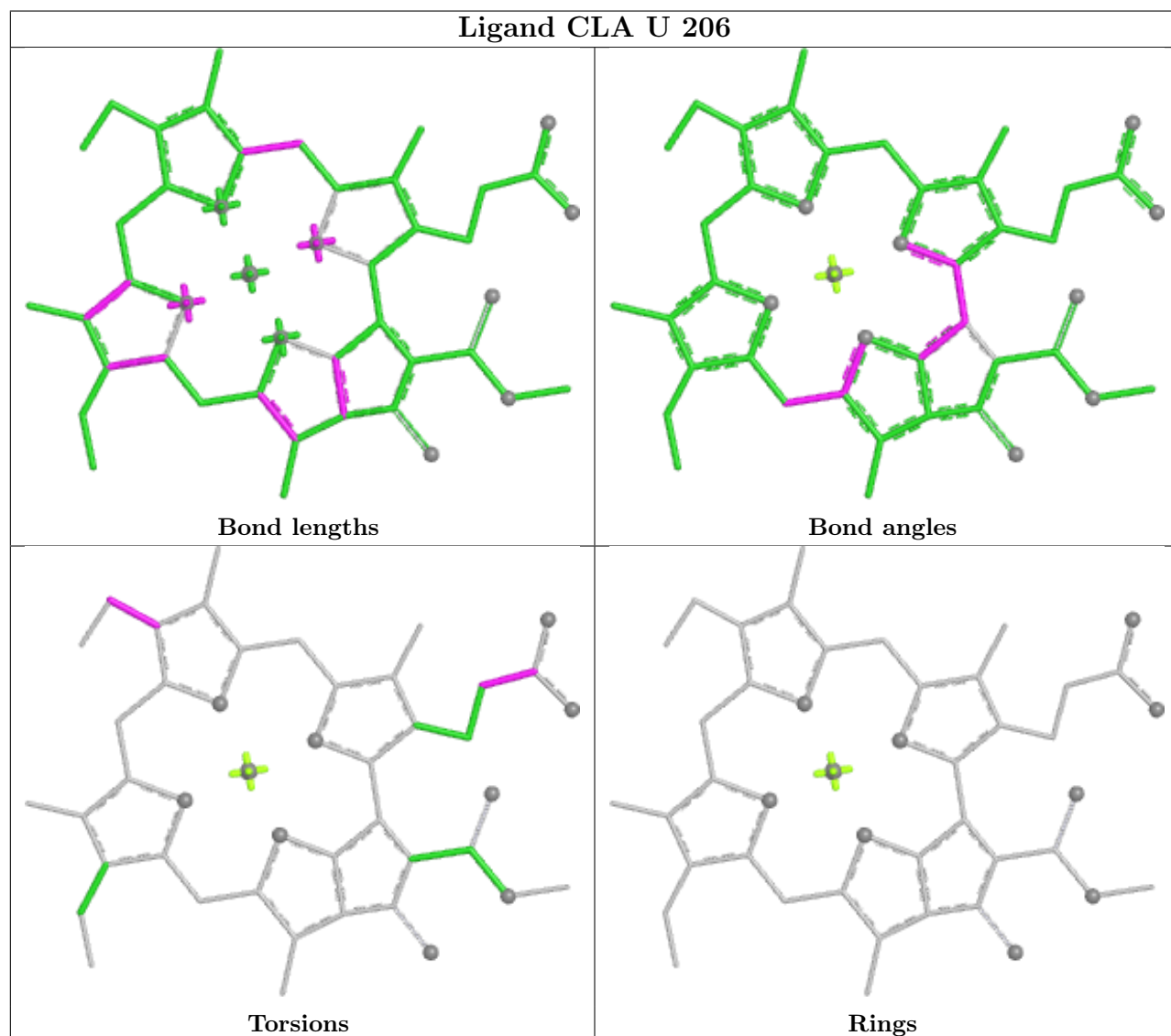
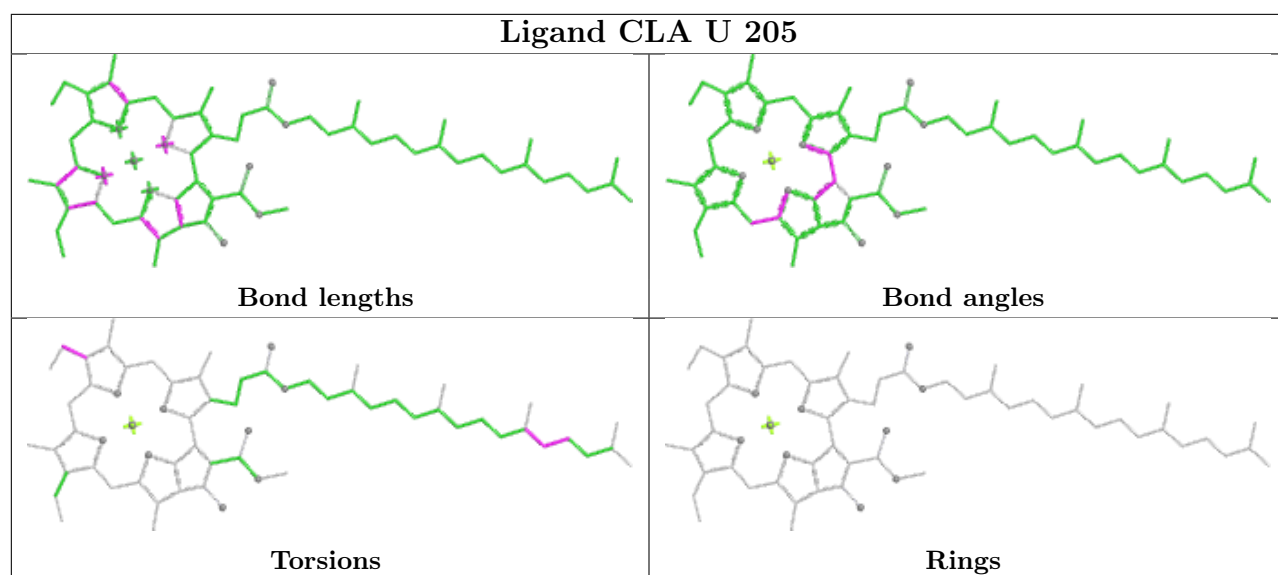


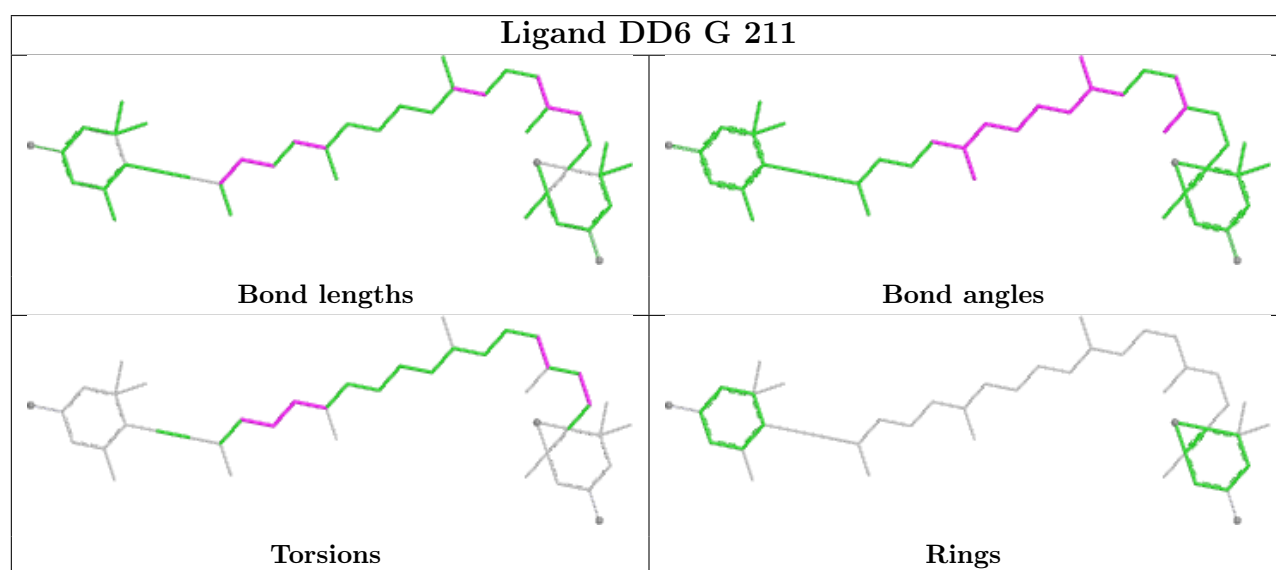
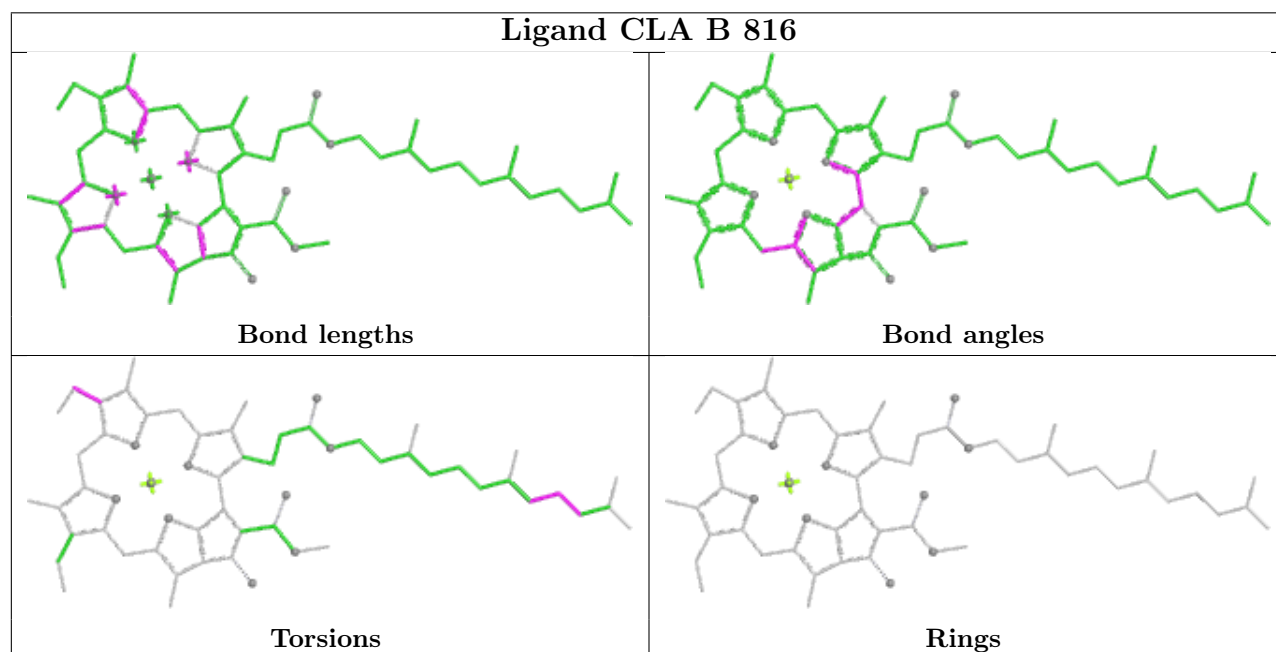
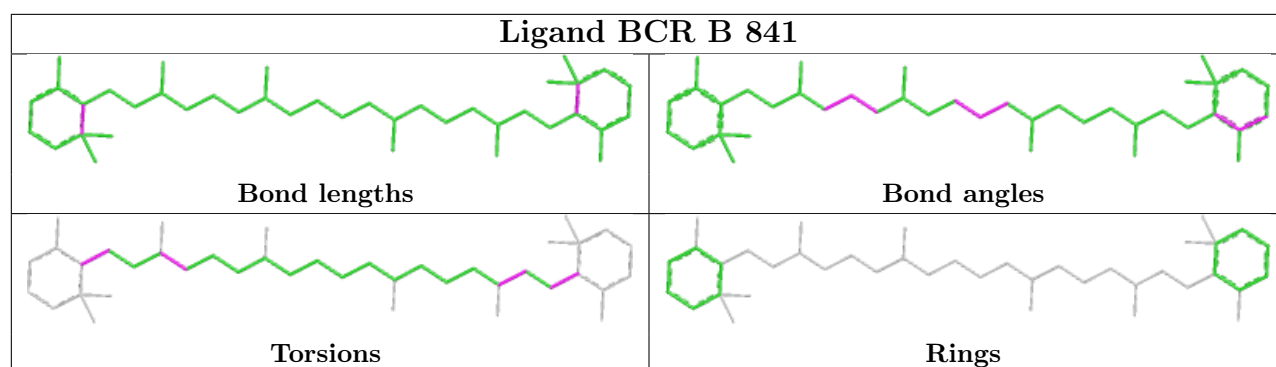




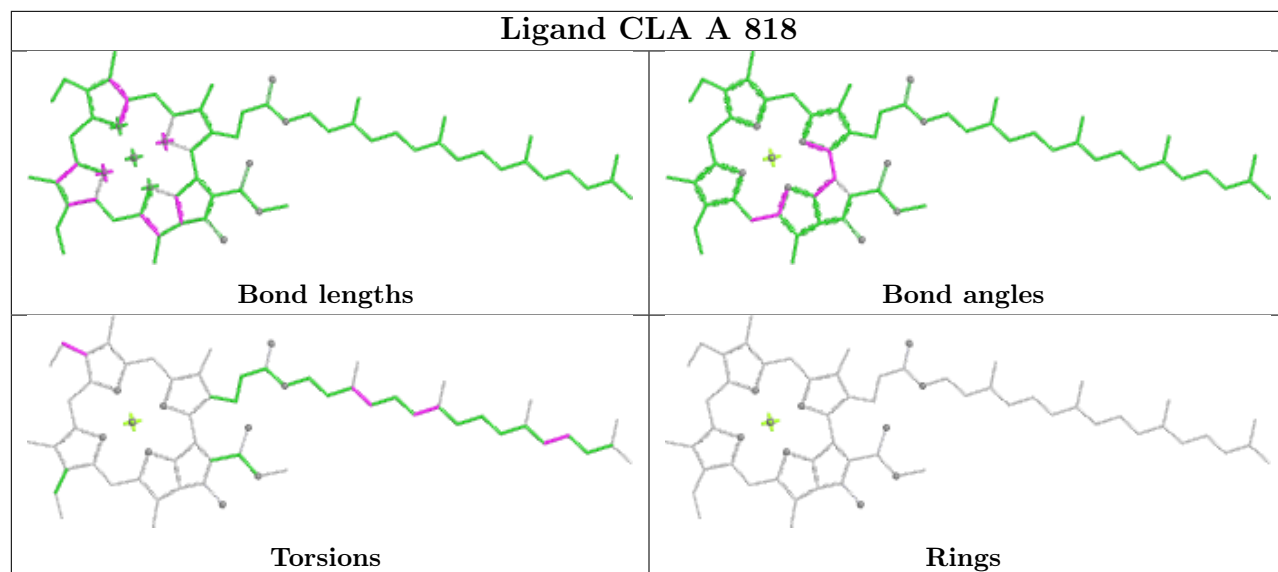




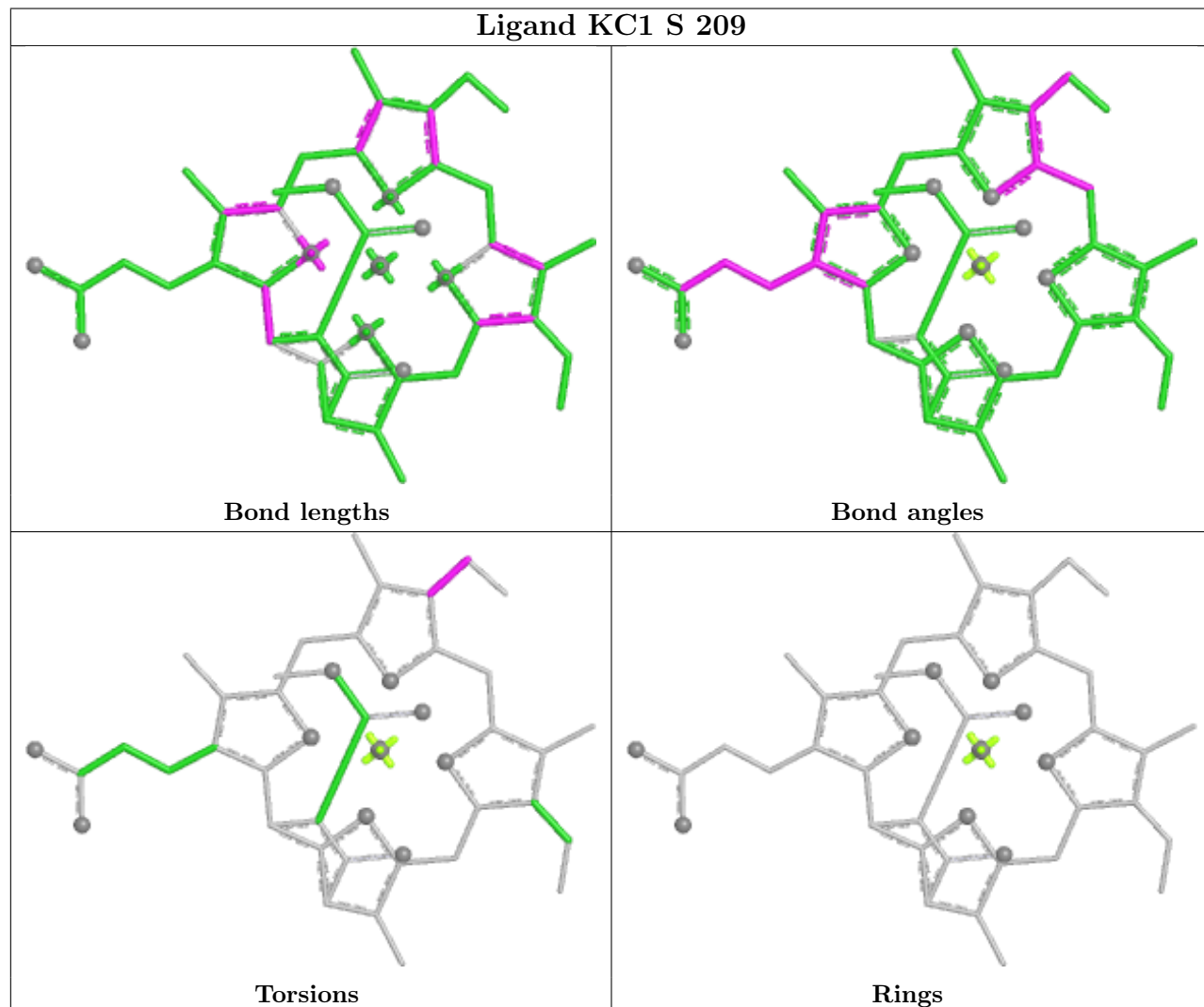


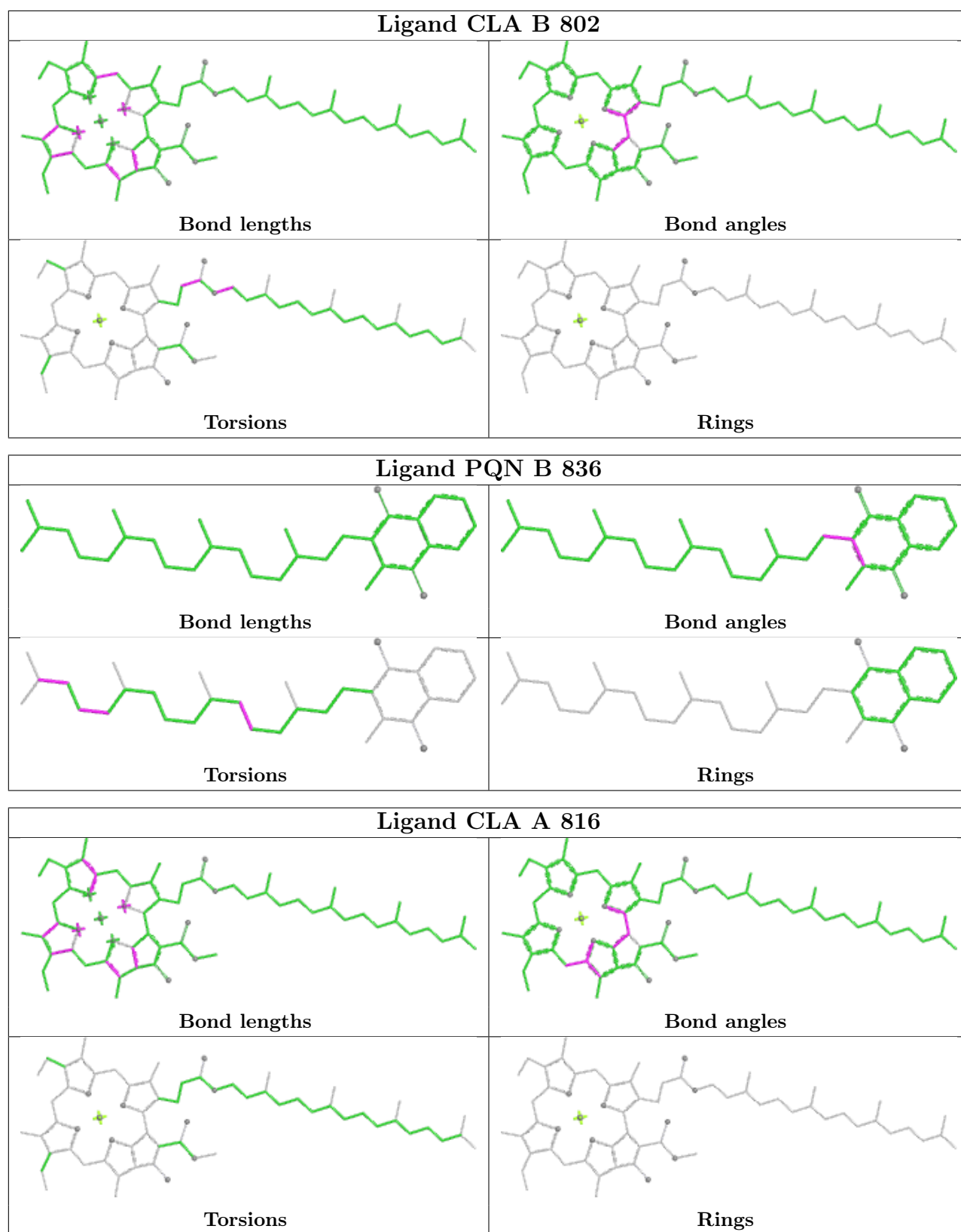


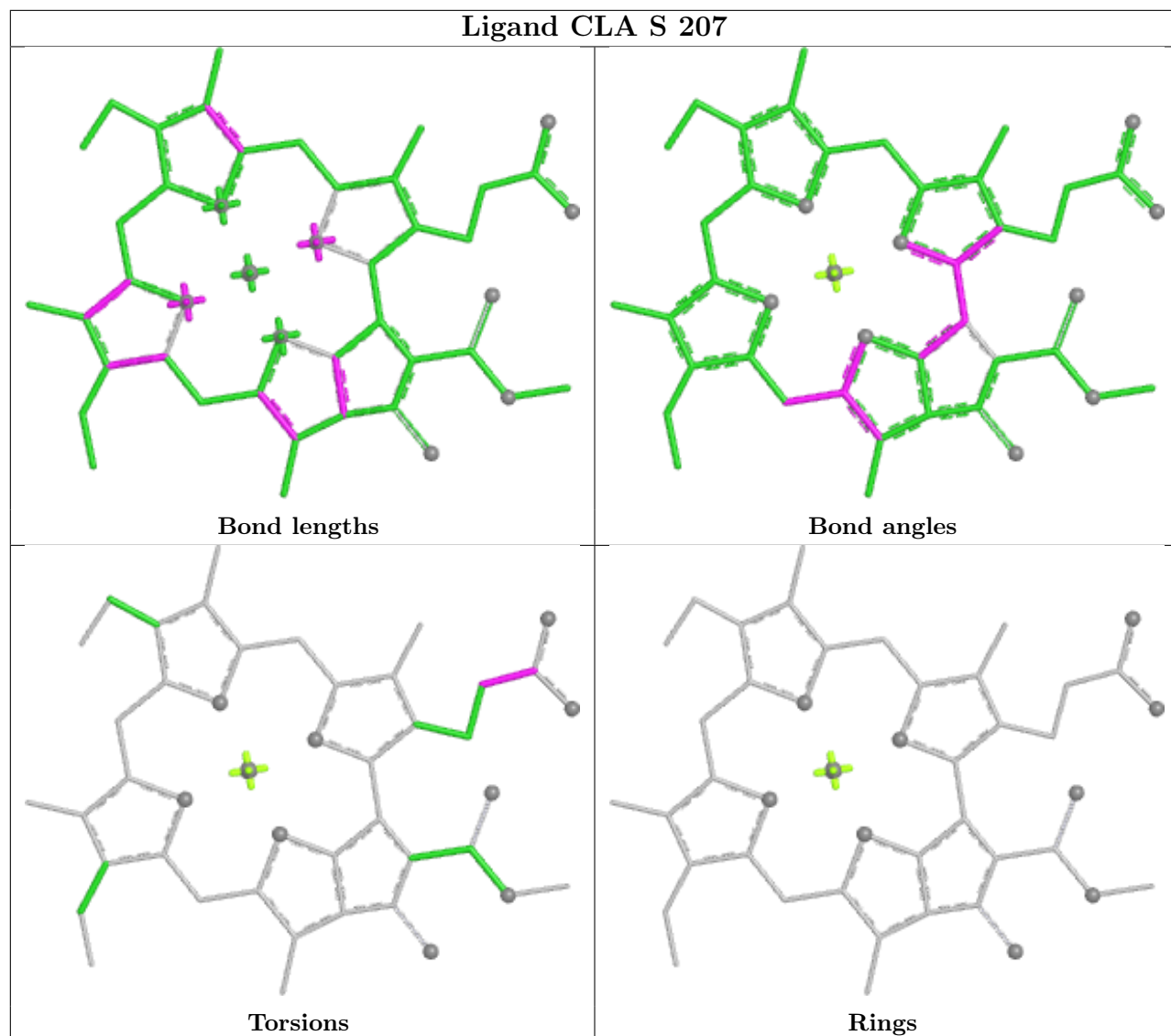
## Ligand CLA A 818

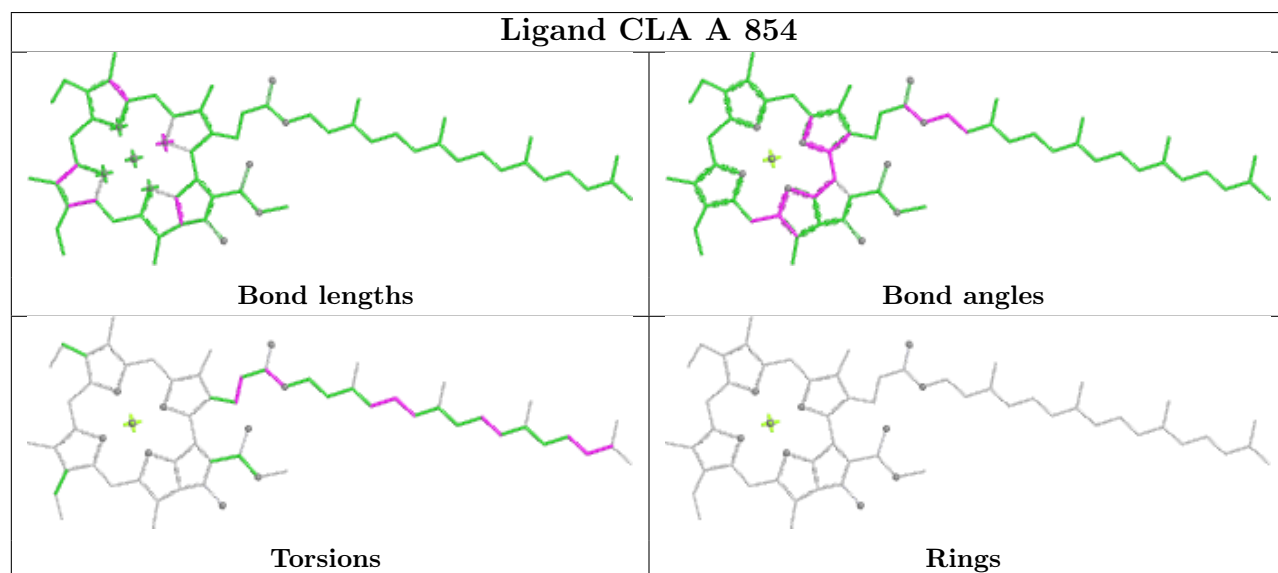
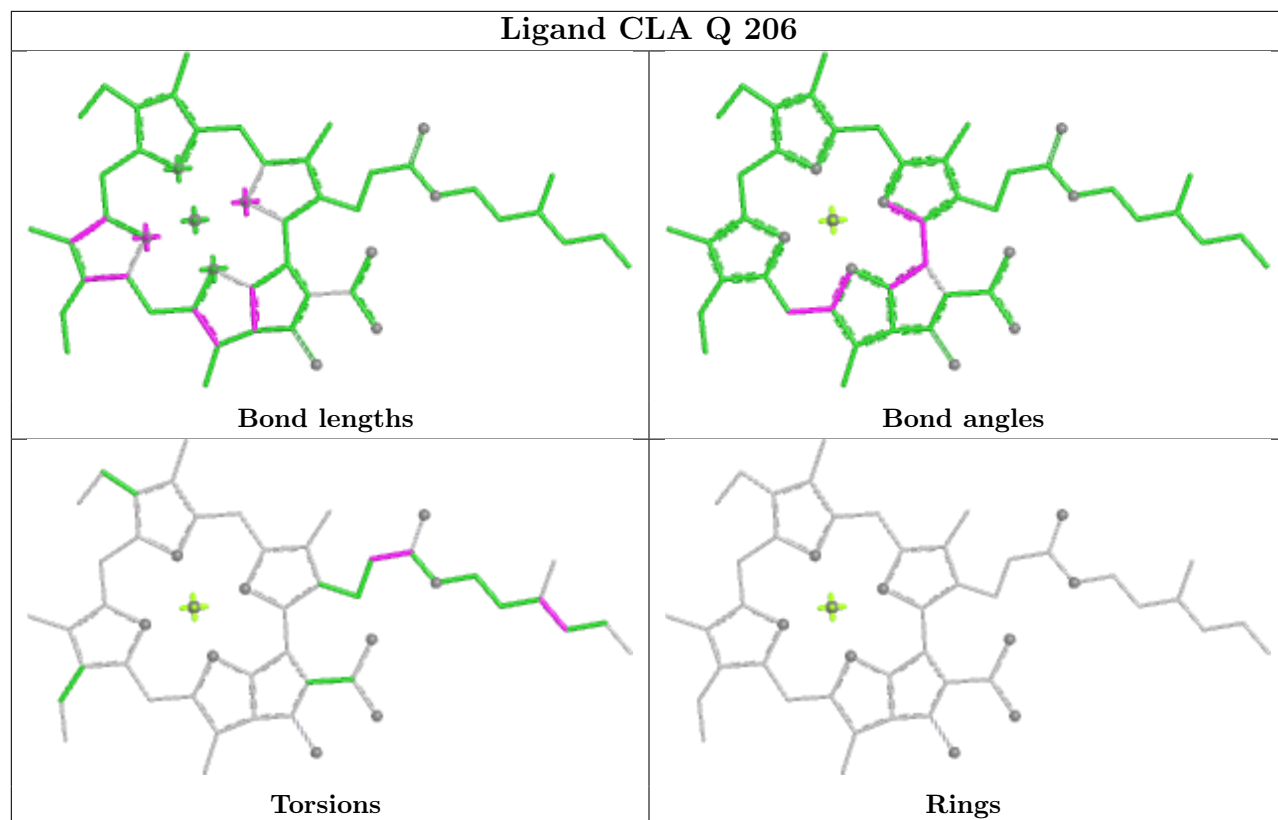


## Ligand KC1 S 209

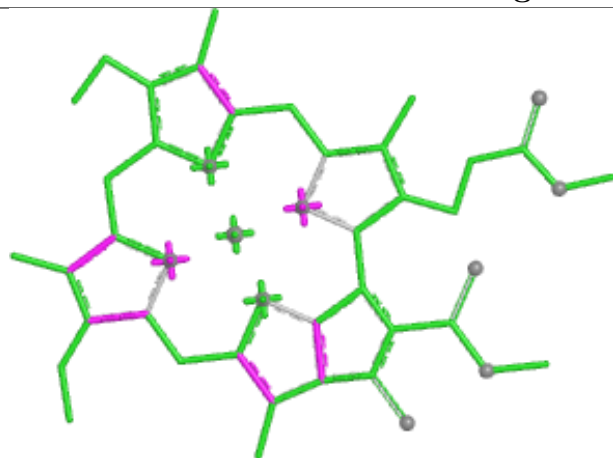




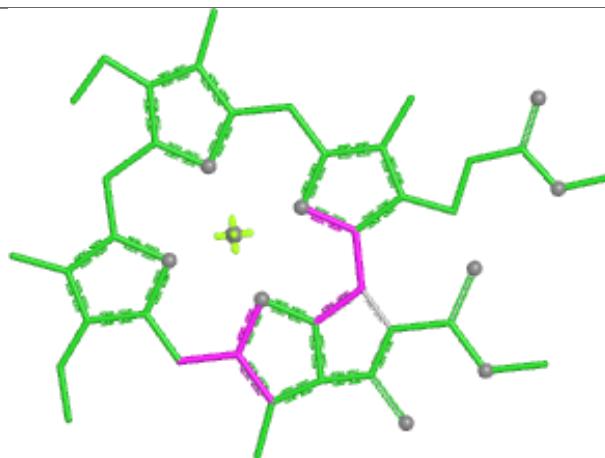




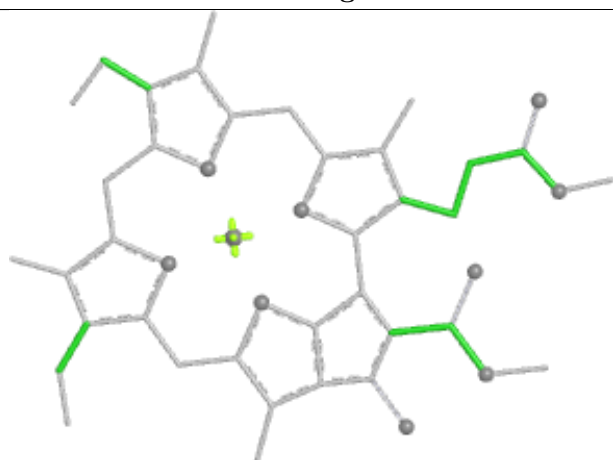
## Ligand CLA O 207



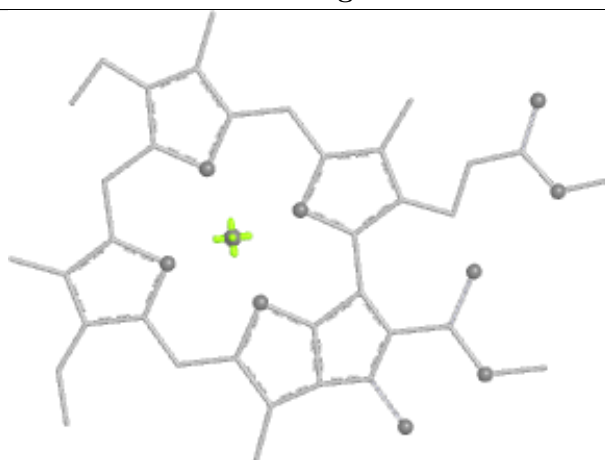
Bond lengths



Bond angles

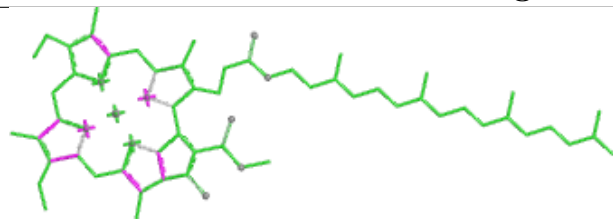


Torsions

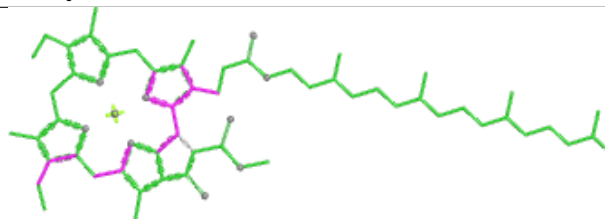


Rings

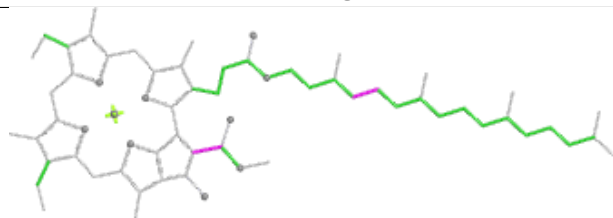
## Ligand CLA Q 212



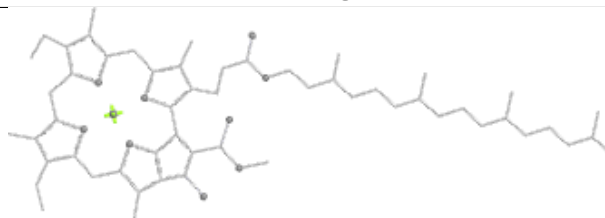
Bond lengths



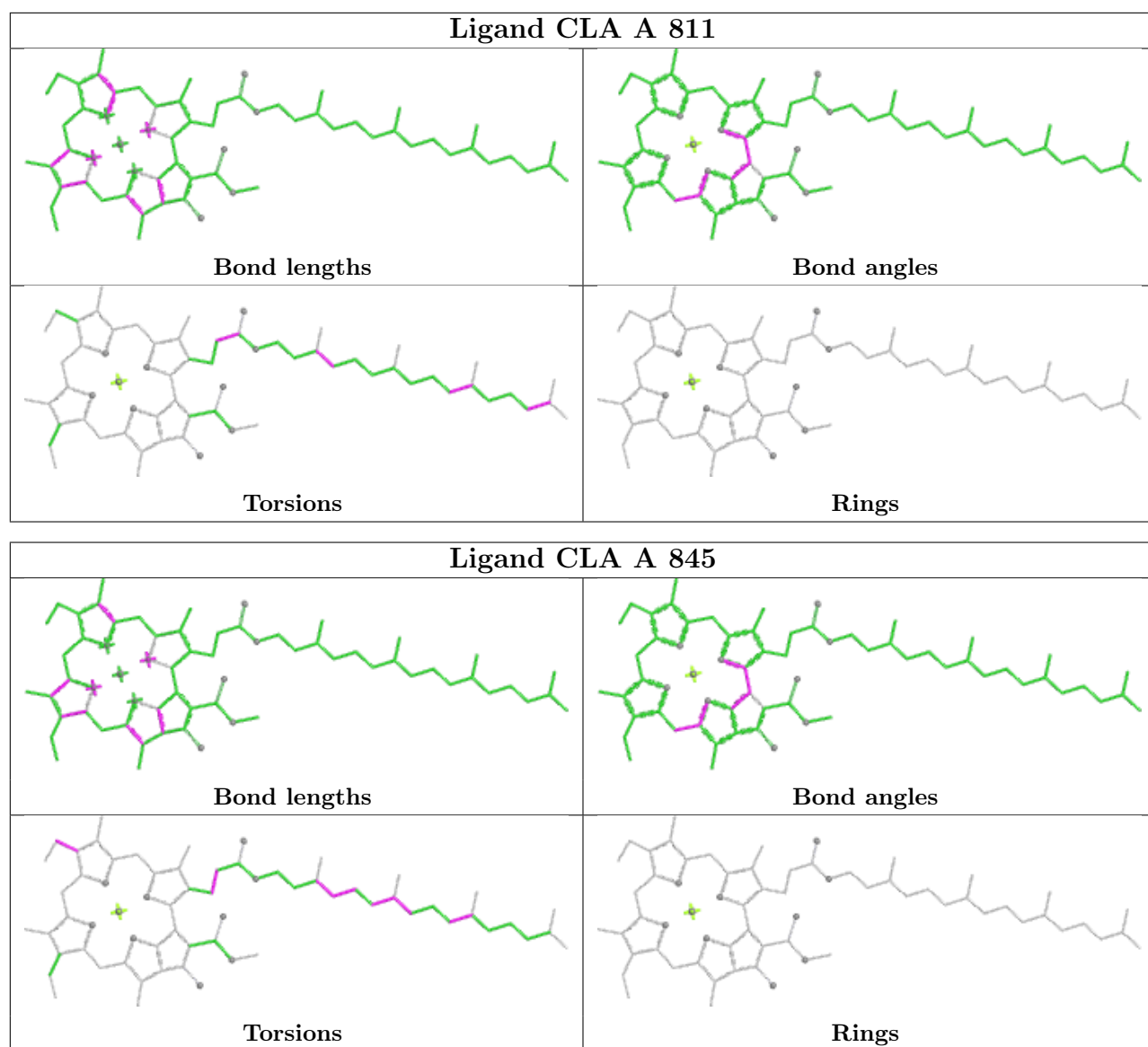
Bond angles



Torsions

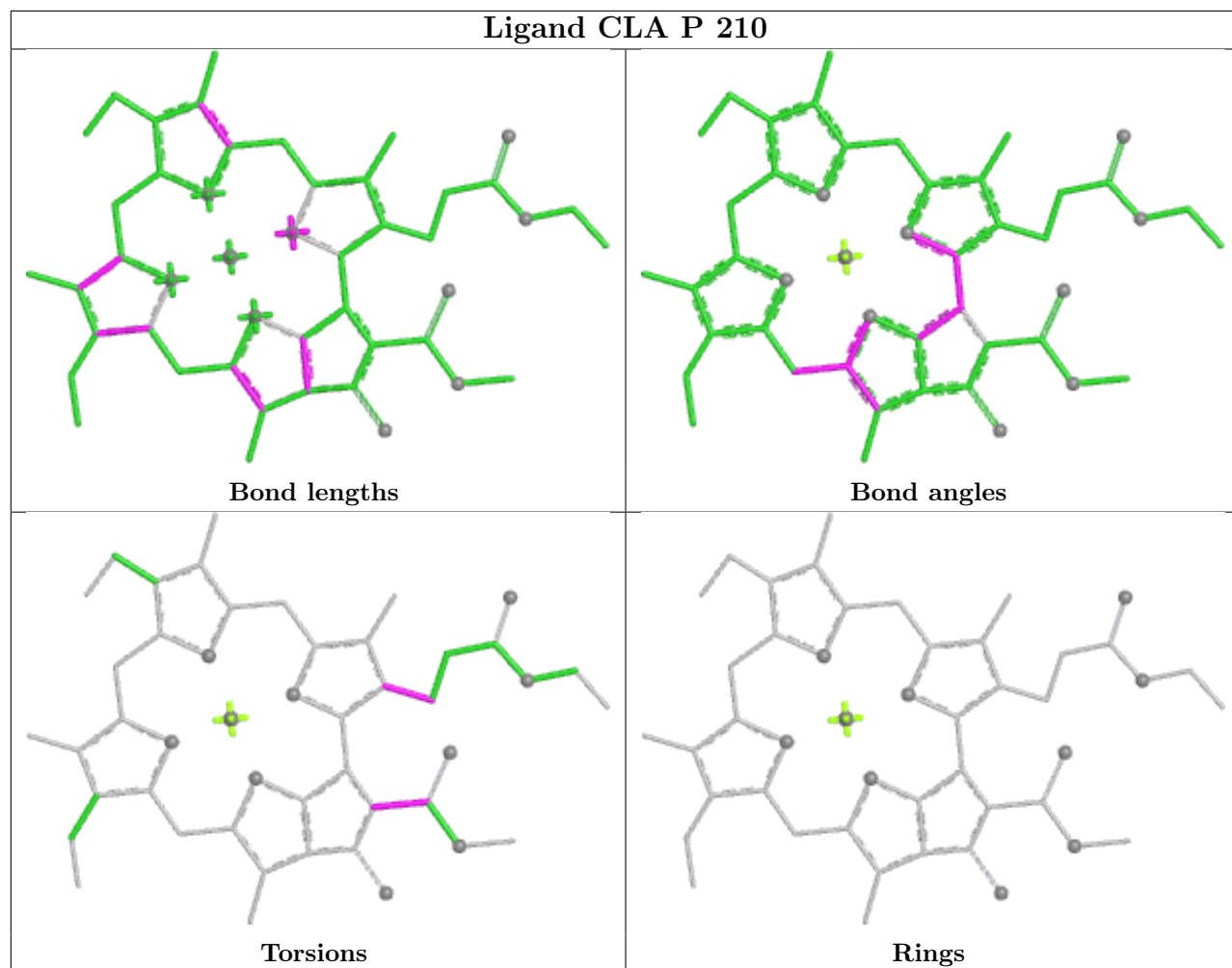


Rings

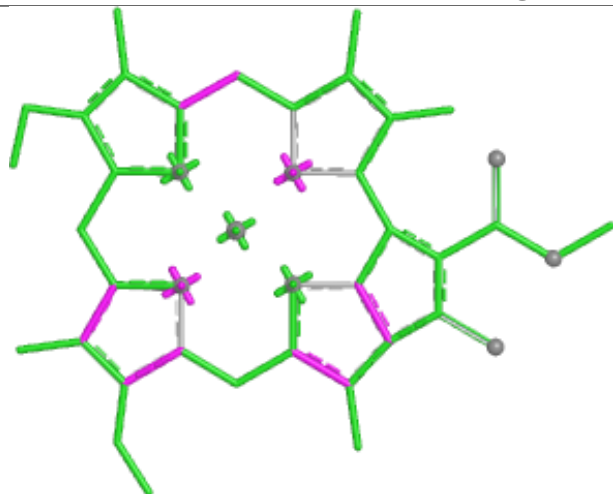




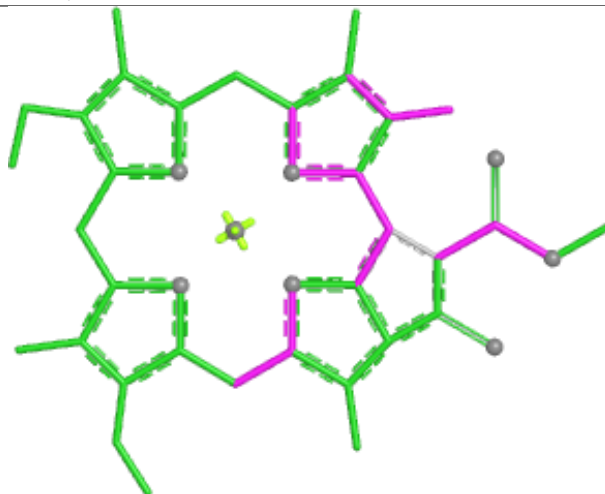
## Ligand CLA P 210



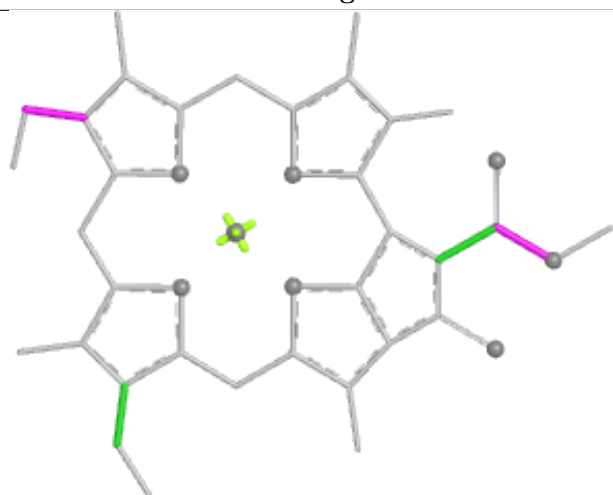
## Ligand CLA Q 211



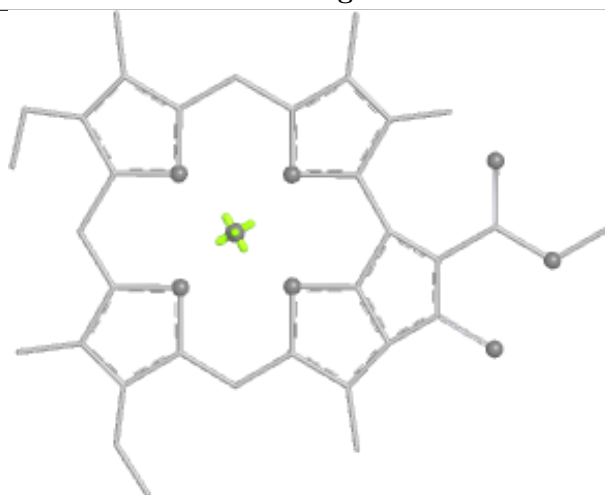
Bond lengths



Bond angles

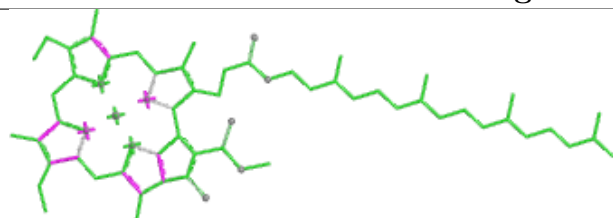


Torsions

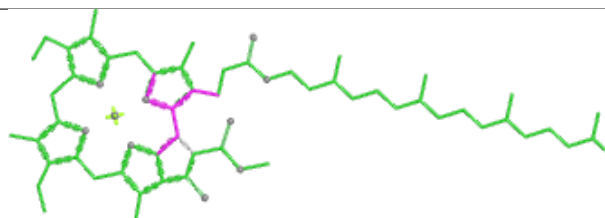


Rings

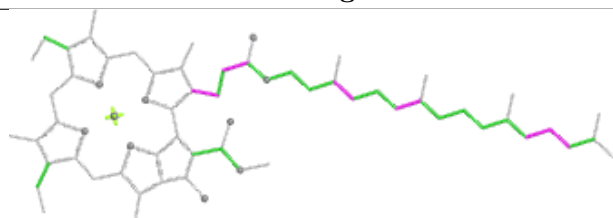
## Ligand CLA B 823



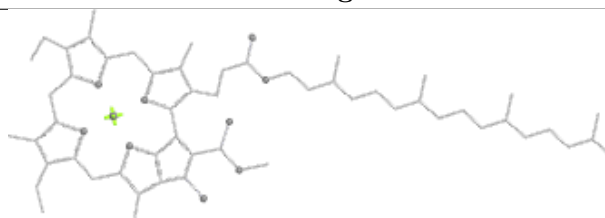
Bond lengths



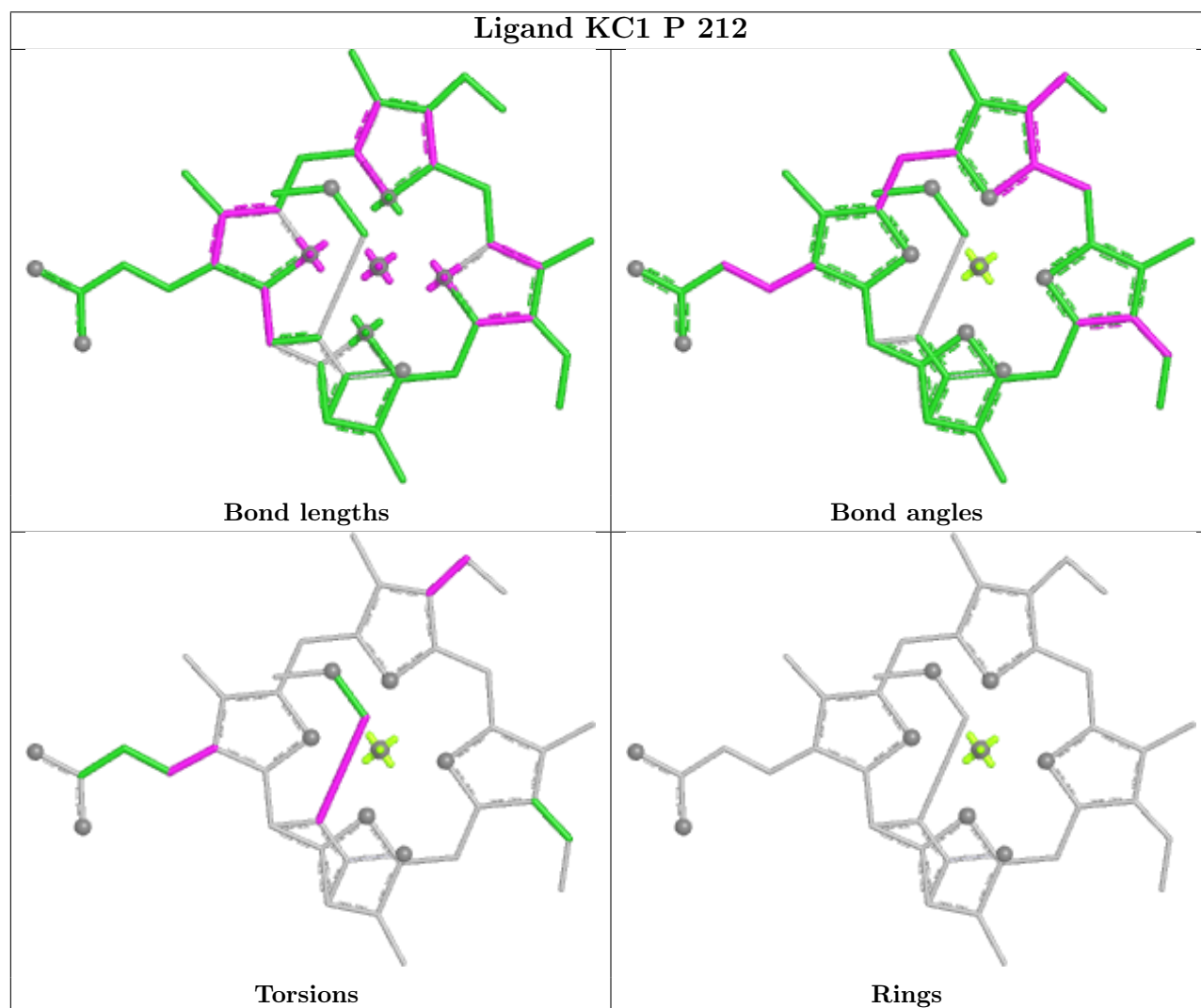
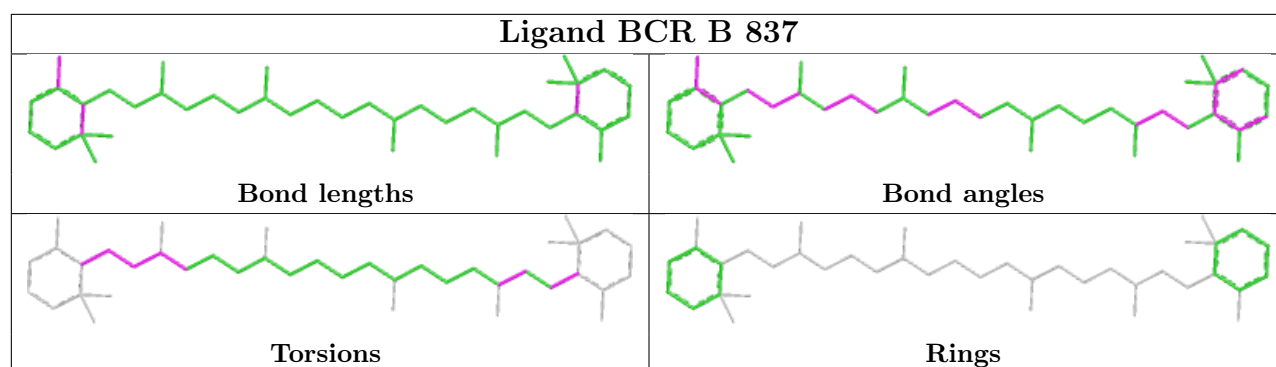
Bond angles



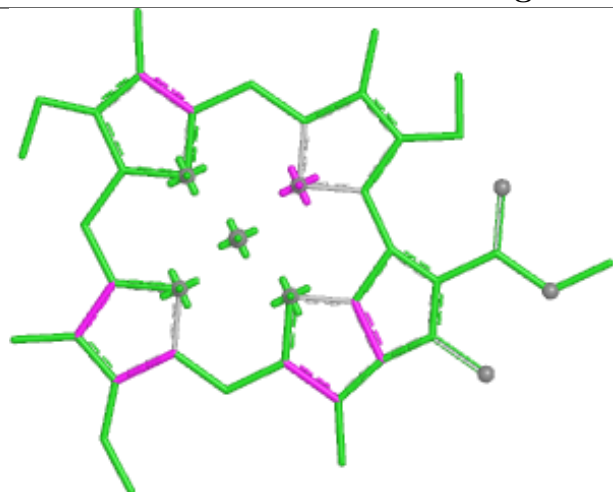
Torsions



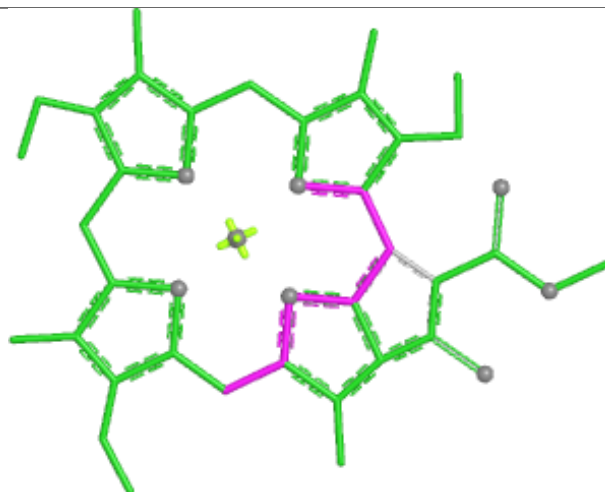
Rings



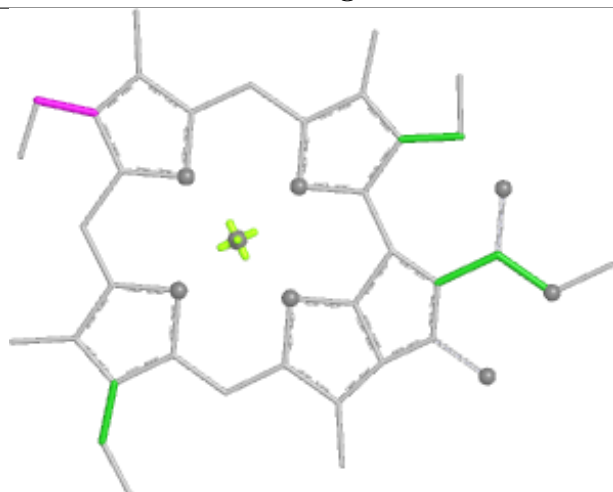
## Ligand CLA T 206



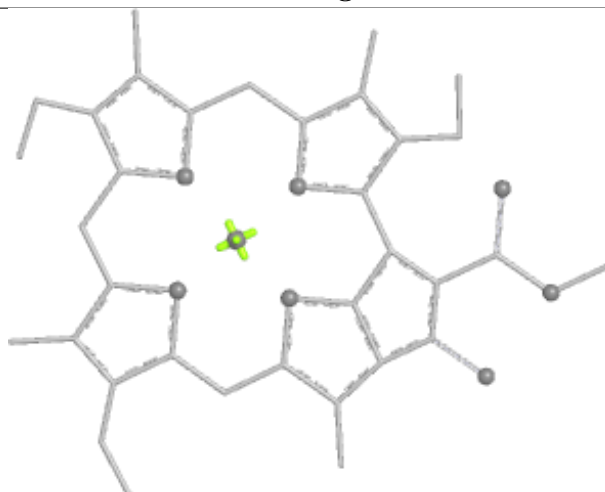
Bond lengths



Bond angles

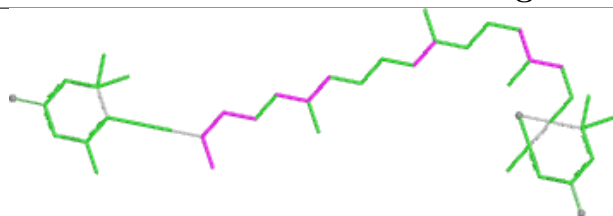


Torsions

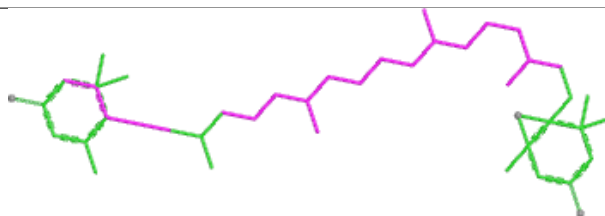


Rings

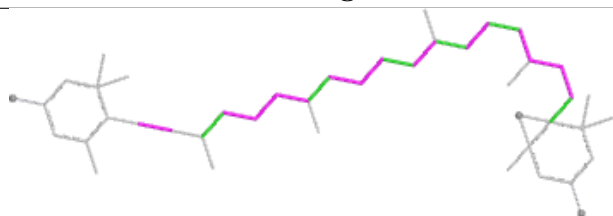
## Ligand DD6 P 220



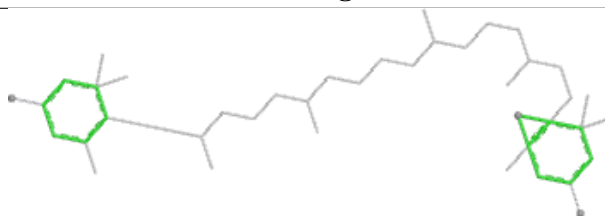
Bond lengths



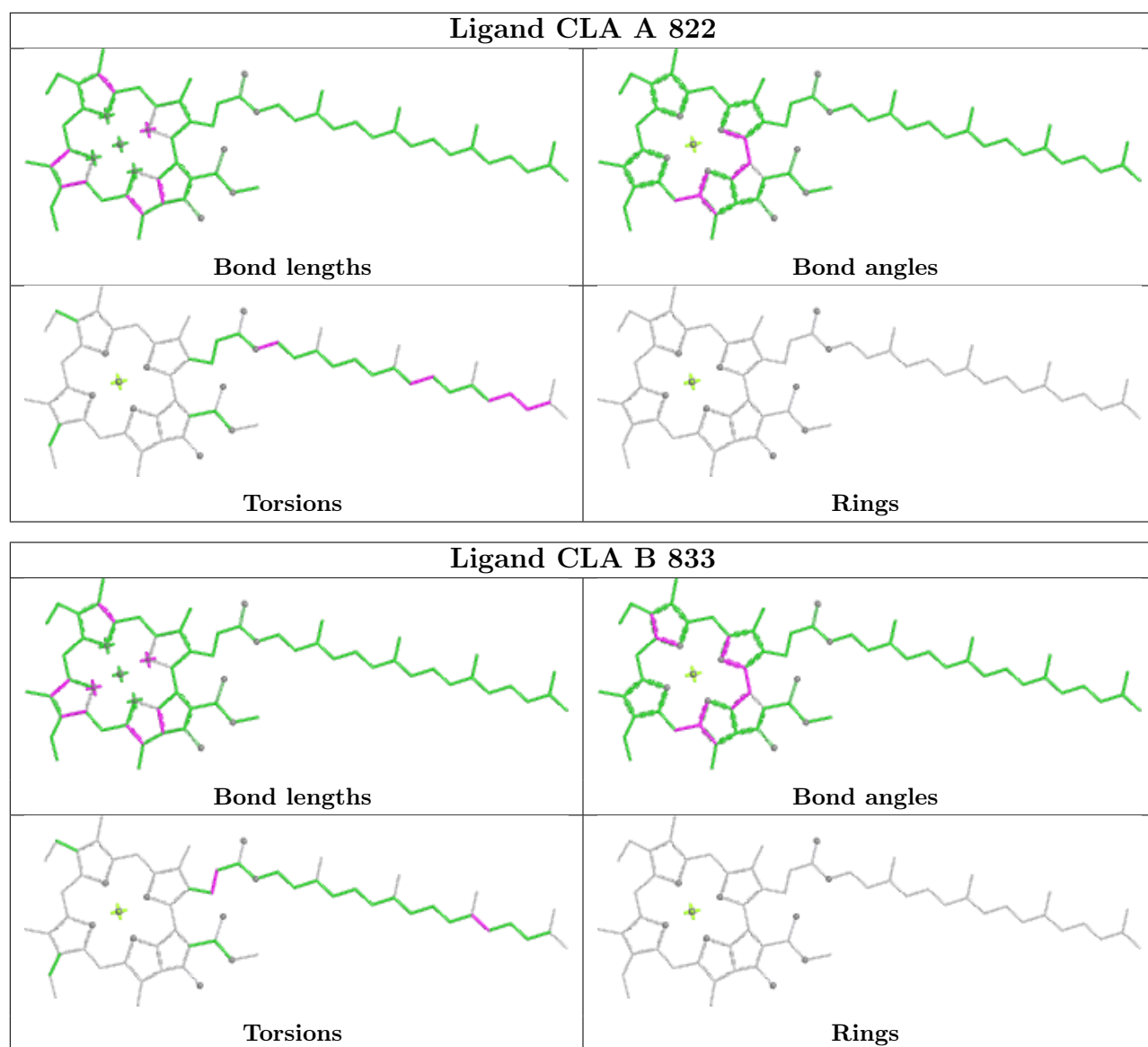
Bond angles



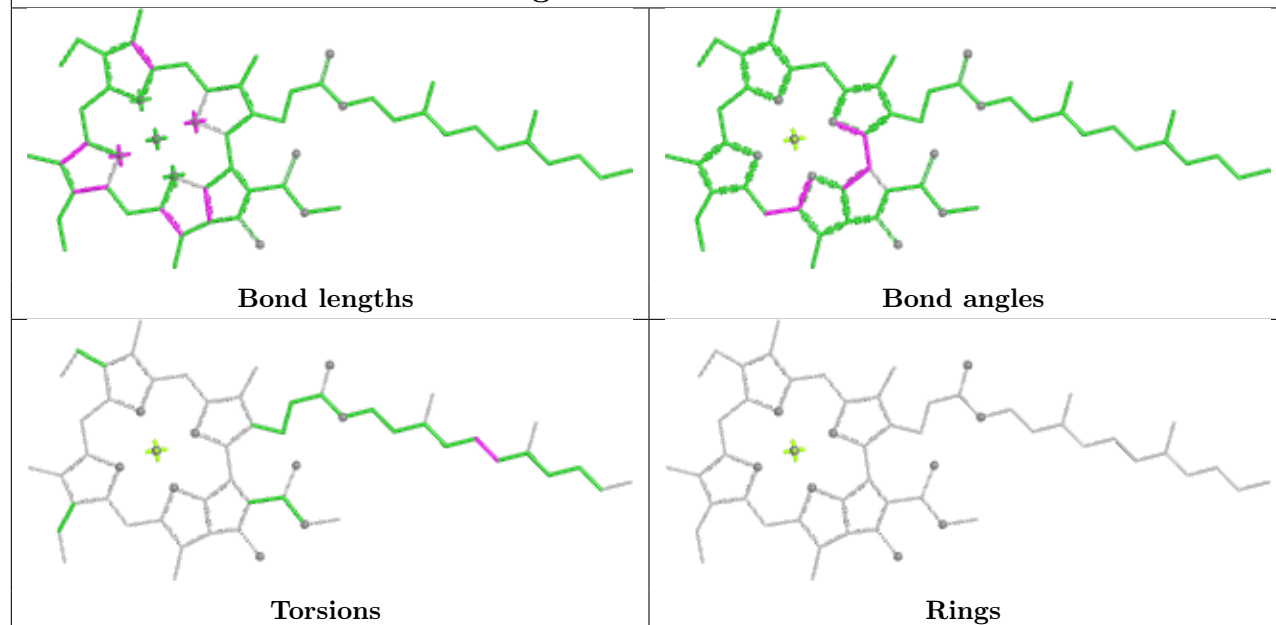
Torsions



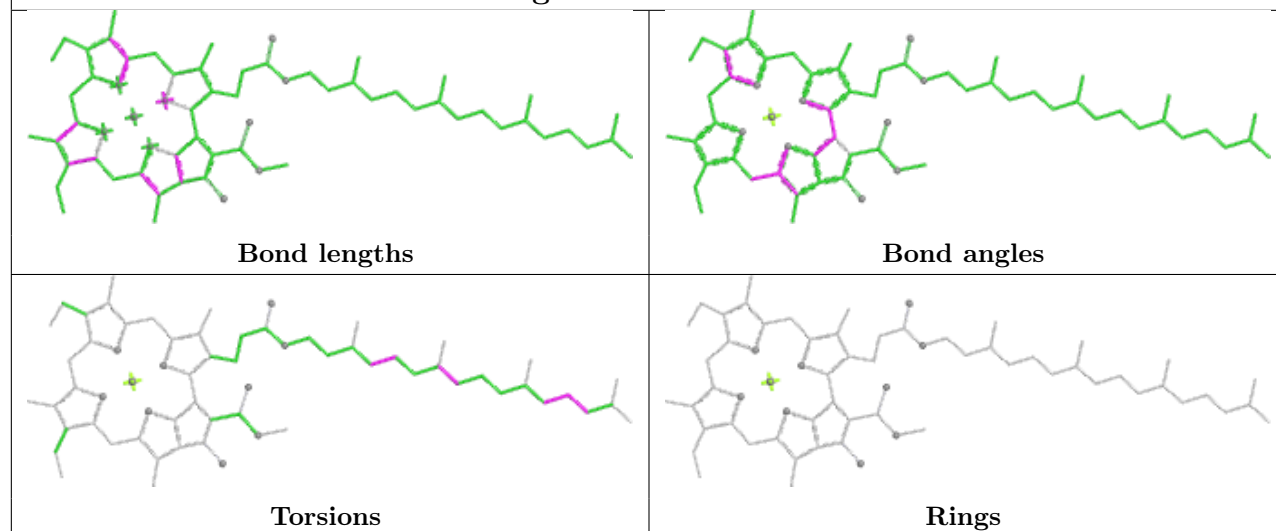
Rings

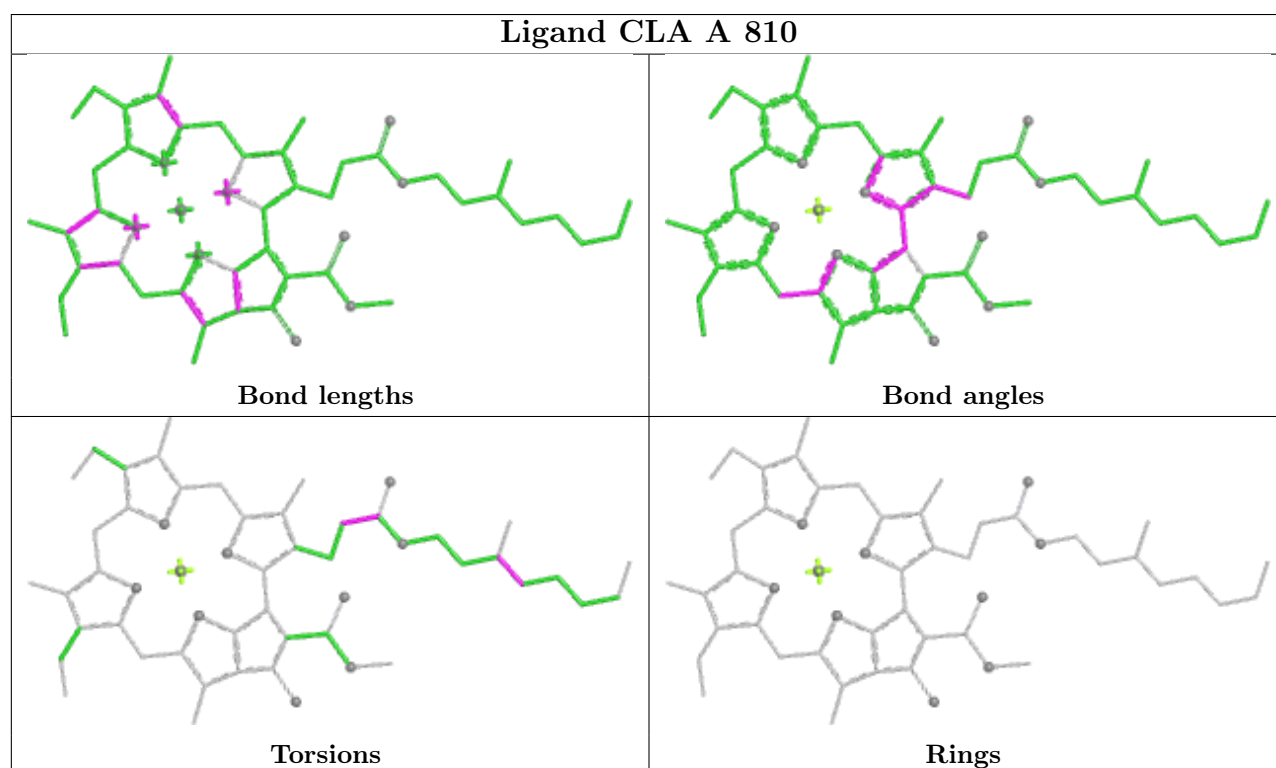
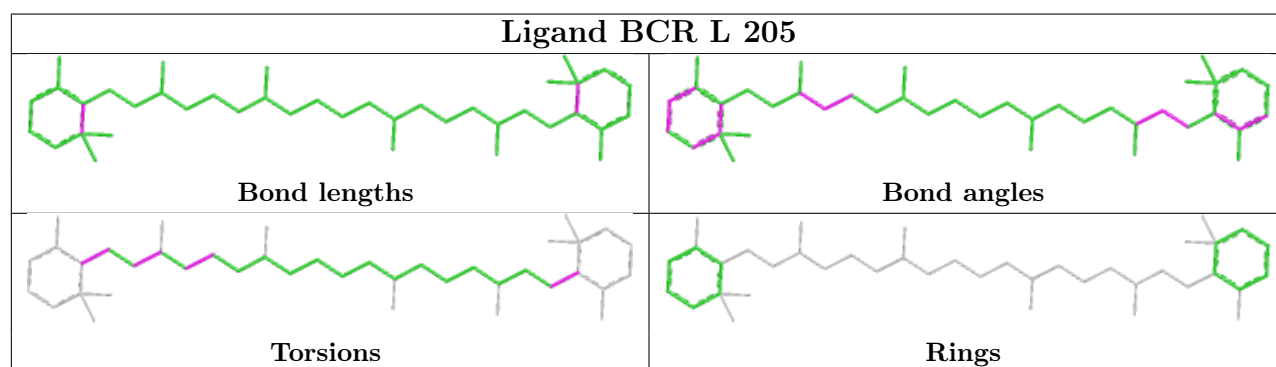
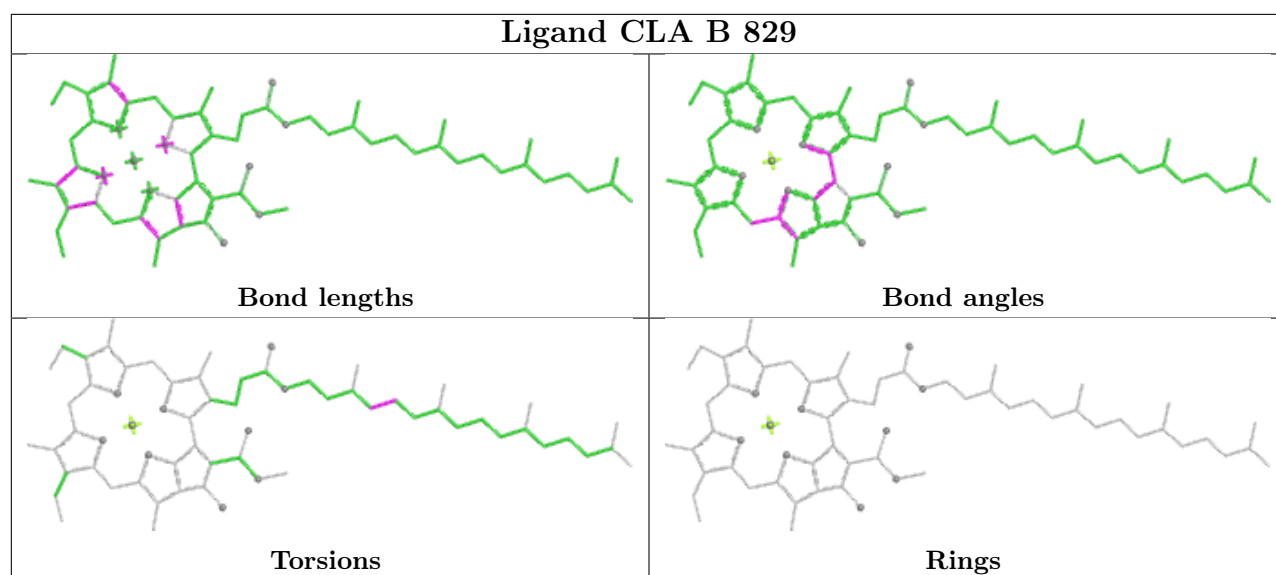


## Ligand CLA B 830

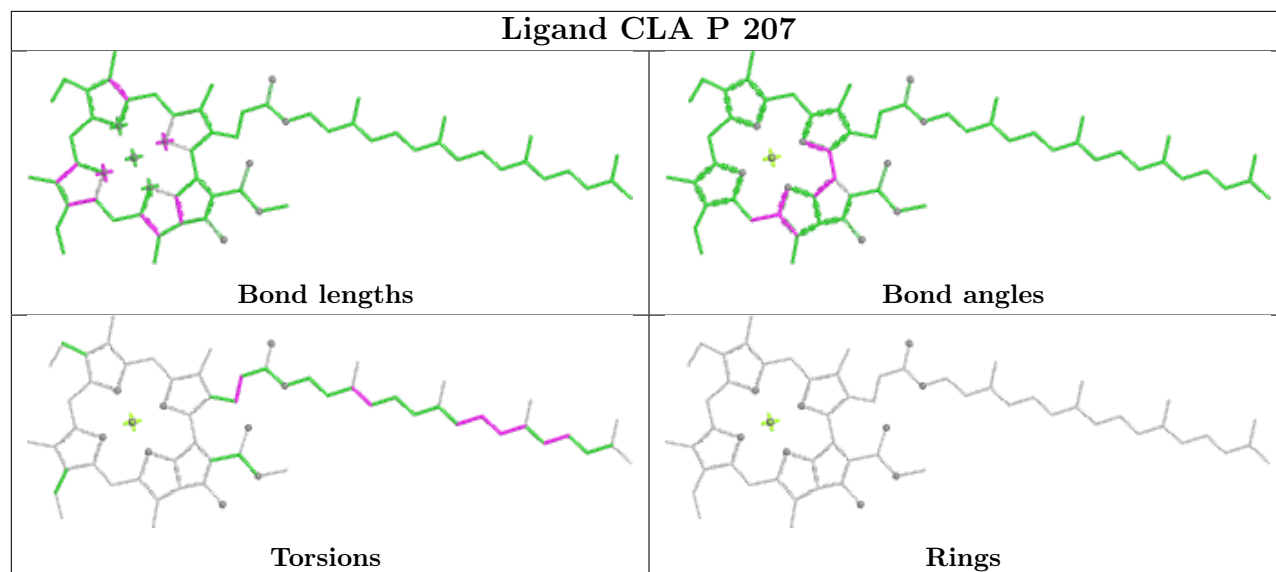


## Ligand CLA B 817

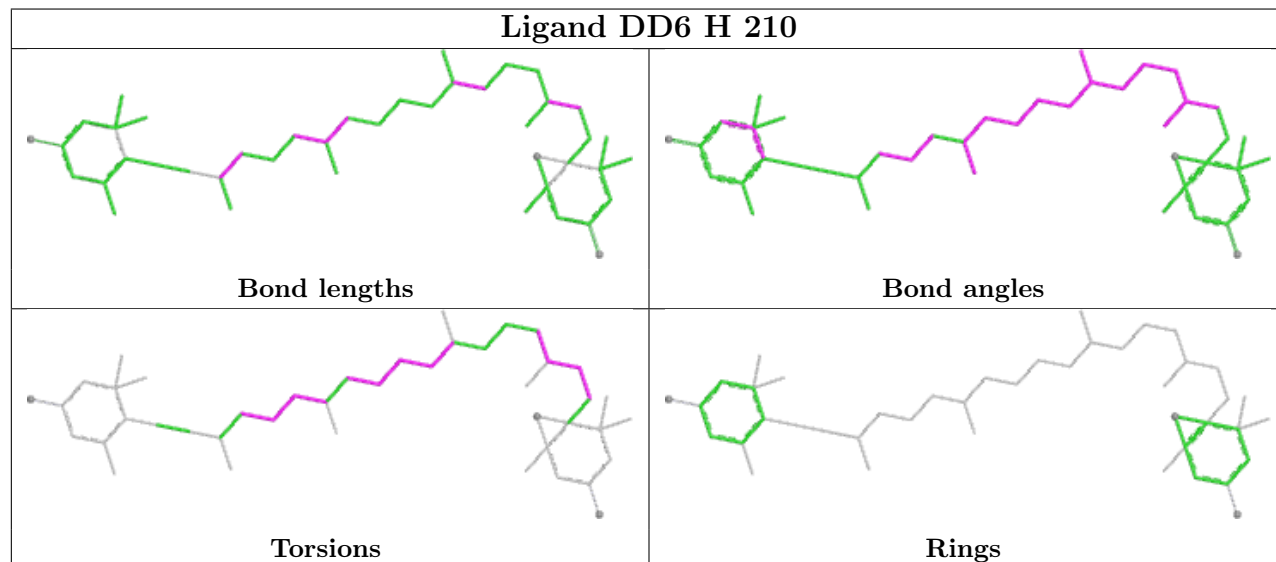




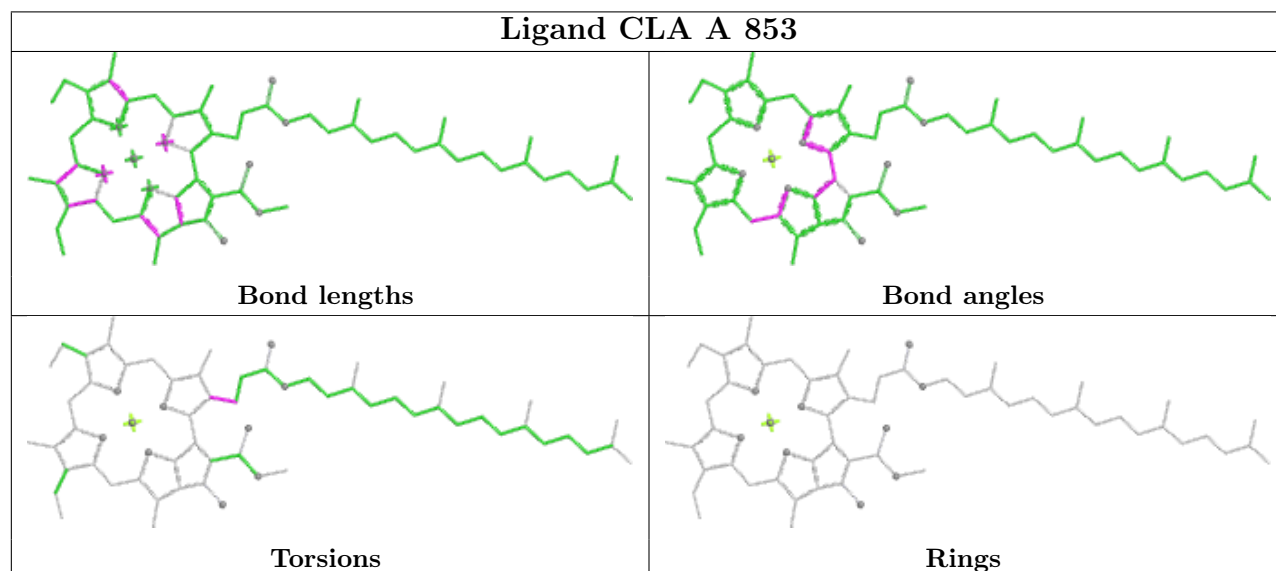
## Ligand CLA P 207



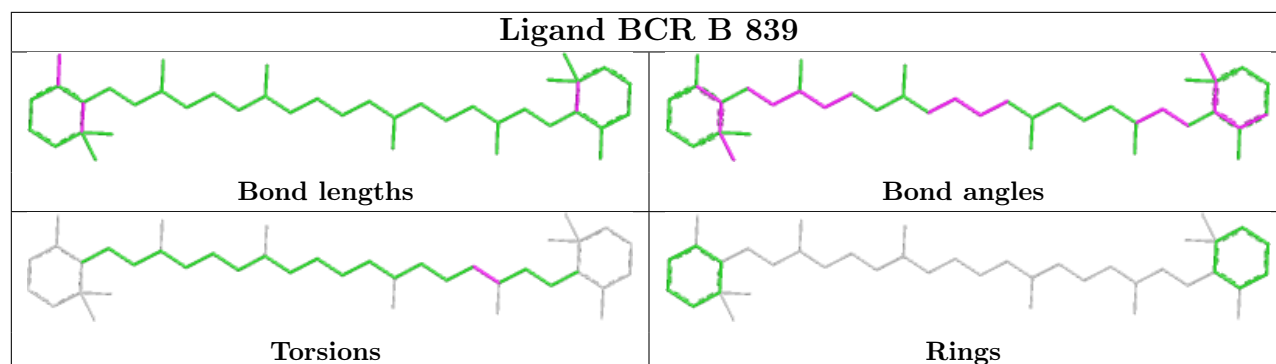
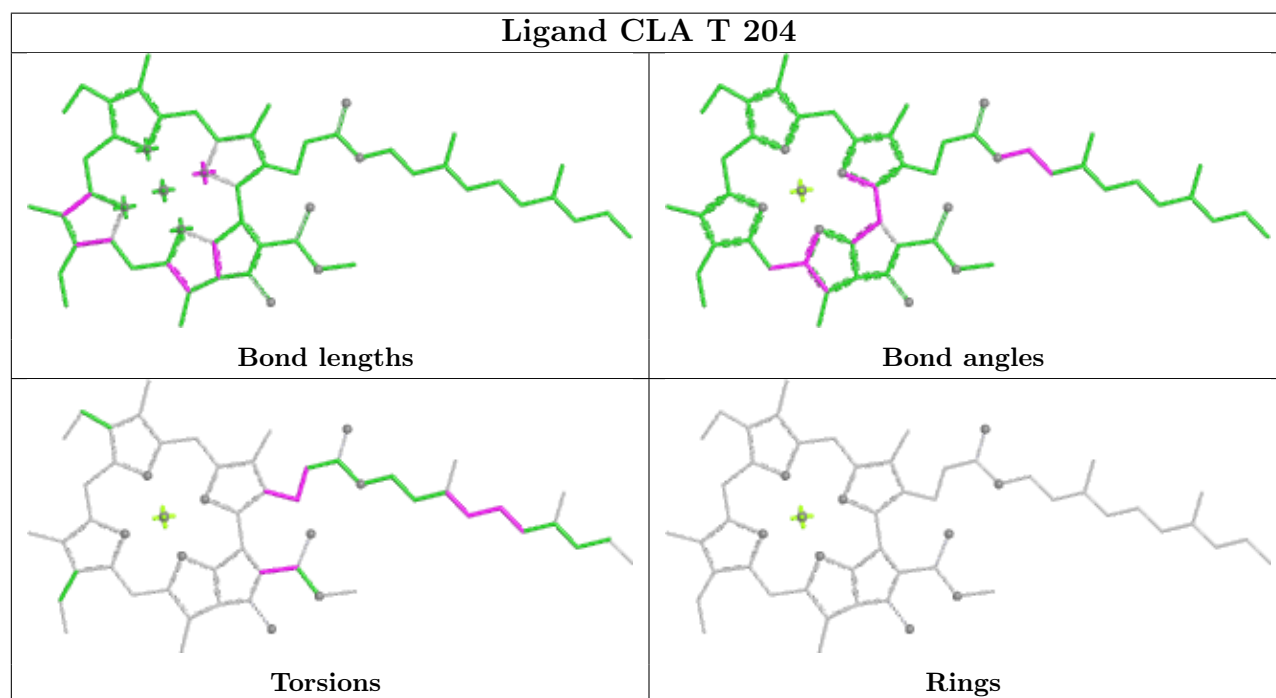
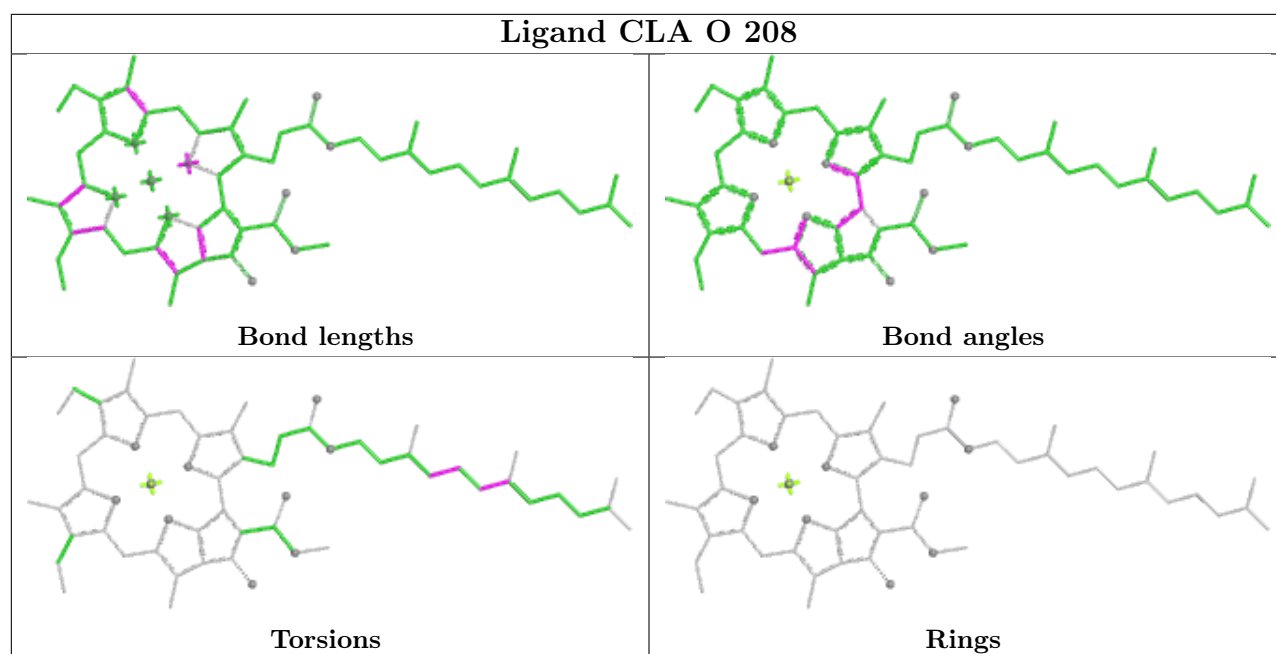
## Ligand DD6 H 210

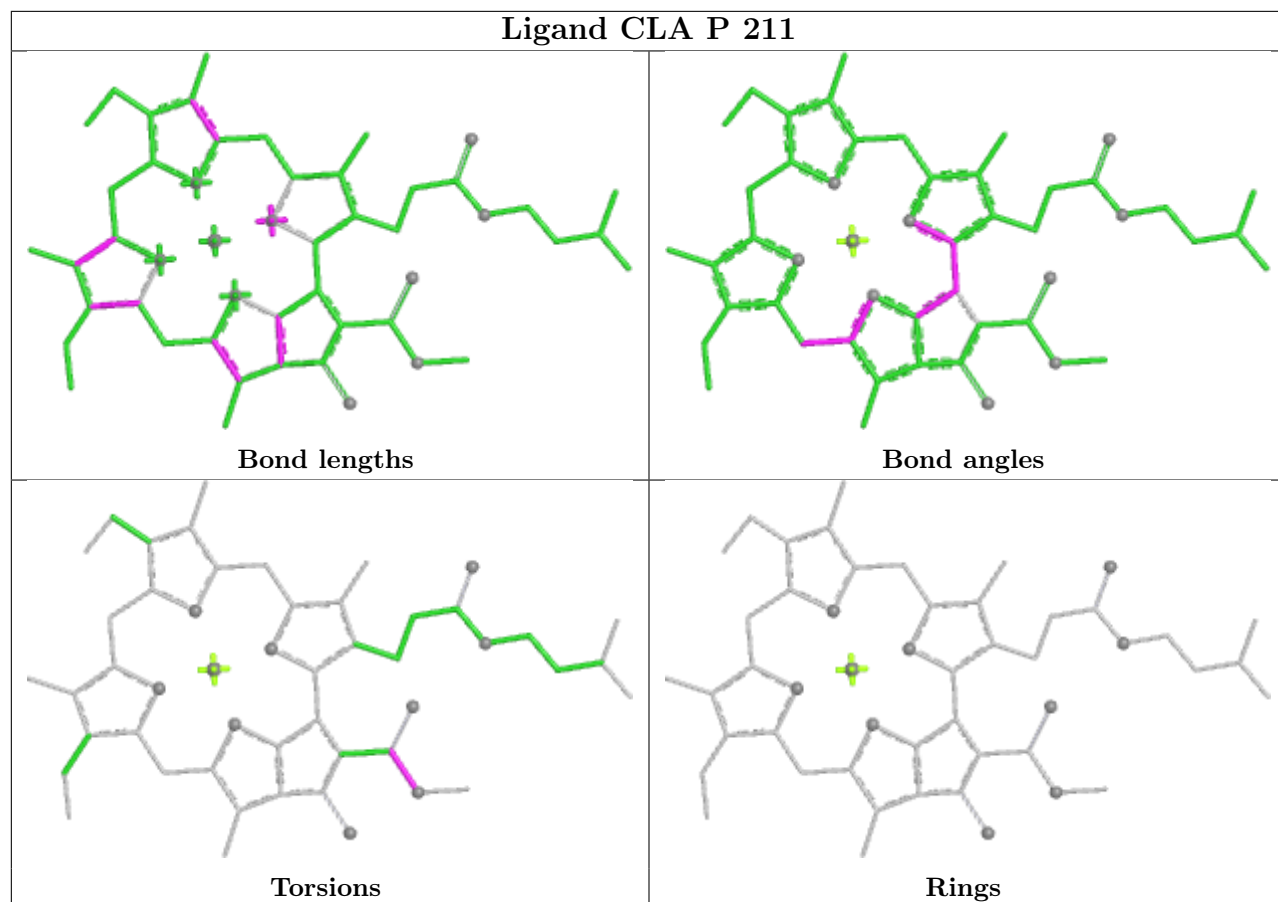


## Ligand CLA A 853

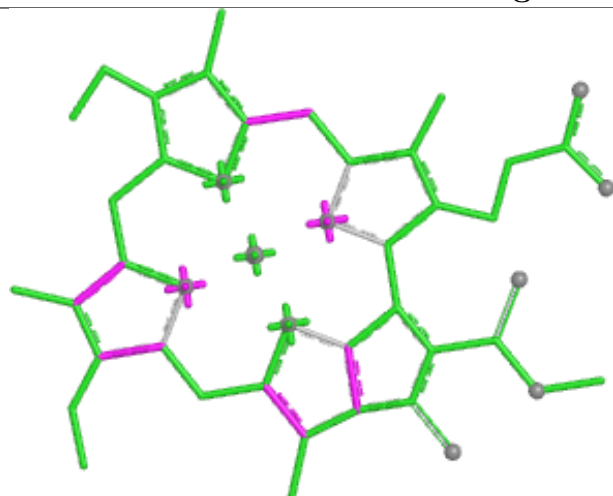




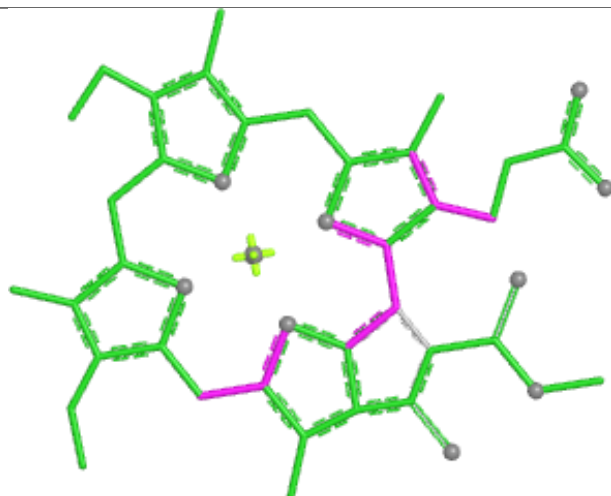




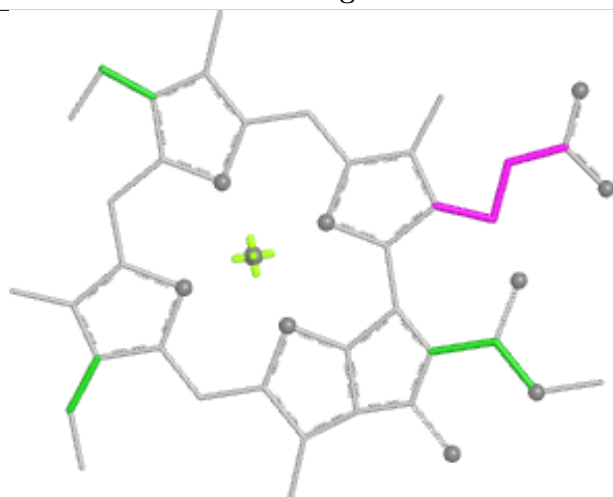
## Ligand CLA H 209



Bond lengths



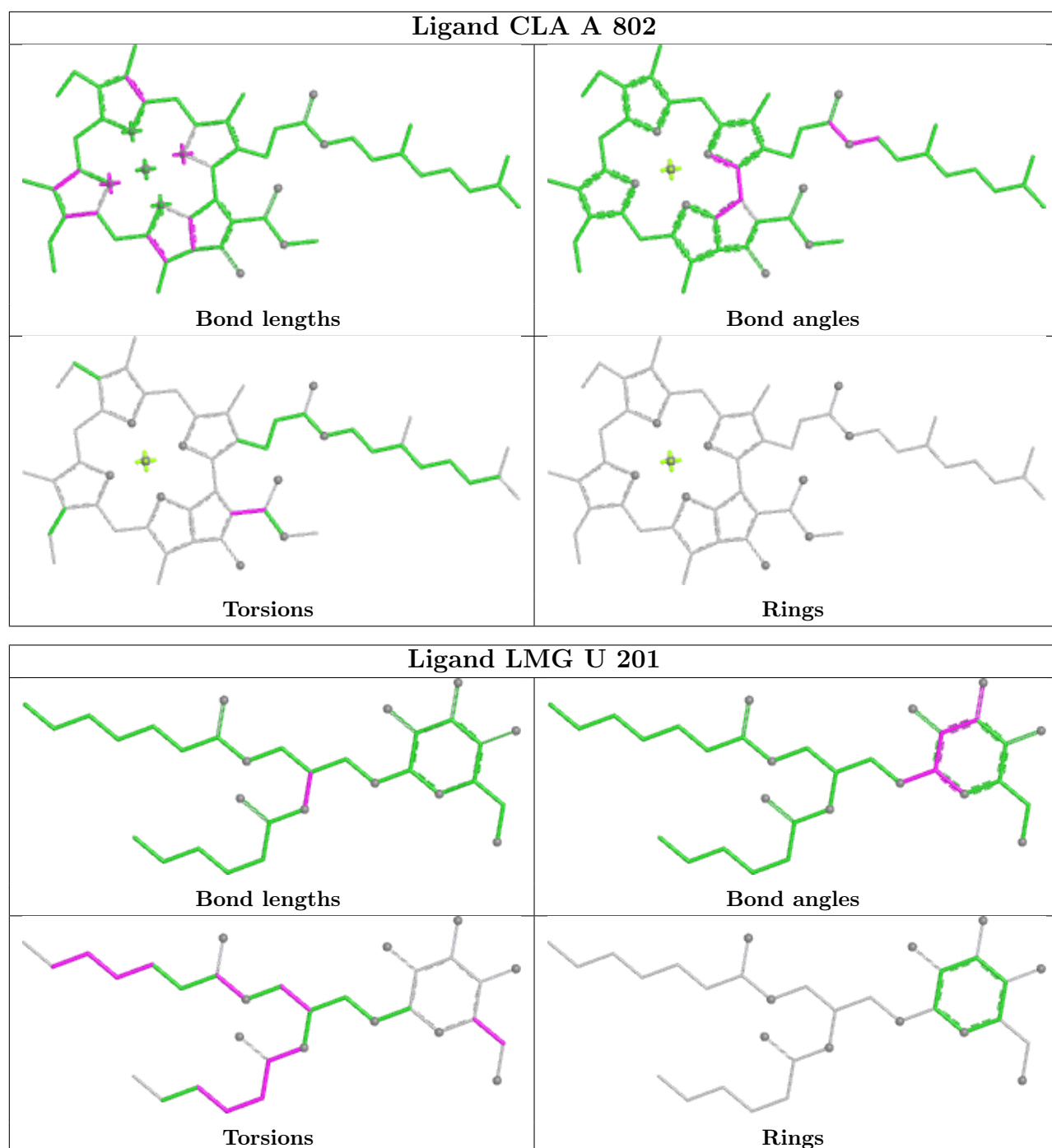
Bond angles



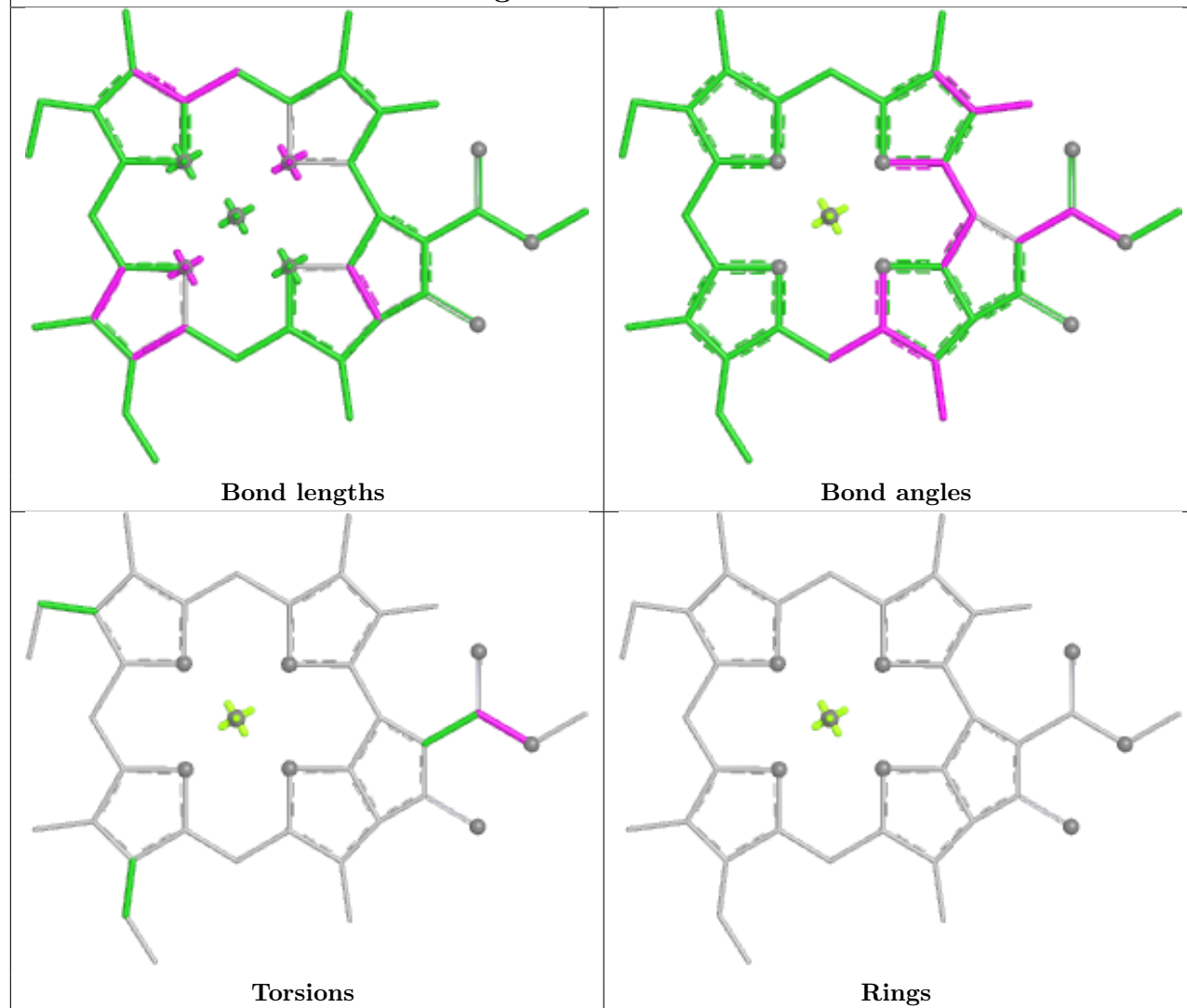
Torsions



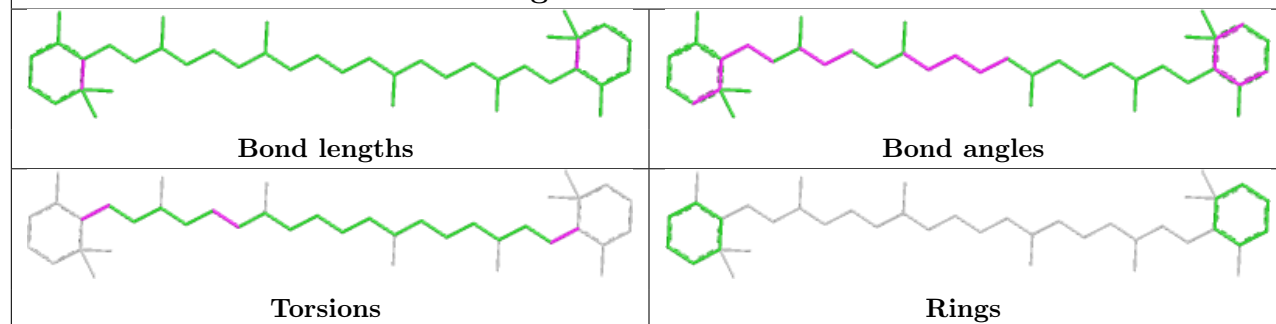
Rings

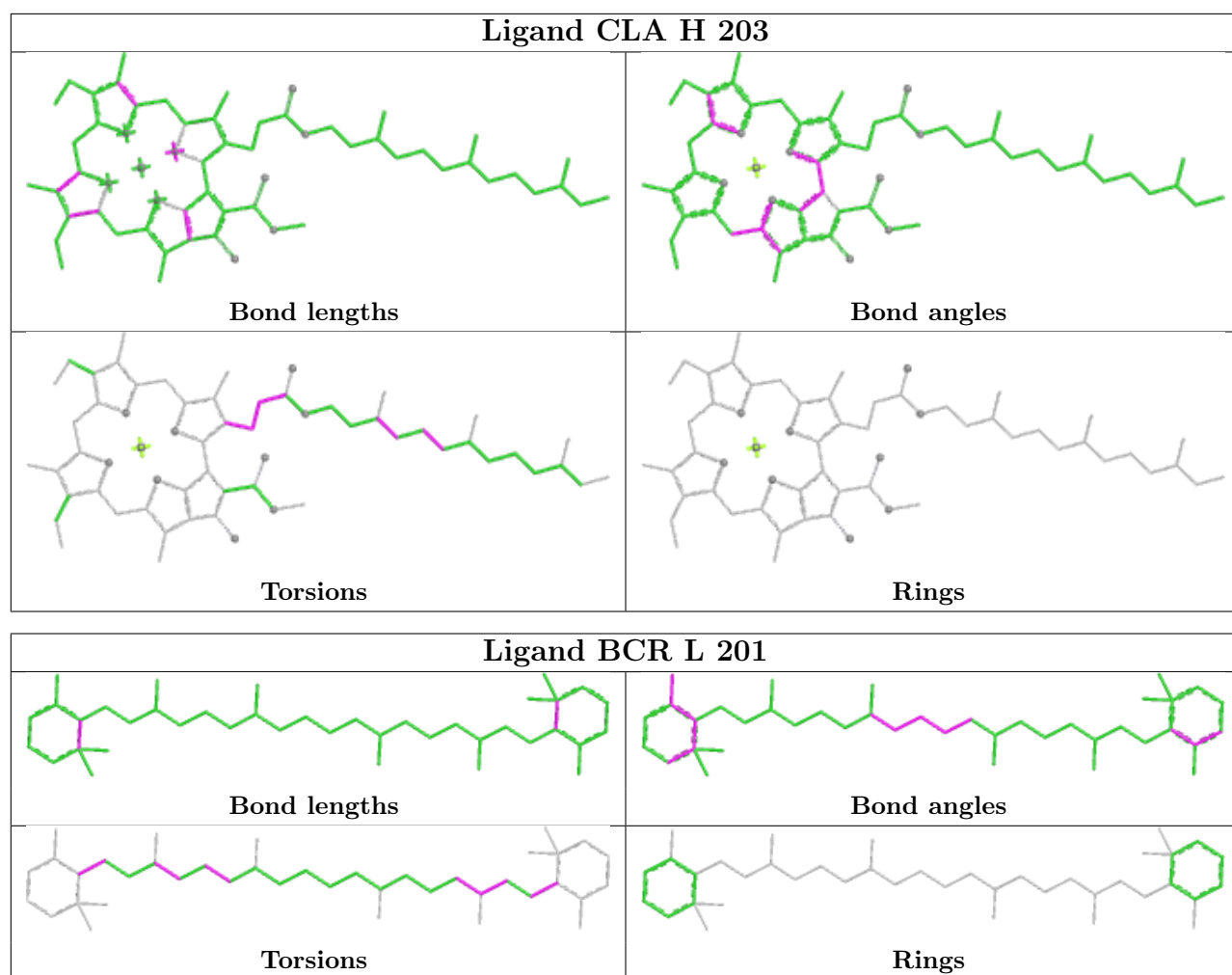


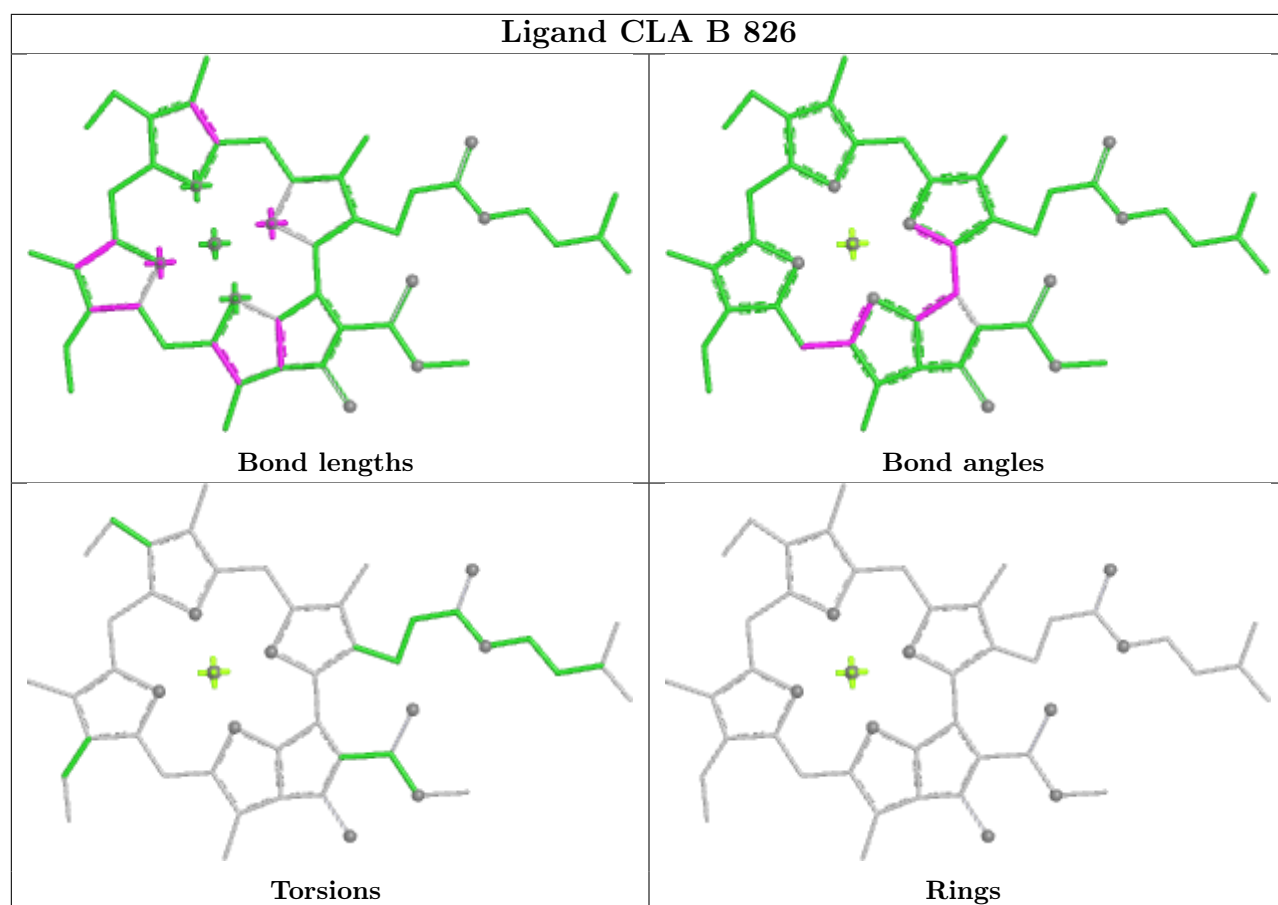
## Ligand CLA H 208



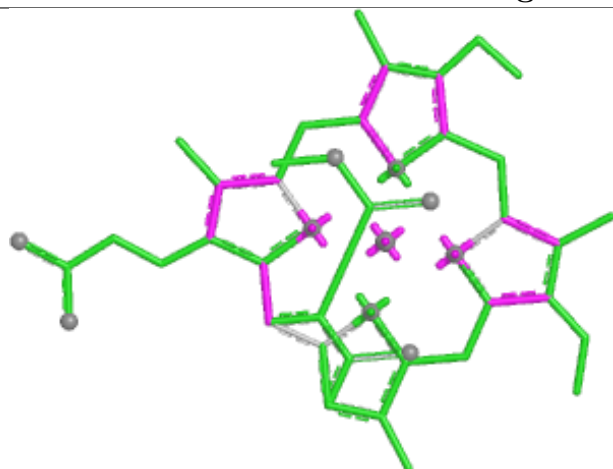
## Ligand BCR B 840



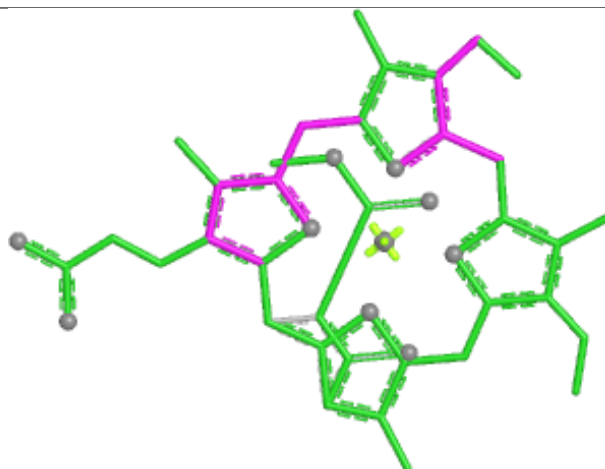




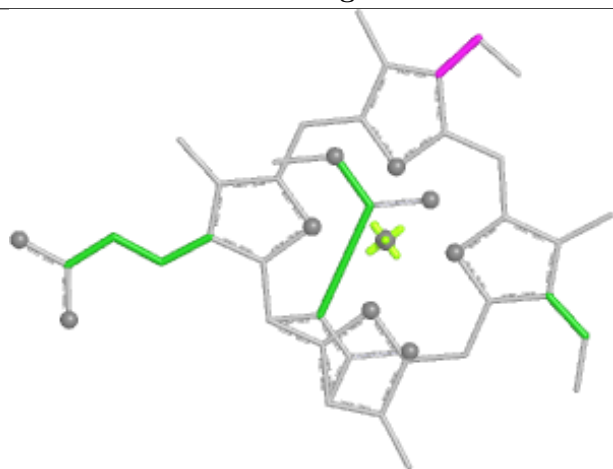
## Ligand KC1 P 203



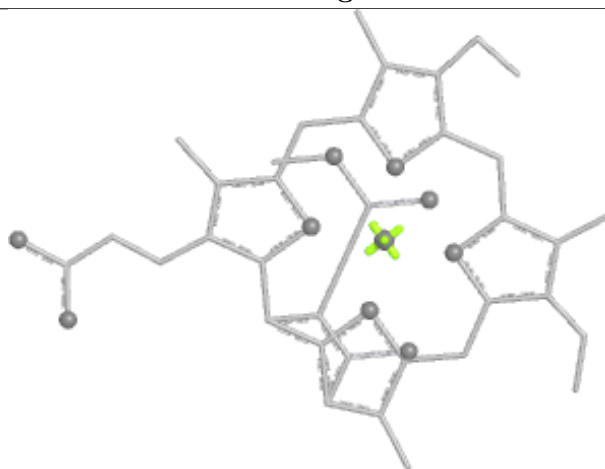
Bond lengths



Bond angles



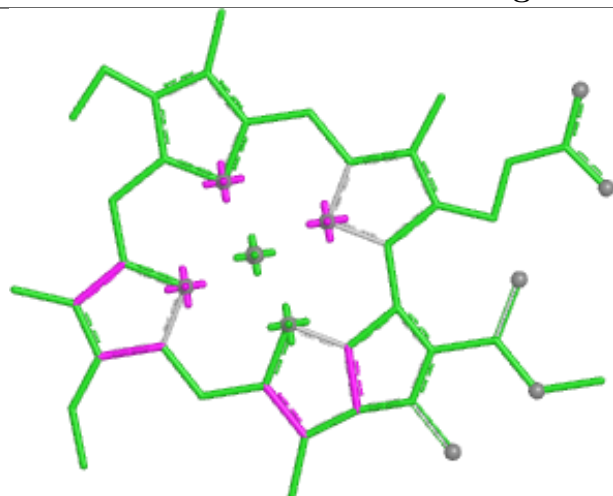
Torsions



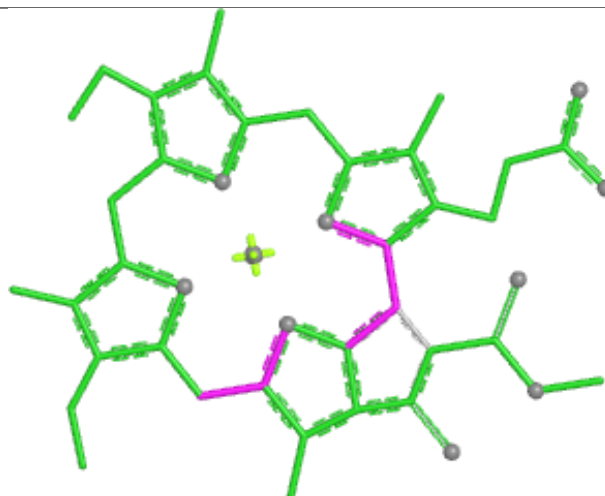
Rings



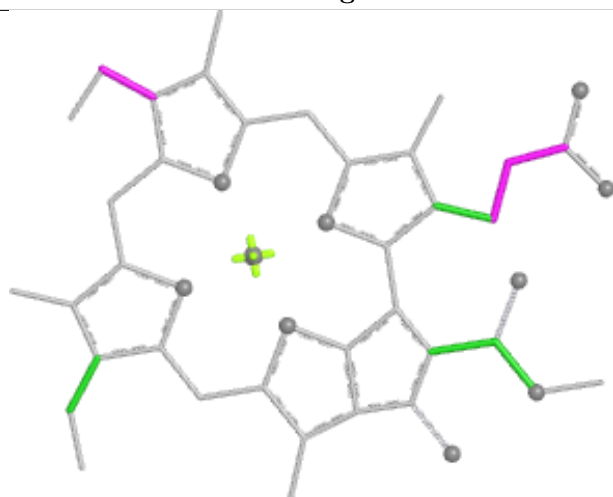
## Ligand CLA G 210



Bond lengths



Bond angles

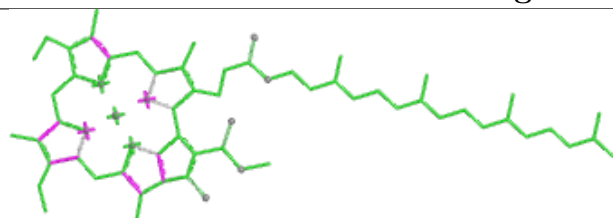


Torsions

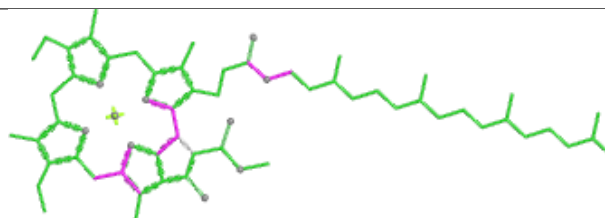


Rings

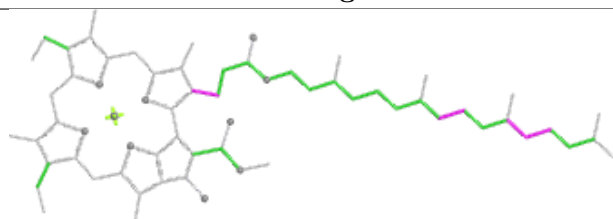
## Ligand CLA B 846



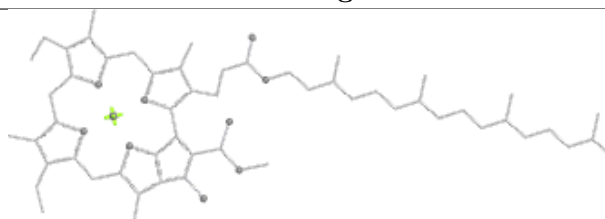
Bond lengths



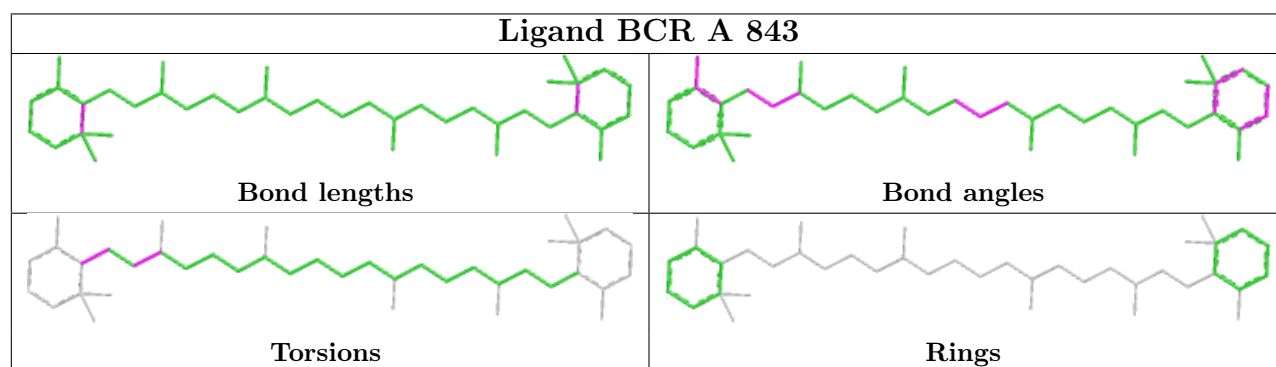
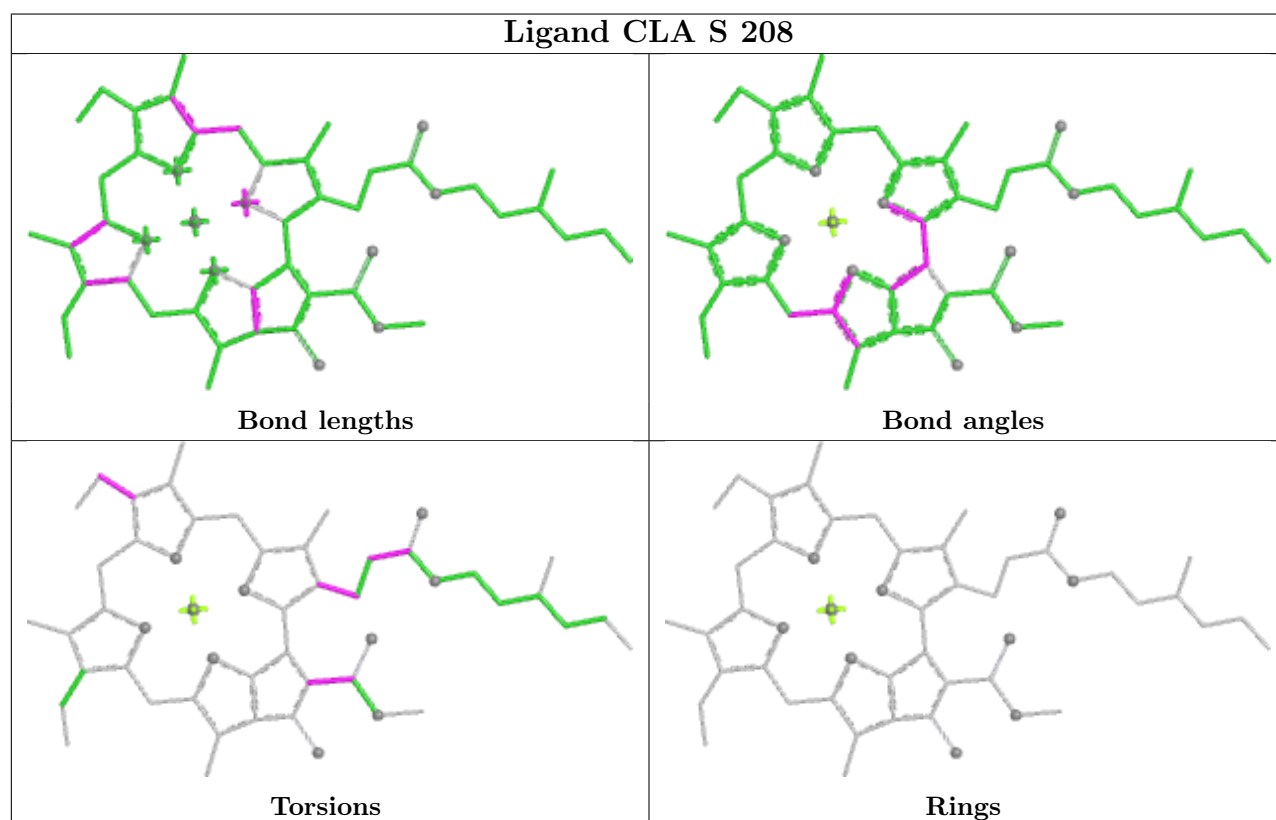
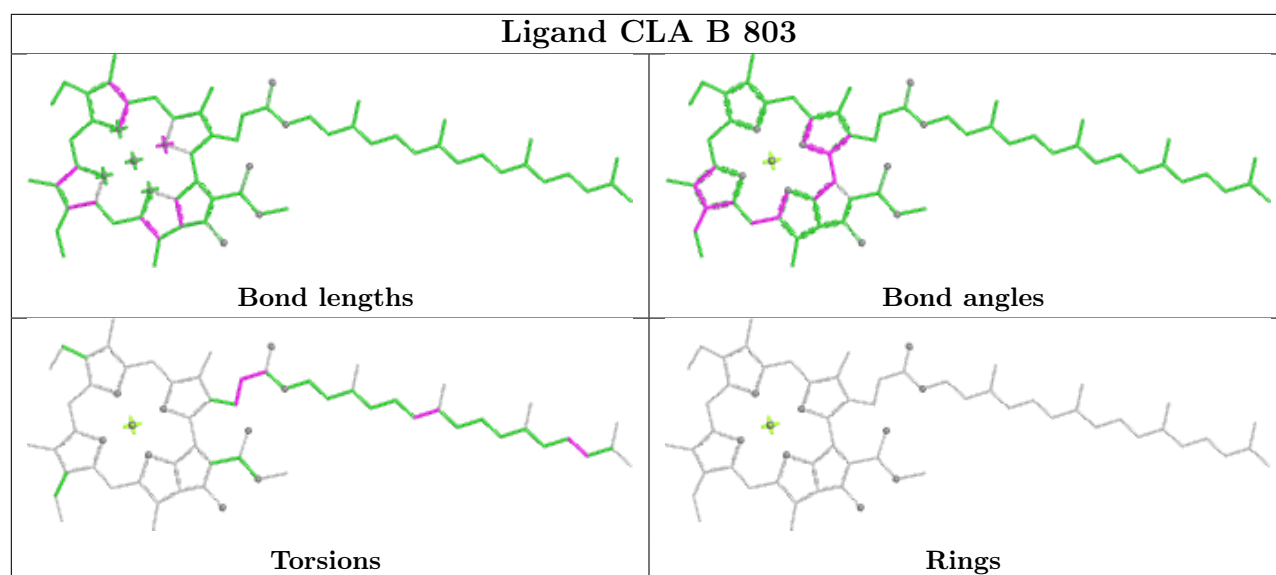
Bond angles

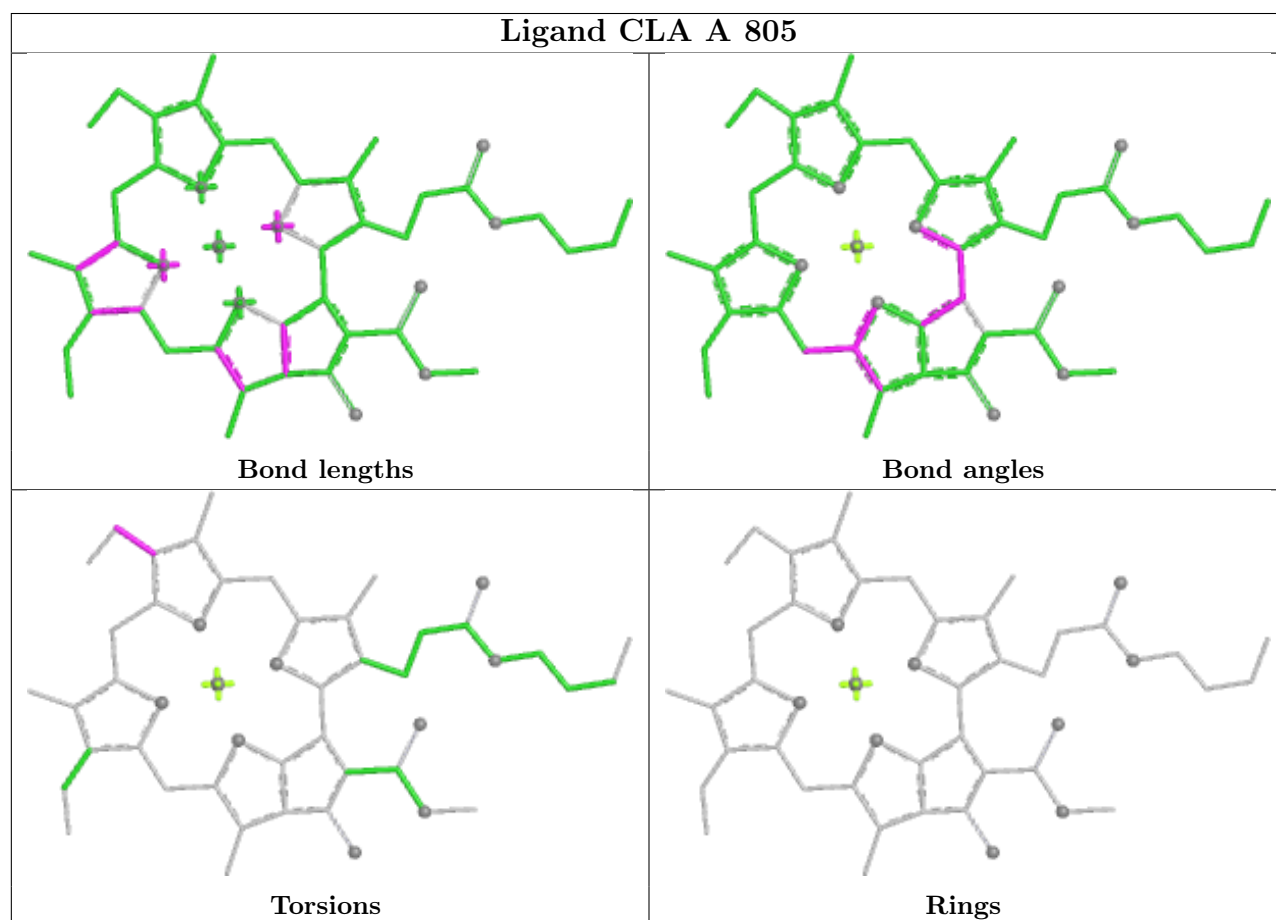
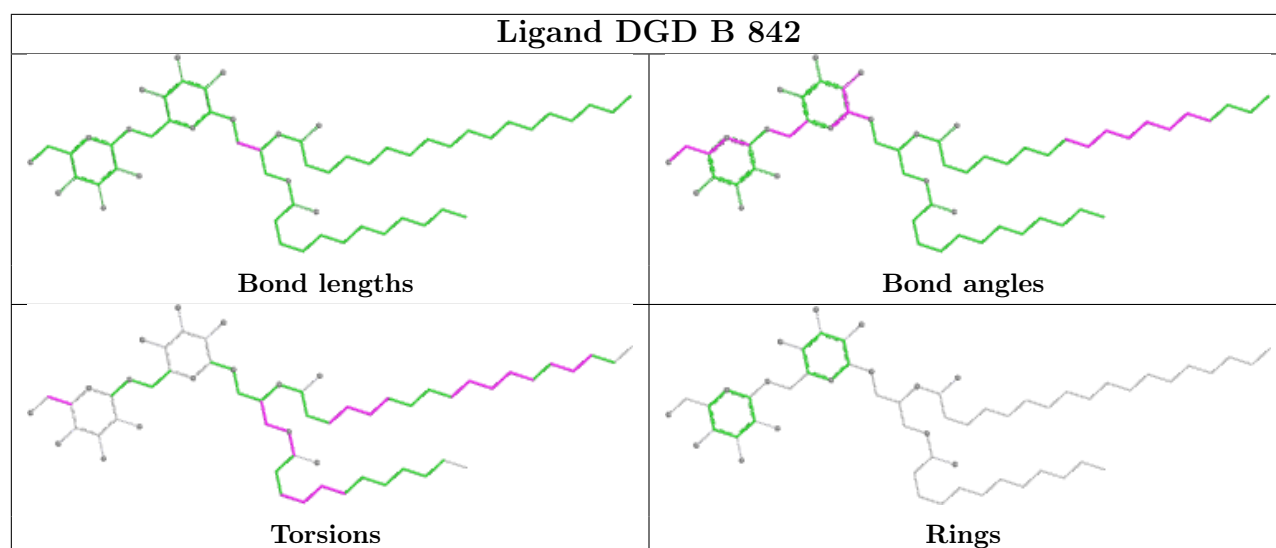


Torsions

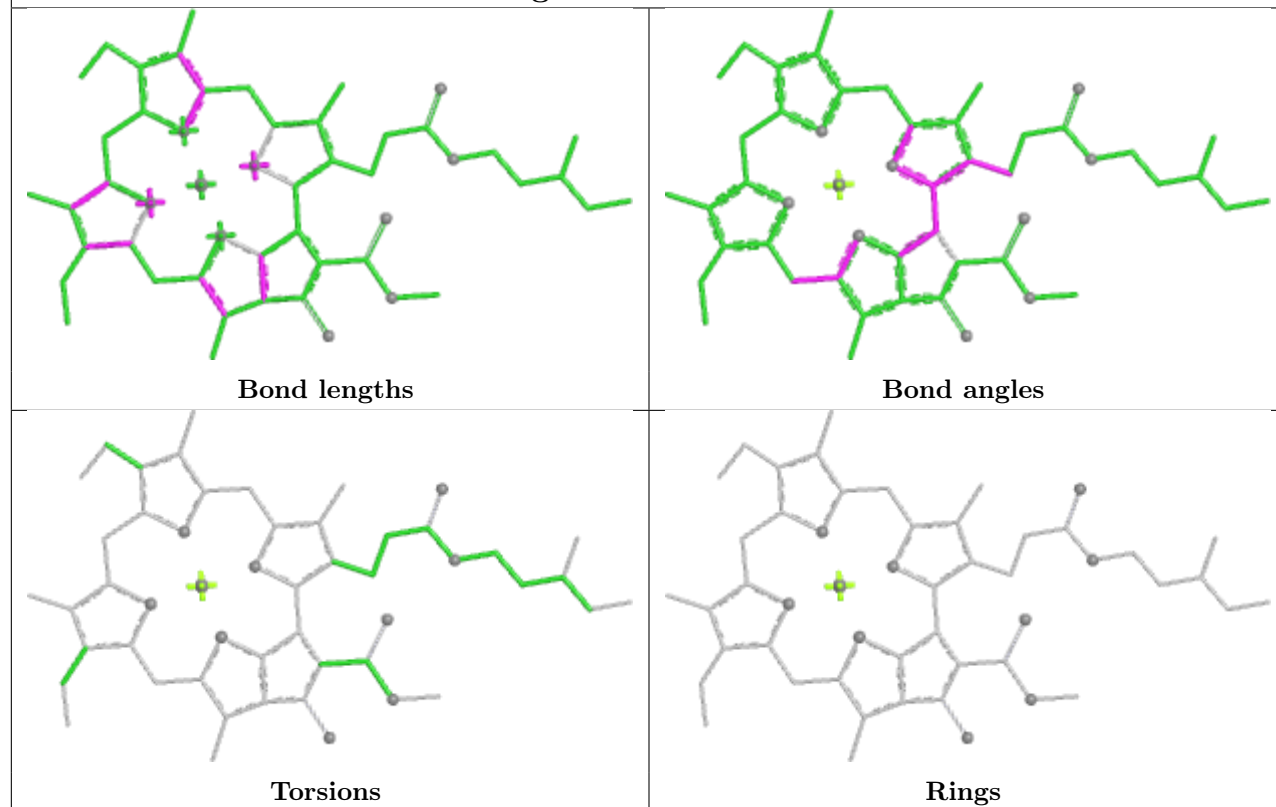


Rings

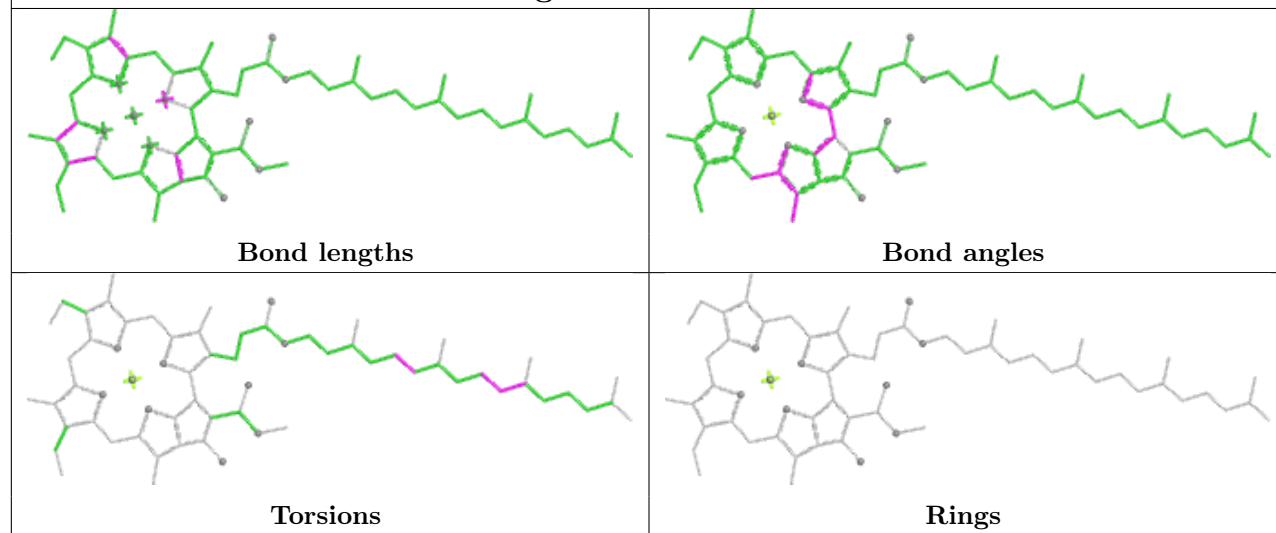


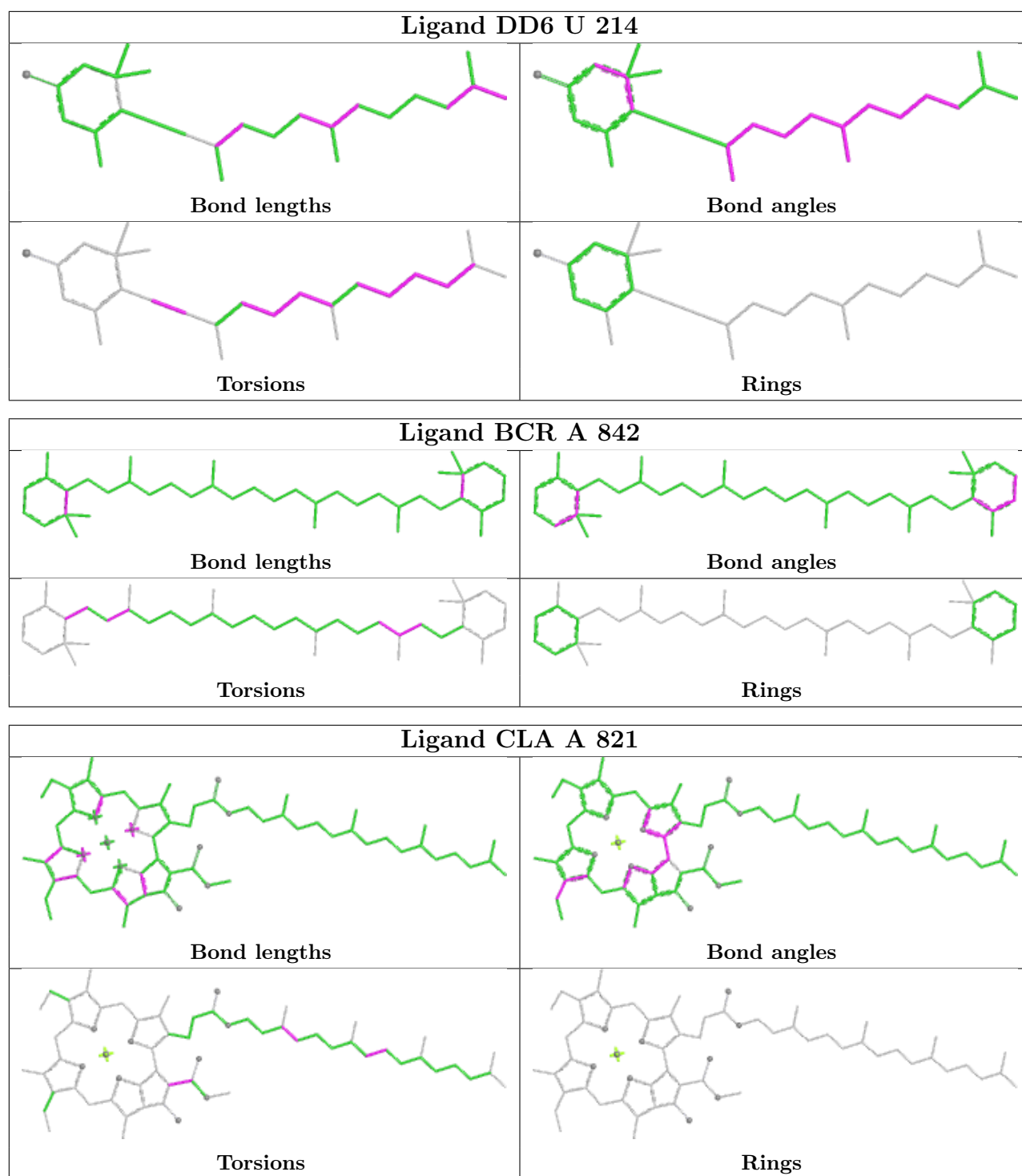


## Ligand CLA A 832

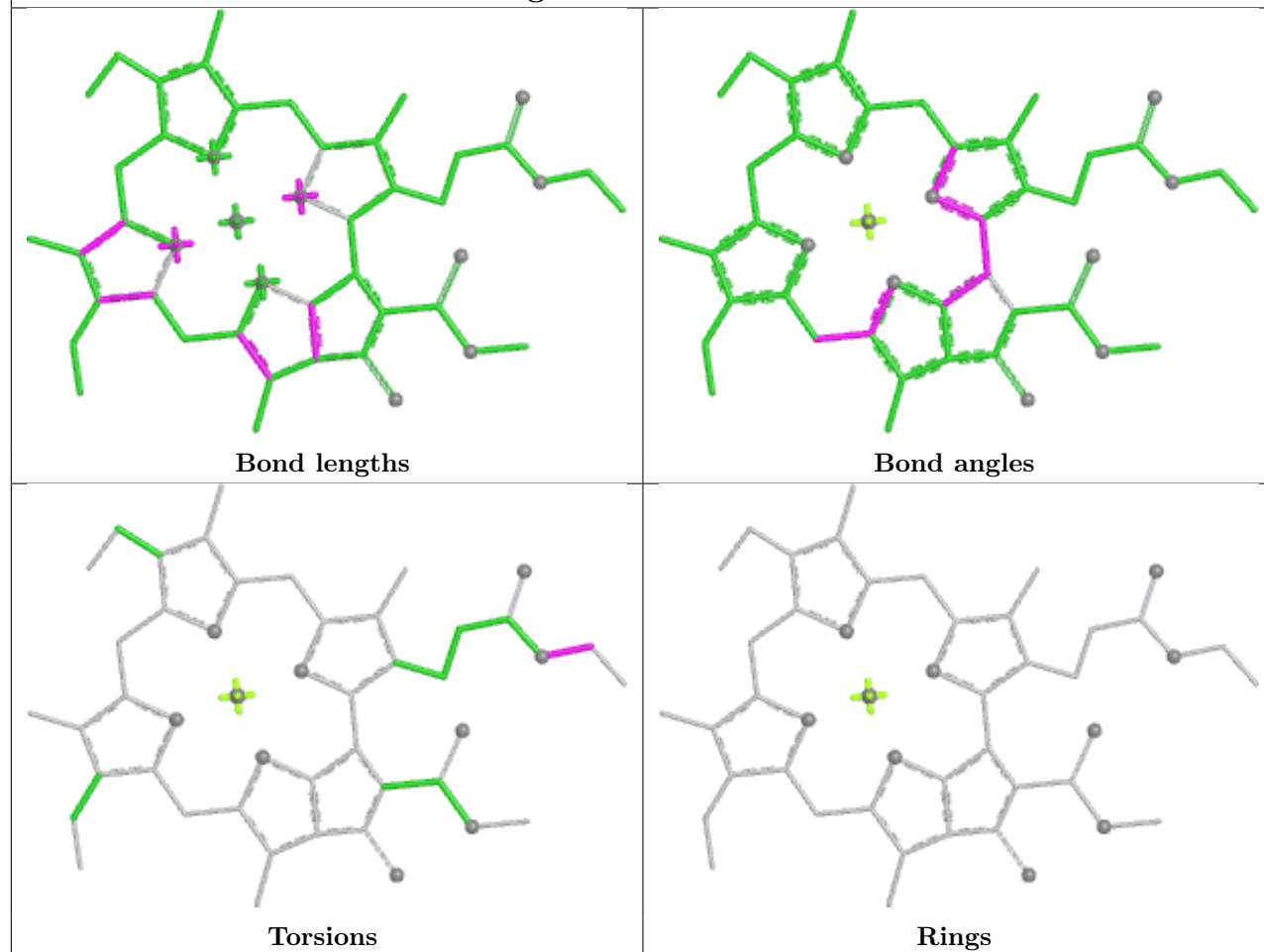


## Ligand CLA S 202

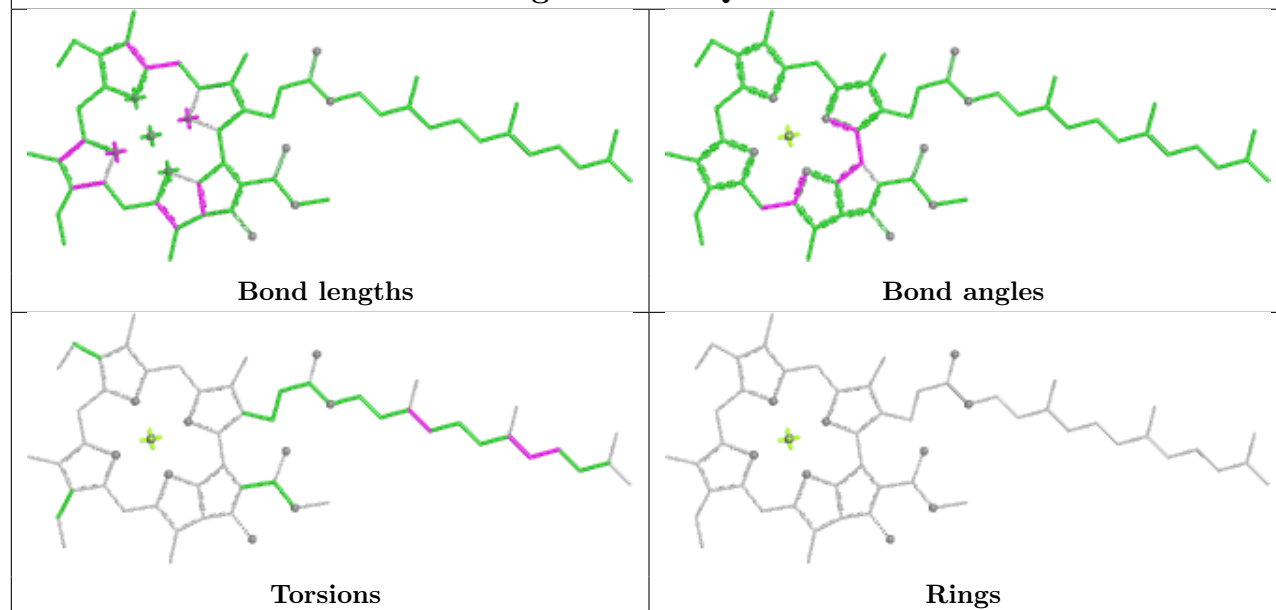


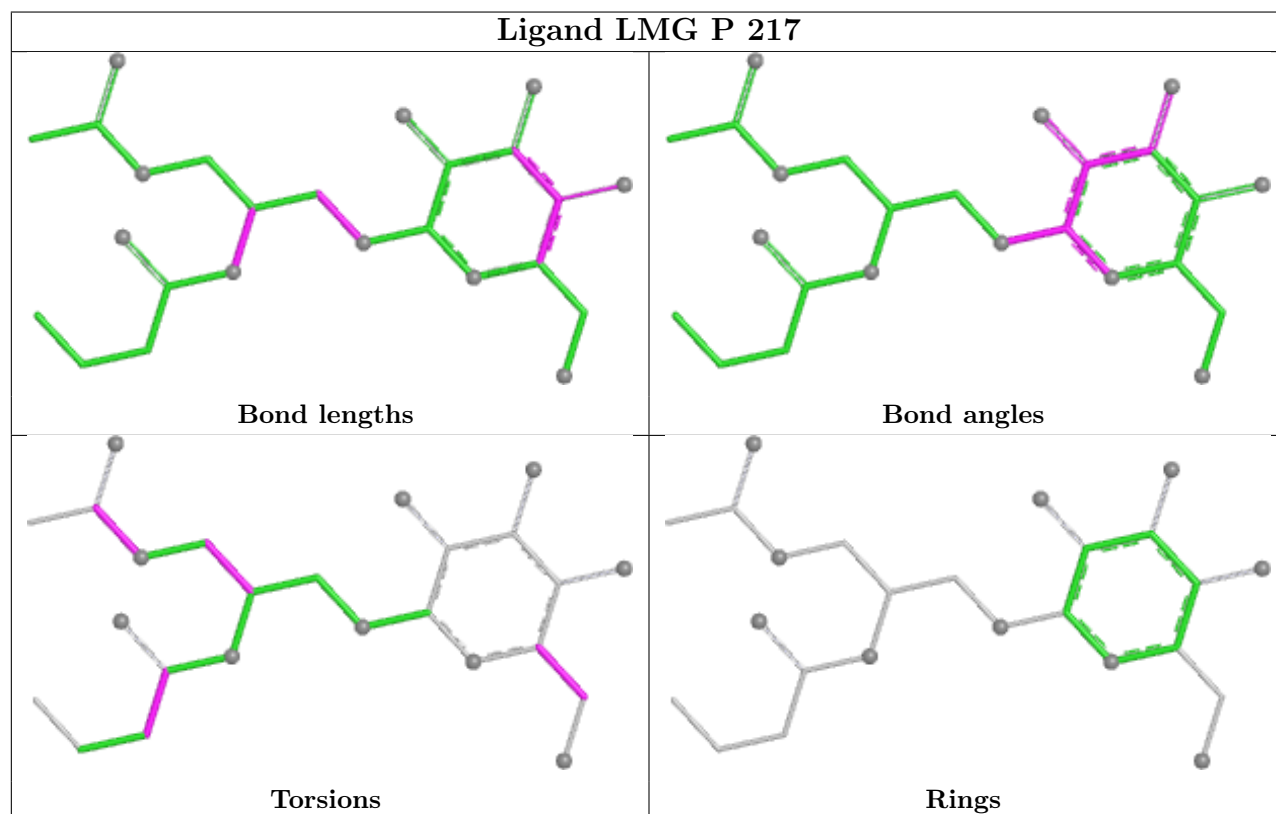
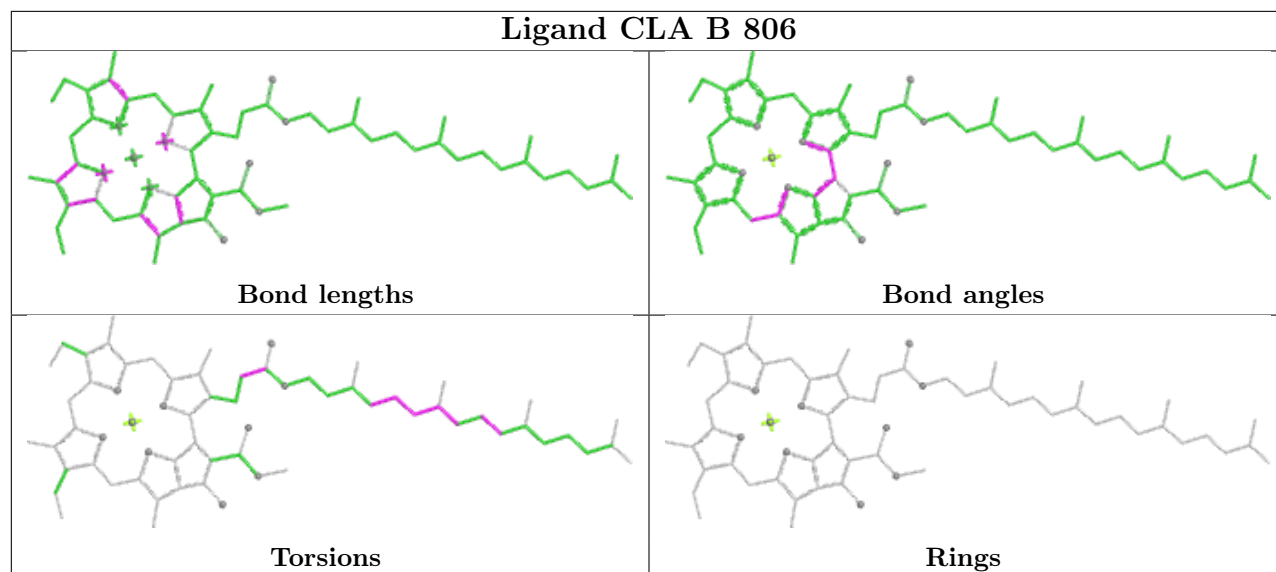


## Ligand CLA B 832

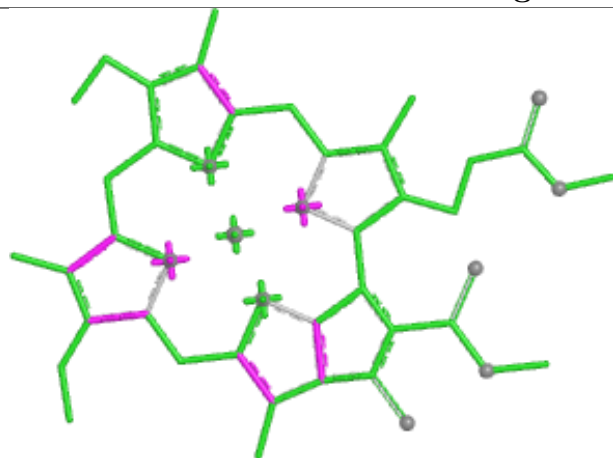


## Ligand CLA Q 205

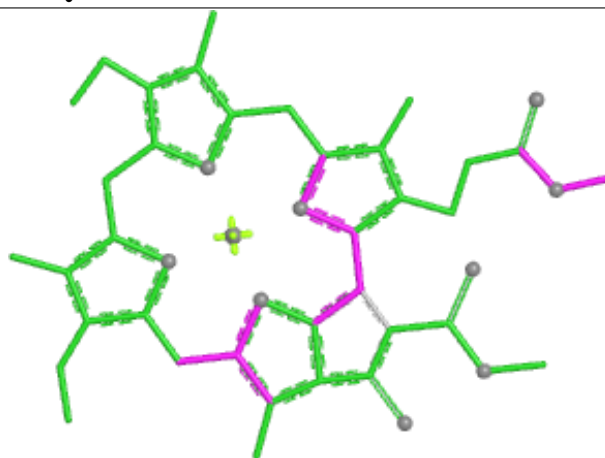




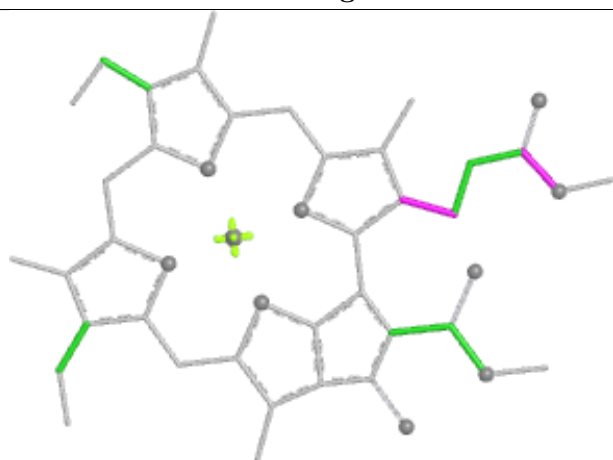
## Ligand CLA Q 207



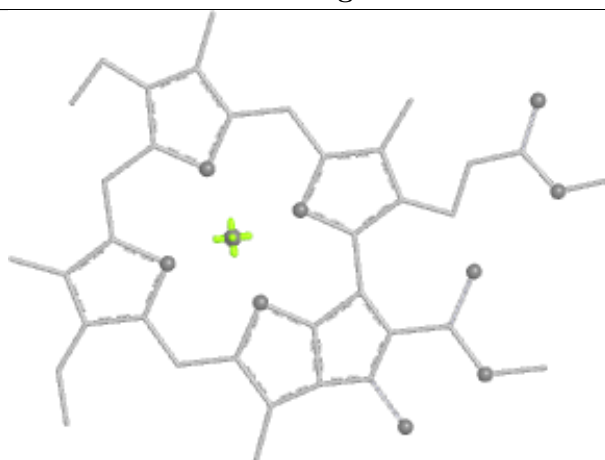
Bond lengths



Bond angles

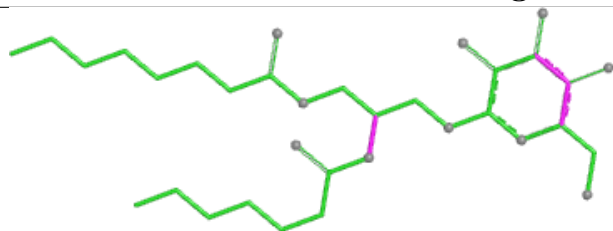


Torsions

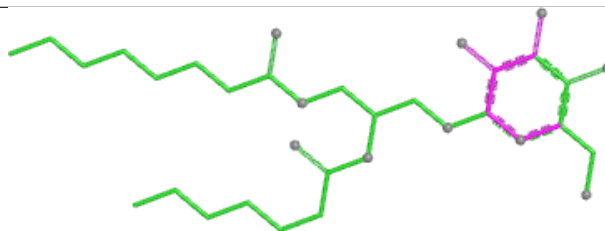


Rings

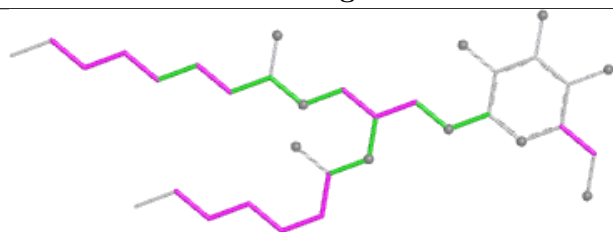
## Ligand LMG P 202



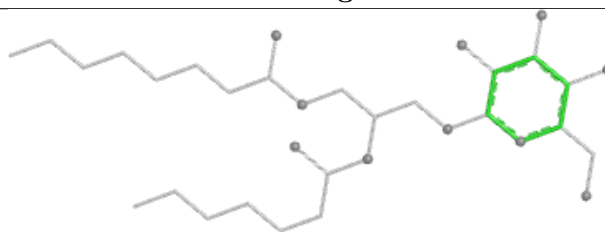
Bond lengths



Bond angles

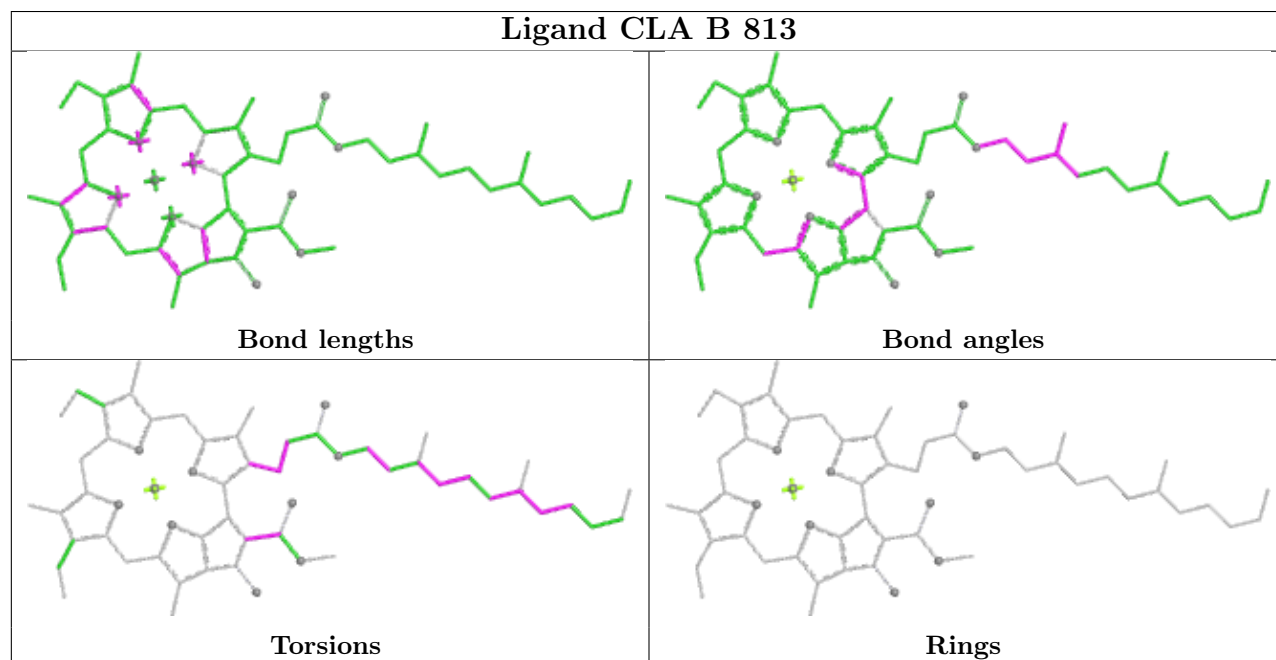
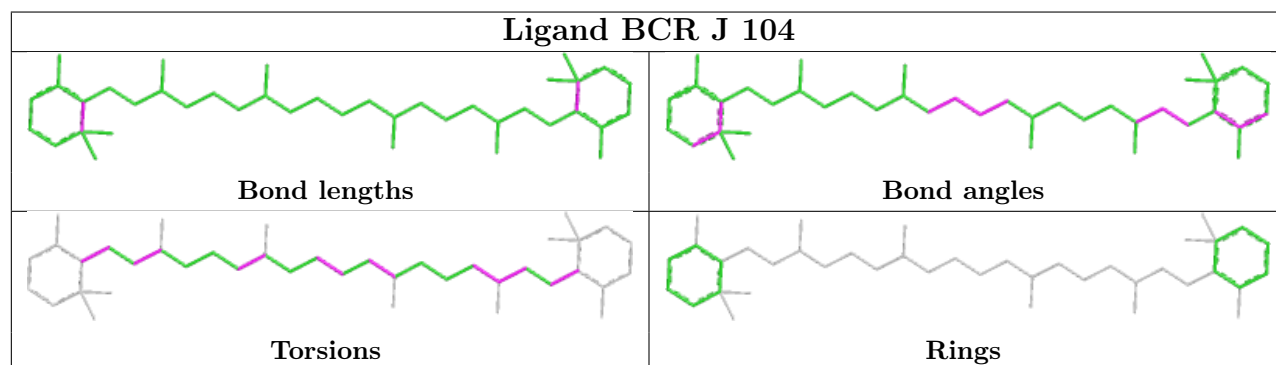
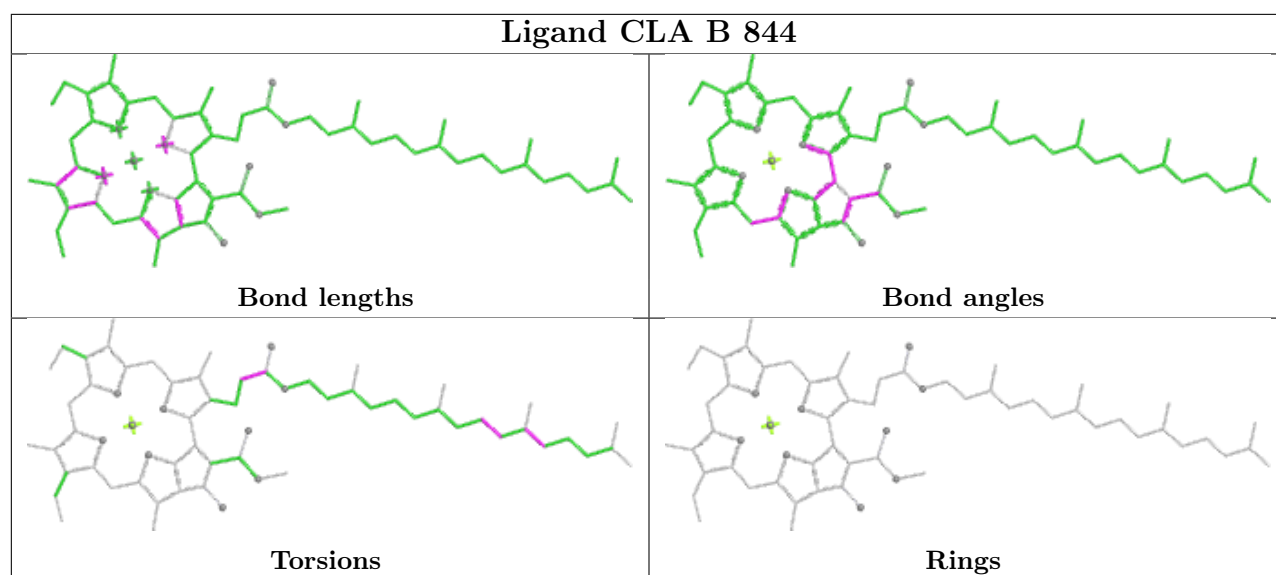


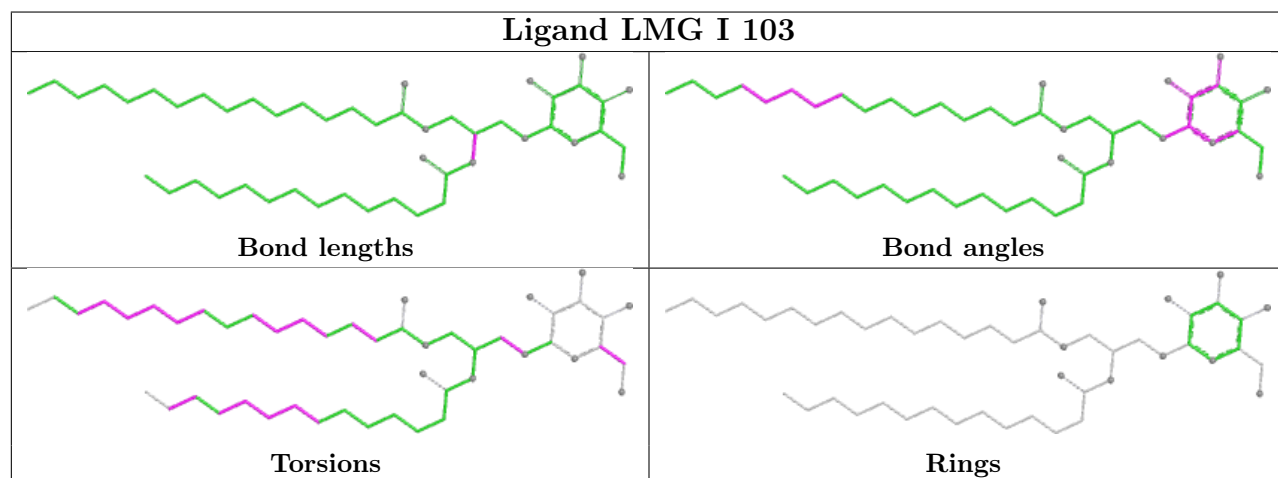
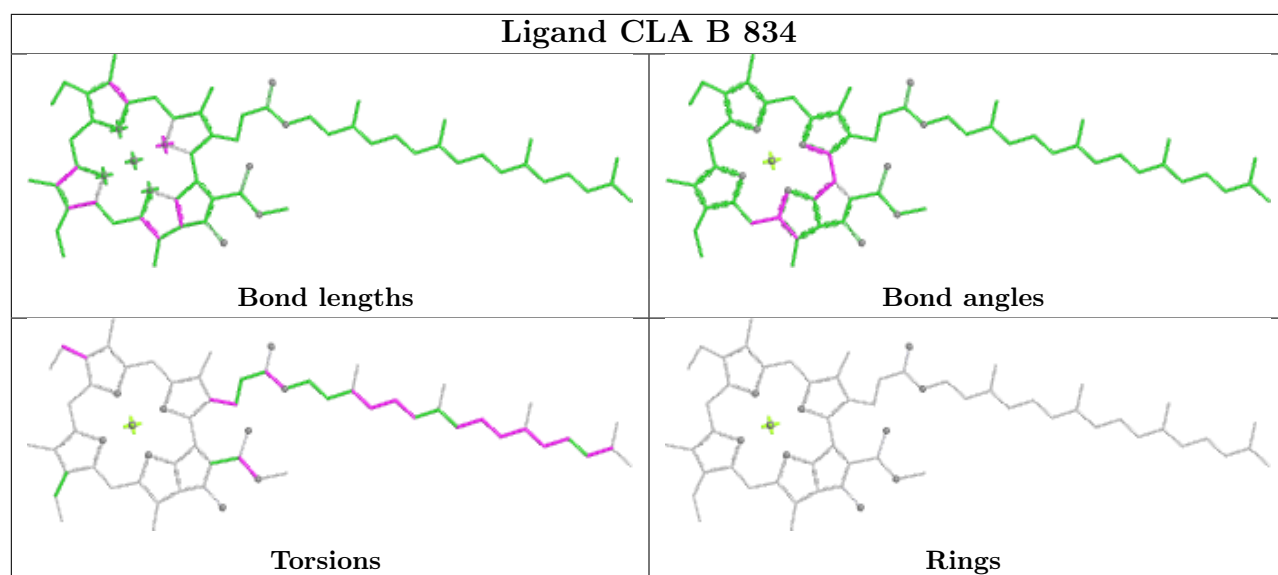
Torsions



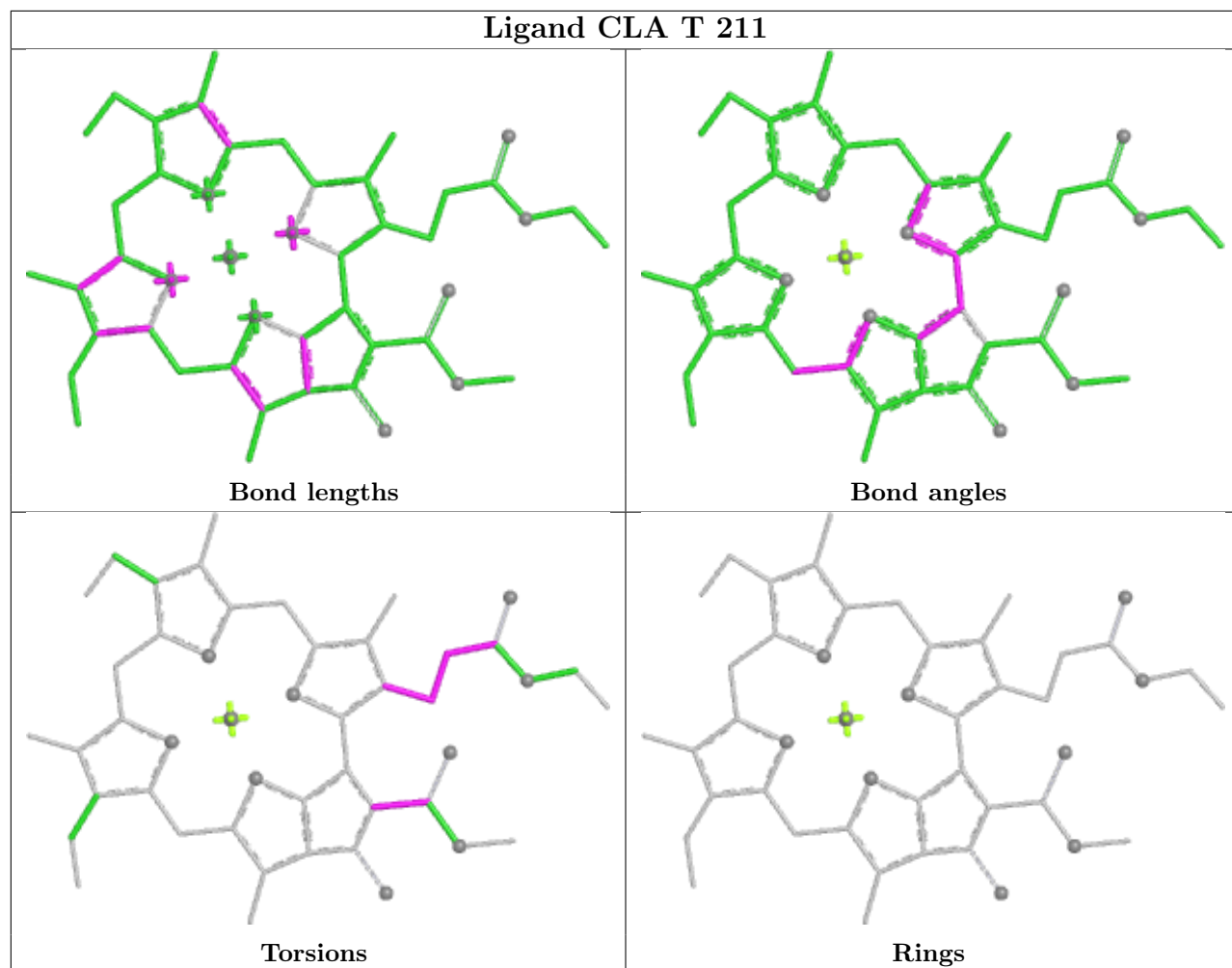
Rings



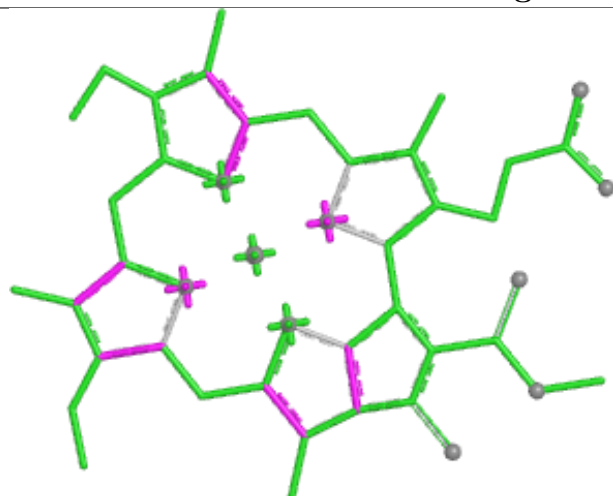




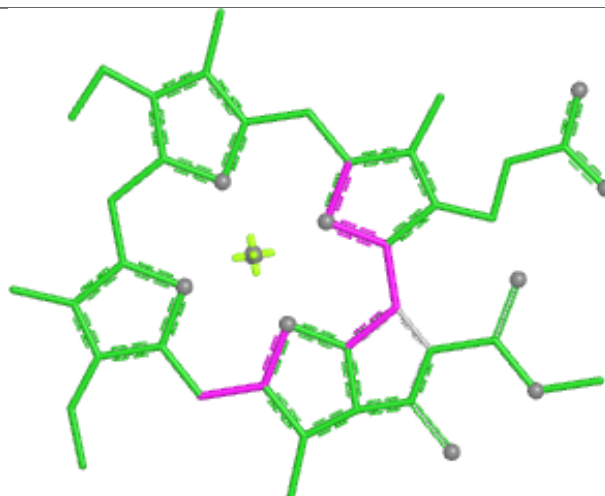
## Ligand CLA T 211



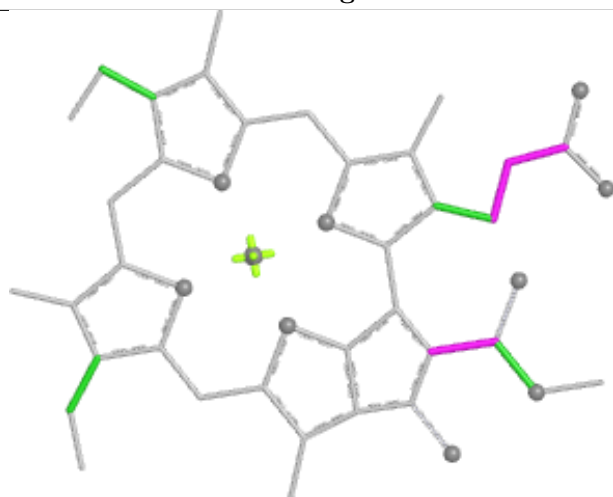
## Ligand CLA B 804



Bond lengths



Bond angles

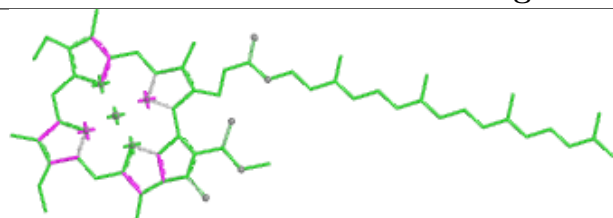


Torsions

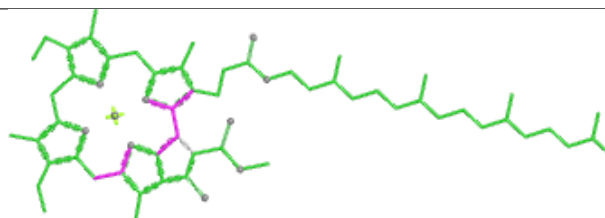


Rings

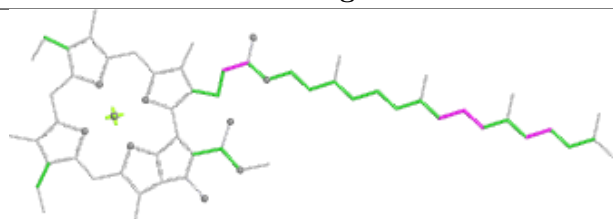
## Ligand CLA A 801



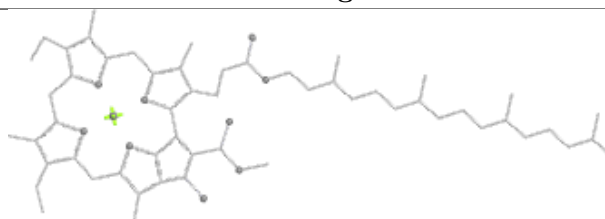
Bond lengths



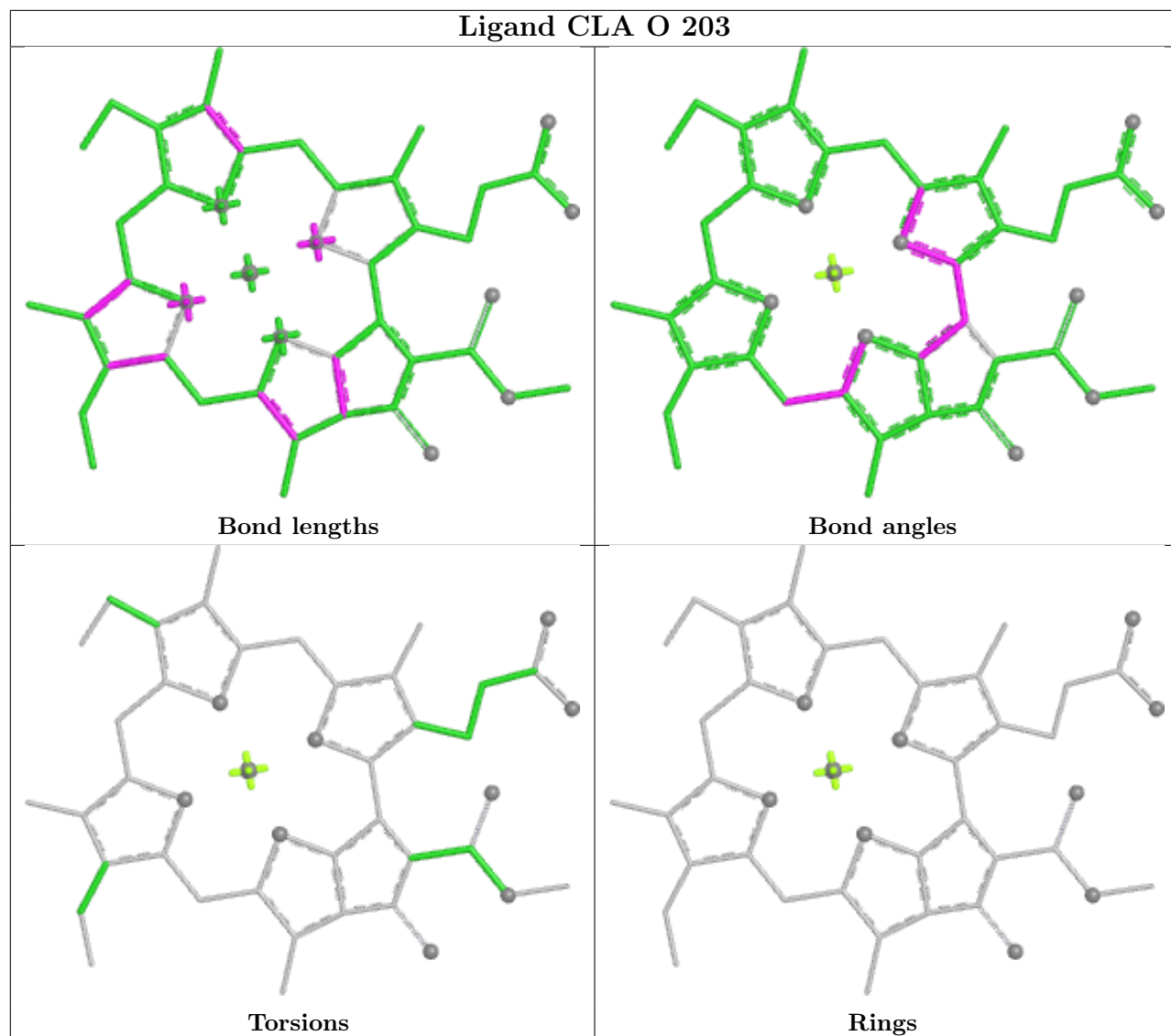
Bond angles

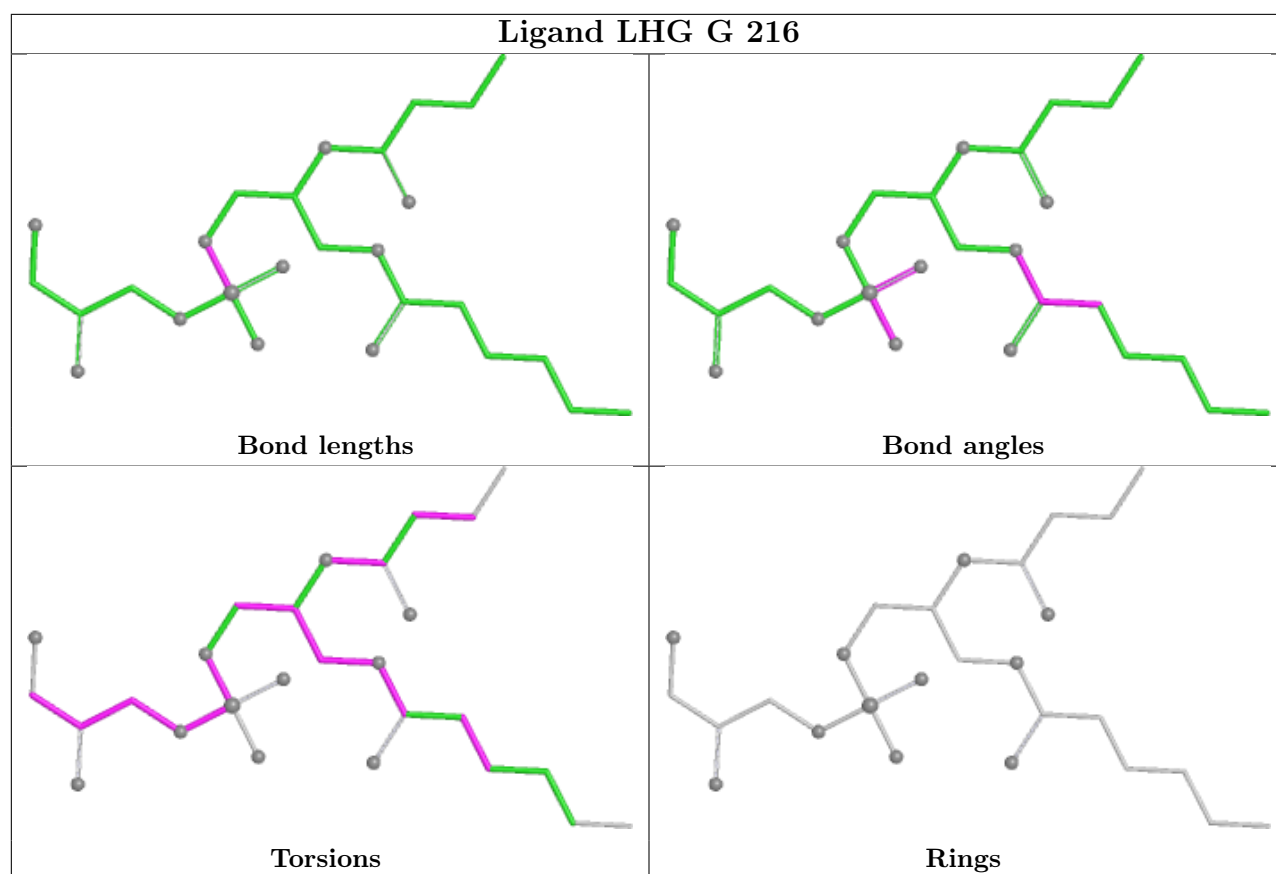


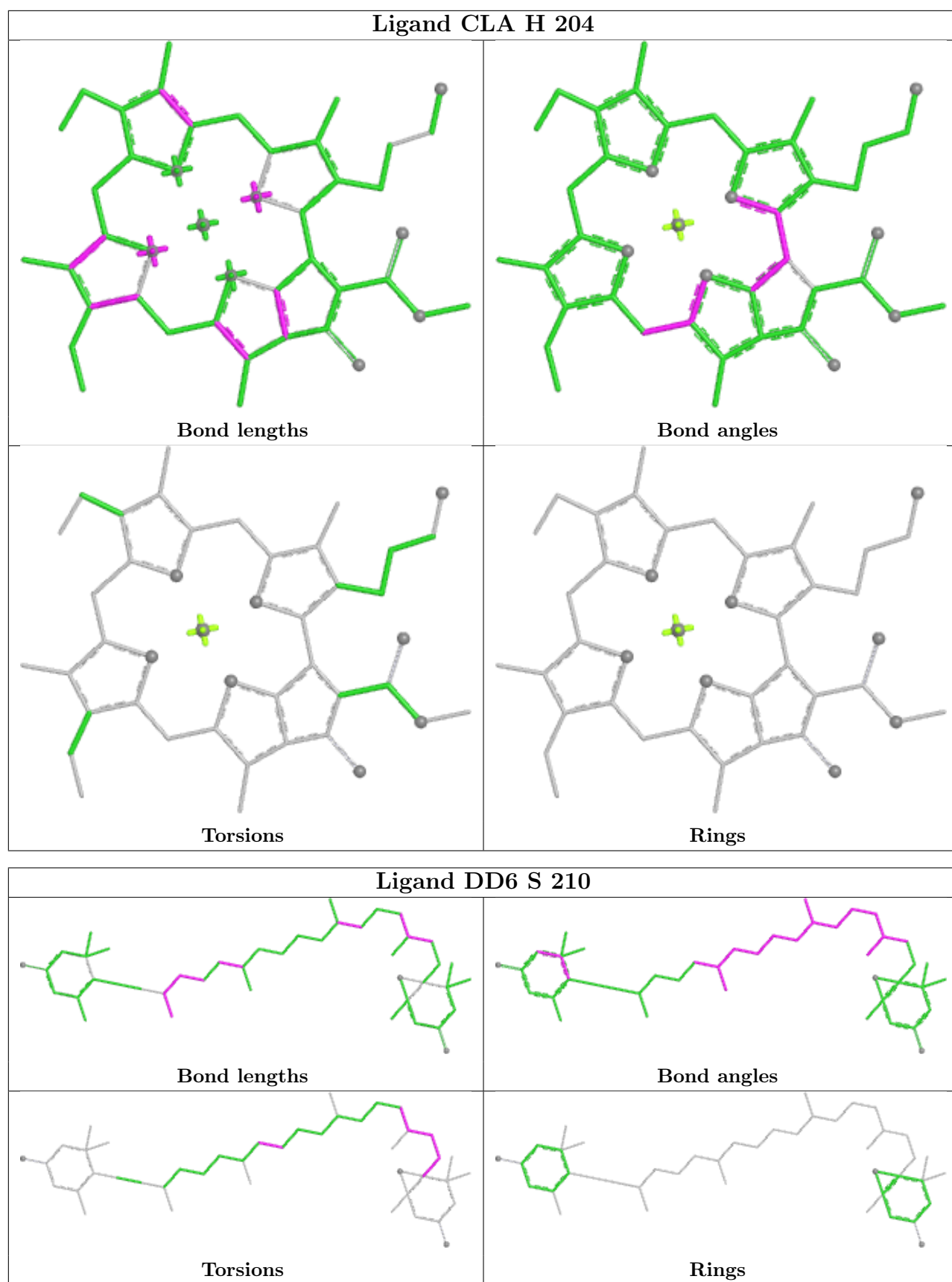
Torsions

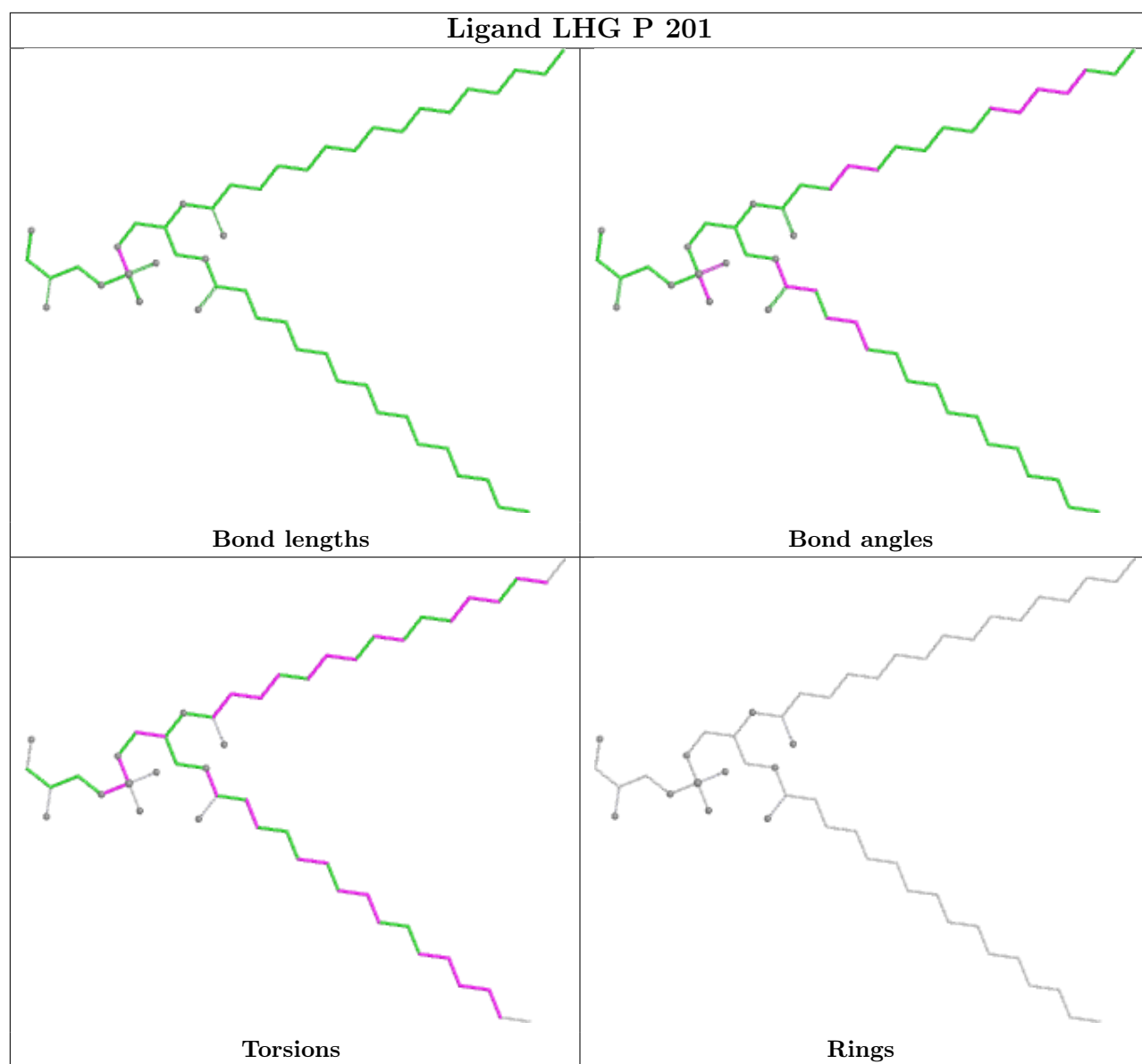


Rings



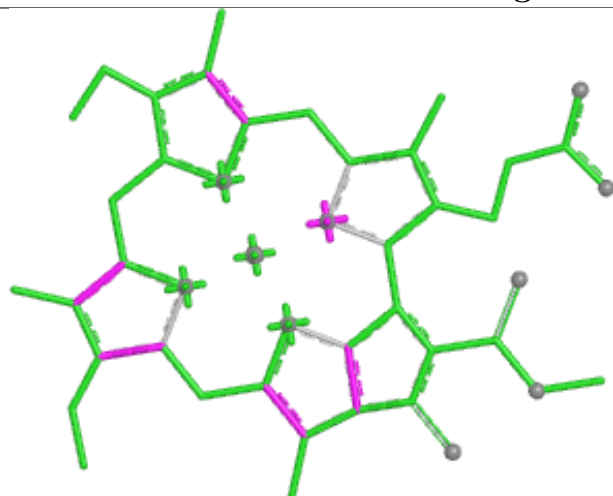




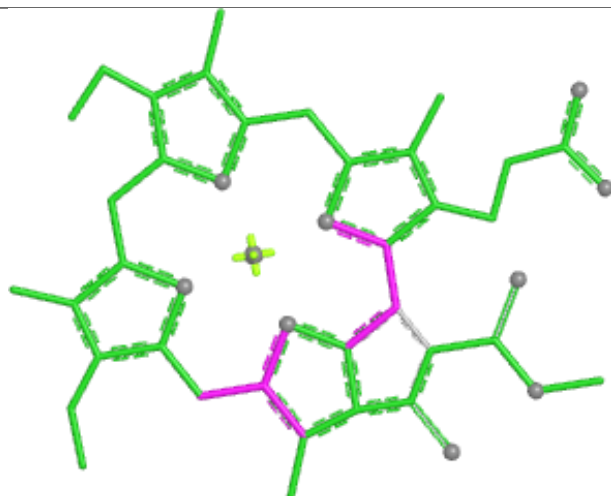




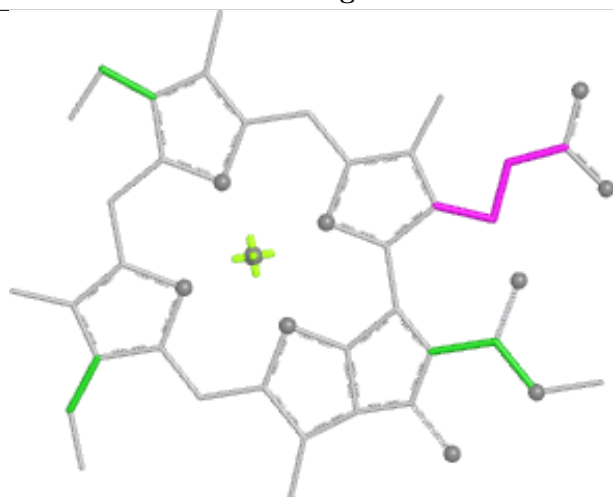
## Ligand CLA A 831



Bond lengths



Bond angles

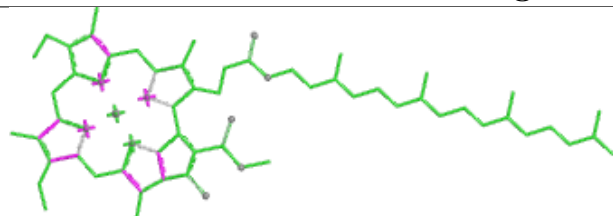


Torsions

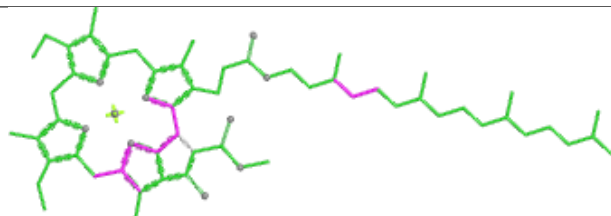


Rings

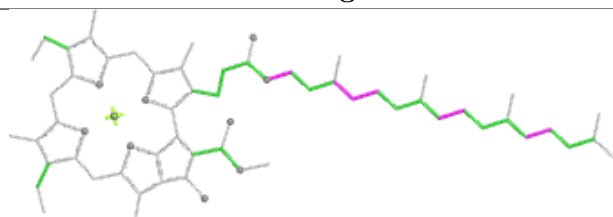
## Ligand CLA A 847



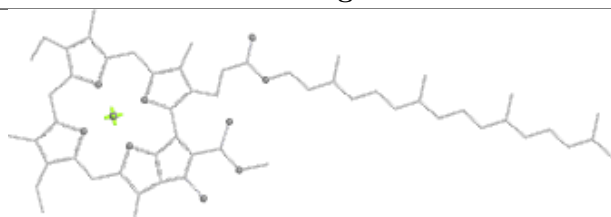
Bond lengths



Bond angles



Torsions



Rings

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

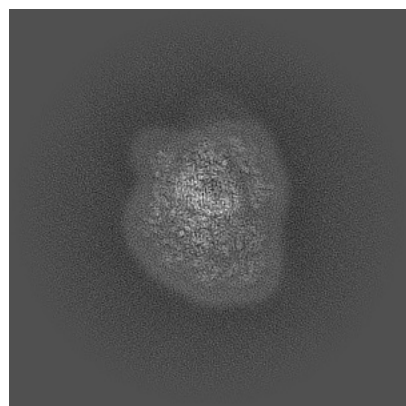
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-64383. These allow visual inspection of the internal detail of the map and identification of artifacts.

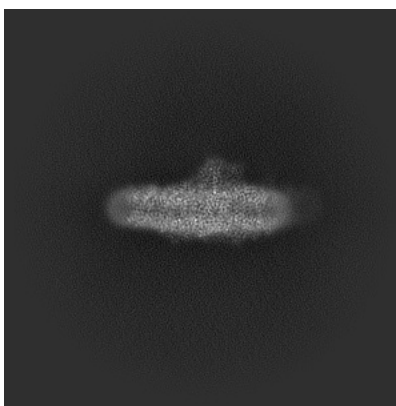
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

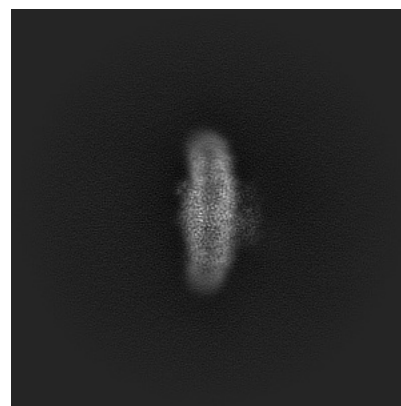
#### 6.1.1 Primary map



X

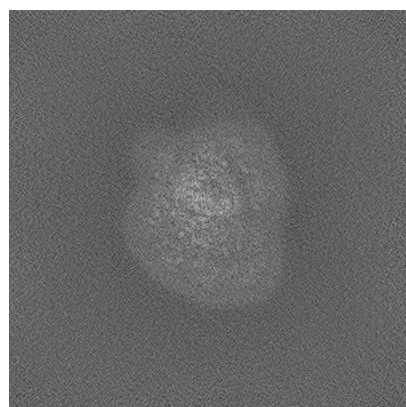


Y

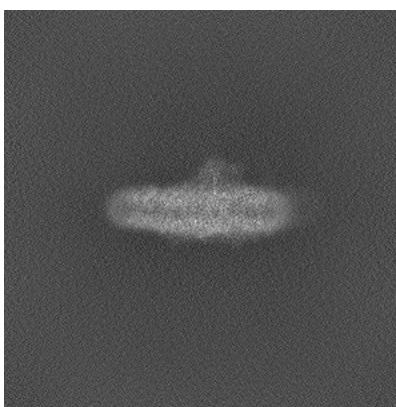


Z

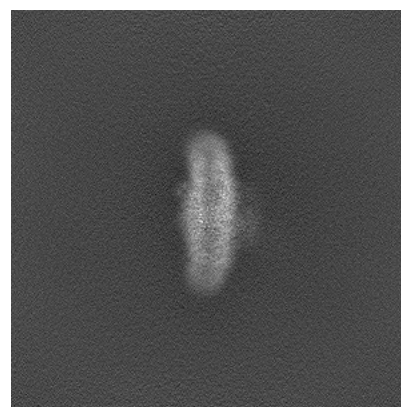
#### 6.1.2 Raw map



X



Y

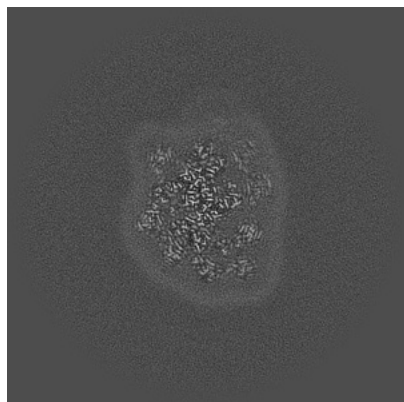


Z

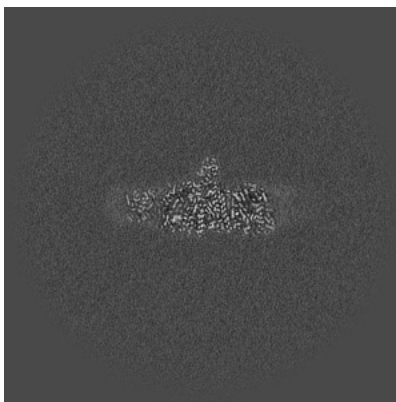
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

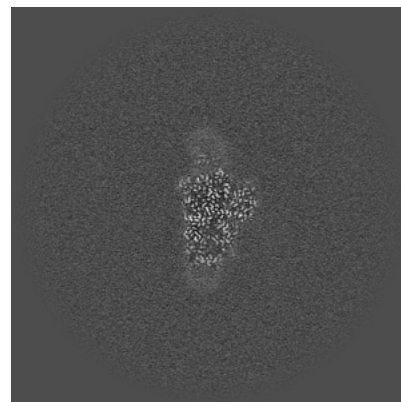
### 6.2.1 Primary map



X Index: 300

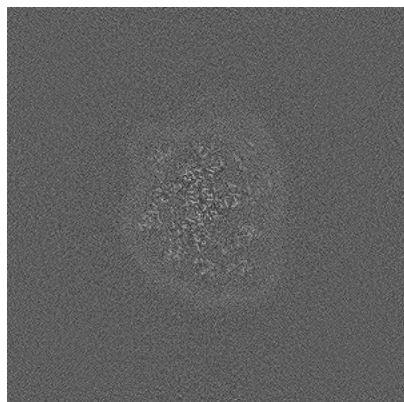


Y Index: 300

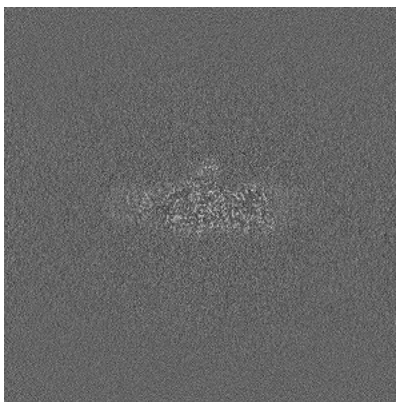


Z Index: 300

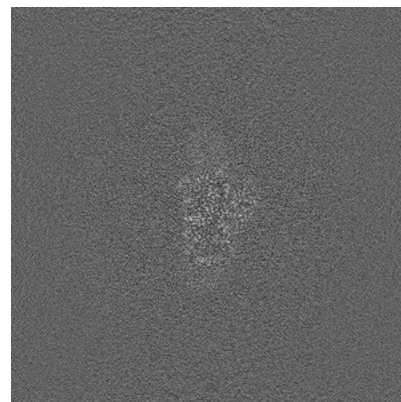
### 6.2.2 Raw map



X Index: 300



Y Index: 300



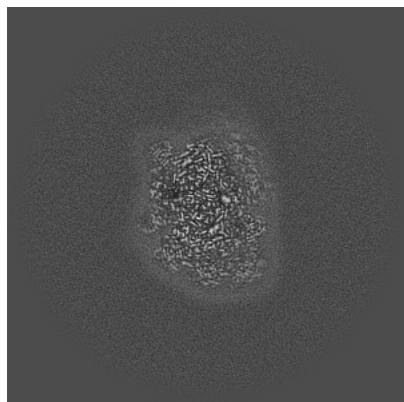
Z Index: 300

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

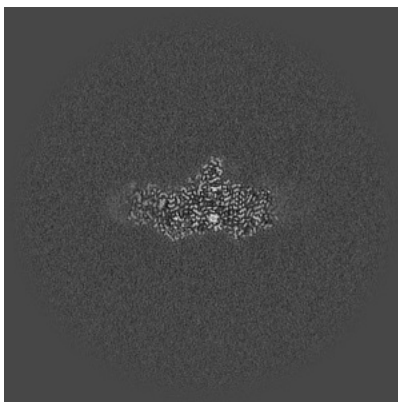


## 6.3 Largest variance slices [i](#)

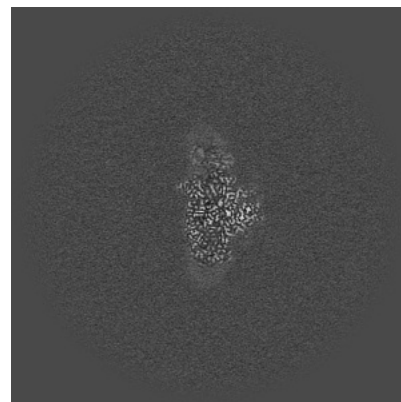
### 6.3.1 Primary map



X Index: 315

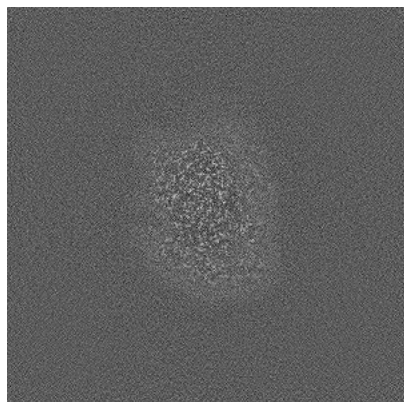


Y Index: 288

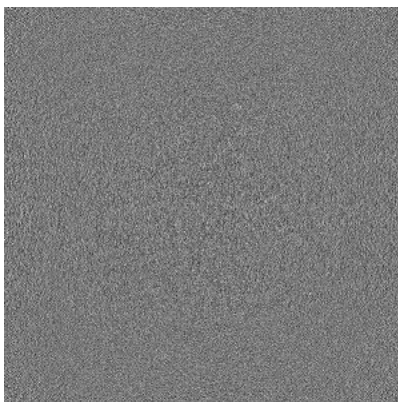


Z Index: 315

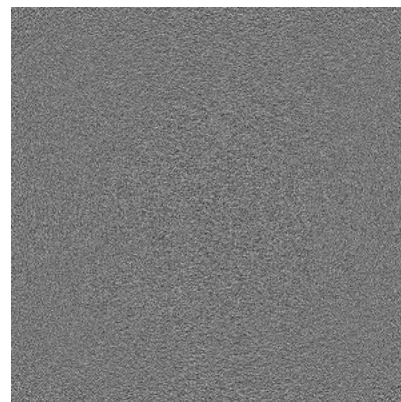
### 6.3.2 Raw map



X Index: 318



Y Index: 0

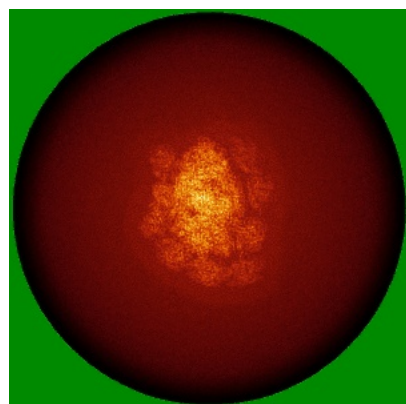


Z Index: 0

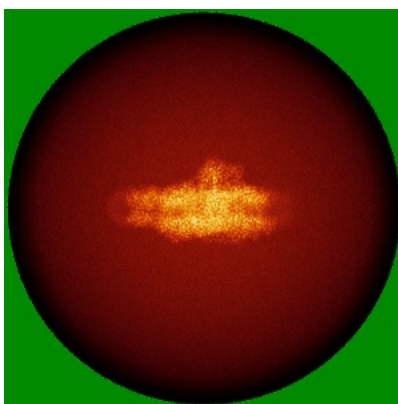
The images above show the largest variance slices of the map in three orthogonal directions.

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

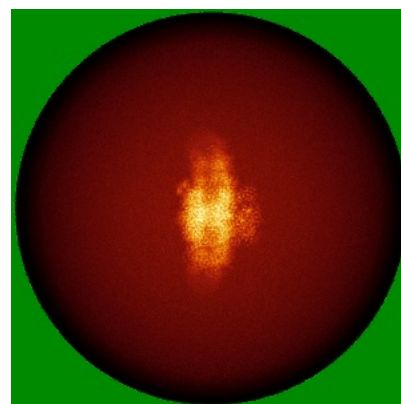
### 6.4.1 Primary map



X

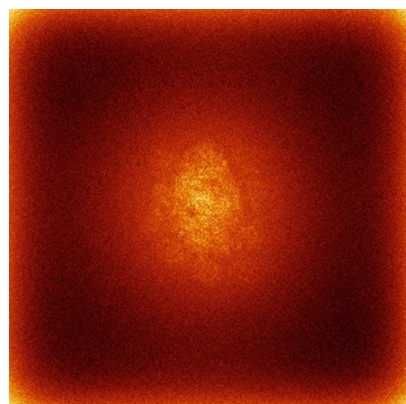


Y

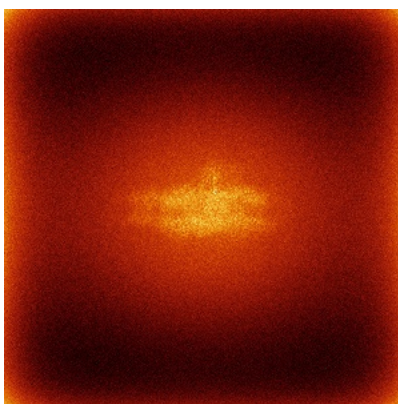


Z

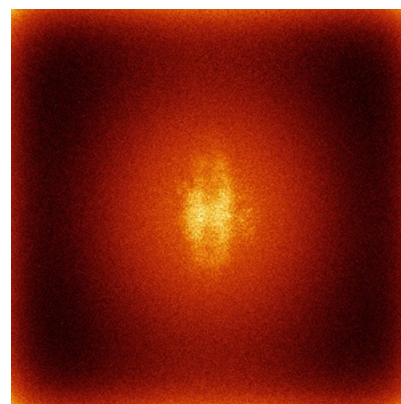
### 6.4.2 Raw map



X



Y

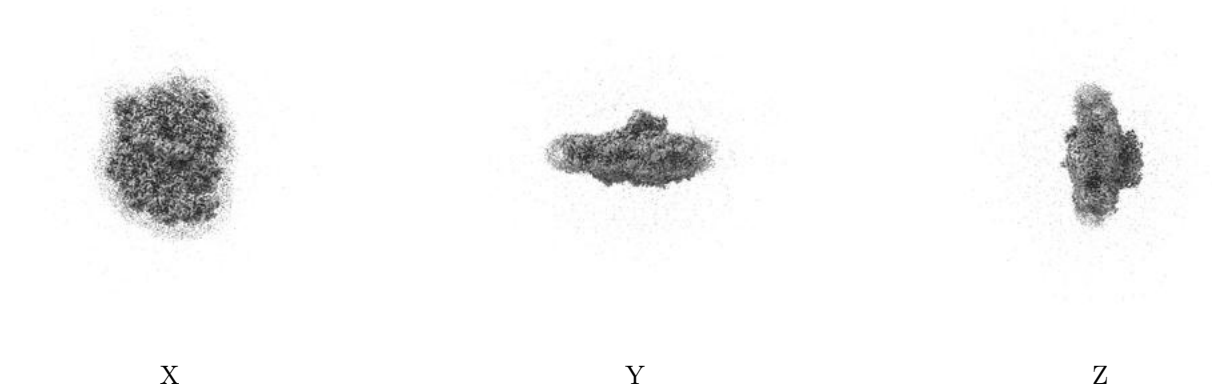


Z

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

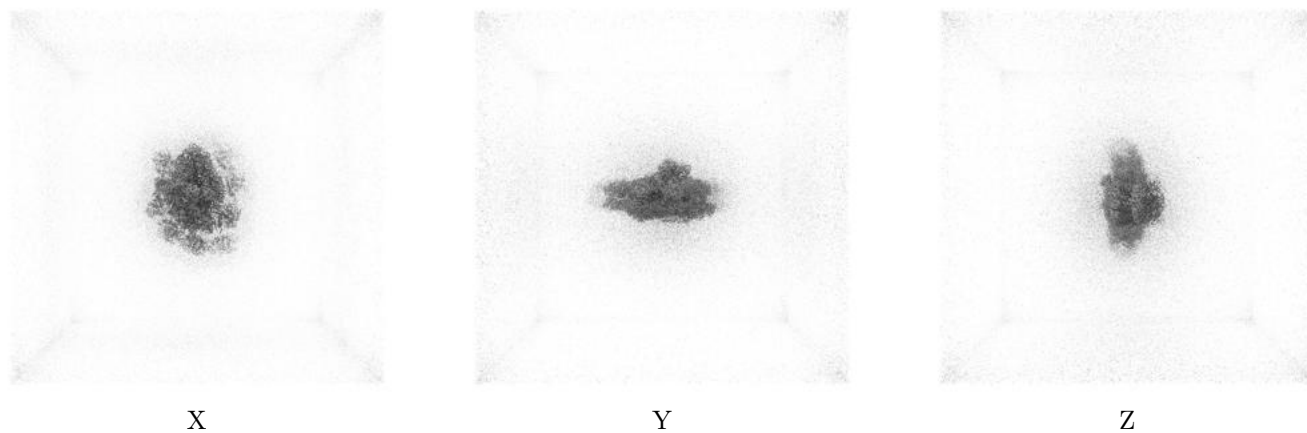
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.07. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



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

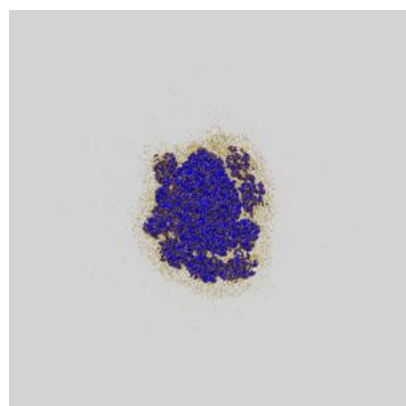
## 6.6 Mask visualisation [i](#)

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

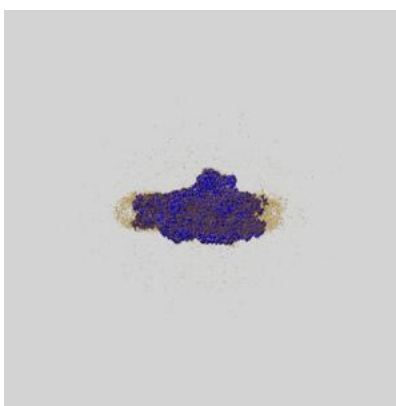
A mask typically either:

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

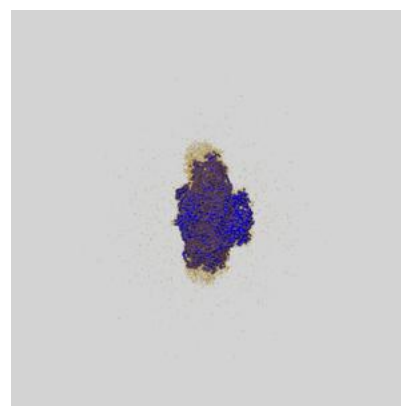
### 6.6.1 emd\_64383\_msk\_1.map [i](#)



X



Y



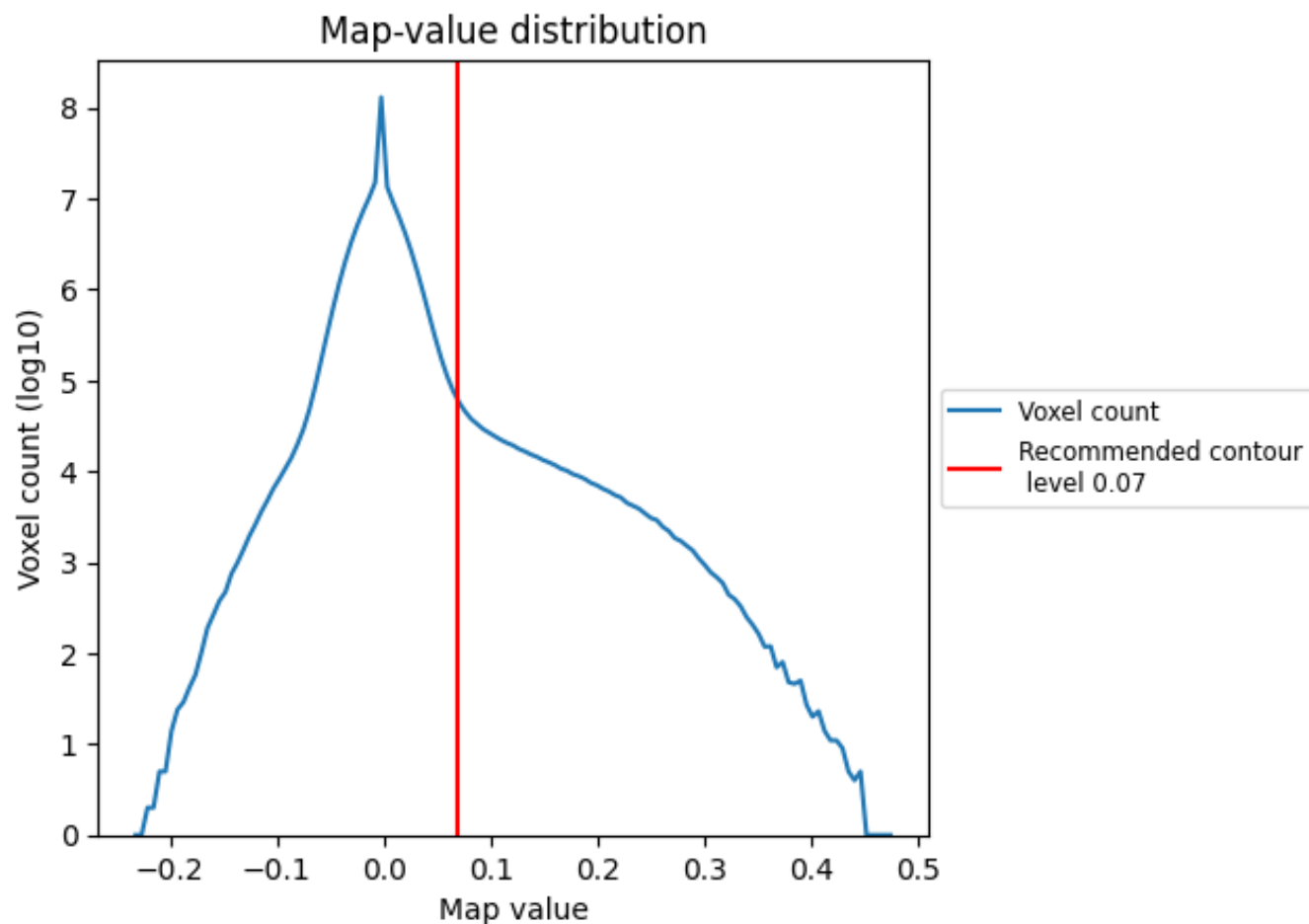
Z



## 7 Map analysis [i](#)

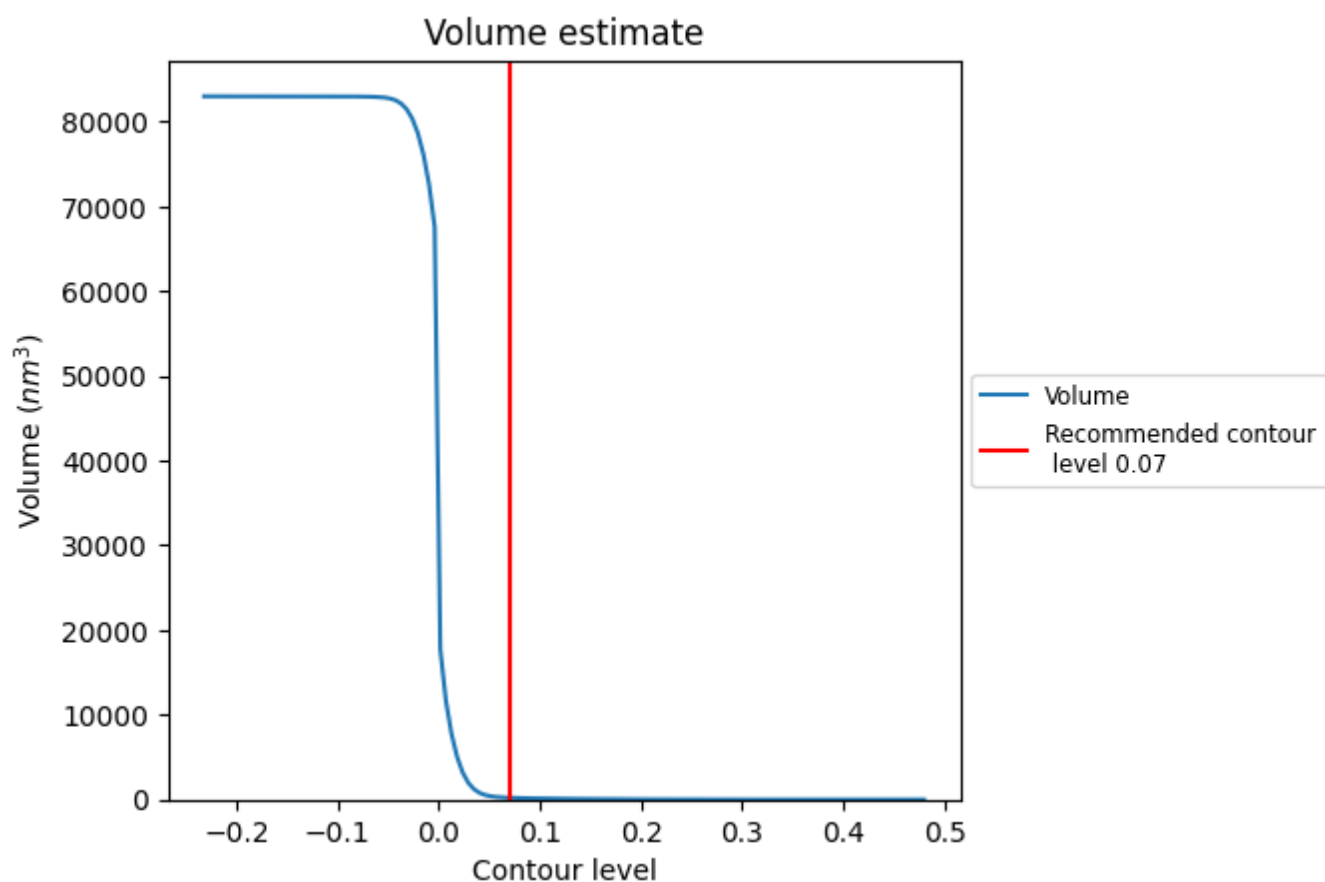
This section contains the results of statistical analysis of the map.

### 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.

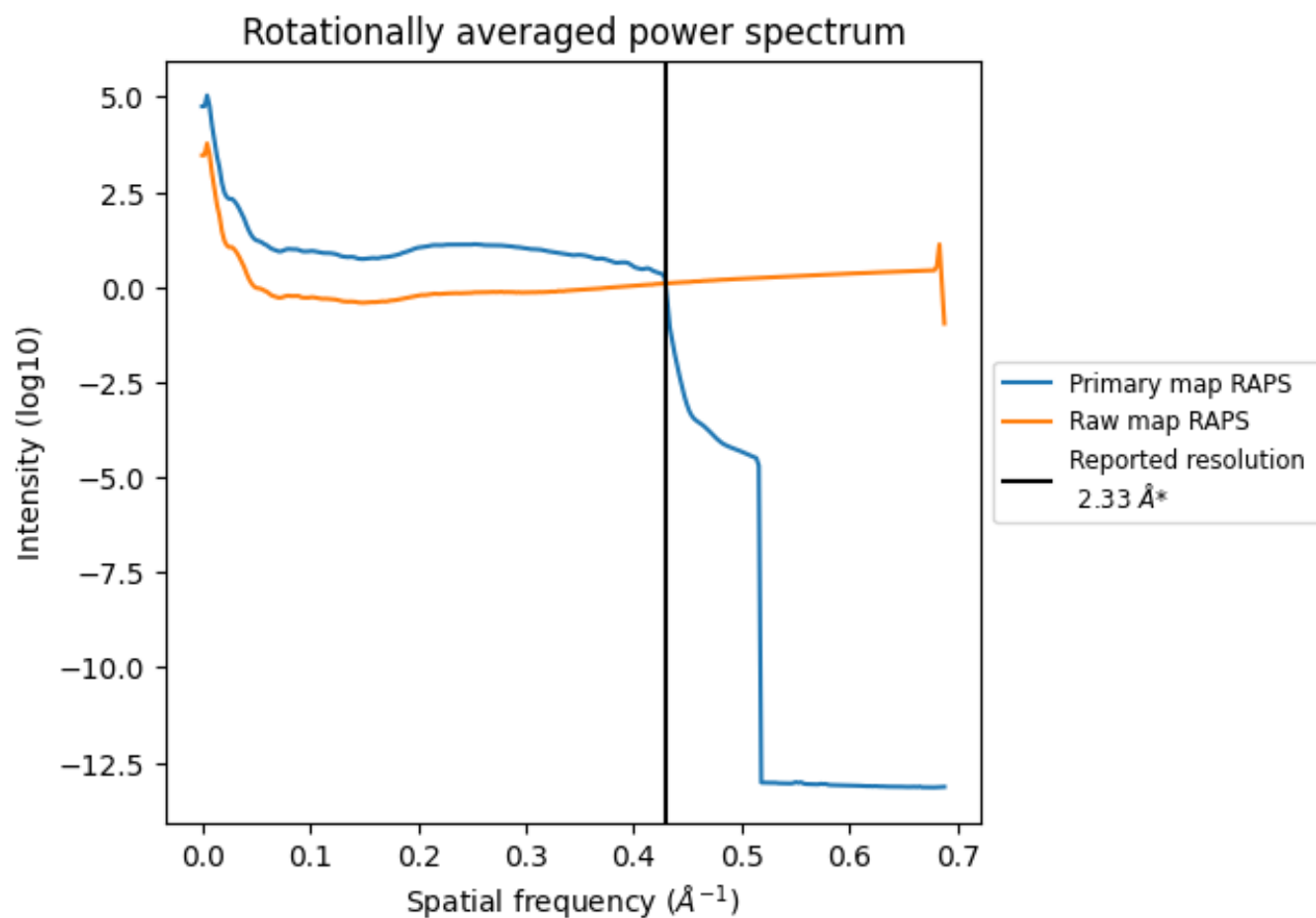
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 212 nm<sup>3</sup>; this corresponds to an approximate mass of 192 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 ⓘ

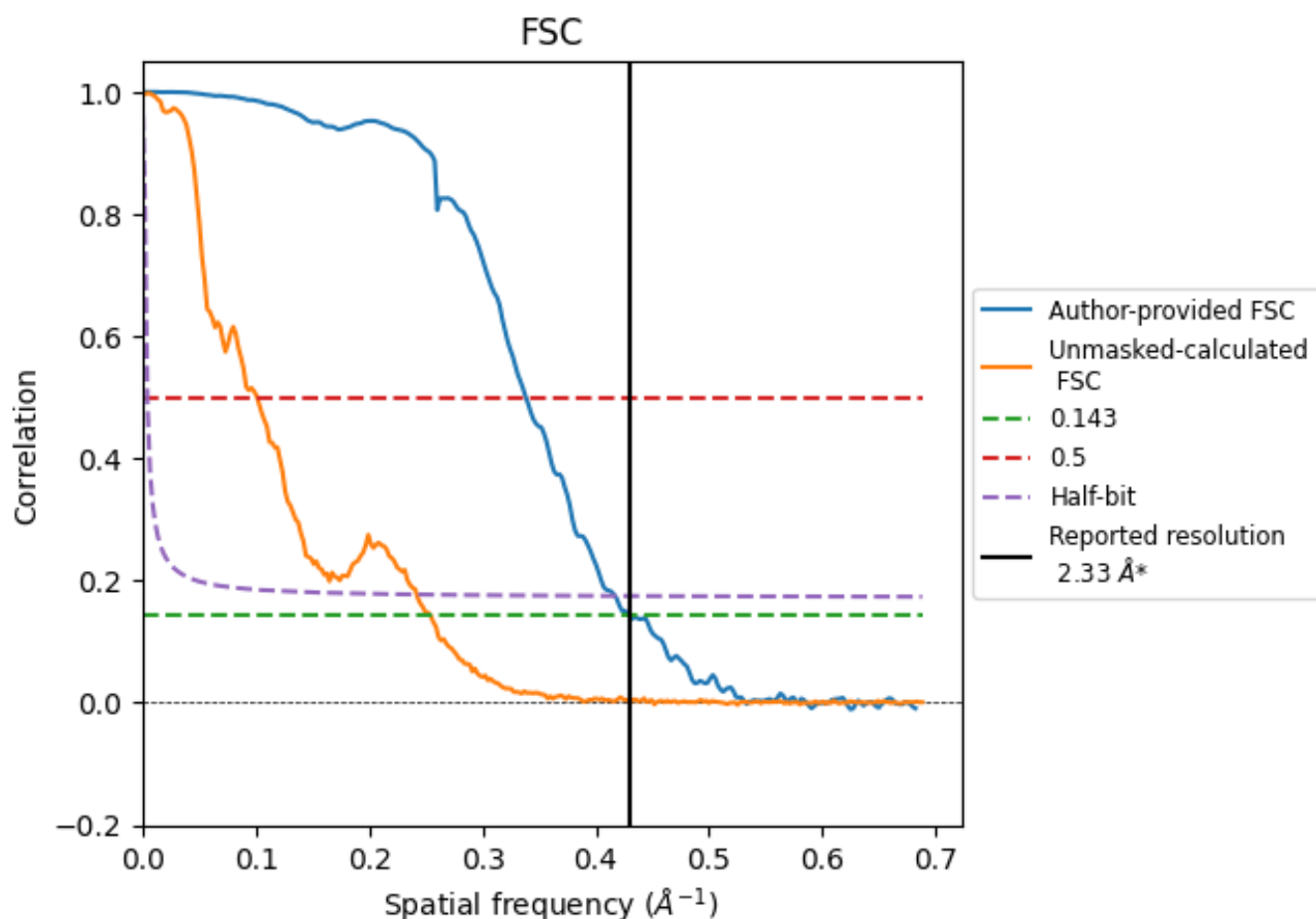


\*Reported resolution corresponds to spatial frequency of 0.429 Å<sup>-1</sup>

## 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 0.429  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

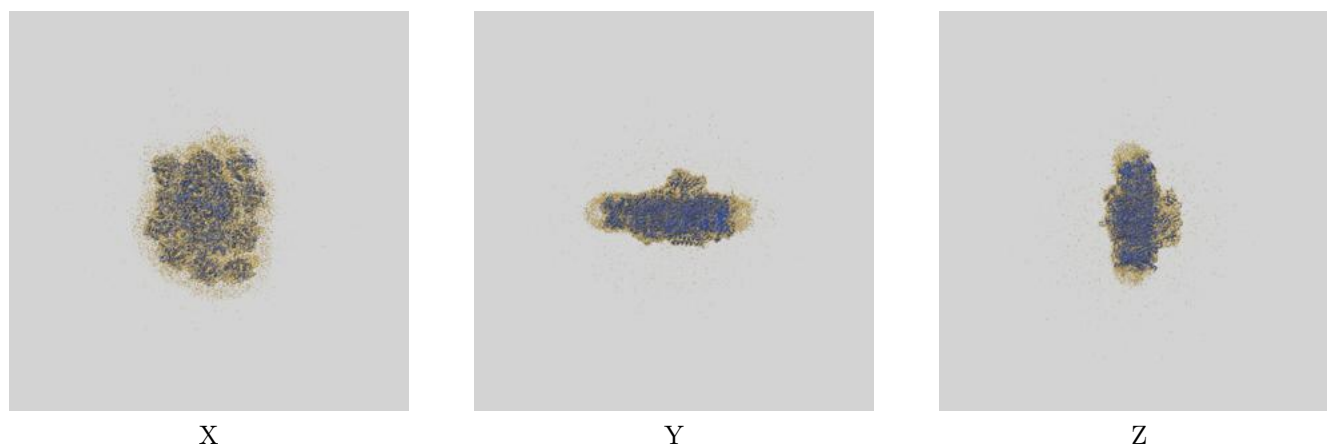
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.33	-	-
Author-provided FSC curve	2.33	2.96	2.40
Unmasked-calculated*	3.94	9.87	4.13

\*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 3.94 differs from the reported value 2.33 by more than 10 %

## 9 Map-model fit [i](#)

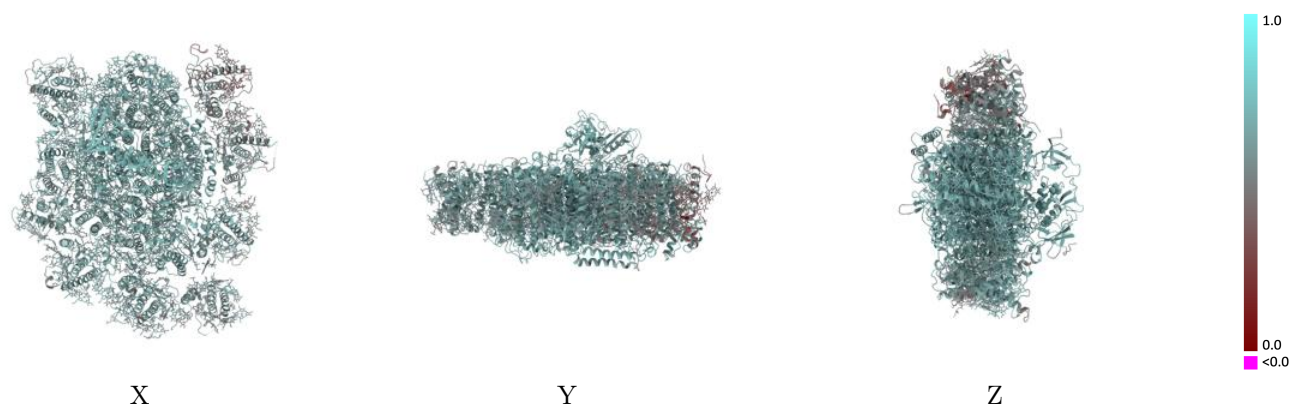
This section contains information regarding the fit between EMDB map EMD-64383 and PDB model 9UOV. Per-residue inclusion information can be found in [section 3](#) on [page 29](#).

### 9.1 Map-model overlay [i](#)



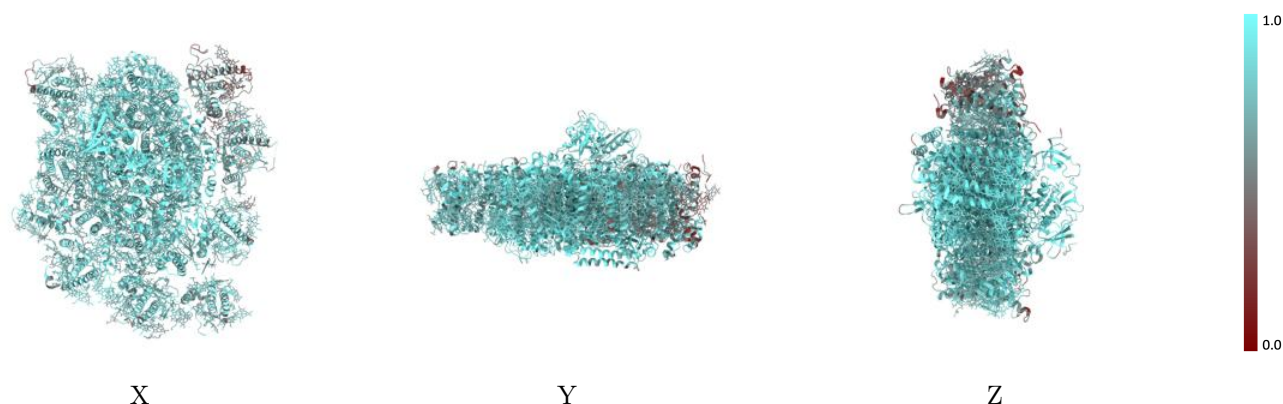
The images above show the 3D surface view of the map at the recommended contour level 0.07 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



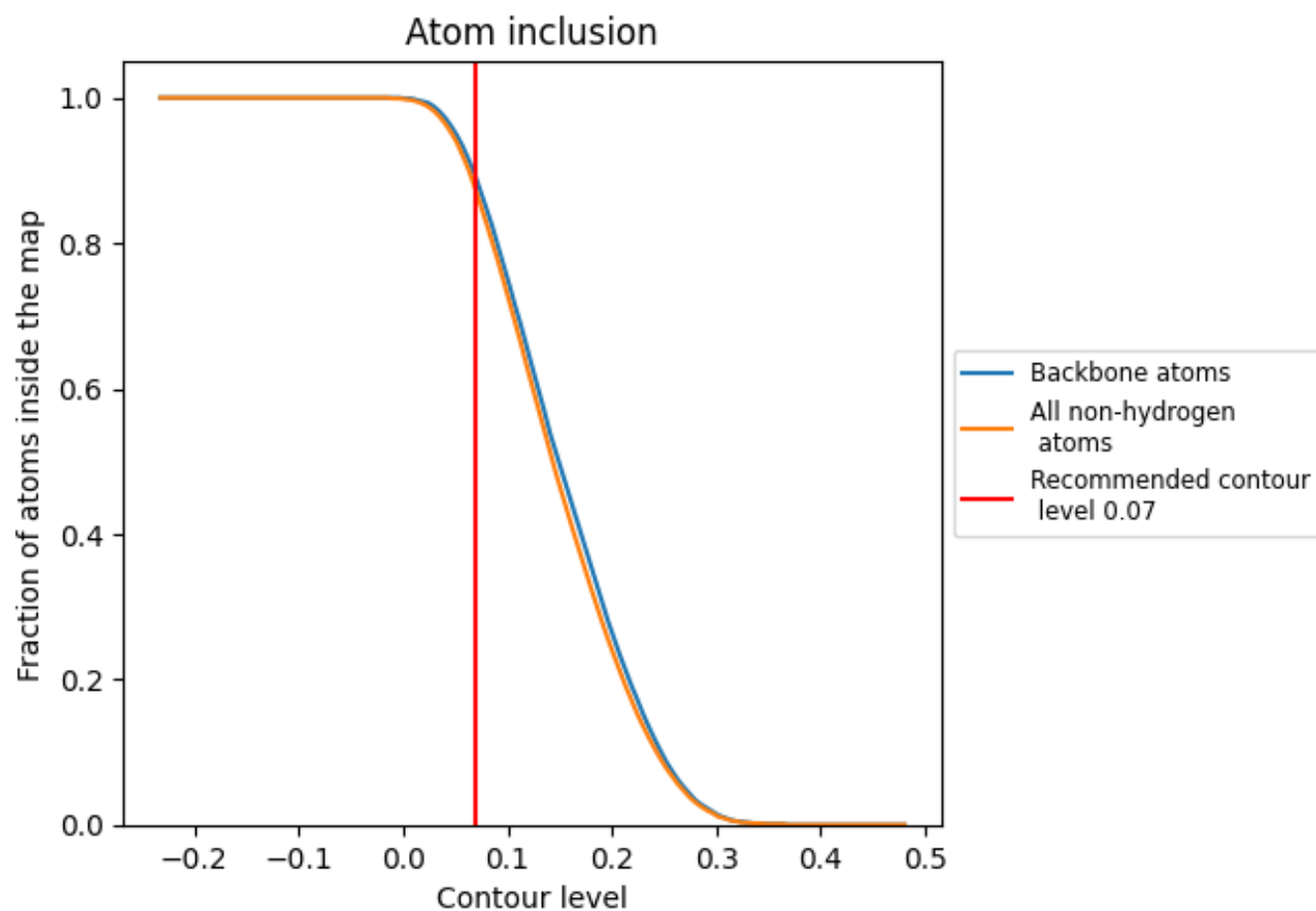
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.07).

## 9.4 Atom inclusion [i](#)











































At the recommended contour level, 89% of all backbone atoms, 87% of all non-hydrogen atoms, are inside the map.



## 9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.07) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8710	 0.6370
A	 0.9380	 0.6710
B	 0.9610	 0.6850
C	 0.9780	 0.6920
D	 0.9050	 0.6540
E	 0.8960	 0.6650
F	 0.9090	 0.6520
G	 0.6840	 0.5460
H	 0.5310	 0.4690
I	 0.9190	 0.6600
J	 0.9090	 0.6610
L	 0.8980	 0.6530
M	 0.9410	 0.6680
O	 0.8350	 0.6150
P	 0.8390	 0.6080
Q	 0.7970	 0.6030
R	 0.8960	 0.6470
S	 0.8330	 0.6200
T	 0.7510	 0.5660
U	 0.7320	 0.5870

