



Full wwPDB EM Validation Report ⓘ

Apr 12, 2026 – 12:31 PM UTC

PDB ID : 9UH3 / pdb_00009uh3
EMDB ID : EMD-64153
Title : PSI-9 FCPI supercomplex from haptophyte *Chrysotila roscoffensis*
Authors : La Rocca, R.; Tsai, P.-C.; Kato, K.; Nakajima, Y.; Akita, F.; Shen, J.-R.
Deposited on : 2025-04-14
Resolution : 1.74 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

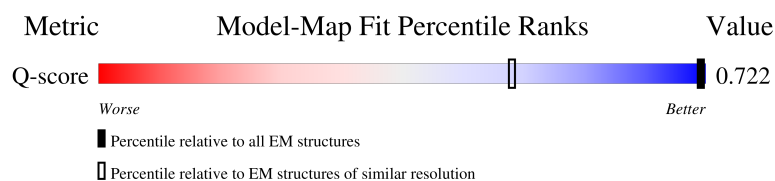
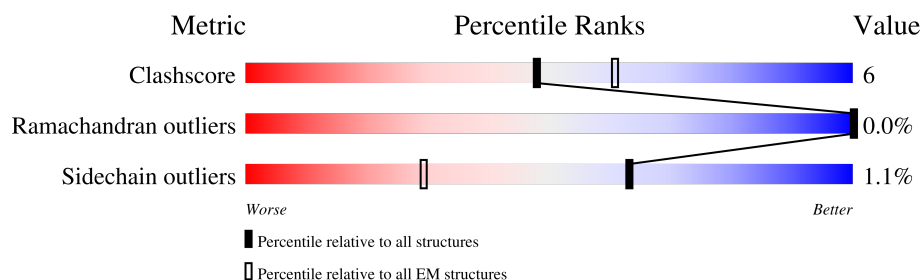
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance

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

The reported resolution of this entry is 1.74 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.








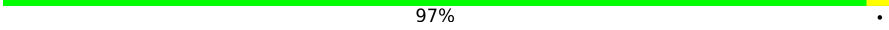





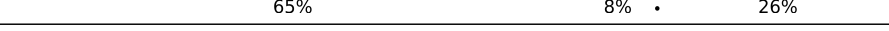





Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	645 (1.25 - 2.24)

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

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

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Mol	Chain	Length	Quality of chain
5	E	67	
6	F	184	
7	I	35	
8	J	39	
9	L	141	
10	M	29	
11	O	201	
12	P	231	
13	Q	197	
14	R	90	
15	S	215	
16	U	191	
17	G	209	
18	H	169	
19	K	200	
20	T	202	
21	k	89	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	A	802	X	-	-	-
22	CLA	A	803	X	-	-	-
22	CLA	A	804	X	-	-	-
22	CLA	A	805	X	-	-	-
22	CLA	A	806	X	-	-	-
22	CLA	A	809	X	-	-	-
22	CLA	A	810	X	-	-	-
22	CLA	A	811	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	A	812	X	-	-	-
22	CLA	A	815	X	-	-	-
22	CLA	A	816	X	-	-	-
22	CLA	A	817	X	-	-	-
22	CLA	A	818	X	-	-	-
22	CLA	A	820	X	-	-	-
22	CLA	A	821	X	-	-	-
22	CLA	A	822	X	-	-	-
22	CLA	A	823	X	-	-	-
22	CLA	A	824	X	-	-	-
22	CLA	A	825	X	-	-	-
22	CLA	A	828	X	-	-	-
22	CLA	A	829	X	-	-	-
22	CLA	A	831	X	-	-	-
22	CLA	A	832	X	-	-	-
22	CLA	A	833	X	-	-	-
22	CLA	A	835	X	-	-	-
22	CLA	A	836	X	-	-	-
22	CLA	A	838	X	-	-	-
22	CLA	A	845	X	-	-	-
22	CLA	A	850	X	-	-	-
22	CLA	A	853	X	-	-	-
22	CLA	A	854	X	-	-	-
22	CLA	A	855	X	-	-	-
22	CLA	A	856	X	-	-	-
22	CLA	B	801	X	-	-	-
22	CLA	B	802	X	-	-	-
22	CLA	B	803	X	-	-	-
22	CLA	B	804	X	-	-	-
22	CLA	B	805	X	-	-	-
22	CLA	B	807	X	-	-	-
22	CLA	B	808	X	-	-	-
22	CLA	B	811	X	-	-	-
22	CLA	B	815	X	-	-	-
22	CLA	B	816	X	-	-	-
22	CLA	B	819	X	-	-	-
22	CLA	B	820	X	-	-	-
22	CLA	B	821	X	-	-	-
22	CLA	B	822	X	-	-	-
22	CLA	B	826	X	-	-	-
22	CLA	B	828	X	-	-	-
22	CLA	B	829	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	B	830	X	-	-	-
22	CLA	B	831	X	-	-	-
22	CLA	B	832	X	-	-	-
22	CLA	B	834	X	-	-	-
22	CLA	B	842	X	-	-	-
22	CLA	B	843	X	-	-	-
22	CLA	B	844	X	-	-	-
22	CLA	B	845	X	-	-	-
22	CLA	B	847	X	-	-	-
22	CLA	F	802	X	-	-	-
22	CLA	F	803	X	-	-	-
22	CLA	F	804	X	-	-	-
22	CLA	G	202	X	-	-	-
22	CLA	G	203	X	-	-	-
22	CLA	G	206	X	-	-	-
22	CLA	G	208	X	-	-	-
22	CLA	G	209	X	-	-	-
22	CLA	G	210	X	-	-	-
22	CLA	G	215	X	-	-	-
22	CLA	H	202	X	-	-	-
22	CLA	H	203	X	-	-	-
22	CLA	H	204	X	-	-	-
22	CLA	H	205	X	-	-	-
22	CLA	H	206	X	-	-	-
22	CLA	H	208	X	-	-	-
22	CLA	H	209	X	-	-	-
22	CLA	H	213	X	-	-	-
22	CLA	J	103	X	-	-	-
22	CLA	K	203	X	-	-	-
22	CLA	K	205	X	-	-	-
22	CLA	K	206	X	-	-	-
22	CLA	L	204	X	-	-	-
22	CLA	O	205	X	-	-	-
22	CLA	O	206	X	-	-	-
22	CLA	O	207	X	-	-	-
22	CLA	O	208	X	-	-	-
22	CLA	P	207	X	-	-	-
22	CLA	P	208	X	-	-	-
22	CLA	P	209	X	-	-	-
22	CLA	P	213	X	-	-	-
22	CLA	P	214	X	-	-	-
22	CLA	P	216	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	Q	204	X	-	-	-
22	CLA	Q	205	X	-	-	-
22	CLA	Q	206	X	-	-	-
22	CLA	Q	207	X	-	-	-
22	CLA	Q	208	X	-	-	-
22	CLA	Q	211	X	-	-	-
22	CLA	Q	213	X	-	-	-
22	CLA	R	101	X	-	-	-
22	CLA	S	202	X	-	-	-
22	CLA	S	206	X	-	-	-
22	CLA	S	207	X	-	-	-
22	CLA	S	208	X	-	-	-
22	CLA	S	216	X	-	-	-
22	CLA	S	217	X	-	-	-
22	CLA	T	201	X	-	-	-
22	CLA	T	202	X	-	-	-
22	CLA	T	203	X	-	-	-
22	CLA	T	204	X	-	-	-
22	CLA	T	205	X	-	-	-
22	CLA	T	211	X	-	-	-
22	CLA	U	204	X	-	-	-
22	CLA	U	206	X	-	-	-
22	CLA	U	207	X	-	-	-
22	CLA	U	208	X	-	-	-
22	CLA	U	211	X	-	-	-
22	CLA	k	102	X	-	-	-
22	CLA	k	103	X	-	-	-

2 Entry composition [i](#)

There are 35 unique types of molecules in this entry. The entry contains 42258 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 IX (FCPI-9).

Mol	Chain	Residues	Atoms					AltConf	Trace
19	K	97	Total	C	N	O	S	0	0
			748	495	121	125	7		

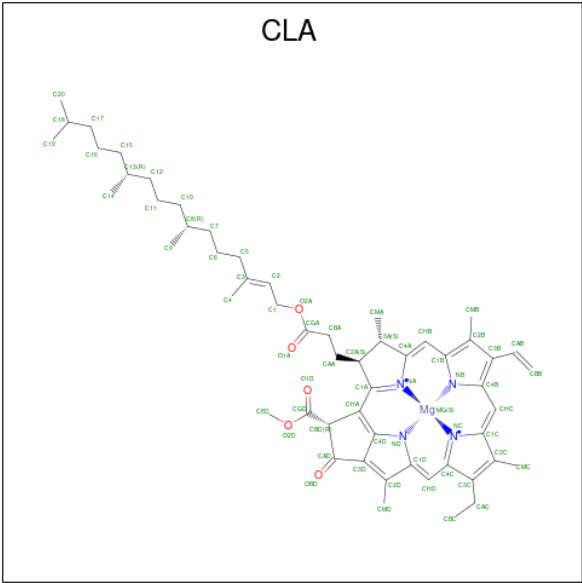
- Molecule 20 is a protein called Fucoxanthin chlorophyll a/c binding protein V (FCPI-5).

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

- Molecule 21 is a protein called Photosystem I reaction center subunit psaK.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	k	55	Total	C	N	O	S	0	0
			379	247	62	67	3		

- Molecule 22 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅).



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

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

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Mol	Chain	Residues	Atoms					AltConf
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 52	C 42	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 40	C 32	Mg 1	N 4	O 3	0
22	A	1	Total 46	C 36	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0

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

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Mol	Chain	Residues	Atoms					AltConf
22	B	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
22	F	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	F	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
22	F	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
22	J	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
22	L	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
22	L	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	L	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
22	O	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
22	O	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	O	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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

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Mol	Chain	Residues	Atoms					AltConf
22	Q	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
22	Q	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	Q	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
22	Q	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	R	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	R	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	S	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	S	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
22	S	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
22	S	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	S	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
22	S	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	S	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	U	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
22	U	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	U	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	U	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	U	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
22	U	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
22	U	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	U	1	Total	C	Mg	N	O	0
			52	42	1	4	5	

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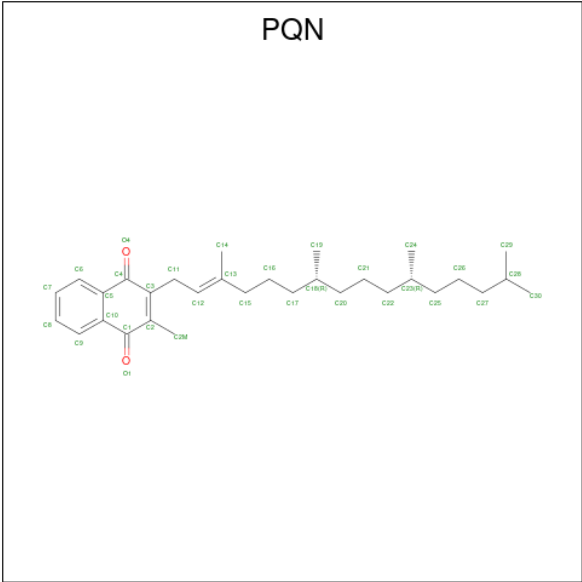
Mol	Chain	Residues	Atoms					AltConf
22	G	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	G	1	Total 41	C 33	Mg 1	N 4	O 3	0
22	G	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	G	1	Total 43	C 35	Mg 1	N 4	O 3	0
22	G	1	Total 61	C 51	Mg 1	N 4	O 5	0
22	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	G	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	G	1	Total 55	C 45	Mg 1	N 4	O 5	0
22	G	1	Total 56	C 46	Mg 1	N 4	O 5	0
22	G	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	G	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	H	1	Total 40	C 32	Mg 1	N 4	O 3	0
22	H	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	H	1	Total 61	C 51	Mg 1	N 4	O 5	0
22	H	1	Total 44	C 35	Mg 1	N 4	O 4	0
22	H	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	H	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	H	1	Total 58	C 48	Mg 1	N 4	O 5	0
22	H	1	Total 41	C 33	Mg 1	N 4	O 3	0
22	H	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	H	1	Total 65	C 55	Mg 1	N 4	O 5	0

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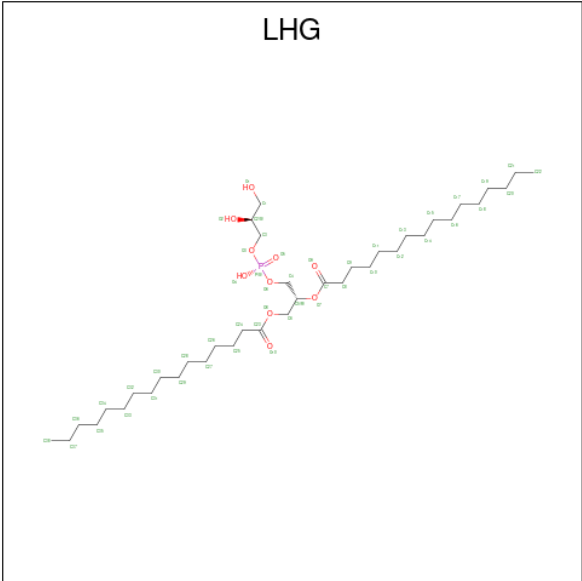
Mol	Chain	Residues	Atoms					AltConf
22	K	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	K	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
22	K	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
22	K	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	K	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
22	T	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
22	T	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
22	T	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
22	T	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
22	T	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
22	T	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
22	T	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	T	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
22	T	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
22	T	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
22	k	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
22	k	1	Total	C	Mg	N	O	0
			55	45	1	4	5	

- Molecule 23 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 24 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).



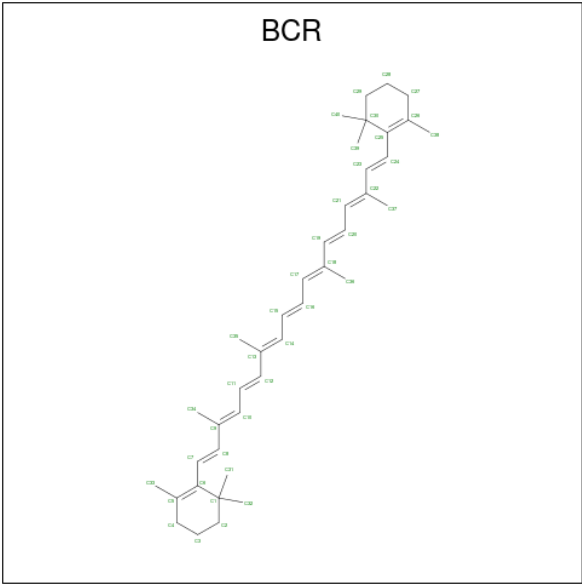
Mol	Chain	Residues	Atoms				AltConf
24	A	1	Total	C	O	P	0
			48	37	10	1	

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Mol	Chain	Residues	Atoms				AltConf
24	A	1	Total	C	O	P	0
			27	16	10	1	
24	P	1	Total	C	O	P	0
			49	38	10	1	
24	G	1	Total	C	O	P	0
			27	16	10	1	

- Molecule 25 is BETA-CAROTENE (CCD ID: BCR) (formula: C₄₀H₅₆).



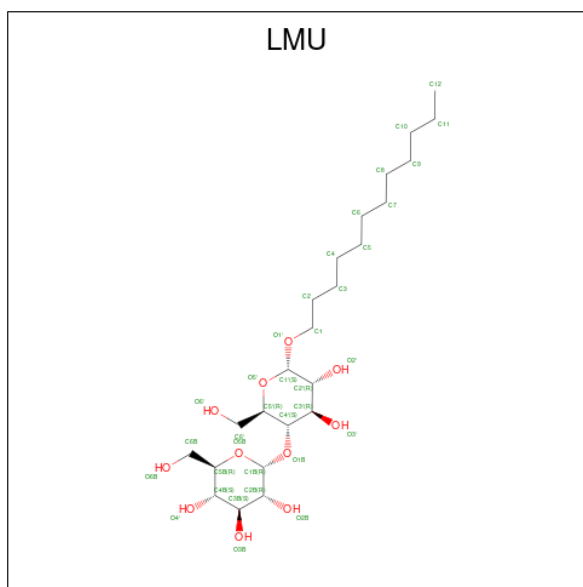
Mol	Chain	Residues	Atoms		AltConf
25	A	1	Total	C	0
			40	40	
25	A	1	Total	C	0
			40	40	
25	A	1	Total	C	0
			40	40	
25	A	1	Total	C	0
			40	40	
25	B	1	Total	C	0
			40	40	
25	B	1	Total	C	0
			40	40	
25	B	1	Total	C	0
			40	40	
25	B	1	Total	C	0
			40	40	

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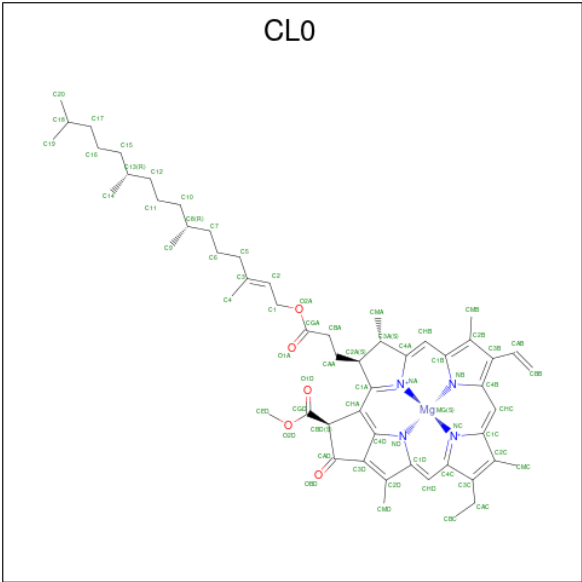
Mol	Chain	Residues	Atoms	AltConf
25	B	1	Total C 40 40	0
25	F	1	Total C 40 40	0
25	F	1	Total C 40 40	0
25	I	1	Total C 40 40	0
25	I	1	Total C 40 40	0
25	J	1	Total C 40 40	0
25	L	1	Total C 40 40	0
25	L	1	Total C 40 40	0
25	M	1	Total C 40 40	0
25	R	1	Total C 39 39	0
25	k	1	Total C 40 40	0

- Molecule 26 is DODECYL-ALPHA-D-MALTOSE (CCD ID: LMU) (formula: $C_{24}H_{46}O_{11}$).



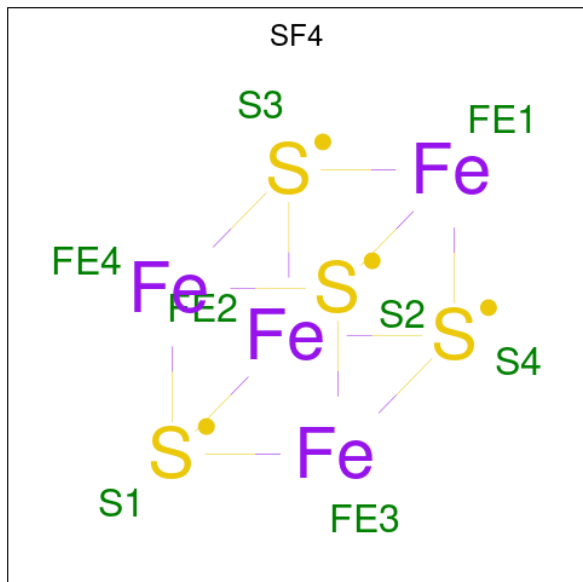
Mol	Chain	Residues	Atoms			AltConf
26	A	1	Total	C	O	0
			35	24	11	
26	A	1	Total	C	O	0
			35	24	11	
26	F	1	Total	C	O	0
			35	24	11	
26	F	1	Total	C	O	0
			35	24	11	
26	L	1	Total	C	O	0
			35	24	11	
26	M	1	Total	C	O	0
			35	24	11	
26	O	1	Total	C	O	0
			35	24	11	
26	P	1	Total	C	O	0
			25	14	11	
26	S	1	Total	C	O	0
			31	20	11	
26	K	1	Total	C	O	0
			35	24	11	
26	K	1	Total	C	O	0
			24	13	11	

- Molecule 27 is CHLOROPHYLL A ISOMER (CCD ID: CL0) (formula: C₅₅H₇₂MgN₄O₅).



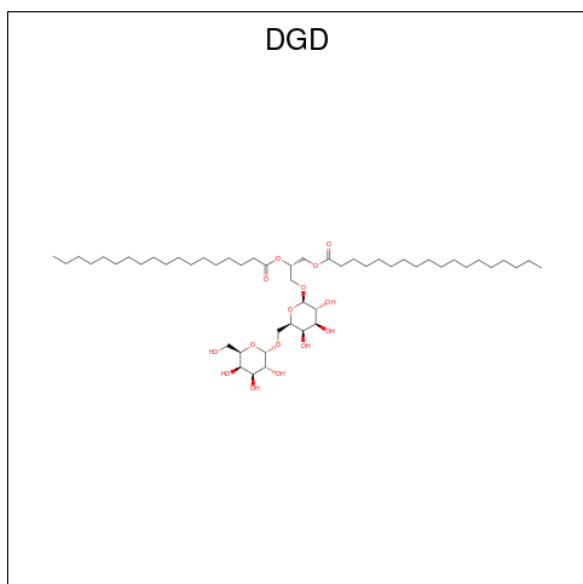
Mol	Chain	Residues	Atoms					AltConf
27	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

- Molecule 28 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).



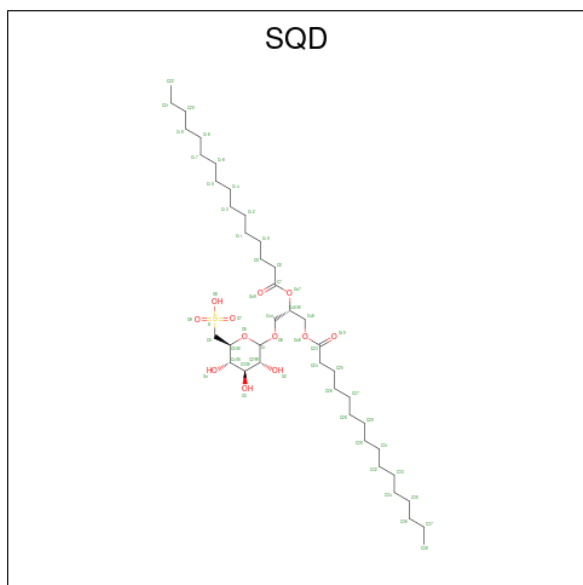
Mol	Chain	Residues	Atoms			AltConf
28	A	1	Total	Fe	S	0
			8	4	4	
28	C	1	Total	Fe	S	0
			8	4	4	
28	C	1	Total	Fe	S	0
			8	4	4	

- Molecule 29 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $\text{C}_{51}\text{H}_{96}\text{O}_{15}$).



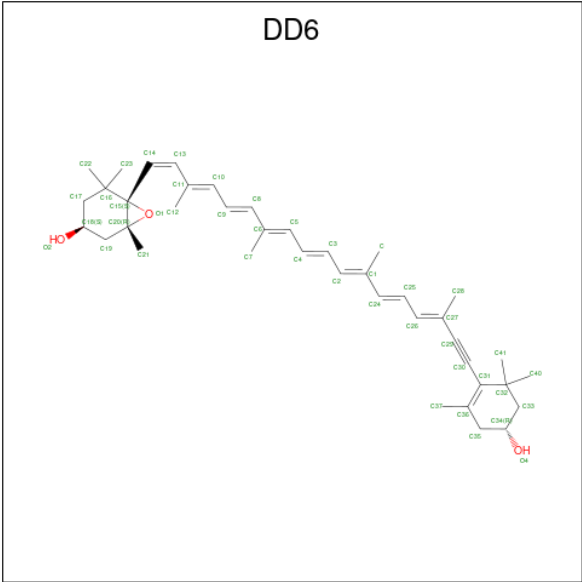
Mol	Chain	Residues	Atoms			AltConf
29	B	1	Total	C	O	0
			60	45	15	

- Molecule 30 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
30	B	1	Total	C	O	S	0
			50	37	12	1	
30	S	1	Total	C	O	S	0
			46	33	12	1	

- Molecule 31 is (3S,3'R,5R,6S,7cis)-7',8'-didehydro-5,6-dihydro-5,6-epoxy-beta,beta-carotene -3,3'-diol (CCD ID: DD6) (formula: $C_{40}H_{54}O_3$).



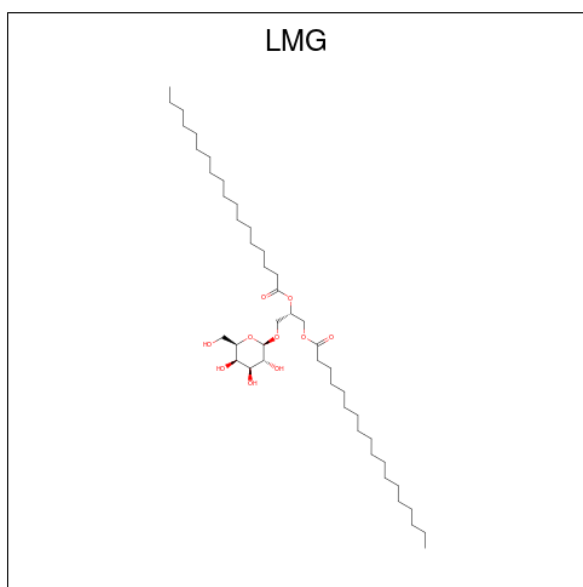
Mol	Chain	Residues	Atoms			AltConf
31	J	1	Total	C	O	0
			43	40	3	
31	O	1	Total	C	O	0
			43	40	3	
31	O	1	Total	C	O	0
			43	40	3	
31	O	1	Total	C	O	0
			43	40	3	
31	O	1	Total	C	O	0
			43	40	3	
31	O	1	Total	C	O	0
			43	40	3	
31	P	1	Total	C	O	0
			43	40	3	
31	P	1	Total	C	O	0
			43	40	3	
31	P	1	Total	C	O	0
			43	40	3	
31	P	1	Total	C	O	0
			43	40	3	
31	Q	1	Total	C	O	0
			43	40	3	
31	Q	1	Total	C	O	0
			43	40	3	
31	S	1	Total	C	O	0
			43	40	3	
31	S	1	Total	C	O	0
			43	40	3	

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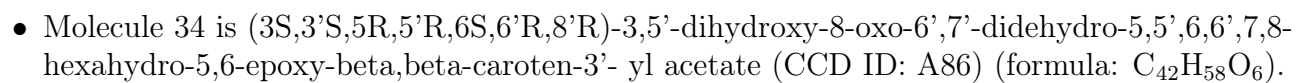
Mol	Chain	Residues	Atoms			AltConf
31	S	1	Total 43	C 40	O 3	0
31	S	1	Total 43	C 40	O 3	0
31	S	1	Total 43	C 40	O 3	0
31	U	1	Total 43	C 40	O 3	0
31	U	1	Total 43	C 40	O 3	0
31	U	1	Total 26	C 25	O 1	0
31	G	1	Total 43	C 40	O 3	0
31	G	1	Total 43	C 40	O 3	0
31	G	1	Total 43	C 40	O 3	0
31	G	1	Total 43	C 40	O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

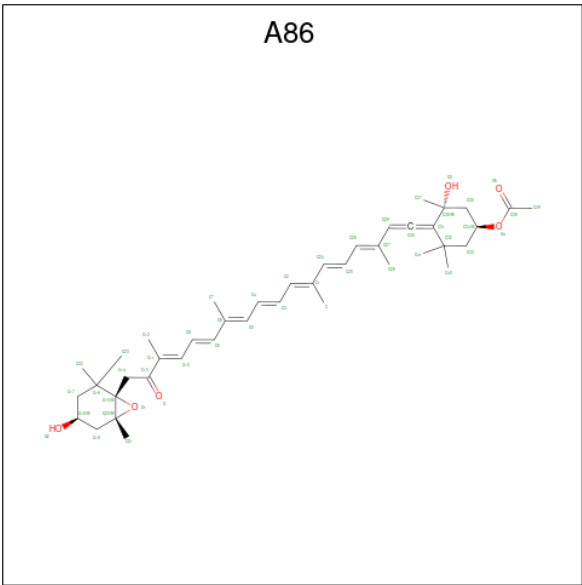
- Molecule 32 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: C₄₅H₈₆O₁₀).



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

- Molecule 33 is Chlorophyll c1 (CCD ID: KC1) (formula: $C_{35}H_{30}MgN_4O_5$).





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

- Molecule 35 is water.

Mol	Chain	Residues	Atoms		AltConf
35	A	117	Total	O	0
			117	117	
35	B	211	Total	O	0
			211	211	
35	C	46	Total	O	0
			46	46	
35	D	21	Total	O	0
			21	21	
35	E	14	Total	O	0
			14	14	

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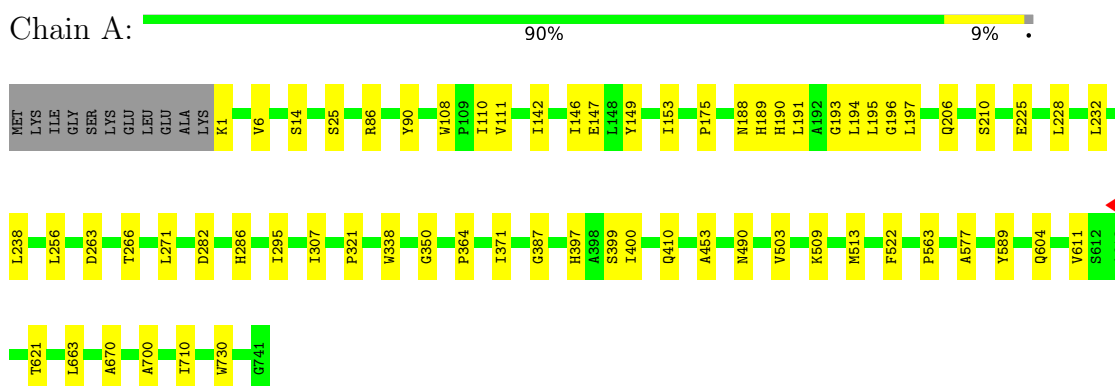
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Mol	Chain	Residues	Atoms		AltConf
35	F	21	Total 21	O 21	0
35	I	2	Total 2	O 2	0
35	J	3	Total 3	O 3	0
35	L	18	Total 18	O 18	0
35	M	2	Total 2	O 2	0
35	O	11	Total 11	O 11	0
35	P	18	Total 18	O 18	0
35	Q	9	Total 9	O 9	0
35	R	4	Total 4	O 4	0
35	S	11	Total 11	O 11	0
35	U	5	Total 5	O 5	0
35	k	1	Total 1	O 1	0

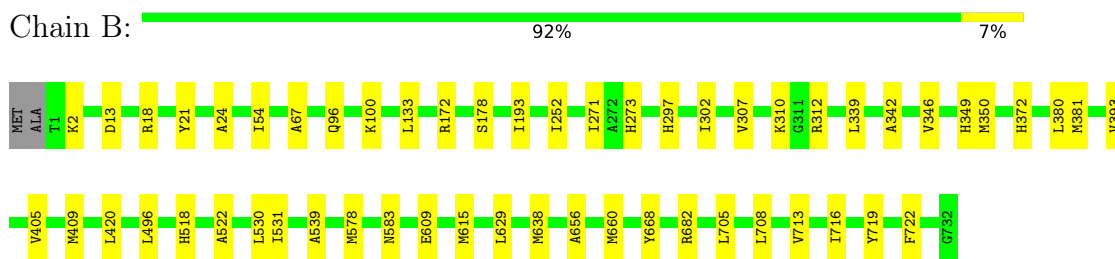
3 Residue-property plots

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

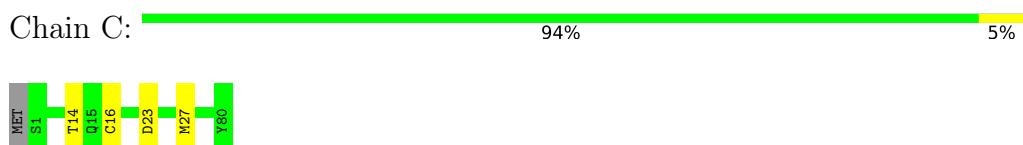
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1 (psaA)



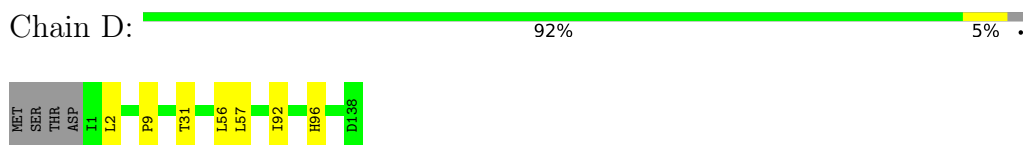
- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2 (psaB)



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



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




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

Chain E:  90% . . .




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

Chain F:  80% 8% 12%




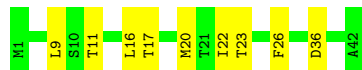
- Molecule 7: Photosystem I reaction center subunit VIII (psaI)

Chain I:  86% 11% .



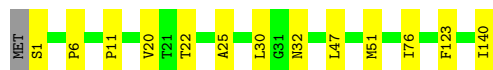
- Molecule 8: Photosystem I reaction center subunit IX (psaJ)

Chain J:  77% 23%



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

Chain L:  90% 9% .




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

Chain M:  97% .




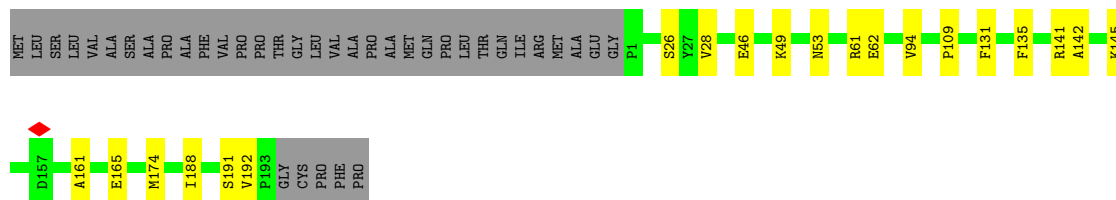
- Molecule 11: Fucoxanthin chlorophyll a/c binding protein III (FCPI-3)

Chain O:  81% 7% 12%




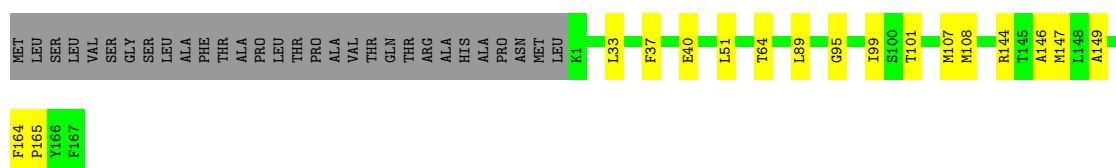
- Molecule 12: Fucoxanthin chlorophyll a/c binding protein VI (FCPI-6)

Chain P:  75% 9% 16%




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

Chain Q:  76% 9% 15%



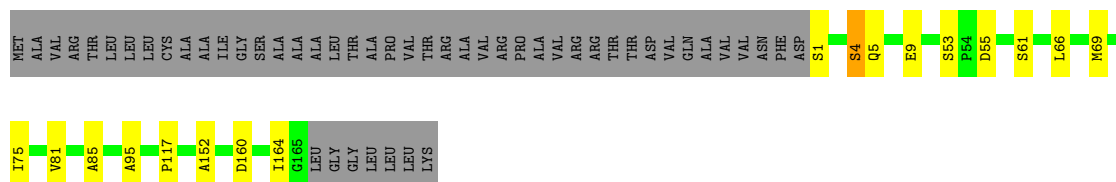
- Molecule 14: Photosystem I reaction center subunit psaR

Chain R:  88% 10% .



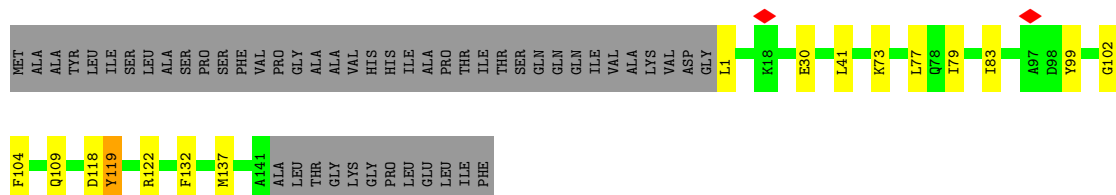
- Molecule 15: Fucoxanthin chlorophyll a/c binding protein II (FCPI-2)

Chain S:  69% 7% 23%



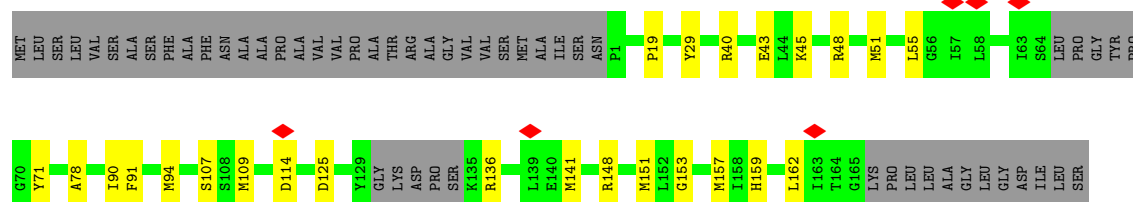
- Molecule 16: Fucoxanthin chlorophyll a/c binding protein I (FCPI-1)

Chain U:  65% 8% 26%



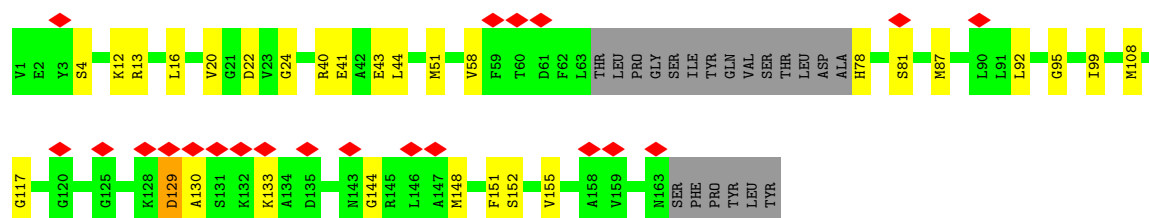
- Molecule 17: Fucoxanthin chlorophyll a/c binding protein VII (FCPI-7)

Chain G: 




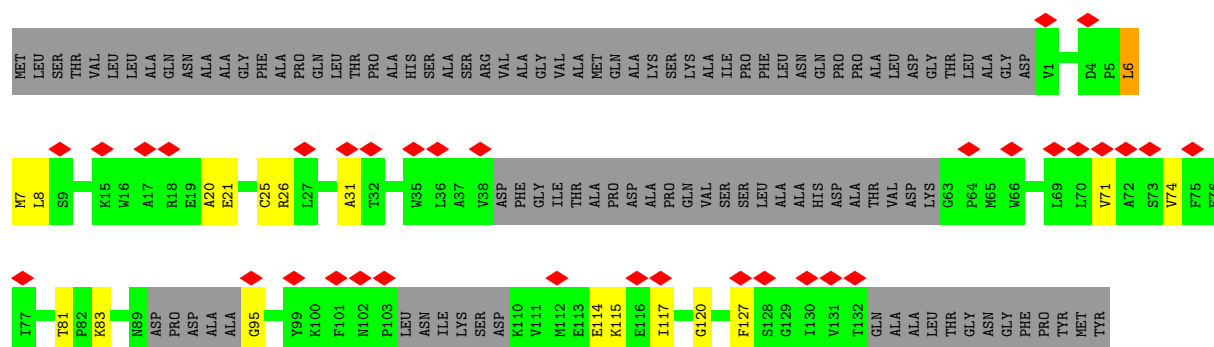
- Molecule 18: Fucoxanthin chlorophyll a/c binding protein VIII (FCPI-8)

Chain H: 



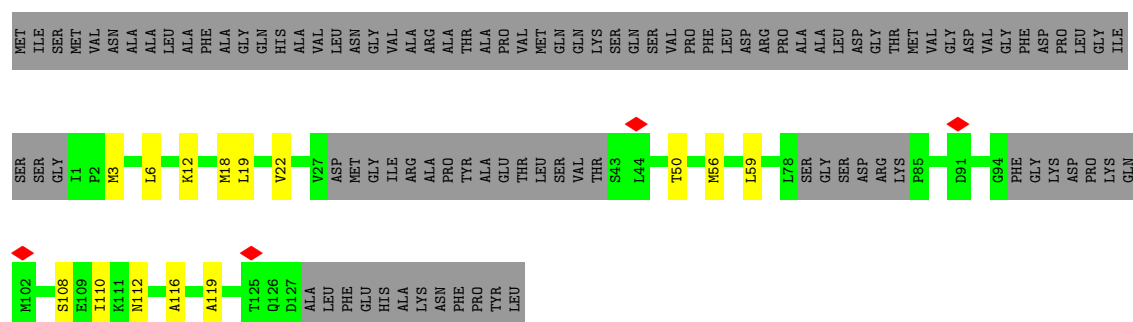
- Molecule 19: Fucoxanthin chlorophyll a/c binding protein IX (FCPI-9)

Chain K: 

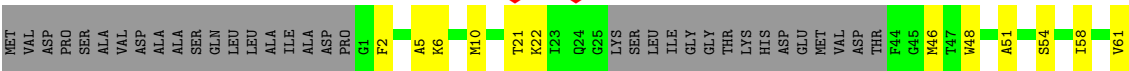


- Molecule 20: Fucoxanthin chlorophyll a/c binding protein V (FCPI-5)

Chain T: 



- Molecule 21: Photosystem I reaction center subunit psaK



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	191444	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	1.885	Depositor
Minimum map value	-0.618	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.020	Depositor
Recommended contour level	0.065	Depositor
Map size (\AA)	436.2, 436.2, 436.2	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	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: BCR, A86, CL0, SQD, DGD, SF4, PQN, KC1, CLA, LHG, DD6, LMG, LMU

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.20	0/6007	0.40	0/8185
2	B	0.22	0/6015	0.41	0/8205
3	C	0.16	0/609	0.38	0/826
4	D	0.15	0/1116	0.38	0/1503
5	E	0.16	0/505	0.31	0/689
6	F	0.21	0/1275	0.42	0/1728
7	I	0.22	0/273	0.48	0/373
8	J	0.43	0/313	0.70	0/427
9	L	0.20	0/1081	0.43	0/1470
10	M	0.19	0/218	0.30	0/295
11	O	0.18	0/1376	0.39	0/1865
12	P	0.20	0/1480	0.37	0/2010
13	Q	0.16	0/1285	0.37	0/1736
14	R	0.19	0/681	0.35	0/930
15	S	0.14	0/1272	0.32	0/1732
16	U	0.24	0/1109	0.47	2/1499 (0.1%)
17	G	0.17	0/1204	0.39	0/1624
18	H	0.20	0/1149	0.41	0/1546
19	K	0.25	0/764	0.52	0/1029
20	T	0.24	0/741	0.44	0/999
21	k	0.14	0/383	0.30	0/519
All	All	0.20	0/28856	0.41	2/39190 (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
11	O	0	1
13	Q	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
19	K	0	1
All	All	0	4

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	U	119	TYR	CA-C-N	5.81	128.54	120.29
16	U	119	TYR	C-N-CA	5.81	128.54	120.29

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
19	K	20	ALA	Peptide
11	O	173	VAL	Peptide
13	Q	164	PHE	Peptide
13	Q	165	PRO	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	49	0
2	B	5805	0	5635	49	0
3	C	599	0	577	3	0
4	D	1092	0	1096	4	0
5	E	494	0	488	2	0
6	F	1246	0	1256	12	0
7	I	266	0	278	4	0
8	J	305	0	310	8	0
9	L	1056	0	1068	10	0
10	M	216	0	234	1	0
11	O	1341	0	1347	14	0
12	P	1441	0	1421	16	0
13	Q	1257	0	1260	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	R	664	0	668	5	0
15	S	1238	0	1217	13	0
16	U	1082	0	1058	12	0
17	G	1179	0	1166	22	0
18	H	1128	0	1134	18	0
19	K	748	0	777	12	0
20	T	731	0	749	23	0
21	k	379	0	409	10	0
22	A	2701	0	2712	65	0
22	B	2344	0	2385	79	0
22	F	159	0	141	4	0
22	G	561	0	486	20	0
22	H	524	0	475	14	0
22	J	42	0	31	1	0
22	K	245	0	201	7	0
22	L	164	0	150	4	0
22	O	495	0	475	13	0
22	P	403	0	337	8	0
22	Q	609	0	566	8	0
22	R	110	0	105	5	0
22	S	384	0	358	9	0
22	T	473	0	379	22	0
22	U	441	0	417	14	0
22	k	97	0	80	4	0
23	A	33	0	46	2	0
23	B	33	0	46	1	0
24	A	75	0	93	3	0
24	G	27	0	24	1	0
24	P	49	0	74	4	0
25	A	160	0	224	5	0
25	B	200	0	280	14	0
25	F	80	0	112	4	0
25	I	80	0	112	5	0
25	J	40	0	56	1	0
25	L	80	0	112	2	0
25	M	40	0	56	1	0
25	R	39	0	53	3	0
25	k	40	0	56	2	0
26	A	70	0	92	1	0
26	F	70	0	92	1	0
26	K	59	0	67	2	0
26	L	35	0	46	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	M	35	0	46	1	0
26	O	35	0	46	0	0
26	P	25	0	23	0	0
26	S	31	0	35	1	0
27	A	65	0	72	3	0
28	A	8	0	0	0	0
28	C	16	0	0	1	0
29	B	60	0	81	9	0
30	B	50	0	67	1	0
30	S	46	0	56	1	0
31	G	172	0	0	3	0
31	H	129	0	0	0	0
31	J	43	0	0	0	0
31	K	43	0	0	0	0
31	O	215	0	0	2	0
31	P	172	0	0	0	0
31	Q	86	0	0	0	0
31	S	215	0	0	0	0
31	T	86	0	0	0	0
31	U	112	0	0	1	0
31	k	43	0	0	0	0
32	J	39	0	48	3	0
32	P	59	0	58	4	0
32	Q	55	0	86	3	0
32	S	49	0	68	2	0
32	U	32	0	34	1	0
33	O	45	0	0	0	0
33	P	179	0	0	0	0
33	Q	45	0	0	0	0
33	S	90	0	0	0	0
33	T	45	0	0	1	0
33	U	45	0	0	0	0
34	P	48	0	0	0	0
34	Q	144	0	0	0	0
34	R	92	0	0	1	0
34	U	48	0	0	0	0
35	A	117	0	0	1	0
35	B	211	0	0	0	0
35	C	46	0	0	0	0
35	D	21	0	0	0	0
35	E	14	0	0	0	0
35	F	21	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	I	2	0	0	0	0
35	J	3	0	0	0	0
35	L	18	0	0	0	0
35	M	2	0	0	0	0
35	O	11	0	0	0	0
35	P	18	0	0	0	0
35	Q	9	0	0	0	0
35	R	4	0	0	0	0
35	S	11	0	0	0	0
35	U	5	0	0	0	0
35	k	1	0	0	0	0
All	All	42258	0	39505	480	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 (480) 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)
19:K:8:LEU:HD21	21:k:46:MET:SD	2.05	0.96
17:G:90:ILE:HG22	17:G:94:MET:HE2	1.50	0.94
12:P:46:GLU:OE2	12:P:49:LYS:HE3	1.68	0.93
20:T:56:MET:HE2	20:T:56:MET:HA	1.56	0.87
22:B:830:CLA:H152	25:F:805:BCR:H23C	1.65	0.78
13:Q:40:GLU:HG3	13:Q:107:MET:HE1	1.64	0.78
1:A:146:ILE:HD12	1:A:147:GLU:N	1.98	0.78
12:P:109:PRO:HG2	22:P:210:CLA:HBC3	1.66	0.77
1:A:149:TYR:CE2	1:A:153:ILE:HD11	2.20	0.76
22:A:822:CLA:H91	25:A:844:BCR:H23C	1.68	0.75
11:O:115:LYS:NZ	11:O:115:LYS:HB2	2.05	0.71
6:F:113:LYS:HE3	6:F:116:GLU:HG3	1.73	0.71
17:G:148:ARG:HA	17:G:151:MET:HE3	1.73	0.70
1:A:522:PHE:HA	22:A:833:CLA:HED1	1.73	0.70
20:T:56:MET:HE3	22:T:204:CLA:CBA	2.22	0.70
20:T:59:LEU:HD23	22:T:210:CLA:CBC	2.22	0.69
2:B:178:SER:HB3	22:B:847:CLA:HAC2	1.75	0.69
22:A:803:CLA:H72	25:A:842:BCR:HC8	1.74	0.69
1:A:232:LEU:HD23	1:A:238:LEU:CD2	2.23	0.69
1:A:321:PRO:HB3	9:L:1:SER:HB2	1.75	0.68
1:A:146:ILE:HD12	1:A:147:GLU:H	1.57	0.68
22:A:808:CLA:HBB2	22:A:811:CLA:HMA3	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:H:206:CLA:HBB2	22:H:213:CLA:H171	1.76	0.67
1:A:149:TYR:CZ	1:A:153:ILE:HD11	2.30	0.67
12:P:46:GLU:CD	12:P:49:LYS:HE3	2.19	0.67
16:U:73:LYS:O	16:U:77:LEU:HD22	1.95	0.67
1:A:193:GLY:O	1:A:197:LEU:HB2	1.95	0.67
9:L:25:ALA:HB2	16:U:104:PHE:HB3	1.76	0.67
22:B:817:CLA:HMD2	25:B:836:BCR:HC7	1.77	0.66
18:H:20:VAL:O	18:H:40:ARG:NH2	2.29	0.66
9:L:47:LEU:O	9:L:51:MET:HG3	1.96	0.65
22:Q:208:CLA:H3A	32:Q:217:LMG:H321	1.77	0.65
17:G:55:LEU:HD23	22:G:209:CLA:CMC	2.27	0.64
25:A:843:BCR:H23C	22:A:848:CLA:HBC2	1.80	0.64
2:B:13:ASP:HB3	2:B:18:ARG:HB2	1.79	0.64
6:F:71:LEU:HD22	6:F:82:GLU:HG2	1.82	0.61
22:B:845:CLA:H43	9:L:76:ILE:HD12	1.82	0.61
6:F:107:PHE:HB2	6:F:129:MET:HE1	1.81	0.61
20:T:56:MET:CE	22:T:204:CLA:HBA2	2.31	0.61
22:B:823:CLA:H11	25:B:837:BCR:H393	1.82	0.61
22:S:206:CLA:HBB2	22:S:216:CLA:HAB	1.83	0.60
22:G:205:CLA:H71	22:G:206:CLA:H72	1.83	0.60
22:B:818:CLA:HBB2	22:B:834:CLA:H52	1.83	0.60
20:T:108:SER:O	20:T:112:ASN:HB2	2.00	0.59
21:k:21:THR:HG21	21:k:48:TRP:HE1	1.66	0.59
22:B:812:CLA:H143	25:B:837:BCR:HC32	1.84	0.59
1:A:206:GLN:HA	1:A:210:SER:HB2	1.83	0.59
11:O:56:MET:HE1	22:O:209:CLA:HHC	1.83	0.59
15:S:1:SER:HB3	15:S:4:SER:HB2	1.84	0.58
22:B:803:CLA:HBC1	29:B:841:DGD:HA92	1.85	0.58
22:B:847:CLA:HBA1	13:Q:101:THR:HG21	1.86	0.58
20:T:56:MET:HE3	22:T:204:CLA:HBA2	1.85	0.58
22:B:820:CLA:H72	22:B:834:CLA:H191	1.86	0.58
10:M:26:ARG:HD2	15:S:9:GLU:HB3	1.86	0.57
21:k:5:ALA:HB1	21:k:73:LEU:HD22	1.87	0.57
12:P:53:ASN:HA	32:P:217:LMG:HC71	1.87	0.57
22:A:801:CLA:H18	25:F:801:BCR:H14C	1.87	0.57
22:B:824:CLA:H102	29:B:841:DGD:HBH1	1.87	0.57
22:A:835:CLA:H101	8:J:17:THR:HG23	1.87	0.56
9:L:32:ASN:HB3	22:L:202:CLA:HAC1	1.87	0.56
2:B:100:LYS:H	2:B:100:LYS:HD2	1.70	0.56
22:B:845:CLA:H42	15:S:66:LEU:HD12	1.87	0.56
1:A:146:ILE:HD12	1:A:147:GLU:HG3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:453:ALA:O	2:B:638:MET:HE3	2.06	0.56
22:A:816:CLA:HBB2	22:A:816:CLA:H151	1.88	0.56
22:A:831:CLA:HBA2	22:k:103:CLA:H11	1.87	0.56
2:B:342:ALA:HB2	22:B:819:CLA:H43	1.88	0.56
22:S:206:CLA:HAA2	22:S:208:CLA:HBC2	1.87	0.55
1:A:86:ARG:HH12	1:A:149:TYR:HD1	1.52	0.55
18:H:41:GLU:OE1	18:H:108:MET:HE1	2.07	0.55
25:B:837:BCR:H16C	22:O:205:CLA:H172	1.88	0.55
22:A:805:CLA:H2	22:A:807:CLA:H52	1.89	0.55
22:A:802:CLA:H41	26:A:847:LMU:H112	1.89	0.55
2:B:24:ALA:HA	22:B:824:CLA:H43	1.87	0.55
12:P:135:PHE:HZ	32:P:217:LMG:HC2	1.72	0.54
22:F:802:CLA:HHC	22:F:802:CLA:HBB1	1.90	0.54
22:A:848:CLA:HHC	22:A:848:CLA:HBB1	1.89	0.54
11:O:54:GLN:HE22	22:O:208:CLA:HHD	1.72	0.54
22:B:806:CLA:HBB1	22:B:807:CLA:H202	1.89	0.54
22:B:829:CLA:H52	22:F:804:CLA:HBB2	1.89	0.54
6:F:123:VAL:HB	32:J:102:LMG:HC72	1.89	0.54
24:P:201:LHG:H192	22:R:104:CLA:H121	1.89	0.54
1:A:86:ARG:HH22	1:A:149:TYR:HB2	1.73	0.54
1:A:338:TRP:HB3	22:A:803:CLA:HAC1	1.89	0.54
1:A:730:TRP:NE1	22:A:824:CLA:O1A	2.40	0.54
22:A:816:CLA:H141	22:A:823:CLA:H193	1.90	0.54
22:A:845:CLA:HBC2	2:B:583:ASN:HB2	1.90	0.54
1:A:190:HIS:O	1:A:194:LEU:HB3	2.08	0.54
22:B:834:CLA:HBB2	22:R:104:CLA:O2A	2.08	0.54
32:J:102:LMG:H161	32:J:102:LMG:H211	1.89	0.54
18:H:151:PHE:O	18:H:155:VAL:HG23	2.07	0.54
21:k:54:SER:O	21:k:58:ILE:HG13	2.08	0.53
22:A:846:CLA:H91	25:k:104:BCR:H291	1.90	0.53
2:B:273:HIS:HB3	22:B:814:CLA:HMB2	1.90	0.53
13:Q:144:ARG:HA	13:Q:147:MET:HE3	1.90	0.53
17:G:29:TYR:HB2	24:G:216:LHG:HC42	1.89	0.53
22:A:824:CLA:H142	22:A:826:CLA:H18	1.90	0.53
2:B:409:MET:HG3	25:R:102:BCR:H402	1.89	0.53
1:A:146:ILE:CD1	1:A:147:GLU:HG3	2.39	0.53
22:A:835:CLA:HHC	22:A:835:CLA:HBB1	1.91	0.53
2:B:297:HIS:HB3	2:B:302:ILE:HD11	1.91	0.53
22:B:845:CLA:HED3	22:B:845:CLA:H51	1.90	0.53
11:O:111:SER:O	11:O:115:LYS:HG3	2.08	0.53
22:B:805:CLA:H91	29:B:841:DGD:HBN2	1.88	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:B:828:CLA:HHC	22:B:828:CLA:HBB1	1.91	0.53
20:T:56:MET:HE3	22:T:204:CLA:HBA1	1.91	0.53
16:U:30:GLU:HG2	22:U:209:CLA:HED1	1.91	0.52
22:S:206:CLA:HHC	22:S:206:CLA:HBB1	1.91	0.52
2:B:310:LYS:HG3	12:P:131:PHE:HE2	1.75	0.52
18:H:40:ARG:NH1	18:H:43:GLU:OE1	2.43	0.52
22:B:826:CLA:HBC3	25:F:805:BCR:H362	1.92	0.52
22:F:804:CLA:HHC	22:F:804:CLA:HBB1	1.91	0.52
12:P:165:GLU:OE1	22:P:211:CLA:HMA2	2.10	0.52
22:B:833:CLA:HHC	22:B:833:CLA:HBB1	1.92	0.52
22:Q:203:CLA:HHC	22:Q:203:CLA:HBB1	1.90	0.52
22:A:815:CLA:HHC	22:A:815:CLA:HBB1	1.91	0.52
17:G:91:PHE:HA	17:G:94:MET:HE3	1.92	0.52
22:B:829:CLA:H122	25:B:839:BCR:H311	1.92	0.52
22:B:830:CLA:H172	22:B:844:CLA:HBC1	1.90	0.52
13:Q:33:LEU:HD11	32:Q:217:LMG:H162	1.91	0.52
18:H:4:SER:HB3	18:H:24:GLY:HA3	1.92	0.52
18:H:155:VAL:HG11	22:H:213:CLA:H93	1.91	0.52
20:T:59:LEU:HD23	22:T:210:CLA:HBC1	1.92	0.52
22:k:102:CLA:HBB1	22:k:102:CLA:HHC	1.91	0.52
22:B:818:CLA:H3A	22:B:834:CLA:HED3	1.90	0.52
19:K:21:GLU:HB2	22:K:207:CLA:C1B	2.39	0.52
20:T:59:LEU:HD23	22:T:210:CLA:HBC2	1.92	0.52
22:T:201:CLA:HHC	22:T:201:CLA:HBB1	1.92	0.52
2:B:96:GLN:O	2:B:100:LYS:HD2	2.11	0.51
8:J:22:ILE:HG23	22:J:103:CLA:HBB2	1.92	0.51
12:P:174:MET:HE3	12:P:174:MET:O	2.10	0.51
17:G:153:GLY:C	17:G:157:MET:HE3	2.35	0.51
1:A:589:TYR:OH	27:A:849:CL0:H9	2.10	0.51
12:P:28:VAL:HG21	12:P:165:GLU:HB2	1.91	0.51
13:Q:89:LEU:HB3	22:Q:212:CLA:HBC1	1.91	0.51
15:S:152:ALA:HA	32:S:213:LMG:HC2	1.92	0.51
22:U:211:CLA:HBB1	22:U:211:CLA:HHC	1.93	0.51
19:K:6:LEU:HD12	21:k:46:MET:SD	2.50	0.51
2:B:719:TYR:HB2	22:B:801:CLA:HED2	1.93	0.51
22:U:204:CLA:H42	22:U:211:CLA:HED2	1.92	0.51
22:U:208:CLA:HHC	22:U:208:CLA:HBB1	1.93	0.51
22:A:828:CLA:H42	22:A:836:CLA:H2	1.92	0.51
22:H:209:CLA:HHC	22:H:209:CLA:HBB1	1.93	0.51
22:B:834:CLA:HAA2	24:P:201:LHG:H351	1.91	0.51
20:T:3:MET:HA	20:T:6:LEU:HB2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:S:160:ASP:O	15:S:164:ILE:HG13	2.11	0.51
11:O:115:LYS:HB2	11:O:115:LYS:HZ3	1.73	0.51
2:B:578:MET:HG3	2:B:708:LEU:HD21	1.93	0.51
22:B:826:CLA:H43	32:P:202:LMG:H291	1.92	0.51
22:B:847:CLA:HHC	22:B:847:CLA:HBB1	1.92	0.51
22:A:835:CLA:H71	22:A:853:CLA:H171	1.92	0.51
22:B:806:CLA:H201	22:B:808:CLA:H192	1.93	0.51
9:L:22:THR:O	16:U:109:GLN:NE2	2.44	0.51
16:U:137:MET:HE2	31:U:212:DD6:O1	2.11	0.51
17:G:55:LEU:HD23	22:G:209:CLA:HAC2	1.93	0.51
22:H:210:CLA:HHC	22:H:210:CLA:HBB1	1.93	0.51
2:B:100:LYS:HD2	2:B:100:LYS:N	2.26	0.50
22:A:831:CLA:HHC	22:A:831:CLA:HBB1	1.93	0.50
22:G:215:CLA:HHC	22:G:215:CLA:HBB1	1.93	0.50
22:A:820:CLA:HHC	22:A:820:CLA:HBB1	1.94	0.50
22:U:207:CLA:H143	22:U:210:CLA:HBC1	1.93	0.50
17:G:55:LEU:HD23	22:G:209:CLA:HMC3	1.94	0.50
22:T:210:CLA:HHC	22:T:210:CLA:HBB1	1.92	0.50
22:H:202:CLA:HHC	22:H:202:CLA:HBB1	1.93	0.50
1:A:256:LEU:HD11	21:k:61:VAL:HG22	1.94	0.50
22:T:205:CLA:HHC	22:T:205:CLA:HBB1	1.93	0.50
22:B:809:CLA:H52	22:B:810:CLA:HBC2	1.92	0.50
22:B:814:CLA:HHC	22:B:814:CLA:HBB1	1.93	0.50
22:A:811:CLA:H111	26:K:201:LMU:H111	1.94	0.50
15:S:69:MET:HE2	15:S:75:ILE:HA	1.94	0.50
18:H:13:ARG:HB2	18:H:16:LEU:HD13	1.93	0.50
19:K:71:VAL:HA	19:K:74:VAL:HG22	1.94	0.50
11:O:115:LYS:NZ	11:O:115:LYS:CB	2.73	0.50
22:A:855:CLA:HHC	22:A:855:CLA:HBB1	1.94	0.50
22:B:807:CLA:HHC	22:B:807:CLA:HBB1	1.93	0.50
22:B:820:CLA:H143	22:B:834:CLA:H192	1.93	0.50
22:B:821:CLA:HHC	22:B:821:CLA:HBB1	1.94	0.50
32:S:213:LMG:H352	22:S:216:CLA:H93	1.93	0.50
17:G:78:ALA:HB1	22:G:209:CLA:HED3	1.94	0.50
18:H:22:ASP:HB2	22:H:207:CLA:HED2	1.94	0.50
2:B:24:ALA:HB2	29:B:841:DGD:HA32	1.94	0.49
22:B:832:CLA:HHC	22:B:832:CLA:HBB1	1.94	0.49
22:P:213:CLA:HHC	22:P:213:CLA:HBB1	1.94	0.49
18:H:129:ASP:OD1	18:H:129:ASP:N	2.38	0.49
22:A:854:CLA:H42	9:L:20:VAL:HG13	1.94	0.49
22:H:203:CLA:HHC	22:H:203:CLA:HBB1	1.92	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:B:818:CLA:HBB	22:B:834:CLA:O1D	2.13	0.49
22:O:207:CLA:HHC	22:O:207:CLA:HBB1	1.94	0.49
6:F:120:ILE:HG12	8:J:11:THR:HG22	1.95	0.49
17:G:55:LEU:HD23	22:G:209:CLA:HMC2	1.94	0.49
22:G:201:CLA:HHC	22:G:201:CLA:HBB1	1.95	0.49
22:H:205:CLA:HHC	22:H:205:CLA:HBB1	1.93	0.49
1:A:266:THR:OG1	1:A:282:ASP:OD1	2.25	0.49
22:B:816:CLA:H141	22:B:828:CLA:H52	1.93	0.49
22:A:810:CLA:HHC	22:A:810:CLA:HBB1	1.94	0.49
4:D:9:PRO:HG2	4:D:57:LEU:HD23	1.94	0.49
5:E:5:SER:HB2	5:E:63:PRO:HD3	1.95	0.49
22:A:817:CLA:HHC	22:A:817:CLA:HBB1	1.94	0.49
22:P:214:CLA:HHC	22:P:214:CLA:HBB1	1.95	0.49
32:U:201:LMG:H321	22:U:211:CLA:H42	1.94	0.49
1:A:397:HIS:HA	1:A:400:ILE:HD12	1.94	0.49
22:B:820:CLA:H43	22:B:828:CLA:HBB2	1.95	0.49
11:O:56:MET:HE3	31:O:212:DD6:C6	2.43	0.49
22:T:209:CLA:HHC	22:T:209:CLA:HBB1	1.95	0.49
4:D:2:LEU:HD23	4:D:92:ILE:HD13	1.94	0.48
17:G:71:TYR:HA	22:G:209:CLA:HED2	1.94	0.48
22:T:211:CLA:HHC	22:T:211:CLA:HBB1	1.94	0.48
22:O:202:CLA:HHC	22:O:202:CLA:HBB1	1.95	0.48
22:O:203:CLA:HHC	22:O:203:CLA:HBB1	1.94	0.48
14:R:49:ASN:ND2	34:R:103:A86:O3	2.46	0.48
19:K:83:LYS:NZ	19:K:95:GLY:O	2.46	0.48
7:I:29:LEU:HD22	30:S:201:SQD:H462	1.93	0.48
19:K:7:MET:SD	19:K:7:MET:N	2.87	0.48
13:Q:37:PHE:HB2	13:Q:108:MET:HE2	1.96	0.48
1:A:110:ILE:HG13	1:A:111:VAL:HG13	1.95	0.48
1:A:196:GLY:HA3	1:A:295:ILE:HG13	1.96	0.48
22:A:814:CLA:HHC	22:A:814:CLA:HBB1	1.94	0.48
22:K:207:CLA:HHC	22:K:207:CLA:HBB1	1.93	0.48
22:H:213:CLA:H51	22:H:213:CLA:HBA2	1.95	0.48
22:A:851:CLA:H172	6:F:101:GLY:HA2	1.95	0.48
2:B:172:ARG:HB2	22:B:842:CLA:HBC2	1.95	0.48
22:B:818:CLA:H42	22:B:819:CLA:H121	1.95	0.48
17:G:114:ASP:N	17:G:114:ASP:OD1	2.46	0.48
22:H:213:CLA:HBA1	22:H:213:CLA:H3A	1.68	0.48
1:A:86:ARG:NH1	1:A:149:TYR:HD1	2.11	0.48
22:B:826:CLA:HHC	22:B:826:CLA:HBB1	1.96	0.48
22:P:210:CLA:HHC	22:P:210:CLA:HBB1	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:K:203:CLA:HHC	22:K:203:CLA:HBB1	1.95	0.48
11:O:130:PHE:HD2	22:O:209:CLA:H11	1.79	0.48
1:A:86:ARG:NH1	1:A:149:TYR:CD1	2.81	0.48
23:A:837:PQN:H141	22:F:802:CLA:HBB2	1.95	0.48
22:P:207:CLA:H61	22:P:207:CLA:H41	1.72	0.48
22:S:208:CLA:HED3	22:S:209:CLA:HBC2	1.96	0.48
22:G:206:CLA:HBB2	31:G:214:DD6:C3	2.44	0.48
20:T:56:MET:CE	22:T:204:CLA:CBA	2.89	0.48
1:A:232:LEU:CD2	1:A:238:LEU:CD2	2.92	0.47
2:B:609:GLU:OE2	6:F:17:ARG:NH2	2.47	0.47
22:B:845:CLA:HBB1	22:B:845:CLA:HHC	1.94	0.47
22:R:104:CLA:HED2	22:R:104:CLA:HAA1	1.95	0.47
19:K:21:GLU:O	19:K:25:CYS:N	2.40	0.47
1:A:232:LEU:HD23	1:A:238:LEU:HD23	1.97	0.47
1:A:307:ILE:HD13	21:k:51:ALA:HB2	1.96	0.47
22:O:205:CLA:HED2	22:O:205:CLA:H72	1.95	0.47
22:G:203:CLA:HHC	22:G:203:CLA:HBB1	1.95	0.47
18:H:148:MET:HE1	22:H:207:CLA:HHC	1.96	0.47
22:A:816:CLA:HBC3	22:A:825:CLA:H121	1.96	0.47
27:A:849:CL0:H32	22:A:850:CLA:C1D	2.44	0.47
19:K:114:GLU:HA	19:K:117:ILE:HD12	1.97	0.47
20:T:59:LEU:CG	22:T:210:CLA:HBC1	2.44	0.47
22:A:850:CLA:H122	25:B:840:BCR:H12C	1.96	0.47
22:T:206:CLA:HHC	22:T:206:CLA:HBB1	1.95	0.47
1:A:108:TRP:CD2	22:A:807:CLA:HED3	2.49	0.47
1:A:563:PRO:HB3	1:A:710:ILE:HB	1.97	0.47
22:A:808:CLA:HBA1	22:A:810:CLA:HMD2	1.97	0.47
22:L:202:CLA:H3A	22:L:202:CLA:HBA2	1.75	0.47
22:U:209:CLA:HHC	22:U:209:CLA:HBB1	1.96	0.47
2:B:393:VAL:HG13	2:B:539:ALA:HB1	1.97	0.47
5:E:1:VAL:HG23	5:E:26:ILE:HD11	1.96	0.47
1:A:263:ASP:N	1:A:263:ASP:OD1	2.44	0.47
22:A:801:CLA:HMD3	2:B:531:ILE:HG12	1.97	0.47
9:L:6:PRO:HB3	9:L:11:PRO:HA	1.96	0.47
22:A:854:CLA:H12	9:L:30:LEU:HD11	1.96	0.46
22:B:802:CLA:H13	25:I:101:BCR:H281	1.96	0.46
20:T:112:ASN:HD22	22:T:207:CLA:HBB1	1.78	0.46
1:A:271:LEU:HD21	1:A:364:PRO:HD2	1.98	0.46
8:J:23:THR:HA	8:J:26:PHE:CE2	2.51	0.46
22:Q:204:CLA:H93	22:Q:204:CLA:H62	1.77	0.46
22:G:208:CLA:HHC	22:G:208:CLA:HBB1	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:T:56:MET:HA	20:T:56:MET:CE	2.37	0.46
2:B:346:VAL:HG21	22:B:823:CLA:HHD	1.98	0.46
11:O:25:PHE:HE1	22:O:202:CLA:HBC3	1.81	0.46
17:G:125:ASP:OD1	31:G:211:DD6:O4	2.34	0.46
20:T:112:ASN:HD22	22:T:207:CLA:CBB	2.28	0.46
23:A:837:PQN:H222	23:A:837:PQN:H18	1.71	0.46
16:U:30:GLU:OE1	16:U:102:GLY:N	2.47	0.46
22:A:813:CLA:HHC	22:A:813:CLA:HBB1	1.96	0.46
16:U:41:LEU:HD22	22:U:207:CLA:H93	1.98	0.46
1:A:90:TYR:OH	1:A:142:ILE:O	2.32	0.46
26:F:806:LMU:H2B	26:F:806:LMU:H4'	1.55	0.46
11:O:126:ASP:OD1	31:O:212:DD6:O2	2.33	0.46
12:P:61:ARG:NH2	22:P:207:CLA:O1D	2.49	0.46
17:G:141:MET:HB3	22:G:202:CLA:HED2	1.98	0.46
26:K:201:LMU:H12	26:K:201:LMU:H42	1.63	0.46
1:A:490:ASN:HB2	22:A:831:CLA:HED2	1.97	0.45
22:B:844:CLA:HHC	22:B:844:CLA:HBB1	1.98	0.45
18:H:152:SER:HB2	22:H:213:CLA:H162	1.97	0.45
19:K:25:CYS:HB3	19:K:120:GLY:HA3	1.98	0.45
1:A:228:LEU:HD22	22:A:814:CLA:HED1	1.97	0.45
6:F:115:ASN:N	6:F:115:ASN:OD1	2.46	0.45
11:O:11:LYS:NZ	11:O:12:PRO:O	2.49	0.45
1:A:399:SER:HB3	1:A:577:ALA:HB1	1.99	0.45
2:B:312:ARG:HB2	32:P:217:LMG:HC3	1.97	0.45
4:D:31:THR:HG22	4:D:56:LEU:HB2	1.99	0.45
22:Q:204:CLA:HHC	22:Q:204:CLA:HBB1	1.98	0.45
22:Q:208:CLA:H3A	32:Q:217:LMG:H342	1.98	0.45
22:A:801:CLA:H162	22:A:801:CLA:H122	1.87	0.45
2:B:339:LEU:HD11	22:B:804:CLA:H51	1.97	0.45
1:A:1:LYS:HD2	1:A:1:LYS:HA	1.69	0.45
18:H:78:HIS:HA	18:H:87:MET:HE3	1.99	0.45
3:C:14:THR:HG22	3:C:27:MET:HG3	1.97	0.45
8:J:20:MET:HA	8:J:20:MET:HE2	1.98	0.45
9:L:123:PHE:HE2	15:S:95:ALA:HA	1.82	0.45
20:T:116:ALA:HA	20:T:119:ALA:HB3	1.98	0.45
2:B:2:LYS:HD3	7:I:34:GLU:HB3	1.98	0.45
25:B:839:BCR:H15C	25:B:839:BCR:H351	1.83	0.45
6:F:96:TRP:HH2	22:G:205:CLA:H42	1.81	0.45
8:J:9:LEU:HB3	32:J:102:LMG:H141	1.99	0.45
14:R:86:ASN:HB3	14:R:88:LYS:HE2	1.99	0.45
15:S:5:GLN:O	15:S:9:GLU:HG3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:350:GLY:HA2	1:A:387:GLY:HA2	1.99	0.45
2:B:271:ILE:HG23	22:B:815:CLA:HMA3	1.99	0.45
2:B:656:ALA:HB3	22:B:802:CLA:HBB2	1.99	0.45
2:B:705:LEU:HD22	29:B:841:DGD:HB22	1.99	0.45
22:B:817:CLA:HHC	22:B:817:CLA:HBB1	1.98	0.45
26:L:206:LMU:H72	15:S:85:ALA:HA	1.98	0.45
2:B:372:HIS:HE2	22:B:823:CLA:C1B	2.30	0.45
25:A:843:BCR:H20C	25:A:843:BCR:H361	1.75	0.44
22:A:845:CLA:H61	22:A:845:CLA:H41	1.76	0.44
22:R:101:CLA:HHC	22:R:101:CLA:HBB1	1.97	0.44
16:U:79:ILE:O	16:U:83:ILE:HG12	2.16	0.44
22:A:824:CLA:H91	22:A:826:CLA:H192	1.97	0.44
22:A:824:CLA:H102	22:A:824:CLA:H61	1.86	0.44
25:B:836:BCR:H20C	25:B:836:BCR:H361	1.85	0.44
26:M:102:LMU:H42	15:S:152:ALA:HB1	1.99	0.44
2:B:405:VAL:O	2:B:409:MET:HG2	2.18	0.44
25:R:102:BCR:H24C	25:R:102:BCR:H371	1.87	0.44
11:O:92:GLY:HA3	26:S:203:LMU:H11	1.99	0.44
24:A:839:LHG:H141	24:A:839:LHG:H112	1.85	0.44
2:B:193:ILE:HG12	2:B:252:ILE:HB	2.00	0.44
22:B:845:CLA:H61	22:B:845:CLA:H41	1.75	0.44
13:Q:146:ALA:HA	13:Q:149:ALA:HB3	1.99	0.44
22:O:209:CLA:H41	22:O:209:CLA:H62	1.65	0.44
12:P:161:ALA:O	12:P:165:GLU:HG2	2.18	0.44
18:H:95:GLY:O	18:H:99:ILE:HG12	2.18	0.44
22:A:838:CLA:HED1	22:U:210:CLA:HAA2	2.00	0.43
2:B:339:LEU:HB3	2:B:380:LEU:HD13	1.98	0.43
22:B:805:CLA:H152	22:B:805:CLA:H102	1.99	0.43
6:F:113:LYS:HE3	6:F:116:GLU:CG	2.45	0.43
2:B:54:ILE:HD11	25:M:101:BCR:HC8	2.00	0.43
2:B:705:LEU:HD23	29:B:841:DGD:HA21	2.00	0.43
22:B:845:CLA:H121	25:L:201:BCR:H271	2.00	0.43
19:K:26:ARG:HB3	22:K:204:CLA:HBC2	2.00	0.43
1:A:700:ALA:O	6:F:109:LYS:NZ	2.44	0.43
22:A:851:CLA:HBB2	6:F:101:GLY:HA3	2.00	0.43
2:B:629:LEU:HD22	2:B:722:PHE:HA	1.99	0.43
12:P:28:VAL:O	12:P:61:ARG:NH1	2.41	0.43
22:T:210:CLA:HED2	22:T:210:CLA:HBD	1.85	0.43
2:B:716:ILE:HG22	22:B:822:CLA:H52	2.01	0.43
25:J:104:BCR:H20C	25:J:104:BCR:H361	1.82	0.43
2:B:420:LEU:HD13	2:B:530:LEU:HA	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:Q:51:LEU:HB3	22:Q:216:CLA:HAB	2.00	0.43
19:K:8:LEU:CD2	21:k:46:MET:SD	2.93	0.43
22:K:204:CLA:HHC	22:K:204:CLA:HBB1	1.99	0.43
1:A:371:ILE:HG23	1:A:509:LYS:HG2	2.00	0.43
22:A:853:CLA:H91	22:A:853:CLA:H112	1.84	0.43
2:B:518:HIS:CG	22:B:830:CLA:HED3	2.54	0.43
2:B:522:ALA:HB2	22:B:830:CLA:HMA1	2.00	0.43
11:O:70:LYS:NZ	11:O:79:VAL:O	2.39	0.43
22:P:208:CLA:H62	22:P:208:CLA:H41	1.88	0.43
22:A:816:CLA:H91	22:A:825:CLA:H162	2.00	0.43
2:B:21:TYR:CE2	29:B:841:DGD:HG32	2.54	0.43
20:T:50:THR:HG21	22:T:204:CLA:H2A	2.00	0.43
22:B:806:CLA:H12	7:I:14:VAL:HG21	2.00	0.43
22:B:815:CLA:H91	22:B:815:CLA:H111	1.87	0.43
3:C:23:ASP:OD2	4:D:96:HIS:ND1	2.44	0.43
17:G:48:ARG:HA	17:G:51:MET:SD	2.58	0.43
25:k:104:BCR:H20C	25:k:104:BCR:H361	1.86	0.43
17:G:153:GLY:O	17:G:157:MET:HG3	2.18	0.43
22:K:205:CLA:C1D	22:K:206:CLA:HMD2	2.49	0.43
20:T:12:LYS:HE3	20:T:12:LYS:HB2	1.81	0.43
22:k:103:CLA:H11	22:k:103:CLA:H51	1.83	0.43
1:A:6:VAL:HA	1:A:175:PRO:HA	2.00	0.42
22:A:829:CLA:HBB1	22:A:829:CLA:HMB3	2.01	0.42
22:U:205:CLA:H92	22:U:206:CLA:HMA1	2.01	0.42
22:K:207:CLA:H61	22:K:207:CLA:H41	1.60	0.42
22:B:826:CLA:H42	25:F:805:BCR:H353	2.02	0.42
26:L:206:LMU:H21	15:S:81:VAL:HG22	2.00	0.42
14:R:81:TRP:O	14:R:85:GLN:HG2	2.18	0.42
22:G:206:CLA:HBB2	31:G:214:DD6:C4	2.49	0.42
22:A:846:CLA:H111	22:A:846:CLA:H72	1.85	0.42
25:I:102:BCR:H15C	25:I:102:BCR:H351	1.84	0.42
16:U:1:LEU:HD23	16:U:1:LEU:HA	1.94	0.42
17:G:136:ARG:HH12	22:G:204:CLA:HMA2	1.84	0.42
20:T:56:MET:CE	22:T:204:CLA:H3A	2.50	0.42
24:P:201:LHG:H261	24:P:201:LHG:H291	1.86	0.42
22:S:202:CLA:HMD2	22:S:216:CLA:HBC2	2.02	0.42
18:H:81:SER:HB2	18:H:87:MET:HE2	2.00	0.42
22:G:206:CLA:HED2	22:G:206:CLA:HBD	1.90	0.42
1:A:286:HIS:HE2	22:A:816:CLA:C2B	2.32	0.42
22:B:816:CLA:H143	22:B:816:CLA:H111	1.86	0.42
25:B:839:BCR:H24C	25:B:839:BCR:H371	1.86	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:U:208:CLA:HED2	22:U:208:CLA:HBD	1.88	0.42
22:A:836:CLA:H122	25:I:102:BCR:H19C	2.01	0.42
22:B:804:CLA:H203	22:B:804:CLA:H162	1.93	0.42
25:B:838:BCR:H15C	25:B:838:BCR:H351	1.89	0.42
22:B:842:CLA:H141	22:B:842:CLA:H162	1.76	0.42
3:C:16:CYS:HB3	28:C:102:SF4:S4	2.60	0.42
25:L:205:BCR:H11C	25:L:205:BCR:H341	1.90	0.42
12:P:188:ILE:O	12:P:191:SER:HB2	2.20	0.42
13:Q:95:GLY:O	13:Q:99:ILE:HG12	2.19	0.42
21:k:22:LYS:HE2	21:k:22:LYS:HB2	1.76	0.42
22:B:832:CLA:HBB2	23:B:835:PQN:H141	2.02	0.42
15:S:66:LEU:HD22	22:S:202:CLA:HMA1	2.00	0.42
15:S:117:PRO:HB2	22:S:217:CLA:HED3	2.01	0.42
16:U:132:PHE:HE1	22:U:205:CLA:H202	1.84	0.42
22:B:816:CLA:H91	22:B:816:CLA:H112	1.74	0.42
17:G:45:LYS:HE3	17:G:45:LYS:HB2	1.75	0.42
22:A:836:CLA:H92	22:A:836:CLA:H61	1.80	0.42
25:I:101:BCR:H361	25:I:101:BCR:H20C	1.80	0.42
1:A:191:LEU:HD23	1:A:195:LEU:HD12	2.00	0.41
24:A:839:LHG:H282	24:A:839:LHG:H312	1.72	0.41
2:B:349:HIS:ND1	22:B:814:CLA:OBD	2.49	0.41
2:B:682:ARG:HA	2:B:682:ARG:HD3	1.87	0.41
14:R:25:VAL:HB	14:R:30:TYR:CE2	2.54	0.41
17:G:107:SER:HB2	17:G:109:MET:HE3	2.02	0.41
17:G:159:HIS:HA	17:G:162:LEU:HD12	2.02	0.41
18:H:44:LEU:HG	18:H:117:GLY:HA3	2.02	0.41
22:H:213:CLA:HBA1	22:H:213:CLA:H12	1.69	0.41
2:B:713:VAL:HG22	29:B:841:DGD:HBV1	2.02	0.41
1:A:188:ASN:HB3	22:A:817:CLA:HMD1	2.02	0.41
1:A:604:GLN:HB3	1:A:621:THR:HG23	2.03	0.41
22:B:806:CLA:H161	22:B:806:CLA:H122	1.76	0.41
14:R:2:LYS:HA	14:R:2:LYS:HD3	1.69	0.41
22:R:104:CLA:H62	22:R:104:CLA:H41	1.76	0.41
1:A:670:ALA:HB3	22:A:801:CLA:HBB2	2.02	0.41
22:A:854:CLA:H41	22:L:203:CLA:H161	2.01	0.41
22:B:833:CLA:H92	22:B:833:CLA:H62	1.92	0.41
20:T:59:LEU:HG	22:T:210:CLA:HBC1	2.02	0.41
24:A:840:LHG:HC61	22:A:848:CLA:HMB1	2.03	0.41
2:B:660:MET:HB2	22:B:802:CLA:C1C	2.50	0.41
22:B:821:CLA:HED1	22:B:828:CLA:HAB	2.03	0.41
25:B:840:BCR:H20C	25:B:840:BCR:H361	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:P:62:GLU:OE1	12:P:141:ARG:NH1	2.46	0.41
18:H:130:ALA:HA	18:H:133:LYS:HB3	2.03	0.41
25:A:841:BCR:H15C	25:A:841:BCR:H351	1.93	0.41
22:A:853:CLA:H93	8:J:16:LEU:HD11	2.02	0.41
2:B:496:LEU:HD23	2:B:496:LEU:HA	1.91	0.41
25:B:837:BCR:H15C	25:B:837:BCR:H351	1.92	0.41
16:U:122:ARG:NH1	22:U:211:CLA:O2D	2.53	0.41
17:G:19:PRO:O	17:G:40:ARG:NH1	2.46	0.41
17:G:43:GLU:HG3	22:G:207:CLA:NB	2.36	0.41
30:B:846:SQD:H151	22:S:217:CLA:H112	2.03	0.41
19:K:31:ALA:HB1	19:K:127:PHE:CZ	2.56	0.41
1:A:663:LEU:HD11	2:B:615:MET:HB2	2.03	0.41
22:A:845:CLA:HHB	22:B:801:CLA:H202	2.02	0.41
27:A:849:CL0:H34	35:A:930:HOH:O	2.20	0.41
2:B:668:TYR:OH	22:B:802:CLA:OBD	2.35	0.41
22:B:805:CLA:H72	22:B:805:CLA:H111	1.93	0.41
22:B:824:CLA:C2D	29:B:841:DGD:HB61	2.51	0.41
25:I:101:BCR:H24C	25:I:101:BCR:H371	1.95	0.41
18:H:51:MET:HG3	18:H:144:GLY:HA2	2.02	0.41
20:T:12:LYS:NZ	22:T:206:CLA:O1D	2.37	0.41
20:T:18:MET:HE1	20:T:112:ASN:HB3	2.02	0.41
20:T:112:ASN:HD21	33:T:208:KC1:C1A	2.34	0.41
22:A:816:CLA:H72	22:A:816:CLA:H111	1.81	0.41
22:A:833:CLA:H51	22:A:833:CLA:H11	1.84	0.41
22:B:826:CLA:HAC1	22:B:831:CLA:HBC3	2.02	0.41
22:L:204:CLA:HED2	22:L:204:CLA:HBD	1.91	0.41
12:P:131:PHE:HB2	24:P:201:LHG:HC92	2.03	0.41
16:U:119:TYR:CE2	22:U:210:CLA:HHB	2.56	0.41
22:G:205:CLA:H72	22:G:206:CLA:H13	2.02	0.41
21:k:10:MET:HG3	22:k:102:CLA:C3D	2.51	0.41
1:A:503:VAL:HG22	1:A:513:MET:HB2	2.03	0.40
18:H:152:SER:HB2	22:H:213:CLA:H141	2.01	0.40
22:B:812:CLA:H91	22:B:812:CLA:H112	1.86	0.40
22:Q:213:CLA:H12	22:Q:213:CLA:H52	1.89	0.40
25:R:102:BCR:H15C	25:R:102:BCR:H351	1.91	0.40
2:B:350:MET:HE2	2:B:350:MET:HB3	1.87	0.40
2:B:381:MET:HE1	25:B:839:BCR:H361	2.03	0.40
22:B:809:CLA:H61	22:O:205:CLA:H93	2.03	0.40
1:A:189:HIS:CE1	22:A:810:CLA:NA	2.89	0.40
2:B:67:ALA:HB2	2:B:133:LEU:HB2	2.04	0.40
11:O:56:MET:HE1	22:O:209:CLA:HAB	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:O:205:CLA:H62	22:O:205:CLA:H41	1.88	0.40
22:G:205:CLA:H62	22:G:205:CLA:H41	1.67	0.40
22:A:826:CLA:H202	22:A:835:CLA:HHB	2.03	0.40
22:A:836:CLA:H191	7:I:24:ALA:HB2	2.04	0.40
22:B:827:CLA:O1D	8:J:36:ASP:HA	2.21	0.40
25:B:838:BCR:H24C	25:B:838:BCR:H371	1.90	0.40
12:P:142:ALA:HB3	12:P:145:LYS:HG3	2.03	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%)	719 (97%)	20 (3%)	0	100	100
2	B	730/734 (100%)	712 (98%)	18 (2%)	0	100	100
3	C	78/81 (96%)	77 (99%)	1 (1%)	0	100	100
4	D	136/142 (96%)	132 (97%)	4 (3%)	0	100	100
5	E	62/67 (92%)	61 (98%)	1 (2%)	0	100	100
6	F	159/184 (86%)	155 (98%)	4 (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%)	137 (99%)	1 (1%)	0	100	100
10	M	27/29 (93%)	27 (100%)	0	0	100	100
11	O	174/201 (87%)	170 (98%)	3 (2%)	1 (1%)	21	8
12	P	191/231 (83%)	188 (98%)	3 (2%)	0	100	100
13	Q	165/197 (84%)	157 (95%)	8 (5%)	0	100	100
14	R	86/90 (96%)	84 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	S	163/215 (76%)	160 (98%)	3 (2%)	0	100	100
16	U	139/191 (73%)	138 (99%)	1 (1%)	0	100	100
17	G	149/209 (71%)	146 (98%)	3 (2%)	0	100	100
18	H	145/169 (86%)	140 (97%)	5 (3%)	0	100	100
19	K	89/200 (44%)	87 (98%)	2 (2%)	0	100	100
20	T	91/202 (45%)	89 (98%)	2 (2%)	0	100	100
21	k	51/89 (57%)	50 (98%)	1 (2%)	0	100	100
All	All	3581/4198 (85%)	3498 (98%)	82 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
11	O	174	PRO

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%)	598 (99%)	5 (1%)	73	64
2	B	590/591 (100%)	589 (100%)	1 (0%)	87	84
3	C	68/69 (99%)	68 (100%)	0	100	100
4	D	118/122 (97%)	118 (100%)	0	100	100
5	E	53/55 (96%)	52 (98%)	1 (2%)	50	28
6	F	133/152 (88%)	132 (99%)	1 (1%)	73	64
7	I	31/32 (97%)	31 (100%)	0	100	100
8	J	32/32 (100%)	32 (100%)	0	100	100
9	L	111/112 (99%)	110 (99%)	1 (1%)	70	59
10	M	21/21 (100%)	21 (100%)	0	100	100
11	O	145/161 (90%)	145 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	P	144/173 (83%)	141 (98%)	3 (2%)	47	24
13	Q	133/157 (85%)	132 (99%)	1 (1%)	73	64
14	R	71/73 (97%)	70 (99%)	1 (1%)	59	41
15	S	125/162 (77%)	121 (97%)	4 (3%)	34	11
16	U	110/148 (74%)	108 (98%)	2 (2%)	51	30
17	G	127/167 (76%)	127 (100%)	0	100	100
18	H	119/137 (87%)	115 (97%)	4 (3%)	32	10
19	K	78/153 (51%)	75 (96%)	3 (4%)	29	8
20	T	73/153 (48%)	70 (96%)	3 (4%)	27	6
21	k	38/65 (58%)	36 (95%)	2 (5%)	20	4
All	All	2923/3347 (87%)	2891 (99%)	32 (1%)	63	50

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	SER
1	A	25	SER
1	A	225	GLU
1	A	410	GLN
1	A	611	VAL
2	B	307	VAL
5	E	5	SER
6	F	44	GLN
9	L	140	ILE
12	P	26	SER
12	P	94	VAL
12	P	192	VAL
13	Q	64	THR
14	R	77	HIS
15	S	4	SER
15	S	53	SER
15	S	55	ASP
15	S	61	SER
16	U	99	TYR
16	U	118	ASP
18	H	12	LYS
18	H	58	VAL
18	H	92	LEU

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Mol	Chain	Res	Type
18	H	129	ASP
19	K	6	LEU
19	K	81	THR
19	K	115	LYS
20	T	19	LEU
20	T	22	VAL
20	T	110	ILE
21	k	2	PHE
21	k	6	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	431	ASN
1	A	627	ASN
2	B	112	ASN
2	B	641	GLN
3	C	3	ASN
4	D	115	ASN
4	D	128	ASN
6	F	44	GLN
9	L	32	ASN
9	L	69	ASN
14	R	86	ASN
17	G	3	ASN
17	G	102	ASN
18	H	157	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

272 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$
22	CLA	A	807	1	69,73,73	1.17	8 (11%)	82,113,113	0.94	4 (4%)
22	CLA	B	828	35	69,73,73	1.17	7 (10%)	82,113,113	0.98	5 (6%)
26	LMU	K	201	-	36,36,36	1.19	3 (8%)	47,47,47	1.61	9 (19%)
22	CLA	P	213	12	45,49,73	1.48	7 (15%)	54,84,113	1.21	4 (7%)
22	CLA	G	208	-	59,63,73	1.24	6 (10%)	70,101,113	1.08	6 (8%)
25	BCR	B	838	-	41,41,41	1.09	3 (7%)	56,56,56	1.27	6 (10%)
22	CLA	S	206	15	50,54,73	1.34	6 (12%)	59,90,113	1.08	4 (6%)
22	CLA	F	803	35	52,56,73	1.40	7 (13%)	61,92,113	1.20	6 (9%)
25	BCR	L	205	-	41,41,41	1.04	2 (4%)	56,56,56	1.31	5 (8%)
22	CLA	Q	205	13	64,68,73	1.21	8 (12%)	76,107,113	0.91	3 (3%)
22	CLA	Q	213	35	61,65,73	1.24	7 (11%)	72,103,113	1.06	7 (9%)
22	CLA	A	822	35	69,73,73	1.12	6 (8%)	82,113,113	0.91	4 (4%)
22	CLA	B	804	2	69,73,73	1.16	7 (10%)	82,113,113	0.91	4 (4%)
25	BCR	J	104	-	41,41,41	1.08	2 (4%)	56,56,56	1.20	4 (7%)
22	CLA	U	211	16	56,60,73	1.33	7 (12%)	65,97,113	1.08	5 (7%)
22	CLA	A	812	1	49,53,73	1.42	8 (16%)	58,89,113	1.04	4 (6%)
31	DD6	J	101	-	40,45,45	1.27	8 (20%)	51,67,67	1.57	9 (17%)
22	CLA	O	205	11	69,73,73	1.22	7 (10%)	82,113,113	0.91	4 (4%)
31	DD6	O	214	-	40,45,45	1.24	7 (17%)	51,67,67	1.54	9 (17%)
25	BCR	F	801	-	41,41,41	1.03	2 (4%)	56,56,56	1.22	2 (3%)
22	CLA	G	210	17	49,53,73	1.51	8 (16%)	58,89,113	1.03	4 (6%)
22	CLA	A	806	1	69,73,73	1.14	8 (11%)	82,113,113	1.00	4 (4%)
22	CLA	B	807	2	69,73,73	1.23	7 (10%)	82,113,113	0.90	3 (3%)
22	CLA	B	813	2	59,63,73	1.40	8 (13%)	70,101,113	0.94	3 (4%)
22	CLA	H	207	18	69,73,73	1.14	8 (11%)	82,113,113	1.13	7 (8%)
23	PQN	B	835	-	34,34,34	0.41	0	43,45,45	0.55	1 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	A	835	1	69,73,73	1.23	7 (10%)	82,113,113	0.92	3 (3%)
31	DD6	O	213	-	40,45,45	1.33	8 (20%)	51,67,67	1.38	8 (15%)
34	A86	Q	214	-	47,50,50	1.37	5 (10%)	51,76,76	1.41	8 (15%)
24	LHG	G	216	-	26,26,48	0.86	1 (3%)	29,32,54	1.20	2 (6%)
22	CLA	A	838	24	56,60,73	1.33	8 (14%)	65,97,113	1.06	5 (7%)
25	BCR	B	839	-	41,41,41	1.06	2 (4%)	56,56,56	1.20	5 (8%)
25	BCR	I	101	-	41,41,41	1.07	2 (4%)	56,56,56	1.29	6 (10%)
26	LMU	O	216	-	36,36,36	1.23	2 (5%)	47,47,47	1.07	2 (4%)
22	CLA	O	204	11	69,73,73	1.19	8 (11%)	82,113,113	0.90	4 (4%)
22	CLA	B	827	2	62,66,73	1.30	7 (11%)	73,104,113	1.00	6 (8%)
22	CLA	A	854	1	69,73,73	1.14	6 (8%)	82,113,113	0.93	6 (7%)
22	CLA	A	816	1	69,73,73	1.17	8 (11%)	82,113,113	0.95	4 (4%)
22	CLA	B	810	2	59,63,73	1.22	7 (11%)	70,101,113	0.96	5 (7%)
22	CLA	A	818	35	69,73,73	1.14	7 (10%)	82,113,113	0.96	5 (6%)
22	CLA	k	103	35	59,63,73	1.30	7 (11%)	70,101,113	0.98	3 (4%)
31	DD6	U	214	-	24,26,45	1.52	5 (20%)	29,35,67	1.59	6 (20%)
32	LMG	P	217	-	25,25,55	1.38	4 (16%)	33,33,63	1.47	7 (21%)
22	CLA	B	806	2	69,73,73	1.17	7 (10%)	82,113,113	0.90	3 (3%)
22	CLA	Q	204	-	65,69,73	1.18	6 (9%)	77,108,113	0.99	4 (5%)
22	CLA	P	216	12	51,55,73	1.39	7 (13%)	60,91,113	1.14	5 (8%)
22	CLA	k	102	21	46,50,73	1.44	7 (15%)	53,85,113	1.08	3 (5%)
22	CLA	B	803	2	49,53,73	1.46	8 (16%)	58,89,113	1.01	3 (5%)
31	DD6	H	201	-	40,45,45	1.42	9 (22%)	51,67,67	1.67	11 (21%)
22	CLA	U	209	16	46,50,73	1.68	8 (17%)	53,85,113	1.05	3 (5%)
31	DD6	P	220	-	40,45,45	1.30	7 (17%)	51,67,67	1.70	12 (23%)
22	CLA	A	848	1	69,73,73	1.20	8 (11%)	82,113,113	1.04	6 (7%)
22	CLA	B	805	2	69,73,73	1.20	8 (11%)	82,113,113	0.86	4 (4%)
22	CLA	B	845	2	69,73,73	1.19	8 (11%)	82,113,113	1.21	9 (10%)
32	LMG	P	202	-	34,34,55	1.02	2 (5%)	42,42,63	1.28	4 (9%)
33	KC1	T	208	20	49,53,53	1.77	10 (20%)	61,89,89	1.06	2 (3%)
26	LMU	M	102	-	36,36,36	1.18	2 (5%)	47,47,47	1.03	2 (4%)
22	CLA	P	207	12	69,73,73	1.14	7 (10%)	82,113,113	0.97	4 (4%)
26	LMU	P	221	-	26,26,36	1.28	2 (7%)	37,37,47	1.36	4 (10%)
22	CLA	T	201	-	46,50,73	1.48	8 (17%)	53,85,113	1.03	3 (5%)
22	CLA	O	211	11	45,49,73	1.45	7 (15%)	54,84,113	1.20	5 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	Q	216	35	69,73,73	1.13	7 (10%)	82,113,113	0.88	4 (4%)
22	CLA	A	830	1	54,58,73	1.34	7 (12%)	64,95,113	0.94	3 (4%)
32	LMG	Q	217	-	55,55,55	0.70	0	63,63,63	1.32	6 (9%)
22	CLA	B	823	2	69,73,73	1.25	7 (10%)	82,113,113	0.97	5 (6%)
22	CLA	S	207	15	50,54,73	1.49	7 (14%)	59,90,113	1.07	5 (8%)
22	CLA	Q	203	13	52,56,73	1.33	7 (13%)	61,92,113	1.04	4 (6%)
25	BCR	F	805	-	41,41,41	1.05	2 (4%)	56,56,56	1.18	5 (8%)
22	CLA	A	819	1	47,51,73	1.42	7 (14%)	55,86,113	1.04	3 (5%)
22	CLA	B	826	2	53,57,73	1.39	7 (13%)	61,93,113	0.99	3 (4%)
22	CLA	L	204	35	54,58,73	1.32	7 (12%)	64,95,113	1.11	6 (9%)
22	CLA	B	812	2	63,67,73	1.27	9 (14%)	74,105,113	0.92	4 (5%)
22	CLA	B	824	2	69,73,73	1.25	7 (10%)	82,113,113	0.85	2 (2%)
26	LMU	A	857	-	36,36,36	0.42	0	47,47,47	0.74	1 (2%)
22	CLA	A	824	1	66,70,73	1.22	7 (10%)	78,109,113	0.97	3 (3%)
31	DD6	U	212	-	40,45,45	1.30	7 (17%)	51,67,67	1.66	10 (19%)
22	CLA	A	820	1	55,59,73	1.36	7 (12%)	64,96,113	1.12	5 (7%)
30	SQD	B	846	-	48,50,54	1.00	5 (10%)	58,61,65	1.55	9 (15%)
22	CLA	G	202	-	45,49,73	1.42	6 (13%)	54,84,113	1.12	5 (9%)
22	CLA	A	833	1	69,73,73	1.22	7 (10%)	82,113,113	0.92	4 (4%)
22	CLA	Q	212	13	69,73,73	1.23	7 (10%)	82,113,113	0.99	7 (8%)
25	BCR	M	101	-	41,41,41	1.09	2 (4%)	56,56,56	1.29	7 (12%)
28	SF4	A	852	1,2	0,12,12	-	-	-	-	-
31	DD6	O	201	-	40,45,45	1.29	7 (17%)	51,67,67	1.46	10 (19%)
22	CLA	Q	209	13	69,73,73	1.21	7 (10%)	82,113,113	0.86	3 (3%)
25	BCR	R	102	-	40,40,41	1.18	2 (5%)	54,54,56	1.43	11 (20%)
22	CLA	A	811	1	69,73,73	1.18	8 (11%)	82,113,113	0.92	3 (3%)
22	CLA	G	205	17	65,69,73	1.15	6 (9%)	77,108,113	1.06	8 (10%)
22	CLA	B	847	2	54,58,73	1.33	7 (12%)	64,95,113	1.02	3 (4%)
22	CLA	H	213	-	69,73,73	1.15	5 (7%)	82,113,113	1.11	7 (8%)
22	CLA	T	206	20	46,50,73	1.83	8 (17%)	53,85,113	1.03	3 (5%)
22	CLA	A	827	1	54,58,73	1.40	7 (12%)	64,95,113	0.97	4 (6%)
22	CLA	A	834	1	69,73,73	1.30	9 (13%)	82,113,113	0.88	4 (4%)
22	CLA	P	210	35	51,55,73	1.35	6 (11%)	60,91,113	1.06	4 (6%)
22	CLA	A	856	-	50,54,73	1.33	7 (14%)	59,90,113	1.04	4 (6%)
29	DGD	B	841	-	61,61,67	0.95	1 (1%)	75,75,81	1.33	7 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	DD6	T	213	-	40,45,45	1.33	6 (15%)	51,67,67	2.05	12 (23%)
22	CLA	B	843	2	69,73,73	1.27	6 (8%)	82,113,113	0.88	3 (3%)
31	DD6	G	211	-	40,45,45	1.31	8 (20%)	51,67,67	1.45	7 (13%)
22	CLA	A	814	35	49,53,73	1.39	7 (14%)	58,89,113	1.11	6 (10%)
22	CLA	P	211	12	54,58,73	1.27	7 (12%)	64,95,113	1.01	4 (6%)
31	DD6	k	101	-	40,45,45	1.30	8 (20%)	51,67,67	1.47	10 (19%)
22	CLA	B	821	2	69,73,73	1.24	7 (10%)	82,113,113	0.90	4 (4%)
22	CLA	U	205	16	69,73,73	1.18	7 (10%)	82,113,113	0.91	3 (3%)
22	CLA	A	810	1	58,62,73	1.27	6 (10%)	68,99,113	1.06	4 (5%)
22	CLA	A	823	1	69,73,73	1.22	7 (10%)	82,113,113	0.87	3 (3%)
33	KC1	P	219	12	49,53,53	1.55	9 (18%)	61,89,89	0.86	1 (1%)
22	CLA	B	808	2	69,73,73	1.19	8 (11%)	82,113,113	0.91	5 (6%)
25	BCR	A	843	-	41,41,41	1.06	2 (4%)	56,56,56	1.23	4 (7%)
26	LMU	F	807	-	36,36,36	1.21	2 (5%)	47,47,47	0.97	2 (4%)
22	CLA	B	814	2	63,67,73	1.20	6 (9%)	74,105,113	1.01	5 (6%)
22	CLA	U	206	16	49,53,73	1.39	7 (14%)	58,89,113	0.99	3 (5%)
22	CLA	H	209	18	45,49,73	1.43	7 (15%)	54,84,113	1.22	4 (7%)
22	CLA	B	829	2	62,66,73	1.27	8 (12%)	73,104,113	1.03	4 (5%)
22	CLA	A	804	1	69,73,73	1.16	7 (10%)	82,113,113	0.91	6 (7%)
27	CL0	A	849	1	58,73,73	0.97	4 (6%)	60,113,113	1.83	10 (16%)
34	A86	Q	201	-	47,50,50	1.32	5 (10%)	51,76,76	1.41	8 (15%)
22	CLA	F	804	6	50,54,73	1.38	7 (14%)	59,90,113	1.06	4 (6%)
32	LMG	J	102	-	39,39,55	0.87	0	47,47,63	1.24	4 (8%)
22	CLA	A	845	35	69,73,73	1.19	7 (10%)	82,113,113	0.87	3 (3%)
22	CLA	A	851	1	69,73,73	1.20	7 (10%)	82,113,113	0.91	3 (3%)
22	CLA	B	815	2	64,68,73	1.23	7 (10%)	76,107,113	0.95	4 (5%)
25	BCR	B	836	-	41,41,41	1.09	2 (4%)	56,56,56	1.18	5 (8%)
22	CLA	B	844	2	69,73,73	1.24	7 (10%)	82,113,113	1.01	4 (4%)
22	CLA	L	203	9	69,73,73	1.15	7 (10%)	82,113,113	0.88	4 (4%)
34	A86	R	103	-	44,46,50	1.50	3 (6%)	49,70,76	1.69	14 (28%)
22	CLA	B	822	2	69,73,73	1.21	6 (8%)	82,113,113	0.92	3 (3%)
22	CLA	Q	208	13	54,58,73	1.33	8 (14%)	64,95,113	1.41	7 (10%)
22	CLA	K	205	19	59,63,73	1.25	7 (11%)	70,101,113	0.98	4 (5%)
31	DD6	S	214	-	40,45,45	1.24	7 (17%)	51,67,67	1.69	10 (19%)
22	CLA	B	818	2	57,61,73	1.26	8 (14%)	67,98,113	0.97	5 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	T	211	-	51,55,73	1.35	7 (13%)	60,91,113	1.16	5 (8%)
25	BCR	k	104	-	41,41,41	1.06	2 (4%)	56,56,56	1.29	6 (10%)
22	CLA	A	831	1	49,53,73	1.38	7 (14%)	58,89,113	1.14	4 (6%)
22	CLA	A	801	-	69,73,73	1.16	8 (11%)	82,113,113	0.86	4 (4%)
22	CLA	T	210	20	50,54,73	1.42	7 (14%)	59,90,113	1.11	5 (8%)
22	CLA	R	101	35	49,53,73	1.43	8 (16%)	58,89,113	1.08	4 (6%)
22	CLA	S	209	15	56,60,73	1.25	4 (7%)	65,97,113	1.04	4 (6%)
22	CLA	H	205	18	47,52,73	1.43	8 (17%)	55,87,113	1.06	3 (5%)
22	CLA	T	202	20	45,49,73	1.41	7 (15%)	54,84,113	1.14	5 (9%)
22	CLA	O	207	11	50,54,73	1.37	7 (14%)	59,90,113	1.11	6 (10%)
22	CLA	S	216	35	69,73,73	1.13	7 (10%)	82,113,113	0.91	4 (4%)
25	BCR	A	842	-	41,41,41	1.08	2 (4%)	56,56,56	1.13	4 (7%)
33	KC1	P	206	12	49,53,53	1.64	11 (22%)	61,89,89	0.80	1 (1%)
31	DD6	P	218	-	40,45,45	1.33	8 (20%)	51,67,67	1.91	11 (21%)
22	CLA	P	208	12	60,64,73	1.27	8 (13%)	71,102,113	0.98	4 (5%)
22	CLA	O	202	11	47,51,73	1.39	6 (12%)	55,86,113	1.14	5 (9%)
32	LMG	U	201	-	32,32,55	0.99	0	40,40,63	1.13	2 (5%)
31	DD6	K	208	-	40,45,45	1.37	9 (22%)	51,67,67	1.60	9 (17%)
22	CLA	F	802	35	69,73,73	1.19	8 (11%)	82,113,113	0.98	4 (4%)
34	A86	P	204	-	47,50,50	1.36	5 (10%)	51,76,76	1.45	9 (17%)
22	CLA	B	825	2	54,58,73	1.42	8 (14%)	64,95,113	0.96	4 (6%)
31	DD6	G	214	-	40,45,45	1.33	7 (17%)	51,67,67	1.63	13 (25%)
22	CLA	B	820	35	68,72,73	1.14	6 (8%)	80,111,113	0.92	4 (5%)
22	CLA	P	214	12	49,53,73	1.46	7 (14%)	58,89,113	1.11	4 (6%)
34	A86	Q	218	-	47,50,50	1.40	5 (10%)	51,76,76	1.42	9 (17%)
22	CLA	A	817	1	49,53,73	1.40	7 (14%)	58,89,113	1.13	4 (6%)
22	CLA	A	836	35	69,73,73	1.16	8 (11%)	82,113,113	0.96	4 (4%)
31	DD6	P	205	-	40,45,45	1.26	7 (17%)	51,67,67	1.58	10 (19%)
22	CLA	A	855	-	44,48,73	1.47	8 (18%)	51,82,113	1.33	7 (13%)
22	CLA	A	850	35	69,73,73	1.14	7 (10%)	82,113,113	0.92	4 (4%)
22	CLA	U	208	16	50,54,73	1.36	7 (14%)	59,90,113	1.16	6 (10%)
22	CLA	A	853	1	69,73,73	1.17	7 (10%)	82,113,113	0.90	3 (3%)
22	CLA	G	215	17	49,53,73	1.35	5 (10%)	58,89,113	1.17	4 (6%)
22	CLA	O	209	11	69,73,73	1.19	7 (10%)	82,113,113	1.03	5 (6%)
22	CLA	S	202	35	69,73,73	1.11	5 (7%)	82,113,113	1.08	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	A	825	1	69,73,73	1.21	7 (10%)	82,113,113	0.87	4 (4%)
22	CLA	G	203	17	49,53,73	1.45	7 (14%)	58,89,113	1.12	4 (6%)
22	CLA	B	809	2	58,62,73	1.40	9 (15%)	71,100,113	0.94	4 (5%)
22	CLA	O	208	11	64,68,73	1.17	7 (10%)	76,107,113	0.93	4 (5%)
22	CLA	P	209	-	56,60,73	1.29	6 (10%)	65,97,113	0.98	5 (7%)
22	CLA	H	210	18	49,53,73	1.49	7 (14%)	58,89,113	1.08	5 (8%)
22	CLA	G	209	17	60,64,73	1.22	6 (10%)	71,102,113	1.08	6 (8%)
22	CLA	G	207	17	64,68,73	1.15	6 (9%)	76,107,113	1.03	4 (5%)
23	PQN	A	837	-	34,34,34	0.40	0	43,45,45	0.59	1 (2%)
28	SF4	C	102	3	0,12,12	-	-	-	-	-
33	KC1	P	212	12	46,52,53	1.70	9 (19%)	59,87,89	1.18	6 (10%)
22	CLA	B	817	2	50,54,73	1.37	7 (14%)	59,90,113	1.08	4 (6%)
24	LHG	A	839	-	47,47,48	0.65	2 (4%)	50,53,54	1.22	5 (10%)
22	CLA	A	805	1	53,57,73	1.40	7 (13%)	61,93,113	0.99	4 (6%)
26	LMU	A	847	-	36,36,36	1.21	2 (5%)	47,47,47	0.89	1 (2%)
25	BCR	L	201	-	41,41,41	1.09	2 (4%)	56,56,56	1.19	4 (7%)
22	CLA	A	826	1	69,73,73	1.29	8 (11%)	82,113,113	0.81	3 (3%)
22	CLA	K	207	19	62,66,73	1.21	6 (9%)	73,104,113	1.18	6 (8%)
22	CLA	B	819	35	67,71,73	1.21	7 (10%)	79,110,113	1.00	5 (6%)
22	CLA	B	811	2	58,62,73	1.32	7 (12%)	68,99,113	0.96	4 (5%)
31	DD6	G	212	-	40,45,45	1.31	7 (17%)	51,67,67	1.53	10 (19%)
33	KC1	S	210	15	49,53,53	1.61	9 (18%)	61,89,89	1.09	4 (6%)
25	BCR	B	840	-	41,41,41	1.08	2 (4%)	56,56,56	1.18	5 (8%)
22	CLA	H	204	18	65,69,73	1.16	6 (9%)	77,108,113	0.98	4 (5%)
22	CLA	K	206	19	49,53,73	1.54	8 (16%)	58,89,113	0.98	3 (5%)
22	CLA	B	801	2	69,73,73	1.24	6 (8%)	82,113,113	0.79	3 (3%)
25	BCR	A	841	-	41,41,41	1.02	2 (4%)	56,56,56	1.26	2 (3%)
22	CLA	B	802	-	69,73,73	1.16	7 (10%)	82,113,113	0.97	7 (8%)
22	CLA	L	202	9	53,57,73	1.35	8 (15%)	61,93,113	1.13	6 (9%)
22	CLA	Q	207	13	50,54,73	1.37	8 (16%)	59,90,113	1.19	7 (11%)
25	BCR	I	102	-	41,41,41	1.06	2 (4%)	56,56,56	1.26	4 (7%)
22	CLA	G	201	17	49,53,73	1.38	6 (12%)	58,89,113	1.07	4 (6%)
31	DD6	S	204	-	40,45,45	1.28	7 (17%)	51,67,67	1.51	9 (17%)
31	DD6	G	213	-	40,45,45	1.29	8 (20%)	51,67,67	1.42	7 (13%)
33	KC1	Q	210	13	49,53,53	1.59	9 (18%)	61,89,89	1.12	6 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	DD6	P	215	-	40,45,45	1.35	7 (17%)	51,67,67	1.83	11 (21%)
22	CLA	A	846	1	64,68,73	1.31	7 (10%)	76,107,113	0.91	4 (5%)
22	CLA	H	202	-	44,48,73	1.43	6 (13%)	51,82,113	1.44	7 (13%)
31	DD6	T	212	-	40,45,45	1.32	7 (17%)	51,67,67	1.67	9 (17%)
22	CLA	B	831	2	51,55,73	1.39	6 (11%)	60,91,113	1.02	4 (6%)
22	CLA	B	816	35	69,73,73	1.18	7 (10%)	82,113,113	0.90	4 (4%)
26	LMU	F	806	-	36,36,36	1.28	3 (8%)	47,47,47	1.55	8 (17%)
22	CLA	A	802	1	59,63,73	1.24	8 (13%)	70,101,113	0.95	4 (5%)
31	DD6	U	203	-	40,45,45	1.34	7 (17%)	51,67,67	1.74	12 (23%)
22	CLA	A	828	1	69,73,73	1.26	7 (10%)	82,113,113	0.85	3 (3%)
22	CLA	A	832	1	55,59,73	1.35	8 (14%)	64,96,113	1.07	5 (7%)
22	CLA	T	209	20	45,49,73	1.46	7 (15%)	54,84,113	1.18	5 (9%)
22	CLA	R	104	14	69,73,73	1.31	8 (11%)	82,113,113	0.92	5 (6%)
22	CLA	T	207	20	69,73,73	1.11	5 (7%)	82,113,113	0.95	5 (6%)
22	CLA	H	203	18	64,68,73	1.24	8 (12%)	76,107,113	0.97	5 (6%)
22	CLA	O	203	-	49,53,73	1.40	8 (16%)	58,89,113	1.11	4 (6%)
34	A86	R	105	-	47,50,50	1.40	5 (10%)	51,76,76	1.28	8 (15%)
22	CLA	S	217	15	69,73,73	1.16	7 (10%)	82,113,113	1.03	6 (7%)
22	CLA	T	205	-	50,54,73	1.34	6 (12%)	59,90,113	1.14	5 (8%)
32	LMG	S	213	-	49,49,55	0.73	1 (2%)	57,57,63	1.29	6 (10%)
33	KC1	S	212	15	49,53,53	1.56	7 (14%)	61,89,89	1.20	6 (9%)
22	CLA	B	832	35	69,73,73	1.19	8 (11%)	82,113,113	0.95	4 (4%)
22	CLA	B	833	2	69,73,73	1.23	7 (10%)	82,113,113	0.90	4 (4%)
22	CLA	A	815	1	69,73,73	1.21	7 (10%)	82,113,113	0.98	5 (6%)
22	CLA	A	809	1	66,70,73	1.19	7 (10%)	78,109,113	0.88	4 (5%)
22	CLA	T	203	20	50,54,73	1.40	7 (14%)	59,90,113	1.00	3 (5%)
34	A86	U	202	-	47,50,50	1.36	5 (10%)	51,76,76	1.39	7 (13%)
25	BCR	B	837	-	41,41,41	1.04	2 (4%)	56,56,56	1.20	3 (5%)
22	CLA	J	103	8	46,50,73	1.40	7 (15%)	53,85,113	1.03	4 (7%)
31	DD6	Q	202	-	40,45,45	1.31	8 (20%)	51,67,67	1.70	14 (27%)
31	DD6	O	215	-	40,45,45	1.29	7 (17%)	51,67,67	1.60	11 (21%)
22	CLA	U	207	35	69,73,73	1.10	6 (8%)	82,113,113	1.08	8 (9%)
31	DD6	H	212	-	40,45,45	1.31	7 (17%)	51,67,67	1.55	11 (21%)
26	LMU	K	202	-	25,25,36	1.24	3 (12%)	36,36,47	1.82	11 (30%)
24	LHG	P	201	-	48,48,48	0.61	2 (4%)	51,54,54	1.26	5 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	LHG	A	840	22	26,26,48	0.88	1 (3%)	29,32,54	1.32	3 (10%)
22	CLA	U	204	35	65,69,73	1.19	7 (10%)	77,108,113	0.96	4 (5%)
22	CLA	A	803	1	69,73,73	1.14	7 (10%)	82,113,113	0.93	4 (4%)
22	CLA	A	813	1	54,58,73	1.40	6 (11%)	64,95,113	1.10	5 (7%)
22	CLA	G	204	17	47,51,73	1.39	7 (14%)	55,86,113	1.08	3 (5%)
31	DD6	S	215	-	40,45,45	1.28	7 (17%)	51,67,67	1.66	10 (19%)
22	CLA	G	206	17	69,73,73	1.31	7 (10%)	82,113,113	0.92	4 (4%)
22	CLA	U	210	16	69,73,73	1.14	6 (8%)	82,113,113	0.92	5 (6%)
22	CLA	A	821	35	69,73,73	1.20	7 (10%)	82,113,113	0.95	4 (4%)
33	KC1	O	210	11	49,53,53	1.60	10 (20%)	61,89,89	1.19	5 (8%)
22	CLA	Q	211	13	45,49,73	1.48	7 (15%)	54,84,113	1.22	5 (9%)
22	CLA	K	204	19	46,50,73	1.42	7 (15%)	53,85,113	1.17	5 (9%)
28	SF4	C	101	3	0,12,12	-	-	-	-	-
31	DD6	Q	215	-	40,45,45	1.27	8 (20%)	51,67,67	1.52	10 (19%)
31	DD6	S	205	-	40,45,45	1.29	8 (20%)	51,67,67	1.49	10 (19%)
22	CLA	K	203	19	49,53,73	1.69	9 (18%)	58,89,113	1.84	12 (20%)
31	DD6	H	211	-	40,45,45	1.29	6 (15%)	51,67,67	1.71	10 (19%)
22	CLA	B	834	35	69,73,73	1.19	8 (11%)	82,113,113	0.95	6 (7%)
33	KC1	U	213	16	49,53,53	1.65	11 (22%)	61,89,89	0.90	3 (4%)
22	CLA	B	842	2	69,73,73	1.23	9 (13%)	82,113,113	0.92	3 (3%)
25	BCR	A	844	-	41,41,41	1.10	2 (4%)	56,56,56	1.21	6 (10%)
22	CLA	S	208	15	49,53,73	1.31	5 (10%)	58,89,113	1.10	5 (8%)
22	CLA	H	208	-	62,66,73	1.20	6 (9%)	73,104,113	0.96	4 (5%)
22	CLA	T	204	-	61,65,73	1.20	5 (8%)	72,103,113	0.98	4 (5%)
33	KC1	P	203	-	49,53,53	1.70	11 (22%)	61,89,89	0.87	1 (1%)
30	SQD	S	201	-	44,46,54	1.03	4 (9%)	54,57,65	1.51	9 (16%)
22	CLA	B	830	2	69,73,73	1.20	6 (8%)	82,113,113	0.88	4 (4%)
31	DD6	O	212	-	40,45,45	1.34	9 (22%)	51,67,67	1.66	10 (19%)
22	CLA	A	808	1	60,64,73	1.27	8 (13%)	71,102,113	0.93	3 (4%)
31	DD6	S	211	-	40,45,45	1.26	7 (17%)	51,67,67	1.45	7 (13%)
26	LMU	S	203	-	32,32,36	1.35	4 (12%)	43,43,47	1.62	6 (13%)
22	CLA	Q	206	13	54,59,73	1.42	7 (12%)	62,96,113	0.96	3 (4%)
22	CLA	H	206	18	49,53,73	1.48	7 (14%)	58,89,113	0.95	3 (5%)
22	CLA	O	206	35	69,73,73	1.17	7 (10%)	82,113,113	0.92	5 (6%)
22	CLA	A	829	1	69,73,73	1.19	6 (8%)	82,113,113	0.90	4 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	LMU	L	206	-	36,36,36	1.18	2 (5%)	47,47,47	1.22	3 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	A	807	1	-	3/39/115/115	-
22	CLA	B	828	35	1/1/15/20	1/39/115/115	-
26	LMU	K	201	-	-	9/21/61/61	0/2/2/2
22	CLA	P	213	12	1/1/10/20	2/10/86/115	-
22	CLA	G	208	-	1/1/13/20	2/27/103/115	-
25	BCR	B	838	-	-	3/29/63/63	0/2/2/2
22	CLA	S	206	15	1/1/11/20	0/17/93/115	-
22	CLA	F	803	35	1/1/11/20	3/19/95/115	-
25	BCR	L	205	-	-	8/29/63/63	0/2/2/2
22	CLA	Q	205	13	1/1/14/20	4/33/109/115	-
22	CLA	Q	213	35	1/1/13/20	7/30/106/115	-
22	CLA	A	822	35	1/1/15/20	3/39/115/115	-
22	CLA	B	804	2	1/1/15/20	8/39/115/115	-
25	BCR	J	104	-	-	7/29/63/63	0/2/2/2
22	CLA	U	211	16	1/1/12/20	6/24/100/115	-
22	CLA	A	812	1	1/1/11/20	0/15/91/115	-
31	DD6	J	101	-	-	5/26/80/80	0/3/3/3
22	CLA	O	205	11	1/1/15/20	9/39/115/115	-
31	DD6	O	214	-	-	8/26/80/80	0/3/3/3
25	BCR	F	801	-	-	4/29/63/63	0/2/2/2
22	CLA	G	210	17	1/1/11/20	4/15/91/115	-
22	CLA	A	806	1	1/1/15/20	7/39/115/115	-
22	CLA	B	807	2	1/1/15/20	5/39/115/115	-
22	CLA	B	813	2	-	2/27/103/115	-
22	CLA	H	207	18	-	11/39/115/115	-
23	PQN	B	835	-	-	1/23/43/43	0/2/2/2
22	CLA	A	835	1	1/1/15/20	1/39/115/115	-
31	DD6	O	213	-	-	11/26/80/80	0/3/3/3
34	A86	Q	214	-	-	11/34/90/90	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	LHG	G	216	-	-	14/31/31/53	-
22	CLA	A	838	24	1/1/12/20	2/24/100/115	-
25	BCR	B	839	-	-	4/29/63/63	0/2/2/2
25	BCR	I	101	-	-	3/29/63/63	0/2/2/2
26	LMU	O	216	-	-	14/21/61/61	0/2/2/2
22	CLA	O	204	11	-	1/39/115/115	-
22	CLA	A	854	1	1/1/15/20	6/39/115/115	-
22	CLA	k	103	35	1/1/13/20	3/27/103/115	-
22	CLA	A	816	1	1/1/15/20	0/39/115/115	-
22	CLA	B	810	2	-	1/27/103/115	-
22	CLA	A	818	35	1/1/15/20	2/39/115/115	-
22	CLA	B	827	2	-	4/31/107/115	-
31	DD6	U	214	-	-	8/14/37/80	0/1/1/3
32	LMG	P	217	-	-	12/19/39/70	0/1/1/1
22	CLA	B	806	2	-	3/39/115/115	-
22	CLA	Q	204	-	1/1/14/20	5/35/111/115	-
22	CLA	P	216	12	1/1/11/20	0/18/94/115	-
22	CLA	k	102	21	1/1/10/20	0/12/88/115	-
22	CLA	B	803	2	1/1/11/20	4/15/91/115	-
31	DD6	H	201	-	-	12/26/80/80	0/3/3/3
22	CLA	U	209	16	-	0/12/88/115	-
31	DD6	P	220	-	-	11/26/80/80	0/3/3/3
22	CLA	B	805	2	1/1/15/20	4/39/115/115	-
22	CLA	B	845	2	1/1/15/20	7/39/115/115	-
22	CLA	A	848	1	-	5/39/115/115	-
32	LMG	P	202	-	-	12/29/49/70	0/1/1/1
33	KC1	T	208	20	-	1/15/71/71	-
26	LMU	M	102	-	-	9/21/61/61	0/2/2/2
22	CLA	P	207	12	1/1/15/20	8/39/115/115	-
26	LMU	P	221	-	-	6/11/51/61	0/2/2/2
22	CLA	T	201	-	1/1/10/20	1/12/88/115	-
22	CLA	O	211	11	-	0/10/86/115	-
22	CLA	Q	216	35	-	7/39/115/115	-
22	CLA	A	830	1	-	1/21/97/115	-
32	LMG	Q	217	-	-	24/50/70/70	0/1/1/1
22	CLA	B	823	2	-	3/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	S	207	15	1/1/11/20	3/17/93/115	-
22	CLA	Q	203	13	-	2/19/95/115	-
25	BCR	F	805	-	-	6/29/63/63	0/2/2/2
22	CLA	A	819	1	-	0/13/89/115	-
22	CLA	B	826	2	1/1/11/20	2/20/96/115	-
22	CLA	L	204	35	1/1/12/20	7/21/97/115	-
22	CLA	B	812	2	-	2/32/108/115	-
22	CLA	B	824	2	-	3/39/115/115	-
26	LMU	A	857	-	-	12/21/61/61	0/2/2/2
22	CLA	A	824	1	1/1/14/20	4/36/112/115	-
31	DD6	U	212	-	-	13/26/80/80	0/3/3/3
22	CLA	A	820	1	1/1/12/20	4/23/99/115	-
30	SQD	B	846	-	-	17/45/65/69	0/1/1/1
22	CLA	G	202	-	1/1/10/20	0/10/86/115	-
22	CLA	A	833	1	1/1/15/20	3/39/115/115	-
22	CLA	Q	212	13	-	8/39/115/115	-
25	BCR	M	101	-	-	6/29/63/63	0/2/2/2
31	DD6	O	201	-	-	6/26/80/80	0/3/3/3
28	SF4	A	852	1,2	-	-	0/6/5/5
22	CLA	Q	209	13	-	10/39/115/115	-
25	BCR	R	102	-	-	10/27/61/63	0/2/2/2
22	CLA	A	811	1	1/1/15/20	3/39/115/115	-
22	CLA	H	213	-	1/1/15/20	10/39/115/115	-
22	CLA	B	847	2	1/1/12/20	4/21/97/115	-
22	CLA	G	205	17	-	9/35/111/115	-
22	CLA	T	206	20	-	0/12/88/115	-
22	CLA	A	827	1	-	3/21/97/115	-
22	CLA	A	834	1	-	5/39/115/115	-
22	CLA	P	210	35	-	4/18/94/115	-
22	CLA	A	856	-	1/1/11/20	4/17/93/115	-
29	DGD	B	841	-	-	19/49/89/95	0/2/2/2
31	DD6	T	213	-	-	12/26/80/80	0/3/3/3
22	CLA	B	843	2	1/1/15/20	3/39/115/115	-
31	DD6	G	211	-	-	8/26/80/80	0/3/3/3
22	CLA	A	814	35	-	5/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	P	211	12	-	2/21/97/115	-
31	DD6	k	101	-	-	10/26/80/80	0/3/3/3
22	CLA	B	821	2	1/1/15/20	0/39/115/115	-
22	CLA	U	205	16	-	4/39/115/115	-
22	CLA	A	810	1	1/1/12/20	0/26/102/115	-
22	CLA	A	823	1	1/1/15/20	2/39/115/115	-
33	KC1	P	219	12	-	3/15/71/71	-
22	CLA	B	808	2	1/1/15/20	4/39/115/115	-
25	BCR	A	843	-	-	3/29/63/63	0/2/2/2
26	LMU	F	807	-	-	7/21/61/61	0/2/2/2
22	CLA	H	209	18	1/1/10/20	2/10/86/115	-
22	CLA	U	206	16	1/1/11/20	3/15/91/115	-
22	CLA	B	814	2	-	6/32/108/115	-
22	CLA	B	829	2	1/1/13/20	3/31/107/115	-
22	CLA	A	804	1	1/1/15/20	9/39/115/115	-
27	CL0	A	849	1	-	8/37/135/135	-
34	A86	Q	201	-	-	13/34/90/90	0/3/3/3
22	CLA	F	804	6	1/1/11/20	3/17/93/115	-
32	LMG	J	102	-	-	27/34/54/70	0/1/1/1
22	CLA	A	845	35	1/1/15/20	6/39/115/115	-
22	CLA	B	815	2	1/1/14/20	2/33/109/115	-
22	CLA	A	851	1	-	4/39/115/115	-
25	BCR	B	836	-	-	8/29/63/63	0/2/2/2
22	CLA	B	844	2	1/1/15/20	2/39/115/115	-
22	CLA	L	203	9	-	0/39/115/115	-
34	A86	R	103	-	-	8/30/84/90	0/3/3/3
22	CLA	B	822	2	1/1/15/20	5/39/115/115	-
22	CLA	Q	208	13	1/1/12/20	1/21/97/115	-
22	CLA	K	205	19	1/1/13/20	4/27/103/115	-
31	DD6	S	214	-	-	16/26/80/80	0/3/3/3
22	CLA	B	818	2	-	1/25/101/115	-
22	CLA	T	211	-	1/1/11/20	4/18/94/115	-
25	BCR	k	104	-	-	8/29/63/63	0/2/2/2
22	CLA	A	831	1	1/1/11/20	2/15/91/115	-
22	CLA	A	801	-	-	3/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	T	210	20	-	4/17/93/115	-
22	CLA	R	101	35	1/1/11/20	0/15/91/115	-
22	CLA	S	209	15	-	3/24/100/115	-
22	CLA	H	205	18	1/1/10/20	2/14/90/115	-
22	CLA	T	202	20	1/1/10/20	1/10/86/115	-
22	CLA	O	207	11	1/1/11/20	4/17/93/115	-
22	CLA	S	216	35	1/1/15/20	0/39/115/115	-
25	BCR	A	842	-	-	8/29/63/63	0/2/2/2
33	KC1	P	206	12	-	2/15/71/71	-
31	DD6	P	218	-	-	11/26/80/80	0/3/3/3
22	CLA	P	208	12	1/1/13/20	5/29/105/115	-
22	CLA	O	202	11	-	1/13/89/115	-
32	LMG	U	201	-	-	14/27/47/70	0/1/1/1
31	DD6	K	208	-	-	10/26/80/80	0/3/3/3
22	CLA	F	802	35	1/1/15/20	0/39/115/115	-
34	A86	P	204	-	-	9/34/90/90	0/3/3/3
22	CLA	B	825	2	-	0/21/97/115	-
31	DD6	G	214	-	-	10/26/80/80	0/3/3/3
22	CLA	B	820	35	1/1/14/20	2/38/114/115	-
22	CLA	P	214	12	1/1/11/20	2/15/91/115	-
34	A86	Q	218	-	-	13/34/90/90	0/3/3/3
22	CLA	A	817	1	1/1/11/20	0/15/91/115	-
22	CLA	A	836	35	1/1/15/20	5/39/115/115	-
31	DD6	P	205	-	-	4/26/80/80	0/3/3/3
22	CLA	A	855	-	1/1/9/20	1/10/82/115	-
22	CLA	A	850	35	1/1/15/20	2/39/115/115	-
22	CLA	U	208	16	1/1/11/20	4/17/93/115	-
22	CLA	A	853	1	1/1/15/20	9/39/115/115	-
22	CLA	G	215	17	1/1/11/20	3/15/91/115	-
22	CLA	G	203	17	1/1/11/20	4/15/91/115	-
22	CLA	S	202	35	1/1/15/20	4/39/115/115	-
22	CLA	A	825	1	1/1/15/20	6/39/115/115	-
22	CLA	O	209	11	-	8/39/115/115	-
22	CLA	P	209	-	1/1/12/20	1/24/100/115	-
22	CLA	O	208	11	1/1/14/20	2/33/109/115	-
22	CLA	B	809	2	-	2/25/101/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	H	210	18	-	4/15/91/115	-
22	CLA	G	209	17	1/1/13/20	4/29/105/115	-
22	CLA	G	207	17	-	5/33/109/115	-
23	PQN	A	837	-	-	3/23/43/43	0/2/2/2
33	KC1	P	212	12	-	4/12/68/71	-
28	SF4	C	102	3	-	-	0/6/5/5
22	CLA	B	817	2	-	1/17/93/115	-
24	LHG	A	839	-	-	15/52/52/53	-
22	CLA	A	805	1	1/1/11/20	3/20/96/115	-
26	LMU	A	847	-	-	10/21/61/61	0/2/2/2
25	BCR	L	201	-	-	10/29/63/63	0/2/2/2
22	CLA	A	826	1	-	3/39/115/115	-
22	CLA	K	207	19	-	7/31/107/115	-
22	CLA	B	819	35	1/1/14/20	4/37/113/115	-
22	CLA	B	811	2	1/1/12/20	2/26/102/115	-
31	DD6	G	212	-	-	5/26/80/80	0/3/3/3
33	KC1	S	210	15	-	1/15/71/71	-
25	BCR	B	840	-	-	8/29/63/63	0/2/2/2
22	CLA	H	204	18	1/1/14/20	3/35/111/115	-
22	CLA	K	206	19	1/1/11/20	4/15/91/115	-
22	CLA	B	801	2	1/1/15/20	3/39/115/115	-
25	BCR	A	841	-	-	7/29/63/63	0/2/2/2
22	CLA	B	802	-	1/1/15/20	4/39/115/115	-
22	CLA	Q	207	13	1/1/11/20	5/17/93/115	-
22	CLA	L	202	9	-	6/20/96/115	-
25	BCR	I	102	-	-	10/29/63/63	0/2/2/2
22	CLA	G	201	17	-	2/15/91/115	-
31	DD6	S	204	-	-	7/26/80/80	0/3/3/3
31	DD6	G	213	-	-	9/26/80/80	0/3/3/3
33	KC1	Q	210	13	-	2/15/71/71	-
31	DD6	P	215	-	-	12/26/80/80	0/3/3/3
22	CLA	A	846	1	-	2/33/109/115	-
22	CLA	H	202	-	1/1/9/20	0/10/82/115	-
31	DD6	T	212	-	-	9/26/80/80	0/3/3/3
22	CLA	B	831	2	1/1/11/20	0/18/94/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	B	816	35	1/1/15/20	6/39/115/115	-
26	LMU	F	806	-	-	15/21/61/61	0/2/2/2
22	CLA	A	802	1	1/1/13/20	3/27/103/115	-
31	DD6	U	203	-	-	12/26/80/80	0/3/3/3
22	CLA	A	828	1	1/1/15/20	3/39/115/115	-
22	CLA	A	832	1	1/1/12/20	1/23/99/115	-
22	CLA	T	209	20	-	0/10/86/115	-
22	CLA	R	104	14	-	6/39/115/115	-
22	CLA	T	207	20	-	5/39/115/115	-
22	CLA	H	203	18	1/1/14/20	9/33/109/115	-
22	CLA	O	203	-	-	0/15/91/115	-
34	A86	R	105	-	-	11/34/90/90	0/3/3/3
22	CLA	S	217	15	1/1/15/20	2/39/115/115	-
22	CLA	T	205	-	1/1/11/20	2/17/93/115	-
32	LMG	S	213	-	-	22/44/64/70	0/1/1/1
33	KC1	S	212	15	-	5/15/71/71	-
22	CLA	B	832	35	1/1/15/20	3/39/115/115	-
22	CLA	B	833	2	-	4/39/115/115	-
22	CLA	A	815	1	1/1/15/20	7/39/115/115	-
22	CLA	A	809	1	1/1/14/20	2/36/112/115	-
22	CLA	T	203	20	1/1/11/20	5/17/93/115	-
34	A86	U	202	-	-	17/34/90/90	0/3/3/3
25	BCR	B	837	-	-	8/29/63/63	0/2/2/2
22	CLA	J	103	8	1/1/10/20	2/12/88/115	-
31	DD6	Q	202	-	-	5/26/80/80	0/3/3/3
31	DD6	O	215	-	-	15/26/80/80	0/3/3/3
22	CLA	U	207	35	1/1/15/20	3/39/115/115	-
31	DD6	H	212	-	-	10/26/80/80	0/3/3/3
26	LMU	K	202	-	-	4/10/50/61	0/2/2/2
24	LHG	P	201	-	-	38/53/53/53	-
24	LHG	A	840	22	-	12/31/31/53	-
22	CLA	U	204	35	1/1/14/20	7/35/111/115	-
22	CLA	A	803	1	1/1/15/20	4/39/115/115	-
22	CLA	A	813	1	-	0/21/97/115	-
22	CLA	G	204	17	-	4/13/89/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	DD6	S	215	-	-	13/26/80/80	0/3/3/3
22	CLA	G	206	17	1/1/15/20	15/39/115/115	-
22	CLA	U	210	16	-	3/39/115/115	-
22	CLA	A	821	35	1/1/15/20	8/39/115/115	-
33	KC1	O	210	11	-	0/15/71/71	-
22	CLA	Q	211	13	1/1/10/20	2/10/86/115	-
22	CLA	K	204	19	-	0/12/88/115	-
31	DD6	Q	215	-	-	9/26/80/80	0/3/3/3
31	DD6	H	211	-	-	13/26/80/80	0/3/3/3
31	DD6	S	205	-	-	10/26/80/80	0/3/3/3
22	CLA	K	203	19	1/1/11/20	2/15/91/115	-
28	SF4	C	101	3	-	-	0/6/5/5
22	CLA	B	834	35	1/1/15/20	1/39/115/115	-
33	KC1	U	213	16	-	0/15/71/71	-
22	CLA	B	842	2	1/1/15/20	4/39/115/115	-
25	BCR	A	844	-	-	8/29/63/63	0/2/2/2
22	CLA	S	208	15	1/1/11/20	0/15/91/115	-
22	CLA	H	208	-	1/1/13/20	5/31/107/115	-
22	CLA	T	204	-	1/1/13/20	10/30/106/115	-
33	KC1	P	203	-	-	1/15/71/71	-
30	SQD	S	201	-	-	21/41/61/69	0/1/1/1
22	CLA	B	830	2	1/1/15/20	1/39/115/115	-
31	DD6	O	212	-	-	10/26/80/80	0/3/3/3
22	CLA	A	808	1	-	2/29/105/115	-
31	DD6	S	211	-	-	13/26/80/80	0/3/3/3
26	LMU	S	203	-	-	10/17/57/61	0/2/2/2
22	CLA	Q	206	13	1/1/12/20	3/22/98/115	-
22	CLA	H	206	18	1/1/11/20	2/15/91/115	-
22	CLA	O	206	35	1/1/15/20	5/39/115/115	-
22	CLA	A	829	1	1/1/15/20	3/39/115/115	-
26	LMU	L	206	-	-	7/21/61/61	0/2/2/2

All (1680) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	R	103	A86	C13-C11	-6.84	1.36	1.49
34	R	105	A86	C13-C11	-6.74	1.36	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	Q	218	A86	C13-C11	-6.70	1.37	1.49
34	Q	214	A86	C13-C11	-6.52	1.37	1.49
22	K	203	CLA	MG-NA	6.36	2.21	2.06
34	P	204	A86	C13-C11	-6.30	1.37	1.49
34	U	202	A86	C13-C11	-6.27	1.37	1.49
34	Q	201	A86	C13-C11	-6.00	1.38	1.49
22	T	206	CLA	MG-NC	5.92	2.20	2.06
22	U	209	CLA	MG-NC	5.56	2.19	2.06
22	G	206	CLA	MG-NA	5.48	2.19	2.06
33	T	208	KC1	MG-NA	5.11	2.18	2.06
22	B	824	CLA	MG-NA	5.09	2.18	2.06
22	A	826	CLA	MG-NA	5.08	2.18	2.06
22	S	207	CLA	MG-NA	5.04	2.18	2.06
22	K	206	CLA	MG-NA	4.97	2.18	2.06
22	H	210	CLA	MG-NA	4.94	2.18	2.06
22	A	834	CLA	MG-NA	4.85	2.17	2.06
22	B	803	CLA	MG-NA	4.83	2.17	2.06
22	A	813	CLA	MG-NA	4.82	2.17	2.06
22	H	206	CLA	MG-NA	4.82	2.17	2.06
22	B	843	CLA	MG-NA	4.81	2.17	2.06
22	B	813	CLA	MG-NA	4.74	2.17	2.06
22	B	844	CLA	MG-NA	4.74	2.17	2.06
22	Q	206	CLA	MG-NA	4.74	2.17	2.06
22	A	825	CLA	MG-NA	4.72	2.17	2.06
22	B	847	CLA	C4C-C3C	-4.71	1.37	1.45
22	G	209	CLA	C1C-C2C	-4.70	1.35	1.44
22	A	808	CLA	C4C-C3C	-4.69	1.37	1.45
22	A	823	CLA	C4C-C3C	-4.68	1.37	1.45
22	A	823	CLA	MG-NA	4.67	2.17	2.06
22	A	828	CLA	MG-NA	4.66	2.17	2.06
22	A	805	CLA	MG-NA	4.66	2.17	2.06
22	B	807	CLA	C4C-C3C	-4.65	1.37	1.45
33	P	206	KC1	C4C-C3C	-4.65	1.37	1.45
22	B	817	CLA	C4C-C3C	-4.64	1.37	1.45
22	R	104	CLA	MG-NA	4.63	2.17	2.06
22	B	822	CLA	C4C-C3C	-4.63	1.37	1.45
22	F	803	CLA	MG-NA	4.62	2.17	2.06
22	P	209	CLA	C4C-C3C	-4.61	1.37	1.45
22	B	811	CLA	C4C-C3C	-4.60	1.37	1.45
22	S	207	CLA	C4C-C3C	-4.60	1.37	1.45
22	A	806	CLA	C4C-C3C	-4.59	1.37	1.45
22	k	103	CLA	C4C-C3C	-4.59	1.37	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	806	CLA	C4C-C3C	-4.58	1.37	1.45
22	B	834	CLA	C4C-C3C	-4.58	1.37	1.45
22	B	821	CLA	MG-NA	4.57	2.17	2.06
22	A	832	CLA	MG-NA	4.57	2.17	2.06
22	G	204	CLA	C4C-C3C	-4.57	1.37	1.45
33	P	203	KC1	MG-NA	4.57	2.17	2.06
22	Q	209	CLA	C4C-C3C	-4.57	1.37	1.45
22	B	826	CLA	MG-NA	4.57	2.17	2.06
22	B	803	CLA	C4C-C3C	-4.56	1.37	1.45
22	B	844	CLA	C4C-C3C	-4.56	1.37	1.45
22	B	842	CLA	MG-NA	4.56	2.17	2.06
22	A	817	CLA	C4C-C3C	-4.56	1.37	1.45
22	B	815	CLA	C4C-C3C	-4.55	1.37	1.45
22	B	833	CLA	C4C-C3C	-4.55	1.37	1.45
22	K	203	CLA	C4C-C3C	-4.55	1.37	1.45
22	A	822	CLA	C4C-C3C	-4.55	1.37	1.45
22	A	853	CLA	C4C-C3C	-4.55	1.37	1.45
22	S	206	CLA	C4C-C3C	-4.55	1.37	1.45
22	O	205	CLA	MG-NA	4.55	2.17	2.06
22	A	809	CLA	C4C-C3C	-4.54	1.37	1.45
22	G	210	CLA	MG-NA	4.54	2.17	2.06
22	A	838	CLA	C4C-C3C	-4.54	1.37	1.45
22	B	801	CLA	C4C-C3C	-4.54	1.37	1.45
22	G	203	CLA	MG-NA	4.54	2.17	2.06
22	G	210	CLA	C4C-C3C	-4.54	1.37	1.45
22	U	210	CLA	C4C-C3C	-4.54	1.37	1.45
22	O	209	CLA	C4C-C3C	-4.54	1.37	1.45
33	Q	210	KC1	C4C-C3C	-4.53	1.37	1.45
22	A	818	CLA	C1C-C2C	-4.53	1.35	1.44
22	B	823	CLA	C4C-C3C	-4.53	1.37	1.45
22	P	208	CLA	C4C-C3C	-4.53	1.37	1.45
22	T	205	CLA	C4C-C3C	-4.53	1.37	1.45
22	T	201	CLA	C4C-C3C	-4.53	1.37	1.45
22	B	827	CLA	C4C-C3C	-4.52	1.37	1.45
22	B	826	CLA	C4C-C3C	-4.52	1.37	1.45
22	R	101	CLA	C4C-C3C	-4.52	1.37	1.45
22	L	203	CLA	C4C-C3C	-4.52	1.37	1.45
22	U	206	CLA	C4C-C3C	-4.51	1.37	1.45
22	Q	212	CLA	C4C-C3C	-4.51	1.37	1.45
22	B	816	CLA	C4C-C3C	-4.51	1.37	1.45
22	A	829	CLA	C4C-C3C	-4.51	1.37	1.45
22	B	805	CLA	C4C-C3C	-4.51	1.37	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	P	214	CLA	C4C-C3C	-4.51	1.37	1.45
22	H	207	CLA	C4C-C3C	-4.51	1.37	1.45
22	O	203	CLA	C4C-C3C	-4.51	1.37	1.45
22	T	202	CLA	C4C-C3C	-4.51	1.37	1.45
22	S	216	CLA	C4C-C3C	-4.51	1.37	1.45
22	A	815	CLA	MG-NA	4.51	2.17	2.06
22	U	207	CLA	C4C-C3C	-4.51	1.37	1.45
22	B	820	CLA	C4C-C3C	-4.50	1.37	1.45
22	H	206	CLA	C4C-C3C	-4.50	1.37	1.45
22	A	821	CLA	MG-NA	4.50	2.17	2.06
22	A	819	CLA	C4C-C3C	-4.50	1.37	1.45
22	A	824	CLA	C4C-C3C	-4.50	1.37	1.45
22	A	834	CLA	C4C-C3C	-4.50	1.37	1.45
22	T	203	CLA	C4C-C3C	-4.50	1.37	1.45
22	H	205	CLA	C4C-C3C	-4.50	1.37	1.45
22	U	205	CLA	C4C-C3C	-4.50	1.37	1.45
22	B	814	CLA	C4C-C3C	-4.50	1.37	1.45
22	Q	207	CLA	C4C-C3C	-4.50	1.37	1.45
22	A	802	CLA	C4C-C3C	-4.49	1.37	1.45
22	R	104	CLA	C4C-C3C	-4.49	1.37	1.45
22	Q	212	CLA	MG-NA	4.49	2.16	2.06
22	A	854	CLA	C4C-C3C	-4.49	1.37	1.45
22	G	206	CLA	C4C-C3C	-4.49	1.37	1.45
22	G	203	CLA	C4C-C3C	-4.49	1.37	1.45
33	S	212	KC1	C4C-C3C	-4.49	1.37	1.45
22	A	828	CLA	C4C-C3C	-4.49	1.37	1.45
22	A	812	CLA	C4C-C3C	-4.48	1.37	1.45
33	O	210	KC1	C4C-C3C	-4.48	1.37	1.45
22	U	204	CLA	C4C-C3C	-4.48	1.37	1.45
22	A	805	CLA	C4C-C3C	-4.48	1.37	1.45
22	B	821	CLA	C4C-C3C	-4.48	1.37	1.45
22	P	213	CLA	C4C-C3C	-4.48	1.37	1.45
22	B	819	CLA	C4C-C3C	-4.48	1.37	1.45
22	T	210	CLA	C4C-C3C	-4.48	1.37	1.45
22	A	813	CLA	C4C-C3C	-4.47	1.37	1.45
22	A	820	CLA	C4C-C3C	-4.47	1.37	1.45
22	U	211	CLA	C4C-C3C	-4.47	1.37	1.45
22	A	811	CLA	C4C-C3C	-4.47	1.37	1.45
22	Q	206	CLA	C4C-C3C	-4.47	1.37	1.45
22	B	831	CLA	C4C-C3C	-4.47	1.37	1.45
22	G	202	CLA	C4C-C3C	-4.47	1.37	1.45
22	B	830	CLA	C4C-C3C	-4.46	1.37	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	G	201	CLA	C4C-C3C	-4.46	1.37	1.45
22	B	813	CLA	C4C-C3C	-4.46	1.37	1.45
22	H	213	CLA	C4C-C3C	-4.45	1.37	1.45
22	B	825	CLA	C4C-C3C	-4.45	1.37	1.45
22	A	836	CLA	C4C-C3C	-4.45	1.37	1.45
22	T	207	CLA	C4C-C3C	-4.45	1.37	1.45
22	k	102	CLA	C4C-C3C	-4.45	1.37	1.45
22	A	832	CLA	C4C-C3C	-4.45	1.37	1.45
22	A	850	CLA	C4C-C3C	-4.45	1.37	1.45
22	B	809	CLA	C4C-C3C	-4.45	1.37	1.45
22	B	825	CLA	MG-NA	4.45	2.16	2.06
22	H	204	CLA	C4C-C3C	-4.44	1.37	1.45
22	B	845	CLA	C4C-C3C	-4.44	1.37	1.45
22	B	823	CLA	MG-NA	4.44	2.16	2.06
22	J	103	CLA	C4C-C3C	-4.44	1.37	1.45
22	Q	205	CLA	C4C-C3C	-4.44	1.37	1.45
22	L	202	CLA	C4C-C3C	-4.44	1.37	1.45
22	P	216	CLA	C4C-C3C	-4.44	1.37	1.45
22	A	814	CLA	C4C-C3C	-4.44	1.37	1.45
22	G	207	CLA	C4C-C3C	-4.43	1.37	1.45
22	G	205	CLA	C4C-C3C	-4.43	1.37	1.45
22	P	211	CLA	C4C-C3C	-4.43	1.37	1.45
22	A	825	CLA	C4C-C3C	-4.43	1.37	1.45
22	G	208	CLA	C4C-C3C	-4.43	1.37	1.45
22	H	208	CLA	C4C-C3C	-4.43	1.37	1.45
22	T	211	CLA	C4C-C3C	-4.43	1.37	1.45
33	U	213	KC1	C4C-C3C	-4.42	1.37	1.45
22	B	812	CLA	C4C-C3C	-4.42	1.37	1.45
22	T	206	CLA	MG-ND	4.42	2.14	2.05
22	O	205	CLA	C4C-C3C	-4.42	1.37	1.45
33	T	208	KC1	C4C-C3C	-4.42	1.37	1.45
22	A	816	CLA	C4C-C3C	-4.42	1.37	1.45
22	O	204	CLA	C4C-C3C	-4.42	1.37	1.45
22	T	204	CLA	C4C-C3C	-4.42	1.37	1.45
33	P	212	KC1	C4C-C3C	-4.42	1.37	1.45
22	Q	216	CLA	C4C-C3C	-4.42	1.37	1.45
22	Q	213	CLA	C4C-C3C	-4.41	1.37	1.45
22	B	822	CLA	MG-NA	4.41	2.16	2.06
22	A	810	CLA	C4C-C3C	-4.41	1.37	1.45
22	H	210	CLA	C4C-C3C	-4.40	1.37	1.45
22	S	209	CLA	C4C-C3C	-4.40	1.37	1.45
22	A	855	CLA	C4C-C3C	-4.40	1.37	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	O	211	CLA	C4C-C3C	-4.40	1.37	1.45
22	P	210	CLA	C4C-C3C	-4.40	1.37	1.45
22	T	209	CLA	C4C-C3C	-4.40	1.37	1.45
22	A	846	CLA	MG-NA	4.40	2.16	2.06
22	P	207	CLA	C4C-C3C	-4.40	1.37	1.45
22	O	206	CLA	C4C-C3C	-4.40	1.37	1.45
22	A	807	CLA	C4C-C3C	-4.39	1.37	1.45
22	H	203	CLA	C4C-C3C	-4.39	1.37	1.45
22	A	826	CLA	C4C-C3C	-4.39	1.37	1.45
22	B	818	CLA	C4C-C3C	-4.39	1.37	1.45
22	B	834	CLA	MG-NA	4.39	2.16	2.06
22	A	856	CLA	C4C-C3C	-4.39	1.37	1.45
22	H	209	CLA	C4C-C3C	-4.39	1.37	1.45
22	A	845	CLA	C4C-C3C	-4.39	1.37	1.45
22	A	833	CLA	C4C-C3C	-4.39	1.37	1.45
22	A	851	CLA	C4C-C3C	-4.39	1.37	1.45
22	A	801	CLA	C4C-C3C	-4.38	1.37	1.45
22	A	827	CLA	C4C-C3C	-4.38	1.37	1.45
22	A	804	CLA	C4C-C3C	-4.38	1.37	1.45
22	K	206	CLA	C4C-C3C	-4.38	1.37	1.45
22	A	827	CLA	MG-NA	4.38	2.16	2.06
22	A	821	CLA	C4C-C3C	-4.38	1.37	1.45
22	F	804	CLA	C4C-C3C	-4.38	1.37	1.45
22	B	827	CLA	MG-NA	4.38	2.16	2.06
22	K	207	CLA	C4C-C3C	-4.38	1.37	1.45
22	A	830	CLA	C4C-C3C	-4.37	1.37	1.45
22	A	846	CLA	C4C-C3C	-4.37	1.37	1.45
22	B	812	CLA	MG-NA	4.37	2.16	2.06
22	A	833	CLA	MG-NA	4.36	2.16	2.06
22	B	828	CLA	C4C-C3C	-4.36	1.37	1.45
22	T	206	CLA	C4C-C3C	-4.36	1.37	1.45
22	S	202	CLA	C4C-C3C	-4.36	1.37	1.45
22	A	831	CLA	C4C-C3C	-4.36	1.37	1.45
22	A	812	CLA	MG-NA	4.36	2.16	2.06
22	B	802	CLA	C4C-C3C	-4.36	1.37	1.45
22	B	804	CLA	C4C-C3C	-4.36	1.37	1.45
22	A	803	CLA	C4C-C3C	-4.35	1.37	1.45
22	K	205	CLA	C4C-C3C	-4.35	1.37	1.45
22	P	216	CLA	MG-NA	4.34	2.16	2.06
22	K	204	CLA	C4C-C3C	-4.34	1.37	1.45
22	T	206	CLA	MG-NA	4.34	2.16	2.06
22	B	808	CLA	C4C-C3C	-4.34	1.37	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	835	CLA	C4C-C3C	-4.34	1.37	1.45
22	Q	208	CLA	C4C-C3C	-4.34	1.37	1.45
22	G	215	CLA	C4C-C3C	-4.34	1.37	1.45
22	O	207	CLA	C4C-C3C	-4.34	1.37	1.45
22	S	217	CLA	C4C-C3C	-4.33	1.37	1.45
33	S	210	KC1	C4C-C3C	-4.33	1.37	1.45
22	B	809	CLA	MG-NA	4.33	2.16	2.06
22	S	208	CLA	C4C-C3C	-4.33	1.37	1.45
22	B	810	CLA	C4C-C3C	-4.32	1.37	1.45
22	U	209	CLA	C4C-C3C	-4.31	1.37	1.45
22	A	815	CLA	C4C-C3C	-4.31	1.37	1.45
22	A	818	CLA	C4C-C3C	-4.31	1.37	1.45
22	B	824	CLA	C4C-C3C	-4.31	1.37	1.45
22	F	802	CLA	C4C-C3C	-4.31	1.37	1.45
22	A	824	CLA	MG-NA	4.30	2.16	2.06
22	U	211	CLA	MG-NA	4.29	2.16	2.06
22	L	204	CLA	C4C-C3C	-4.28	1.37	1.45
22	Q	211	CLA	C4C-C3C	-4.28	1.37	1.45
22	B	843	CLA	C4C-C3C	-4.28	1.37	1.45
22	B	829	CLA	C4C-C3C	-4.27	1.37	1.45
22	O	208	CLA	C4C-C3C	-4.27	1.37	1.45
22	O	202	CLA	C4C-C3C	-4.27	1.37	1.45
22	Q	203	CLA	C4C-C3C	-4.27	1.37	1.45
22	T	210	CLA	MG-NA	4.26	2.16	2.06
22	B	833	CLA	MG-NA	4.26	2.16	2.06
22	U	208	CLA	C4C-C3C	-4.26	1.37	1.45
22	B	832	CLA	C4C-C3C	-4.25	1.37	1.45
33	P	203	KC1	C4C-C3C	-4.25	1.37	1.45
22	R	104	CLA	MG-NC	4.25	2.16	2.06
22	T	203	CLA	MG-NA	4.24	2.16	2.06
22	B	819	CLA	C1C-C2C	-4.23	1.35	1.44
22	A	829	CLA	MG-NA	4.23	2.16	2.06
22	A	807	CLA	MG-NA	4.22	2.16	2.06
22	B	829	CLA	MG-NA	4.22	2.16	2.06
22	G	209	CLA	C4C-C3C	-4.22	1.37	1.45
22	Q	209	CLA	MG-NA	4.22	2.16	2.06
22	B	832	CLA	MG-NA	4.21	2.16	2.06
33	P	219	KC1	C4C-C3C	-4.21	1.37	1.45
22	B	811	CLA	MG-NA	4.21	2.16	2.06
22	B	842	CLA	C4C-C3C	-4.21	1.37	1.45
22	A	851	CLA	C1C-C2C	-4.21	1.36	1.44
22	B	805	CLA	MG-NA	4.18	2.16	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	Q	212	CLA	C1C-C2C	-4.18	1.36	1.44
22	Q	204	CLA	C4C-C3C	-4.18	1.37	1.45
22	Q	204	CLA	C1C-C2C	-4.18	1.36	1.44
22	O	202	CLA	C1C-C2C	-4.17	1.36	1.44
22	F	803	CLA	C4C-C3C	-4.17	1.38	1.45
22	A	803	CLA	C1C-C2C	-4.17	1.36	1.44
22	P	214	CLA	MG-NA	4.17	2.16	2.06
22	A	848	CLA	C1C-C2C	-4.16	1.36	1.44
22	B	807	CLA	C1C-C2C	-4.16	1.36	1.44
22	B	831	CLA	MG-NA	4.16	2.16	2.06
22	A	834	CLA	MG-NC	4.15	2.16	2.06
22	B	815	CLA	MG-NA	4.15	2.16	2.06
22	B	815	CLA	C1C-C2C	-4.15	1.36	1.44
22	k	102	CLA	C1C-C2C	-4.15	1.36	1.44
22	K	207	CLA	C1C-C2C	-4.15	1.36	1.44
22	A	808	CLA	C1C-C2C	-4.15	1.36	1.44
22	B	819	CLA	MG-NA	4.15	2.16	2.06
22	A	823	CLA	C1C-C2C	-4.15	1.36	1.44
22	A	829	CLA	C1C-C2C	-4.14	1.36	1.44
22	L	203	CLA	C1C-C2C	-4.14	1.36	1.44
22	A	846	CLA	C1C-C2C	-4.14	1.36	1.44
22	B	807	CLA	MG-NA	4.13	2.16	2.06
22	B	834	CLA	C1C-C2C	-4.13	1.36	1.44
22	S	202	CLA	C1C-C2C	-4.13	1.36	1.44
22	B	802	CLA	C1C-C2C	-4.13	1.36	1.44
22	H	203	CLA	C1C-C2C	-4.13	1.36	1.44
22	P	208	CLA	MG-NA	4.12	2.16	2.06
33	P	203	KC1	C1C-C2C	-4.12	1.36	1.44
22	B	808	CLA	C1C-C2C	-4.12	1.36	1.44
22	H	202	CLA	C1C-C2C	-4.12	1.36	1.44
22	H	202	CLA	C4C-C3C	-4.12	1.38	1.45
22	B	842	CLA	C1C-C2C	-4.12	1.36	1.44
22	B	828	CLA	C1C-C2C	-4.12	1.36	1.44
33	P	212	KC1	C1C-C2C	-4.12	1.36	1.44
33	Q	210	KC1	C1C-C2C	-4.12	1.36	1.44
22	P	209	CLA	C1C-C2C	-4.11	1.36	1.44
22	L	202	CLA	C1C-C2C	-4.11	1.36	1.44
22	U	210	CLA	C1C-C2C	-4.10	1.36	1.44
22	A	817	CLA	MG-NA	4.10	2.16	2.06
22	A	845	CLA	MG-NA	4.10	2.16	2.06
22	T	210	CLA	C1C-C2C	-4.10	1.36	1.44
22	O	205	CLA	C1C-C2C	-4.10	1.36	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	811	CLA	MG-NA	4.10	2.16	2.06
22	B	818	CLA	C1C-C2C	-4.10	1.36	1.44
22	Q	211	CLA	C1C-C2C	-4.09	1.36	1.44
22	A	811	CLA	C1C-C2C	-4.09	1.36	1.44
33	T	208	KC1	C1C-C2C	-4.09	1.36	1.44
22	B	827	CLA	C1C-C2C	-4.09	1.36	1.44
22	A	820	CLA	C1C-C2C	-4.09	1.36	1.44
22	Q	203	CLA	C1C-C2C	-4.09	1.36	1.44
22	B	801	CLA	MG-NC	4.09	2.16	2.06
22	O	208	CLA	C1C-C2C	-4.09	1.36	1.44
22	A	809	CLA	C1C-C2C	-4.09	1.36	1.44
33	S	212	KC1	C1C-C2C	-4.09	1.36	1.44
22	U	206	CLA	C1C-C2C	-4.09	1.36	1.44
22	P	210	CLA	C1C-C2C	-4.08	1.36	1.44
22	A	853	CLA	C1C-C2C	-4.08	1.36	1.44
22	L	202	CLA	MG-NA	4.08	2.16	2.06
33	O	210	KC1	C4A-C3A	-4.08	1.36	1.44
22	B	823	CLA	C1C-C2C	-4.08	1.36	1.44
22	B	825	CLA	C1C-C2C	-4.08	1.36	1.44
22	B	833	CLA	C1C-C2C	-4.08	1.36	1.44
22	B	821	CLA	C1C-C2C	-4.08	1.36	1.44
22	T	204	CLA	C1C-C2C	-4.08	1.36	1.44
33	U	213	KC1	C3B-C4B	-4.08	1.38	1.46
22	K	203	CLA	C1C-C2C	-4.08	1.36	1.44
22	H	210	CLA	C1C-C2C	-4.07	1.36	1.44
22	A	835	CLA	MG-NA	4.07	2.15	2.06
22	H	209	CLA	C1C-C2C	-4.07	1.36	1.44
33	P	219	KC1	C1C-C2C	-4.07	1.36	1.44
22	Q	213	CLA	C1C-C2C	-4.07	1.36	1.44
22	A	817	CLA	C1C-C2C	-4.07	1.36	1.44
22	Q	208	CLA	MG-NA	4.07	2.15	2.06
22	O	211	CLA	C1C-C2C	-4.07	1.36	1.44
22	O	209	CLA	MG-NA	4.06	2.15	2.06
22	S	207	CLA	C1C-C2C	-4.06	1.36	1.44
22	A	813	CLA	C1C-C2C	-4.06	1.36	1.44
22	Q	216	CLA	C1C-C2C	-4.06	1.36	1.44
22	G	210	CLA	C1C-C2C	-4.06	1.36	1.44
22	B	801	CLA	MG-NA	4.06	2.15	2.06
22	Q	205	CLA	C1C-C2C	-4.06	1.36	1.44
22	B	812	CLA	C1C-C2C	-4.05	1.36	1.44
33	P	203	KC1	C3B-C4B	-4.05	1.39	1.46
22	B	804	CLA	C1C-C2C	-4.05	1.36	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	P	208	CLA	C1C-C2C	-4.05	1.36	1.44
22	P	211	CLA	C1C-C2C	-4.05	1.36	1.44
22	A	827	CLA	C1C-C2C	-4.05	1.36	1.44
22	A	812	CLA	C1C-C2C	-4.05	1.36	1.44
22	R	104	CLA	C1C-C2C	-4.05	1.36	1.44
22	S	217	CLA	C1C-C2C	-4.05	1.36	1.44
22	O	206	CLA	C1C-C2C	-4.04	1.36	1.44
22	G	215	CLA	C1C-C2C	-4.04	1.36	1.44
22	A	848	CLA	MG-NA	4.04	2.15	2.06
22	T	207	CLA	C1C-C2C	-4.04	1.36	1.44
22	O	203	CLA	C1C-C2C	-4.04	1.36	1.44
22	T	205	CLA	C1C-C2C	-4.04	1.36	1.44
22	F	803	CLA	C1C-C2C	-4.03	1.36	1.44
22	A	816	CLA	C1C-C2C	-4.03	1.36	1.44
22	H	213	CLA	C1C-C2C	-4.03	1.36	1.44
22	A	828	CLA	C1C-C2C	-4.03	1.36	1.44
22	A	820	CLA	MG-NA	4.03	2.15	2.06
22	A	830	CLA	C1C-C2C	-4.03	1.36	1.44
22	S	206	CLA	C1C-C2C	-4.03	1.36	1.44
22	K	206	CLA	C1C-C2C	-4.03	1.36	1.44
22	O	204	CLA	C1C-C2C	-4.03	1.36	1.44
22	A	826	CLA	C1C-C2C	-4.03	1.36	1.44
22	B	830	CLA	C1C-C2C	-4.03	1.36	1.44
22	U	211	CLA	C1C-C2C	-4.03	1.36	1.44
22	A	830	CLA	MG-NA	4.03	2.15	2.06
22	P	207	CLA	C1C-C2C	-4.03	1.36	1.44
22	O	204	CLA	MG-NA	4.02	2.15	2.06
22	Q	209	CLA	C1C-C2C	-4.02	1.36	1.44
22	P	216	CLA	C1C-C2C	-4.02	1.36	1.44
22	S	208	CLA	C1C-C2C	-4.02	1.36	1.44
22	A	855	CLA	C1C-C2C	-4.02	1.36	1.44
22	B	843	CLA	C1C-C2C	-4.02	1.36	1.44
33	S	210	KC1	C1C-C2C	-4.02	1.36	1.44
33	U	213	KC1	C1C-C2C	-4.01	1.36	1.44
22	k	103	CLA	C1C-C2C	-4.01	1.36	1.44
22	Q	207	CLA	C1C-C2C	-4.01	1.36	1.44
33	O	210	KC1	C1C-C2C	-4.01	1.36	1.44
22	A	801	CLA	C1C-C2C	-4.01	1.36	1.44
22	B	810	CLA	C1C-C2C	-4.01	1.36	1.44
22	A	822	CLA	C1C-C2C	-4.01	1.36	1.44
22	A	825	CLA	C1C-C2C	-4.01	1.36	1.44
22	A	804	CLA	C1C-C2C	-4.01	1.36	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	810	CLA	C1C-C2C	-4.01	1.36	1.44
22	T	209	CLA	MG-NA	4.01	2.15	2.06
22	A	856	CLA	C1C-C2C	-4.00	1.36	1.44
22	O	203	CLA	MG-NA	4.00	2.15	2.06
22	G	201	CLA	C1C-C2C	-4.00	1.36	1.44
22	A	838	CLA	MG-NA	4.00	2.15	2.06
22	U	208	CLA	C1C-C2C	-4.00	1.36	1.44
22	T	209	CLA	C1C-C2C	-4.00	1.36	1.44
22	U	207	CLA	C1C-C2C	-4.00	1.36	1.44
22	T	203	CLA	C1C-C2C	-4.00	1.36	1.44
22	A	814	CLA	MG-NA	4.00	2.15	2.06
22	B	847	CLA	C1C-C2C	-4.00	1.36	1.44
33	P	206	KC1	C3B-C4B	-3.99	1.39	1.46
22	Q	206	CLA	C1C-C2C	-3.99	1.36	1.44
22	P	213	CLA	C1C-C2C	-3.99	1.36	1.44
22	A	819	CLA	C1C-C2C	-3.99	1.36	1.44
22	B	826	CLA	C1C-C2C	-3.99	1.36	1.44
22	O	207	CLA	MG-NA	3.99	2.15	2.06
22	G	203	CLA	C1C-C2C	-3.99	1.36	1.44
22	G	206	CLA	C1C-C2C	-3.99	1.36	1.44
26	S	203	LMU	O5'-C1'	3.99	1.52	1.41
22	F	804	CLA	C1C-C2C	-3.98	1.36	1.44
22	Q	208	CLA	C1C-C2C	-3.98	1.36	1.44
22	T	211	CLA	C1C-C2C	-3.98	1.36	1.44
22	B	820	CLA	C1C-C2C	-3.98	1.36	1.44
22	B	845	CLA	C1C-C2C	-3.98	1.36	1.44
22	H	205	CLA	C1C-C2C	-3.98	1.36	1.44
33	P	206	KC1	C1C-C2C	-3.98	1.36	1.44
22	A	855	CLA	MG-NA	3.98	2.15	2.06
22	B	832	CLA	C1C-C2C	-3.98	1.36	1.44
22	A	805	CLA	C1C-C2C	-3.98	1.36	1.44
22	U	205	CLA	MG-NA	3.98	2.15	2.06
22	A	806	CLA	C1C-C2C	-3.98	1.36	1.44
22	B	824	CLA	C1C-C2C	-3.98	1.36	1.44
22	T	202	CLA	C1C-C2C	-3.97	1.36	1.44
22	k	103	CLA	MG-NA	3.97	2.15	2.06
22	A	833	CLA	C1C-C2C	-3.97	1.36	1.44
22	J	103	CLA	C1C-C2C	-3.97	1.36	1.44
22	H	208	CLA	C1C-C2C	-3.97	1.36	1.44
22	O	207	CLA	C1C-C2C	-3.97	1.36	1.44
22	B	829	CLA	C1C-C2C	-3.97	1.36	1.44
22	G	204	CLA	C1C-C2C	-3.97	1.36	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	P	214	CLA	C1C-C2C	-3.96	1.36	1.44
22	T	201	CLA	C1C-C2C	-3.96	1.36	1.44
22	A	854	CLA	C1C-C2C	-3.96	1.36	1.44
22	T	201	CLA	MG-NA	3.96	2.15	2.06
33	P	219	KC1	C3B-C4B	-3.96	1.39	1.46
22	A	814	CLA	C1C-C2C	-3.96	1.36	1.44
22	P	213	CLA	MG-NA	3.96	2.15	2.06
22	H	205	CLA	MG-NA	3.96	2.15	2.06
22	A	819	CLA	MG-NA	3.95	2.15	2.06
22	G	202	CLA	C1C-C2C	-3.95	1.36	1.44
22	A	807	CLA	C1C-C2C	-3.95	1.36	1.44
22	T	211	CLA	MG-NA	3.95	2.15	2.06
22	Q	207	CLA	MG-NA	3.95	2.15	2.06
22	B	814	CLA	C1C-C2C	-3.95	1.36	1.44
22	S	209	CLA	C1C-C2C	-3.95	1.36	1.44
22	S	216	CLA	C1C-C2C	-3.95	1.36	1.44
22	T	206	CLA	C1C-C2C	-3.95	1.36	1.44
22	A	821	CLA	C1C-C2C	-3.95	1.36	1.44
22	U	205	CLA	C1C-C2C	-3.95	1.36	1.44
22	U	204	CLA	C1C-C2C	-3.94	1.36	1.44
22	A	831	CLA	C1C-C2C	-3.94	1.36	1.44
22	A	835	CLA	C1C-C2C	-3.94	1.36	1.44
22	B	813	CLA	C1C-C2C	-3.94	1.36	1.44
22	H	203	CLA	MG-NA	3.94	2.15	2.06
22	K	205	CLA	C1C-C2C	-3.94	1.36	1.44
22	F	802	CLA	C1C-C2C	-3.94	1.36	1.44
22	G	205	CLA	C1C-C2C	-3.94	1.36	1.44
22	L	204	CLA	C1C-C2C	-3.94	1.36	1.44
22	B	813	CLA	MG-NC	3.94	2.15	2.06
22	A	834	CLA	C1C-C2C	-3.93	1.36	1.44
22	B	817	CLA	C1C-C2C	-3.93	1.36	1.44
26	F	806	LMU	O5'-C1'	3.93	1.52	1.41
22	B	811	CLA	C1C-C2C	-3.93	1.36	1.44
22	L	204	CLA	MG-NA	3.93	2.15	2.06
22	A	836	CLA	C1C-C2C	-3.93	1.36	1.44
22	B	805	CLA	C1C-C2C	-3.93	1.36	1.44
22	A	802	CLA	C1C-C2C	-3.93	1.36	1.44
33	O	210	KC1	C3B-C4B	-3.93	1.39	1.46
22	A	848	CLA	C4C-C3C	-3.93	1.38	1.45
22	G	207	CLA	C1C-C2C	-3.93	1.36	1.44
22	K	204	CLA	MG-NA	3.93	2.15	2.06
22	G	208	CLA	C1C-C2C	-3.93	1.36	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	H	204	CLA	C1C-C2C	-3.93	1.36	1.44
22	A	832	CLA	C1C-C2C	-3.93	1.36	1.44
22	B	801	CLA	C1C-C2C	-3.92	1.36	1.44
22	Q	213	CLA	MG-NA	3.92	2.15	2.06
22	B	844	CLA	C1C-C2C	-3.92	1.36	1.44
22	B	806	CLA	C1C-C2C	-3.92	1.36	1.44
33	S	212	KC1	C1B-C2B	-3.92	1.37	1.45
22	A	815	CLA	C1C-C2C	-3.92	1.36	1.44
22	B	809	CLA	C1C-C2C	-3.92	1.36	1.44
22	B	816	CLA	C1C-C2C	-3.91	1.36	1.44
22	Q	211	CLA	MG-NA	3.91	2.15	2.06
22	H	213	CLA	MG-NA	3.90	2.15	2.06
22	F	804	CLA	MG-NA	3.90	2.15	2.06
22	B	822	CLA	C1C-C2C	-3.89	1.36	1.44
22	A	853	CLA	MG-NA	3.89	2.15	2.06
22	R	101	CLA	C1C-C2C	-3.89	1.36	1.44
22	A	838	CLA	C1C-C2C	-3.89	1.36	1.44
22	B	831	CLA	C1C-C2C	-3.87	1.36	1.44
22	K	205	CLA	MG-NA	3.87	2.15	2.06
22	B	843	CLA	MG-NC	3.87	2.15	2.06
22	F	802	CLA	MG-NA	3.87	2.15	2.06
22	B	803	CLA	C1C-C2C	-3.87	1.36	1.44
22	A	850	CLA	C1C-C2C	-3.86	1.36	1.44
22	H	206	CLA	C1C-C2C	-3.86	1.36	1.44
22	B	806	CLA	MG-NA	3.86	2.15	2.06
22	R	101	CLA	MG-NA	3.86	2.15	2.06
33	P	212	KC1	C4A-C3A	-3.86	1.36	1.44
22	K	206	CLA	MG-NC	3.84	2.15	2.06
22	k	102	CLA	MG-NA	3.84	2.15	2.06
22	A	845	CLA	C1C-C2C	-3.84	1.36	1.44
22	O	206	CLA	MG-NA	3.83	2.15	2.06
22	U	206	CLA	MG-NA	3.83	2.15	2.06
33	P	206	KC1	MG-NA	3.83	2.15	2.06
22	U	209	CLA	C1C-C2C	-3.83	1.36	1.44
33	S	210	KC1	C1B-C2B	-3.83	1.37	1.45
33	U	213	KC1	MG-NA	3.81	2.15	2.06
33	T	208	KC1	C3B-C4B	-3.81	1.39	1.46
22	K	204	CLA	C1C-C2C	-3.81	1.36	1.44
22	A	827	CLA	MG-NC	3.81	2.15	2.06
22	T	206	CLA	MG-NB	3.80	2.13	2.05
33	S	210	KC1	C4A-C3A	-3.80	1.36	1.44
22	A	809	CLA	MG-NA	3.80	2.15	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	H	207	CLA	C1C-C2C	-3.80	1.36	1.44
22	U	208	CLA	MG-NA	3.79	2.15	2.06
22	P	210	CLA	MG-NA	3.79	2.15	2.06
22	Q	205	CLA	MG-NA	3.79	2.15	2.06
22	J	103	CLA	MG-NA	3.79	2.15	2.06
33	S	212	KC1	C3B-C4B	-3.78	1.39	1.46
22	O	202	CLA	MG-NA	3.77	2.15	2.06
22	H	202	CLA	MG-NA	3.77	2.15	2.06
22	B	830	CLA	MG-NA	3.77	2.15	2.06
22	A	804	CLA	MG-NA	3.77	2.15	2.06
22	G	208	CLA	MG-NA	3.77	2.15	2.06
22	S	217	CLA	MG-NA	3.77	2.15	2.06
22	B	825	CLA	MG-NC	3.76	2.15	2.06
22	G	201	CLA	MG-NA	3.76	2.15	2.06
22	A	850	CLA	MG-NA	3.76	2.15	2.06
33	Q	210	KC1	C3B-C4B	-3.75	1.39	1.46
33	P	212	KC1	C3B-C4B	-3.75	1.39	1.46
22	O	209	CLA	C1C-C2C	-3.75	1.36	1.44
22	O	211	CLA	MG-NA	3.74	2.15	2.06
33	S	210	KC1	C3B-C4B	-3.73	1.39	1.46
22	A	824	CLA	C1C-C2C	-3.73	1.37	1.44
22	Q	204	CLA	MG-NA	3.72	2.15	2.06
33	P	212	KC1	MG-NA	3.72	2.15	2.06
33	P	203	KC1	C4A-C3A	-3.72	1.37	1.44
33	T	208	KC1	C1B-C2B	-3.71	1.38	1.45
22	A	810	CLA	MG-NA	3.70	2.15	2.06
33	T	208	KC1	C4A-C3A	-3.70	1.37	1.44
22	B	847	CLA	MG-NA	3.70	2.15	2.06
22	Q	203	CLA	MG-NA	3.68	2.15	2.06
33	P	212	KC1	C1B-C2B	-3.68	1.38	1.45
22	B	845	CLA	MG-NA	3.67	2.15	2.06
33	Q	210	KC1	C1B-C2B	-3.66	1.38	1.45
22	G	204	CLA	MG-NA	3.66	2.15	2.06
22	A	831	CLA	MG-NA	3.65	2.14	2.06
22	U	204	CLA	MG-NA	3.65	2.14	2.06
22	P	209	CLA	MG-NA	3.64	2.14	2.06
33	O	210	KC1	C1B-C2B	-3.64	1.38	1.45
22	P	207	CLA	MG-NA	3.63	2.14	2.06
22	B	808	CLA	MG-NA	3.63	2.14	2.06
22	U	209	CLA	MG-NB	3.63	2.13	2.05
22	H	209	CLA	MG-NA	3.63	2.14	2.06
22	G	202	CLA	MG-NA	3.62	2.14	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	801	CLA	MG-NA	3.62	2.14	2.06
22	A	816	CLA	MG-NA	3.62	2.14	2.06
22	G	206	CLA	MG-NC	3.61	2.14	2.06
26	F	807	LMU	O5'-C1'	3.61	1.51	1.41
33	Q	210	KC1	MG-NA	3.61	2.14	2.06
33	U	213	KC1	C4A-C3A	-3.61	1.37	1.44
33	P	206	KC1	C4A-C3A	-3.60	1.37	1.44
22	A	846	CLA	MG-NC	3.60	2.14	2.06
22	B	804	CLA	MG-NA	3.59	2.14	2.06
22	B	817	CLA	MG-NA	3.59	2.14	2.06
26	P	221	LMU	O5'-C1'	3.59	1.51	1.41
33	P	206	KC1	C1B-C2B	-3.58	1.38	1.45
22	A	808	CLA	MG-NA	3.57	2.14	2.06
26	O	216	LMU	O5'-C1'	3.57	1.51	1.41
22	B	802	CLA	MG-NA	3.57	2.14	2.06
33	P	219	KC1	C4A-C3A	-3.57	1.37	1.44
25	R	102	BCR	C30-C25	-3.57	1.49	1.53
33	S	212	KC1	C4A-C3A	-3.56	1.37	1.44
26	A	847	LMU	O5'-C1'	3.55	1.51	1.41
22	H	207	CLA	MG-NA	3.55	2.14	2.06
22	A	856	CLA	MG-NA	3.55	2.14	2.06
22	U	209	CLA	MG-NA	3.54	2.14	2.06
22	A	854	CLA	MG-NA	3.54	2.14	2.06
26	F	806	LMU	O5B-C1B	3.54	1.50	1.41
22	A	828	CLA	MG-NC	3.54	2.14	2.06
33	P	203	KC1	C1B-C2B	-3.53	1.38	1.45
31	H	211	DD6	C26-C27	3.53	1.44	1.37
22	A	851	CLA	MG-NA	3.53	2.14	2.06
22	B	828	CLA	MG-NA	3.52	2.14	2.06
33	P	219	KC1	C1B-C2B	-3.52	1.38	1.45
22	H	208	CLA	MG-NA	3.51	2.14	2.06
22	S	209	CLA	MG-NA	3.51	2.14	2.06
22	G	215	CLA	MG-NA	3.51	2.14	2.06
22	A	835	CLA	MG-NC	3.50	2.14	2.06
25	B	836	BCR	C1-C6	-3.49	1.49	1.53
22	A	836	CLA	MG-NA	3.49	2.14	2.06
33	U	213	KC1	C1B-C2B	-3.49	1.38	1.45
22	T	202	CLA	MG-NA	3.47	2.14	2.06
33	Q	210	KC1	C4A-C3A	-3.45	1.37	1.44
22	B	814	CLA	MG-NA	3.43	2.14	2.06
31	U	214	DD6	C8-C6	-3.43	1.41	1.50
25	A	844	BCR	C1-C6	-3.43	1.49	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	U	203	DD6	C26-C27	3.40	1.44	1.37
33	S	210	KC1	MG-NA	3.39	2.14	2.06
31	G	214	DD6	C26-C27	3.39	1.44	1.37
26	L	206	LMU	O5'-C1'	3.39	1.50	1.41
26	K	202	LMU	O5B-C1B	3.39	1.50	1.41
26	O	216	LMU	O5B-C1B	3.39	1.50	1.41
26	M	102	LMU	O5'-C1'	3.38	1.50	1.41
22	Q	216	CLA	MG-NA	3.37	2.14	2.06
22	T	204	CLA	MG-NA	3.37	2.14	2.06
22	S	216	CLA	MG-NA	3.37	2.14	2.06
26	P	221	LMU	O5B-C1B	3.37	1.50	1.41
22	U	210	CLA	MG-NA	3.35	2.14	2.06
33	O	210	KC1	MG-NA	3.33	2.14	2.06
25	R	102	BCR	C1-C6	-3.33	1.49	1.53
22	K	207	CLA	MG-NA	3.33	2.14	2.06
22	T	205	CLA	MG-NA	3.33	2.14	2.06
26	A	847	LMU	O5B-C1B	3.33	1.50	1.41
22	S	202	CLA	MG-NA	3.32	2.14	2.06
31	P	215	DD6	C26-C27	3.32	1.44	1.37
26	L	206	LMU	O5B-C1B	3.32	1.50	1.41
26	K	201	LMU	O5B-C1B	3.31	1.50	1.41
31	K	208	DD6	C26-C27	3.30	1.43	1.37
22	A	826	CLA	MG-NC	3.30	2.14	2.06
33	T	208	KC1	MG-NC	3.29	2.14	2.06
22	A	802	CLA	MG-NA	3.29	2.14	2.06
31	U	214	DD6	C26-C27	3.29	1.43	1.37
22	A	803	CLA	MG-NA	3.29	2.14	2.06
22	B	829	CLA	MG-NC	3.28	2.14	2.06
33	S	212	KC1	MG-NA	3.28	2.14	2.06
26	S	203	LMU	O5B-C1B	3.28	1.50	1.41
31	Q	202	DD6	C26-C27	3.28	1.43	1.37
33	T	208	KC1	MG-NB	3.27	2.12	2.05
22	B	816	CLA	MG-NA	3.26	2.14	2.06
31	O	213	DD6	C26-C27	3.25	1.43	1.37
22	A	851	CLA	MG-NC	3.25	2.14	2.06
22	H	206	CLA	MG-NC	3.25	2.14	2.06
31	G	212	DD6	C26-C27	3.24	1.43	1.37
22	Q	206	CLA	MG-NC	3.23	2.13	2.06
22	H	204	CLA	MG-NA	3.22	2.13	2.06
22	S	206	CLA	MG-NA	3.22	2.13	2.06
32	P	217	LMG	C4-C5	3.21	1.59	1.53
26	K	201	LMU	O5'-C1'	3.21	1.50	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	P	218	DD6	C26-C27	3.21	1.43	1.37
25	J	104	BCR	C30-C25	-3.21	1.49	1.53
22	B	810	CLA	MG-NA	3.21	2.13	2.06
22	B	818	CLA	MG-NA	3.21	2.13	2.06
31	H	201	DD6	C24-C1	-3.20	1.39	1.46
26	F	807	LMU	O5B-C1B	3.20	1.50	1.41
22	G	205	CLA	MG-NA	3.20	2.13	2.06
22	O	208	CLA	MG-NA	3.18	2.13	2.06
33	P	219	KC1	MG-NA	3.18	2.13	2.06
31	T	213	DD6	C26-C27	3.16	1.43	1.37
22	B	831	CLA	MG-NC	3.16	2.13	2.06
31	O	212	DD6	C26-C27	3.15	1.43	1.37
22	G	207	CLA	MG-NA	3.14	2.13	2.06
31	S	215	DD6	C26-C27	3.14	1.43	1.37
25	B	840	BCR	C30-C25	-3.14	1.49	1.53
22	B	820	CLA	MG-NA	3.13	2.13	2.06
31	H	212	DD6	C26-C27	3.13	1.43	1.37
22	L	203	CLA	MG-NA	3.13	2.13	2.06
25	B	838	BCR	C1-C6	-3.13	1.49	1.53
22	A	806	CLA	MG-NA	3.12	2.13	2.06
32	P	217	LMG	C4-C3	3.12	1.60	1.52
25	M	101	BCR	C30-C25	-3.12	1.49	1.53
30	S	201	SQD	O48-C23	3.11	1.42	1.33
27	A	849	CL0	MG-ND	-3.11	1.99	2.05
22	B	830	CLA	MG-NC	3.11	2.13	2.06
26	M	102	LMU	O5B-C1B	3.11	1.49	1.41
31	P	220	DD6	C26-C27	3.11	1.43	1.37
25	A	842	BCR	C30-C25	-3.10	1.49	1.53
22	B	824	CLA	MG-NC	3.10	2.13	2.06
25	L	201	BCR	C1-C6	-3.09	1.49	1.53
22	A	845	CLA	MG-NC	3.08	2.13	2.06
26	K	202	LMU	O5'-C1'	3.08	1.49	1.41
31	T	212	DD6	C26-C27	3.07	1.43	1.37
31	P	218	DD6	C10-C11	3.07	1.42	1.35
25	A	842	BCR	C1-C6	-3.06	1.49	1.53
33	P	203	KC1	MG-NC	3.06	2.13	2.06
22	A	833	CLA	MG-NC	3.06	2.13	2.06
31	O	201	DD6	C26-C27	3.06	1.43	1.37
22	B	809	CLA	MG-NC	3.06	2.13	2.06
22	P	211	CLA	MG-NA	3.03	2.13	2.06
22	B	842	CLA	MG-NC	3.03	2.13	2.06
25	A	843	BCR	C1-C6	-3.03	1.49	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	T	207	CLA	MG-NA	3.03	2.13	2.06
22	A	848	CLA	MG-NC	3.03	2.13	2.06
25	F	805	BCR	C1-C6	-3.03	1.49	1.53
22	A	822	CLA	MG-NA	3.02	2.13	2.06
22	S	208	CLA	MG-NA	3.01	2.13	2.06
25	k	104	BCR	C1-C6	-3.01	1.49	1.53
25	L	201	BCR	C30-C25	-3.00	1.49	1.53
25	I	102	BCR	C1-C6	-3.00	1.49	1.53
22	F	803	CLA	MG-NC	2.99	2.13	2.06
31	Q	215	DD6	C26-C27	2.99	1.43	1.37
31	T	213	DD6	C8-C6	-2.99	1.39	1.46
30	B	846	SQD	O48-C23	2.98	1.42	1.33
31	U	212	DD6	C26-C27	2.98	1.43	1.37
22	G	210	CLA	MG-NC	2.98	2.13	2.06
22	Q	212	CLA	MG-NC	2.97	2.13	2.06
25	M	101	BCR	C1-C6	-2.97	1.50	1.53
25	I	101	BCR	C1-C6	-2.97	1.50	1.53
22	F	802	CLA	MG-NC	2.96	2.13	2.06
25	B	839	BCR	C1-C6	-2.96	1.50	1.53
25	B	840	BCR	C1-C6	-2.94	1.50	1.53
22	G	209	CLA	MG-NA	2.93	2.13	2.06
22	B	811	CLA	MG-NC	2.93	2.13	2.06
25	I	102	BCR	C30-C25	-2.93	1.50	1.53
22	A	805	CLA	MG-NC	2.93	2.13	2.06
31	S	205	DD6	C26-C27	2.93	1.43	1.37
22	K	203	CLA	MG-NC	2.93	2.13	2.06
31	k	101	DD6	C26-C27	2.92	1.43	1.37
22	B	822	CLA	MG-NC	2.92	2.13	2.06
22	T	201	CLA	C1D-C2D	-2.90	1.39	1.45
31	O	215	DD6	C26-C27	2.90	1.43	1.37
31	G	211	DD6	C26-C27	2.89	1.43	1.37
22	P	214	CLA	MG-NC	2.89	2.13	2.06
22	A	824	CLA	MG-NC	2.89	2.13	2.06
22	A	838	CLA	MG-NC	2.89	2.13	2.06
22	B	816	CLA	C1B-C2B	-2.88	1.36	1.43
31	G	213	DD6	C26-C27	2.87	1.43	1.37
25	F	801	BCR	C1-C6	-2.87	1.50	1.53
22	U	209	CLA	MG-ND	2.87	2.11	2.05
31	J	101	DD6	C26-C27	2.84	1.43	1.37
33	S	210	KC1	C2A-C3A	2.83	1.42	1.37
34	R	103	A86	C8-C6	-2.83	1.39	1.46
22	B	807	CLA	MG-NC	2.83	2.13	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B	839	BCR	C30-C25	-2.82	1.50	1.53
25	L	205	BCR	C30-C25	-2.82	1.50	1.53
22	B	808	CLA	MG-NC	2.82	2.13	2.06
22	A	821	CLA	MG-NC	2.82	2.13	2.06
31	H	201	DD6	C26-C27	2.81	1.42	1.37
30	B	846	SQD	O47-C7	2.80	1.42	1.34
22	B	823	CLA	MG-NC	2.80	2.12	2.06
25	J	104	BCR	C1-C6	-2.80	1.50	1.53
22	B	833	CLA	MG-NC	2.80	2.12	2.06
22	G	210	CLA	MG-NB	2.78	2.11	2.05
30	S	201	SQD	O47-C7	2.78	1.42	1.34
22	A	818	CLA	MG-NA	2.77	2.12	2.06
22	A	818	CLA	C1B-NB	-2.77	1.34	1.37
22	B	803	CLA	MG-NC	2.77	2.12	2.06
22	B	823	CLA	MG-NB	2.76	2.11	2.05
31	H	201	DD6	C25-C26	-2.76	1.34	1.43
27	A	849	CL0	MG-NB	-2.76	2.00	2.05
22	S	207	CLA	MG-NC	2.75	2.12	2.06
22	O	205	CLA	MG-NC	2.75	2.12	2.06
22	B	826	CLA	MG-NC	2.75	2.12	2.06
25	B	838	BCR	C30-C25	-2.74	1.50	1.53
31	S	204	DD6	C26-C27	2.74	1.42	1.37
22	k	103	CLA	C1D-C2D	-2.74	1.39	1.45
22	A	815	CLA	MG-NC	2.74	2.12	2.06
22	A	832	CLA	MG-NC	2.73	2.12	2.06
22	A	836	CLA	MG-NC	2.72	2.12	2.06
25	B	837	BCR	C1-C6	-2.71	1.50	1.53
25	L	205	BCR	C1-C6	-2.70	1.50	1.53
22	K	203	CLA	C4D-CHA	2.70	1.47	1.38
31	S	211	DD6	C13-C11	-2.70	1.40	1.46
31	P	205	DD6	C26-C27	2.69	1.42	1.37
27	A	849	CL0	C3B-C4B	-2.69	1.38	1.41
33	U	213	KC1	C2A-C3A	2.69	1.42	1.37
22	G	203	CLA	MG-NC	2.69	2.12	2.06
33	P	203	KC1	C2A-C3A	2.69	1.42	1.37
22	U	207	CLA	MG-NA	2.69	2.12	2.06
31	S	211	DD6	C24-C1	-2.67	1.40	1.46
31	S	214	DD6	C26-C27	2.67	1.42	1.37
22	A	820	CLA	C3D-C4D	-2.66	1.38	1.44
25	F	805	BCR	C30-C25	-2.66	1.50	1.53
31	O	213	DD6	C8-C6	-2.66	1.40	1.46
33	U	213	KC1	C1A-CHA	2.65	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	845	CLA	MG-NC	2.65	2.12	2.06
32	P	202	LMG	C4-C5	2.64	1.58	1.53
22	A	820	CLA	MG-NC	2.64	2.12	2.06
22	A	812	CLA	MG-NC	2.63	2.12	2.06
25	A	844	BCR	C30-C25	-2.63	1.50	1.53
25	B	837	BCR	C30-C25	-2.63	1.50	1.53
31	k	101	DD6	C8-C6	-2.63	1.40	1.46
22	G	210	CLA	C3D-C4D	-2.63	1.38	1.44
25	B	836	BCR	C30-C25	-2.62	1.50	1.53
22	B	827	CLA	C1D-C2D	-2.62	1.40	1.45
22	R	101	CLA	MG-NC	2.62	2.12	2.06
25	k	104	BCR	C30-C25	-2.62	1.50	1.53
31	O	214	DD6	C26-C27	2.61	1.42	1.37
22	P	214	CLA	MG-NB	2.61	2.11	2.05
22	O	209	CLA	C3D-C4D	-2.60	1.38	1.44
22	Q	209	CLA	MG-NC	2.60	2.12	2.06
22	B	843	CLA	C3D-C4D	-2.59	1.38	1.44
31	O	215	DD6	C24-C1	-2.59	1.40	1.46
22	G	206	CLA	C3D-C4D	-2.59	1.38	1.44
33	T	208	KC1	C2A-C3A	2.59	1.42	1.37
22	P	216	CLA	MG-NC	2.58	2.12	2.06
22	B	816	CLA	C3D-C4D	-2.58	1.38	1.44
22	B	845	CLA	C3D-C4D	-2.58	1.38	1.44
24	A	840	LHG	O7-C5	-2.57	1.40	1.46
22	B	816	CLA	C1D-C2D	-2.57	1.40	1.45
22	Q	206	CLA	C3D-C4D	-2.57	1.38	1.44
33	T	208	KC1	C1A-CHA	2.57	1.46	1.40
22	K	203	CLA	C1D-C2D	-2.57	1.40	1.45
22	k	103	CLA	MG-NC	2.57	2.12	2.06
22	B	805	CLA	MG-NC	2.56	2.12	2.06
25	A	841	BCR	C1-C6	-2.56	1.50	1.53
31	P	218	DD6	C2-C1	2.56	1.41	1.35
31	S	204	DD6	C24-C1	-2.56	1.40	1.46
33	P	206	KC1	C1A-CHA	2.56	1.46	1.40
25	I	101	BCR	C30-C25	-2.56	1.50	1.53
22	R	101	CLA	C1D-C2D	-2.56	1.40	1.45
33	S	210	KC1	C1A-CHA	2.56	1.46	1.40
31	P	215	DD6	C5-C6	2.56	1.41	1.35
31	O	212	DD6	C10-C11	2.56	1.41	1.35
33	P	212	KC1	C1A-CHA	2.55	1.46	1.40
22	A	815	CLA	C1B-C2B	-2.55	1.37	1.43
31	k	101	DD6	C13-C11	-2.55	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	O	209	CLA	C1D-C2D	-2.55	1.40	1.45
22	B	806	CLA	C3D-C4D	-2.55	1.38	1.44
22	A	830	CLA	MG-NC	2.55	2.12	2.06
31	P	215	DD6	C2-C1	2.55	1.41	1.35
34	Q	214	A86	C24-C1	-2.54	1.40	1.46
22	B	821	CLA	C3D-C4D	-2.54	1.38	1.44
22	B	832	CLA	C3D-C4D	-2.54	1.38	1.44
31	G	211	DD6	C24-C1	-2.53	1.40	1.46
22	R	101	CLA	C1B-C2B	-2.53	1.37	1.43
22	A	813	CLA	C3D-C4D	-2.53	1.38	1.44
33	P	203	KC1	C1A-CHA	2.53	1.46	1.40
22	P	211	CLA	C3D-C4D	-2.53	1.38	1.44
22	B	844	CLA	MG-NC	2.52	2.12	2.06
22	U	208	CLA	C3D-C4D	-2.52	1.38	1.44
31	P	218	DD6	C5-C6	2.52	1.41	1.35
22	A	819	CLA	MG-NC	2.52	2.12	2.06
34	R	105	A86	C24-C1	-2.52	1.40	1.46
31	T	212	DD6	C10-C11	2.52	1.41	1.35
22	B	820	CLA	C3D-C4D	-2.52	1.38	1.44
22	S	206	CLA	C3D-C4D	-2.52	1.38	1.44
31	T	213	DD6	C13-C11	-2.51	1.40	1.46
22	B	821	CLA	C1D-C2D	-2.51	1.40	1.45
22	H	210	CLA	MG-NC	2.51	2.12	2.06
22	O	205	CLA	C3D-C4D	-2.51	1.38	1.44
22	B	813	CLA	C3D-C4D	-2.51	1.38	1.44
22	L	202	CLA	MG-NC	2.51	2.12	2.06
31	J	101	DD6	C24-C1	-2.51	1.40	1.46
22	B	814	CLA	C1B-C2B	-2.51	1.37	1.43
31	O	213	DD6	C13-C11	-2.51	1.40	1.46
34	U	202	A86	C5-C6	2.51	1.41	1.35
22	Q	211	CLA	C3D-C4D	-2.50	1.38	1.44
25	F	801	BCR	C30-C25	-2.50	1.50	1.53
31	k	101	DD6	C24-C1	-2.50	1.40	1.46
22	A	801	CLA	C1B-C2B	-2.50	1.37	1.43
31	P	205	DD6	C13-C11	-2.50	1.40	1.46
22	G	207	CLA	C3D-C4D	-2.50	1.38	1.44
22	B	833	CLA	C3D-C4D	-2.50	1.38	1.44
22	P	213	CLA	MG-NC	2.50	2.12	2.06
22	A	828	CLA	C3D-C4D	-2.50	1.38	1.44
22	B	813	CLA	MG-NB	2.50	2.10	2.05
22	B	823	CLA	C3D-C4D	-2.49	1.38	1.44
22	B	804	CLA	C3D-C4D	-2.49	1.38	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	818	CLA	C3D-C4D	-2.49	1.38	1.44
22	L	203	CLA	C3D-C4D	-2.49	1.38	1.44
22	A	830	CLA	C3D-C4D	-2.49	1.38	1.44
22	B	824	CLA	C3D-C4D	-2.49	1.38	1.44
22	B	801	CLA	C1D-C2D	-2.49	1.40	1.45
22	A	803	CLA	C3D-C4D	-2.49	1.38	1.44
31	Q	215	DD6	C10-C11	2.49	1.41	1.35
22	A	831	CLA	C3D-C4D	-2.49	1.38	1.44
22	B	811	CLA	C3D-C4D	-2.49	1.38	1.44
22	B	812	CLA	C3D-C4D	-2.49	1.38	1.44
22	A	809	CLA	C3D-C4D	-2.49	1.38	1.44
22	B	830	CLA	C3D-C4D	-2.49	1.38	1.44
22	R	104	CLA	MG-NB	2.48	2.10	2.05
31	P	215	DD6	C10-C11	2.48	1.41	1.35
22	B	818	CLA	MG-NC	2.48	2.12	2.06
22	Q	209	CLA	C3D-C4D	-2.48	1.38	1.44
22	H	202	CLA	C3D-C4D	-2.48	1.38	1.44
22	Q	211	CLA	MG-NC	2.48	2.12	2.06
25	A	841	BCR	C30-C25	-2.48	1.50	1.53
22	T	207	CLA	C3D-C4D	-2.48	1.38	1.44
25	A	843	BCR	C30-C25	-2.47	1.50	1.53
22	A	827	CLA	C3D-C4D	-2.47	1.38	1.44
22	A	807	CLA	MG-NC	2.47	2.12	2.06
22	G	215	CLA	C3D-C4D	-2.47	1.38	1.44
33	Q	210	KC1	C1A-CHA	2.47	1.46	1.40
22	O	207	CLA	C3D-C4D	-2.47	1.38	1.44
31	O	213	DD6	C24-C1	-2.47	1.40	1.46
31	K	208	DD6	C5-C6	2.47	1.41	1.35
22	B	827	CLA	MG-NC	2.47	2.12	2.06
22	U	211	CLA	MG-NC	2.47	2.12	2.06
22	T	203	CLA	MG-NC	2.46	2.12	2.06
22	R	104	CLA	C3D-C4D	-2.46	1.38	1.44
33	U	213	KC1	MG-NC	2.46	2.12	2.06
22	B	809	CLA	C3D-C4D	-2.46	1.38	1.44
22	A	827	CLA	C1D-C2D	-2.46	1.40	1.45
22	A	838	CLA	C1D-C2D	-2.46	1.40	1.45
22	B	802	CLA	MG-NC	2.46	2.12	2.06
22	H	206	CLA	C3D-C4D	-2.46	1.38	1.44
31	G	212	DD6	C2-C1	2.46	1.41	1.35
22	L	204	CLA	C3D-C4D	-2.46	1.38	1.44
22	A	829	CLA	MG-NC	2.46	2.12	2.06
22	B	805	CLA	C3D-C4D	-2.46	1.38	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	k	102	CLA	C3D-C4D	-2.46	1.38	1.44
22	S	209	CLA	C3D-C4D	-2.46	1.38	1.44
22	P	208	CLA	C3D-C4D	-2.46	1.38	1.44
22	U	207	CLA	C3D-C4D	-2.46	1.38	1.44
22	A	846	CLA	C3D-C4D	-2.45	1.38	1.44
22	Q	208	CLA	MG-NC	2.45	2.12	2.06
22	T	210	CLA	MG-NC	2.45	2.12	2.06
22	A	813	CLA	C1B-C2B	-2.45	1.37	1.43
22	O	208	CLA	C3D-C4D	-2.45	1.38	1.44
22	A	802	CLA	C3D-C4D	-2.45	1.38	1.44
22	A	810	CLA	C3D-C4D	-2.45	1.38	1.44
22	Q	207	CLA	C3D-C4D	-2.45	1.38	1.44
22	B	807	CLA	C1D-C2D	-2.45	1.40	1.45
31	G	214	DD6	C8-C6	-2.45	1.40	1.46
31	T	212	DD6	C2-C1	2.45	1.41	1.35
22	B	814	CLA	C3D-C4D	-2.45	1.38	1.44
22	O	202	CLA	C3D-C4D	-2.45	1.38	1.44
22	T	205	CLA	C3D-C4D	-2.45	1.38	1.44
22	K	207	CLA	C3D-C4D	-2.44	1.38	1.44
22	Q	207	CLA	MG-NC	2.44	2.12	2.06
22	A	813	CLA	MG-NC	2.44	2.12	2.06
22	F	804	CLA	C3D-C4D	-2.44	1.38	1.44
22	A	838	CLA	C3D-C4D	-2.44	1.38	1.44
22	T	201	CLA	MG-NC	2.44	2.12	2.06
22	B	810	CLA	C3D-C4D	-2.44	1.38	1.44
34	U	202	A86	C2-C1	2.44	1.41	1.35
22	A	818	CLA	C3D-C4D	-2.44	1.38	1.44
22	P	207	CLA	C3D-C4D	-2.44	1.38	1.44
22	H	204	CLA	C3D-C4D	-2.44	1.38	1.44
31	G	212	DD6	C5-C6	2.44	1.41	1.35
22	A	802	CLA	MG-NC	2.43	2.12	2.06
33	P	206	KC1	MG-NC	2.43	2.12	2.06
22	P	216	CLA	C3D-C4D	-2.43	1.38	1.44
24	G	216	LHG	P-O6	2.43	1.68	1.59
22	Q	216	CLA	C3D-C4D	-2.43	1.38	1.44
22	J	103	CLA	C3D-C4D	-2.43	1.38	1.44
22	A	825	CLA	C3D-C4D	-2.43	1.38	1.44
22	U	206	CLA	C3D-C4D	-2.43	1.38	1.44
22	U	210	CLA	C3D-C4D	-2.42	1.38	1.44
31	U	212	DD6	C10-C11	2.42	1.41	1.35
22	A	815	CLA	C3D-C4D	-2.42	1.38	1.44
31	O	212	DD6	C2-C1	2.42	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	817	CLA	C3D-C4D	-2.42	1.38	1.44
22	Q	205	CLA	C3D-C4D	-2.42	1.38	1.44
22	Q	213	CLA	C3D-C4D	-2.42	1.38	1.44
31	K	208	DD6	C2-C1	2.42	1.41	1.35
22	Q	203	CLA	C3D-C4D	-2.42	1.38	1.44
22	K	206	CLA	MG-NB	2.42	2.10	2.05
22	A	822	CLA	C3D-C4D	-2.42	1.38	1.44
22	T	204	CLA	C3D-C4D	-2.42	1.38	1.44
31	H	211	DD6	C2-C1	2.42	1.41	1.35
22	B	806	CLA	MG-NC	2.42	2.12	2.06
31	P	205	DD6	C24-C1	-2.42	1.40	1.46
31	G	211	DD6	C10-C11	2.42	1.41	1.35
22	A	826	CLA	C3D-C4D	-2.42	1.38	1.44
22	B	815	CLA	C3D-C4D	-2.42	1.38	1.44
22	S	216	CLA	C3D-C4D	-2.42	1.38	1.44
31	K	208	DD6	C10-C11	2.42	1.41	1.35
22	A	854	CLA	C3D-C4D	-2.42	1.38	1.44
22	H	207	CLA	C3D-C4D	-2.42	1.38	1.44
22	K	205	CLA	C3D-C4D	-2.42	1.38	1.44
22	Q	212	CLA	C1D-C2D	-2.42	1.40	1.45
22	H	203	CLA	C3D-C4D	-2.41	1.38	1.44
22	P	210	CLA	C3D-C4D	-2.41	1.38	1.44
22	A	817	CLA	C3D-C4D	-2.41	1.38	1.44
22	S	202	CLA	C3D-C4D	-2.41	1.38	1.44
31	S	204	DD6	C8-C6	-2.41	1.40	1.46
22	A	804	CLA	C3D-C4D	-2.41	1.38	1.44
32	S	213	LMG	O7-C8	-2.41	1.40	1.46
22	A	853	CLA	C3D-C4D	-2.41	1.38	1.44
22	S	208	CLA	C3D-C4D	-2.41	1.38	1.44
22	B	847	CLA	C3D-C4D	-2.41	1.38	1.44
22	U	205	CLA	C3D-C4D	-2.41	1.38	1.44
22	P	213	CLA	C3D-C4D	-2.41	1.38	1.44
22	O	206	CLA	C3D-C4D	-2.41	1.38	1.44
22	B	844	CLA	C1B-C2B	-2.41	1.37	1.43
31	S	215	DD6	C5-C6	2.41	1.41	1.35
31	Q	202	DD6	C10-C11	2.41	1.41	1.35
22	O	203	CLA	C3D-C4D	-2.40	1.38	1.44
22	H	208	CLA	C3D-C4D	-2.40	1.38	1.44
33	P	212	KC1	C2A-C3A	2.40	1.42	1.37
22	A	801	CLA	C1D-C2D	-2.40	1.40	1.45
22	A	814	CLA	C1B-C2B	-2.40	1.37	1.43
22	G	201	CLA	C1B-C2B	-2.40	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	T	212	DD6	C5-C6	2.40	1.41	1.35
31	G	214	DD6	C13-C11	-2.40	1.40	1.46
31	G	214	DD6	C5-C6	2.40	1.41	1.35
22	P	209	CLA	C3D-C4D	-2.40	1.38	1.44
22	T	203	CLA	C3D-C4D	-2.40	1.38	1.44
22	H	210	CLA	C3D-C4D	-2.40	1.38	1.44
22	A	819	CLA	C3D-C4D	-2.40	1.38	1.44
22	A	805	CLA	C3D-C4D	-2.40	1.38	1.44
22	B	826	CLA	C3D-C4D	-2.40	1.38	1.44
22	S	217	CLA	C3D-C4D	-2.40	1.38	1.44
22	B	825	CLA	C3D-C4D	-2.40	1.38	1.44
31	H	201	DD6	C5-C6	2.40	1.41	1.35
22	S	207	CLA	C3D-C4D	-2.40	1.38	1.44
31	O	201	DD6	C8-C6	-2.40	1.40	1.46
31	T	212	DD6	C24-C1	-2.40	1.40	1.46
22	P	208	CLA	MG-NC	2.40	2.12	2.06
22	A	816	CLA	C3D-C4D	-2.40	1.38	1.44
22	B	809	CLA	CAB-C3B	-2.39	1.45	1.50
22	A	806	CLA	C3D-C4D	-2.39	1.38	1.44
22	T	209	CLA	C3D-C4D	-2.39	1.38	1.44
22	G	209	CLA	C3D-C4D	-2.39	1.38	1.44
22	A	816	CLA	C1B-C2B	-2.39	1.37	1.43
22	O	204	CLA	C3D-C4D	-2.39	1.38	1.44
31	O	214	DD6	C24-C1	-2.39	1.40	1.46
22	G	205	CLA	C3D-C4D	-2.39	1.38	1.44
31	P	205	DD6	C8-C6	-2.39	1.40	1.46
22	A	823	CLA	C3D-C4D	-2.39	1.38	1.44
22	K	204	CLA	C3D-C4D	-2.39	1.38	1.44
22	A	807	CLA	C3D-C4D	-2.39	1.38	1.44
22	A	811	CLA	C3D-C4D	-2.39	1.38	1.44
22	B	808	CLA	C3D-C4D	-2.39	1.38	1.44
22	Q	204	CLA	C3D-C4D	-2.39	1.38	1.44
22	U	211	CLA	C3D-C4D	-2.39	1.38	1.44
31	O	215	DD6	C8-C6	-2.39	1.40	1.46
31	H	212	DD6	C5-C6	2.39	1.41	1.35
22	G	209	CLA	C1D-C2D	-2.39	1.40	1.45
22	A	835	CLA	C3D-C4D	-2.39	1.38	1.44
22	B	829	CLA	C3D-C4D	-2.39	1.38	1.44
22	L	204	CLA	MG-NC	2.39	2.11	2.06
22	B	824	CLA	C1D-C2D	-2.39	1.40	1.45
34	R	105	A86	C8-C6	-2.39	1.40	1.46
31	S	214	DD6	C10-C11	2.39	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	O	204	CLA	MG-NC	2.39	2.11	2.06
22	A	823	CLA	C1D-C2D	-2.39	1.40	1.45
31	H	212	DD6	C13-C11	-2.38	1.40	1.46
22	G	204	CLA	C3D-C4D	-2.38	1.38	1.44
22	K	206	CLA	C3D-C4D	-2.38	1.38	1.44
31	S	211	DD6	C8-C6	-2.38	1.40	1.46
22	B	844	CLA	C3D-C4D	-2.38	1.38	1.44
22	L	202	CLA	C3D-C4D	-2.38	1.38	1.44
31	G	213	DD6	C24-C1	-2.38	1.40	1.46
22	P	211	CLA	C1D-C2D	-2.38	1.40	1.45
22	H	209	CLA	C3D-C4D	-2.38	1.38	1.44
22	U	204	CLA	C3D-C4D	-2.38	1.38	1.44
22	G	206	CLA	C1D-C2D	-2.38	1.40	1.45
22	B	808	CLA	C1B-NB	-2.38	1.34	1.37
22	A	832	CLA	C1B-C2B	-2.38	1.37	1.43
22	A	829	CLA	C3D-C4D	-2.38	1.38	1.44
22	B	828	CLA	C3D-C4D	-2.38	1.38	1.44
31	U	214	DD6	C5-C6	2.38	1.41	1.34
22	A	832	CLA	C3D-C4D	-2.37	1.38	1.44
22	B	801	CLA	C3D-C4D	-2.37	1.38	1.44
31	H	212	DD6	C2-C1	2.37	1.41	1.35
22	B	844	CLA	C1D-C2D	-2.37	1.40	1.45
31	G	213	DD6	C13-C11	-2.37	1.40	1.46
22	A	818	CLA	C1B-C2B	-2.37	1.37	1.43
22	B	818	CLA	C1D-C2D	-2.37	1.40	1.45
22	B	826	CLA	C1B-C2B	-2.37	1.37	1.43
22	A	848	CLA	C3D-C4D	-2.37	1.38	1.44
33	O	210	KC1	MG-NC	2.37	2.11	2.06
34	P	204	A86	C2-C1	2.37	1.41	1.35
22	B	819	CLA	C3D-C4D	-2.37	1.38	1.44
22	A	814	CLA	C3D-C4D	-2.37	1.38	1.44
22	k	103	CLA	C3D-C4D	-2.37	1.38	1.44
31	G	213	DD6	C8-C6	-2.37	1.40	1.46
22	B	809	CLA	MG-NB	2.37	2.10	2.05
22	A	836	CLA	C3D-C4D	-2.37	1.38	1.44
22	A	850	CLA	C3D-C4D	-2.37	1.38	1.44
31	S	204	DD6	C13-C11	-2.37	1.40	1.46
22	B	828	CLA	MG-NC	2.36	2.11	2.06
22	O	206	CLA	MG-NC	2.36	2.11	2.06
33	P	206	KC1	C2A-C3A	2.36	1.42	1.37
22	A	855	CLA	C3D-C4D	-2.36	1.38	1.44
22	O	211	CLA	C3D-C4D	-2.36	1.38	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	T	210	CLA	C3D-C4D	-2.36	1.38	1.44
22	T	202	CLA	C3D-C4D	-2.36	1.38	1.44
22	A	851	CLA	C3D-C4D	-2.36	1.38	1.44
34	P	204	A86	C5-C6	2.36	1.41	1.35
22	U	204	CLA	MG-NC	2.36	2.11	2.06
31	G	211	DD6	C8-C6	-2.36	1.40	1.46
22	B	827	CLA	C3D-C4D	-2.36	1.38	1.44
31	H	201	DD6	C2-C1	2.36	1.41	1.35
33	P	219	KC1	C1A-CHA	2.35	1.46	1.40
31	G	212	DD6	C10-C11	2.35	1.41	1.35
22	H	205	CLA	C3D-C4D	-2.35	1.38	1.44
22	A	808	CLA	C3D-C4D	-2.35	1.38	1.44
22	A	825	CLA	MG-NC	2.35	2.11	2.06
22	B	834	CLA	C1D-C2D	-2.35	1.40	1.45
22	B	812	CLA	MG-NC	2.35	2.11	2.06
22	Q	204	CLA	C1B-C2B	-2.35	1.37	1.43
22	B	802	CLA	C1D-C2D	-2.35	1.40	1.45
22	A	833	CLA	MG-NB	2.35	2.10	2.05
22	A	834	CLA	C3D-C4D	-2.35	1.38	1.44
32	P	217	LMG	O4-C4	-2.35	1.37	1.43
22	H	210	CLA	MG-NB	2.35	2.10	2.05
22	A	809	CLA	MG-NC	2.35	2.11	2.06
22	A	831	CLA	MG-NC	2.35	2.11	2.06
31	U	203	DD6	C10-C11	2.34	1.41	1.35
22	Q	208	CLA	C3D-C4D	-2.34	1.38	1.44
31	S	214	DD6	C24-C1	-2.34	1.40	1.46
31	O	212	DD6	C28-C27	-2.34	1.49	1.50
33	S	212	KC1	C1A-CHA	2.34	1.46	1.40
31	Q	202	DD6	C5-C6	2.34	1.41	1.35
22	F	802	CLA	C3D-C4D	-2.34	1.38	1.44
22	K	203	CLA	C1B-C2B	-2.34	1.37	1.43
22	G	203	CLA	C1D-C2D	-2.34	1.40	1.45
22	B	834	CLA	C3D-C4D	-2.34	1.38	1.44
22	B	831	CLA	C3D-C4D	-2.34	1.38	1.44
31	H	201	DD6	C10-C11	2.34	1.41	1.35
31	Q	215	DD6	C24-C1	-2.34	1.41	1.46
22	A	833	CLA	C3D-C4D	-2.34	1.38	1.44
31	S	205	DD6	C8-C6	-2.34	1.41	1.46
22	A	824	CLA	C3D-C4D	-2.34	1.38	1.44
22	Q	208	CLA	C1D-C2D	-2.34	1.40	1.45
22	O	211	CLA	MG-NC	2.34	2.11	2.06
22	G	201	CLA	C3D-C4D	-2.34	1.38	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	821	CLA	C1D-C2D	-2.33	1.40	1.45
22	A	856	CLA	C3D-C4D	-2.33	1.38	1.44
22	B	822	CLA	C3D-C4D	-2.33	1.38	1.44
31	Q	202	DD6	C2-C1	2.33	1.41	1.35
22	G	202	CLA	C3D-C4D	-2.33	1.38	1.44
22	K	205	CLA	MG-NC	2.33	2.11	2.06
31	O	213	DD6	C28-C27	-2.33	1.49	1.50
31	S	215	DD6	C2-C1	2.33	1.41	1.35
22	B	817	CLA	C1B-C2B	-2.33	1.37	1.43
22	B	832	CLA	MG-NC	2.33	2.11	2.06
31	O	201	DD6	C24-C1	-2.33	1.41	1.46
22	A	814	CLA	MG-NC	2.33	2.11	2.06
22	B	843	CLA	C1D-C2D	-2.33	1.40	1.45
22	H	203	CLA	MG-NC	2.33	2.11	2.06
22	B	847	CLA	C1D-C2D	-2.33	1.40	1.45
22	F	802	CLA	C1D-C2D	-2.33	1.40	1.45
31	Q	215	DD6	C5-C6	2.33	1.41	1.35
31	U	214	DD6	C2-C1	2.33	1.41	1.35
22	R	101	CLA	C3D-C4D	-2.33	1.39	1.44
31	Q	215	DD6	C2-C1	2.32	1.41	1.35
22	A	825	CLA	C1D-C2D	-2.32	1.40	1.45
22	O	207	CLA	C1B-C2B	-2.32	1.37	1.43
22	B	829	CLA	C1D-C2D	-2.32	1.40	1.45
31	P	220	DD6	C10-C11	2.32	1.41	1.35
31	O	212	DD6	C24-C1	-2.32	1.41	1.46
22	B	805	CLA	C1D-C2D	-2.32	1.40	1.45
22	B	845	CLA	C1B-C2B	-2.32	1.37	1.43
22	B	819	CLA	C1D-C2D	-2.32	1.40	1.45
22	G	206	CLA	C1B-C2B	-2.32	1.37	1.43
31	H	211	DD6	C13-C11	-2.32	1.41	1.46
22	A	817	CLA	C1D-C2D	-2.32	1.40	1.45
31	J	101	DD6	C13-C11	-2.32	1.41	1.46
31	G	214	DD6	C2-C1	2.32	1.41	1.35
22	G	210	CLA	C1D-C2D	-2.32	1.40	1.45
31	H	201	DD6	C36-C31	-2.32	1.32	1.35
22	F	804	CLA	MG-NC	2.32	2.11	2.06
33	O	210	KC1	C1A-CHA	2.32	1.46	1.40
22	A	806	CLA	C1D-C2D	-2.32	1.40	1.45
34	Q	218	A86	C2-C1	2.31	1.41	1.35
22	F	804	CLA	C1B-C2B	-2.31	1.37	1.43
22	G	208	CLA	C3D-C4D	-2.31	1.39	1.44
22	G	208	CLA	C1B-C2B	-2.31	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	S	205	DD6	C24-C1	-2.31	1.41	1.46
22	A	812	CLA	C3D-C4D	-2.31	1.39	1.44
31	S	215	DD6	C10-C11	2.31	1.41	1.35
22	G	204	CLA	C1D-C2D	-2.31	1.40	1.45
22	B	821	CLA	C1B-C2B	-2.31	1.37	1.43
22	S	206	CLA	C1B-C2B	-2.31	1.37	1.43
22	G	203	CLA	C3D-C4D	-2.30	1.39	1.44
31	P	205	DD6	C10-C11	2.30	1.41	1.35
22	T	206	CLA	C3D-C4D	-2.30	1.39	1.44
31	P	220	DD6	C8-C6	-2.30	1.41	1.46
31	O	201	DD6	C13-C11	-2.30	1.41	1.46
22	O	204	CLA	C1D-C2D	-2.30	1.40	1.45
31	P	220	DD6	C13-C11	-2.30	1.41	1.46
22	H	205	CLA	C1D-C2D	-2.30	1.40	1.45
22	B	819	CLA	MG-NC	2.30	2.11	2.06
22	A	846	CLA	C1D-C2D	-2.30	1.40	1.45
31	S	214	DD6	C9-C8	2.30	1.40	1.34
22	O	202	CLA	C1B-C2B	-2.30	1.37	1.43
22	Q	212	CLA	C3D-C4D	-2.30	1.39	1.44
31	S	215	DD6	C8-C6	-2.30	1.41	1.46
31	J	101	DD6	C10-C11	2.30	1.41	1.35
22	B	807	CLA	C3D-C4D	-2.30	1.39	1.44
22	B	822	CLA	C1D-C2D	-2.30	1.40	1.45
22	O	209	CLA	C1B-C2B	-2.30	1.37	1.43
31	O	214	DD6	C5-C6	2.30	1.41	1.35
22	T	209	CLA	C1B-C2B	-2.30	1.37	1.43
22	B	812	CLA	MG-NB	2.30	2.10	2.05
33	Q	210	KC1	C2A-C3A	2.30	1.41	1.37
31	U	203	DD6	C5-C6	2.29	1.41	1.35
22	B	842	CLA	C3D-C4D	-2.29	1.39	1.44
31	S	214	DD6	C2-C1	2.29	1.41	1.35
22	G	203	CLA	C1B-C2B	-2.29	1.37	1.43
31	S	205	DD6	C13-C11	-2.29	1.41	1.46
22	A	803	CLA	C1B-NB	-2.29	1.34	1.37
31	U	212	DD6	C5-C6	2.29	1.41	1.35
22	A	819	CLA	C1D-C2D	-2.29	1.40	1.45
31	P	220	DD6	C5-C6	2.29	1.41	1.35
22	P	211	CLA	C1B-NB	-2.29	1.34	1.37
31	O	214	DD6	C10-C11	2.29	1.41	1.35
33	O	210	KC1	C3B-C2B	2.29	1.41	1.37
22	A	820	CLA	C1B-C2B	-2.29	1.37	1.43
31	P	220	DD6	C2-C1	2.29	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	K	204	CLA	C1B-C2B	-2.29	1.37	1.43
22	A	831	CLA	C1B-C2B	-2.28	1.37	1.43
31	H	211	DD6	C10-C11	2.28	1.41	1.35
22	B	832	CLA	C1B-C2B	-2.28	1.37	1.43
22	P	214	CLA	C3D-C4D	-2.28	1.39	1.44
22	B	803	CLA	C3D-C4D	-2.28	1.39	1.44
22	P	209	CLA	C1D-C2D	-2.28	1.40	1.45
22	B	821	CLA	MG-NC	2.28	2.11	2.06
22	B	803	CLA	C1D-C2D	-2.28	1.40	1.45
22	F	803	CLA	C3D-C4D	-2.28	1.39	1.44
31	H	201	DD6	C13-C11	-2.28	1.41	1.46
34	R	103	A86	C24-C1	-2.28	1.41	1.46
22	H	213	CLA	C3D-C4D	-2.28	1.39	1.44
22	A	830	CLA	C1D-C2D	-2.28	1.40	1.45
22	G	205	CLA	C1D-C2D	-2.28	1.40	1.45
22	A	811	CLA	C1D-C2D	-2.28	1.40	1.45
22	Q	211	CLA	C1D-C2D	-2.28	1.40	1.45
22	H	205	CLA	MG-NC	2.28	2.11	2.06
22	T	211	CLA	C3D-C4D	-2.28	1.39	1.44
22	B	806	CLA	C1D-C2D	-2.28	1.40	1.45
22	B	808	CLA	C1D-C2D	-2.28	1.40	1.45
31	U	203	DD6	C8-C6	-2.28	1.41	1.46
22	T	201	CLA	C3D-C4D	-2.28	1.39	1.44
33	S	210	KC1	C1B-NB	-2.27	1.34	1.37
22	R	104	CLA	C1D-C2D	-2.27	1.40	1.45
34	Q	201	A86	C24-C1	-2.27	1.41	1.46
31	H	212	DD6	C8-C6	-2.27	1.41	1.46
31	G	213	DD6	C10-C11	2.27	1.41	1.35
22	A	803	CLA	C1B-C2B	-2.27	1.37	1.43
22	A	816	CLA	MG-NC	2.27	2.11	2.06
22	A	801	CLA	C3D-C4D	-2.27	1.39	1.44
22	K	204	CLA	MG-NC	2.27	2.11	2.06
31	H	212	DD6	C24-C1	-2.27	1.41	1.46
22	U	205	CLA	C1B-C2B	-2.27	1.37	1.43
22	A	801	CLA	MG-NC	2.27	2.11	2.06
31	H	211	DD6	C8-C6	-2.27	1.41	1.46
22	B	804	CLA	MG-NC	2.27	2.11	2.06
22	G	209	CLA	C1B-NB	-2.27	1.34	1.37
31	U	214	DD6	C24-C1	-2.27	1.41	1.46
22	A	828	CLA	C1D-C2D	-2.26	1.40	1.45
34	Q	201	A86	C8-C6	-2.26	1.41	1.46
31	J	101	DD6	C8-C6	-2.26	1.41	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	U	212	DD6	C2-C1	2.26	1.41	1.35
22	B	802	CLA	C1B-C2B	-2.26	1.37	1.43
22	B	807	CLA	C1B-C2B	-2.26	1.37	1.43
22	Q	209	CLA	C1D-C2D	-2.26	1.40	1.45
22	A	846	CLA	MG-NB	2.26	2.10	2.05
34	Q	218	A86	C5-C6	2.26	1.41	1.35
22	A	807	CLA	C1D-C2D	-2.26	1.40	1.45
31	G	214	DD6	C24-C1	-2.26	1.41	1.46
22	B	802	CLA	C3D-C4D	-2.25	1.39	1.44
22	S	206	CLA	C1D-C2D	-2.25	1.40	1.45
34	Q	201	A86	C2-C1	2.25	1.41	1.35
22	A	804	CLA	C1D-C2D	-2.25	1.40	1.45
34	Q	218	A86	C24-C1	-2.25	1.41	1.46
22	A	826	CLA	C1D-C2D	-2.25	1.40	1.45
22	B	833	CLA	C1B-C2B	-2.25	1.37	1.43
26	K	202	LMU	O5B-C5B	2.25	1.49	1.44
22	A	821	CLA	C3D-C4D	-2.25	1.39	1.44
31	S	215	DD6	C13-C11	-2.25	1.41	1.46
31	H	211	DD6	C5-C6	2.25	1.41	1.35
22	Q	206	CLA	C1D-C2D	-2.25	1.40	1.45
22	U	208	CLA	C1B-C2B	-2.25	1.37	1.43
22	U	211	CLA	C1D-C2D	-2.25	1.40	1.45
26	S	203	LMU	O5'-C5'	2.25	1.49	1.44
22	U	211	CLA	C1B-C2B	-2.25	1.37	1.43
31	O	212	DD6	C5-C6	2.24	1.41	1.35
22	A	810	CLA	C1B-C2B	-2.24	1.37	1.43
22	A	845	CLA	C1D-C2D	-2.24	1.40	1.45
22	P	216	CLA	C1D-C2D	-2.24	1.40	1.45
33	U	213	KC1	C1B-NB	-2.24	1.34	1.37
22	B	834	CLA	C1B-C2B	-2.24	1.37	1.43
22	A	826	CLA	C1B-NB	-2.24	1.34	1.37
22	A	850	CLA	C1B-C2B	-2.24	1.37	1.43
22	B	820	CLA	C1B-NB	-2.24	1.34	1.37
22	U	205	CLA	MG-NC	2.24	2.11	2.06
22	B	825	CLA	MG-NB	2.23	2.10	2.05
26	S	203	LMU	O5B-C5B	2.23	1.49	1.44
31	T	213	DD6	C24-C1	-2.23	1.41	1.46
31	S	205	DD6	C10-C11	2.23	1.41	1.35
22	A	817	CLA	C1B-C2B	-2.23	1.37	1.43
22	B	847	CLA	C1B-C2B	-2.23	1.37	1.43
22	P	214	CLA	C1B-C2B	-2.23	1.37	1.43
22	S	207	CLA	C1D-C2D	-2.23	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	O	201	DD6	C5-C6	2.23	1.41	1.35
22	A	851	CLA	C1D-C2D	-2.23	1.40	1.45
31	G	211	DD6	C2-C1	2.23	1.41	1.35
31	O	214	DD6	C2-C1	2.23	1.41	1.35
22	B	833	CLA	C1D-C2D	-2.23	1.40	1.45
22	P	210	CLA	C1B-C2B	-2.23	1.37	1.43
34	P	204	A86	C24-C1	-2.23	1.41	1.46
22	A	848	CLA	MG-NB	2.23	2.10	2.05
31	G	211	DD6	C5-C6	2.22	1.40	1.35
22	U	208	CLA	MG-NC	2.22	2.11	2.06
22	B	831	CLA	C1D-C2D	-2.22	1.40	1.45
31	U	203	DD6	C13-C11	-2.22	1.41	1.46
31	U	203	DD6	C2-C1	2.22	1.40	1.35
22	O	204	CLA	C1B-C2B	-2.22	1.37	1.43
22	A	836	CLA	C1D-C2D	-2.22	1.40	1.45
22	K	207	CLA	C1B-C2B	-2.22	1.37	1.43
26	F	806	LMU	O5B-C5B	2.22	1.49	1.44
22	B	812	CLA	C1D-C2D	-2.22	1.40	1.45
22	H	209	CLA	C1B-C2B	-2.22	1.37	1.43
22	B	830	CLA	C1D-C2D	-2.22	1.40	1.45
22	A	810	CLA	C1D-C2D	-2.22	1.40	1.45
34	Q	214	A86	C8-C6	-2.22	1.41	1.46
22	A	829	CLA	C1B-C2B	-2.22	1.37	1.43
34	U	202	A86	C24-C1	-2.22	1.41	1.46
22	P	211	CLA	C1B-C2B	-2.22	1.37	1.43
22	P	213	CLA	C1B-C2B	-2.22	1.37	1.43
22	S	217	CLA	C1D-C2D	-2.21	1.41	1.45
22	H	210	CLA	C1B-C2B	-2.21	1.37	1.43
22	J	103	CLA	C1D-C2D	-2.21	1.41	1.45
31	H	212	DD6	C10-C11	2.21	1.40	1.35
22	Q	205	CLA	C1D-C2D	-2.21	1.41	1.45
22	k	102	CLA	C1D-C2D	-2.21	1.41	1.45
31	P	220	DD6	C24-C1	-2.21	1.41	1.46
22	U	209	CLA	C1B-C2B	-2.21	1.37	1.43
31	O	212	DD6	C13-C11	-2.21	1.41	1.46
22	B	823	CLA	C1D-C2D	-2.21	1.41	1.45
33	P	219	KC1	MG-NC	2.21	2.11	2.06
31	K	208	DD6	C8-C6	-2.21	1.41	1.46
22	B	845	CLA	MG-NB	2.21	2.10	2.05
22	A	850	CLA	MG-NC	2.21	2.11	2.06
22	A	835	CLA	C1D-C2D	-2.21	1.41	1.45
22	B	826	CLA	C1D-C2D	-2.21	1.41	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	808	CLA	MG-NC	2.20	2.11	2.06
22	B	811	CLA	C1B-C2B	-2.20	1.38	1.43
22	H	206	CLA	C1D-C2D	-2.20	1.41	1.45
34	Q	218	A86	C8-C6	-2.20	1.41	1.46
27	A	849	CL0	C3D-C4D	-2.20	1.38	1.41
22	A	855	CLA	MG-NC	2.20	2.11	2.06
22	A	835	CLA	C1B-C2B	-2.20	1.38	1.43
22	A	856	CLA	MG-NC	2.20	2.11	2.06
22	U	205	CLA	C1D-C2D	-2.20	1.41	1.45
22	A	812	CLA	C1B-NB	-2.20	1.35	1.37
29	B	841	DGD	O1G-C1G	-2.20	1.40	1.45
34	Q	201	A86	C5-C6	2.20	1.40	1.35
22	A	854	CLA	C1B-C2B	-2.20	1.38	1.43
22	H	206	CLA	C1B-C2B	-2.20	1.38	1.43
30	B	846	SQD	O3-C3	-2.19	1.37	1.43
22	B	847	CLA	MG-NC	2.19	2.11	2.06
22	A	853	CLA	MG-NC	2.19	2.11	2.06
22	A	845	CLA	C3D-C4D	-2.19	1.39	1.44
22	k	102	CLA	MG-NC	2.19	2.11	2.06
22	T	209	CLA	MG-NC	2.19	2.11	2.06
31	U	212	DD6	C24-C1	-2.19	1.41	1.46
31	G	214	DD6	C10-C11	2.19	1.40	1.35
22	B	828	CLA	C1D-C2D	-2.19	1.41	1.45
22	U	206	CLA	MG-NC	2.19	2.11	2.06
22	A	804	CLA	C1B-NB	-2.19	1.35	1.37
31	S	214	DD6	C5-C6	2.19	1.40	1.35
22	A	815	CLA	C1D-C2D	-2.19	1.41	1.45
22	B	808	CLA	C1B-C2B	-2.19	1.38	1.43
22	H	203	CLA	C1B-C2B	-2.19	1.38	1.43
31	G	212	DD6	C8-C6	-2.19	1.41	1.46
22	B	803	CLA	C1B-C2B	-2.19	1.38	1.43
22	A	808	CLA	C1D-C2D	-2.19	1.41	1.45
22	B	815	CLA	C1D-C2D	-2.18	1.41	1.45
31	O	214	DD6	C8-C6	-2.18	1.41	1.46
22	U	204	CLA	C1D-C2D	-2.18	1.41	1.45
22	G	215	CLA	C1B-C2B	-2.18	1.38	1.43
34	R	105	A86	C2-C1	2.18	1.40	1.35
22	Q	203	CLA	C1B-C2B	-2.18	1.38	1.43
22	G	204	CLA	C1B-C2B	-2.18	1.38	1.43
31	G	212	DD6	C13-C11	-2.18	1.41	1.46
31	S	204	DD6	C10-C11	2.18	1.40	1.35
22	B	825	CLA	C1D-C2D	-2.18	1.41	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	P	215	DD6	C28-C27	-2.18	1.49	1.50
31	K	208	DD6	C28-C27	-2.18	1.49	1.50
31	P	205	DD6	C2-C1	2.18	1.40	1.35
22	Q	213	CLA	MG-NC	2.18	2.11	2.06
22	B	813	CLA	C1D-C2D	-2.18	1.41	1.45
22	Q	213	CLA	C1D-C2D	-2.17	1.41	1.45
31	O	201	DD6	C10-C11	2.17	1.40	1.35
22	A	806	CLA	C1B-NB	-2.17	1.35	1.37
22	T	206	CLA	C1B-C2B	-2.17	1.38	1.43
22	O	211	CLA	C1D-C2D	-2.17	1.41	1.45
22	A	819	CLA	C1B-C2B	-2.17	1.38	1.43
22	G	202	CLA	MG-NC	2.17	2.11	2.06
22	A	801	CLA	C1B-NB	-2.17	1.35	1.37
22	Q	207	CLA	C1D-C2D	-2.17	1.41	1.45
22	A	806	CLA	MG-NC	2.17	2.11	2.06
31	O	212	DD6	C8-C6	-2.17	1.41	1.46
33	P	206	KC1	C1B-NB	-2.17	1.35	1.37
22	U	206	CLA	C1D-C2D	-2.17	1.41	1.45
22	A	845	CLA	C1B-C2B	-2.17	1.38	1.43
22	A	824	CLA	C1D-C2D	-2.17	1.41	1.45
22	A	824	CLA	C1B-C2B	-2.17	1.38	1.43
22	T	211	CLA	C1B-C2B	-2.17	1.38	1.43
31	P	215	DD6	C24-C1	-2.17	1.41	1.46
31	O	213	DD6	C2-C1	2.16	1.40	1.35
22	H	202	CLA	MG-NC	2.16	2.11	2.06
32	P	217	LMG	O7-C8	-2.16	1.41	1.46
22	A	812	CLA	C1B-C2B	-2.16	1.38	1.43
22	B	813	CLA	C1B-C2B	-2.16	1.38	1.43
22	H	205	CLA	C1B-C2B	-2.16	1.38	1.43
22	Q	205	CLA	MG-NC	2.16	2.11	2.06
22	S	217	CLA	MG-NC	2.16	2.11	2.06
22	A	812	CLA	C1D-C2D	-2.16	1.41	1.45
22	A	853	CLA	C1D-C2D	-2.16	1.41	1.45
34	P	204	A86	C8-C6	-2.16	1.41	1.46
31	P	218	DD6	C8-C6	-2.16	1.41	1.46
22	B	829	CLA	C1B-C2B	-2.16	1.38	1.43
22	B	842	CLA	C1D-C2D	-2.16	1.41	1.45
31	G	212	DD6	C24-C1	-2.16	1.41	1.46
31	T	213	DD6	C9-C10	-2.16	1.36	1.43
22	A	848	CLA	C1B-C2B	-2.15	1.38	1.43
22	O	203	CLA	C1B-C2B	-2.15	1.38	1.43
31	S	211	DD6	C5-C6	2.15	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	838	CLA	CHB-C1B	2.15	1.44	1.39
22	B	828	CLA	C1B-C2B	-2.15	1.38	1.43
22	B	832	CLA	C1D-C2D	-2.15	1.41	1.45
22	U	207	CLA	C1D-C2D	-2.15	1.41	1.45
22	B	824	CLA	C1B-C2B	-2.15	1.38	1.43
22	A	854	CLA	C1D-C2D	-2.15	1.41	1.45
22	H	207	CLA	C1D-C2D	-2.15	1.41	1.45
31	O	215	DD6	C2-C1	2.15	1.40	1.35
22	B	810	CLA	C1B-NB	-2.15	1.35	1.37
22	T	210	CLA	C1B-C2B	-2.15	1.38	1.43
22	Q	203	CLA	C1D-C2D	-2.15	1.41	1.45
31	O	215	DD6	C25-C26	-2.15	1.36	1.43
22	A	811	CLA	C1B-NB	-2.15	1.35	1.37
22	B	804	CLA	C1B-NB	-2.15	1.35	1.37
22	A	811	CLA	C1B-C2B	-2.15	1.38	1.43
31	J	101	DD6	C5-C6	2.14	1.40	1.35
24	P	201	LHG	P-O6	2.14	1.67	1.59
22	T	203	CLA	C1B-C2B	-2.14	1.38	1.43
30	B	846	SQD	O2-C2	-2.14	1.37	1.43
22	F	802	CLA	CHB-C1B	2.14	1.44	1.39
22	B	845	CLA	C1D-C2D	-2.14	1.41	1.45
31	S	211	DD6	C26-C27	2.14	1.41	1.37
22	A	820	CLA	C1D-C2D	-2.14	1.41	1.45
22	B	820	CLA	C1D-C2D	-2.14	1.41	1.45
22	A	802	CLA	C1D-C2D	-2.14	1.41	1.45
22	A	855	CLA	C1B-C2B	-2.14	1.38	1.43
31	P	205	DD6	C5-C6	2.14	1.40	1.35
22	A	832	CLA	C1D-C2D	-2.14	1.41	1.45
22	H	202	CLA	C1B-C2B	-2.14	1.38	1.43
24	P	201	LHG	O7-C5	-2.14	1.41	1.46
22	A	832	CLA	C1B-NB	-2.14	1.35	1.37
22	T	205	CLA	C1B-C2B	-2.14	1.38	1.43
22	B	827	CLA	MG-NB	2.14	2.10	2.05
32	P	202	LMG	O8-C9	-2.14	1.40	1.45
22	B	815	CLA	C1B-C2B	-2.14	1.38	1.43
26	K	201	LMU	O5B-C5B	2.13	1.49	1.44
22	B	816	CLA	C1B-NB	-2.13	1.35	1.37
22	A	822	CLA	C1B-NB	-2.13	1.35	1.37
33	Q	210	KC1	MG-NC	2.13	2.11	2.06
34	U	202	A86	C8-C6	-2.13	1.41	1.46
34	Q	214	A86	C5-C6	2.13	1.40	1.35
22	H	203	CLA	MG-NB	2.13	2.10	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	Q	202	DD6	C24-C1	-2.13	1.41	1.46
31	P	218	DD6	C13-C11	-2.13	1.41	1.46
31	P	218	DD6	C24-C1	-2.13	1.41	1.46
22	T	201	CLA	C1B-C2B	-2.13	1.38	1.43
22	O	209	CLA	C1B-NB	-2.12	1.35	1.37
22	H	207	CLA	MG-NC	2.12	2.11	2.06
22	T	204	CLA	C1D-C2D	-2.12	1.41	1.45
22	L	202	CLA	C1D-C2D	-2.12	1.41	1.45
22	P	208	CLA	C1D-C2D	-2.12	1.41	1.45
22	A	816	CLA	C1B-NB	-2.12	1.35	1.37
22	K	204	CLA	C1D-C2D	-2.12	1.41	1.45
22	T	203	CLA	C1D-C2D	-2.12	1.41	1.45
22	O	203	CLA	C1D-C2D	-2.12	1.41	1.45
22	Q	204	CLA	MG-NC	2.12	2.11	2.06
31	S	205	DD6	C5-C6	2.12	1.40	1.35
31	Q	202	DD6	C28-C27	-2.12	1.49	1.50
31	K	208	DD6	C13-C11	-2.12	1.41	1.46
22	A	826	CLA	C1B-C2B	-2.12	1.38	1.43
31	J	101	DD6	C2-C1	2.12	1.40	1.35
22	L	202	CLA	C1B-NB	-2.12	1.35	1.37
22	B	810	CLA	C1B-C2B	-2.12	1.38	1.43
22	A	818	CLA	C1D-C2D	-2.12	1.41	1.45
22	T	211	CLA	MG-NC	2.12	2.11	2.06
33	P	203	KC1	C1B-NB	-2.12	1.35	1.37
22	U	207	CLA	C1B-C2B	-2.11	1.38	1.43
22	A	807	CLA	C1B-C2B	-2.11	1.38	1.43
22	B	806	CLA	C1B-C2B	-2.11	1.38	1.43
33	O	210	KC1	C1B-NB	-2.11	1.35	1.37
22	Q	203	CLA	MG-NC	2.11	2.11	2.06
22	F	804	CLA	C1D-C2D	-2.11	1.41	1.45
22	G	205	CLA	C1B-C2B	-2.11	1.38	1.43
22	H	207	CLA	C1B-C2B	-2.11	1.38	1.43
31	G	213	DD6	C5-C6	2.11	1.40	1.35
22	R	104	CLA	C1B-C2B	-2.11	1.38	1.43
31	S	211	DD6	C10-C11	2.11	1.40	1.35
31	S	204	DD6	C5-C6	2.11	1.40	1.35
22	U	206	CLA	C1B-C2B	-2.11	1.38	1.43
31	U	212	DD6	C8-C6	-2.11	1.41	1.46
22	O	204	CLA	C1B-NB	-2.11	1.35	1.37
22	Q	212	CLA	C1B-NB	-2.11	1.35	1.37
22	A	834	CLA	MG-NB	2.11	2.10	2.05
22	B	842	CLA	MG-NB	2.11	2.10	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	P	206	KC1	C3B-C2B	2.11	1.41	1.37
22	B	817	CLA	MG-NC	2.11	2.11	2.06
22	B	825	CLA	C1B-C2B	-2.11	1.38	1.43
22	A	808	CLA	C1B-C2B	-2.10	1.38	1.43
31	G	211	DD6	C25-C26	-2.10	1.36	1.43
22	Q	209	CLA	C1B-C2B	-2.10	1.38	1.43
31	G	213	DD6	C2-C1	2.10	1.40	1.35
31	k	101	DD6	C5-C6	2.10	1.40	1.35
31	Q	215	DD6	C8-C6	-2.10	1.41	1.46
34	Q	214	A86	C2-C1	2.10	1.40	1.35
22	P	207	CLA	C1D-C2D	-2.10	1.41	1.45
22	J	103	CLA	C1B-C2B	-2.10	1.38	1.43
22	A	808	CLA	C1B-NB	-2.10	1.35	1.37
31	H	201	DD6	C8-C6	-2.10	1.41	1.46
22	A	814	CLA	C1D-C2D	-2.10	1.41	1.45
22	B	842	CLA	C1B-NB	-2.10	1.35	1.37
22	O	207	CLA	MG-NC	2.10	2.11	2.06
30	S	201	SQD	O4-C4	-2.10	1.37	1.43
22	F	802	CLA	C1B-C2B	-2.10	1.38	1.43
22	k	102	CLA	C1B-C2B	-2.10	1.38	1.43
22	F	803	CLA	C1D-C2D	-2.10	1.41	1.45
22	H	204	CLA	C1D-C2D	-2.10	1.41	1.45
22	K	203	CLA	C1B-NB	-2.10	1.35	1.37
33	P	212	KC1	C1B-NB	-2.10	1.35	1.37
31	G	213	DD6	C25-C26	-2.10	1.36	1.43
22	A	816	CLA	C1D-C2D	-2.10	1.41	1.45
22	A	802	CLA	C1B-C2B	-2.09	1.38	1.43
22	K	206	CLA	C1D-C2D	-2.09	1.41	1.45
22	Q	216	CLA	C1B-NB	-2.09	1.35	1.37
22	O	207	CLA	C1D-C2D	-2.09	1.41	1.45
22	P	213	CLA	C1D-C2D	-2.09	1.41	1.45
31	O	201	DD6	C2-C1	2.09	1.40	1.35
22	B	832	CLA	C1B-NB	-2.09	1.35	1.37
22	Q	216	CLA	C1D-C2D	-2.09	1.41	1.45
31	P	215	DD6	C8-C6	-2.09	1.41	1.46
22	B	812	CLA	C1B-C2B	-2.09	1.38	1.43
22	S	216	CLA	C1B-C2B	-2.09	1.38	1.43
22	S	207	CLA	MG-NB	2.09	2.09	2.05
22	A	823	CLA	C1B-C2B	-2.09	1.38	1.43
22	G	201	CLA	C1D-C2D	-2.09	1.41	1.45
22	A	807	CLA	C1B-NB	-2.09	1.35	1.37
22	Q	216	CLA	C1B-C2B	-2.09	1.38	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	U	203	DD6	C24-C1	-2.09	1.41	1.46
22	S	202	CLA	MG-NC	2.09	2.11	2.06
31	T	213	DD6	C28-C27	-2.09	1.49	1.50
31	S	204	DD6	C25-C26	-2.09	1.36	1.43
22	k	103	CLA	CHB-C1B	2.09	1.44	1.39
31	Q	202	DD6	C8-C6	-2.09	1.41	1.46
22	U	210	CLA	C1D-C2D	-2.08	1.41	1.45
22	U	210	CLA	CHB-C1B	2.08	1.44	1.39
31	Q	215	DD6	C13-C11	-2.08	1.41	1.46
22	B	815	CLA	MG-NC	2.08	2.11	2.06
22	O	205	CLA	C1B-C2B	-2.08	1.38	1.43
22	A	811	CLA	MG-NC	2.08	2.11	2.06
31	U	212	DD6	C28-C27	-2.08	1.49	1.50
22	B	818	CLA	C1B-NB	-2.08	1.35	1.37
22	B	819	CLA	C1B-NB	-2.08	1.35	1.37
22	B	809	CLA	C1B-C2B	-2.08	1.38	1.43
22	P	207	CLA	C1B-C2B	-2.08	1.38	1.43
22	G	207	CLA	CHB-C1B	2.08	1.44	1.39
22	Q	205	CLA	C1B-C2B	-2.08	1.38	1.43
22	Q	213	CLA	C1B-C2B	-2.07	1.38	1.43
31	O	214	DD6	C13-C11	-2.07	1.41	1.46
22	A	809	CLA	C1D-C2D	-2.07	1.41	1.45
22	L	204	CLA	C1D-C2D	-2.07	1.41	1.45
22	A	855	CLA	CHB-C1B	2.07	1.44	1.39
22	L	202	CLA	C1B-C2B	-2.07	1.38	1.43
22	A	855	CLA	C1D-C2D	-2.07	1.41	1.45
22	G	204	CLA	MG-NC	2.07	2.11	2.06
22	A	822	CLA	C1B-C2B	-2.07	1.38	1.43
31	S	205	DD6	C2-C1	2.07	1.40	1.35
31	S	211	DD6	C2-C1	2.07	1.40	1.35
22	T	205	CLA	C1D-C2D	-2.07	1.41	1.45
22	T	201	CLA	CHB-C1B	2.07	1.44	1.39
22	A	823	CLA	C1B-NB	-2.07	1.35	1.37
24	A	839	LHG	O7-C5	-2.07	1.41	1.46
22	H	204	CLA	C1B-C2B	-2.07	1.38	1.43
22	B	814	CLA	C1D-C2D	-2.07	1.41	1.45
22	A	851	CLA	C1B-NB	-2.07	1.35	1.37
31	k	101	DD6	C25-C26	-2.07	1.36	1.43
31	G	211	DD6	C13-C11	-2.07	1.41	1.46
22	T	207	CLA	C1D-C2D	-2.07	1.41	1.45
22	B	818	CLA	C1B-C2B	-2.07	1.38	1.43
22	O	208	CLA	C1B-NB	-2.07	1.35	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	U	213	KC1	C3B-C2B	2.07	1.41	1.37
34	R	105	A86	C5-C6	2.07	1.40	1.35
22	L	203	CLA	MG-NC	2.06	2.11	2.06
22	A	833	CLA	C1B-C2B	-2.06	1.38	1.43
31	J	101	DD6	C25-C26	-2.06	1.36	1.43
22	A	804	CLA	MG-NC	2.06	2.11	2.06
25	B	838	BCR	C33-C5	-2.06	1.47	1.50
22	G	208	CLA	C1D-C2D	-2.06	1.41	1.45
22	O	203	CLA	MG-NC	2.06	2.11	2.06
22	A	836	CLA	C1B-C2B	-2.06	1.38	1.43
22	B	809	CLA	C1D-C2D	-2.06	1.41	1.45
22	T	202	CLA	C1D-C2D	-2.06	1.41	1.45
31	O	215	DD6	C10-C11	2.06	1.40	1.35
22	A	831	CLA	C1D-C2D	-2.06	1.41	1.45
22	L	203	CLA	C1D-C2D	-2.06	1.41	1.45
22	O	208	CLA	C1D-C2D	-2.06	1.41	1.45
22	U	208	CLA	C1D-C2D	-2.06	1.41	1.45
22	P	208	CLA	C1B-C2B	-2.06	1.38	1.43
22	A	836	CLA	CHB-C1B	2.06	1.44	1.39
22	P	209	CLA	MG-NC	2.06	2.11	2.06
31	K	208	DD6	C24-C1	-2.06	1.41	1.46
22	G	210	CLA	C1B-C2B	-2.06	1.38	1.43
31	Q	202	DD6	C13-C11	-2.06	1.41	1.46
31	O	213	DD6	C25-C26	-2.06	1.36	1.43
22	T	209	CLA	C1D-C2D	-2.06	1.41	1.45
22	K	205	CLA	C1D-C2D	-2.05	1.41	1.45
22	B	803	CLA	C1B-NB	-2.05	1.35	1.37
22	B	829	CLA	C1B-NB	-2.05	1.35	1.37
22	A	806	CLA	C1B-C2B	-2.05	1.38	1.43
22	P	207	CLA	MG-NC	2.05	2.11	2.06
22	A	821	CLA	CHB-C1B	2.05	1.44	1.39
31	P	218	DD6	C9-C8	2.05	1.40	1.34
22	B	804	CLA	C1B-C2B	-2.05	1.38	1.43
22	Q	207	CLA	CHB-C1B	2.05	1.44	1.39
22	H	209	CLA	CHB-C1B	2.05	1.44	1.39
22	O	206	CLA	C1D-C2D	-2.05	1.41	1.45
22	K	205	CLA	C1B-C2B	-2.05	1.38	1.43
31	k	101	DD6	C10-C11	2.05	1.40	1.35
22	P	210	CLA	C1D-C2D	-2.05	1.41	1.45
22	G	207	CLA	C1D-C2D	-2.05	1.41	1.45
31	O	213	DD6	C5-C6	2.05	1.40	1.35
22	H	207	CLA	CHB-C1B	2.05	1.44	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	834	CLA	C1B-C2B	-2.05	1.38	1.43
22	B	805	CLA	C1B-NB	-2.05	1.35	1.37
22	B	842	CLA	C1B-C2B	-2.05	1.38	1.43
22	O	203	CLA	CHB-C1B	2.05	1.44	1.39
22	B	810	CLA	C1D-C2D	-2.05	1.41	1.45
22	O	205	CLA	C1D-C2D	-2.05	1.41	1.45
22	G	202	CLA	C1D-C2D	-2.05	1.41	1.45
22	A	834	CLA	C1B-NB	-2.05	1.35	1.37
31	K	208	DD6	C25-C26	-2.05	1.36	1.43
22	T	202	CLA	MG-NC	2.04	2.11	2.06
31	T	212	DD6	C8-C6	-2.04	1.41	1.46
22	B	834	CLA	C1B-NB	-2.04	1.35	1.37
22	L	203	CLA	C1B-NB	-2.04	1.35	1.37
22	A	834	CLA	C1D-C2D	-2.04	1.41	1.45
22	A	856	CLA	C1D-C2D	-2.04	1.41	1.45
22	O	202	CLA	C1D-C2D	-2.04	1.41	1.45
30	S	201	SQD	O2-C2	-2.04	1.37	1.43
22	A	817	CLA	MG-NC	2.04	2.11	2.06
22	K	206	CLA	CHB-C1B	2.04	1.44	1.39
22	T	210	CLA	C1D-C2D	-2.04	1.41	1.45
22	A	853	CLA	C1B-C2B	-2.04	1.38	1.43
24	A	839	LHG	P-O6	2.04	1.67	1.59
22	A	805	CLA	C1B-C2B	-2.03	1.38	1.43
22	H	213	CLA	C1D-C2D	-2.03	1.41	1.45
22	A	809	CLA	C1B-C2B	-2.03	1.38	1.43
22	L	204	CLA	C1B-NB	-2.03	1.35	1.37
22	B	817	CLA	C1D-C2D	-2.03	1.41	1.45
22	A	825	CLA	C1B-C2B	-2.03	1.38	1.43
22	H	205	CLA	CHB-C1B	2.03	1.44	1.39
22	S	216	CLA	C1D-C2D	-2.03	1.41	1.45
22	H	209	CLA	C1D-C2D	-2.03	1.41	1.45
22	R	101	CLA	C1B-NB	-2.03	1.35	1.37
33	P	203	KC1	C3B-C2B	2.03	1.41	1.37
22	H	208	CLA	MG-NC	2.03	2.11	2.06
22	A	803	CLA	C1D-C2D	-2.03	1.41	1.45
33	P	219	KC1	C3B-C2B	2.03	1.41	1.37
22	T	211	CLA	CHB-C1B	2.03	1.44	1.39
22	A	828	CLA	C1B-C2B	-2.03	1.38	1.43
22	K	207	CLA	C1D-C2D	-2.03	1.41	1.45
31	O	212	DD6	C25-C26	-2.03	1.36	1.43
22	Q	205	CLA	CHB-C1B	2.03	1.44	1.39
31	S	214	DD6	C25-C26	-2.03	1.36	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	812	CLA	C1B-NB	-2.03	1.35	1.37
31	S	205	DD6	C28-C27	-2.03	1.49	1.50
22	U	209	CLA	C3D-C4D	-2.02	1.39	1.44
31	Q	215	DD6	C25-C26	-2.02	1.36	1.43
22	O	211	CLA	C1B-C2B	-2.02	1.38	1.43
22	U	204	CLA	C1B-C2B	-2.02	1.38	1.43
22	O	208	CLA	C1B-C2B	-2.02	1.38	1.43
22	Q	208	CLA	C1B-NB	-2.02	1.35	1.37
22	F	803	CLA	C1B-C2B	-2.02	1.38	1.43
31	O	215	DD6	C5-C6	2.02	1.40	1.35
22	B	834	CLA	MG-NC	2.02	2.11	2.06
22	A	830	CLA	C1B-NB	-2.02	1.35	1.37
22	A	802	CLA	C1B-NB	-2.02	1.35	1.37
22	K	203	CLA	MG-NB	2.02	2.09	2.05
22	A	827	CLA	C1B-C2B	-2.02	1.38	1.43
22	Q	206	CLA	C1B-C2B	-2.02	1.38	1.43
22	S	216	CLA	MG-NC	2.02	2.11	2.06
22	P	208	CLA	C1B-NB	-2.02	1.35	1.37
22	A	805	CLA	C1D-C2D	-2.01	1.41	1.45
31	S	215	DD6	C24-C1	-2.01	1.41	1.46
22	B	811	CLA	C1D-C2D	-2.01	1.41	1.45
22	Q	208	CLA	C1B-C2B	-2.01	1.38	1.43
22	P	216	CLA	C1B-NB	-2.01	1.35	1.37
30	B	846	SQD	O4-C4	-2.01	1.38	1.43
22	S	217	CLA	C1B-C2B	-2.01	1.38	1.43
22	J	103	CLA	MG-NC	2.01	2.11	2.06
22	A	850	CLA	C1B-NB	-2.01	1.35	1.37
31	T	212	DD6	C25-C26	-2.01	1.37	1.43
22	Q	211	CLA	C1B-NB	-2.01	1.35	1.37
22	S	208	CLA	C1B-C2B	-2.01	1.38	1.43
22	B	805	CLA	C1B-C2B	-2.00	1.38	1.43
22	Q	207	CLA	C1B-C2B	-2.00	1.38	1.43
31	k	101	DD6	C2-C1	2.00	1.40	1.35
22	O	206	CLA	C1B-C2B	-2.00	1.38	1.43
22	T	202	CLA	C1B-C2B	-2.00	1.38	1.43
22	H	203	CLA	C1D-C2D	-2.00	1.41	1.45
22	A	856	CLA	CHB-C1B	2.00	1.43	1.39
22	H	208	CLA	CHB-C1B	2.00	1.43	1.39
22	A	838	CLA	C1B-C2B	-2.00	1.38	1.43
22	A	848	CLA	C1B-NB	-2.00	1.35	1.37

All (1406) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	A	849	CL0	C1B-CHB-C4A	9.33	127.33	121.32
31	T	213	DD6	C10-C9-C8	6.72	142.68	123.20
22	Q	208	CLA	C1-O2A-CGA	6.47	132.31	116.65
22	K	203	CLA	CAA-C2A-C3A	-6.14	96.40	113.00
31	P	218	DD6	C10-C9-C8	5.49	139.10	123.20
31	U	212	DD6	C3-C4-C5	5.27	134.31	123.52
26	S	203	LMU	O1B-C4'-C5'	5.24	123.22	109.48
31	O	212	DD6	C4-C3-C2	5.24	134.23	123.52
31	P	218	DD6	C4-C3-C2	5.04	133.82	123.52
31	T	213	DD6	C8-C6-C5	5.02	126.91	119.01
31	P	218	DD6	C9-C10-C11	4.85	134.08	127.28
22	K	203	CLA	C1D-ND-C4D	4.83	109.70	106.31
31	H	211	DD6	C4-C3-C2	4.81	133.35	123.52
31	H	201	DD6	C4-C3-C2	4.79	133.33	123.52
31	T	213	DD6	C4-C3-C2	4.66	133.05	123.52
31	U	203	DD6	C4-C3-C2	4.65	133.03	123.52
31	P	215	DD6	C3-C4-C5	4.65	133.03	123.52
22	H	202	CLA	C3A-C2A-C1A	-4.62	101.57	106.30
34	Q	201	A86	C3-C4-C5	4.60	132.94	123.52
31	P	218	DD6	C3-C4-C5	4.60	132.93	123.52
31	P	215	DD6	C4-C3-C2	4.59	132.92	123.52
31	T	212	DD6	C3-C4-C5	4.52	132.76	123.52
26	S	203	LMU	O5B-C5B-C4B	4.49	117.78	109.70
26	K	201	LMU	C1B-O1B-C4'	-4.48	107.37	117.98
31	O	212	DD6	C3-C4-C5	4.47	132.67	123.52
31	S	214	DD6	C3-C4-C5	4.36	132.45	123.52
31	G	214	DD6	C24-C1-C2	4.34	125.84	119.01
24	P	201	LHG	O4-P-O5	4.32	132.56	112.44
31	S	211	DD6	C3-C4-C5	4.31	132.33	123.52
31	P	220	DD6	C13-C11-C10	4.30	125.77	119.01
31	S	214	DD6	C12-C11-C10	-4.30	115.85	122.82
24	A	840	LHG	O4-P-O5	4.30	132.44	112.44
33	O	210	KC1	C2A-C3A-C4A	4.28	109.63	106.41
24	G	216	LHG	O4-P-O5	4.28	132.34	112.44
22	K	203	CLA	C4D-CHA-C1A	4.27	126.34	121.24
31	Q	202	DD6	C3-C4-C5	4.27	132.25	123.52
31	H	211	DD6	C3-C4-C5	4.26	132.23	123.52
24	A	839	LHG	O4-P-O5	4.24	132.16	112.44
22	Q	207	CLA	C4D-CHA-C1A	4.21	126.27	121.24
25	F	801	BCR	C2-C1-C6	4.19	116.53	110.44
31	Q	215	DD6	C4-C3-C2	4.19	132.09	123.52
25	A	841	BCR	C2-C1-C6	4.18	116.50	110.44
22	B	829	CLA	C4D-CHA-C1A	4.17	126.22	121.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	K	203	CLA	C2A-C1A-CHA	4.13	131.04	123.87
30	S	201	SQD	O9-S-O7	-4.10	100.48	113.82
31	K	208	DD6	C3-C4-C5	4.07	131.85	123.52
30	B	846	SQD	O9-S-O7	-4.07	100.58	113.82
26	K	202	LMU	O5B-C5B-C4B	4.07	117.03	109.70
31	O	215	DD6	C12-C11-C10	-4.05	116.26	122.82
34	U	202	A86	C3-C4-C5	4.05	131.80	123.52
22	H	207	CLA	C4D-CHA-C1A	4.05	126.07	121.24
26	K	202	LMU	C2'-C3'-C4'	4.04	118.85	109.68
22	G	209	CLA	C4D-CHA-C1A	4.04	126.06	121.24
26	F	806	LMU	C3B-C4B-C5B	4.01	117.50	110.23
22	A	855	CLA	C3A-C2A-C1A	-4.00	102.20	106.30
31	S	215	DD6	C4-C3-C2	4.00	131.69	123.52
22	A	831	CLA	C4D-CHA-C1A	3.99	126.00	121.24
31	T	212	DD6	C13-C11-C10	3.98	125.27	119.01
25	k	104	BCR	C2-C1-C6	3.98	116.22	110.44
26	F	806	LMU	O5B-C5B-C4B	3.97	116.85	109.70
22	A	850	CLA	C4D-CHA-C1A	3.97	125.98	121.24
30	B	846	SQD	O47-C7-C8	3.97	120.06	111.48
31	H	212	DD6	C3-C4-C5	3.97	131.64	123.52
31	P	220	DD6	C3-C4-C5	3.96	131.63	123.52
31	P	220	DD6	C12-C11-C10	-3.96	116.40	122.82
34	Q	218	A86	C3-C4-C5	3.96	131.61	123.52
22	B	845	CLA	C1-O2A-CGA	3.95	126.21	116.65
27	A	849	CL0	C3D-C4D-CHA	3.95	114.54	108.54
31	T	212	DD6	C12-C11-C10	-3.93	116.44	122.82
22	A	838	CLA	C4D-CHA-C1A	3.92	125.92	121.24
26	K	201	LMU	O1'-C1'-C2'	3.92	114.22	108.27
34	P	204	A86	C3-C4-C5	3.92	131.53	123.52
26	K	202	LMU	C3B-C4B-C5B	3.92	117.33	110.23
31	P	220	DD6	C4-C3-C2	3.91	131.53	123.52
22	P	207	CLA	C4D-CHA-C1A	3.91	125.91	121.24
31	J	101	DD6	C3-C4-C5	3.91	131.51	123.52
22	K	203	CLA	CHA-C1A-NA	-3.90	117.55	126.39
34	U	202	A86	C4-C3-C2	3.90	131.50	123.52
31	H	211	DD6	C8-C6-C5	3.90	125.14	119.01
31	T	213	DD6	C3-C4-C5	3.90	131.49	123.52
22	B	815	CLA	C4D-CHA-C1A	3.89	125.89	121.24
22	F	803	CLA	C4D-CHA-C1A	3.89	125.89	121.24
22	H	207	CLA	O2A-C1-C2	3.88	123.04	108.11
30	S	201	SQD	O9-S-C6	3.88	112.55	106.76
26	P	221	LMU	C1B-O1B-C4'	-3.88	108.79	117.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	816	CLA	C4D-CHA-C1A	3.87	125.86	121.24
25	M	101	BCR	C2-C1-C6	3.86	116.04	110.44
22	K	207	CLA	O2A-C1-C2	3.86	122.95	108.11
26	L	206	LMU	C2'-C3'-C4'	3.85	118.42	109.68
22	F	804	CLA	C4D-CHA-C1A	3.85	125.83	121.24
22	O	206	CLA	C4D-CHA-C1A	3.84	125.83	121.24
31	P	215	DD6	C12-C11-C10	-3.84	116.59	122.82
31	U	214	DD6	C4-C3-C2	3.84	131.37	123.52
30	S	201	SQD	O47-C7-C8	3.83	119.77	111.48
22	B	817	CLA	C4D-CHA-C1A	3.82	125.81	121.24
31	T	213	DD6	C12-C11-C10	-3.82	116.62	122.82
34	Q	214	A86	C3-C4-C5	3.82	131.34	123.52
31	G	212	DD6	C4-C3-C2	3.82	131.34	123.52
22	B	813	CLA	C4D-CHA-C1A	3.82	125.80	121.24
31	U	214	DD6	C3-C4-C5	3.82	131.33	123.52
22	A	819	CLA	C4D-CHA-C1A	3.82	125.80	121.24
22	Q	204	CLA	C4D-CHA-C1A	3.82	125.80	121.24
31	O	214	DD6	C12-C11-C10	-3.81	116.64	122.82
22	T	202	CLA	C4D-CHA-C1A	3.81	125.79	121.24
22	B	806	CLA	C4D-CHA-C1A	3.81	125.78	121.24
22	B	831	CLA	C4D-CHA-C1A	3.80	125.78	121.24
22	H	204	CLA	C4D-CHA-C1A	3.80	125.78	121.24
22	G	207	CLA	C4D-CHA-C1A	3.79	125.77	121.24
31	G	212	DD6	C3-C4-C5	3.79	131.28	123.52
31	O	214	DD6	C4-C3-C2	3.79	131.27	123.52
22	U	204	CLA	C4D-CHA-C1A	3.78	125.75	121.24
22	Q	208	CLA	O2A-C1-C2	3.77	122.62	108.11
22	L	203	CLA	C4D-CHA-C1A	3.77	125.74	121.24
31	S	205	DD6	C3-C4-C5	3.77	131.23	123.52
22	A	811	CLA	C4D-CHA-C1A	3.77	125.74	121.24
22	P	214	CLA	C4D-CHA-C1A	3.77	125.74	121.24
22	T	211	CLA	C4D-CHA-C1A	3.76	125.73	121.24
31	O	214	DD6	C3-C4-C5	3.76	131.21	123.52
31	J	101	DD6	C13-C11-C10	3.75	124.92	119.01
22	K	207	CLA	C4D-CHA-C1A	3.75	125.72	121.24
22	A	851	CLA	C4D-CHA-C1A	3.75	125.71	121.24
22	Q	203	CLA	C4D-CHA-C1A	3.75	125.71	121.24
22	S	206	CLA	C4D-CHA-C1A	3.74	125.71	121.24
22	G	204	CLA	C4D-CHA-C1A	3.74	125.70	121.24
31	G	211	DD6	C4-C3-C2	3.74	131.17	123.52
22	S	202	CLA	C4D-CHA-C1A	3.74	125.70	121.24
22	U	208	CLA	C4D-CHA-C1A	3.74	125.70	121.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	T	212	DD6	C4-C3-C2	3.74	131.16	123.52
22	B	825	CLA	C4D-CHA-C1A	3.73	125.69	121.24
22	A	814	CLA	C4D-CHA-C1A	3.72	125.68	121.24
31	S	215	DD6	C3-C4-C5	3.71	131.11	123.52
31	K	208	DD6	C4-C3-C2	3.71	131.10	123.52
31	U	203	DD6	C24-C1-C2	3.70	124.83	119.01
22	F	802	CLA	C4D-CHA-C1A	3.70	125.66	121.24
22	A	854	CLA	C4D-CHA-C1A	3.70	125.66	121.24
22	A	822	CLA	C4D-CHA-C1A	3.70	125.66	121.24
22	A	836	CLA	C4D-CHA-C1A	3.70	125.66	121.24
22	B	842	CLA	C4D-CHA-C1A	3.69	125.65	121.24
22	A	829	CLA	C4D-CHA-C1A	3.69	125.65	121.24
31	P	205	DD6	C3-C4-C5	3.68	131.06	123.52
22	A	855	CLA	C4D-CHA-C1A	3.68	125.63	121.24
22	A	848	CLA	C4D-CHA-C1A	3.68	125.63	121.24
31	G	213	DD6	C4-C3-C2	3.67	131.03	123.52
22	H	203	CLA	C4D-CHA-C1A	3.67	125.62	121.24
22	P	209	CLA	C4D-CHA-C1A	3.67	125.62	121.24
31	J	101	DD6	C12-C11-C10	-3.66	116.89	122.82
31	U	203	DD6	C3-C4-C5	3.65	130.99	123.52
31	O	213	DD6	C4-C3-C2	3.65	130.99	123.52
22	G	208	CLA	C4D-CHA-C1A	3.65	125.59	121.24
22	B	828	CLA	C4D-CHA-C1A	3.64	125.59	121.24
31	U	212	DD6	C8-C6-C5	3.64	124.73	119.01
22	A	856	CLA	C4D-CHA-C1A	3.63	125.58	121.24
22	O	204	CLA	C4D-CHA-C1A	3.63	125.58	121.24
26	K	201	LMU	C2'-C3'-C4'	3.62	117.90	109.68
31	S	214	DD6	C10-C9-C8	3.62	133.68	123.20
22	R	101	CLA	C4D-CHA-C1A	3.61	125.55	121.24
32	P	202	LMG	C1-C2-C3	-3.61	102.42	110.01
34	R	103	A86	C28-C27-C26	-3.61	116.97	122.82
22	H	209	CLA	C4D-CHA-C1A	3.60	125.54	121.24
22	O	211	CLA	C4D-CHA-C1A	3.60	125.53	121.24
31	Q	202	DD6	C12-C11-C10	-3.59	116.99	122.82
31	S	204	DD6	C3-C4-C5	3.59	130.87	123.52
31	S	205	DD6	C12-C11-C10	-3.58	117.01	122.82
31	O	201	DD6	C12-C11-C10	-3.58	117.02	122.82
26	S	203	LMU	C3B-C4B-C5B	3.58	116.71	110.23
22	H	208	CLA	C4D-CHA-C1A	3.57	125.50	121.24
22	G	205	CLA	CAA-C2A-C3A	-3.57	103.35	113.00
22	A	833	CLA	C4D-CHA-C1A	3.57	125.50	121.24
22	B	847	CLA	C4D-CHA-C1A	3.57	125.50	121.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	P	205	DD6	C12-C11-C10	-3.56	117.04	122.82
31	P	215	DD6	C8-C6-C5	3.56	124.61	119.01
22	S	216	CLA	C4D-CHA-C1A	3.56	125.49	121.24
22	A	835	CLA	C4D-CHA-C1A	3.55	125.48	121.24
22	U	211	CLA	C4D-CHA-C1A	3.54	125.47	121.24
34	R	103	A86	C4-C3-C2	3.54	130.76	123.52
31	Q	215	DD6	C12-C11-C10	-3.54	117.08	122.82
31	G	214	DD6	C-C1-C2	-3.53	117.09	122.82
22	B	822	CLA	C4D-CHA-C1A	3.53	125.46	121.24
22	A	803	CLA	C4D-CHA-C1A	3.53	125.45	121.24
31	S	214	DD6	C7-C6-C5	-3.53	117.10	122.82
22	B	823	CLA	C1-O2A-CGA	3.53	125.19	116.65
22	T	209	CLA	C4D-CHA-C1A	3.52	125.44	121.24
22	U	207	CLA	CAA-C2A-C3A	-3.51	103.51	113.00
34	Q	218	A86	C4-C3-C2	3.51	130.71	123.52
22	H	202	CLA	C4D-CHA-C1A	3.51	125.43	121.24
31	P	215	DD6	C23-C16-C17	-3.51	102.81	108.97
22	K	203	CLA	CAA-C2A-C1A	3.51	123.46	111.97
22	B	844	CLA	C4D-CHA-C1A	3.50	125.42	121.24
22	S	209	CLA	C4D-CHA-C1A	3.50	125.42	121.24
31	P	215	DD6	C15-C14-C13	3.50	133.39	125.99
22	G	202	CLA	C4D-CHA-C1A	3.50	125.42	121.24
26	P	221	LMU	C1B-C2B-C3B	3.50	117.37	110.01
31	G	211	DD6	C3-C4-C5	3.49	130.67	123.52
31	O	201	DD6	C4-C3-C2	3.49	130.67	123.52
31	G	214	DD6	C12-C11-C10	-3.49	117.16	122.82
30	B	846	SQD	O9-S-C6	3.49	111.97	106.76
22	A	825	CLA	C4D-CHA-C1A	3.48	125.40	121.24
31	H	211	DD6	C12-C11-C10	-3.48	117.18	122.82
22	H	213	CLA	C4D-CHA-C1A	3.48	125.40	121.24
31	P	205	DD6	C4-C3-C2	3.48	130.64	123.52
22	B	830	CLA	C4D-CHA-C1A	3.47	125.38	121.24
22	G	215	CLA	C4D-CHA-C1A	3.47	125.38	121.24
31	T	212	DD6	C8-C6-C5	3.46	124.46	119.01
22	B	811	CLA	C4D-CHA-C1A	3.46	125.37	121.24
22	O	207	CLA	C4D-CHA-C1A	3.46	125.37	121.24
22	L	204	CLA	C4D-CHA-C1A	3.46	125.36	121.24
34	R	105	A86	C4-C3-C2	3.45	130.59	123.52
25	L	205	BCR	C2-C1-C6	3.45	115.45	110.44
22	T	204	CLA	C4D-CHA-C1A	3.45	125.36	121.24
33	O	210	KC1	CAA-C2A-C1A	3.45	139.74	124.64
34	R	103	A86	C-C1-C2	-3.44	117.23	122.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	U	212	DD6	C12-C11-C10	-3.44	117.24	122.82
31	H	201	DD6	C3-C4-C5	3.44	130.56	123.52
22	G	206	CLA	C4D-CHA-C1A	3.44	125.35	121.24
31	k	101	DD6	C3-C4-C5	3.44	130.56	123.52
31	G	212	DD6	C12-C11-C10	-3.44	117.25	122.82
31	K	208	DD6	C12-C11-C10	-3.44	117.25	122.82
31	S	215	DD6	C24-C1-C2	3.44	124.41	119.01
31	S	204	DD6	C12-C11-C10	-3.44	117.25	122.82
22	B	810	CLA	C4D-CHA-C1A	3.43	125.34	121.24
31	H	212	DD6	C4-C3-C2	3.43	130.54	123.52
22	Q	209	CLA	C4D-CHA-C1A	3.43	125.34	121.24
22	A	815	CLA	C4D-CHA-C1A	3.43	125.33	121.24
31	H	201	DD6	C12-C11-C10	-3.42	117.27	122.82
31	G	211	DD6	C12-C11-C10	-3.42	117.27	122.82
31	G	213	DD6	C12-C11-C10	-3.42	117.27	122.82
22	S	207	CLA	C4D-CHA-C1A	3.42	125.32	121.24
31	U	203	DD6	C-C1-C2	-3.42	117.28	122.82
22	Q	205	CLA	C4D-CHA-C1A	3.42	125.32	121.24
31	U	203	DD6	C12-C11-C10	-3.42	117.28	122.82
22	T	205	CLA	C4D-CHA-C1A	3.41	125.32	121.24
22	U	206	CLA	C4D-CHA-C1A	3.41	125.31	121.24
22	P	216	CLA	C4D-CHA-C1A	3.41	125.31	121.24
31	O	215	DD6	C4-C3-C2	3.40	130.49	123.52
22	G	203	CLA	C4D-CHA-C1A	3.40	125.31	121.24
22	B	814	CLA	C4D-CHA-C1A	3.40	125.30	121.24
22	A	808	CLA	C4D-CHA-C1A	3.40	125.30	121.24
31	Q	202	DD6	C4-C3-C2	3.40	130.48	123.52
22	A	846	CLA	C4D-CHA-C1A	3.40	125.30	121.24
22	Q	213	CLA	C4D-CHA-C1A	3.40	125.30	121.24
25	J	104	BCR	C2-C1-C6	3.40	115.38	110.44
31	k	101	DD6	C4-C3-C2	3.40	130.47	123.52
22	Q	206	CLA	C4D-CHA-C1A	3.40	125.30	121.24
31	P	215	DD6	C13-C11-C10	3.40	124.35	119.01
22	S	202	CLA	CHD-C1D-ND	-3.40	120.02	124.80
34	P	204	A86	C4-C3-C2	3.38	130.44	123.52
22	A	827	CLA	C4D-CHA-C1A	3.38	125.28	121.24
22	B	823	CLA	C4D-CHA-C1A	3.38	125.28	121.24
31	k	101	DD6	C12-C11-C10	-3.38	117.34	122.82
31	O	213	DD6	C12-C11-C10	-3.37	117.36	122.82
22	A	830	CLA	C4D-CHA-C1A	3.37	125.26	121.24
31	S	204	DD6	C4-C3-C2	3.37	130.41	123.52
22	B	827	CLA	C4D-CHA-C1A	3.37	125.26	121.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	L	206	LMU	C1B-O1B-C4'	-3.36	110.01	117.98
22	T	207	CLA	C4D-CHA-C1A	3.36	125.25	121.24
31	S	215	DD6	C12-C11-C10	-3.36	117.37	122.82
22	A	813	CLA	C4D-CHA-C1A	3.36	125.25	121.24
22	O	208	CLA	C4D-CHA-C1A	3.36	125.25	121.24
27	A	849	CL0	C1C-CHC-C4B	3.36	128.08	116.07
22	A	805	CLA	C4D-CHA-C1A	3.35	125.24	121.24
31	T	213	DD6	C-C1-C2	-3.35	117.38	122.82
22	A	810	CLA	C4D-CHA-C1A	3.35	125.24	121.24
22	A	845	CLA	C4D-CHA-C1A	3.34	125.23	121.24
31	S	211	DD6	C12-C11-C10	-3.34	117.41	122.82
22	Q	208	CLA	C4D-CHA-C1A	3.34	125.22	121.24
22	A	832	CLA	C4D-CHA-C1A	3.34	125.22	121.24
22	B	832	CLA	C4D-CHA-C1A	3.33	125.22	121.24
22	A	812	CLA	C4D-CHA-C1A	3.33	125.22	121.24
31	T	213	DD6	C7-C6-C5	-3.33	117.42	122.82
27	A	849	CL0	C1A-CHA-C4D	3.33	124.53	118.98
22	B	809	CLA	C4D-CHA-C1A	3.33	125.21	121.24
31	U	203	DD6	C26-C25-C24	3.32	132.83	123.20
22	k	102	CLA	C4D-CHA-C1A	3.32	125.21	121.24
22	H	210	CLA	C4D-CHA-C1A	3.31	125.19	121.24
22	K	204	CLA	C4D-CHA-C1A	3.31	125.19	121.24
22	K	203	CLA	CAA-CBA-CGA	3.31	121.31	112.49
22	T	210	CLA	C4D-CHA-C1A	3.30	125.19	121.24
22	S	217	CLA	C4D-CHA-C1A	3.30	125.18	121.24
31	P	218	DD6	C8-C6-C5	3.29	124.18	119.01
22	A	853	CLA	C4D-CHA-C1A	3.29	125.17	121.24
25	I	102	BCR	C27-C26-C25	3.29	127.15	122.70
31	S	214	DD6	C13-C11-C10	3.28	124.18	119.01
22	O	203	CLA	C4D-CHA-C1A	3.28	125.16	121.24
22	O	205	CLA	C4D-CHA-C1A	3.28	125.16	121.24
22	U	205	CLA	C4D-CHA-C1A	3.28	125.16	121.24
34	Q	201	A86	C8-C6-C5	3.28	124.17	119.01
22	O	202	CLA	C4D-CHA-C1A	3.28	125.15	121.24
22	A	809	CLA	C4D-CHA-C1A	3.28	125.15	121.24
31	O	215	DD6	C14-C13-C11	3.27	130.61	125.53
31	H	211	DD6	C10-C9-C8	3.27	132.69	123.20
31	O	215	DD6	C3-C4-C5	3.27	130.21	123.52
25	B	839	BCR	C15-C16-C17	-3.27	116.83	123.52
22	L	202	CLA	C4D-CHA-C1A	3.27	125.14	121.24
22	P	216	CLA	C4A-NA-C1A	3.27	108.17	106.68
22	T	203	CLA	C4D-CHA-C1A	3.27	125.14	121.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	G	214	DD6	C8-C6-C5	3.26	124.14	119.01
22	A	818	CLA	C4D-CHA-C1A	3.26	125.13	121.24
22	Q	216	CLA	C4D-CHA-C1A	3.26	125.13	121.24
22	B	845	CLA	C4D-CHA-C1A	3.25	125.12	121.24
22	B	834	CLA	C4D-CHA-C1A	3.25	125.12	121.24
25	L	205	BCR	C3-C4-C5	-3.25	108.26	114.06
22	P	213	CLA	C4D-CHA-C1A	3.25	125.12	121.24
31	H	211	DD6	C7-C6-C5	-3.25	117.56	122.82
22	A	834	CLA	C4D-CHA-C1A	3.25	125.12	121.24
22	k	103	CLA	C4A-NA-C1A	3.25	108.16	106.68
31	O	201	DD6	C3-C4-C5	3.24	130.15	123.52
22	H	205	CLA	C4D-CHA-C1A	3.24	125.11	121.24
22	k	103	CLA	C4D-CHA-C1A	3.24	125.11	121.24
22	A	806	CLA	C4D-CHA-C1A	3.24	125.11	121.24
31	P	220	DD6	C24-C1-C2	3.24	124.10	119.01
22	A	820	CLA	C4D-CHA-C1A	3.23	125.10	121.24
31	H	201	DD6	C28-C27-C26	-3.23	117.91	124.18
22	U	207	CLA	C4D-CHA-C1A	3.23	125.09	121.24
22	B	804	CLA	C4D-CHA-C1A	3.22	125.08	121.24
22	A	824	CLA	C4D-CHA-C1A	3.22	125.08	121.24
31	H	212	DD6	C12-C11-C10	-3.21	117.61	122.82
31	P	205	DD6	C8-C6-C5	3.21	124.06	119.01
22	R	104	CLA	C4D-CHA-C1A	3.21	125.07	121.24
22	B	833	CLA	C4D-CHA-C1A	3.20	125.06	121.24
22	B	821	CLA	C4D-CHA-C1A	3.19	125.05	121.24
31	U	212	DD6	C7-C6-C5	-3.19	117.64	122.82
26	F	806	LMU	O1B-C4'-C5'	3.19	117.85	109.48
22	U	210	CLA	C4D-CHA-C1A	3.19	125.05	121.24
31	H	211	DD6	C24-C1-C2	3.19	124.02	119.01
22	A	828	CLA	C4D-CHA-C1A	3.18	125.04	121.24
31	J	101	DD6	C4-C3-C2	3.17	130.01	123.52
31	H	211	DD6	C-C1-C2	-3.17	117.68	122.82
22	P	210	CLA	C4D-CHA-C1A	3.17	125.03	121.24
22	Q	211	CLA	C4D-CHA-C1A	3.17	125.03	121.24
34	Q	201	A86	C7-C6-C5	-3.17	117.68	122.82
22	B	819	CLA	CHA-C1A-NA	-3.16	119.24	126.39
22	K	205	CLA	C4D-CHA-C1A	3.15	125.00	121.24
31	S	215	DD6	C26-C25-C24	3.15	132.33	123.20
31	Q	202	DD6	O1-C15-C14	-3.15	107.85	116.88
34	R	103	A86	C26-C25-C24	3.15	132.32	123.20
31	S	215	DD6	C-C1-C2	-3.13	117.74	122.82
22	B	826	CLA	C4D-CHA-C1A	3.12	124.97	121.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	808	CLA	C4D-CHA-C1A	3.12	124.96	121.24
31	k	101	DD6	C24-C1-C2	3.12	123.91	119.01
27	A	849	CL0	C4D-ND-C1D	3.12	107.58	105.22
31	G	212	DD6	C24-C1-C2	3.11	123.90	119.01
29	B	841	DGD	O5D-C6D-C5D	-3.11	102.41	109.42
31	O	212	DD6	C12-C11-C10	-3.11	117.78	122.82
26	O	216	LMU	C2'-C3'-C4'	3.10	116.73	109.68
22	A	821	CLA	CHA-C1A-NA	-3.10	119.37	126.39
34	Q	214	A86	C4-C3-C2	3.10	129.85	123.52
31	P	215	DD6	C7-C6-C5	-3.09	117.80	122.82
31	G	214	DD6	C3-C4-C5	3.09	129.85	123.52
31	T	213	DD6	C24-C1-C2	3.09	123.87	119.01
31	H	212	DD6	C24-C1-C2	3.09	123.86	119.01
31	P	205	DD6	C10-C9-C8	3.08	132.14	123.20
22	A	804	CLA	C4D-CHA-C1A	3.08	124.92	121.24
31	J	101	DD6	C8-C6-C5	3.08	123.85	119.01
22	A	817	CLA	C4D-CHA-C1A	3.08	124.92	121.24
31	P	218	DD6	C24-C1-C2	3.08	123.85	119.01
31	S	205	DD6	C8-C6-C5	3.08	123.85	119.01
31	T	212	DD6	C7-C6-C5	-3.08	117.83	122.82
31	H	201	DD6	C37-C36-C31	-3.07	118.41	124.16
31	P	205	DD6	C13-C11-C10	3.07	123.84	119.01
22	H	213	CLA	C4A-NA-C1A	3.06	108.08	106.68
22	G	207	CLA	CHD-C1D-ND	-3.06	120.49	124.80
22	A	802	CLA	C4D-CHA-C1A	3.06	124.90	121.24
22	P	208	CLA	C4D-CHA-C1A	3.06	124.89	121.24
25	M	101	BCR	C3-C4-C5	-3.06	108.60	114.06
26	K	202	LMU	C4B-C3B-C2B	3.06	116.20	110.83
22	B	843	CLA	C4D-CHA-C1A	3.06	124.89	121.24
34	R	105	A86	C3-C4-C5	3.06	129.77	123.52
22	Q	212	CLA	C4A-NA-C1A	3.05	108.07	106.68
31	O	212	DD6	C8-C6-C5	3.05	123.81	119.01
22	Q	212	CLA	CHA-C1A-NA	-3.05	119.49	126.39
31	P	220	DD6	C8-C6-C5	3.05	123.80	119.01
22	B	807	CLA	C4D-CHA-C1A	3.05	124.88	121.24
31	O	214	DD6	C8-C6-C5	3.05	123.80	119.01
31	Q	202	DD6	C8-C6-C5	3.04	123.80	119.01
31	T	213	DD6	C9-C10-C11	-3.04	123.01	127.28
31	G	213	DD6	C3-C4-C5	3.04	129.74	123.52
22	B	817	CLA	CHD-C1D-ND	-3.04	120.53	124.80
22	J	103	CLA	C4D-CHA-C1A	3.03	124.86	121.24
30	B	846	SQD	C44-O6-C1	3.03	120.30	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	B	846	SQD	O8-S-C6	3.03	111.83	105.97
31	Q	215	DD6	C3-C4-C5	3.03	129.71	123.52
22	A	822	CLA	CHD-C1D-ND	-3.02	120.55	124.80
24	A	840	LHG	O8-C23-C24	3.02	120.31	111.15
34	R	103	A86	C24-C1-C2	3.02	123.75	119.01
31	P	220	DD6	C-C1-C2	-3.02	117.93	122.82
22	P	214	CLA	CHD-C1D-ND	-3.01	120.56	124.80
22	G	205	CLA	C4D-CHA-C1A	3.01	124.84	121.24
22	A	807	CLA	C4D-CHA-C1A	3.01	124.84	121.24
31	O	212	DD6	C7-C6-C5	-3.01	117.94	122.82
22	B	816	CLA	C4D-CHA-C1A	3.01	124.83	121.24
31	P	205	DD6	C7-C6-C5	-3.01	117.95	122.82
31	S	204	DD6	C24-C1-C2	3.00	123.73	119.01
34	P	204	A86	C8-C6-C5	3.00	123.72	119.01
31	U	212	DD6	C4-C3-C2	3.00	129.65	123.52
31	K	208	DD6	C8-C6-C5	3.00	123.72	119.01
22	H	206	CLA	C4D-CHA-C1A	2.99	124.81	121.24
34	Q	214	A86	C7-C6-C5	-2.99	117.97	122.82
22	T	211	CLA	CHD-C1D-ND	-2.99	120.60	124.80
22	B	820	CLA	C4D-CHA-C1A	2.99	124.81	121.24
25	L	205	BCR	C11-C10-C9	-2.99	123.09	127.28
22	H	210	CLA	CHD-C1D-ND	-2.98	120.60	124.80
22	G	201	CLA	C4D-CHA-C1A	2.98	124.80	121.24
22	B	814	CLA	CHD-C1D-ND	-2.98	120.60	124.80
31	Q	202	DD6	C7-C6-C5	-2.98	117.98	122.82
31	P	218	DD6	C7-C6-C5	-2.98	117.99	122.82
22	G	210	CLA	C4D-CHA-C1A	2.98	124.79	121.24
31	Q	202	DD6	C24-C1-C2	2.98	123.69	119.01
25	M	101	BCR	C11-C10-C9	-2.97	123.11	127.28
22	B	802	CLA	C4D-CHA-C1A	2.97	124.79	121.24
34	Q	214	A86	C8-C6-C5	2.97	123.68	119.01
24	P	201	LHG	O8-C23-C24	2.97	120.88	111.83
34	U	202	A86	C8-C6-C5	2.97	123.67	119.01
22	L	203	CLA	CHD-C1D-ND	-2.96	120.63	124.80
31	S	205	DD6	C7-C6-C5	-2.96	118.02	122.82
22	S	208	CLA	CHD-C1D-ND	-2.96	120.64	124.80
31	J	101	DD6	C7-C6-C5	-2.96	118.02	122.82
31	k	101	DD6	C-C1-C2	-2.96	118.02	122.82
32	J	102	LMG	O6-C1-O1	-2.96	103.06	110.04
22	Q	208	CLA	CHA-C1A-NA	-2.96	119.70	126.39
25	I	102	BCR	C15-C16-C17	-2.95	117.47	123.52
22	B	827	CLA	C4A-NA-C1A	2.95	108.03	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	P	216	CLA	CHA-C1A-NA	-2.95	119.71	126.39
34	Q	214	A86	C35-C34-C33	2.95	115.18	109.89
22	H	213	CLA	CHA-C1A-NA	-2.95	119.72	126.39
31	G	214	DD6	C26-C25-C24	2.94	131.73	123.20
25	I	101	BCR	C2-C1-C6	2.94	114.71	110.44
22	G	215	CLA	CHD-C1D-ND	-2.94	120.66	124.80
22	K	206	CLA	C4D-CHA-C1A	2.94	124.75	121.24
22	Q	212	CLA	C4D-CHA-C1A	2.94	124.75	121.24
31	U	214	DD6	C24-C1-C2	2.94	123.63	119.01
34	Q	218	A86	C8-C6-C5	2.94	123.63	119.01
22	k	103	CLA	CHA-C1A-NA	-2.94	119.74	126.39
31	H	201	DD6	C35-C36-C31	2.94	126.61	120.50
25	k	104	BCR	C27-C26-C25	2.94	126.67	122.70
31	O	214	DD6	C7-C6-C5	-2.94	118.06	122.82
31	S	214	DD6	C4-C3-C2	2.93	129.52	123.52
26	L	206	LMU	C1'-C2'-C3'	2.93	116.18	110.01
31	U	212	DD6	C24-C1-C2	2.93	123.62	119.01
22	O	211	CLA	CAA-C2A-C3A	-2.93	109.51	116.23
22	B	805	CLA	C4D-CHA-C1A	2.93	124.74	121.24
31	G	212	DD6	C-C1-C2	-2.93	118.07	122.82
31	S	211	DD6	C8-C6-C5	2.93	123.61	119.01
22	H	202	CLA	CHD-C1D-ND	-2.93	120.68	124.80
31	S	215	DD6	C28-C27-C26	-2.92	118.50	124.18
22	A	825	CLA	CHA-C1A-NA	-2.92	119.77	126.39
22	B	822	CLA	CHA-C1A-NA	-2.92	119.77	126.39
31	K	208	DD6	C24-C1-C2	2.91	123.59	119.01
27	A	849	CL0	C4C-CHD-C1D	2.91	126.49	116.07
26	K	201	LMU	O5'-C5'-C4'	2.91	115.74	109.72
22	A	815	CLA	CHA-C1A-NA	-2.90	119.81	126.39
22	A	834	CLA	CHA-C1A-NA	-2.90	119.82	126.39
22	A	845	CLA	CHA-C1A-NA	-2.90	119.82	126.39
31	G	213	DD6	C24-C1-C2	2.90	123.57	119.01
22	B	827	CLA	CHA-C1A-NA	-2.90	119.82	126.39
31	G	211	DD6	C24-C1-C2	2.90	123.57	119.01
31	K	208	DD6	C-C1-C2	-2.90	118.12	122.82
22	A	817	CLA	CHA-C1A-NA	-2.90	119.83	126.39
31	O	213	DD6	C3-C4-C5	2.90	129.45	123.52
22	T	201	CLA	CHA-C1A-NA	-2.89	119.84	126.39
26	P	221	LMU	O5B-C1B-C2B	2.89	116.31	110.37
31	P	220	DD6	C7-C6-C5	-2.89	118.13	122.82
22	K	207	CLA	CHD-C1D-ND	-2.89	120.73	124.80
34	P	204	A86	C7-C6-C5	-2.89	118.13	122.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	Q	208	CLA	CAA-CBA-CGA	2.89	121.42	113.21
31	S	211	DD6	C7-C6-C5	-2.89	118.14	122.82
31	H	212	DD6	C-C1-C2	-2.89	118.14	122.82
22	L	202	CLA	CHA-C1A-NA	-2.89	119.85	126.39
31	O	215	DD6	C24-C1-C2	2.89	123.55	119.01
31	U	214	DD6	C-C1-C2	-2.89	118.14	122.82
22	B	802	CLA	CHA-C1A-NA	-2.88	119.86	126.39
22	K	203	CLA	C4A-NA-C1A	2.88	108.00	106.68
31	O	214	DD6	C24-C1-C2	2.88	123.54	119.01
31	S	215	DD6	C8-C6-C5	2.88	123.54	119.01
22	S	209	CLA	CHD-C1D-ND	-2.88	120.75	124.80
22	A	807	CLA	CHA-C1A-NA	-2.88	119.87	126.39
31	K	208	DD6	C7-C6-C5	-2.88	118.16	122.82
22	A	829	CLA	CHD-C1D-ND	-2.88	120.75	124.80
31	U	212	DD6	C-C1-C2	-2.87	118.16	122.82
22	S	216	CLA	CHD-C1D-ND	-2.87	120.76	124.80
22	Q	213	CLA	C1-O2A-CGA	2.87	123.60	116.65
32	P	217	LMG	O1-C1-C2	-2.87	103.91	108.27
31	Q	202	DD6	C-C1-C2	-2.87	118.17	122.82
31	S	204	DD6	C-C1-C2	-2.87	118.17	122.82
22	A	810	CLA	C4A-NA-C1A	2.87	107.99	106.68
22	F	803	CLA	CHA-C1A-NA	-2.87	119.90	126.39
25	B	838	BCR	C27-C26-C25	2.87	126.58	122.70
22	F	802	CLA	C4A-NA-C1A	2.86	107.99	106.68
22	A	803	CLA	CHD-C1D-ND	-2.86	120.78	124.80
31	Q	215	DD6	C8-C6-C5	2.86	123.51	119.01
22	S	202	CLA	CMD-C2D-C1D	2.86	129.76	124.73
22	G	203	CLA	CHA-C1A-NA	-2.86	119.92	126.39
25	L	201	BCR	C15-C16-C17	-2.86	117.67	123.52
22	A	823	CLA	C4D-CHA-C1A	2.86	124.65	121.24
34	Q	218	A86	C7-C6-C5	-2.86	118.19	122.82
22	U	207	CLA	CHD-C1D-ND	-2.85	120.79	124.80
31	Q	215	DD6	C-C1-C2	-2.85	118.19	122.82
31	S	204	DD6	C7-C6-C5	-2.85	118.19	122.82
31	S	215	DD6	C7-C6-C5	-2.85	118.19	122.82
22	B	801	CLA	CHA-C1A-NA	-2.85	119.94	126.39
22	B	844	CLA	CHA-C1A-NA	-2.85	119.94	126.39
22	B	812	CLA	C4D-CHA-C1A	2.85	124.64	121.24
31	O	214	DD6	C-C1-C2	-2.85	118.20	122.82
26	F	806	LMU	O1B-C1B-C2B	2.85	115.09	108.09
31	U	203	DD6	C33-C32-C31	2.84	115.09	109.49
31	Q	215	DD6	C7-C6-C5	-2.84	118.21	122.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	T	211	CLA	CHA-C1A-NA	-2.84	119.95	126.39
31	S	204	DD6	C8-C6-C5	2.84	123.48	119.01
22	O	209	CLA	C4D-CHA-C1A	2.84	124.63	121.24
22	U	211	CLA	CHA-C1A-NA	-2.84	119.96	126.39
22	B	804	CLA	CHD-C1D-ND	-2.84	120.80	124.80
22	A	807	CLA	C4A-NA-C1A	2.84	107.97	106.68
31	P	215	DD6	C24-C1-C2	2.84	123.47	119.01
22	A	812	CLA	CHA-C1A-NA	-2.84	119.97	126.39
22	R	101	CLA	CHA-C1A-NA	-2.83	119.97	126.39
22	T	206	CLA	C4D-CHA-C1A	2.83	124.62	121.24
26	K	202	LMU	O1B-C4'-C3'	2.83	114.43	107.23
34	U	202	A86	C7-C6-C5	-2.83	118.23	122.82
22	U	210	CLA	CHD-C1D-ND	-2.83	120.82	124.80
33	T	208	KC1	CAB-C3B-C4B	2.83	131.58	124.82
22	A	838	CLA	CHA-C1A-NA	-2.83	119.98	126.39
34	Q	218	A86	C24-C1-C2	2.83	123.46	119.01
22	B	808	CLA	CHA-C1A-NA	-2.83	119.98	126.39
22	B	834	CLA	CHA-C1A-NA	-2.83	119.99	126.39
22	A	813	CLA	CHA-C1A-NA	-2.83	119.99	126.39
22	B	826	CLA	CHA-C1A-NA	-2.83	119.99	126.39
22	B	833	CLA	CHA-C1A-NA	-2.83	119.99	126.39
22	B	844	CLA	C4A-NA-C1A	2.83	107.97	106.68
22	T	207	CLA	CHD-C1D-ND	-2.82	120.83	124.80
31	O	201	DD6	C24-C1-C2	2.82	123.45	119.01
22	A	810	CLA	CHA-C1A-NA	-2.82	120.01	126.39
22	Q	207	CLA	CHA-C1A-NA	-2.82	120.01	126.39
31	Q	215	DD6	C24-C1-C2	2.82	123.44	119.01
22	B	818	CLA	CHA-C1A-NA	-2.82	120.01	126.39
22	P	211	CLA	C4D-CHA-C1A	2.82	124.60	121.24
25	R	102	BCR	C39-C30-C25	-2.82	105.83	110.24
22	R	104	CLA	CHA-C1A-NA	-2.82	120.02	126.39
25	R	102	BCR	C19-C18-C17	-2.81	118.21	124.72
22	T	205	CLA	CHD-C1D-ND	-2.81	120.84	124.80
22	S	217	CLA	CHA-C1A-NA	-2.81	120.03	126.39
22	F	803	CLA	C1-O2A-CGA	2.81	123.45	116.65
32	P	217	LMG	C4-C3-C2	2.81	115.76	110.83
31	P	218	DD6	C-C1-C2	-2.81	118.27	122.82
31	O	212	DD6	C22-C16-C17	-2.81	104.03	108.97
22	A	805	CLA	CHD-C1D-ND	-2.81	120.85	124.80
22	S	207	CLA	CHA-C1A-NA	-2.81	120.03	126.39
31	O	201	DD6	C-C1-C2	-2.81	118.27	122.82
22	G	206	CLA	CHA-C1A-NA	-2.81	120.04	126.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	B	841	DGD	CDB-CCB-CBB	-2.80	100.19	114.37
30	S	201	SQD	O7-S-C6	2.80	110.94	106.76
26	K	201	LMU	C3'-C4'-C5'	2.80	117.14	110.93
22	Q	211	CLA	CAA-C2A-C3A	-2.80	109.81	116.23
31	G	213	DD6	C-C1-C2	-2.80	118.28	122.82
22	A	835	CLA	CHA-C1A-NA	-2.80	120.05	126.39
31	Q	215	DD6	C13-C11-C10	2.80	123.41	119.01
31	H	201	DD6	C25-C26-C27	2.80	134.44	126.61
34	R	103	A86	C3-C4-C5	2.79	129.24	123.52
22	B	818	CLA	C4D-CHA-C1A	2.79	124.58	121.24
22	Q	207	CLA	CHD-C1D-ND	-2.79	120.87	124.80
34	R	103	A86	C28-C27-C29	-2.79	112.74	118.94
31	P	205	DD6	C-C1-C2	-2.79	118.30	122.82
22	G	201	CLA	CHA-C1A-NA	-2.79	120.08	126.39
31	H	212	DD6	C7-C6-C5	-2.79	118.30	122.82
31	G	212	DD6	C8-C6-C5	2.79	123.39	119.01
31	S	205	DD6	C4-C3-C2	2.79	129.22	123.52
22	A	828	CLA	CHA-C1A-NA	-2.78	120.09	126.39
22	Q	211	CLA	CHA-C1A-NA	-2.78	120.09	126.39
31	G	211	DD6	C7-C6-C5	-2.78	118.31	122.82
22	A	827	CLA	CHA-C1A-NA	-2.78	120.09	126.39
31	U	203	DD6	C7-C6-C5	-2.78	118.31	122.82
22	F	802	CLA	CHA-C1A-NA	-2.78	120.09	126.39
31	U	203	DD6	C8-C6-C5	2.78	123.39	119.01
22	B	805	CLA	CHA-C1A-NA	-2.78	120.09	126.39
22	A	848	CLA	CHA-C1A-NA	-2.78	120.10	126.39
22	B	831	CLA	CHA-C1A-NA	-2.78	120.10	126.39
22	B	842	CLA	CHA-C1A-NA	-2.78	120.10	126.39
22	H	206	CLA	CHA-C1A-NA	-2.78	120.10	126.39
31	O	215	DD6	C-C1-C2	-2.78	118.32	122.82
33	S	210	KC1	CAB-C3B-C4B	2.78	131.45	124.82
34	Q	218	A86	C-C1-C2	-2.78	118.32	122.82
22	K	206	CLA	CHA-C1A-NA	-2.78	120.10	126.39
22	B	832	CLA	CHA-C1A-NA	-2.78	120.11	126.39
22	H	205	CLA	CHA-C1A-NA	-2.78	120.11	126.39
22	B	803	CLA	CHA-C1A-NA	-2.77	120.11	126.39
22	H	207	CLA	CHD-C1D-ND	-2.77	120.90	124.80
22	A	850	CLA	CHA-C1A-NA	-2.77	120.11	126.39
22	B	811	CLA	CHD-C1D-ND	-2.77	120.90	124.80
22	B	803	CLA	C4D-CHA-C1A	2.77	124.55	121.24
31	P	215	DD6	C-C1-C2	-2.77	118.33	122.82
22	T	210	CLA	CHA-C1A-NA	-2.77	120.13	126.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	U	201	LMG	O6-C1-O1	-2.77	103.51	110.04
22	P	208	CLA	CHA-C1A-NA	-2.77	120.13	126.39
22	L	204	CLA	C4A-NA-C1A	2.76	107.94	106.68
22	O	211	CLA	CHA-C1A-NA	-2.76	120.13	126.39
22	A	821	CLA	C4A-NA-C1A	2.76	107.94	106.68
25	R	102	BCR	C29-C30-C25	2.76	114.45	110.44
22	A	832	CLA	CHA-C1A-NA	-2.76	120.14	126.39
31	G	211	DD6	C-C1-C2	-2.76	118.34	122.82
22	L	204	CLA	CHA-C1A-NA	-2.76	120.14	126.39
34	R	103	A86	C29-C30-C31	-2.76	174.41	177.66
22	U	209	CLA	CHA-C1A-NA	-2.76	120.15	126.39
22	O	203	CLA	CHA-C1A-NA	-2.76	120.15	126.39
22	B	847	CLA	CHA-C1A-NA	-2.76	120.15	126.39
22	G	208	CLA	CHD-C1D-ND	-2.75	120.93	124.80
34	Q	201	A86	C4-C3-C2	2.75	129.16	123.52
22	K	204	CLA	CHA-C1A-NA	-2.75	120.16	126.39
22	P	207	CLA	CHD-C1D-ND	-2.75	120.93	124.80
22	B	824	CLA	CHA-C1A-NA	-2.75	120.16	126.39
25	J	104	BCR	C24-C23-C22	-2.75	122.16	126.23
25	L	205	BCR	C27-C26-C25	2.75	126.42	122.70
22	B	828	CLA	CHA-C1A-NA	-2.75	120.16	126.39
22	T	202	CLA	CHD-C1D-ND	-2.75	120.93	124.80
22	O	204	CLA	CHA-C1A-NA	-2.75	120.17	126.39
25	F	801	BCR	C27-C26-C25	2.75	126.42	122.70
32	P	217	LMG	O6-C5-C4	2.75	114.65	109.70
22	B	843	CLA	CHA-C1A-NA	-2.75	120.17	126.39
31	G	212	DD6	C7-C6-C5	-2.75	118.37	122.82
31	H	212	DD6	C8-C6-C5	2.75	123.33	119.01
22	B	806	CLA	CHD-C1D-ND	-2.75	120.94	124.80
26	K	201	LMU	O5B-C5B-C4B	2.74	114.64	109.70
30	B	846	SQD	C1-O5-C5	2.74	119.08	113.72
22	A	811	CLA	CHA-C1A-NA	-2.74	120.18	126.39
26	K	202	LMU	O1B-C4'-C5'	-2.74	102.28	109.48
22	A	830	CLA	CHA-C1A-NA	-2.74	120.18	126.39
22	A	817	CLA	C4A-NA-C1A	2.74	107.93	106.68
31	G	211	DD6	C8-C6-C5	2.74	123.32	119.01
22	A	801	CLA	CHA-C1A-NA	-2.74	120.18	126.39
22	A	821	CLA	C4D-CHA-C1A	2.74	124.51	121.24
22	G	209	CLA	C4A-NA-C1A	2.74	107.93	106.68
31	P	205	DD6	C24-C1-C2	2.74	123.32	119.01
31	G	214	DD6	C7-C6-C5	-2.74	118.38	122.82
22	P	213	CLA	CHA-C1A-NA	-2.74	120.19	126.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	Q	204	CLA	CHD-C1D-ND	-2.74	120.95	124.80
22	F	803	CLA	C4A-NA-C1A	2.74	107.93	106.68
34	R	105	A86	C24-C1-C2	2.73	123.31	119.01
34	R	105	A86	C7-C6-C5	-2.73	118.39	122.82
22	S	202	CLA	CHD-C1D-C2D	2.73	131.16	125.49
22	O	209	CLA	CHA-C1A-NA	-2.73	120.22	126.39
22	B	815	CLA	CHD-C1D-ND	-2.73	120.97	124.80
22	B	819	CLA	C4D-CHA-C1A	2.73	124.50	121.24
25	L	201	BCR	C27-C26-C25	2.73	126.39	122.70
22	O	209	CLA	C7-C6-C5	2.73	120.53	113.26
22	A	854	CLA	CHA-C1A-NA	-2.72	120.22	126.39
22	Q	213	CLA	CHA-C1A-NA	-2.72	120.22	126.39
22	K	205	CLA	CHA-C1A-NA	-2.72	120.22	126.39
25	A	843	BCR	C2-C1-C6	2.72	114.39	110.44
22	O	202	CLA	CHD-C1D-ND	-2.72	120.97	124.80
22	L	202	CLA	C1-O2A-CGA	2.72	123.24	116.65
34	R	105	A86	C-C1-C2	-2.72	118.41	122.82
22	O	207	CLA	CHD-C1D-ND	-2.72	120.97	124.80
22	O	202	CLA	CHA-C1A-NA	-2.72	120.24	126.39
22	B	812	CLA	CHD-C1D-ND	-2.71	120.98	124.80
34	P	204	A86	C-C1-C2	-2.71	118.42	122.82
22	U	209	CLA	C4D-CHA-C1A	2.71	124.48	121.24
22	A	831	CLA	CHD-C1D-ND	-2.71	120.99	124.80
31	O	215	DD6	C7-C6-C5	-2.71	118.42	122.82
26	M	102	LMU	C1B-O1B-C4'	-2.71	111.55	117.98
22	A	850	CLA	CHD-C1D-ND	-2.71	120.99	124.80
22	A	804	CLA	CHA-C1A-NA	-2.71	120.25	126.39
26	F	806	LMU	C4B-C3B-C2B	2.71	115.59	110.83
22	A	820	CLA	CHA-C1A-NA	-2.71	120.25	126.39
31	S	214	DD6	C8-C6-C5	2.71	123.27	119.01
22	A	851	CLA	CHA-C1A-NA	-2.71	120.26	126.39
31	H	201	DD6	C7-C6-C5	-2.71	118.43	122.82
22	Q	212	CLA	CAA-C2A-C1A	2.71	120.85	111.97
31	k	101	DD6	C7-C6-C5	-2.71	118.43	122.82
22	H	204	CLA	CHD-C1D-ND	-2.71	120.99	124.80
25	R	102	BCR	C19-C20-C21	-2.71	117.98	123.52
22	A	814	CLA	CHA-C1A-NA	-2.70	120.27	126.39
31	S	215	DD6	C29-C30-C31	-2.70	169.18	175.48
30	B	846	SQD	O7-S-C6	2.70	110.79	106.76
25	I	102	BCR	C15-C14-C13	-2.70	123.49	127.28
22	Q	206	CLA	CHA-C1A-NA	-2.70	120.27	126.39
22	U	205	CLA	CHA-C1A-NA	-2.70	120.28	126.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	S	214	DD6	C-C1-C2	-2.70	118.44	122.82
22	B	821	CLA	CHA-C1A-NA	-2.70	120.28	126.39
22	A	854	CLA	CHD-C1D-ND	-2.70	121.00	124.80
31	S	214	DD6	C24-C1-C2	2.70	123.25	119.01
22	H	208	CLA	CHD-C1D-ND	-2.70	121.01	124.80
34	U	202	A86	C-C1-C2	-2.70	118.45	122.82
31	O	215	DD6	O1-C20-C19	-2.70	110.96	113.49
22	A	846	CLA	CHA-C1A-NA	-2.70	120.28	126.39
22	G	204	CLA	CHA-C1A-NA	-2.70	120.28	126.39
22	O	203	CLA	C4A-NA-C1A	2.70	107.91	106.68
27	A	849	CL0	C4D-CHA-CBD	-2.69	106.25	108.97
22	P	210	CLA	CHA-C1A-NA	-2.69	120.29	126.39
22	A	802	CLA	CHD-C1D-ND	-2.69	121.01	124.80
26	F	806	LMU	C3'-C4'-C5'	-2.69	104.96	110.93
22	B	812	CLA	CHA-C1A-NA	-2.69	120.30	126.39
31	k	101	DD6	C8-C6-C5	2.69	123.24	119.01
33	P	212	KC1	CAB-C3B-C4B	2.69	131.24	124.82
22	J	103	CLA	CHA-C1A-NA	-2.69	120.30	126.39
22	k	102	CLA	CHA-C1A-NA	-2.69	120.30	126.39
22	U	206	CLA	CHA-C1A-NA	-2.69	120.30	126.39
31	O	213	DD6	C-C1-C2	-2.69	118.46	122.82
22	G	210	CLA	CHA-C1A-NA	-2.69	120.31	126.39
22	U	211	CLA	C4A-NA-C1A	2.69	107.90	106.68
31	G	213	DD6	C7-C6-C5	-2.69	118.47	122.82
22	H	210	CLA	CHA-C1A-NA	-2.68	120.31	126.39
30	S	201	SQD	O6-C1-C2	2.68	112.35	108.27
22	G	208	CLA	CHA-C1A-NA	-2.68	120.31	126.39
22	A	823	CLA	CHA-C1A-NA	-2.68	120.32	126.39
32	Q	217	LMG	O6-C1-O1	-2.68	103.71	110.04
22	A	824	CLA	CHA-C1A-NA	-2.68	120.32	126.39
34	R	105	A86	C8-C6-C5	2.68	123.22	119.01
22	T	205	CLA	CHA-C1A-NA	-2.68	120.33	126.39
22	G	202	CLA	CHA-C1A-NA	-2.68	120.33	126.39
22	G	209	CLA	CHA-C1A-NA	-2.68	120.33	126.39
22	B	806	CLA	CHA-C1A-NA	-2.68	120.33	126.39
22	B	810	CLA	CHD-C1D-ND	-2.67	121.04	124.80
22	T	203	CLA	CHA-C1A-NA	-2.67	120.33	126.39
25	B	839	BCR	C15-C14-C13	-2.67	123.53	127.28
22	F	804	CLA	CHA-C1A-NA	-2.67	120.33	126.39
22	G	205	CLA	CHA-C1A-NA	-2.67	120.33	126.39
22	B	829	CLA	CHA-C1A-NA	-2.67	120.34	126.39
22	U	210	CLA	CHA-C1A-NA	-2.67	120.34	126.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	O	213	DD6	C24-C1-C2	2.67	123.21	119.01
22	B	845	CLA	O2A-C1-C2	-2.67	97.83	108.11
22	S	206	CLA	CHD-C1D-ND	-2.67	121.04	124.80
22	A	826	CLA	C4D-CHA-C1A	2.67	124.43	121.24
22	A	855	CLA	CHA-C1A-NA	-2.67	120.25	126.33
22	B	823	CLA	CHA-C1A-NA	-2.67	120.35	126.39
26	M	102	LMU	O5'-C5'-C4'	2.67	115.24	109.72
22	Q	204	CLA	CHA-C1A-NA	-2.67	120.35	126.39
34	P	204	A86	C24-C1-C2	2.67	123.20	119.01
22	O	208	CLA	CHD-C1D-ND	-2.66	121.05	124.80
22	B	815	CLA	CHA-C1A-NA	-2.66	120.36	126.39
22	B	845	CLA	CHA-C1A-NA	-2.66	120.36	126.39
22	O	211	CLA	C4A-NA-C1A	2.66	107.89	106.68
22	B	830	CLA	CHA-C1A-NA	-2.66	120.37	126.39
33	S	212	KC1	CAB-C3B-C4B	2.66	131.17	124.82
22	P	209	CLA	CHA-C1A-NA	-2.66	120.37	126.39
31	S	204	DD6	C28-C27-C26	-2.66	119.02	124.18
22	G	215	CLA	CHA-C1A-NA	-2.66	120.37	126.39
22	A	856	CLA	CHA-C1A-NA	-2.66	120.37	126.39
22	U	204	CLA	CHA-C1A-NA	-2.66	120.37	126.39
26	K	201	LMU	C4B-C3B-C2B	2.66	115.49	110.83
31	O	214	DD6	C13-C11-C10	2.66	123.19	119.01
22	O	205	CLA	CHD-C1D-ND	-2.66	121.07	124.80
22	H	209	CLA	CHA-C1A-NA	-2.65	120.38	126.39
34	Q	201	A86	C-C1-C2	-2.65	118.52	122.82
22	A	813	CLA	CHD-C1D-ND	-2.65	121.07	124.80
22	P	211	CLA	CHA-C1A-NA	-2.65	120.39	126.39
22	A	831	CLA	CHA-C1A-NA	-2.65	120.39	126.39
22	O	207	CLA	CHA-C1A-NA	-2.65	120.39	126.39
22	Q	205	CLA	CHA-C1A-NA	-2.65	120.39	126.39
31	J	101	DD6	C10-C9-C8	2.65	130.88	123.20
22	B	816	CLA	CHA-C1A-NA	-2.65	120.40	126.39
22	S	208	CLA	C4D-CHA-C1A	2.65	124.40	121.24
22	B	820	CLA	CHD-C1D-ND	-2.65	121.08	124.80
24	A	839	LHG	O8-C23-C24	2.64	119.90	111.83
22	T	209	CLA	CHA-C1A-NA	-2.64	120.40	126.39
31	J	101	DD6	C-C1-C2	-2.64	118.53	122.82
31	O	201	DD6	C7-C6-C5	-2.64	118.53	122.82
22	A	833	CLA	CHD-C1D-ND	-2.64	121.08	124.80
22	A	819	CLA	CHA-C1A-NA	-2.64	120.41	126.39
22	H	208	CLA	CHA-C1A-NA	-2.64	120.41	126.39
22	B	811	CLA	CHA-C1A-NA	-2.64	120.42	126.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	829	CLA	CHA-C1A-NA	-2.64	120.42	126.39
22	B	810	CLA	CHA-C1A-NA	-2.64	120.42	126.39
33	Q	210	KC1	CAB-C3B-C4B	2.63	131.11	124.82
31	P	220	DD6	C9-C10-C11	2.63	130.97	127.28
22	G	209	CLA	CHD-C1D-ND	-2.63	121.10	124.80
22	P	214	CLA	CHA-C1A-NA	-2.63	120.43	126.39
22	B	830	CLA	CHD-C1D-ND	-2.63	121.10	124.80
22	S	202	CLA	CHA-C1A-NA	-2.63	120.43	126.39
22	A	809	CLA	CHA-C1A-NA	-2.63	120.43	126.39
22	O	206	CLA	CHA-C1A-NA	-2.63	120.43	126.39
22	S	209	CLA	CHA-C1A-NA	-2.63	120.43	126.39
22	Q	207	CLA	C4A-NA-C1A	2.63	107.88	106.68
22	U	208	CLA	CHA-C1A-NA	-2.63	120.44	126.39
22	T	204	CLA	CHD-C1D-ND	-2.63	121.10	124.80
22	Q	213	CLA	CHD-C1D-ND	-2.63	121.10	124.80
22	A	818	CLA	CHA-C1A-NA	-2.63	120.44	126.39
31	T	212	DD6	C24-C1-C2	2.63	123.14	119.01
33	Q	210	KC1	CBA-CAA-C2A	2.63	136.00	125.45
22	B	825	CLA	CHA-C1A-NA	-2.63	120.44	126.39
22	O	206	CLA	CHD-C1D-ND	-2.63	121.11	124.80
22	K	205	CLA	CHD-C1D-ND	-2.62	121.11	124.80
25	B	840	BCR	C27-C26-C25	2.62	126.25	122.70
22	T	202	CLA	CHA-C1A-NA	-2.62	120.45	126.39
31	U	214	DD6	C26-C25-C24	2.62	130.79	123.20
22	A	826	CLA	CHA-C1A-NA	-2.62	120.46	126.39
22	T	206	CLA	CHA-C1A-NA	-2.62	120.46	126.39
31	S	205	DD6	C13-C11-C10	2.62	123.13	119.01
22	Q	203	CLA	CHD-C1D-ND	-2.62	121.11	124.80
31	Q	202	DD6	C15-C14-C13	2.62	131.53	125.99
22	H	207	CLA	CHA-C1A-NA	-2.62	120.46	126.39
22	H	213	CLA	CHD-C1D-ND	-2.62	121.12	124.80
31	J	101	DD6	C24-C1-C2	2.62	123.13	119.01
23	A	837	PQN	C11-C3-C2	-2.62	120.41	124.89
22	T	211	CLA	C4A-NA-C1A	2.61	107.87	106.68
22	A	809	CLA	CHD-C1D-ND	-2.61	121.12	124.80
25	k	104	BCR	C15-C16-C17	-2.61	118.17	123.52
22	B	816	CLA	C3B-C4B-NB	-2.61	108.20	110.53
30	B	846	SQD	O48-C23-C24	2.61	119.80	111.83
22	K	207	CLA	CHA-C1A-NA	-2.61	120.48	126.39
22	B	804	CLA	CHA-C1A-NA	-2.61	120.48	126.39
26	P	221	LMU	C4B-C3B-C2B	2.61	115.41	110.83
22	A	814	CLA	CHD-C1D-ND	-2.61	121.13	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	805	CLA	CHA-C1A-NA	-2.61	120.48	126.39
22	A	855	CLA	C4A-NA-C1A	2.61	107.87	106.68
22	A	836	CLA	CHA-C1A-NA	-2.61	120.48	126.39
22	A	816	CLA	CHA-C1A-NA	-2.61	120.49	126.39
25	J	104	BCR	C27-C26-C25	2.61	126.23	122.70
33	S	212	KC1	C2A-C3A-C4A	2.61	108.37	106.41
22	A	806	CLA	CHA-C1A-NA	-2.61	120.49	126.39
22	Q	216	CLA	CHD-C1D-ND	-2.61	121.14	124.80
22	P	207	CLA	CHA-C1A-NA	-2.61	120.49	126.39
22	Q	203	CLA	CHA-C1A-NA	-2.61	120.49	126.39
22	T	204	CLA	CHA-C1A-NA	-2.60	120.50	126.39
22	A	848	CLA	C4A-NA-C1A	2.60	107.87	106.68
25	B	836	BCR	C7-C8-C9	-2.60	122.39	126.23
22	B	820	CLA	CHA-C1A-NA	-2.60	120.50	126.39
22	A	801	CLA	C4D-CHA-C1A	2.60	124.34	121.24
22	B	809	CLA	CHA-C1A-NA	-2.60	120.51	126.39
31	O	215	DD6	C12-C11-C13	2.60	122.06	118.09
22	A	820	CLA	CHD-C1D-ND	-2.60	121.15	124.80
22	H	202	CLA	CHA-C1A-NA	-2.60	120.42	126.33
31	Q	202	DD6	C13-C11-C10	2.59	123.09	119.01
22	H	203	CLA	CHA-C1A-NA	-2.59	120.52	126.39
25	A	842	BCR	C27-C26-C25	2.59	126.21	122.70
22	Q	216	CLA	CHA-C1A-NA	-2.59	120.52	126.39
34	Q	214	A86	C28-C27-C26	-2.59	118.62	122.82
34	U	202	A86	C24-C1-C2	2.59	123.08	119.01
22	T	209	CLA	CHD-C1D-ND	-2.59	121.16	124.80
22	B	813	CLA	CHA-C1A-NA	-2.58	120.54	126.39
22	S	208	CLA	CHA-C1A-NA	-2.58	120.54	126.39
22	Q	211	CLA	C4A-NA-C1A	2.58	107.86	106.68
31	O	215	DD6	C8-C6-C5	2.58	123.07	119.01
22	B	809	CLA	CHD-C1D-ND	-2.58	121.17	124.80
22	A	808	CLA	CHA-C1A-NA	-2.58	120.55	126.39
22	H	203	CLA	CHD-C1D-ND	-2.58	121.17	124.80
34	Q	214	A86	C-C1-C2	-2.58	118.64	122.82
22	B	817	CLA	CHA-C1A-NA	-2.58	120.55	126.39
31	G	213	DD6	C8-C6-C5	2.57	123.06	119.01
34	R	103	A86	C10-C9-C8	2.57	130.66	123.20
22	S	216	CLA	CHA-C1A-NA	-2.57	120.56	126.39
22	A	816	CLA	CHD-C1D-ND	-2.57	121.19	124.80
22	G	202	CLA	CHD-C1D-ND	-2.57	121.19	124.80
25	B	836	BCR	C29-C30-C25	2.57	114.17	110.44
25	M	101	BCR	C15-C14-C13	-2.57	123.68	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	844	BCR	C28-C27-C26	-2.57	109.48	114.06
22	T	210	CLA	CHD-C1D-ND	-2.56	121.19	124.80
32	S	213	LMG	O6-C1-O1	-2.56	103.99	110.04
31	T	212	DD6	C-C1-C2	-2.56	118.67	122.82
22	A	833	CLA	CHA-C1A-NA	-2.56	120.59	126.39
22	T	201	CLA	C4D-CHA-C1A	2.56	124.30	121.24
30	S	201	SQD	O48-C23-C24	2.56	119.63	111.83
25	F	805	BCR	C27-C26-C25	2.56	126.16	122.70
25	F	805	BCR	C2-C1-C6	2.56	114.15	110.44
22	L	203	CLA	CHA-C1A-NA	-2.55	120.61	126.39
22	L	202	CLA	C4A-NA-C1A	2.55	107.84	106.68
31	S	205	DD6	C-C1-C2	-2.55	118.68	122.82
22	H	202	CLA	CHD-C1D-C2D	2.55	130.79	125.49
22	A	802	CLA	CHA-C1A-NA	-2.55	120.62	126.39
31	U	203	DD6	C13-C11-C10	2.55	123.02	119.01
25	R	102	BCR	C40-C30-C25	2.55	114.24	110.24
22	A	855	CLA	CHD-C1D-ND	-2.55	121.22	124.80
22	G	205	CLA	CHD-C1D-ND	-2.55	121.22	124.80
22	L	204	CLA	CHD-C1D-ND	-2.54	121.22	124.80
22	B	825	CLA	CHD-C1D-ND	-2.54	121.22	124.80
22	P	210	CLA	CHD-C1D-ND	-2.54	121.23	124.80
26	S	203	LMU	O1'-C1'-C2'	2.54	112.13	108.27
22	A	803	CLA	CHA-C1A-NA	-2.54	120.65	126.39
22	B	813	CLA	CHD-C1D-ND	-2.54	121.23	124.80
22	H	204	CLA	CHA-C1A-NA	-2.54	120.65	126.39
22	O	205	CLA	CHA-C1A-NA	-2.53	120.66	126.39
31	T	212	DD6	C9-C10-C11	2.53	130.83	127.28
24	A	840	LHG	C11-C10-C9	-2.53	101.57	114.37
22	O	208	CLA	CHA-C1A-NA	-2.53	120.67	126.39
24	P	201	LHG	C11-C10-C9	-2.53	101.60	114.37
25	M	101	BCR	C27-C26-C25	2.52	126.12	122.70
22	A	856	CLA	CHD-C1D-ND	-2.52	121.25	124.80
22	B	824	CLA	C4D-CHA-C1A	2.52	124.25	121.24
25	M	101	BCR	C15-C16-C17	-2.52	118.36	123.52
22	B	814	CLA	CHA-C1A-NA	-2.52	120.69	126.39
22	K	203	CLA	CHA-C4D-ND	2.52	137.74	132.55
22	A	853	CLA	CHA-C1A-NA	-2.52	120.69	126.39
22	K	204	CLA	CHD-C1D-ND	-2.52	121.26	124.80
22	U	207	CLA	CAA-CBA-CGA	2.51	120.35	113.21
22	J	103	CLA	CHD-C1D-ND	-2.51	121.26	124.80
22	A	819	CLA	CHD-C1D-ND	-2.51	121.27	124.80
22	A	806	CLA	C1-O2A-CGA	2.51	122.73	116.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	G	207	CLA	CHA-C1A-NA	-2.51	120.71	126.39
22	B	807	CLA	CHA-C1A-NA	-2.51	120.71	126.39
22	B	845	CLA	CAA-C2A-C3A	-2.51	106.22	113.00
25	L	201	BCR	C15-C14-C13	-2.51	123.76	127.28
22	P	208	CLA	CHD-C1D-ND	-2.51	121.27	124.80
22	A	848	CLA	CHD-C1D-ND	-2.51	121.28	124.80
22	S	217	CLA	C7-C6-C5	-2.51	106.58	113.26
22	T	207	CLA	CHA-C1A-NA	-2.50	120.72	126.39
26	K	202	LMU	C1'-C2'-C3'	2.50	115.27	110.01
25	I	101	BCR	C16-C15-C14	-2.50	118.41	123.52
22	A	824	CLA	CHD-C1D-ND	-2.50	121.29	124.80
22	G	207	CLA	CHD-C1D-C2D	2.49	130.67	125.49
22	B	845	CLA	CHD-C1D-ND	-2.49	121.29	124.80
22	H	213	CLA	CAA-CBA-CGA	2.49	120.29	113.21
22	S	207	CLA	CHD-C1D-ND	-2.49	121.30	124.80
31	O	201	DD6	C8-C6-C5	2.49	122.92	119.01
31	O	213	DD6	C7-C6-C5	-2.49	118.79	122.82
26	S	203	LMU	O5'-C1'-O1'	2.49	115.92	110.04
31	H	201	DD6	C8-C6-C5	2.49	122.92	119.01
22	F	804	CLA	CHD-C1D-ND	-2.48	121.31	124.80
31	O	201	DD6	C13-C11-C10	2.48	122.92	119.01
25	B	840	BCR	C16-C15-C14	-2.48	118.44	123.52
22	A	846	CLA	C4A-NA-C1A	2.48	107.81	106.68
22	S	206	CLA	CHA-C1A-NA	-2.48	120.77	126.39
31	S	211	DD6	C13-C11-C10	2.48	122.91	119.01
31	H	201	DD6	C24-C1-C2	2.48	122.91	119.01
22	A	818	CLA	CHD-C1D-ND	-2.48	121.31	124.80
22	U	209	CLA	CHD-C1D-ND	-2.48	121.31	124.80
22	A	853	CLA	CHD-C1D-ND	-2.48	121.32	124.80
33	P	212	KC1	CHC-C4B-NB	-2.48	121.32	124.80
22	B	823	CLA	CHD-C1D-ND	-2.48	121.32	124.80
22	Q	209	CLA	CHA-C1A-NA	-2.47	120.79	126.39
27	A	849	CL0	CHA-C1A-C2A	-2.47	127.50	133.31
22	T	201	CLA	C4A-NA-C1A	2.47	107.81	106.68
22	A	806	CLA	CHD-C1D-ND	-2.47	121.32	124.80
22	P	209	CLA	CHD-C1D-ND	-2.47	121.33	124.80
22	G	204	CLA	CHD-C1D-ND	-2.47	121.33	124.80
31	Q	202	DD6	C23-C16-C17	-2.47	104.63	108.97
22	B	847	CLA	CHD-C1D-ND	-2.47	121.33	124.80
23	B	835	PQN	C11-C3-C2	-2.47	120.66	124.89
22	P	213	CLA	CHD-C1D-ND	-2.47	121.33	124.80
22	A	815	CLA	CHD-C1D-ND	-2.46	121.34	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	G	203	CLA	C4A-NA-C1A	2.46	107.80	106.68
22	U	205	CLA	CHD-C1D-ND	-2.46	121.34	124.80
31	Q	202	DD6	C28-C27-C26	-2.46	119.41	124.18
22	U	204	CLA	CHD-C1D-ND	-2.46	121.35	124.80
22	T	203	CLA	CHD-C1D-ND	-2.46	121.35	124.80
25	B	839	BCR	C27-C26-C25	2.45	126.02	122.70
22	H	209	CLA	CHD-C1D-ND	-2.45	121.35	124.80
31	S	205	DD6	C33-C32-C31	2.45	114.32	109.49
27	A	849	CL0	C3C-C4C-NC	-2.45	108.66	114.65
34	Q	218	A86	C22-C16-C17	-2.45	104.66	108.97
26	F	807	LMU	C1B-O1B-C4'	-2.45	112.17	117.98
26	F	807	LMU	C2'-C3'-C4'	2.45	115.24	109.68
25	A	842	BCR	C2-C1-C6	2.45	114.00	110.44
31	k	101	DD6	C28-C27-C26	-2.45	119.43	124.18
22	G	201	CLA	CHD-C1D-ND	-2.45	121.36	124.80
25	B	840	BCR	C2-C1-C6	2.45	113.99	110.44
33	S	212	KC1	CAA-C2A-C1A	2.44	135.35	124.64
22	A	804	CLA	CHD-C1D-ND	-2.44	121.36	124.80
25	B	836	BCR	C33-C5-C6	-2.44	121.82	124.48
25	A	844	BCR	C15-C16-C17	-2.44	118.53	123.52
22	G	209	CLA	CHC-C1C-NC	2.44	127.98	124.31
22	O	203	CLA	CHD-C1D-ND	-2.44	121.37	124.80
22	H	213	CLA	C1-O2A-CGA	2.44	122.55	116.65
22	L	202	CLA	CHD-C1D-ND	-2.44	121.37	124.80
22	A	832	CLA	CHD-C1D-ND	-2.44	121.38	124.80
24	A	839	LHG	C11-C10-C9	-2.44	102.06	114.37
34	Q	201	A86	C24-C1-C2	2.43	122.83	119.01
22	P	213	CLA	CAA-C2A-C3A	-2.43	110.66	116.23
22	A	832	CLA	C4A-NA-C1A	2.43	107.79	106.68
25	A	843	BCR	C29-C30-C25	2.43	113.96	110.44
26	S	203	LMU	C1B-O5B-C5B	2.42	118.45	113.72
34	R	103	A86	C7-C6-C5	-2.42	118.89	122.82
34	Q	214	A86	C24-C1-C2	2.42	122.81	119.01
22	B	843	CLA	CGD-CBD-CAD	-2.42	103.02	110.85
22	A	808	CLA	CHD-C1D-ND	-2.42	121.40	124.80
33	S	210	KC1	CHC-C4B-C3B	2.41	129.28	125.21
22	A	815	CLA	C3B-C4B-NB	-2.41	108.38	110.53
32	P	217	LMG	O3-C3-C2	-2.41	104.69	110.38
22	U	208	CLA	CHD-C1D-ND	-2.41	121.41	124.80
22	B	831	CLA	CHD-C1D-ND	-2.41	121.42	124.80
22	G	215	CLA	CHD-C1D-C2D	2.40	130.49	125.49
25	I	102	BCR	C2-C1-C6	2.40	113.93	110.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	G	205	CLA	C2A-C1A-CHA	2.40	128.03	123.87
22	B	819	CLA	C4A-NA-C1A	2.40	107.77	106.68
22	B	828	CLA	CHD-C1D-ND	-2.40	121.43	124.80
22	Q	206	CLA	CHD-C1D-ND	-2.39	121.43	124.80
22	A	848	CLA	C1D-ND-C4D	2.39	107.99	106.31
22	K	203	CLA	CHD-C1D-ND	-2.39	121.44	124.80
34	U	202	A86	C28-C27-C26	-2.39	118.95	122.82
34	R	103	A86	C19-C18-C17	2.39	115.25	110.79
22	Q	212	CLA	CAA-C2A-C3A	-2.39	106.55	113.00
22	T	206	CLA	CHD-C1D-ND	-2.38	121.45	124.80
31	T	213	DD6	C12-C11-C13	2.38	121.72	118.09
31	T	213	DD6	C29-C30-C31	-2.38	169.94	175.48
22	Q	209	CLA	CHD-C1D-ND	-2.38	121.45	124.80
22	B	833	CLA	C4A-NA-C1A	2.38	107.76	106.68
31	U	212	DD6	C28-C27-C26	-2.38	119.56	124.18
31	U	203	DD6	C28-C27-C26	-2.38	119.57	124.18
22	B	833	CLA	CHD-C1D-ND	-2.38	121.46	124.80
22	B	834	CLA	CHD-C1D-ND	-2.38	121.46	124.80
22	Q	211	CLA	CHD-C1D-ND	-2.37	121.47	124.80
22	Q	208	CLA	C4A-NA-C1A	2.37	107.76	106.68
22	A	812	CLA	C4A-NA-C1A	2.36	107.76	106.68
22	A	822	CLA	CHA-C1A-NA	-2.36	121.04	126.39
22	S	217	CLA	CHD-C1D-ND	-2.36	121.48	124.80
22	O	204	CLA	CHD-C1D-ND	-2.36	121.48	124.80
25	R	102	BCR	C17-C16-C15	-2.36	119.26	124.72
33	P	212	KC1	CHC-C4B-C3B	2.36	129.19	125.21
22	O	211	CLA	CHD-C1D-ND	-2.36	121.48	124.80
22	B	829	CLA	C4A-NA-C1A	2.36	107.75	106.68
22	B	801	CLA	C4D-CHA-C1A	2.36	124.06	121.24
22	O	202	CLA	CHD-C1D-C2D	2.36	130.39	125.49
34	Q	218	A86	C19-C18-C17	2.35	115.19	110.79
22	B	814	CLA	CHD-C1D-C2D	2.35	130.38	125.49
25	B	840	BCR	C10-C11-C12	-2.35	116.38	123.20
26	A	847	LMU	C1B-O1B-C4'	-2.35	112.40	117.98
22	U	207	CLA	CHA-C1A-NA	-2.35	121.07	126.39
33	S	212	KC1	CHC-C4B-C3B	2.35	129.17	125.21
25	A	841	BCR	C27-C26-C25	2.35	125.88	122.70
22	U	206	CLA	CHD-C1D-ND	-2.35	121.50	124.80
31	S	211	DD6	C-C1-C2	-2.35	119.02	122.82
31	O	212	DD6	C4-C5-C6	2.35	130.57	127.28
31	O	212	DD6	C-C1-C2	-2.34	119.02	122.82
25	I	101	BCR	C29-C30-C25	2.34	113.84	110.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	Q	210	KC1	C1A-C2A-C3A	-2.34	105.13	107.28
22	A	823	CLA	CHD-C1D-ND	-2.34	121.50	124.80
22	A	830	CLA	CHD-C1D-ND	-2.34	121.51	124.80
25	B	837	BCR	C28-C27-C26	-2.34	109.88	114.06
25	B	837	BCR	C15-C16-C17	-2.34	118.73	123.52
25	R	102	BCR	C33-C5-C6	-2.34	121.93	124.48
31	P	220	DD6	C26-C25-C24	2.34	129.97	123.20
22	B	818	CLA	CHD-C1D-ND	-2.33	121.52	124.80
33	P	212	KC1	C1B-CHB-C4A	2.33	130.98	126.02
22	T	211	CLA	CHD-C1D-C2D	2.33	130.34	125.49
25	B	839	BCR	C2-C1-C6	2.33	113.82	110.44
22	H	202	CLA	CMD-C2D-C1D	2.33	128.83	124.73
29	B	841	DGD	O6D-C1D-O3G	-2.33	104.55	110.04
25	B	838	BCR	C2-C1-C6	2.33	113.82	110.44
22	A	811	CLA	CHD-C1D-ND	-2.33	121.53	124.80
31	S	205	DD6	C24-C1-C2	2.32	122.67	119.01
22	S	209	CLA	CHD-C1D-C2D	2.32	130.32	125.49
22	A	836	CLA	CHD-C1D-ND	-2.32	121.53	124.80
22	B	844	CLA	CHD-C1D-ND	-2.32	121.53	124.80
22	U	204	CLA	O2A-C1-C2	2.32	117.05	108.11
32	Q	217	LMG	O1-C7-C8	-2.32	105.17	110.82
22	B	832	CLA	C4A-NA-C1A	2.32	107.74	106.68
22	U	210	CLA	C4A-NA-C1A	2.32	107.74	106.68
32	P	202	LMG	C1-O6-C5	-2.32	109.19	113.72
22	A	801	CLA	CHD-C1D-ND	-2.32	121.54	124.80
22	O	207	CLA	C1-O2A-CGA	2.32	123.49	116.07
25	A	844	BCR	C29-C30-C25	2.32	113.80	110.44
25	A	843	BCR	C28-C27-C26	-2.32	109.93	114.06
31	G	214	DD6	C3-C2-C1	2.31	130.52	127.28
31	U	214	DD6	C33-C32-C31	2.31	114.05	109.49
22	A	822	CLA	CHD-C1D-C2D	2.31	130.30	125.49
34	Q	218	A86	C28-C27-C26	-2.31	119.07	122.82
22	Q	212	CLA	CHD-C1D-ND	-2.31	121.55	124.80
22	A	810	CLA	CHD-C1D-ND	-2.31	121.55	124.80
31	O	213	DD6	C8-C6-C5	2.31	122.64	119.01
22	Q	207	CLA	C1-O2A-CGA	2.31	123.47	116.07
22	Q	204	CLA	CHD-C1D-C2D	2.31	130.29	125.49
34	Q	201	A86	C28-C27-C26	-2.31	119.08	122.82
22	B	827	CLA	C1D-ND-C4D	2.31	107.93	106.31
32	S	213	LMG	C40-C39-C38	-2.31	102.71	114.37
22	A	838	CLA	C4A-NA-C1A	2.31	107.73	106.68
31	P	215	DD6	C22-C16-C17	-2.31	104.92	108.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	H	210	CLA	CAA-CBA-CGA	2.31	118.64	112.49
26	K	201	LMU	C1-O1'-C1'	-2.30	109.74	113.68
22	Q	205	CLA	CHD-C1D-ND	-2.30	121.56	124.80
31	H	212	DD6	C33-C32-C31	2.30	114.03	109.49
22	S	216	CLA	CHD-C1D-C2D	2.30	130.27	125.49
29	B	841	DGD	CFB-CEB-CDB	-2.30	102.74	114.37
30	B	846	SQD	C4-C3-C2	2.30	114.86	110.83
31	H	212	DD6	C12-C11-C13	2.30	121.59	118.09
22	B	808	CLA	C4A-NA-C1A	2.29	107.73	106.68
22	B	802	CLA	CAC-C3C-C4C	2.29	127.77	124.79
33	P	212	KC1	C1A-C2A-C3A	-2.29	105.17	107.28
22	A	834	CLA	CHD-C1D-ND	-2.29	121.58	124.80
31	G	214	DD6	C10-C9-C8	2.29	129.84	123.20
25	R	102	BCR	C27-C26-C25	2.29	125.80	122.70
22	A	829	CLA	CHD-C1D-C2D	2.29	130.25	125.49
31	U	203	DD6	C22-C16-C17	-2.29	104.95	108.97
22	S	202	CLA	C4A-NA-C1A	2.29	107.72	106.68
24	G	216	LHG	O8-C23-C24	2.29	118.81	111.83
22	B	845	CLA	CGD-CBD-CAD	-2.28	103.45	110.85
22	A	838	CLA	CHD-C1D-ND	-2.28	121.59	124.80
22	B	834	CLA	O2A-C1-C2	2.28	116.88	108.11
22	B	826	CLA	CHD-C1D-ND	-2.28	121.60	124.80
22	A	846	CLA	CHD-C1D-ND	-2.27	121.60	124.80
33	S	210	KC1	CHC-C4B-NB	-2.27	121.60	124.80
34	R	103	A86	O3-C36-C35	-2.27	104.05	107.70
22	H	202	CLA	C2A-C1A-CHA	2.27	126.23	122.71
22	O	202	CLA	C1D-ND-C4D	2.27	107.91	106.31
25	A	844	BCR	C11-C10-C9	-2.27	124.09	127.28
22	H	206	CLA	CHD-C1D-ND	-2.27	121.61	124.80
33	O	210	KC1	C1A-C2A-C3A	-2.27	105.20	107.28
22	A	851	CLA	CHD-C1D-ND	-2.27	121.61	124.80
31	S	214	DD6	C9-C8-C6	2.27	132.57	126.36
22	S	208	CLA	CHD-C1D-C2D	2.26	130.20	125.49
22	B	829	CLA	CHD-C1D-ND	-2.26	121.62	124.80
31	O	201	DD6	C26-C25-C24	2.26	129.76	123.20
31	H	211	DD6	C13-C11-C10	2.26	122.57	119.01
22	A	835	CLA	CHD-C1D-ND	-2.26	121.62	124.80
22	B	818	CLA	C2A-C1A-CHA	2.26	127.79	123.87
22	R	104	CLA	CHD-C1D-ND	-2.26	121.63	124.80
22	P	214	CLA	CHD-C1D-C2D	2.25	130.18	125.49
22	B	832	CLA	CHD-C1D-ND	-2.25	121.63	124.80
22	A	825	CLA	CHD-C1D-ND	-2.25	121.64	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	P	217	LMG	C6-C5-C4	-2.25	107.50	113.02
22	B	817	CLA	CHD-C1D-C2D	2.25	130.16	125.49
22	H	207	CLA	CAA-C2A-C3A	2.25	119.07	113.00
22	P	211	CLA	CHD-C1D-ND	-2.25	121.64	124.80
31	Q	202	DD6	O1-C20-C19	-2.25	111.39	113.49
22	B	810	CLA	CHD-C1D-C2D	2.25	130.16	125.49
32	Q	217	LMG	O3-C3-C2	-2.24	105.08	110.38
25	B	839	BCR	C8-C7-C6	-2.24	121.00	127.00
31	G	212	DD6	C26-C25-C24	2.24	129.70	123.20
34	P	204	A86	C28-C27-C26	-2.24	119.18	122.82
31	S	204	DD6	C26-C25-C24	2.24	129.69	123.20
22	A	803	CLA	CHD-C1D-C2D	2.24	130.15	125.49
25	F	805	BCR	C11-C10-C9	-2.24	124.14	127.28
22	A	831	CLA	CHD-C1D-C2D	2.24	130.14	125.49
31	O	214	DD6	C10-C9-C8	2.24	129.69	123.20
25	B	838	BCR	C30-C25-C26	-2.24	119.58	122.64
32	S	213	LMG	O3-C3-C2	-2.23	105.11	110.38
34	R	103	A86	C22-C16-C17	-2.23	105.04	108.97
31	G	212	DD6	C13-C11-C10	2.23	122.52	119.01
22	B	819	CLA	C2A-C1A-CHA	2.23	127.74	123.87
25	k	104	BCR	C15-C14-C13	-2.23	124.15	127.28
22	A	820	CLA	CHD-C1D-C2D	2.23	130.13	125.49
25	M	101	BCR	C24-C23-C22	-2.23	122.94	126.23
22	T	207	CLA	CHD-C1D-C2D	2.23	130.12	125.49
22	A	854	CLA	C4A-NA-C1A	2.23	107.70	106.68
22	F	802	CLA	CHD-C1D-ND	-2.23	121.67	124.80
22	B	808	CLA	C1D-ND-C4D	2.23	107.88	106.31
22	G	202	CLA	CAA-C2A-C3A	-2.23	111.13	116.23
22	K	206	CLA	CHD-C1D-ND	-2.22	121.67	124.80
22	U	207	CLA	C3A-C2A-C1A	-2.22	98.01	101.34
31	O	215	DD6	C23-C16-C17	-2.22	105.07	108.97
22	K	204	CLA	C3B-C4B-NB	-2.22	108.55	110.53
22	T	205	CLA	CHD-C1D-C2D	2.22	130.10	125.49
24	P	201	LHG	C20-C19-C18	-2.22	103.17	114.37
31	G	214	DD6	C13-C11-C10	2.22	122.50	119.01
34	R	105	A86	C23-C16-C17	-2.22	105.07	108.97
22	P	216	CLA	CHD-C1D-ND	-2.21	121.69	124.80
32	P	217	LMG	O6-C1-O1	-2.21	104.81	110.04
22	Q	213	CLA	C4A-NA-C1A	2.21	107.69	106.68
22	G	208	CLA	C4A-NA-C1A	2.21	107.69	106.68
25	A	842	BCR	C15-C16-C17	-2.21	118.99	123.52
34	R	105	A86	C28-C27-C26	-2.21	119.23	122.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	S	213	LMG	C38-C37-C36	-2.21	103.18	114.37
22	U	207	CLA	CHD-C1D-C2D	2.21	130.09	125.49
22	B	814	CLA	C3B-C4B-NB	-2.21	108.56	110.53
31	P	205	DD6	C33-C32-C31	2.21	113.85	109.49
22	H	205	CLA	CHD-C1D-ND	-2.21	121.69	124.80
25	B	836	BCR	C28-C27-C26	-2.21	110.12	114.06
31	T	213	DD6	C26-C25-C24	2.21	129.60	123.20
22	A	807	CLA	CHD-C1D-ND	-2.21	121.69	124.80
22	A	804	CLA	C1D-ND-C4D	2.21	107.86	106.31
25	k	104	BCR	C3-C4-C5	-2.21	110.12	114.06
22	A	814	CLA	C4A-NA-C1A	2.21	107.69	106.68
26	K	202	LMU	C1B-O5B-C5B	2.21	118.03	113.72
22	A	813	CLA	CHD-C1D-C2D	2.21	130.07	125.49
22	P	207	CLA	CHD-C1D-C2D	2.21	130.07	125.49
22	B	803	CLA	CHD-C1D-ND	-2.21	121.70	124.80
22	A	818	CLA	CHC-C1C-NC	2.20	127.63	124.31
22	B	804	CLA	CHD-C1D-C2D	2.20	130.07	125.49
22	A	812	CLA	CHD-C1D-ND	-2.20	121.70	124.80
26	A	857	LMU	O1'-C1'-C2'	2.20	111.62	108.27
22	U	207	CLA	C2A-C3A-C4A	-2.20	98.31	101.87
24	A	839	LHG	C27-C26-C25	-2.20	103.24	114.37
22	K	205	CLA	CHD-C1D-C2D	2.20	130.06	125.49
32	Q	217	LMG	C40-C39-C38	-2.20	103.25	114.37
25	L	201	BCR	C33-C5-C6	-2.20	122.08	124.48
22	H	204	CLA	CHD-C1D-C2D	2.20	130.06	125.49
22	O	209	CLA	O2D-CGD-CBD	2.20	115.07	111.23
22	Q	208	CLA	CHD-C1D-ND	-2.20	121.71	124.80
22	B	820	CLA	CHD-C1D-C2D	2.19	130.05	125.49
30	S	201	SQD	O8-S-C6	2.19	110.21	105.97
22	A	834	CLA	C4A-NA-C1A	2.19	107.68	106.68
22	H	208	CLA	CHD-C1D-C2D	2.19	130.05	125.49
22	Q	212	CLA	C2A-C1A-CHA	2.19	127.67	123.87
22	Q	207	CLA	CHD-C1D-C2D	2.19	130.04	125.49
33	P	212	KC1	CBA-CAA-C2A	2.19	134.25	125.45
22	k	102	CLA	CHD-C1D-ND	-2.19	121.72	124.80
31	U	212	DD6	C26-C25-C24	2.19	129.54	123.20
22	S	217	CLA	C4A-NA-C1A	2.19	107.68	106.68
29	B	841	DGD	CAB-C9B-C8B	-2.19	103.31	114.37
26	F	806	LMU	O1B-C4'-C3'	2.19	112.79	107.23
22	F	803	CLA	CHD-C1D-ND	-2.19	121.72	124.80
22	A	848	CLA	CHD-C1D-C2D	2.18	130.03	125.49
22	A	855	CLA	C2A-C1A-CHA	2.18	126.10	122.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	O	212	DD6	C24-C1-C2	2.18	122.44	119.01
22	B	819	CLA	CHD-C1D-ND	-2.18	121.73	124.80
22	H	207	CLA	C1-O2A-CGA	-2.18	111.37	116.65
25	A	842	BCR	C15-C14-C13	-2.18	124.22	127.28
22	K	207	CLA	CHD-C1D-C2D	2.18	130.02	125.49
22	U	210	CLA	CHD-C1D-C2D	2.18	130.02	125.49
22	B	827	CLA	CHD-C1D-ND	-2.18	121.74	124.80
32	Q	217	LMG	C38-C37-C36	-2.18	103.37	114.37
22	L	204	CLA	CHD-C1D-C2D	2.18	130.01	125.49
25	B	837	BCR	C29-C30-C25	2.17	113.60	110.44
22	B	802	CLA	C4A-NA-C1A	2.17	107.67	106.68
33	T	208	KC1	CBA-CAA-C2A	2.17	134.18	125.45
22	B	812	CLA	CHD-C1D-C2D	2.17	130.00	125.49
31	Q	202	DD6	C26-C25-C24	2.17	129.49	123.20
22	A	817	CLA	CHD-C1D-ND	-2.17	121.75	124.80
22	O	208	CLA	CHD-C1D-C2D	2.17	130.00	125.49
22	O	209	CLA	CHD-C1D-ND	-2.17	121.75	124.80
22	O	205	CLA	CHD-C1D-C2D	2.17	130.00	125.49
32	J	102	LMG	O3-C3-C2	-2.17	105.27	110.38
33	P	206	KC1	CBA-CAA-C2A	2.16	134.15	125.45
26	K	202	LMU	O5'-C5'-C4'	2.16	114.20	109.72
22	B	831	CLA	C4A-NA-C1A	2.16	107.67	106.68
22	B	802	CLA	C2A-C1A-CHA	2.16	127.62	123.87
22	U	211	CLA	CHD-C1D-ND	-2.16	121.76	124.80
22	A	854	CLA	CHD-C1D-C2D	2.16	129.98	125.49
22	B	811	CLA	CHD-C1D-C2D	2.16	129.97	125.49
22	L	203	CLA	CHD-C1D-C2D	2.16	129.97	125.49
22	B	815	CLA	CHD-C1D-C2D	2.15	129.97	125.49
32	S	213	LMG	C6-C5-C4	-2.15	107.73	113.02
22	S	207	CLA	C4A-NA-C1A	2.15	107.66	106.68
22	U	208	CLA	O2D-CGD-CBD	2.15	115.00	111.23
24	P	201	LHG	C27-C26-C25	-2.15	103.48	114.37
22	Q	213	CLA	CHD-C1D-C2D	2.15	129.97	125.49
30	S	201	SQD	C4-C3-C2	2.15	114.61	110.83
25	R	102	BCR	C40-C30-C39	-2.15	102.47	108.63
22	P	216	CLA	C1D-ND-C4D	2.15	107.82	106.31
22	Q	203	CLA	CHD-C1D-C2D	2.15	129.96	125.49
22	B	805	CLA	C4A-NA-C1A	2.15	107.66	106.68
22	H	210	CLA	CHD-C1D-C2D	2.15	129.96	125.49
31	K	208	DD6	C13-C11-C10	2.15	122.39	119.01
34	R	103	A86	C8-C6-C5	2.15	122.39	119.01
22	T	202	CLA	CHD-C1D-C2D	2.15	129.96	125.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	G	214	DD6	C33-C32-C31	2.15	113.72	109.49
25	B	838	BCR	C31-C1-C6	2.15	113.61	110.24
33	S	212	KC1	O2D-CGD-CBD	2.15	114.98	111.23
22	B	828	CLA	C1D-ND-C4D	2.14	107.82	106.31
25	I	101	BCR	C10-C11-C12	-2.14	116.98	123.20
22	A	805	CLA	CHD-C1D-C2D	2.14	129.95	125.49
22	B	834	CLA	C4A-NA-C1A	2.14	107.66	106.68
22	A	820	CLA	O2D-CGD-CBD	2.14	114.98	111.23
33	Q	210	KC1	CHC-C4B-NB	-2.14	121.79	124.80
31	P	218	DD6	C12-C11-C10	-2.14	119.34	122.82
22	B	834	CLA	C1D-ND-C4D	2.14	107.81	106.31
25	J	104	BCR	C15-C16-C17	-2.14	119.14	123.52
22	R	101	CLA	C1D-ND-C4D	2.14	107.81	106.31
25	F	805	BCR	C16-C15-C14	-2.14	119.14	123.52
22	O	206	CLA	CHD-C1D-C2D	2.14	129.93	125.49
25	B	840	BCR	C15-C16-C17	-2.14	119.15	123.52
31	k	101	DD6	C26-C25-C24	2.14	129.39	123.20
22	G	208	CLA	CHD-C1D-C2D	2.13	129.92	125.49
22	A	821	CLA	C2A-C1A-CHA	2.13	127.57	123.87
22	B	808	CLA	CHD-C1D-ND	-2.13	121.80	124.80
22	H	213	CLA	CHD-C1D-C2D	2.13	129.92	125.49
22	A	813	CLA	C3B-C4B-NB	-2.13	108.63	110.53
26	F	806	LMU	C6B-C5B-C4B	-2.13	107.79	113.02
22	B	816	CLA	CHD-C1D-ND	-2.13	121.81	124.80
33	Q	210	KC1	CHC-C4B-C3B	2.13	128.80	125.21
32	P	217	LMG	O2-C2-C1	-2.13	105.01	110.08
22	T	209	CLA	CHD-C1D-C2D	2.12	129.91	125.49
22	O	206	CLA	C4A-NA-C1A	2.12	107.65	106.68
22	T	204	CLA	CHD-C1D-C2D	2.12	129.90	125.49
26	K	201	LMU	C1'-O5'-C5'	-2.12	109.58	113.72
22	B	842	CLA	CHD-C1D-ND	-2.12	121.82	124.80
22	Q	216	CLA	CHD-C1D-C2D	2.12	129.90	125.49
22	G	210	CLA	CHD-C1D-ND	-2.12	121.82	124.80
22	T	210	CLA	C4A-NA-C1A	2.12	107.65	106.68
22	A	814	CLA	C3B-C4B-NB	-2.12	108.64	110.53
22	B	822	CLA	CHD-C1D-ND	-2.12	121.82	124.80
31	Q	215	DD6	C22-C16-C17	-2.12	105.25	108.97
22	S	206	CLA	CHD-C1D-C2D	2.12	129.89	125.49
22	A	804	CLA	C4A-NA-C1A	2.12	107.64	106.68
22	A	845	CLA	CHD-C1D-ND	-2.12	121.82	124.80
22	Q	213	CLA	O2D-CGD-CBD	2.12	114.93	111.23
31	H	212	DD6	C23-C16-C17	-2.12	105.25	108.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	P	218	DD6	C26-C25-C24	2.12	129.33	123.20
34	P	204	A86	C35-C34-C33	2.11	113.68	109.89
22	B	802	CLA	C1D-ND-C4D	2.11	107.80	106.31
31	Q	215	DD6	C33-C32-C31	2.11	113.65	109.49
31	U	212	DD6	C34-C35-C36	2.11	117.44	112.18
31	k	101	DD6	C12-C11-C13	2.11	121.31	118.09
22	P	210	CLA	CHD-C1D-C2D	2.11	129.87	125.49
22	H	209	CLA	CAA-C2A-C3A	-2.11	111.39	116.23
29	B	841	DGD	O2D-C2D-C1D	-2.11	105.05	110.08
22	H	207	CLA	CHD-C1D-C2D	2.11	129.87	125.49
22	T	209	CLA	CAA-C2A-C3A	-2.11	111.40	116.23
22	H	203	CLA	C4A-NA-C1A	2.11	107.64	106.68
22	G	205	CLA	C2A-C3A-C4A	-2.11	98.47	101.87
33	Q	210	KC1	CMD-C2D-C1D	2.10	128.62	125.42
25	L	205	BCR	C15-C14-C13	-2.10	124.33	127.28
22	A	818	CLA	CHD-C1D-C2D	2.10	129.86	125.49
22	B	821	CLA	CHD-C1D-ND	-2.10	121.84	124.80
22	U	208	CLA	CHD-C1D-C2D	2.10	129.86	125.49
22	B	805	CLA	CHD-C1D-ND	-2.10	121.84	124.80
22	A	833	CLA	CHD-C1D-C2D	2.10	129.86	125.49
32	P	202	LMG	O6-C1-O1	-2.10	105.08	110.04
22	A	801	CLA	C2A-C1A-CHA	2.10	127.51	123.87
22	O	207	CLA	CHD-C1D-C2D	2.10	129.85	125.49
22	A	827	CLA	C4A-NA-C1A	2.10	107.64	106.68
22	A	854	CLA	C1D-ND-C4D	2.09	107.78	106.31
24	A	839	LHG	C18-C17-C16	-2.09	103.79	114.37
22	A	832	CLA	CAA-C2A-C1A	2.09	118.83	111.97
32	Q	217	LMG	C42-C41-C40	-2.09	103.80	114.37
22	O	204	CLA	C1D-ND-C4D	2.09	107.78	106.31
22	A	816	CLA	CHD-C1D-C2D	2.09	129.84	125.49
32	J	102	LMG	C9-C8-C7	-2.09	106.91	111.78
31	G	214	DD6	C4-C3-C2	2.09	127.79	123.52
34	P	204	A86	C23-C16-C17	-2.09	105.30	108.97
25	k	104	BCR	C40-C30-C25	2.09	113.52	110.24
25	R	102	BCR	C7-C8-C9	-2.09	123.15	126.23
32	J	102	LMG	C1-C2-C3	-2.08	105.63	110.01
22	A	802	CLA	CHD-C1D-C2D	2.08	129.82	125.49
25	R	102	BCR	C24-C23-C22	-2.08	123.16	126.23
25	A	844	BCR	C15-C14-C13	-2.08	124.36	127.28
22	B	801	CLA	C2A-C1A-CHA	2.08	127.47	123.87
22	A	814	CLA	CHD-C1D-C2D	2.08	129.81	125.49
22	A	856	CLA	CHD-C1D-C2D	2.08	129.81	125.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	P	202	LMG	O1-C7-C8	-2.08	105.77	110.82
22	G	203	CLA	CHD-C1D-ND	-2.08	121.88	124.80
22	K	203	CLA	CHC-C4B-NB	-2.08	120.94	124.05
22	B	845	CLA	CHD-C1D-C2D	2.08	129.80	125.49
33	O	210	KC1	CHB-C4A-NA	2.08	127.45	124.23
33	U	213	KC1	C1B-CHB-C4A	2.08	130.43	126.02
22	G	202	CLA	CHD-C1D-C2D	2.07	129.80	125.49
31	G	214	DD6	C28-C27-C26	-2.07	120.16	124.18
25	I	101	BCR	C28-C27-C26	-2.07	110.36	114.06
31	O	213	DD6	C12-C11-C13	2.07	121.25	118.09
22	T	202	CLA	CAA-C2A-C3A	-2.07	111.48	116.23
22	H	203	CLA	CHD-C1D-C2D	2.07	129.80	125.49
26	K	202	LMU	O3'-C3'-C2'	-2.07	105.50	110.38
26	K	202	LMU	C3'-C4'-C5'	2.07	115.51	110.93
22	P	208	CLA	CHD-C1D-C2D	2.07	129.79	125.49
22	A	827	CLA	CHD-C1D-ND	-2.07	121.89	124.80
22	A	809	CLA	CHD-C1D-C2D	2.07	129.78	125.49
25	B	836	BCR	C27-C26-C25	2.07	125.50	122.70
22	G	206	CLA	O2D-CGD-CBD	2.07	114.84	111.23
33	S	212	KC1	CHC-C4B-NB	-2.07	121.90	124.80
22	A	836	CLA	C1D-ND-C4D	2.07	107.76	106.31
22	A	850	CLA	CHD-C1D-C2D	2.06	129.78	125.49
31	S	211	DD6	O1-C20-C19	-2.06	111.56	113.49
22	B	821	CLA	C4A-NA-C1A	2.06	107.62	106.68
33	U	213	KC1	CBA-CAA-C2A	2.06	133.72	125.45
31	H	201	DD6	C13-C11-C10	2.06	122.25	119.01
22	B	802	CLA	CHD-C1D-ND	-2.06	121.91	124.80
29	B	841	DGD	CBB-CAB-C9B	-2.06	103.97	114.37
22	B	809	CLA	CHD-C1D-C2D	2.06	129.76	125.49
22	K	203	CLA	C3D-C4D-ND	-2.06	106.64	109.99
22	U	208	CLA	C3B-C4B-NB	-2.05	108.70	110.53
33	O	210	KC1	CBA-CAA-C2A	2.05	133.70	125.45
32	S	213	LMG	O2-C2-C1	-2.05	105.18	110.08
22	A	855	CLA	CHD-C1D-C2D	2.05	129.76	125.49
32	U	201	LMG	O3-C3-C2	-2.05	105.54	110.38
22	G	205	CLA	CHD-C1D-C2D	2.05	129.75	125.49
22	P	209	CLA	C4A-NA-C1A	2.05	107.61	106.68
22	A	838	CLA	O2D-CGD-CBD	2.05	114.82	111.23
22	B	827	CLA	CAA-C2A-C1A	2.05	118.69	111.97
22	R	104	CLA	O2D-CGD-CBD	2.05	114.81	111.23
22	B	823	CLA	CHD-C1D-C2D	2.05	129.75	125.49
22	T	210	CLA	CHD-C1D-C2D	2.05	129.75	125.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	P	203	KC1	C1A-C2A-C3A	-2.05	105.40	107.28
22	S	208	CLA	C2A-C1A-CHA	2.05	127.42	123.87
22	P	211	CLA	O2D-CGD-CBD	2.05	114.81	111.23
22	A	815	CLA	CHD-C1D-C2D	2.05	129.74	125.49
22	R	104	CLA	C4A-NA-C1A	2.04	107.61	106.68
31	K	208	DD6	C34-C35-C36	2.04	117.26	112.18
31	O	212	DD6	C3-C2-C1	2.04	130.14	127.28
22	T	207	CLA	O2D-CGD-CBD	2.04	114.80	111.23
31	O	201	DD6	C23-C16-C17	-2.04	105.39	108.97
25	I	101	BCR	C15-C16-C17	-2.04	119.35	123.52
22	G	210	CLA	O2D-CGD-CBD	2.04	114.79	111.23
22	F	804	CLA	CHD-C1D-C2D	2.03	129.72	125.49
22	A	828	CLA	CHD-C1D-ND	-2.03	121.94	124.80
22	O	207	CLA	C3B-C4B-NB	-2.03	108.72	110.53
31	P	220	DD6	C28-C27-C26	-2.03	120.24	124.18
22	B	830	CLA	CHD-C1D-C2D	2.03	129.71	125.49
22	S	207	CLA	O2D-CGD-CBD	2.03	114.78	111.23
25	A	844	BCR	C33-C5-C6	-2.03	122.27	124.48
31	P	218	DD6	C23-C16-C17	-2.03	105.40	108.97
22	G	201	CLA	CHD-C1D-C2D	2.03	129.71	125.49
22	B	818	CLA	CHD-C1D-C2D	2.03	129.71	125.49
25	A	843	BCR	C16-C15-C14	-2.03	119.37	123.52
31	H	211	DD6	C33-C32-C31	2.02	113.48	109.49
34	Q	201	A86	C10-C9-C8	2.02	129.07	123.20
31	P	220	DD6	C33-C32-C31	2.02	113.47	109.49
22	B	810	CLA	C1D-ND-C4D	2.02	107.73	106.31
30	S	201	SQD	C44-O6-C1	2.02	118.13	113.80
22	K	204	CLA	CHD-C1D-C2D	2.02	129.69	125.49
33	U	213	KC1	CGD-CBD-CAD	-2.02	104.31	110.85
22	J	103	CLA	CHD-C1D-C2D	2.02	129.69	125.49
22	F	803	CLA	C1D-ND-C4D	2.02	107.73	106.31
22	L	202	CLA	CHD-C1D-C2D	2.02	129.68	125.49
22	S	217	CLA	C6-C5-C3	2.02	118.38	113.47
22	L	204	CLA	O2D-CGD-CBD	2.02	114.75	111.23
22	T	205	CLA	O2D-CGD-CBD	2.02	114.75	111.23
22	K	207	CLA	C3B-C4B-NB	-2.02	108.73	110.53
22	G	206	CLA	CHD-C1D-ND	-2.01	121.97	124.80
22	A	826	CLA	CHD-C1D-ND	-2.01	121.97	124.80
22	B	825	CLA	CHD-C1D-C2D	2.01	129.68	125.49
22	G	209	CLA	CAC-C3C-C4C	2.01	127.41	124.79
22	G	208	CLA	C3B-C4B-NB	-2.01	108.73	110.53
22	A	825	CLA	C1D-ND-C4D	2.01	107.72	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	R	101	CLA	CHD-C1D-ND	-2.01	121.97	124.80
33	S	210	KC1	CHB-C4A-NA	2.01	127.35	124.23
31	H	212	DD6	C26-C25-C24	2.01	129.03	123.20
22	B	807	CLA	CHD-C1D-ND	-2.01	121.97	124.80
25	B	838	BCR	C15-C14-C13	-2.01	124.46	127.28
31	S	205	DD6	C23-C16-C15	2.01	115.47	110.05
33	P	219	KC1	CMD-C2D-C1D	2.01	128.47	125.42
22	Q	207	CLA	CMD-C2D-C1D	2.01	128.26	124.73
25	B	838	BCR	C40-C30-C25	2.01	113.39	110.24
22	G	205	CLA	C1D-ND-C4D	2.01	107.72	106.31
27	A	849	CL0	CGD-CBD-CAD	-2.01	104.35	110.85
22	P	209	CLA	CHD-C1D-C2D	2.01	129.66	125.49
22	U	211	CLA	CAA-C2A-C1A	2.01	118.55	111.97
22	B	828	CLA	CHD-C1D-C2D	2.01	129.66	125.49
25	F	805	BCR	C35-C13-C14	-2.00	119.57	122.82
26	O	216	LMU	O5'-C5'-C4'	2.00	113.86	109.72
22	A	804	CLA	CHD-C1D-C2D	2.00	129.65	125.49
22	B	845	CLA	C2A-C1A-CHA	2.00	127.34	123.87
31	G	212	DD6	C28-C27-C26	-2.00	120.30	124.18

All (119) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
22	A	802	CLA	ND
22	A	803	CLA	ND
22	A	804	CLA	ND
22	A	805	CLA	ND
22	A	806	CLA	ND
22	A	809	CLA	ND
22	A	810	CLA	ND
22	A	811	CLA	ND
22	A	812	CLA	ND
22	A	815	CLA	ND
22	A	816	CLA	ND
22	A	817	CLA	ND
22	A	818	CLA	ND
22	A	820	CLA	ND
22	A	821	CLA	ND
22	A	822	CLA	ND
22	A	823	CLA	ND
22	A	824	CLA	ND
22	A	825	CLA	ND

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Mol	Chain	Res	Type	Atom
22	A	828	CLA	ND
22	A	829	CLA	ND
22	A	831	CLA	ND
22	A	832	CLA	ND
22	A	833	CLA	ND
22	A	835	CLA	ND
22	A	836	CLA	ND
22	A	838	CLA	ND
22	A	845	CLA	ND
22	A	850	CLA	ND
22	A	853	CLA	ND
22	A	854	CLA	ND
22	A	855	CLA	ND
22	A	856	CLA	ND
22	B	801	CLA	ND
22	B	802	CLA	ND
22	B	803	CLA	ND
22	B	804	CLA	ND
22	B	805	CLA	ND
22	B	807	CLA	ND
22	B	808	CLA	ND
22	B	811	CLA	ND
22	B	815	CLA	ND
22	B	816	CLA	ND
22	B	819	CLA	ND
22	B	820	CLA	ND
22	B	821	CLA	ND
22	B	822	CLA	ND
22	B	826	CLA	ND
22	B	828	CLA	ND
22	B	829	CLA	ND
22	B	830	CLA	ND
22	B	831	CLA	ND
22	B	832	CLA	ND
22	B	834	CLA	ND
22	B	842	CLA	ND
22	B	843	CLA	ND
22	B	844	CLA	ND
22	B	845	CLA	ND
22	B	847	CLA	ND
22	F	802	CLA	ND
22	F	803	CLA	ND

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Mol	Chain	Res	Type	Atom
22	F	804	CLA	ND
22	J	103	CLA	ND
22	L	204	CLA	ND
22	O	205	CLA	ND
22	O	206	CLA	ND
22	O	207	CLA	ND
22	O	208	CLA	ND
22	P	207	CLA	ND
22	P	208	CLA	ND
22	P	209	CLA	ND
22	P	213	CLA	ND
22	P	214	CLA	ND
22	P	216	CLA	ND
22	Q	204	CLA	ND
22	Q	205	CLA	ND
22	Q	206	CLA	ND
22	Q	207	CLA	ND
22	Q	208	CLA	ND
22	Q	211	CLA	ND
22	Q	213	CLA	ND
22	R	101	CLA	ND
22	S	202	CLA	ND
22	S	206	CLA	ND
22	S	207	CLA	ND
22	S	208	CLA	ND
22	S	216	CLA	ND
22	S	217	CLA	ND
22	U	204	CLA	ND
22	U	206	CLA	ND
22	U	207	CLA	ND
22	U	208	CLA	ND
22	U	211	CLA	ND
22	G	202	CLA	ND
22	G	203	CLA	ND
22	G	206	CLA	ND
22	G	208	CLA	ND
22	G	209	CLA	ND
22	G	210	CLA	ND
22	G	215	CLA	ND
22	H	202	CLA	ND
22	H	203	CLA	ND
22	H	204	CLA	ND

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Mol	Chain	Res	Type	Atom
22	H	205	CLA	ND
22	H	206	CLA	ND
22	H	208	CLA	ND
22	H	209	CLA	ND
22	H	213	CLA	ND
22	K	203	CLA	ND
22	K	205	CLA	ND
22	K	206	CLA	ND
22	T	201	CLA	ND
22	T	202	CLA	ND
22	T	203	CLA	ND
22	T	204	CLA	ND
22	T	205	CLA	ND
22	T	211	CLA	ND
22	k	102	CLA	ND
22	k	103	CLA	ND

All (1495) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	A	803	CLA	CAD-CBD-CGD-O2D
22	A	804	CLA	C1A-C2A-CAA-CBA
22	A	804	CLA	C3A-C2A-CAA-CBA
22	A	806	CLA	CBA-CGA-O2A-C1
22	A	806	CLA	O1A-CGA-O2A-C1
22	A	806	CLA	CHA-CBD-CGD-O1D
22	A	806	CLA	CHA-CBD-CGD-O2D
22	A	815	CLA	C3A-C2A-CAA-CBA
22	A	820	CLA	CBD-CGD-O2D-CED
22	A	820	CLA	O1D-CGD-O2D-CED
22	A	820	CLA	C4-C3-C5-C6
22	A	821	CLA	CHA-CBD-CGD-O1D
22	A	821	CLA	CHA-CBD-CGD-O2D
22	A	826	CLA	CHA-CBD-CGD-O1D
22	A	826	CLA	CHA-CBD-CGD-O2D
22	A	829	CLA	CHA-CBD-CGD-O1D
22	A	829	CLA	CHA-CBD-CGD-O2D
22	A	838	CLA	CBD-CGD-O2D-CED
22	A	838	CLA	O1D-CGD-O2D-CED
22	A	853	CLA	CHA-CBD-CGD-O1D
22	A	853	CLA	CHA-CBD-CGD-O2D
22	A	856	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
22	B	803	CLA	CHA-CBD-CGD-O2D
22	B	807	CLA	CHA-CBD-CGD-O1D
22	B	807	CLA	CHA-CBD-CGD-O2D
22	B	819	CLA	CHA-CBD-CGD-O1D
22	B	819	CLA	CHA-CBD-CGD-O2D
22	B	820	CLA	CHA-CBD-CGD-O1D
22	B	820	CLA	CHA-CBD-CGD-O2D
22	B	823	CLA	CBA-CGA-O2A-C1
22	B	823	CLA	O1A-CGA-O2A-C1
22	B	824	CLA	CHA-CBD-CGD-O1D
22	B	824	CLA	CHA-CBD-CGD-O2D
22	B	845	CLA	C1A-C2A-CAA-CBA
22	B	847	CLA	C1A-C2A-CAA-CBA
22	B	847	CLA	C3A-C2A-CAA-CBA
22	F	803	CLA	CBA-CGA-O2A-C1
22	F	803	CLA	O1A-CGA-O2A-C1
22	F	804	CLA	C1A-C2A-CAA-CBA
22	J	103	CLA	CAD-CBD-CGD-O2D
22	L	202	CLA	C1A-C2A-CAA-CBA
22	L	202	CLA	CBA-CGA-O2A-C1
22	L	202	CLA	O1A-CGA-O2A-C1
22	L	204	CLA	CBD-CGD-O2D-CED
22	L	204	CLA	O1D-CGD-O2D-CED
22	O	205	CLA	CHA-CBD-CGD-O1D
22	O	205	CLA	CHA-CBD-CGD-O2D
22	O	209	CLA	CBD-CGD-O2D-CED
22	O	209	CLA	O1D-CGD-O2D-CED
22	P	208	CLA	C1A-C2A-CAA-CBA
22	P	210	CLA	CHA-CBD-CGD-O1D
22	P	210	CLA	CHA-CBD-CGD-O2D
22	P	211	CLA	CBD-CGD-O2D-CED
22	P	211	CLA	O1D-CGD-O2D-CED
22	P	213	CLA	CBD-CGD-O2D-CED
22	P	213	CLA	O1D-CGD-O2D-CED
22	Q	207	CLA	C1A-C2A-CAA-CBA
22	Q	208	CLA	C2-C1-O2A-CGA
22	Q	209	CLA	CHA-CBD-CGD-O2D
22	Q	211	CLA	CBD-CGD-O2D-CED
22	Q	211	CLA	O1D-CGD-O2D-CED
22	Q	212	CLA	CHA-CBD-CGD-O1D
22	Q	212	CLA	CHA-CBD-CGD-O2D
22	Q	213	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
22	Q	213	CLA	O1A-CGA-O2A-C1
22	Q	213	CLA	CBD-CGD-O2D-CED
22	Q	213	CLA	O1D-CGD-O2D-CED
22	R	104	CLA	CBD-CGD-O2D-CED
22	R	104	CLA	O1D-CGD-O2D-CED
22	S	207	CLA	CBD-CGD-O2D-CED
22	S	207	CLA	O1D-CGD-O2D-CED
22	U	204	CLA	C1A-C2A-CAA-CBA
22	U	204	CLA	C3A-C2A-CAA-CBA
22	U	208	CLA	CBD-CGD-O2D-CED
22	U	208	CLA	O1D-CGD-O2D-CED
22	U	210	CLA	CHA-CBD-CGD-O2D
22	G	203	CLA	C1A-C2A-CAA-CBA
22	G	203	CLA	C3A-C2A-CAA-CBA
22	G	204	CLA	C1A-C2A-CAA-CBA
22	G	204	CLA	C3A-C2A-CAA-CBA
22	G	206	CLA	C1A-C2A-CAA-CBA
22	G	206	CLA	C3A-C2A-CAA-CBA
22	G	206	CLA	CBD-CGD-O2D-CED
22	G	206	CLA	O1D-CGD-O2D-CED
22	G	210	CLA	CBD-CGD-O2D-CED
22	G	210	CLA	O1D-CGD-O2D-CED
22	H	203	CLA	C1A-C2A-CAA-CBA
22	H	203	CLA	C3A-C2A-CAA-CBA
22	H	203	CLA	CHA-CBD-CGD-O1D
22	H	203	CLA	CHA-CBD-CGD-O2D
22	H	205	CLA	CAA-CBA-CGA-O1A
22	H	207	CLA	C3A-C2A-CAA-CBA
22	H	208	CLA	CAD-CBD-CGD-O1D
22	H	208	CLA	CAD-CBD-CGD-O2D
22	H	209	CLA	CBD-CGD-O2D-CED
22	H	209	CLA	O1D-CGD-O2D-CED
22	H	210	CLA	C1A-C2A-CAA-CBA
22	H	213	CLA	C1A-C2A-CAA-CBA
22	H	213	CLA	C3A-C2A-CAA-CBA
22	H	213	CLA	CBA-CGA-O2A-C1
22	H	213	CLA	O1A-CGA-O2A-C1
22	H	213	CLA	C11-C10-C8-C9
22	K	203	CLA	CHA-CBD-CGD-O1D
22	K	203	CLA	CHA-CBD-CGD-O2D
22	T	204	CLA	C1A-C2A-CAA-CBA
22	T	205	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
22	T	205	CLA	O1D-CGD-O2D-CED
22	T	207	CLA	CBD-CGD-O2D-CED
22	T	207	CLA	O1D-CGD-O2D-CED
22	T	210	CLA	CBD-CGD-O2D-CED
22	T	210	CLA	O1D-CGD-O2D-CED
24	A	839	LHG	C4-O6-P-O4
24	A	840	LHG	C3-O3-P-O5
24	A	840	LHG	C4-O6-P-O4
24	P	201	LHG	O2-C2-C3-O3
24	P	201	LHG	C3-O3-P-O4
24	P	201	LHG	C4-O6-P-O3
24	P	201	LHG	C4-O6-P-O4
24	P	201	LHG	C4-O6-P-O5
24	G	216	LHG	C1-C2-C3-O3
24	G	216	LHG	C3-O3-P-O4
24	G	216	LHG	C3-O3-P-O6
24	G	216	LHG	C4-O6-P-O3
24	G	216	LHG	C4-O6-P-O5
25	A	841	BCR	C20-C21-C22-C37
25	A	841	BCR	C21-C22-C23-C24
25	A	842	BCR	C7-C8-C9-C34
25	A	842	BCR	C21-C22-C23-C24
25	A	844	BCR	C21-C22-C23-C24
25	A	844	BCR	C37-C22-C23-C24
25	B	837	BCR	C6-C7-C8-C9
25	B	837	BCR	C7-C8-C9-C34
25	B	837	BCR	C21-C22-C23-C24
25	B	837	BCR	C37-C22-C23-C24
25	F	801	BCR	C7-C8-C9-C10
25	F	801	BCR	C7-C8-C9-C34
25	F	801	BCR	C37-C22-C23-C24
25	I	102	BCR	C7-C8-C9-C34
25	I	102	BCR	C23-C24-C25-C26
25	I	102	BCR	C23-C24-C25-C30
25	J	104	BCR	C7-C8-C9-C34
25	J	104	BCR	C11-C12-C13-C14
25	J	104	BCR	C21-C22-C23-C24
25	L	201	BCR	C21-C22-C23-C24
25	L	201	BCR	C37-C22-C23-C24
25	L	205	BCR	C22-C23-C24-C25
25	M	101	BCR	C7-C8-C9-C10
25	M	101	BCR	C7-C8-C9-C34

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Mol	Chain	Res	Type	Atoms
25	M	101	BCR	C21-C22-C23-C24
25	R	102	BCR	C7-C8-C9-C10
25	R	102	BCR	C7-C8-C9-C34
25	R	102	BCR	C20-C21-C22-C37
25	k	104	BCR	C6-C7-C8-C9
25	k	104	BCR	C7-C8-C9-C10
25	k	104	BCR	C7-C8-C9-C34
26	A	857	LMU	O5'-C1'-O1'-C1
26	F	806	LMU	C2B-C1B-O1B-C4'
26	O	216	LMU	O5'-C1'-O1'-C1
26	O	216	LMU	C2-C1-O1'-C1'
26	S	203	LMU	C2-C1-O1'-C1'
27	A	849	CL0	C1-C2-C3-C4
27	A	849	CL0	C1-C2-C3-C5
29	B	841	DGD	O2G-C2G-C3G-O3G
30	B	846	SQD	C5-C6-S-O8
30	B	846	SQD	C5-C6-S-O9
30	S	201	SQD	O5-C1-O6-C44
30	S	201	SQD	O6-C44-C45-O47
30	S	201	SQD	O5-C5-C6-S
31	O	201	DD6	C10-C11-C13-C14
31	O	201	DD6	C12-C11-C13-C14
31	O	201	DD6	C13-C14-C15-O1
31	O	212	DD6	C1-C2-C3-C4
31	O	212	DD6	C2-C3-C4-C5
31	O	212	DD6	C3-C4-C5-C6
31	O	212	DD6	C4-C5-C6-C7
31	O	212	DD6	C4-C5-C6-C8
31	O	213	DD6	C9-C10-C11-C12
31	O	213	DD6	C9-C10-C11-C13
31	O	213	DD6	C10-C11-C13-C14
31	O	213	DD6	C2-C3-C4-C5
31	O	213	DD6	C5-C6-C8-C9
31	O	213	DD6	C7-C6-C8-C9
31	O	214	DD6	C10-C11-C13-C14
31	O	214	DD6	C12-C11-C13-C14
31	O	214	DD6	C11-C13-C14-C15
31	O	214	DD6	C2-C3-C4-C5
31	O	214	DD6	C4-C5-C6-C7
31	O	214	DD6	C4-C5-C6-C8
31	O	215	DD6	C2-C1-C24-C25
31	O	215	DD6	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
31	O	215	DD6	C9-C10-C11-C13
31	O	215	DD6	C11-C13-C14-C15
31	O	215	DD6	C24-C25-C26-C27
31	O	215	DD6	C2-C3-C4-C5
31	O	215	DD6	C4-C5-C6-C7
31	O	215	DD6	C4-C5-C6-C8
31	O	215	DD6	C5-C6-C8-C9
31	O	215	DD6	C7-C6-C8-C9
31	P	205	DD6	C13-C14-C15-O1
31	P	215	DD6	C9-C10-C11-C12
31	P	215	DD6	C9-C10-C11-C13
31	P	215	DD6	C11-C13-C14-C15
31	P	215	DD6	C13-C14-C15-C16
31	P	215	DD6	C13-C14-C15-C20
31	P	215	DD6	C13-C14-C15-O1
31	P	215	DD6	C2-C3-C4-C5
31	P	215	DD6	C4-C5-C6-C7
31	P	215	DD6	C4-C5-C6-C8
31	P	218	DD6	C10-C11-C13-C14
31	P	218	DD6	C11-C13-C14-C15
31	P	218	DD6	C13-C14-C15-O1
31	P	218	DD6	C2-C3-C4-C5
31	P	218	DD6	C4-C5-C6-C7
31	P	218	DD6	C4-C5-C6-C8
31	P	220	DD6	C9-C10-C11-C12
31	P	220	DD6	C9-C10-C11-C13
31	P	220	DD6	C11-C13-C14-C15
31	P	220	DD6	C1-C24-C25-C26
31	P	220	DD6	C24-C25-C26-C27
31	Q	215	DD6	C2-C1-C24-C25
31	Q	215	DD6	C9-C10-C11-C12
31	Q	215	DD6	C9-C10-C11-C13
31	Q	215	DD6	C10-C11-C13-C14
31	Q	215	DD6	C12-C11-C13-C14
31	Q	215	DD6	C11-C13-C14-C15
31	S	204	DD6	C2-C3-C4-C5
31	S	204	DD6	C4-C5-C6-C7
31	S	204	DD6	C4-C5-C6-C8
31	S	205	DD6	C10-C11-C13-C14
31	S	205	DD6	C12-C11-C13-C14
31	S	205	DD6	C2-C3-C4-C5
31	S	205	DD6	C4-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
31	S	205	DD6	C4-C5-C6-C8
31	S	205	DD6	C5-C6-C8-C9
31	S	205	DD6	C7-C6-C8-C9
31	S	211	DD6	C-C1-C24-C25
31	S	211	DD6	C2-C1-C24-C25
31	S	211	DD6	C11-C13-C14-C15
31	S	211	DD6	C13-C14-C15-O1
31	S	214	DD6	C9-C10-C11-C12
31	S	214	DD6	C9-C10-C11-C13
31	S	214	DD6	C11-C13-C14-C15
31	S	214	DD6	C5-C6-C8-C9
31	S	215	DD6	C9-C10-C11-C12
31	S	215	DD6	C9-C10-C11-C13
31	S	215	DD6	C10-C11-C13-C14
31	S	215	DD6	C12-C11-C13-C14
31	S	215	DD6	C11-C13-C14-C15
31	S	215	DD6	C2-C3-C4-C5
31	S	215	DD6	C4-C5-C6-C7
31	S	215	DD6	C4-C5-C6-C8
31	U	203	DD6	C1-C2-C3-C4
31	U	203	DD6	C1-C24-C25-C26
31	U	203	DD6	C2-C3-C4-C5
31	U	212	DD6	C10-C11-C13-C14
31	U	212	DD6	C11-C13-C14-C15
31	U	212	DD6	C2-C3-C4-C5
31	U	212	DD6	C5-C6-C8-C9
31	U	212	DD6	C7-C6-C8-C9
31	U	214	DD6	C-C1-C24-C25
31	U	214	DD6	C2-C1-C24-C25
31	U	214	DD6	C24-C25-C26-C27
31	U	214	DD6	C2-C3-C4-C5
31	U	214	DD6	C3-C4-C5-C6
31	U	214	DD6	C4-C5-C6-C7
31	G	211	DD6	C11-C13-C14-C15
31	G	211	DD6	C4-C5-C6-C7
31	G	211	DD6	C4-C5-C6-C8
31	G	212	DD6	C2-C1-C24-C25
31	G	212	DD6	C2-C3-C4-C5
31	G	212	DD6	C4-C5-C6-C7
31	G	212	DD6	C4-C5-C6-C8
31	G	213	DD6	C2-C1-C24-C25
31	G	213	DD6	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
31	G	213	DD6	C4-C5-C6-C7
31	G	213	DD6	C4-C5-C6-C8
31	G	214	DD6	C1-C24-C25-C26
31	H	201	DD6	C10-C11-C13-C14
31	H	201	DD6	C12-C11-C13-C14
31	H	201	DD6	C11-C13-C14-C15
31	H	211	DD6	C9-C10-C11-C12
31	H	211	DD6	C9-C10-C11-C13
31	H	211	DD6	C11-C13-C14-C15
31	H	211	DD6	C1-C2-C3-C4
31	H	212	DD6	C9-C10-C11-C12
31	H	212	DD6	C9-C10-C11-C13
31	H	212	DD6	C10-C11-C13-C14
31	H	212	DD6	C12-C11-C13-C14
31	H	212	DD6	C13-C14-C15-O1
31	H	212	DD6	C4-C5-C6-C7
31	H	212	DD6	C4-C5-C6-C8
31	H	212	DD6	C5-C6-C8-C9
31	K	208	DD6	C-C1-C24-C25
31	K	208	DD6	C2-C1-C24-C25
31	K	208	DD6	C2-C3-C4-C5
31	K	208	DD6	C4-C5-C6-C7
31	K	208	DD6	C4-C5-C6-C8
31	K	208	DD6	C5-C6-C8-C9
31	K	208	DD6	C7-C6-C8-C9
31	T	212	DD6	C9-C10-C11-C12
31	T	212	DD6	C9-C10-C11-C13
31	T	212	DD6	C3-C4-C5-C6
31	T	212	DD6	C4-C5-C6-C7
31	T	212	DD6	C4-C5-C6-C8
31	T	213	DD6	C9-C10-C11-C12
31	T	213	DD6	C9-C10-C11-C13
31	T	213	DD6	C11-C13-C14-C15
31	T	213	DD6	C1-C2-C3-C4
31	T	213	DD6	C1-C24-C25-C26
31	T	213	DD6	C24-C25-C26-C27
31	T	213	DD6	C3-C4-C5-C6
31	k	101	DD6	C10-C11-C13-C14
31	k	101	DD6	C12-C11-C13-C14
31	k	101	DD6	C5-C6-C8-C9
31	k	101	DD6	C7-C6-C8-C9
32	J	102	LMG	O6-C1-O1-C7

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Mol	Chain	Res	Type	Atoms
32	J	102	LMG	O9-C10-O7-C8
32	U	201	LMG	C11-C10-O7-C8
33	P	206	KC1	C2A-CAA-CBA-CGA
33	P	212	KC1	CAD-CBD-CGD-O2D
33	P	212	KC1	CHA-CBD-CGD-O2D
33	P	219	KC1	C1A-C2A-CAA-CBA
33	Q	210	KC1	C2A-CAA-CBA-CGA
33	S	212	KC1	C3A-C2A-CAA-CBA
33	S	212	KC1	CBD-CGD-O2D-CED
33	S	212	KC1	O1D-CGD-O2D-CED
34	P	204	A86	C-C1-C2-C3
34	P	204	A86	C24-C1-C2-C3
34	P	204	A86	C2-C3-C4-C5
34	Q	201	A86	C9-C10-C11-C12
34	Q	201	A86	C10-C11-C13-O
34	Q	201	A86	C12-C11-C13-O
34	Q	201	A86	C5-C6-C8-C9
34	Q	201	A86	C7-C6-C8-C9
34	Q	201	A86	C6-C8-C9-C10
34	Q	214	A86	C2-C3-C4-C5
34	Q	214	A86	C39-C38-O4-C34
34	Q	214	A86	O5-C38-O4-C34
34	Q	214	A86	C4-C5-C6-C7
34	Q	214	A86	C4-C5-C6-C8
34	Q	214	A86	C5-C6-C8-C9
34	Q	214	A86	C6-C8-C9-C10
34	Q	218	A86	C-C1-C24-C25
34	Q	218	A86	C2-C1-C24-C25
34	Q	218	A86	C1-C2-C3-C4
34	Q	218	A86	C1-C24-C25-C26
34	Q	218	A86	C26-C27-C29-C30
34	Q	218	A86	C28-C27-C29-C30
34	Q	218	A86	C4-C5-C6-C7
34	Q	218	A86	C4-C5-C6-C8
34	Q	218	A86	C6-C8-C9-C10
34	R	103	A86	C6-C8-C9-C10
34	R	105	A86	O-C13-C14-C15
34	R	105	A86	C2-C3-C4-C5
34	R	105	A86	C39-C38-O4-C34
34	R	105	A86	O5-C38-O4-C34
34	U	202	A86	C10-C11-C13-O
34	U	202	A86	C12-C11-C13-O

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Mol	Chain	Res	Type	Atoms
34	U	202	A86	C2-C3-C4-C5
34	U	202	A86	C4-C5-C6-C7
34	U	202	A86	C4-C5-C6-C8
34	U	202	A86	C5-C6-C8-C9
34	U	202	A86	C6-C8-C9-C10
26	S	203	LMU	C5'-C4'-O1B-C1B
34	P	204	A86	C39-C38-O4-C34
26	F	806	LMU	O5B-C1B-O1B-C4'
34	U	202	A86	C39-C38-O4-C34
34	P	204	A86	C35-C34-O4-C38
34	Q	201	A86	C39-C38-O4-C34
22	O	207	CLA	O1A-CGA-O2A-C1
22	Q	207	CLA	O1A-CGA-O2A-C1
26	K	202	LMU	C3'-C4'-O1B-C1B
22	O	207	CLA	CBA-CGA-O2A-C1
22	Q	207	CLA	CBA-CGA-O2A-C1
22	A	836	CLA	C3-C5-C6-C7
22	B	816	CLA	C3-C5-C6-C7
22	O	209	CLA	C3-C5-C6-C7
22	Q	204	CLA	C3-C5-C6-C7
22	Q	213	CLA	C3-C5-C6-C7
22	U	205	CLA	C3-C5-C6-C7
22	K	205	CLA	C3-C5-C6-C7
22	T	204	CLA	C3-C5-C6-C7
34	P	204	A86	O5-C38-O4-C34
22	A	845	CLA	C4-C3-C5-C6
22	B	809	CLA	C4-C3-C5-C6
22	O	209	CLA	C4-C3-C5-C6
22	P	207	CLA	C4-C3-C5-C6
22	P	208	CLA	C4-C3-C5-C6
22	Q	209	CLA	C4-C3-C5-C6
22	G	205	CLA	C4-C3-C5-C6
22	G	207	CLA	C4-C3-C5-C6
22	K	205	CLA	C4-C3-C5-C6
22	K	207	CLA	C4-C3-C5-C6
22	B	809	CLA	C2-C3-C5-C6
22	B	845	CLA	C2-C3-C5-C6
22	O	209	CLA	C2-C3-C5-C6
22	P	207	CLA	C2-C3-C5-C6
22	Q	209	CLA	C2-C3-C5-C6
22	K	205	CLA	C2-C3-C5-C6
22	K	207	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
26	L	206	LMU	O5'-C5'-C6'-O6'
26	M	102	LMU	O5'-C5'-C6'-O6'
26	O	216	LMU	O5B-C5B-C6B-O6B
26	O	216	LMU	C4'-C5'-C6'-O6'
22	A	814	CLA	C2A-CAA-CBA-CGA
31	P	218	DD6	C11-C10-C9-C8
31	Q	215	DD6	C24-C25-C26-C27
31	S	211	DD6	C24-C25-C26-C27
31	U	203	DD6	C3-C4-C5-C6
31	U	212	DD6	C24-C25-C26-C27
31	H	201	DD6	C24-C25-C26-C27
31	K	208	DD6	C24-C25-C26-C27
32	U	201	LMG	O9-C10-O7-C8
26	O	216	LMU	O5'-C5'-C6'-O6'
22	B	814	CLA	C3-C5-C6-C7
22	B	833	CLA	C3-C5-C6-C7
22	Q	205	CLA	C3-C5-C6-C7
26	P	221	LMU	O5'-C5'-C6'-O6'
24	A	840	LHG	C8-C7-O7-C5
32	S	213	LMG	O6-C5-C6-O5
31	G	214	DD6	C2-C3-C4-C5
26	O	216	LMU	C2B-C1B-O1B-C4'
32	J	102	LMG	O6-C5-C6-O5
22	B	813	CLA	C4-C3-C5-C6
22	O	205	CLA	C4-C3-C5-C6
22	H	204	CLA	C4-C3-C5-C6
22	B	813	CLA	C2-C3-C5-C6
22	O	205	CLA	C2-C3-C5-C6
22	P	208	CLA	C2-C3-C5-C6
22	H	203	CLA	C2-C3-C5-C6
22	H	204	CLA	C2-C3-C5-C6
24	A	840	LHG	O9-C7-O7-C5
29	B	841	DGD	O6E-C5E-C6E-O5E
26	O	216	LMU	C4B-C5B-C6B-O6B
32	S	213	LMG	C4-C5-C6-O5
24	A	839	LHG	C23-C24-C25-C26
26	F	807	LMU	O5'-C5'-C6'-O6'
32	Q	217	LMG	O6-C1-O1-C7
32	U	201	LMG	O6-C1-O1-C7
26	S	203	LMU	O5'-C5'-C6'-O6'
32	J	102	LMG	C29-C28-O8-C9
26	L	206	LMU	O5B-C5B-C6B-O6B

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Mol	Chain	Res	Type	Atoms
26	L	206	LMU	C4'-C5'-C6'-O6'
26	F	806	LMU	O5'-C5'-C6'-O6'
26	M	102	LMU	C4'-C5'-C6'-O6'
24	A	839	LHG	C28-C29-C30-C31
31	P	218	DD6	C1-C2-C3-C4
31	S	214	DD6	C24-C25-C26-C27
31	S	214	DD6	C3-C4-C5-C6
27	A	849	CL0	CBA-CGA-O2A-C1
26	P	221	LMU	C4'-C5'-C6'-O6'
32	P	217	LMG	C29-C28-O8-C9
22	H	203	CLA	C4-C3-C5-C6
22	A	845	CLA	C2-C3-C5-C6
22	G	205	CLA	C2-C3-C5-C6
22	G	207	CLA	C2-C3-C5-C6
22	B	816	CLA	C14-C13-C15-C16
22	Q	204	CLA	C6-C7-C8-C9
22	Q	212	CLA	C11-C12-C13-C14
26	S	203	LMU	C2'-C1'-O1'-C1
32	J	102	LMG	C2-C1-O1-C7
32	Q	217	LMG	C2-C1-O1-C7
32	U	201	LMG	C2-C1-O1-C7
24	G	216	LHG	O2-C2-C3-O3
26	F	806	LMU	C4'-C5'-C6'-O6'
25	A	842	BCR	C37-C22-C23-C24
25	A	843	BCR	C7-C8-C9-C34
25	A	844	BCR	C11-C12-C13-C35
25	B	836	BCR	C37-C22-C23-C24
25	B	840	BCR	C37-C22-C23-C24
25	F	805	BCR	C7-C8-C9-C34
25	F	805	BCR	C37-C22-C23-C24
25	I	102	BCR	C37-C22-C23-C24
25	J	104	BCR	C11-C12-C13-C35
25	J	104	BCR	C37-C22-C23-C24
25	M	101	BCR	C37-C22-C23-C24
31	J	101	DD6	C12-C11-C13-C14
31	O	212	DD6	C-C1-C24-C25
31	O	213	DD6	C12-C11-C13-C14
31	O	215	DD6	C-C1-C24-C25
31	O	215	DD6	C12-C11-C13-C14
31	P	218	DD6	C12-C11-C13-C14
31	P	220	DD6	C-C1-C24-C25
31	Q	215	DD6	C-C1-C24-C25

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Mol	Chain	Res	Type	Atoms
31	S	211	DD6	C12-C11-C13-C14
31	S	214	DD6	C12-C11-C13-C14
31	S	214	DD6	C7-C6-C8-C9
31	S	215	DD6	C-C1-C24-C25
31	U	203	DD6	C-C1-C24-C25
31	U	212	DD6	C12-C11-C13-C14
31	G	212	DD6	C-C1-C24-C25
31	G	213	DD6	C-C1-C24-C25
31	H	211	DD6	C12-C11-C13-C14
31	H	212	DD6	C7-C6-C8-C9
31	T	212	DD6	C7-C6-C8-C9
31	T	213	DD6	C12-C11-C13-C14
34	Q	214	A86	C7-C6-C8-C9
34	U	202	A86	C7-C6-C8-C9
34	U	202	A86	O5-C38-O4-C34
25	B	837	BCR	C7-C8-C9-C10
25	I	102	BCR	C21-C22-C23-C24
31	J	101	DD6	C10-C11-C13-C14
31	O	215	DD6	C10-C11-C13-C14
31	P	220	DD6	C2-C1-C24-C25
31	S	211	DD6	C10-C11-C13-C14
31	S	214	DD6	C10-C11-C13-C14
31	S	215	DD6	C2-C1-C24-C25
31	U	203	DD6	C2-C1-C24-C25
31	H	201	DD6	C2-C1-C24-C25
31	H	211	DD6	C10-C11-C13-C14
31	T	212	DD6	C5-C6-C8-C9
31	T	213	DD6	C10-C11-C13-C14
26	S	203	LMU	C4'-C5'-C6'-O6'
24	P	201	LHG	C24-C23-O8-C6
26	O	216	LMU	O5B-C1B-O1B-C4'
31	Q	215	DD6	C2-C3-C4-C5
34	Q	201	A86	O5-C38-O4-C34
26	A	857	LMU	O5'-C5'-C6'-O6'
32	P	217	LMG	O10-C28-O8-C9
31	P	218	DD6	C3-C4-C5-C6
31	P	220	DD6	C3-C4-C5-C6
31	U	203	DD6	C24-C25-C26-C27
31	G	213	DD6	C24-C25-C26-C27
31	H	211	DD6	C24-C25-C26-C27
31	H	211	DD6	C3-C4-C5-C6
34	Q	218	A86	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
26	F	807	LMU	C4'-C5'-C6'-O6'
26	M	102	LMU	O5B-C5B-C6B-O6B
30	S	201	SQD	C7-C8-C9-C10
32	Q	217	LMG	C28-C29-C30-C31
27	A	849	CL0	O1A-CGA-O2A-C1
22	A	811	CLA	C10-C11-C12-C13
22	A	824	CLA	C10-C11-C12-C13
22	B	812	CLA	C5-C6-C7-C8
22	Q	216	CLA	C5-C6-C7-C8
22	G	209	CLA	C5-C6-C7-C8
26	K	202	LMU	O5B-C5B-C6B-O6B
22	A	807	CLA	C2A-CAA-CBA-CGA
22	L	204	CLA	C2A-CAA-CBA-CGA
25	k	104	BCR	C10-C11-C12-C13
31	J	101	DD6	C1-C24-C25-C26
31	O	214	DD6	C1-C24-C25-C26
31	S	215	DD6	C1-C24-C25-C26
22	A	809	CLA	C8-C10-C11-C12
22	Q	212	CLA	C10-C11-C12-C13
32	Q	217	LMG	O6-C5-C6-O5
26	M	102	LMU	C4B-C5B-C6B-O6B
24	A	840	LHG	C7-C8-C9-C10
24	P	201	LHG	O10-C23-O8-C6
32	J	102	LMG	O10-C28-O8-C9
22	B	819	CLA	C3-C5-C6-C7
26	A	857	LMU	C3'-C4'-O1B-C1B
26	P	221	LMU	O5'-C1'-O1'-C1
26	S	203	LMU	O5'-C1'-O1'-C1
22	A	822	CLA	C13-C15-C16-C17
22	T	204	CLA	C5-C6-C7-C8
32	P	217	LMG	O6-C5-C6-O5
22	B	816	CLA	C8-C10-C11-C12
22	A	853	CLA	C8-C10-C11-C12
22	B	830	CLA	C13-C15-C16-C17
32	J	102	LMG	C4-C5-C6-O5
26	M	102	LMU	O1'-C1-C2-C3
22	Q	203	CLA	O2A-C1-C2-C3
33	S	212	KC1	C2A-CAA-CBA-CGA
22	B	845	CLA	C3-C5-C6-C7
31	P	220	DD6	C1-C2-C3-C4
31	S	215	DD6	C24-C25-C26-C27
34	Q	201	A86	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
22	A	854	CLA	C15-C16-C17-C18
22	H	213	CLA	C5-C6-C7-C8
24	P	201	LHG	C1-C2-C3-O3
22	A	825	CLA	C2A-CAA-CBA-CGA
22	A	845	CLA	C2A-CAA-CBA-CGA
22	H	203	CLA	C2A-CAA-CBA-CGA
31	H	201	DD6	C2-C3-C4-C5
22	B	844	CLA	C13-C15-C16-C17
22	Q	204	CLA	C5-C6-C7-C8
22	Q	209	CLA	C5-C6-C7-C8
22	U	205	CLA	C5-C6-C7-C8
22	H	213	CLA	C8-C10-C11-C12
32	J	102	LMG	C11-C10-O7-C8
26	A	857	LMU	C2'-C1'-O1'-C1
26	P	221	LMU	C2'-C1'-O1'-C1
24	P	201	LHG	C23-C24-C25-C26
25	A	842	BCR	C20-C21-C22-C37
25	L	201	BCR	C16-C17-C18-C36
31	J	101	DD6	C4-C5-C6-C7
31	O	213	DD6	C4-C5-C6-C7
31	Q	202	DD6	C4-C5-C6-C7
31	S	205	DD6	C9-C10-C11-C12
31	S	211	DD6	C4-C5-C6-C7
31	S	214	DD6	C4-C5-C6-C7
31	U	203	DD6	C4-C5-C6-C7
31	U	212	DD6	C4-C5-C6-C7
31	G	213	DD6	C9-C10-C11-C12
31	G	214	DD6	C9-C10-C11-C12
31	H	201	DD6	C4-C5-C6-C7
31	H	211	DD6	C4-C5-C6-C7
31	k	101	DD6	C9-C10-C11-C12
34	R	103	A86	C25-C26-C27-C28
34	R	105	A86	C-C1-C2-C3
34	U	202	A86	C-C1-C2-C3
26	S	203	LMU	O5B-C5B-C6B-O6B
22	H	207	CLA	C13-C15-C16-C17
25	B	836	BCR	C7-C8-C9-C34
25	L	201	BCR	C11-C12-C13-C35
31	Q	202	DD6	C12-C11-C13-C14
31	S	214	DD6	C-C1-C24-C25
31	H	201	DD6	C-C1-C24-C25
31	H	211	DD6	C-C1-C24-C25

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Mol	Chain	Res	Type	Atoms
31	T	213	DD6	C-C1-C24-C25
25	B	836	BCR	C7-C8-C9-C10
31	Q	202	DD6	C10-C11-C13-C14
31	S	214	DD6	C2-C1-C24-C25
31	H	211	DD6	C2-C1-C24-C25
31	T	213	DD6	C2-C1-C24-C25
22	A	806	CLA	C2A-CAA-CBA-CGA
22	B	819	CLA	C2A-CAA-CBA-CGA
22	B	847	CLA	C2A-CAA-CBA-CGA
22	G	215	CLA	C2A-CAA-CBA-CGA
24	P	201	LHG	O1-C1-C2-C3
26	A	847	LMU	C1-C2-C3-C4
25	A	841	BCR	C20-C21-C22-C23
25	I	101	BCR	C16-C17-C18-C19
25	I	102	BCR	C20-C21-C22-C23
31	J	101	DD6	C4-C5-C6-C8
31	O	213	DD6	C4-C5-C6-C8
31	Q	202	DD6	C4-C5-C6-C8
31	S	205	DD6	C9-C10-C11-C13
31	S	211	DD6	C4-C5-C6-C8
31	S	214	DD6	C4-C5-C6-C8
31	U	203	DD6	C4-C5-C6-C8
31	U	212	DD6	C4-C5-C6-C8
31	G	213	DD6	C9-C10-C11-C13
31	G	214	DD6	C9-C10-C11-C13
31	H	201	DD6	C4-C5-C6-C8
31	H	211	DD6	C4-C5-C6-C8
31	k	101	DD6	C9-C10-C11-C13
34	R	103	A86	C25-C26-C27-C29
34	R	105	A86	C24-C1-C2-C3
34	U	202	A86	C24-C1-C2-C3
32	P	217	LMG	O6-C1-O1-C7
22	A	834	CLA	C3-C5-C6-C7
34	Q	201	A86	C9-C10-C11-C13
34	R	103	A86	C9-C10-C11-C13
34	R	105	A86	C9-C10-C11-C13
34	U	202	A86	C9-C10-C11-C13
26	M	102	LMU	C1-C2-C3-C4
26	O	216	LMU	C1-C2-C3-C4
31	Q	202	DD6	C2-C3-C4-C5
31	S	214	DD6	C2-C3-C4-C5
31	G	211	DD6	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
31	H	212	DD6	C2-C3-C4-C5
34	Q	201	A86	C2-C3-C4-C5
34	Q	218	A86	C2-C3-C4-C5
26	F	806	LMU	C6-C7-C8-C9
32	S	213	LMG	C31-C32-C33-C34
32	S	213	LMG	C28-C29-C30-C31
22	B	827	CLA	C5-C6-C7-C8
32	J	102	LMG	C14-C15-C16-C17
26	F	807	LMU	O1'-C1-C2-C3
24	P	201	LHG	O1-C1-C2-O2
24	P	201	LHG	C11-C10-C9-C8
30	S	201	SQD	C12-C13-C14-C15
32	P	202	LMG	C31-C32-C33-C34
22	P	207	CLA	C16-C17-C18-C20
22	A	856	CLA	C2A-CAA-CBA-CGA
24	A	839	LHG	C24-C25-C26-C27
30	S	201	SQD	C29-C30-C31-C32
32	Q	217	LMG	C29-C28-O8-C9
24	P	201	LHG	C33-C34-C35-C36
32	S	213	LMG	C33-C34-C35-C36
22	B	845	CLA	C4-C3-C5-C6
22	F	804	CLA	C3A-C2A-CAA-CBA
22	P	208	CLA	C3A-C2A-CAA-CBA
22	Q	207	CLA	C3A-C2A-CAA-CBA
22	K	206	CLA	C3A-C2A-CAA-CBA
22	T	203	CLA	C3A-C2A-CAA-CBA
24	P	201	LHG	C10-C11-C12-C13
22	A	846	CLA	C8-C10-C11-C12
24	G	216	LHG	C7-C8-C9-C10
32	P	217	LMG	C10-C11-C12-C13
31	S	214	DD6	C1-C2-C3-C4
22	P	207	CLA	C16-C17-C18-C19
22	K	207	CLA	CBA-CGA-O2A-C1
26	L	206	LMU	C3-C4-C5-C6
29	B	841	DGD	C4B-C5B-C6B-C7B
24	P	201	LHG	C28-C29-C30-C31
32	Q	217	LMG	C15-C16-C17-C18
26	K	201	LMU	C3-C4-C5-C6
30	B	846	SQD	C32-C33-C34-C35
32	J	102	LMG	C15-C16-C17-C18
26	A	857	LMU	C5'-C4'-O1B-C1B
29	B	841	DGD	C4E-C5E-C6E-O5E

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Mol	Chain	Res	Type	Atoms
30	B	846	SQD	C13-C14-C15-C16
25	A	844	BCR	C23-C24-C25-C26
25	A	844	BCR	C23-C24-C25-C30
25	R	102	BCR	C1-C6-C7-C8
25	R	102	BCR	C5-C6-C7-C8
30	S	201	SQD	C26-C27-C28-C29
32	J	102	LMG	C13-C14-C15-C16
24	P	201	LHG	C8-C7-O7-C5
23	B	835	PQN	C23-C25-C26-C27
24	P	201	LHG	C14-C15-C16-C17
24	P	201	LHG	C29-C30-C31-C32
22	B	832	CLA	C2A-CAA-CBA-CGA
24	P	201	LHG	C7-C8-C9-C10
22	B	815	CLA	C8-C10-C11-C12
29	B	841	DGD	C5A-C6A-C7A-C8A
31	O	212	DD6	C1-C24-C25-C26
31	O	215	DD6	C1-C24-C25-C26
34	P	204	A86	C1-C24-C25-C26
34	U	202	A86	C1-C24-C25-C26
26	F	807	LMU	C4-C5-C6-C7
26	F	807	LMU	C5-C6-C7-C8
32	S	213	LMG	C34-C35-C36-C37
22	U	204	CLA	C10-C11-C12-C13
26	F	806	LMU	C7-C8-C9-C10
30	S	201	SQD	C11-C12-C13-C14
26	A	857	LMU	C7-C8-C9-C10
22	B	802	CLA	C13-C15-C16-C17
26	A	847	LMU	C11-C10-C9-C8
32	U	201	LMG	C29-C30-C31-C32
24	P	201	LHG	C17-C18-C19-C20
32	Q	217	LMG	C31-C32-C33-C34
26	M	102	LMU	C11-C10-C9-C8
31	G	211	DD6	C24-C25-C26-C27
32	P	217	LMG	C11-C10-O7-C8
26	O	216	LMU	C4-C5-C6-C7
29	B	841	DGD	CAB-CBB-CCB-CDB
34	Q	218	A86	C39-C38-O4-C34
25	I	101	BCR	C37-C22-C23-C24
31	P	205	DD6	C12-C11-C13-C14
31	P	220	DD6	C7-C6-C8-C9
31	S	204	DD6	C7-C6-C8-C9
30	S	201	SQD	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
25	L	205	BCR	C7-C8-C9-C10
31	P	205	DD6	C10-C11-C13-C14
31	P	220	DD6	C5-C6-C8-C9
26	F	806	LMU	C2-C3-C4-C5
30	B	846	SQD	C28-C29-C30-C31
22	A	824	CLA	C5-C6-C7-C8
26	A	847	LMU	C4'-C5'-C6'-O6'
26	A	847	LMU	C5-C6-C7-C8
26	F	806	LMU	O1'-C1-C2-C3
22	K	207	CLA	O1A-CGA-O2A-C1
24	A	840	LHG	O6-C4-C5-O7
22	Q	212	CLA	C8-C10-C11-C12
22	G	205	CLA	C8-C10-C11-C12
33	P	212	KC1	C4B-C3B-CAB-CBB
33	P	219	KC1	C2A-CAA-CBA-CGA
33	Q	210	KC1	C4B-C3B-CAB-CBB
33	S	212	KC1	C4B-C3B-CAB-CBB
32	J	102	LMG	O7-C8-C9-O8
26	A	847	LMU	C4-C5-C6-C7
32	Q	217	LMG	C32-C33-C34-C35
24	A	839	LHG	C27-C28-C29-C30
32	S	213	LMG	C30-C31-C32-C33
22	B	814	CLA	C4-C3-C5-C6
22	G	209	CLA	C3-C5-C6-C7
22	O	206	CLA	C2-C3-C5-C6
24	P	201	LHG	C9-C10-C11-C12
32	P	202	LMG	C29-C28-O8-C9
22	O	208	CLA	C5-C6-C7-C8
26	A	857	LMU	C11-C10-C9-C8
32	P	202	LMG	C12-C13-C14-C15
32	Q	217	LMG	C23-C24-C25-C26
22	A	807	CLA	C1A-C2A-CAA-CBA
22	A	815	CLA	C1A-C2A-CAA-CBA
22	B	822	CLA	C1A-C2A-CAA-CBA
22	H	207	CLA	C1A-C2A-CAA-CBA
22	K	206	CLA	C1A-C2A-CAA-CBA
22	T	203	CLA	C1A-C2A-CAA-CBA
26	K	202	LMU	C4B-C5B-C6B-O6B
24	P	201	LHG	C24-C25-C26-C27
32	J	102	LMG	C19-C20-C21-C22
22	B	844	CLA	C15-C16-C17-C18
34	R	103	A86	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
34	R	105	A86	C9-C10-C11-C12
24	A	840	LHG	O6-C4-C5-C6
24	P	201	LHG	C16-C17-C18-C19
29	B	841	DGD	CDB-CEB-CFB-CGB
22	A	804	CLA	C11-C12-C13-C15
22	B	822	CLA	C6-C7-C8-C10
22	O	206	CLA	C12-C13-C15-C16
22	Q	209	CLA	C11-C10-C8-C7
22	Q	212	CLA	C11-C12-C13-C15
22	Q	216	CLA	C12-C13-C15-C16
22	S	202	CLA	C11-C12-C13-C15
22	A	804	CLA	C8-C10-C11-C12
24	A	839	LHG	C9-C10-C11-C12
22	O	206	CLA	C4-C3-C5-C6
22	G	208	CLA	C2-C3-C5-C6
22	B	842	CLA	C10-C11-C12-C13
22	A	804	CLA	C11-C12-C13-C14
22	Q	205	CLA	C6-C7-C8-C9
22	Q	216	CLA	C14-C13-C15-C16
22	K	207	CLA	C11-C10-C8-C9
24	A	839	LHG	C30-C31-C32-C33
31	S	215	DD6	C1-C2-C3-C4
32	U	201	LMG	C29-C28-O8-C9
22	O	205	CLA	C8-C10-C11-C12
26	A	847	LMU	O5B-C5B-C6B-O6B
26	F	806	LMU	C2'-C1'-O1'-C1
26	O	216	LMU	C2'-C1'-O1'-C1
29	B	841	DGD	C1G-C2G-C3G-O3G
30	B	846	SQD	C44-C45-C46-O48
32	P	217	LMG	C7-C8-C9-O8
32	Q	217	LMG	O1-C7-C8-C9
32	S	213	LMG	C7-C8-C9-O8
22	T	207	CLA	C10-C11-C12-C13
24	A	839	LHG	C10-C11-C12-C13
26	F	806	LMU	O5B-C5B-C6B-O6B
24	P	201	LHG	C13-C14-C15-C16
32	P	202	LMG	C30-C31-C32-C33
26	K	202	LMU	C5'-C4'-O1B-C1B
25	A	842	BCR	C16-C17-C18-C36
25	B	840	BCR	C11-C10-C9-C34
25	I	102	BCR	C20-C21-C22-C37
31	G	211	DD6	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
22	A	821	CLA	C15-C16-C17-C18
22	A	821	CLA	C4-C3-C5-C6
22	G	208	CLA	C4-C3-C5-C6
22	A	821	CLA	C2-C3-C5-C6
22	A	823	CLA	C2-C3-C5-C6
22	S	217	CLA	C2-C3-C5-C6
25	L	205	BCR	C7-C8-C9-C34
31	U	203	DD6	C12-C11-C13-C14
24	A	839	LHG	C32-C33-C34-C35
32	U	201	LMG	C4-C5-C6-O5
24	A	839	LHG	C26-C27-C28-C29
25	F	801	BCR	C21-C22-C23-C24
31	U	203	DD6	C10-C11-C13-C14
24	P	201	LHG	C30-C31-C32-C33
31	H	211	DD6	C1-C24-C25-C26
24	G	216	LHG	C24-C25-C26-C27
26	O	216	LMU	C11-C10-C9-C8
25	A	842	BCR	C20-C21-C22-C23
25	A	844	BCR	C20-C21-C22-C23
25	I	101	BCR	C20-C21-C22-C23
31	G	211	DD6	C9-C10-C11-C13
26	F	806	LMU	C4-C5-C6-C7
29	B	841	DGD	C9B-CAB-CBB-CCB
30	B	846	SQD	C27-C28-C29-C30
32	Q	217	LMG	C41-C42-C43-C44
30	S	201	SQD	C13-C14-C15-C16
32	P	202	LMG	C13-C14-C15-C16
29	B	841	DGD	CEB-CFB-CGB-CHB
32	S	213	LMG	C39-C40-C41-C42
26	A	857	LMU	C9-C10-C11-C12
30	S	201	SQD	C32-C33-C34-C35
32	Q	217	LMG	O7-C8-C9-O8
32	U	201	LMG	O1-C7-C8-O7
32	P	202	LMG	C32-C33-C34-C35
26	O	216	LMU	C3-C4-C5-C6
32	U	201	LMG	C31-C32-C33-C34
26	A	857	LMU	C2-C3-C4-C5
22	L	204	CLA	CAA-CBA-CGA-O2A
22	A	822	CLA	C3-C5-C6-C7
26	L	206	LMU	C9-C10-C11-C12
32	U	201	LMG	C12-C13-C14-C15
32	J	102	LMG	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
30	S	201	SQD	C27-C28-C29-C30
24	A	839	LHG	C29-C30-C31-C32
32	Q	217	LMG	C24-C25-C26-C27
22	A	823	CLA	C4-C3-C5-C6
22	A	825	CLA	C4-C3-C5-C6
26	A	847	LMU	C3-C4-C5-C6
26	A	857	LMU	C2-C1-O1'-C1'
31	O	213	DD6	C27-C29-C30-C31
31	S	211	DD6	C27-C29-C30-C31
31	G	214	DD6	C27-C29-C30-C31
31	T	213	DD6	C27-C29-C30-C31
22	B	822	CLA	C6-C7-C8-C9
22	B	845	CLA	C11-C12-C13-C14
22	O	206	CLA	C14-C13-C15-C16
22	U	204	CLA	C6-C7-C8-C9
30	S	201	SQD	C25-C26-C27-C28
22	B	829	CLA	C5-C6-C7-C8
26	L	206	LMU	C2-C3-C4-C5
22	A	853	CLA	C13-C15-C16-C17
24	P	201	LHG	O6-C4-C5-C6
22	A	825	CLA	C12-C13-C15-C16
22	Q	205	CLA	C6-C7-C8-C10
22	U	204	CLA	C6-C7-C8-C10
22	G	206	CLA	C6-C7-C8-C10
22	H	213	CLA	C11-C10-C8-C7
23	A	837	PQN	C17-C18-C20-C21
26	A	847	LMU	C9-C10-C11-C12
32	J	102	LMG	C29-C30-C31-C32
29	B	841	DGD	O1B-C1B-O2G-C2G
22	U	204	CLA	C3-C5-C6-C7
22	A	854	CLA	C4-C3-C5-C6
22	L	202	CLA	C3A-C2A-CAA-CBA
22	Q	216	CLA	C4-C3-C5-C6
22	G	209	CLA	C4-C3-C5-C6
22	T	204	CLA	C3A-C2A-CAA-CBA
22	G	206	CLA	C2-C3-C5-C6
26	K	201	LMU	C5-C6-C7-C8
31	O	201	DD6	C24-C25-C26-C27
31	O	212	DD6	C24-C25-C26-C27
31	O	214	DD6	C24-C25-C26-C27
31	S	211	DD6	C1-C2-C3-C4
31	k	101	DD6	C3-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
22	B	807	CLA	C3-C5-C6-C7
24	P	201	LHG	C32-C33-C34-C35
32	Q	217	LMG	C35-C36-C37-C38
22	A	836	CLA	C5-C6-C7-C8
30	B	846	SQD	O6-C44-C45-C46
30	S	201	SQD	O6-C44-C45-C46
32	P	202	LMG	O1-C7-C8-C9
32	S	213	LMG	O1-C7-C8-C9
32	U	201	LMG	O1-C7-C8-C9
26	S	203	LMU	C4B-C5B-C6B-O6B
29	B	841	DGD	C5B-C6B-C7B-C8B
22	B	804	CLA	C15-C16-C17-C18
32	S	213	LMG	C36-C37-C38-C39
22	A	806	CLA	C4-C3-C5-C6
32	S	213	LMG	C37-C38-C39-C40
26	L	206	LMU	C4B-C5B-C6B-O6B
24	P	201	LHG	C11-C12-C13-C14
25	A	841	BCR	C23-C24-C25-C30
25	A	844	BCR	C1-C6-C7-C8
25	B	836	BCR	C1-C6-C7-C8
25	B	836	BCR	C5-C6-C7-C8
25	B	837	BCR	C1-C6-C7-C8
25	B	839	BCR	C23-C24-C25-C30
25	L	201	BCR	C1-C6-C7-C8
25	L	205	BCR	C23-C24-C25-C30
25	R	102	BCR	C23-C24-C25-C30
25	k	104	BCR	C1-C6-C7-C8
24	P	201	LHG	C2-C3-O3-P
26	K	201	LMU	C2B-C1B-O1B-C4'
31	G	213	DD6	C1-C2-C3-C4
29	B	841	DGD	C4A-C5A-C6A-C7A
22	T	204	CLA	C2A-CAA-CBA-CGA
32	S	213	LMG	O7-C8-C9-O8
26	P	221	LMU	C2-C1-O1'-C1'
22	S	217	CLA	C4-C3-C5-C6
22	G	206	CLA	C4-C3-C5-C6
22	Q	216	CLA	C2-C3-C5-C6
22	G	209	CLA	C2-C3-C5-C6
29	B	841	DGD	C2A-C3A-C4A-C5A
22	H	207	CLA	C1-C2-C3-C5
32	U	201	LMG	C30-C31-C32-C33
22	A	825	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
22	B	804	CLA	C11-C10-C8-C9
22	H	213	CLA	C6-C7-C8-C9
24	P	201	LHG	C18-C19-C20-C21
25	L	205	BCR	C6-C7-C8-C9
25	R	102	BCR	C22-C23-C24-C25
26	A	857	LMU	C4'-C5'-C6'-O6'
32	J	102	LMG	C11-C12-C13-C14
30	S	201	SQD	C24-C23-O48-C46
26	F	806	LMU	C5-C6-C7-C8
31	U	212	DD6	C3-C4-C5-C6
22	A	825	CLA	C2-C3-C5-C6
22	Q	209	CLA	C13-C15-C16-C17
31	O	201	DD6	C9-C10-C11-C12
31	S	204	DD6	C9-C10-C11-C12
31	S	211	DD6	C9-C10-C11-C12
31	H	201	DD6	C9-C10-C11-C12
34	R	103	A86	C-C1-C2-C3
34	R	105	A86	C4-C5-C6-C7
24	G	216	LHG	C2-C3-O3-P
31	P	215	DD6	C-C1-C24-C25
31	U	212	DD6	C-C1-C24-C25
31	T	212	DD6	C12-C11-C13-C14
22	B	804	CLA	C11-C10-C8-C7
22	O	209	CLA	C6-C7-C8-C10
22	P	207	CLA	C11-C12-C13-C15
22	Q	204	CLA	C6-C7-C8-C10
22	G	205	CLA	C11-C10-C8-C7
22	G	206	CLA	C11-C12-C13-C15
30	S	201	SQD	C23-C24-C25-C26
32	U	201	LMG	O6-C5-C6-O5
25	B	836	BCR	C21-C22-C23-C24
25	I	102	BCR	C7-C8-C9-C10
31	O	212	DD6	C2-C1-C24-C25
31	T	212	DD6	C10-C11-C13-C14
31	U	214	DD6	C4-C5-C6-C8
22	A	850	CLA	C2A-CAA-CBA-CGA
32	J	102	LMG	C20-C21-C22-C23
32	Q	217	LMG	C18-C19-C20-C21
32	P	217	LMG	O9-C10-O7-C8
22	A	815	CLA	CAA-CBA-CGA-O2A
22	T	207	CLA	C8-C10-C11-C12
26	M	102	LMU	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
26	K	201	LMU	O1'-C1-C2-C3
22	S	202	CLA	O2A-C1-C2-C3
32	J	102	LMG	C7-C8-O7-C10
22	A	828	CLA	C16-C17-C18-C20
26	S	203	LMU	C1-C2-C3-C4
26	A	847	LMU	O5'-C5'-C6'-O6'
22	A	821	CLA	C8-C10-C11-C12
34	Q	218	A86	O5-C38-O4-C34
34	R	105	A86	C4-C5-C6-C8
24	P	201	LHG	O6-C4-C5-O7
32	J	102	LMG	C7-C8-C9-O8
33	S	210	KC1	C4B-C3B-CAB-CBB
33	T	208	KC1	C4B-C3B-CAB-CBB
22	A	818	CLA	C4-C3-C5-C6
22	A	834	CLA	C4-C3-C5-C6
22	B	814	CLA	CAA-CBA-CGA-O2A
22	R	104	CLA	C2-C3-C5-C6
34	P	204	A86	C28-C27-C29-C30
24	A	840	LHG	C11-C10-C9-C8
32	P	202	LMG	O1-C7-C8-O7
22	B	805	CLA	C10-C11-C12-C13
22	B	842	CLA	C11-C10-C8-C9
22	R	104	CLA	C11-C10-C8-C9
26	F	807	LMU	C3-C4-C5-C6
30	S	201	SQD	C30-C31-C32-C33
22	B	845	CLA	C13-C15-C16-C17
34	Q	201	A86	C13-C14-C15-O1
34	Q	214	A86	C13-C14-C15-O1
34	R	105	A86	C13-C14-C15-O1
34	U	202	A86	C13-C14-C15-O1
33	P	212	KC1	CBD-CGD-O2D-CED
34	P	204	A86	C11-C10-C9-C8
22	A	854	CLA	C2-C3-C5-C6
22	G	206	CLA	C2A-CAA-CBA-CGA
22	A	815	CLA	C8-C10-C11-C12
22	K	207	CLA	C3-C5-C6-C7
26	F	807	LMU	C2-C1-O1'-C1'
31	O	215	DD6	C27-C29-C30-C31
31	P	205	DD6	C27-C29-C30-C31
31	U	203	DD6	C27-C29-C30-C31
31	K	208	DD6	C27-C29-C30-C31
22	L	202	CLA	O2A-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
22	A	814	CLA	C1A-C2A-CAA-CBA
24	A	839	LHG	C24-C23-O8-C6
22	B	822	CLA	C4-C3-C5-C6
22	R	104	CLA	C4-C3-C5-C6
31	S	204	DD6	C5-C6-C8-C9
31	U	212	DD6	C2-C1-C24-C25
34	U	202	A86	C9-C10-C11-C12
29	B	841	DGD	C3B-C4B-C5B-C6B
22	A	820	CLA	C2-C3-C5-C6
30	B	846	SQD	C5-C6-S-O7
26	A	847	LMU	C7-C8-C9-C10
22	Q	216	CLA	C11-C10-C8-C7
22	H	207	CLA	C11-C12-C13-C15
32	S	213	LMG	C29-C30-C31-C32
32	S	213	LMG	C17-C18-C19-C20
22	Q	206	CLA	C4-C3-C5-C6
22	A	834	CLA	C2-C3-C5-C6
22	B	822	CLA	C2-C3-C5-C6
26	P	221	LMU	O5B-C1B-O1B-C4'
22	A	854	CLA	C11-C10-C8-C9
22	G	205	CLA	C11-C10-C8-C9
23	A	837	PQN	C19-C18-C20-C21
25	R	102	BCR	C19-C20-C21-C22
31	G	214	DD6	C24-C25-C26-C27
22	G	207	CLA	C8-C10-C11-C12
22	A	805	CLA	C1-C2-C3-C4
22	B	826	CLA	C1-C2-C3-C4
33	P	219	KC1	C3A-C2A-CAA-CBA
30	B	846	SQD	O6-C44-C45-O47
30	B	846	SQD	O47-C45-C46-O48
32	P	217	LMG	O7-C8-C9-O8
32	Q	217	LMG	O1-C7-C8-O7
32	S	213	LMG	O1-C7-C8-O7
32	P	217	LMG	C2-C1-O1-C7
32	Q	217	LMG	C36-C37-C38-C39
22	A	833	CLA	C13-C15-C16-C17
22	A	853	CLA	C10-C11-C12-C13
22	B	804	CLA	CAD-CBD-CGD-O2D
22	T	204	CLA	CAD-CBD-CGD-O2D
22	T	211	CLA	CAD-CBD-CGD-O2D
22	B	815	CLA	C10-C11-C12-C13
30	B	846	SQD	C34-C35-C36-C37

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Mol	Chain	Res	Type	Atoms
26	K	201	LMU	O5B-C1B-O1B-C4'
26	K	201	LMU	O5'-C5'-C6'-O6'
22	A	802	CLA	CHA-CBD-CGD-O1D
22	A	802	CLA	CHA-CBD-CGD-O2D
22	A	803	CLA	CAD-CBD-CGD-O1D
22	A	814	CLA	CAD-CBD-CGD-O1D
22	A	827	CLA	CHA-CBD-CGD-O1D
22	A	827	CLA	CHA-CBD-CGD-O2D
22	A	855	CLA	CHA-CBD-CGD-O1D
22	B	803	CLA	CHA-CBD-CGD-O1D
22	B	804	CLA	CAD-CBD-CGD-O1D
22	B	827	CLA	CHA-CBD-CGD-O1D
22	B	827	CLA	CHA-CBD-CGD-O2D
22	J	103	CLA	CAD-CBD-CGD-O1D
22	O	202	CLA	CHA-CBD-CGD-O2D
22	Q	209	CLA	CHA-CBD-CGD-O1D
22	U	207	CLA	CAD-CBD-CGD-O1D
22	U	210	CLA	CHA-CBD-CGD-O1D
22	G	204	CLA	CHA-CBD-CGD-O2D
22	T	204	CLA	CAD-CBD-CGD-O1D
22	T	211	CLA	CAD-CBD-CGD-O1D
24	P	201	LHG	C3-O3-P-O5
24	P	201	LHG	C3-O3-P-O6
27	A	849	CL0	CHA-CBD-CGD-O1D
27	A	849	CL0	CHA-CBD-CGD-O2D
31	O	213	DD6	C1-C2-C3-C4
31	P	215	DD6	C1-C2-C3-C4
25	L	205	BCR	C1-C6-C7-C8
22	A	806	CLA	C2-C3-C5-C6
30	S	201	SQD	O48-C23-C24-C25
34	U	202	A86	C12-C11-C13-C14
31	S	214	DD6	C6-C8-C9-C10
32	S	213	LMG	C16-C17-C18-C19
22	G	207	CLA	C11-C12-C13-C15
22	P	207	CLA	C11-C12-C13-C14
22	G	206	CLA	C6-C7-C8-C9
22	G	206	CLA	C11-C12-C13-C14
32	J	102	LMG	C17-C18-C19-C20
29	B	841	DGD	CBB-CCB-CDB-CEB
25	J	104	BCR	C12-C13-C14-C15
25	R	102	BCR	C20-C21-C22-C23
31	S	204	DD6	C9-C10-C11-C13

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Mol	Chain	Res	Type	Atoms
31	S	211	DD6	C9-C10-C11-C13
29	B	841	DGD	O6D-C1D-O3G-C3G
26	K	201	LMU	C4-C5-C6-C7
32	J	102	LMG	C28-C29-C30-C31
26	M	102	LMU	C6-C7-C8-C9
22	O	205	CLA	C16-C17-C18-C20
24	G	216	LHG	O7-C5-C6-O8
31	U	212	DD6	C1-C2-C3-C4
31	k	101	DD6	C1-C2-C3-C4
32	P	202	LMG	C29-C30-C31-C32
22	A	829	CLA	C15-C16-C17-C18
29	B	841	DGD	C3A-C4A-C5A-C6A
22	B	807	CLA	C4-C3-C5-C6
32	J	102	LMG	O1-C7-C8-C9
26	F	806	LMU	C1-C2-C3-C4
26	O	216	LMU	C9-C10-C11-C12
22	A	828	CLA	C16-C17-C18-C19
31	P	215	DD6	C2-C1-C24-C25
24	A	840	LHG	O10-C23-C24-C25
32	Q	217	LMG	C8-C7-O1-C1
24	P	201	LHG	C27-C28-C29-C30
32	J	102	LMG	C21-C22-C23-C24
22	B	807	CLA	C2-C3-C5-C6
22	L	204	CLA	CAA-CBA-CGA-O1A
22	A	848	CLA	C4C-C3C-CAC-CBC
22	B	806	CLA	C4-C3-C5-C6
22	B	811	CLA	C4-C3-C5-C6
34	R	103	A86	C11-C10-C9-C8
22	A	834	CLA	C6-C7-C8-C10
22	A	845	CLA	C11-C10-C8-C7
22	B	842	CLA	C11-C10-C8-C7
22	H	207	CLA	C12-C13-C15-C16
26	K	201	LMU	C2-C3-C4-C5
22	U	206	CLA	CAA-CBA-CGA-O2A
22	A	856	CLA	C3A-C2A-CAA-CBA
22	B	845	CLA	C3A-C2A-CAA-CBA
22	A	831	CLA	CAA-CBA-CGA-O1A
25	B	838	BCR	C20-C21-C22-C37
25	F	805	BCR	C35-C13-C14-C15
25	L	201	BCR	C11-C10-C9-C34
31	G	214	DD6	C-C1-C2-C3
31	K	208	DD6	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
32	S	213	LMG	C38-C39-C40-C41
22	A	807	CLA	C2-C1-O2A-CGA
22	O	208	CLA	C2-C1-O2A-CGA
34	Q	201	A86	C3-C4-C5-C6
22	U	206	CLA	CAA-CBA-CGA-O1A
22	A	814	CLA	CAA-CBA-CGA-O1A
22	B	803	CLA	CAA-CBA-CGA-O2A
25	B	840	BCR	C21-C22-C23-C24
22	U	211	CLA	C4-C3-C5-C6
22	A	818	CLA	C2-C3-C5-C6
22	A	834	CLA	C13-C15-C16-C17
24	A	840	LHG	C10-C11-C12-C13
30	B	846	SQD	C12-C13-C14-C15
22	A	801	CLA	C11-C12-C13-C14
22	A	824	CLA	C14-C13-C15-C16
22	B	802	CLA	C6-C7-C8-C9
22	O	209	CLA	C11-C10-C8-C9
22	S	202	CLA	C11-C10-C8-C9
32	S	213	LMG	C18-C19-C20-C21
22	A	848	CLA	C2C-C3C-CAC-CBC
22	O	206	CLA	C13-C15-C16-C17
31	S	205	DD6	C24-C25-C26-C27
31	G	211	DD6	C3-C4-C5-C6
22	H	206	CLA	CAA-CBA-CGA-O1A
22	A	848	CLA	C4-C3-C5-C6
22	T	204	CLA	C4-C3-C5-C6
22	B	806	CLA	C2-C3-C5-C6
22	B	811	CLA	C1A-C2A-CAA-CBA
22	B	818	CLA	C1A-C2A-CAA-CBA
22	B	824	CLA	C1A-C2A-CAA-CBA
25	B	838	BCR	C20-C21-C22-C23
25	B	840	BCR	C20-C21-C22-C23
25	F	805	BCR	C12-C13-C14-C15
25	L	201	BCR	C11-C10-C9-C8
31	O	201	DD6	C9-C10-C11-C13
31	G	214	DD6	C24-C1-C2-C3
22	H	207	CLA	CBA-CGA-O2A-C1
24	A	840	LHG	O8-C23-C24-C25
25	A	841	BCR	C1-C6-C7-C8
25	A	841	BCR	C23-C24-C25-C26
25	A	843	BCR	C1-C6-C7-C8
25	A	843	BCR	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
25	A	844	BCR	C5-C6-C7-C8
25	B	836	BCR	C23-C24-C25-C30
25	B	837	BCR	C5-C6-C7-C8
25	B	839	BCR	C1-C6-C7-C8
25	B	839	BCR	C23-C24-C25-C26
25	B	840	BCR	C1-C6-C7-C8
25	B	840	BCR	C23-C24-C25-C30
25	F	805	BCR	C1-C6-C7-C8
25	F	805	BCR	C5-C6-C7-C8
25	L	201	BCR	C5-C6-C7-C8
25	L	201	BCR	C23-C24-C25-C30
25	L	205	BCR	C5-C6-C7-C8
25	L	205	BCR	C23-C24-C25-C26
25	R	102	BCR	C23-C24-C25-C26
25	k	104	BCR	C5-C6-C7-C8
25	k	104	BCR	C23-C24-C25-C30
22	A	831	CLA	CAA-CBA-CGA-O2A
22	P	214	CLA	CAA-CBA-CGA-O2A
22	A	804	CLA	C4-C3-C5-C6
22	A	851	CLA	C4-C3-C5-C6
22	B	808	CLA	C4-C3-C5-C6
32	Q	217	LMG	C17-C18-C19-C20
22	G	205	CLA	C5-C6-C7-C8
22	B	816	CLA	C12-C13-C15-C16
22	R	104	CLA	C11-C12-C13-C15
22	A	846	CLA	C2A-CAA-CBA-CGA
22	H	208	CLA	C2A-CAA-CBA-CGA
24	P	201	LHG	O7-C5-C6-O8
22	A	814	CLA	CAA-CBA-CGA-O2A
22	B	832	CLA	C16-C17-C18-C20
31	G	214	DD6	C-C1-C24-C25
22	B	816	CLA	C4-C3-C5-C6
22	Q	204	CLA	C4-C3-C5-C6
22	A	833	CLA	C10-C11-C12-C13
22	A	836	CLA	C15-C16-C17-C18
22	G	206	CLA	C5-C6-C7-C8
22	A	804	CLA	C2-C3-C5-C6
22	A	851	CLA	C2-C3-C5-C6
22	P	214	CLA	CAA-CBA-CGA-O1A
22	G	206	CLA	C13-C15-C16-C17
22	B	803	CLA	CAA-CBA-CGA-O1A
22	A	850	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
22	B	827	CLA	C4-C3-C5-C6
22	U	205	CLA	C4-C3-C5-C6
22	U	211	CLA	C2-C3-C5-C6
22	H	207	CLA	O1A-CGA-O2A-C1
32	Q	217	LMG	O10-C28-O8-C9
24	G	216	LHG	C4-C5-C6-O8
22	O	209	CLA	C5-C6-C7-C8
22	P	207	CLA	C2A-CAA-CBA-CGA
22	H	206	CLA	CAA-CBA-CGA-O2A
22	B	832	CLA	C15-C16-C17-C18
23	A	837	PQN	C18-C20-C21-C22
31	O	212	DD6	C27-C29-C30-C31
31	P	218	DD6	C27-C29-C30-C31
31	U	214	DD6	C27-C29-C30-C31
22	A	845	CLA	C10-C11-C12-C13
22	H	207	CLA	C15-C16-C17-C18
22	G	203	CLA	CAA-CBA-CGA-O1A
22	G	203	CLA	CAA-CBA-CGA-O2A
22	O	205	CLA	C16-C17-C18-C19
34	Q	214	A86	C-C1-C2-C3
22	S	209	CLA	CAA-CBA-CGA-O2A
26	S	203	LMU	C3-C4-C5-C6
22	B	805	CLA	C4-C3-C5-C6
22	G	201	CLA	CAA-CBA-CGA-O1A
22	T	204	CLA	C2-C3-C5-C6
22	S	202	CLA	C5-C6-C7-C8
22	K	206	CLA	CAA-CBA-CGA-O2A
22	G	201	CLA	CAA-CBA-CGA-O2A
22	A	851	CLA	C11-C10-C8-C9
22	Q	216	CLA	C11-C10-C8-C9
22	Q	206	CLA	C2A-CAA-CBA-CGA
22	Q	213	CLA	C2A-CAA-CBA-CGA
22	A	830	CLA	C2-C1-O2A-CGA
22	A	836	CLA	C2-C1-O2A-CGA
22	U	207	CLA	C2-C1-O2A-CGA
22	U	211	CLA	C2-C1-O2A-CGA
22	G	206	CLA	C2-C1-O2A-CGA
22	A	804	CLA	C10-C11-C12-C13
22	A	853	CLA	C3A-C2A-CAA-CBA
22	O	207	CLA	C3A-C2A-CAA-CBA
22	H	205	CLA	C3A-C2A-CAA-CBA
22	H	210	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
22	B	808	CLA	C2-C3-C5-C6
22	B	814	CLA	C2-C3-C5-C6
22	A	824	CLA	O2A-C1-C2-C3
26	K	201	LMU	C1-C2-C3-C4
22	G	207	CLA	C11-C12-C13-C14
24	A	839	LHG	C34-C35-C36-C37
34	R	103	A86	C24-C1-C2-C3
30	S	201	SQD	C10-C11-C12-C13
22	B	826	CLA	O2A-C1-C2-C3
26	F	806	LMU	O5'-C1'-O1'-C1
22	K	206	CLA	CAA-CBA-CGA-O1A
32	Q	217	LMG	C7-C8-C9-O8
24	P	201	LHG	C25-C26-C27-C28
30	B	846	SQD	C25-C26-C27-C28
22	B	828	CLA	C4-C3-C5-C6
26	F	806	LMU	C11-C10-C9-C8
29	B	841	DGD	C1B-C2B-C3B-C4B
32	S	213	LMG	C32-C33-C34-C35
32	J	102	LMG	O1-C7-C8-O7
22	A	801	CLA	C8-C10-C11-C12
22	Q	209	CLA	C11-C10-C8-C9
22	Q	212	CLA	C11-C10-C8-C9
22	H	207	CLA	C11-C12-C13-C14
22	A	808	CLA	C4-C3-C5-C6
32	P	202	LMG	C4-C5-C6-O5
22	A	801	CLA	C11-C12-C13-C15
22	H	213	CLA	C6-C7-C8-C10
22	K	207	CLA	C11-C10-C8-C7
22	A	805	CLA	C2B-C3B-CAB-CBB
22	A	825	CLA	C2B-C3B-CAB-CBB
22	A	832	CLA	C2B-C3B-CAB-CBB
22	A	833	CLA	C2B-C3B-CAB-CBB
22	A	851	CLA	C2B-C3B-CAB-CBB
22	A	853	CLA	C2B-C3B-CAB-CBB
22	A	854	CLA	C2B-C3B-CAB-CBB
22	A	856	CLA	C2B-C3B-CAB-CBB
22	B	804	CLA	C2B-C3B-CAB-CBB
22	B	810	CLA	C2B-C3B-CAB-CBB
22	B	823	CLA	C2B-C3B-CAB-CBB
22	B	834	CLA	C2B-C3B-CAB-CBB
22	L	202	CLA	C2B-C3B-CAB-CBB
22	L	204	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
22	O	205	CLA	C2B-C3B-CAB-CBB
22	P	209	CLA	C2B-C3B-CAB-CBB
22	Q	207	CLA	C2B-C3B-CAB-CBB
22	Q	213	CLA	C2B-C3B-CAB-CBB
22	S	207	CLA	C2B-C3B-CAB-CBB
22	S	209	CLA	C2B-C3B-CAB-CBB
22	U	204	CLA	C2B-C3B-CAB-CBB
22	U	206	CLA	C2B-C3B-CAB-CBB
22	U	210	CLA	C2B-C3B-CAB-CBB
22	G	204	CLA	C2B-C3B-CAB-CBB
22	H	204	CLA	C2B-C3B-CAB-CBB
22	K	205	CLA	C2B-C3B-CAB-CBB
22	T	202	CLA	C2B-C3B-CAB-CBB
22	T	203	CLA	C2B-C3B-CAB-CBB
22	k	103	CLA	C2B-C3B-CAB-CBB
25	A	841	BCR	C5-C6-C7-C8
25	A	842	BCR	C23-C24-C25-C26
25	A	842	BCR	C23-C24-C25-C30
25	B	836	BCR	C23-C24-C25-C26
25	B	838	BCR	C5-C6-C7-C8
25	B	839	BCR	C5-C6-C7-C8
25	B	840	BCR	C5-C6-C7-C8
25	B	840	BCR	C23-C24-C25-C26
25	I	102	BCR	C1-C6-C7-C8
25	I	102	BCR	C5-C6-C7-C8
25	L	201	BCR	C23-C24-C25-C26
25	M	101	BCR	C5-C6-C7-C8
25	M	101	BCR	C23-C24-C25-C30
25	k	104	BCR	C23-C24-C25-C26
22	A	827	CLA	C2-C1-O2A-CGA
22	B	801	CLA	C2-C1-O2A-CGA
22	P	210	CLA	CAA-CBA-CGA-O2A
32	P	217	LMG	O7-C10-C11-C12
24	A	839	LHG	O8-C23-C24-C25
22	A	808	CLA	C2-C3-C5-C6
22	Q	212	CLA	C15-C16-C17-C18
22	A	811	CLA	CAA-CBA-CGA-O2A
32	P	202	LMG	O7-C10-C11-C12
22	A	804	CLA	C3-C5-C6-C7
24	P	201	LHG	C15-C16-C17-C18
22	B	808	CLA	CAA-CBA-CGA-O2A
22	U	208	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
22	A	822	CLA	C15-C16-C17-C18
22	Q	206	CLA	C2-C3-C5-C6
22	G	215	CLA	CAA-CBA-CGA-O2A
31	k	101	DD6	C4-C5-C6-C7
22	B	833	CLA	C10-C11-C12-C13
24	A	840	LHG	C9-C10-C11-C12
22	B	843	CLA	CAA-CBA-CGA-O2A
22	A	815	CLA	CAA-CBA-CGA-O1A
22	B	814	CLA	CAA-CBA-CGA-O1A
31	H	201	DD6	C27-C29-C30-C31
31	k	101	DD6	C27-C29-C30-C31
22	G	210	CLA	CAA-CBA-CGA-O1A
32	S	213	LMG	C40-C41-C42-C43
22	B	816	CLA	C11-C10-C8-C9
22	U	211	CLA	CAA-CBA-CGA-O2A
22	G	205	CLA	CAA-CBA-CGA-O2A
22	T	211	CLA	CAA-CBA-CGA-O2A
22	k	103	CLA	CAA-CBA-CGA-O2A
22	A	809	CLA	C1A-C2A-CAA-CBA
22	A	853	CLA	C1A-C2A-CAA-CBA
22	B	804	CLA	C1A-C2A-CAA-CBA
22	B	842	CLA	C1A-C2A-CAA-CBA
22	O	207	CLA	C1A-C2A-CAA-CBA
22	U	211	CLA	C4B-C3B-CAB-CBB
22	H	203	CLA	C4B-C3B-CAB-CBB
22	T	201	CLA	C4B-C3B-CAB-CBB
34	Q	214	A86	O-C13-C14-C15
22	H	210	CLA	CAA-CBA-CGA-O1A
22	T	210	CLA	CAA-CBA-CGA-O2A
22	A	848	CLA	C2-C3-C5-C6
31	G	214	DD6	C2-C1-C24-C25
22	H	210	CLA	CAA-CBA-CGA-O2A
22	A	821	CLA	CAA-CBA-CGA-O2A
22	B	805	CLA	CAA-CBA-CGA-O2A
22	H	208	CLA	CAA-CBA-CGA-O2A
22	A	815	CLA	C2A-CAA-CBA-CGA
22	B	802	CLA	C2A-CAA-CBA-CGA
22	B	804	CLA	C2A-CAA-CBA-CGA
22	T	203	CLA	C2A-CAA-CBA-CGA
26	A	857	LMU	C6-C7-C8-C9
22	A	815	CLA	C13-C15-C16-C17
22	A	845	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
22	T	207	CLA	C2-C1-O2A-CGA
27	A	849	CL0	C2-C1-O2A-CGA
24	G	216	LHG	O7-C7-C8-C9
22	Q	209	CLA	C6-C7-C8-C10
22	B	833	CLA	C16-C17-C18-C19
22	O	204	CLA	C16-C17-C18-C19
24	G	216	LHG	C23-C24-C25-C26
22	A	836	CLA	O2A-C1-C2-C3
22	A	802	CLA	CAA-CBA-CGA-O2A
22	B	806	CLA	C2A-CAA-CBA-CGA
22	U	205	CLA	C2A-CAA-CBA-CGA
22	Q	205	CLA	C5-C6-C7-C8
22	B	843	CLA	C16-C17-C18-C20
22	H	203	CLA	CAA-CBA-CGA-O2A
22	P	210	CLA	CAA-CBA-CGA-O1A
22	T	204	CLA	C8-C10-C11-C12
22	B	814	CLA	C5-C6-C7-C8
22	G	210	CLA	CAA-CBA-CGA-O2A
22	B	829	CLA	C10-C11-C12-C13
22	S	209	CLA	C3A-C2A-CAA-CBA
22	U	207	CLA	C3A-C2A-CAA-CBA
22	G	205	CLA	C3A-C2A-CAA-CBA
25	B	837	BCR	C11-C10-C9-C8
31	H	201	DD6	C9-C10-C11-C13
22	G	215	CLA	CAA-CBA-CGA-O1A
22	P	207	CLA	C15-C16-C17-C18
30	B	846	SQD	O49-C7-C8-C9
30	S	201	SQD	O10-C23-C24-C25
32	J	102	LMG	O9-C10-C11-C12
32	Q	217	LMG	C22-C23-C24-C25
22	B	801	CLA	C15-C16-C17-C18
30	S	201	SQD	C11-C10-C9-C8
22	F	804	CLA	CAA-CBA-CGA-O2A
22	A	811	CLA	CAA-CBA-CGA-O1A
22	k	103	CLA	CAA-CBA-CGA-O1A
30	B	846	SQD	C14-C15-C16-C17
24	P	201	LHG	C31-C32-C33-C34
22	B	808	CLA	CAA-CBA-CGA-O1A
22	B	843	CLA	CAA-CBA-CGA-O1A
22	U	208	CLA	CAA-CBA-CGA-O1A
32	Q	217	LMG	O10-C28-C29-C30
22	B	847	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
22	A	853	CLA	C2-C3-C5-C6
33	P	203	KC1	C3A-C2A-CAA-CBA
22	A	854	CLA	C5-C6-C7-C8
22	O	205	CLA	C15-C16-C17-C18
25	J	104	BCR	C7-C8-C9-C10
22	B	805	CLA	CAA-CBA-CGA-O1A
32	J	102	LMG	C8-C7-O1-C1
22	U	211	CLA	CAA-CBA-CGA-O1A
22	H	208	CLA	CAA-CBA-CGA-O1A
24	G	216	LHG	O9-C7-C8-C9
32	P	217	LMG	O9-C10-C11-C12
22	A	803	CLA	C2A-CAA-CBA-CGA
32	U	201	LMG	C7-C8-C9-O8
22	G	205	CLA	CAA-CBA-CGA-O1A
22	T	210	CLA	CAA-CBA-CGA-O1A
27	A	849	CL0	C4-C3-C5-C6
22	G	206	CLA	CAA-CBA-CGA-O2A
22	A	828	CLA	C10-C11-C12-C13
22	A	848	CLA	C10-C11-C12-C13
22	A	805	CLA	CAD-CBD-CGD-O2D
22	A	826	CLA	CAD-CBD-CGD-O2D
22	A	835	CLA	CAD-CBD-CGD-O2D
22	B	812	CLA	CAD-CBD-CGD-O2D
22	B	829	CLA	CAD-CBD-CGD-O2D
22	F	803	CLA	CAD-CBD-CGD-O2D
22	T	203	CLA	CAD-CBD-CGD-O2D
33	P	206	KC1	CAD-CBD-CGD-O2D
22	B	817	CLA	CAA-CBA-CGA-O2A
32	Q	217	LMG	O8-C28-C29-C30
24	A	839	LHG	O10-C23-C24-C25
22	L	204	CLA	C2-C1-O2A-CGA
32	P	202	LMG	O9-C10-C11-C12
22	H	207	CLA	C1-C2-C3-C4
22	B	833	CLA	C16-C17-C18-C20
22	T	211	CLA	CAA-CBA-CGA-O1A
22	A	803	CLA	CAA-CBA-CGA-O2A
22	B	801	CLA	CAA-CBA-CGA-O2A
22	B	802	CLA	CAA-CBA-CGA-O2A
30	B	846	SQD	O47-C7-C8-C9
32	J	102	LMG	O7-C10-C11-C12
22	Q	209	CLA	C10-C11-C12-C13
22	P	208	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
22	Q	203	CLA	CAA-CBA-CGA-O2A
22	A	821	CLA	CAA-CBA-CGA-O1A
32	S	213	LMG	O9-C10-C11-C12

There are no ring outliers.

190 monomers are involved in 325 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	A	807	CLA	2	0
22	B	828	CLA	4	0
26	K	201	LMU	2	0
22	P	213	CLA	1	0
22	G	208	CLA	1	0
25	B	838	BCR	2	0
22	S	206	CLA	3	0
25	L	205	BCR	1	0
22	Q	213	CLA	1	0
22	A	822	CLA	1	0
22	B	804	CLA	2	0
25	J	104	BCR	1	0
22	U	211	CLA	4	0
22	O	205	CLA	4	0
25	F	801	BCR	1	0
22	B	807	CLA	2	0
22	H	207	CLA	2	0
23	B	835	PQN	1	0
22	A	835	CLA	4	0
24	G	216	LHG	1	0
22	A	838	CLA	1	0
25	B	839	BCR	4	0
25	I	101	BCR	3	0
22	B	827	CLA	1	0
22	A	854	CLA	3	0
22	A	816	CLA	6	0
22	B	810	CLA	1	0
22	k	103	CLA	2	0
32	P	217	LMG	3	0
22	B	806	CLA	4	0
22	Q	204	CLA	2	0
22	k	102	CLA	2	0
22	B	803	CLA	1	0
22	U	209	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	A	848	CLA	3	0
22	B	805	CLA	3	0
22	B	845	CLA	6	0
32	P	202	LMG	1	0
33	T	208	KC1	1	0
26	M	102	LMU	1	0
22	P	207	CLA	2	0
22	T	201	CLA	1	0
22	Q	216	CLA	1	0
32	Q	217	LMG	3	0
22	B	823	CLA	3	0
22	Q	203	CLA	1	0
25	F	805	BCR	3	0
22	B	826	CLA	5	0
22	L	204	CLA	1	0
22	B	812	CLA	2	0
22	B	824	CLA	3	0
22	A	824	CLA	4	0
31	U	212	DD6	1	0
22	A	820	CLA	1	0
30	B	846	SQD	1	0
22	G	202	CLA	1	0
22	A	833	CLA	2	0
22	Q	212	CLA	1	0
25	M	101	BCR	1	0
25	R	102	BCR	3	0
22	A	811	CLA	2	0
22	G	205	CLA	4	0
22	B	847	CLA	3	0
22	H	213	CLA	7	0
22	T	206	CLA	2	0
22	P	210	CLA	2	0
29	B	841	DGD	9	0
31	G	211	DD6	1	0
22	A	814	CLA	2	0
22	P	211	CLA	1	0
22	B	821	CLA	2	0
22	U	205	CLA	2	0
22	A	810	CLA	3	0
22	A	823	CLA	1	0
22	B	808	CLA	1	0
25	A	843	BCR	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	B	814	CLA	3	0
22	U	206	CLA	1	0
22	H	209	CLA	1	0
22	B	829	CLA	2	0
27	A	849	CL0	3	0
22	F	804	CLA	2	0
32	J	102	LMG	3	0
22	A	845	CLA	3	0
22	A	851	CLA	2	0
22	B	815	CLA	2	0
25	B	836	BCR	2	0
22	B	844	CLA	2	0
22	L	203	CLA	1	0
34	R	103	A86	1	0
22	B	822	CLA	1	0
22	Q	208	CLA	2	0
22	K	205	CLA	1	0
22	B	818	CLA	4	0
22	T	211	CLA	1	0
25	k	104	BCR	2	0
22	A	831	CLA	3	0
22	A	801	CLA	4	0
22	T	210	CLA	7	0
22	R	101	CLA	1	0
22	S	209	CLA	1	0
22	H	205	CLA	1	0
22	O	207	CLA	1	0
22	S	216	CLA	3	0
25	A	842	BCR	1	0
22	P	208	CLA	1	0
22	O	202	CLA	2	0
32	U	201	LMG	1	0
22	F	802	CLA	2	0
31	G	214	DD6	2	0
22	B	820	CLA	3	0
22	P	214	CLA	1	0
22	A	817	CLA	2	0
22	A	836	CLA	4	0
22	A	855	CLA	1	0
22	A	850	CLA	2	0
22	U	208	CLA	2	0
22	A	853	CLA	3	0

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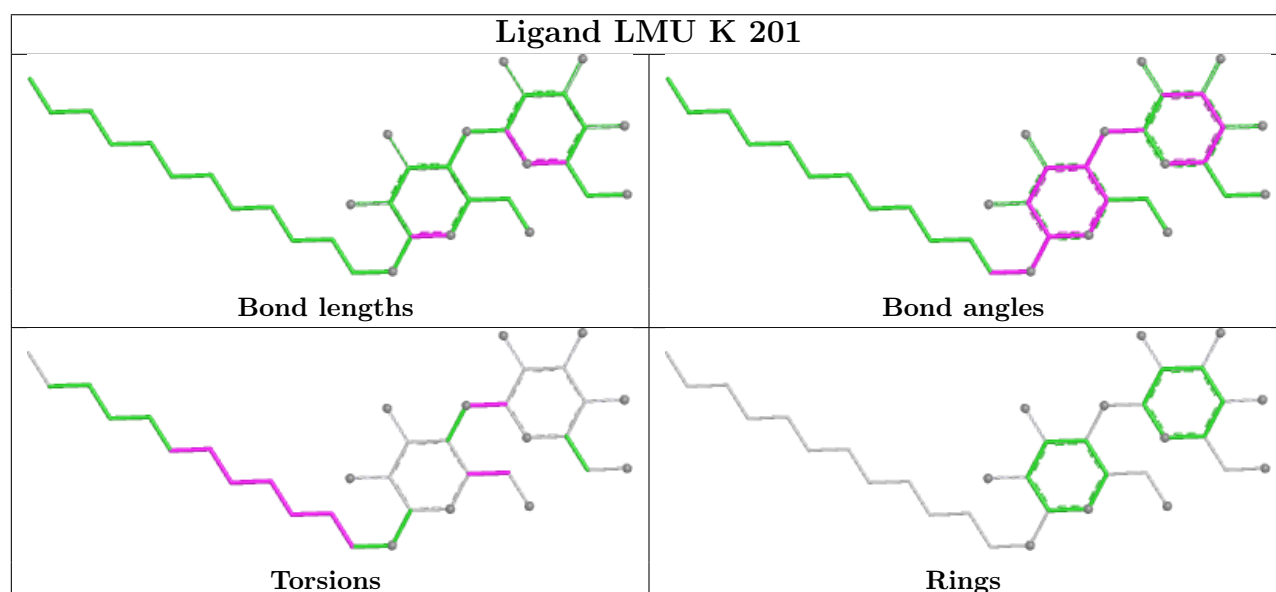
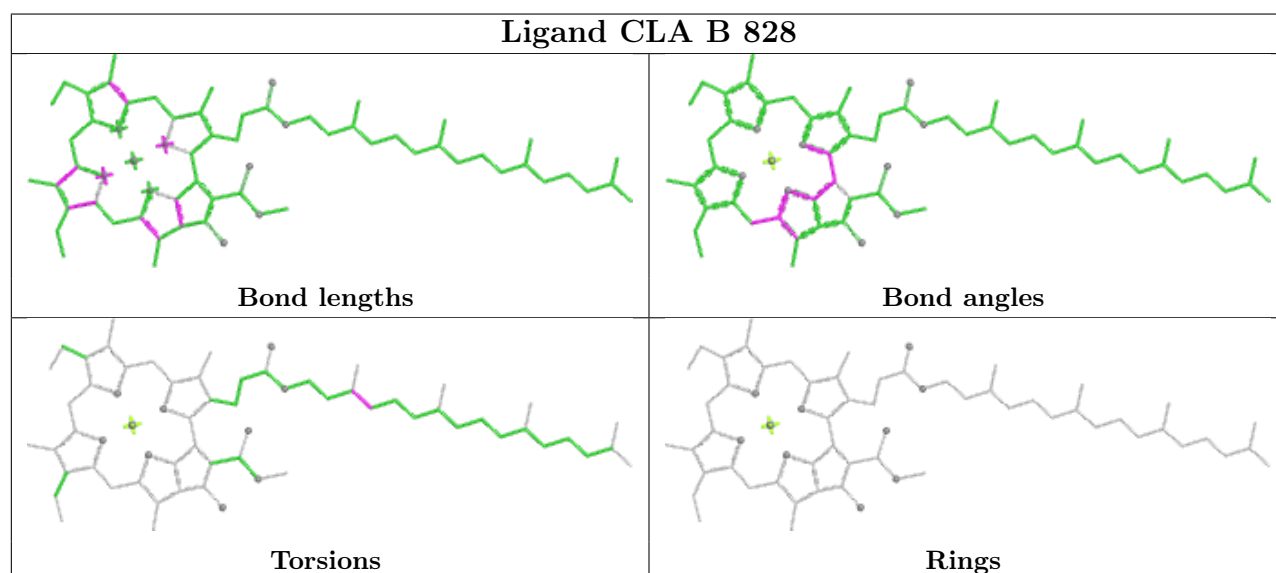
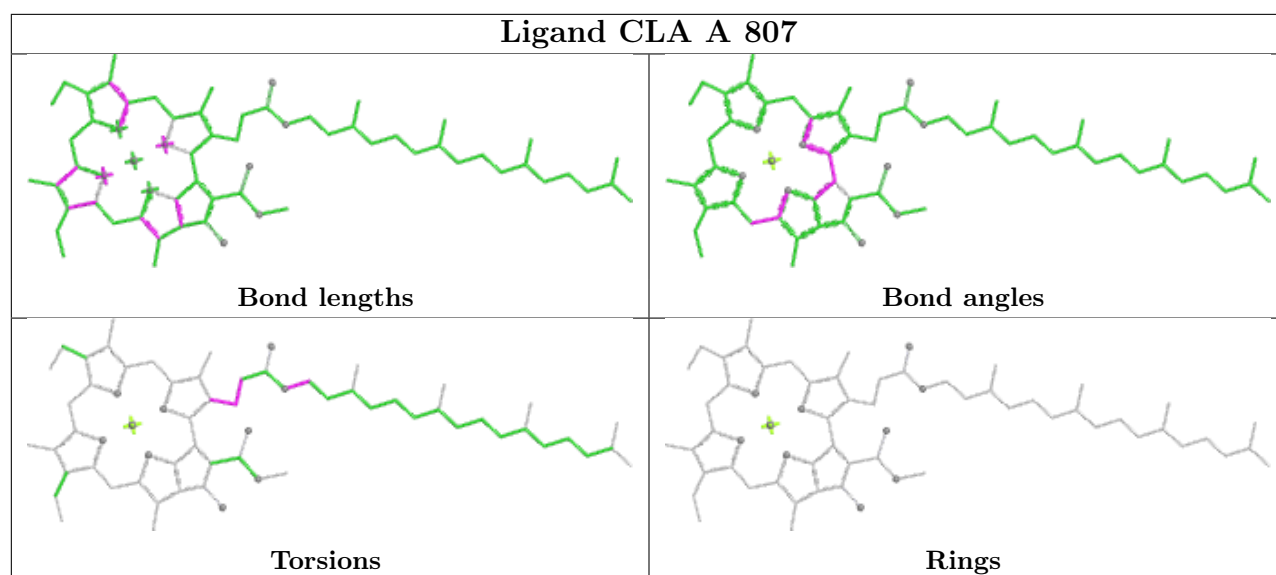
Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	G	215	CLA	1	0
22	O	209	CLA	4	0
22	S	202	CLA	2	0
22	A	825	CLA	2	0
22	G	203	CLA	1	0
22	B	809	CLA	2	0
22	O	208	CLA	1	0
22	H	210	CLA	1	0
22	G	209	CLA	6	0
22	G	207	CLA	1	0
23	A	837	PQN	2	0
28	C	102	SF4	1	0
22	B	817	CLA	2	0
24	A	839	LHG	2	0
22	A	805	CLA	1	0
26	A	847	LMU	1	0
25	L	201	BCR	1	0
22	A	826	CLA	3	0
22	K	207	CLA	3	0
22	B	819	CLA	2	0
25	B	840	BCR	2	0
22	K	206	CLA	1	0
22	B	801	CLA	2	0
25	A	841	BCR	1	0
22	B	802	CLA	4	0
22	L	202	CLA	2	0
25	I	102	BCR	2	0
22	G	201	CLA	1	0
22	A	846	CLA	2	0
22	H	202	CLA	1	0
22	B	831	CLA	1	0
22	B	816	CLA	3	0
26	F	806	LMU	1	0
22	A	802	CLA	1	0
22	A	828	CLA	1	0
22	T	209	CLA	1	0
22	R	104	CLA	4	0
22	T	207	CLA	2	0
22	H	203	CLA	1	0
22	O	203	CLA	1	0
22	S	217	CLA	2	0
22	T	205	CLA	1	0

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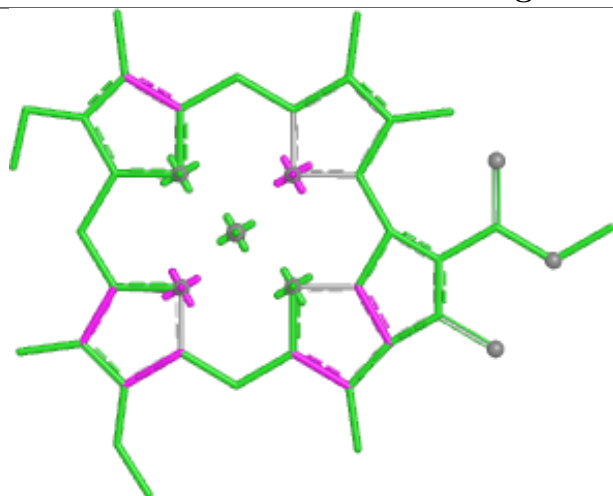
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	S	213	LMG	2	0
22	B	832	CLA	2	0
22	B	833	CLA	2	0
22	A	815	CLA	1	0
25	B	837	BCR	4	0
22	J	103	CLA	1	0
22	U	207	CLA	2	0
24	P	201	LHG	4	0
24	A	840	LHG	1	0
22	U	204	CLA	1	0
22	A	803	CLA	2	0
22	A	813	CLA	1	0
22	G	204	CLA	1	0
22	G	206	CLA	5	0
22	U	210	CLA	3	0
22	K	204	CLA	2	0
22	K	203	CLA	1	0
22	B	834	CLA	7	0
22	B	842	CLA	2	0
25	A	844	BCR	1	0
22	S	208	CLA	2	0
22	T	204	CLA	7	0
30	S	201	SQD	1	0
22	B	830	CLA	4	0
31	O	212	DD6	2	0
22	A	808	CLA	2	0
26	S	203	LMU	1	0
22	H	206	CLA	1	0
22	A	829	CLA	1	0
26	L	206	LMU	2	0

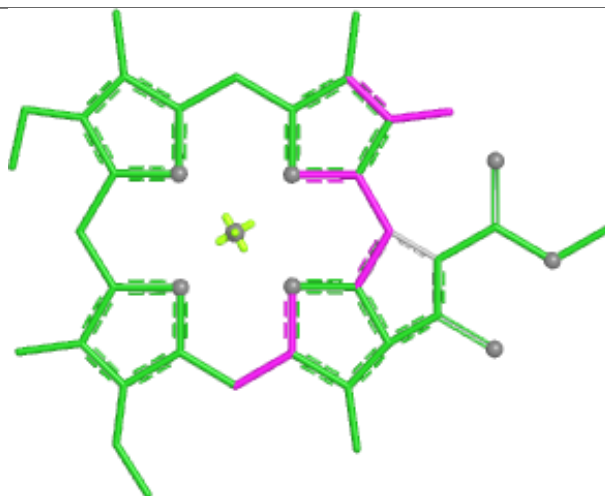
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



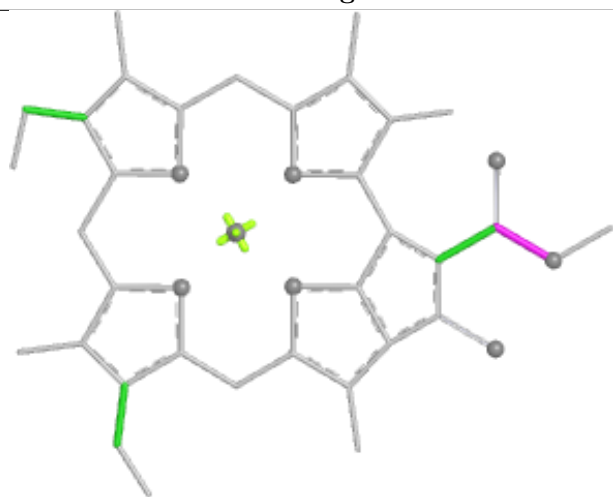
Ligand CLA P 213



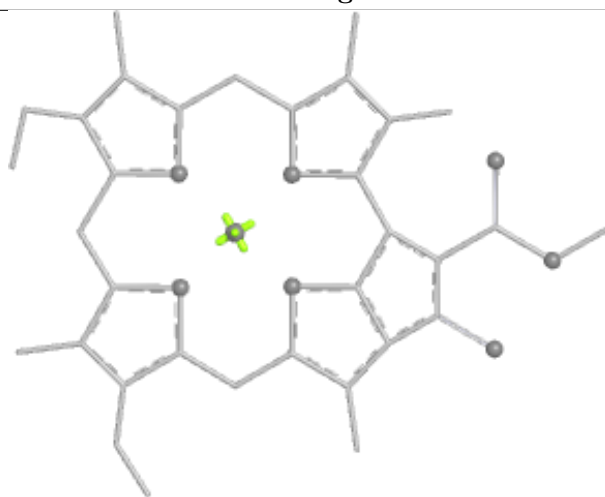
Bond lengths



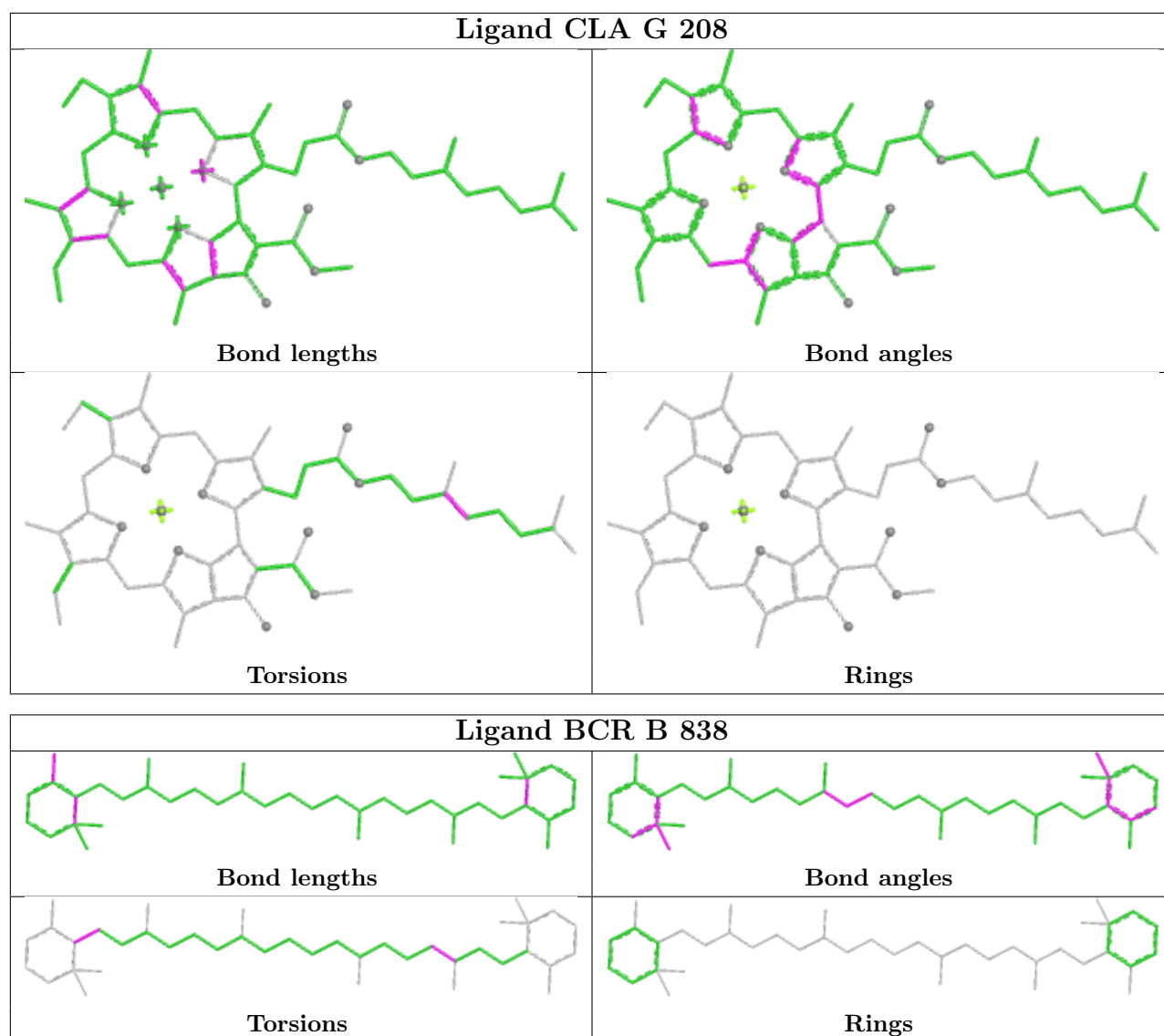
Bond angles



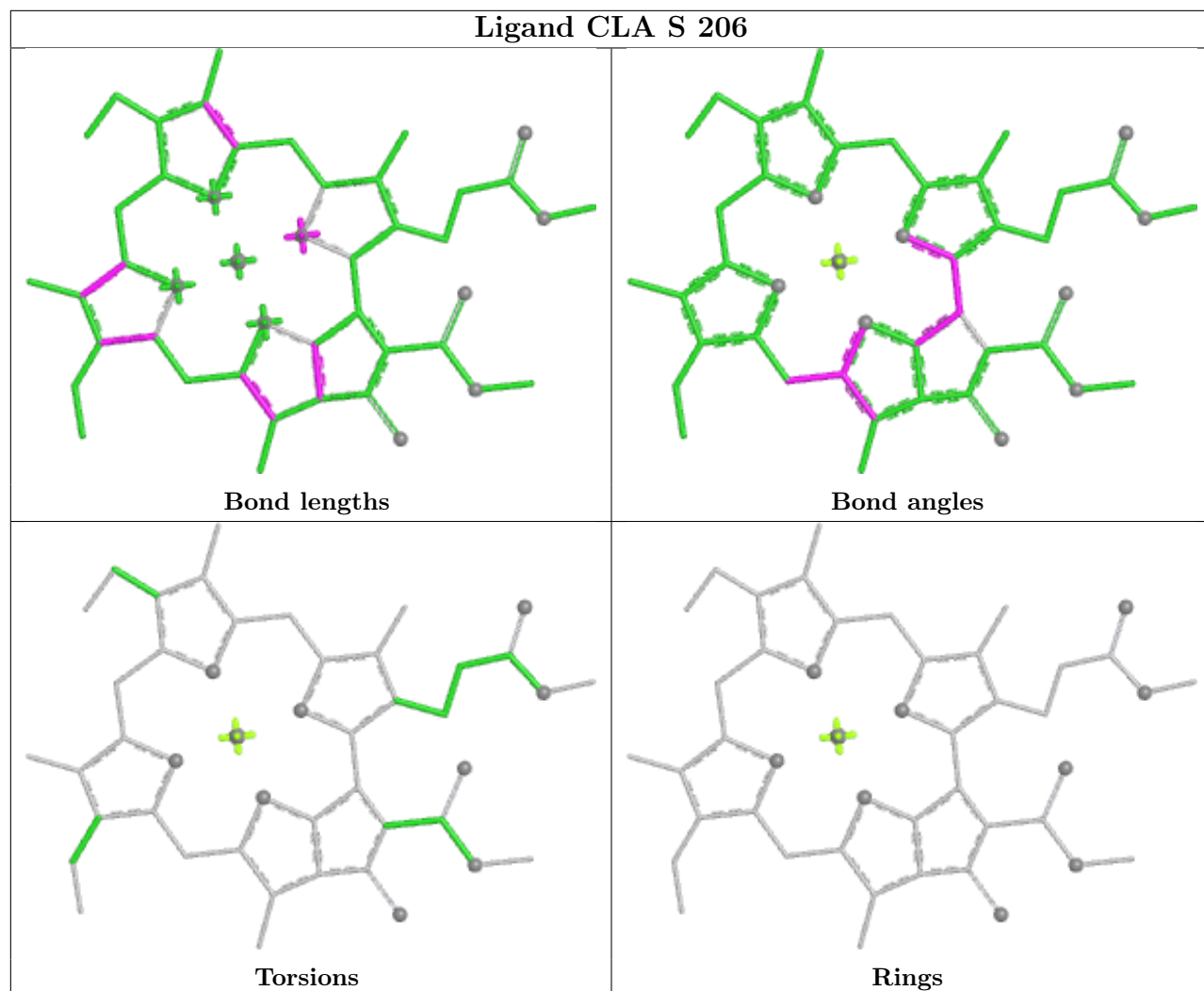
Torsions



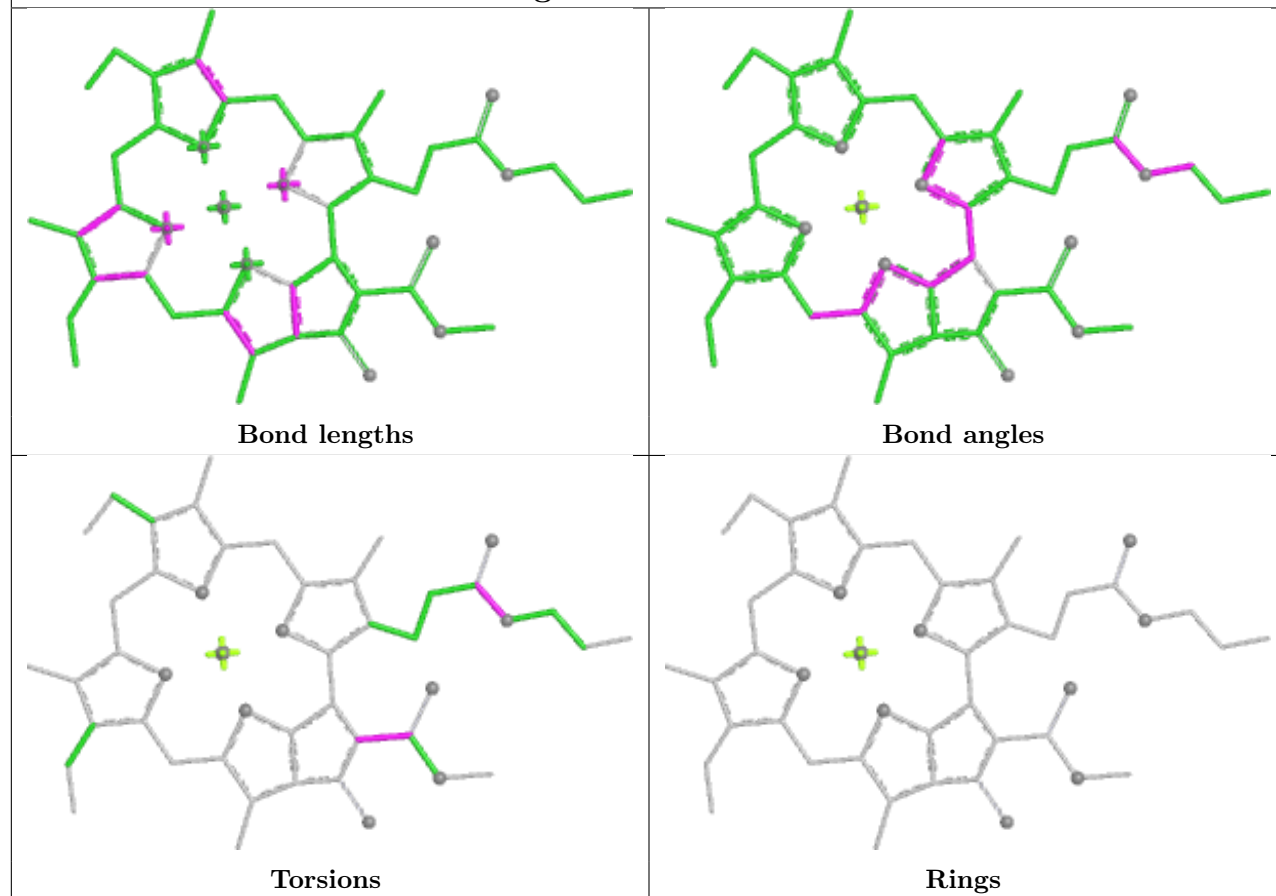
Rings



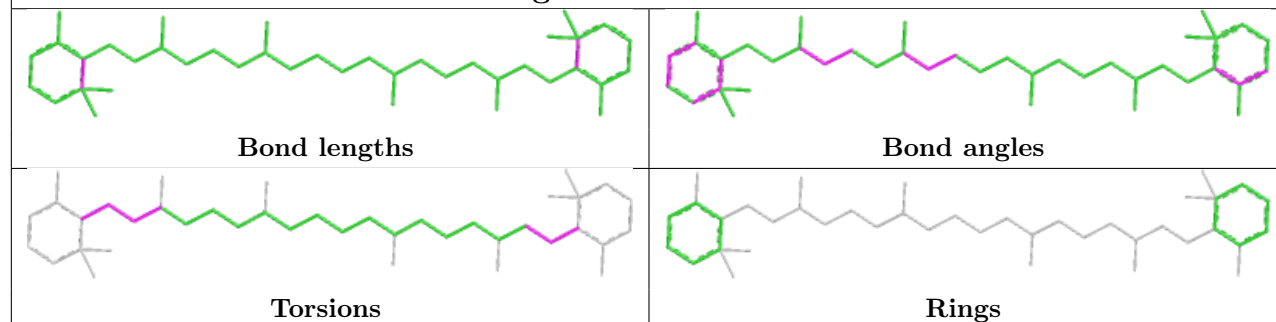
Ligand CLA S 206



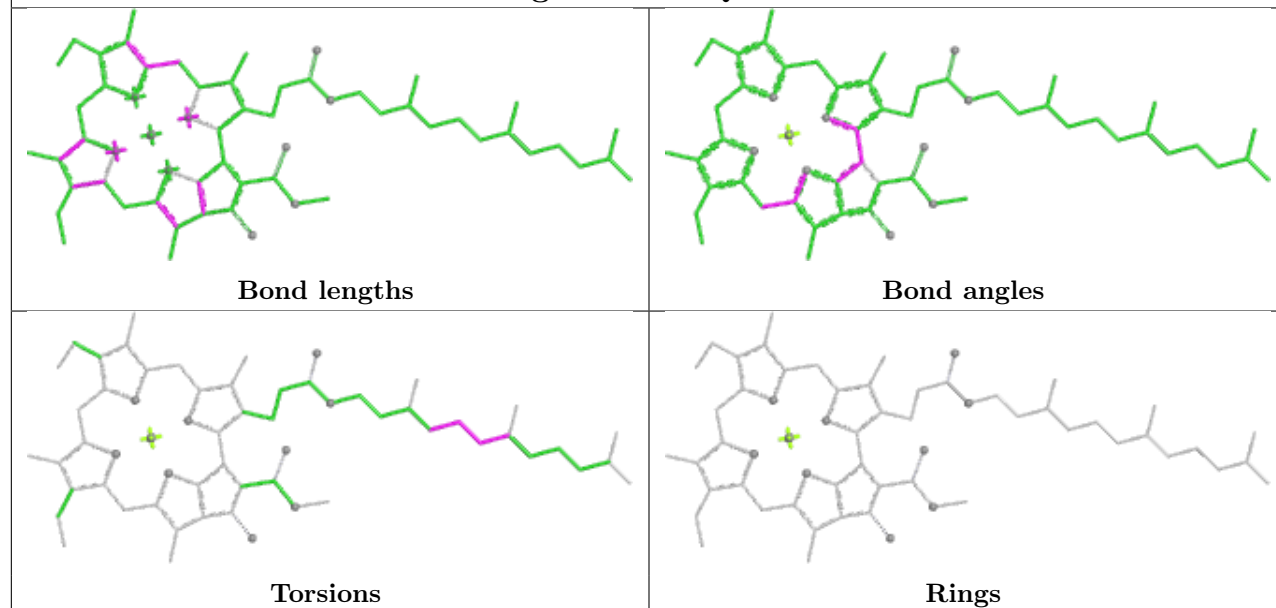
Ligand CLA F 803



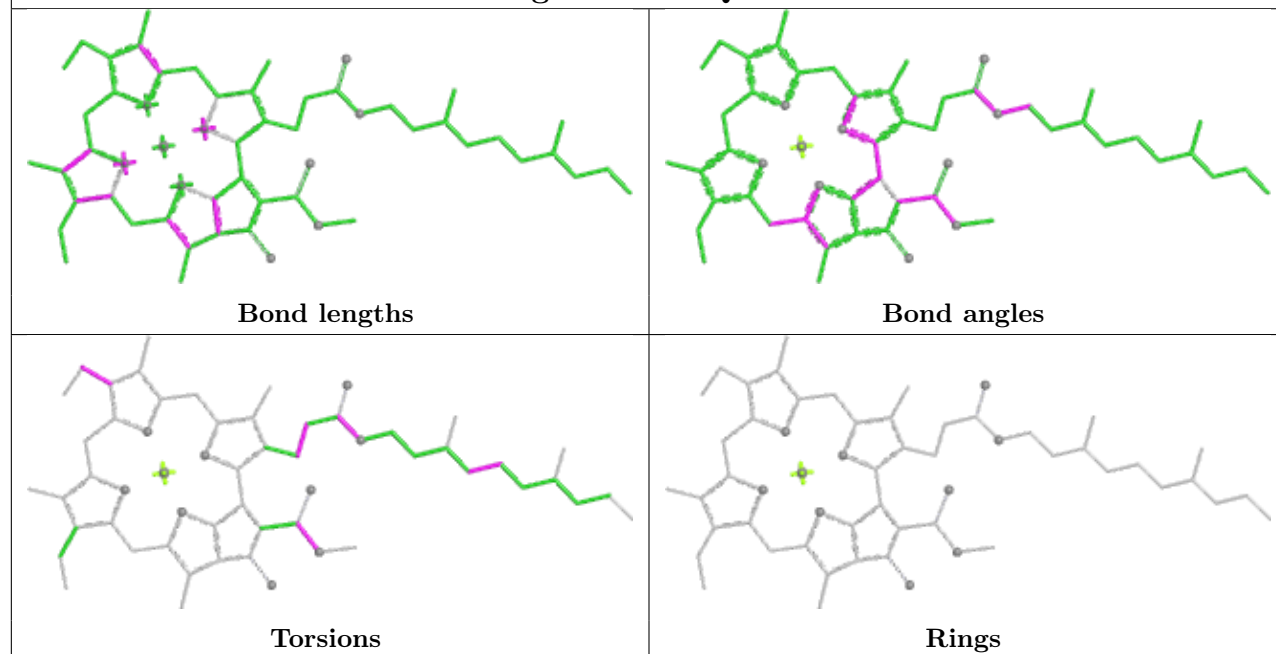
Ligand BCR L 205

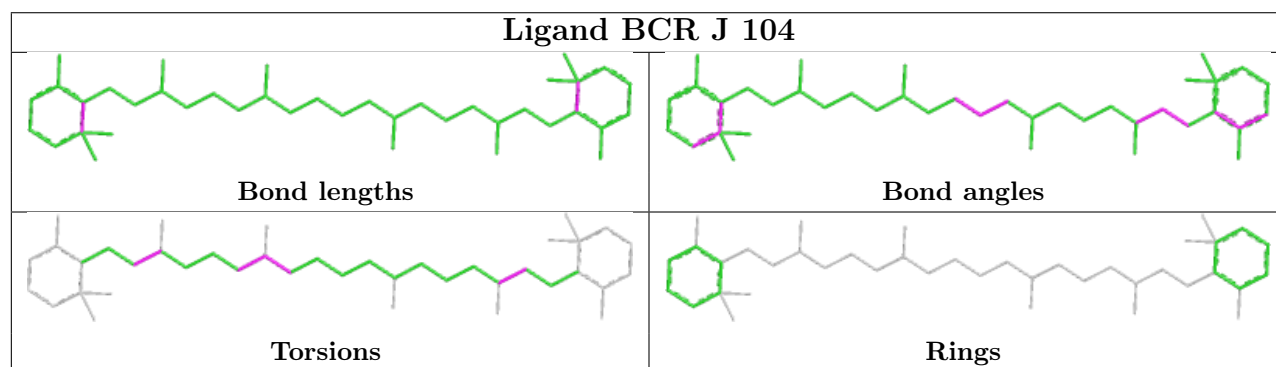
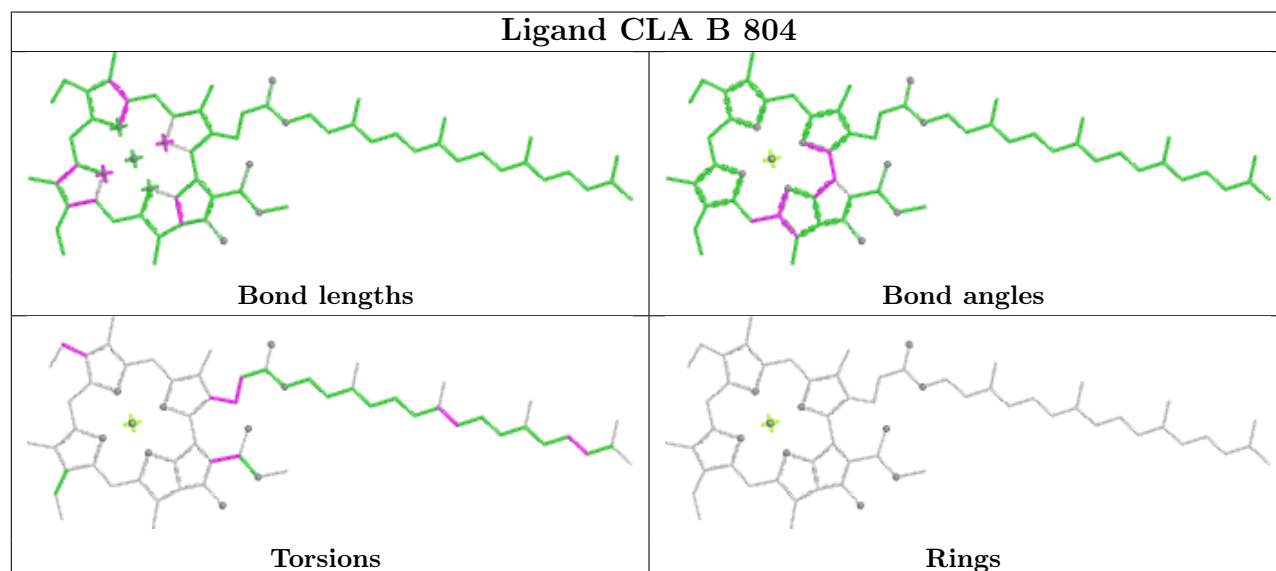
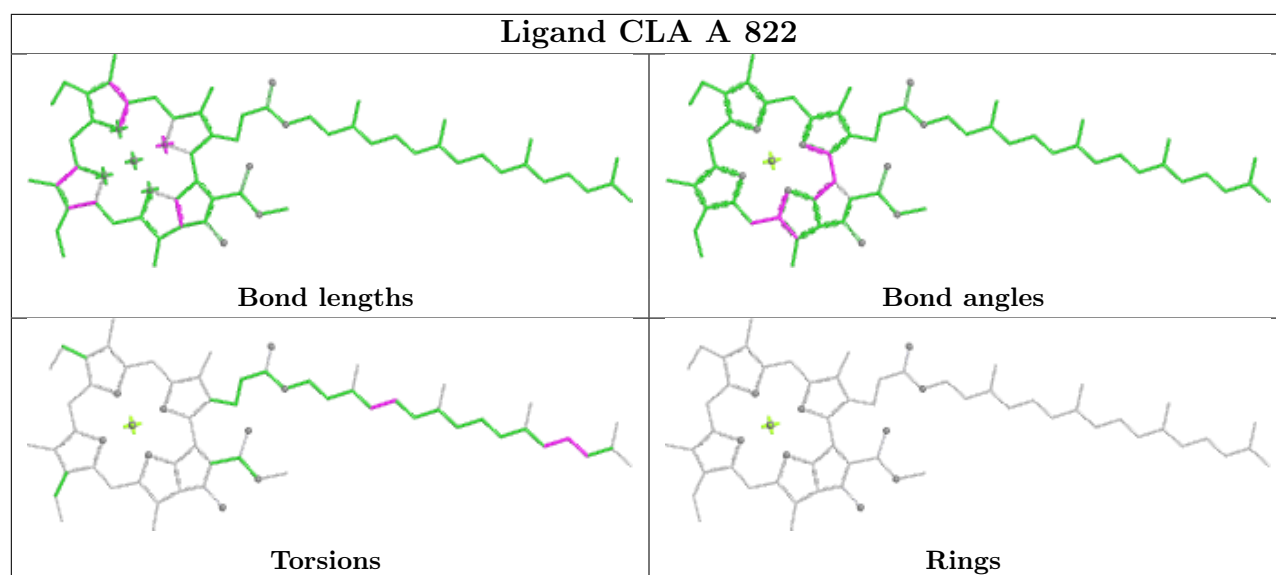


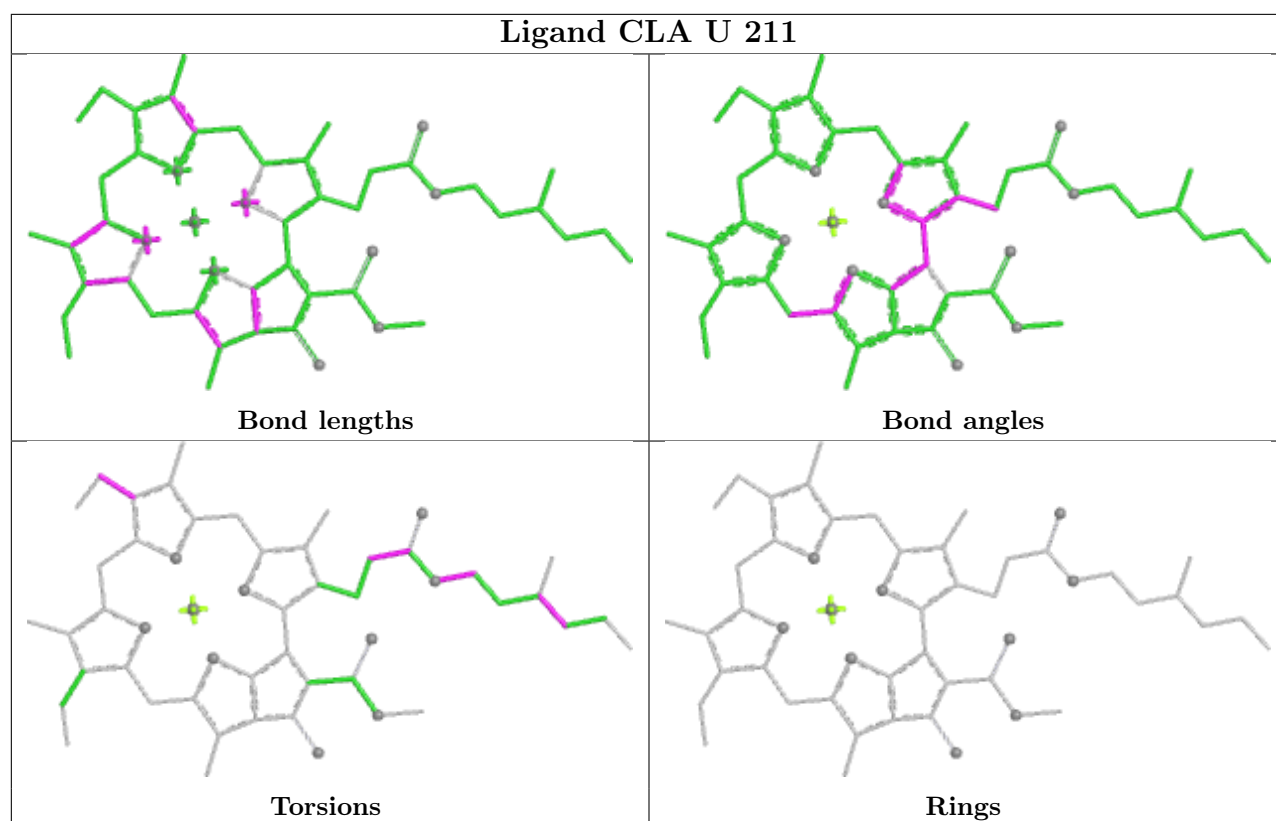
Ligand CLA Q 205



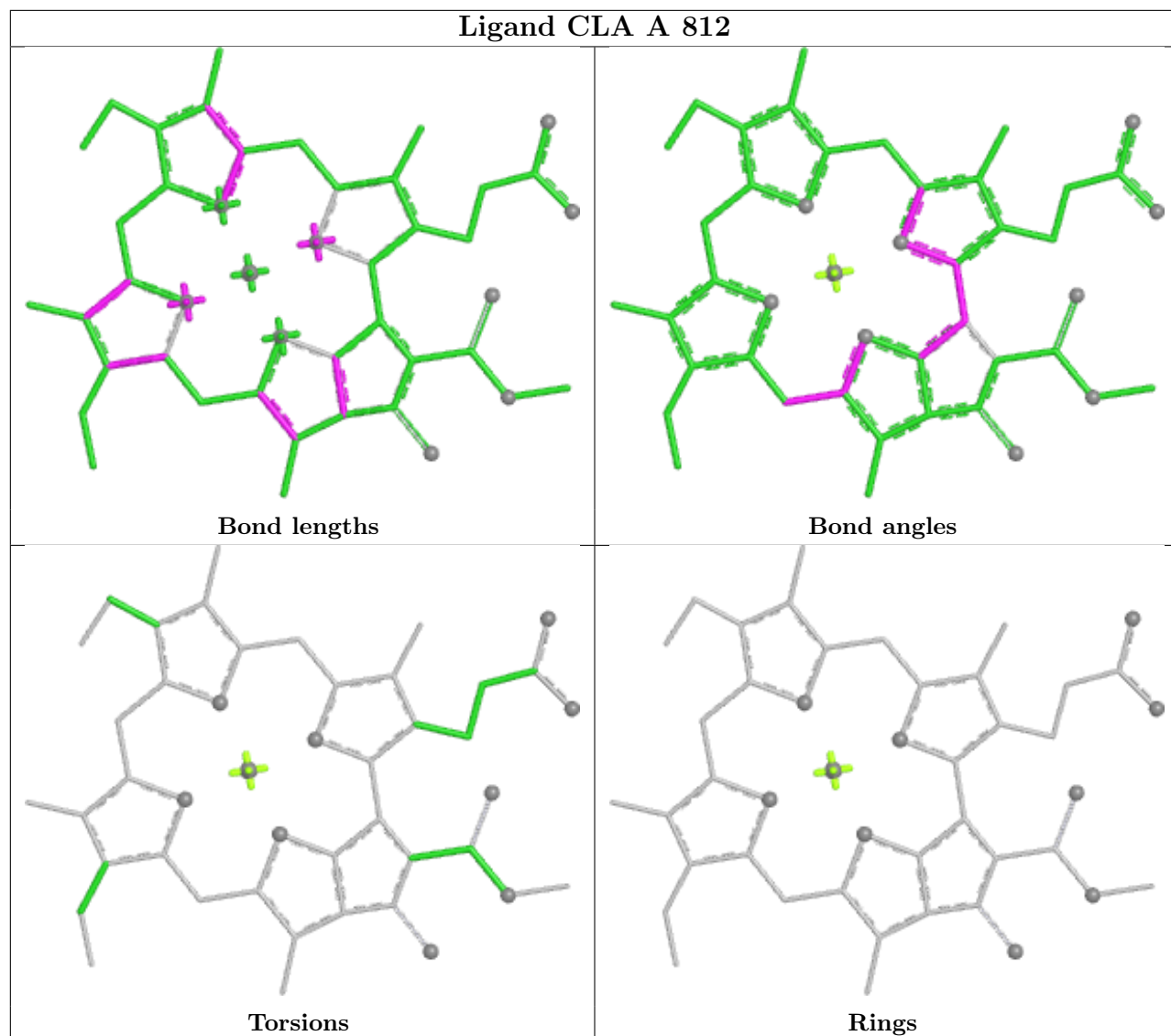
Ligand CLA Q 213



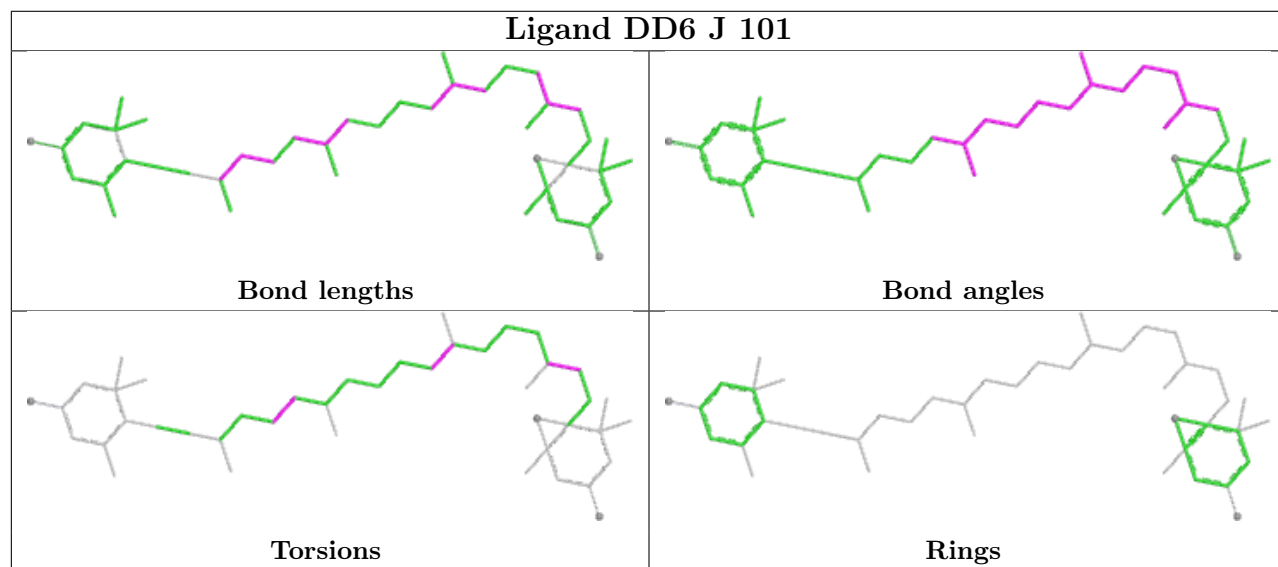


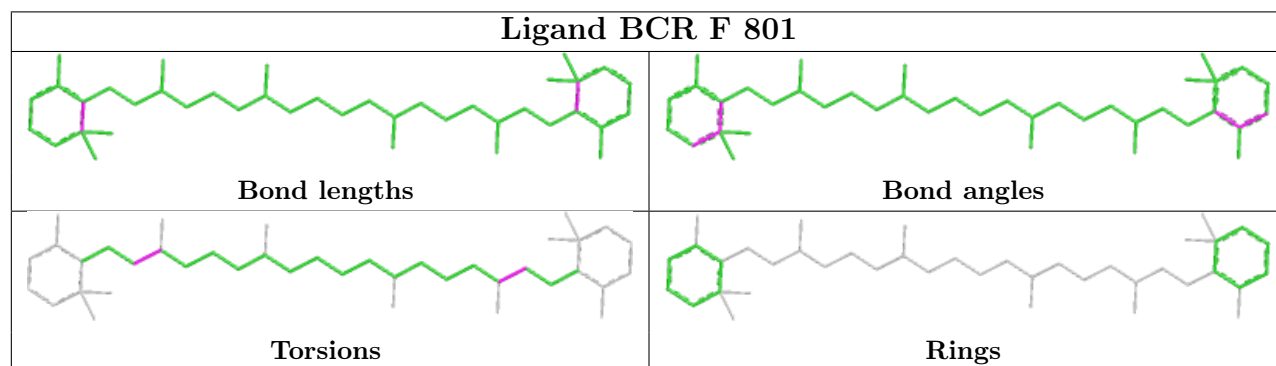
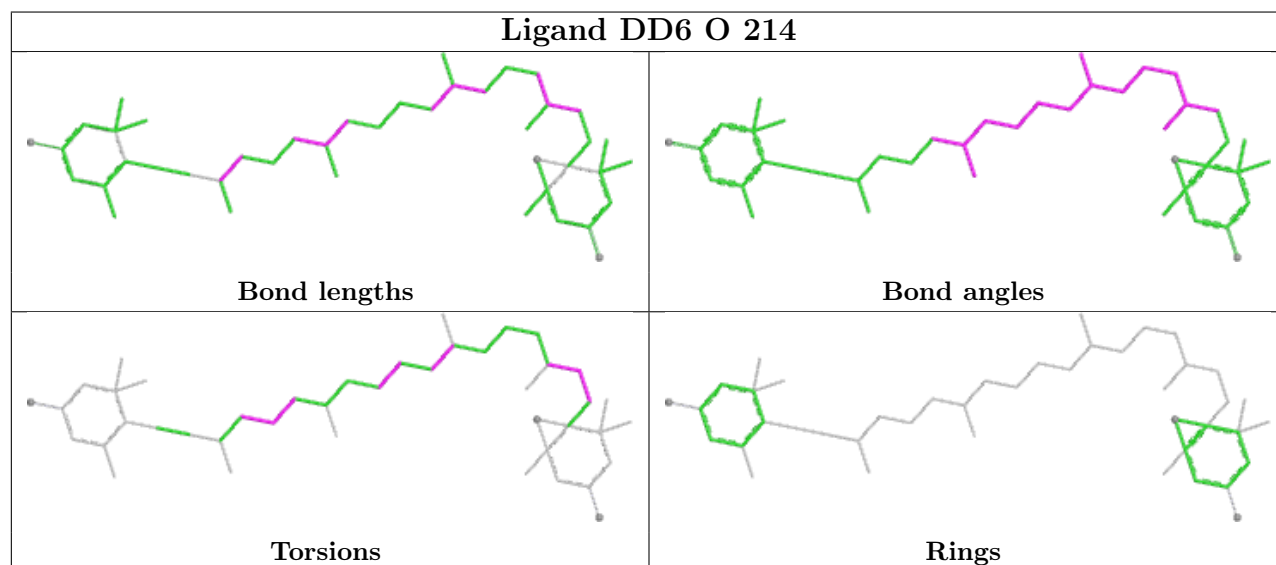
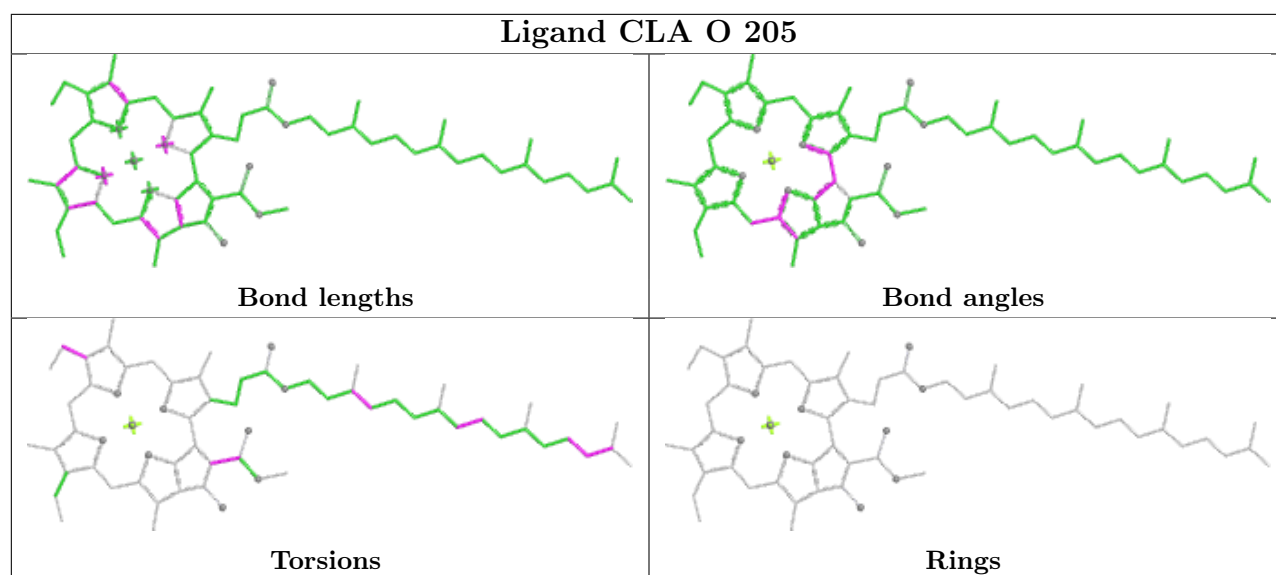


Ligand CLA A 812

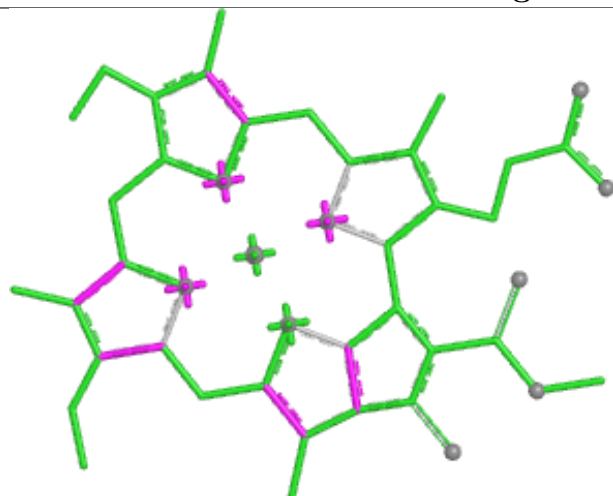


Ligand DD6 J 101

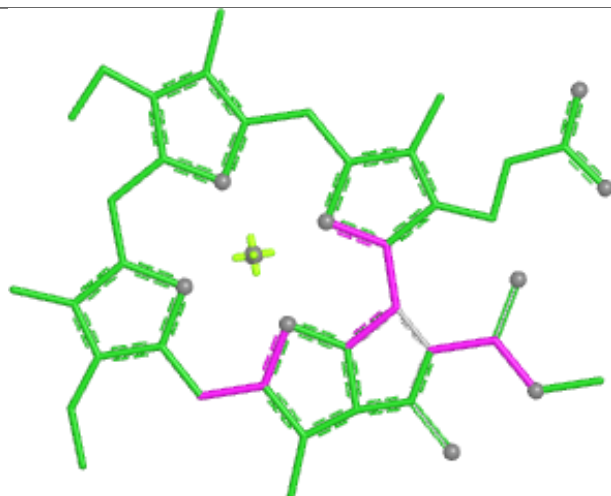




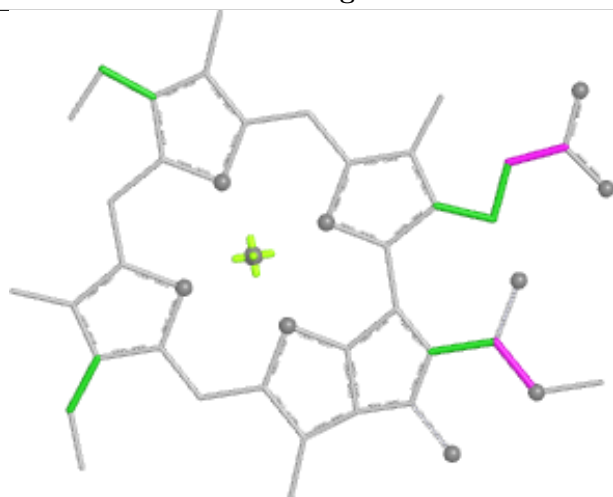
Ligand CLA G 210



Bond lengths



Bond angles

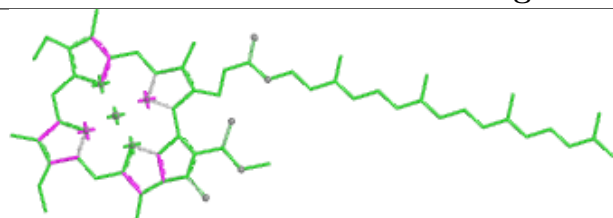


Torsions

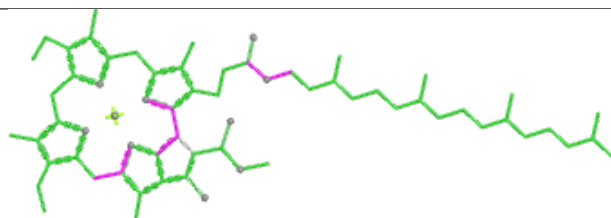


Rings

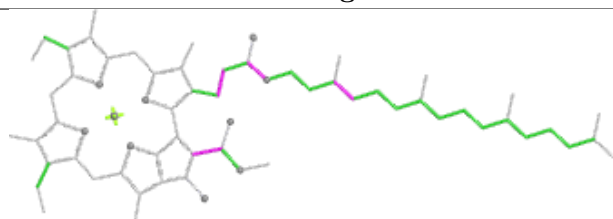
Ligand CLA A 806



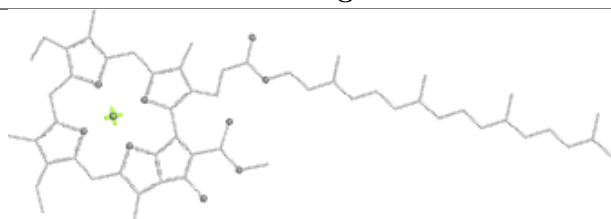
Bond lengths



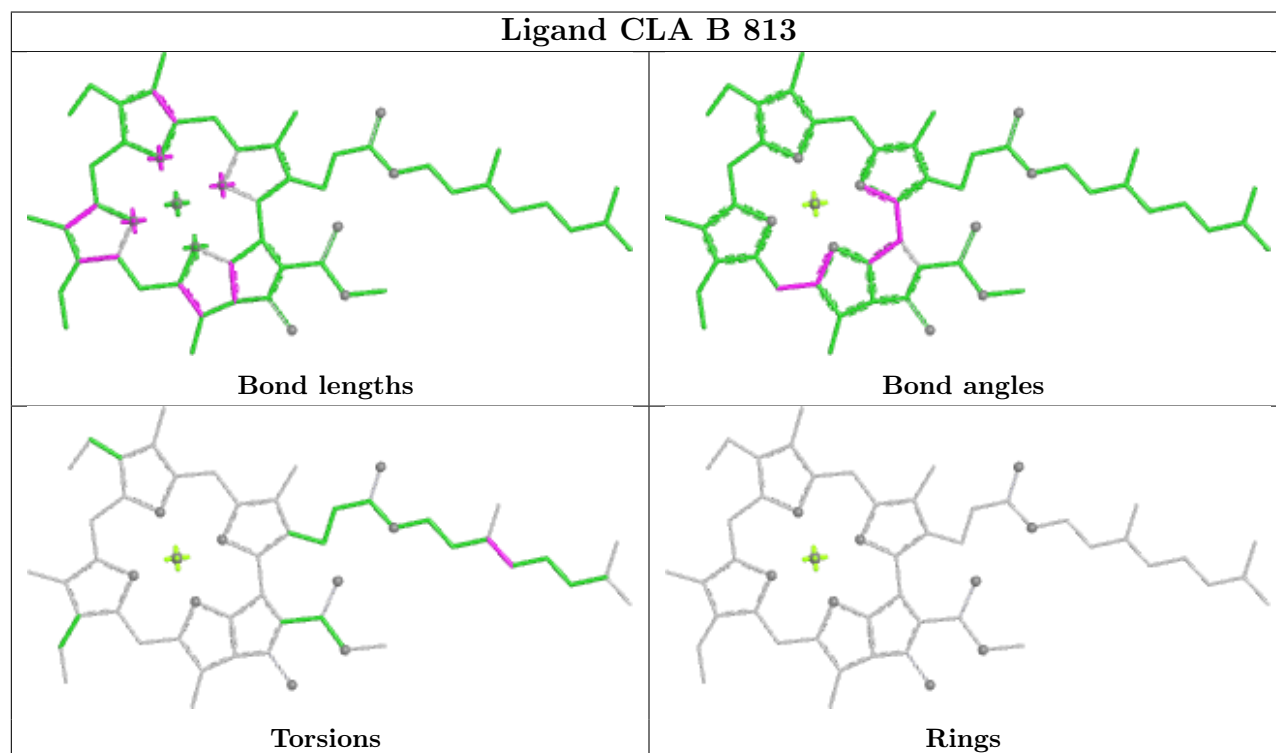
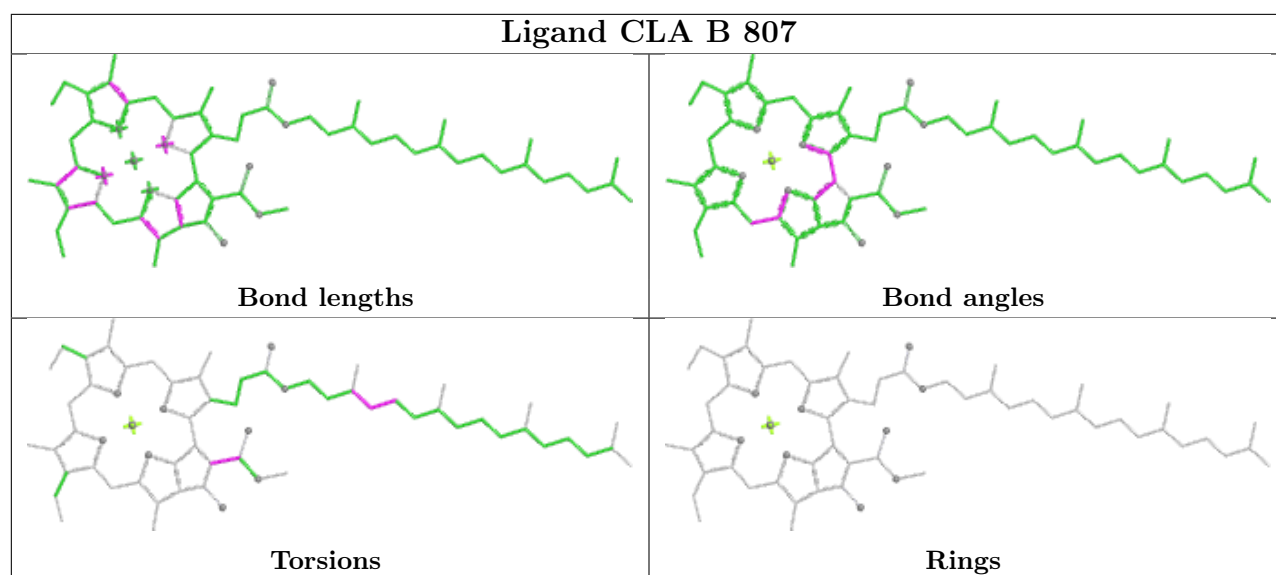
Bond angles

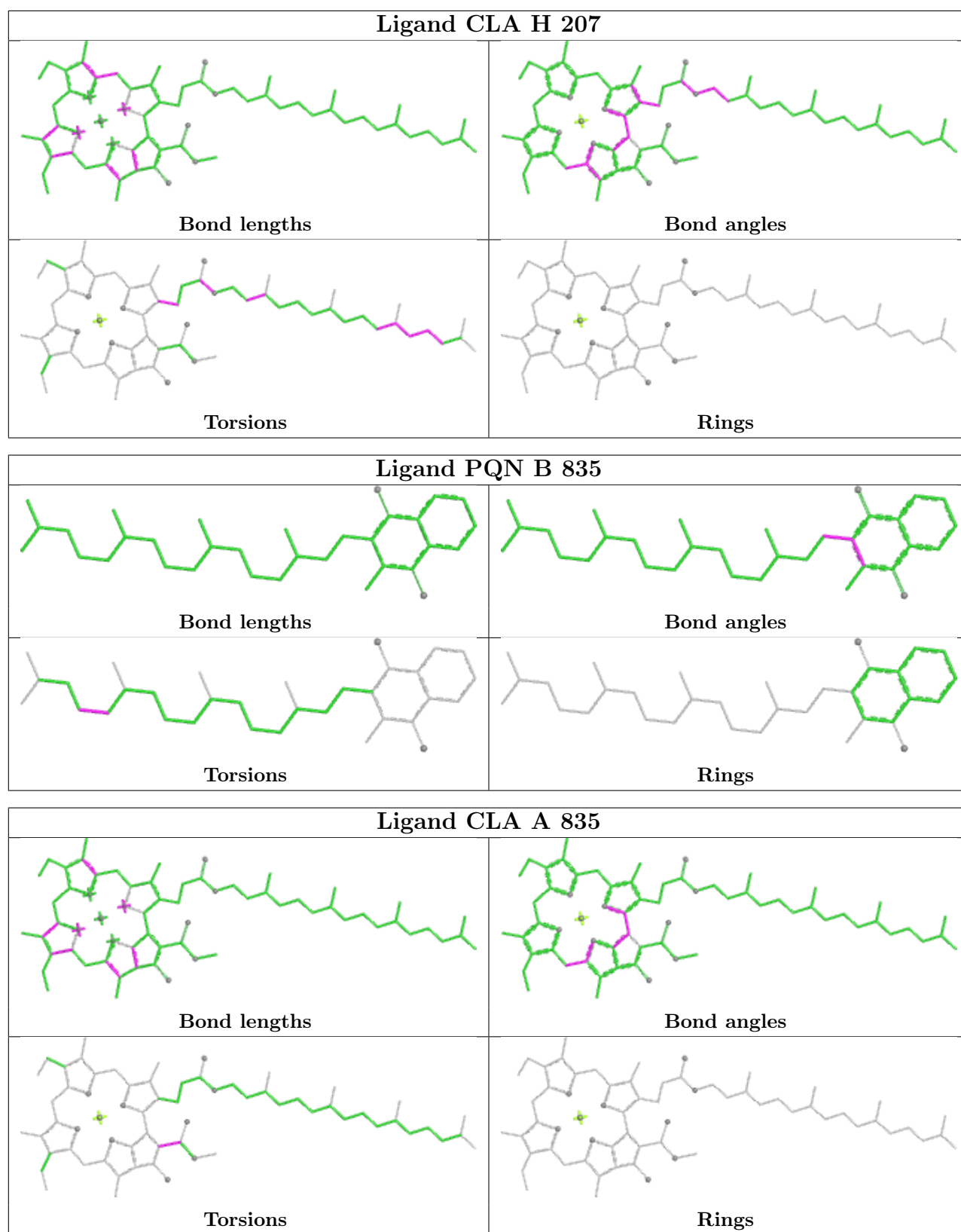


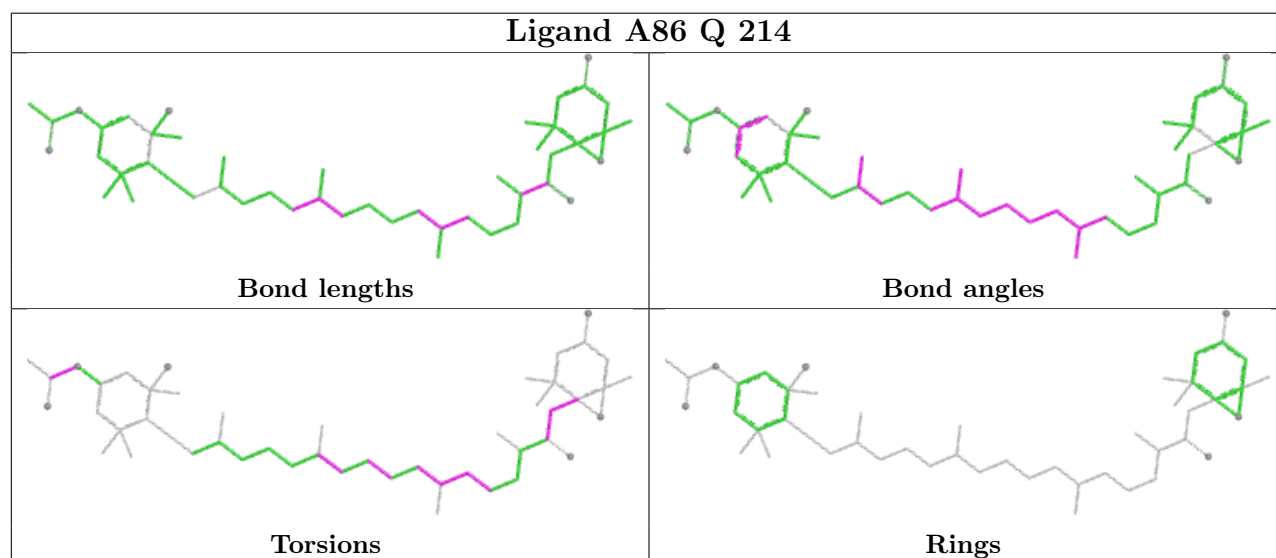
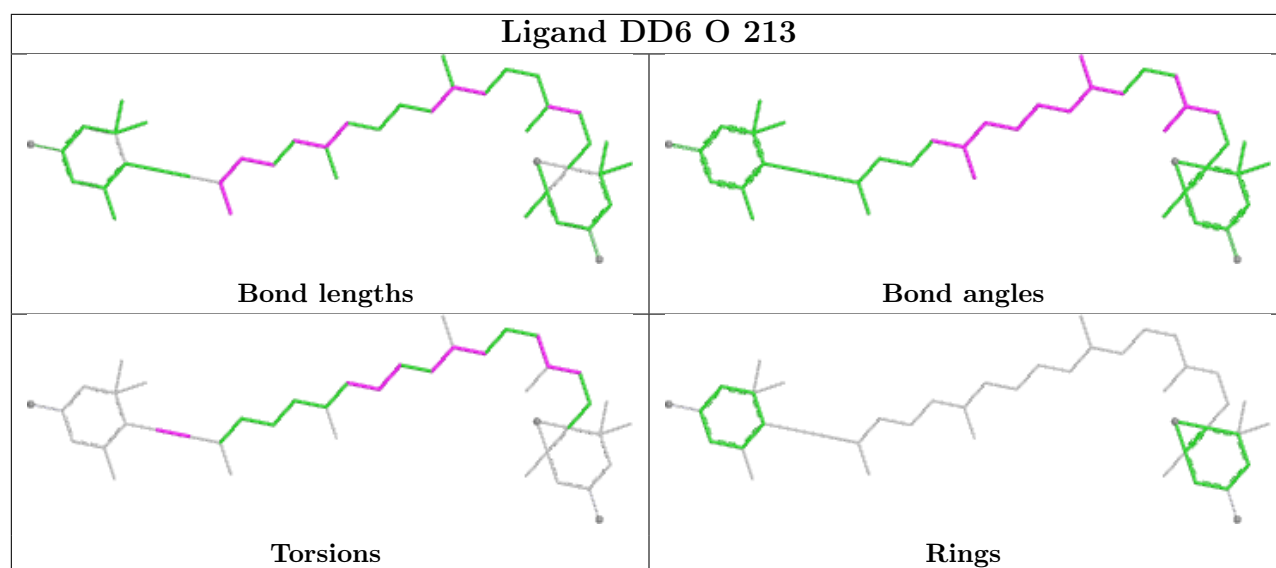
Torsions

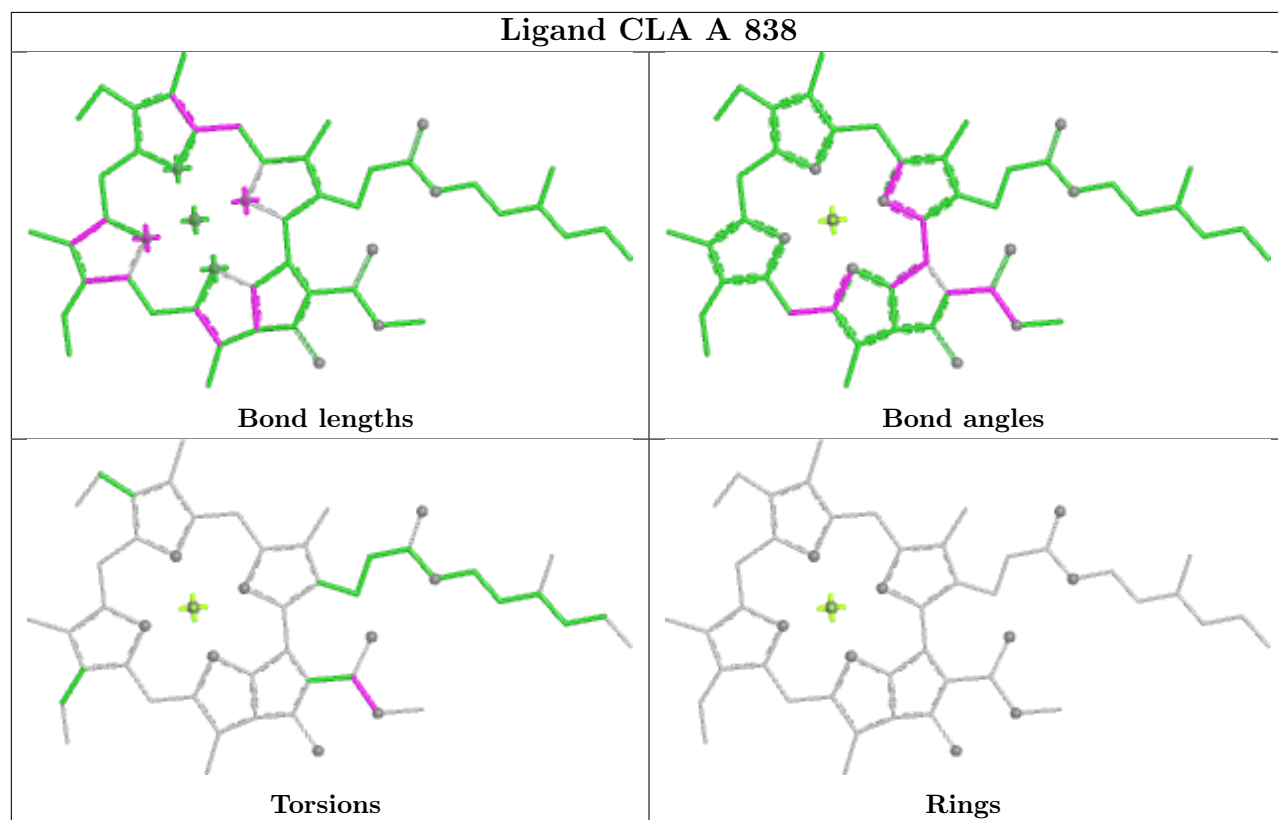
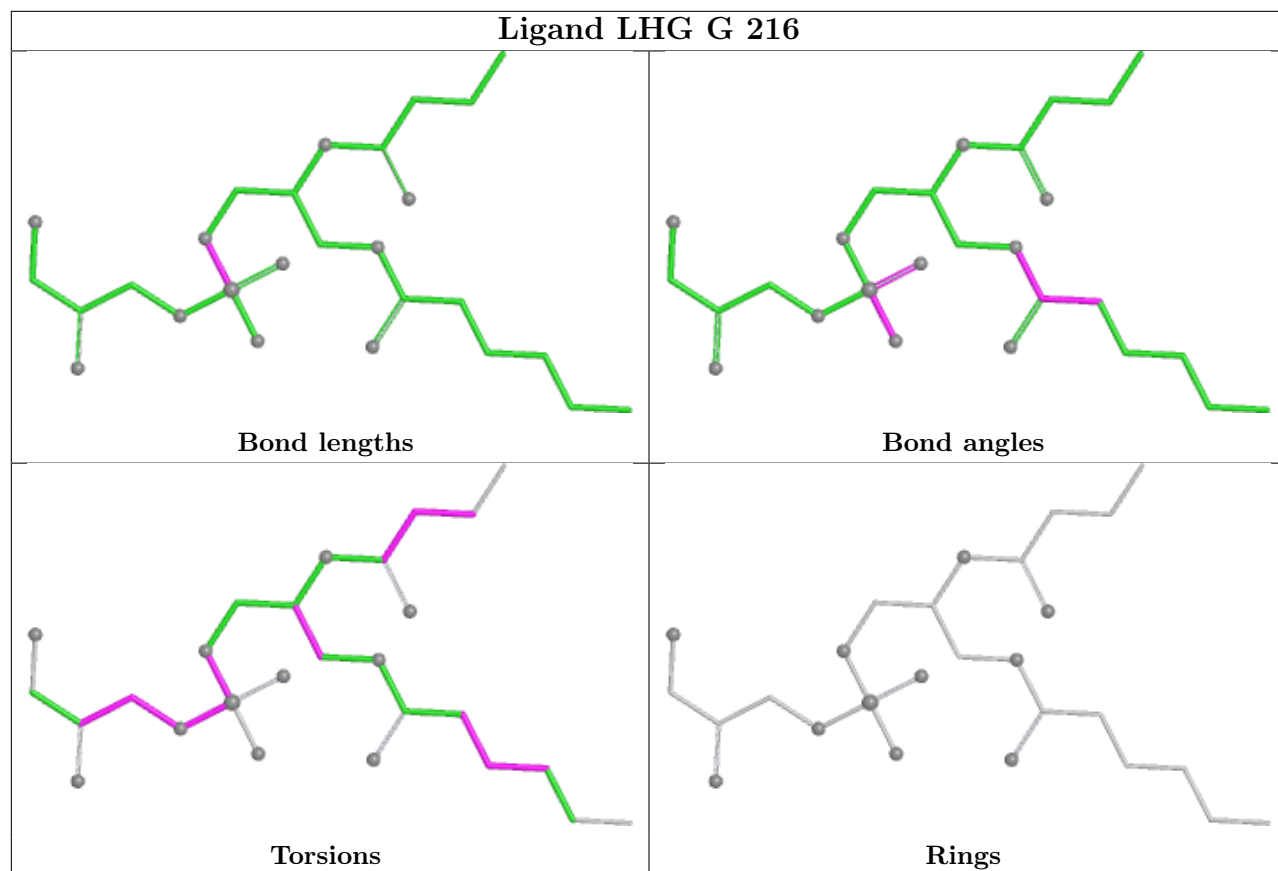


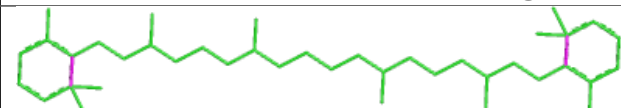
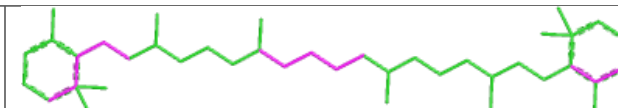
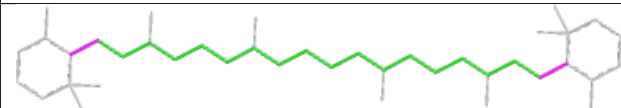
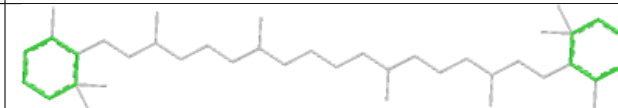
Rings


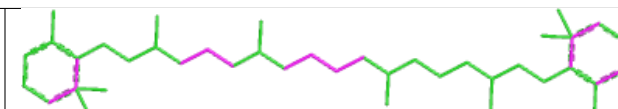
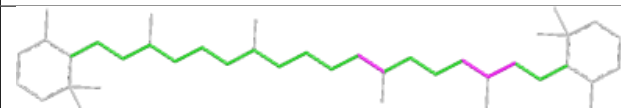
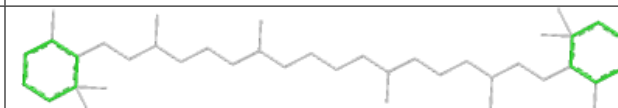


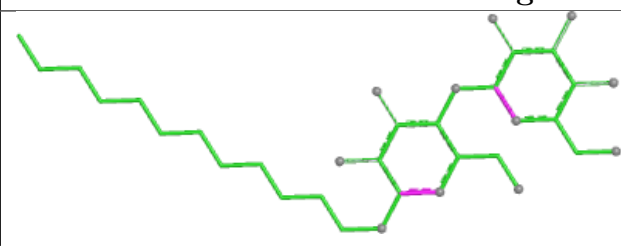
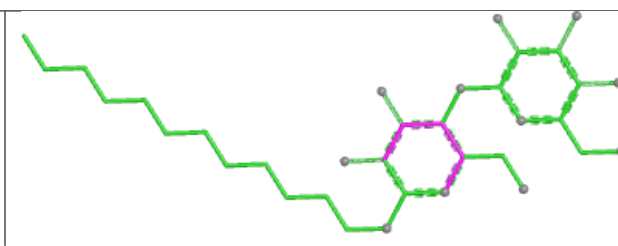
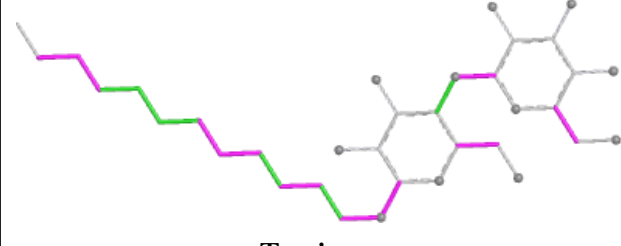
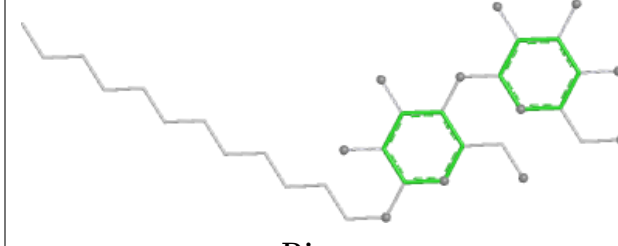


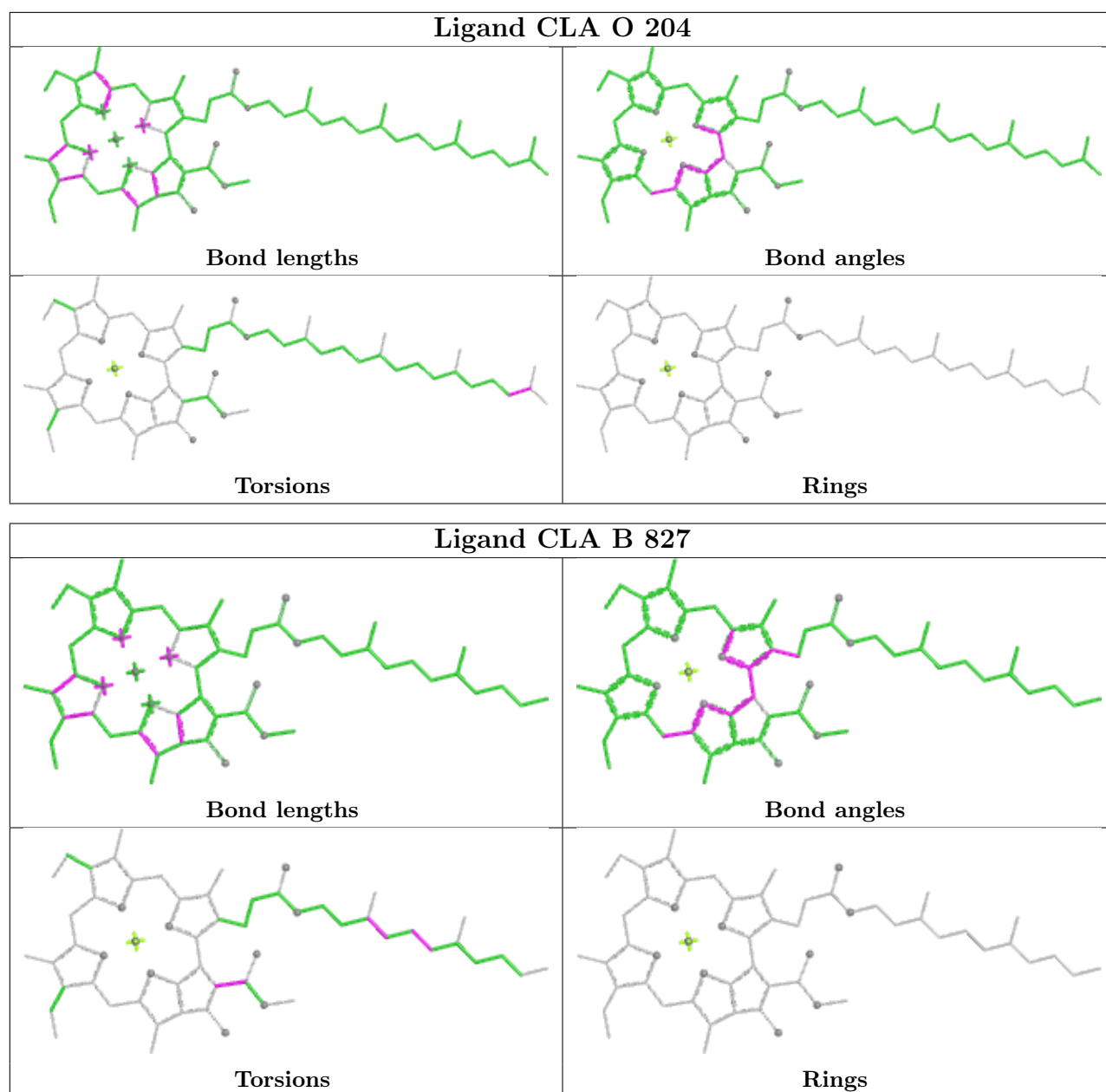


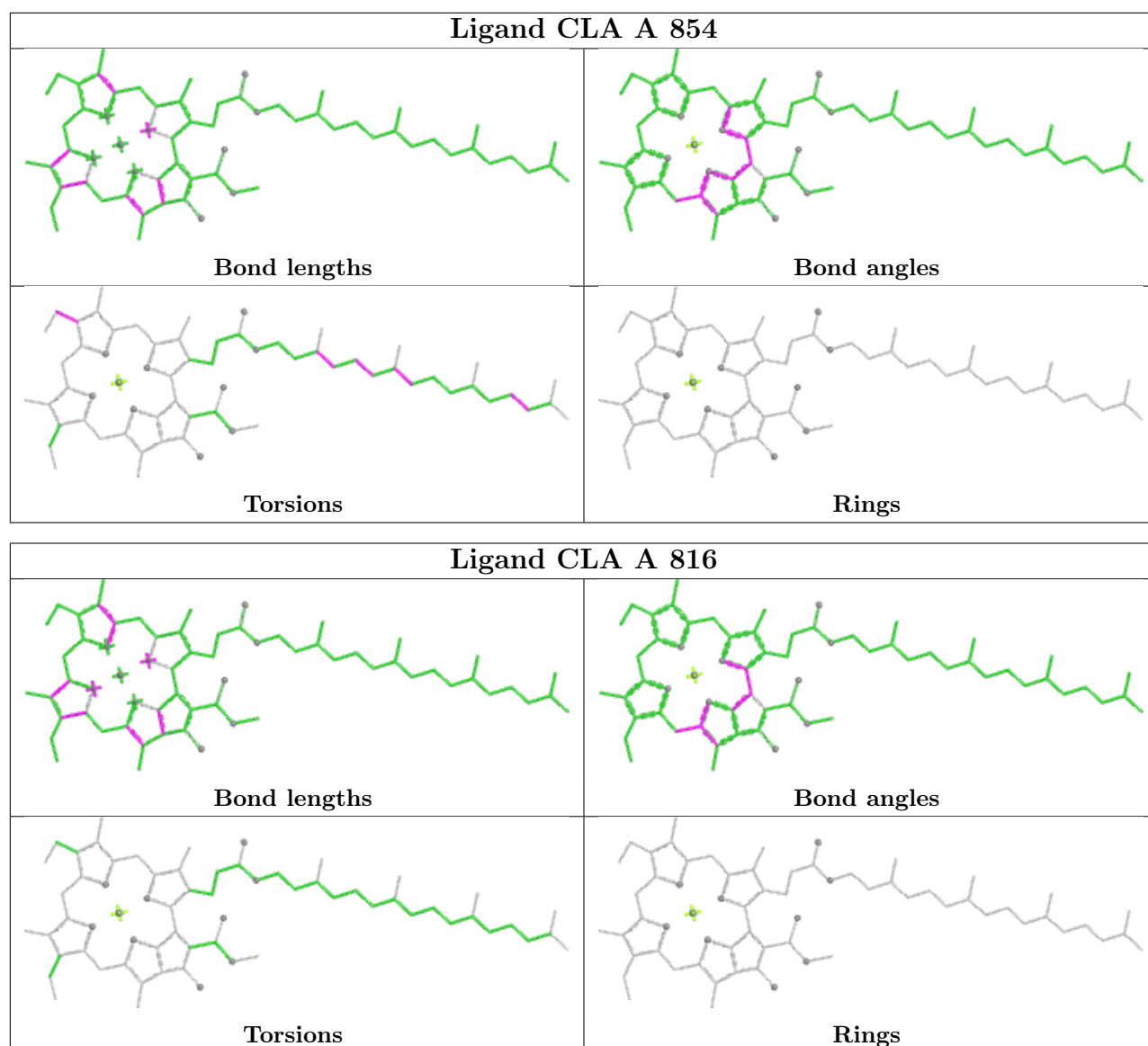


Ligand BCR B 839	
	
Bond lengths	Bond angles
	
Torsions	Rings

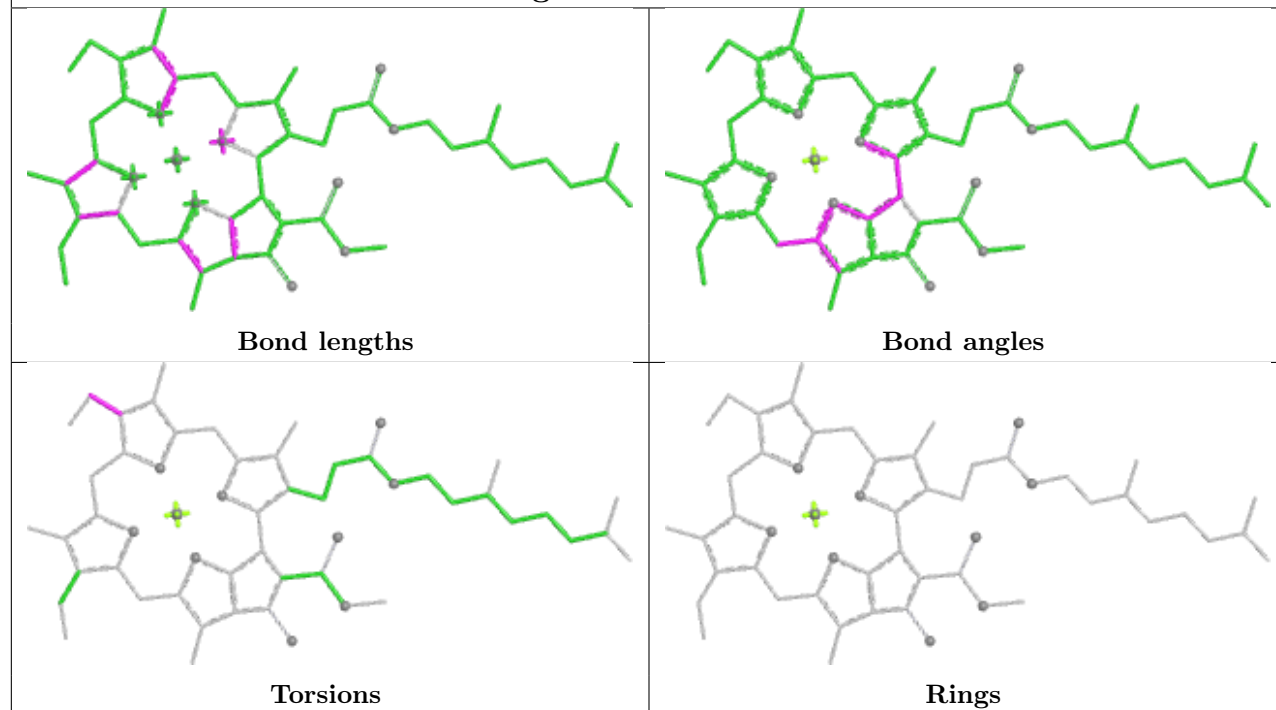
Ligand BCR I 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand LMU O 216	
	
Bond lengths	Bond angles
	
Torsions	Rings

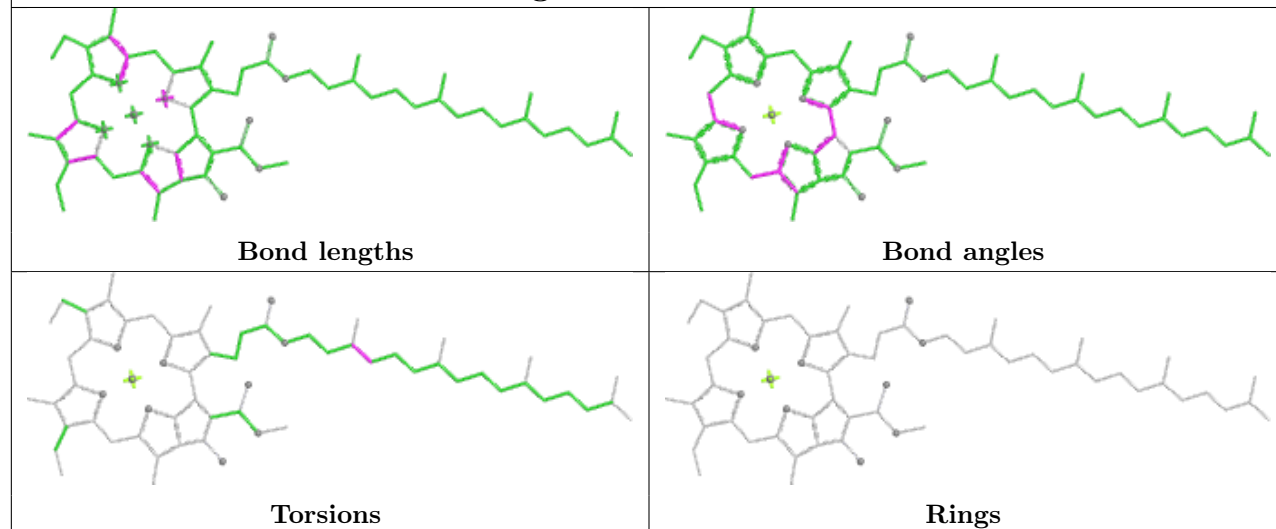




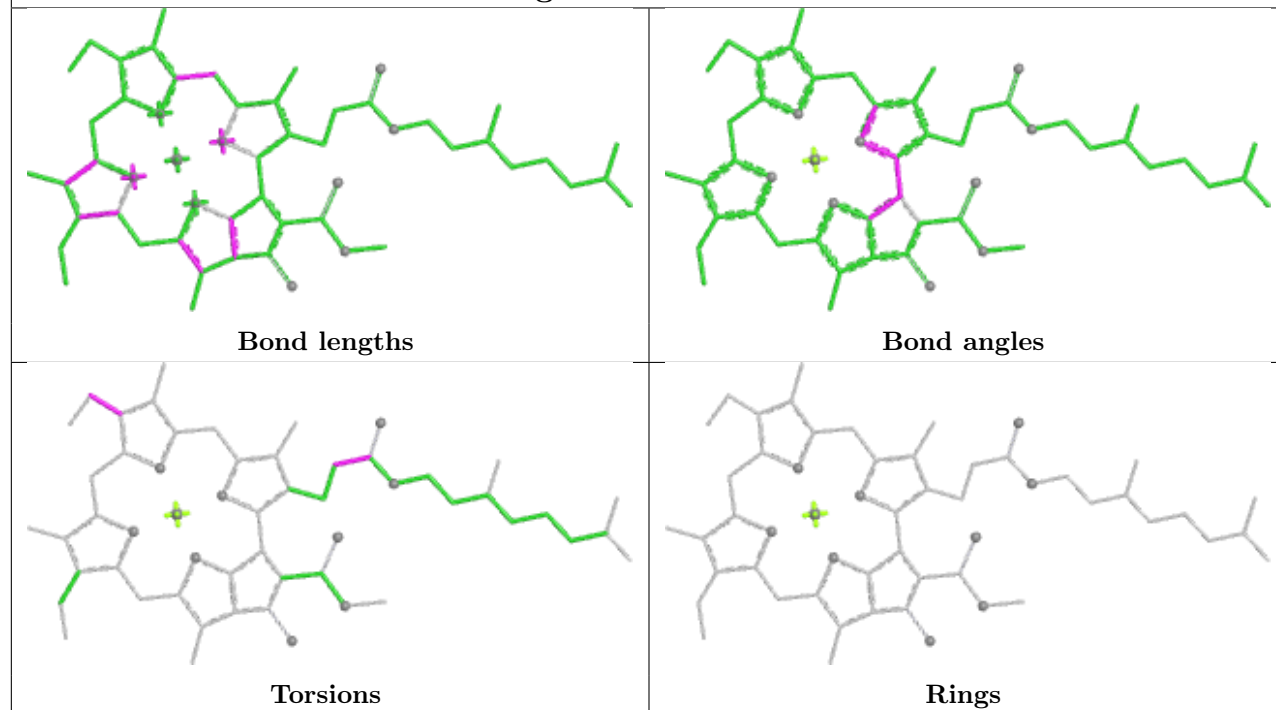
Ligand CLA B 810



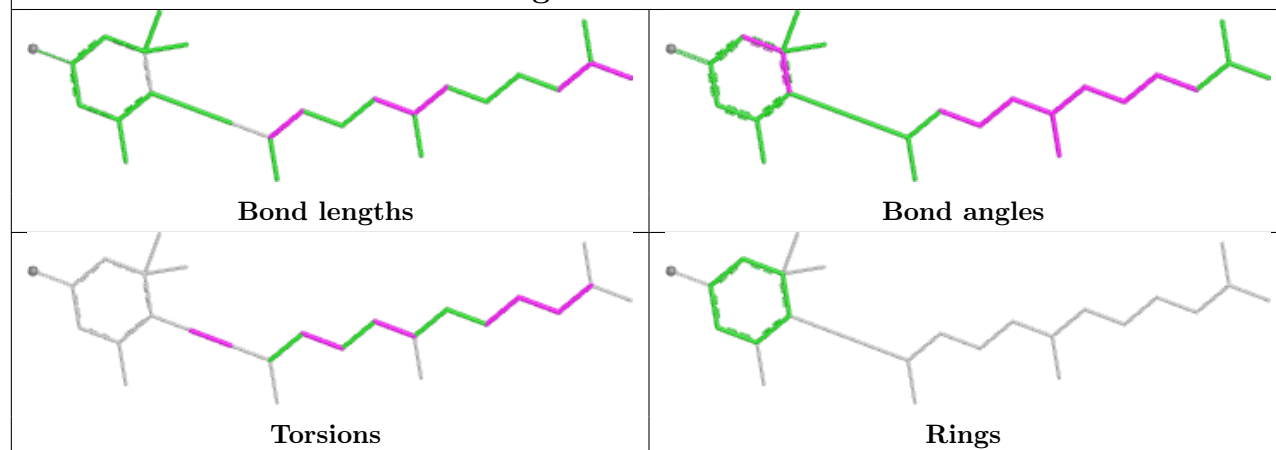
Ligand CLA A 818

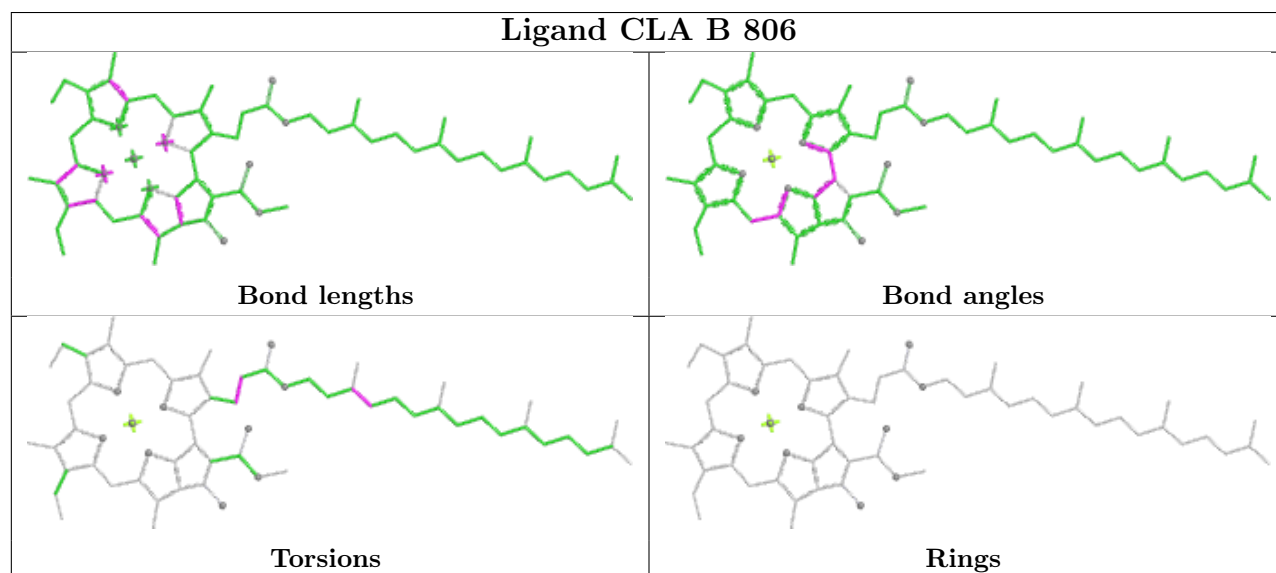
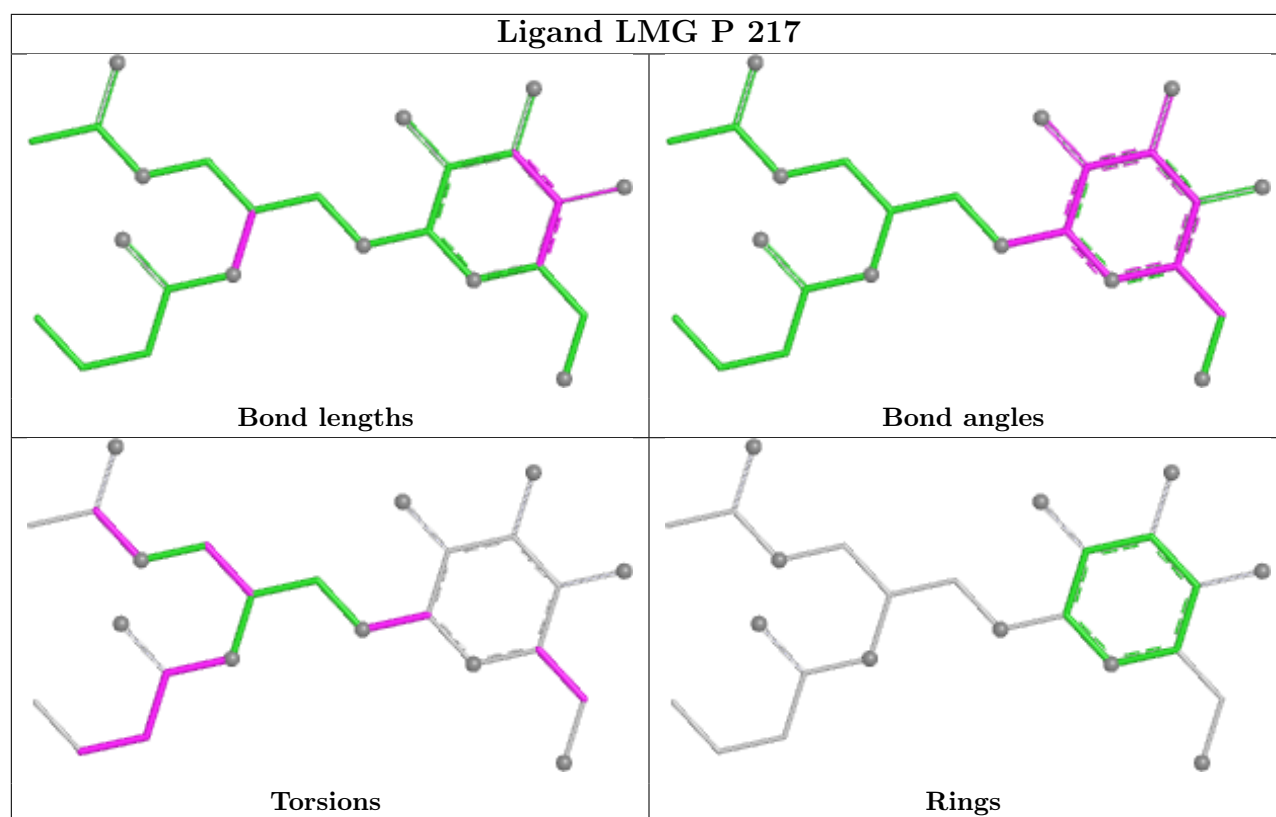


Ligand CLA k 103

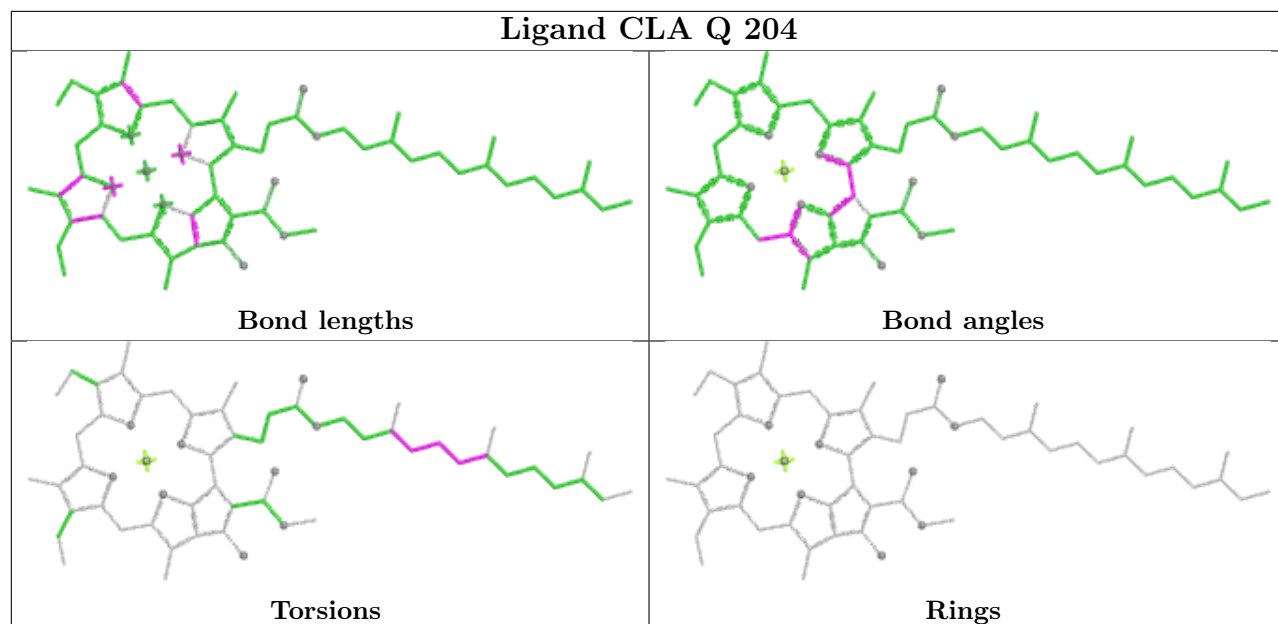


Ligand DD6 U 214

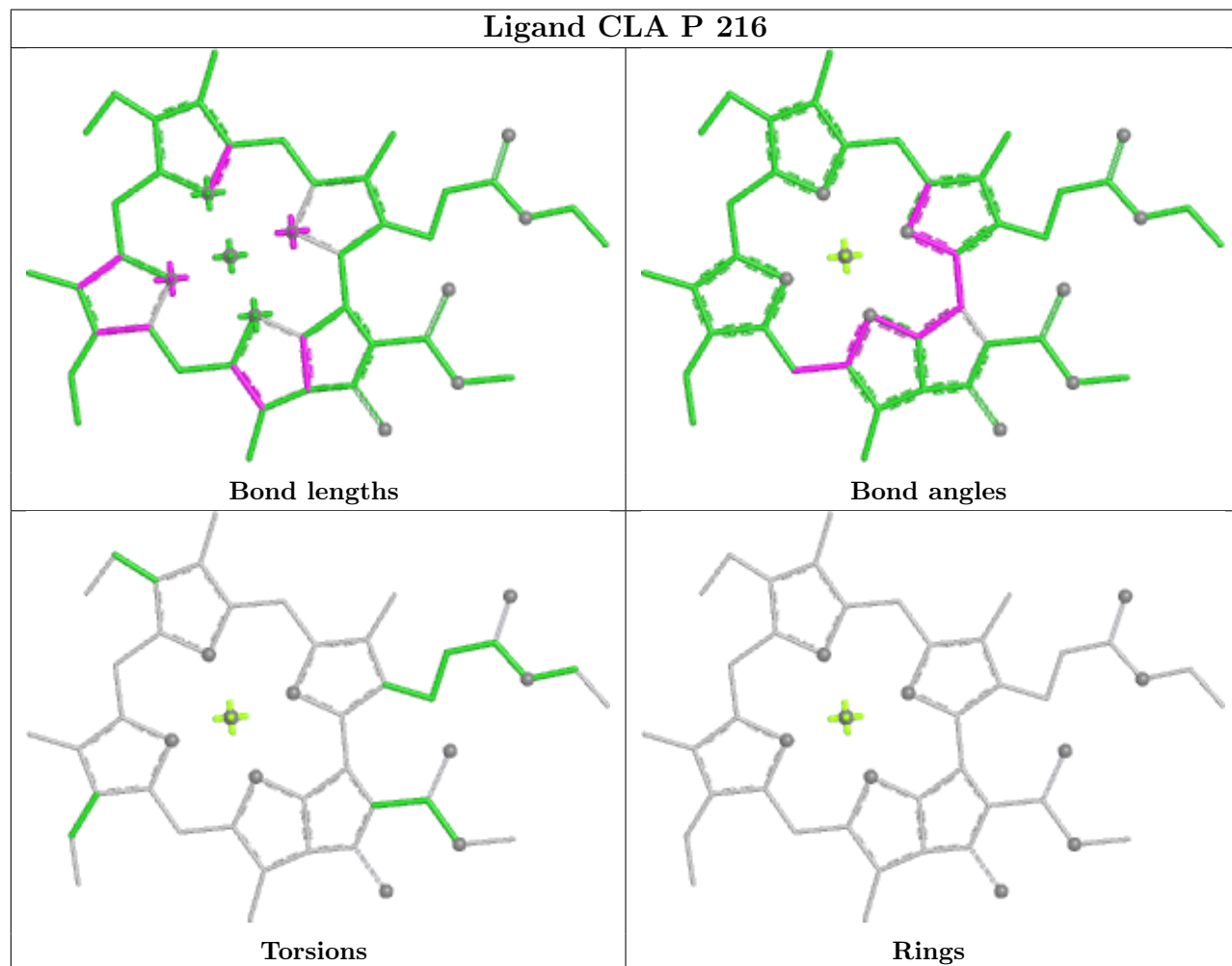




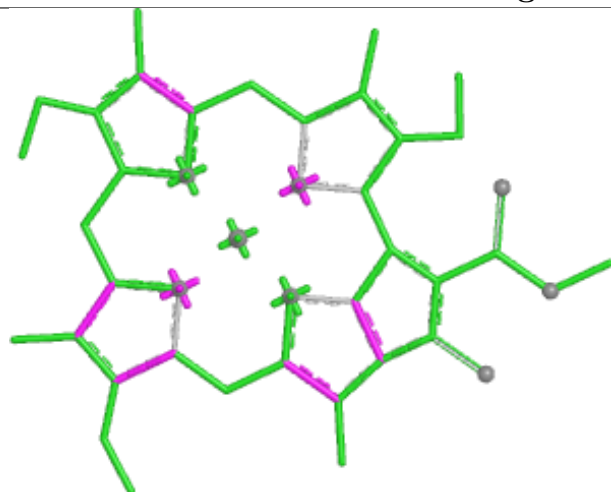
Ligand CLA Q 204



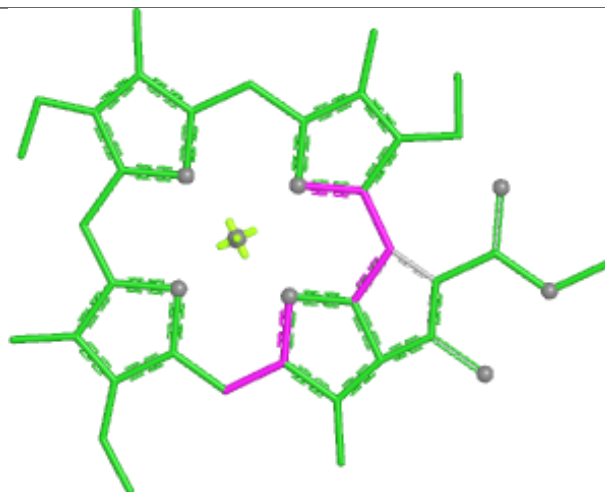
Ligand CLA P 216



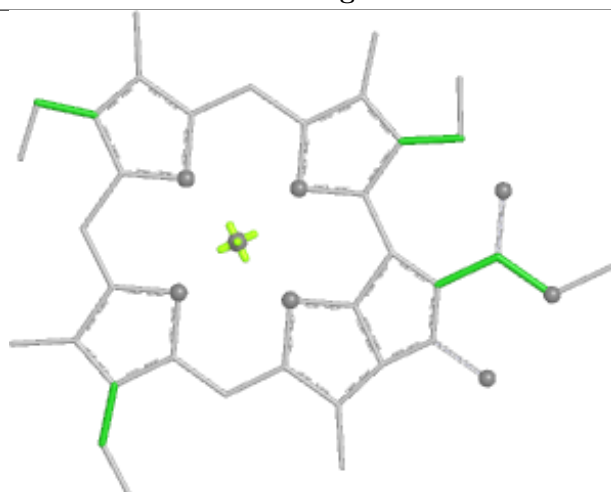
Ligand CLA k 102



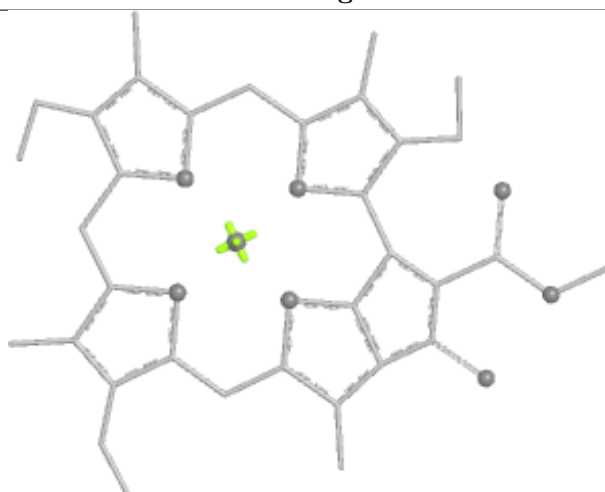
Bond lengths



Bond angles

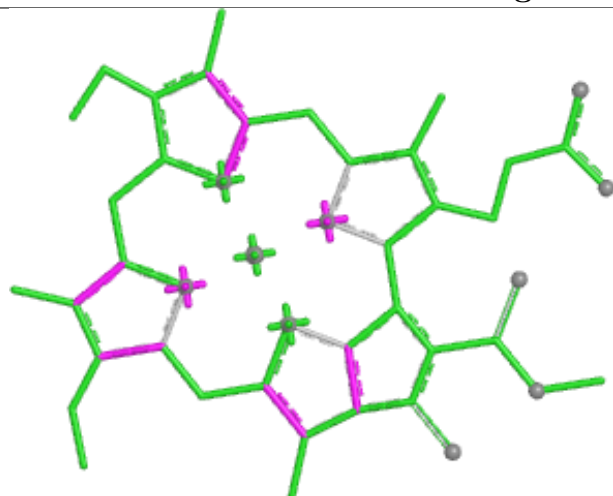


Torsions

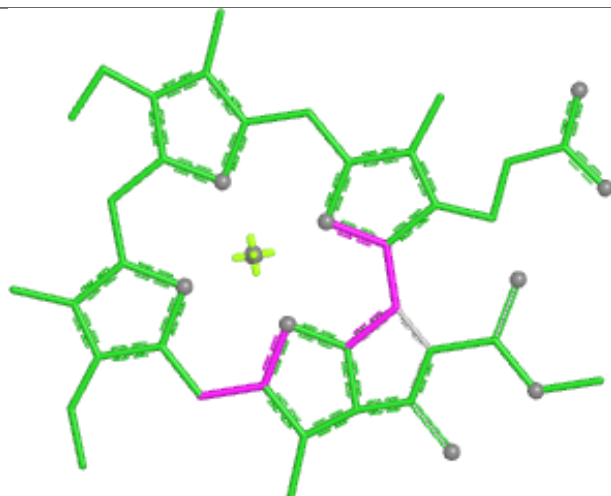


Rings

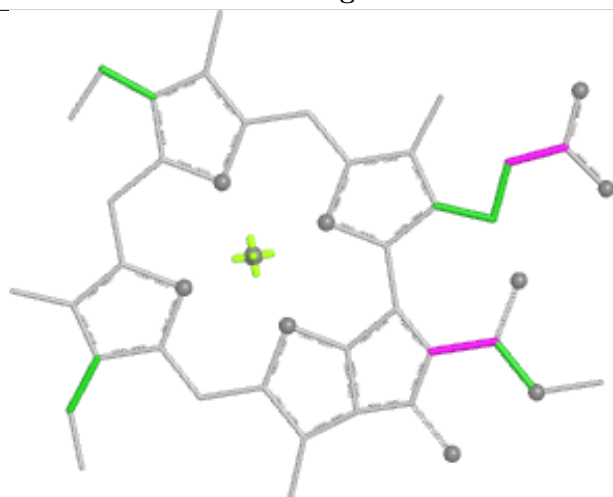
Ligand CLA B 803



Bond lengths



Bond angles

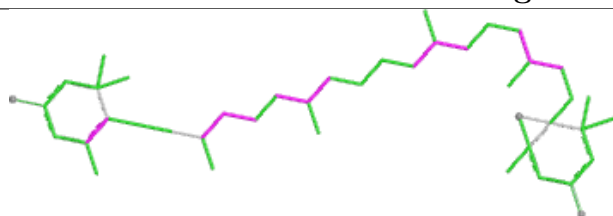


Torsions

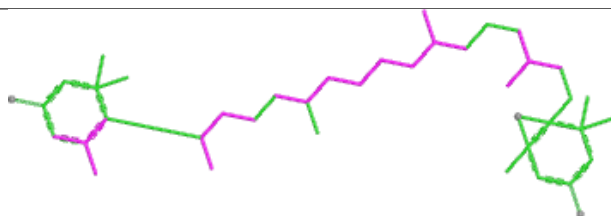


Rings

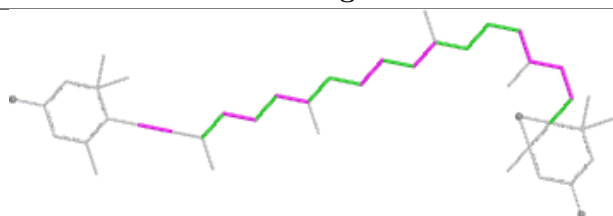
Ligand DD6 H 201



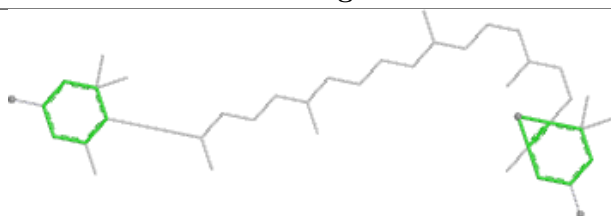
Bond lengths



Bond angles

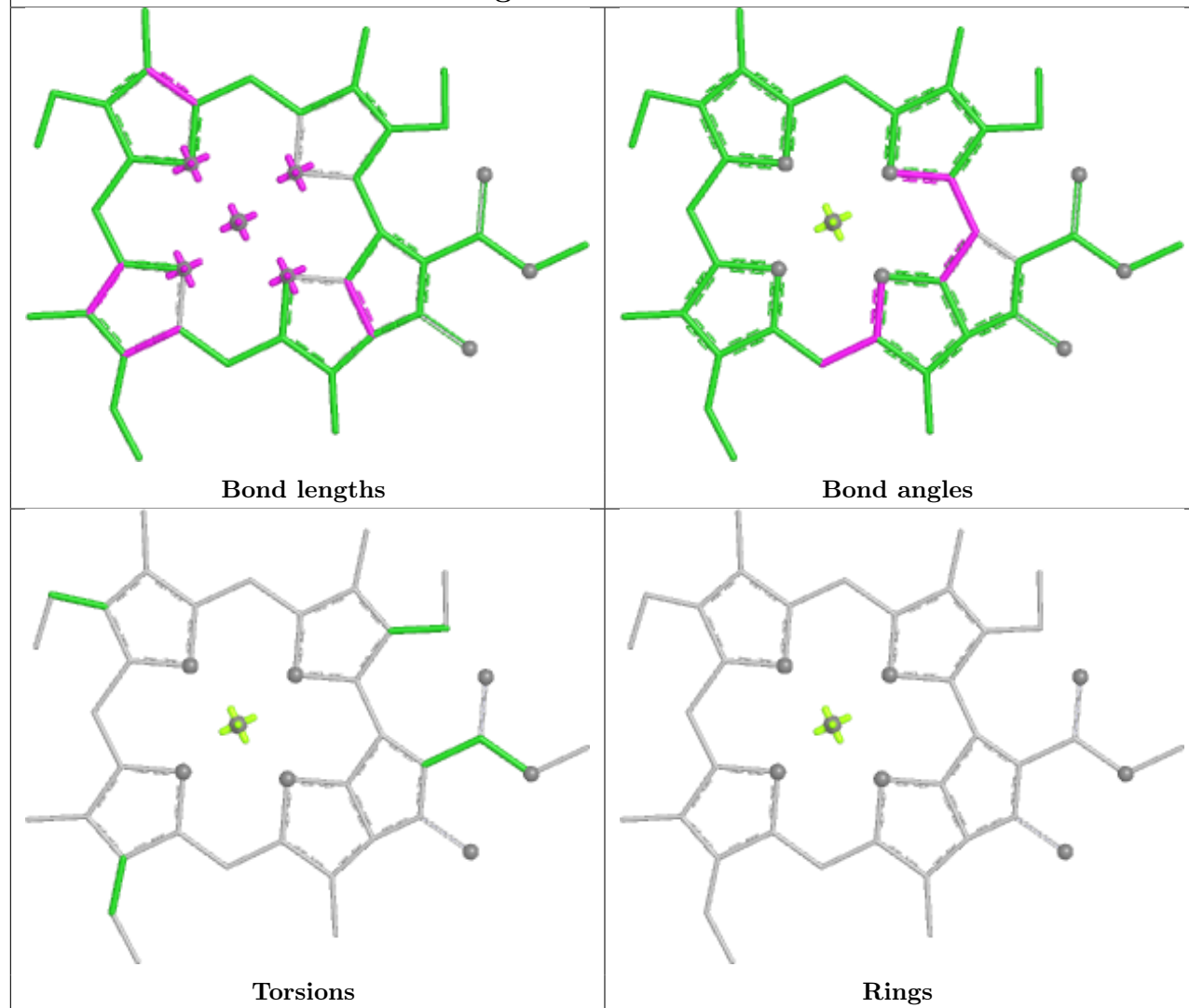


Torsions

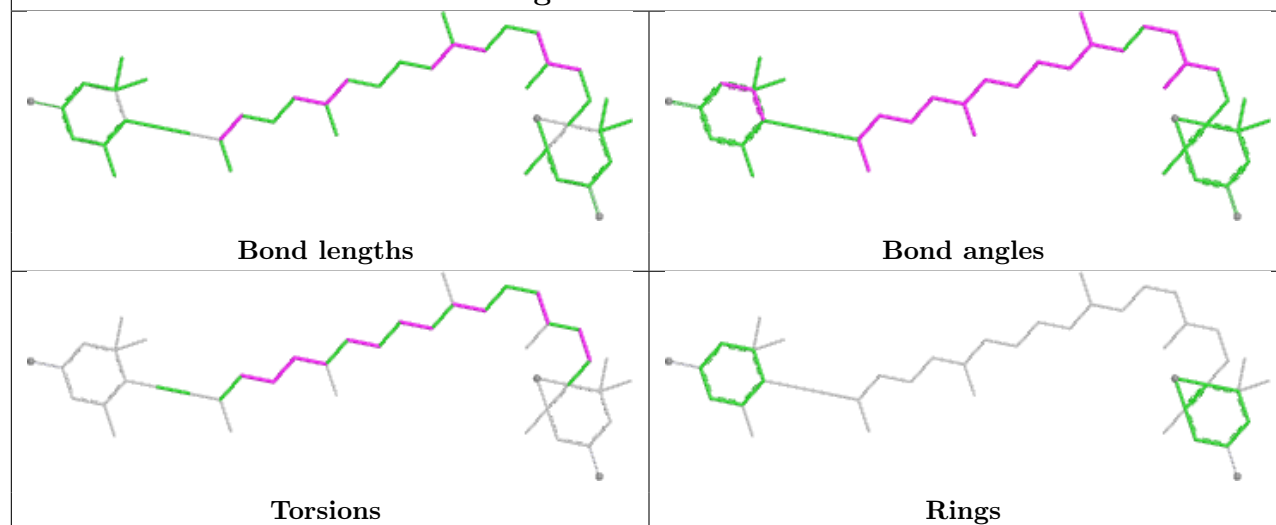


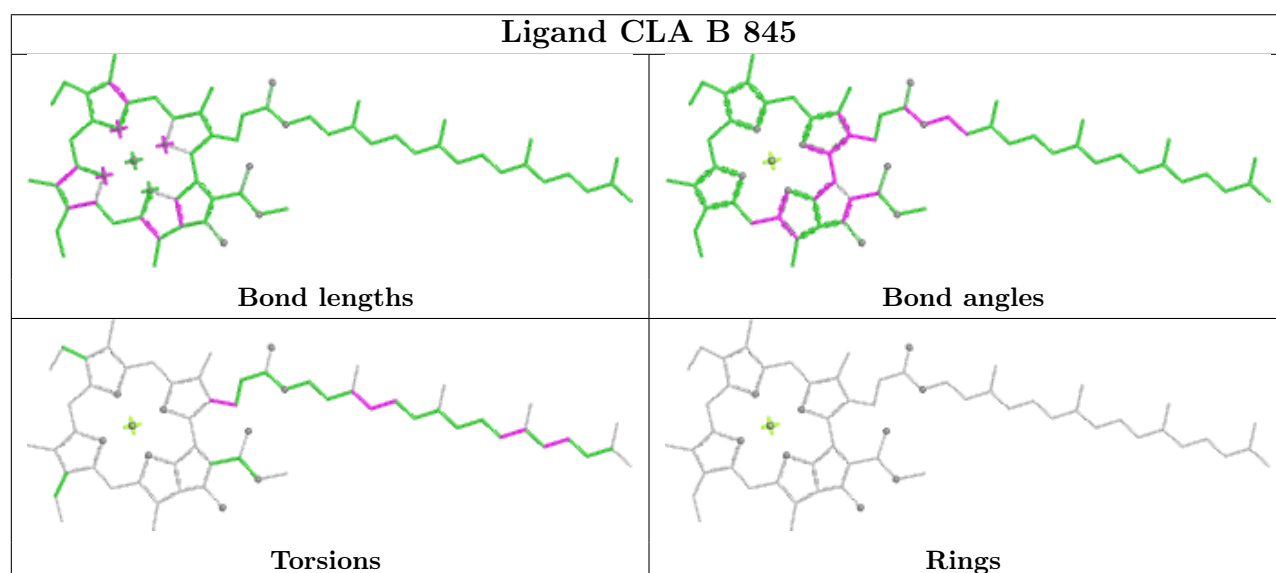
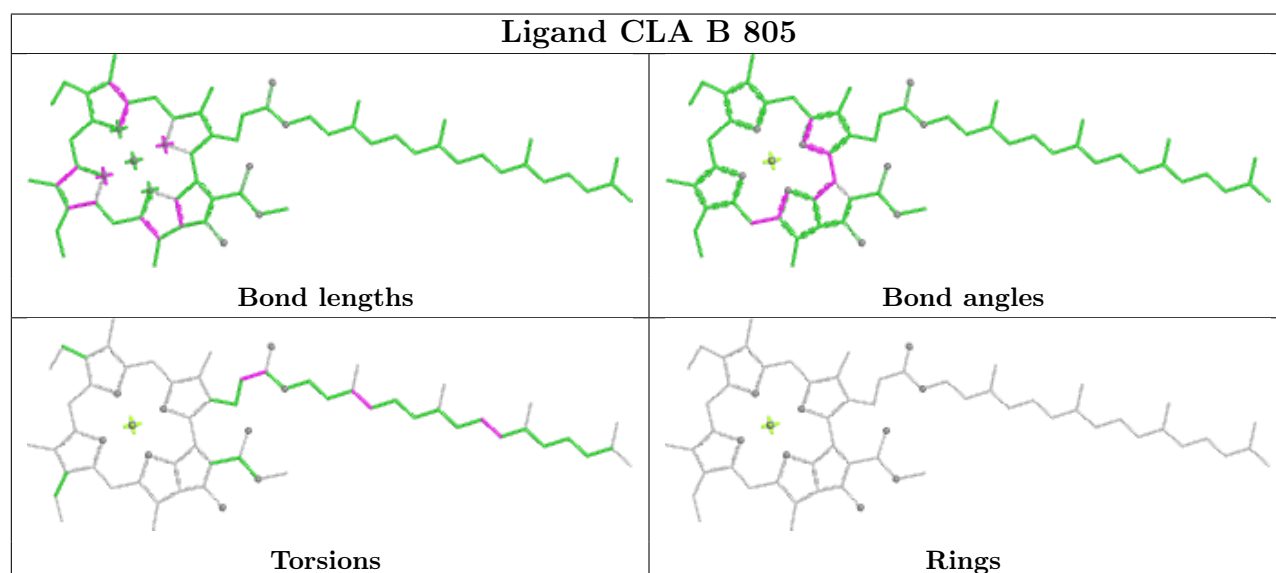
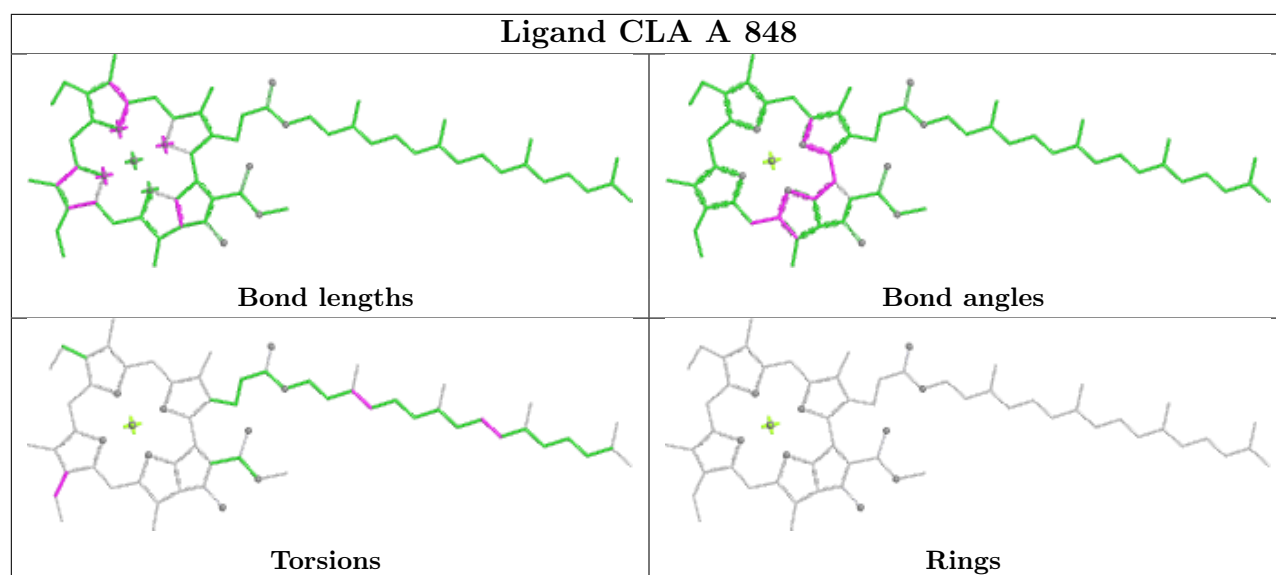
Rings

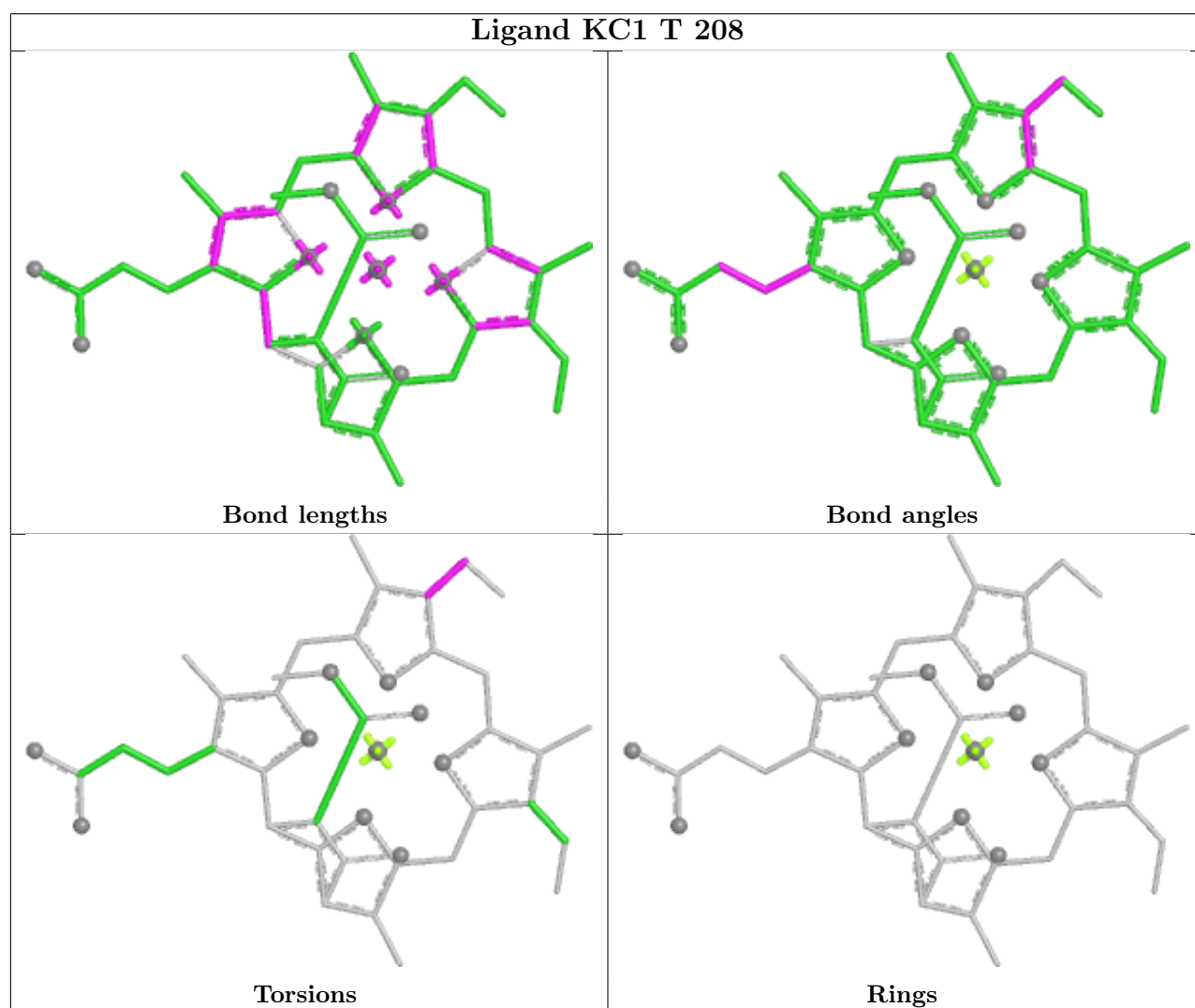
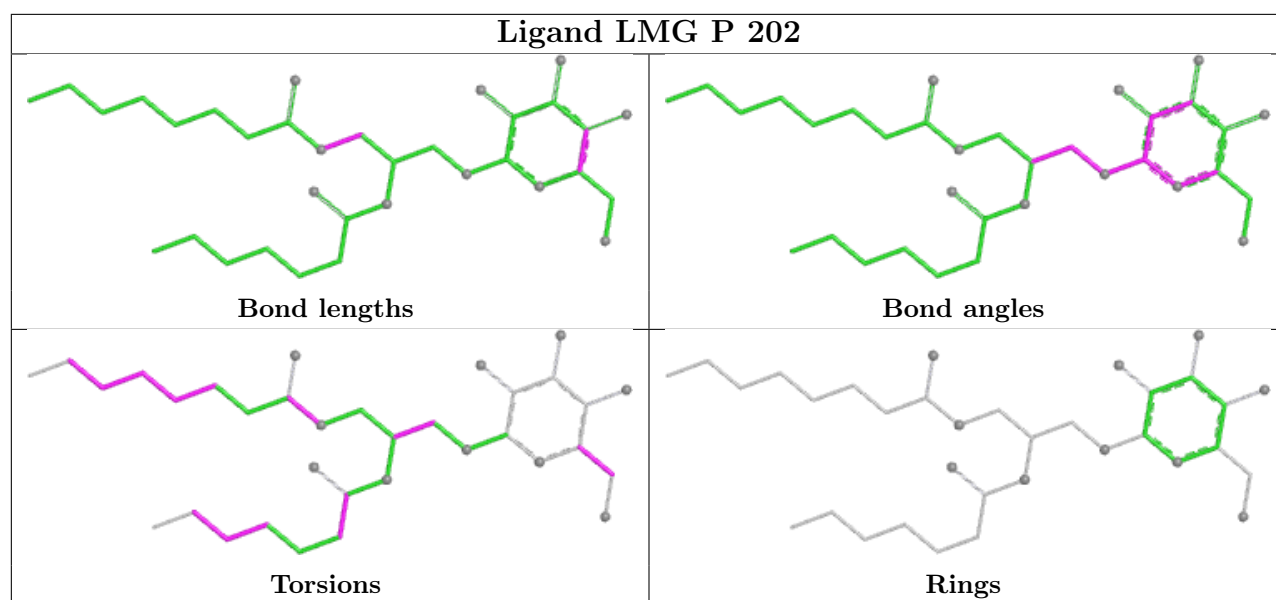
Ligand CLA U 209

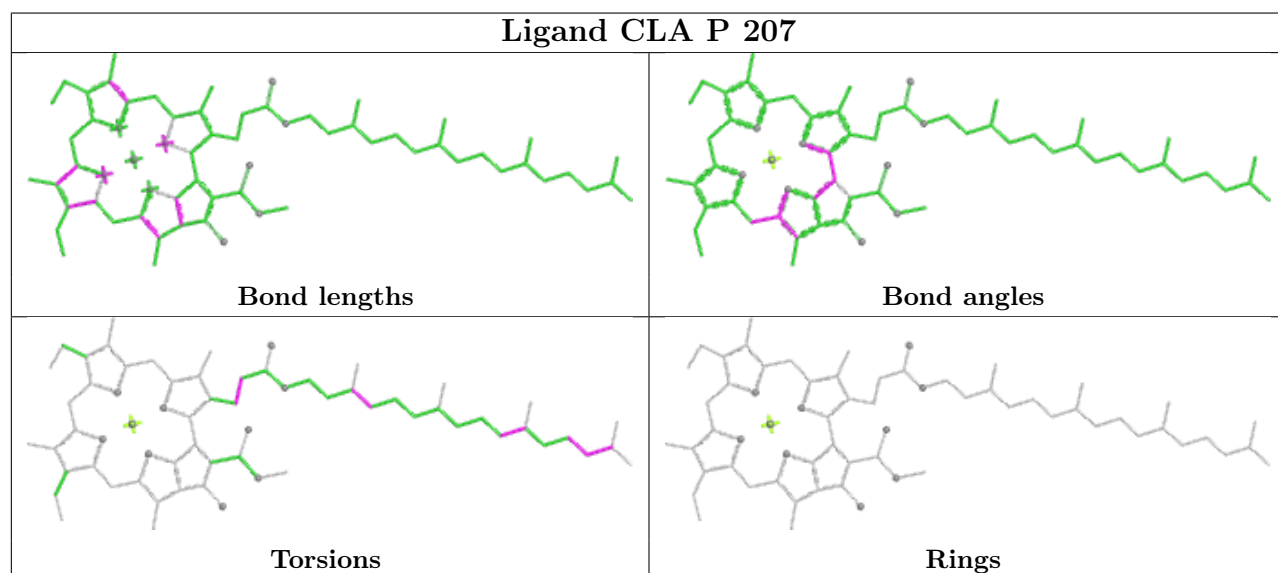
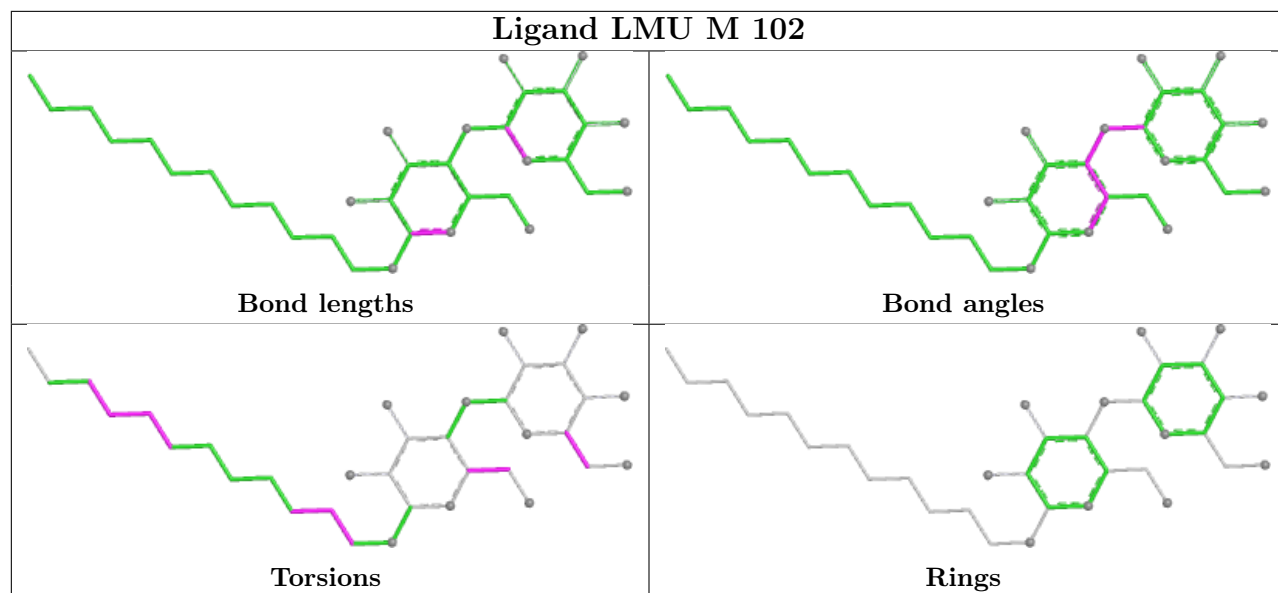


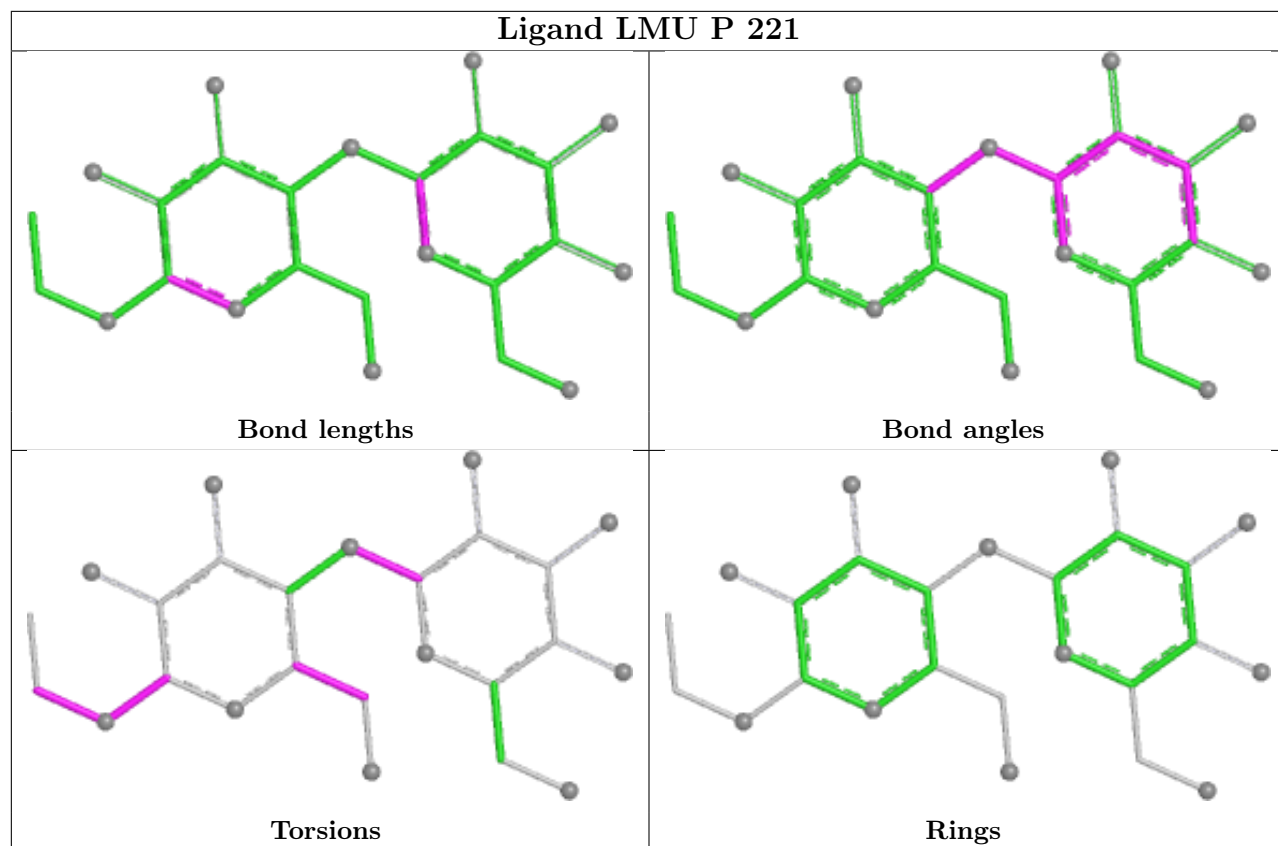
Ligand DD6 P 220



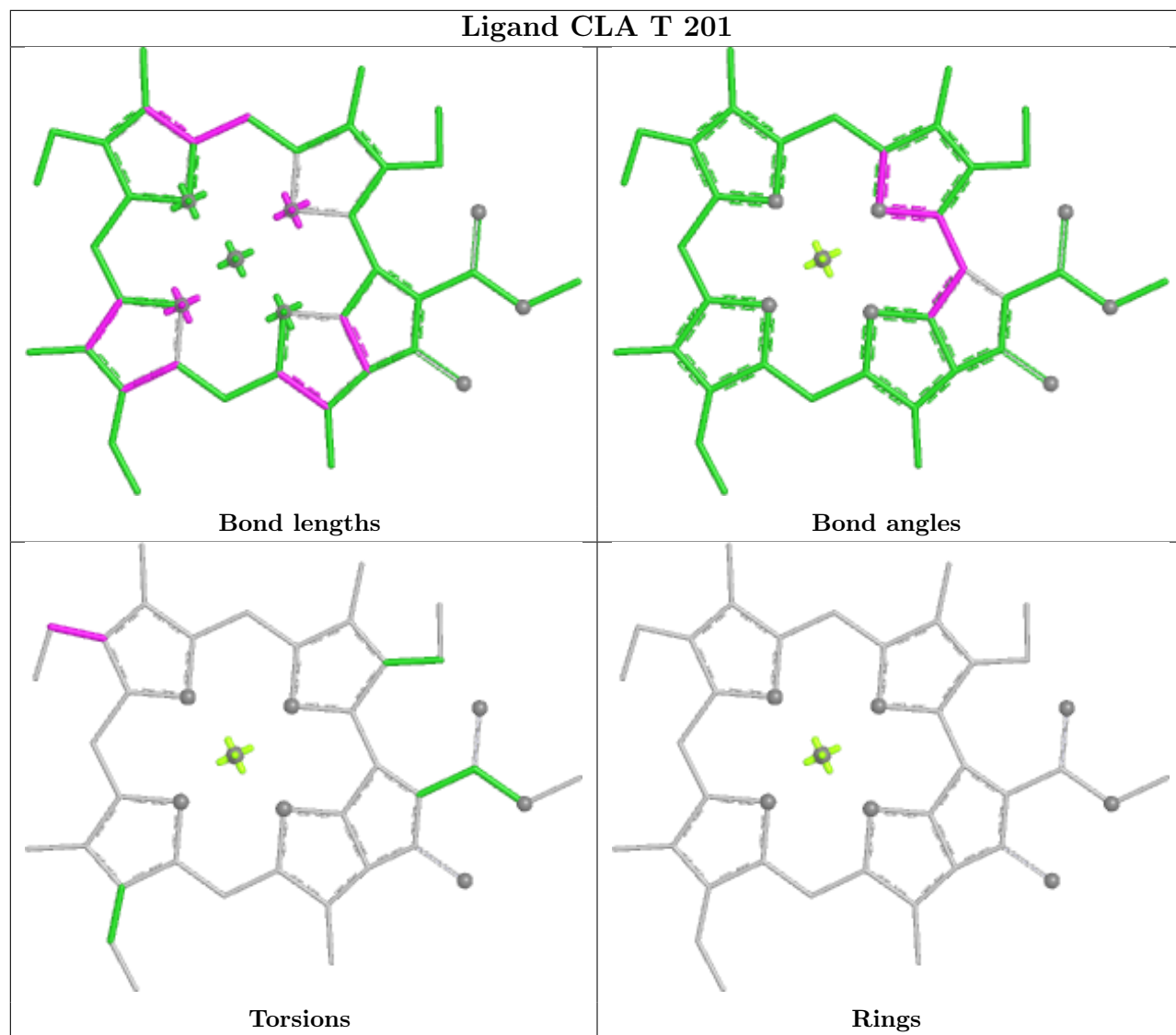




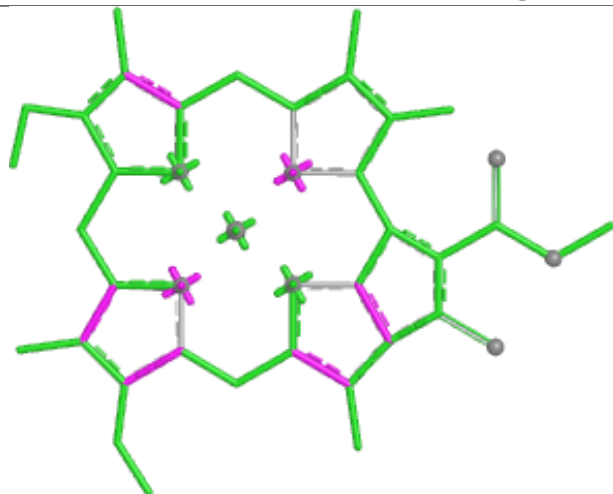




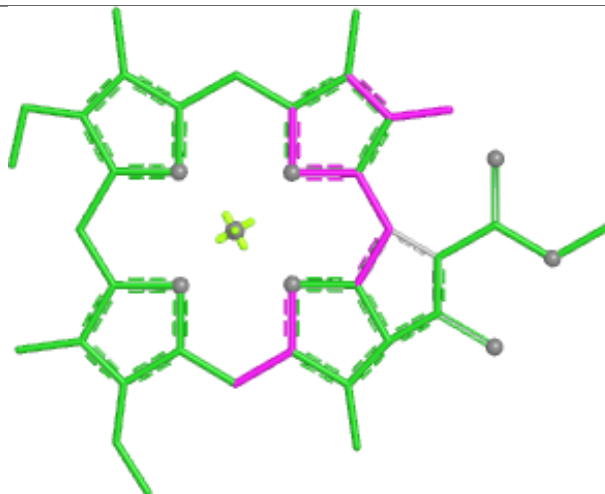
Ligand CLA T 201



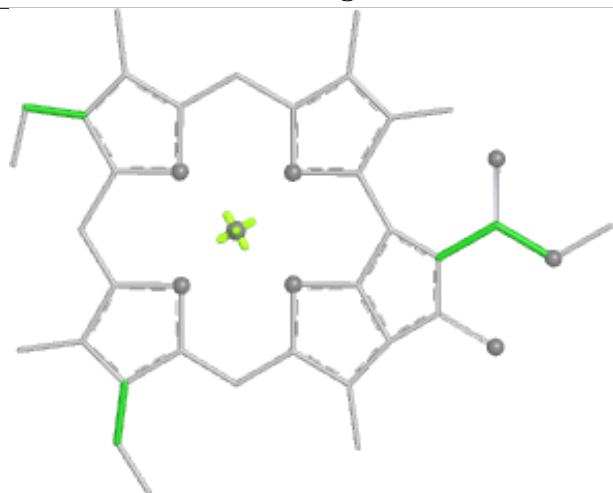
Ligand CLA O 211



Bond lengths



Bond angles

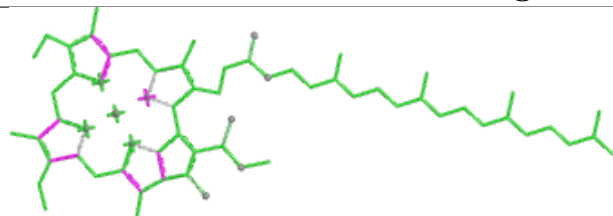


Torsions

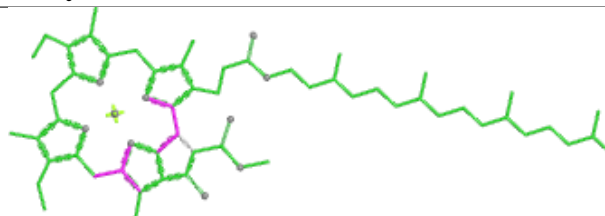


Rings

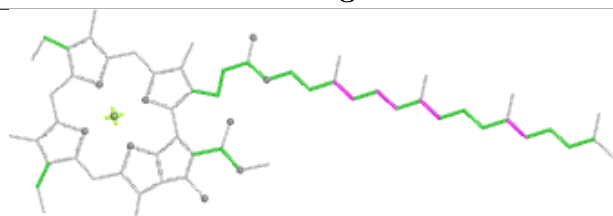
Ligand CLA Q 216



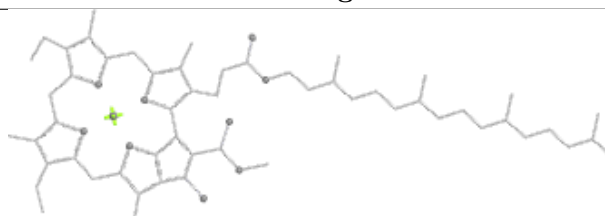
Bond lengths



Bond angles

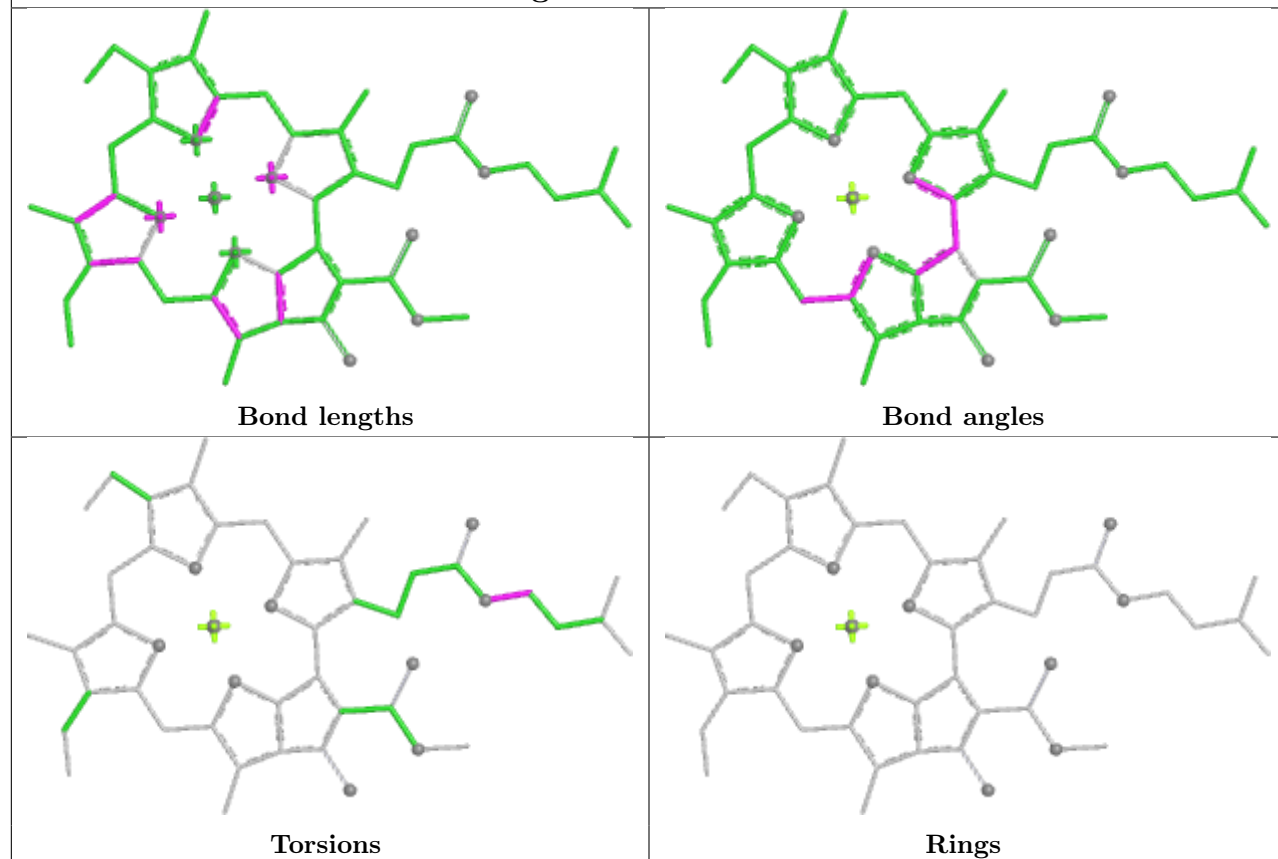


Torsions

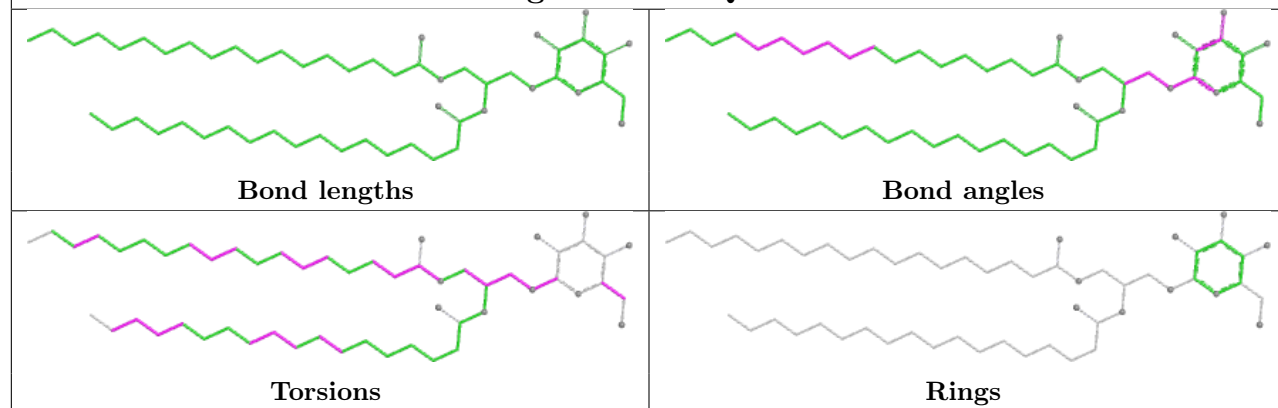


Rings

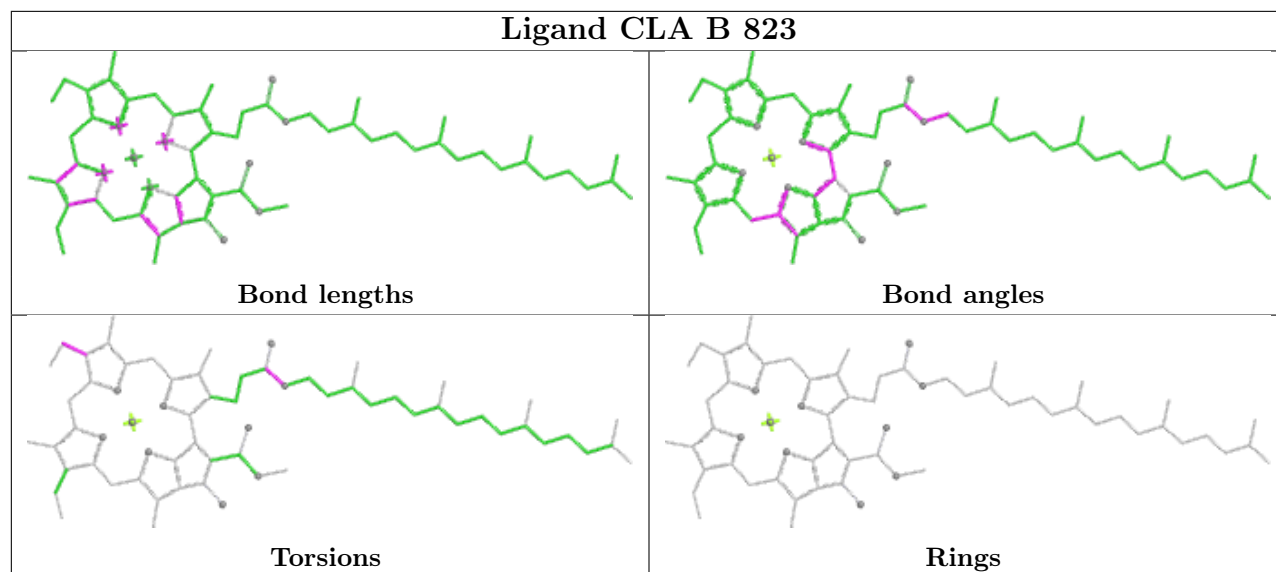
Ligand CLA A 830



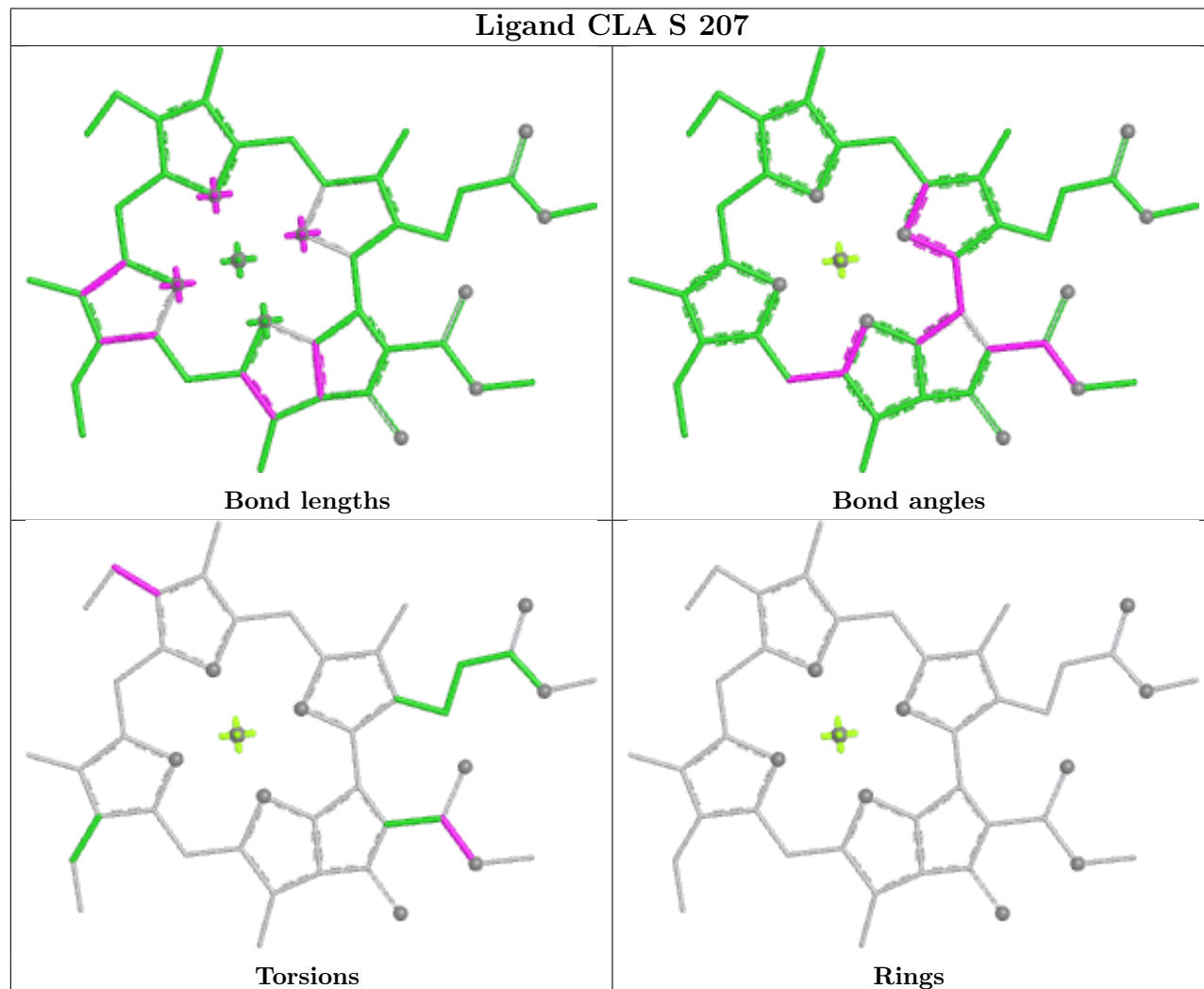
Ligand LMG Q 217

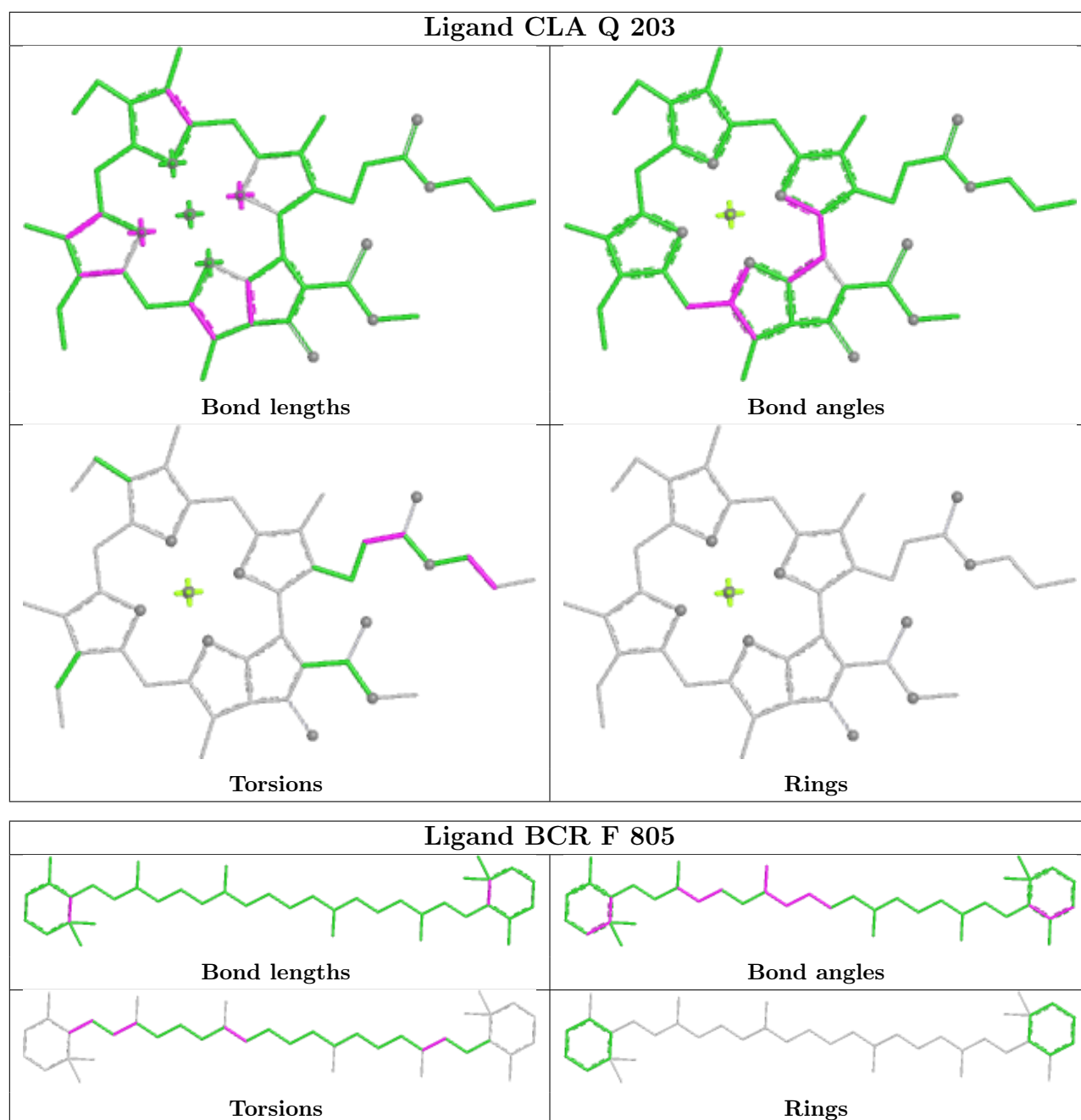


Ligand CLA B 823

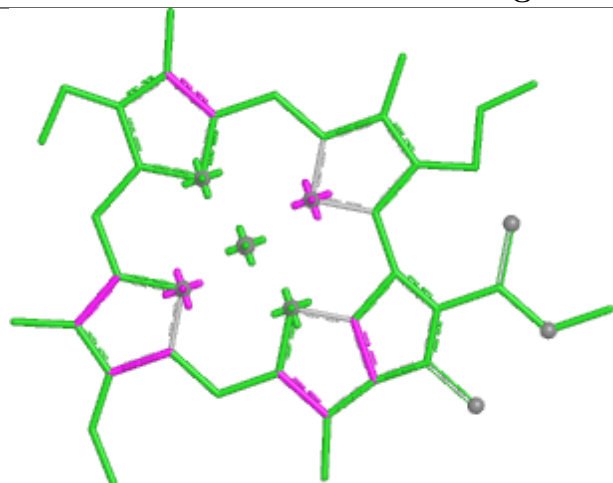


Ligand CLA S 207

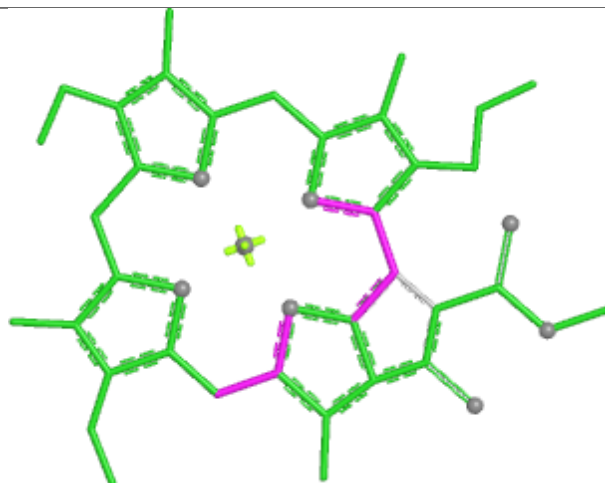




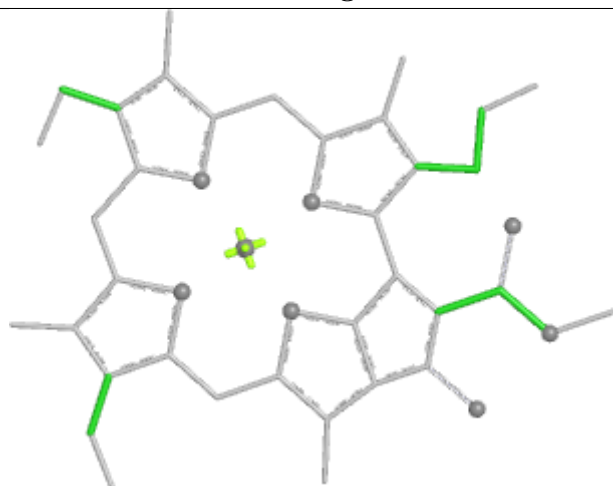
Ligand CLA A 819



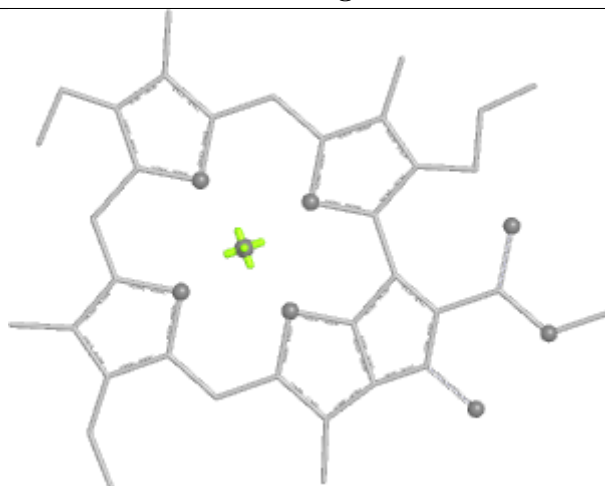
Bond lengths



Bond angles

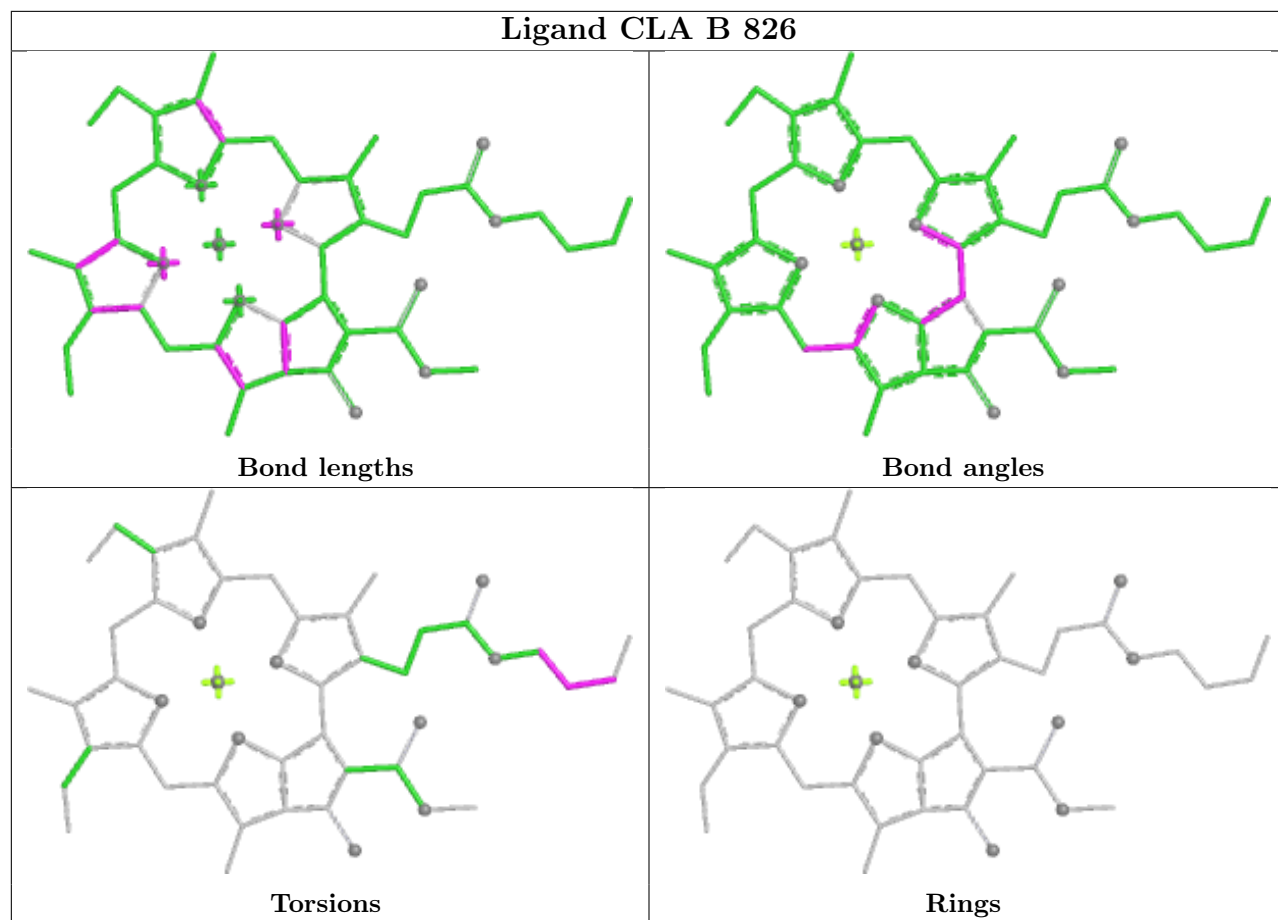


Torsions

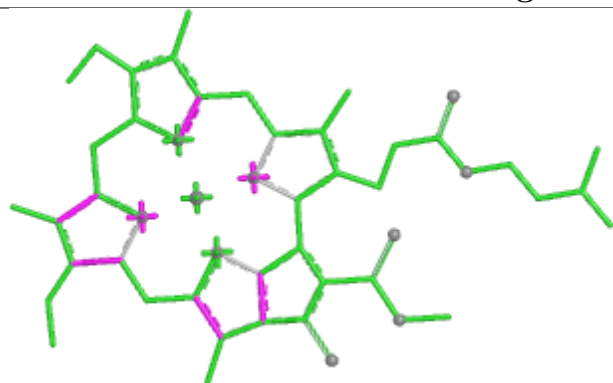


Rings

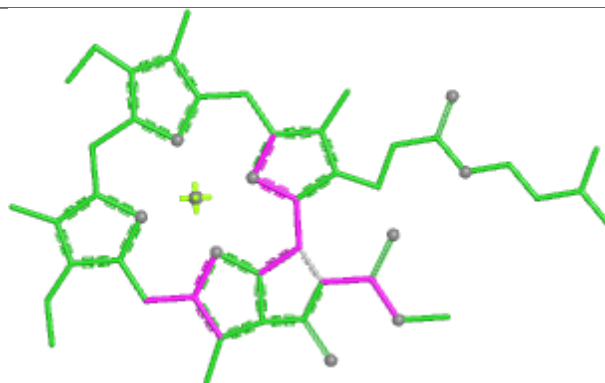
Ligand CLA B 826



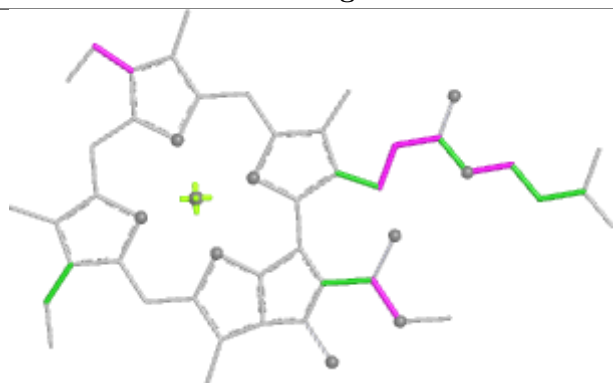
Ligand CLA L 204



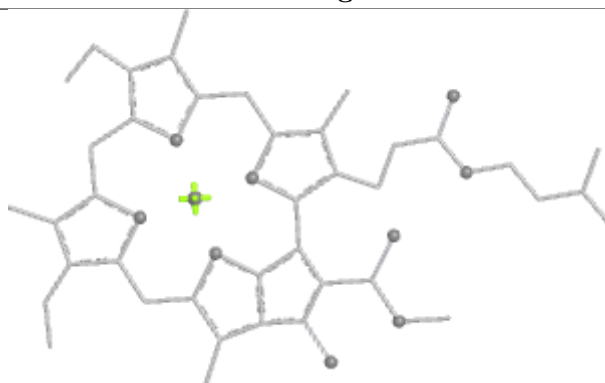
Bond lengths



Bond angles

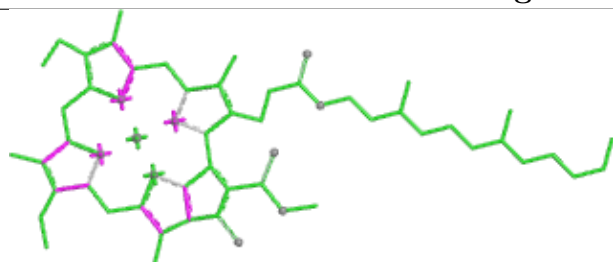


Torsions

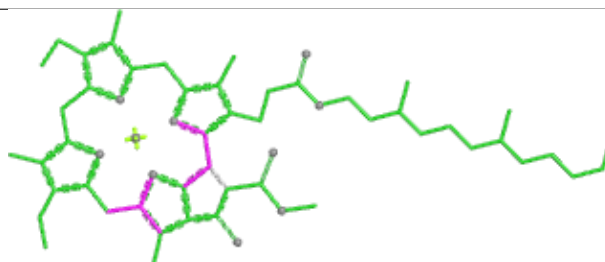


Rings

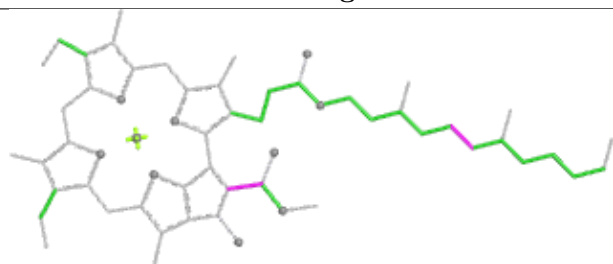
Ligand CLA B 812



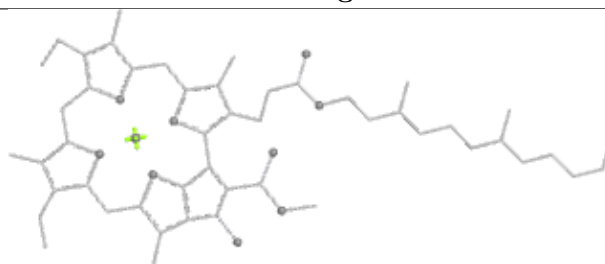
Bond lengths



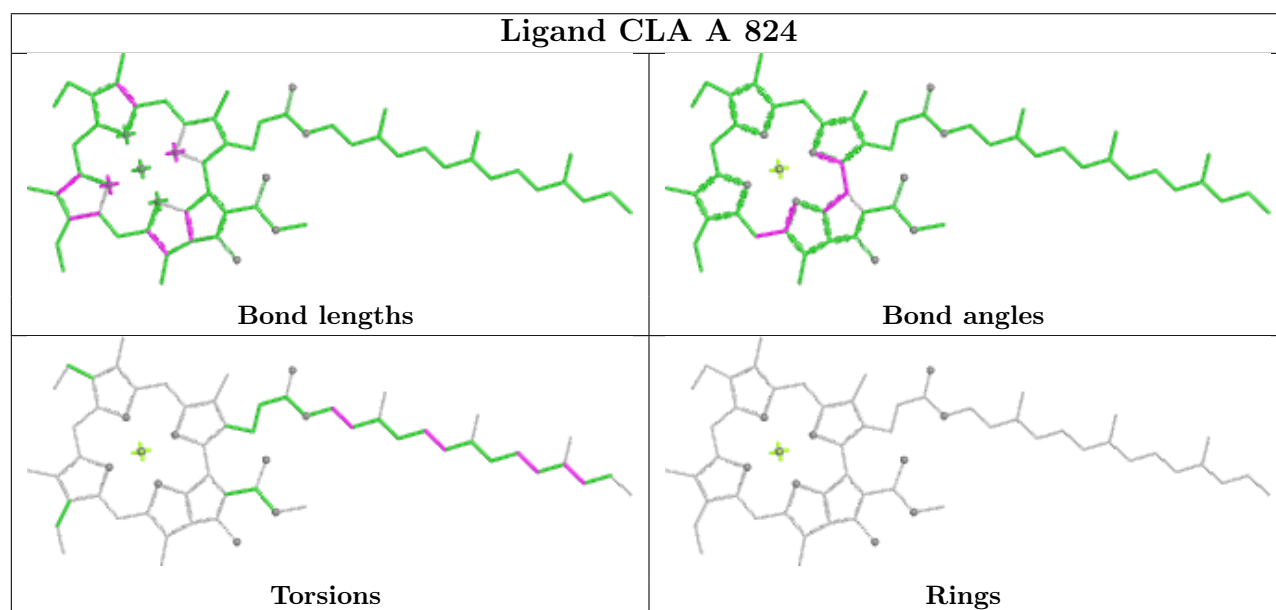
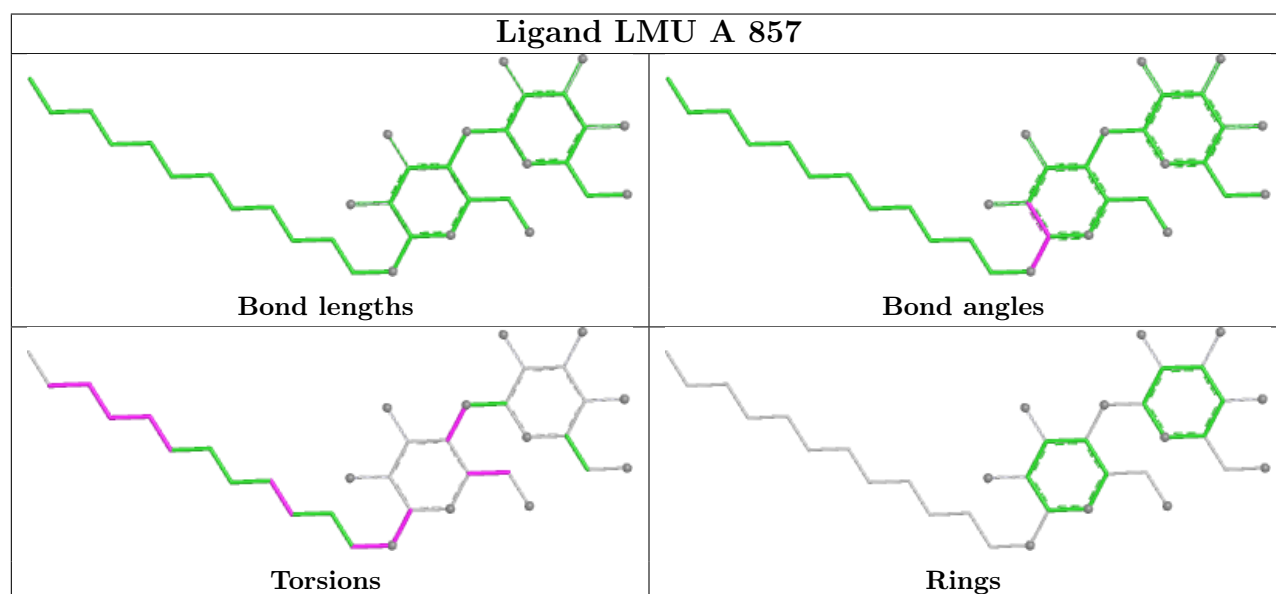
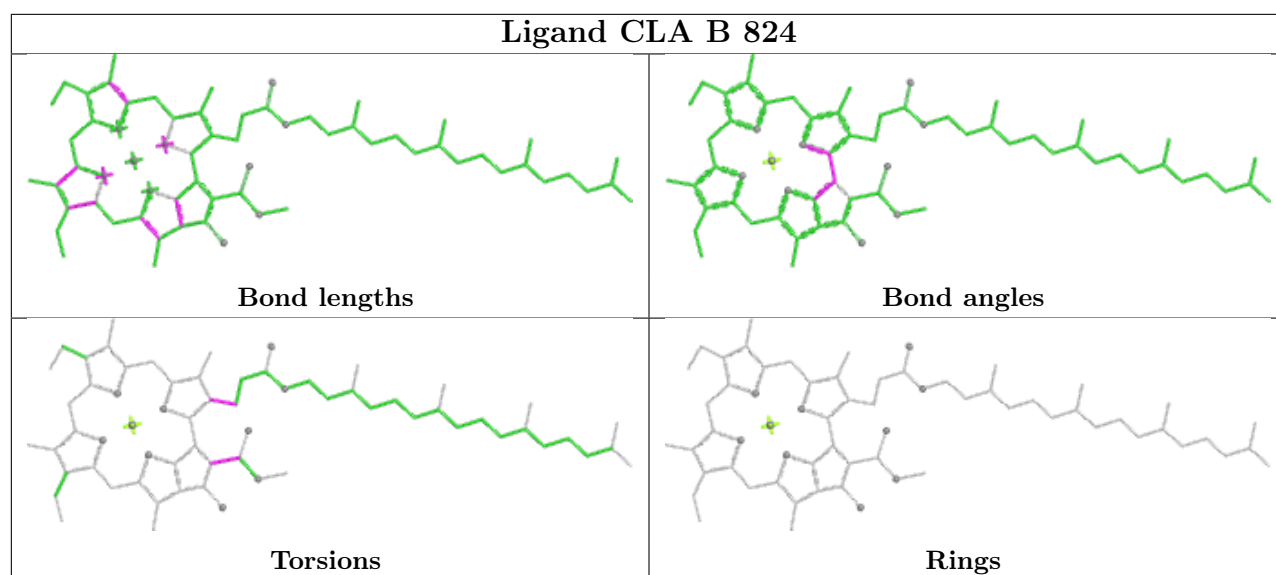
Bond angles

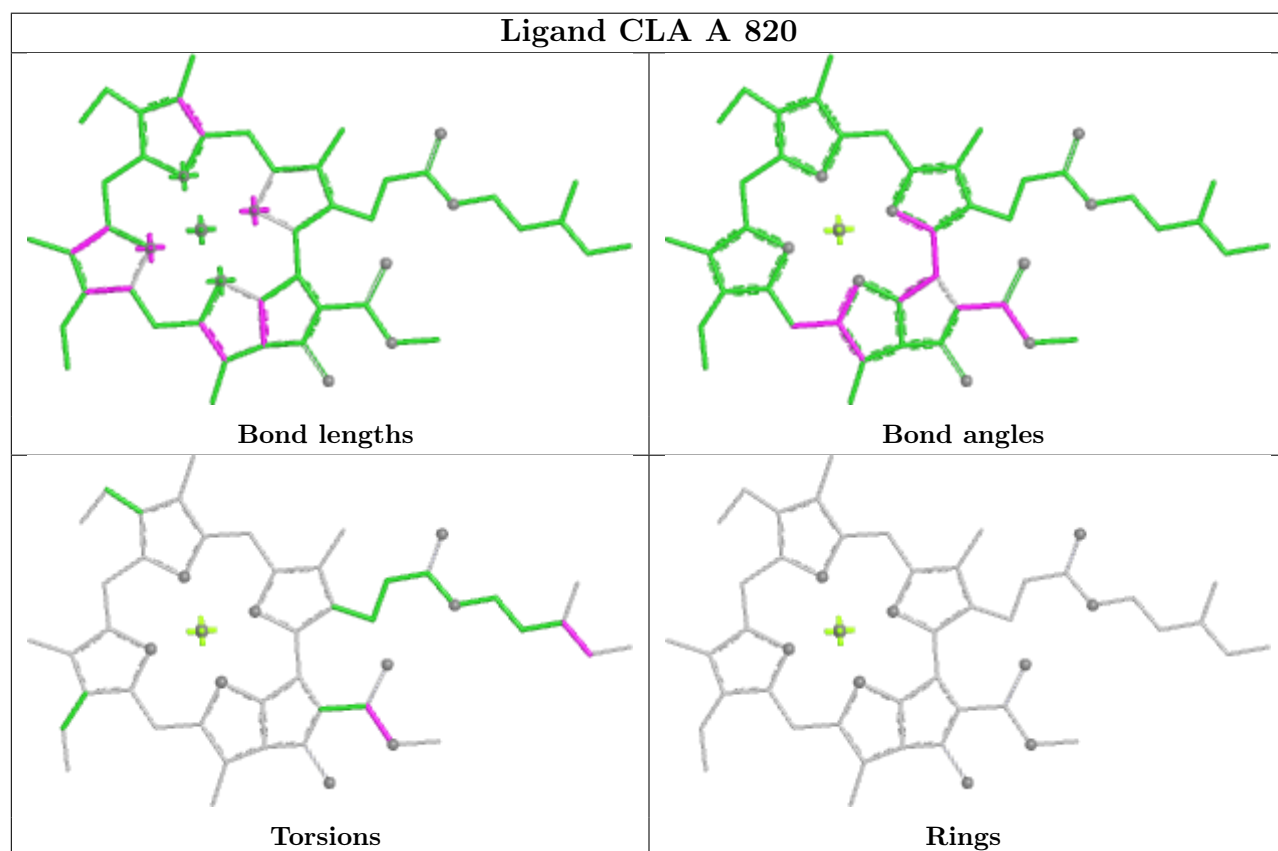
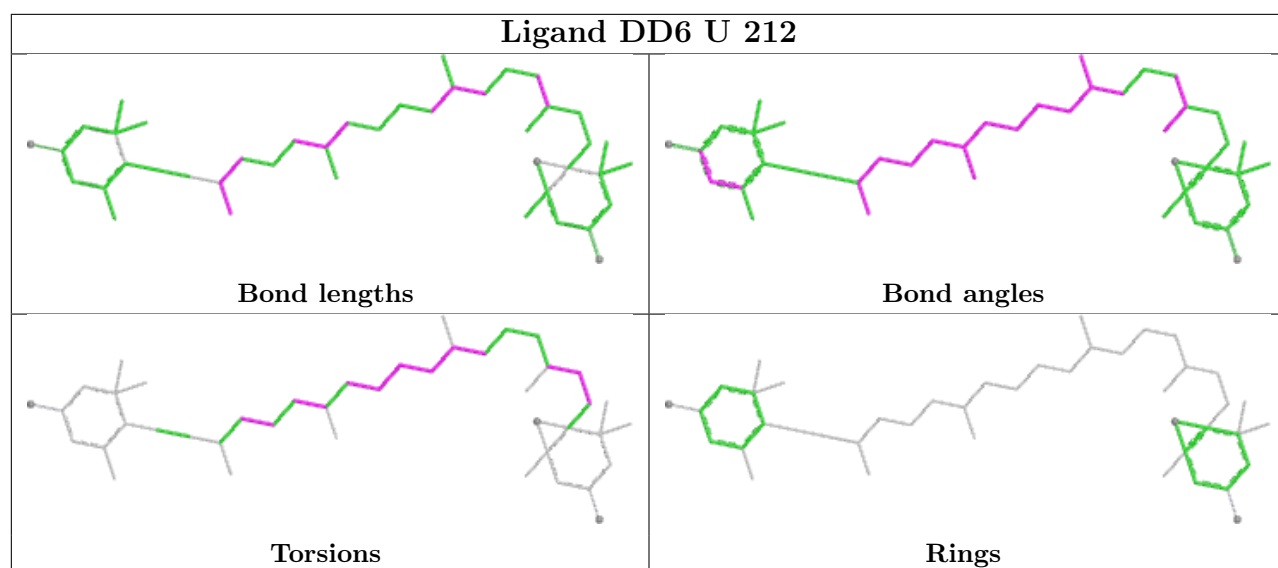


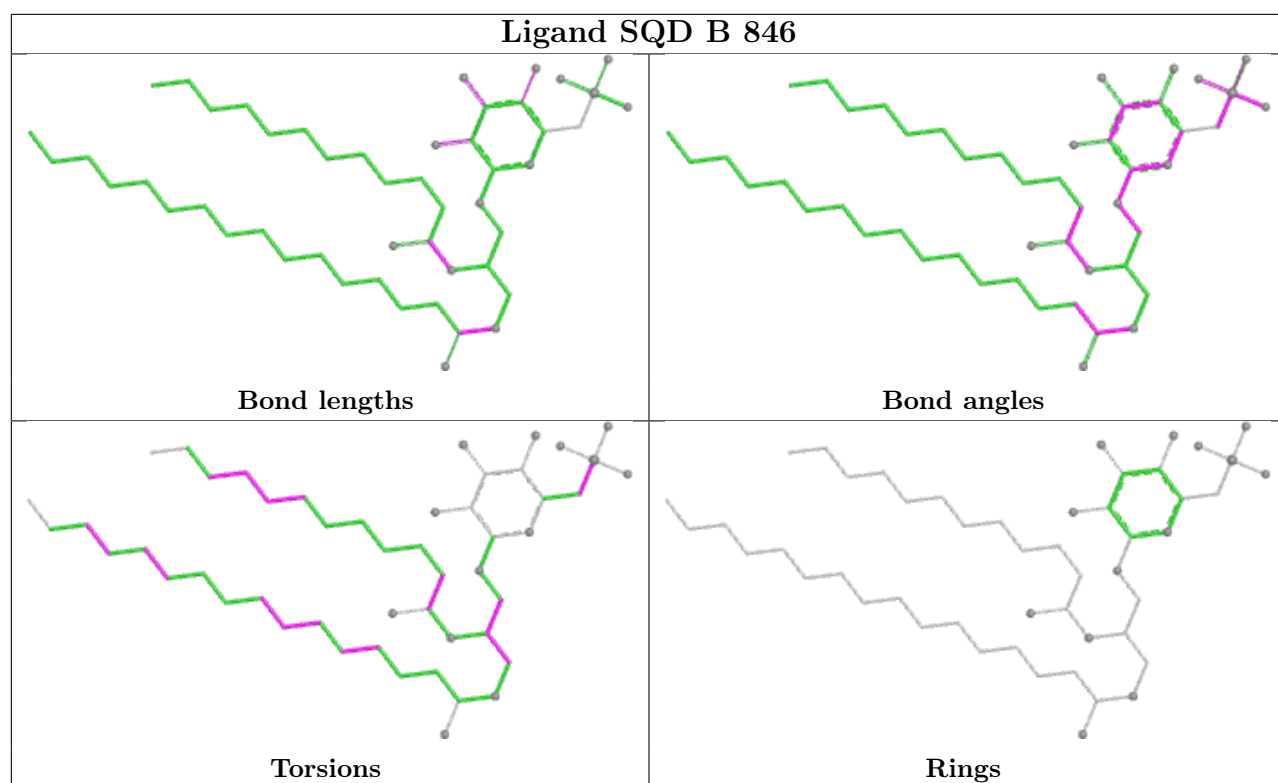
Torsions



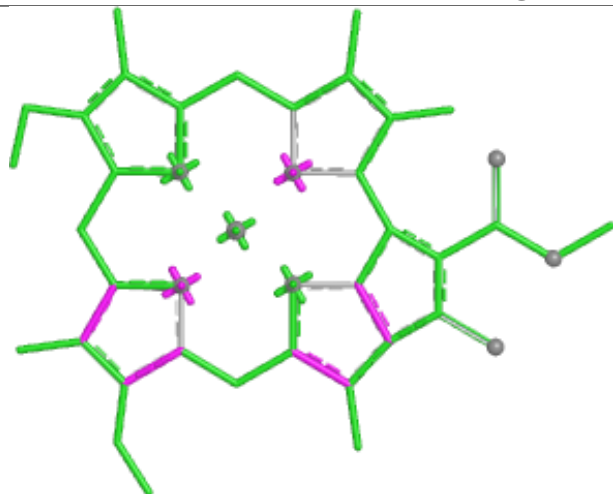
Rings



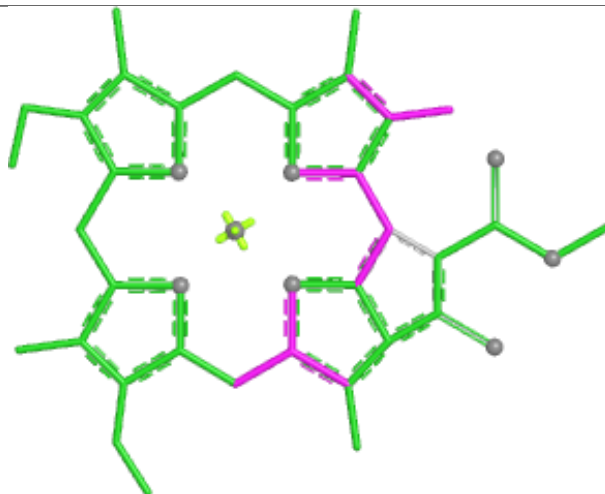




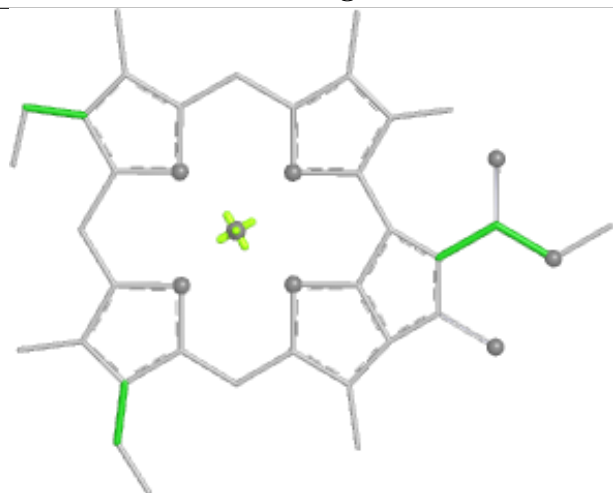
Ligand CLA G 202



Bond lengths



Bond angles

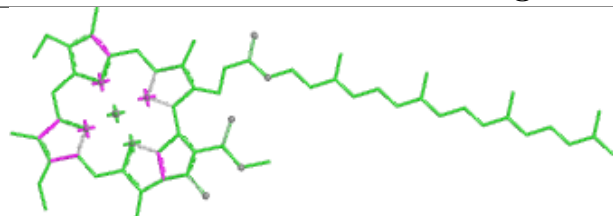


Torsions

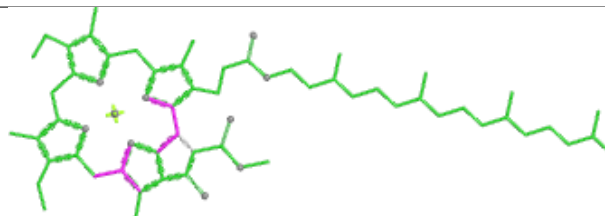


Rings

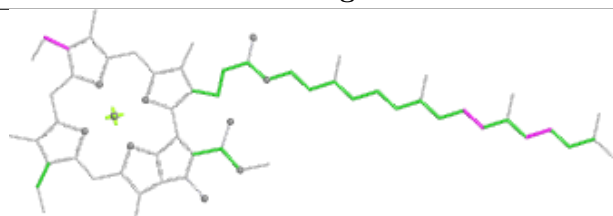
Ligand CLA A 833



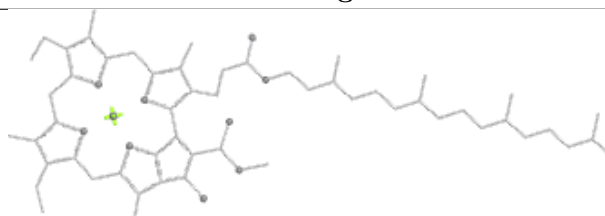
Bond lengths



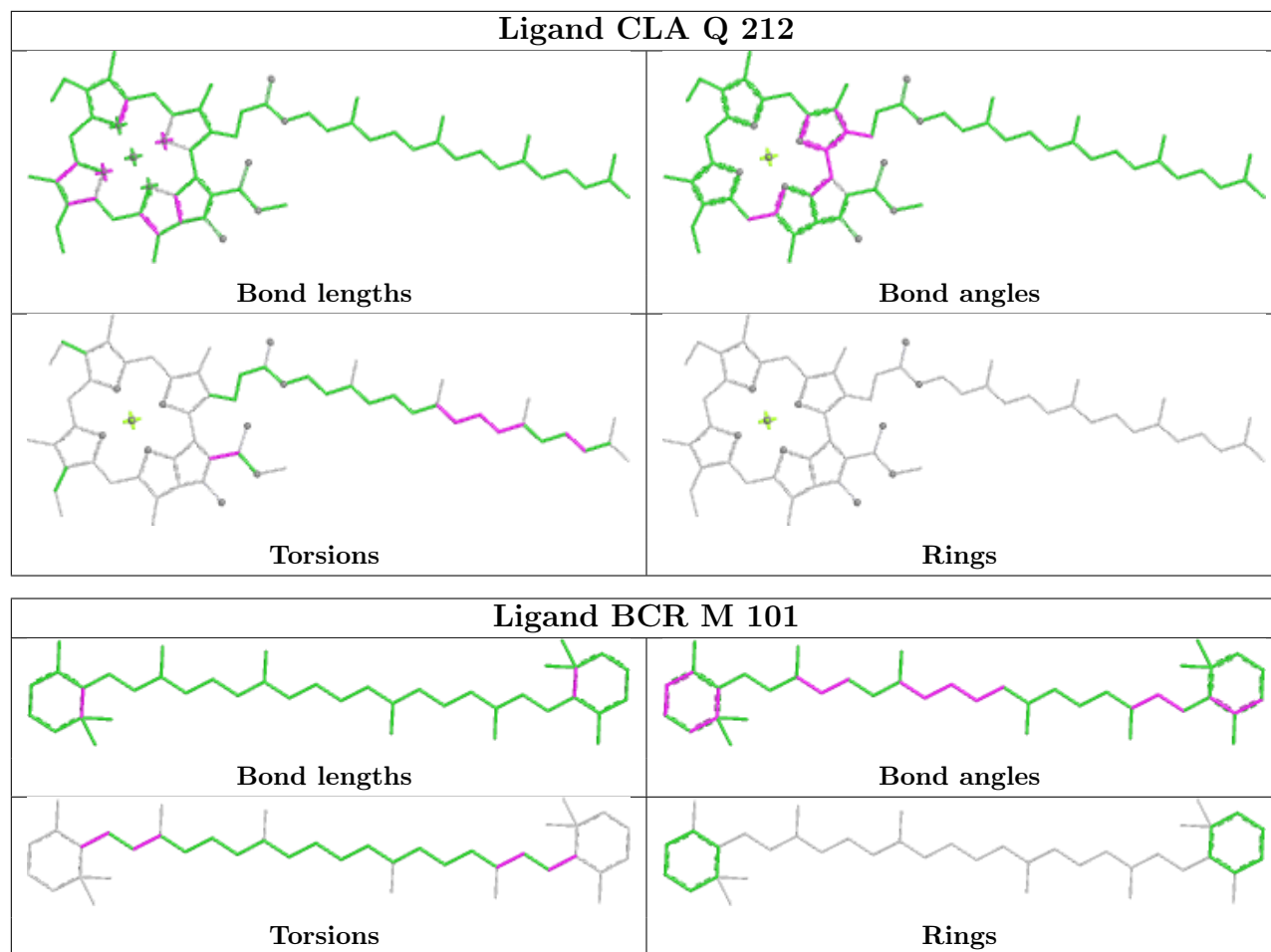
Bond angles

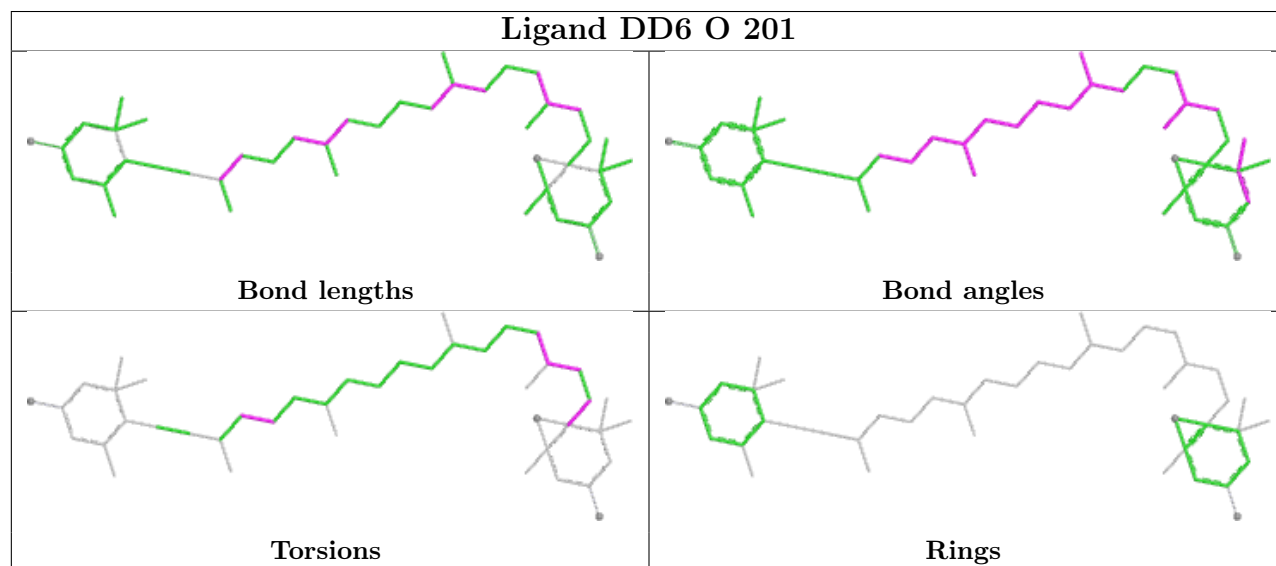
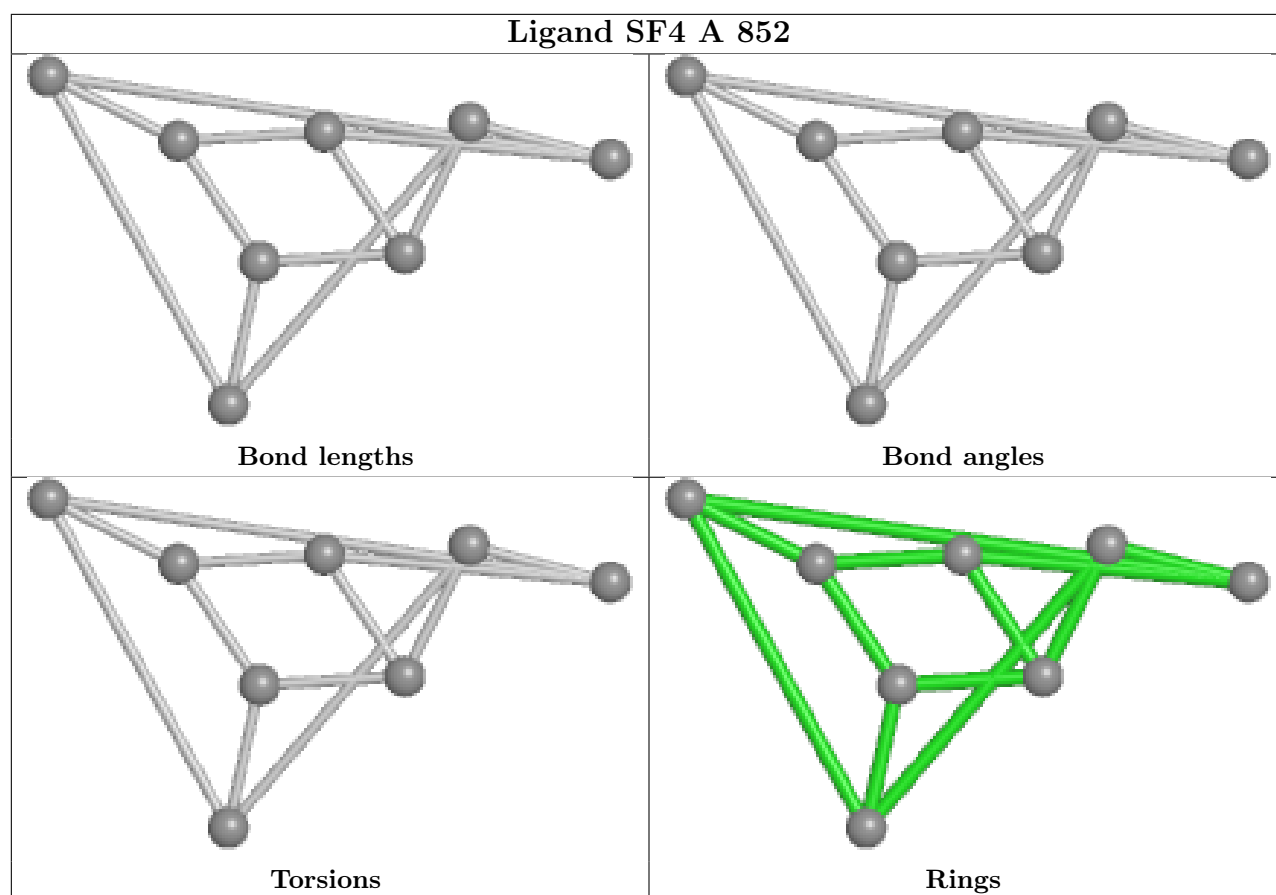


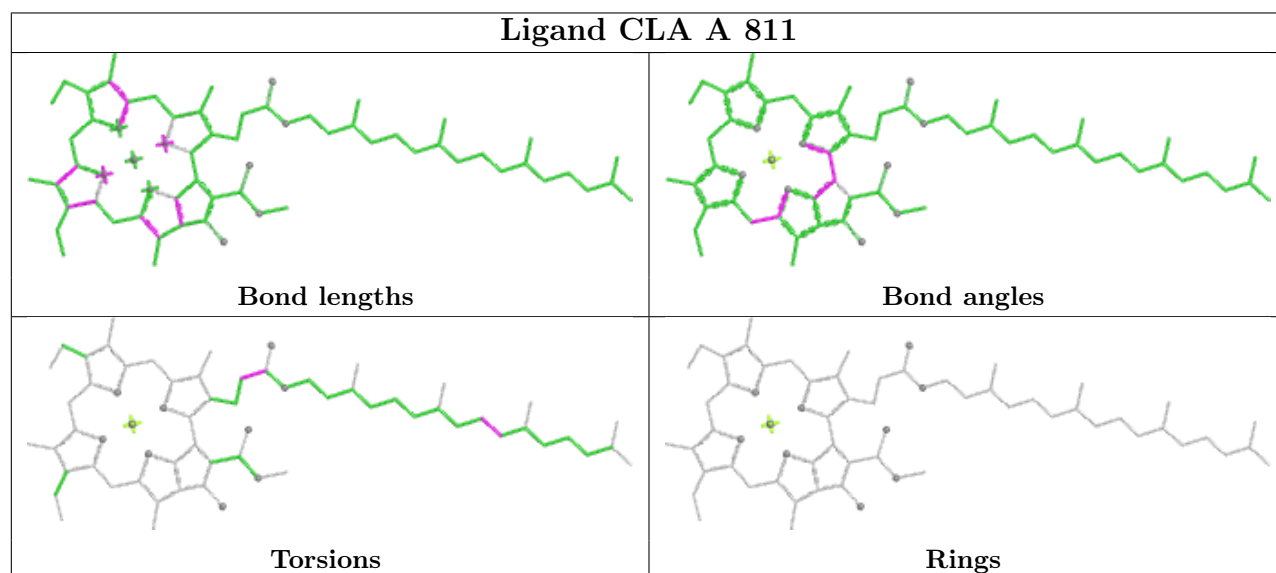
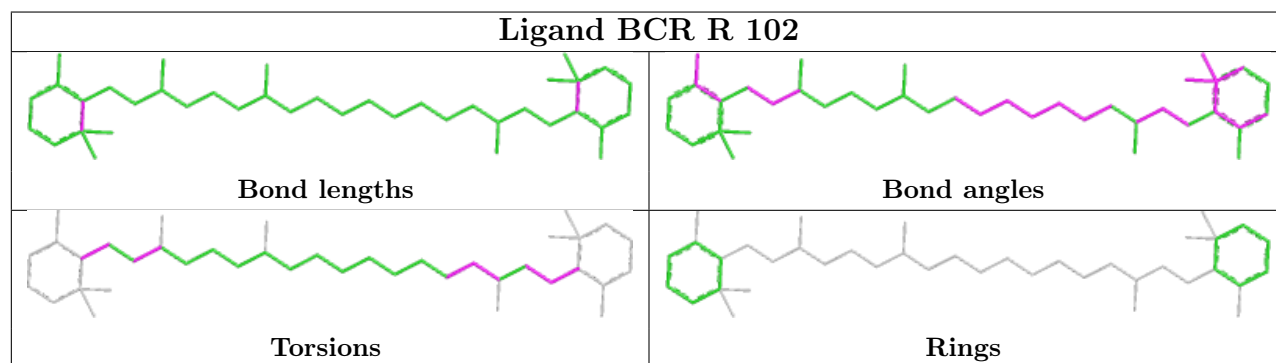
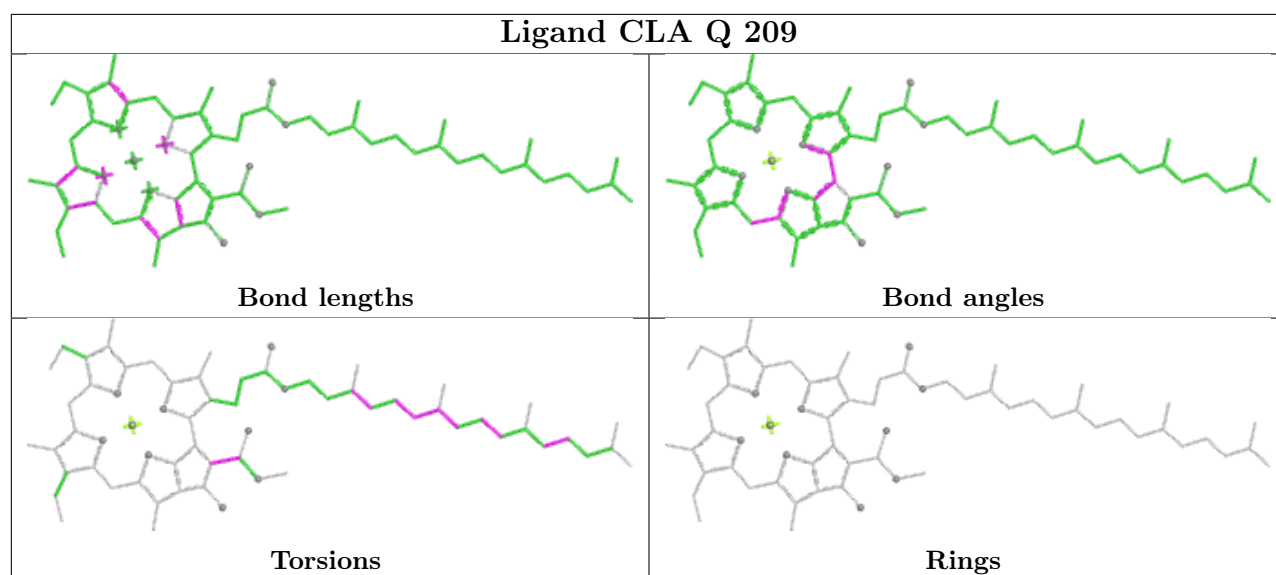
Torsions

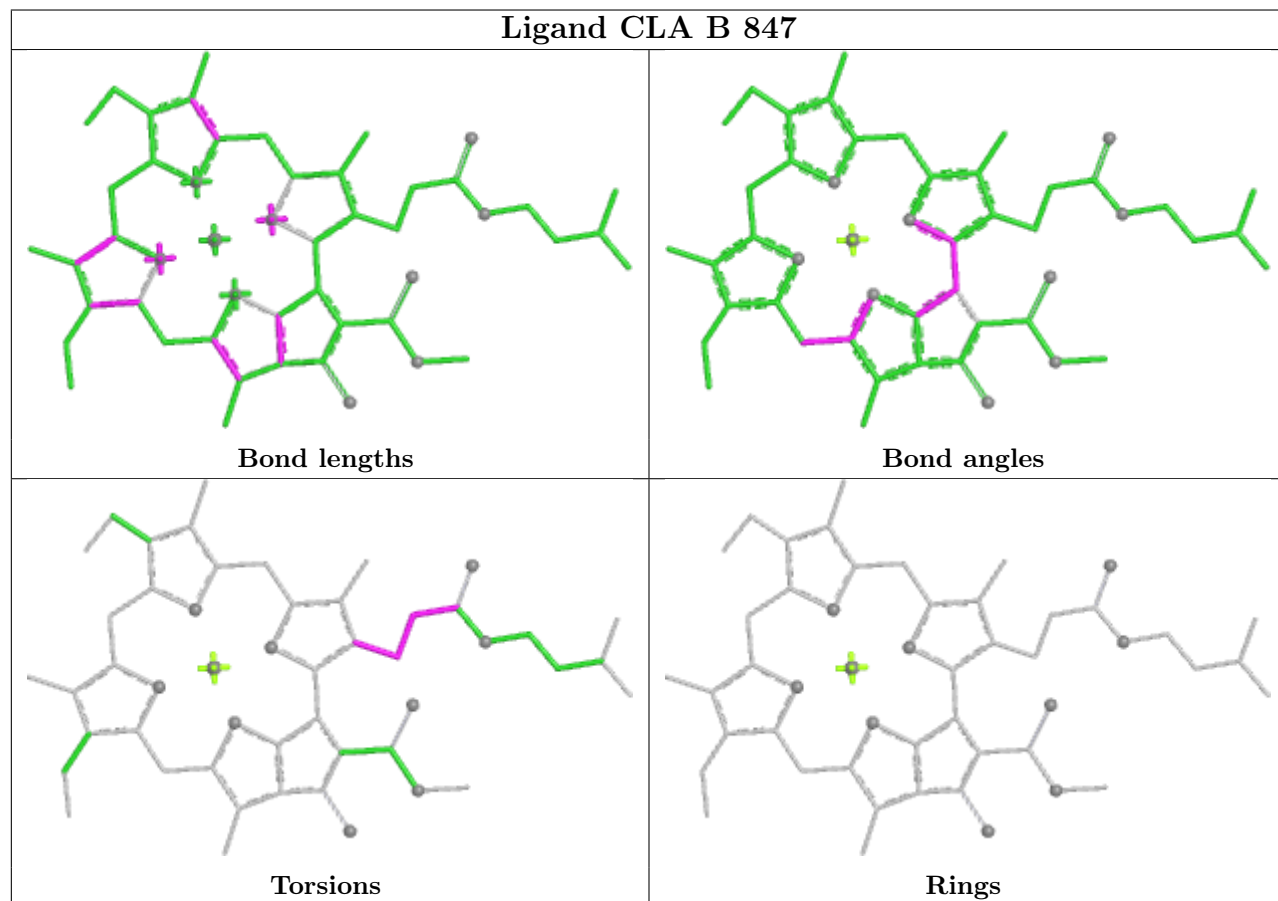
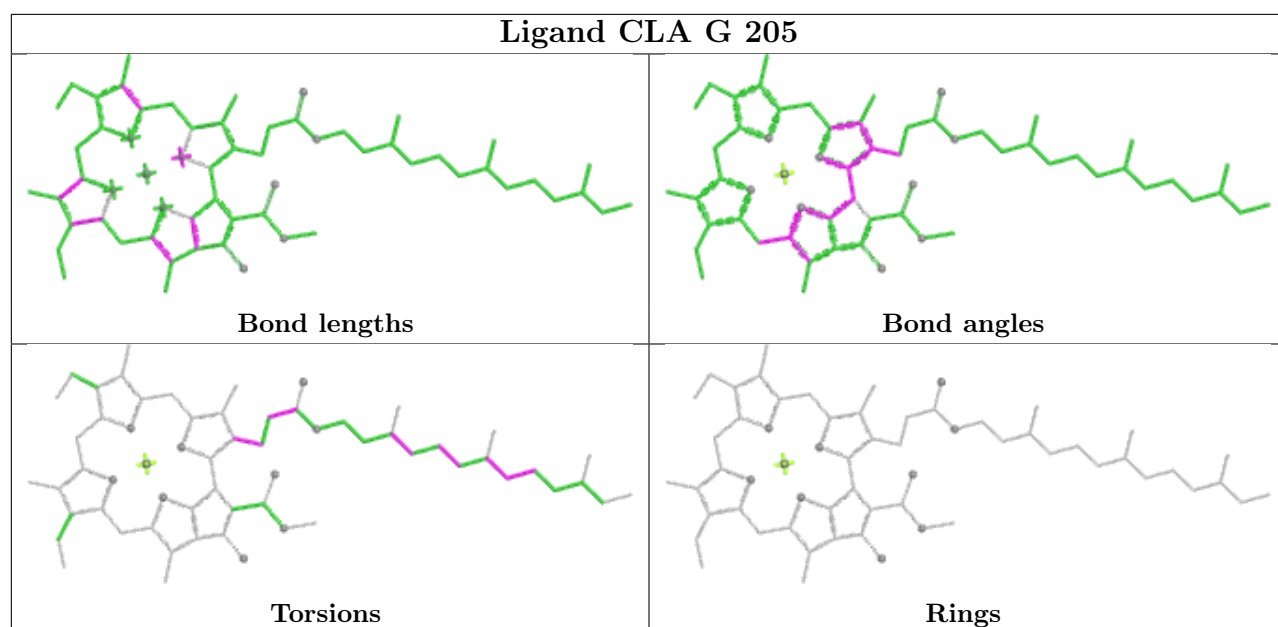


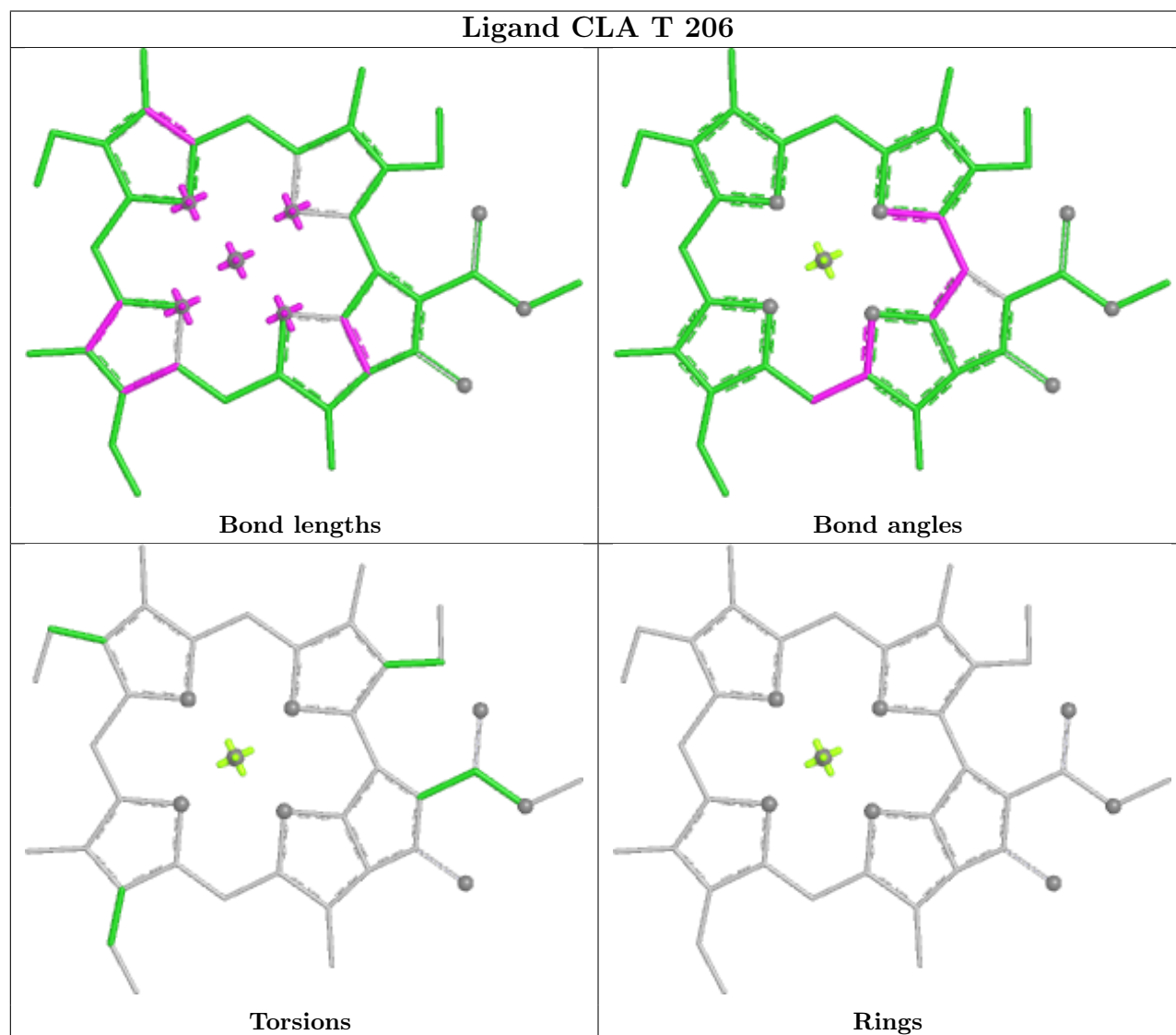
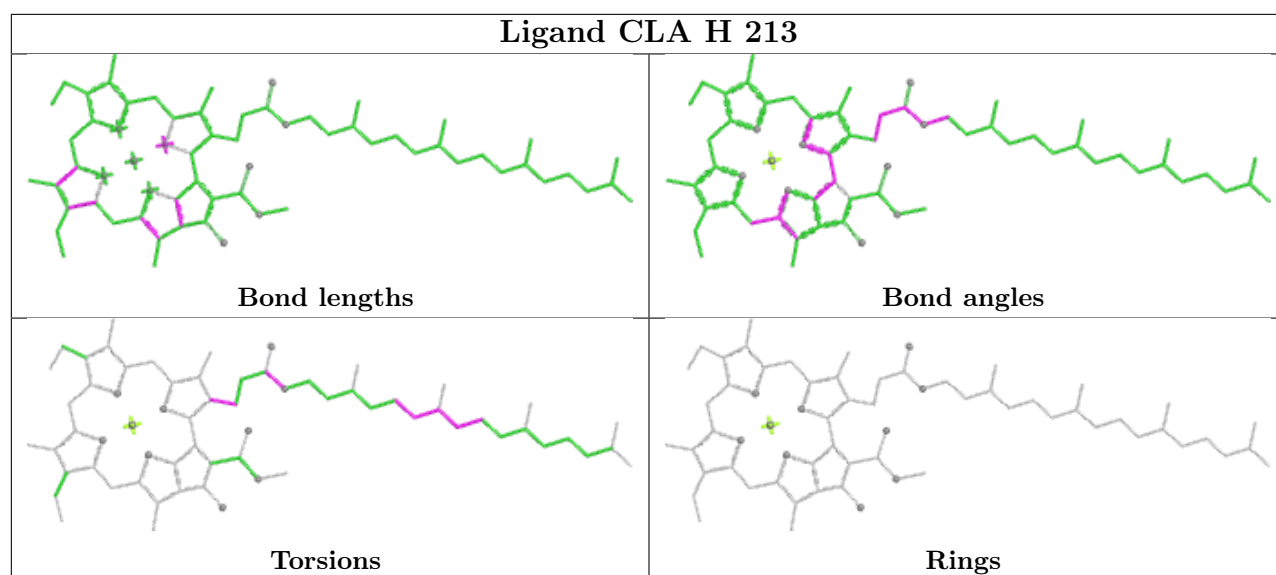
Rings



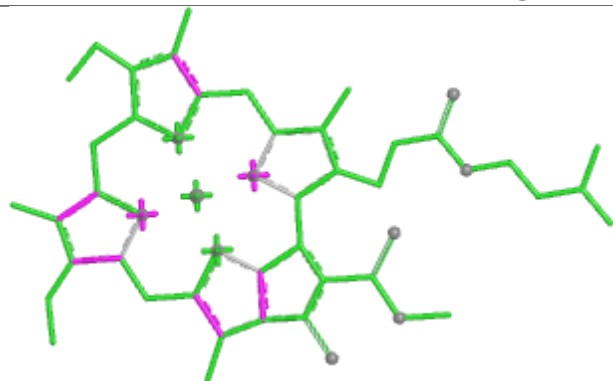




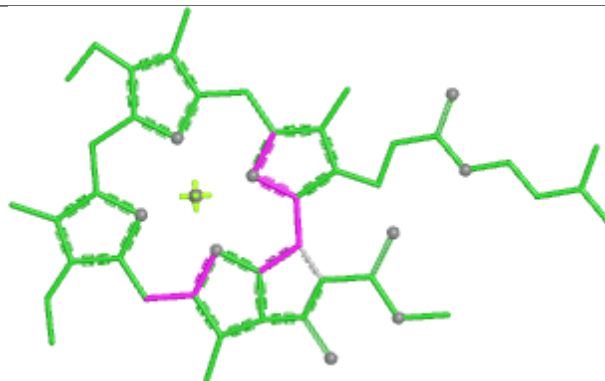




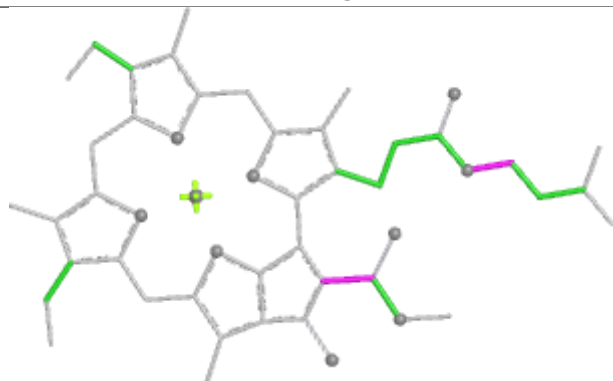
Ligand CLA A 827



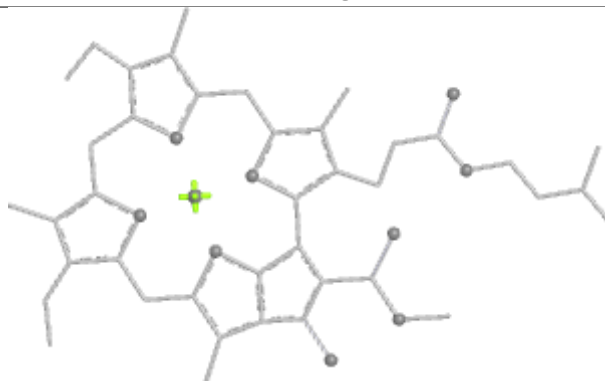
Bond lengths



Bond angles

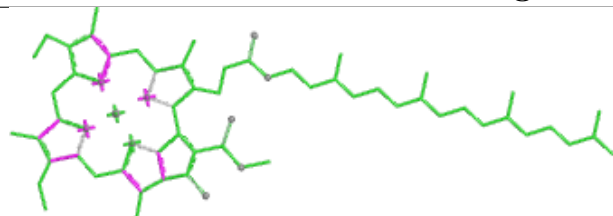


Torsions

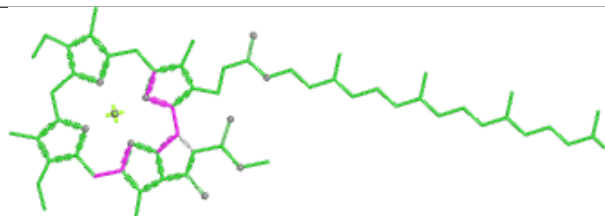


Rings

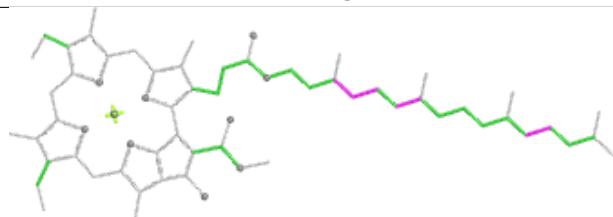
Ligand CLA A 834



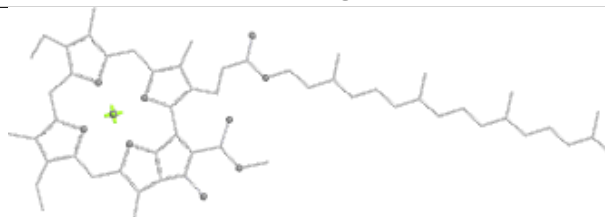
Bond lengths



Bond angles

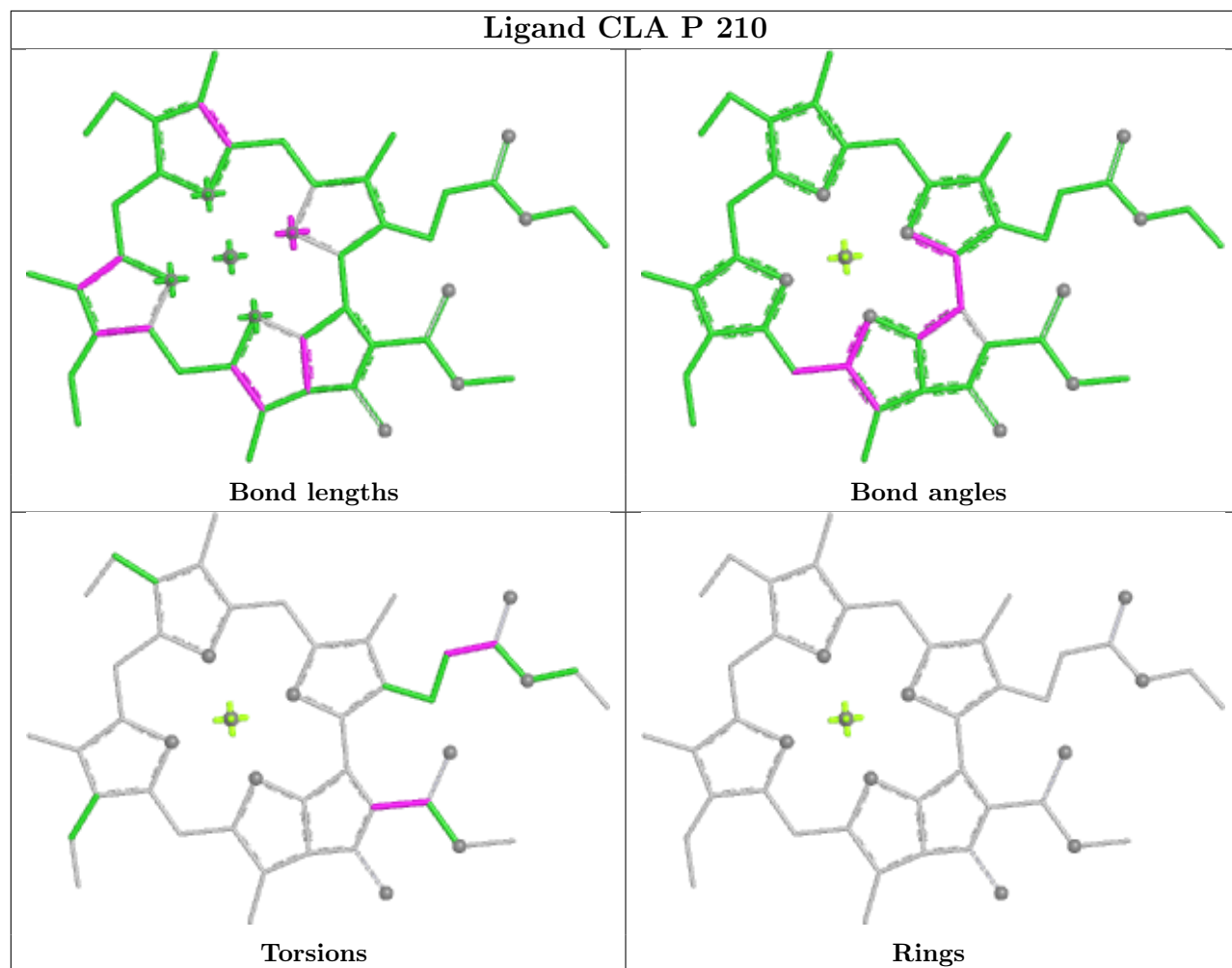


Torsions

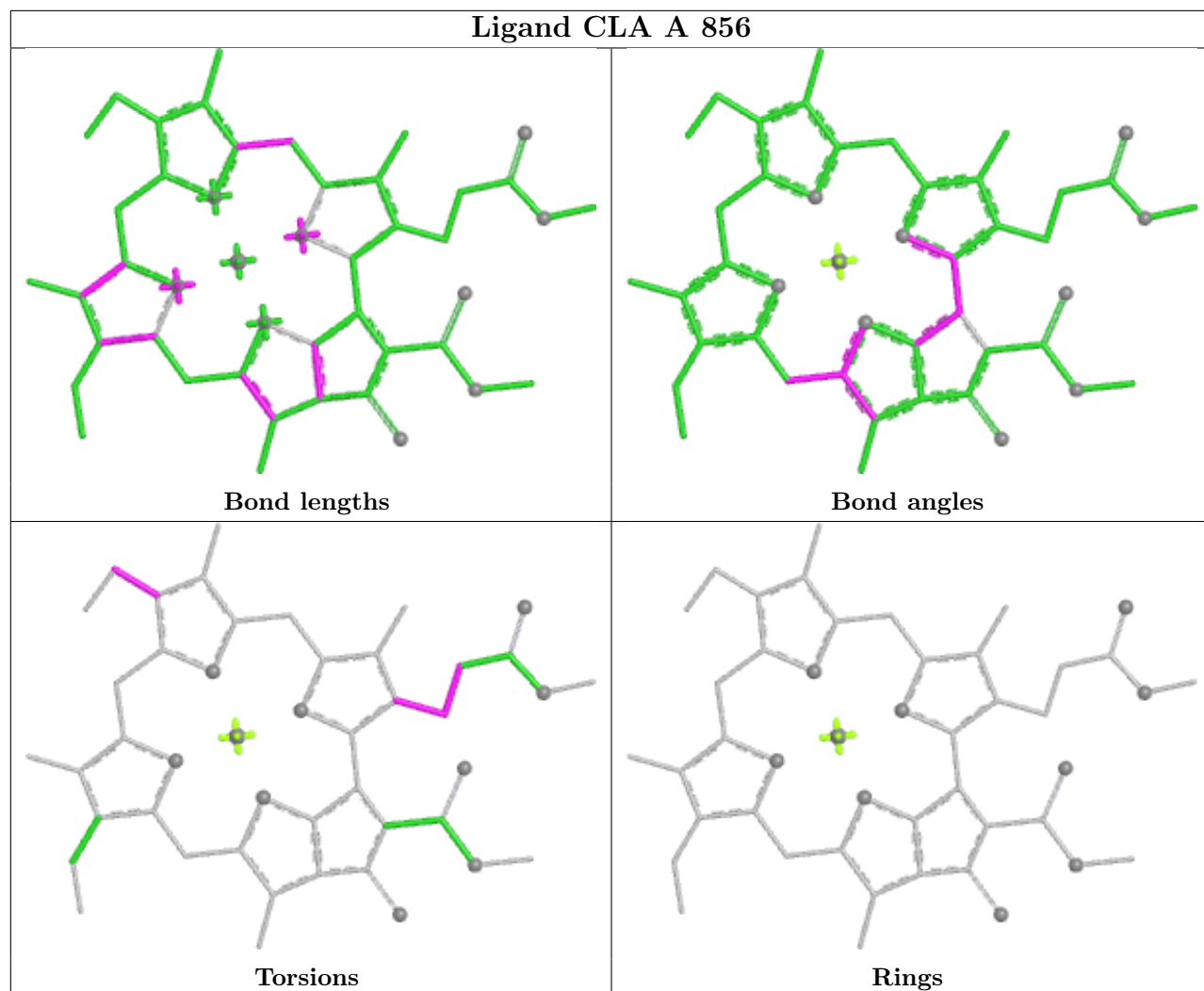


Rings

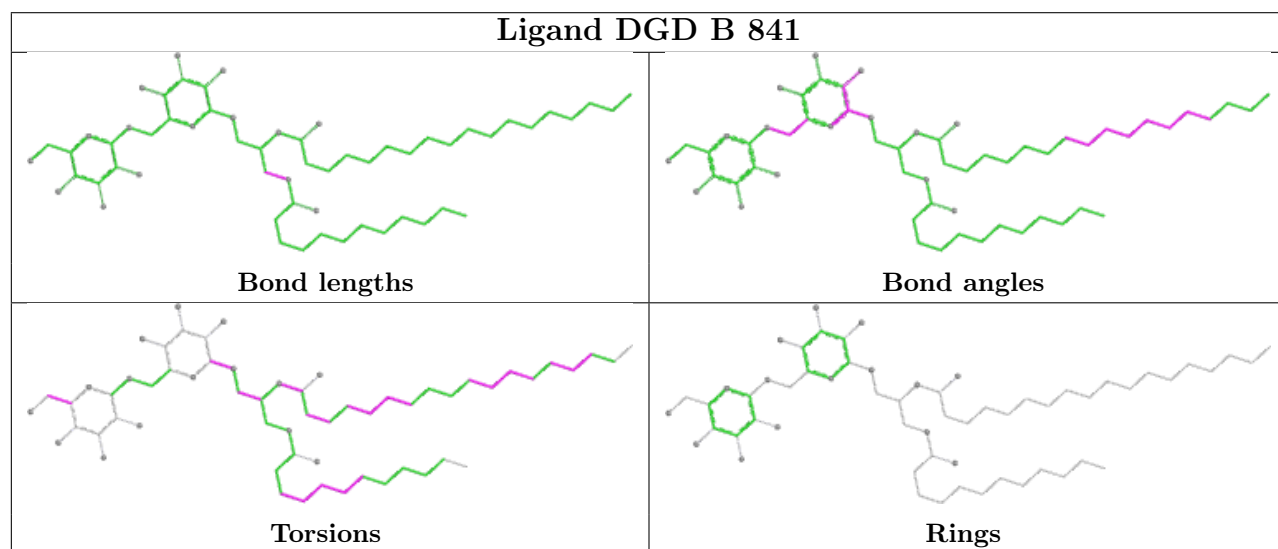
Ligand CLA P 210



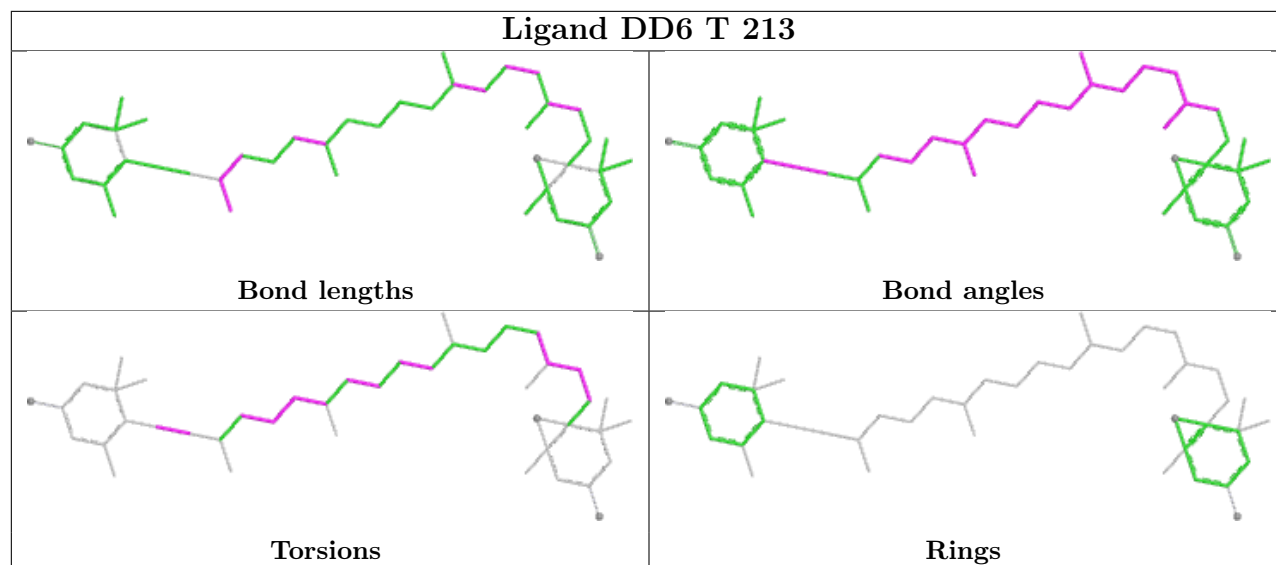
Ligand CLA A 856



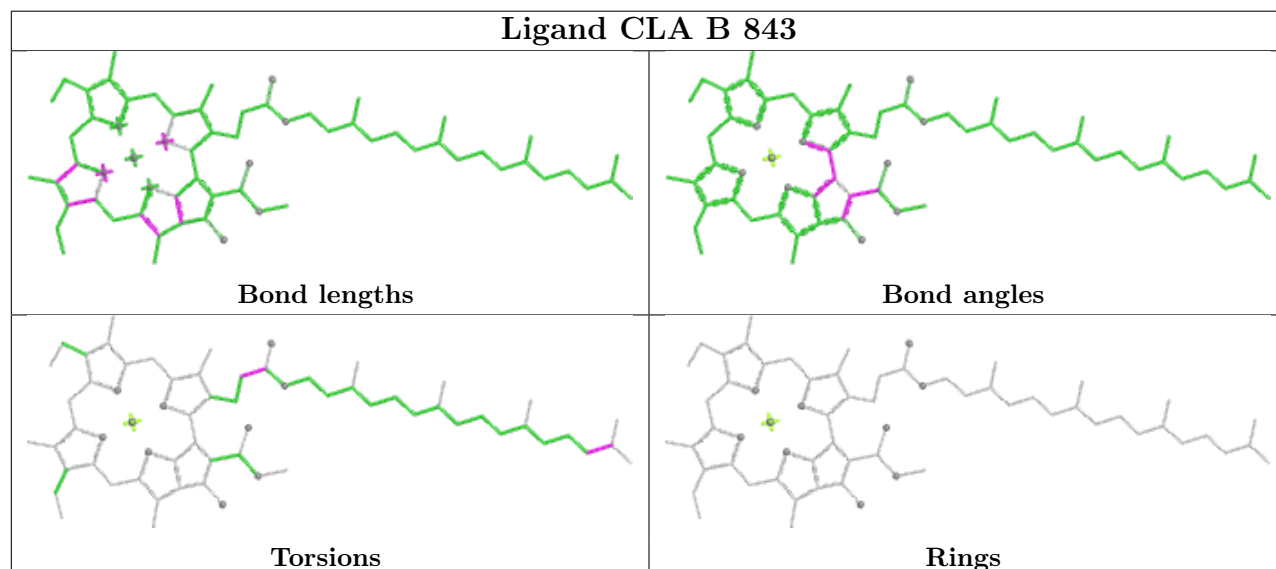
Ligand DGD B 841



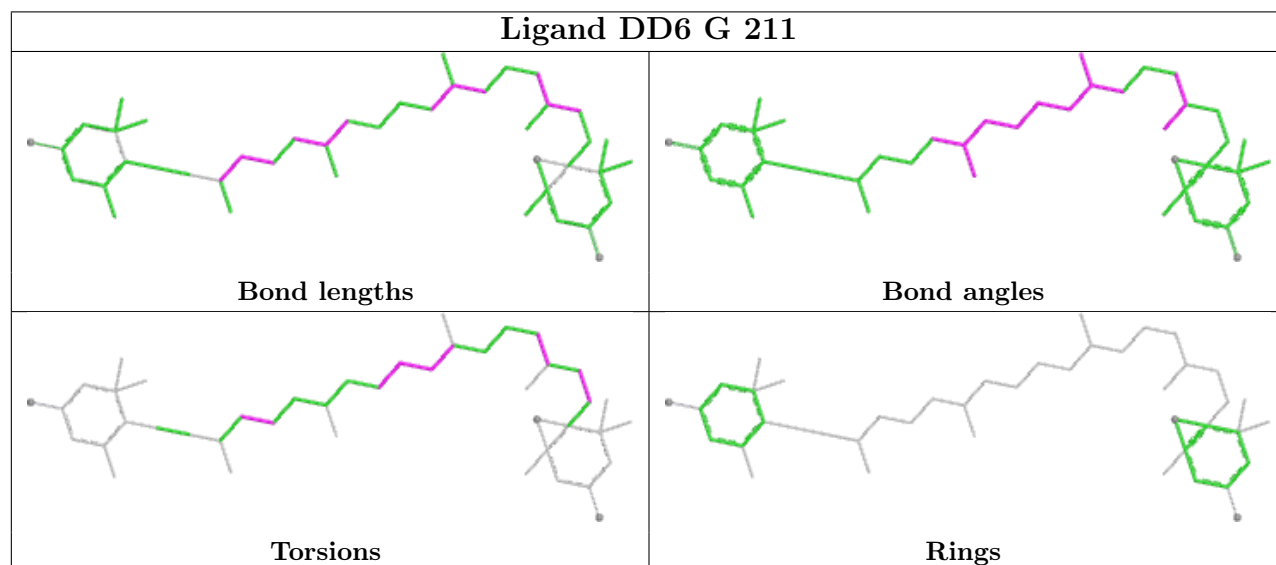
Ligand DD6 T 213

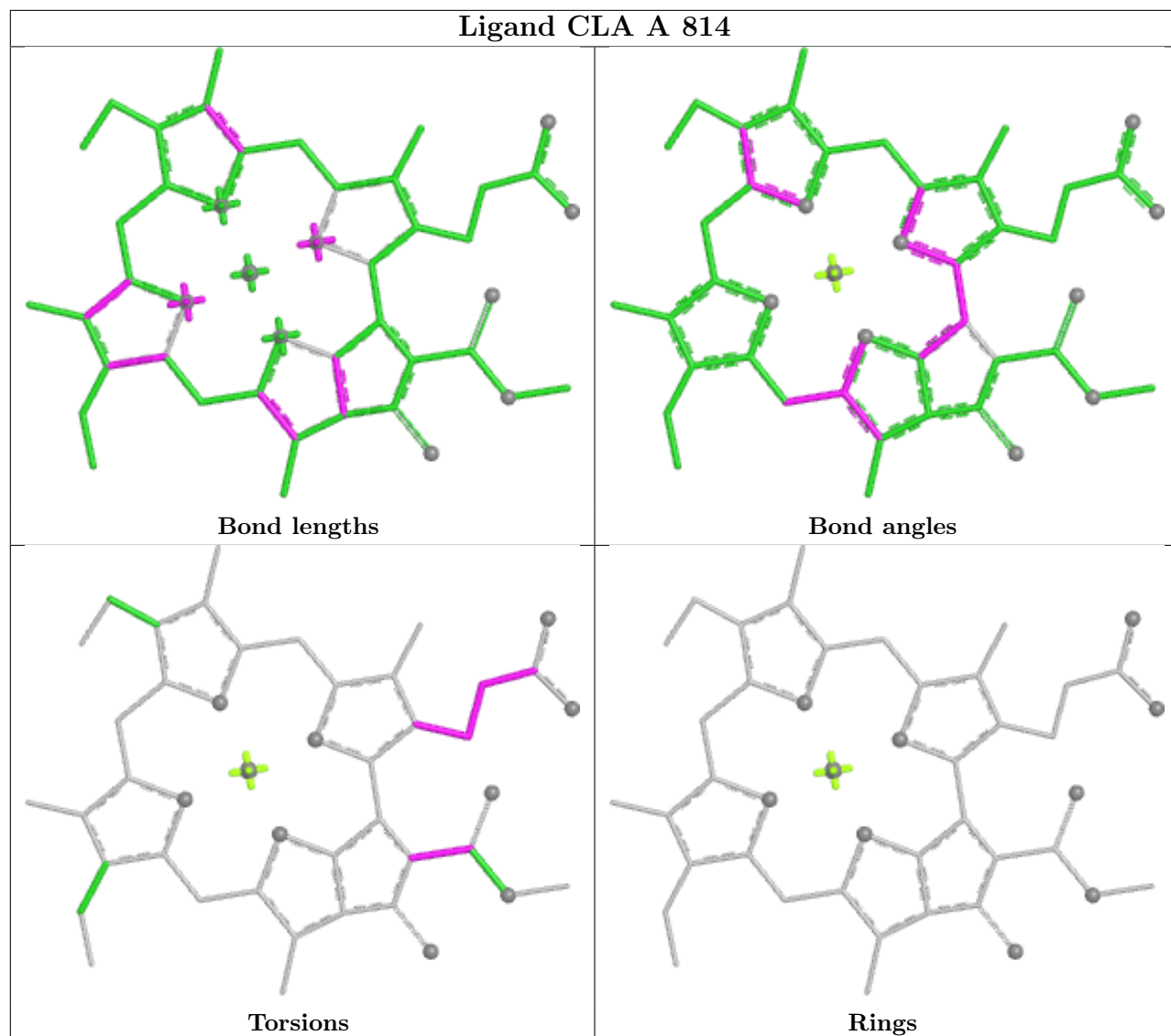


Ligand CLA B 843

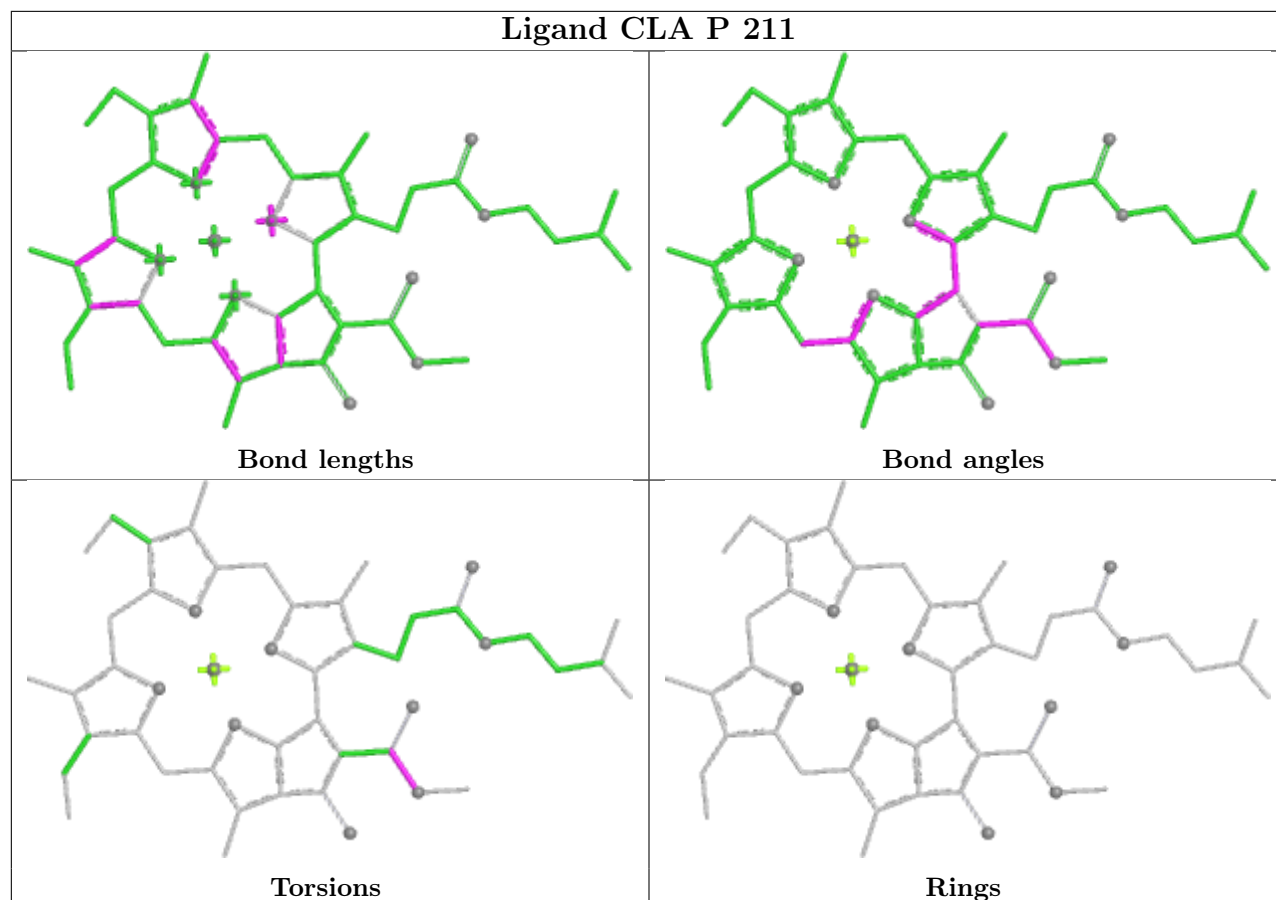


Ligand DD6 G 211

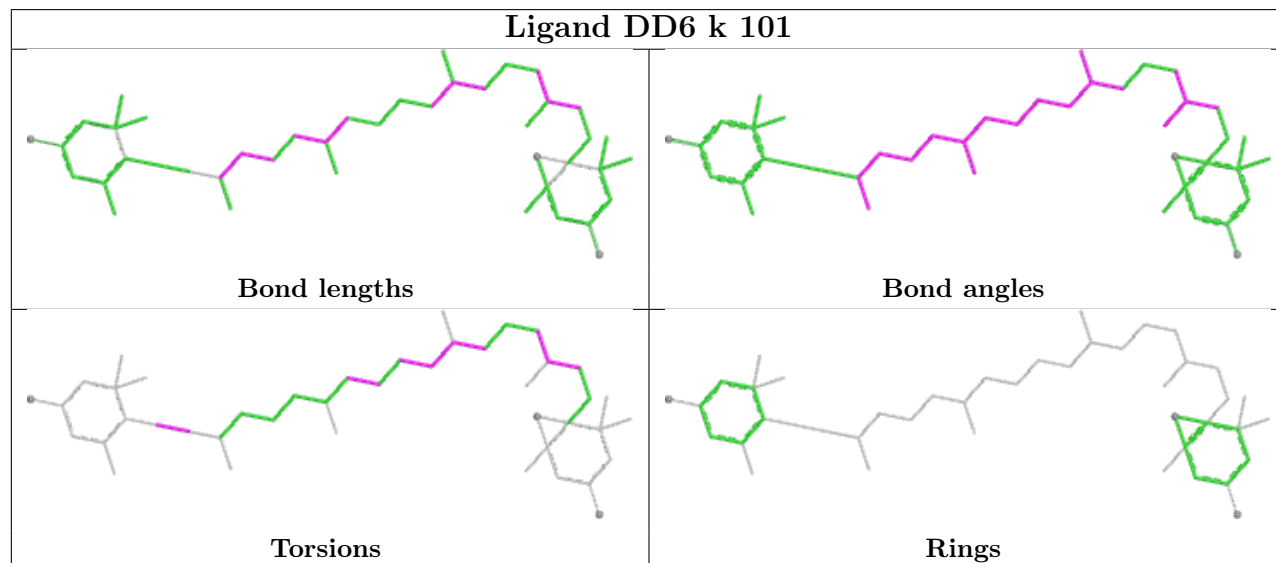


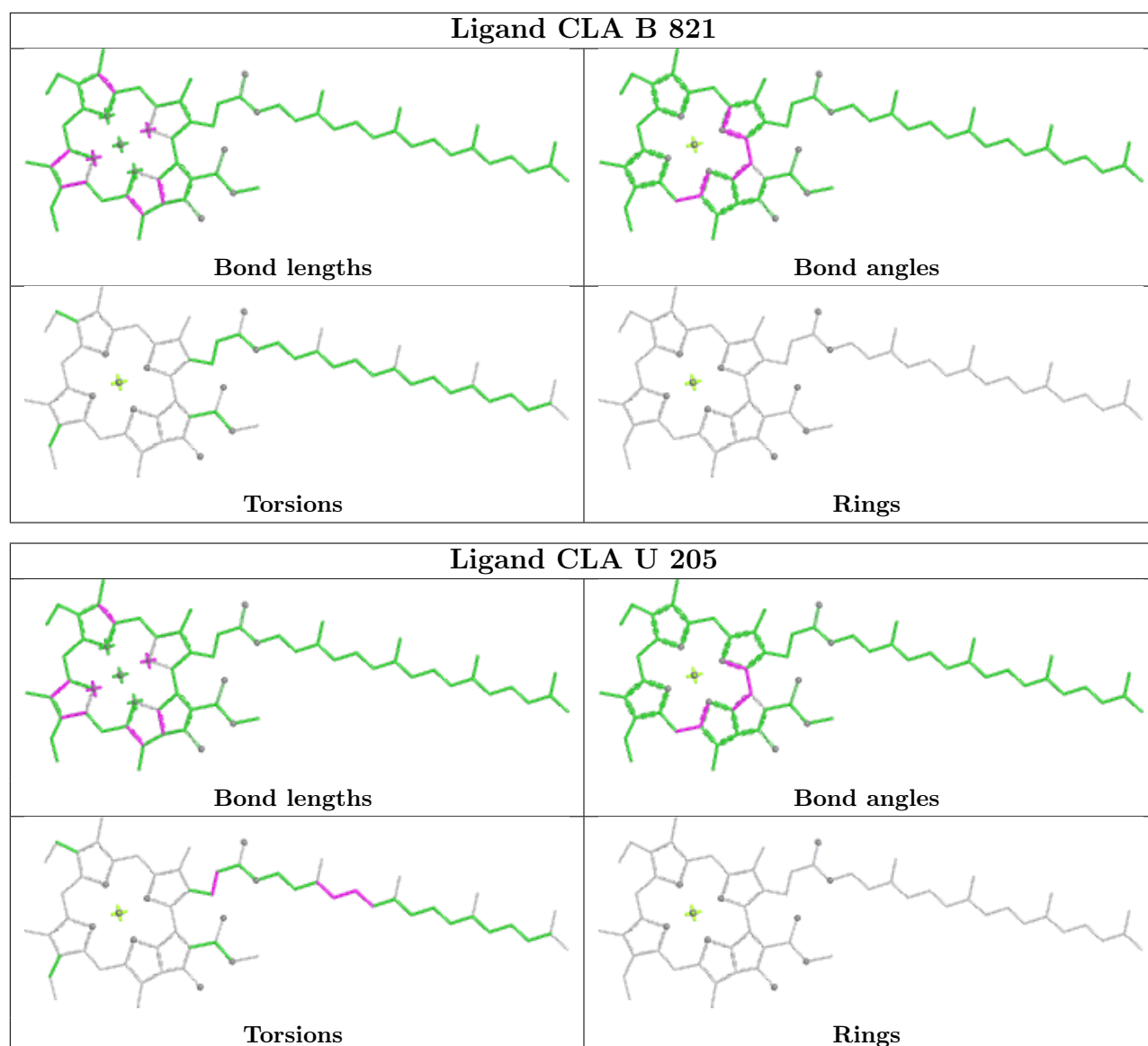


Ligand CLA P 211

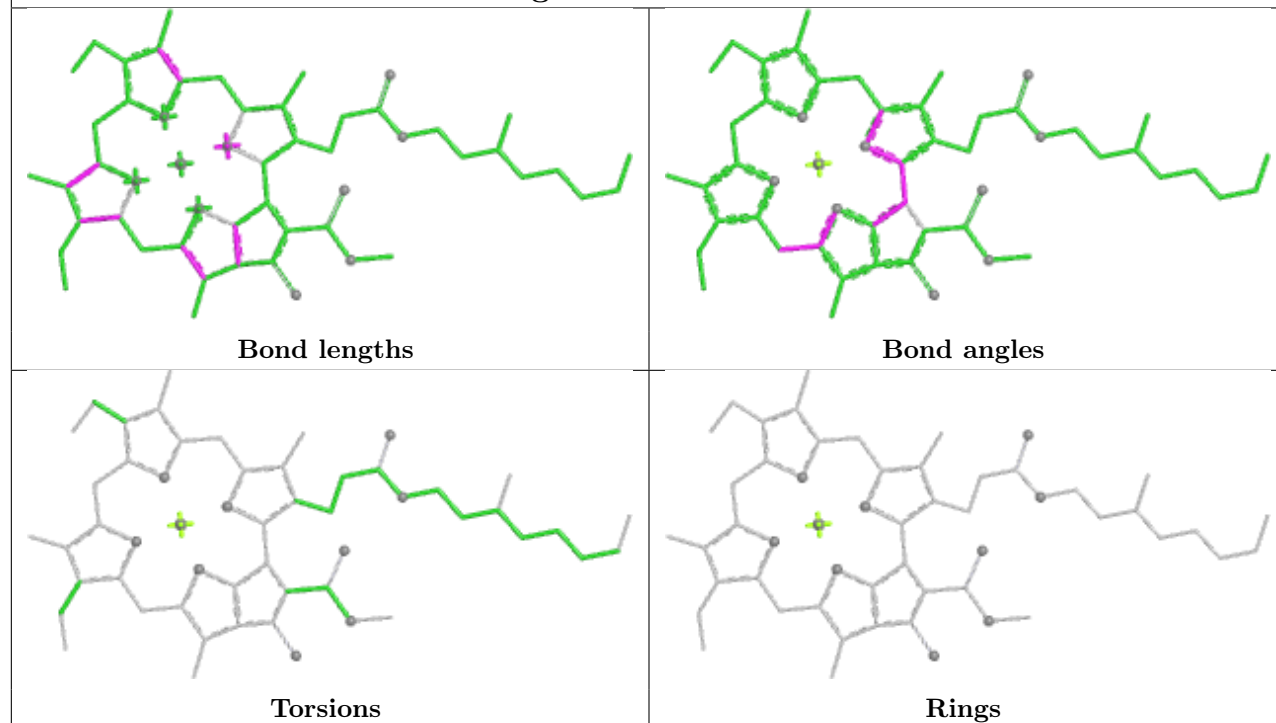


Ligand DD6 k 101

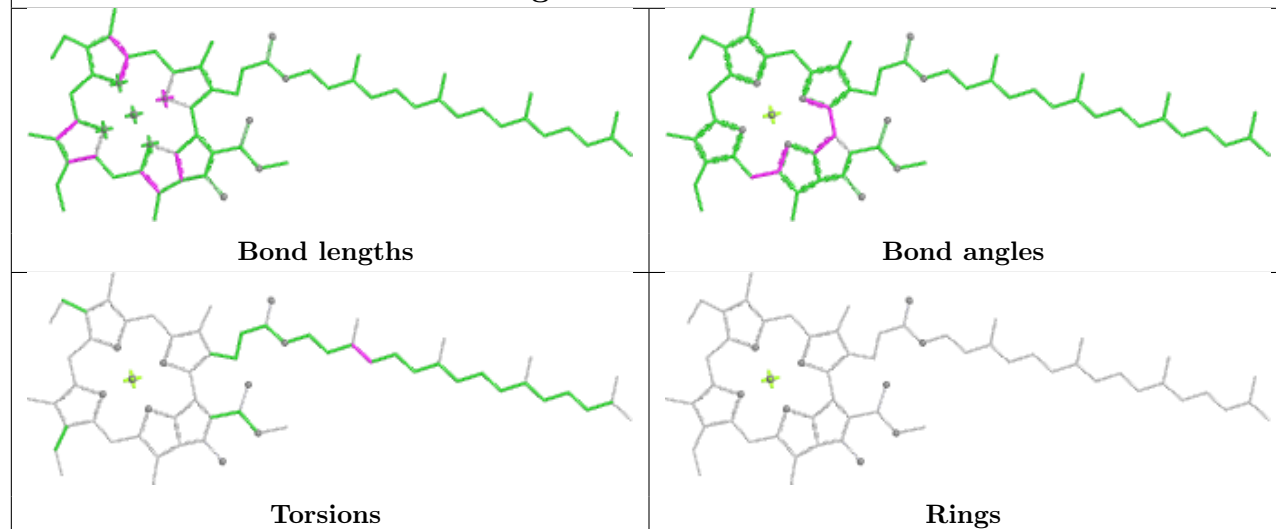




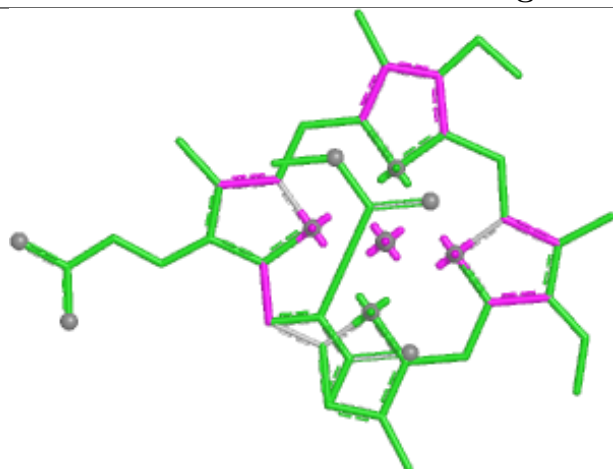
Ligand CLA A 810



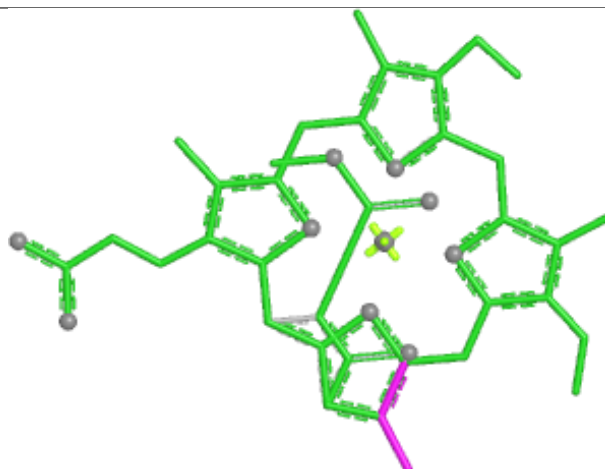
Ligand CLA A 823



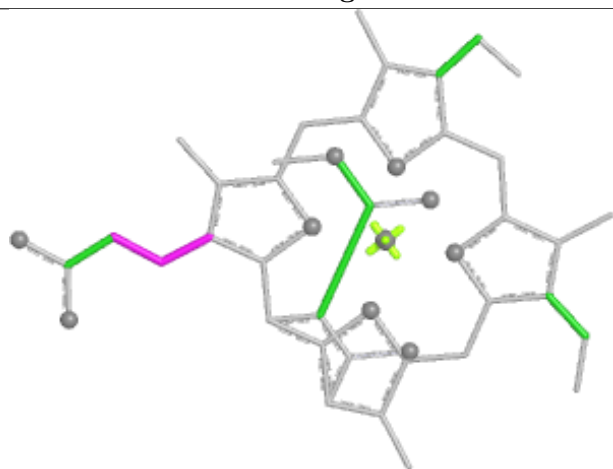
Ligand KC1 P 219



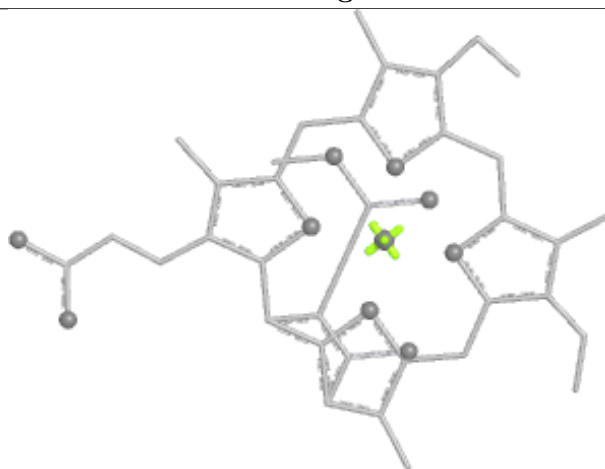
Bond lengths



Bond angles

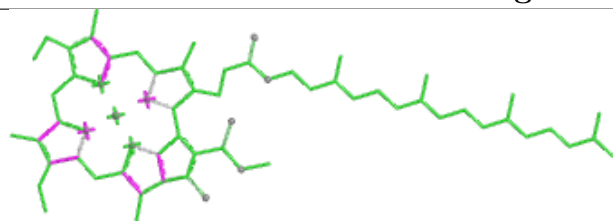


Torsions

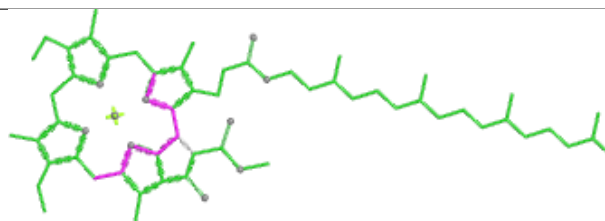


Rings

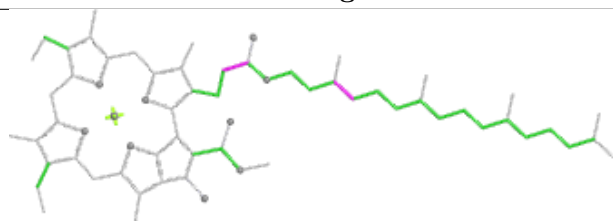
Ligand CLA B 808



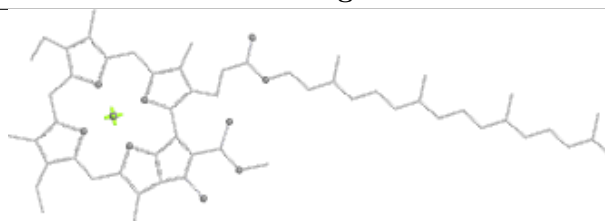
Bond lengths



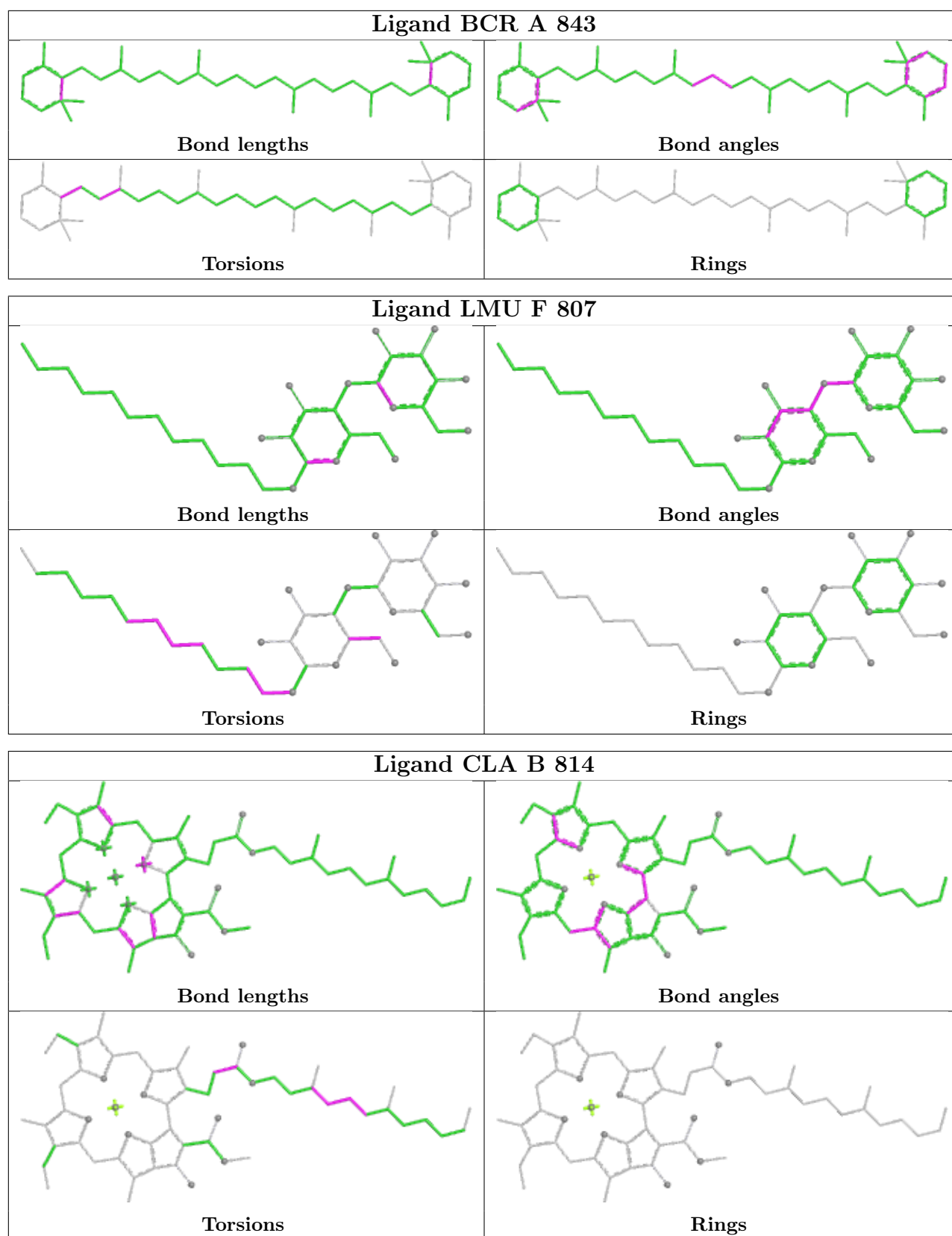
Bond angles

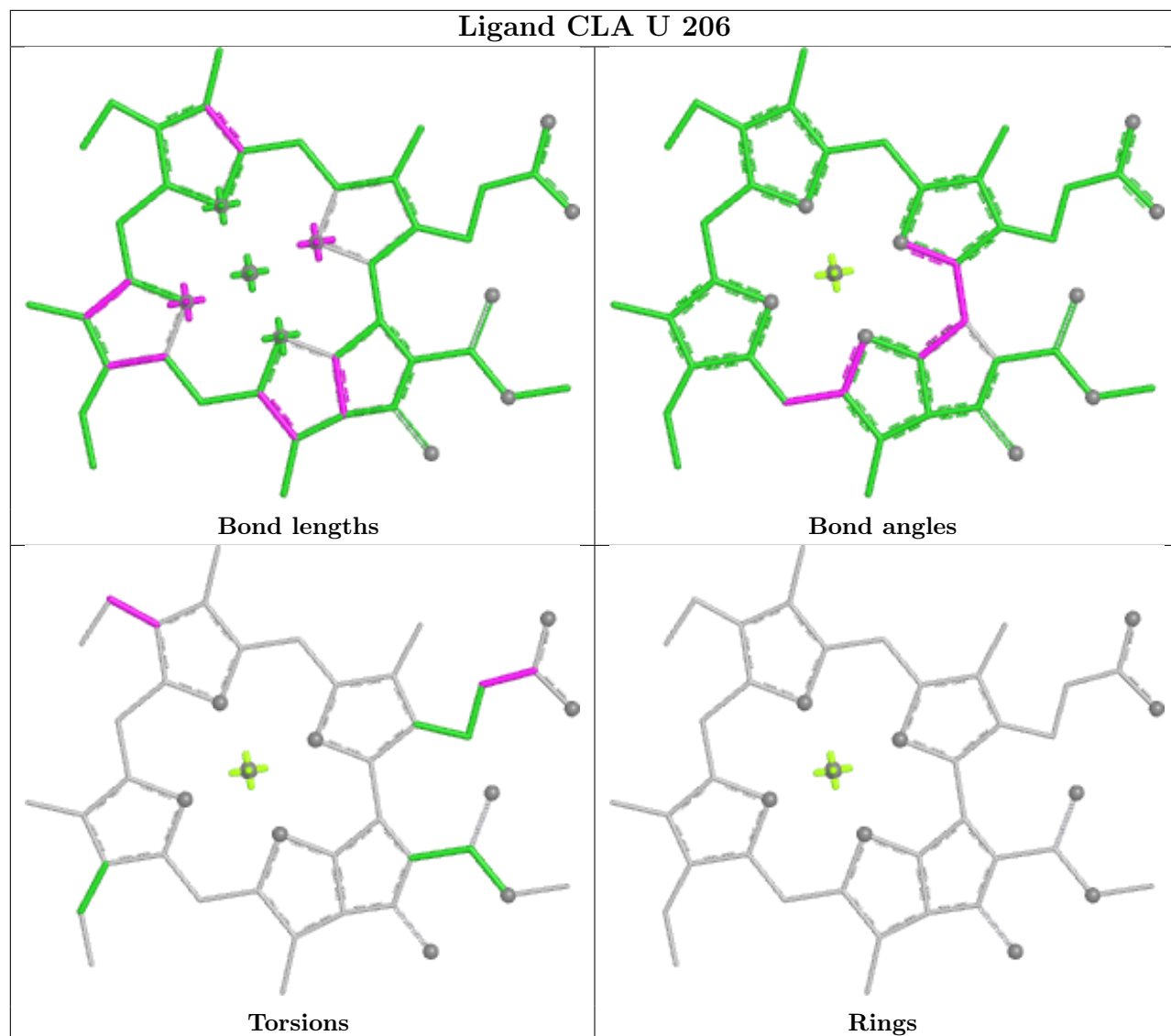


Torsions

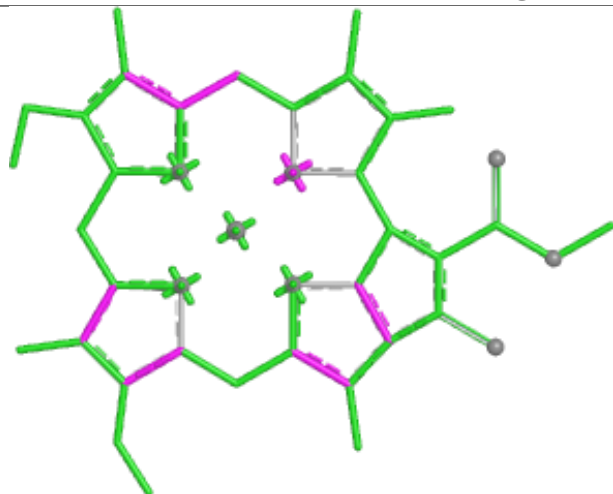


Rings

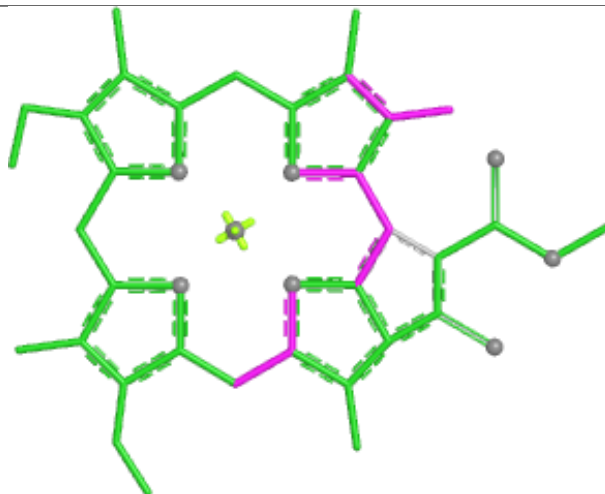




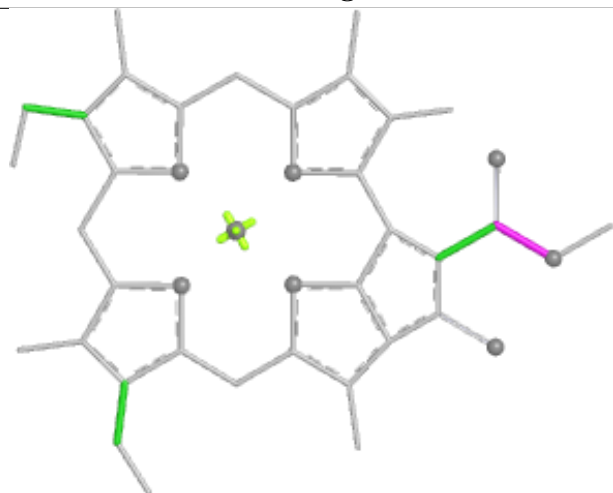
Ligand CLA H 209



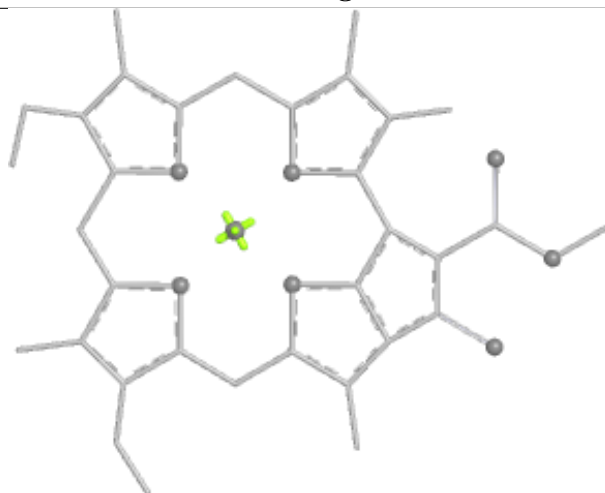
Bond lengths



Bond angles

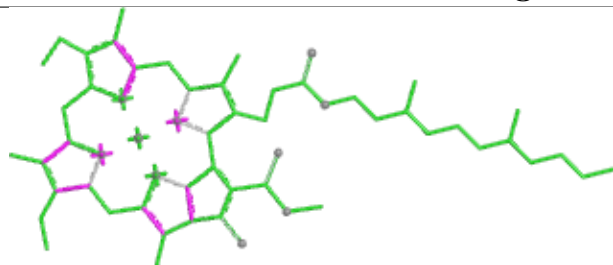


Torsions

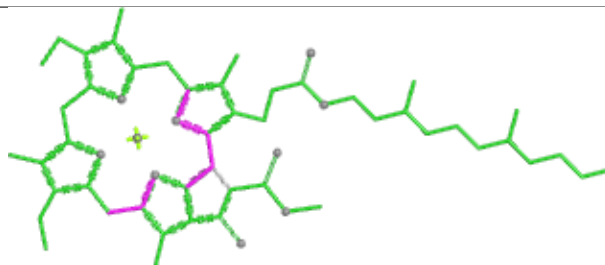


Rings

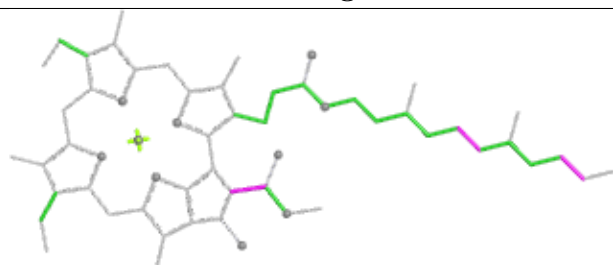
Ligand CLA B 829



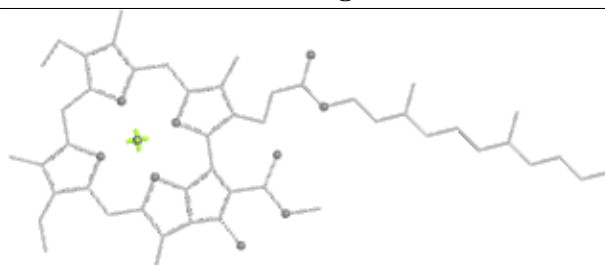
Bond lengths



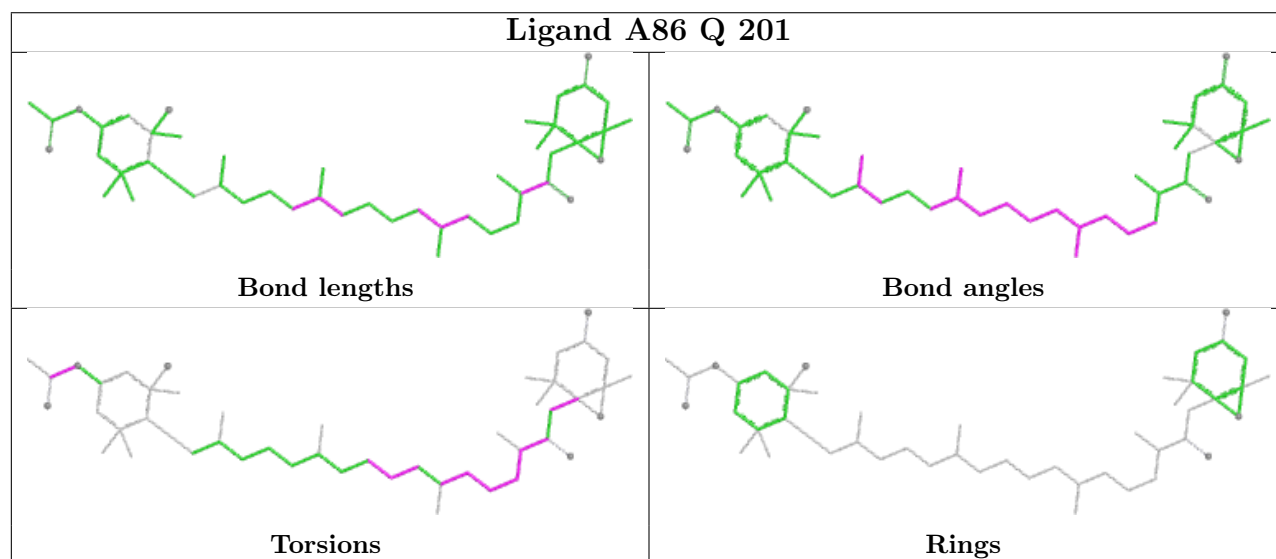
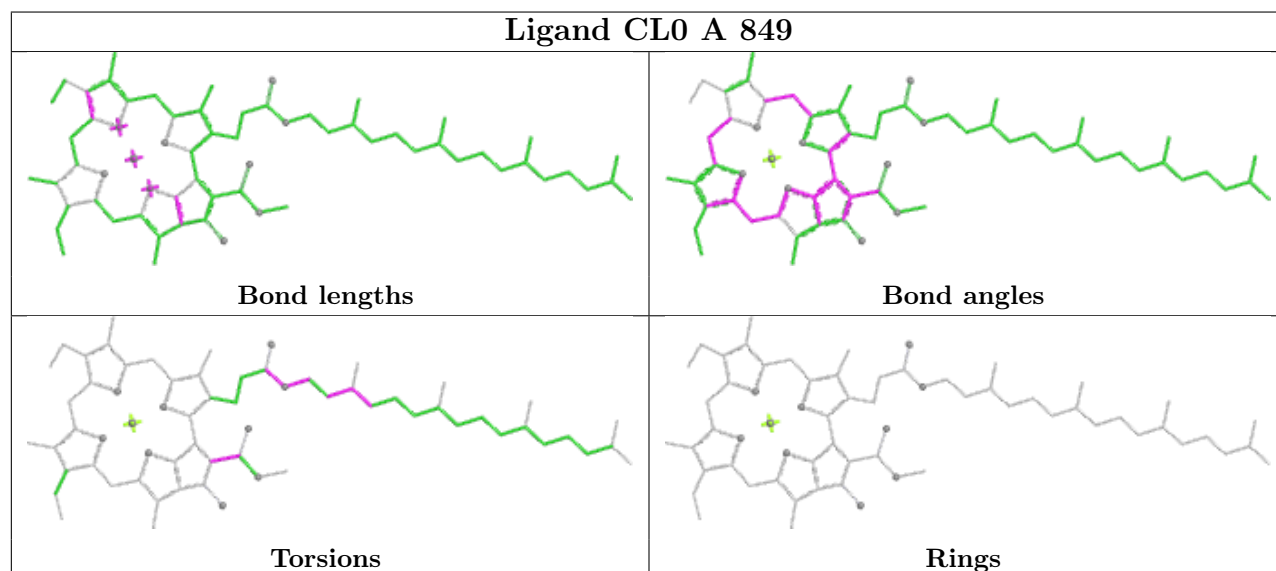
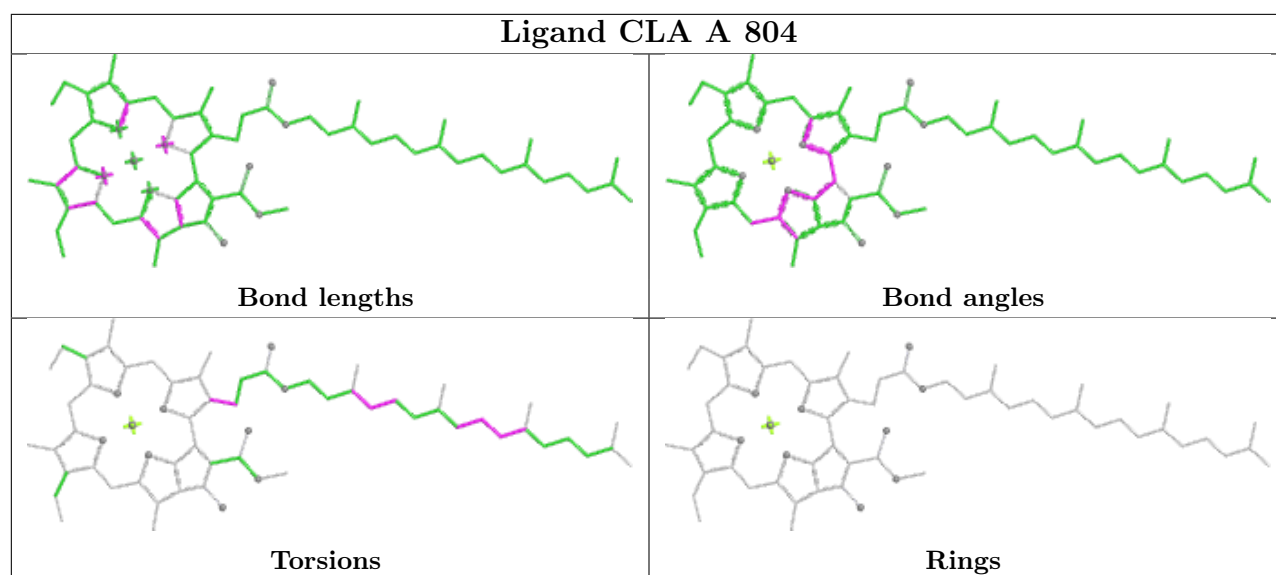
Bond angles



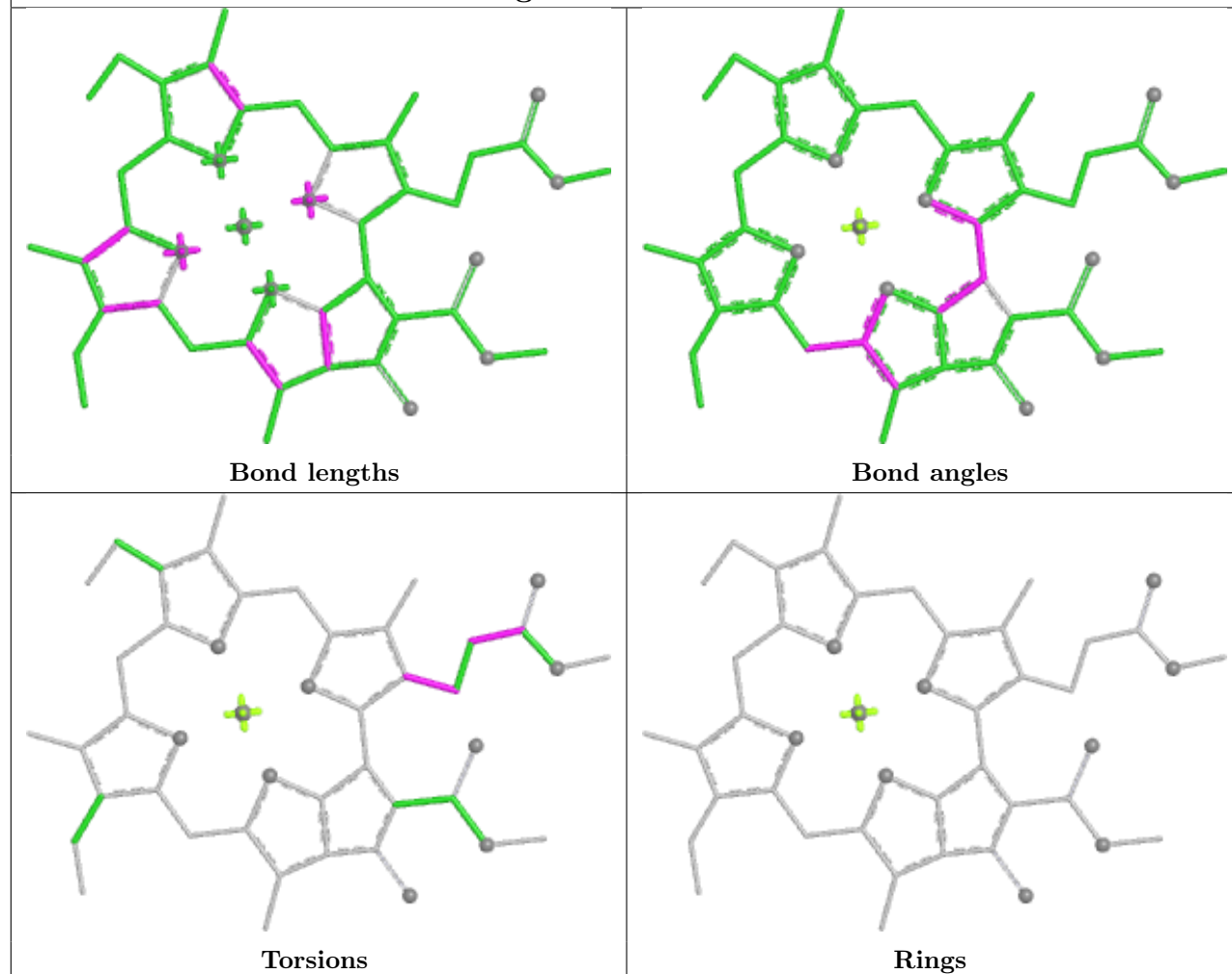
Torsions



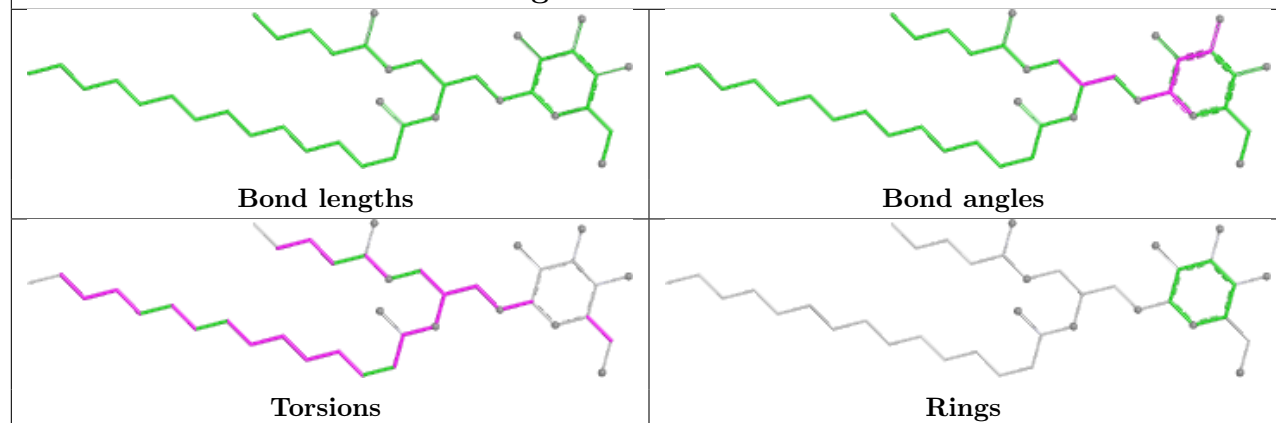
Rings

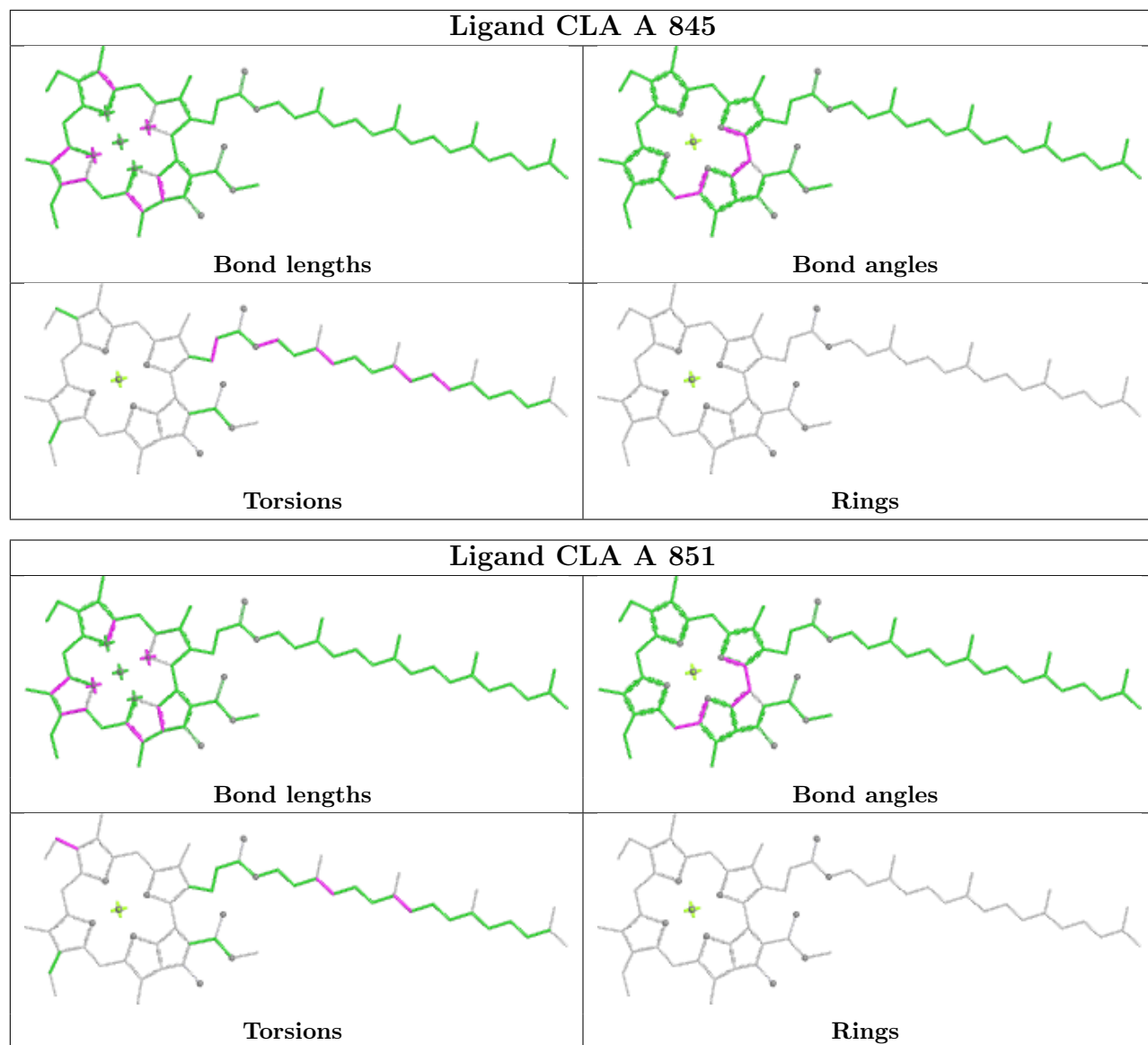


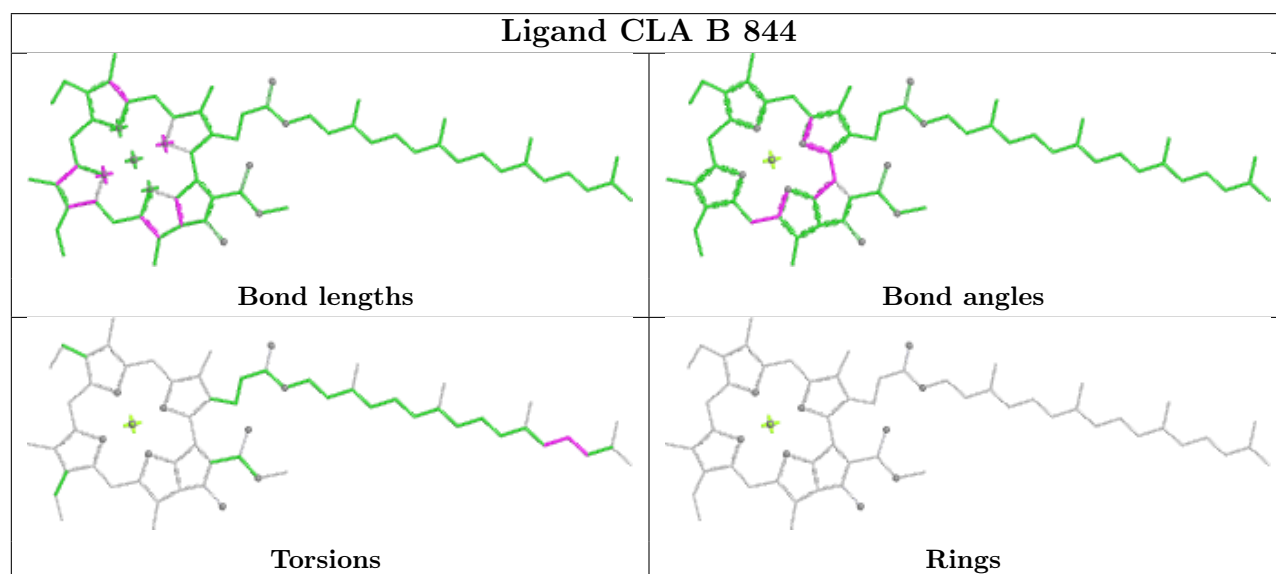
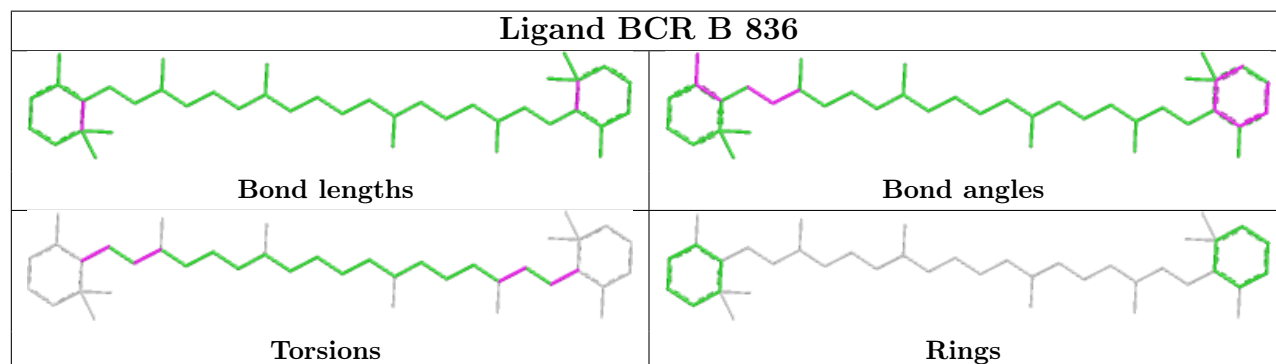
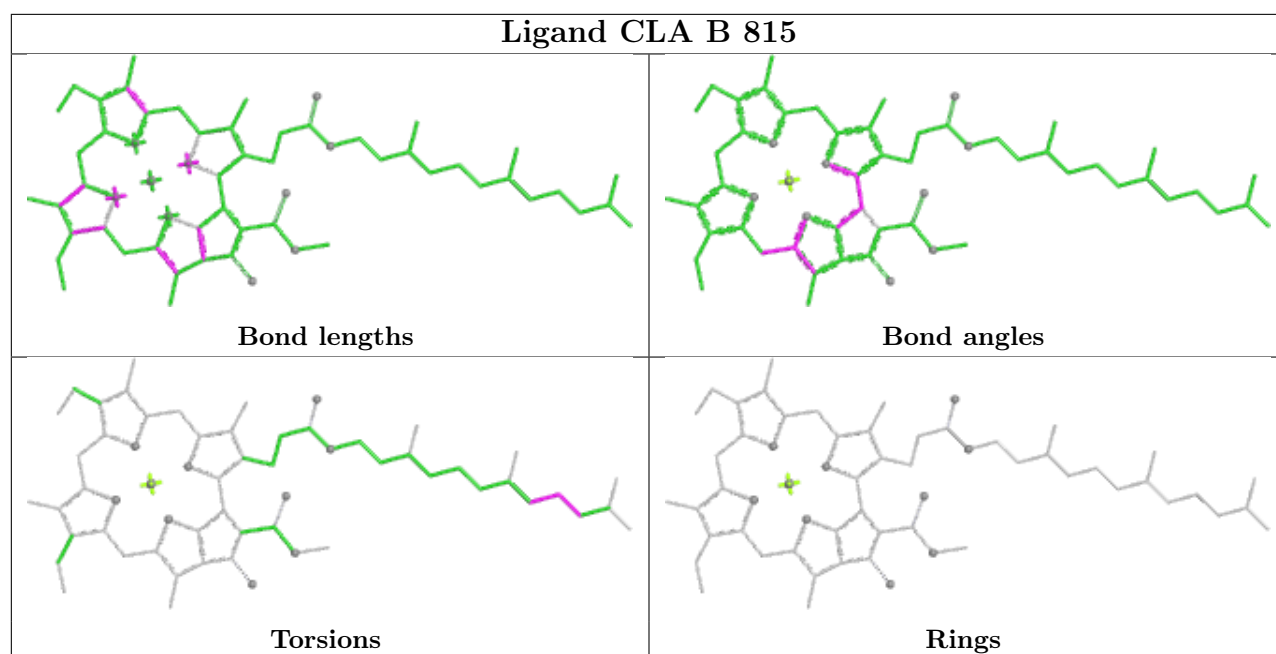
Ligand CLA F 804



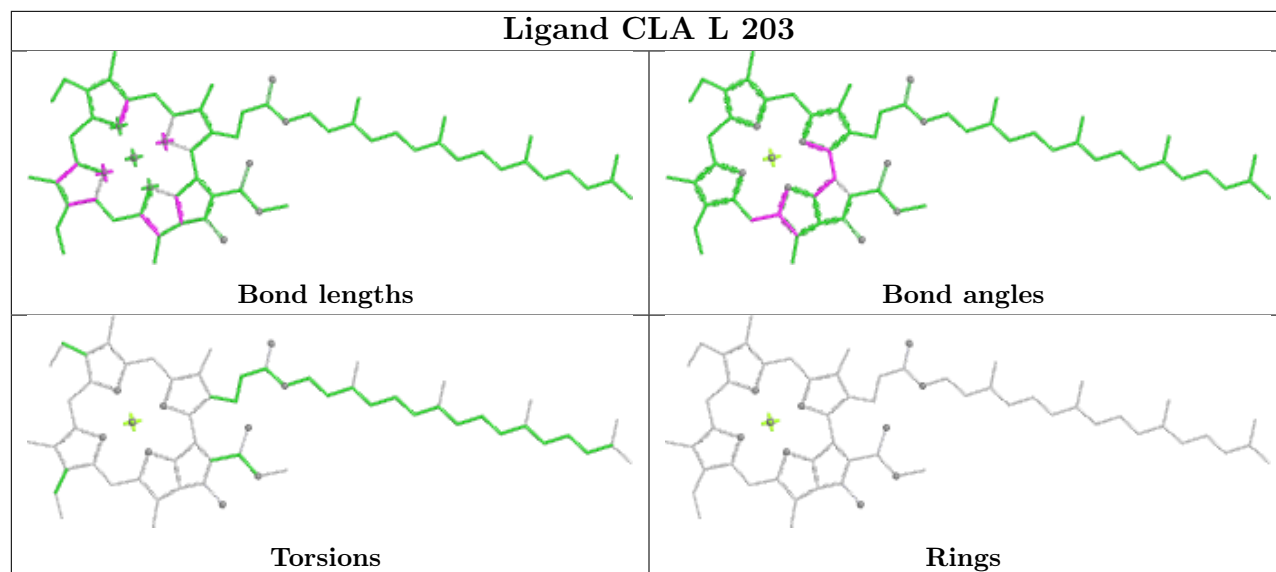
Ligand LMG J 102



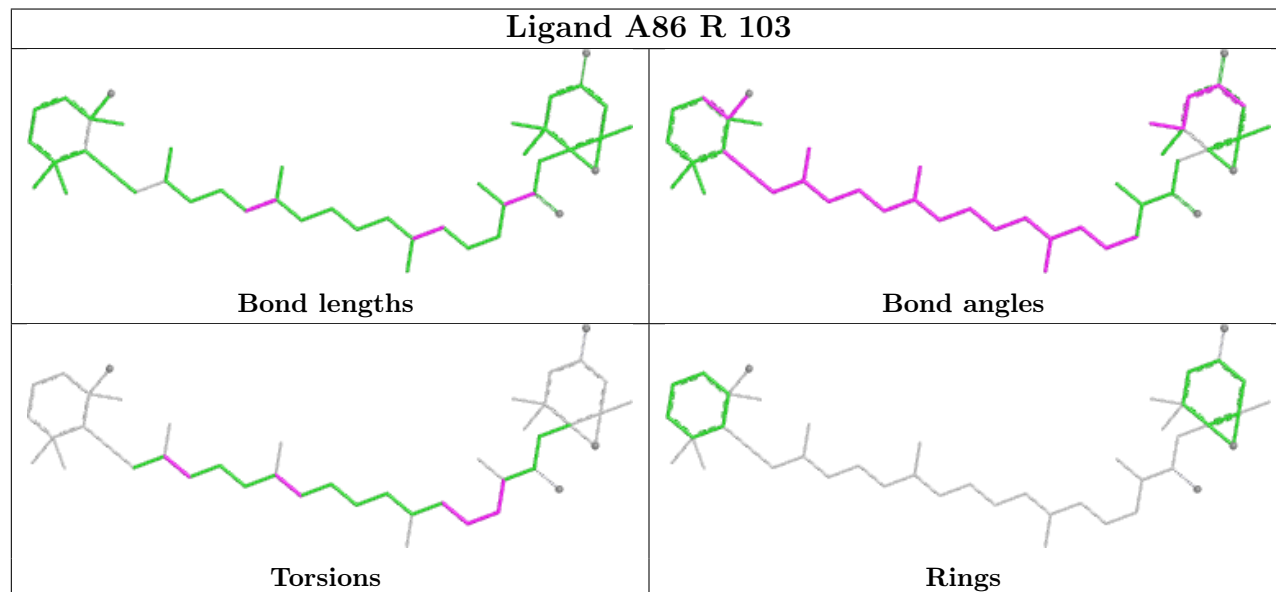




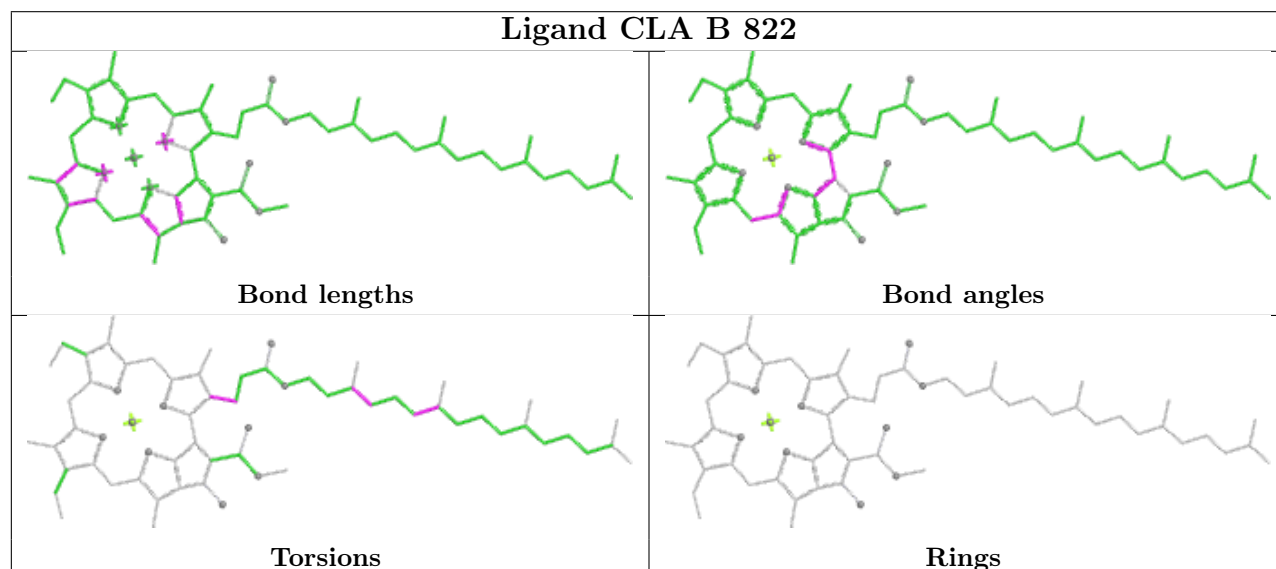
Ligand CLA L 203



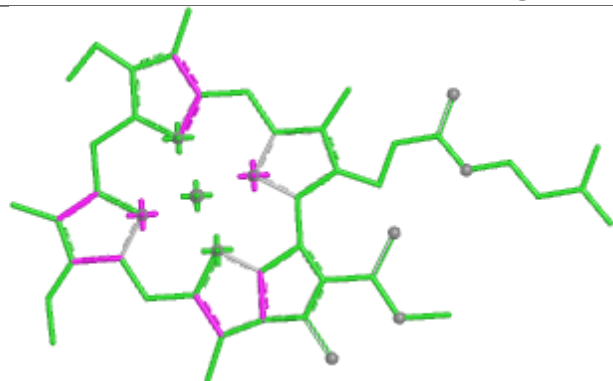
Ligand A86 R 103



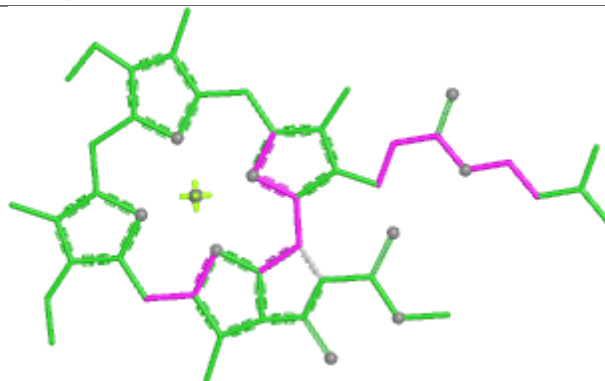
Ligand CLA B 822



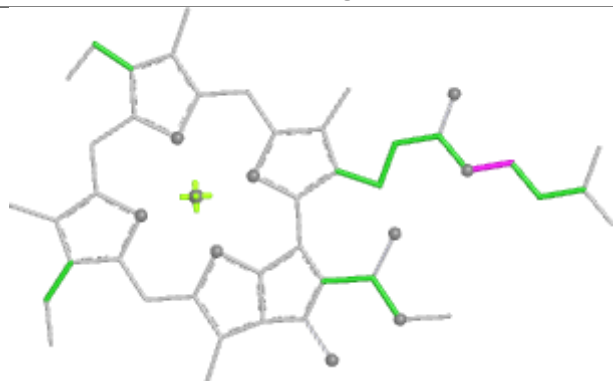
Ligand CLA Q 208



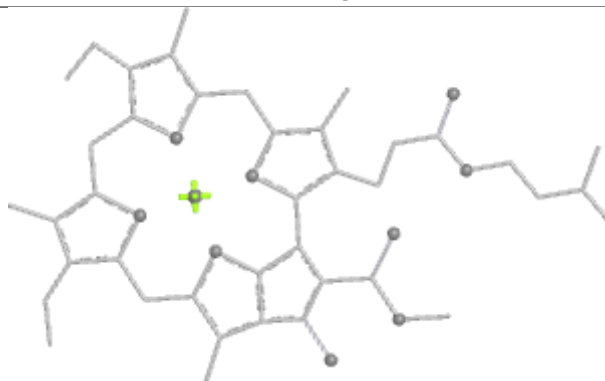
Bond lengths



Bond angles

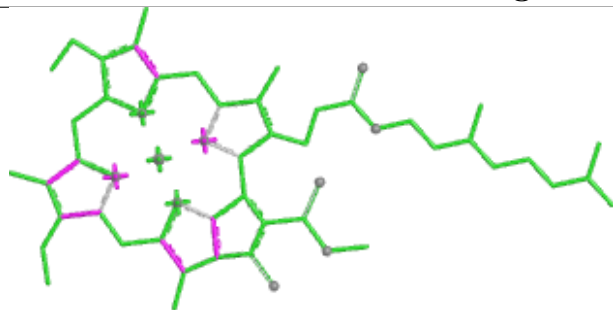


Torsions

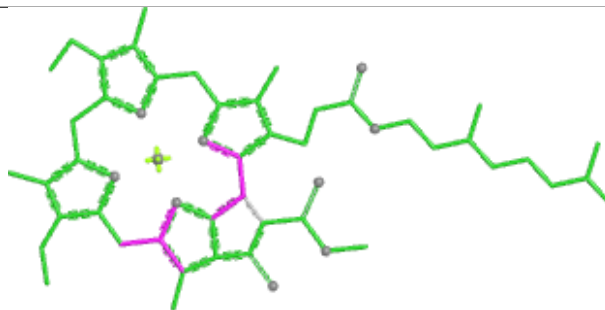


Rings

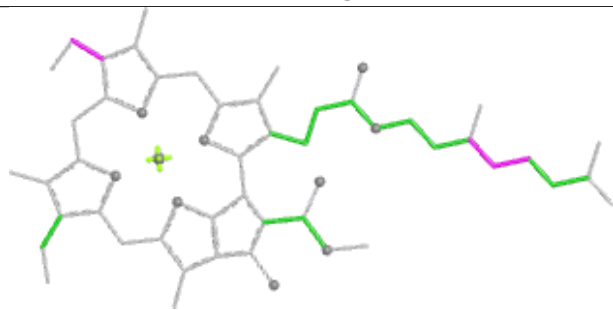
Ligand CLA K 205



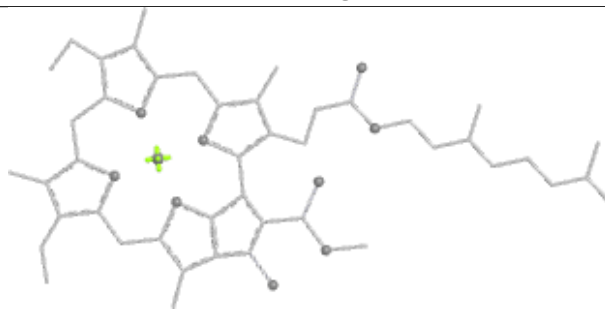
Bond lengths



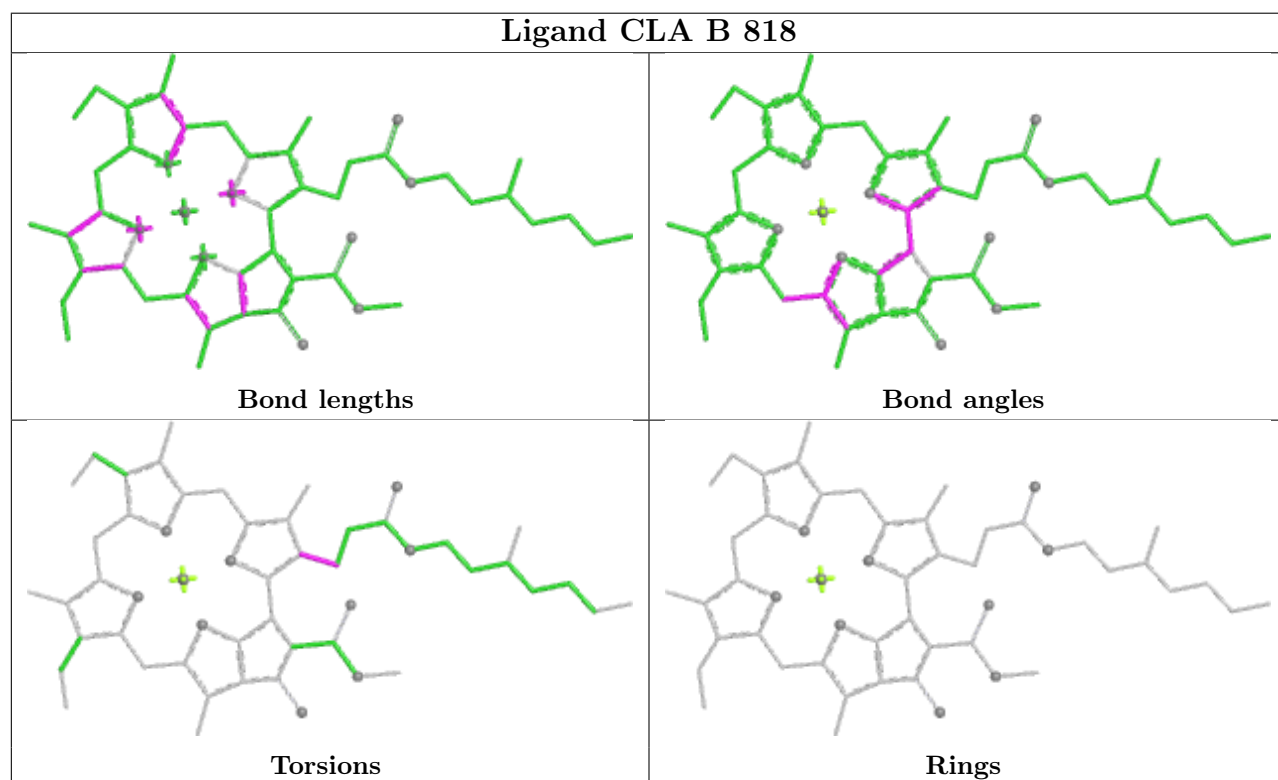
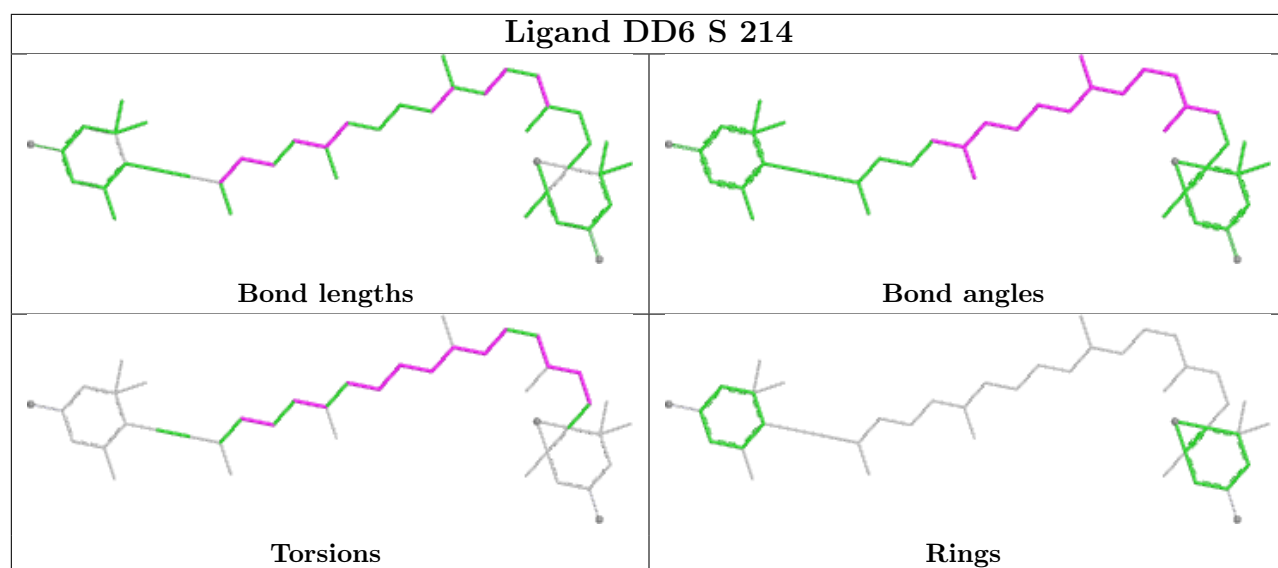
Bond angles



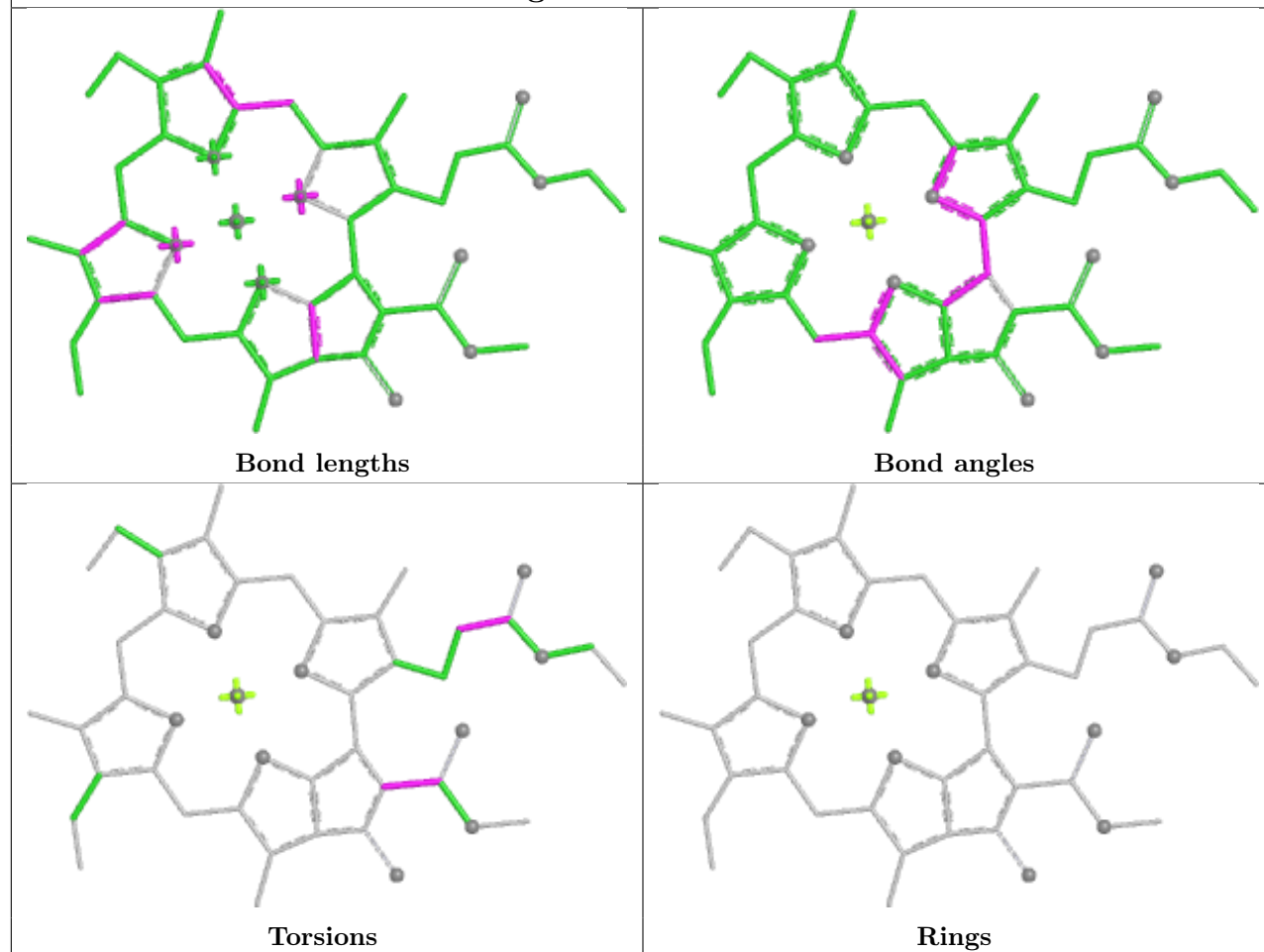
Torsions



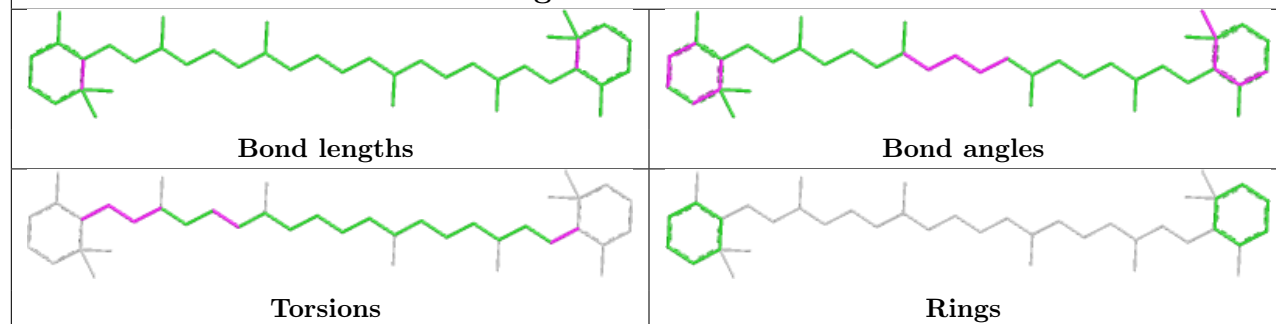
Rings



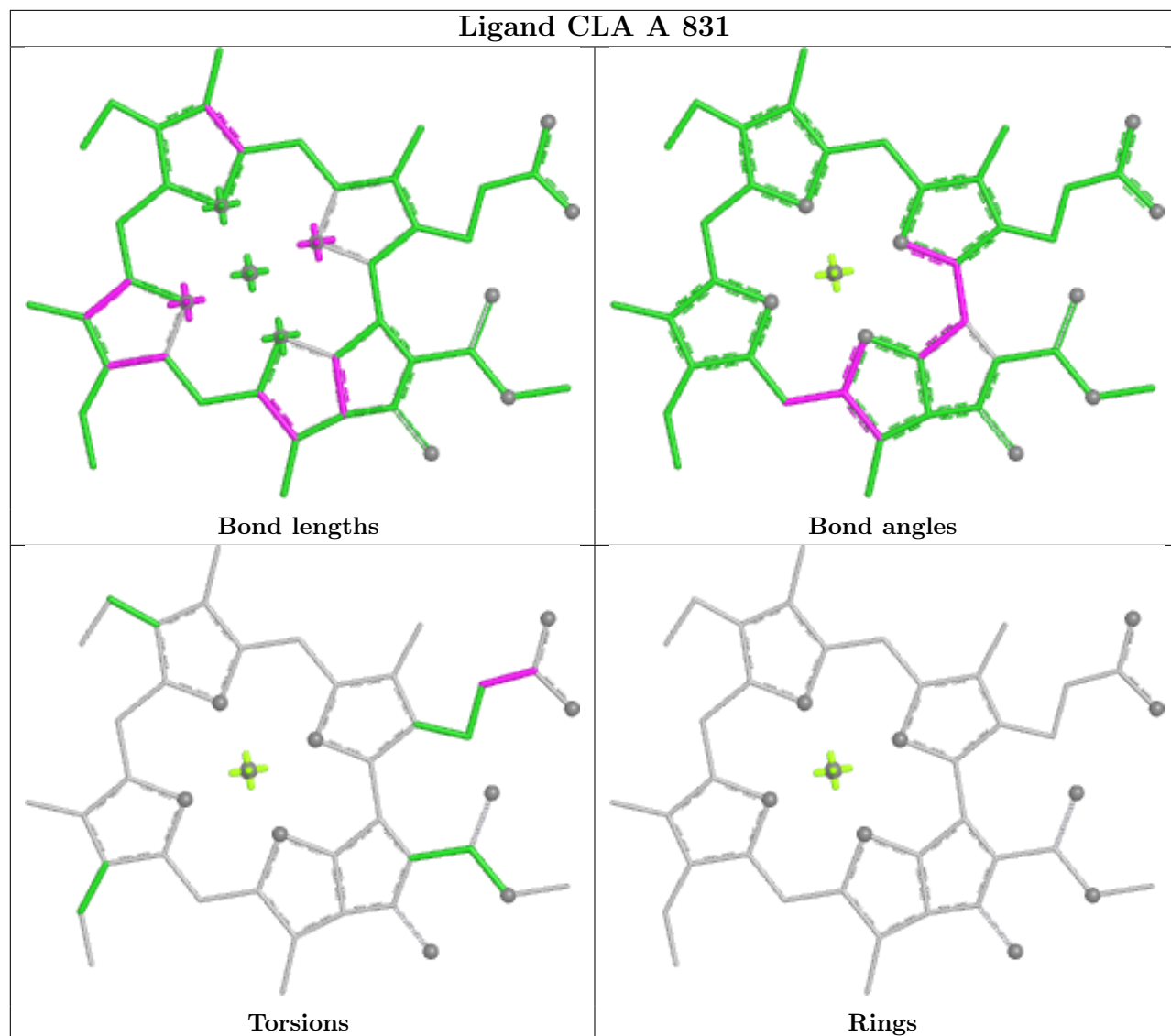
Ligand CLA T 211



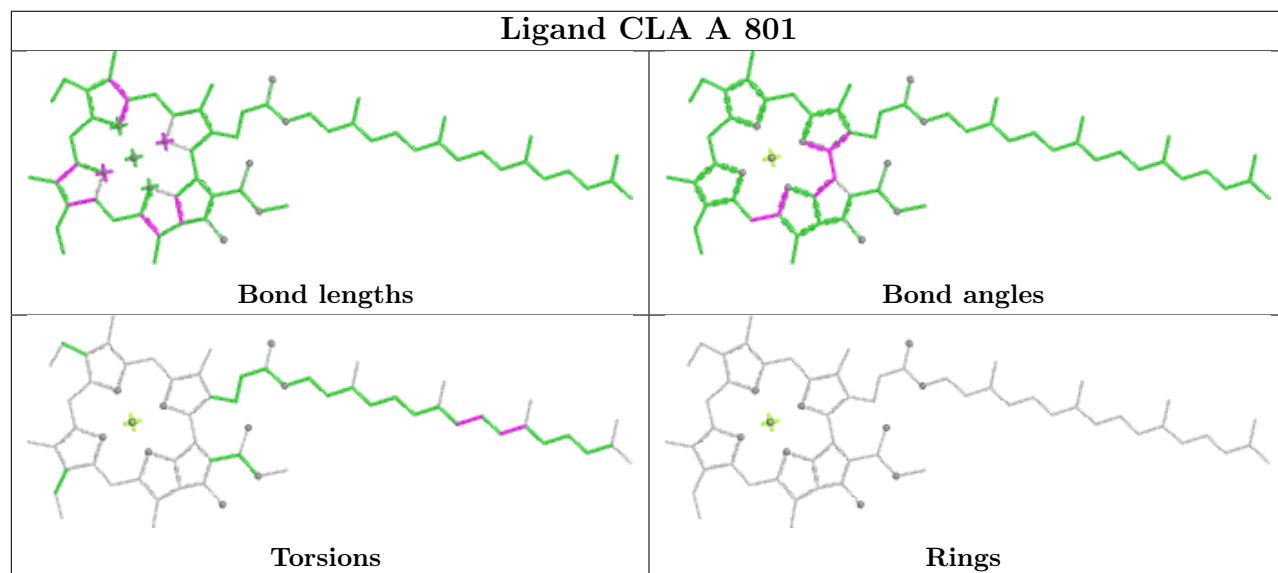
Ligand BCR k 104



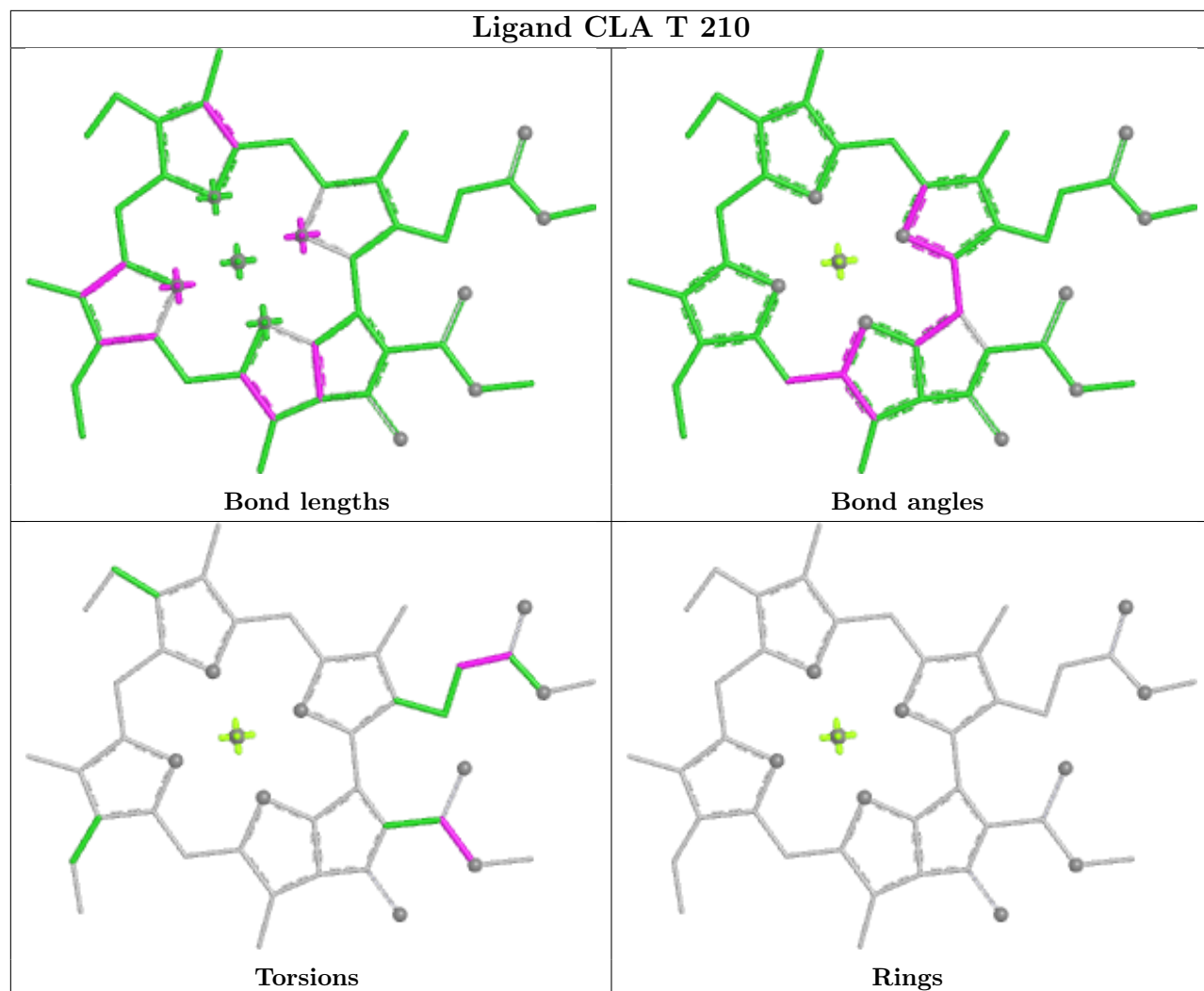
Ligand CLA A 831



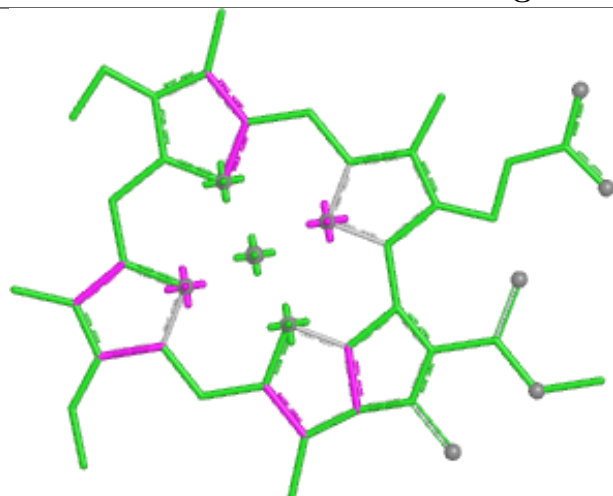
Ligand CLA A 801



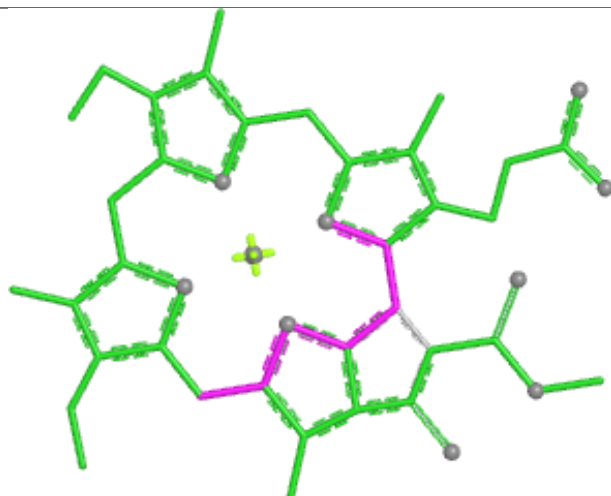
Ligand CLA T 210



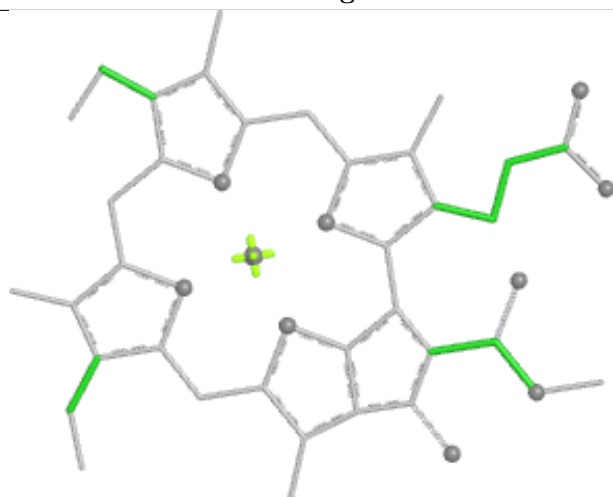
Ligand CLA R 101



Bond lengths



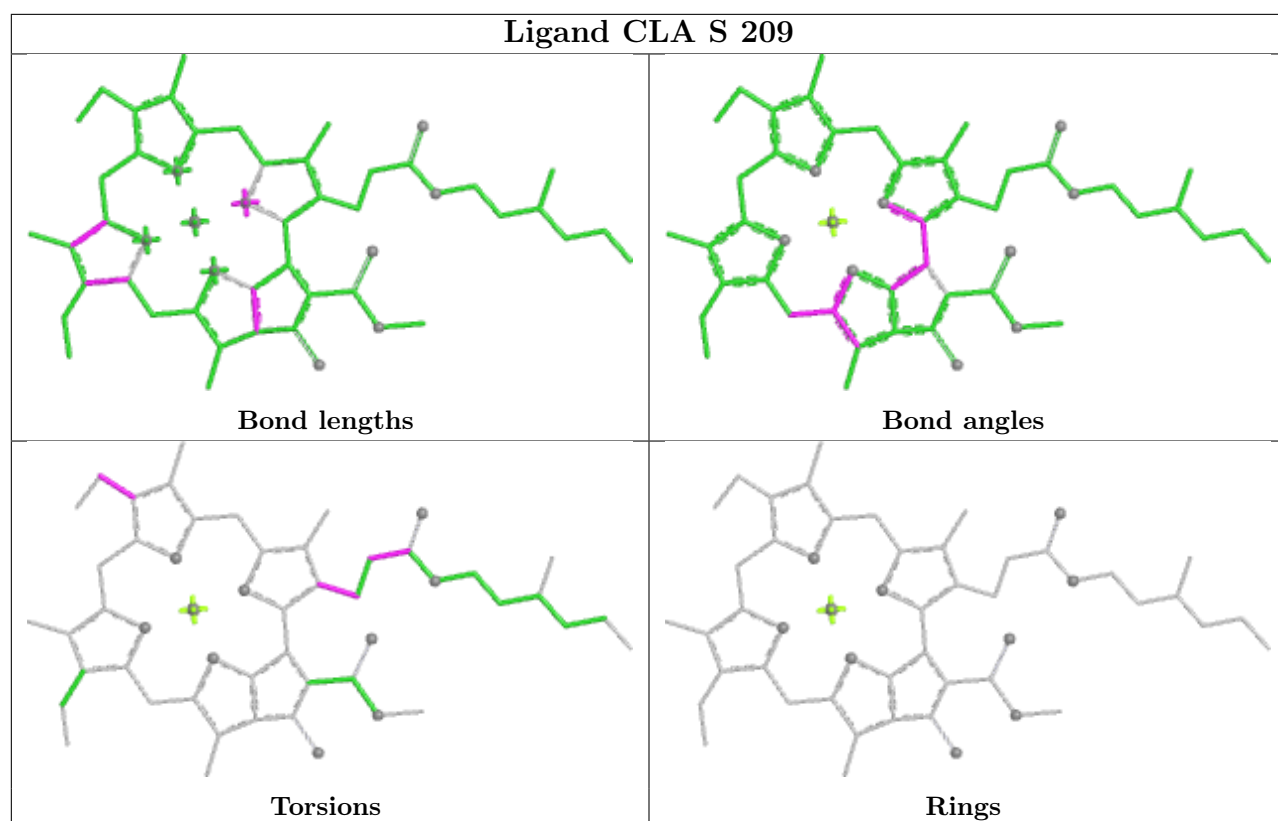
Bond angles

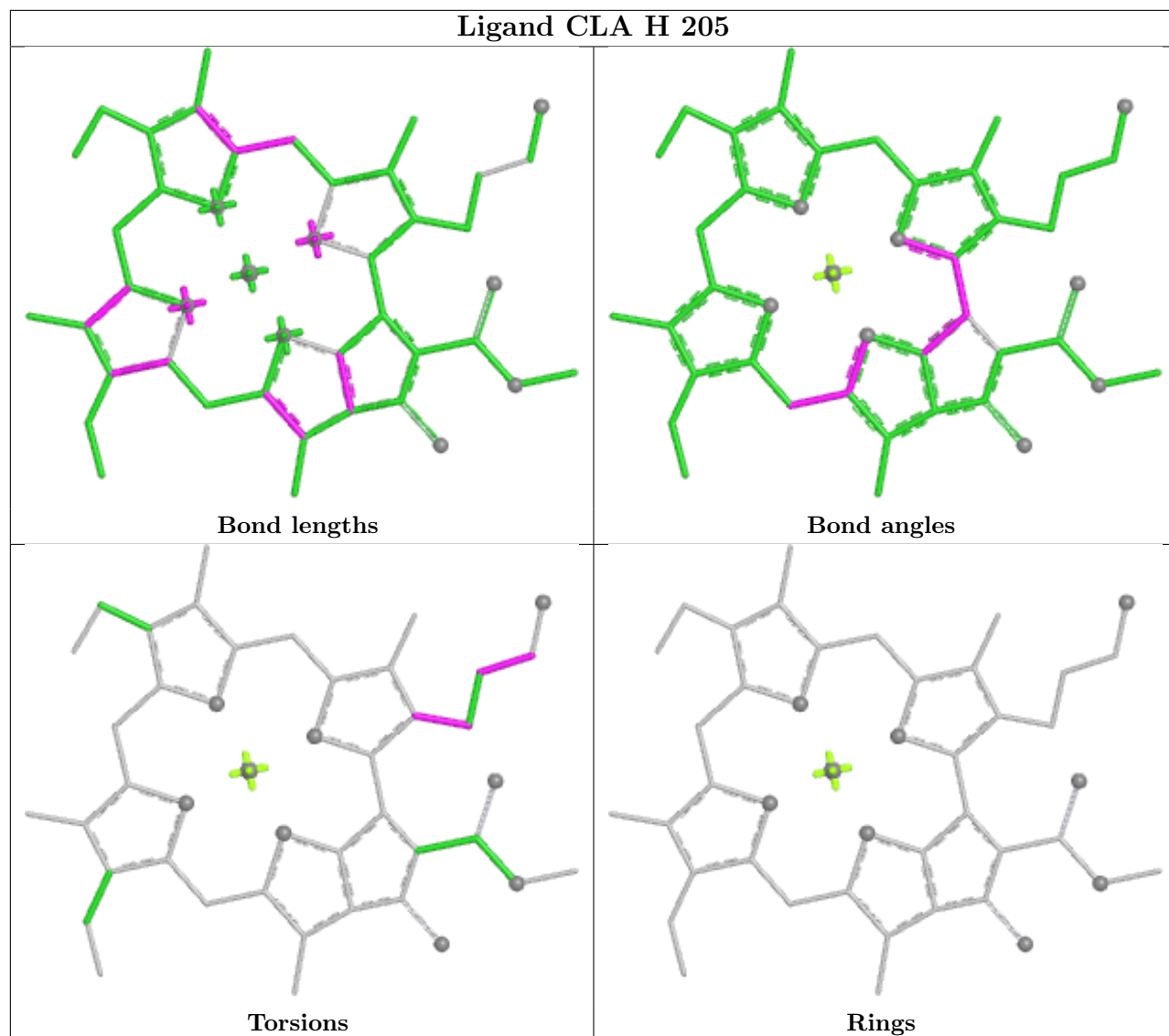


Torsions

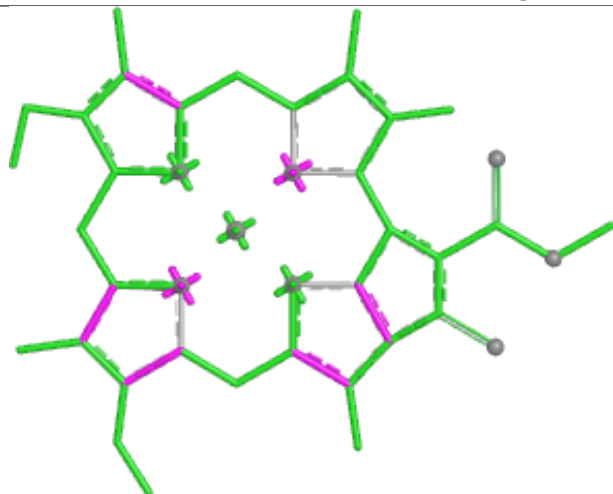


Rings

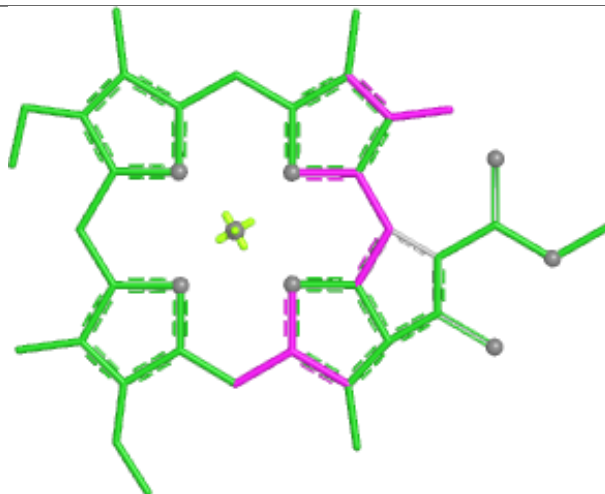




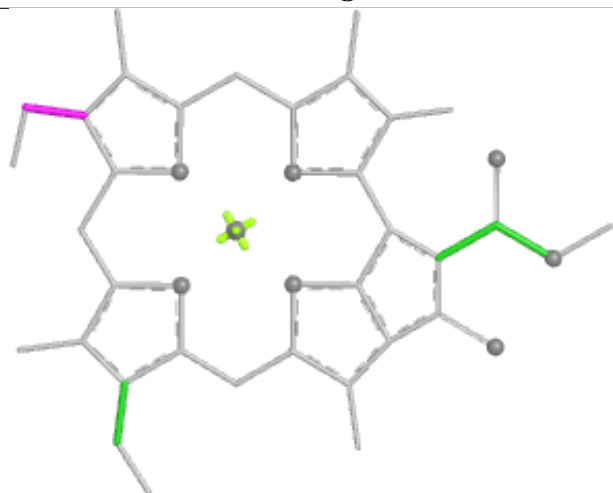
Ligand CLA T 202



Bond lengths



Bond angles

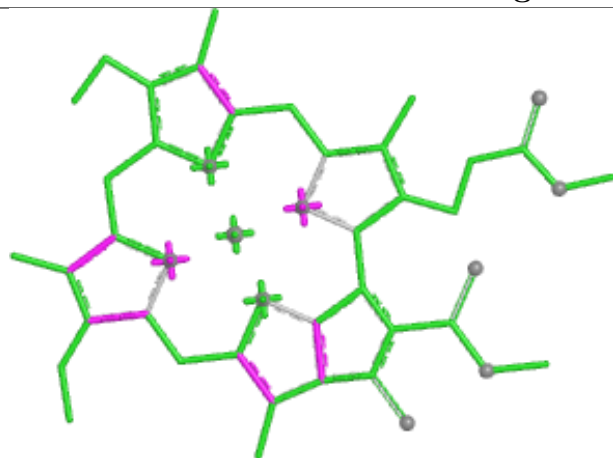


Torsions

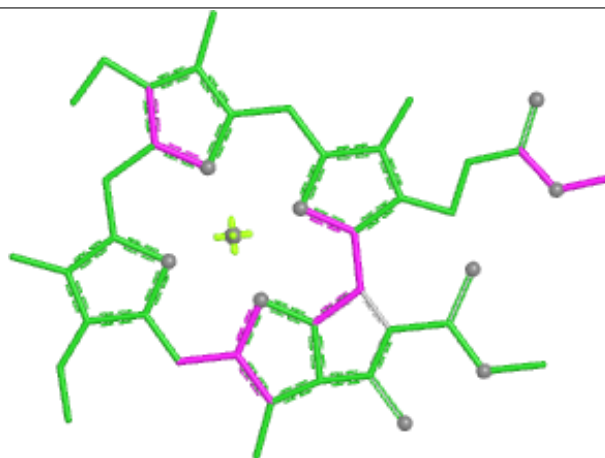


Rings

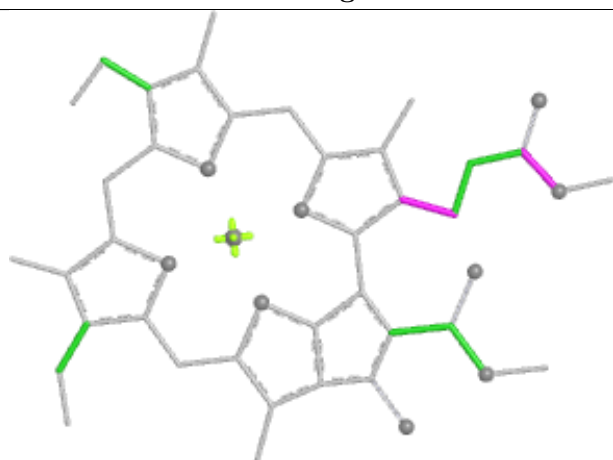
Ligand CLA O 207



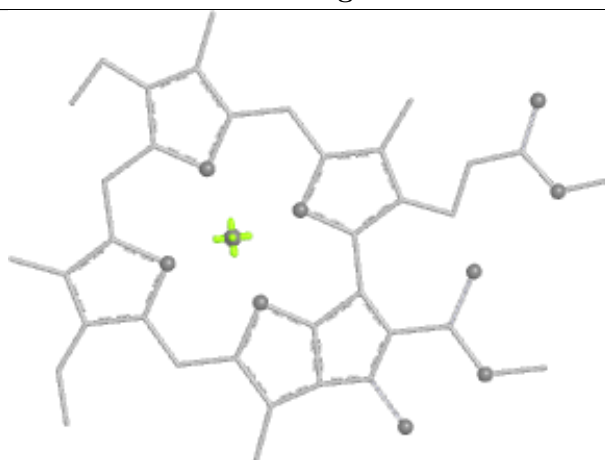
Bond lengths



Bond angles

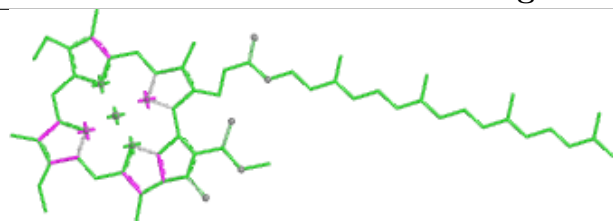


Torsions

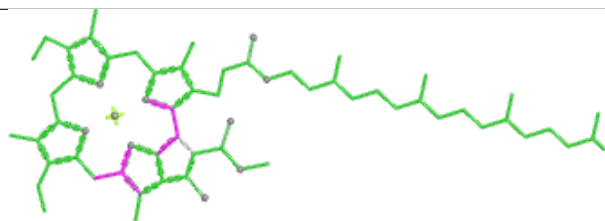


Rings

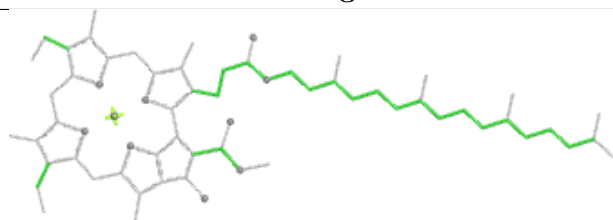
Ligand CLA S 216



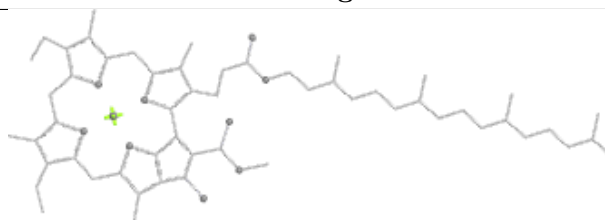
Bond lengths



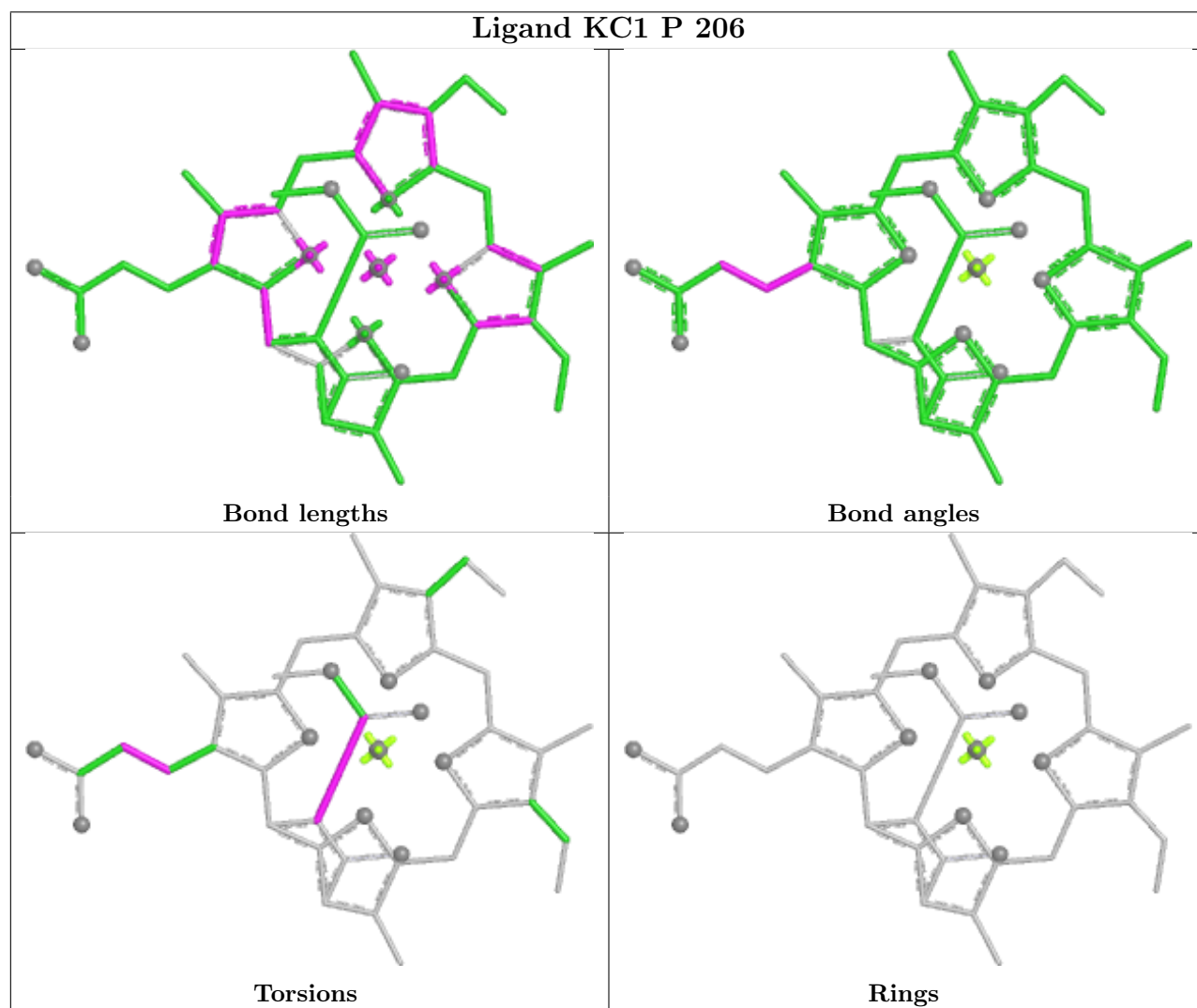
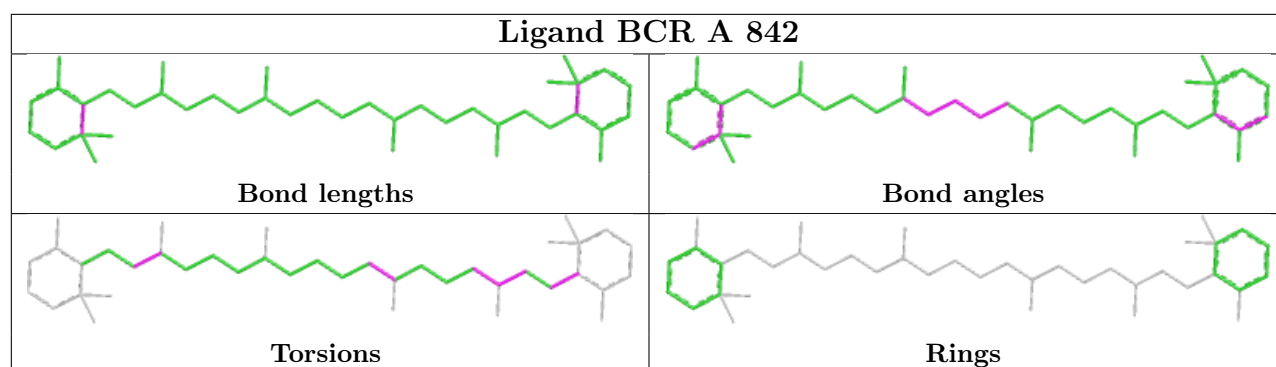
Bond angles



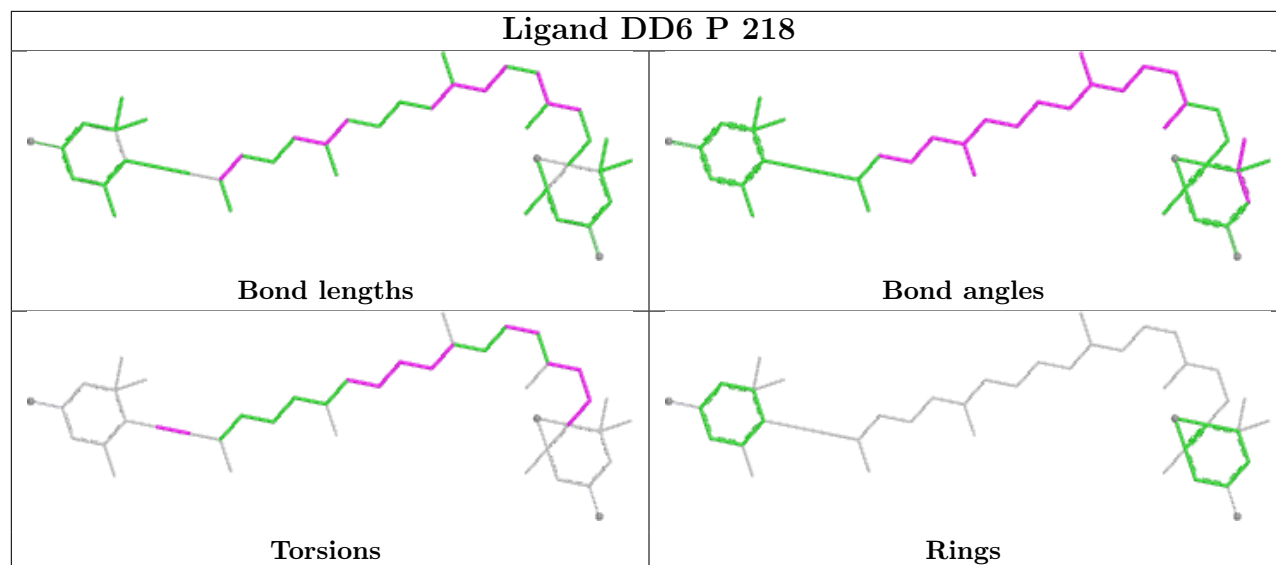
Torsions



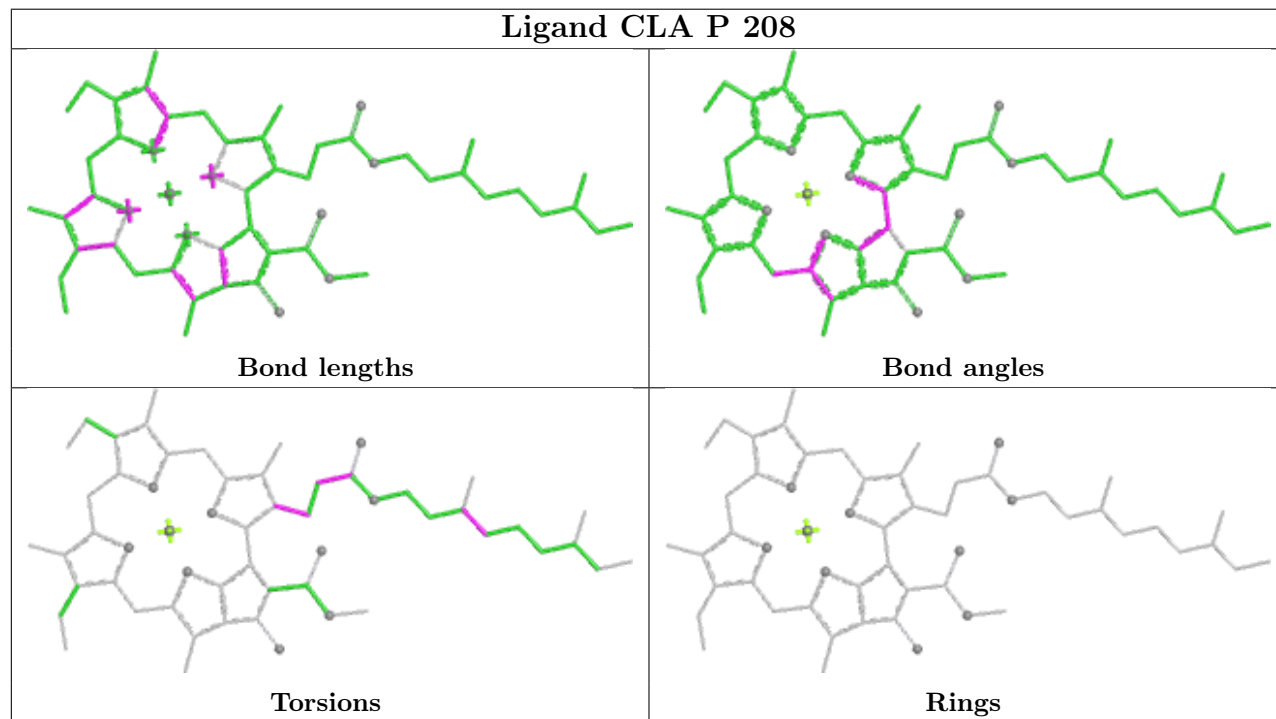
Rings



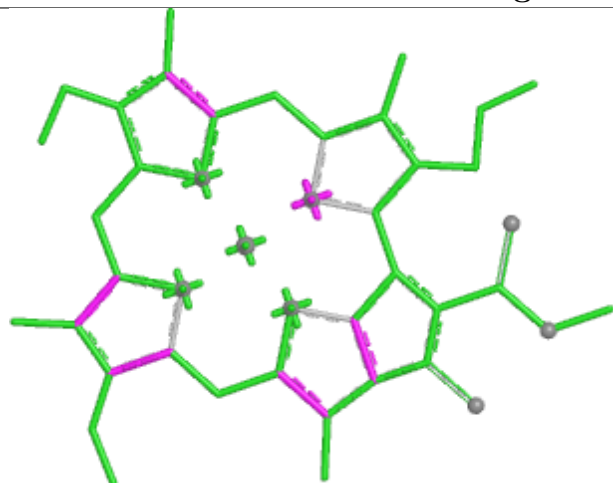
Ligand DD6 P 218



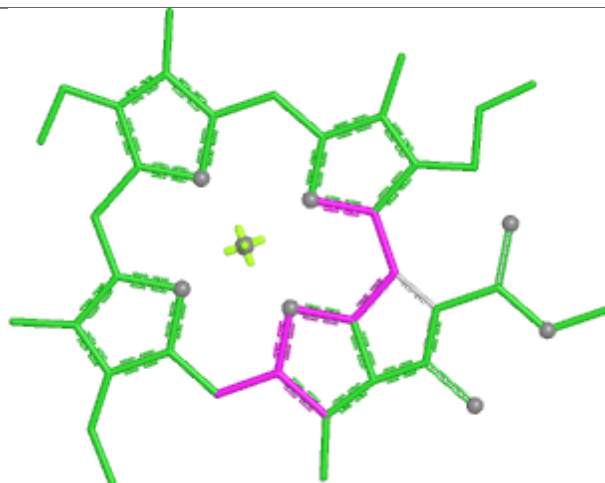
Ligand CLA P 208



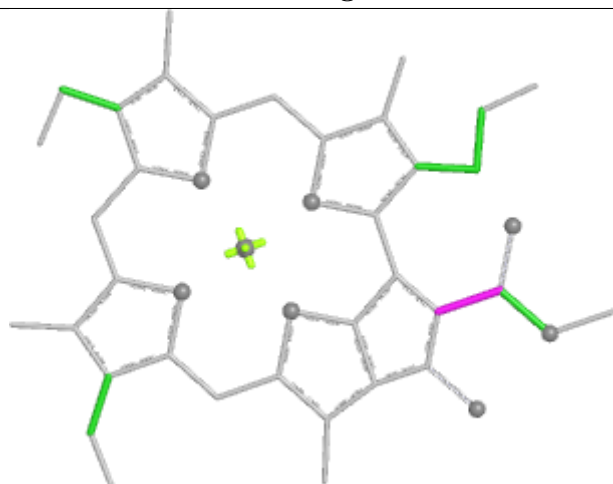
Ligand CLA O 202



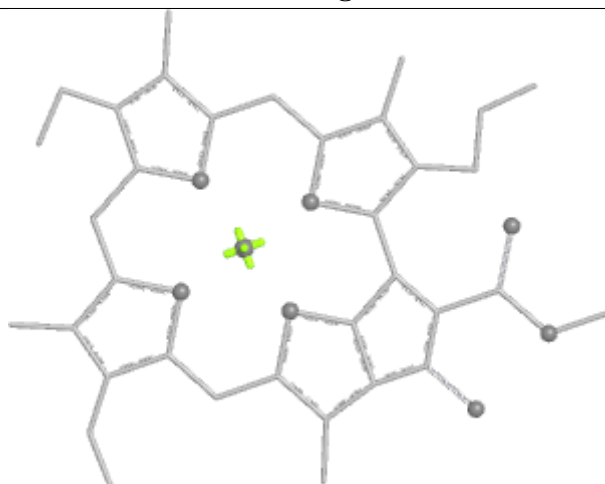
Bond lengths



Bond angles

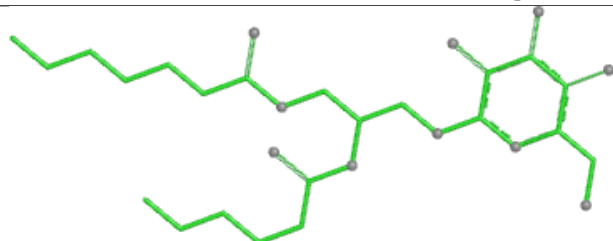


Torsions

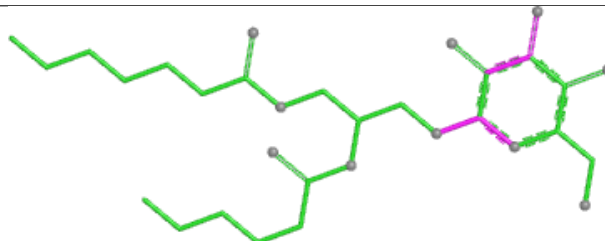


Rings

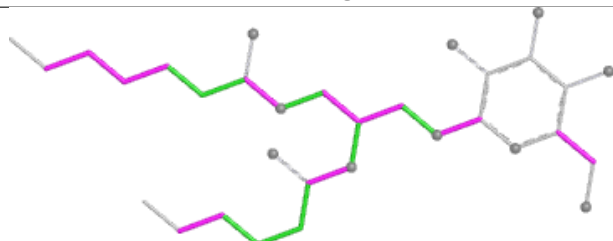
Ligand LMG U 201



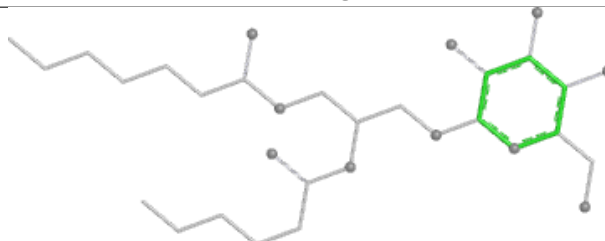
Bond lengths



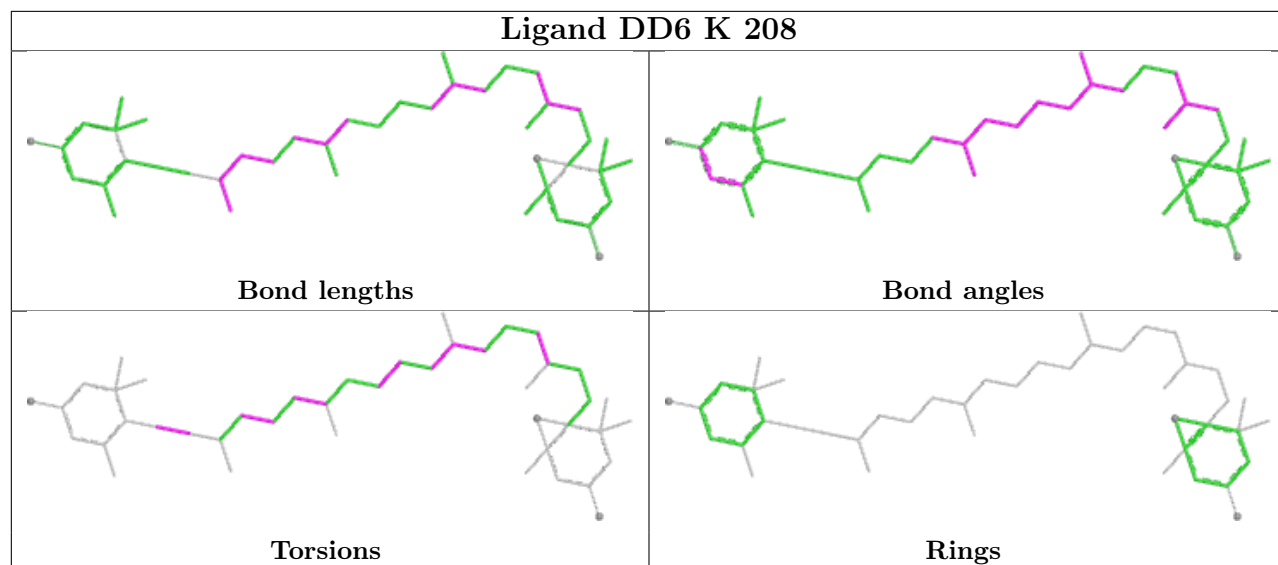
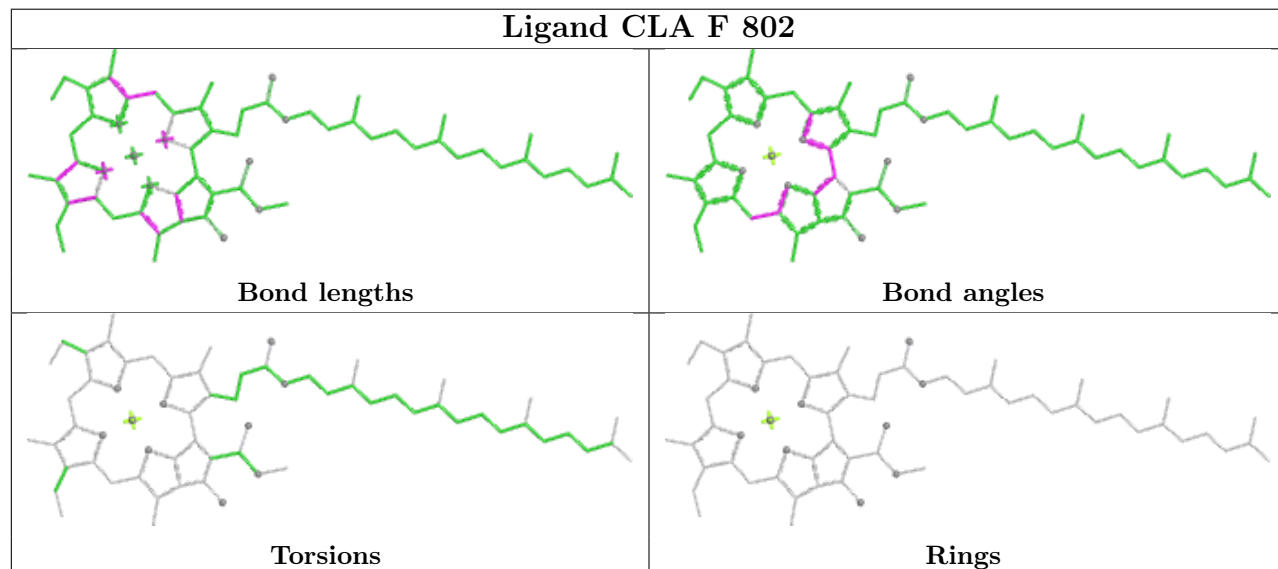
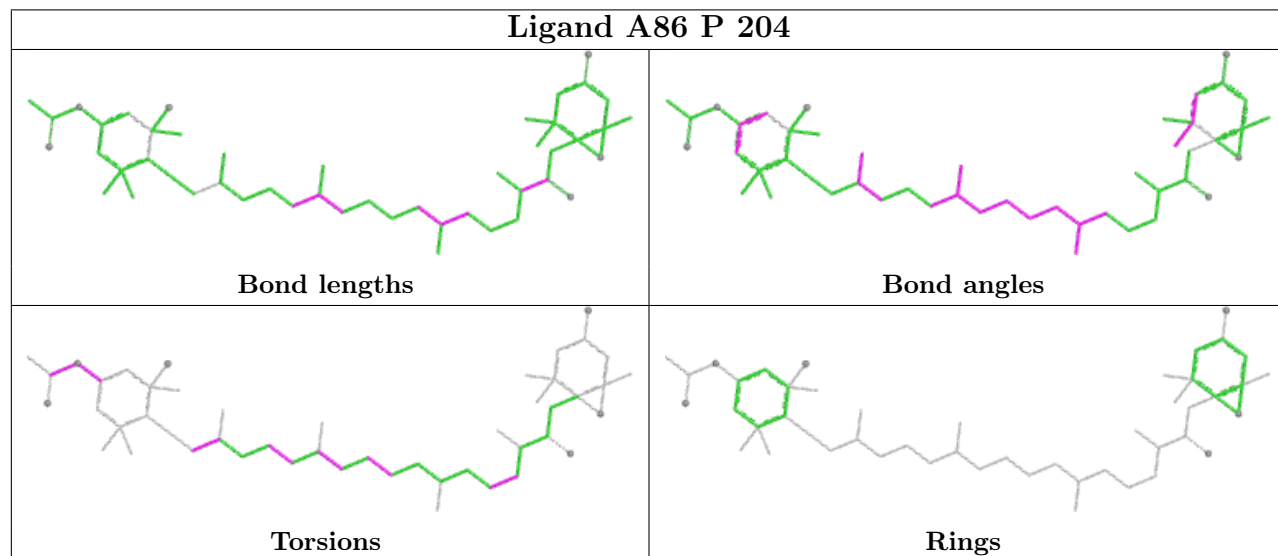
Bond angles



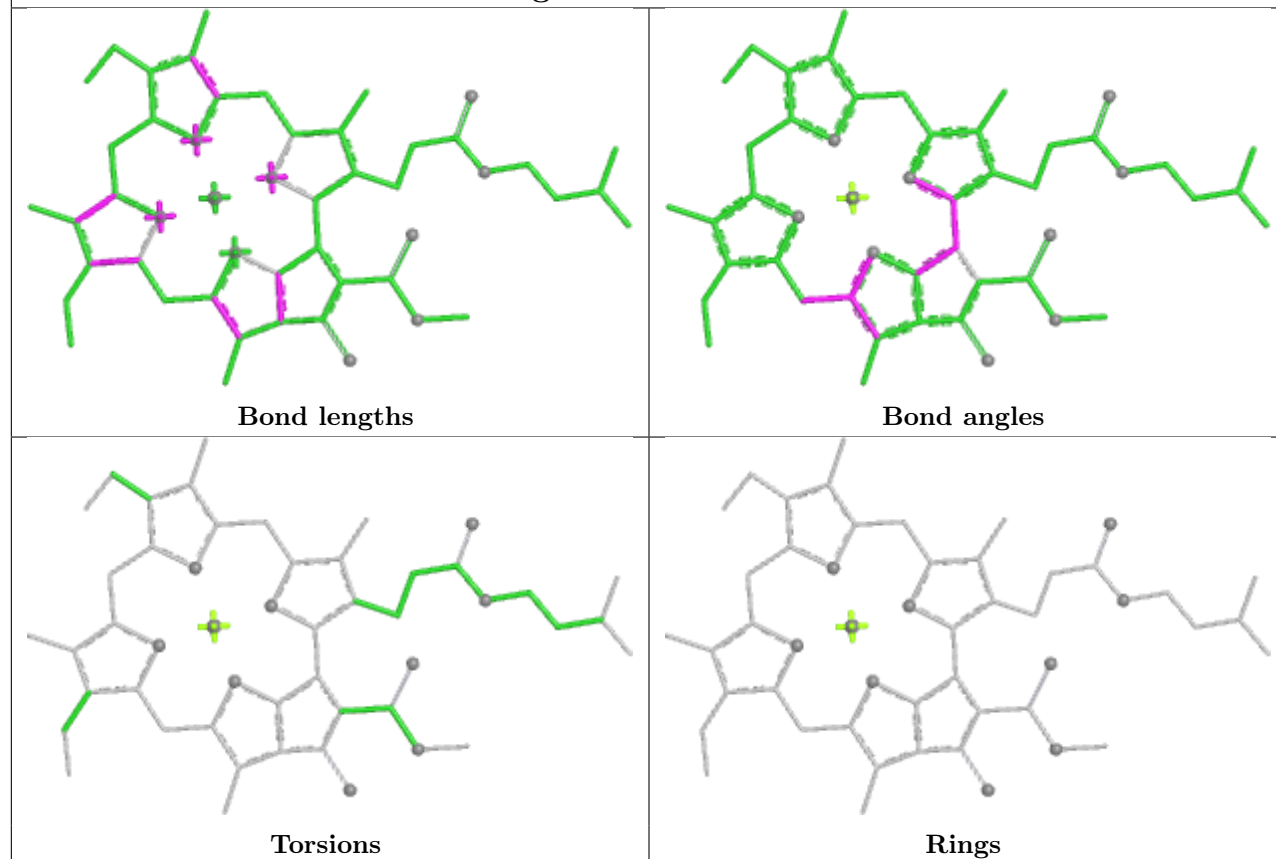
Torsions



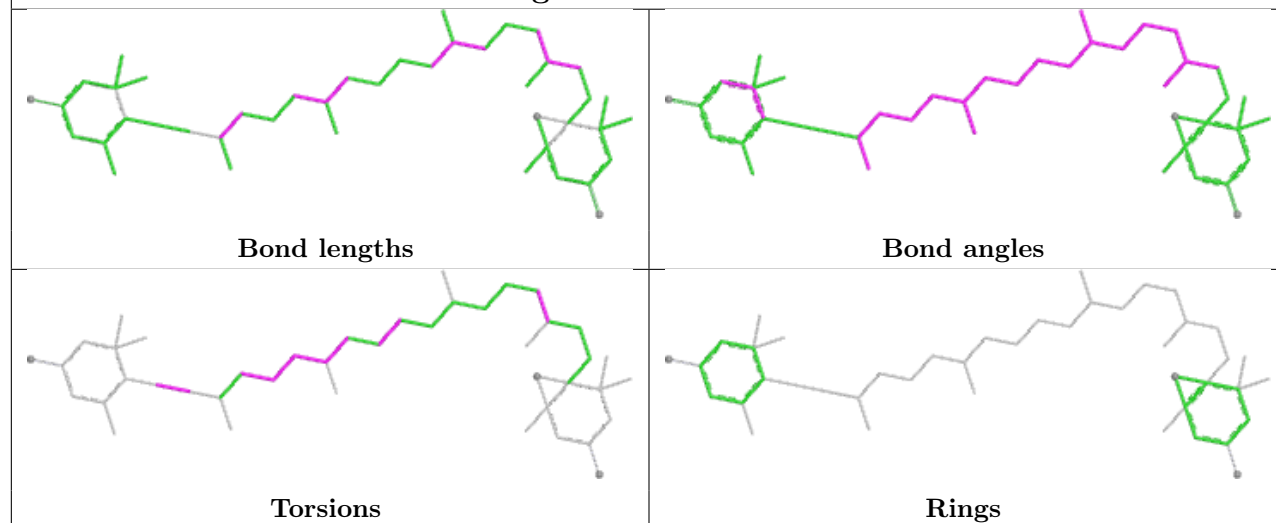
Rings

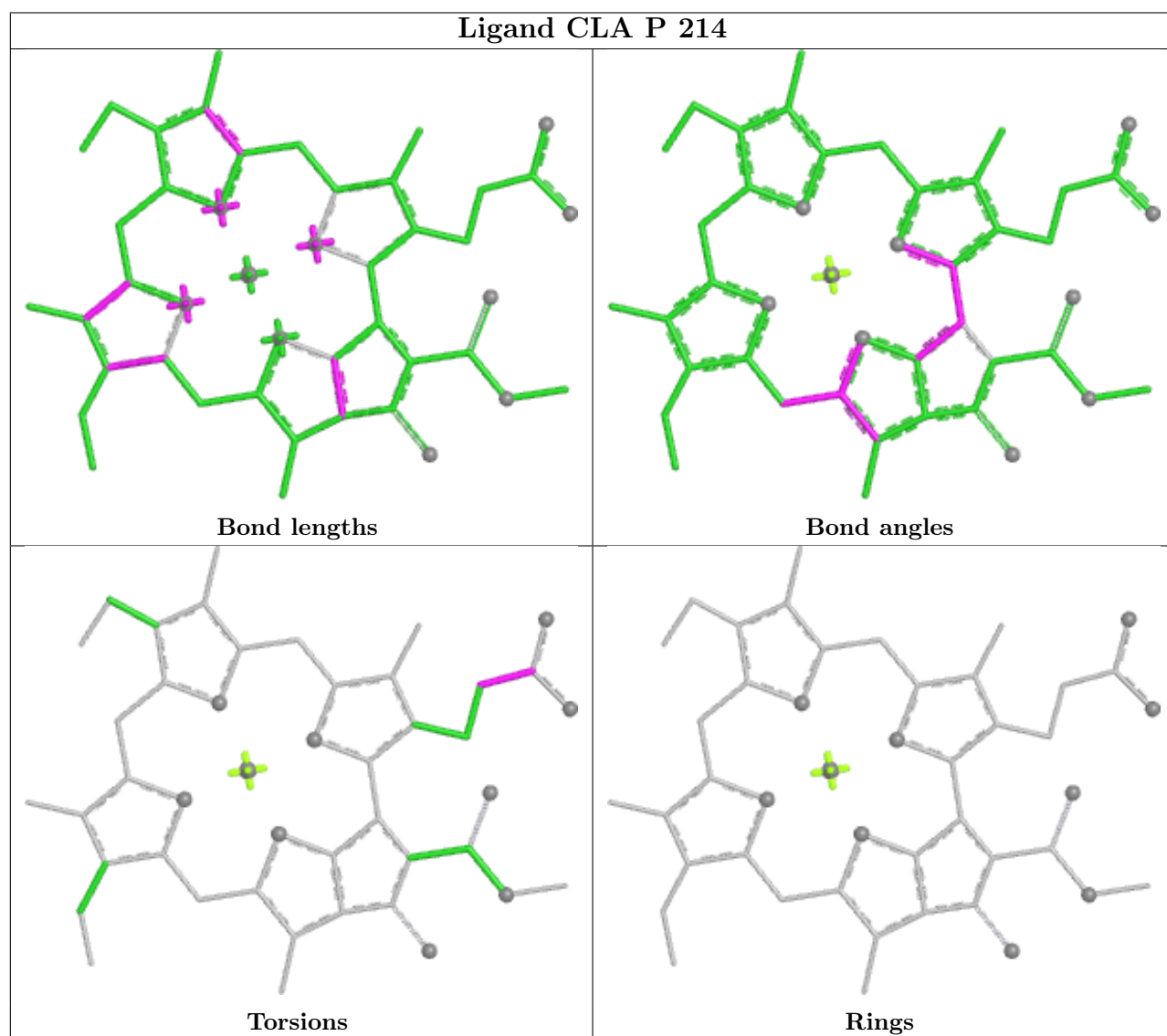
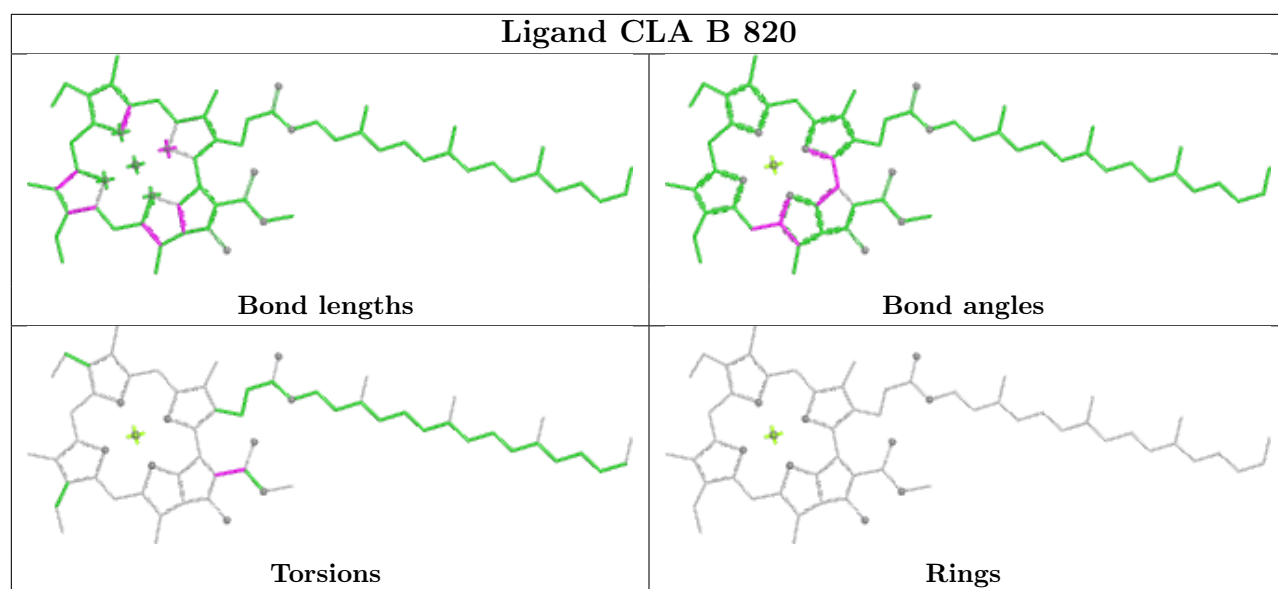
Ligand DD6 K 208**Ligand CLA F 802****Ligand A86 P 204**

Ligand CLA B 825

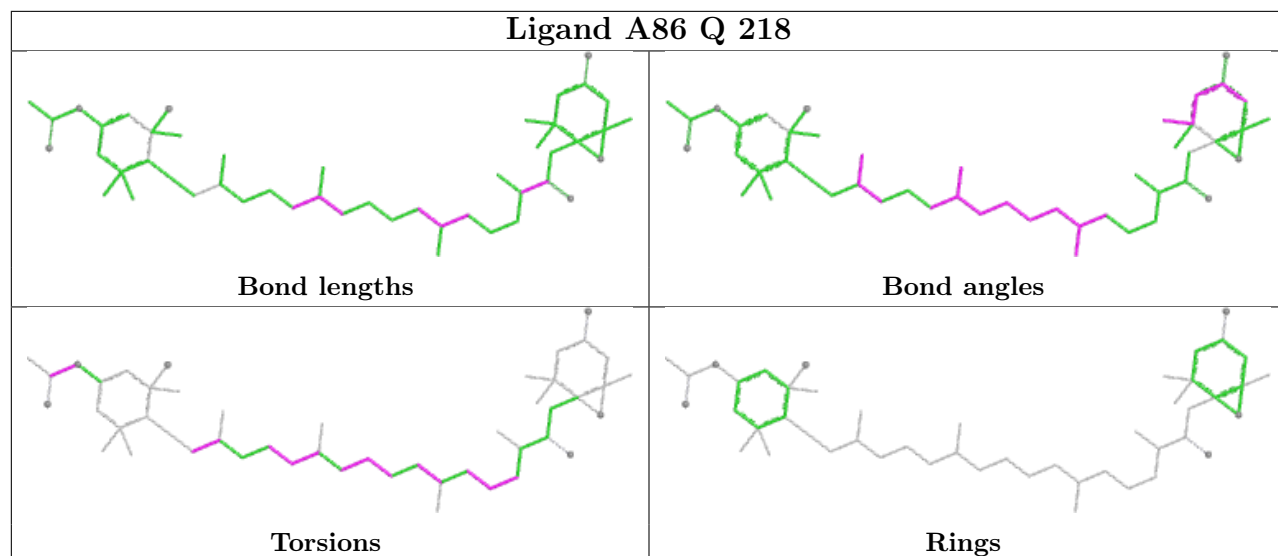


Ligand DD6 G 214

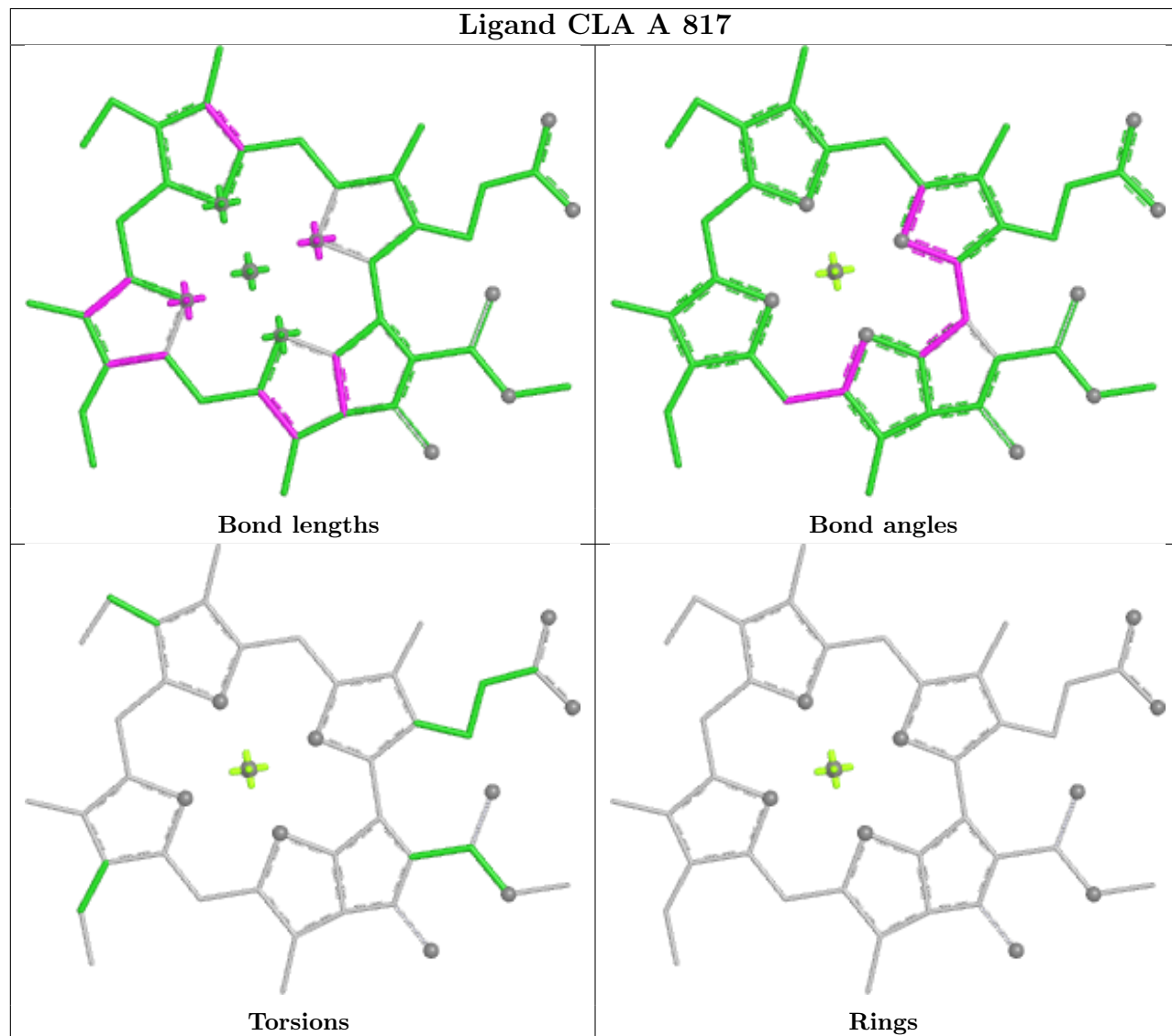


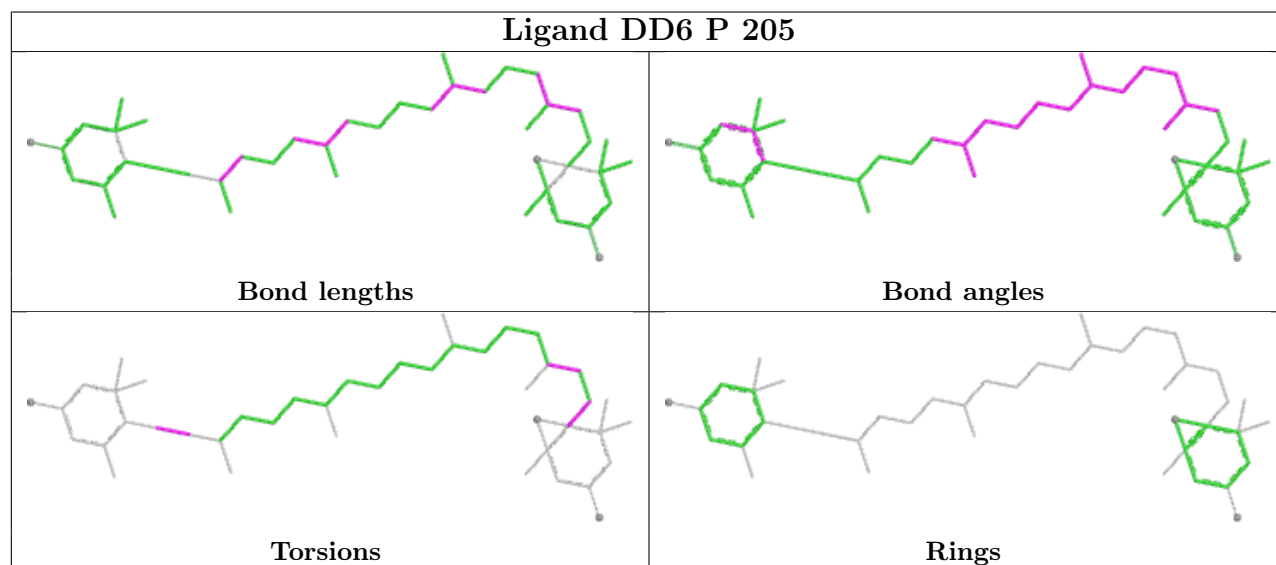
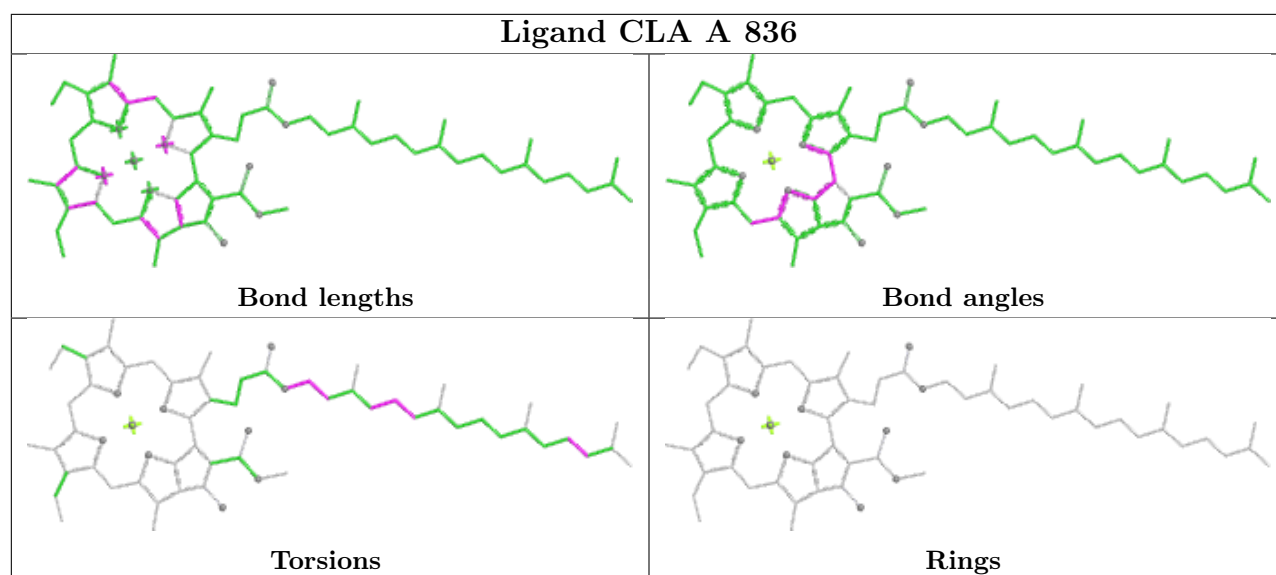


Ligand A86 Q 218

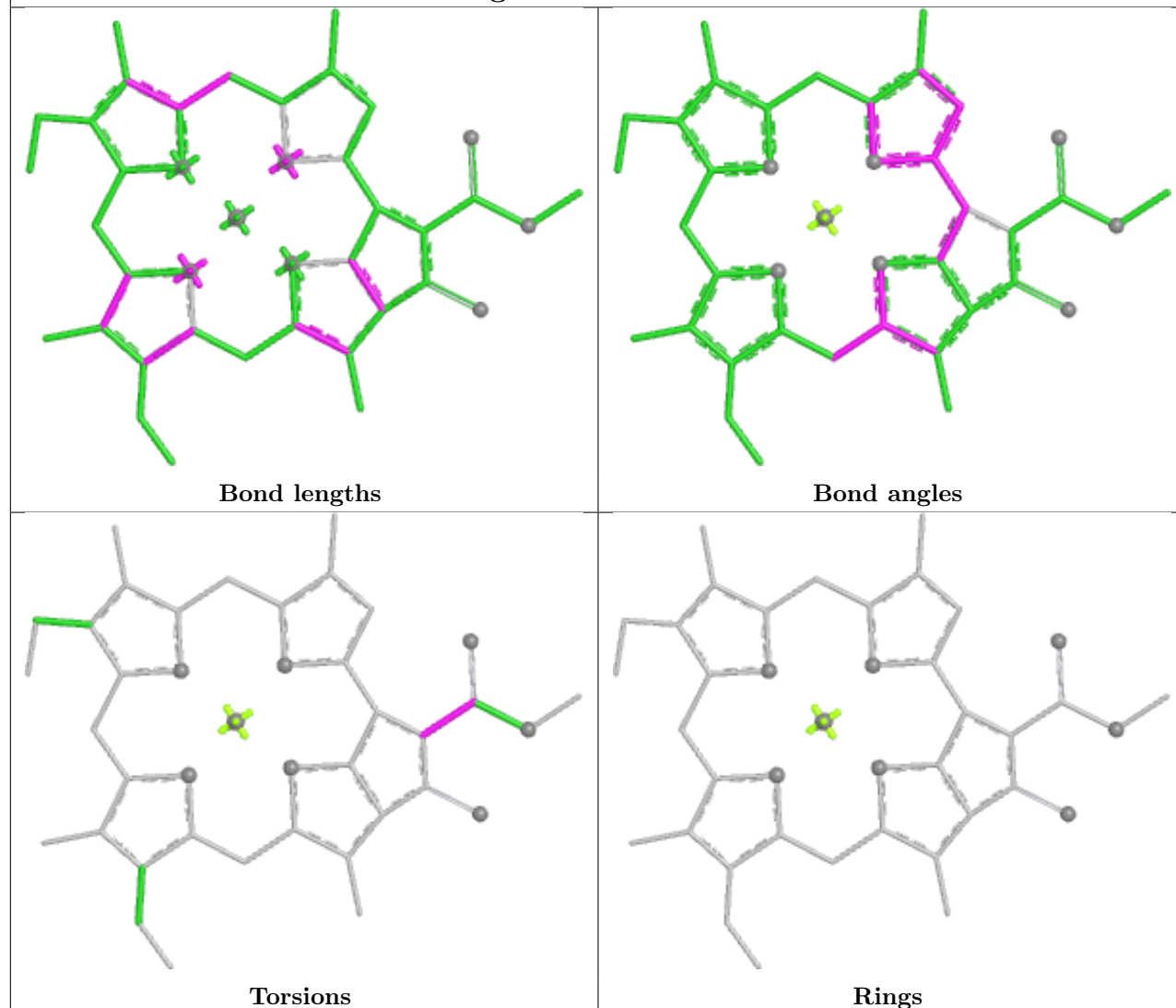


Ligand CLA A 817

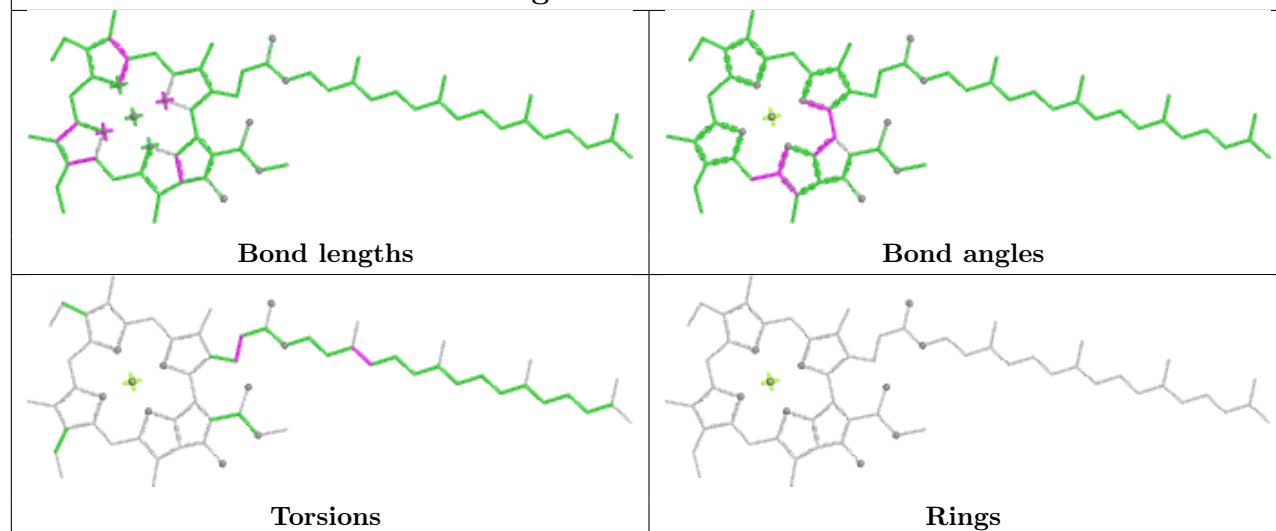




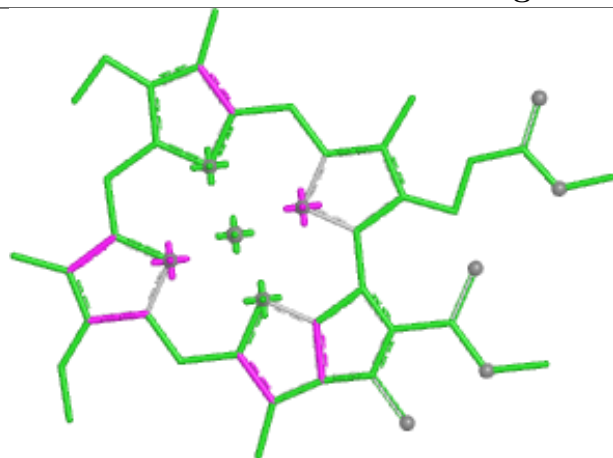
Ligand CLA A 855



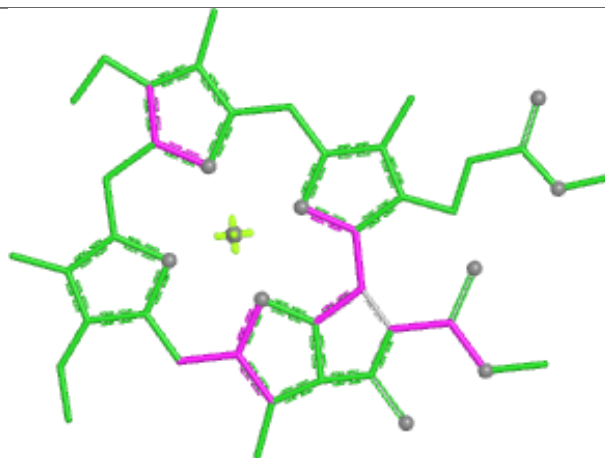
Ligand CLA A 850



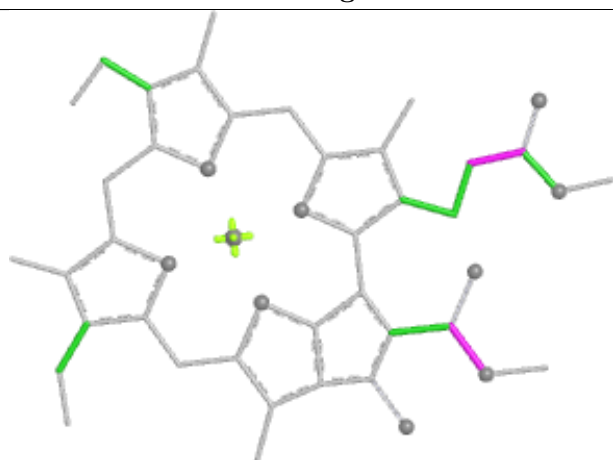
Ligand CLA U 208



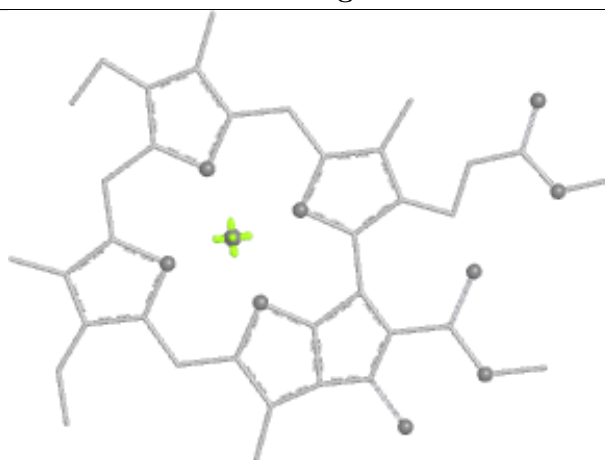
Bond lengths



Bond angles

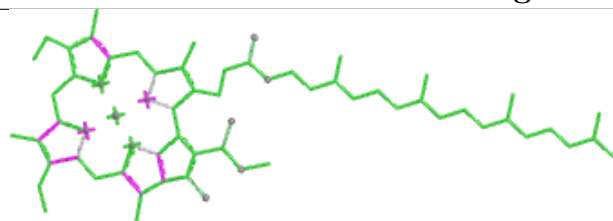


Torsions

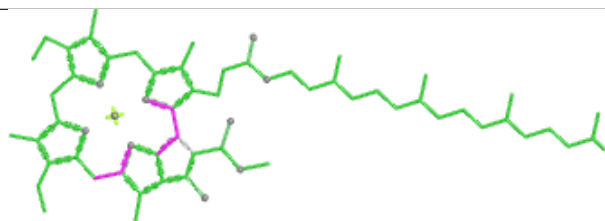


Rings

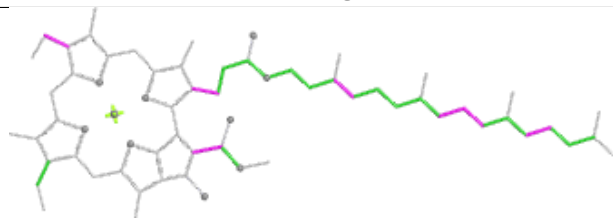
Ligand CLA A 853



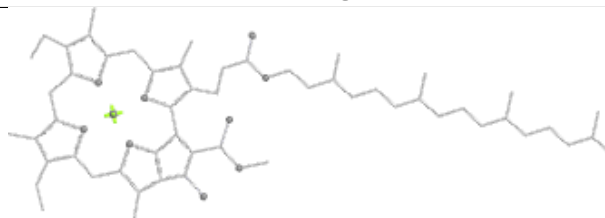
Bond lengths



Bond angles

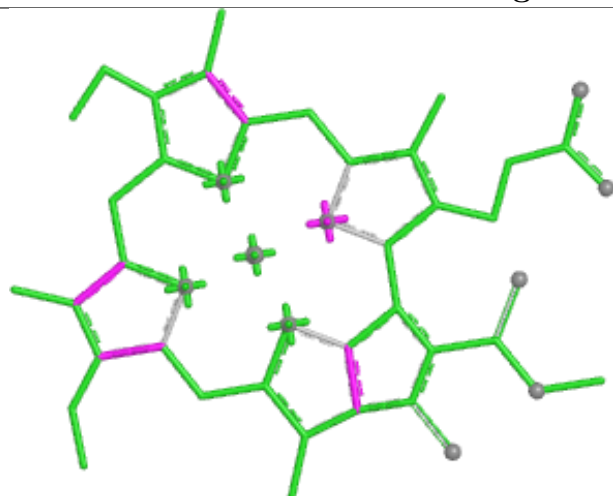


Torsions

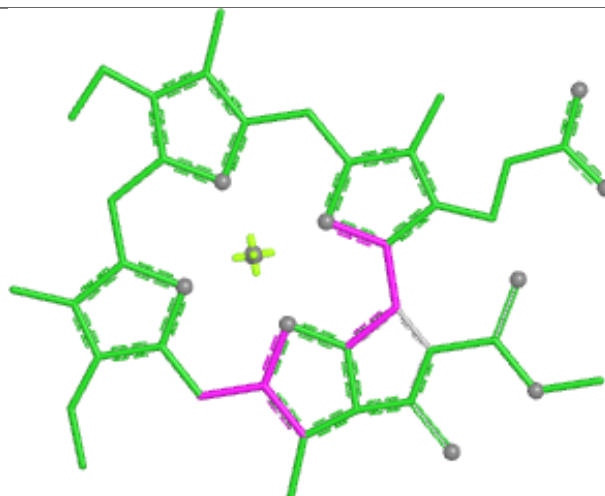


Rings

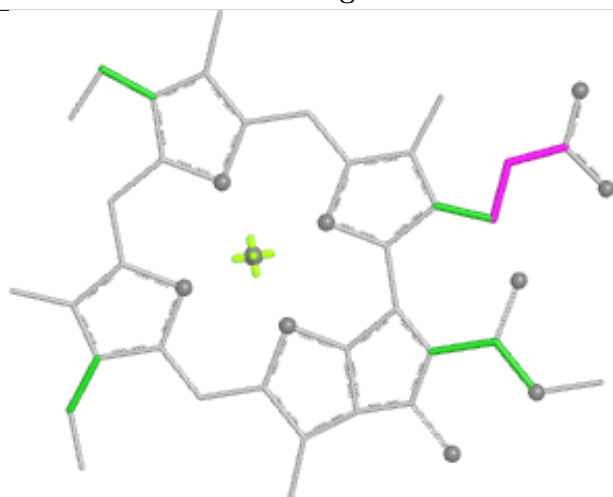
Ligand CLA G 215



Bond lengths



Bond angles

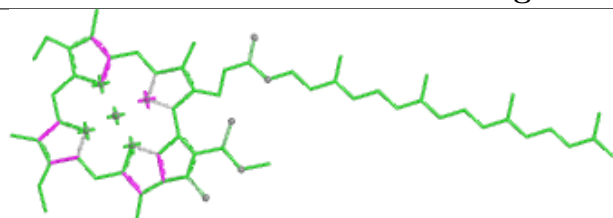


Torsions

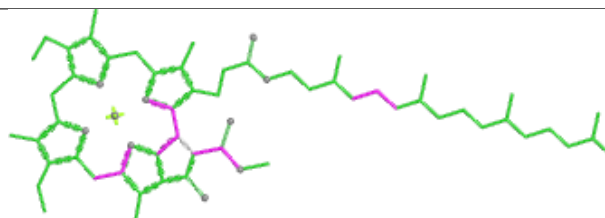


Rings

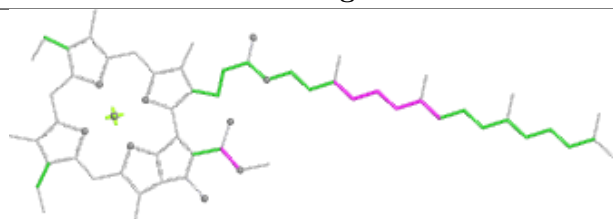
Ligand CLA O 209



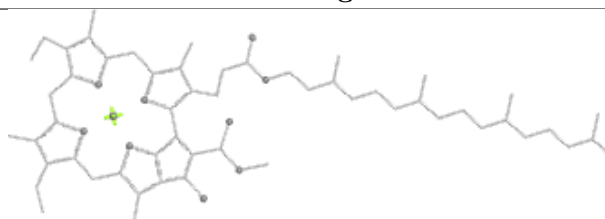
Bond lengths



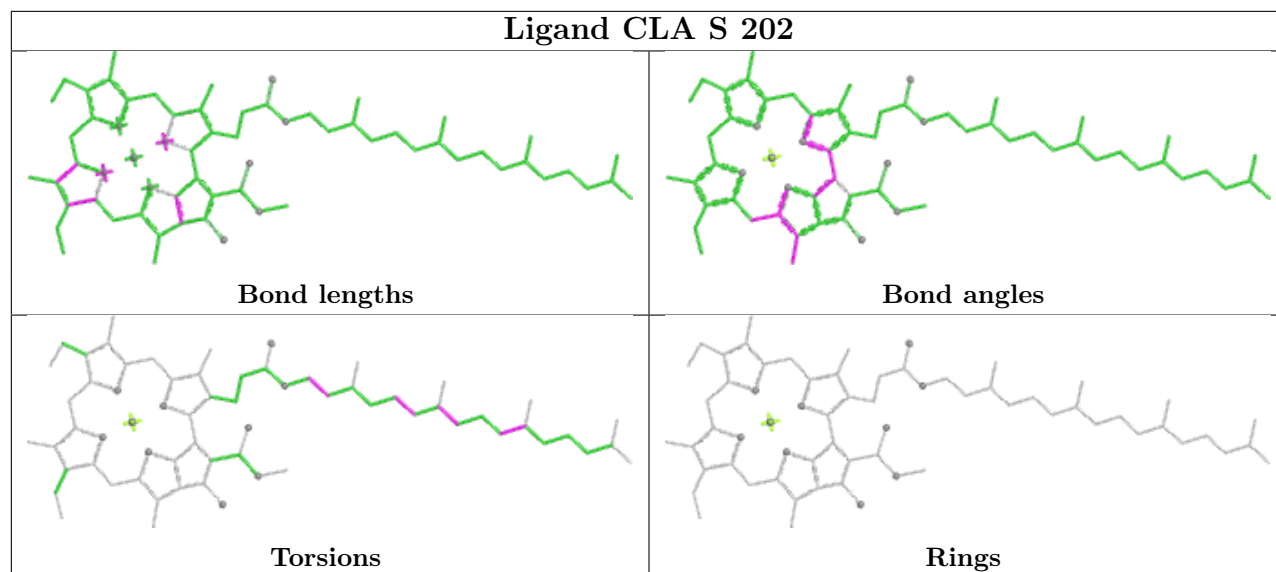
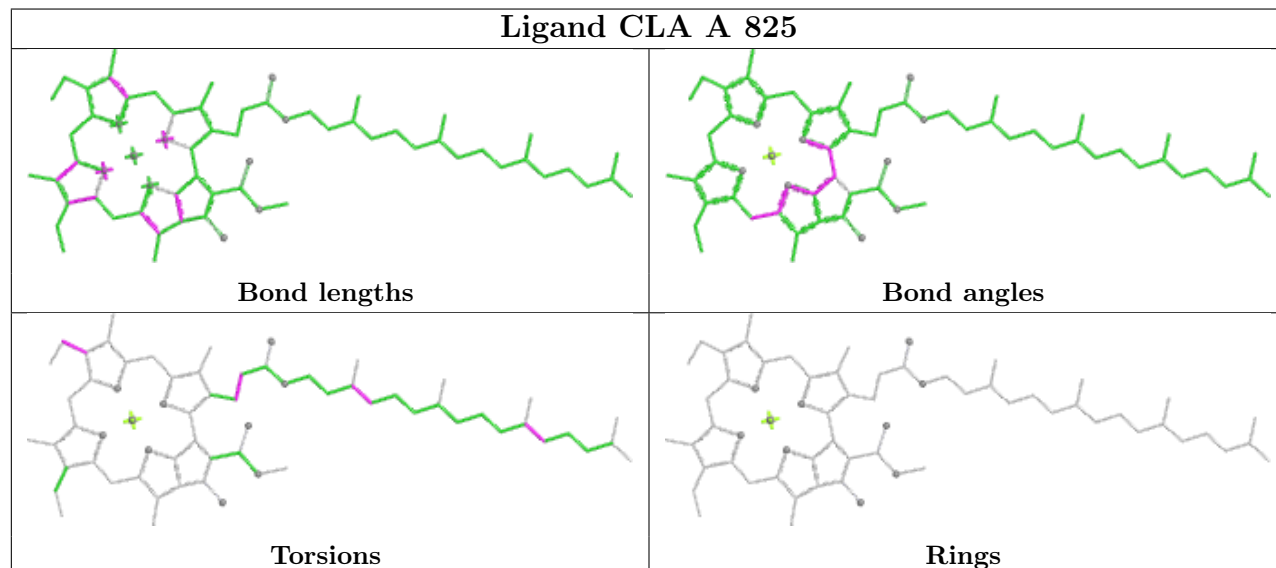
Bond angles

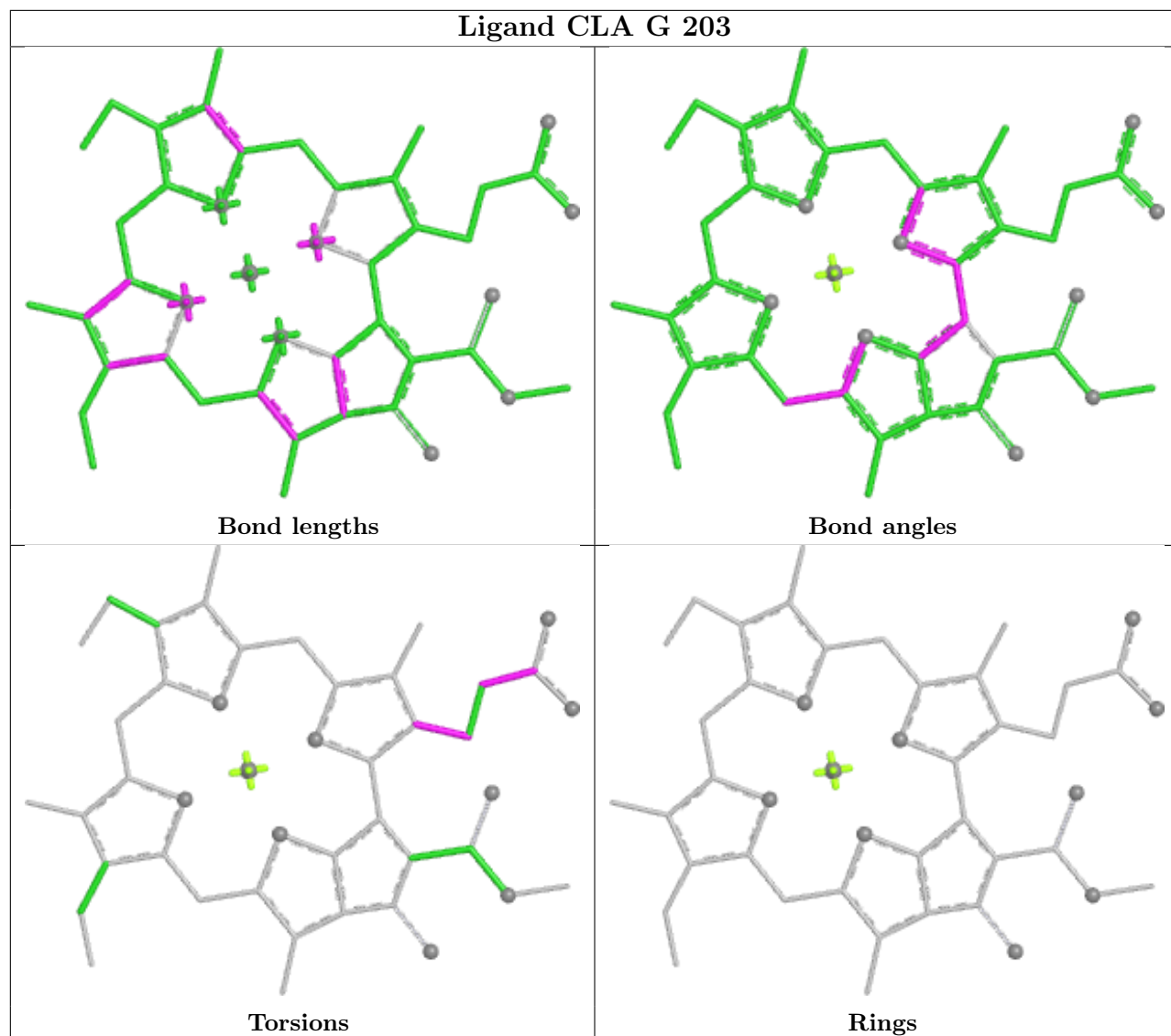


Torsions

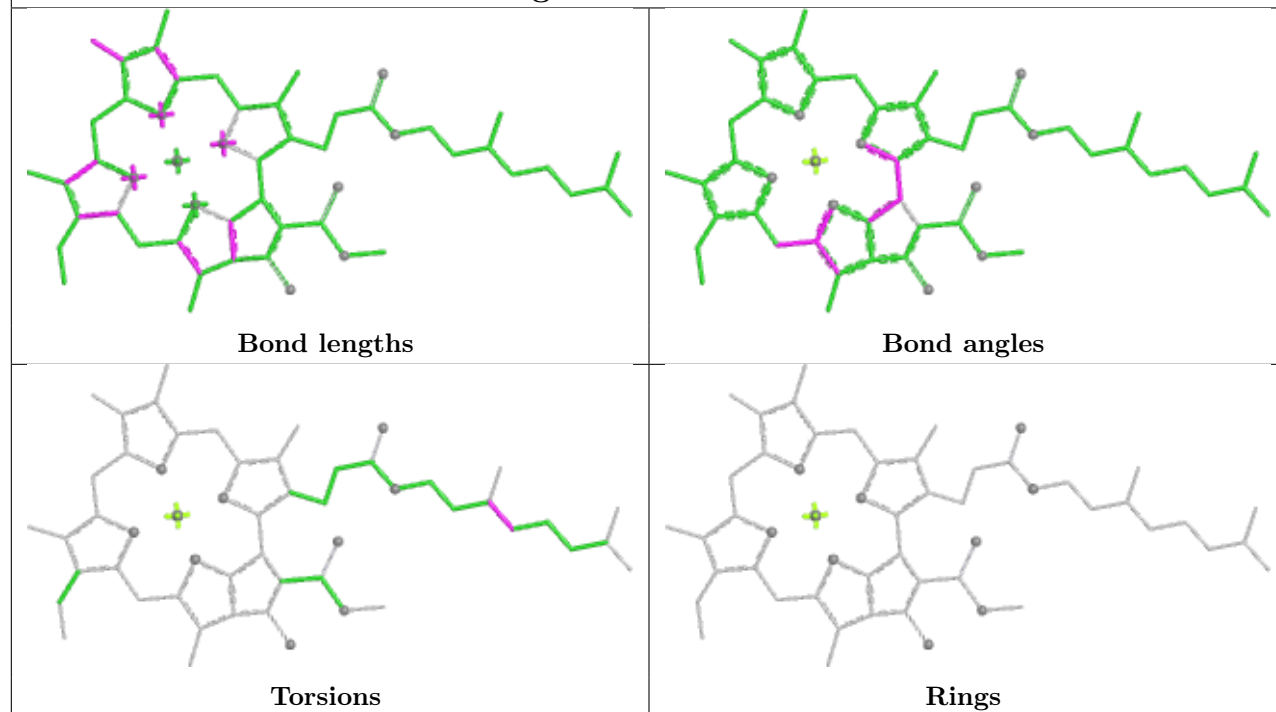


Rings

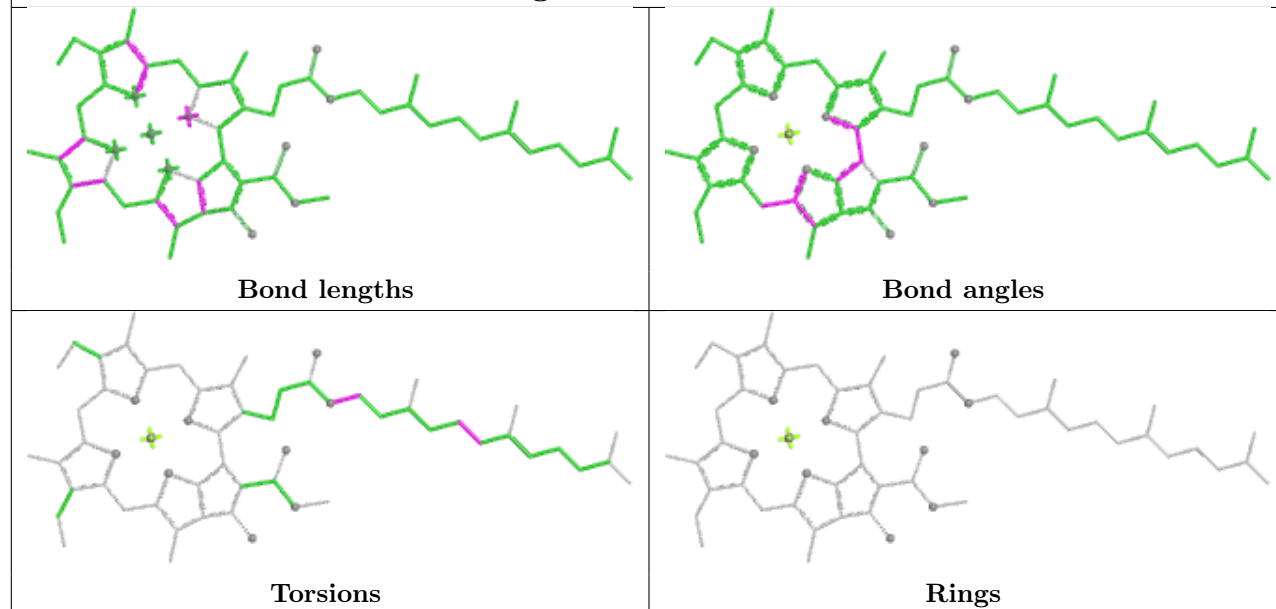
Ligand CLA S 202**Ligand CLA A 825**

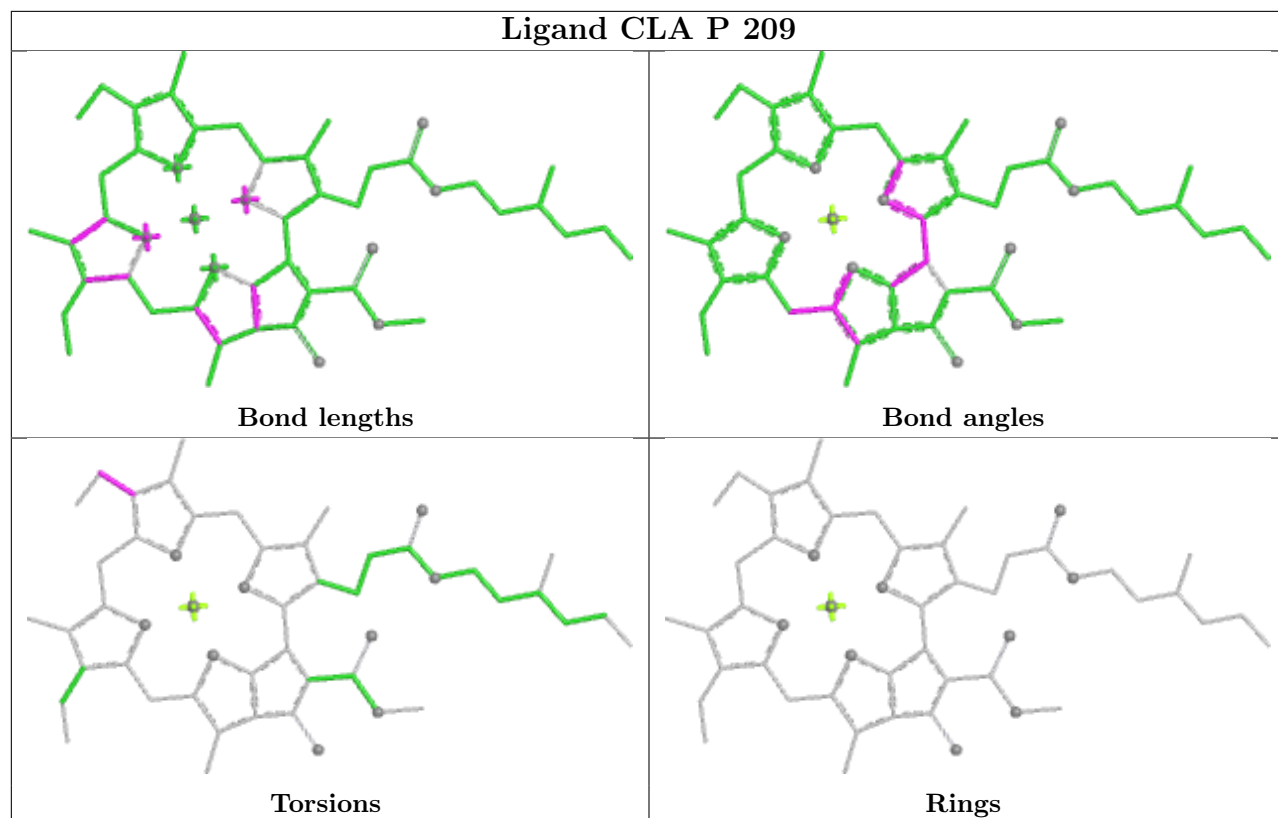


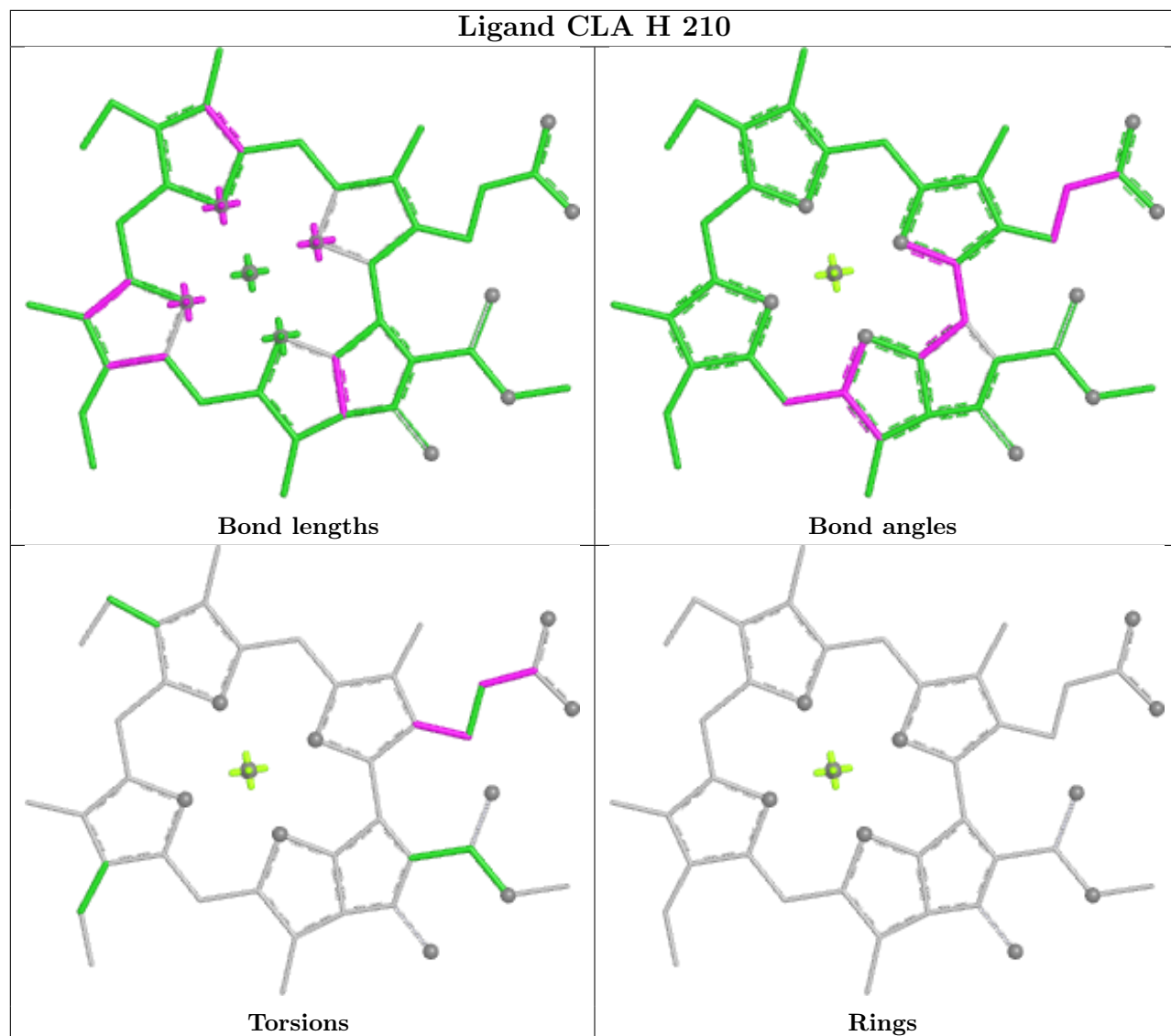
Ligand CLA B 809

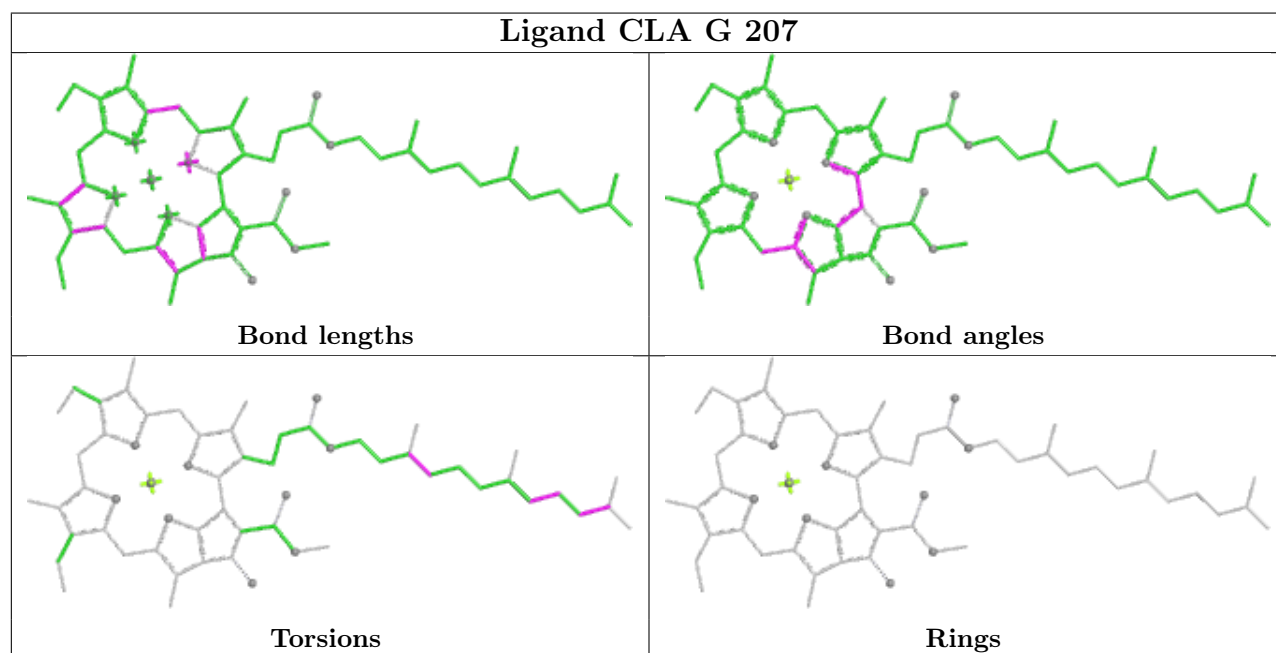
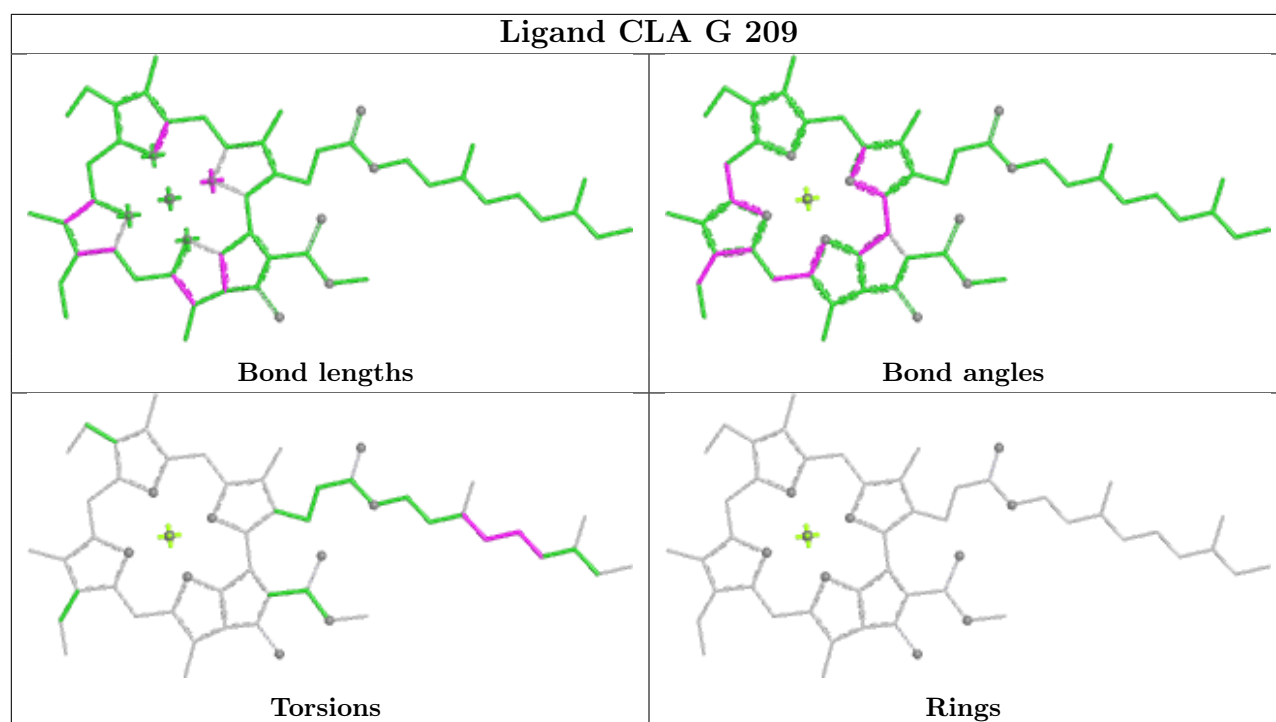


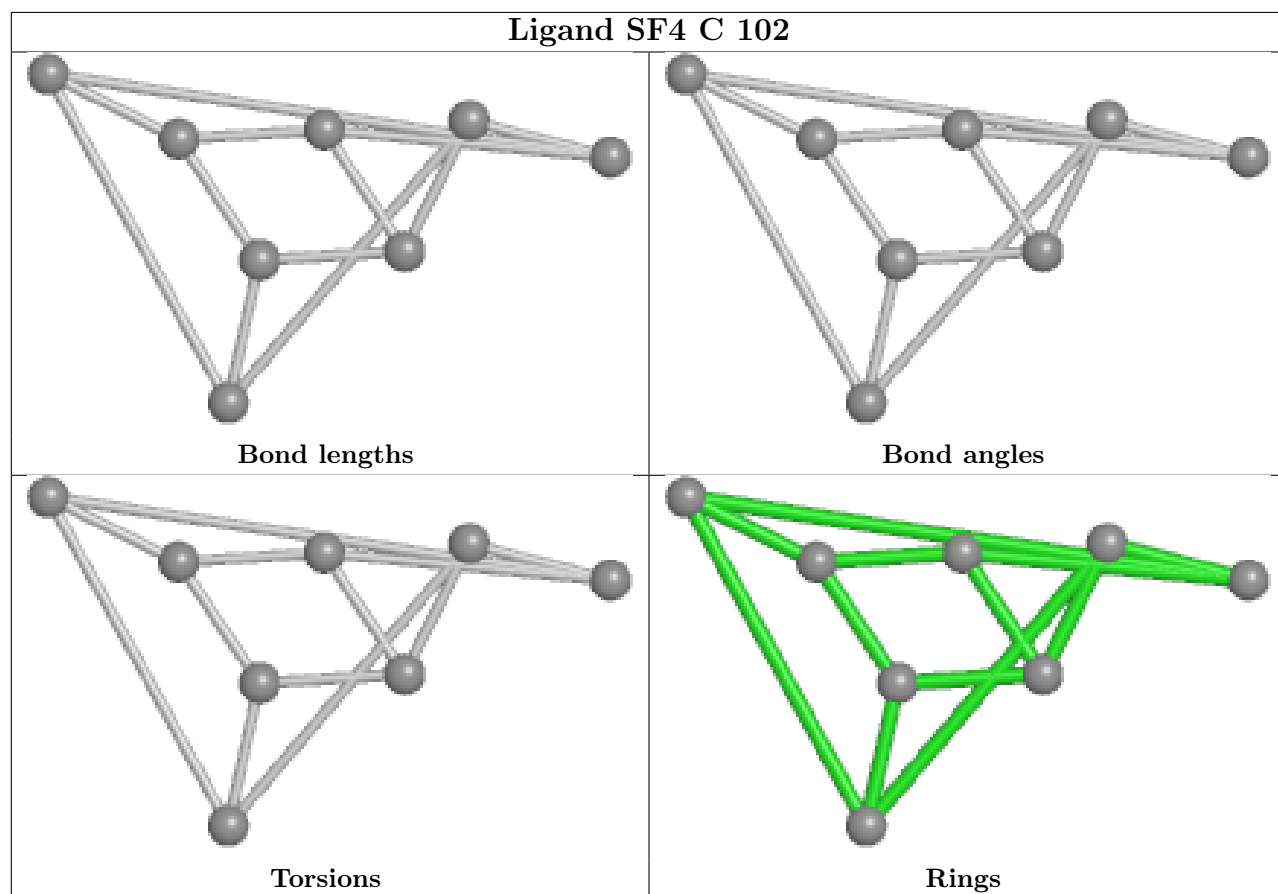
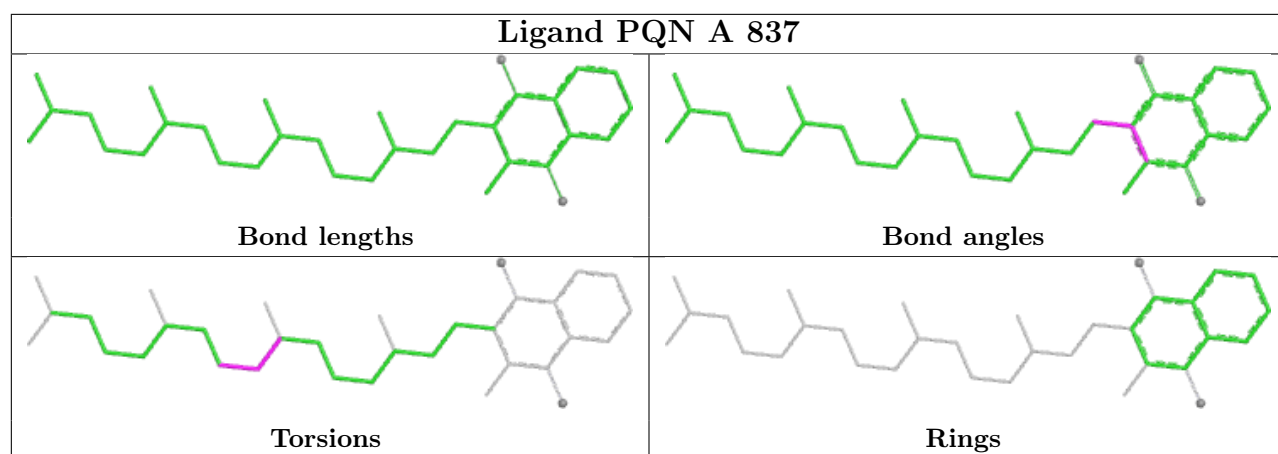
Ligand CLA O 208



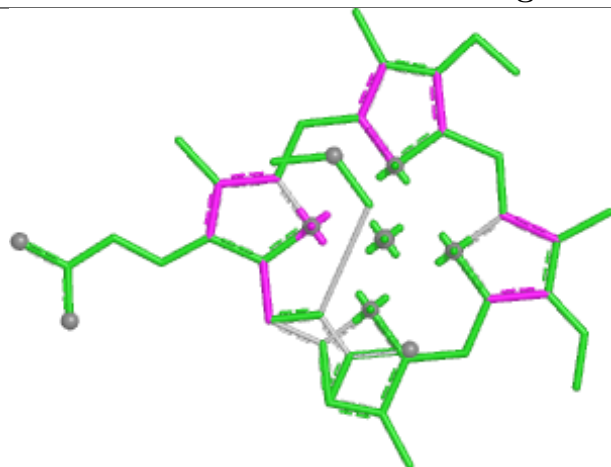




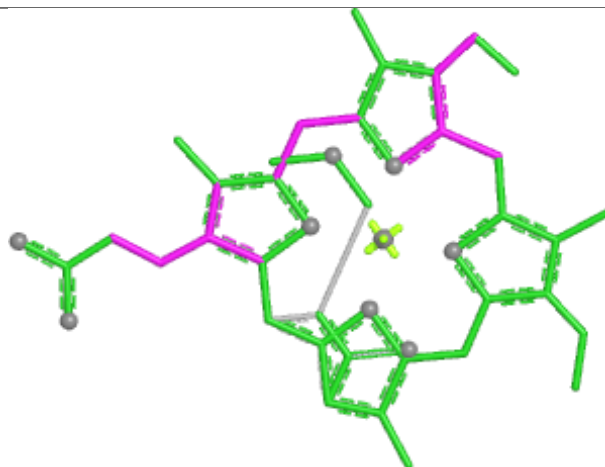




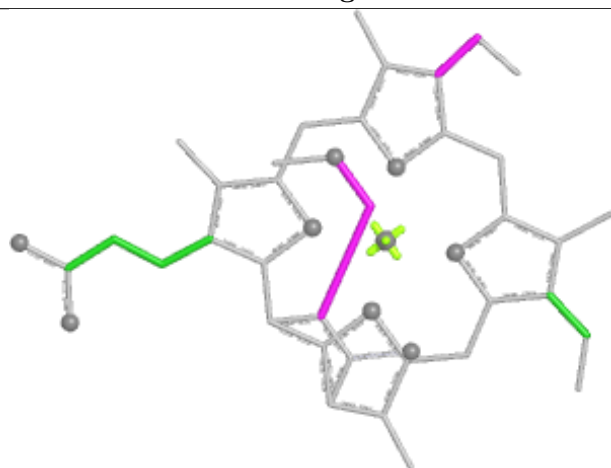
Ligand KC1 P 212



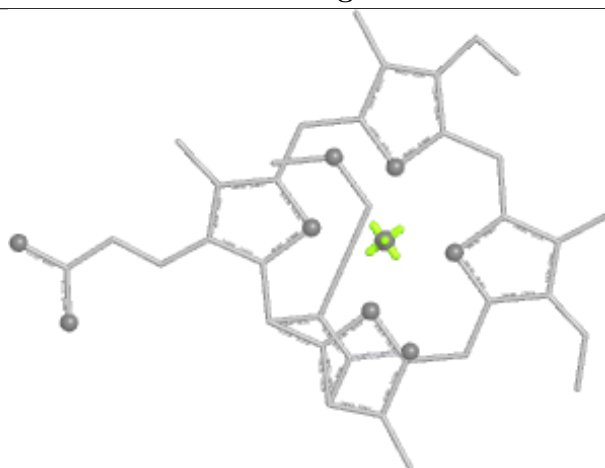
Bond lengths



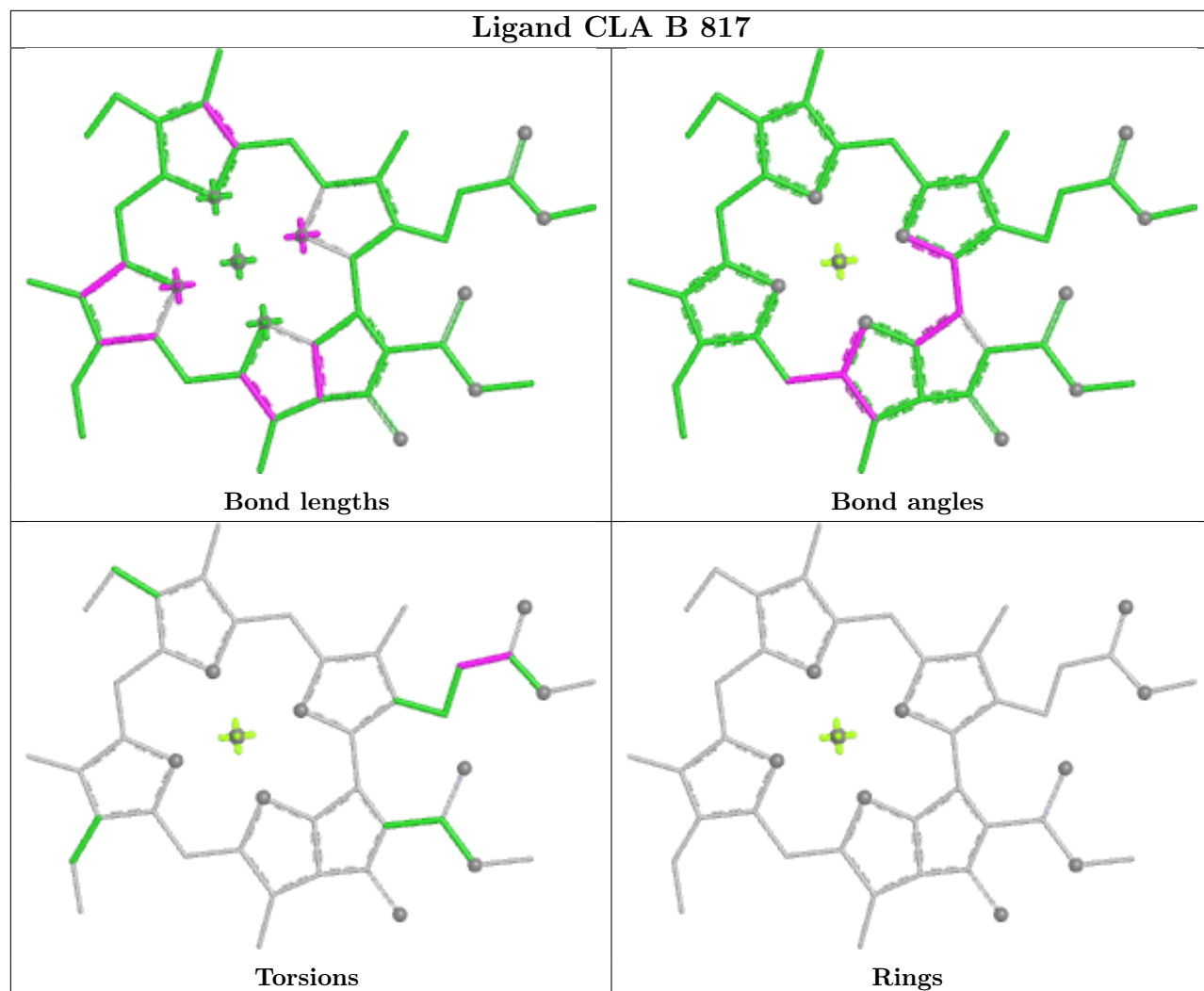
Bond angles

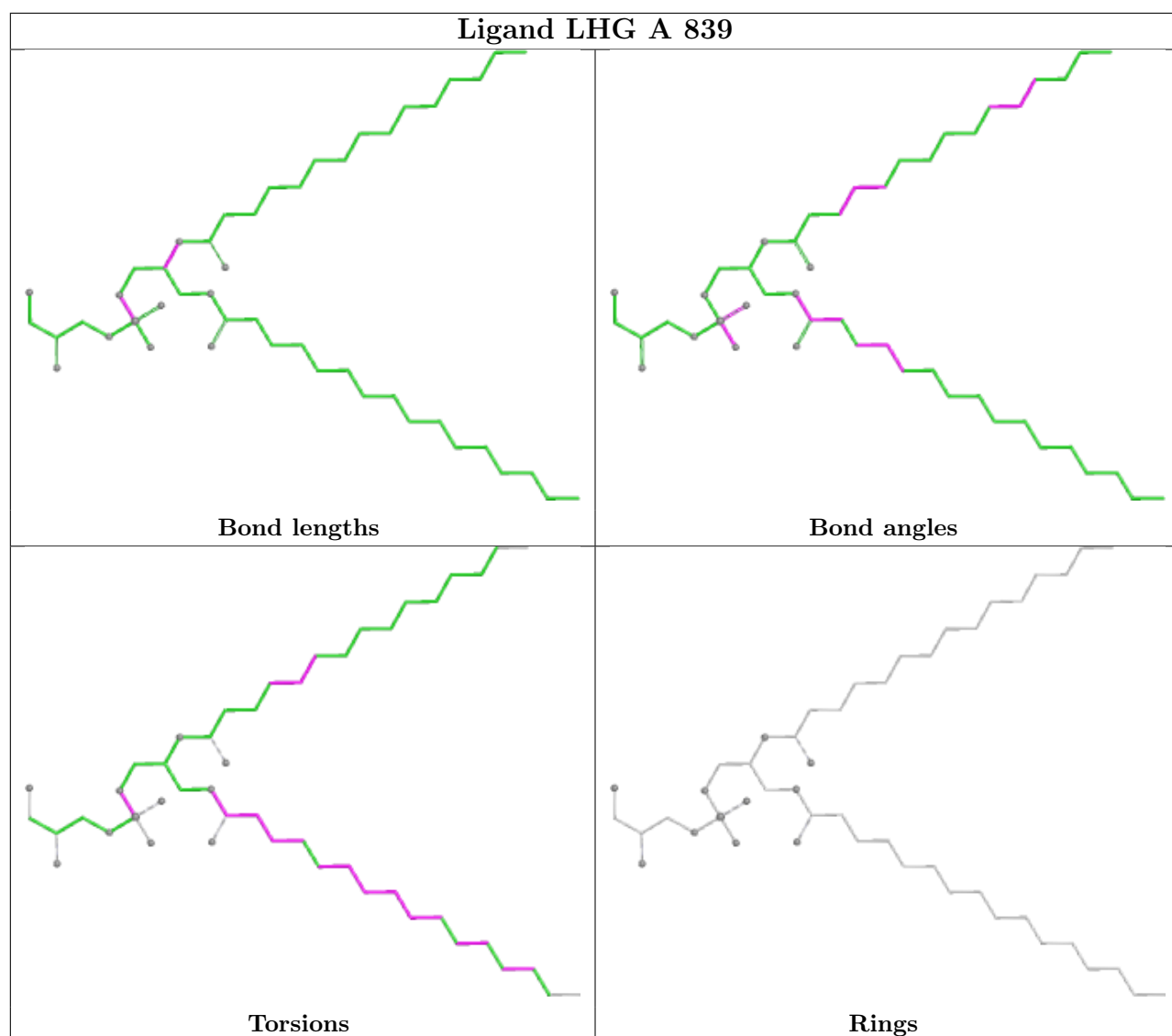


Torsions

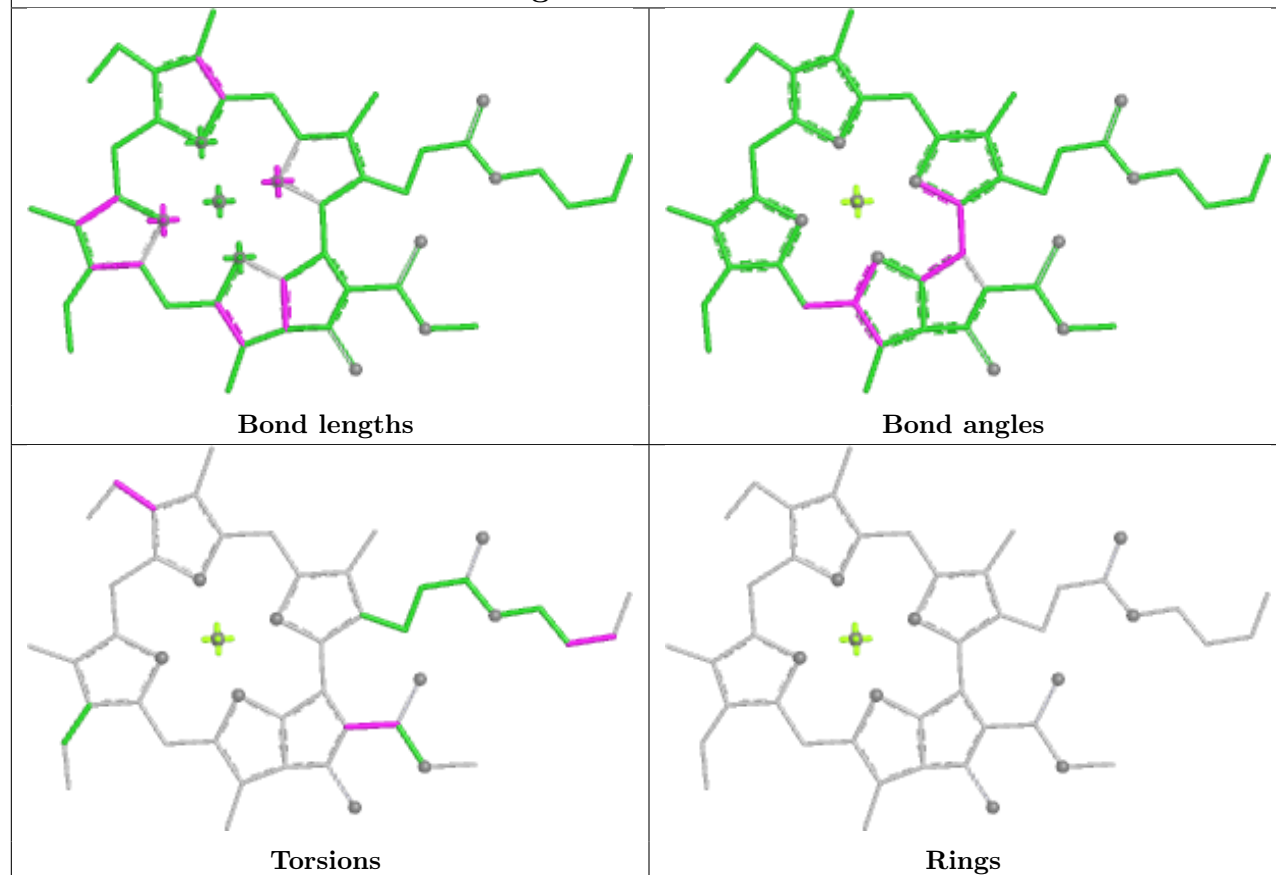


Rings

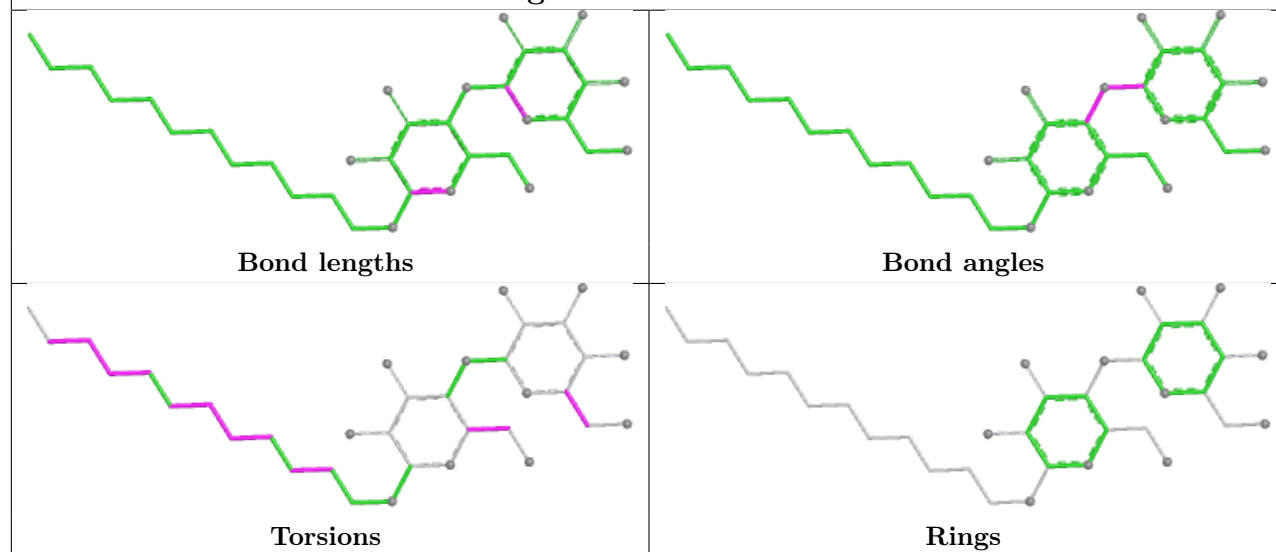




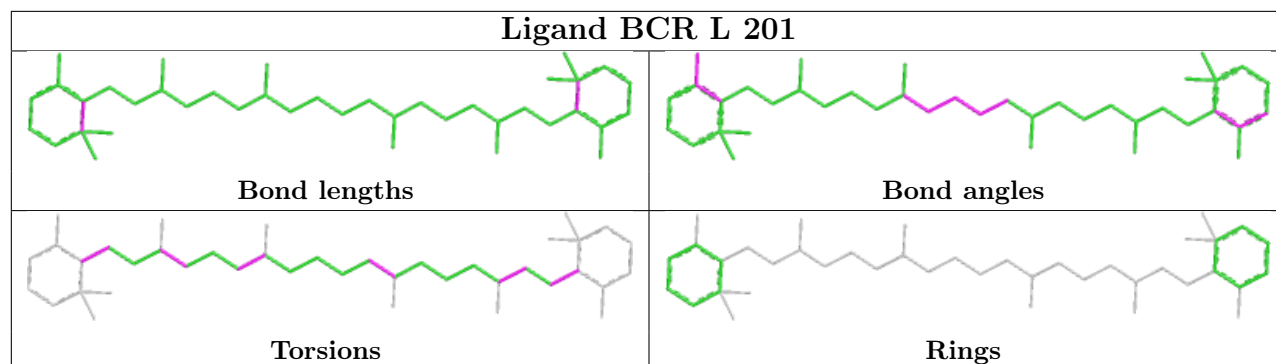
Ligand CLA A 805



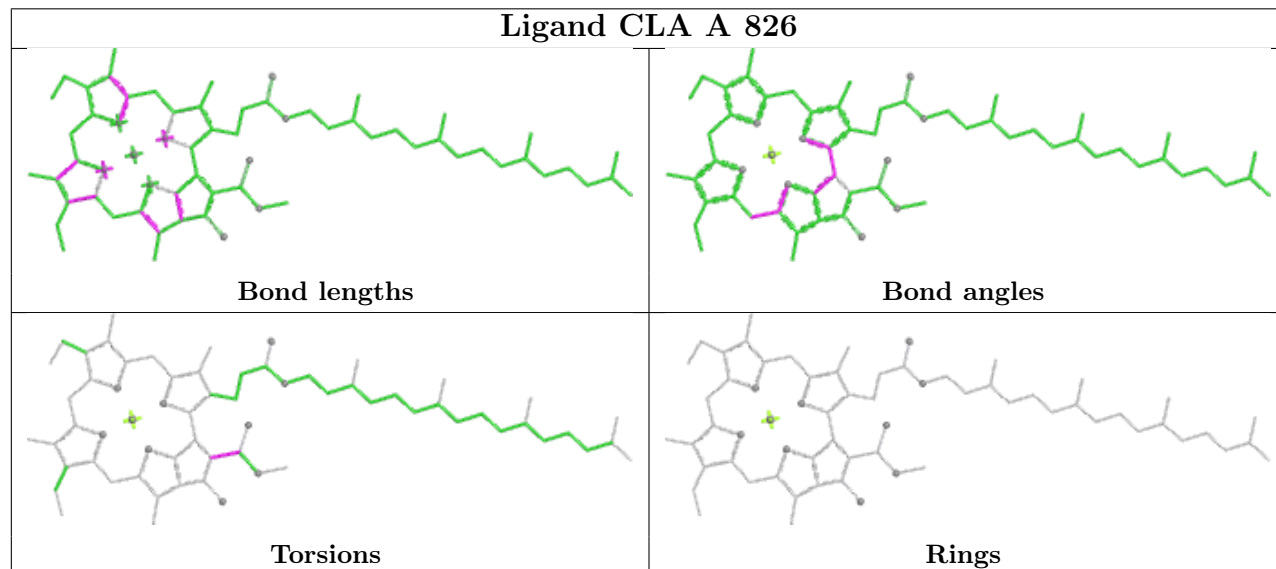
Ligand LMU A 847



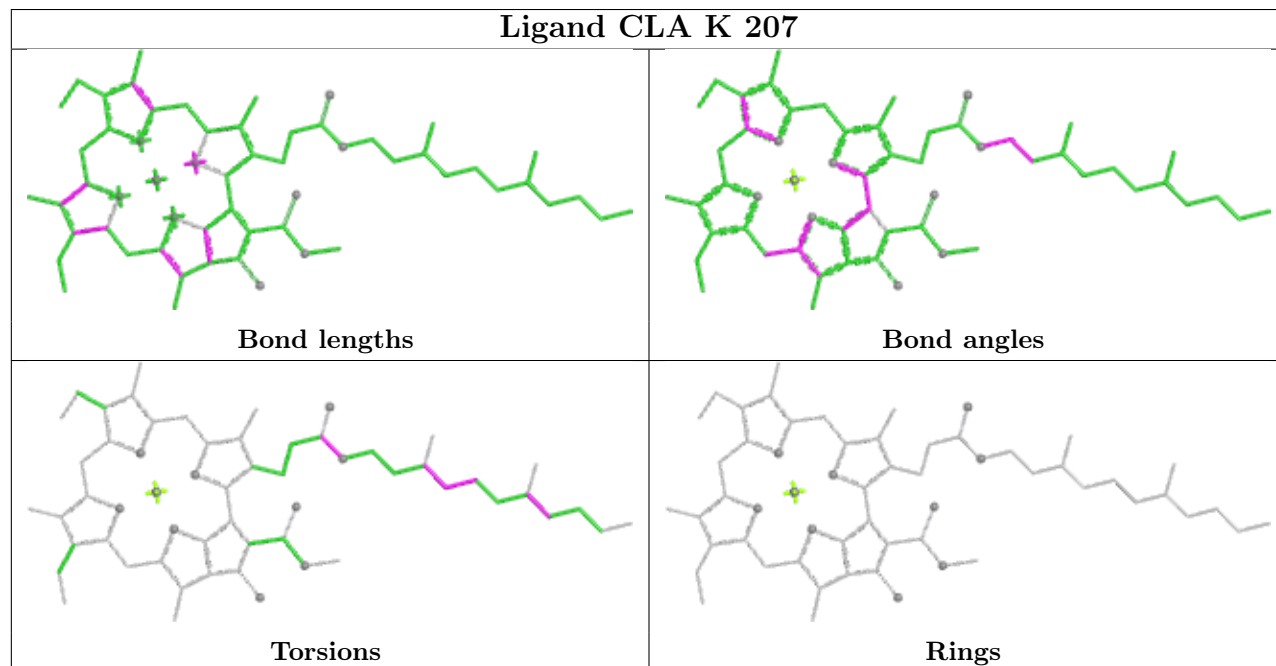
Ligand BCR L 201

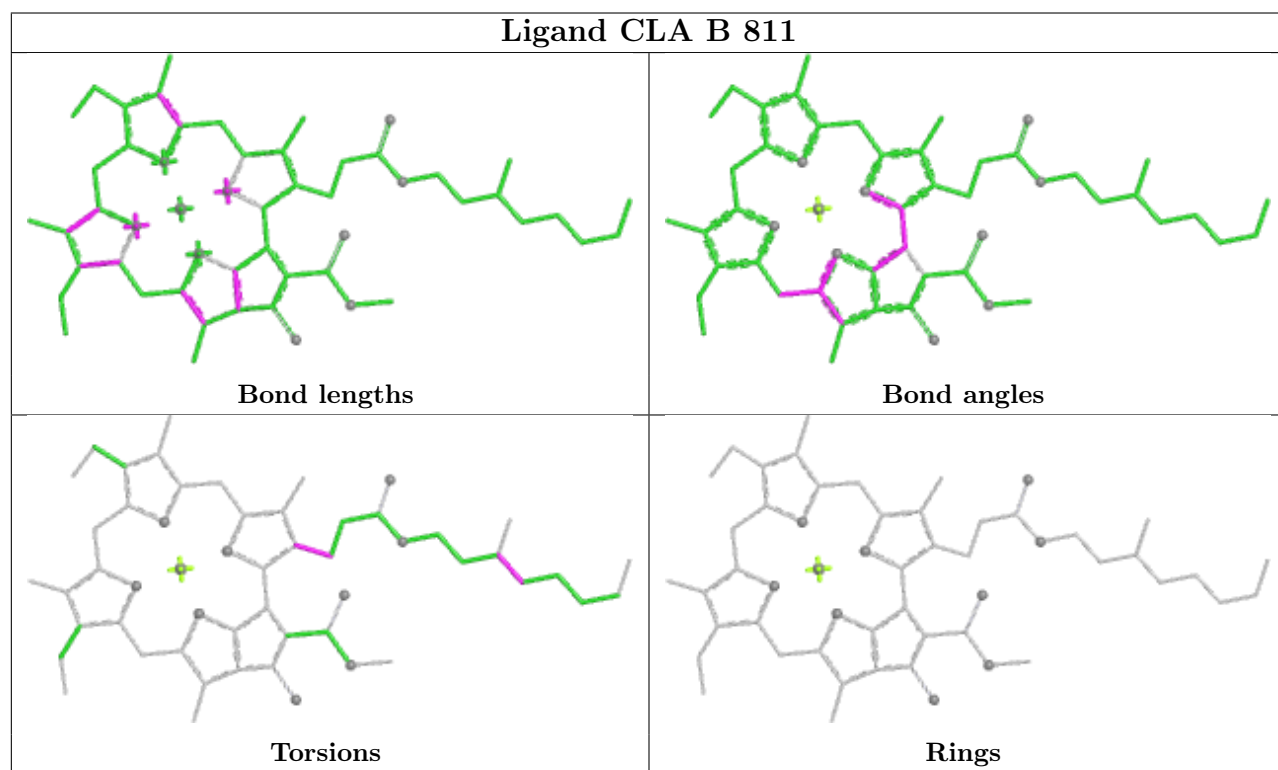
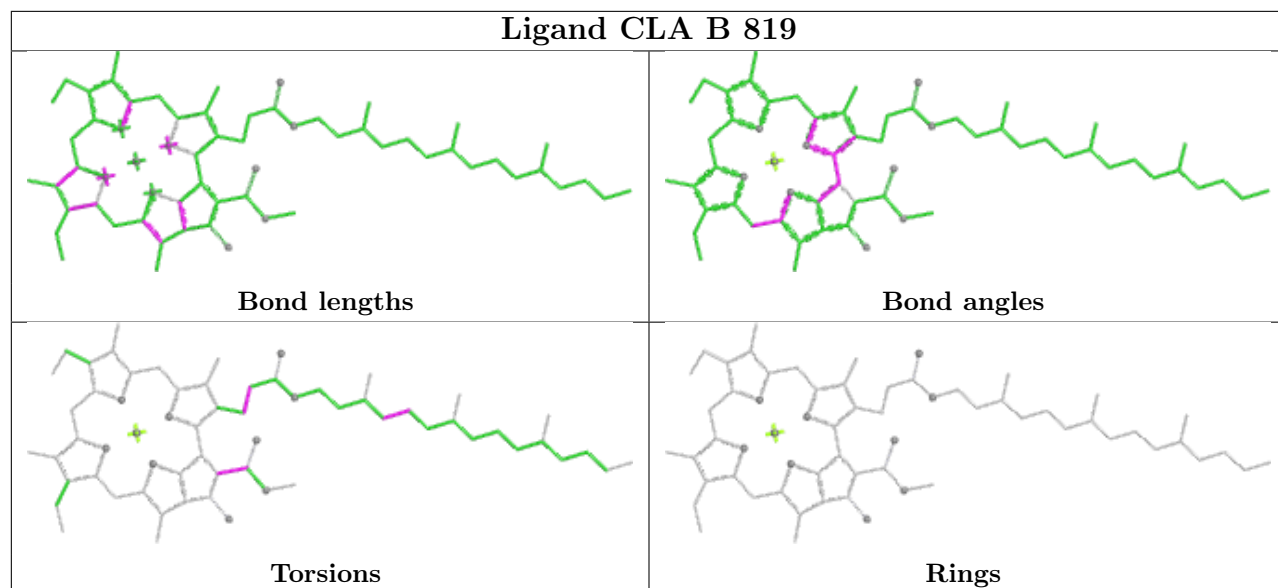


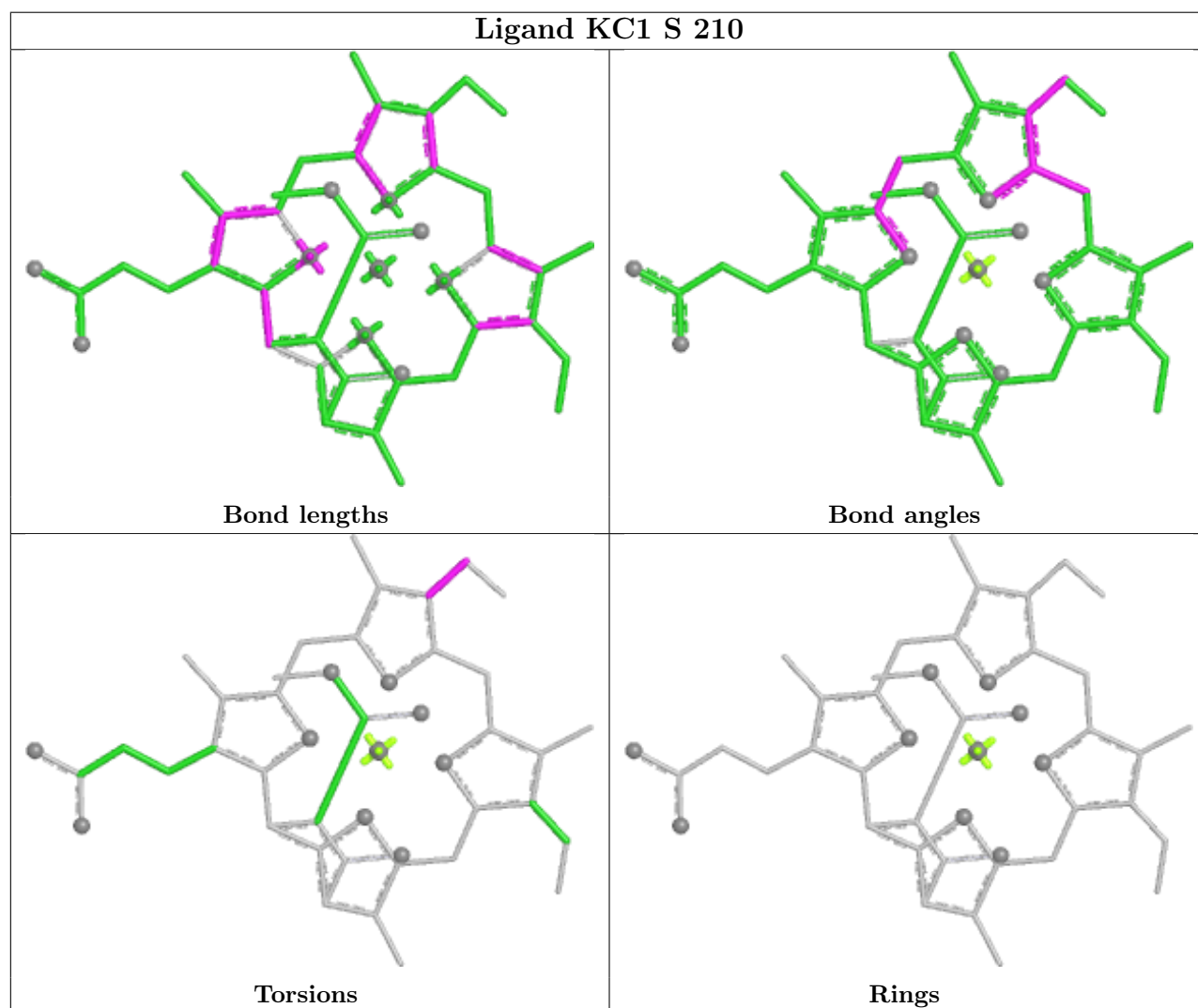
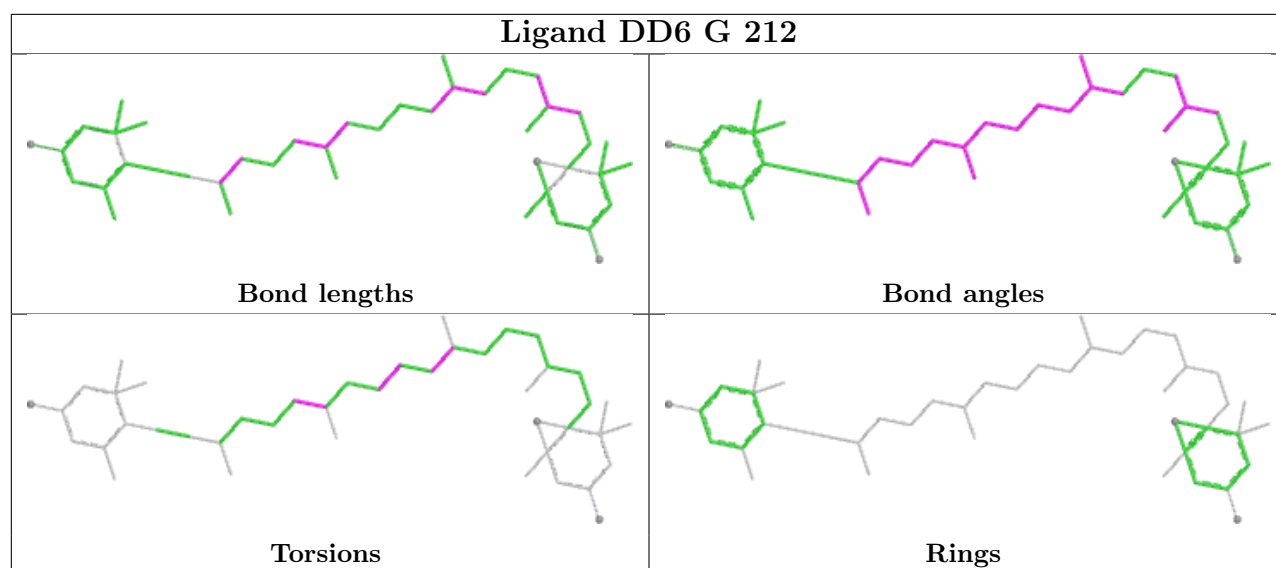
Ligand CLA A 826

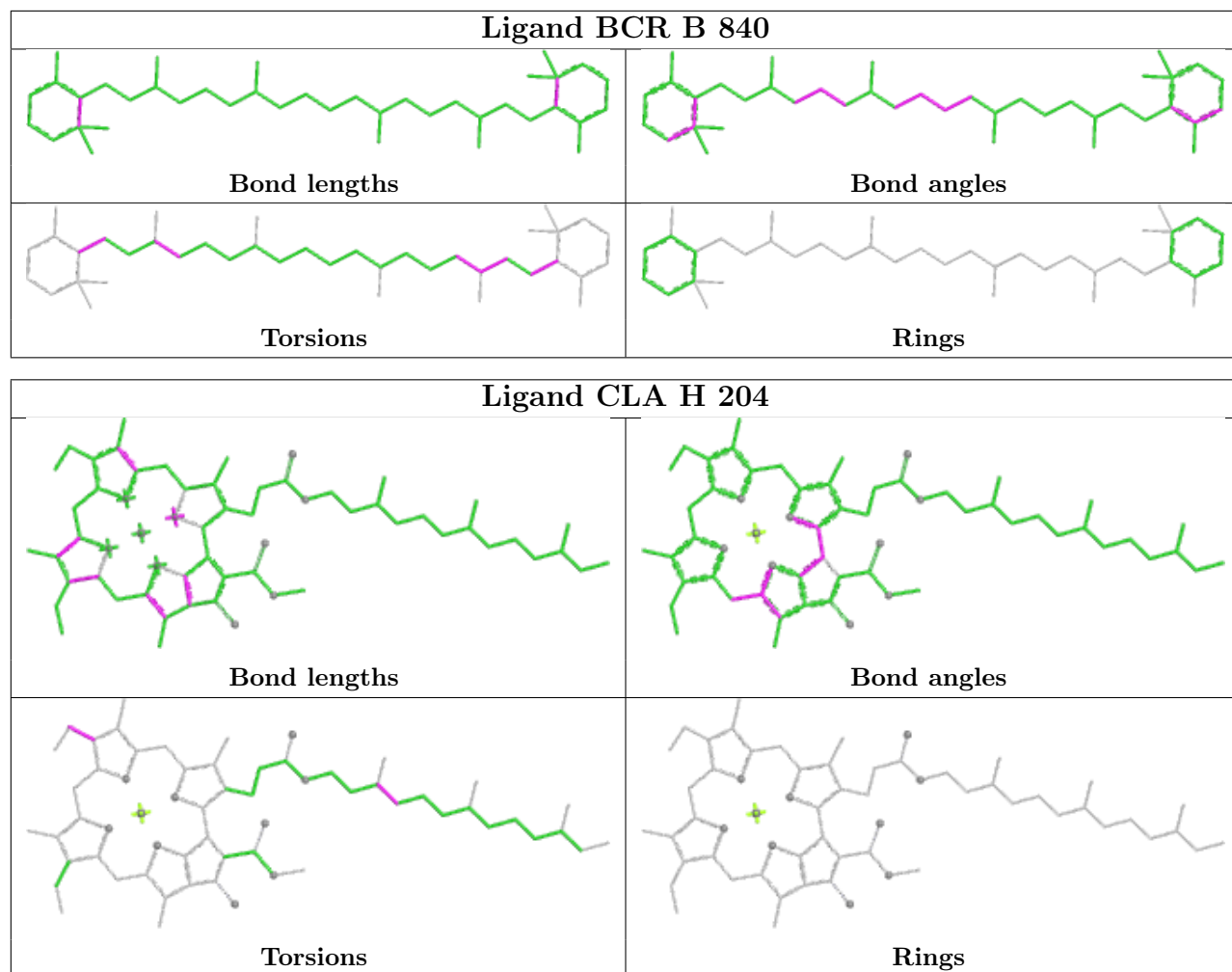


Ligand CLA K 207

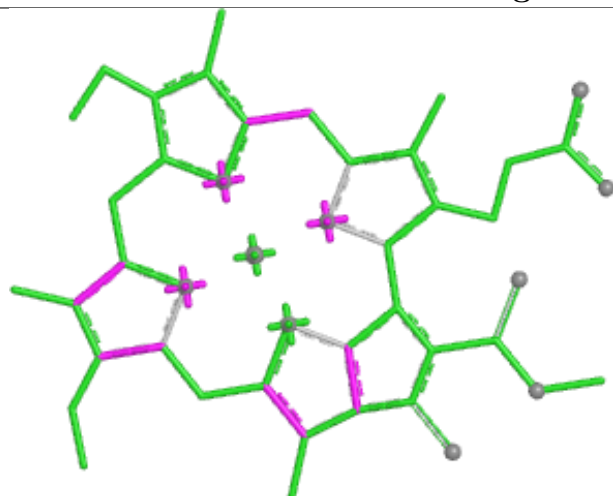




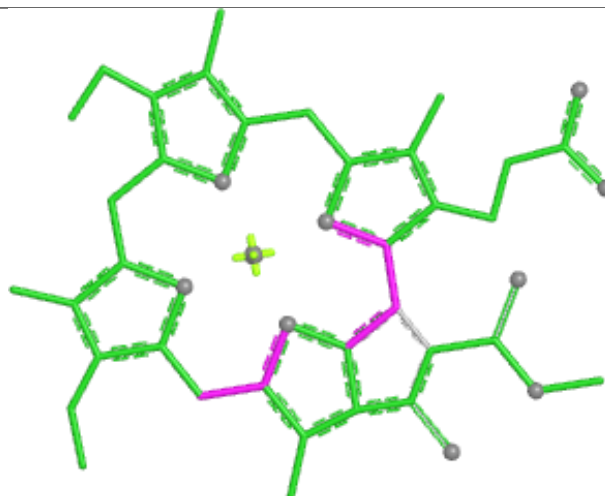




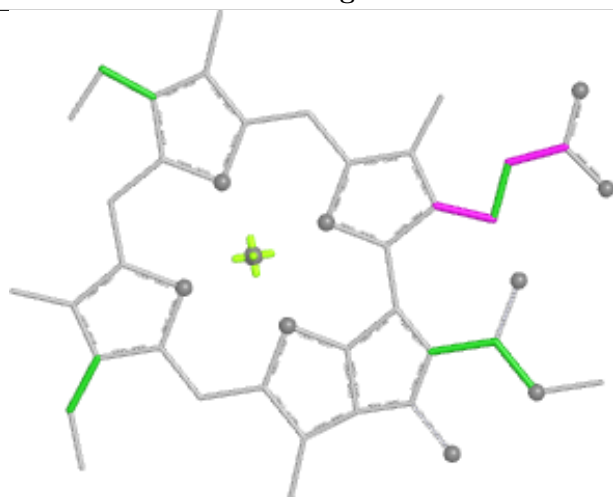
Ligand CLA K 206



Bond lengths



Bond angles

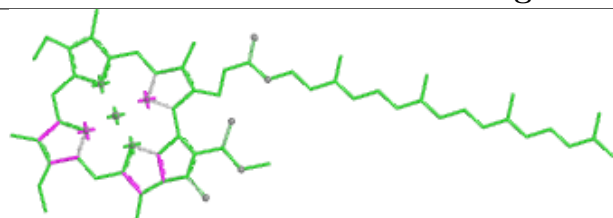


Torsions

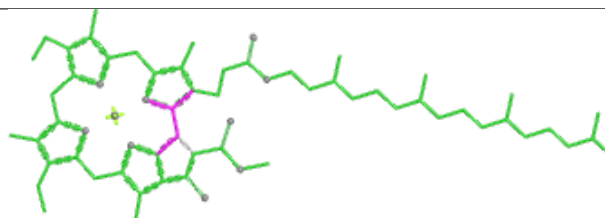


Rings

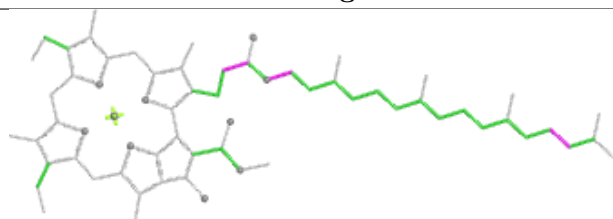
Ligand CLA B 801



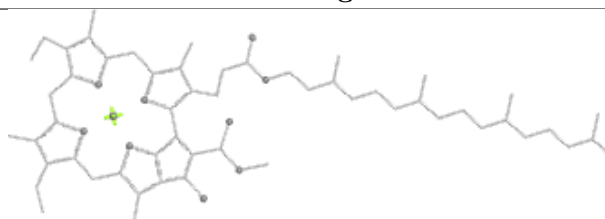
Bond lengths



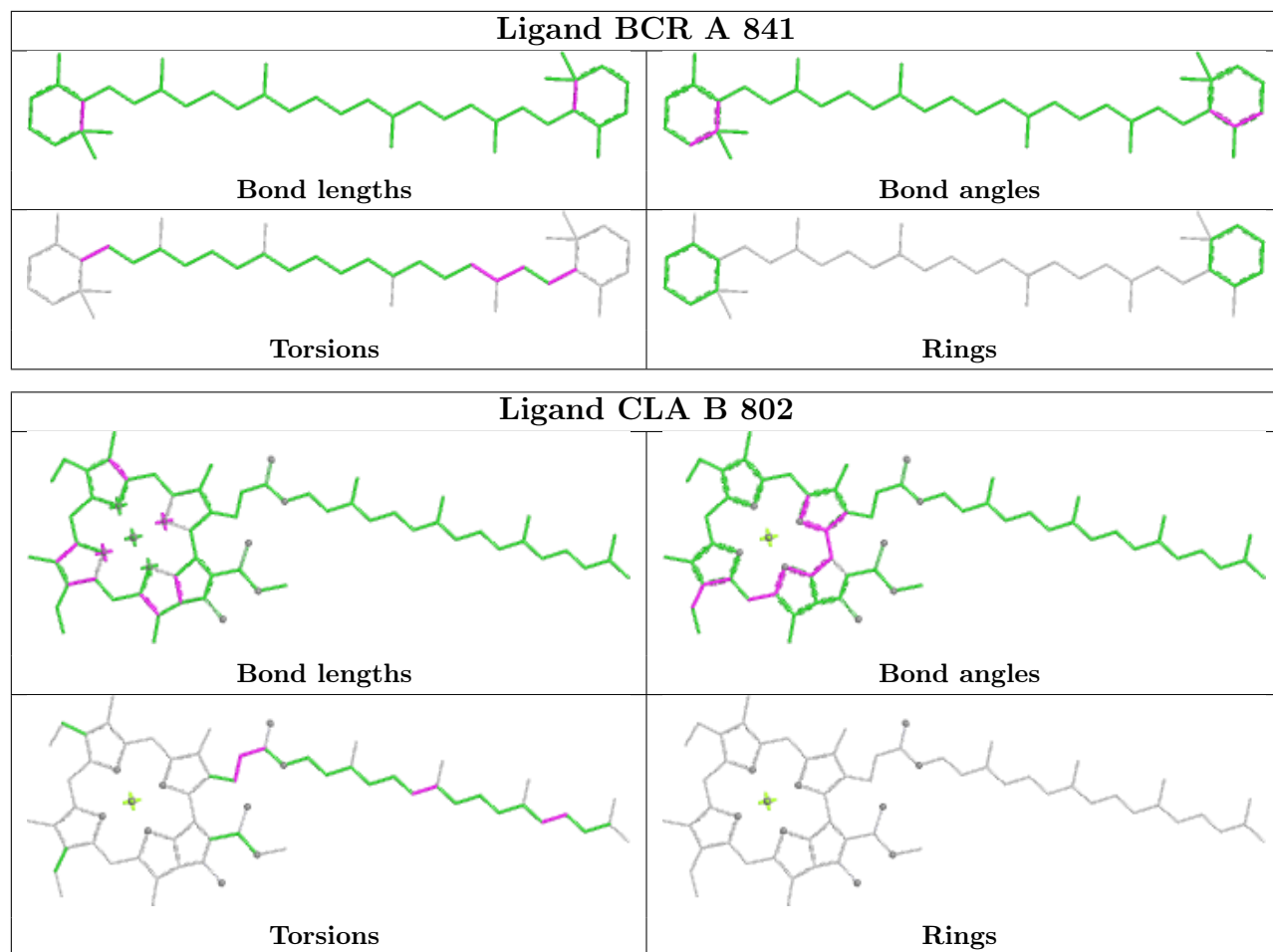
Bond angles

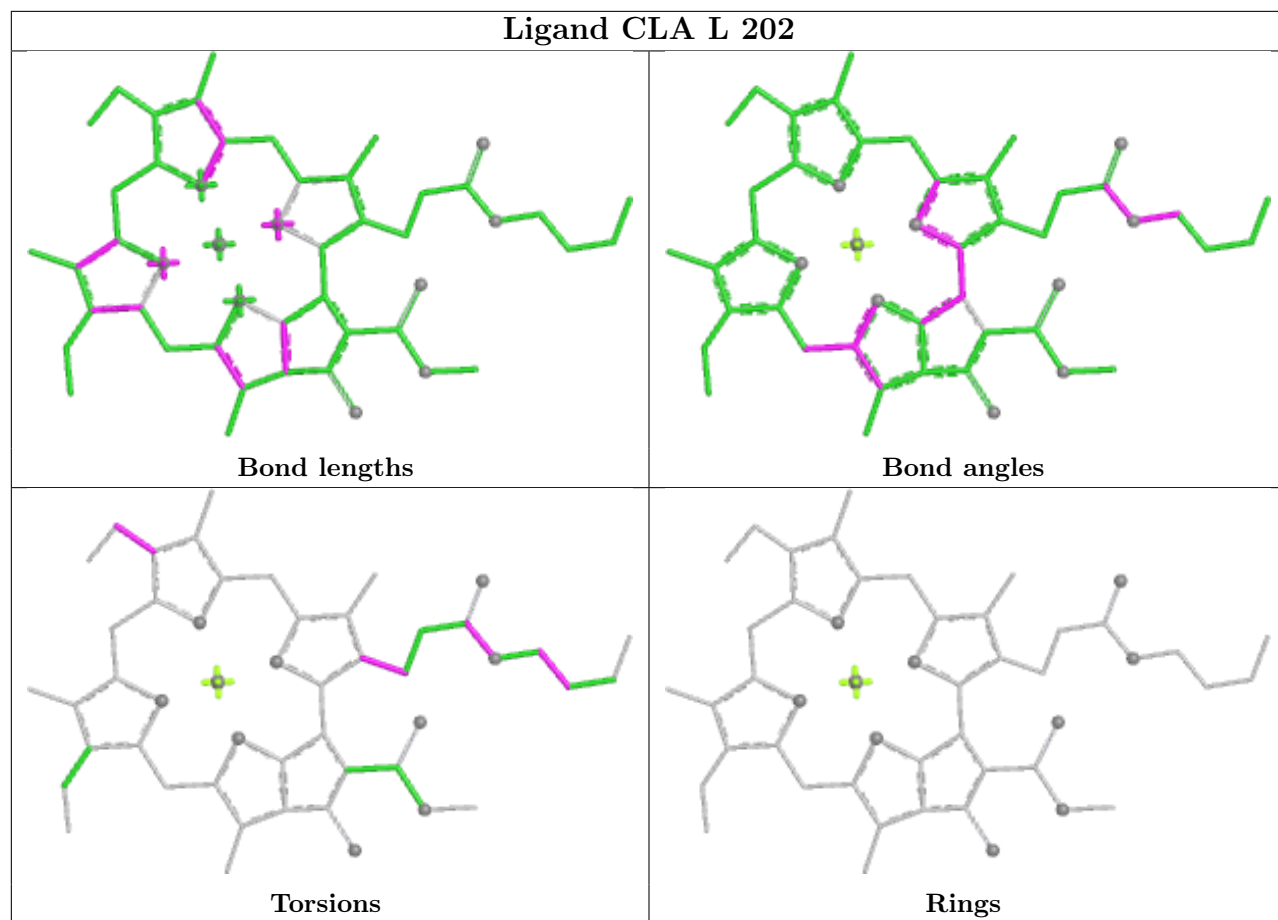


Torsions

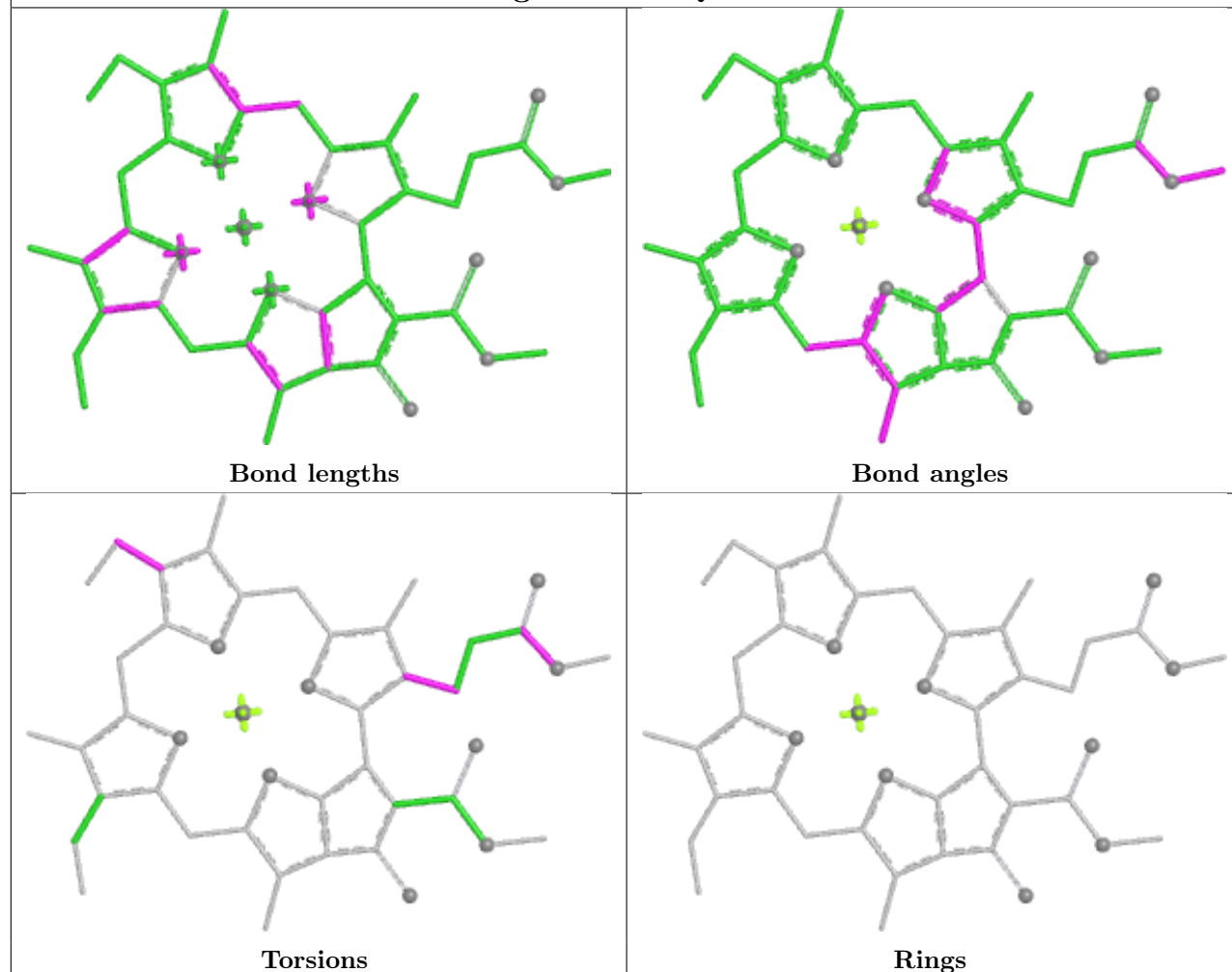


Rings

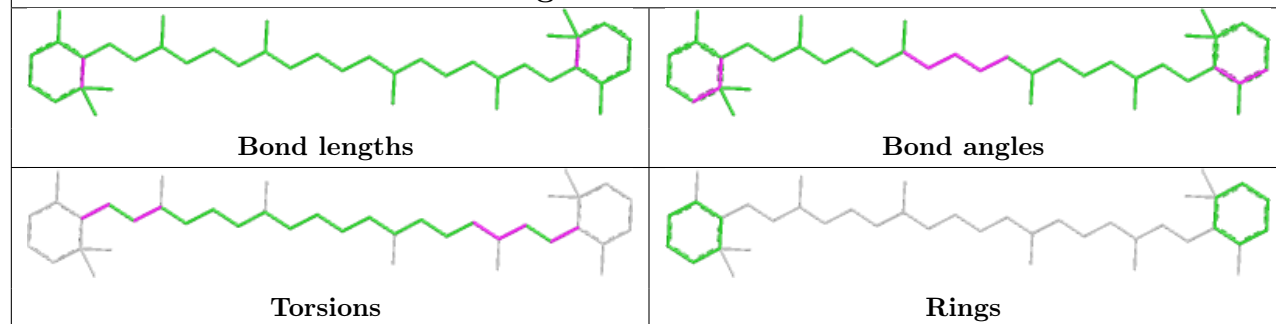




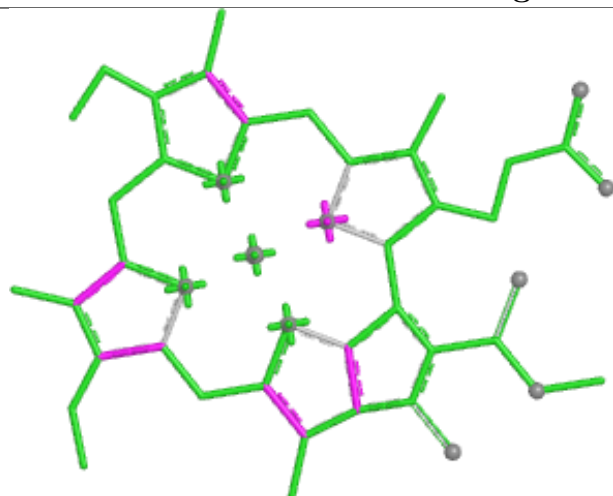
Ligand CLA Q 207



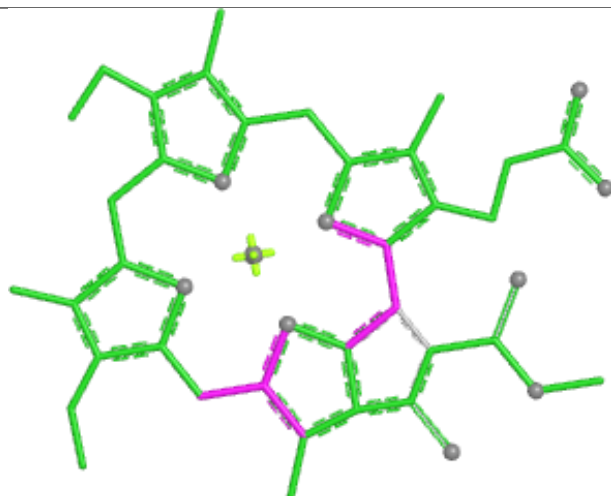
Ligand BCR I 102



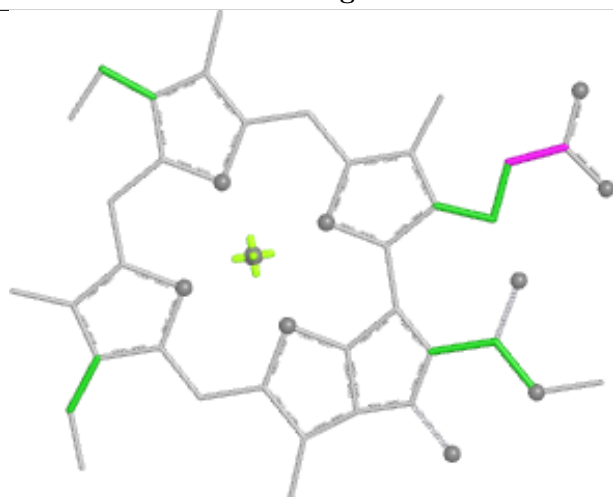
Ligand CLA G 201



Bond lengths



Bond angles

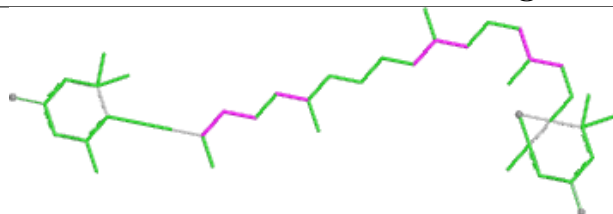


Torsions

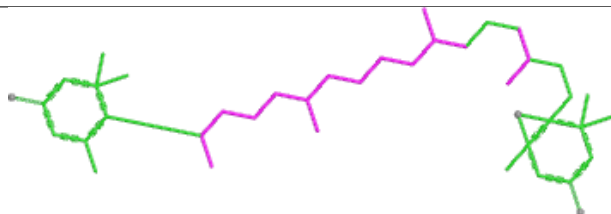


Rings

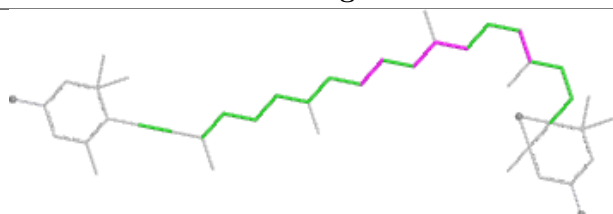
Ligand DD6 S 204



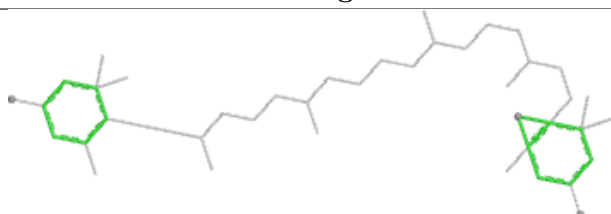
Bond lengths



Bond angles

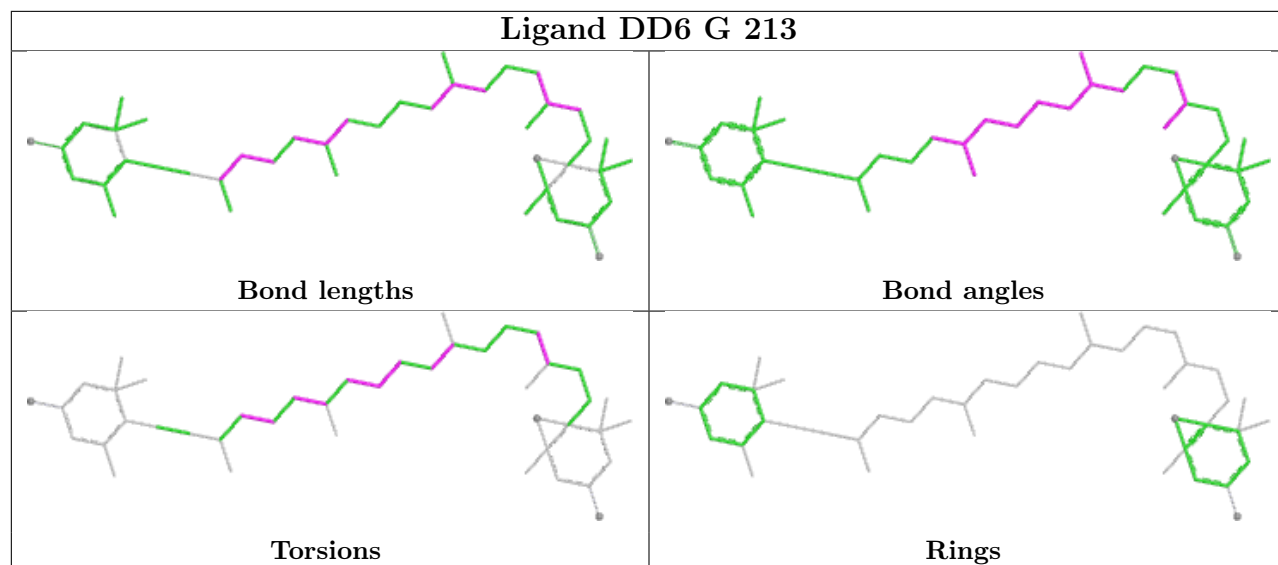


Torsions

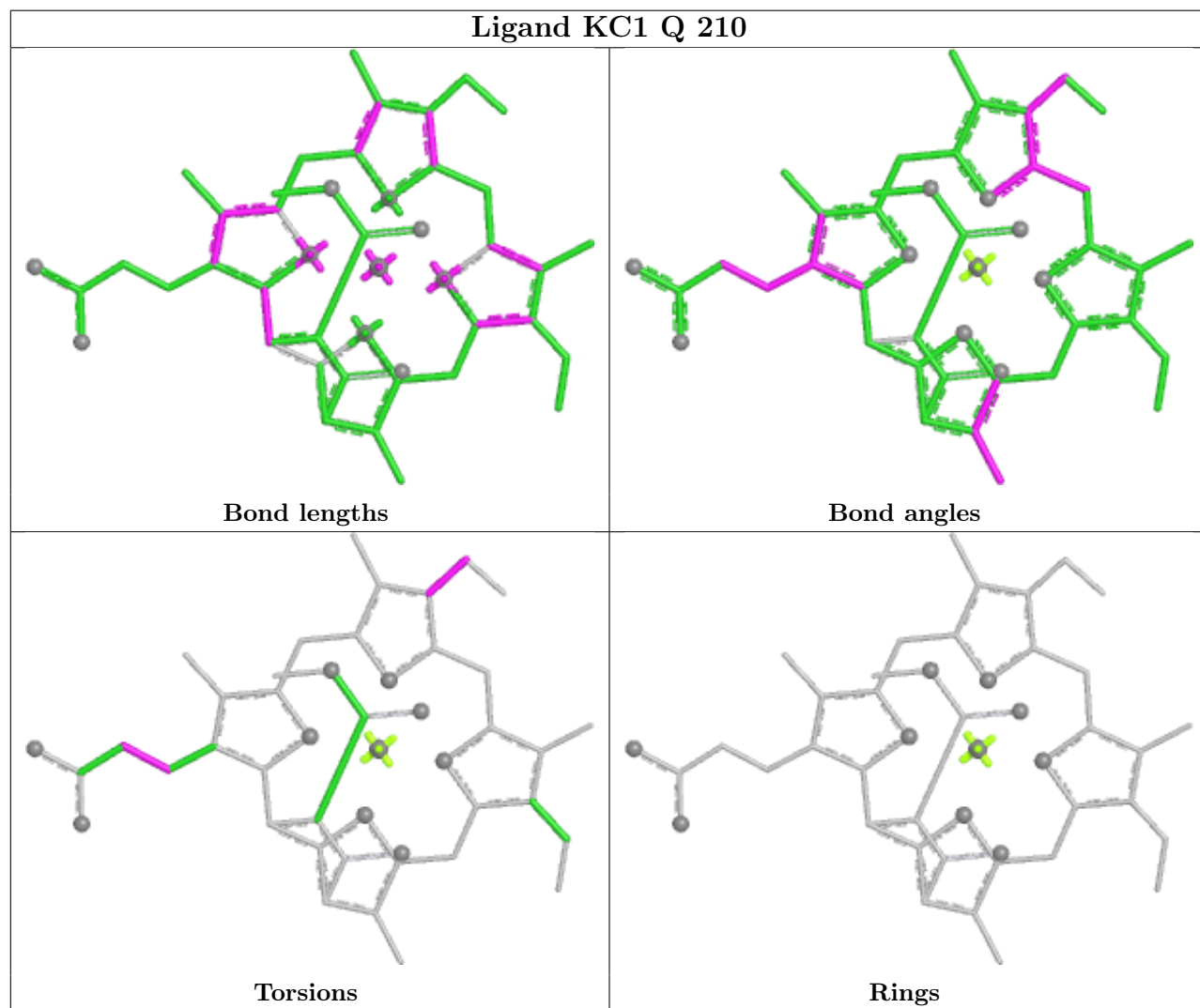


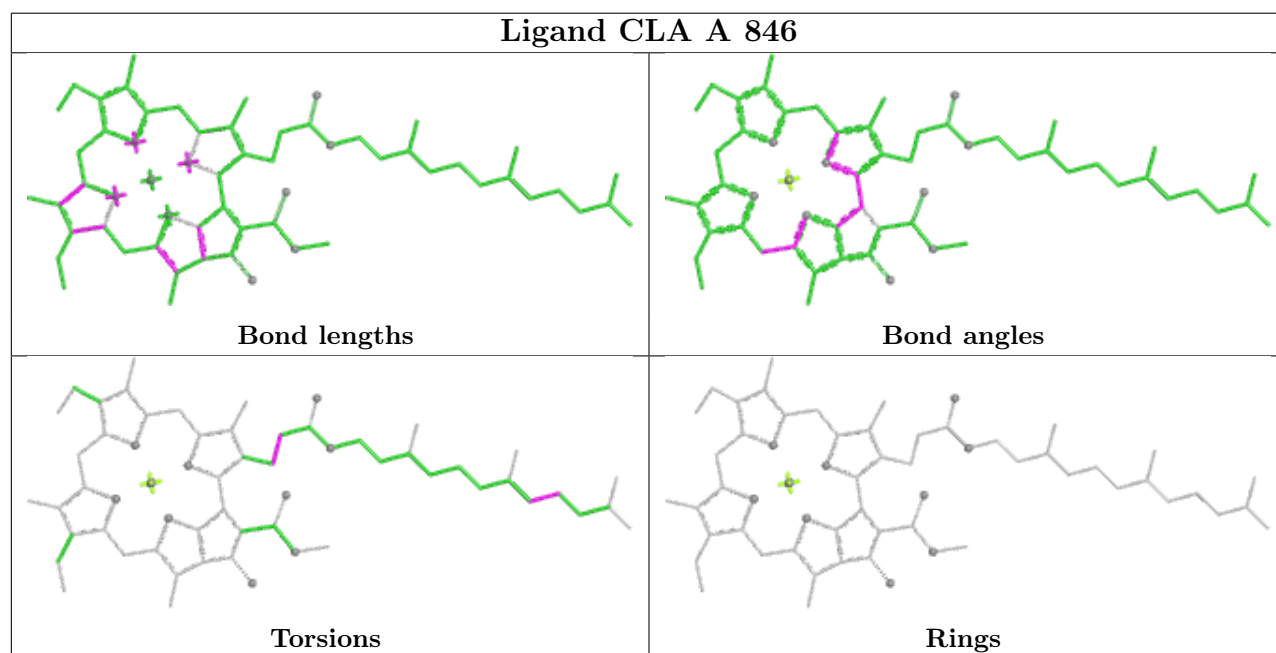
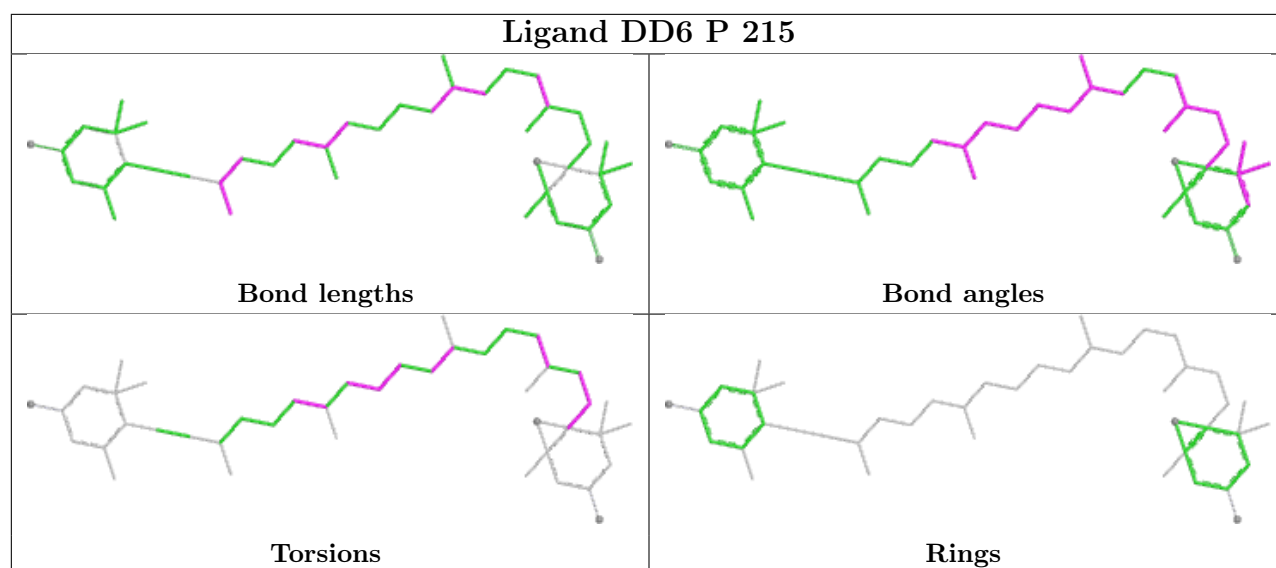
Rings

Ligand DD6 G 213

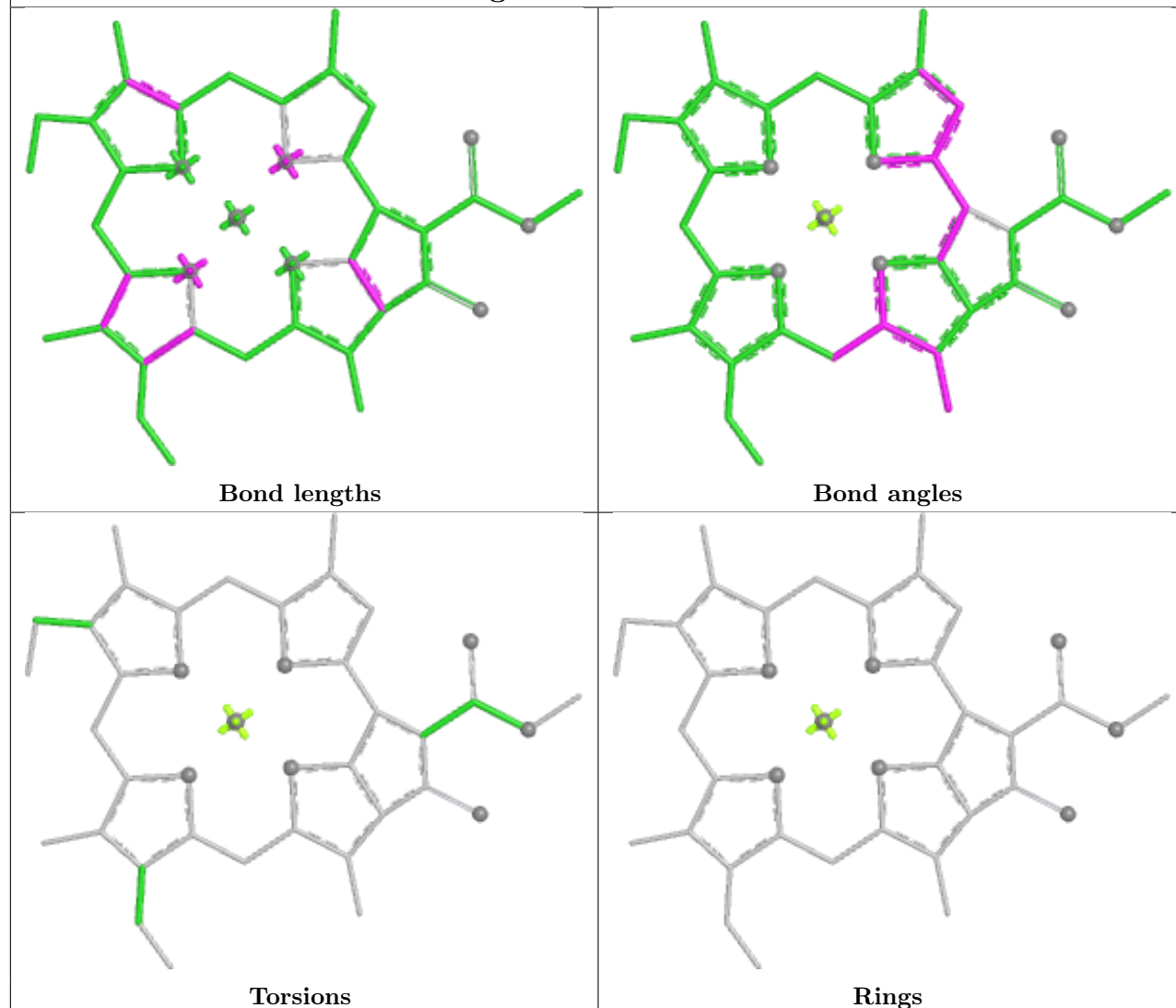


Ligand KC1 Q 210

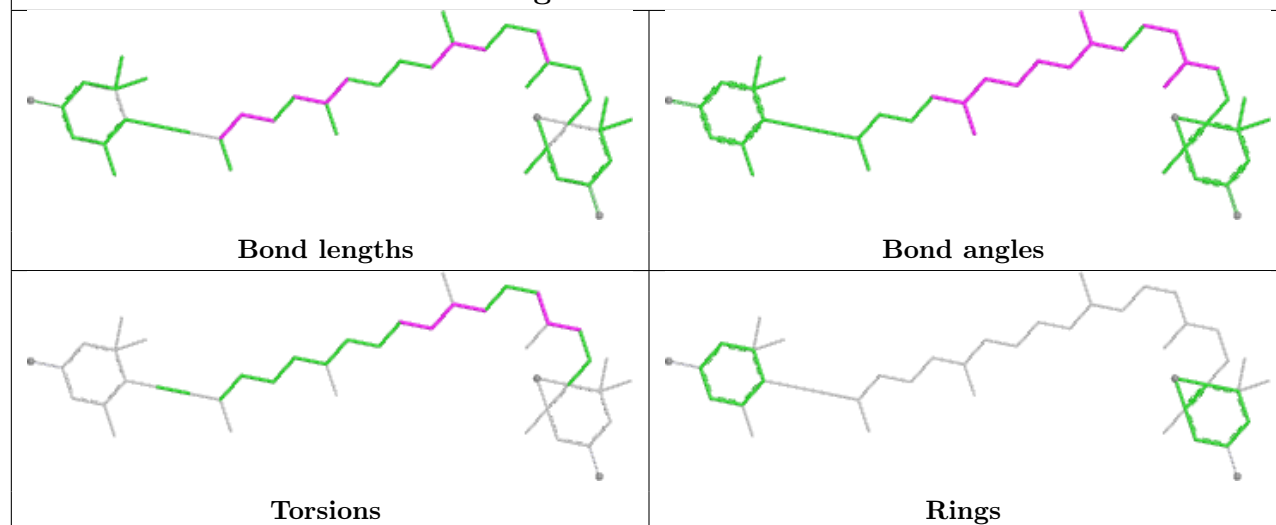




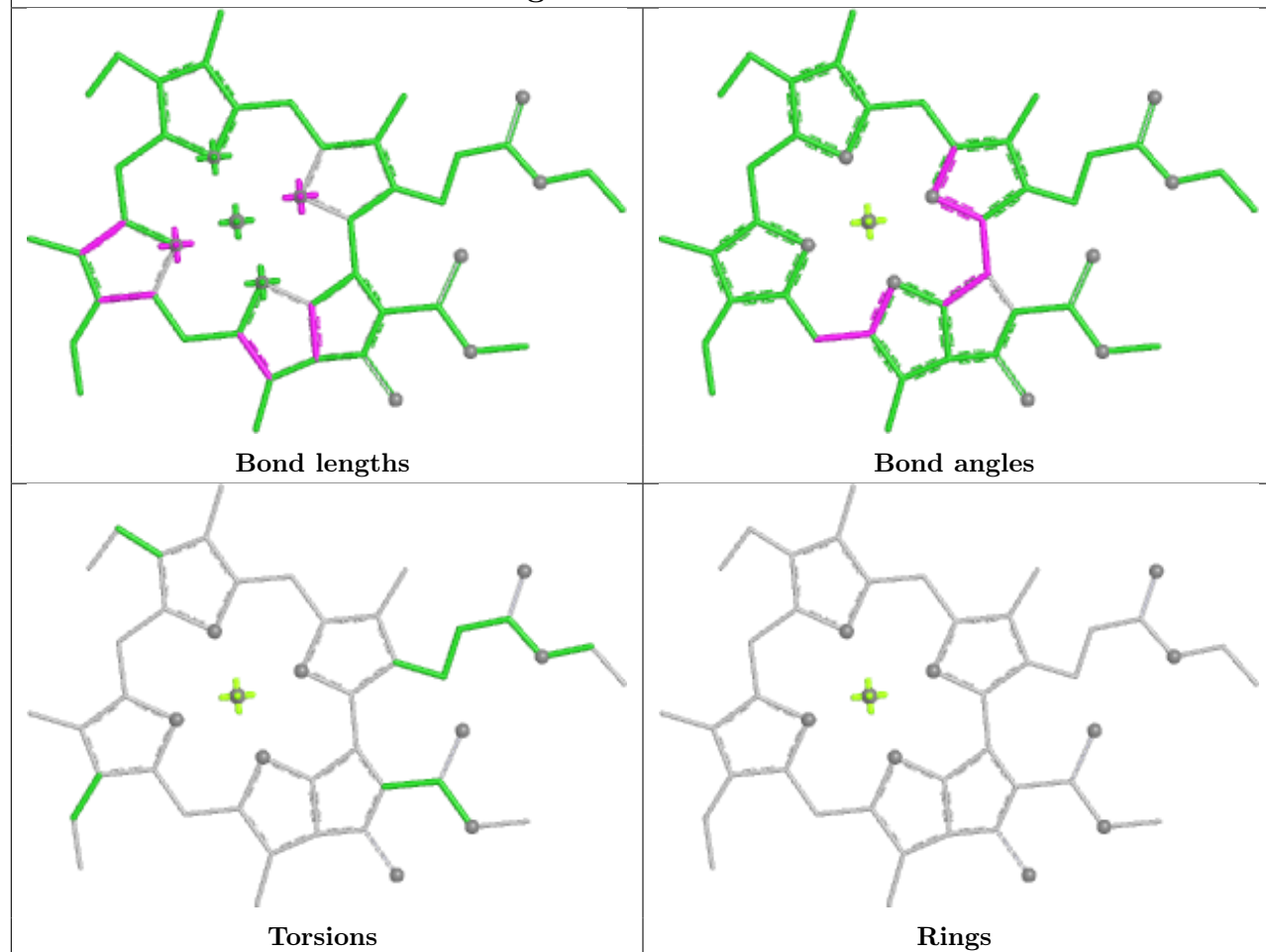
Ligand CLA H 202



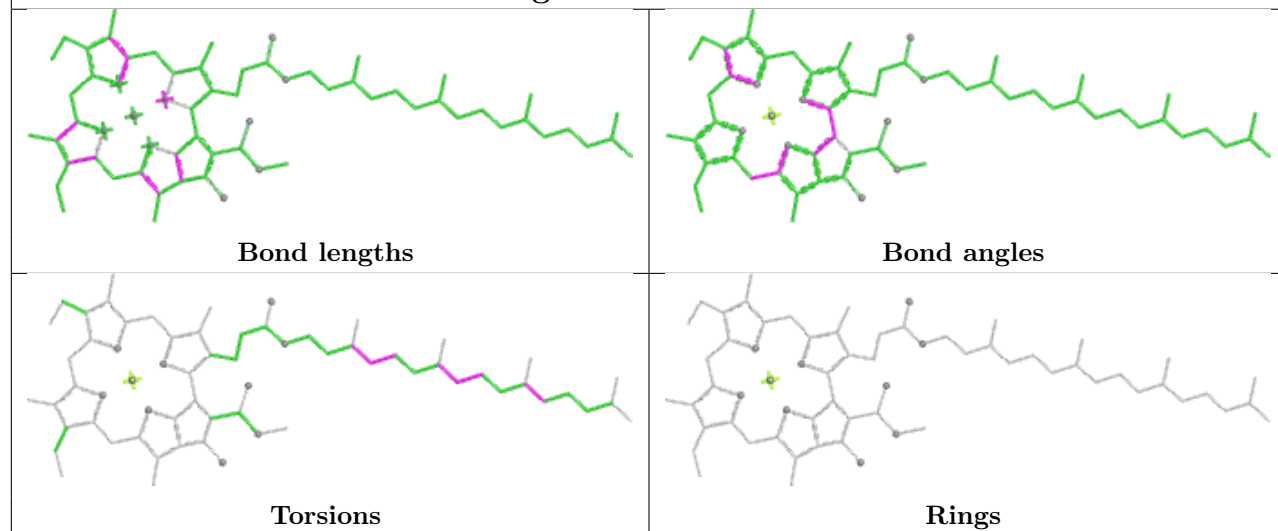
Ligand DD6 T 212

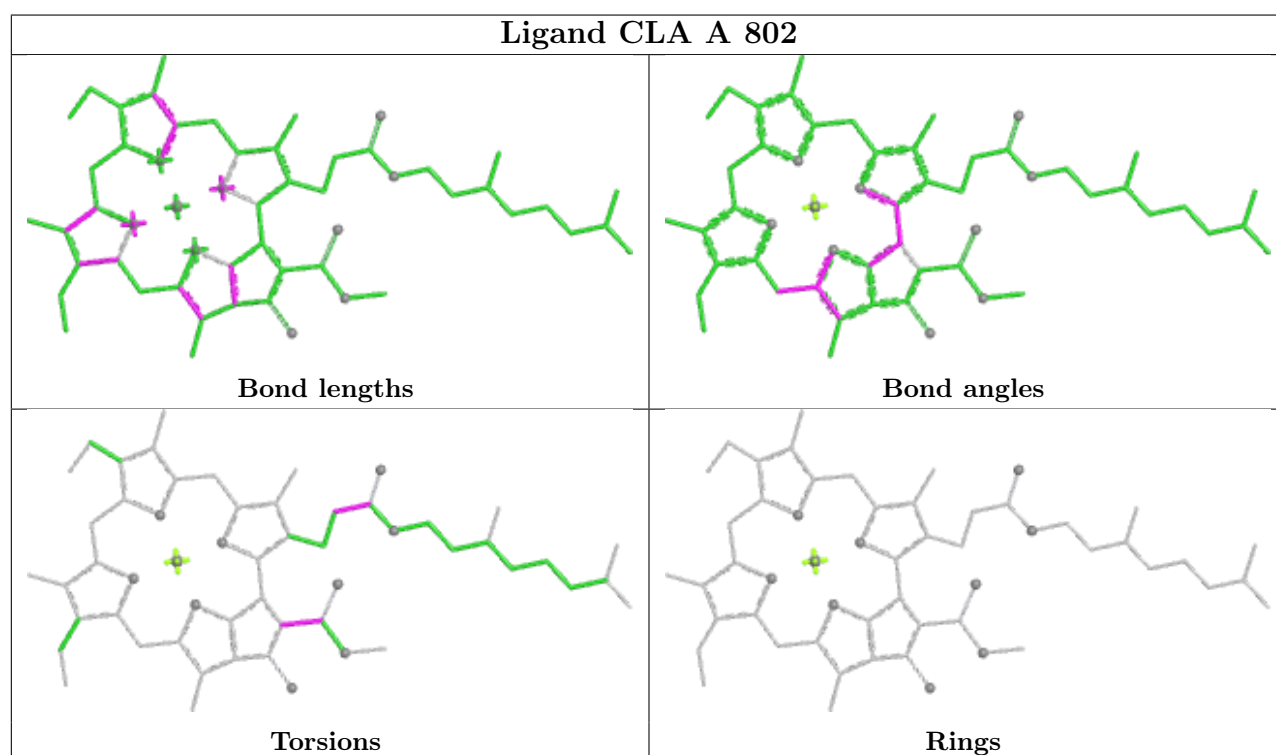
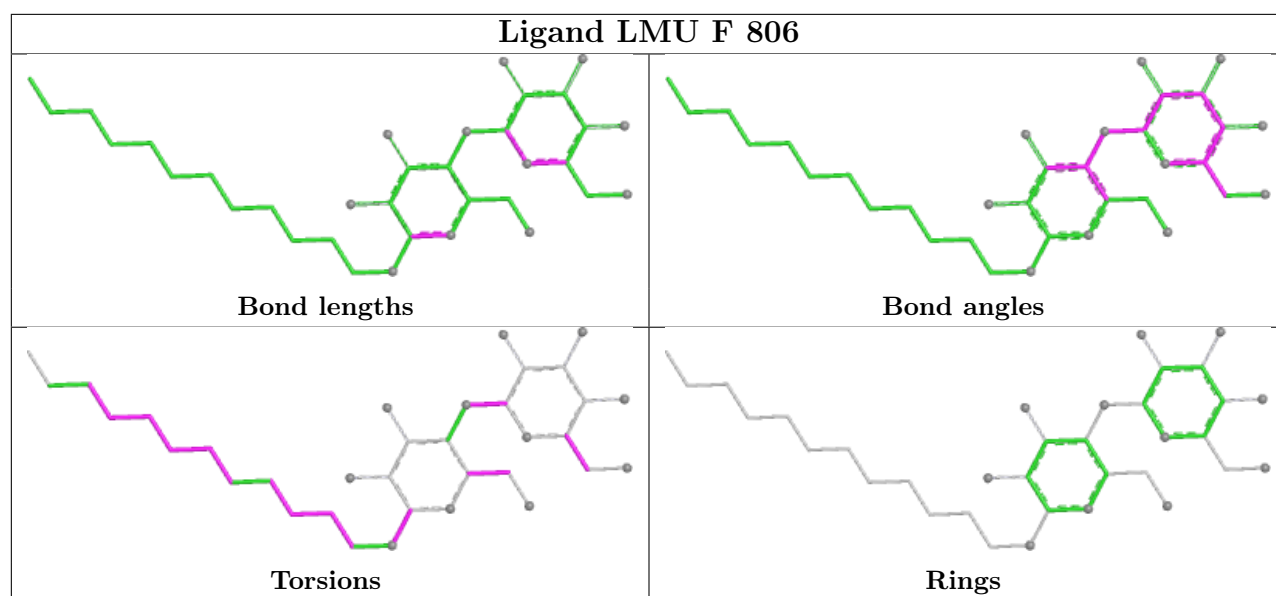


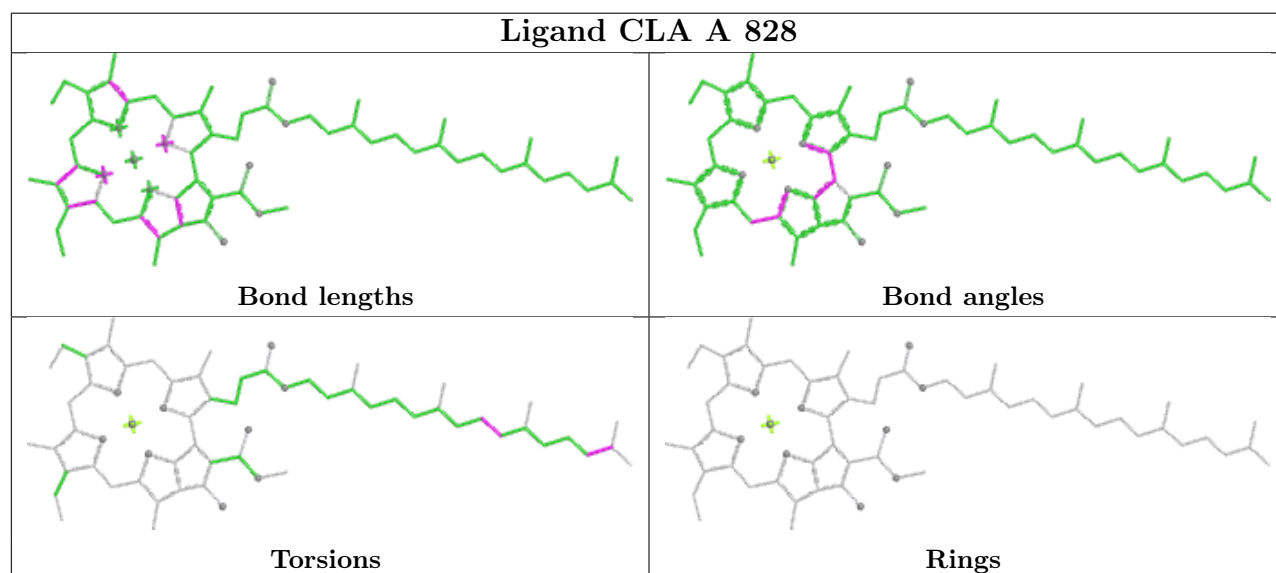
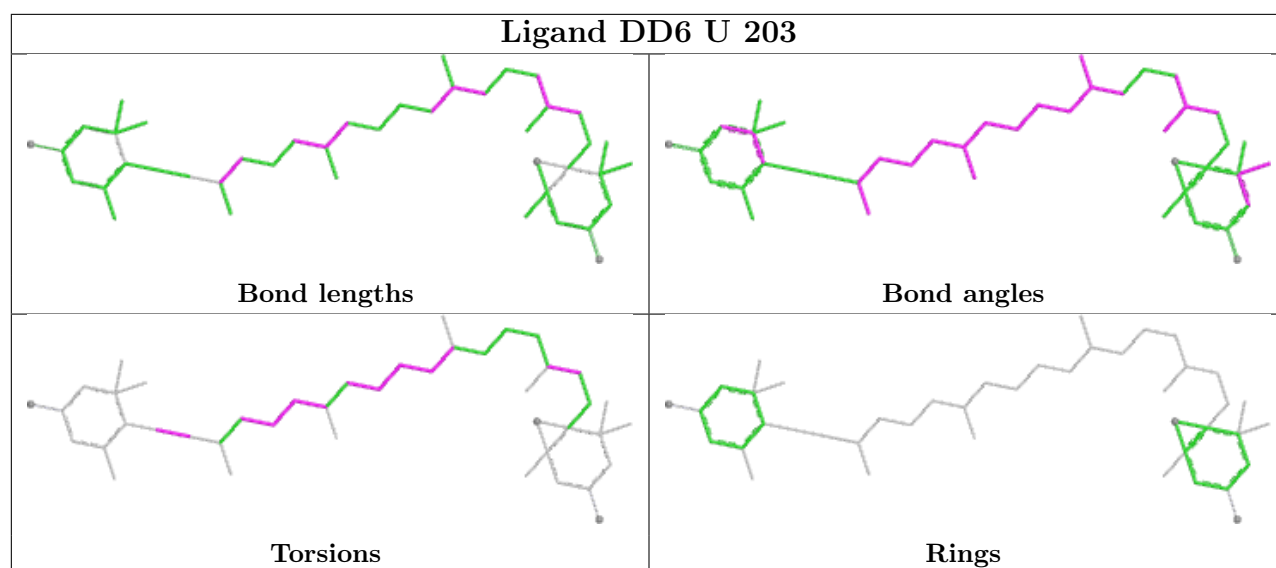
Ligand CLA B 831

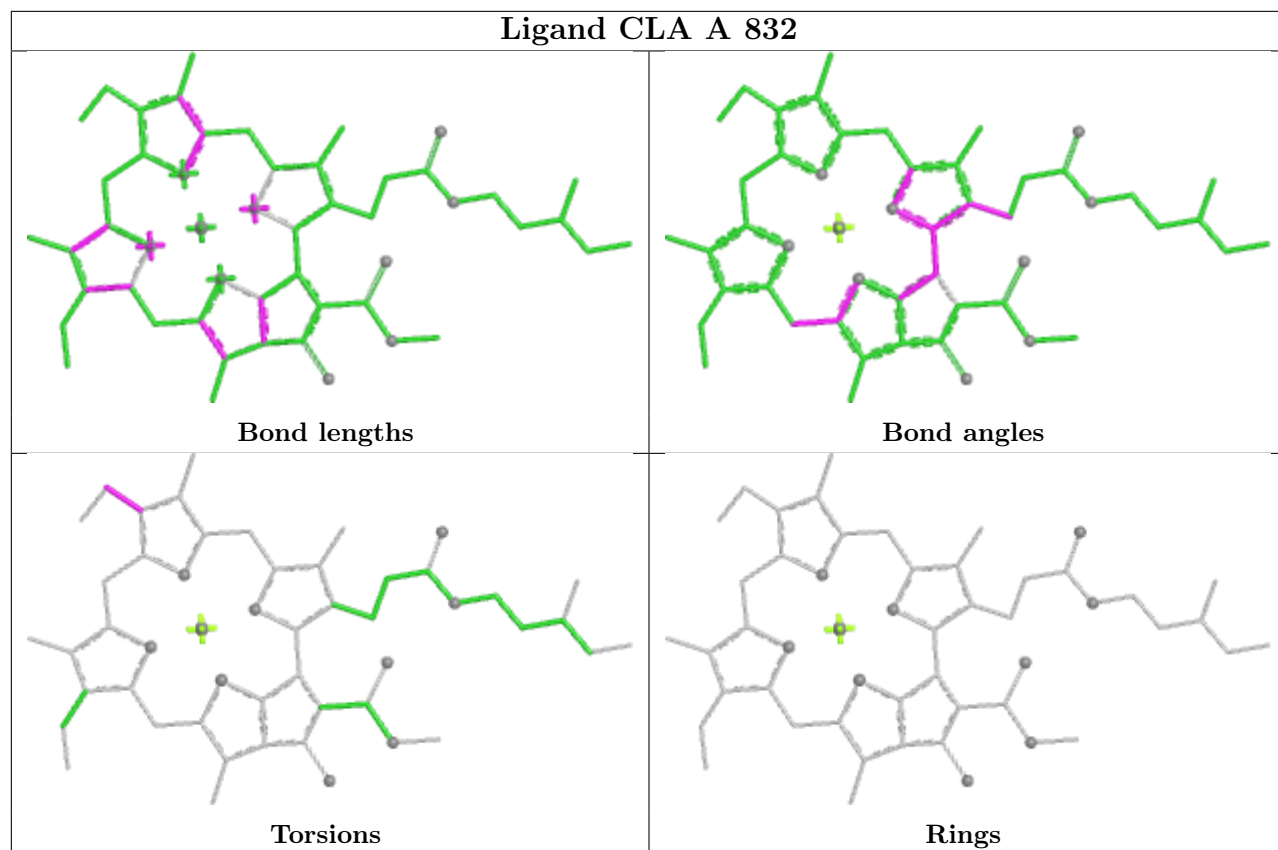


Ligand CLA B 816

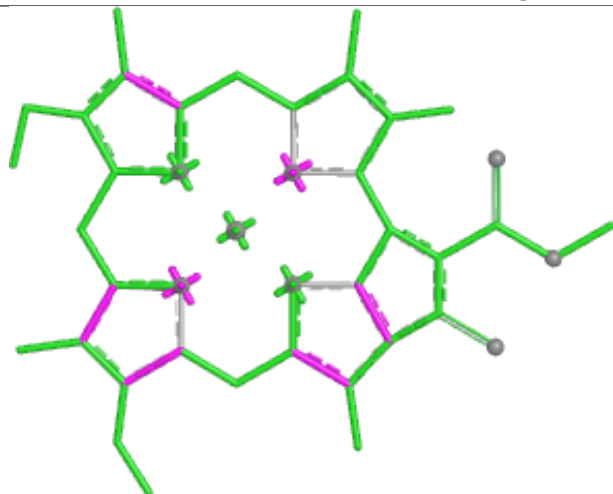




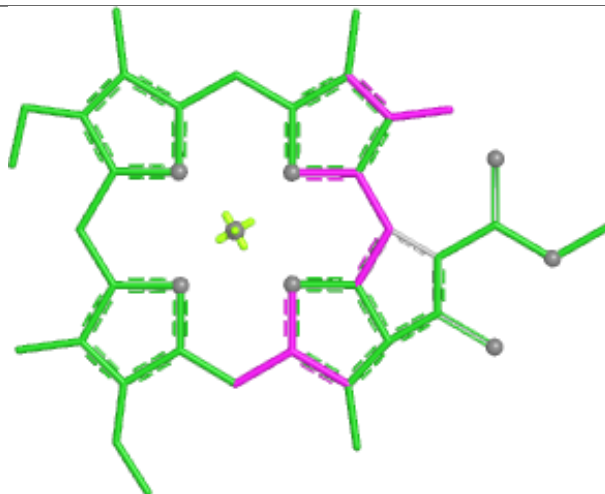




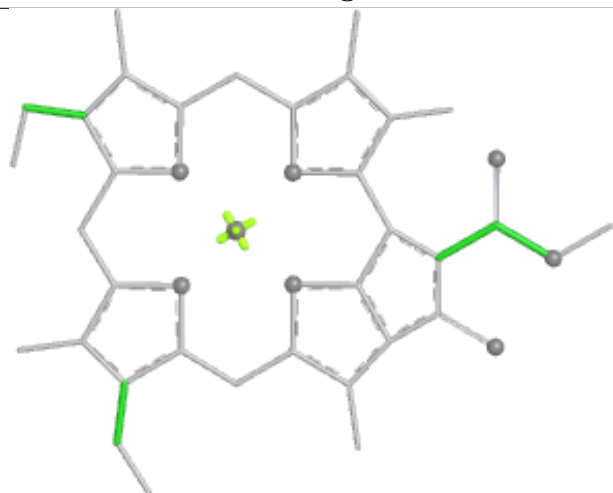
Ligand CLA T 209



Bond lengths



Bond angles

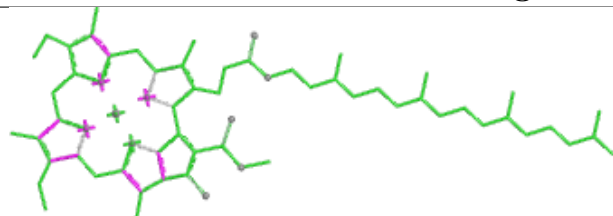


Torsions

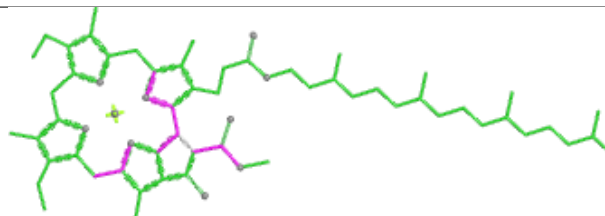


Rings

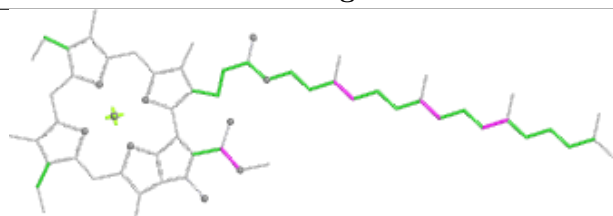
Ligand CLA R 104



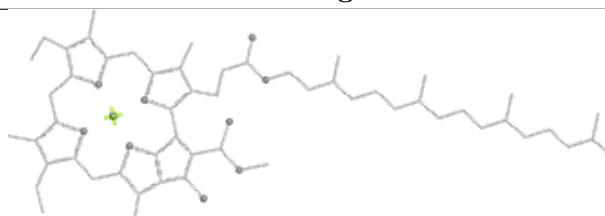
Bond lengths



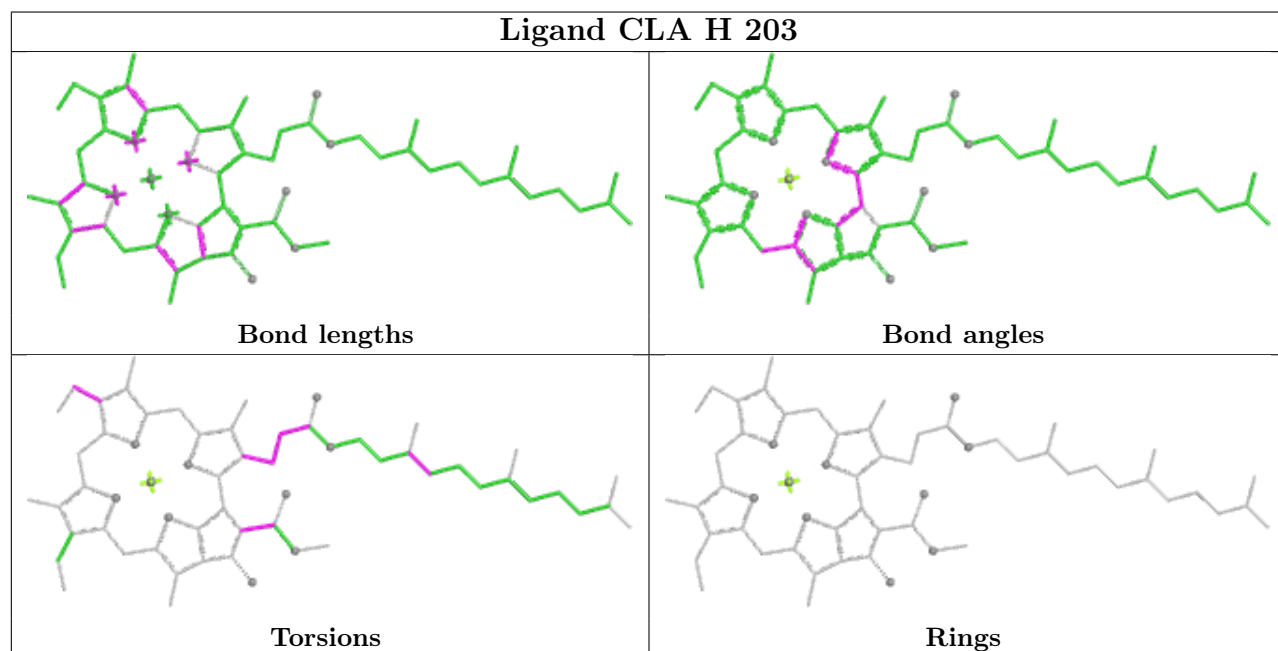
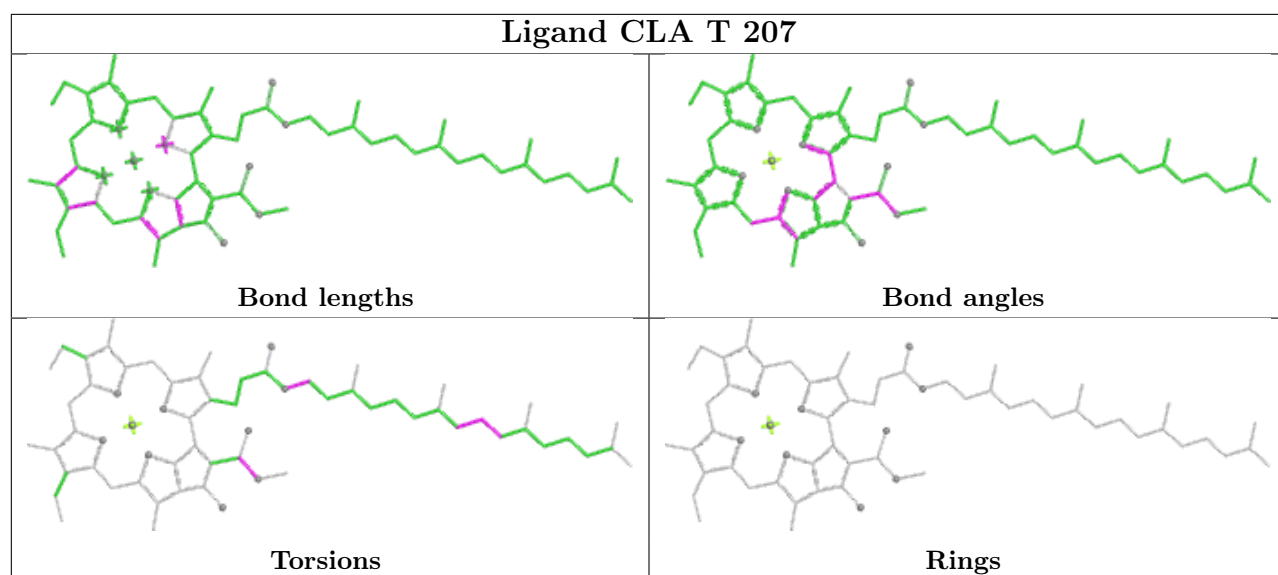
Bond angles



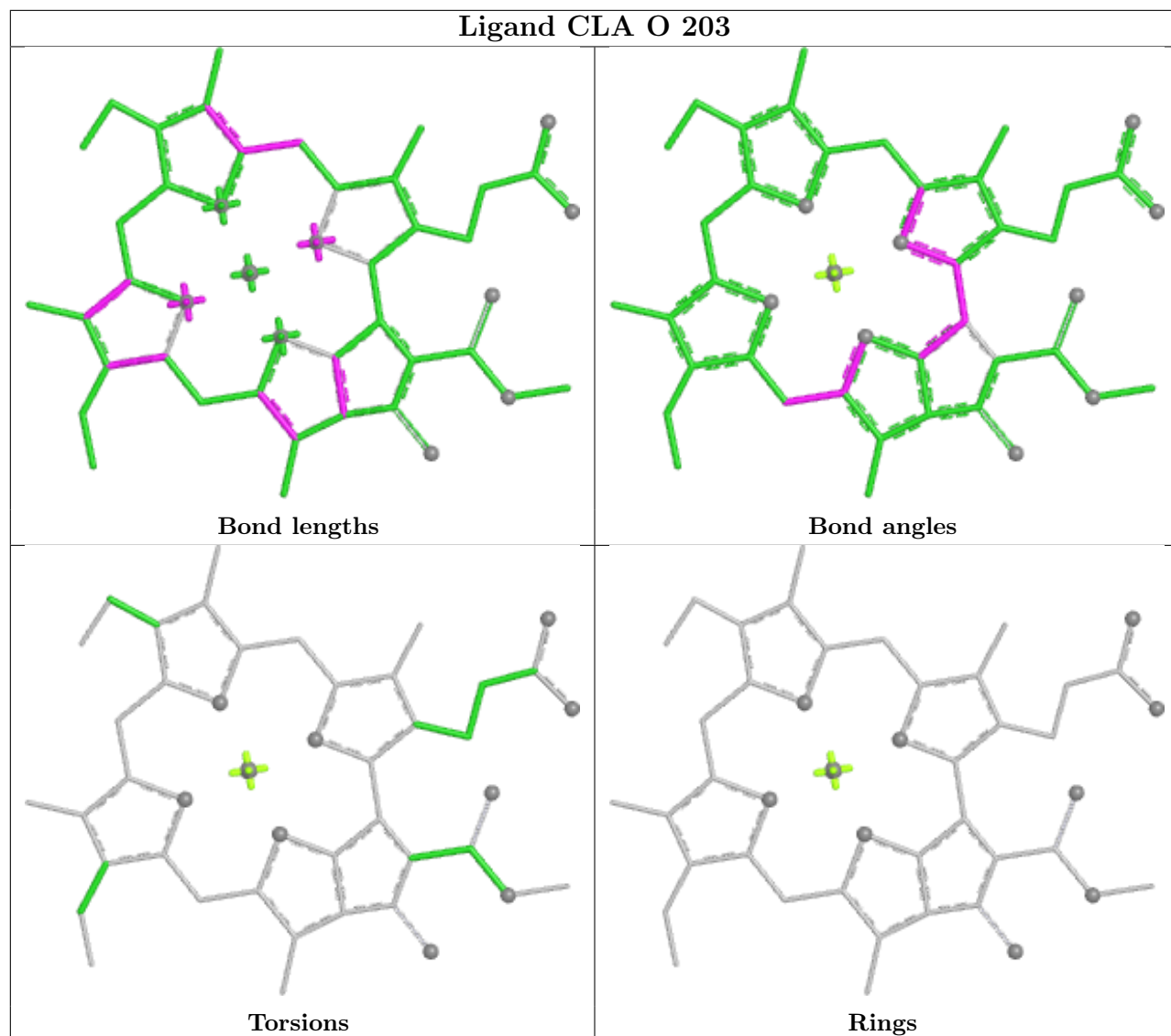
Torsions



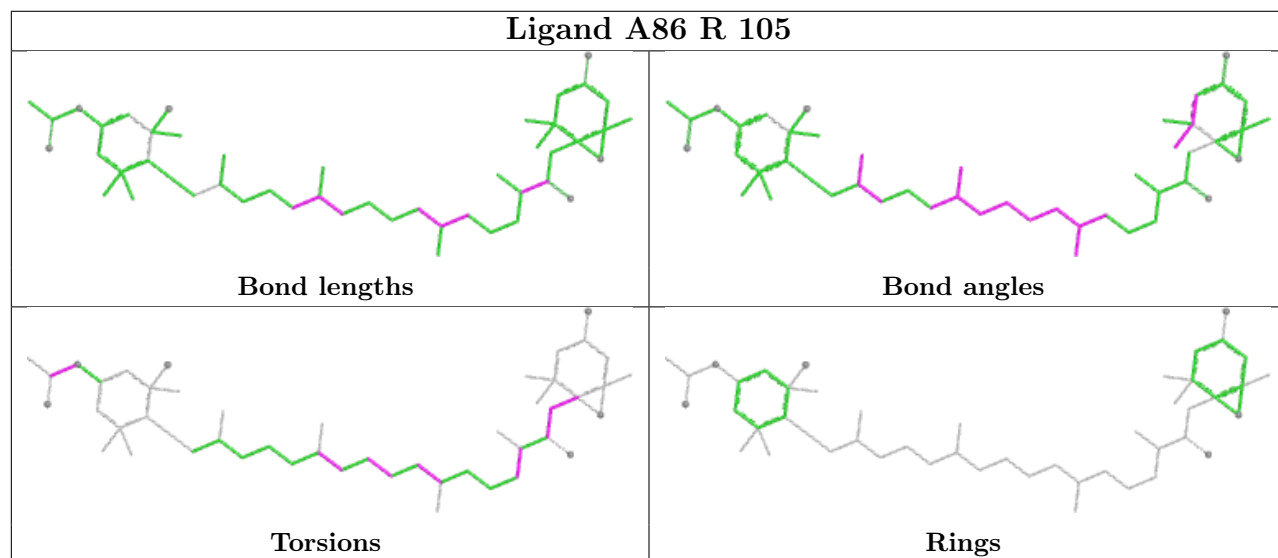
Rings



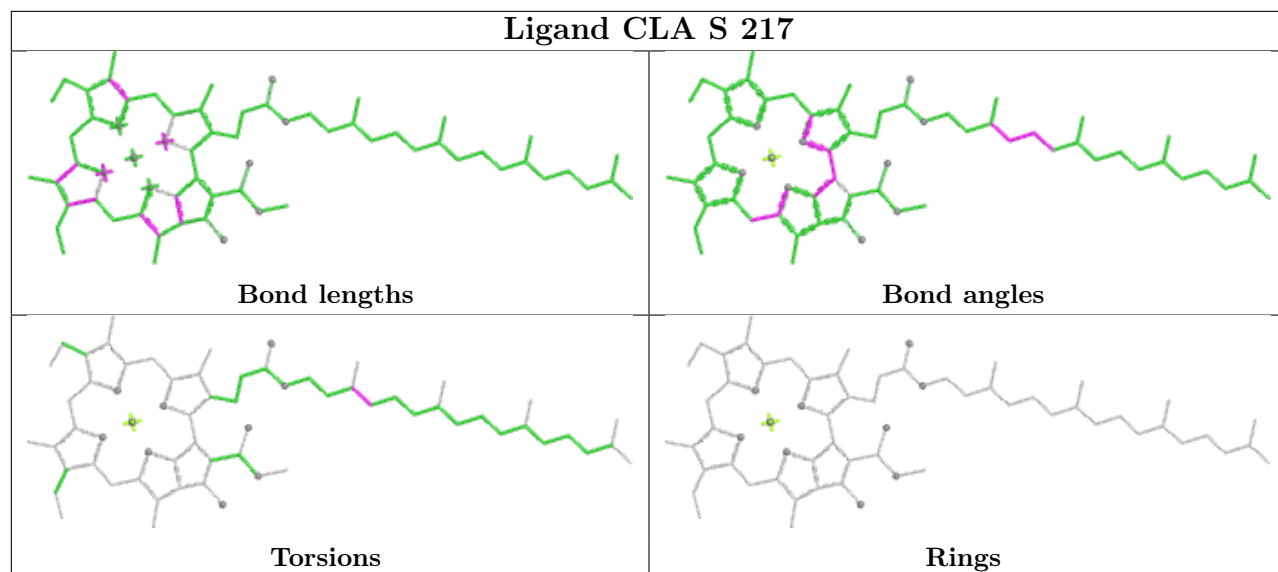
Ligand CLA O 203



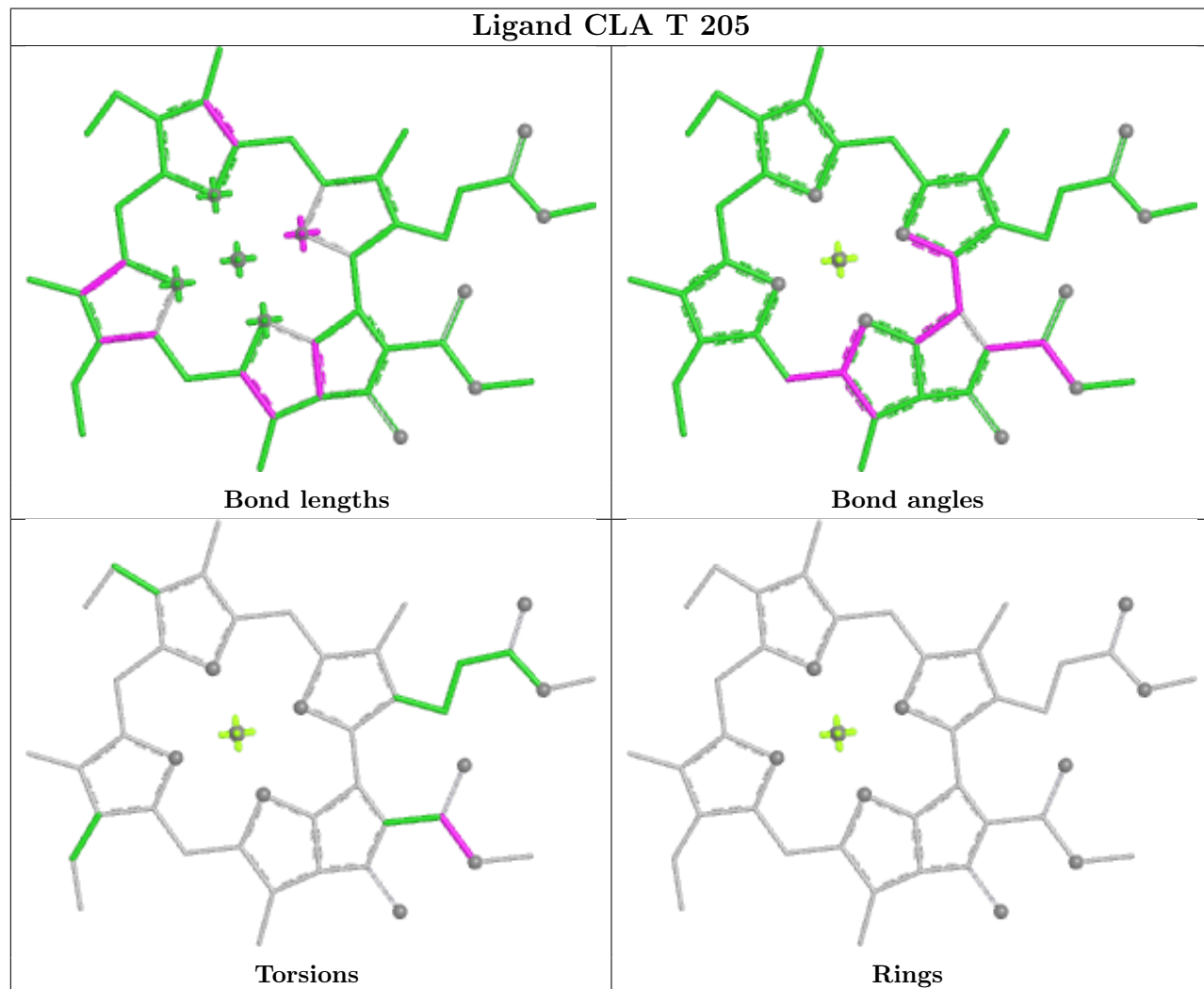
Ligand A86 R 105

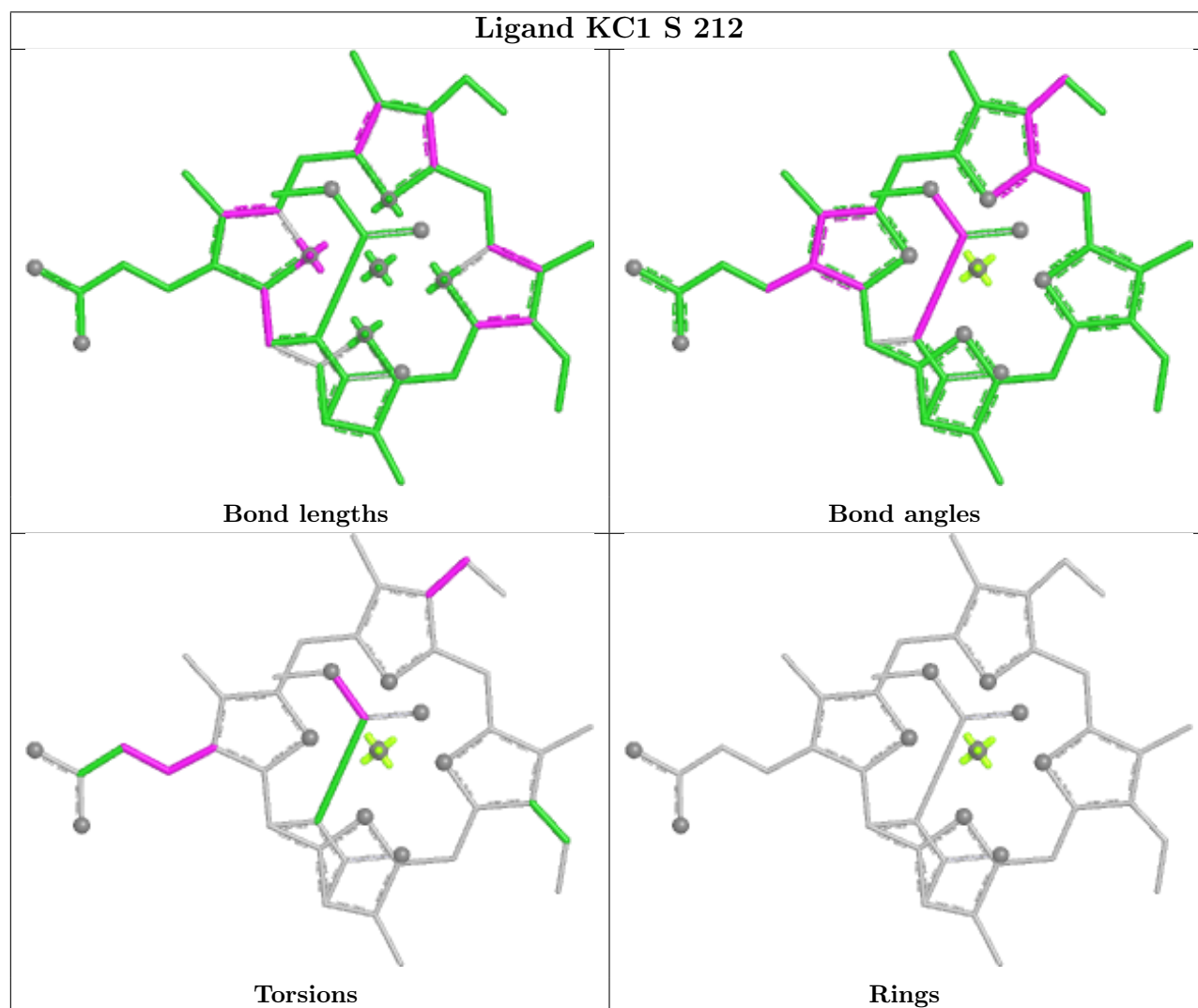
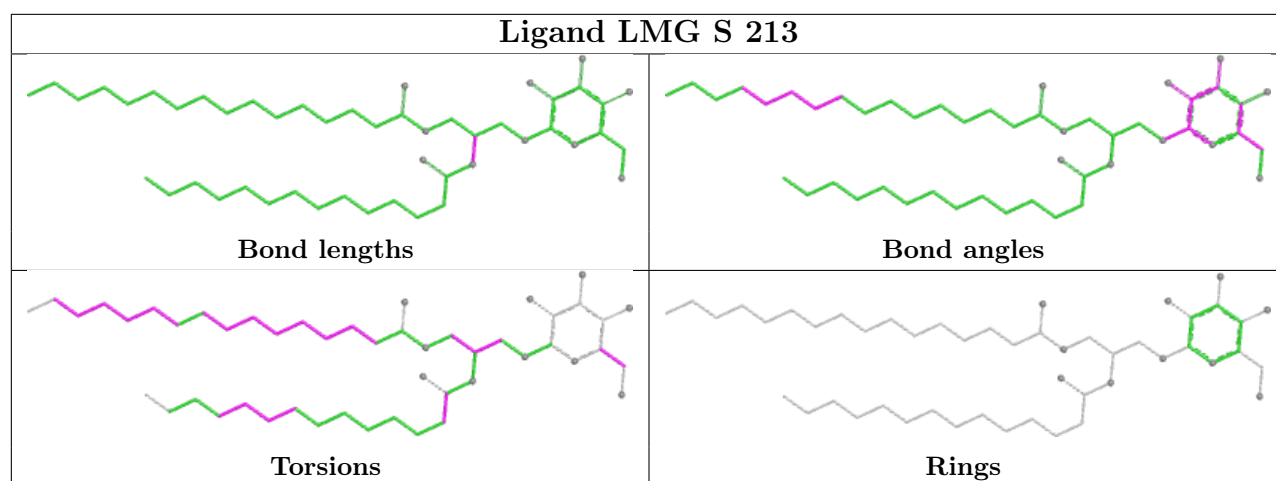


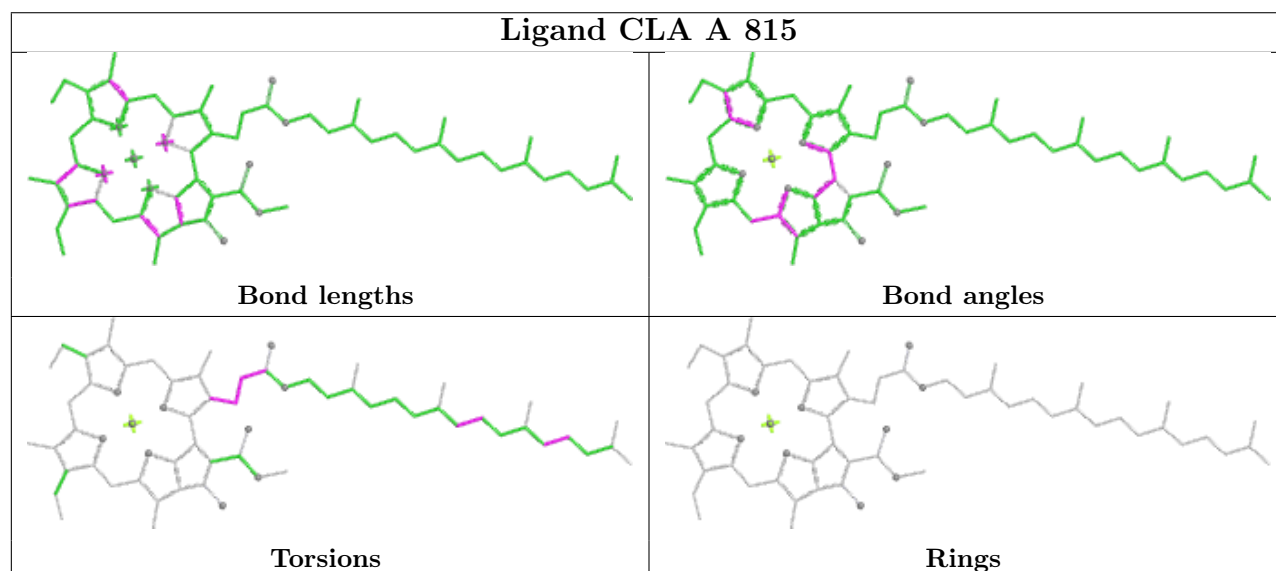
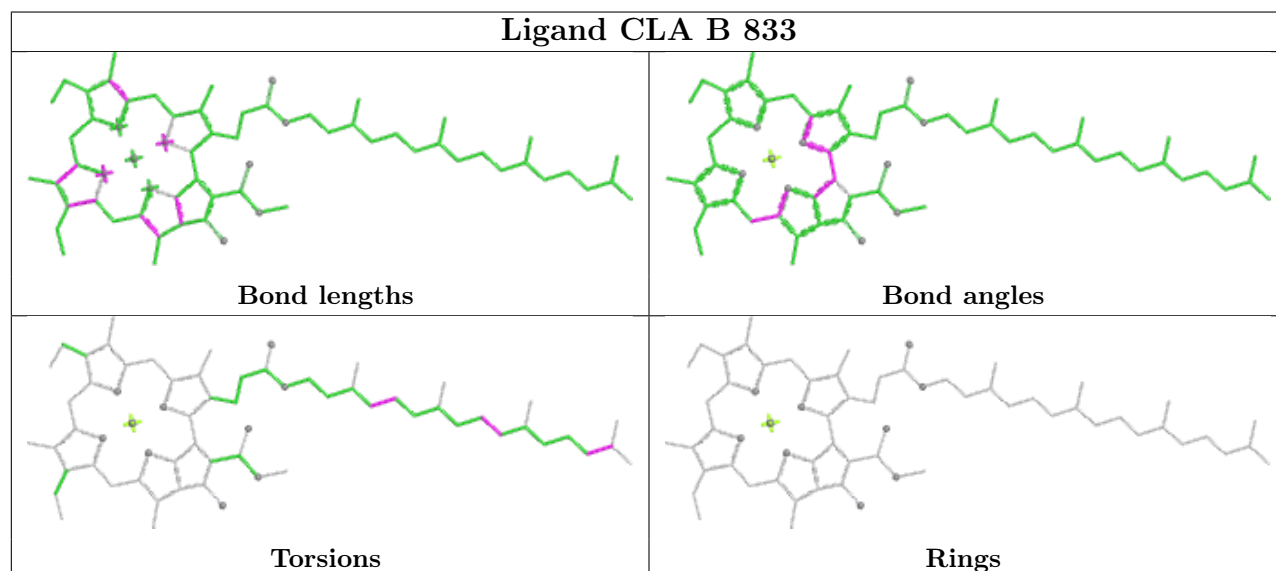
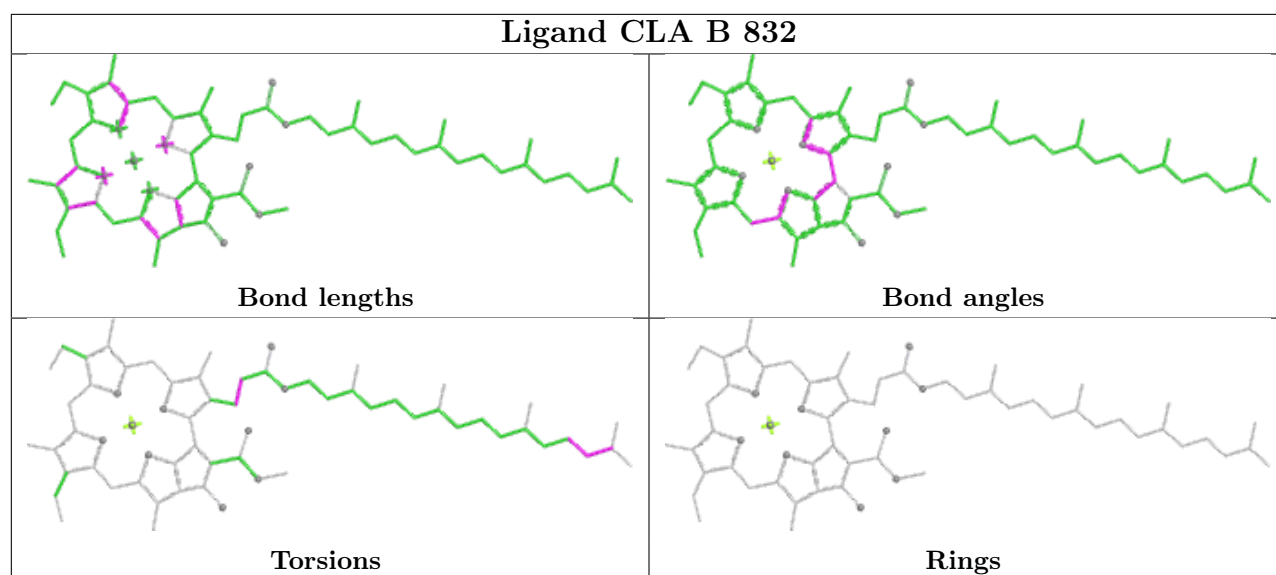
Ligand CLA S 217



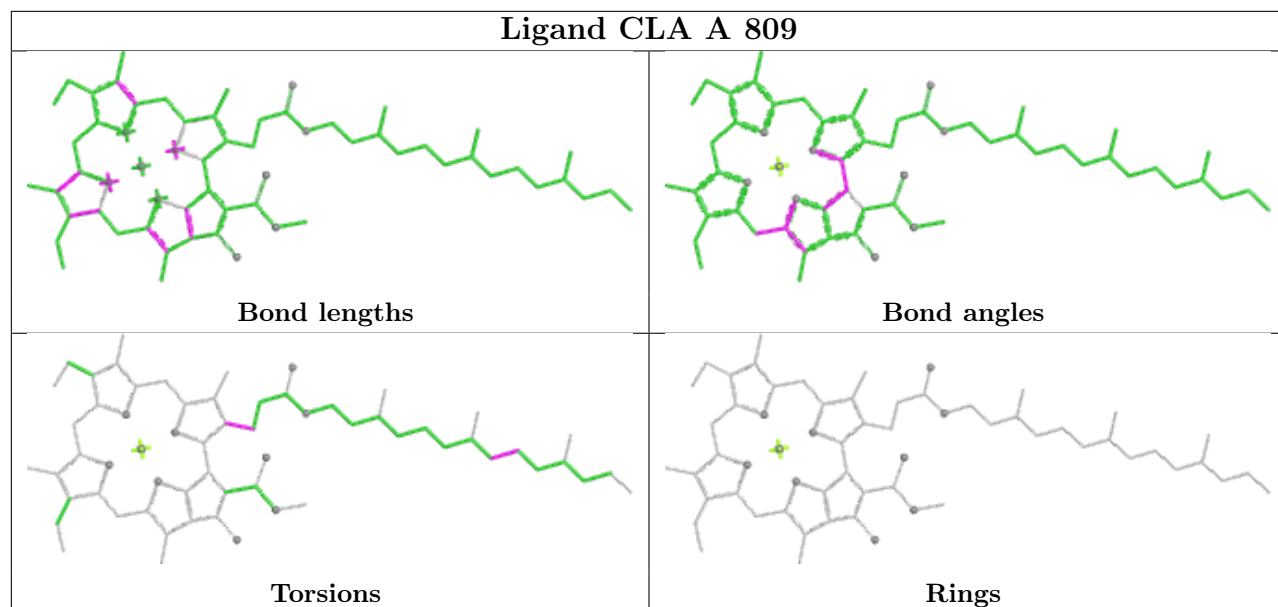
Ligand CLA T 205



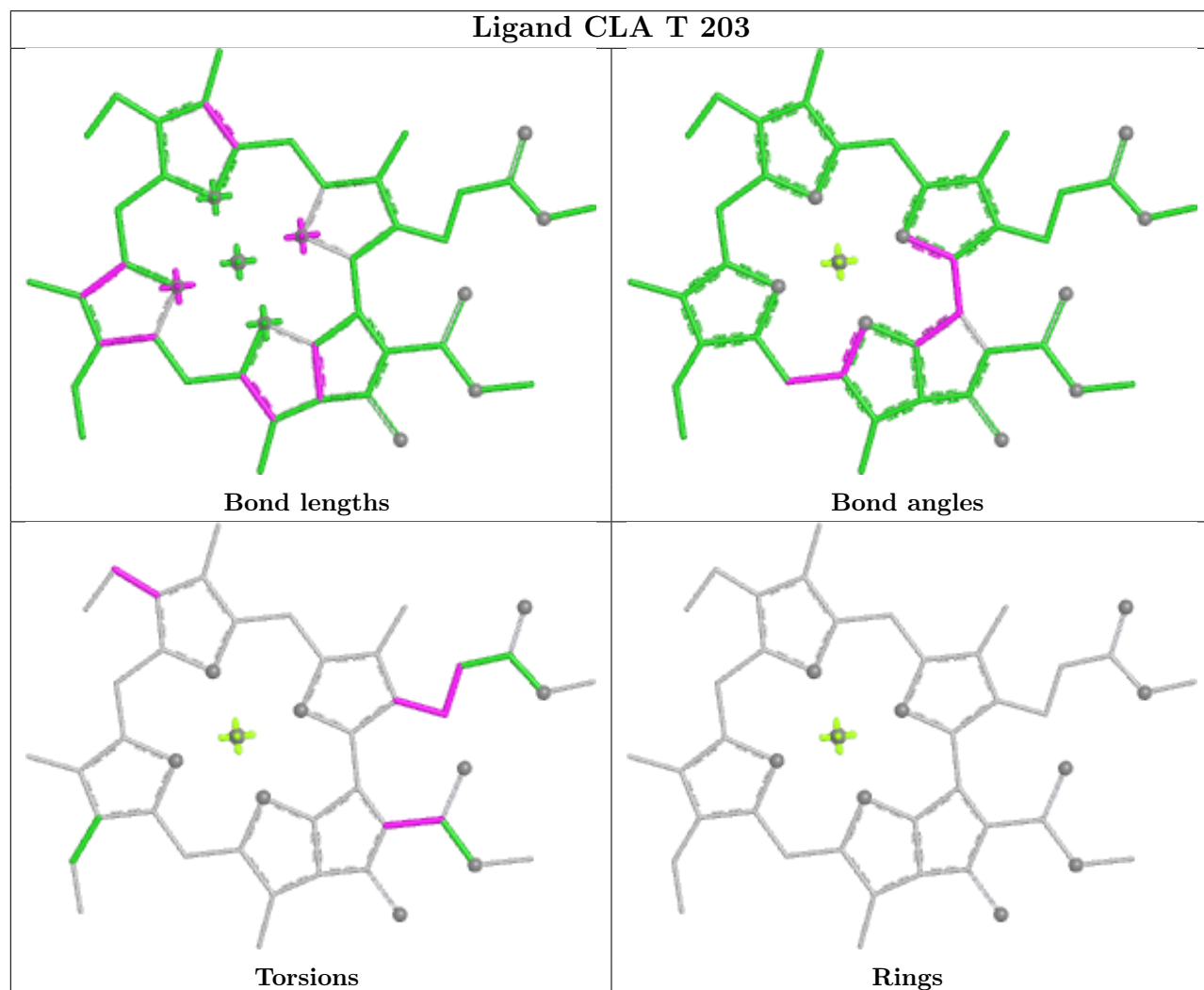


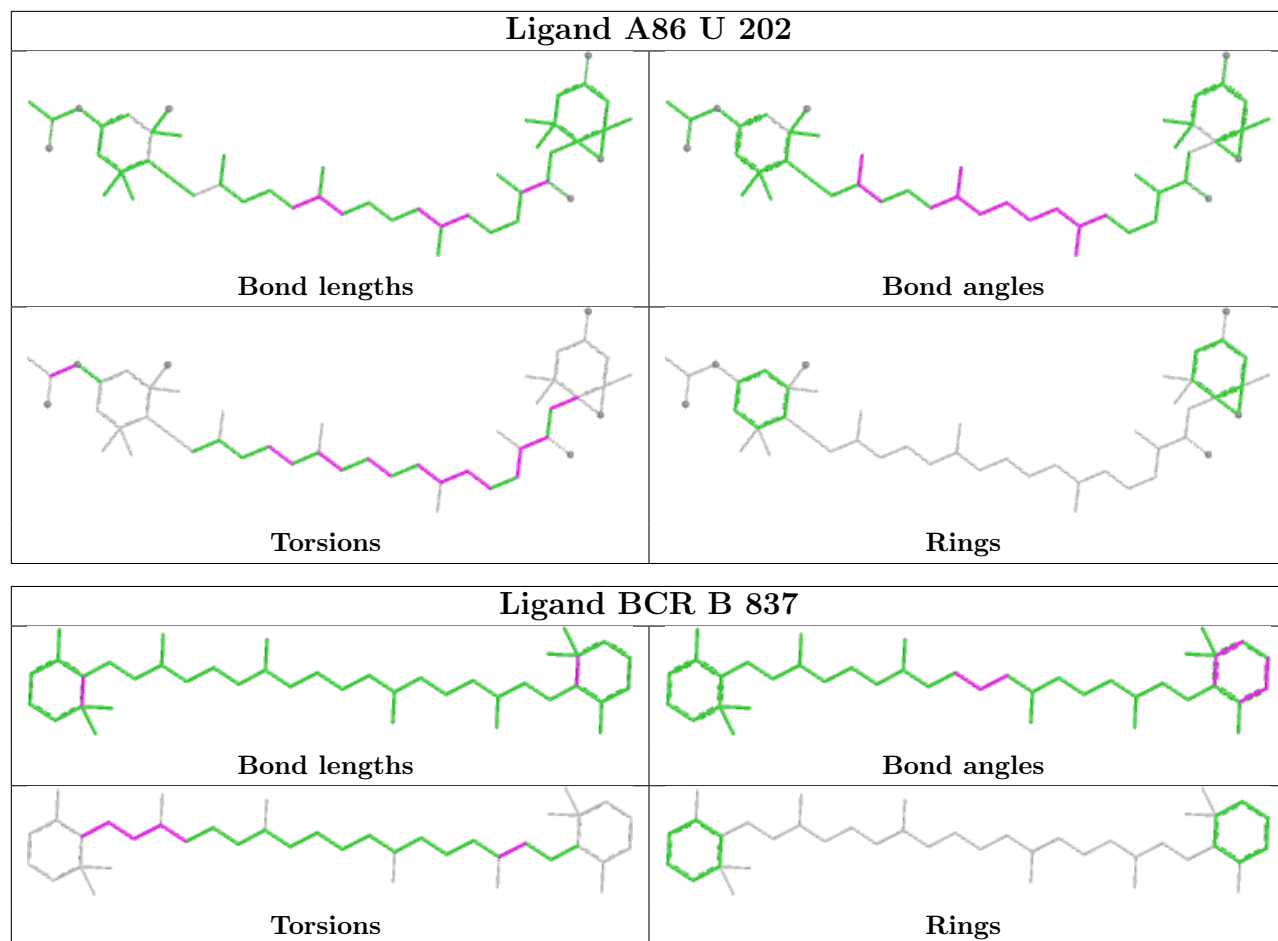


Ligand CLA A 809

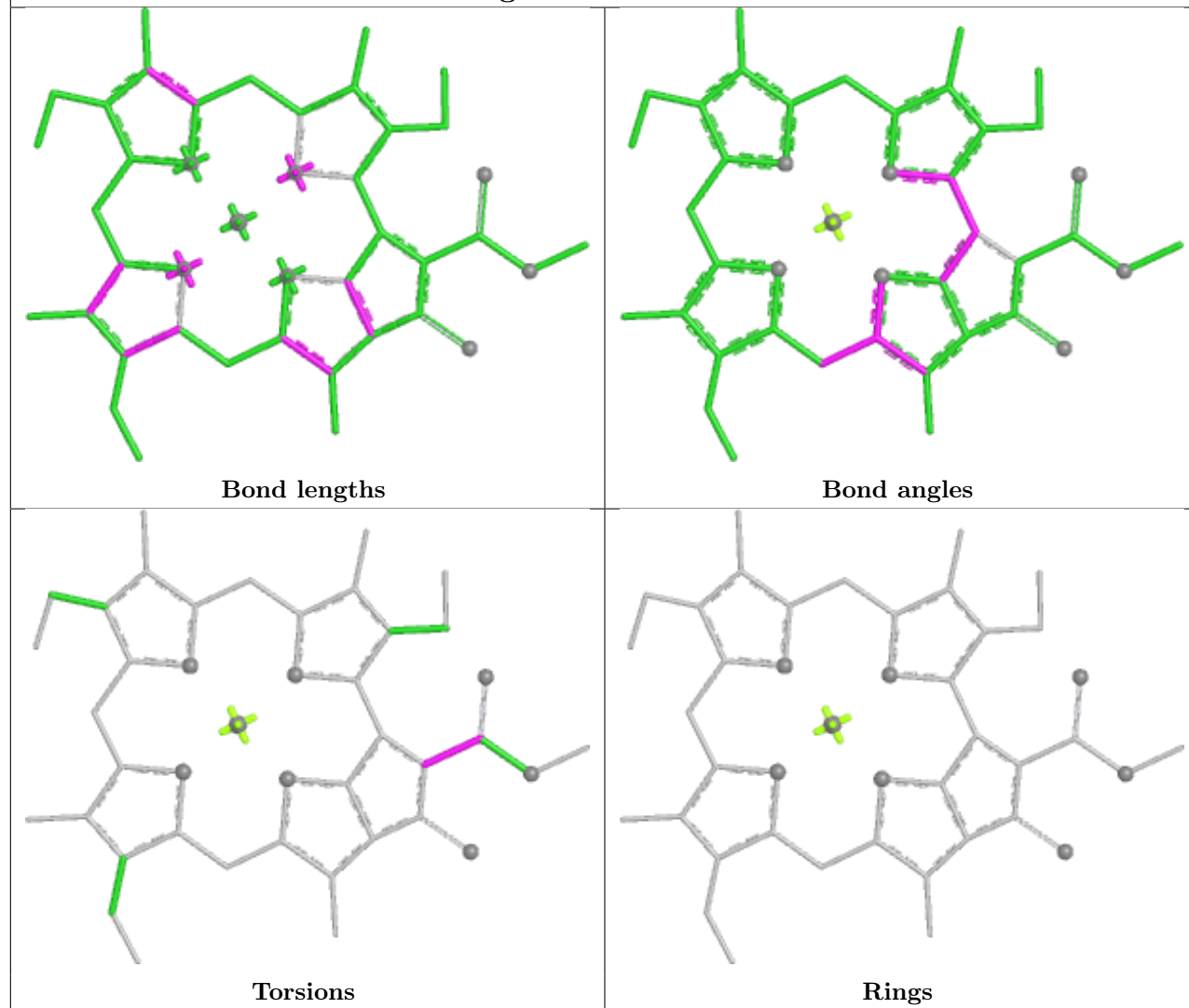


Ligand CLA T 203

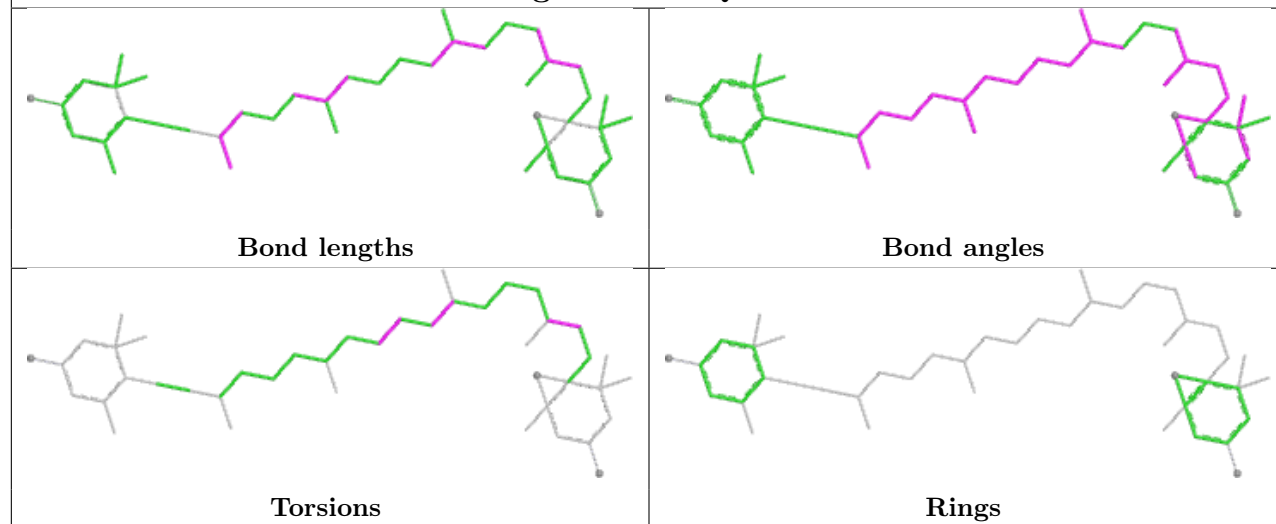




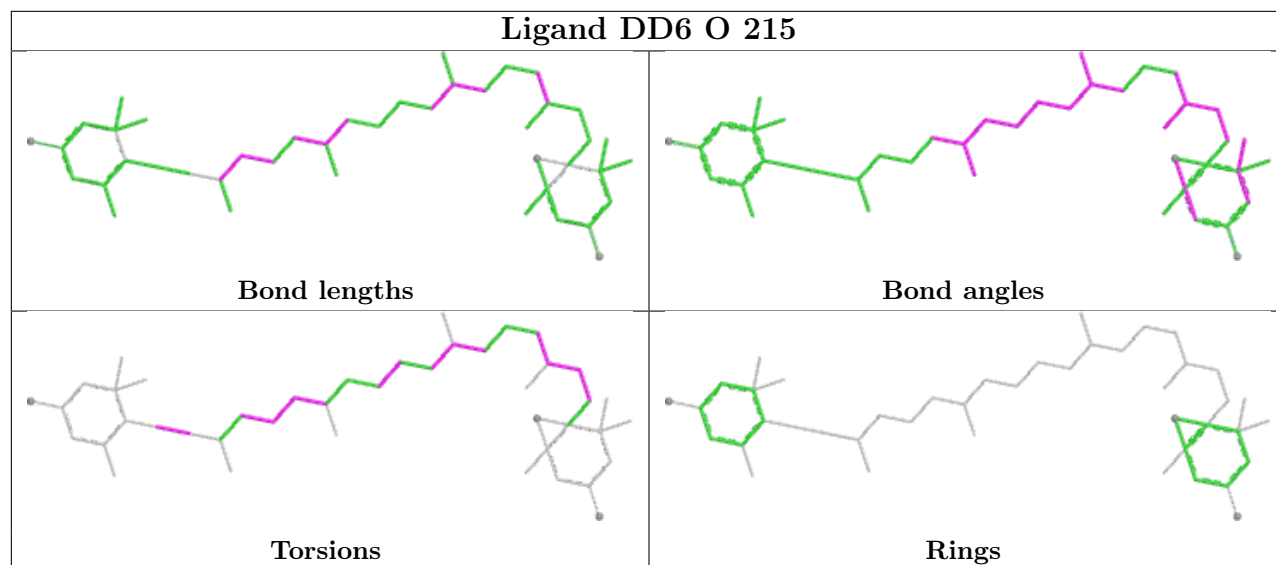
Ligand CLA J 103



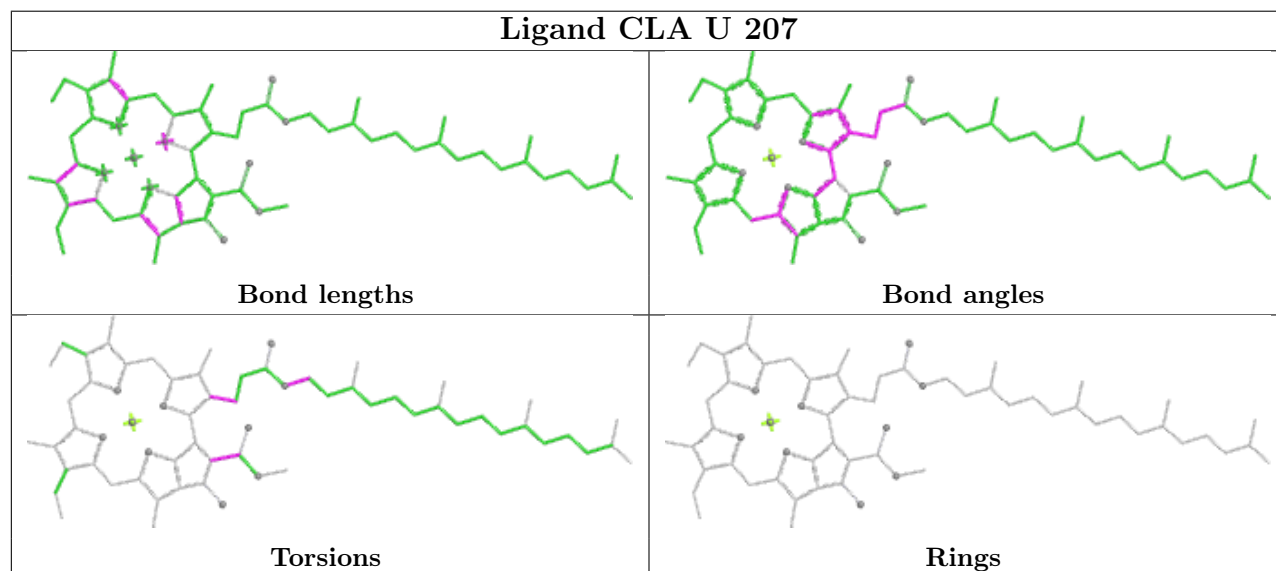
Ligand DD6 Q 202



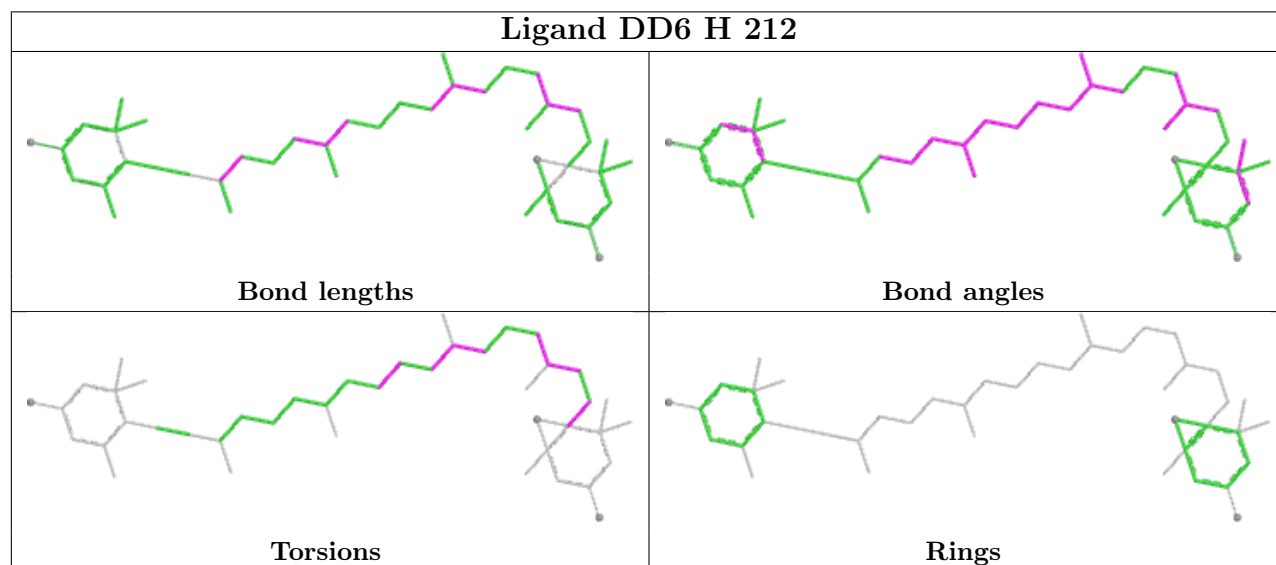
Ligand DD6 O 215

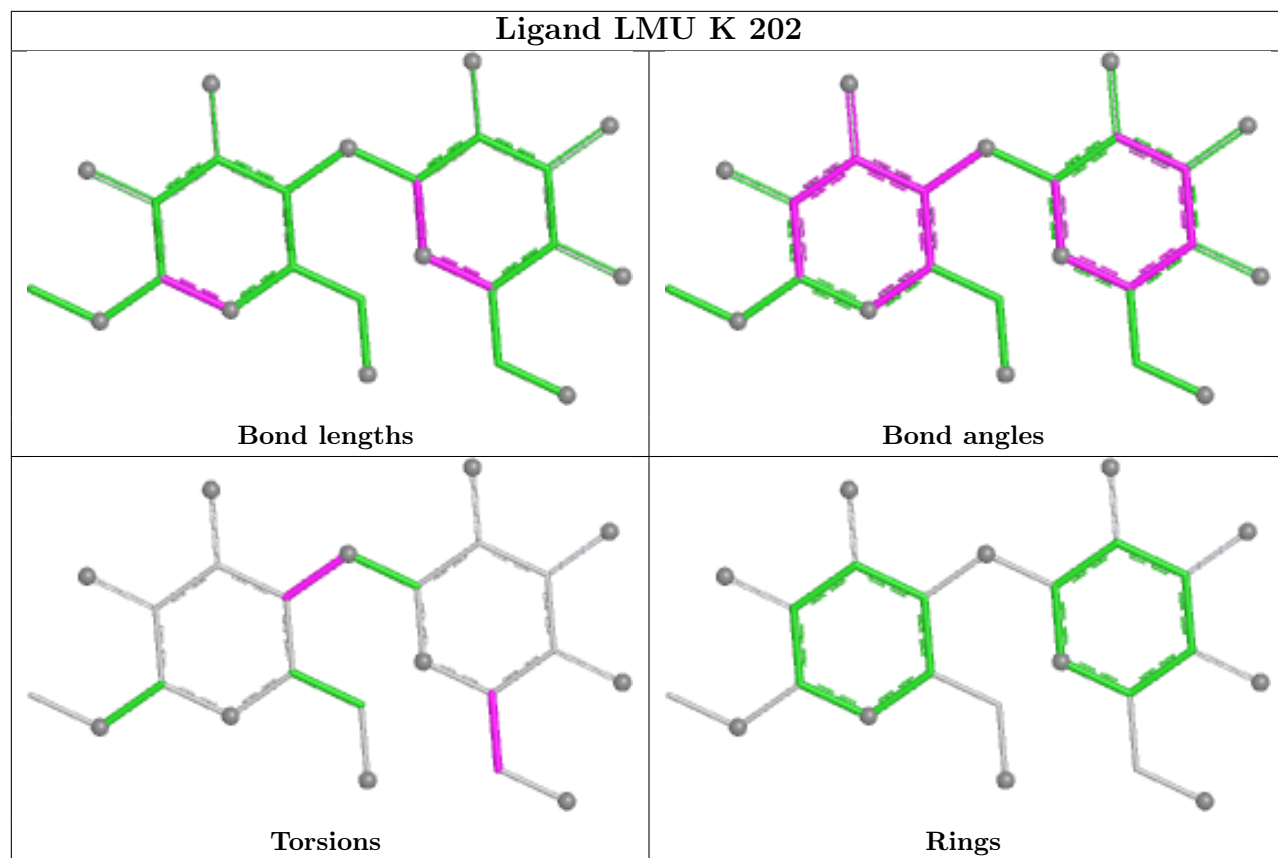


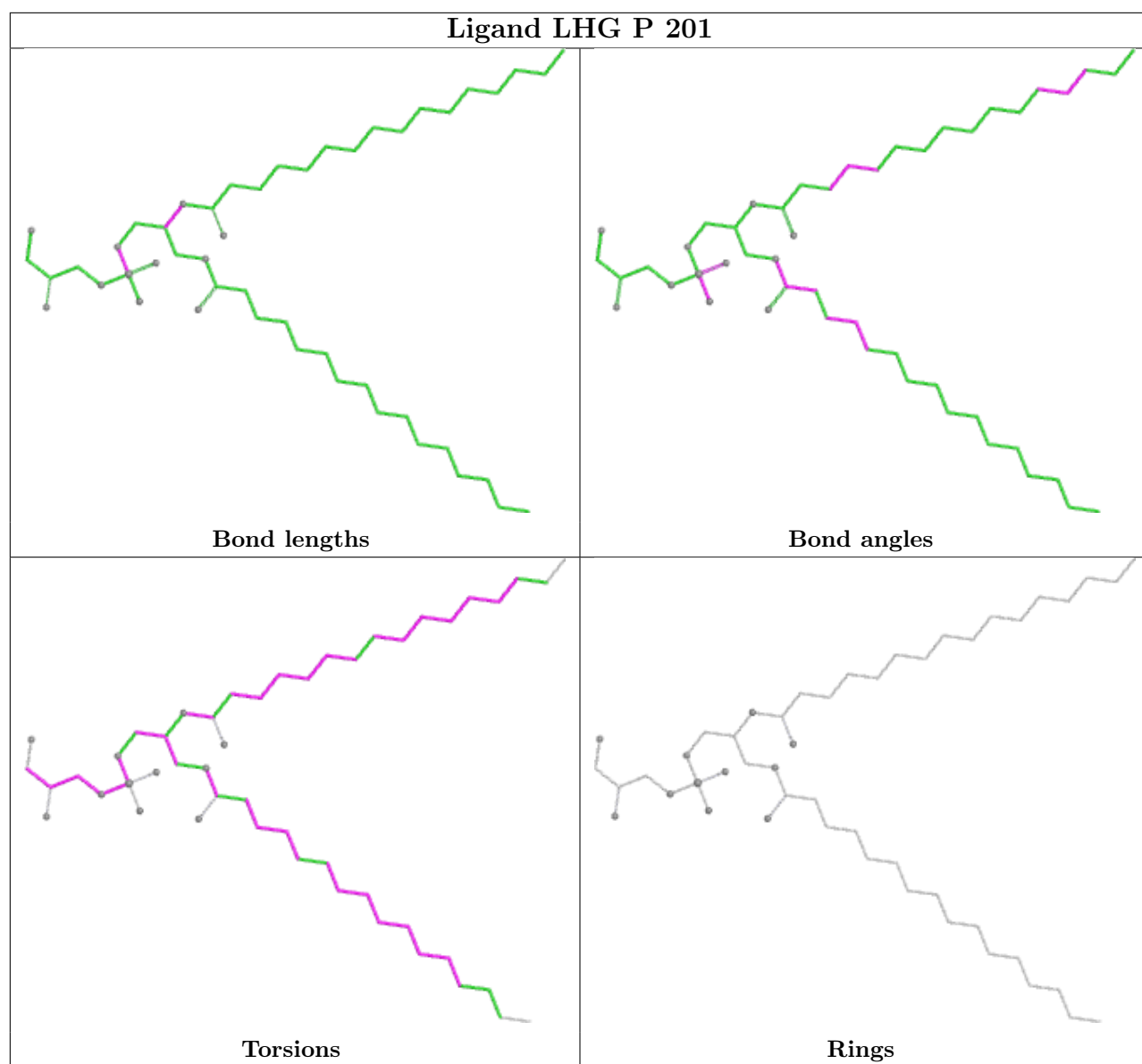
Ligand CLA U 207

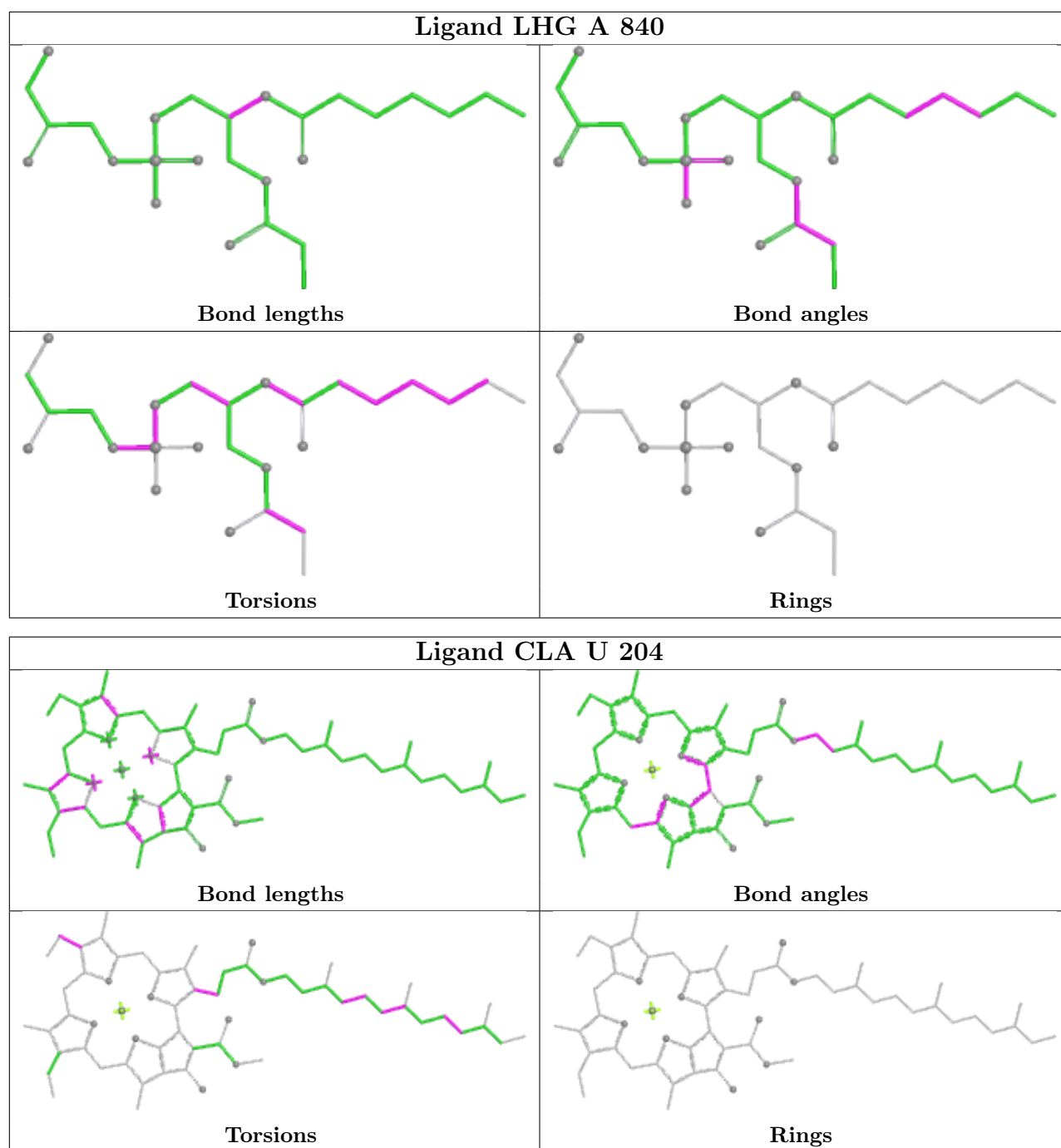


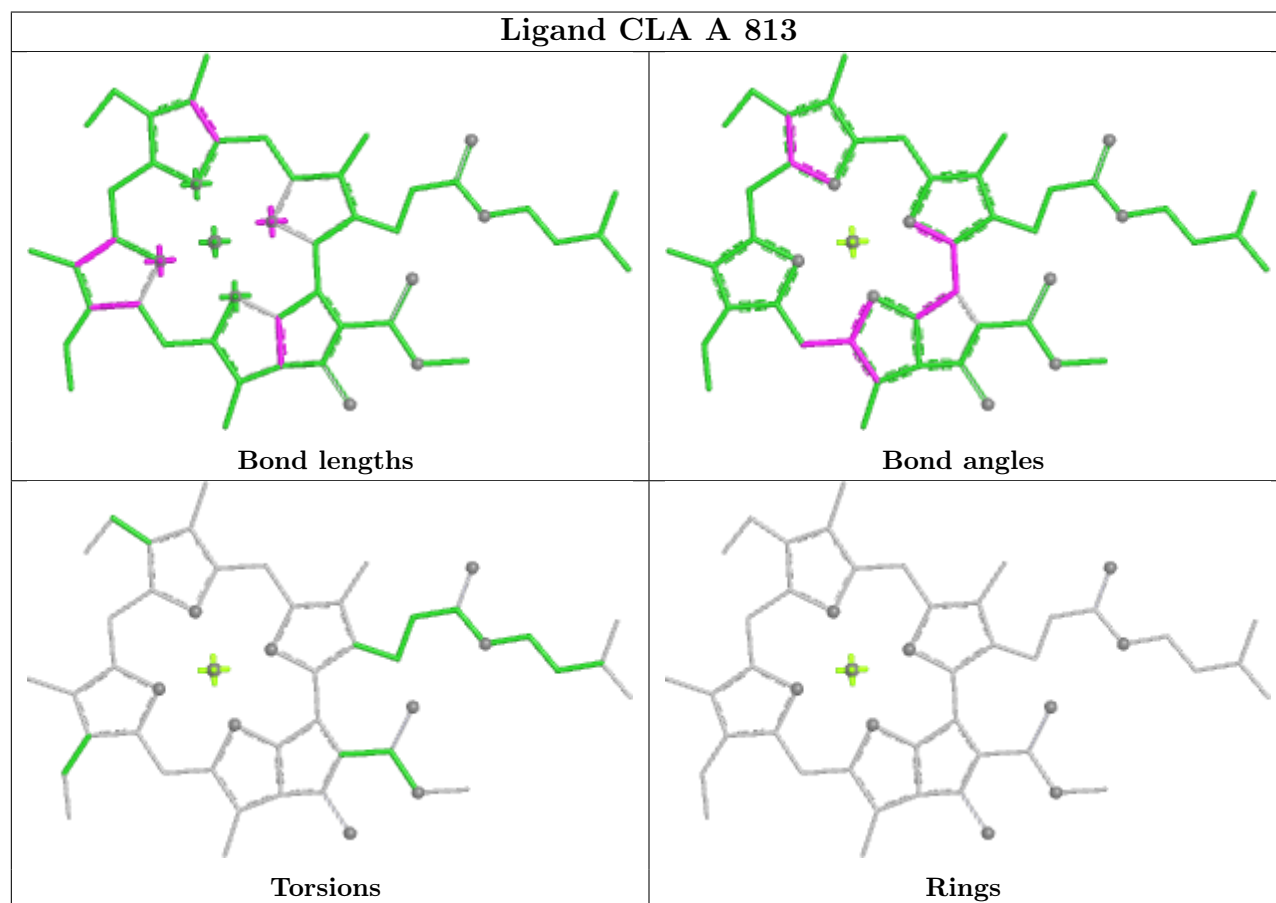
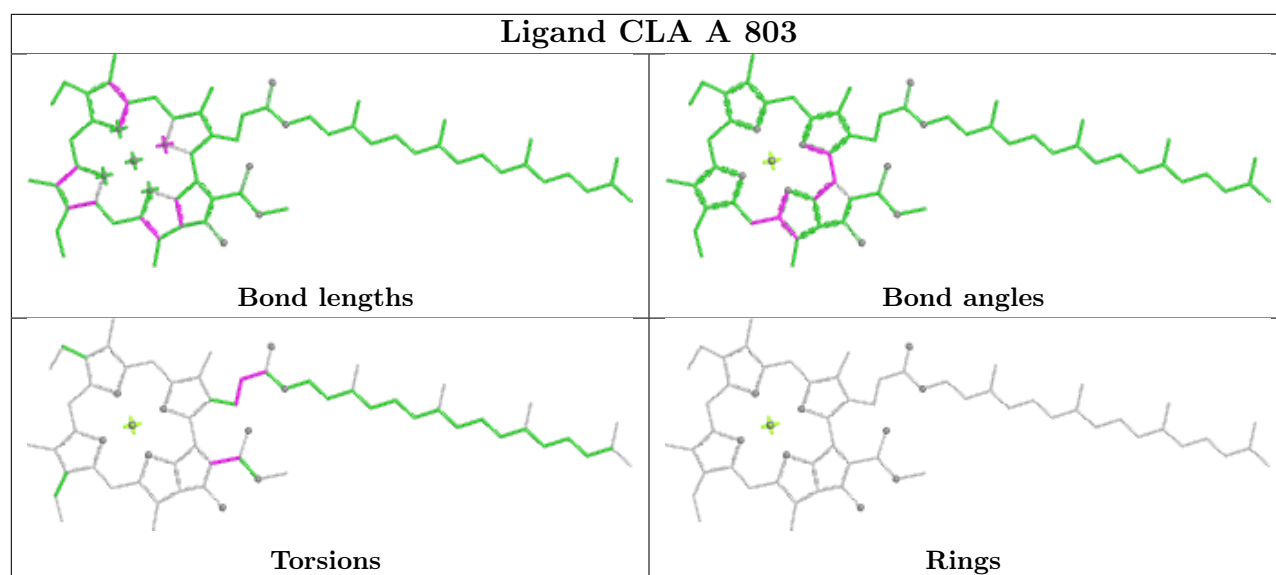
Ligand DD6 H 212



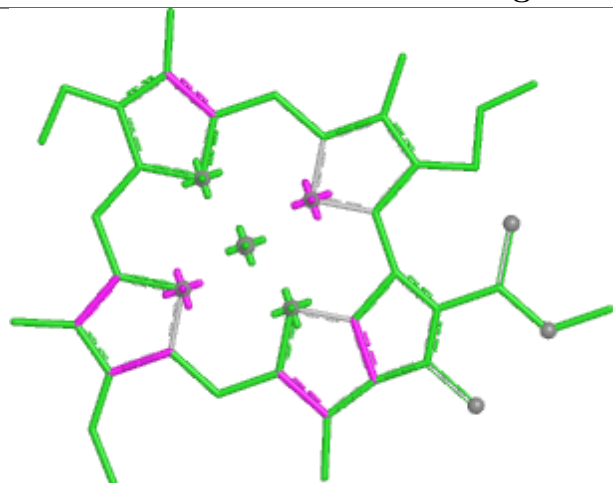




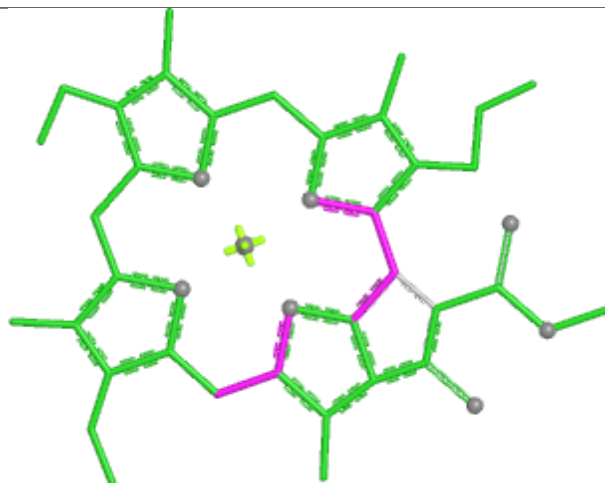




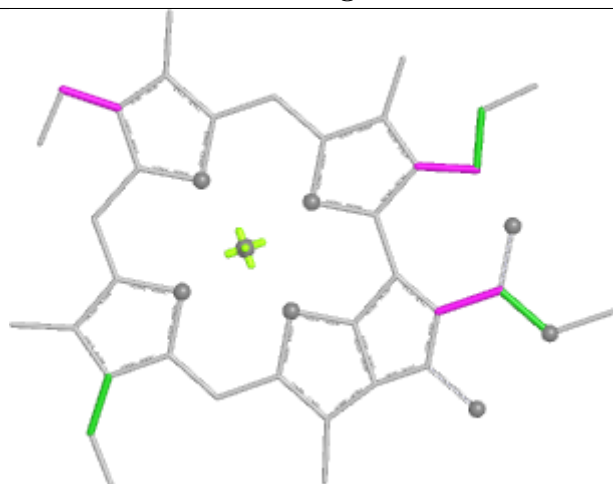
Ligand CLA G 204



Bond lengths



Bond angles

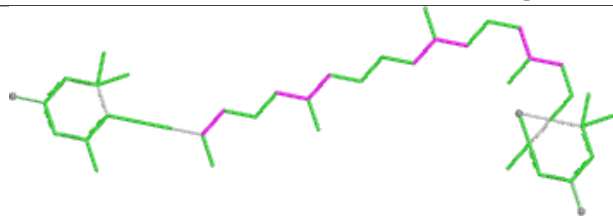


Torsions

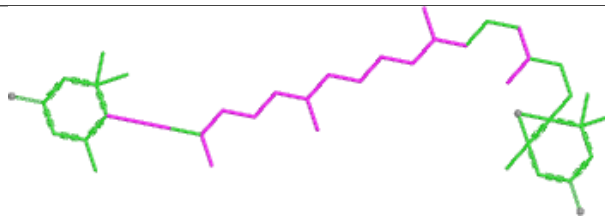


Rings

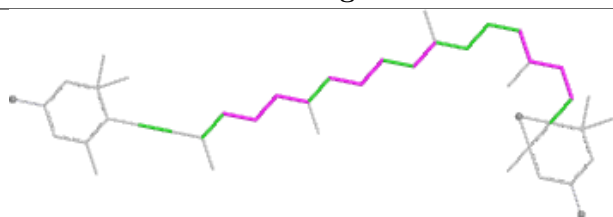
Ligand DD6 S 215



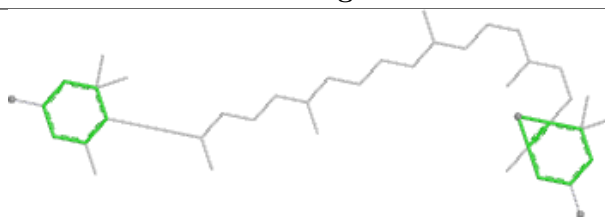
Bond lengths



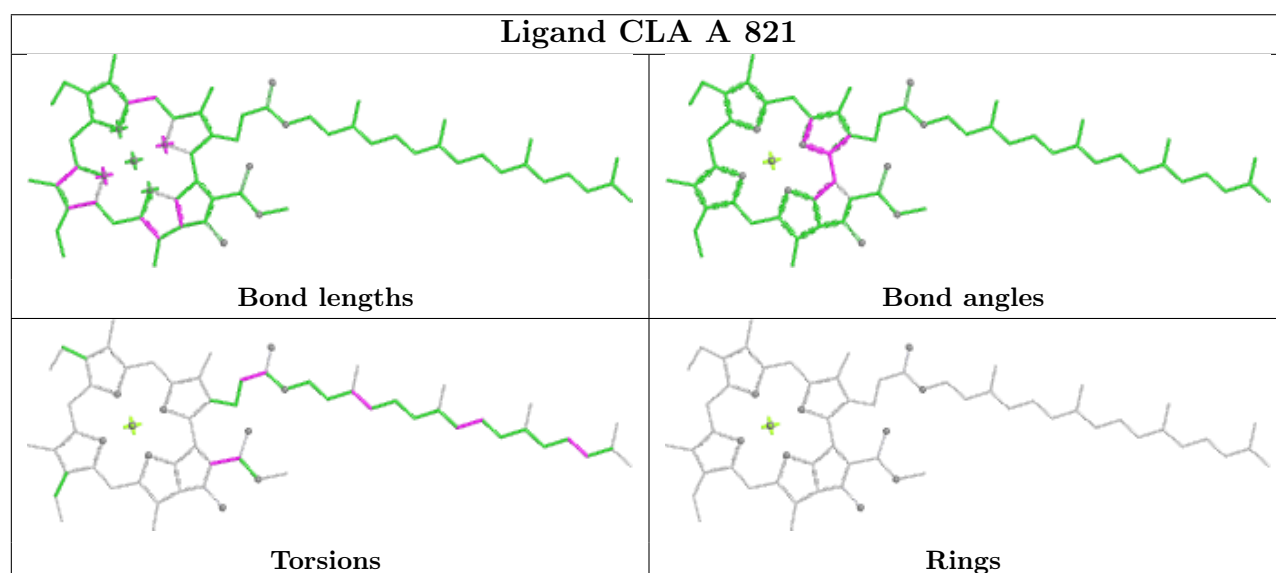
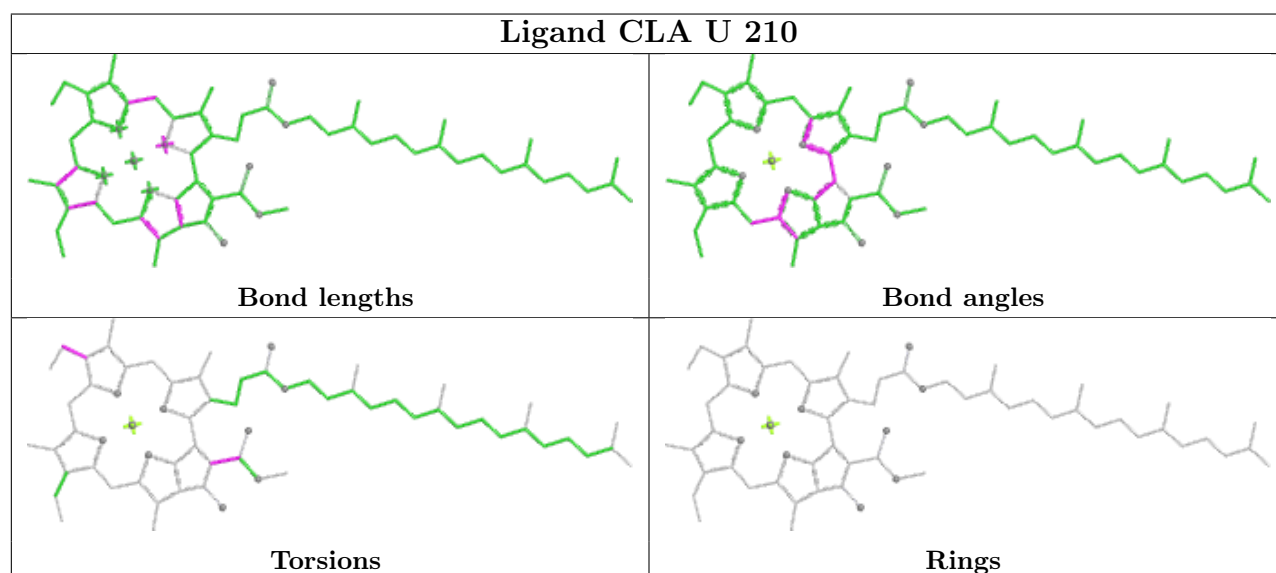
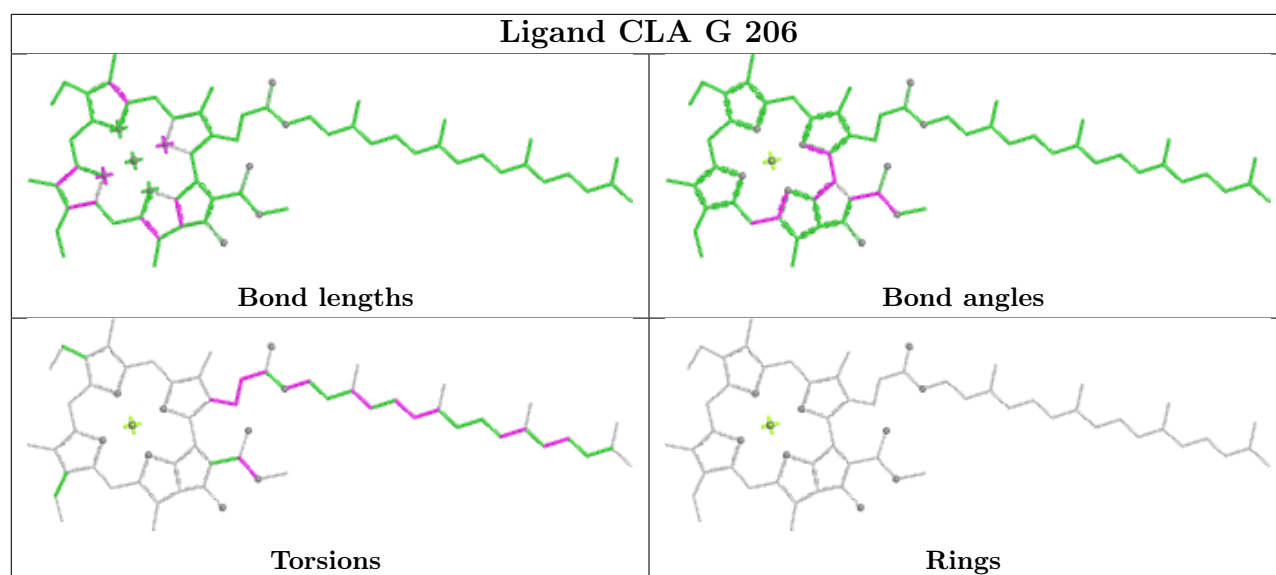
Bond angles



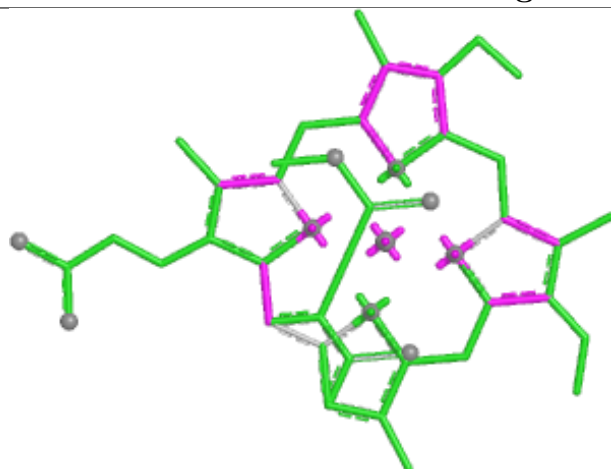
Torsions



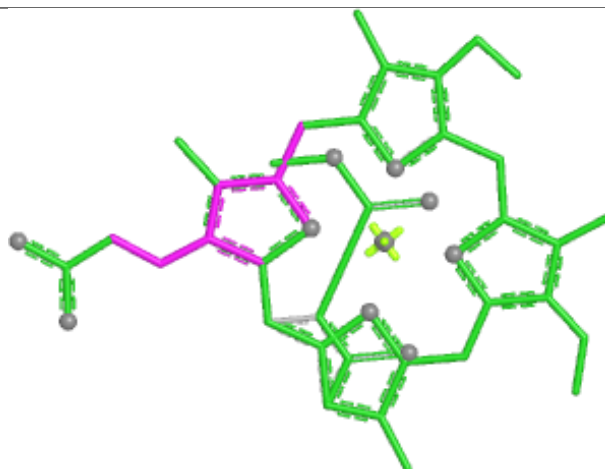
Rings



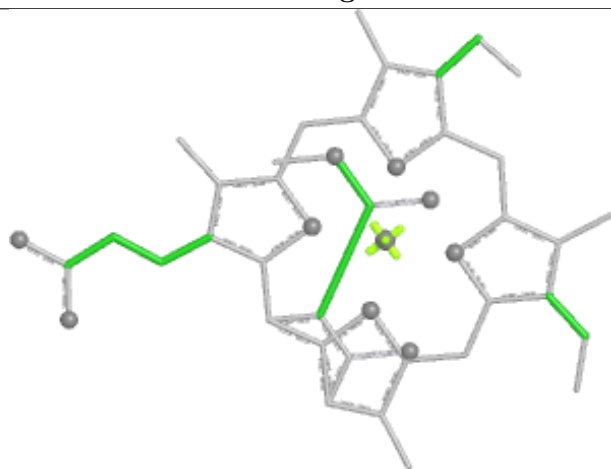
Ligand KC1 O 210



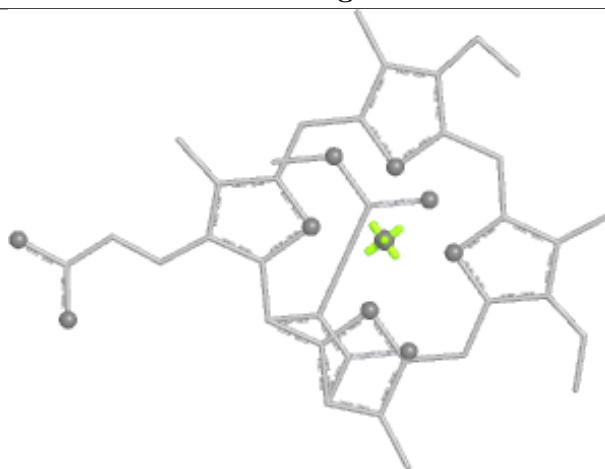
Bond lengths



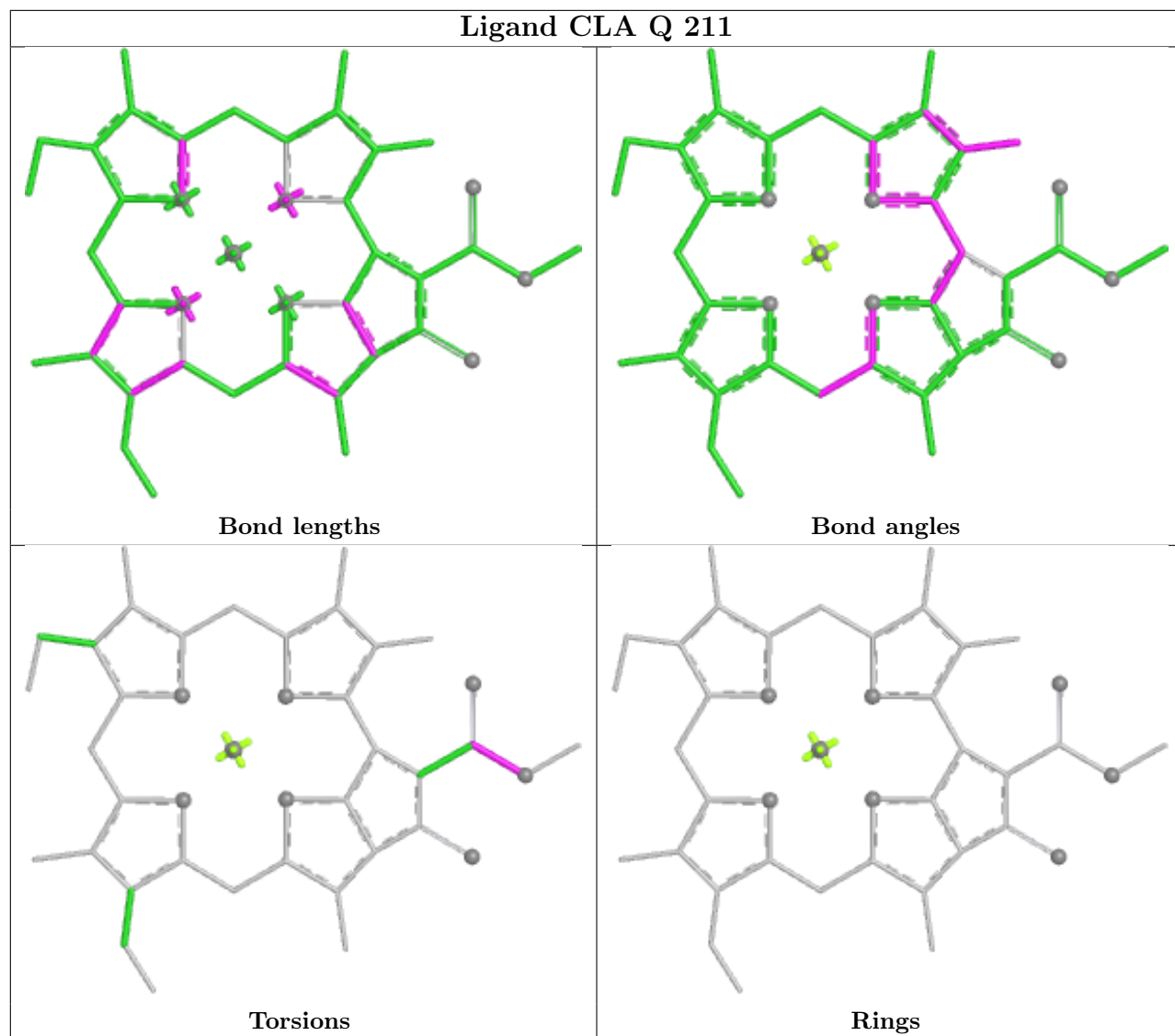
Bond angles

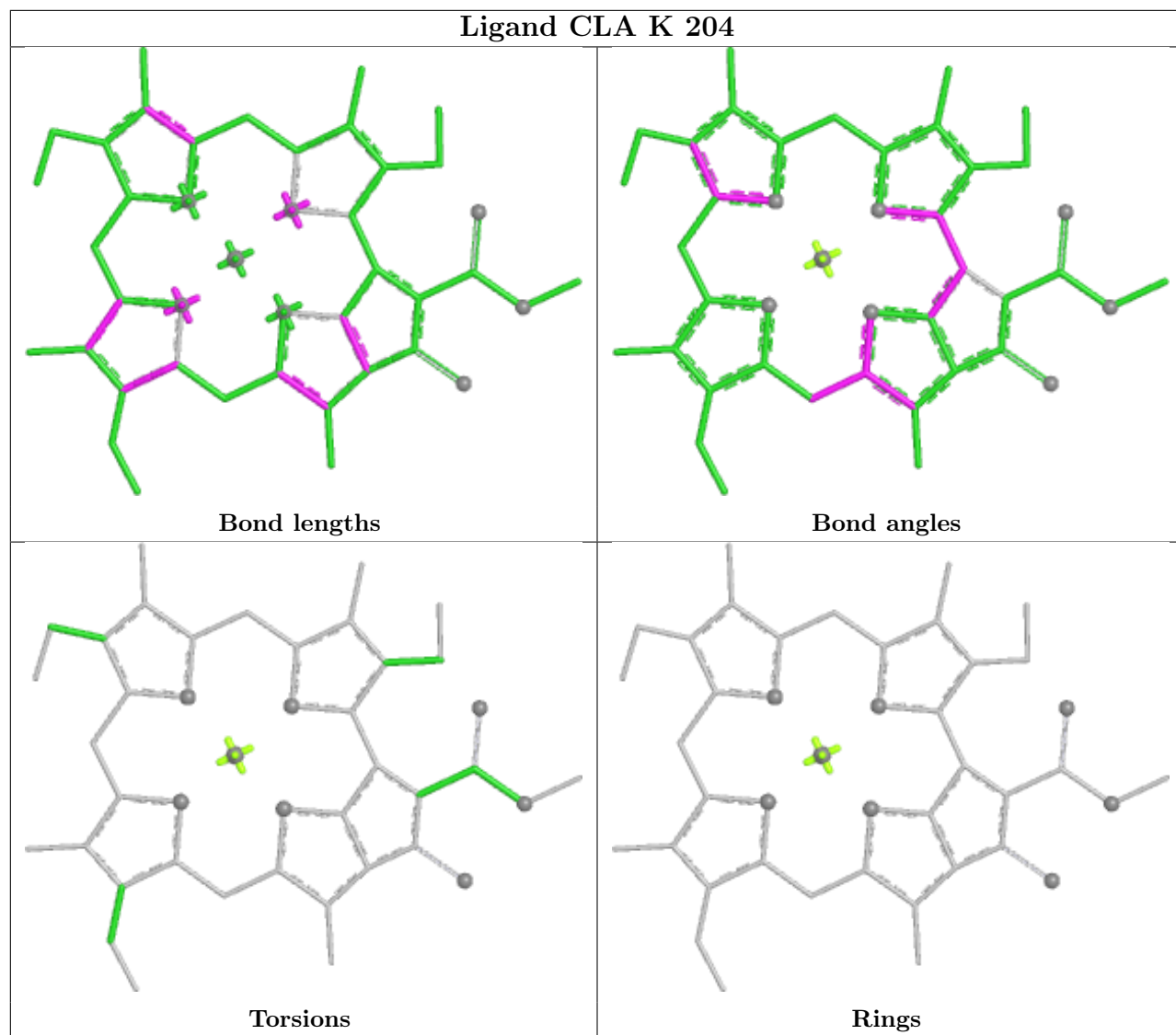


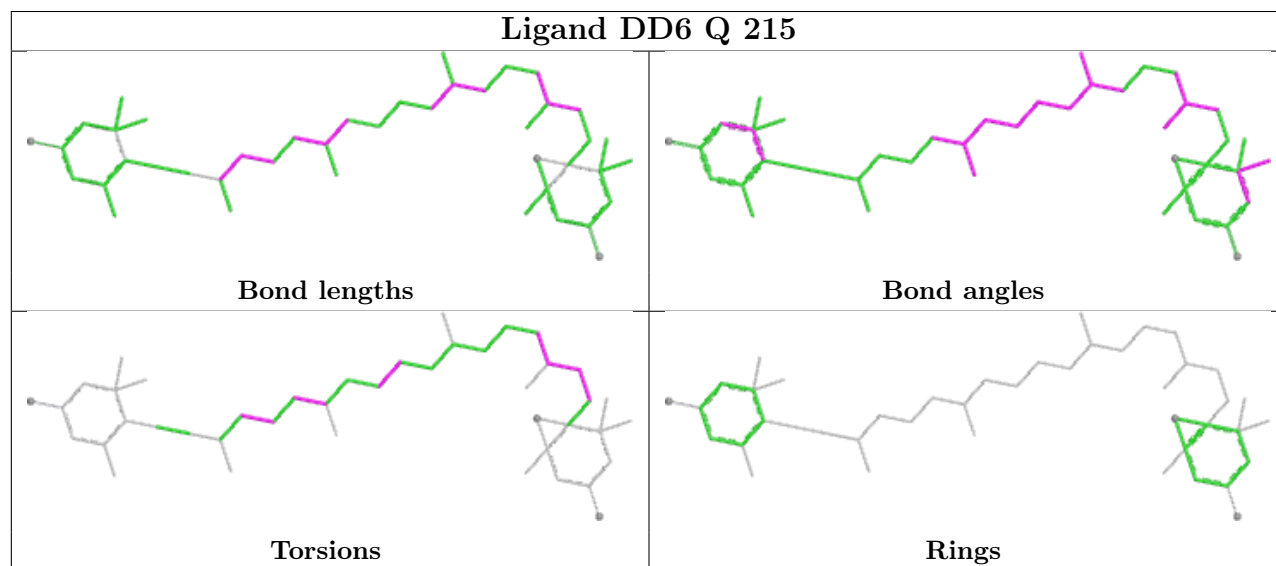
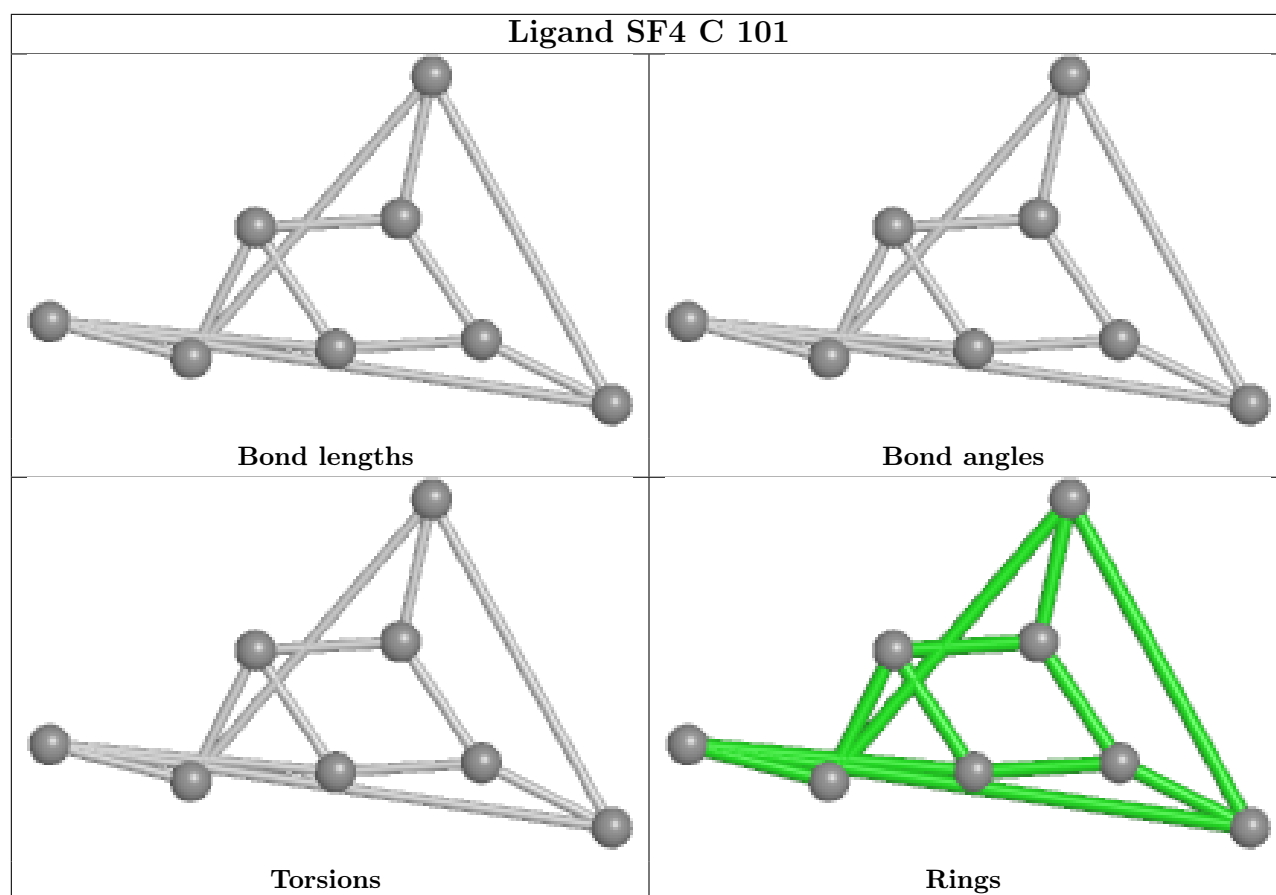
Torsions



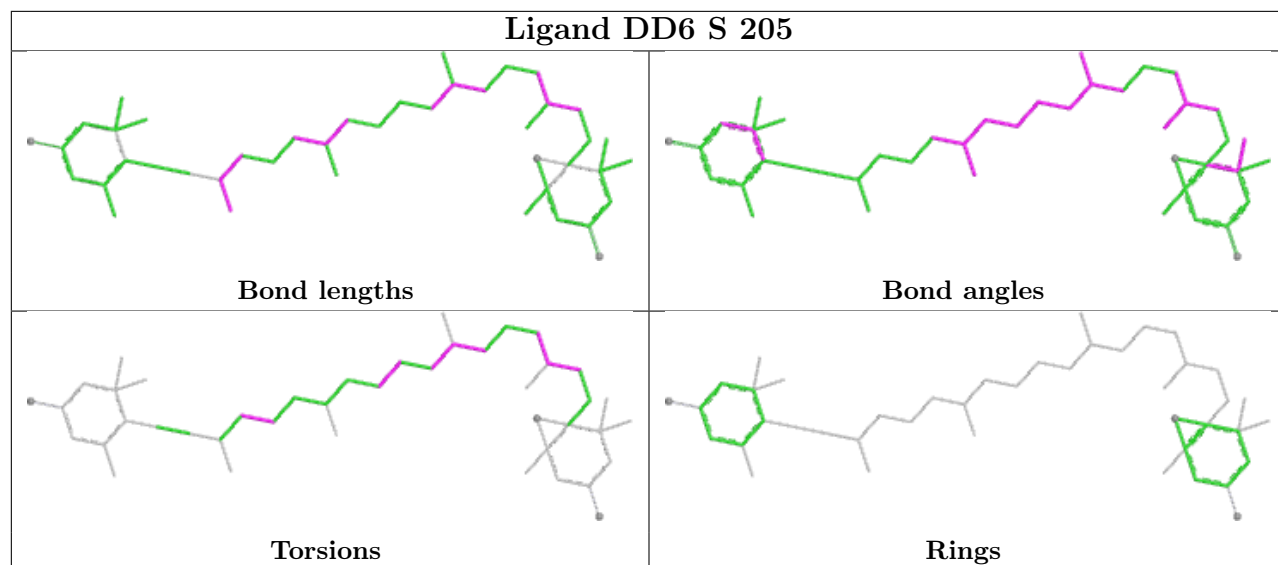
Rings



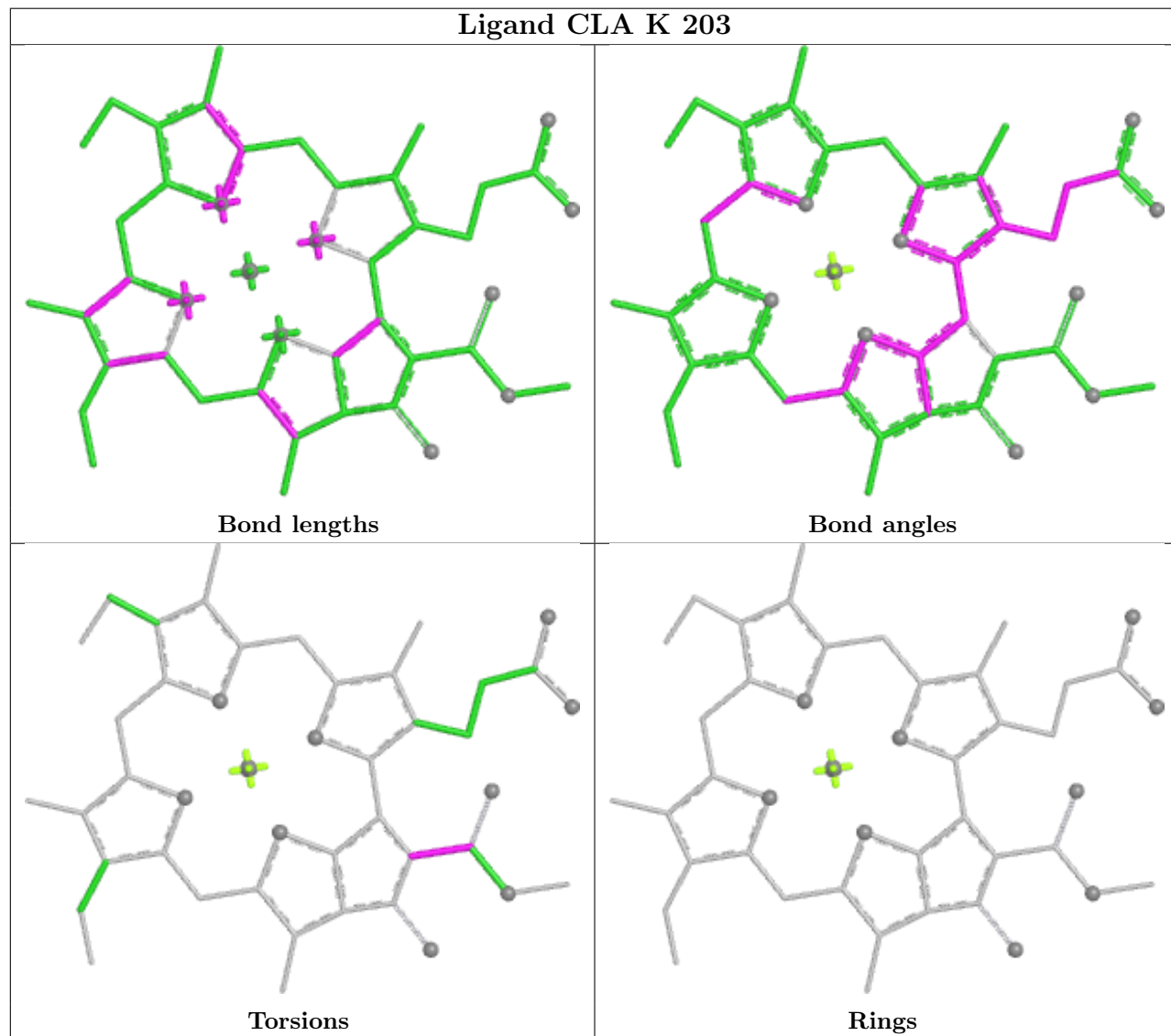


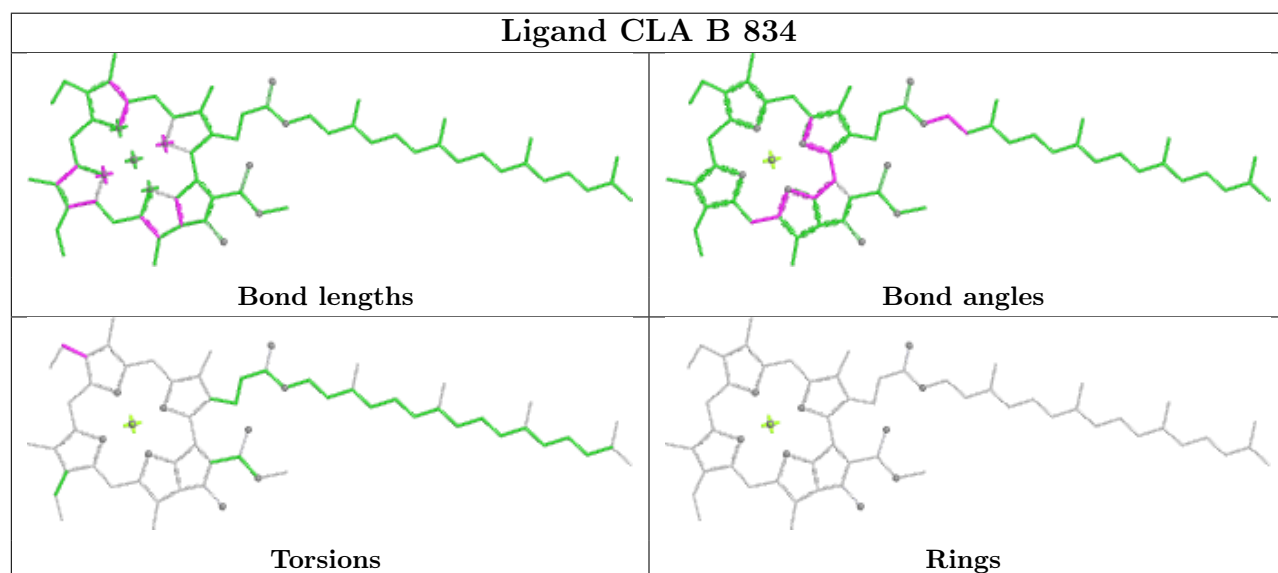
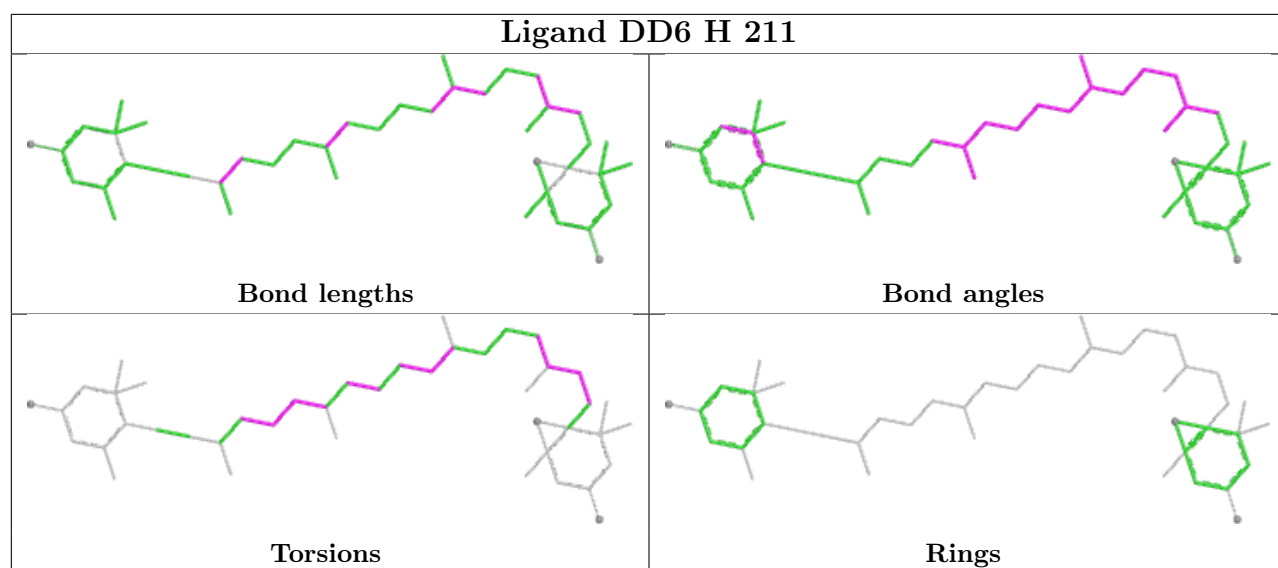


Ligand DD6 S 205

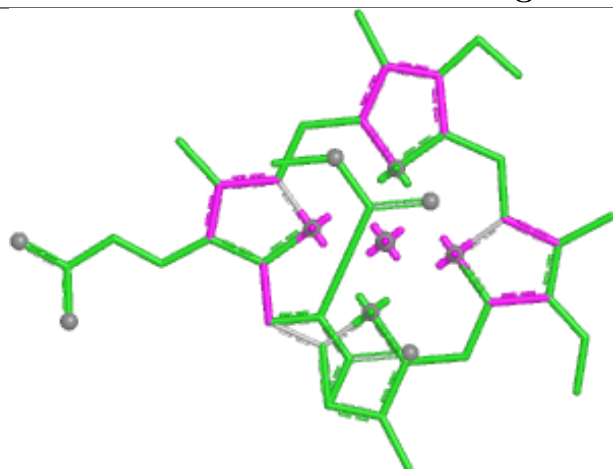


Ligand CLA K 203

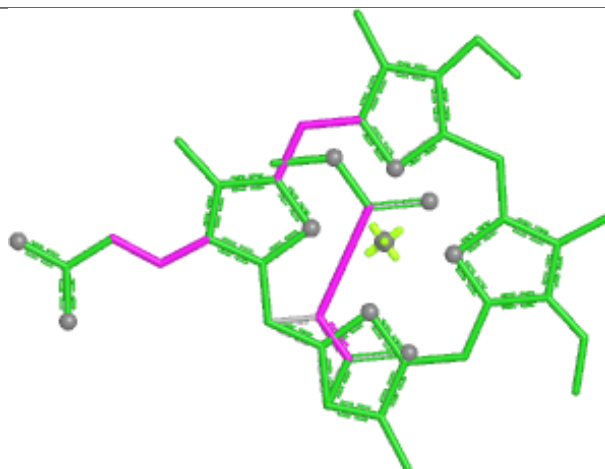




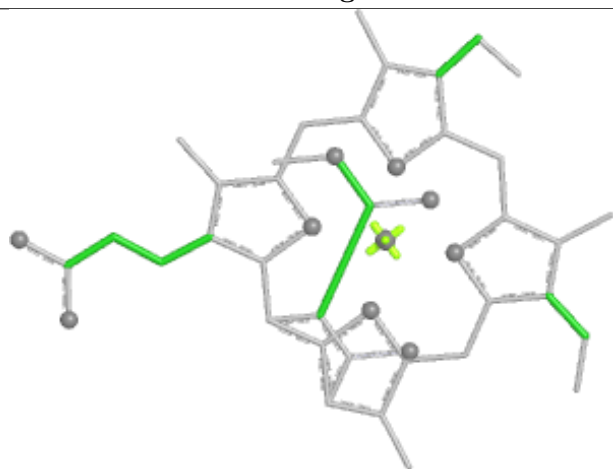
Ligand KC1 U 213



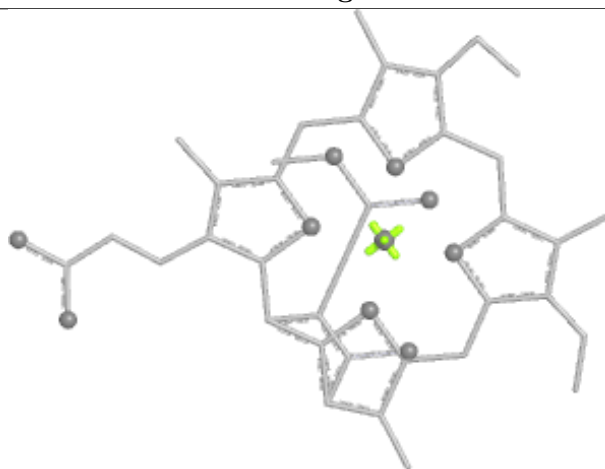
Bond lengths



Bond angles

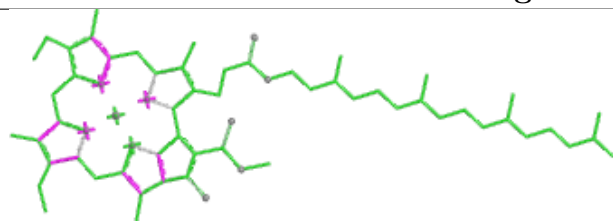


Torsions

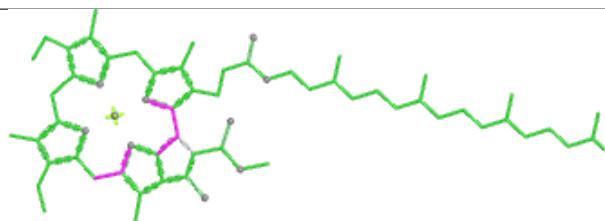


Rings

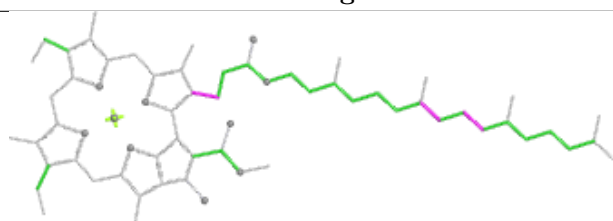
Ligand CLA B 842



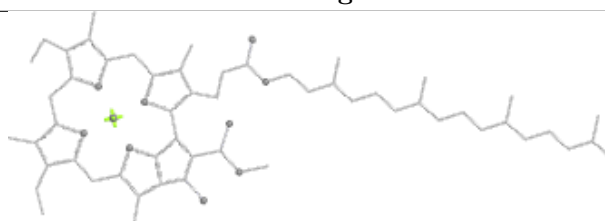
Bond lengths



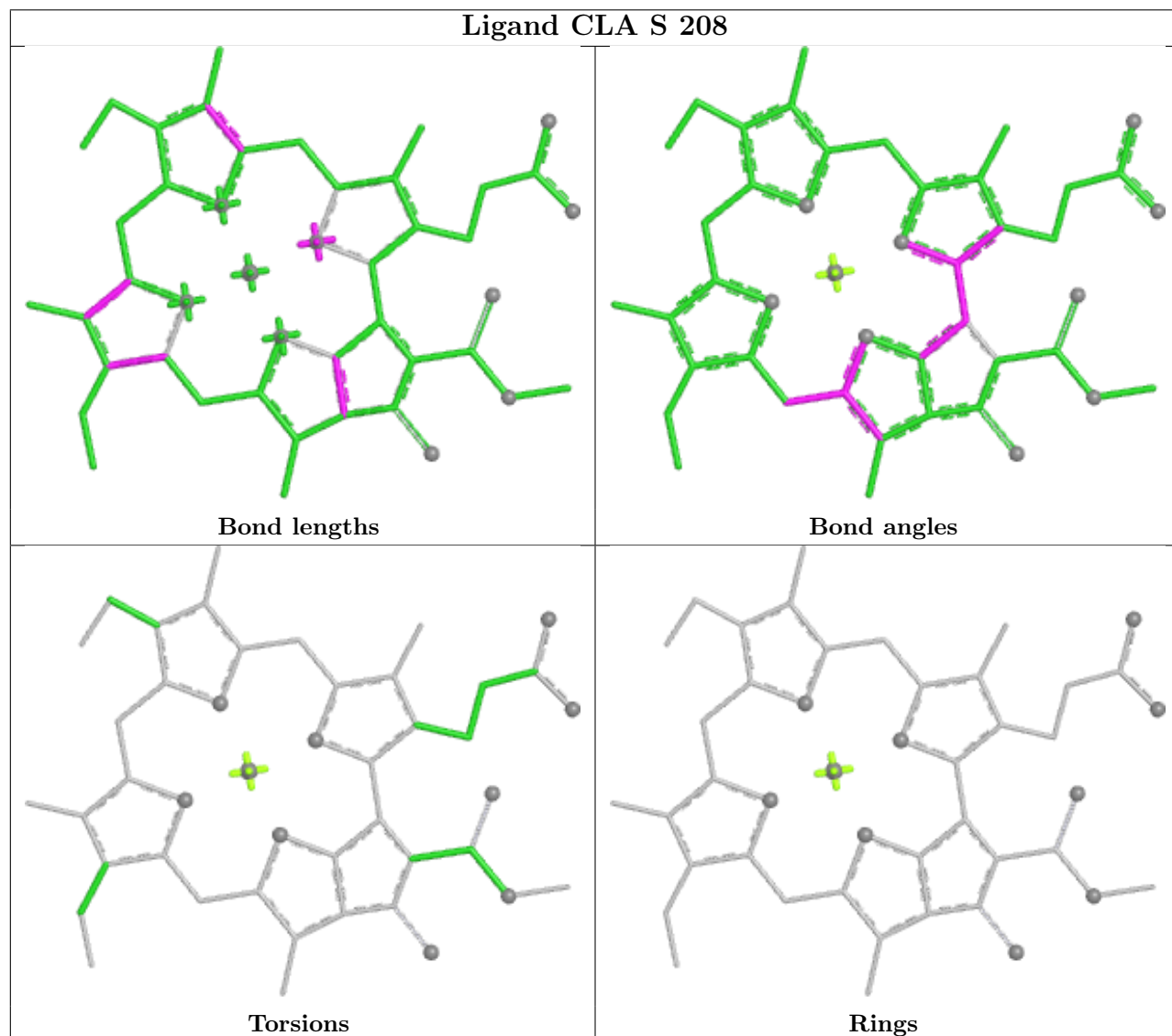
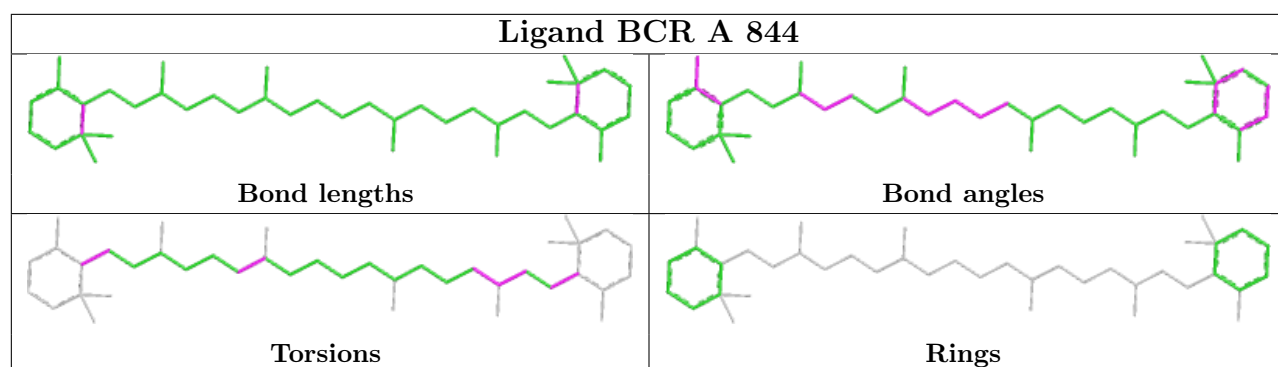
Bond angles



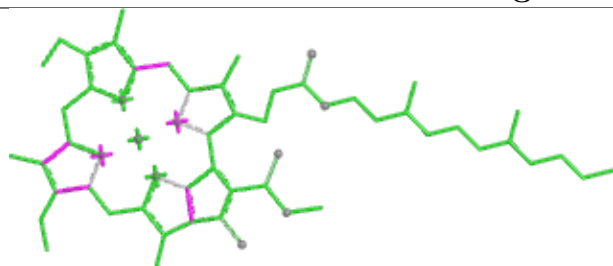
Torsions



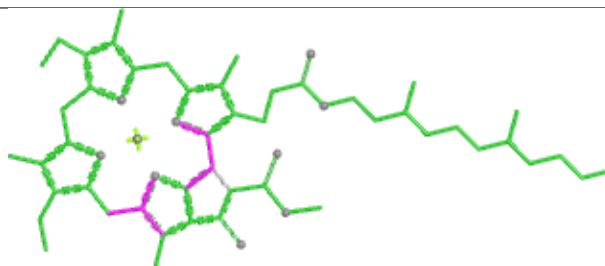
Rings



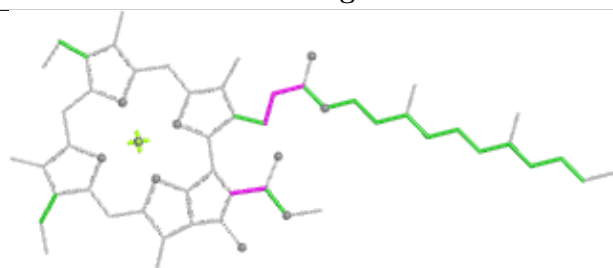
Ligand CLA H 208



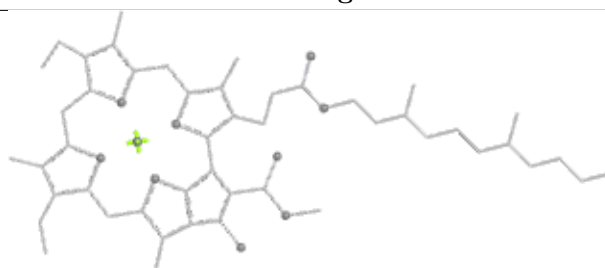
Bond lengths



Bond angles

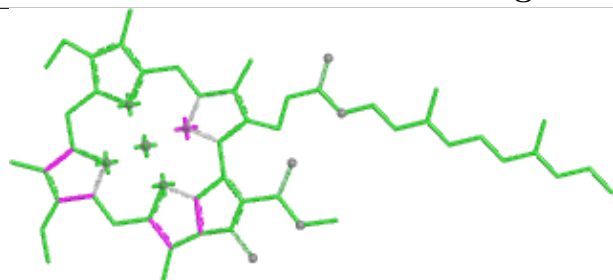


Torsions

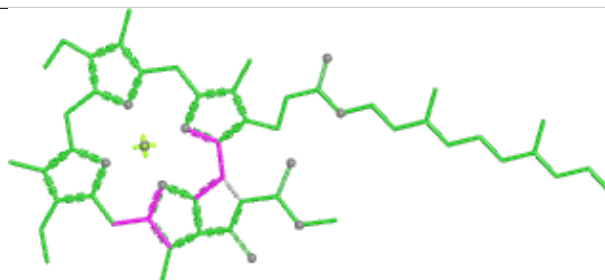


Rings

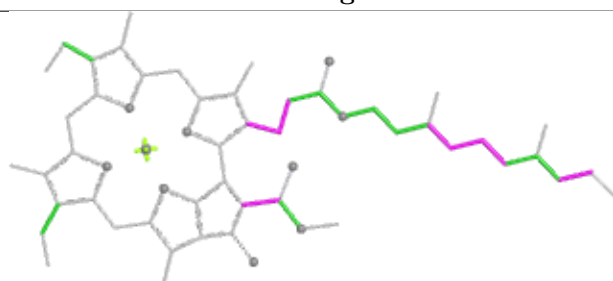
Ligand CLA T 204



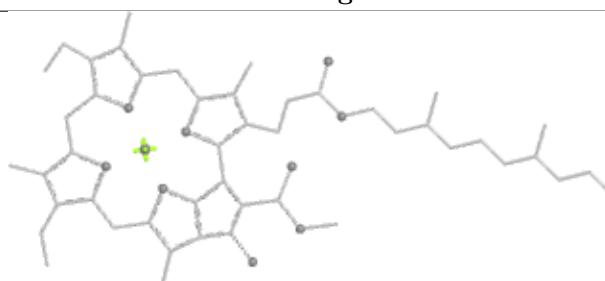
Bond lengths



Bond angles

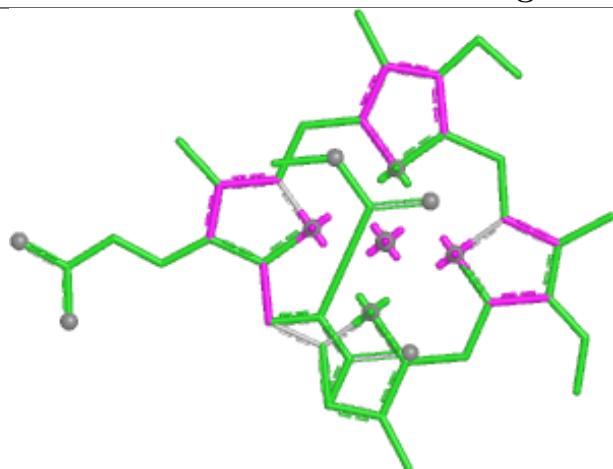


Torsions

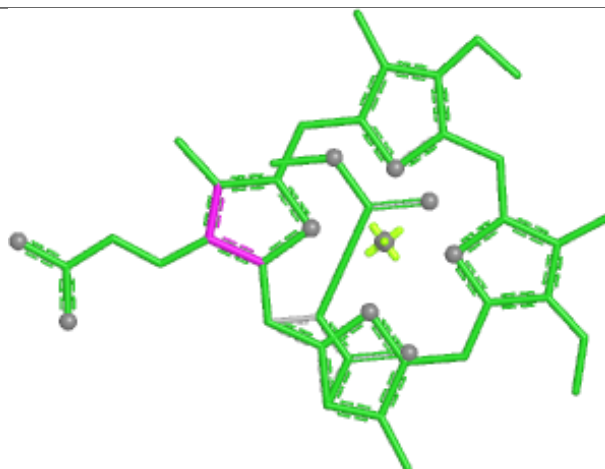


Rings

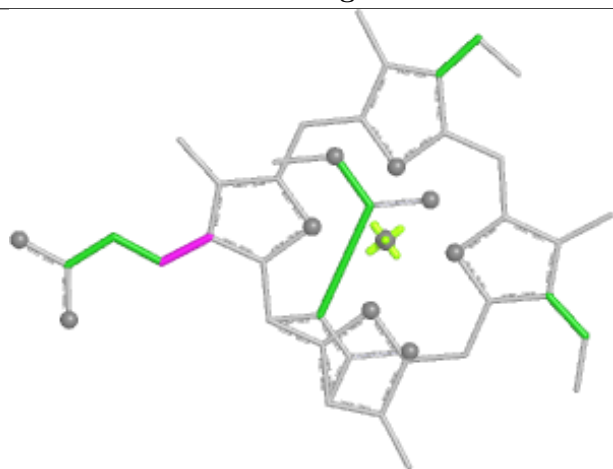
Ligand KC1 P 203



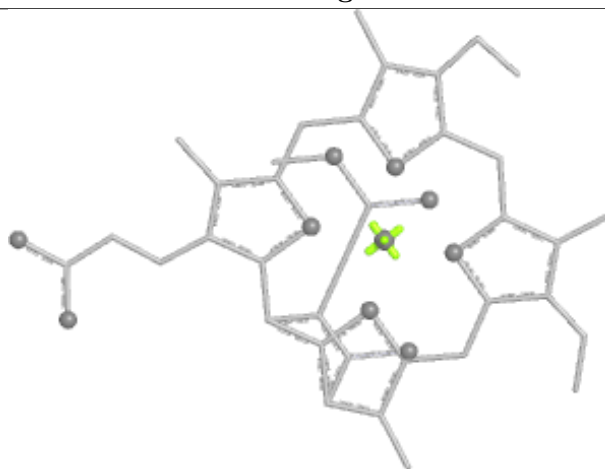
Bond lengths



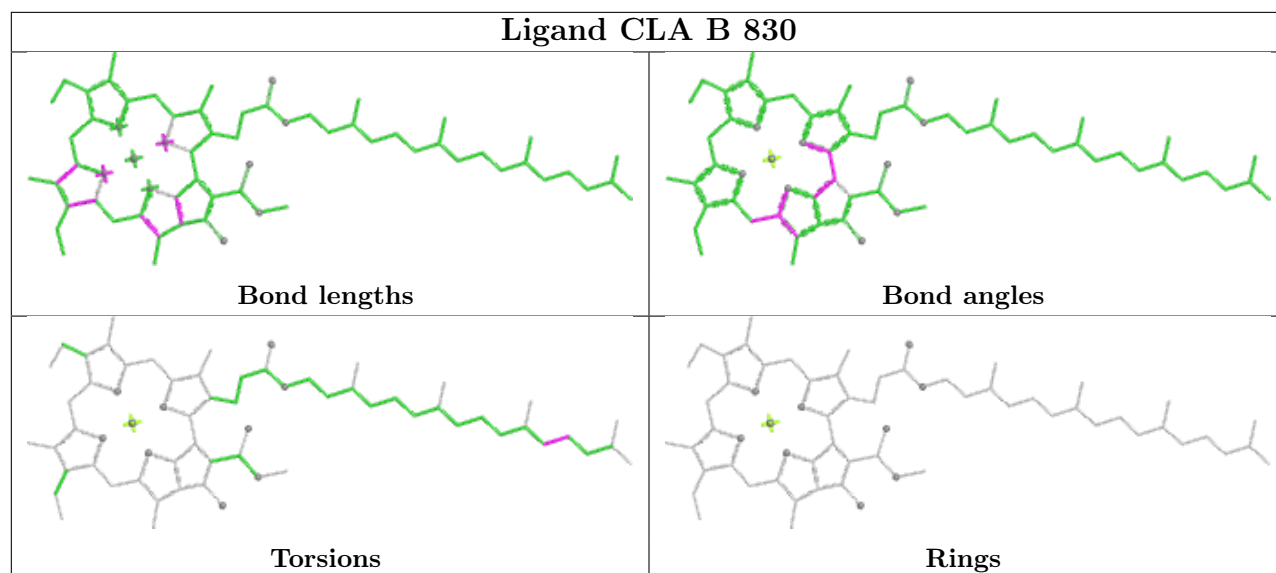
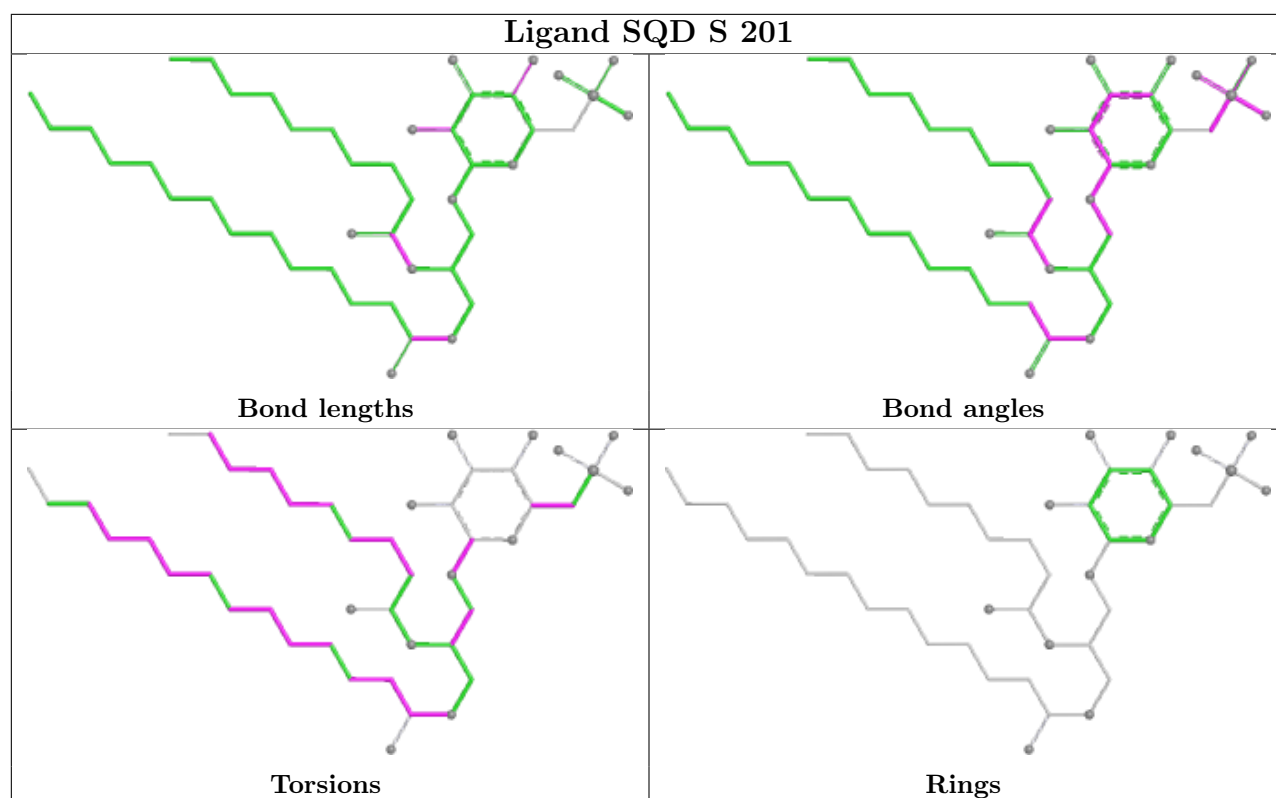
Bond angles

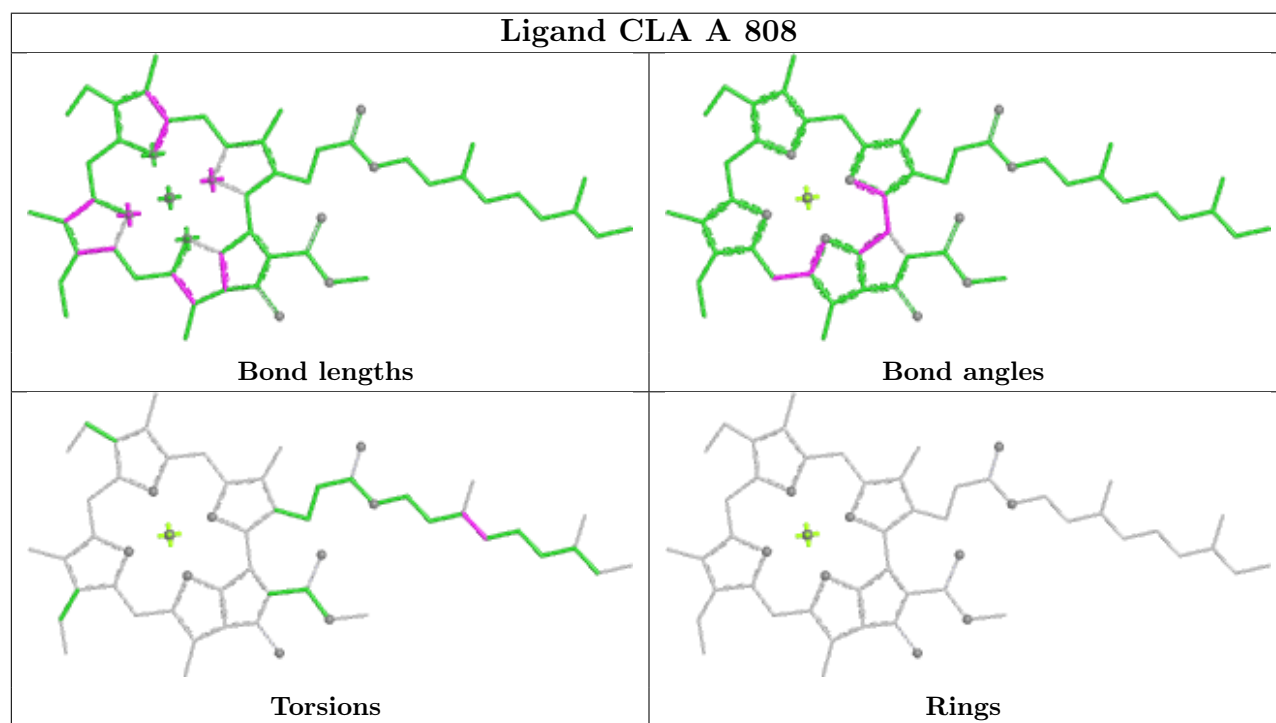
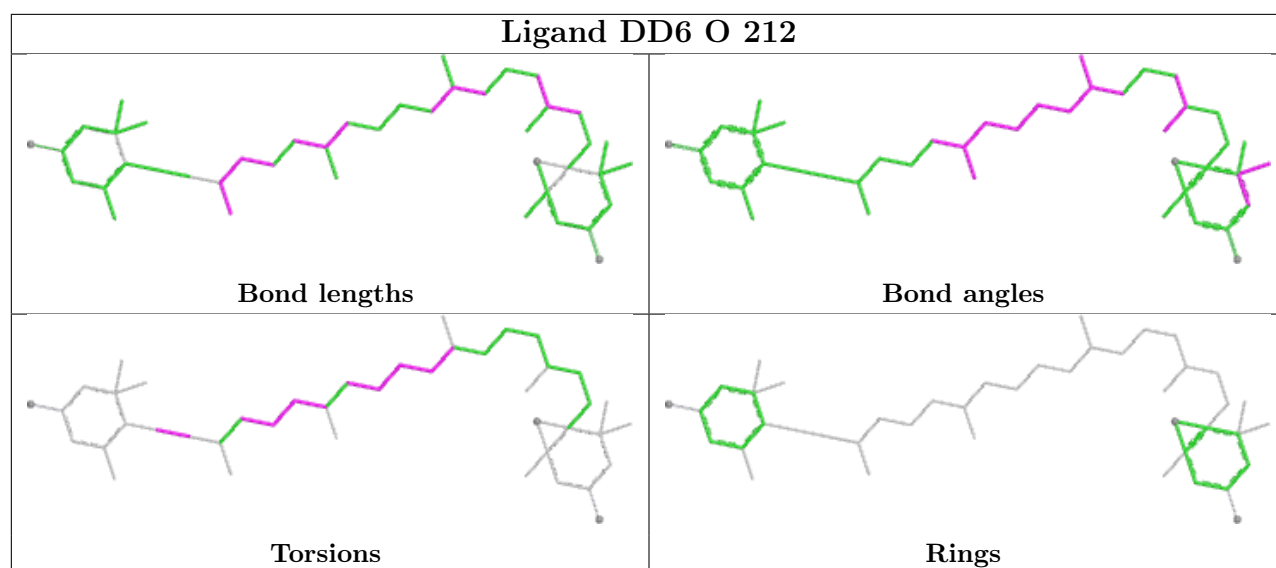


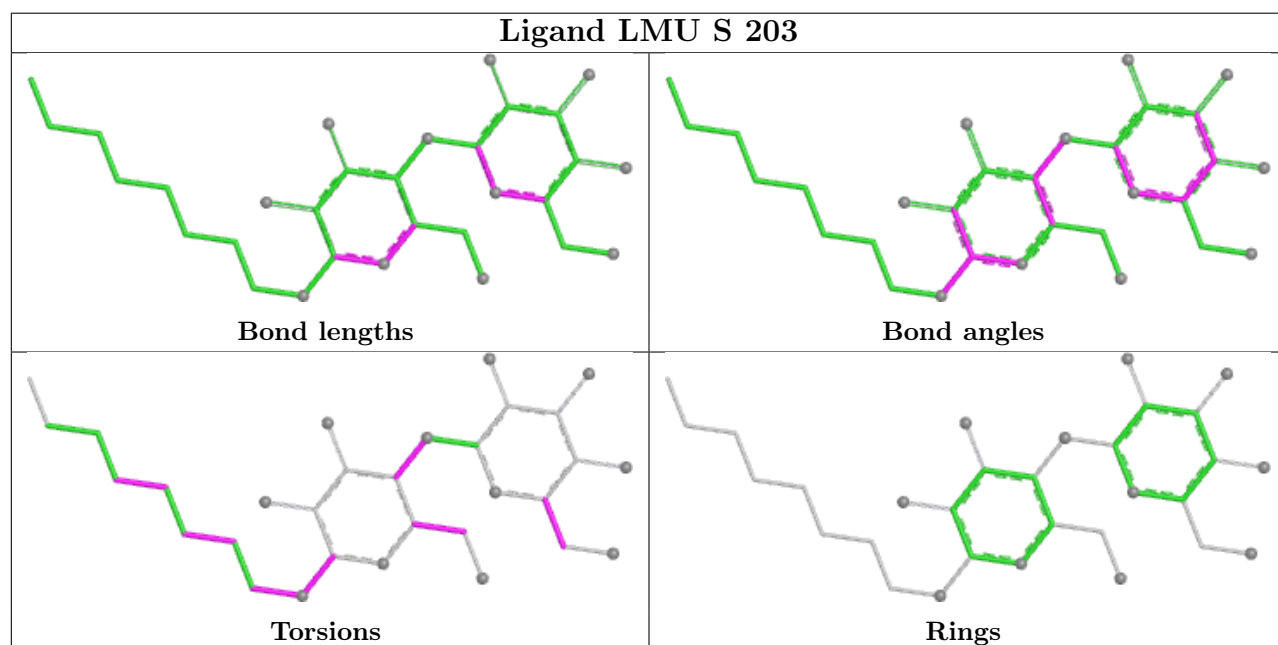
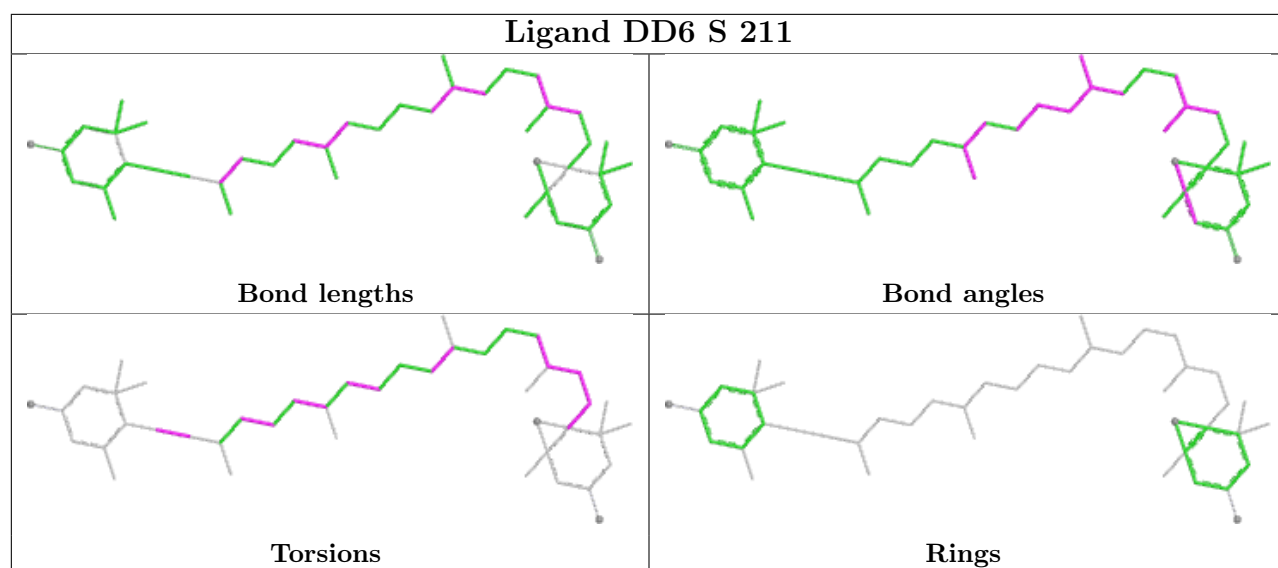
Torsions

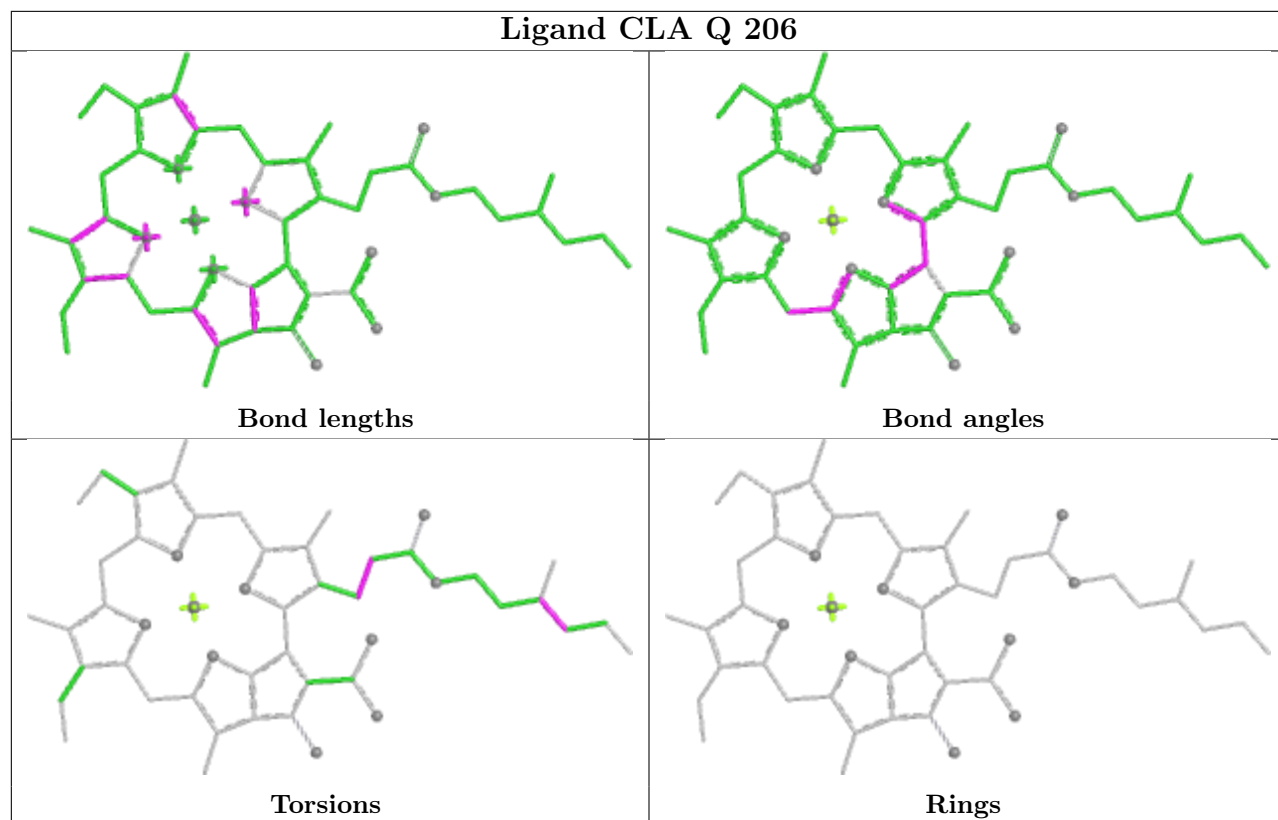


Rings

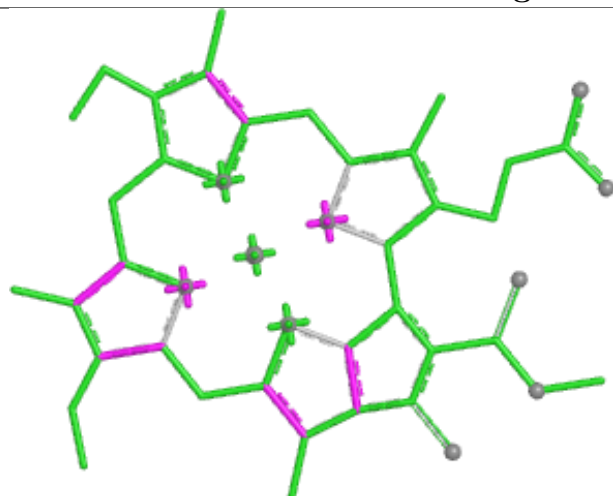




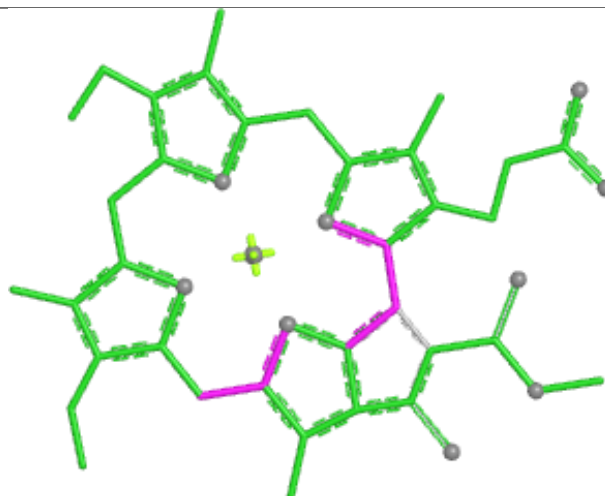




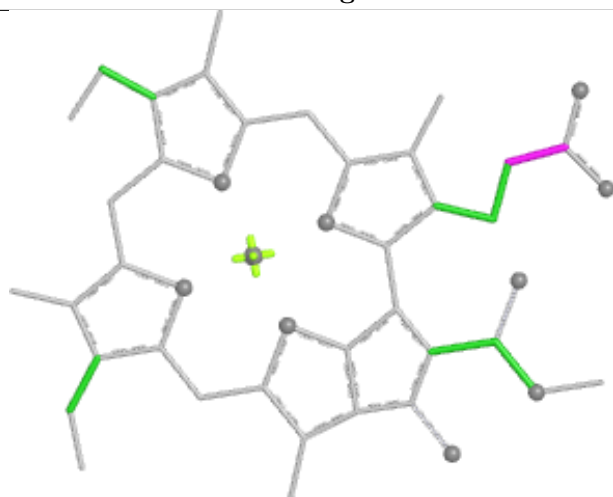
Ligand CLA H 206



Bond lengths



Bond angles

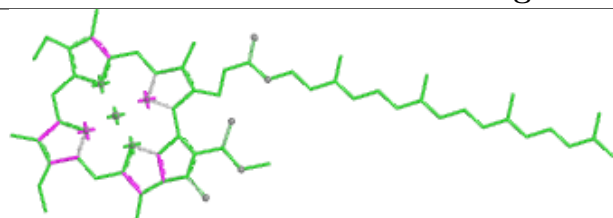


Torsions

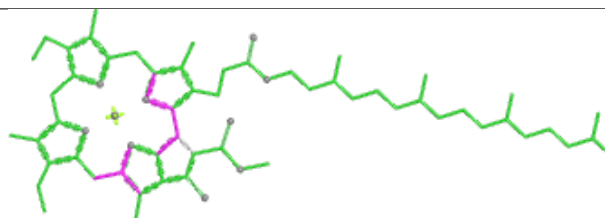


Rings

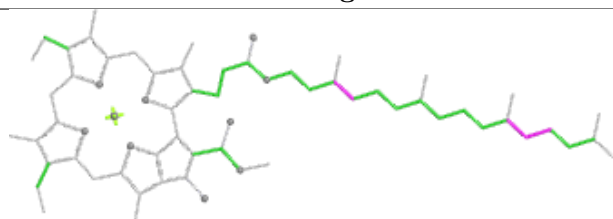
Ligand CLA O 206



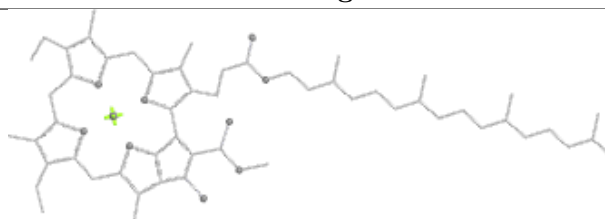
Bond lengths



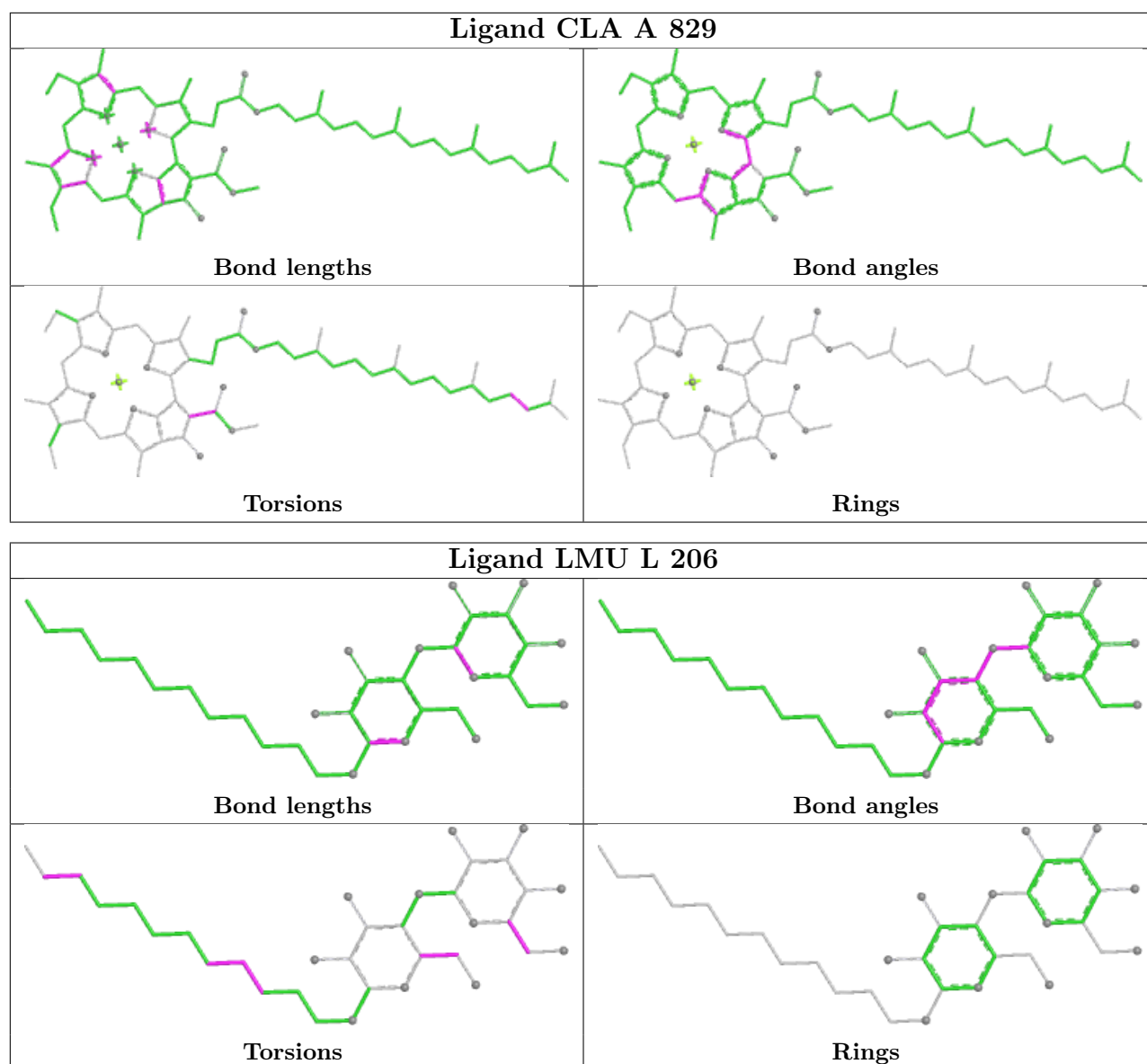
Bond angles



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.

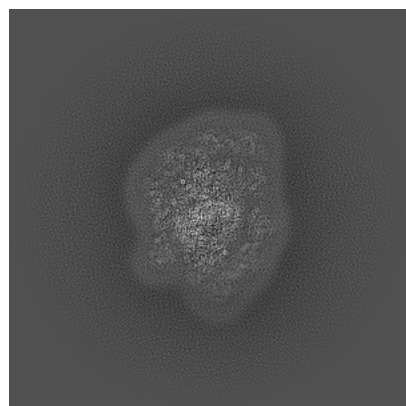
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-64153. These allow visual inspection of the internal detail of the map and identification of artifacts.

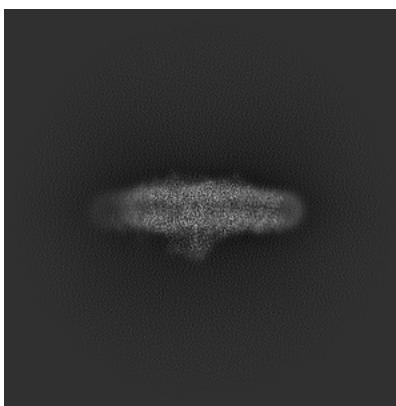
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

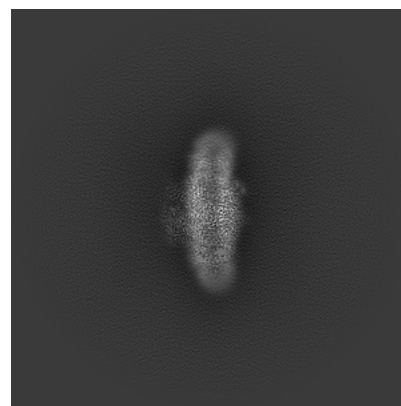
6.1.1 Primary map



X

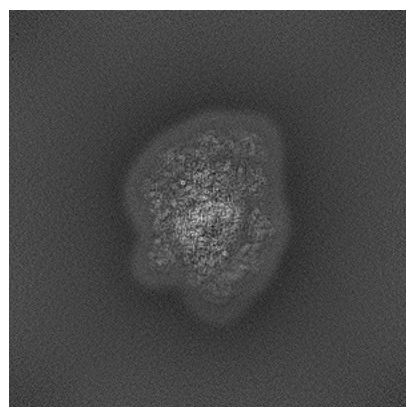


Y

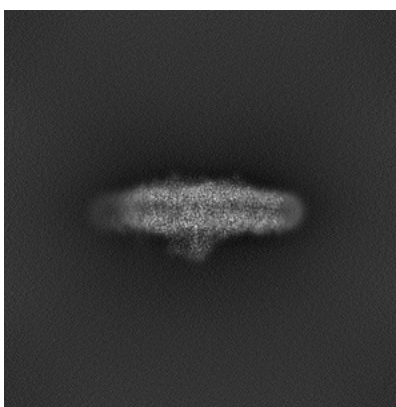


Z

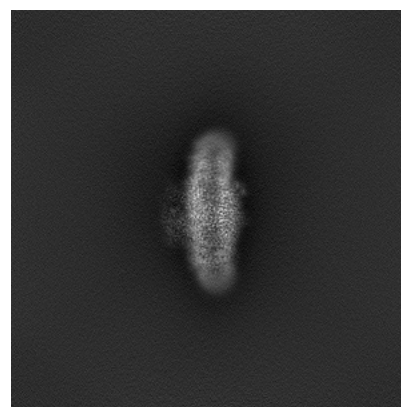
6.1.2 Raw map



X



Y

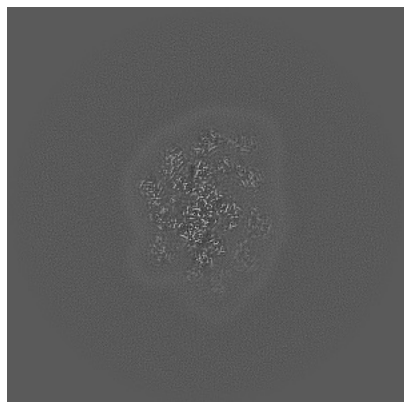


Z

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

6.2 Central slices [i](#)

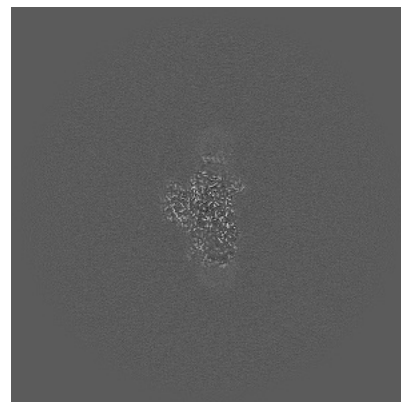
6.2.1 Primary map



X Index: 300

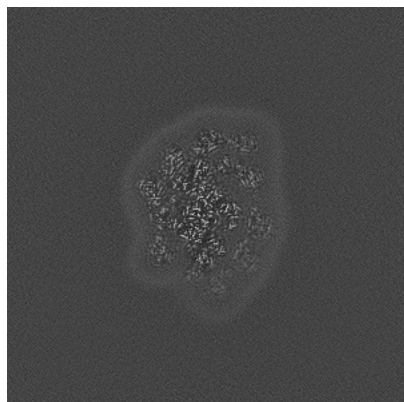


Y Index: 300

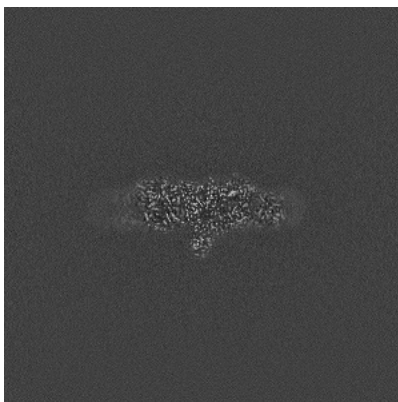


Z Index: 300

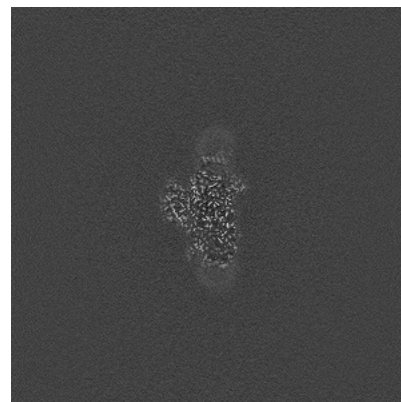
6.2.2 Raw map



X Index: 300



Y Index: 300

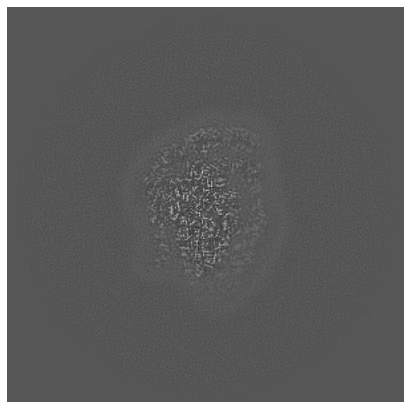


Z Index: 300

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

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 316

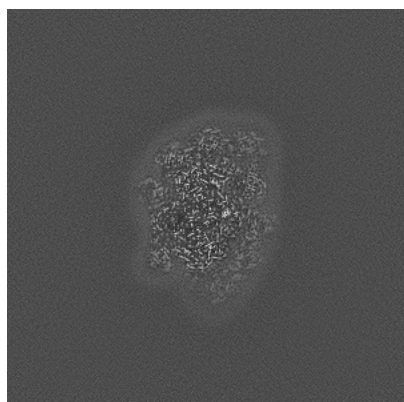


Y Index: 290

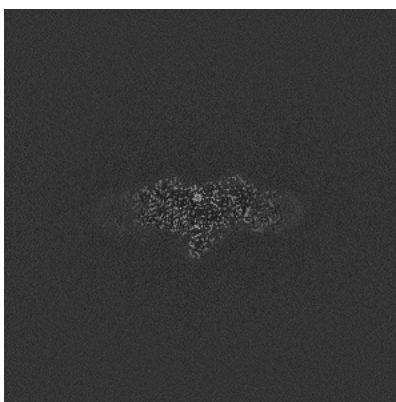


Z Index: 288

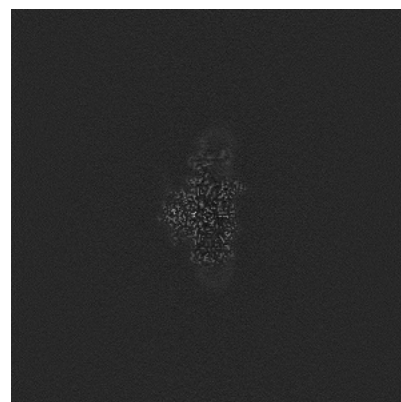
6.3.2 Raw map



X Index: 285



Y Index: 289

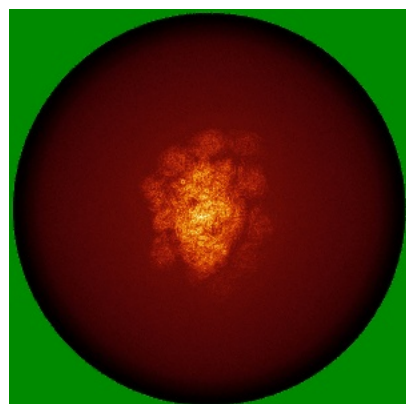


Z Index: 288

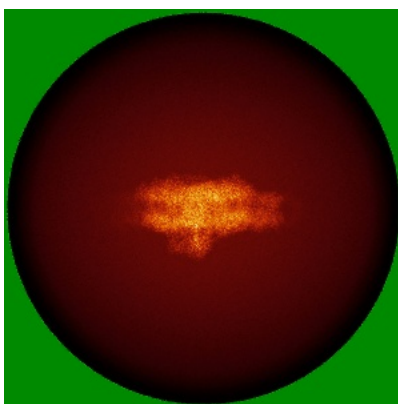
The images above show the largest variance slices of the map in three orthogonal directions.

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

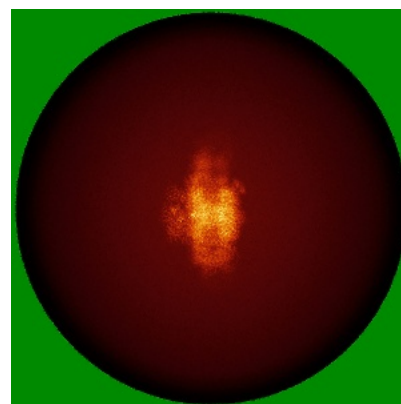
6.4.1 Primary map



X

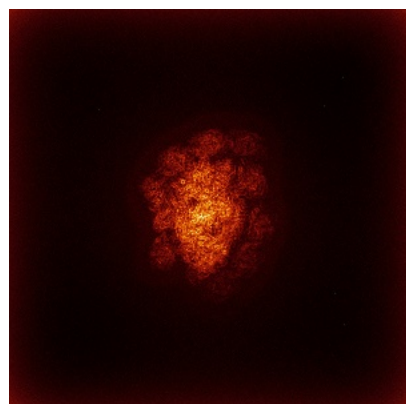


Y



Z

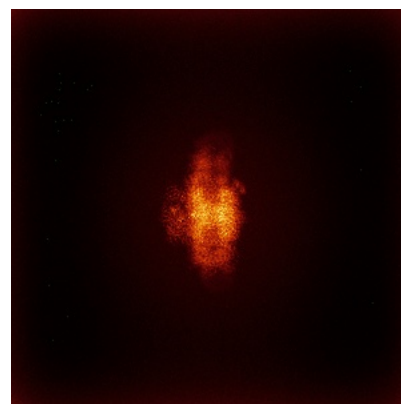
6.4.2 Raw map



X



Y

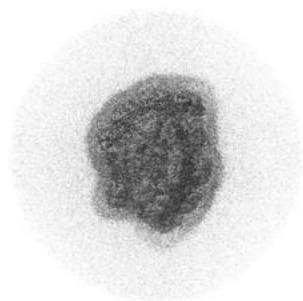


Z

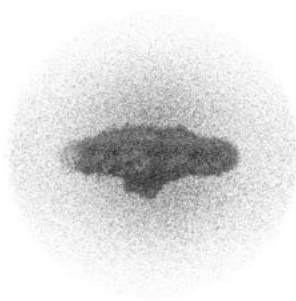
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



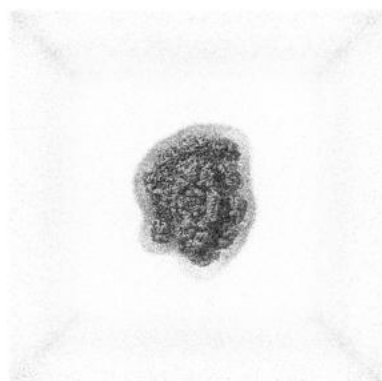
Y



Z

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

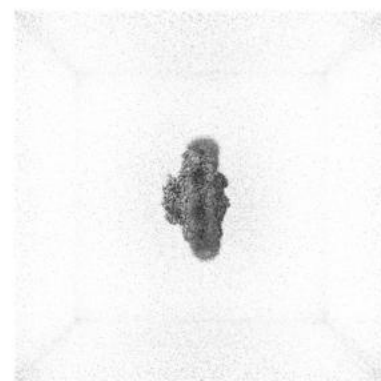
6.5.2 Raw map



X



Y



Z

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.

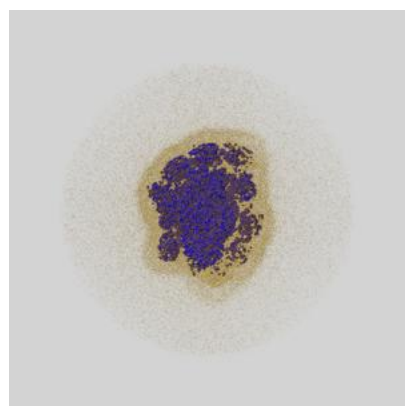
6.6 Mask visualisation [i](#)

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

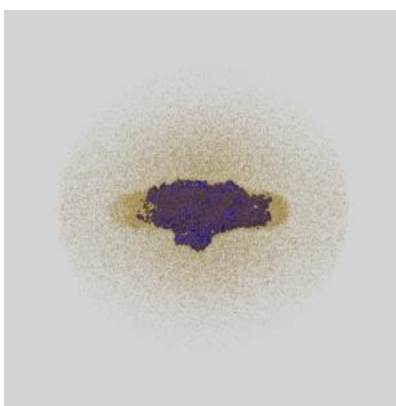
A mask typically either:

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

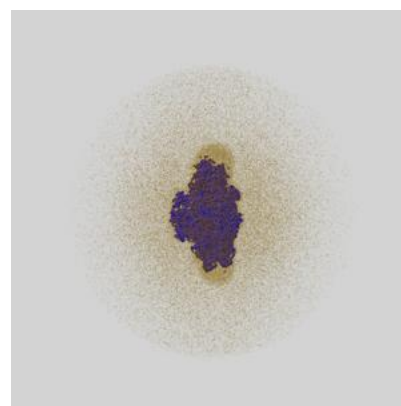
6.6.1 emd_64153_msk_1.map [i](#)



X



Y

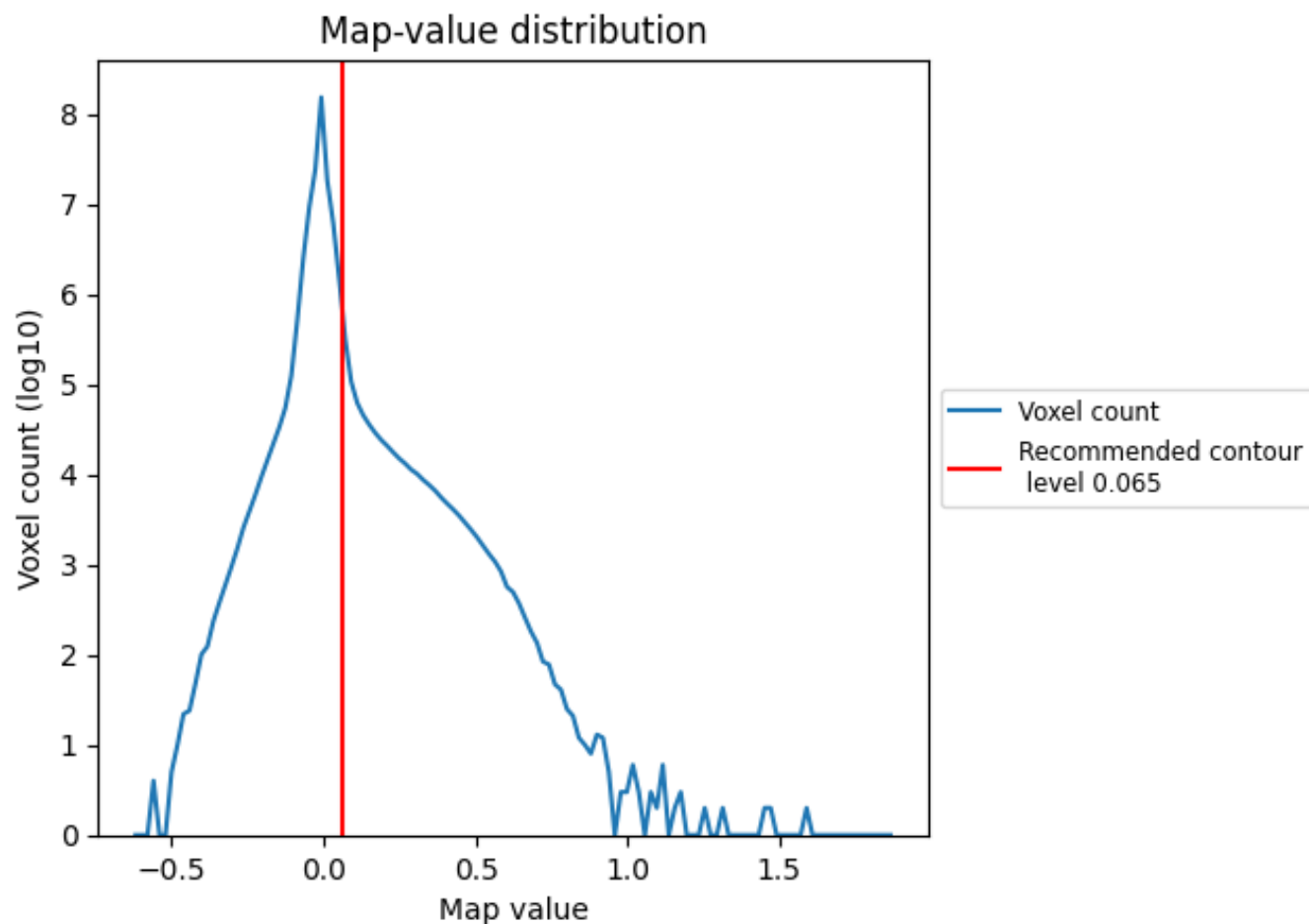


Z

7 Map analysis [i](#)

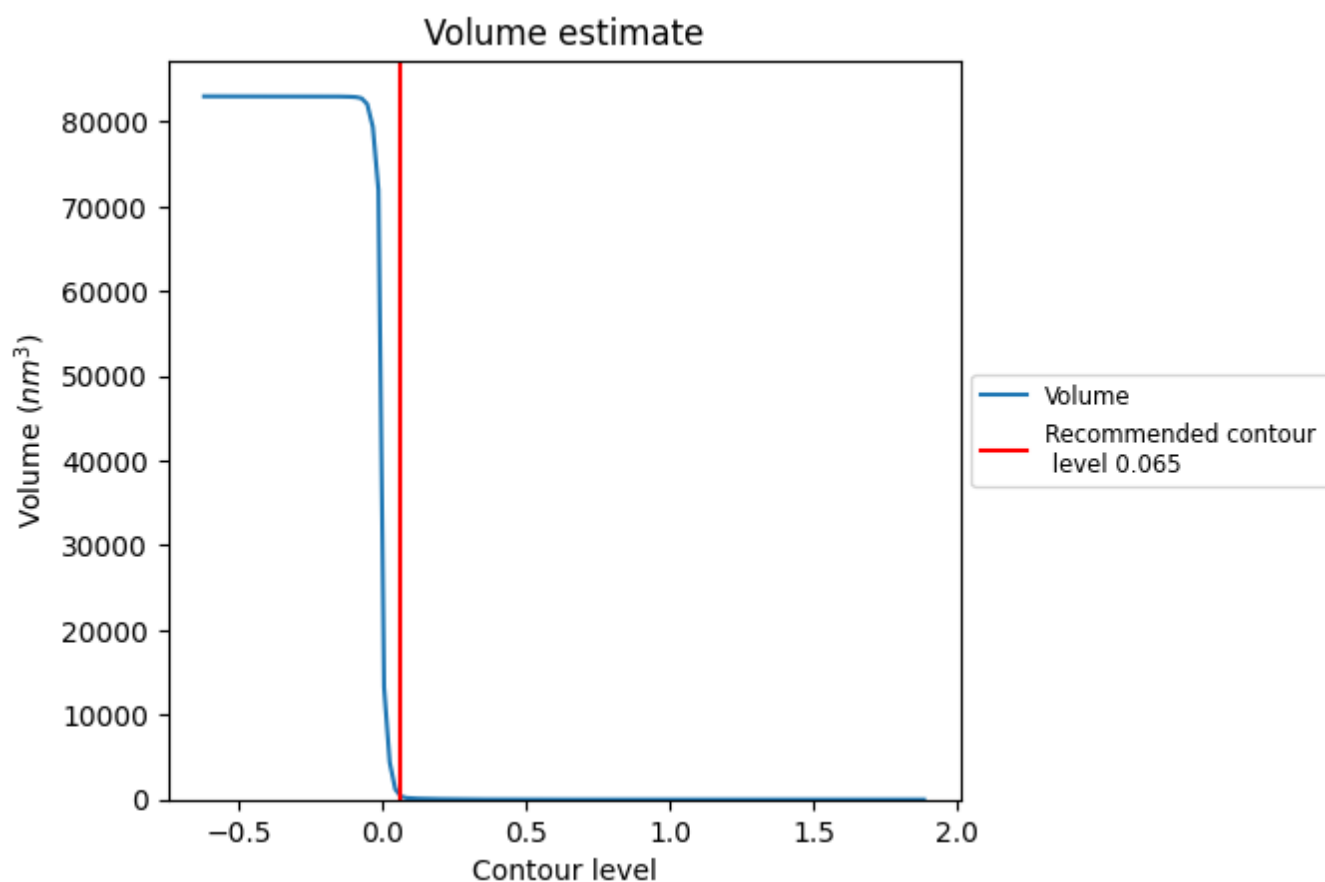
This section contains the results of statistical analysis of the map.

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.

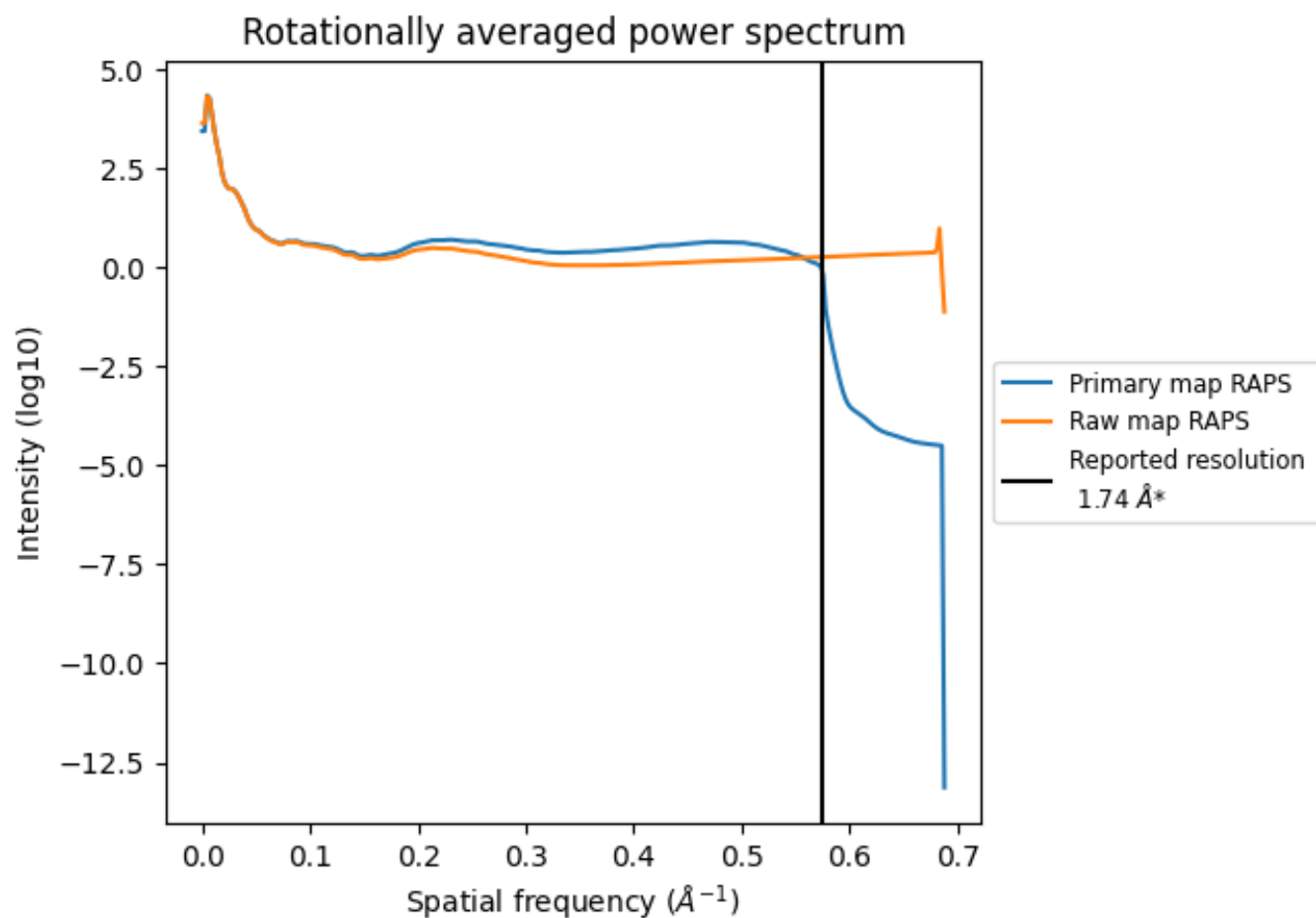
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 416 nm^3 ; this corresponds to an approximate mass of 375 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 ⓘ

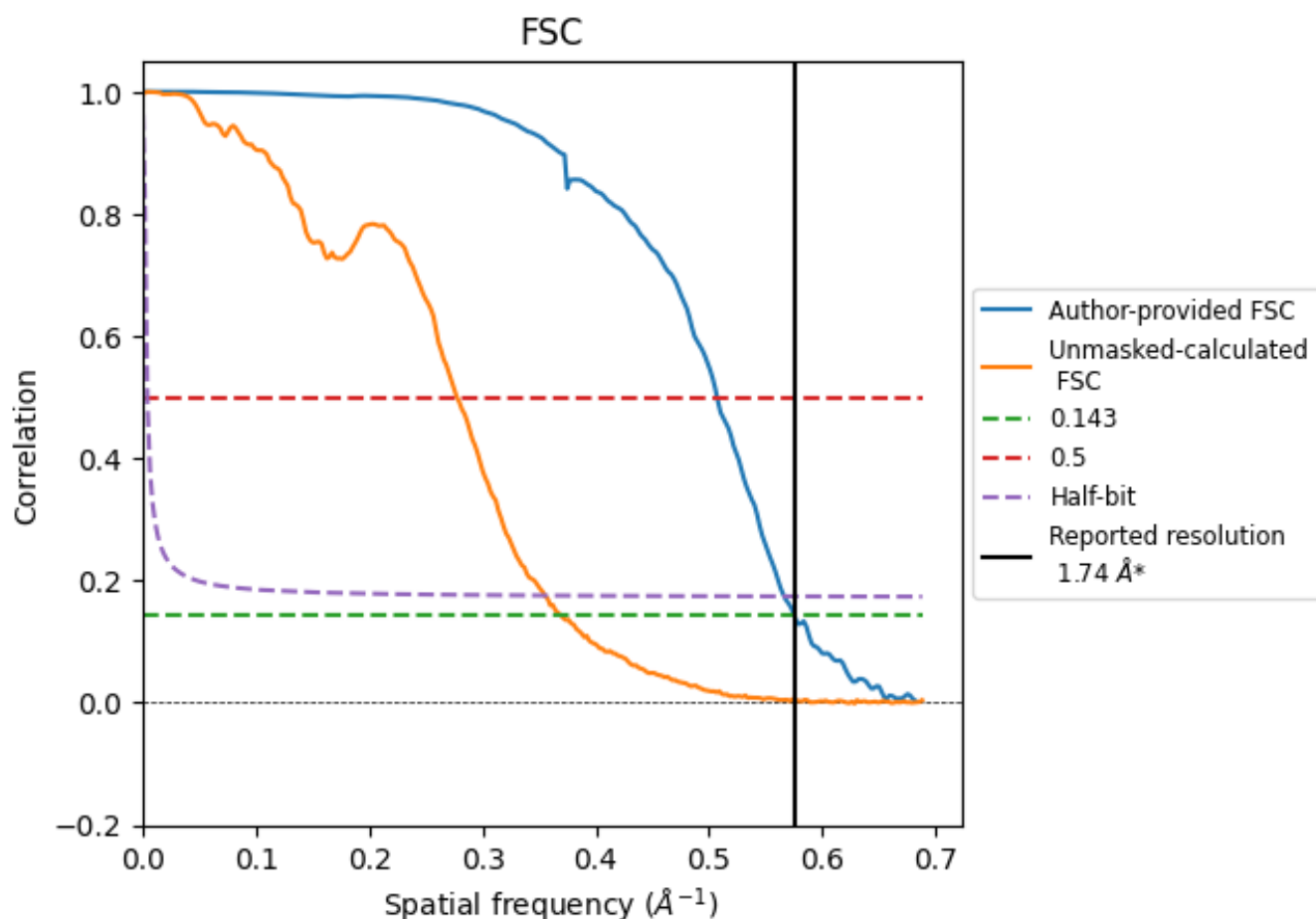


*Reported resolution corresponds to spatial frequency of 0.575 \AA^{-1}

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.575 \AA^{-1}

8.2 Resolution estimates [i](#)

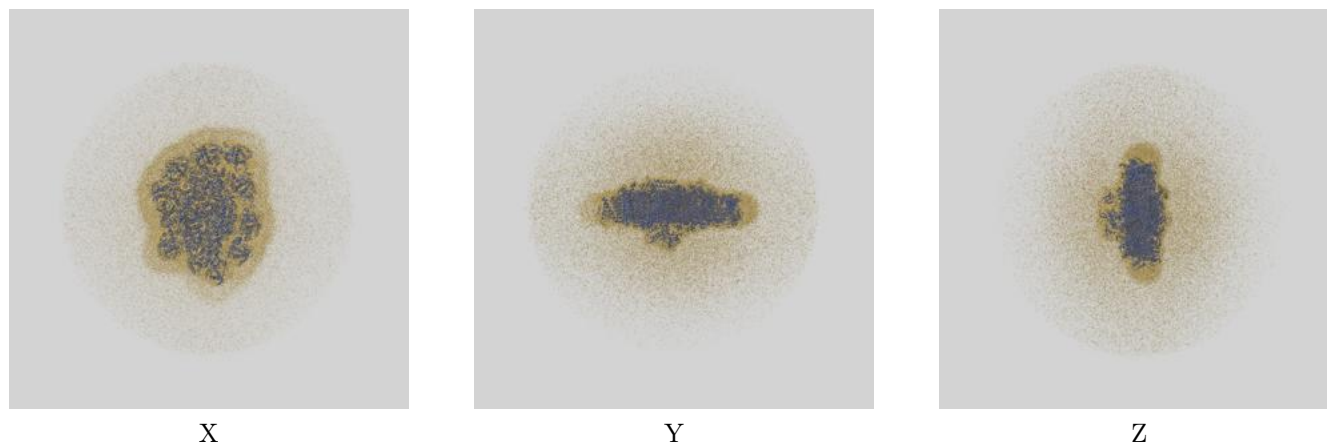
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	1.74	-	-
Author-provided FSC curve	1.74	1.97	1.77
Unmasked-calculated*	2.71	3.60	2.82

*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 2.71 differs from the reported value 1.74 by more than 10 %

9 Map-model fit [i](#)

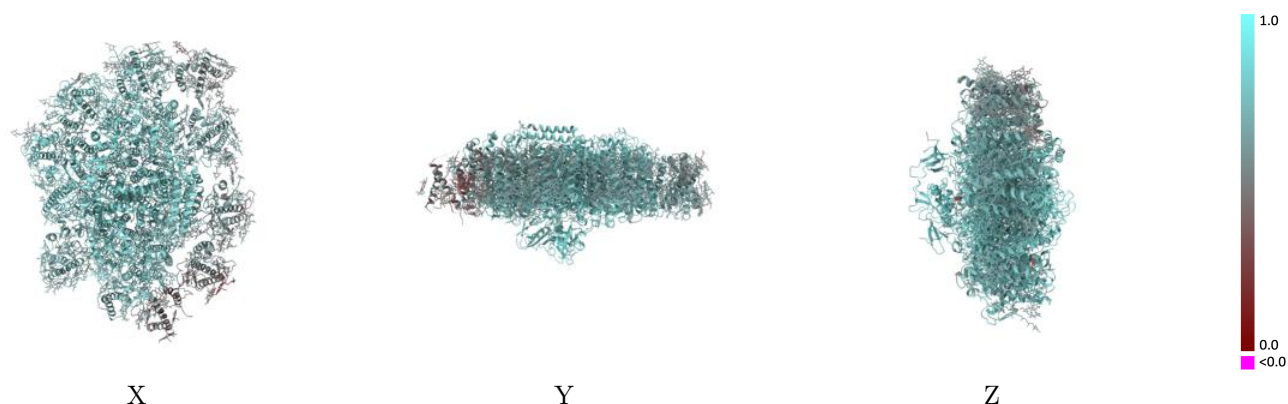
This section contains information regarding the fit between EMDB map EMD-64153 and PDB model 9UH3. Per-residue inclusion information can be found in [section 3](#) on [page 31](#).

9.1 Map-model overlay [i](#)



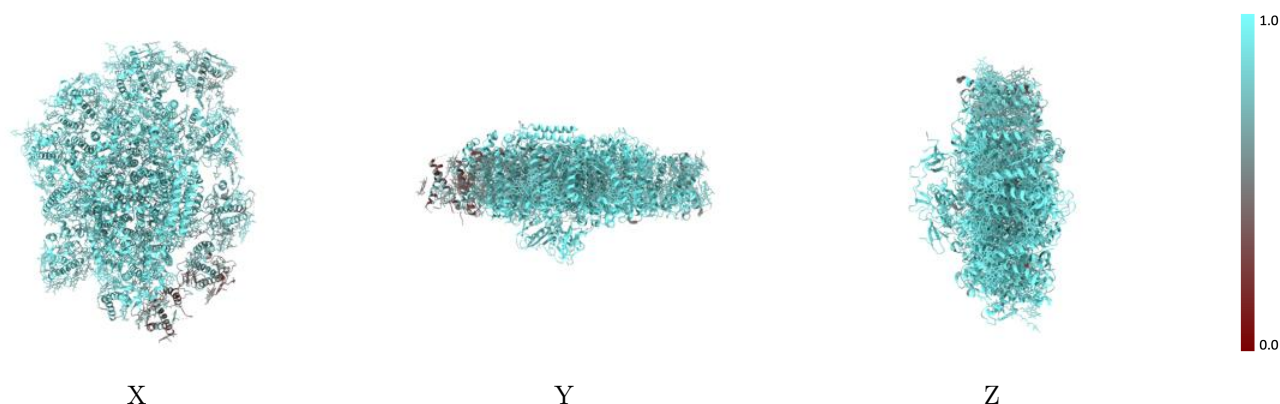
The images above show the 3D surface view of the map at the recommended contour level 0.065 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



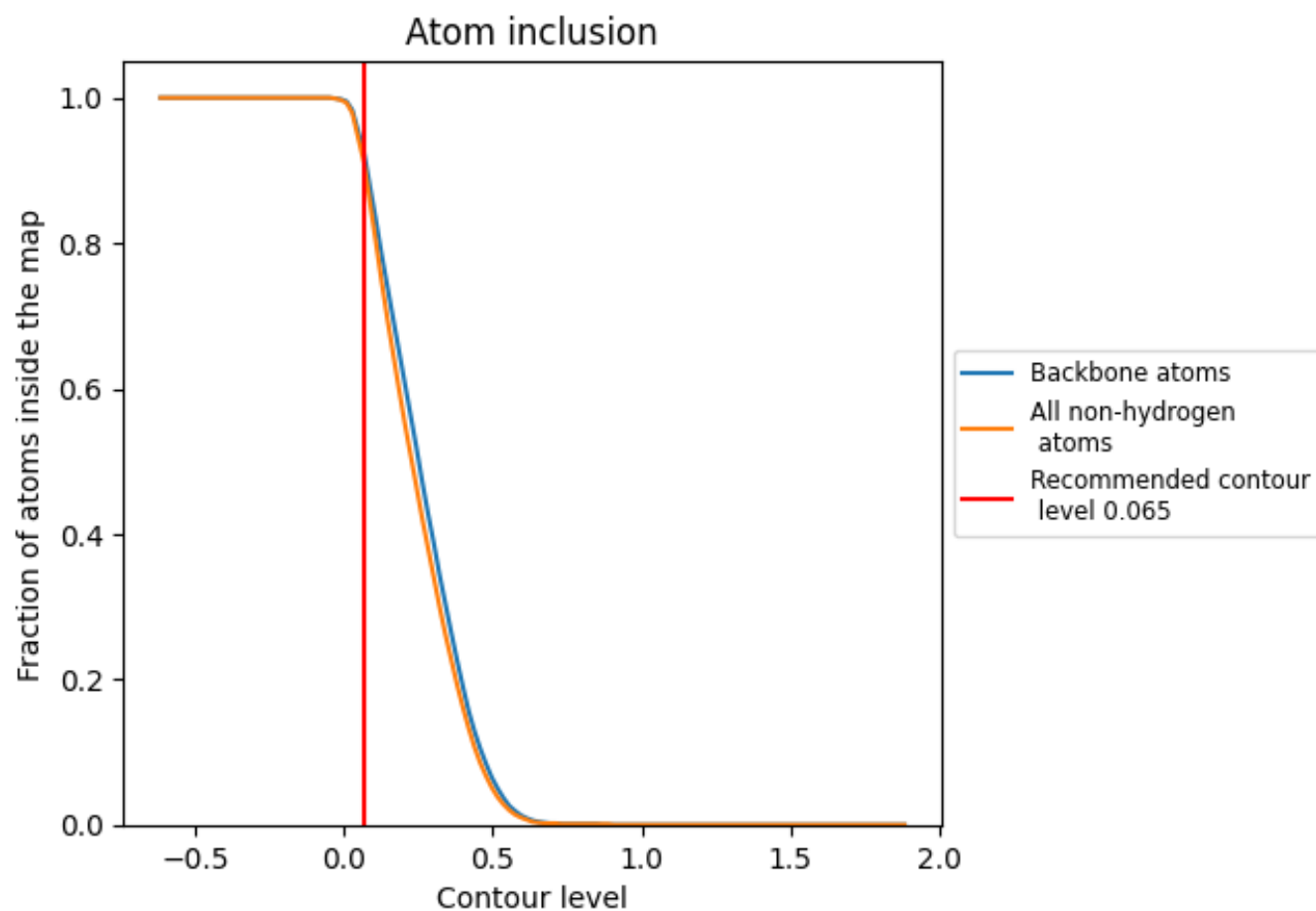
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.065).













































9.4 Atom inclusion [i](#)



At the recommended contour level, 93% of all backbone atoms, 91% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

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

Chain	Atom inclusion	Q-score
All	 0.9140	 0.7220
A	 0.9690	 0.7790
B	 0.9840	 0.8090
C	 0.9980	 0.8330
D	 0.9700	 0.7820
E	 0.9520	 0.7730
F	 0.9550	 0.7550
G	 0.7920	 0.5830
H	 0.6390	 0.5150
I	 0.9860	 0.8110
J	 0.9650	 0.7480
K	 0.4900	 0.4410
L	 0.9560	 0.7740
M	 0.9790	 0.7990
O	 0.9340	 0.7160
P	 0.8940	 0.6600
Q	 0.8910	 0.6650
R	 0.9550	 0.7440
S	 0.9440	 0.7330
T	 0.7520	 0.5480
U	 0.8730	 0.6620
k	 0.8200	 0.6270

