



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 03:56 PM UTC

PDB ID : 8J7B / pdb_00008j7b
EMDB ID : EMD-36037
Title : Coordinates of Cryo-EM structure of the Arabidopsis thaliana PSI in state 2 (PSI-ST2)
Authors : Chen, S.J.B.; Wu, J.H.; Sui, S.F.; Zhang, L.X.
Deposited on : 2023-04-27
Resolution : 3.22 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

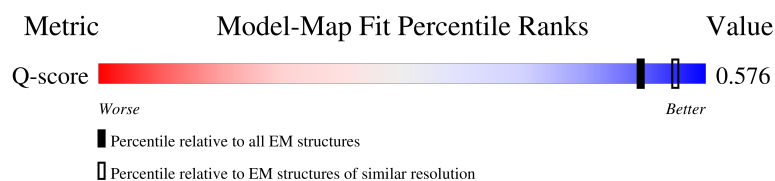
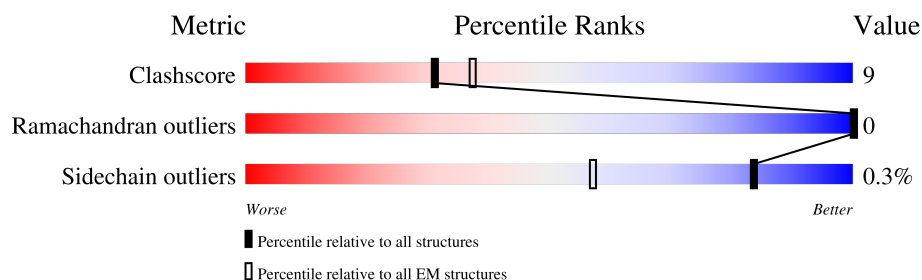
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.22 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	14612 (2.72 - 3.72)

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	1	241	 65% 15% 20%
2	2	257	 69% 9% 22%
3	3	273	 70% 10% 20%
4	4	251	 67% 11% 22%

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Mol	Chain	Length	Quality of chain
5	A	750	
6	B	734	
7	C	81	
8	D	204	
9	E	143	
10	F	221	
11	G	160	
12	H	145	
13	I	37	
14	J	44	
15	K	130	
16	L	219	

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
17	CHL	1	601	X	-	-	-
17	CHL	1	606	X	-	-	-
17	CHL	2	601	X	-	-	-
17	CHL	2	605	X	-	-	-
17	CHL	2	606	X	-	-	-
17	CHL	2	607	X	-	-	-
17	CHL	2	615	X	-	-	-
17	CHL	3	606	X	-	-	-
17	CHL	4	605	X	-	-	-
17	CHL	4	606	X	-	-	-
17	CHL	4	607	X	-	-	-
17	CHL	4	615	X	-	-	-
18	CLA	1	602	X	-	-	-
18	CLA	1	603	X	-	-	-
18	CLA	1	604	X	-	-	-
18	CLA	1	605	X	-	-	-
18	CLA	1	607	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
18	CLA	1	608	X	-	-	-
18	CLA	1	609	X	-	-	-
18	CLA	1	610	X	-	-	-
18	CLA	1	611	X	-	-	-
18	CLA	1	612	X	-	-	-
18	CLA	1	613	X	-	-	-
18	CLA	2	602	X	-	-	-
18	CLA	2	603	X	-	-	-
18	CLA	2	604	X	-	-	-
18	CLA	2	608	X	-	-	-
18	CLA	2	609	X	-	-	-
18	CLA	2	610	X	-	-	-
18	CLA	2	611	X	-	-	-
18	CLA	2	612	X	-	-	-
18	CLA	2	613	X	-	-	-
18	CLA	3	601	X	-	-	-
18	CLA	3	602	X	-	-	-
18	CLA	3	603	X	-	-	-
18	CLA	3	604	X	-	-	-
18	CLA	3	605	X	-	-	-
18	CLA	3	607	X	-	-	-
18	CLA	3	608	X	-	-	-
18	CLA	3	609	X	-	-	-
18	CLA	3	610	X	-	-	-
18	CLA	3	611	X	-	-	-
18	CLA	3	612	X	-	-	-
18	CLA	4	601	X	-	-	-
18	CLA	4	602	X	-	-	-
18	CLA	4	603	X	-	-	-
18	CLA	4	604	X	-	-	-
18	CLA	4	608	X	-	-	-
18	CLA	4	609	X	-	-	-
18	CLA	4	610	X	-	-	-
18	CLA	4	611	X	-	-	-
18	CLA	4	612	X	-	-	-
18	CLA	4	613	X	-	-	-
18	CLA	4	614	X	-	-	-
18	CLA	A	802	X	-	-	-
18	CLA	A	803	X	-	-	-
18	CLA	A	804	X	-	-	-
18	CLA	A	805	X	-	-	-
18	CLA	A	806	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
18	CLA	A	807	X	-	-	-
18	CLA	A	808	X	-	-	-
18	CLA	A	809	X	-	-	-
18	CLA	A	810	X	-	-	-
18	CLA	A	811	X	-	-	-
18	CLA	A	812	X	-	-	-
18	CLA	A	813	X	-	-	-
18	CLA	A	814	X	-	-	-
18	CLA	A	815	X	-	-	-
18	CLA	A	816	X	-	-	-
18	CLA	A	817	X	-	-	-
18	CLA	A	818	X	-	-	-
18	CLA	A	819	X	-	-	-
18	CLA	A	820	X	-	-	-
18	CLA	A	821	X	-	-	-
18	CLA	A	822	X	-	-	-
18	CLA	A	823	X	-	-	-
18	CLA	A	824	X	-	-	-
18	CLA	A	825	X	-	-	-
18	CLA	A	826	X	-	-	-
18	CLA	A	827	X	-	-	-
18	CLA	A	828	X	-	-	-
18	CLA	A	829	X	-	-	-
18	CLA	A	830	X	-	-	-
18	CLA	A	831	X	-	-	-
18	CLA	A	832	X	-	-	-
18	CLA	A	833	X	-	-	-
18	CLA	A	834	X	-	-	-
18	CLA	A	835	X	-	-	-
18	CLA	A	836	X	-	-	-
18	CLA	A	837	X	-	-	-
18	CLA	A	838	X	-	-	-
18	CLA	A	839	X	-	-	-
18	CLA	A	840	X	-	-	-
18	CLA	A	841	X	-	-	-
18	CLA	A	842	X	-	-	-
18	CLA	A	843	X	-	-	-
18	CLA	A	844	X	-	-	-
18	CLA	A	845	X	-	-	-
18	CLA	B	802	X	-	-	-
18	CLA	B	803	X	-	-	-
18	CLA	B	804	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
18	CLA	B	805	X	-	-	-
18	CLA	B	806	X	-	-	-
18	CLA	B	807	X	-	-	-
18	CLA	B	808	X	-	-	-
18	CLA	B	809	X	-	-	-
18	CLA	B	810	X	-	-	-
18	CLA	B	811	X	-	-	-
18	CLA	B	812	X	-	-	-
18	CLA	B	813	X	-	-	-
18	CLA	B	814	X	-	-	-
18	CLA	B	815	X	-	-	-
18	CLA	B	816	X	-	-	-
18	CLA	B	817	X	-	-	-
18	CLA	B	818	X	-	-	-
18	CLA	B	819	X	-	-	-
18	CLA	B	820	X	-	-	-
18	CLA	B	821	X	-	-	-
18	CLA	B	822	X	-	-	-
18	CLA	B	823	X	-	-	-
18	CLA	B	824	X	-	-	-
18	CLA	B	825	X	-	-	-
18	CLA	B	826	X	-	-	-
18	CLA	B	827	X	-	-	-
18	CLA	B	828	X	-	-	-
18	CLA	B	829	X	-	-	-
18	CLA	B	830	X	-	-	-
18	CLA	B	831	X	-	-	-
18	CLA	B	832	X	-	-	-
18	CLA	B	833	X	-	-	-
18	CLA	B	834	X	-	-	-
18	CLA	B	835	X	-	-	-
18	CLA	B	836	X	-	-	-
18	CLA	B	837	X	-	-	-
18	CLA	B	838	X	-	-	-
18	CLA	B	839	X	-	-	-
18	CLA	B	840	X	-	-	-
18	CLA	B	841	X	-	-	-
18	CLA	F	301	X	-	-	-
18	CLA	F	302	X	-	-	-
18	CLA	F	303	X	-	-	-
18	CLA	G	201	X	-	-	-
18	CLA	G	202	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
18	CLA	G	203	X	-	-	-
18	CLA	H	201	X	-	-	-
18	CLA	J	101	X	-	-	-
18	CLA	K	201	X	-	-	-
18	CLA	K	203	X	-	-	-
18	CLA	K	204	X	-	-	-
18	CLA	K	206	X	-	-	-
18	CLA	L	302	X	-	-	-
18	CLA	L	303	X	-	-	-
18	CLA	L	304	X	-	-	-
24	CL0	A	801	X	-	-	-

2 Entry composition

There are 27 unique types of molecules in this entry. The entry contains 35077 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 Chlorophyll a-b binding protein 6, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	193	Total	C	N	O	S	0	0
			1496	975	248	268	5		

- Molecule 2 is a protein called Photosystem I chlorophyll a/b-binding protein 2, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	201	Total	C	N	O	S	0	0
			1566	1024	256	282	4		

- Molecule 3 is a protein called Photosystem I chlorophyll a/b-binding protein 3-1, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	3	218	Total	C	N	O	S	0	0
			1666	1088	270	303	5		

- Molecule 4 is a protein called Chlorophyll a-b binding protein 4, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	4	196	Total	C	N	O	S	0	0
			1551	1013	253	282	3		

- Molecule 5 is a protein called Photosystem I P700 chlorophyll a apoprotein A1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	A	737	Total	C	N	O	S	0	0
			5807	3807	986	996	18		

- Molecule 6 is a protein called Photosystem I P700 chlorophyll a apoprotein A2.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	B	732	Total	C	N	O	S	0	0
			5854	3842	997	1001	14		

- Molecule 7 is a protein called Photosystem I iron-sulfur center.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	C	80	Total	C	N	O	S	0	0
			616	381	107	117	11		

- Molecule 8 is a protein called Photosystem I reaction center subunit II-2, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	D	143	Total	C	N	O	S	0	0
			1128	723	195	206	4		

- Molecule 9 is a protein called Photosystem I reaction center subunit IV A, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	E	64	Total	C	N	O		0	0
			517	331	92	94			

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	F	152	Total	C	N	O	S	0	0
			1208	789	207	209	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	G	91	Total	C	N	O		0	0
			708	458	118	132			

- Molecule 12 is a protein called Photosystem I reaction center subunit VI-2, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	H	90	Total	C	N	O		0	0
			693	451	112	130			

- Molecule 13 is a protein called Photosystem I reaction center subunit VIII.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	I	31	Total	C	N	O	S	0	0
			239	162	39	37	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	J	41	Total	C	N	O	S	0	0
			327	221	50	55	1		

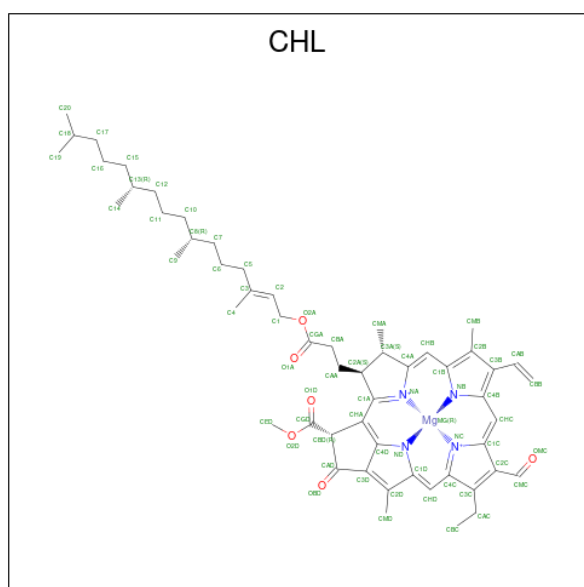
- Molecule 15 is a protein called Photosystem I reaction center subunit psaK, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	K	84	Total	C	N	O	S	0	0
			593	373	104	113	3		

- Molecule 16 is a protein called Photosystem I reaction center subunit XI, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	L	160	Total	C	N	O	S	0	0
			1207	799	191	215	2		

- Molecule 17 is CHLOROPHYLL B (CCD ID: CHL) (formula: $C_{55}H_{70}MgN_4O_6$) (labeled as "Ligand of Interest" by depositor).



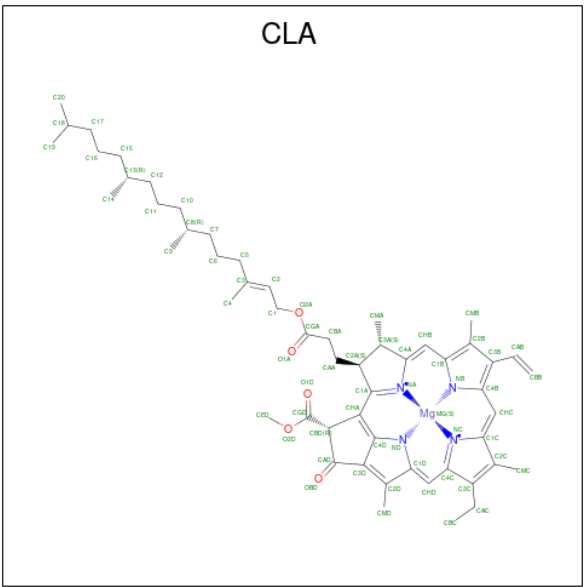
Mol	Chain	Residues	Atoms					AltConf
17	1	1	Total	C	Mg	N	O	0
			52	41	1	4	6	
17	1	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
17	2	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
17	2	1	Total	C	Mg	N	O	0
			43	34	1	4	4	

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Mol	Chain	Residues	Atoms					AltConf
17	2	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
17	2	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
17	2	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
17	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
17	4	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
17	4	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
17	4	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
17	4	1	Total	C	Mg	N	O	0
			46	35	1	4	6	

- Molecule 18 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
18	1	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
18	1	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
18	1	1	Total	C	Mg	N	O	0
			49	39	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
18	1	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
18	1	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
18	1	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
18	1	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
18	1	1	Total	C	Mg	N	O	0
			38	30	1	4	3	
18	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	1	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
18	1	1	Total	C	Mg	N	O	0
			38	30	1	4	3	
18	2	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
18	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	2	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
18	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	2	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
18	2	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
18	2	1	Total	C	Mg	N	O	0
			38	30	1	4	3	
18	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	2	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
18	3	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
18	3	1	Total	C	Mg	N	O	0
			36	30	1	4	1	
18	3	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
18	3	1	Total	C	Mg	N	O	0
			54	44	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
18	3	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
18	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	3	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
18	3	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
18	3	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
18	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	3	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
18	4	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
18	4	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
18	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	4	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
18	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	4	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
18	4	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
18	4	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
18	4	1	Total	C	Mg	N	O	0
			43	33	1	4	5	
18	4	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
18	4	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			52	42	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
18	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	A	1	Total 60	C 50	Mg 1	N 4	O 5	0
18	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
18	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	A	1	Total 54	C 44	Mg 1	N 4	O 5	0
18	A	1	Total 50	C 40	Mg 1	N 4	O 5	0
18	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	A	1	Total 50	C 40	Mg 1	N 4	O 5	0
18	A	1	Total 42	C 34	Mg 1	N 4	O 3	0
18	A	1	Total 41	C 33	Mg 1	N 4	O 3	0
18	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	A	1	Total 52	C 42	Mg 1	N 4	O 5	0
18	A	1	Total 50	C 40	Mg 1	N 4	O 5	0
18	A	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
18	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
18	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
18	B	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
18	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
18	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
18	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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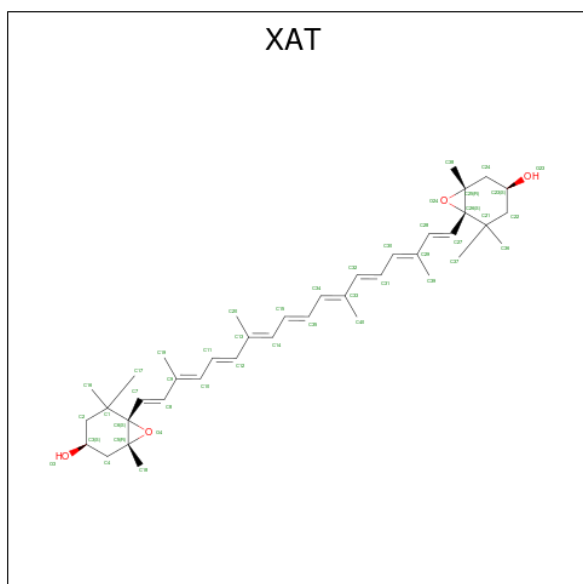
Mol	Chain	Residues	Atoms					AltConf
18	B	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
18	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
18	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
18	B	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
18	F	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
18	F	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
18	F	1	Total	C	Mg	N	O	0
			51	41	1	4	5	

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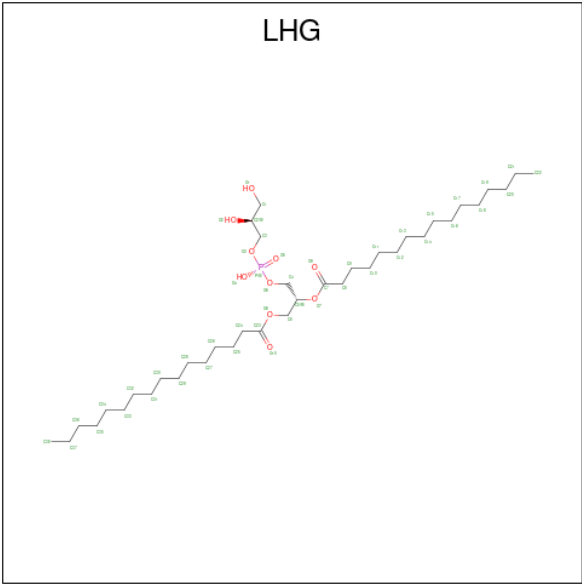
Mol	Chain	Residues	Atoms					AltConf
18	G	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	G	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
18	G	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	H	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
18	J	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
18	K	1	Total	C	Mg	N	O	0
			39	31	1	4	3	
18	K	1	Total	C	Mg	N	O	0
			37	31	1	4	1	
18	K	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
18	K	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	L	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	L	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	L	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

- Molecule 19 is (3S,5R,6S,3'S,5'R,6'S)-5,6,5',6'-DIEPOXY-5,6,5',6'- TETRAHYDRO-BETA ,BETA-CAROTENE-3,3'-DIOL (CCD ID: XAT) (formula: C₄₀H₅₆O₄).



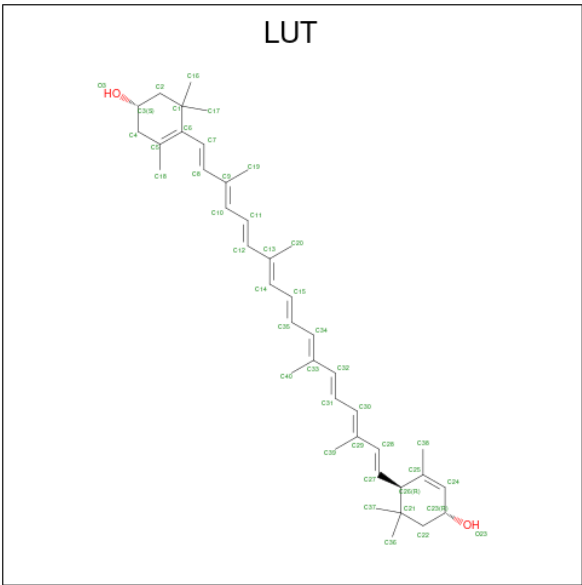
Mol	Chain	Residues	Atoms			AltConf
19	1	1	Total	C	O	0
			44	40	4	
19	2	1	Total	C	O	0
			44	40	4	
19	4	1	Total	C	O	0
			44	40	4	

- Molecule 20 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).



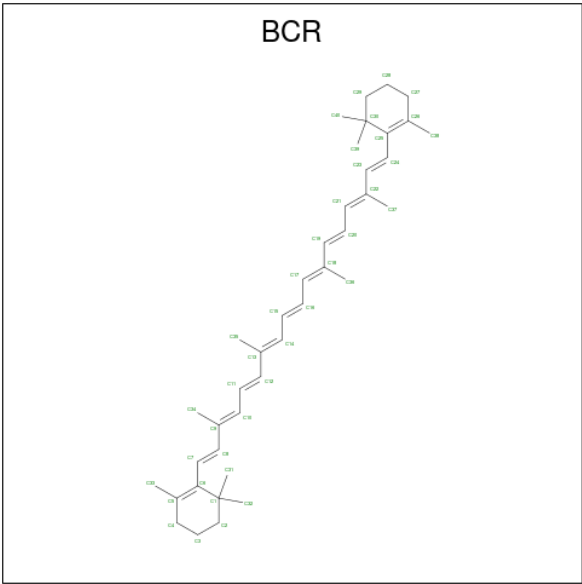
Mol	Chain	Residues	Atoms				AltConf
20	1	1	Total	C	O	P	0
			49	38	10	1	
20	2	1	Total	C	O	P	0
			37	26	10	1	
20	A	1	Total	C	O	P	0
			30	19	10	1	
20	A	1	Total	C	O	P	0
			49	38	10	1	
20	B	1	Total	C	O	P	0
			38	27	10	1	
20	B	1	Total	C	O	P	0
			49	38	10	1	

- Molecule 21 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (CCD ID: LUT) (formula: C₄₀H₅₆O₂).



Mol	Chain	Residues	Atoms			AltConf
21	1	1	Total	C	O	0
			42	40	2	
21	2	1	Total	C	O	0
			42	40	2	
21	2	1	Total	C	O	0
			42	40	2	
21	3	1	Total	C	O	0
			42	40	2	
21	4	1	Total	C	O	0
			42	40	2	

- Molecule 22 is BETA-CAROTENE (CCD ID: BCR) (formula: C₄₀H₅₆).



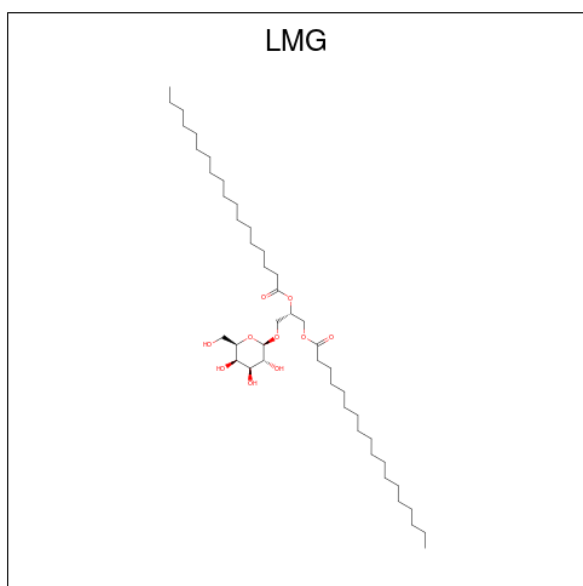
Mol	Chain	Residues	Atoms	AltConf
22	3	1	Total C 40 40	0
22	4	1	Total C 40 40	0
22	A	1	Total C 40 40	0
22	A	1	Total C 40 40	0
22	A	1	Total C 40 40	0
22	A	1	Total C 40 40	0
22	A	1	Total C 40 40	0
22	A	1	Total C 40 40	0
22	B	1	Total C 40 40	0
22	B	1	Total C 40 40	0
22	B	1	Total C 40 40	0
22	B	1	Total C 40 40	0
22	B	1	Total C 40 40	0
22	B	1	Total C 40 40	0
22	B	1	Total C 40 40	0
22	B	1	Total C 40 40	0
22	F	1	Total C 40 40	0
22	G	1	Total C 40 40	0
22	I	1	Total C 40 40	0
22	J	1	Total C 40 40	0
22	K	1	Total C 40 40	0
22	K	1	Total C 40 40	0

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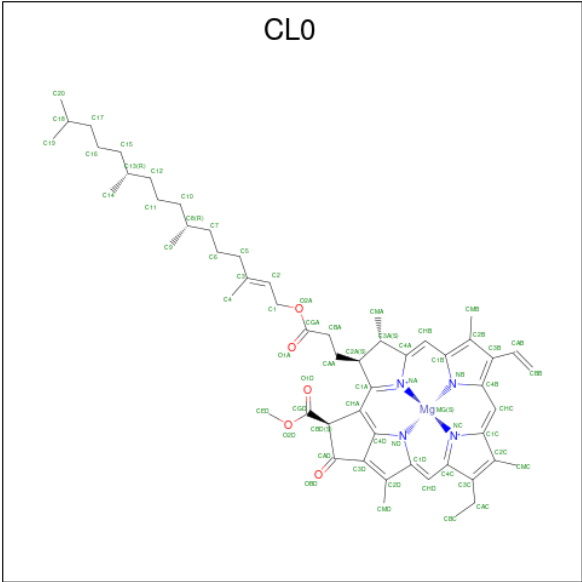
Mol	Chain	Residues	Atoms		AltConf
22	L	1	Total	C	0
			40	40	
22	L	1	Total	C	0
			40	40	
22	L	1	Total	C	0
			40	40	

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



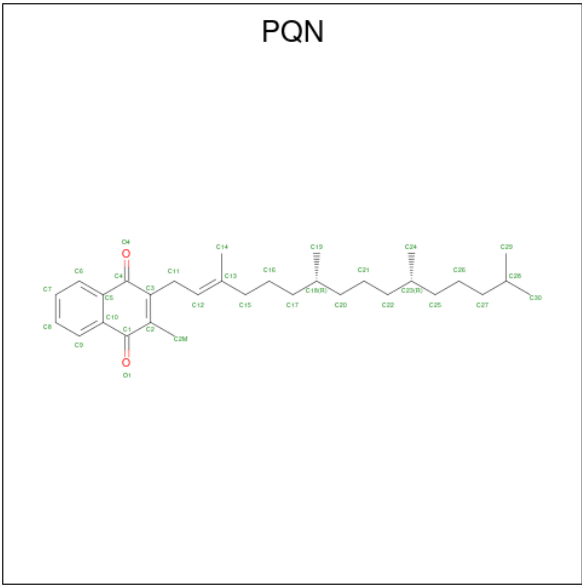
Mol	Chain	Residues	Atoms			AltConf
23	4	1	Total	C	O	0
			39	29	10	
23	4	1	Total	C	O	0
			33	23	10	

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



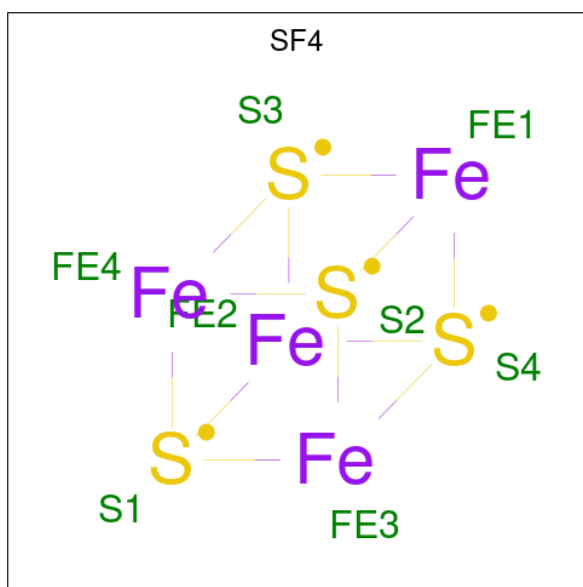
Mol	Chain	Residues	Atoms					AltConf
24	A	1	Total	C	Mg	N	O	0
			60	52	1	4	3	

- Molecule 25 is PHYLLOQUINONE (CCD ID: PQN) (formula: C₃₁H₄₆O₂).



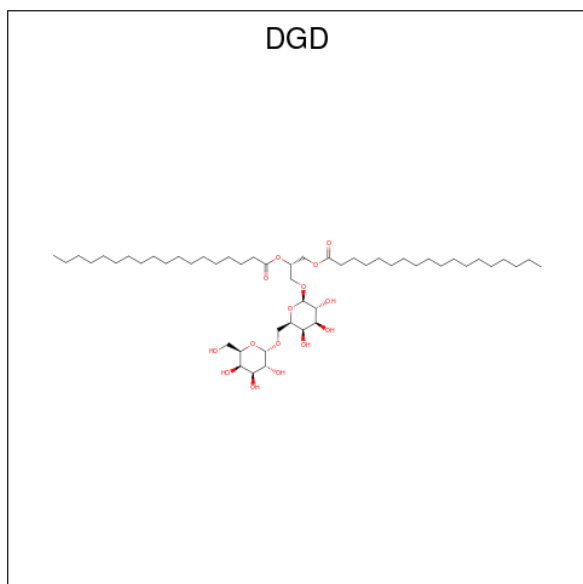
Mol	Chain	Residues	Atoms			AltConf
25	A	1	Total	C	O	0
			33	31	2	
25	B	1	Total	C	O	0
			33	31	2	

- Molecule 26 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



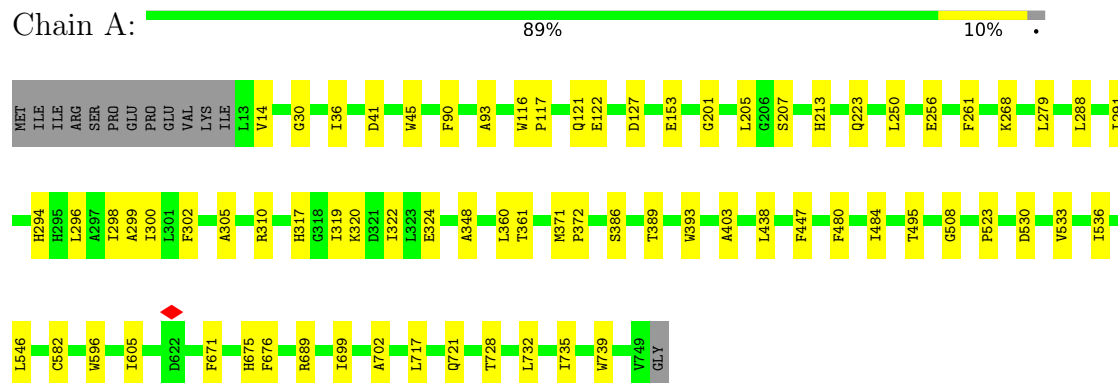
Mol	Chain	Residues	Atoms			AltConf
26	A	1	Total	Fe	S	0
			8	4	4	
26	C	1	Total	Fe	S	0
			8	4	4	
26	C	1	Total	Fe	S	0
			8	4	4	

- Molecule 27 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).

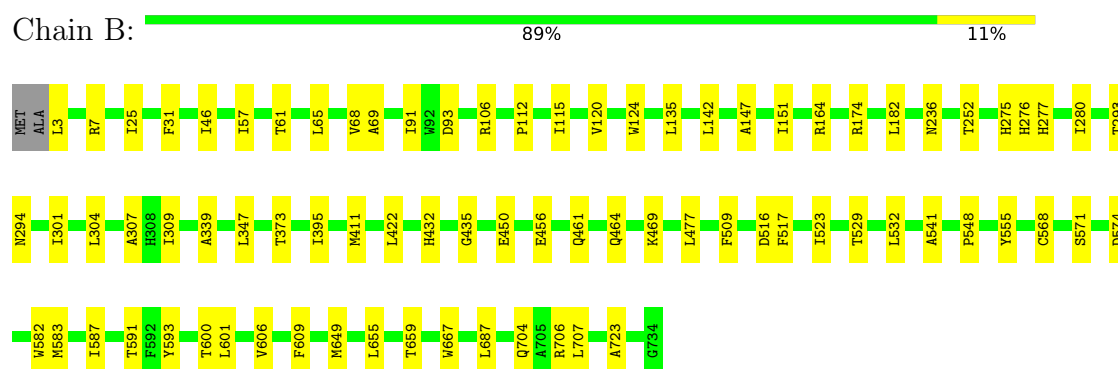


Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
27	B	1	66	51	15	0

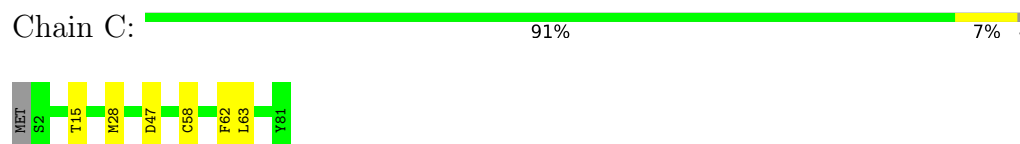
- Molecule 5: Photosystem I P700 chlorophyll a apoprotein A1



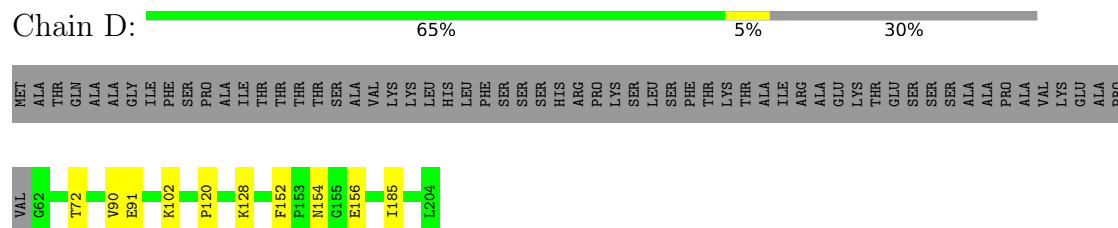
- Molecule 6: Photosystem I P700 chlorophyll a apoprotein A2



- Molecule 7: Photosystem I iron-sulfur center

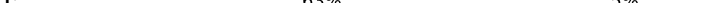


- Molecule 8: Photosystem I reaction center subunit II-2, chloroplatic

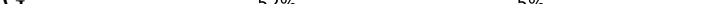


- Molecule 9: Photosystem I reaction center subunit IV A, chloroplastic

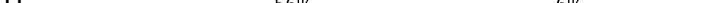
[illegible]

- Chain F:  63% 5% 31%

[illegible]

- Chain G:  52% 5% 43%

[illegible]

- Chain H:  56% 6% 38%

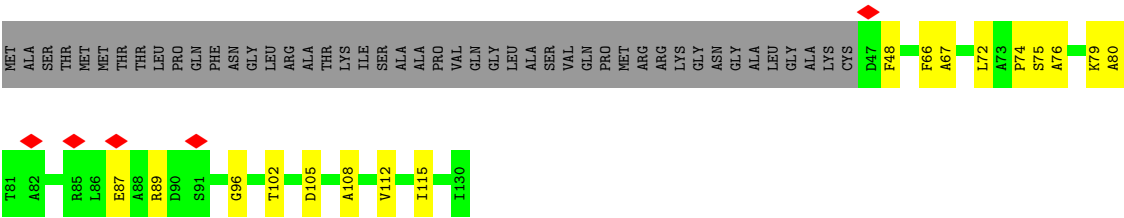
Sequence logo for the 100th position of the 100th protein. The y-axis represents information content in bits, ranging from 0 to 1.5. The x-axis shows the amino acid sequence: MET, ALA, SER, PHE, THR, ILE, ALA, VAL, GLN, PRO, SER, ALA, VAL, LYS, GLY, LEU, GLY, SER, SER, LEU, ALA, GLY, ALA, LYS, LEU, PHE, ILE, LYS, PRO, SER, ARG, GLN, SER, PHE, LYS, THR, LYS, SER, THR, ARG, ALA, GLY, ALA, VAL, VAL, ALA, LYS, TYR, GLY, ASP, LYS. The sequence is color-coded: MET (grey), ALA (light blue), SER (light green), PHE (light orange), THR (light yellow), ILE (light green), ALA (light blue), VAL (light orange), GLN (light yellow), PRO (light green), SER (light orange), ALA (light blue), VAL (light orange), LYS (light green), GLY (light yellow), LEU (light orange), GLY (light yellow), SER (light orange), SER (light orange), LEU (light orange), ALA (light blue), GLY (light yellow), ALA (light blue), LYS (light green), LEU (light orange), PHE (light orange), ILE (light green), LYS (light green), PRO (light green), SER (light orange), ARG (light orange), GLN (light yellow), SER (light orange), PHE (light orange), LYS (light green), THR (light yellow), LYS (light green), SER (light orange), THR (light yellow), ARG (light orange), ALA (light blue), GLY (light yellow), ALA (light blue), VAL (light orange), VAL (light orange), ALA (light blue), LYS (light green), TYR (light yellow), GLY (light yellow), ASP (light orange), LYS (light green). The sequence is flanked by two yellow bars labeled 'S56' and 'S57'.

- Chain I:  76% 8% 16%

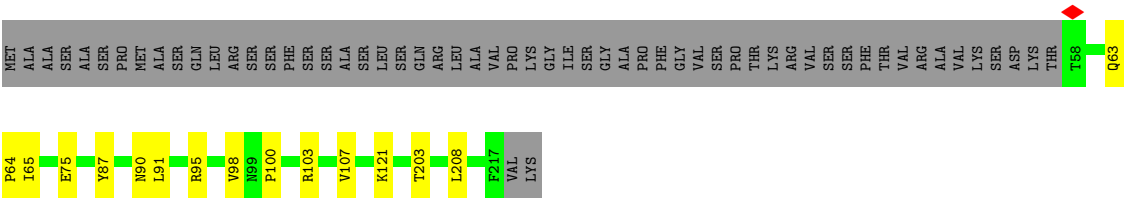
MET
THR
THR
PHE
N5
I10
M24
L27
K35
ILE
PHE

- Chain J:  77% 16% 7%

● Molecule 15: Photosystem I reaction center subunit psaK, chloroplastic



● Molecule 16: Photosystem I reaction center subunit XI, chloroplastic



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	137602	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50.5	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	35.714	Depositor
Minimum map value	-22.642	Depositor
Average map value	0.012	Depositor
Map value standard deviation	1.070	Depositor
Recommended contour level	3.21	Depositor
Map size ($\text{\AA}$)	365.232, 365.232, 365.232	wwPDB
Map dimensions	336, 336, 336	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.087, 1.087, 1.087	Depositor

5 Model quality

5.1 Standard geometry

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

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	1	0.12	0/1546	0.32	0/2110
2	2	0.12	0/1622	0.28	0/2219
3	3	0.13	0/1717	0.30	0/2336
4	4	0.12	0/1599	0.29	0/2178
5	A	0.10	0/6005	0.25	0/8194
6	B	0.11	0/6065	0.28	1/8279 (0.0%)
7	C	0.12	0/629	0.38	0/852
8	D	0.10	0/1157	0.30	0/1563
9	E	0.08	0/528	0.23	0/715
10	F	0.11	0/1238	0.26	0/1670
11	G	0.08	0/724	0.25	0/981
12	H	0.10	0/713	0.27	0/968
13	I	0.12	0/245	0.29	0/333
14	J	0.10	0/336	0.25	0/458
15	K	0.16	0/599	0.50	3/809 (0.4%)
16	L	0.10	0/1244	0.27	0/1700
All	All	0.11	0/25967	0.28	4/35365 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	K	74	PRO	CA-N-CD	-7.69	101.24	112.00
15	K	74	PRO	N-CD-CG	-5.20	95.41	103.20
6	B	477	LEU	CB-CA-C	-5.12	110.26	117.23
15	K	74	PRO	CB-CG-CD	-5.12	89.72	106.10

There are no chirality outliers.

There are no planarity outliers.

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	1	1496	0	1471	30	0
2	2	1566	0	1519	22	0
3	3	1666	0	1627	19	0
4	4	1551	0	1508	24	0
5	A	5807	0	5659	55	0
6	B	5854	0	5646	63	0
7	C	616	0	600	5	0
8	D	1128	0	1134	8	0
9	E	517	0	526	1	0
10	F	1208	0	1243	9	0
11	G	708	0	700	6	0
12	H	693	0	690	6	0
13	I	239	0	258	3	0
14	J	327	0	342	7	0
15	K	593	0	614	13	0
16	L	1207	0	1209	13	0
17	1	93	0	62	10	0
17	2	226	0	150	12	0
17	3	45	0	30	1	0
17	4	169	0	100	3	0
18	1	496	0	354	24	0
18	2	434	0	352	25	0
18	3	498	0	377	13	0
18	4	527	0	412	18	0
18	A	2533	0	2495	104	0
18	B	2284	0	2242	93	0
18	F	149	0	123	6	0
18	G	132	0	97	1	0
18	H	60	0	59	2	0
18	J	51	0	41	2	0
18	K	167	0	116	2	0
18	L	155	0	138	7	0
19	1	44	0	56	18	0
19	2	44	0	56	7	0
19	4	44	0	56	5	0
20	1	49	0	74	13	0
20	2	37	0	44	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	A	79	0	104	6	0
20	B	87	0	120	5	0
21	1	42	0	56	3	0
21	2	84	0	112	10	0
21	3	42	0	56	6	0
21	4	42	0	56	4	0
22	3	40	0	56	4	0
22	4	40	0	56	4	0
22	A	240	0	336	27	0
22	B	320	0	448	44	0
22	F	40	0	56	2	0
22	G	40	0	56	2	0
22	I	40	0	56	1	0
22	J	40	0	56	6	0
22	K	80	0	112	7	0
22	L	120	0	168	18	0
23	4	72	0	84	1	0
24	A	60	0	68	5	0
25	A	33	0	46	3	0
25	B	33	0	46	2	0
26	A	8	0	0	0	0
26	C	16	0	0	0	0
27	B	66	0	96	5	0
All	All	35077	0	34424	610	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 9.

All (610) 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)
18:B:814:CLA:H3A	22:B:845:BCR:H393	1.51	0.91
17:1:601:CHL:HBB1	20:1:615:LHG:H252	1.57	0.84
21:2:619:LUT:H8	21:2:619:LUT:H181	1.60	0.82
22:B:801:BCR:H12C	22:B:801:BCR:H341	1.63	0.81
3:3:79:LEU:HD13	18:A:813:CLA:H2	1.63	0.81
2:2:143:VAL:HG22	18:4:613:CLA:HBA2	1.61	0.80
4:4:104:MET:HE1	18:4:609:CLA:HAB	1.64	0.80
22:A:853:BCR:H12C	22:A:853:BCR:H341	1.68	0.76
1:1:202:PHE:CE1	19:1:614:XAT:H10	2.20	0.76
22:B:845:BCR:H16C	22:B:845:BCR:H20C	1.68	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:L:306:BCR:H321	22:L:306:BCR:HC8	1.68	0.75
18:3:612:CLA:HAB	18:3:607:CLA:HBA1	1.66	0.75
18:1:602:CLA:H51	19:1:614:XAT:H373	1.69	0.75
3:3:170:ARG:NH2	18:3:607:CLA:O1D	2.21	0.74
6:B:411:MET:HE2	22:B:846:BCR:H402	1.68	0.74
22:A:850:BCR:H16C	22:A:850:BCR:H351	1.69	0.74
18:A:814:CLA:HHC	18:A:814:CLA:HBB1	1.69	0.72
17:1:601:CHL:HBB1	17:1:601:CHL:HHC	1.72	0.72
18:B:812:CLA:HHC	18:B:812:CLA:HBB1	1.68	0.72
21:3:613:LUT:H401	21:3:613:LUT:H15	1.72	0.72
8:D:154:ASN:ND2	8:D:156:GLU:OE2	2.19	0.71
18:1:602:CLA:CBB	19:1:614:XAT:H32	2.21	0.71
17:4:605:CHL:HHC	17:4:605:CHL:HBB1	1.73	0.71
6:B:304:LEU:HA	18:B:822:CLA:HED1	1.72	0.70
21:4:616:LUT:H8	21:4:616:LUT:H171	1.73	0.70
18:1:602:CLA:HBB2	19:1:614:XAT:H32	1.73	0.69
17:1:601:CHL:HHC	20:1:615:LHG:H252	1.75	0.69
22:3:614:BCR:H403	22:3:614:BCR:H23C	1.74	0.69
3:3:256:ASP:O	3:3:264:ASN:ND2	2.26	0.69
18:A:805:CLA:H43	18:A:812:CLA:HBB1	1.73	0.68
3:3:215:GLU:N	3:3:215:GLU:OE2	2.23	0.68
1:1:97:ALA:HA	19:1:614:XAT:H181	1.76	0.68
3:3:81:LEU:HD13	18:3:601:CLA:H42	1.76	0.68
18:A:804:CLA:H191	18:A:844:CLA:H203	1.75	0.68
2:2:98:CYS:O	2:2:102:MET:HG3	1.93	0.67
1:1:172:PHE:HB2	18:1:609:CLA:HMD1	1.75	0.67
22:A:853:BCR:HC8	22:A:853:BCR:H311	1.75	0.67
16:L:107:VAL:HA	18:L:303:CLA:HED1	1.74	0.67
12:H:87:SER:O	12:H:91:GLU:HG3	1.95	0.67
18:A:829:CLA:H202	22:J:102:BCR:H19C	1.76	0.66
22:L:301:BCR:H21C	22:L:301:BCR:H361	1.77	0.66
1:1:187:LEU:HD13	18:1:609:CLA:HAA2	1.78	0.66
6:B:65:LEU:HD11	22:B:845:BCR:H282	1.75	0.66
18:B:805:CLA:H52	18:B:813:CLA:H61	1.78	0.66
13:I:24:MET:HE3	22:L:305:BCR:H352	1.78	0.65
18:A:804:CLA:HBD	18:A:804:CLA:HBA2	1.78	0.65
5:A:393:TRP:CD1	18:A:829:CLA:HAB	2.31	0.65
18:2:613:CLA:H2A	18:2:613:CLA:HED2	1.78	0.65
6:B:164:ARG:NH2	11:G:108:GLY:O	2.30	0.65
6:B:517:PHE:HA	18:B:837:CLA:HED1	1.79	0.65
18:B:828:CLA:H171	22:B:845:BCR:H362	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:J:102:BCR:HC8	22:J:102:BCR:H311	1.79	0.65
5:A:320:LYS:NZ	5:A:324:GLU:OE2	2.31	0.64
18:A:803:CLA:HBA2	6:B:655:LEU:HB2	1.79	0.64
25:A:855:PQN:H172	22:B:801:BCR:H382	1.78	0.64
18:A:802:CLA:H202	18:A:842:CLA:H2	1.80	0.64
16:L:65:ILE:HA	16:L:75:GLU:HG3	1.81	0.64
22:B:848:BCR:H403	22:B:848:BCR:H23C	1.80	0.63
22:B:847:BCR:HC8	22:B:847:BCR:H311	1.80	0.63
22:A:851:BCR:H16C	22:A:851:BCR:H351	1.80	0.63
22:K:205:BCR:H403	22:K:205:BCR:H23C	1.80	0.63
1:1:116:GLN:HG2	18:1:605:CLA:HBB2	1.80	0.63
22:B:801:BCR:HC8	22:B:801:BCR:H331	1.80	0.63
18:A:842:CLA:HBC2	25:A:855:PQN:H192	1.81	0.62
4:4:165:GLY:HA2	4:4:168:ASN:HD22	1.63	0.62
22:A:849:BCR:H383	22:A:849:BCR:H23C	1.80	0.62
6:B:574:ASP:OD1	6:B:706:ARG:NH1	2.31	0.62
6:B:307:ALA:HB3	18:B:822:CLA:HED3	1.80	0.62
18:B:841:CLA:HED1	18:B:822:CLA:HAB	1.80	0.62
2:2:119:ILE:HG22	2:2:120:LEU:HD12	1.81	0.61
18:3:607:CLA:HHC	18:3:607:CLA:HBB1	1.82	0.61
6:B:57:ILE:HA	18:B:806:CLA:HBC3	1.83	0.61
22:B:846:BCR:H343	18:B:822:CLA:HBB2	1.83	0.61
15:K:75:SER:OG	15:K:76:ALA:N	2.33	0.61
15:K:75:SER:O	15:K:89:ARG:NH2	2.34	0.61
1:1:73:LEU:HD12	19:1:614:XAT:H221	1.81	0.60
5:A:302:PHE:HE1	18:A:822:CLA:HAB	1.66	0.60
16:L:100:PRO:HA	16:L:103:ARG:HD3	1.83	0.60
22:A:851:BCR:H23C	22:A:851:BCR:H403	1.82	0.60
22:L:305:BCR:H321	22:L:305:BCR:HC8	1.82	0.60
22:G:204:BCR:HC8	22:G:204:BCR:H311	1.82	0.60
5:A:508:GLY:HA2	5:A:523:PRO:HB3	1.81	0.60
24:A:801:CL0:H15	24:A:801:CL0:H2	1.84	0.60
21:1:616:LUT:H391	21:1:616:LUT:H32	1.81	0.60
6:B:469:LYS:NZ	6:B:509:PHE:O	2.33	0.60
22:B:846:BCR:HC8	22:B:846:BCR:H311	1.84	0.60
4:4:100:GLY:O	4:4:104:MET:HG3	2.02	0.60
4:4:216:PHE:CD2	19:4:617:XAT:H14	2.37	0.60
18:1:609:CLA:HHC	18:1:609:CLA:HBB1	1.84	0.59
20:1:615:LHG:H151	18:4:614:CLA:HED3	1.83	0.59
22:K:205:BCR:H321	22:K:205:BCR:HC8	1.82	0.59
6:B:293:THR:HG22	6:B:294:ASN:H	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:732:LEU:HA	20:A:846:LHG:H383	1.83	0.59
18:A:821:CLA:HHC	18:A:821:CLA:HBB1	1.85	0.59
6:B:432:HIS:HB2	22:B:849:BCR:H402	1.84	0.59
12:H:117:TYR:O	12:H:121:ASN:ND2	2.30	0.59
18:4:613:CLA:HBD	18:4:613:CLA:HBA1	1.85	0.59
22:A:852:BCR:H403	22:A:852:BCR:H23C	1.85	0.59
6:B:68:VAL:HG11	6:B:124:TRP:HZ3	1.68	0.59
17:1:601:CHL:O1A	4:4:151:HIS:ND1	2.35	0.58
18:A:822:CLA:H2	18:A:826:CLA:HBB1	1.85	0.58
14:J:10:VAL:HG12	14:J:12:PRO:HD2	1.85	0.58
6:B:571:SER:OG	6:B:574:ASP:OD2	2.21	0.58
21:2:619:LUT:H172	18:4:610:CLA:HHC	1.84	0.58
6:B:600:THR:HG21	6:B:609:PHE:HB2	1.85	0.58
7:C:15:THR:HA	7:C:28:MET:HE3	1.86	0.58
22:4:618:BCR:HC8	22:4:618:BCR:H321	1.85	0.58
18:A:831:CLA:H172	20:A:846:LHG:H182	1.85	0.58
1:1:125:GLN:NE2	1:1:133:VAL:O	2.31	0.58
5:A:348:ALA:HB1	22:A:850:BCR:H393	1.86	0.58
17:1:601:CHL:HAA1	20:1:615:LHG:H141	1.85	0.58
5:A:288:LEU:HD23	5:A:291:ILE:HD12	1.86	0.58
6:B:147:ALA:O	6:B:151:ILE:HG13	2.04	0.58
4:4:178:LEU:HD21	4:4:189:ILE:HG22	1.86	0.57
18:A:820:CLA:H91	18:A:820:CLA:H151	1.86	0.57
5:A:36:ILE:O	5:A:45:TRP:NE1	2.29	0.57
5:A:438:LEU:HG	5:A:546:LEU:HB2	1.86	0.57
18:A:809:CLA:HAB	18:A:829:CLA:H122	1.86	0.57
18:A:809:CLA:H201	20:A:846:LHG:H211	1.86	0.57
2:2:104:GLY:HA2	19:2:617:XAT:H181	1.87	0.57
4:4:169:GLN:NE2	4:4:174:LYS:O	2.38	0.57
22:A:850:BCR:H311	22:A:850:BCR:HC8	1.86	0.57
3:3:186:LEU:HD11	22:3:614:BCR:H343	1.87	0.56
5:A:117:PRO:HB3	5:A:122:GLU:HB3	1.86	0.56
6:B:516:ASP:OD2	6:B:593:TYR:OH	2.21	0.56
22:B:843:BCR:H16C	22:B:843:BCR:H351	1.87	0.56
5:A:739:TRP:HH2	18:A:809:CLA:HBC2	1.70	0.56
15:K:102:THR:OG1	15:K:105:ASP:OD2	2.23	0.56
5:A:495:THR:OG1	18:A:836:CLA:OBD	2.21	0.56
4:4:82:LEU:HD13	18:4:602:CLA:H42	1.86	0.56
3:3:217:SER:O	3:3:221:LEU:HD12	2.06	0.56
5:A:294:HIS:HB2	18:A:819:CLA:C1B	2.36	0.56
6:B:707:LEU:HD11	27:B:850:DGD:HB81	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:395:ILE:HG13	6:B:541:ALA:HB1	1.89	0.55
18:A:825:CLA:H41	22:A:851:BCR:H15C	1.87	0.55
6:B:523:ILE:HG21	18:B:836:CLA:HAB	1.89	0.55
16:L:90:ASN:O	16:L:95:ARG:NH1	2.38	0.55
5:A:735:ILE:HD12	20:A:846:LHG:H382	1.87	0.55
18:H:201:CLA:HAA2	22:L:306:BCR:H342	1.89	0.55
5:A:279:LEU:HD21	5:A:372:PRO:HD2	1.89	0.55
18:A:808:CLA:H2	18:A:810:CLA:H42	1.87	0.55
17:2:615:CHL:HHC	17:2:615:CHL:HBB1	1.88	0.55
25:B:842:PQN:H272	18:B:840:CLA:H42	1.89	0.55
18:B:824:CLA:H141	18:B:824:CLA:H193	1.87	0.55
20:1:615:LHG:H171	20:1:615:LHG:H342	1.89	0.55
5:A:296:LEU:O	5:A:300:ILE:HG12	2.07	0.55
5:A:728:THR:HG23	20:A:846:LHG:H341	1.88	0.55
8:D:72:THR:HG23	8:D:120:PRO:HB2	1.88	0.55
6:B:704:GLN:HG3	27:B:850:DGD:HA22	1.89	0.54
18:B:831:CLA:HBC2	18:B:838:CLA:HMC3	1.89	0.54
6:B:373:THR:HG23	6:B:591:THR:HG21	1.90	0.54
13:I:27:LEU:HD22	22:L:305:BCR:H323	1.89	0.54
18:1:602:CLA:H2	19:1:614:XAT:H221	1.89	0.54
5:A:360:LEU:HD11	18:A:820:CLA:H8	1.90	0.54
22:A:853:BCR:H23C	22:A:853:BCR:H393	1.89	0.54
6:B:276:HIS:HB2	18:B:817:CLA:C1B	2.38	0.54
22:F:304:BCR:H14C	22:F:304:BCR:H10C	1.90	0.54
18:A:842:CLA:HBD	18:A:842:CLA:HBA1	1.90	0.53
1:1:95:MET:HE3	18:1:609:CLA:HAB	1.89	0.53
21:3:613:LUT:H161	21:3:613:LUT:H8	1.89	0.53
18:B:808:CLA:O1A	18:B:827:CLA:HBD	2.09	0.53
16:L:63:GLN:HG2	16:L:64:PRO:HD2	1.90	0.53
4:4:116:PHE:O	4:4:120:GLY:N	2.30	0.53
22:4:618:BCR:H383	22:4:618:BCR:H23C	1.91	0.53
18:B:805:CLA:H101	18:B:824:CLA:HBA1	1.89	0.53
1:1:237:VAL:HG13	1:1:238:ILE:HG23	1.90	0.53
18:A:830:CLA:CHA	18:A:830:CLA:HBA1	2.38	0.53
20:B:851:LHG:H261	20:B:851:LHG:H302	1.90	0.53
20:B:852:LHG:H121	18:B:822:CLA:H52	1.90	0.53
6:B:659:THR:HA	18:B:803:CLA:HAB	1.89	0.53
6:B:707:LEU:HD23	27:B:850:DGD:HA21	1.91	0.53
5:A:689:ARG:H	6:B:568:CYS:HB2	1.74	0.53
4:4:191:ASN:OD1	21:4:616:LUT:O23	2.27	0.53
1:1:64:GLY:HA3	1:1:192:ILE:HG21	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:25:ILE:HG21	27:B:850:DGD:HA72	1.91	0.52
18:B:828:CLA:H122	22:B:845:BCR:H372	1.91	0.52
22:B:849:BCR:H10C	14:J:38:THR:O	2.09	0.52
1:1:69:ASP:HA	19:1:614:XAT:O23	2.10	0.52
18:A:841:CLA:H143	18:F:302:CLA:HBC1	1.92	0.52
3:3:61:GLN:O	3:3:64:SER:OG	2.26	0.52
18:A:812:CLA:H141	18:A:812:CLA:H203	1.91	0.52
17:2:605:CHL:HHB	21:2:619:LUT:H392	1.91	0.52
18:A:844:CLA:HMB2	18:B:802:CLA:H203	1.90	0.52
5:A:389:THR:HG23	5:A:605:ILE:HG21	1.92	0.52
5:A:536:ILE:HG23	24:A:801:CL0:H70	1.92	0.52
4:4:170:ASP:OD1	4:4:173:PHE:N	2.42	0.52
5:A:403:ALA:HB2	22:A:851:BCR:H323	1.92	0.52
18:A:843:CLA:HMD3	22:B:848:BCR:H393	1.91	0.52
18:B:840:CLA:H122	22:L:305:BCR:H351	1.92	0.52
5:A:14:VAL:HG11	18:A:811:CLA:HED3	1.91	0.52
18:A:803:CLA:H2	6:B:655:LEU:HD22	1.92	0.52
25:B:842:PQN:H272	18:B:840:CLA:H11	1.91	0.52
16:L:90:ASN:HB3	18:L:302:CLA:HAC1	1.92	0.52
22:B:843:BCR:H311	22:B:843:BCR:HC8	1.92	0.51
5:A:699:ILE:HA	18:A:841:CLA:HED1	1.92	0.51
18:A:841:CLA:H72	18:B:832:CLA:H42	1.92	0.51
2:2:80:LEU:HD13	18:2:602:CLA:H71	1.92	0.51
3:3:214:ASP:OD1	3:3:216:LYS:N	2.44	0.51
5:A:256:GLU:OE2	5:A:268:LYS:NZ	2.44	0.51
18:A:806:CLA:H51	18:A:814:CLA:H12	1.93	0.51
7:C:47:ASP:OD2	8:D:128:LYS:NZ	2.41	0.51
6:B:236:ASN:HB3	6:B:252:THR:HG22	1.93	0.51
22:B:844:BCR:H382	22:B:844:BCR:H23C	1.93	0.51
2:2:167:THR:HG22	2:2:175:LYS:HD3	1.93	0.51
1:1:156:ARG:NH2	18:1:608:CLA:O1D	2.38	0.51
17:2:605:CHL:C2C	18:2:604:CLA:HBB2	2.41	0.51
18:B:832:CLA:HHC	18:B:832:CLA:HBB1	1.93	0.51
19:1:614:XAT:H242	19:1:614:XAT:H362	1.93	0.51
14:J:28:GLU:HG3	18:J:101:CLA:CHA	2.40	0.50
18:A:809:CLA:H202	18:A:809:CLA:H91	1.93	0.50
11:G:68:ILE:HG21	11:G:147:LEU:HG	1.93	0.50
15:K:108:ALA:O	15:K:112:VAL:HG23	2.10	0.50
12:H:80:SER:HB2	16:L:98:VAL:HG13	1.93	0.50
18:B:838:CLA:HHC	18:B:838:CLA:HBB1	1.93	0.50
18:1:602:CLA:ND	19:1:614:XAT:H382	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:104:MET:HE1	18:4:609:CLA:CAB	2.40	0.50
6:B:69:ALA:HB2	6:B:135:LEU:HB2	1.92	0.50
17:2:601:CHL:HHC	17:2:601:CHL:HBB1	1.94	0.49
18:A:811:CLA:H2A	18:A:811:CLA:HED2	1.93	0.49
6:B:450:GLU:OE2	10:F:119:ARG:NH1	2.44	0.49
6:B:120:VAL:HG21	18:B:808:CLA:HED1	1.94	0.49
18:4:614:CLA:CED	18:4:614:CLA:H2A	2.42	0.49
6:B:422:LEU:HD13	6:B:532:LEU:HA	1.94	0.49
2:2:104:GLY:HA3	19:2:617:XAT:H192	1.93	0.49
4:4:175:GLN:OE1	4:4:175:GLN:N	2.28	0.49
22:B:844:BCR:H352	18:B:828:CLA:H192	1.94	0.49
8:D:90:VAL:HG12	8:D:91:GLU:HG3	1.94	0.49
10:F:210:GLU:HG3	10:F:215:ASP:HB3	1.95	0.49
18:4:609:CLA:CGA	18:4:609:CLA:H3A	2.42	0.49
1:1:149:ILE:HA	1:1:152:VAL:HG22	1.94	0.49
5:A:447:PHE:O	18:A:835:CLA:HBB2	2.13	0.49
2:2:99:ARG:NH1	17:2:607:CHL:OBD	2.34	0.49
2:2:213:GLY:O	2:2:217:MET:HG3	2.12	0.49
18:A:844:CLA:H3A	18:A:844:CLA:O1A	2.13	0.49
18:B:819:CLA:HBB1	18:B:824:CLA:H93	1.95	0.49
5:A:261:PHE:HE1	18:A:818:CLA:HBB1	1.77	0.48
18:A:843:CLA:H152	22:L:301:BCR:H16C	1.95	0.48
6:B:395:ILE:HD13	6:B:555:TYR:HA	1.94	0.48
8:D:152:PHE:HB2	8:D:156:GLU:HG2	1.94	0.48
1:1:238:ILE:HD12	23:4:620:LMG:H132	1.94	0.48
21:2:616:LUT:H401	21:2:616:LUT:H15	1.95	0.48
15:K:79:LYS:O	15:K:87:GLU:N	2.45	0.48
17:2:605:CHL:C4C	18:2:604:CLA:HAB	2.44	0.48
6:B:91:ILE:HB	6:B:112:PRO:HB2	1.96	0.48
5:A:361:THR:HA	18:A:830:CLA:HBC2	1.96	0.48
5:A:739:TRP:CH2	18:A:809:CLA:HBC2	2.47	0.48
18:A:802:CLA:H202	18:A:802:CLA:H162	1.70	0.48
16:L:203:THR:HB	22:L:306:BCR:H333	1.94	0.48
17:1:601:CHL:NB	20:1:615:LHG:H131	2.29	0.48
10:F:199:ARG:HE	10:F:199:ARG:HB2	1.53	0.48
2:2:201:LYS:HE3	2:2:205:LEU:HD11	1.95	0.48
4:4:199:GLN:O	4:4:203:GLU:HG3	2.14	0.48
16:L:87:TYR:OH	18:L:303:CLA:O1A	2.30	0.48
1:1:177:TYR:HB2	18:1:609:CLA:HBA2	1.96	0.48
5:A:41:ASP:OD1	5:A:41:ASP:N	2.46	0.48
18:A:809:CLA:H151	18:A:804:CLA:H161	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:A:812:CLA:H92	18:A:812:CLA:H62	1.71	0.48
1:1:190:LYS:HD3	18:1:611:CLA:HAA2	1.95	0.48
17:1:601:CHL:H12	20:1:615:LHG:H181	1.96	0.48
19:2:617:XAT:H401	19:2:617:XAT:H15	1.95	0.48
5:A:717:LEU:HB3	5:A:721:GLN:HG2	1.95	0.48
18:A:806:CLA:H192	22:A:849:BCR:H363	1.96	0.48
25:A:855:PQN:H271	18:A:841:CLA:H91	1.96	0.48
3:3:220:GLU:O	3:3:224:LYS:HG3	2.14	0.47
4:4:151:HIS:HA	18:4:608:CLA:HAB	1.96	0.47
18:4:612:CLA:H91	18:4:612:CLA:H111	1.70	0.47
18:B:821:CLA:HBA1	18:B:821:CLA:HBD	1.95	0.47
4:4:157:ARG:NH2	18:4:608:CLA:O1D	2.33	0.47
18:B:830:CLA:HBC2	18:B:823:CLA:HBB1	1.96	0.47
15:K:48:PHE:HZ	18:K:204:CLA:HBC3	1.80	0.47
18:A:802:CLA:HBA1	18:A:802:CLA:H3A	1.43	0.47
18:B:814:CLA:H121	22:B:845:BCR:H363	1.97	0.47
6:B:106:ARG:HG3	6:B:115:ILE:HD11	1.95	0.47
18:B:805:CLA:H2	18:B:805:CLA:H61	1.58	0.47
11:G:64:PRO:HG2	11:G:67:VAL:HB	1.97	0.47
6:B:277:HIS:HA	6:B:280:ILE:HG12	1.95	0.47
18:B:818:CLA:H3A	18:B:818:CLA:HBA2	1.42	0.47
5:A:702:ALA:HB3	18:A:841:CLA:HED3	1.96	0.47
12:H:104:LEU:O	12:H:108:ILE:HG12	2.15	0.47
22:L:301:BCR:H361	22:L:301:BCR:C21	2.41	0.47
18:2:602:CLA:H192	18:2:602:CLA:H162	1.74	0.47
18:B:834:CLA:HBA1	18:B:834:CLA:H3A	1.57	0.47
18:F:302:CLA:H11	18:F:302:CLA:H52	1.72	0.47
18:1:602:CLA:CBB	19:1:614:XAT:H30	2.45	0.47
18:F:301:CLA:H62	18:F:301:CLA:H41	1.56	0.47
5:A:393:TRP:HD1	18:A:829:CLA:HAB	1.78	0.47
22:A:848:BCR:H403	22:A:848:BCR:H23C	1.96	0.47
2:2:102:MET:HE1	18:2:609:CLA:CBB	2.45	0.46
17:2:606:CHL:HHC	17:2:606:CHL:HBB1	1.97	0.46
3:3:90:PHE:HB2	18:3:602:CLA:H43	1.97	0.46
5:A:207:SER:HB3	5:A:299:ALA:HB2	1.97	0.46
6:B:31:PHE:HE1	18:B:804:CLA:HED1	1.80	0.46
10:F:128:LEU:HD21	14:J:38:THR:HG21	1.96	0.46
6:B:456:GLU:OE1	6:B:461:GLN:NE2	2.48	0.46
18:A:833:CLA:H61	18:A:833:CLA:H41	1.44	0.46
18:1:612:CLA:O2D	18:1:612:CLA:H2A	2.15	0.46
6:B:182:LEU:HD21	18:B:813:CLA:O1A	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:H:116:THR:HG23	13:I:10:ILE:HG23	1.97	0.46
21:1:616:LUT:H35	21:1:616:LUT:H401	1.79	0.46
18:A:805:CLA:H3A	18:A:805:CLA:HBA2	1.38	0.46
18:B:832:CLA:HBB2	22:B:801:BCR:H312	1.98	0.46
1:1:109:TYR:HE1	1:1:129:LEU:HA	1.80	0.46
21:2:616:LUT:H22	18:2:609:CLA:H12	1.98	0.46
18:A:820:CLA:HMB1	18:A:820:CLA:HBB1	1.98	0.46
6:B:46:ILE:HG21	18:B:805:CLA:H202	1.96	0.46
5:A:386:SER:HB3	18:A:829:CLA:HMA1	1.97	0.46
18:A:835:CLA:H161	18:A:835:CLA:H202	1.69	0.46
16:L:87:TYR:OH	18:L:302:CLA:HBB2	2.16	0.46
6:B:435:GLY:HA3	18:B:833:CLA:HAB	1.98	0.46
18:B:840:CLA:HBA1	18:B:840:CLA:H3A	1.66	0.46
18:1:603:CLA:H41	18:1:603:CLA:H62	1.67	0.46
22:K:202:BCR:H23C	22:K:202:BCR:H392	1.97	0.46
18:A:845:CLA:H3A	18:A:845:CLA:HBA1	1.46	0.46
6:B:548:PRO:HD2	7:C:62:PHE:CZ	2.51	0.46
10:F:138:LEU:HD22	10:F:149:GLU:HG2	1.98	0.46
1:1:238:ILE:O	1:1:238:ILE:HG13	2.15	0.45
18:B:837:CLA:H3A	18:B:837:CLA:HBA2	1.72	0.45
18:A:828:CLA:OBD	18:A:827:CLA:HAA2	2.16	0.45
18:A:833:CLA:HBA1	18:A:833:CLA:H3A	1.86	0.45
18:B:818:CLA:HBB1	18:B:818:CLA:HMB1	1.98	0.45
3:3:260:ASP:OD2	3:3:264:ASN:ND2	2.49	0.45
24:A:801:CL0:H51	24:A:801:CL0:H59	1.67	0.45
18:A:804:CLA:H143	22:A:853:BCR:H19C	1.98	0.45
18:H:201:CLA:H93	18:H:201:CLA:H62	1.78	0.45
1:1:212:TYR:HD1	1:1:220:ASN:HD21	1.62	0.45
20:1:615:LHG:H341	20:1:615:LHG:H371	1.50	0.45
2:2:194:TRP:HB2	18:2:609:CLA:O2A	2.16	0.45
3:3:119:ILE:HG13	3:3:120:LEU:HD23	1.98	0.45
22:A:853:BCR:H343	14:J:27:ILE:HG21	1.99	0.45
22:A:851:BCR:H351	22:A:851:BCR:C16	2.42	0.45
6:B:61:THR:HB	6:B:142:LEU:HD13	1.97	0.45
1:1:119:ALA:HB1	1:1:138:LEU:HD12	1.98	0.45
3:3:260:ASP:HA	3:3:261:PRO:HD3	1.86	0.45
21:3:613:LUT:H12	21:3:613:LUT:H191	1.98	0.45
6:B:301:ILE:HG21	18:B:824:CLA:HAC1	1.98	0.45
18:B:806:CLA:H72	18:B:806:CLA:H111	1.52	0.45
18:B:808:CLA:H141	18:B:808:CLA:H162	1.62	0.45
10:F:180:LYS:HB3	10:F:180:LYS:HE3	1.78	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:B:805:CLA:H61	18:B:805:CLA:H93	1.66	0.45
18:B:827:CLA:H152	18:B:827:CLA:H111	1.39	0.45
7:C:62:PHE:HD2	8:D:185:ILE:HG21	1.82	0.45
21:2:619:LUT:H31	21:2:619:LUT:H391	1.82	0.45
6:B:339:ALA:HB2	22:B:847:BCR:H372	1.99	0.45
22:B:846:BCR:H332	20:B:852:LHG:H351	1.98	0.45
22:B:801:BCR:H383	22:B:801:BCR:H23C	1.99	0.45
1:1:190:LYS:O	1:1:194:ASN:ND2	2.42	0.45
5:A:201:GLY:O	5:A:205:LEU:HB2	2.16	0.45
18:A:806:CLA:HBA1	18:A:806:CLA:H3A	1.45	0.45
18:A:841:CLA:HBA2	18:A:841:CLA:H3A	1.41	0.44
18:B:805:CLA:HBA1	18:B:805:CLA:H3A	1.44	0.44
22:A:853:BCR:HC7	22:A:853:BCR:H331	1.82	0.44
6:B:687:LEU:HD11	16:L:91:LEU:HD13	1.99	0.44
2:2:81:SER:O	2:2:81:SER:OG	2.30	0.44
18:A:820:CLA:H62	18:A:820:CLA:H92	1.67	0.44
7:C:58:CYS:HB3	7:C:63:LEU:HD23	2.00	0.44
15:K:96:GLY:O	18:K:201:CLA:H3A	2.18	0.44
1:1:97:ALA:HA	19:1:614:XAT:C18	2.46	0.44
20:1:615:LHG:H342	20:1:615:LHG:H192	1.99	0.44
18:2:602:CLA:H41	18:2:602:CLA:H62	1.51	0.44
4:4:101:ARG:NH1	17:4:607:CHL:OBD	2.43	0.44
18:A:803:CLA:HBA1	18:A:803:CLA:H3A	1.63	0.44
18:A:842:CLA:H102	18:A:842:CLA:H62	1.78	0.44
18:2:612:CLA:H112	18:2:612:CLA:H71	1.68	0.44
18:2:602:CLA:H62	18:2:602:CLA:H102	1.83	0.44
18:4:602:CLA:H92	18:4:603:CLA:HBB	1.99	0.44
5:A:90:PHE:CG	18:A:808:CLA:HBC3	2.53	0.44
20:1:615:LHG:H261	20:1:615:LHG:H292	1.32	0.44
4:4:104:MET:HE1	18:4:609:CLA:HHC	1.99	0.44
9:E:89:ILE:HG22	9:E:91:ARG:H	1.82	0.44
11:G:120:LYS:HB3	11:G:120:LYS:HE3	1.71	0.44
18:G:201:CLA:CGA	18:G:201:CLA:H3A	2.48	0.44
22:K:202:BCR:H24C	22:K:202:BCR:H371	1.77	0.44
1:1:140:THR:O	1:1:144:ILE:HG13	2.17	0.44
18:1:609:CLA:HHC	18:1:609:CLA:CBB	2.47	0.44
22:B:847:BCR:H11C	22:B:847:BCR:H341	1.89	0.44
18:B:826:CLA:H102	18:B:826:CLA:H61	1.74	0.44
18:A:822:CLA:H141	18:A:822:CLA:H162	1.71	0.44
18:A:840:CLA:HMC2	18:A:833:CLA:HBC2	2.00	0.44
15:K:66:PHE:CD1	15:K:66:PHE:C	2.96	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:2:619:LUT:H35	21:2:619:LUT:H401	1.82	0.44
5:A:582:CYS:HB2	6:B:667:TRP:HB3	2.00	0.44
8:D:156:GLU:OE2	8:D:156:GLU:N	2.51	0.44
19:1:614:XAT:H35	19:1:614:XAT:H401	1.87	0.43
18:2:602:CLA:CGA	18:2:602:CLA:H3A	2.48	0.43
4:4:165:GLY:HA2	4:4:168:ASN:ND2	2.31	0.43
18:A:819:CLA:H3A	18:A:819:CLA:HBA2	1.63	0.43
22:A:853:BCR:H15C	22:A:853:BCR:H351	1.85	0.43
6:B:517:PHE:HE1	22:B:849:BCR:H271	1.83	0.43
22:B:846:BCR:H11C	22:B:846:BCR:H341	1.81	0.43
22:B:847:BCR:HC7	22:B:847:BCR:H331	1.85	0.43
18:B:825:CLA:H3A	18:B:825:CLA:HBA1	1.43	0.43
1:1:238:ILE:HD11	4:4:140:SER:HB3	1.99	0.43
2:2:57:PRO:O	3:3:172:GLN:HG2	2.19	0.43
18:3:601:CLA:H8	18:3:601:CLA:H51	1.74	0.43
6:B:395:ILE:HD12	6:B:555:TYR:HD1	1.82	0.43
18:3:603:CLA:HBA1	18:3:603:CLA:H3A	1.30	0.43
21:3:613:LUT:H181	21:3:613:LUT:H7	1.72	0.43
4:4:222:GLN:HE22	21:4:616:LUT:H41	1.83	0.43
5:A:371:MET:HE2	18:A:819:CLA:HAA2	2.00	0.43
15:K:67:ALA:HA	15:K:72:LEU:HD12	2.00	0.43
1:1:184:LEU:HD11	18:1:609:CLA:O2D	2.18	0.43
18:1:604:CLA:C1B	19:1:614:XAT:H42	2.48	0.43
4:4:134:GLN:OE1	4:4:134:GLN:C	2.61	0.43
5:A:317:HIS:HB3	5:A:322:ILE:HD11	1.99	0.43
5:A:676:PHE:CD2	22:A:852:BCR:H363	2.52	0.43
6:B:93:ASP:H	12:H:129:ILE:HD13	1.84	0.43
6:B:174:ARG:HB2	18:B:813:CLA:HBC2	2.00	0.43
18:B:822:CLA:H91	18:B:822:CLA:H111	1.82	0.43
18:3:609:CLA:HMB1	21:3:613:LUT:H26	2.01	0.43
5:A:480:PHE:O	5:A:484:ILE:HG12	2.18	0.43
18:A:825:CLA:H3A	18:A:825:CLA:HBA2	1.40	0.43
18:B:809:CLA:H92	18:B:809:CLA:H62	1.72	0.43
5:A:294:HIS:CE1	5:A:298:ILE:HG13	2.54	0.43
18:B:827:CLA:H193	27:B:850:DGD:HAN2	2.01	0.43
18:B:803:CLA:H61	18:B:803:CLA:H93	1.78	0.43
15:K:115:ILE:HG12	22:K:205:BCR:H313	2.01	0.43
20:2:618:LHG:O4	20:2:618:LHG:O2	2.33	0.43
5:A:93:ALA:HA	5:A:153:GLU:HG2	1.99	0.43
5:A:371:MET:HE2	18:A:819:CLA:HBD	2.00	0.43
1:1:128:TYR:HD1	18:1:604:CLA:HBA1	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:1:602:CLA:H72	19:1:614:XAT:C37	2.49	0.43
2:2:171:PHE:HE2	17:2:615:CHL:HHB	1.84	0.43
19:4:617:XAT:H31	19:4:617:XAT:H391	1.92	0.43
5:A:530:ASP:HA	5:A:533:VAL:HG12	2.01	0.43
22:L:306:BCR:H373	18:L:303:CLA:HMA2	2.00	0.43
3:3:219:LYS:HA	3:3:219:LYS:HD2	1.83	0.43
5:A:223:GLN:HG2	5:A:250:LEU:HD21	2.01	0.43
22:B:846:BCR:H15C	22:B:846:BCR:H351	1.81	0.43
18:B:809:CLA:H41	18:B:809:CLA:H61	1.64	0.43
18:B:841:CLA:H121	18:B:841:CLA:H161	1.75	0.43
17:1:601:CHL:C2C	20:1:615:LHG:HC81	2.49	0.42
18:2:612:CLA:H142	18:2:612:CLA:H111	1.74	0.42
21:2:619:LUT:H181	21:2:619:LUT:C8	2.37	0.42
18:A:807:CLA:H93	18:A:807:CLA:H112	1.88	0.42
22:J:102:BCR:H11C	22:J:102:BCR:H341	1.83	0.42
18:L:303:CLA:H142	18:L:303:CLA:H111	1.72	0.42
2:2:168:ASP:HB3	2:2:171:PHE:O	2.19	0.42
20:2:618:LHG:HC81	20:2:618:LHG:HC41	2.01	0.42
17:4:615:CHL:HMC	17:4:607:CHL:OMC	2.18	0.42
18:A:835:CLA:H3A	18:A:835:CLA:HBA1	1.77	0.42
18:A:835:CLA:HHB	18:A:834:CLA:HAB	2.01	0.42
22:A:848:BCR:H11C	22:A:848:BCR:H341	1.90	0.42
6:B:583:MET:O	6:B:587:ILE:HG12	2.19	0.42
20:B:852:LHG:H121	18:B:822:CLA:H41	2.01	0.42
22:B:801:BCR:HC21	18:F:302:CLA:H51	2.00	0.42
22:B:845:BCR:H21C	22:B:845:BCR:H24C	1.78	0.42
10:F:203:TRP:CG	10:F:204:PRO:HD3	2.54	0.42
18:F:302:CLA:HAA2	14:J:22:LEU:HD11	2.02	0.42
18:1:604:CLA:C3B	19:1:614:XAT:H183	2.49	0.42
2:2:101:ALA:CB	2:2:217:MET:HG2	2.49	0.42
2:2:139:THR:O	2:2:143:VAL:HG23	2.19	0.42
21:3:613:LUT:H191	21:3:613:LUT:C12	2.48	0.42
4:4:221:VAL:HG11	18:4:612:CLA:HAC2	2.00	0.42
18:A:807:CLA:H193	18:A:807:CLA:H161	1.87	0.42
18:A:809:CLA:H71	22:J:102:BCR:H343	2.00	0.42
18:A:817:CLA:HBA1	18:A:817:CLA:H3A	1.65	0.42
22:A:851:BCR:H371	22:A:851:BCR:H24C	1.69	0.42
6:B:529:THR:HG21	6:B:582:TRP:CZ2	2.54	0.42
22:L:305:BCR:H24C	22:L:305:BCR:H371	1.81	0.42
18:A:807:CLA:HBA1	18:A:807:CLA:H3A	1.79	0.42
6:B:347:LEU:HD23	18:B:818:CLA:H72	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:1:614:XAT:H42	19:1:614:XAT:H162	2.01	0.42
21:2:616:LUT:H373	18:2:612:CLA:C2B	2.50	0.42
24:A:801:CL0:H51	24:A:801:CL0:H42	1.79	0.42
18:A:823:CLA:HAA2	15:K:80:ALA:HB3	2.02	0.42
18:A:834:CLA:HMA2	22:I:101:BCR:H272	2.02	0.42
6:B:649:MET:HE2	6:B:723:ALA:HB2	2.02	0.42
18:B:808:CLA:C1A	18:B:808:CLA:CGA	2.97	0.42
18:B:828:CLA:H3A	18:B:828:CLA:HBA2	1.30	0.42
22:B:801:BCR:H15C	22:B:801:BCR:H351	1.87	0.42
1:1:73:LEU:O	20:B:851:LHG:O1	2.28	0.42
18:A:804:CLA:O1D	18:A:804:CLA:H2A	2.19	0.42
6:B:373:THR:HB	18:B:827:CLA:HMB2	2.01	0.42
10:F:203:TRP:CD1	10:F:204:PRO:HD3	2.54	0.42
5:A:30:GLY:HA3	5:A:36:ILE:HG22	2.01	0.42
22:B:848:BCR:H403	22:B:848:BCR:C23	2.49	0.42
22:K:202:BCR:H351	22:K:202:BCR:H15C	1.80	0.42
18:3:605:CLA:O1D	18:3:605:CLA:H2A	2.20	0.42
22:B:846:BCR:H373	18:B:826:CLA:H121	2.01	0.42
22:B:801:BCR:H341	22:B:801:BCR:C12	2.37	0.42
22:L:305:BCR:H393	22:L:305:BCR:H23C	2.01	0.42
18:2:602:CLA:H122	19:2:617:XAT:H371	2.00	0.42
18:2:604:CLA:HBA1	18:2:604:CLA:H3A	1.92	0.42
6:B:294:ASN:HB2	11:G:114:GLU:HA	2.02	0.42
22:L:305:BCR:H20C	22:L:305:BCR:H361	1.88	0.42
1:1:65:ASP:OD2	1:1:65:ASP:C	2.62	0.42
18:B:840:CLA:H93	18:B:840:CLA:H61	1.91	0.42
1:1:227:ASP:OD2	1:1:230:HIS:HB2	2.20	0.41
2:2:102:MET:HE1	18:2:609:CLA:HBB2	2.01	0.41
18:A:844:CLA:H12	18:A:844:CLA:H52	1.84	0.41
18:A:839:CLA:H61	18:A:839:CLA:H41	1.77	0.41
22:A:851:BCR:H331	22:A:851:BCR:C8	2.49	0.41
6:B:275:HIS:HB3	18:B:817:CLA:HMB2	2.02	0.41
18:B:825:CLA:H93	18:B:825:CLA:H111	1.85	0.41
22:B:801:BCR:H24C	22:B:801:BCR:H371	1.87	0.41
8:D:102:LYS:HB2	8:D:102:LYS:HE2	1.91	0.41
17:1:601:CHL:C3B	20:1:615:LHG:H282	2.50	0.41
19:4:617:XAT:H32	18:4:602:CLA:HAB	2.00	0.41
5:A:310:ARG:HH22	15:K:79:LYS:HD3	1.85	0.41
18:A:804:CLA:HBA2	18:A:804:CLA:CBD	2.46	0.41
18:A:842:CLA:HBA2	20:A:846:LHG:H162	2.01	0.41
18:A:812:CLA:H111	18:A:812:CLA:H91	1.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:B:817:CLA:CGA	18:B:817:CLA:H3A	2.50	0.41
22:L:305:BCR:H23C	22:L:305:BCR:H402	2.02	0.41
21:1:616:LUT:H391	21:1:616:LUT:C32	2.49	0.41
18:2:609:CLA:HMD2	17:2:607:CHL:HBA2	2.01	0.41
19:2:617:XAT:H201	19:2:617:XAT:H35	2.02	0.41
18:2:608:CLA:H3A	18:2:608:CLA:HBA2	1.22	0.41
5:A:213:HIS:HB2	18:A:815:CLA:CHC	2.50	0.41
18:A:813:CLA:HBA2	18:A:813:CLA:H3A	1.75	0.41
18:A:830:CLA:H41	18:A:830:CLA:H62	1.68	0.41
18:B:824:CLA:H62	18:B:824:CLA:H41	1.55	0.41
18:A:821:CLA:HHC	18:A:821:CLA:CBB	2.50	0.41
18:A:809:CLA:H92	18:A:809:CLA:H62	1.77	0.41
18:A:830:CLA:H11	18:A:830:CLA:HBA2	1.55	0.41
22:B:848:BCR:H11C	22:B:848:BCR:H341	1.95	0.41
18:B:840:CLA:H111	18:B:840:CLA:H151	1.83	0.41
3:3:169:ARG:HB3	17:3:606:CHL:CMC	2.51	0.41
18:3:601:CLA:H2	18:3:601:CLA:H62	1.76	0.41
18:4:602:CLA:CGA	18:4:602:CLA:H3A	2.51	0.41
22:4:618:BCR:H11C	22:4:618:BCR:H341	1.92	0.41
22:A:851:BCR:H321	22:A:851:BCR:HC7	1.86	0.41
22:B:848:BCR:H20C	22:B:848:BCR:H361	1.92	0.41
18:B:818:CLA:H62	18:B:818:CLA:H41	1.77	0.41
18:B:823:CLA:HBA1	18:B:823:CLA:H3A	1.72	0.41
18:B:832:CLA:H143	18:B:832:CLA:H161	1.80	0.41
21:2:616:LUT:H11	21:2:616:LUT:H191	1.87	0.41
18:2:604:CLA:C2C	19:2:617:XAT:H183	2.50	0.41
18:3:602:CLA:H92	18:A:811:CLA:HMD1	2.02	0.41
19:4:617:XAT:H35	19:4:617:XAT:H401	1.89	0.41
21:4:616:LUT:H15	21:4:616:LUT:H201	1.96	0.41
18:A:825:CLA:HBB1	18:A:832:CLA:HBC2	2.02	0.41
18:B:809:CLA:H142	18:B:809:CLA:H111	1.91	0.41
18:B:802:CLA:HHC	18:B:802:CLA:HBB1	2.02	0.41
20:1:615:LHG:HC12	22:4:618:BCR:H291	2.03	0.41
18:A:805:CLA:HBA1	18:A:812:CLA:C1D	2.50	0.41
18:A:835:CLA:H93	18:A:835:CLA:H111	1.71	0.41
22:A:848:BCR:H23C	22:A:848:BCR:H392	2.02	0.41
22:A:850:BCR:H331	22:A:850:BCR:HC7	1.77	0.41
18:B:828:CLA:HBB1	18:B:806:CLA:HAB	2.03	0.41
18:B:828:CLA:H142	18:B:828:CLA:H112	1.90	0.41
22:B:845:BCR:H15C	22:B:845:BCR:H351	1.94	0.41
14:J:32:LEU:HD21	18:J:101:CLA:HBA2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:156:TRP:CD2	18:2:608:CLA:HMA2	2.55	0.41
2:2:171:PHE:CE2	17:2:615:CHL:HHB	2.55	0.41
5:A:596:TRP:HE1	18:B:803:CLA:C1D	2.33	0.41
18:A:813:CLA:H2A	18:A:813:CLA:O2D	2.21	0.41
18:A:829:CLA:H72	18:A:829:CLA:H111	1.35	0.41
18:B:802:CLA:HBA1	18:B:802:CLA:H3A	1.29	0.41
18:B:820:CLA:C4B	22:B:843:BCR:H15C	2.50	0.41
22:G:204:BCR:HC7	22:G:204:BCR:H331	1.84	0.41
22:J:102:BCR:H15C	22:J:102:BCR:H351	1.82	0.41
22:L:301:BCR:H15C	22:L:301:BCR:H351	1.72	0.41
18:1:607:CLA:HBA2	18:1:607:CLA:H3A	1.23	0.41
18:2:602:CLA:HMC2	19:2:617:XAT:H391	2.03	0.41
5:A:116:TRP:O	5:A:121:GLN:NE2	2.38	0.41
5:A:305:ALA:HB2	18:A:822:CLA:HBC2	2.02	0.41
24:A:801:CL0:H12	18:B:802:CLA:CHB	2.51	0.41
18:A:813:CLA:H2A	18:A:813:CLA:CED	2.51	0.41
18:A:834:CLA:H162	18:A:834:CLA:H141	1.82	0.41
22:A:850:BCR:H11C	22:A:850:BCR:H341	1.84	0.41
18:A:812:CLA:H172	18:A:812:CLA:H13	1.73	0.41
6:B:464:GLN:NE2	18:B:836:CLA:OBD	2.44	0.41
6:B:601:LEU:HA	6:B:606:VAL:HG12	2.03	0.41
18:B:832:CLA:H62	18:B:832:CLA:H2	1.70	0.41
18:B:803:CLA:H202	18:B:803:CLA:H162	1.76	0.41
18:F:302:CLA:O1D	18:F:302:CLA:H2A	2.20	0.41
22:J:102:BCR:HC7	22:J:102:BCR:H331	1.90	0.41
16:L:121:LYS:HB3	16:L:121:LYS:HE3	1.84	0.41
16:L:208:LEU:HD23	16:L:208:LEU:HA	1.92	0.41
22:L:306:BCR:H15C	22:L:306:BCR:H351	1.84	0.41
2:2:174:ASN:HD22	17:2:615:CHL:C4D	2.33	0.41
4:4:155:ILE:HD13	4:4:155:ILE:HA	1.92	0.41
19:4:617:XAT:H11	19:4:617:XAT:H191	1.84	0.41
18:B:820:CLA:HBA2	18:B:820:CLA:H3A	1.32	0.41
22:L:305:BCR:H11C	22:L:305:BCR:H341	1.88	0.41
17:1:601:CHL:H61	17:1:601:CHL:H41	1.70	0.40
18:1:602:CLA:CGA	18:1:602:CLA:H3A	2.51	0.40
17:2:615:CHL:HBB1	17:2:615:CHL:CHC	2.50	0.40
18:2:612:CLA:H3A	18:2:612:CLA:HBA2	1.81	0.40
18:2:604:CLA:HED2	18:2:604:CLA:H2A	2.03	0.40
18:B:808:CLA:HAB	18:B:809:CLA:HAA2	2.03	0.40
18:B:814:CLA:H162	18:B:814:CLA:H141	1.81	0.40
18:B:824:CLA:H91	18:B:824:CLA:H112	1.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:K:75:SER:OG	15:K:105:ASP:OD1	2.27	0.40
22:3:614:BCR:H11C	22:3:614:BCR:H341	1.90	0.40
18:4:602:CLA:H91	18:4:602:CLA:H112	1.81	0.40
18:B:822:CLA:O1D	18:B:822:CLA:HBA1	2.21	0.40
18:3:601:CLA:H91	18:3:601:CLA:H112	1.87	0.40
5:A:319:ILE:HG21	18:A:826:CLA:HAC1	2.03	0.40
6:B:3:LEU:HD13	6:B:7:ARG:HH21	1.85	0.40
18:B:826:CLA:H111	18:B:826:CLA:H142	1.83	0.40
18:B:827:CLA:HBA2	18:B:827:CLA:H3A	1.39	0.40
22:B:843:BCR:H331	22:B:843:BCR:HC7	1.78	0.40
18:L:303:CLA:H112	18:L:303:CLA:H71	1.72	0.40
1:1:162:PRO:HA	1:1:165:LYS:HG3	2.03	0.40
19:1:614:XAT:H183	19:1:614:XAT:H7	1.85	0.40
18:2:602:CLA:H91	18:2:602:CLA:H111	1.82	0.40
20:2:618:LHG:HC91	22:3:614:BCR:HC41	2.04	0.40
5:A:671:PHE:O	5:A:675:HIS:ND1	2.54	0.40
18:A:809:CLA:H101	18:A:809:CLA:H13	1.92	0.40
18:B:813:CLA:O2D	18:B:813:CLA:H2A	2.22	0.40
18:B:832:CLA:CBB	22:B:801:BCR:H312	2.51	0.40
3:3:109:LEU:HD22	18:3:603:CLA:HBC1	2.04	0.40
3:3:167:GLU:OE1	3:3:170:ARG:NH1	2.54	0.40
6:B:432:HIS:CB	22:B:849:BCR:H402	2.49	0.40
10:F:195:ARG:HD2	10:F:195:ARG:HA	1.96	0.40
22:F:304:BCR:H361	22:F:304:BCR:H20C	1.80	0.40
11:G:74:LEU:HD12	11:G:74:LEU:HA	1.97	0.40
22:K:205:BCR:H24C	22:K:205:BCR:H371	1.90	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	1	191/241 (79%)	190 (100%)	1 (0%)	0	100	100
2	2	199/257 (77%)	198 (100%)	1 (0%)	0	100	100
3	3	216/273 (79%)	213 (99%)	3 (1%)	0	100	100
4	4	194/251 (77%)	191 (98%)	3 (2%)	0	100	100
5	A	735/750 (98%)	725 (99%)	10 (1%)	0	100	100
6	B	730/734 (100%)	716 (98%)	14 (2%)	0	100	100
7	C	78/81 (96%)	74 (95%)	4 (5%)	0	100	100
8	D	141/204 (69%)	137 (97%)	4 (3%)	0	100	100
9	E	62/143 (43%)	61 (98%)	1 (2%)	0	100	100
10	F	150/221 (68%)	149 (99%)	1 (1%)	0	100	100
11	G	89/160 (56%)	88 (99%)	1 (1%)	0	100	100
12	H	88/145 (61%)	88 (100%)	0	0	100	100
13	I	29/37 (78%)	28 (97%)	1 (3%)	0	100	100
14	J	39/44 (89%)	38 (97%)	1 (3%)	0	100	100
15	K	82/130 (63%)	82 (100%)	0	0	100	100
16	L	158/219 (72%)	155 (98%)	3 (2%)	0	100	100
All	All	3181/3890 (82%)	3133 (98%)	48 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	1	153/190 (80%)	151 (99%)	2 (1%)	61	75
2	2	163/205 (80%)	163 (100%)	0	100	100
3	3	167/211 (79%)	166 (99%)	1 (1%)	78	83
4	4	163/210 (78%)	162 (99%)	1 (1%)	78	83
5	A	598/610 (98%)	597 (100%)	1 (0%)	87	88

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	B	599/600 (100%)	598 (100%)	1 (0%)	87	88
7	C	70/71 (99%)	70 (100%)	0	100	100
8	D	121/170 (71%)	121 (100%)	0	100	100
9	E	57/114 (50%)	57 (100%)	0	100	100
10	F	125/185 (68%)	124 (99%)	1 (1%)	73	80
11	G	77/133 (58%)	77 (100%)	0	100	100
12	H	75/113 (66%)	75 (100%)	0	100	100
13	I	27/33 (82%)	27 (100%)	0	100	100
14	J	36/39 (92%)	36 (100%)	0	100	100
15	K	61/95 (64%)	61 (100%)	0	100	100
16	L	126/174 (72%)	126 (100%)	0	100	100
All	All	2618/3153 (83%)	2611 (100%)	7 (0%)	84	87

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	59	ASP
1	1	220	ASN
3	3	136	GLN
4	4	132	LYS
5	A	127	ASP
6	B	309	ILE
10	F	96	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	131	ASN
1	1	220	ASN
3	3	242	GLN
3	3	263	ASN
3	3	265	ASN
4	4	168	ASN
4	4	194	ASN
4	4	222	GLN
4	4	224	ASN
4	4	236	GLN

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Mol	Chain	Res	Type
4	4	244	ASN
5	A	179	HIS
5	A	213	HIS
5	A	307	HIS
5	A	349	GLN
5	A	421	ASN
6	B	114	ASN
6	B	178	HIS
6	B	193	HIS
6	B	214	ASN
6	B	289	HIS
6	B	319	HIS
6	B	333	GLN
6	B	502	ASN
8	D	67	GLN
8	D	99	ASN
11	G	99	GLN
11	G	140	HIS
16	L	90	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

201 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	$\# Z > 2$
18	CLA	B	806	6	69,73,73	1.17	8 (11%)	82,113,113	1.27	5 (6%)
18	CLA	1	603	-	58,62,73	1.28	8 (13%)	68,99,113	1.37	5 (7%)
18	CLA	B	836	-	54,58,73	1.32	8 (14%)	64,95,113	3.34	9 (14%)
18	CLA	A	829	-	69,73,73	1.16	7 (10%)	82,113,113	1.27	5 (6%)
18	CLA	B	823	-	49,53,73	1.39	8 (16%)	58,89,113	1.42	4 (6%)
18	CLA	A	844	-	69,73,73	1.17	7 (10%)	82,113,113	1.29	6 (7%)
18	CLA	B	840	-	69,73,73	1.18	8 (11%)	82,113,113	1.26	4 (4%)
18	CLA	B	833	-	49,53,73	1.39	7 (14%)	58,89,113	1.49	6 (10%)
18	CLA	3	604	-	44,49,73	1.44	8 (18%)	50,84,113	1.41	4 (8%)
22	BCR	A	849	-	41,41,41	1.38	8 (19%)	56,56,56	1.93	15 (26%)
18	CLA	4	613	-	49,53,73	1.39	7 (14%)	58,89,113	1.58	5 (8%)
22	BCR	3	614	-	41,41,41	1.39	8 (19%)	56,56,56	1.49	11 (19%)
18	CLA	B	834	-	64,68,73	1.22	7 (10%)	76,107,113	1.32	6 (7%)
18	CLA	B	838	-	51,55,73	1.36	7 (13%)	60,91,113	1.40	5 (8%)
18	CLA	A	821	-	49,53,73	1.40	7 (14%)	58,89,113	1.42	4 (6%)
18	CLA	3	612	-	43,48,73	1.44	7 (16%)	51,83,113	1.51	5 (9%)
18	CLA	A	826	-	69,73,73	1.18	6 (8%)	82,113,113	1.27	5 (6%)
20	LHG	B	852	-	48,48,48	0.28	0	51,54,54	0.34	0
18	CLA	A	845	20	54,58,73	1.33	8 (14%)	64,95,113	1.39	6 (9%)
22	BCR	A	851	-	41,41,41	1.43	7 (17%)	56,56,56	2.41	19 (33%)
23	LMG	4	620	-	33,33,55	0.24	0	41,41,63	0.34	0
18	CLA	J	101	-	55,59,73	1.33	7 (12%)	64,96,113	1.38	5 (7%)
18	CLA	B	825	-	66,70,73	1.19	6 (9%)	78,109,113	1.34	9 (11%)
25	PQN	B	842	-	34,34,34	0.44	0	43,45,45	0.54	1 (2%)
18	CLA	A	814	-	69,73,73	1.18	8 (11%)	82,113,113	1.26	5 (6%)
18	CLA	3	601	-	64,68,73	1.22	7 (10%)	76,107,113	1.32	6 (7%)
21	LUT	2	616	-	42,43,43	1.28	8 (19%)	51,60,60	1.99	13 (25%)
18	CLA	A	810	5	54,58,73	1.33	8 (14%)	64,95,113	1.51	9 (14%)
18	CLA	B	821	-	51,55,73	1.34	7 (13%)	60,91,113	1.55	7 (11%)
18	CLA	A	842	-	69,73,73	1.18	8 (11%)	82,113,113	1.35	7 (8%)
21	LUT	1	616	-	42,43,43	1.28	7 (16%)	51,60,60	2.11	15 (29%)
18	CLA	4	604	-	47,51,73	1.52	9 (19%)	58,87,113	1.46	6 (10%)
18	CLA	4	610	-	46,50,73	1.40	8 (17%)	53,85,113	1.43	4 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	CLA	A	813	-	58,62,73	1.28	7 (12%)	68,99,113	1.40	6 (8%)
18	CLA	B	822	-	69,73,73	1.18	8 (11%)	82,113,113	1.37	8 (9%)
18	CLA	A	817	-	49,53,73	1.40	7 (14%)	58,89,113	1.42	4 (6%)
18	CLA	A	838	-	55,59,73	1.32	8 (14%)	64,96,113	1.40	6 (9%)
18	CLA	4	601	4	50,54,73	1.36	8 (16%)	59,90,113	1.42	4 (6%)
21	LUT	2	619	-	42,43,43	1.29	8 (19%)	51,60,60	1.82	13 (25%)
17	CHL	1	606	-	35,49,74	4.56	17 (48%)	28,84,114	1.67	9 (32%)
18	CLA	B	818	-	64,68,73	1.22	6 (9%)	76,107,113	1.33	8 (10%)
18	CLA	A	827	-	63,67,73	1.23	7 (11%)	74,105,113	1.35	6 (8%)
20	LHG	A	847	18	29,29,48	0.33	0	32,35,54	0.44	0
18	CLA	2	604	-	46,51,73	1.41	8 (17%)	54,86,113	1.46	4 (7%)
18	CLA	A	811	-	69,73,73	1.17	7 (10%)	82,113,113	1.27	6 (7%)
22	BCR	B	843	-	41,41,41	1.39	8 (19%)	56,56,56	1.86	14 (25%)
18	CLA	A	819	-	63,67,73	1.23	8 (12%)	74,105,113	1.34	6 (8%)
27	DGD	B	850	-	67,67,67	0.85	2 (2%)	81,81,81	0.94	4 (4%)
17	CHL	2	601	2	41,55,74	4.16	18 (43%)	35,91,114	2.39	11 (31%)
18	CLA	3	608	-	45,49,73	1.40	7 (15%)	54,84,113	1.55	6 (11%)
18	CLA	1	613	-	41,46,73	1.60	9 (21%)	51,81,113	1.55	7 (13%)
18	CLA	4	608	4	49,53,73	1.39	8 (16%)	58,89,113	1.44	4 (6%)
18	CLA	A	824	-	45,49,73	1.43	7 (15%)	54,84,113	1.48	5 (9%)
19	XAT	2	617	-	41,47,47	1.30	7 (17%)	54,74,74	2.00	14 (25%)
18	CLA	B	832	-	69,73,73	1.17	6 (8%)	82,113,113	1.24	4 (4%)
18	CLA	1	608	1	44,48,73	1.53	9 (20%)	55,83,113	1.53	8 (14%)
18	CLA	2	602	2	69,73,73	1.17	8 (11%)	82,113,113	1.26	5 (6%)
18	CLA	G	202	-	46,50,73	1.41	7 (15%)	53,85,113	1.43	4 (7%)
18	CLA	B	812	-	47,51,73	1.40	7 (14%)	55,86,113	1.41	4 (7%)
17	CHL	4	606	-	35,49,74	3.97	15 (42%)	33,84,114	2.38	11 (33%)
18	CLA	A	804	-	69,73,73	1.18	8 (11%)	82,113,113	1.37	7 (8%)
22	BCR	J	102	-	41,41,41	1.38	8 (19%)	56,56,56	1.69	14 (25%)
22	BCR	A	848	-	41,41,41	1.38	8 (19%)	56,56,56	1.52	11 (19%)
20	LHG	1	615	18	48,48,48	0.93	2 (4%)	51,54,54	1.04	3 (5%)
22	BCR	A	853	-	41,41,41	1.41	8 (19%)	56,56,56	1.71	15 (26%)
18	CLA	1	612	-	50,54,73	1.36	8 (16%)	59,90,113	1.48	5 (8%)
18	CLA	A	830	-	69,73,73	1.17	6 (8%)	82,113,113	1.38	7 (8%)
18	CLA	B	819	-	59,63,73	1.27	8 (13%)	70,101,113	1.37	6 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	CLA	A	807	-	69,73,73	1.18	7 (10%)	82,113,113	1.24	6 (7%)
22	BCR	A	850	-	41,41,41	1.41	8 (19%)	56,56,56	1.85	13 (23%)
18	CLA	4	603	-	48,52,73	1.50	9 (18%)	59,88,113	1.46	6 (10%)
17	CHL	4	615	4	36,49,74	4.28	16 (44%)	30,84,114	2.06	9 (30%)
18	CLA	F	301	-	61,65,73	1.25	8 (13%)	72,103,113	1.30	5 (6%)
18	CLA	2	612	2	69,73,73	1.17	7 (10%)	82,113,113	1.29	7 (8%)
18	CLA	3	607	-	49,53,73	1.40	7 (14%)	58,89,113	1.43	4 (6%)
18	CLA	A	835	-	69,73,73	1.17	7 (10%)	82,113,113	1.29	7 (8%)
18	CLA	B	804	-	45,49,73	1.41	7 (15%)	54,84,113	1.54	6 (11%)
22	BCR	B	801	-	41,41,41	1.42	8 (19%)	56,56,56	1.71	13 (23%)
18	CLA	A	828	-	69,73,73	1.18	8 (11%)	82,113,113	1.30	7 (8%)
18	CLA	A	822	-	69,73,73	1.18	8 (11%)	82,113,113	1.26	5 (6%)
18	CLA	2	610	20	40,45,73	2.62	10 (25%)	46,76,113	1.33	6 (13%)
22	BCR	B	846	-	41,41,41	1.38	8 (19%)	56,56,56	1.62	11 (19%)
18	CLA	B	830	-	47,51,73	1.39	8 (17%)	55,86,113	1.44	4 (7%)
19	XAT	1	614	-	41,47,47	0.89	2 (4%)	54,74,74	3.01	17 (31%)
18	CLA	K	201	15	41,45,73	1.47	8 (19%)	50,78,113	1.46	4 (8%)
22	BCR	B	844	-	41,41,41	1.37	8 (19%)	56,56,56	1.72	12 (21%)
18	CLA	1	604	-	53,57,73	1.33	8 (15%)	61,93,113	1.46	5 (8%)
18	CLA	A	815	-	49,53,73	1.38	7 (14%)	58,89,113	1.44	4 (6%)
18	CLA	2	611	-	48,52,73	1.41	7 (14%)	57,88,113	1.48	5 (8%)
17	CHL	4	605	-	35,49,74	4.11	17 (48%)	30,84,114	2.09	12 (40%)
18	CLA	B	829	-	60,64,73	1.26	8 (13%)	71,102,113	1.33	5 (7%)
18	CLA	B	835	-	46,50,73	1.41	8 (17%)	53,85,113	1.43	4 (7%)
22	BCR	B	849	-	41,41,41	1.38	8 (19%)	56,56,56	1.73	13 (23%)
18	CLA	A	820	-	69,73,73	1.18	7 (10%)	82,113,113	1.28	6 (7%)
22	BCR	F	304	-	41,41,41	1.39	7 (17%)	56,56,56	2.11	16 (28%)
18	CLA	A	831	-	69,73,73	1.17	7 (10%)	82,113,113	1.28	6 (7%)
18	CLA	4	609	-	58,62,73	1.27	9 (15%)	68,99,113	1.37	6 (8%)
18	CLA	A	808	-	54,58,73	1.33	8 (14%)	64,95,113	1.41	6 (9%)
18	CLA	4	602	4	64,68,73	1.21	7 (10%)	76,107,113	1.32	7 (9%)
18	CLA	A	837	5	49,53,73	1.40	7 (14%)	58,89,113	1.42	4 (6%)
21	LUT	3	613	-	42,43,43	1.30	8 (19%)	51,60,60	1.92	17 (33%)
17	CHL	2	607	-	45,59,74	3.93	19 (42%)	40,96,114	2.28	15 (37%)
18	CLA	B	826	-	66,70,73	1.20	7 (10%)	78,109,113	1.31	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	CLA	A	840	-	56,60,73	1.31	7 (12%)	65,97,113	1.39	6 (9%)
18	CLA	1	609	-	46,50,73	1.40	8 (17%)	54,85,113	1.50	4 (7%)
18	CLA	F	303	10	45,49,73	1.43	6 (13%)	54,84,113	1.50	5 (9%)
23	LMG	4	619	-	39,39,55	0.22	0	47,47,63	0.25	0
18	CLA	A	833	-	60,64,73	1.25	7 (11%)	71,102,113	1.34	4 (5%)
22	BCR	L	306	-	41,41,41	1.37	8 (19%)	56,56,56	1.83	16 (28%)
26	SF4	A	854	-	0,12,12	-	-	-	-	-
18	CLA	A	803	-	69,73,73	1.18	7 (10%)	82,113,113	1.25	5 (6%)
18	CLA	3	611	-	40,44,73	1.51	9 (22%)	49,77,113	1.47	4 (8%)
18	CLA	B	814	-	69,73,73	1.16	6 (8%)	82,113,113	1.28	6 (7%)
18	CLA	K	203	-	49,53,73	1.39	7 (14%)	58,89,113	1.46	5 (8%)
18	CLA	B	820	-	54,58,73	1.32	7 (12%)	64,95,113	1.42	6 (9%)
18	CLA	L	304	-	49,53,73	1.40	7 (14%)	58,89,113	1.45	4 (6%)
18	CLA	4	611	-	44,49,73	1.45	8 (18%)	50,84,113	1.42	4 (8%)
18	CLA	L	303	-	69,73,73	1.16	6 (8%)	82,113,113	1.30	6 (7%)
22	BCR	I	101	-	41,41,41	1.38	8 (19%)	56,56,56	1.42	10 (17%)
17	CHL	3	606	-	38,53,74	3.94	18 (47%)	36,89,114	2.34	11 (30%)
18	CLA	B	808	-	69,73,73	1.16	9 (13%)	82,113,113	1.31	6 (7%)
18	CLA	A	825	-	59,63,73	1.27	7 (11%)	70,101,113	1.33	6 (8%)
18	CLA	2	609	-	51,55,73	1.34	8 (15%)	60,91,113	1.43	6 (10%)
18	CLA	B	837	-	69,73,73	1.17	6 (8%)	82,113,113	1.30	6 (7%)
18	CLA	B	810	-	69,73,73	1.18	6 (8%)	82,113,113	1.26	5 (6%)
19	XAT	4	617	-	41,47,47	1.28	8 (19%)	54,74,74	1.66	12 (22%)
22	BCR	B	845	-	41,41,41	1.41	8 (19%)	56,56,56	1.74	14 (25%)
18	CLA	4	612	-	61,65,73	1.24	7 (11%)	72,103,113	1.35	6 (8%)
25	PQN	A	855	-	34,34,34	0.42	0	43,45,45	0.57	1 (2%)
18	CLA	A	809	-	69,73,73	1.17	7 (10%)	82,113,113	1.29	6 (7%)
18	CLA	B	817	-	63,67,73	1.23	9 (14%)	74,105,113	1.32	6 (8%)
18	CLA	K	206	15	42,47,73	1.50	7 (16%)	48,81,113	1.48	5 (10%)
18	CLA	A	841	-	69,73,73	1.18	7 (10%)	82,113,113	1.27	6 (7%)
17	CHL	1	601	1	46,60,74	3.94	18 (39%)	40,97,114	1.86	13 (32%)
18	CLA	B	803	-	69,73,73	1.16	8 (11%)	82,113,113	1.30	5 (6%)
18	CLA	A	843	-	69,73,73	1.17	6 (8%)	82,113,113	1.29	4 (4%)
18	CLA	A	816	-	46,50,73	1.41	8 (17%)	53,85,113	1.44	4 (7%)
22	BCR	B	847	-	41,41,41	1.39	8 (19%)	56,56,56	1.49	11 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	CLA	3	610	-	43,48,73	1.46	7 (16%)	51,83,113	1.48	5 (9%)
18	CLA	B	827	-	69,73,73	1.18	8 (11%)	82,113,113	1.30	6 (7%)
18	CLA	1	605	-	50,54,73	1.37	8 (16%)	59,90,113	1.41	4 (6%)
18	CLA	G	201	-	49,53,73	1.40	7 (14%)	58,89,113	1.42	5 (8%)
18	CLA	B	811	-	58,62,73	1.36	9 (15%)	71,100,113	1.41	7 (9%)
18	CLA	B	802	-	69,73,73	1.18	7 (10%)	82,113,113	1.25	5 (6%)
22	BCR	K	205	-	41,41,41	1.38	8 (19%)	56,56,56	1.90	17 (30%)
18	CLA	3	602	-	59,63,73	1.28	8 (13%)	70,101,113	1.32	5 (7%)
18	CLA	B	809	6	69,73,73	1.17	7 (10%)	82,113,113	1.28	6 (7%)
18	CLA	3	605	-	45,49,73	1.51	9 (20%)	54,84,113	1.52	6 (11%)
18	CLA	A	818	-	64,68,73	1.21	7 (10%)	76,107,113	5.01	7 (9%)
18	CLA	2	603	-	47,52,73	1.42	8 (17%)	55,88,113	1.42	4 (7%)
18	CLA	G	203	11	49,53,73	1.39	7 (14%)	58,89,113	1.44	5 (8%)
18	CLA	H	201	-	64,68,73	1.22	8 (12%)	76,107,113	1.30	4 (5%)
18	CLA	B	841	20	69,73,73	1.17	8 (11%)	82,113,113	1.29	5 (6%)
17	CHL	2	605	-	36,50,74	4.10	17 (47%)	31,85,114	2.30	10 (32%)
18	CLA	B	824	-	69,73,73	1.17	7 (10%)	82,113,113	1.29	6 (7%)
18	CLA	A	805	-	56,60,73	1.30	6 (10%)	65,97,113	1.39	5 (7%)
22	BCR	L	305	-	41,41,41	1.40	8 (19%)	56,56,56	1.68	15 (26%)
18	CLA	B	816	-	59,63,73	1.26	7 (11%)	70,101,113	1.36	6 (8%)
17	CHL	4	607	-	40,54,74	4.13	19 (47%)	34,90,114	2.49	12 (35%)
20	LHG	B	851	18	37,37,48	0.30	0	40,43,54	0.49	0
18	CLA	3	609	-	57,62,73	1.30	8 (14%)	67,100,113	1.32	5 (7%)
26	SF4	C	102	-	0,12,12	-	-	-	-	-
22	BCR	B	848	-	41,41,41	1.39	8 (19%)	56,56,56	1.51	12 (21%)
18	CLA	1	602	1	58,62,73	1.28	7 (12%)	68,99,113	1.35	5 (7%)
20	LHG	2	618	18	36,36,48	0.31	0	39,42,54	0.54	1 (2%)
24	CL0	A	801	-	53,67,73	3.01	17 (32%)	47,102,113	2.28	12 (25%)
22	BCR	G	204	-	41,41,41	1.38	8 (19%)	56,56,56	1.57	12 (21%)
18	CLA	A	832	-	54,58,73	1.31	7 (12%)	64,95,113	1.42	6 (9%)
20	LHG	A	846	-	48,48,48	0.27	0	51,54,54	0.34	0
17	CHL	2	606	-	37,51,74	4.35	17 (45%)	30,86,114	2.45	12 (40%)
18	CLA	B	807	-	56,60,73	1.30	6 (10%)	65,97,113	1.39	5 (7%)
22	BCR	A	852	-	41,41,41	1.38	8 (19%)	56,56,56	1.83	15 (26%)
18	CLA	2	608	-	49,53,73	1.38	6 (12%)	58,89,113	1.44	4 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	CLA	A	812	-	69,73,73	1.18	8 (11%)	82,113,113	1.26	5 (6%)
18	CLA	B	805	-	69,73,73	1.18	7 (10%)	82,113,113	1.24	5 (6%)
22	BCR	4	618	-	41,41,41	1.38	8 (19%)	56,56,56	1.63	10 (17%)
22	BCR	K	202	-	41,41,41	1.38	8 (19%)	56,56,56	1.85	14 (25%)
18	CLA	2	613	-	47,51,73	1.40	8 (17%)	55,86,113	1.42	4 (7%)
18	CLA	F	302	-	55,59,73	1.32	8 (14%)	64,96,113	1.43	6 (9%)
18	CLA	1	610	20	41,46,73	1.60	9 (21%)	51,81,113	1.54	7 (13%)
18	CLA	A	823	-	46,50,73	1.40	6 (13%)	53,85,113	1.45	5 (9%)
18	CLA	B	828	-	69,73,73	1.18	7 (10%)	82,113,113	1.26	5 (6%)
17	CHL	2	615	2	37,51,74	4.37	17 (45%)	30,86,114	2.30	10 (33%)
18	CLA	1	611	-	49,53,73	1.40	8 (16%)	58,89,113	1.42	4 (6%)
18	CLA	1	607	-	47,52,73	1.42	7 (14%)	55,88,113	1.42	4 (7%)
22	BCR	L	301	-	41,41,41	1.39	8 (19%)	56,56,56	2.10	12 (21%)
18	CLA	3	603	-	49,53,73	1.39	8 (16%)	58,89,113	1.43	5 (8%)
18	CLA	A	806	-	69,73,73	1.17	8 (11%)	82,113,113	1.29	5 (6%)
18	CLA	A	802	-	69,73,73	1.17	9 (13%)	82,113,113	1.32	5 (6%)
18	CLA	A	836	-	49,53,73	1.41	8 (16%)	58,89,113	1.43	4 (6%)
18	CLA	B	839	-	69,73,73	1.17	8 (11%)	82,113,113	1.27	5 (6%)
18	CLA	L	302	-	49,53,73	1.39	8 (16%)	58,89,113	1.45	4 (6%)
18	CLA	B	813	-	69,73,73	1.18	8 (11%)	82,113,113	1.35	8 (9%)
18	CLA	B	815	-	47,51,73	1.38	7 (14%)	55,86,113	1.44	4 (7%)
18	CLA	K	204	-	50,54,73	1.37	9 (18%)	59,90,113	1.43	4 (6%)
18	CLA	A	839	-	59,63,73	1.26	7 (11%)	70,101,113	1.35	6 (8%)
18	CLA	A	834	-	69,73,73	1.18	8 (11%)	82,113,113	1.28	6 (7%)
18	CLA	4	614	-	54,58,73	1.32	8 (14%)	64,95,113	1.44	6 (9%)
26	SF4	C	101	-	0,12,12	-	-	-	-	-
21	LUT	4	616	-	42,43,43	1.28	8 (19%)	51,60,60	1.49	11 (21%)
18	CLA	B	831	-	47,51,73	1.39	7 (14%)	55,86,113	1.45	4 (7%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	B	806	6	1/1/15/20	11/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	1	603	-	1/1/12/20	8/26/102/115	-
18	CLA	B	836	-	1/1/12/20	7/21/97/115	-
18	CLA	A	829	-	1/1/15/20	15/39/115/115	-
18	CLA	B	823	-	1/1/11/20	6/15/91/115	-
18	CLA	A	844	-	1/1/15/20	12/39/115/115	-
18	CLA	B	840	-	1/1/15/20	18/39/115/115	-
18	CLA	B	833	-	1/1/11/20	4/15/91/115	-
18	CLA	3	604	-	1/1/10/20	2/10/86/115	-
22	BCR	A	849	-	-	6/29/63/63	0/2/2/2
18	CLA	4	613	-	1/1/11/20	2/15/91/115	-
22	BCR	3	614	-	-	3/29/63/63	0/2/2/2
18	CLA	B	834	-	1/1/14/20	9/33/109/115	-
18	CLA	B	838	-	1/1/11/20	0/18/94/115	-
18	CLA	A	821	-	1/1/11/20	1/15/91/115	-
18	CLA	3	612	-	1/1/10/20	2/8/84/115	-
18	CLA	A	826	-	1/1/15/20	7/39/115/115	-
20	LHG	B	852	-	-	13/53/53/53	-
18	CLA	A	845	20	1/1/12/20	6/21/97/115	-
22	BCR	A	851	-	-	7/29/63/63	0/2/2/2
23	LMG	4	620	-	-	7/28/48/70	0/1/1/1
18	CLA	J	101	-	1/1/12/20	7/23/99/115	-
18	CLA	B	825	-	1/1/14/20	10/36/112/115	-
25	PQN	B	842	-	-	6/23/43/43	0/2/2/2
18	CLA	A	814	-	1/1/15/20	11/39/115/115	-
18	CLA	3	601	-	1/1/14/20	13/33/109/115	-
21	LUT	2	616	-	-	4/29/67/67	0/2/2/2
18	CLA	A	810	5	1/1/12/20	4/21/97/115	-
18	CLA	B	821	-	1/1/11/20	3/18/94/115	-
18	CLA	A	842	-	1/1/15/20	16/39/115/115	-
21	LUT	1	616	-	-	2/29/67/67	0/2/2/2
18	CLA	4	604	-	1/1/11/20	6/11/87/115	-
18	CLA	4	610	-	1/1/10/20	2/12/88/115	-
18	CLA	A	813	-	1/1/12/20	11/26/102/115	-
18	CLA	B	822	-	1/1/15/20	15/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	A	817	-	1/1/11/20	4/15/91/115	-
18	CLA	A	838	-	1/1/12/20	7/23/99/115	-
18	CLA	4	601	4	1/1/11/20	5/17/93/115	-
21	LUT	2	619	-	-	5/29/67/67	0/2/2/2
17	CHL	1	606	-	3/3/15/26	0/8/106/137	-
18	CLA	B	818	-	1/1/14/20	8/33/109/115	-
18	CLA	A	827	-	1/1/13/20	2/32/108/115	-
20	LHG	A	847	18	-	1/34/34/53	-
18	CLA	2	604	-	1/1/10/20	9/12/88/115	-
18	CLA	A	811	-	1/1/15/20	9/39/115/115	-
22	BCR	B	843	-	-	1/29/63/63	0/2/2/2
18	CLA	A	819	-	1/1/13/20	17/32/108/115	-
27	DGD	B	850	-	-	11/55/95/95	0/2/2/2
17	CHL	2	601	2	3/3/16/26	6/17/115/137	-
18	CLA	3	608	-	1/1/10/20	2/10/86/115	-
18	CLA	1	613	-	1/1/10/20	0/4/80/115	-
18	CLA	4	608	4	1/1/11/20	6/15/91/115	-
18	CLA	A	824	-	1/1/10/20	4/10/86/115	-
19	XAT	2	617	-	-	17/31/93/93	0/4/4/4
18	CLA	B	832	-	1/1/15/20	13/39/115/115	-
18	CLA	1	608	1	1/1/10/20	2/8/84/115	-
18	CLA	2	602	2	1/1/15/20	16/39/115/115	-
18	CLA	G	202	-	1/1/10/20	4/12/88/115	-
18	CLA	B	812	-	1/1/10/20	0/13/89/115	-
17	CHL	4	606	-	3/3/15/26	4/10/106/137	-
18	CLA	A	804	-	1/1/15/20	17/39/115/115	-
22	BCR	J	102	-	-	2/29/63/63	0/2/2/2
22	BCR	A	848	-	-	0/29/63/63	0/2/2/2
20	LHG	1	615	18	-	34/53/53/53	-
22	BCR	A	853	-	-	3/29/63/63	0/2/2/2
18	CLA	1	612	-	1/1/11/20	8/17/93/115	-
18	CLA	A	830	-	1/1/15/20	13/39/115/115	-
18	CLA	B	819	-	1/1/13/20	11/27/103/115	-
18	CLA	A	807	-	1/1/15/20	12/39/115/115	-
22	BCR	A	850	-	-	4/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	4	603	-	1/1/11/20	5/13/89/115	-
17	CHL	4	615	4	3/3/15/26	0/10/106/137	-
18	CLA	F	301	-	1/1/13/20	14/30/106/115	-
18	CLA	2	612	2	1/1/15/20	14/39/115/115	-
18	CLA	3	607	-	1/1/11/20	3/15/91/115	-
18	CLA	A	835	-	1/1/15/20	18/39/115/115	-
18	CLA	B	804	-	1/1/10/20	2/10/86/115	-
22	BCR	B	801	-	-	4/29/63/63	0/2/2/2
18	CLA	A	828	-	1/1/15/20	7/39/115/115	-
18	CLA	A	822	-	1/1/15/20	11/39/115/115	-
18	CLA	2	610	20	1/1/7/20	5/10/70/115	-
22	BCR	B	846	-	-	8/29/63/63	0/2/2/2
18	CLA	B	830	-	1/1/10/20	2/13/89/115	-
19	XAT	1	614	-	-	8/31/93/93	0/4/4/4
18	CLA	K	201	15	1/1/8/20	2/4/76/115	-
22	BCR	B	844	-	-	11/29/63/63	0/2/2/2
18	CLA	1	604	-	1/1/11/20	6/20/96/115	-
18	CLA	A	815	-	1/1/11/20	5/15/91/115	-
18	CLA	2	611	-	1/1/11/20	5/13/89/115	-
17	CHL	4	605	-	3/3/15/26	3/8/106/137	-
18	CLA	B	829	-	1/1/13/20	3/29/105/115	-
18	CLA	B	835	-	1/1/10/20	6/12/88/115	-
22	BCR	B	849	-	-	7/29/63/63	0/2/2/2
18	CLA	A	820	-	1/1/15/20	12/39/115/115	-
22	BCR	F	304	-	-	12/29/63/63	0/2/2/2
18	CLA	A	831	-	1/1/15/20	11/39/115/115	-
18	CLA	4	609	-	1/1/12/20	7/26/102/115	-
18	CLA	A	808	-	1/1/12/20	4/21/97/115	-
18	CLA	4	602	4	1/1/14/20	5/33/109/115	-
18	CLA	A	837	5	1/1/11/20	3/15/91/115	-
21	LUT	3	613	-	-	6/29/67/67	0/2/2/2
17	CHL	2	607	-	3/3/17/26	8/21/119/137	-
18	CLA	B	826	-	1/1/14/20	6/36/112/115	-
18	CLA	A	840	-	1/1/12/20	6/24/100/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	1	609	-	1/1/10/20	4/11/87/115	-
18	CLA	F	303	10	1/1/10/20	4/10/86/115	-
23	LMG	4	619	-	-	5/34/54/70	0/1/1/1
18	CLA	A	833	-	1/1/13/20	7/29/105/115	-
22	BCR	L	306	-	-	5/29/63/63	0/2/2/2
26	SF4	A	854	-	-	-	0/6/5/5
18	CLA	A	803	-	1/1/15/20	19/39/115/115	-
18	CLA	3	611	-	1/1/8/20	2/2/74/115	-
18	CLA	B	814	-	1/1/15/20	14/39/115/115	-
18	CLA	K	203	-	1/1/11/20	6/15/91/115	-
18	CLA	B	820	-	1/1/12/20	5/21/97/115	-
18	CLA	L	304	-	1/1/11/20	3/15/91/115	-
18	CLA	4	611	-	1/1/10/20	6/10/86/115	-
18	CLA	L	303	-	1/1/15/20	10/39/115/115	-
22	BCR	I	101	-	-	0/29/63/63	0/2/2/2
17	CHL	3	606	-	3/3/16/26	5/13/111/137	-
18	CLA	B	808	-	1/1/15/20	16/39/115/115	-
18	CLA	A	825	-	1/1/13/20	7/27/103/115	-
18	CLA	2	609	-	1/1/11/20	7/18/94/115	-
18	CLA	B	837	-	1/1/15/20	10/39/115/115	-
18	CLA	B	810	-	1/1/15/20	10/39/115/115	-
19	XAT	4	617	-	-	3/31/93/93	0/4/4/4
22	BCR	B	845	-	-	9/29/63/63	0/2/2/2
18	CLA	4	612	-	1/1/13/20	11/30/106/115	-
25	PQN	A	855	-	-	1/23/43/43	0/2/2/2
18	CLA	A	809	-	1/1/15/20	14/39/115/115	-
18	CLA	B	817	-	1/1/13/20	11/32/108/115	-
18	CLA	K	206	15	1/1/9/20	1/8/80/115	-
18	CLA	A	841	-	1/1/15/20	13/39/115/115	-
17	CHL	1	601	1	3/3/17/26	9/22/120/137	-
18	CLA	B	803	-	1/1/15/20	9/39/115/115	-
18	CLA	A	843	-	1/1/15/20	11/39/115/115	-
18	CLA	A	816	-	1/1/10/20	4/12/88/115	-
22	BCR	B	847	-	-	2/29/63/63	0/2/2/2
18	CLA	3	610	-	1/1/10/20	3/8/84/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	B	827	-	1/1/15/20	21/39/115/115	-
18	CLA	1	605	-	1/1/11/20	7/17/93/115	-
18	CLA	G	201	-	1/1/11/20	9/15/91/115	-
18	CLA	B	811	-	1/1/13/20	11/25/101/115	-
18	CLA	B	802	-	1/1/15/20	14/39/115/115	-
22	BCR	K	205	-	-	9/29/63/63	0/2/2/2
18	CLA	3	602	-	1/1/13/20	11/27/103/115	-
18	CLA	B	809	6	1/1/15/20	18/39/115/115	-
18	CLA	3	605	-	1/1/10/20	6/10/86/115	-
18	CLA	A	818	-	1/1/14/20	13/33/109/115	-
18	CLA	2	603	-	1/1/11/20	3/13/89/115	-
18	CLA	G	203	11	1/1/11/20	3/15/91/115	-
18	CLA	H	201	-	1/1/14/20	14/33/109/115	-
18	CLA	B	841	20	1/1/15/20	20/39/115/115	-
17	CHL	2	605	-	3/3/15/26	4/10/108/137	-
18	CLA	B	824	-	1/1/15/20	12/39/115/115	-
18	CLA	A	805	-	1/1/12/20	5/24/100/115	-
22	BCR	L	305	-	-	2/29/63/63	0/2/2/2
18	CLA	B	816	-	1/1/13/20	6/27/103/115	-
17	CHL	4	607	-	3/3/16/26	4/15/113/137	-
20	LHG	B	851	18	-	5/42/42/53	-
18	CLA	3	609	-	1/1/13/20	8/25/101/115	-
26	SF4	C	102	-	-	-	0/6/5/5
22	BCR	B	848	-	-	0/29/63/63	0/2/2/2
18	CLA	1	602	1	1/1/12/20	5/26/102/115	-
24	CL0	A	801	-	2/2/16/25	8/31/115/135	-
20	LHG	2	618	18	-	9/41/41/53	-
22	BCR	G	204	-	-	2/29/63/63	0/2/2/2
18	CLA	A	832	-	1/1/12/20	4/21/97/115	-
20	LHG	A	846	-	-	4/53/53/53	-
17	CHL	2	606	-	3/3/15/26	4/12/110/137	-
18	CLA	B	807	-	1/1/12/20	5/24/100/115	-
22	BCR	A	852	-	-	14/29/63/63	0/2/2/2
18	CLA	2	608	-	1/1/11/20	7/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	A	812	-	1/1/15/20	19/39/115/115	-
18	CLA	B	805	-	1/1/15/20	16/39/115/115	-
22	BCR	4	618	-	-	6/29/63/63	0/2/2/2
22	BCR	K	202	-	-	2/29/63/63	0/2/2/2
18	CLA	2	613	-	1/1/10/20	5/13/89/115	-
18	CLA	F	302	-	1/1/12/20	6/23/99/115	-
18	CLA	1	610	20	1/1/10/20	1/4/80/115	-
18	CLA	A	823	-	1/1/10/20	4/12/88/115	-
18	CLA	B	828	-	1/1/15/20	17/39/115/115	-
17	CHL	2	615	2	3/3/15/26	2/12/110/137	-
18	CLA	1	611	-	1/1/11/20	6/15/91/115	-
18	CLA	1	607	-	1/1/11/20	8/13/89/115	-
22	BCR	L	301	-	-	3/29/63/63	0/2/2/2
18	CLA	3	603	-	1/1/11/20	9/15/91/115	-
18	CLA	A	806	-	1/1/15/20	18/39/115/115	-
18	CLA	A	802	-	1/1/15/20	17/39/115/115	-
18	CLA	A	836	-	1/1/11/20	9/15/91/115	-
18	CLA	B	839	-	1/1/15/20	9/39/115/115	-
18	CLA	L	302	-	1/1/11/20	2/15/91/115	-
18	CLA	B	813	-	1/1/15/20	15/39/115/115	-
18	CLA	B	815	-	1/1/10/20	2/13/89/115	-
18	CLA	K	204	-	1/1/11/20	12/17/93/115	-
18	CLA	A	839	-	1/1/13/20	9/27/103/115	-
18	CLA	A	834	-	1/1/15/20	9/39/115/115	-
18	CLA	4	614	-	1/1/12/20	10/21/97/115	-
26	SF4	C	101	-	-	-	0/6/5/5
21	LUT	4	616	-	-	2/29/67/67	0/2/2/2
18	CLA	B	831	-	1/1/10/20	0/13/89/115	-

All (1538) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	2	610	CLA	C1A-NA	13.18	1.40	1.29
17	1	606	CHL	C2C-C3C	11.26	1.47	1.36
17	1	601	CHL	C2C-C3C	10.85	1.46	1.36
17	2	615	CHL	C2C-C3C	10.85	1.46	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	2	606	CHL	C2C-C3C	10.85	1.46	1.36
17	2	601	CHL	C2C-C3C	10.80	1.46	1.36
17	4	615	CHL	C2C-C3C	10.63	1.46	1.36
17	1	606	CHL	C1D-C2D	10.62	1.51	1.39
17	2	607	CHL	C2C-C3C	10.59	1.46	1.36
17	2	606	CHL	C1D-C2D	10.50	1.51	1.39
17	1	601	CHL	C1D-C2D	10.40	1.51	1.39
17	3	606	CHL	C1D-C2D	10.35	1.51	1.39
17	4	605	CHL	C1D-C2D	10.33	1.51	1.39
17	2	615	CHL	C1D-C2D	10.32	1.51	1.39
17	4	607	CHL	C2C-C3C	10.32	1.46	1.36
17	4	615	CHL	C1D-C2D	10.31	1.51	1.39
17	2	601	CHL	C1D-C2D	10.30	1.51	1.39
17	2	607	CHL	C1D-C2D	10.19	1.51	1.39
17	4	606	CHL	C1D-C2D	10.19	1.51	1.39
17	2	605	CHL	C1D-C2D	10.18	1.51	1.39
17	4	607	CHL	C1D-C2D	10.12	1.51	1.39
24	A	801	CL0	C1D-C2D	9.20	1.50	1.39
17	1	606	CHL	C1B-C2B	8.57	1.49	1.39
17	2	606	CHL	C1B-C2B	8.55	1.49	1.39
17	2	601	CHL	C1B-C2B	8.54	1.49	1.39
17	4	606	CHL	C1B-C2B	8.54	1.49	1.39
17	3	606	CHL	C1B-C2B	8.48	1.49	1.39
17	4	605	CHL	C1B-C2B	8.48	1.49	1.39
17	4	615	CHL	C1B-C2B	8.46	1.49	1.39
17	2	605	CHL	C1B-C2B	8.44	1.49	1.39
17	2	615	CHL	C1B-C2B	8.37	1.49	1.39
17	1	601	CHL	C1B-C2B	8.32	1.49	1.39
17	4	607	CHL	C1B-C2B	8.29	1.49	1.39
17	2	615	CHL	C3B-C4B	8.22	1.49	1.41
17	1	601	CHL	C3B-C4B	8.19	1.49	1.41
17	2	607	CHL	C1B-C2B	8.18	1.48	1.39
24	A	801	CL0	C1B-C2B	8.13	1.48	1.39
17	1	606	CHL	C3B-C4B	7.98	1.49	1.41
17	4	605	CHL	C3B-C4B	7.96	1.49	1.41
17	2	605	CHL	C3B-C4B	7.96	1.49	1.41
17	4	606	CHL	C4B-C3B	7.94	1.48	1.39
17	4	615	CHL	C4B-C3B	7.90	1.48	1.39
17	2	601	CHL	C3B-C4B	7.83	1.49	1.41
24	A	801	CL0	C3B-C4B	7.80	1.49	1.41
17	2	605	CHL	C1A-CHA	7.79	1.48	1.40
17	2	606	CHL	C3B-C4B	7.74	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	2	615	CHL	C1A-CHA	7.74	1.48	1.40
17	3	606	CHL	C3B-C4B	7.54	1.48	1.41
17	4	607	CHL	C3B-C4B	7.49	1.48	1.41
17	2	607	CHL	C3B-C4B	7.44	1.48	1.41
17	3	606	CHL	C1A-CHA	7.42	1.48	1.40
17	4	606	CHL	C1A-CHA	7.40	1.48	1.40
17	1	601	CHL	C1A-CHA	7.36	1.48	1.40
17	4	615	CHL	C1A-CHA	7.34	1.48	1.40
17	1	606	CHL	C1A-CHA	7.30	1.48	1.40
17	2	601	CHL	C1A-CHA	7.28	1.48	1.40
17	2	607	CHL	C1A-CHA	7.23	1.48	1.40
17	2	606	CHL	C1A-CHA	7.22	1.48	1.40
17	4	605	CHL	C1A-CHA	7.20	1.48	1.40
17	4	607	CHL	C1A-CHA	7.18	1.48	1.40
24	A	801	CL0	C3D-C4D	-6.97	1.34	1.41
24	A	801	CL0	CHB-C4A	-6.93	1.30	1.38
24	A	801	CL0	CHA-C1A	5.81	1.45	1.38
17	1	606	CHL	C3B-C2B	5.45	1.47	1.40
24	A	801	CL0	C3A-C2A	-5.40	1.50	1.54
17	1	606	CHL	CHC-C4B	5.26	1.48	1.39
17	1	606	CHL	C3D-C4D	-5.22	1.33	1.41
17	4	605	CHL	C3D-C4D	-5.20	1.33	1.41
17	2	601	CHL	C3D-C4D	-5.17	1.33	1.41
17	2	607	CHL	C3D-C4D	-5.17	1.33	1.41
17	1	601	CHL	C3D-C4D	-5.16	1.33	1.41
17	4	607	CHL	C3D-C4D	-5.16	1.33	1.41
17	1	606	CHL	CHD-C1D	5.14	1.47	1.39
17	1	606	CHL	CHD-C4C	5.14	1.49	1.39
17	3	606	CHL	C3D-C4D	-5.13	1.33	1.41
17	2	606	CHL	O2D-CGD	5.13	1.45	1.33
17	2	615	CHL	C3B-C2B	5.12	1.47	1.40
17	4	606	CHL	O2D-CGD	5.12	1.45	1.33
17	2	606	CHL	C3D-C4D	-5.11	1.33	1.41
17	2	605	CHL	CHC-C4B	5.11	1.47	1.39
17	2	605	CHL	O2D-CGD	5.10	1.45	1.33
17	2	605	CHL	C3D-C4D	-5.10	1.33	1.41
17	4	607	CHL	O2D-CGD	5.10	1.45	1.33
17	2	615	CHL	O2D-CGD	5.09	1.45	1.33
17	2	606	CHL	C3B-C2B	5.09	1.47	1.40
17	2	601	CHL	C3B-C2B	5.08	1.47	1.40
17	4	615	CHL	C3D-C4D	-5.08	1.33	1.41
17	2	607	CHL	O2D-CGD	5.06	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	2	615	CHL	C3D-C4D	-5.06	1.33	1.41
17	4	605	CHL	OBD-CAD	5.05	1.28	1.22
17	2	605	CHL	C3B-C2B	5.05	1.47	1.40
17	2	606	CHL	OBD-CAD	5.05	1.28	1.22
17	1	601	CHL	CHC-C4B	5.04	1.47	1.39
17	4	606	CHL	OBD-CAD	5.04	1.28	1.22
17	1	601	CHL	C3B-C2B	5.03	1.47	1.40
17	2	601	CHL	O2D-CGD	5.03	1.45	1.33
17	2	615	CHL	OBD-CAD	5.03	1.28	1.22
17	2	601	CHL	OBD-CAD	5.02	1.28	1.22
17	3	606	CHL	OBD-CAD	5.02	1.28	1.22
17	3	606	CHL	O2D-CGD	5.01	1.45	1.33
17	4	615	CHL	OBD-CAD	5.00	1.28	1.22
17	2	615	CHL	CHC-C4B	4.99	1.47	1.39
17	1	606	CHL	OBD-CAD	4.99	1.28	1.22
17	1	601	CHL	OBD-CAD	4.98	1.28	1.22
17	4	606	CHL	C3D-C4D	-4.98	1.33	1.41
17	2	605	CHL	OBD-CAD	4.98	1.28	1.22
17	2	607	CHL	CHC-C4B	4.97	1.47	1.39
17	1	606	CHL	CHB-C1B	4.96	1.47	1.39
17	2	606	CHL	CHC-C4B	4.96	1.47	1.39
17	4	607	CHL	OBD-CAD	4.95	1.28	1.22
17	2	601	CHL	CHC-C4B	4.94	1.47	1.39
17	3	606	CHL	C3B-C2B	4.93	1.47	1.40
17	4	605	CHL	C3B-C2B	4.93	1.47	1.40
17	2	607	CHL	OBD-CAD	4.92	1.28	1.22
17	2	606	CHL	CHD-C4C	4.89	1.48	1.39
17	1	606	CHL	C3D-C2D	4.88	1.48	1.39
17	2	615	CHL	CHD-C4C	4.87	1.48	1.39
17	4	605	CHL	CHC-C4B	4.86	1.47	1.39
17	4	605	CHL	CHD-C4C	4.84	1.48	1.39
17	2	601	CHL	CHD-C4C	4.83	1.48	1.39
17	4	606	CHL	CHC-C4B	4.83	1.47	1.39
17	4	607	CHL	CHC-C4B	4.83	1.47	1.39
17	2	605	CHL	CHD-C4C	4.82	1.48	1.39
17	2	615	CHL	CHD-C1D	4.82	1.47	1.39
17	2	606	CHL	CHD-C1D	4.81	1.47	1.39
17	1	601	CHL	CHD-C1D	4.80	1.47	1.39
17	1	601	CHL	CHD-C4C	4.79	1.48	1.39
17	2	607	CHL	CHD-C4C	4.78	1.48	1.39
17	4	615	CHL	O2D-CGD	4.76	1.45	1.30
17	1	606	CHL	O2D-CGD	4.76	1.45	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	4	605	CHL	O2D-CGD	4.76	1.45	1.30
17	1	606	CHL	CHC-C1C	4.76	1.48	1.39
17	3	606	CHL	CHD-C4C	4.75	1.48	1.39
17	3	606	CHL	CHC-C4B	4.74	1.47	1.39
17	1	601	CHL	O2D-CGD	4.73	1.45	1.30
17	4	615	CHL	CHC-C4B	4.73	1.47	1.39
17	2	605	CHL	C2C-C3C	4.73	1.46	1.37
17	2	607	CHL	C3B-C2B	4.72	1.46	1.40
17	2	601	CHL	CHB-C1B	4.71	1.47	1.39
17	1	601	CHL	CHB-C1B	4.71	1.47	1.39
17	4	615	CHL	CHD-C4C	4.71	1.48	1.39
17	4	607	CHL	C3B-C2B	4.69	1.46	1.40
17	2	601	CHL	CHD-C1D	4.69	1.47	1.39
17	4	605	CHL	C2C-C3C	4.69	1.46	1.37
17	4	606	CHL	CHD-C4C	4.69	1.48	1.39
17	2	606	CHL	CHB-C1B	4.68	1.47	1.39
17	4	605	CHL	CHD-C1D	4.66	1.47	1.39
17	2	606	CHL	C3D-C2D	4.66	1.47	1.39
17	2	605	CHL	CHB-C1B	4.66	1.47	1.39
17	4	605	CHL	CHB-C1B	4.65	1.47	1.39
17	4	607	CHL	CHD-C4C	4.65	1.48	1.39
17	4	615	CHL	CHB-C4A	-4.64	1.33	1.38
17	2	607	CHL	CHD-C1D	4.63	1.47	1.39
17	4	607	CHL	CHB-C4A	-4.62	1.33	1.38
17	2	605	CHL	CHD-C1D	4.62	1.47	1.39
17	2	615	CHL	CHB-C1B	4.59	1.47	1.39
17	3	606	CHL	O2A-CGA	4.59	1.46	1.30
17	2	607	CHL	CHB-C1B	4.58	1.47	1.39
17	3	606	CHL	CHB-C1B	4.58	1.47	1.39
17	2	607	CHL	CHB-C4A	-4.57	1.33	1.38
17	4	615	CHL	CHD-C1D	4.57	1.47	1.39
17	2	601	CHL	C3D-C2D	4.56	1.47	1.39
17	2	605	CHL	C3D-C2D	4.56	1.47	1.39
17	4	606	CHL	CHB-C4A	-4.56	1.33	1.38
17	4	606	CHL	CHB-C1B	4.55	1.47	1.39
17	2	615	CHL	C3D-C2D	4.55	1.47	1.39
17	3	606	CHL	CHB-C4A	-4.55	1.33	1.38
17	4	606	CHL	CHD-C1D	4.55	1.47	1.39
17	2	607	CHL	C3D-C2D	4.53	1.47	1.39
17	4	607	CHL	O2A-CGA	4.53	1.45	1.30
17	2	605	CHL	CHC-C1C	4.53	1.48	1.39
17	3	606	CHL	CHD-C1D	4.53	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	2	615	CHL	CHC-C1C	4.53	1.48	1.39
17	4	606	CHL	C3D-C2D	4.53	1.47	1.39
17	1	601	CHL	CHC-C1C	4.52	1.48	1.39
17	2	607	CHL	CHC-C1C	4.52	1.48	1.39
17	2	615	CHL	CHB-C4A	-4.50	1.33	1.38
17	1	601	CHL	C3D-C2D	4.49	1.47	1.39
17	2	601	CHL	CHC-C1C	4.48	1.48	1.39
17	2	606	CHL	CHC-C1C	4.48	1.48	1.39
17	4	615	CHL	CHB-C1B	4.47	1.46	1.39
17	4	607	CHL	CHB-C1B	4.46	1.46	1.39
17	2	605	CHL	CHB-C4A	-4.44	1.33	1.38
17	4	615	CHL	C3A-C2A	-4.43	1.50	1.54
17	4	607	CHL	CHD-C1D	4.43	1.46	1.39
17	2	601	CHL	CHB-C4A	-4.42	1.33	1.38
17	1	601	CHL	CHB-C4A	-4.41	1.33	1.38
17	3	606	CHL	C3D-C2D	4.41	1.47	1.39
17	4	605	CHL	CHC-C1C	4.40	1.47	1.39
17	4	615	CHL	C3D-C2D	4.38	1.47	1.39
17	4	607	CHL	C3D-C2D	4.38	1.47	1.39
17	2	606	CHL	CHB-C4A	-4.38	1.33	1.38
17	4	605	CHL	CHB-C4A	-4.37	1.33	1.38
17	4	605	CHL	C3D-C2D	4.37	1.47	1.39
17	3	606	CHL	C3A-C2A	-4.36	1.50	1.54
17	4	606	CHL	CHC-C1C	4.36	1.47	1.39
17	4	607	CHL	CHC-C1C	4.34	1.47	1.39
17	2	607	CHL	O2A-CGA	4.33	1.46	1.33
17	4	615	CHL	CHC-C1C	4.33	1.47	1.39
17	1	601	CHL	O2A-CGA	4.25	1.45	1.33
20	1	615	LHG	O8-C23	4.23	1.45	1.33
17	4	607	CHL	C3A-C2A	-4.23	1.51	1.54
27	B	850	DGD	O1G-C1A	4.21	1.45	1.33
17	4	606	CHL	C3A-C2A	-4.21	1.51	1.54
24	A	801	CL0	O2A-CGA	4.19	1.45	1.33
17	3	606	CHL	CHC-C1C	4.17	1.47	1.39
17	2	607	CHL	C3A-C2A	-4.14	1.51	1.54
20	1	615	LHG	O7-C7	4.13	1.46	1.34
17	2	601	CHL	O2A-CGA	4.11	1.45	1.33
27	B	850	DGD	O2G-C1B	4.10	1.45	1.34
17	1	606	CHL	CHB-C4A	-4.06	1.33	1.38
24	A	801	CL0	C3D-C2D	4.01	1.45	1.40
24	A	801	CL0	C3B-C2B	3.97	1.45	1.40
17	4	605	CHL	C3A-C2A	-3.97	1.51	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	2	605	CHL	C3A-C2A	-3.95	1.51	1.54
17	2	615	CHL	C3A-C2A	-3.91	1.51	1.54
17	2	606	CHL	C3A-C2A	-3.86	1.51	1.54
17	1	601	CHL	C3A-C2A	-3.79	1.51	1.54
18	L	304	CLA	C1D-ND	3.69	1.42	1.37
18	A	826	CLA	C1D-ND	3.64	1.42	1.37
18	F	303	CLA	C1D-ND	3.64	1.42	1.37
18	2	611	CLA	C1D-ND	3.63	1.42	1.37
18	3	609	CLA	C1D-ND	3.63	1.42	1.37
18	4	614	CLA	C1D-ND	3.62	1.42	1.37
18	A	836	CLA	C1D-ND	3.62	1.42	1.37
18	B	837	CLA	C1D-ND	3.62	1.42	1.37
18	B	834	CLA	C1D-ND	3.61	1.42	1.37
18	B	820	CLA	C1D-ND	3.60	1.42	1.37
18	A	816	CLA	C1D-ND	3.60	1.42	1.37
18	G	201	CLA	C1D-ND	3.60	1.42	1.37
18	A	820	CLA	C1D-ND	3.60	1.42	1.37
18	K	206	CLA	C1D-ND	3.60	1.42	1.37
18	1	611	CLA	C1D-ND	3.60	1.42	1.37
18	4	613	CLA	C1D-ND	3.60	1.42	1.37
18	4	611	CLA	C1D-ND	3.60	1.42	1.37
18	A	840	CLA	C1D-ND	3.59	1.42	1.37
18	A	817	CLA	C1D-ND	3.59	1.42	1.37
18	1	610	CLA	C1D-ND	3.59	1.42	1.37
18	1	613	CLA	C1D-ND	3.59	1.42	1.37
18	B	840	CLA	C1D-ND	3.59	1.42	1.37
18	K	201	CLA	C1D-ND	3.59	1.42	1.37
18	A	845	CLA	C1D-ND	3.59	1.42	1.37
18	3	611	CLA	C1D-ND	3.59	1.42	1.37
18	H	201	CLA	C1D-ND	3.59	1.42	1.37
18	3	604	CLA	C1D-ND	3.59	1.42	1.37
18	A	825	CLA	C1D-ND	3.59	1.42	1.37
18	A	813	CLA	C1D-ND	3.59	1.42	1.37
18	B	833	CLA	C1D-ND	3.59	1.42	1.37
18	A	804	CLA	C1D-ND	3.59	1.42	1.37
18	A	824	CLA	C1D-ND	3.59	1.42	1.37
18	3	603	CLA	C1D-ND	3.59	1.42	1.37
18	A	835	CLA	C1D-ND	3.59	1.42	1.37
18	1	607	CLA	C1D-ND	3.58	1.42	1.37
18	3	610	CLA	C1D-ND	3.58	1.42	1.37
18	2	602	CLA	C1D-ND	3.58	1.42	1.37
18	B	827	CLA	C1D-ND	3.58	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	G	202	CLA	C1D-ND	3.58	1.42	1.37
18	2	604	CLA	C1D-ND	3.58	1.42	1.37
18	3	601	CLA	C1D-ND	3.58	1.42	1.37
18	F	302	CLA	C1D-ND	3.57	1.42	1.37
18	A	832	CLA	C1D-ND	3.57	1.42	1.37
18	4	612	CLA	C1D-ND	3.57	1.42	1.37
18	2	612	CLA	C1D-ND	3.57	1.42	1.37
18	3	607	CLA	C1D-ND	3.57	1.42	1.37
18	2	613	CLA	C1D-ND	3.57	1.42	1.37
18	A	809	CLA	C1D-ND	3.57	1.42	1.37
18	2	603	CLA	C1D-ND	3.57	1.42	1.37
18	B	831	CLA	C1D-ND	3.57	1.42	1.37
18	A	821	CLA	C1D-ND	3.56	1.42	1.37
18	B	841	CLA	C1D-ND	3.56	1.42	1.37
18	A	806	CLA	C1D-ND	3.56	1.42	1.37
18	J	101	CLA	C1D-ND	3.56	1.42	1.37
18	A	823	CLA	C1D-ND	3.56	1.42	1.37
18	B	818	CLA	C1D-ND	3.56	1.42	1.37
18	1	612	CLA	C1D-ND	3.56	1.42	1.37
18	B	804	CLA	C1D-ND	3.56	1.42	1.37
18	3	602	CLA	C1D-ND	3.56	1.42	1.37
18	B	835	CLA	C1D-ND	3.56	1.42	1.37
18	A	808	CLA	C1D-ND	3.55	1.42	1.37
18	A	833	CLA	C1D-ND	3.55	1.42	1.37
18	B	830	CLA	C1D-ND	3.55	1.42	1.37
18	1	605	CLA	C1D-ND	3.55	1.42	1.37
18	A	837	CLA	C1D-ND	3.55	1.42	1.37
18	B	824	CLA	C1D-ND	3.55	1.42	1.37
18	B	810	CLA	C1D-ND	3.55	1.42	1.37
18	A	839	CLA	C1D-ND	3.55	1.42	1.37
18	B	812	CLA	C1D-ND	3.55	1.42	1.37
18	1	604	CLA	C1D-ND	3.55	1.42	1.37
18	A	841	CLA	C1D-ND	3.55	1.42	1.37
18	B	819	CLA	C1D-ND	3.55	1.42	1.37
18	G	203	CLA	C1D-ND	3.55	1.42	1.37
18	4	604	CLA	C1D-ND	3.54	1.42	1.37
18	A	838	CLA	C1D-ND	3.54	1.42	1.37
18	F	301	CLA	C1D-ND	3.54	1.42	1.37
18	A	807	CLA	C1D-ND	3.54	1.42	1.37
18	A	828	CLA	C1D-ND	3.54	1.42	1.37
18	B	822	CLA	C1D-ND	3.54	1.42	1.37
18	K	203	CLA	C1D-ND	3.53	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	839	CLA	C1D-ND	3.53	1.42	1.37
18	A	834	CLA	C1D-ND	3.53	1.42	1.37
18	3	605	CLA	C1D-ND	3.53	1.42	1.37
18	A	810	CLA	C1D-ND	3.53	1.42	1.37
18	B	815	CLA	C1D-ND	3.53	1.42	1.37
18	A	819	CLA	C1D-ND	3.52	1.42	1.37
18	3	612	CLA	C1D-ND	3.52	1.42	1.37
18	B	817	CLA	C1D-ND	3.52	1.42	1.37
18	A	822	CLA	C1D-ND	3.52	1.42	1.37
18	A	811	CLA	C1D-ND	3.52	1.42	1.37
18	2	608	CLA	C1D-ND	3.52	1.42	1.37
18	L	303	CLA	C1D-ND	3.52	1.42	1.37
18	A	818	CLA	C1D-ND	3.52	1.42	1.37
18	A	843	CLA	C1D-ND	3.52	1.42	1.37
18	B	813	CLA	C1D-ND	3.51	1.42	1.37
18	A	812	CLA	C1D-ND	3.51	1.42	1.37
18	A	805	CLA	C1D-ND	3.51	1.42	1.37
18	B	809	CLA	C1D-ND	3.51	1.42	1.37
18	B	821	CLA	C1D-ND	3.51	1.42	1.37
18	B	811	CLA	C1D-ND	3.51	1.42	1.37
18	B	807	CLA	C1D-ND	3.51	1.42	1.37
18	B	805	CLA	C1D-ND	3.51	1.42	1.37
18	B	814	CLA	C1D-ND	3.51	1.42	1.37
18	A	827	CLA	C1D-ND	3.51	1.42	1.37
18	4	603	CLA	C1D-ND	3.50	1.42	1.37
18	A	814	CLA	C1D-ND	3.50	1.42	1.37
17	2	601	CHL	C3A-C2A	-3.50	1.51	1.54
18	A	844	CLA	C1D-ND	3.50	1.42	1.37
18	B	829	CLA	C1D-ND	3.49	1.42	1.37
18	2	610	CLA	C1D-ND	3.49	1.42	1.37
18	4	608	CLA	C1D-ND	3.49	1.42	1.37
18	4	610	CLA	C1D-ND	3.49	1.42	1.37
18	A	802	CLA	C1D-ND	3.49	1.42	1.37
18	A	831	CLA	C1D-ND	3.49	1.42	1.37
18	B	823	CLA	C1D-ND	3.49	1.42	1.37
18	A	815	CLA	C1D-ND	3.49	1.42	1.37
18	B	836	CLA	C1D-ND	3.48	1.42	1.37
18	B	816	CLA	C1D-ND	3.48	1.42	1.37
18	A	829	CLA	C1D-ND	3.48	1.42	1.37
18	B	838	CLA	C1D-ND	3.47	1.42	1.37
18	K	204	CLA	C1D-ND	3.47	1.42	1.37
18	1	602	CLA	C1D-ND	3.47	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	825	CLA	C1D-ND	3.47	1.42	1.37
18	4	602	CLA	C1D-ND	3.47	1.42	1.37
18	L	302	CLA	C1D-ND	3.47	1.42	1.37
18	1	603	CLA	C1D-ND	3.46	1.42	1.37
18	B	826	CLA	C1D-ND	3.46	1.42	1.37
18	B	802	CLA	C1D-ND	3.46	1.42	1.37
18	3	608	CLA	C1D-ND	3.46	1.42	1.37
18	A	842	CLA	C1D-ND	3.46	1.42	1.37
18	2	609	CLA	C1D-ND	3.46	1.42	1.37
18	B	806	CLA	C1D-ND	3.46	1.42	1.37
18	4	601	CLA	C1D-ND	3.45	1.42	1.37
18	4	609	CLA	C1D-ND	3.45	1.42	1.37
18	1	608	CLA	C1D-ND	3.45	1.42	1.37
18	A	830	CLA	C1D-ND	3.45	1.42	1.37
18	B	803	CLA	C1D-ND	3.45	1.42	1.37
18	A	803	CLA	C1D-ND	3.45	1.42	1.37
18	B	832	CLA	C1D-ND	3.42	1.42	1.37
18	B	812	CLA	C4B-NB	3.38	1.42	1.37
18	B	828	CLA	C1D-ND	3.36	1.42	1.37
18	B	808	CLA	C1D-ND	3.35	1.42	1.37
18	B	805	CLA	C4B-NB	3.30	1.42	1.37
17	1	606	CHL	C2A-C3A	-3.30	1.52	1.54
18	B	838	CLA	C4B-NB	3.27	1.42	1.37
18	A	821	CLA	C4B-NB	3.26	1.42	1.37
18	1	609	CLA	C1D-ND	3.23	1.42	1.37
18	A	814	CLA	C4B-NB	3.21	1.42	1.37
18	3	607	CLA	C4B-NB	3.21	1.42	1.37
18	1	610	CLA	CAB-C3B	-3.20	1.44	1.50
18	3	611	CLA	C4B-NB	3.20	1.42	1.37
18	A	836	CLA	C4B-NB	3.20	1.42	1.37
18	2	610	CLA	CAB-C3B	-3.18	1.44	1.50
18	B	828	CLA	C4B-NB	3.18	1.42	1.37
18	1	608	CLA	CAB-C3B	-3.18	1.44	1.50
18	J	101	CLA	C4B-NB	3.18	1.42	1.37
18	B	802	CLA	C4B-NB	3.16	1.42	1.37
18	A	807	CLA	C4B-NB	3.16	1.42	1.37
18	4	604	CLA	CAB-C3B	-3.16	1.44	1.50
18	4	603	CLA	CAB-C3B	-3.16	1.44	1.50
18	B	832	CLA	C4B-NB	3.16	1.42	1.37
18	F	301	CLA	C4B-NB	3.15	1.42	1.37
18	A	817	CLA	C4B-NB	3.15	1.42	1.37
18	1	613	CLA	CAB-C3B	-3.15	1.44	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	837	CLA	C4B-NB	3.15	1.42	1.37
18	4	611	CLA	C4B-NB	3.14	1.42	1.37
18	B	835	CLA	C4B-NB	3.14	1.42	1.37
18	A	819	CLA	C4B-NB	3.14	1.42	1.37
18	A	845	CLA	C4B-NB	3.14	1.42	1.37
18	B	811	CLA	CAB-C3B	-3.14	1.44	1.50
18	3	605	CLA	CAB-C3B	-3.14	1.44	1.50
18	1	607	CLA	C4B-NB	3.14	1.42	1.37
18	1	605	CLA	C4B-NB	3.12	1.42	1.37
18	L	302	CLA	C4B-NB	3.12	1.42	1.37
18	B	836	CLA	C4B-NB	3.12	1.42	1.37
18	F	303	CLA	C4B-NB	3.12	1.42	1.37
18	1	604	CLA	C4B-NB	3.12	1.42	1.37
18	3	610	CLA	C4B-NB	3.12	1.42	1.37
18	A	838	CLA	C4B-NB	3.11	1.42	1.37
18	3	605	CLA	C4B-NB	3.11	1.41	1.37
18	B	823	CLA	C4B-NB	3.10	1.41	1.37
18	K	201	CLA	C4B-NB	3.10	1.41	1.37
18	A	812	CLA	C4B-NB	3.10	1.41	1.37
18	4	610	CLA	C4B-NB	3.10	1.41	1.37
18	F	302	CLA	C4B-NB	3.10	1.41	1.37
18	G	201	CLA	C4B-NB	3.10	1.41	1.37
18	B	819	CLA	C4B-NB	3.09	1.41	1.37
18	3	602	CLA	C4B-NB	3.09	1.41	1.37
18	B	810	CLA	C4B-NB	3.09	1.41	1.37
18	3	604	CLA	C4B-NB	3.09	1.41	1.37
18	A	828	CLA	C4B-NB	3.08	1.41	1.37
18	2	613	CLA	C4B-NB	3.08	1.41	1.37
18	K	204	CLA	C4B-NB	3.08	1.41	1.37
18	4	601	CLA	C4B-NB	3.08	1.41	1.37
18	1	611	CLA	C4B-NB	3.08	1.41	1.37
18	A	841	CLA	C4B-NB	3.08	1.41	1.37
18	A	840	CLA	C4B-NB	3.07	1.41	1.37
18	3	609	CLA	C4B-NB	3.07	1.41	1.37
18	4	614	CLA	C4B-NB	3.07	1.41	1.37
18	A	834	CLA	C4B-NB	3.07	1.41	1.37
18	B	840	CLA	C4B-NB	3.07	1.41	1.37
18	A	808	CLA	C4B-NB	3.07	1.41	1.37
18	G	202	CLA	C4B-NB	3.07	1.41	1.37
18	B	834	CLA	C4B-NB	3.06	1.41	1.37
18	B	829	CLA	C4B-NB	3.06	1.41	1.37
18	2	611	CLA	C4B-NB	3.06	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	4	603	CLA	C4B-NB	3.06	1.41	1.37
18	B	811	CLA	C4B-NB	3.06	1.41	1.37
18	1	603	CLA	C4B-NB	3.06	1.41	1.37
18	B	826	CLA	C4B-NB	3.06	1.41	1.37
18	A	827	CLA	C4B-NB	3.05	1.41	1.37
18	B	827	CLA	C4B-NB	3.05	1.41	1.37
18	1	610	CLA	C4B-NB	3.05	1.41	1.37
18	K	206	CLA	C4B-NB	3.05	1.41	1.37
18	2	610	CLA	C4B-NB	3.04	1.41	1.37
18	B	815	CLA	C4B-NB	3.04	1.41	1.37
18	A	822	CLA	C4B-NB	3.04	1.41	1.37
18	1	612	CLA	C4B-NB	3.04	1.41	1.37
18	B	839	CLA	C4B-NB	3.04	1.41	1.37
18	A	816	CLA	C4B-NB	3.03	1.41	1.37
18	B	818	CLA	C4B-NB	3.03	1.41	1.37
18	B	817	CLA	C4B-NB	3.03	1.41	1.37
18	4	604	CLA	C4B-NB	3.03	1.41	1.37
18	A	825	CLA	C4B-NB	3.03	1.41	1.37
18	3	603	CLA	C4B-NB	3.03	1.41	1.37
18	A	813	CLA	C4B-NB	3.02	1.41	1.37
18	A	824	CLA	C4B-NB	3.02	1.41	1.37
18	A	820	CLA	C4B-NB	3.02	1.41	1.37
18	1	608	CLA	C4B-NB	3.02	1.41	1.37
18	1	613	CLA	C4B-NB	3.02	1.41	1.37
18	B	813	CLA	C4B-NB	3.02	1.41	1.37
18	L	303	CLA	C4B-NB	3.02	1.41	1.37
18	1	609	CLA	C4B-NB	3.01	1.41	1.37
24	A	801	CL0	CHC-C4B	3.01	1.44	1.39
18	A	810	CLA	C4B-NB	3.01	1.41	1.37
18	A	803	CLA	C4B-NB	3.01	1.41	1.37
18	B	830	CLA	C4B-NB	3.01	1.41	1.37
18	B	807	CLA	C4B-NB	3.01	1.41	1.37
18	A	843	CLA	C4B-NB	3.00	1.41	1.37
18	A	844	CLA	C4B-NB	3.00	1.41	1.37
18	L	304	CLA	C4B-NB	3.00	1.41	1.37
18	G	203	CLA	C4B-NB	3.00	1.41	1.37
18	K	203	CLA	C4B-NB	3.00	1.41	1.37
18	4	602	CLA	C4B-NB	3.00	1.41	1.37
18	A	831	CLA	C4B-NB	2.99	1.41	1.37
18	B	837	CLA	C4B-NB	2.99	1.41	1.37
18	4	608	CLA	C4B-NB	2.99	1.41	1.37
18	A	802	CLA	C4B-NB	2.99	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	805	CLA	C4B-NB	2.99	1.41	1.37
18	B	803	CLA	C4B-NB	2.98	1.41	1.37
18	1	602	CLA	C4B-NB	2.98	1.41	1.37
22	B	845	BCR	C23-C22	-2.98	1.39	1.46
18	B	831	CLA	C4B-NB	2.98	1.41	1.37
18	B	825	CLA	C4B-NB	2.98	1.41	1.37
18	B	804	CLA	C4B-NB	2.98	1.41	1.37
18	B	820	CLA	C4B-NB	2.98	1.41	1.37
18	B	841	CLA	C4B-NB	2.98	1.41	1.37
18	2	603	CLA	C4B-NB	2.97	1.41	1.37
18	4	613	CLA	C4B-NB	2.97	1.41	1.37
18	A	826	CLA	C4B-NB	2.97	1.41	1.37
18	B	814	CLA	C4B-NB	2.97	1.41	1.37
18	B	822	CLA	C4B-NB	2.97	1.41	1.37
18	A	842	CLA	C4B-NB	2.97	1.41	1.37
18	H	201	CLA	C4B-NB	2.96	1.41	1.37
18	A	823	CLA	C4B-NB	2.96	1.41	1.37
24	A	801	CL0	CHD-C4C	2.96	1.45	1.39
18	3	601	CLA	C4B-NB	2.96	1.41	1.37
18	A	804	CLA	C4B-NB	2.95	1.41	1.37
18	A	833	CLA	C4B-NB	2.95	1.41	1.37
18	2	602	CLA	C4B-NB	2.95	1.41	1.37
18	A	832	CLA	C4B-NB	2.95	1.41	1.37
18	A	806	CLA	C4B-NB	2.95	1.41	1.37
18	A	830	CLA	C4B-NB	2.94	1.41	1.37
18	B	824	CLA	C4B-NB	2.94	1.41	1.37
18	B	806	CLA	C4B-NB	2.94	1.41	1.37
18	B	821	CLA	C4B-NB	2.93	1.41	1.37
18	B	808	CLA	C4B-NB	2.93	1.41	1.37
18	B	816	CLA	C4B-NB	2.93	1.41	1.37
18	A	839	CLA	C4B-NB	2.92	1.41	1.37
18	A	818	CLA	C4B-NB	2.92	1.41	1.37
18	4	612	CLA	C4B-NB	2.92	1.41	1.37
22	A	853	BCR	C10-C9	2.91	1.42	1.35
18	A	835	CLA	C4B-NB	2.91	1.41	1.37
18	B	833	CLA	C4B-NB	2.91	1.41	1.37
22	A	850	BCR	C23-C22	-2.91	1.39	1.46
18	B	809	CLA	C4B-NB	2.91	1.41	1.37
22	B	801	BCR	C8-C9	-2.91	1.39	1.46
24	A	801	CL0	CHB-C1B	2.91	1.44	1.39
22	I	101	BCR	C23-C22	-2.89	1.39	1.46
18	2	604	CLA	C4B-NB	2.89	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	3	612	CLA	C4B-NB	2.89	1.41	1.37
18	2	608	CLA	C4B-NB	2.89	1.41	1.37
18	4	609	CLA	C4B-NB	2.89	1.41	1.37
22	B	801	BCR	C10-C9	2.89	1.42	1.35
18	A	829	CLA	C4B-NB	2.88	1.41	1.37
18	2	612	CLA	C4B-NB	2.88	1.41	1.37
22	B	849	BCR	C23-C22	-2.87	1.39	1.46
22	F	304	BCR	C21-C22	2.87	1.42	1.35
18	A	809	CLA	C4B-NB	2.87	1.41	1.37
18	A	815	CLA	C4B-NB	2.87	1.41	1.37
22	B	847	BCR	C23-C22	-2.87	1.39	1.46
22	B	848	BCR	C23-C22	-2.86	1.39	1.46
22	F	304	BCR	C17-C18	2.86	1.42	1.35
22	B	845	BCR	C21-C22	2.86	1.42	1.35
18	3	608	CLA	C4B-NB	2.85	1.41	1.37
18	A	811	CLA	C4B-NB	2.84	1.41	1.37
22	3	614	BCR	C23-C22	-2.83	1.39	1.46
18	2	609	CLA	C4B-NB	2.82	1.41	1.37
18	2	613	CLA	C1B-C2B	2.82	1.49	1.43
18	4	603	CLA	C1B-C2B	2.82	1.49	1.43
22	A	852	BCR	C8-C9	-2.81	1.39	1.46
22	B	846	BCR	C8-C9	-2.80	1.40	1.46
18	B	818	CLA	C1B-C2B	2.80	1.49	1.43
18	1	612	CLA	C1B-C2B	2.80	1.49	1.43
22	I	101	BCR	C8-C9	-2.80	1.40	1.46
18	A	829	CLA	C1B-C2B	2.80	1.49	1.43
22	A	852	BCR	C23-C22	-2.80	1.40	1.46
18	B	814	CLA	C1B-C2B	2.79	1.49	1.43
22	B	849	BCR	C8-C9	-2.79	1.40	1.46
22	G	204	BCR	C8-C9	-2.79	1.40	1.46
22	A	850	BCR	C14-C13	2.79	1.42	1.35
18	B	806	CLA	C1B-C2B	2.79	1.49	1.43
22	4	618	BCR	C8-C9	-2.79	1.40	1.46
22	B	845	BCR	C8-C9	-2.79	1.40	1.46
21	4	616	LUT	C8-C9	-2.79	1.40	1.46
18	H	201	CLA	C1B-C2B	2.79	1.49	1.43
21	3	613	LUT	C10-C9	2.79	1.42	1.35
18	1	608	CLA	C4B-C3B	2.78	1.49	1.43
18	A	843	CLA	C1B-C2B	2.78	1.49	1.43
22	A	849	BCR	C23-C22	-2.78	1.40	1.46
18	2	608	CLA	C1B-C2B	2.78	1.49	1.43
18	1	610	CLA	C1B-C2B	2.78	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	820	CLA	C1B-C2B	2.78	1.49	1.43
18	1	613	CLA	C4B-C3B	2.77	1.49	1.43
18	A	804	CLA	C1B-C2B	2.77	1.49	1.43
21	3	613	LUT	C8-C9	-2.77	1.40	1.46
18	A	824	CLA	C1B-C2B	2.77	1.49	1.43
18	3	601	CLA	C1B-C2B	2.77	1.49	1.43
18	4	614	CLA	C1B-C2B	2.77	1.49	1.43
18	2	610	CLA	C1B-C2B	2.77	1.49	1.43
22	A	848	BCR	C23-C22	-2.77	1.40	1.46
18	A	826	CLA	C1B-C2B	2.77	1.49	1.43
22	3	614	BCR	C8-C9	-2.77	1.40	1.46
18	4	602	CLA	C1B-C2B	2.77	1.49	1.43
22	A	851	BCR	C14-C13	2.77	1.42	1.35
18	A	806	CLA	C1B-C2B	2.76	1.49	1.43
18	A	809	CLA	C1B-C2B	2.76	1.49	1.43
18	A	845	CLA	C1B-C2B	2.76	1.49	1.43
18	B	807	CLA	C1B-C2B	2.76	1.49	1.43
22	G	204	BCR	C23-C22	-2.76	1.40	1.46
18	3	605	CLA	C1B-C2B	2.76	1.49	1.43
18	3	610	CLA	C1B-C2B	2.76	1.49	1.43
18	1	605	CLA	C1B-C2B	2.76	1.49	1.43
22	L	305	BCR	C8-C9	-2.76	1.40	1.46
18	A	817	CLA	C1B-C2B	2.76	1.49	1.43
18	1	603	CLA	C1B-C2B	2.76	1.49	1.43
18	B	841	CLA	C1B-C2B	2.75	1.49	1.43
18	A	827	CLA	C1B-C2B	2.75	1.49	1.43
18	B	826	CLA	C1B-C2B	2.75	1.49	1.43
18	1	602	CLA	C1B-C2B	2.75	1.49	1.43
18	2	611	CLA	C1B-C2B	2.75	1.49	1.43
18	A	818	CLA	C1B-C2B	2.75	1.49	1.43
22	A	851	BCR	C21-C22	2.75	1.42	1.35
18	3	602	CLA	C1B-C2B	2.75	1.49	1.43
18	A	830	CLA	C1B-C2B	2.75	1.49	1.43
18	B	831	CLA	C1B-C2B	2.75	1.49	1.43
18	A	833	CLA	C1B-C2B	2.75	1.49	1.43
22	B	847	BCR	C8-C9	-2.75	1.40	1.46
18	B	837	CLA	C1B-C2B	2.74	1.49	1.43
18	K	204	CLA	C1B-C2B	2.74	1.49	1.43
18	A	823	CLA	C1B-C2B	2.74	1.49	1.43
18	B	823	CLA	C1B-C2B	2.74	1.49	1.43
18	1	607	CLA	C1B-C2B	2.74	1.49	1.43
18	G	201	CLA	C1B-C2B	2.74	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	1	616	LUT	C30-C29	2.74	1.42	1.35
22	L	305	BCR	C23-C22	-2.74	1.40	1.46
18	B	833	CLA	C1B-C2B	2.74	1.49	1.43
18	B	819	CLA	C1B-C2B	2.74	1.49	1.43
18	J	101	CLA	C1B-C2B	2.74	1.49	1.43
18	L	304	CLA	C1B-C2B	2.74	1.49	1.43
18	G	203	CLA	C1B-C2B	2.74	1.49	1.43
18	K	206	CLA	C1B-C2B	2.73	1.49	1.43
18	K	203	CLA	C1B-C2B	2.73	1.49	1.43
18	A	831	CLA	C1B-C2B	2.73	1.49	1.43
18	A	832	CLA	C1B-C2B	2.73	1.49	1.43
18	3	611	CLA	C1B-C2B	2.73	1.49	1.43
18	A	834	CLA	C1B-C2B	2.73	1.49	1.43
18	A	825	CLA	C1B-C2B	2.73	1.49	1.43
18	4	612	CLA	C1B-C2B	2.73	1.49	1.43
18	A	816	CLA	C1B-C2B	2.73	1.49	1.43
18	3	605	CLA	C4B-C3B	2.73	1.49	1.43
18	B	811	CLA	C4B-C3B	2.73	1.49	1.43
18	B	804	CLA	C1B-C2B	2.73	1.49	1.43
18	3	609	CLA	C1B-C2B	2.73	1.49	1.43
18	B	815	CLA	C1B-C2B	2.73	1.49	1.43
22	A	853	BCR	C23-C22	-2.73	1.40	1.46
18	2	603	CLA	C1B-C2B	2.73	1.49	1.43
18	A	814	CLA	C3B-C4B	2.73	1.50	1.42
18	1	611	CLA	C1B-C2B	2.73	1.49	1.43
22	B	848	BCR	C8-C9	-2.73	1.40	1.46
18	A	811	CLA	C1B-C2B	2.72	1.49	1.43
18	B	811	CLA	C1B-C2B	2.72	1.49	1.43
18	B	827	CLA	C1B-C2B	2.72	1.49	1.43
22	4	618	BCR	C23-C22	-2.72	1.40	1.46
18	1	604	CLA	C1B-C2B	2.72	1.49	1.43
22	L	301	BCR	C8-C9	-2.72	1.40	1.46
18	3	612	CLA	C1B-C2B	2.72	1.49	1.43
18	3	608	CLA	C1B-C2B	2.72	1.49	1.43
18	A	840	CLA	C1B-C2B	2.72	1.49	1.43
18	B	821	CLA	C1B-C2B	2.72	1.49	1.43
22	B	844	BCR	C23-C22	-2.72	1.40	1.46
18	B	840	CLA	C1B-C2B	2.72	1.49	1.43
22	K	205	BCR	C8-C9	-2.72	1.40	1.46
18	1	610	CLA	C4B-C3B	2.71	1.49	1.43
18	1	613	CLA	C1B-C2B	2.71	1.49	1.43
18	B	816	CLA	C1B-C2B	2.71	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	853	BCR	C8-C9	-2.71	1.40	1.46
18	G	202	CLA	C1B-C2B	2.71	1.49	1.43
18	B	830	CLA	C1B-C2B	2.71	1.49	1.43
18	B	809	CLA	C1B-C2B	2.71	1.49	1.43
18	A	841	CLA	C1B-C2B	2.71	1.49	1.43
18	A	836	CLA	C1B-C2B	2.71	1.49	1.43
18	B	835	CLA	C1B-C2B	2.71	1.49	1.43
18	L	303	CLA	C1B-C2B	2.71	1.49	1.43
18	4	613	CLA	C1B-C2B	2.71	1.49	1.43
18	A	839	CLA	C1B-C2B	2.71	1.49	1.43
21	2	619	LUT	C8-C9	-2.71	1.40	1.46
22	A	848	BCR	C8-C9	-2.71	1.40	1.46
18	4	608	CLA	C1B-C2B	2.71	1.49	1.43
18	1	608	CLA	C1B-C2B	2.71	1.49	1.43
18	A	837	CLA	C1B-C2B	2.71	1.49	1.43
18	A	819	CLA	C1B-C2B	2.71	1.49	1.43
18	A	813	CLA	C1B-C2B	2.70	1.49	1.43
18	A	805	CLA	C1B-C2B	2.70	1.49	1.43
22	A	849	BCR	C21-C22	2.70	1.42	1.35
18	K	201	CLA	C1B-C2B	2.70	1.49	1.43
18	B	829	CLA	C1B-C2B	2.70	1.49	1.43
18	A	820	CLA	C1B-C2B	2.70	1.49	1.43
18	F	301	CLA	C1B-C2B	2.70	1.49	1.43
18	F	303	CLA	C1B-C2B	2.70	1.49	1.43
22	J	102	BCR	C23-C22	-2.70	1.40	1.46
18	1	609	CLA	C1B-C2B	2.70	1.49	1.43
18	B	824	CLA	C1B-C2B	2.70	1.49	1.43
18	4	610	CLA	C1B-C2B	2.69	1.49	1.43
22	L	306	BCR	C23-C22	-2.69	1.40	1.46
19	2	617	XAT	C34-C33	2.69	1.42	1.35
18	3	607	CLA	C3B-C4B	2.69	1.50	1.42
18	3	604	CLA	C1B-C2B	2.69	1.49	1.43
18	4	604	CLA	C1B-C2B	2.69	1.49	1.43
22	A	850	BCR	C17-C18	2.69	1.42	1.35
18	A	838	CLA	C1B-C2B	2.69	1.49	1.43
18	A	812	CLA	C1B-C2B	2.69	1.49	1.43
22	K	205	BCR	C23-C22	-2.69	1.40	1.46
18	A	835	CLA	C1B-C2B	2.69	1.49	1.43
22	B	801	BCR	C23-C22	-2.69	1.40	1.46
18	B	834	CLA	C1B-C2B	2.69	1.49	1.43
18	B	838	CLA	C1B-C2B	2.69	1.49	1.43
18	B	813	CLA	C1B-C2B	2.69	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	1	616	LUT	C8-C9	-2.69	1.40	1.46
18	B	810	CLA	C1B-C2B	2.69	1.49	1.43
18	2	604	CLA	C1B-C2B	2.69	1.49	1.43
18	3	603	CLA	C1B-C2B	2.69	1.49	1.43
18	A	828	CLA	C1B-C2B	2.69	1.49	1.43
18	B	805	CLA	C1B-C2B	2.69	1.49	1.43
22	A	850	BCR	C8-C9	-2.68	1.40	1.46
22	J	102	BCR	C8-C9	-2.68	1.40	1.46
18	B	817	CLA	C1B-C2B	2.68	1.49	1.43
18	4	611	CLA	C1B-C2B	2.68	1.49	1.43
18	2	609	CLA	C1B-C2B	2.68	1.49	1.43
18	F	302	CLA	C1B-C2B	2.68	1.49	1.43
19	2	617	XAT	C14-C13	2.68	1.42	1.35
18	4	601	CLA	C1B-C2B	2.68	1.49	1.43
18	A	808	CLA	C1B-C2B	2.68	1.49	1.43
18	B	825	CLA	C1B-C2B	2.68	1.49	1.43
18	B	812	CLA	C3B-C4B	2.68	1.50	1.42
22	F	304	BCR	C8-C9	-2.68	1.40	1.46
18	4	603	CLA	C4B-C3B	2.68	1.49	1.43
18	A	815	CLA	C1B-C2B	2.67	1.49	1.43
22	A	851	BCR	C17-C18	2.67	1.42	1.35
18	B	808	CLA	C1B-C2B	2.67	1.49	1.43
18	B	839	CLA	C1B-C2B	2.67	1.49	1.43
22	B	844	BCR	C8-C9	-2.67	1.40	1.46
18	B	802	CLA	C1B-C2B	2.67	1.49	1.43
22	K	202	BCR	C23-C22	-2.67	1.40	1.46
18	4	604	CLA	C4B-C3B	2.67	1.49	1.43
18	A	822	CLA	C1B-C2B	2.67	1.49	1.43
22	B	846	BCR	C23-C22	-2.67	1.40	1.46
18	2	612	CLA	C1B-C2B	2.66	1.49	1.43
22	A	849	BCR	C8-C9	-2.66	1.40	1.46
18	A	807	CLA	C1B-C2B	2.65	1.49	1.43
18	B	836	CLA	C1B-C2B	2.65	1.49	1.43
22	K	202	BCR	C8-C9	-2.65	1.40	1.46
18	A	821	CLA	C1B-C2B	2.64	1.49	1.43
18	2	602	CLA	C1B-C2B	2.64	1.49	1.43
18	2	610	CLA	C4B-C3B	2.64	1.49	1.43
24	A	801	CL0	CHC-C1C	2.64	1.44	1.39
22	A	849	BCR	C17-C18	2.63	1.41	1.35
18	B	803	CLA	C1B-C2B	2.63	1.49	1.43
18	L	302	CLA	C1B-C2B	2.63	1.49	1.43
22	L	301	BCR	C23-C22	-2.63	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	803	CLA	C1B-C2B	2.63	1.49	1.43
22	L	306	BCR	C8-C9	-2.62	1.40	1.46
18	B	812	CLA	C1B-C2B	2.62	1.49	1.43
22	B	843	BCR	C14-C13	2.60	1.41	1.35
22	B	843	BCR	C8-C9	-2.60	1.40	1.46
18	A	810	CLA	C1B-C2B	2.60	1.49	1.43
18	B	828	CLA	C1B-C2B	2.59	1.49	1.43
21	3	613	LUT	C34-C33	2.59	1.41	1.35
18	B	805	CLA	C3B-C4B	2.59	1.50	1.42
18	B	832	CLA	C3B-C4B	2.58	1.50	1.42
22	B	843	BCR	C23-C22	-2.58	1.40	1.46
18	B	828	CLA	C3B-C4B	2.58	1.50	1.42
18	B	802	CLA	C3B-C4B	2.57	1.50	1.42
18	B	832	CLA	C1B-C2B	2.57	1.49	1.43
18	A	842	CLA	C1B-C2B	2.57	1.49	1.43
21	2	616	LUT	C34-C33	2.57	1.41	1.35
18	A	802	CLA	C1B-C2B	2.57	1.49	1.43
18	4	609	CLA	C1B-C2B	2.56	1.49	1.43
18	A	821	CLA	C3B-C4B	2.56	1.50	1.42
18	B	822	CLA	C1B-C2B	2.56	1.49	1.43
18	B	838	CLA	C3B-C4B	2.56	1.50	1.42
18	3	607	CLA	C1B-C2B	2.56	1.49	1.43
22	A	851	BCR	C10-C9	2.54	1.41	1.35
22	A	851	BCR	C8-C9	-2.52	1.40	1.46
18	A	807	CLA	C3B-C4B	2.51	1.50	1.42
18	A	844	CLA	C1B-C2B	2.51	1.49	1.43
22	B	845	BCR	C17-C18	2.49	1.41	1.35
18	A	814	CLA	C1B-C2B	2.49	1.49	1.43
18	A	828	CLA	C3B-C4B	2.48	1.50	1.42
18	4	609	CLA	C3B-C4B	2.47	1.49	1.42
22	B	844	BCR	C21-C22	2.47	1.41	1.35
18	1	609	CLA	C3B-C4B	2.46	1.49	1.42
18	B	810	CLA	C3B-C4B	2.46	1.49	1.42
18	A	828	CLA	CHC-C1C	2.46	1.43	1.38
22	F	304	BCR	C14-C13	2.45	1.41	1.35
24	A	801	CL0	CHD-C1D	2.45	1.43	1.39
18	F	301	CLA	C3B-C4B	2.44	1.49	1.42
22	B	843	BCR	C17-C18	2.44	1.41	1.35
18	4	611	CLA	C3B-C4B	2.44	1.49	1.42
18	A	808	CLA	C3B-C4B	2.44	1.49	1.42
22	A	851	BCR	C23-C22	-2.44	1.40	1.46
22	F	304	BCR	C10-C9	2.44	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	K	205	BCR	C21-C22	2.43	1.41	1.35
22	L	301	BCR	C17-C18	2.43	1.41	1.35
21	2	616	LUT	C8-C9	-2.43	1.40	1.46
18	3	604	CLA	C3B-C4B	2.43	1.49	1.42
18	A	810	CLA	C3B-C4B	2.42	1.49	1.42
22	L	301	BCR	C21-C22	2.42	1.41	1.35
18	4	609	CLA	CHC-C1C	2.42	1.43	1.38
19	4	617	XAT	C34-C33	2.42	1.41	1.35
22	L	306	BCR	C17-C18	2.42	1.41	1.35
22	B	849	BCR	C14-C13	2.41	1.41	1.35
18	G	202	CLA	C3B-C4B	2.41	1.49	1.42
22	B	843	BCR	C21-C22	2.41	1.41	1.35
18	A	837	CLA	C3B-C4B	2.41	1.49	1.42
22	J	102	BCR	C10-C9	2.41	1.41	1.35
22	A	849	BCR	C14-C13	2.41	1.41	1.35
21	1	616	LUT	C34-C33	2.41	1.41	1.35
18	J	101	CLA	C3B-C4B	2.41	1.49	1.42
18	1	611	CLA	C3B-C4B	2.41	1.49	1.42
18	1	609	CLA	CMD-C2D	-2.41	1.45	1.50
22	L	306	BCR	C10-C9	2.41	1.41	1.35
18	A	824	CLA	C3B-C4B	2.40	1.49	1.42
22	L	306	BCR	C21-C22	2.40	1.41	1.35
19	4	617	XAT	C10-C9	2.40	1.41	1.35
18	A	836	CLA	C3B-C4B	2.40	1.49	1.42
22	K	202	BCR	C10-C9	2.40	1.41	1.35
18	3	609	CLA	C3B-C4B	2.40	1.49	1.42
18	F	303	CLA	C3B-C4B	2.40	1.49	1.42
22	B	843	BCR	C10-C9	2.40	1.41	1.35
21	2	616	LUT	C14-C13	2.40	1.41	1.35
18	B	834	CLA	C3B-C4B	2.40	1.49	1.42
19	2	617	XAT	C30-C29	2.40	1.41	1.35
18	B	840	CLA	C3B-C4B	2.39	1.49	1.42
18	G	201	CLA	C3B-C4B	2.39	1.49	1.42
18	F	301	CLA	CHC-C1C	2.39	1.43	1.38
18	A	840	CLA	C3B-C4B	2.39	1.49	1.42
22	L	301	BCR	C14-C13	2.39	1.41	1.35
21	1	616	LUT	C14-C13	2.39	1.41	1.35
19	2	617	XAT	C10-C9	2.39	1.41	1.35
19	4	617	XAT	C30-C29	2.39	1.41	1.35
18	A	844	CLA	CHC-C1C	2.39	1.43	1.38
22	K	205	BCR	C10-C9	2.39	1.41	1.35
22	J	102	BCR	C14-C13	2.39	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	836	CLA	C3B-C4B	2.39	1.49	1.42
18	B	825	CLA	CHC-C1C	2.38	1.43	1.38
18	A	819	CLA	C3B-C4B	2.38	1.49	1.42
18	A	802	CLA	C3B-C4B	2.38	1.49	1.42
22	B	801	BCR	C14-C13	2.38	1.41	1.35
22	B	846	BCR	C21-C22	2.38	1.41	1.35
18	A	814	CLA	CHC-C1C	2.38	1.43	1.38
22	A	850	BCR	C10-C9	2.38	1.41	1.35
18	3	610	CLA	C3B-C4B	2.38	1.49	1.42
18	A	823	CLA	C3B-C4B	2.38	1.49	1.42
19	4	617	XAT	C14-C13	2.38	1.41	1.35
18	3	611	CLA	C3B-C4B	2.38	1.49	1.42
18	A	813	CLA	C3B-C4B	2.37	1.49	1.42
22	J	102	BCR	C17-C18	2.37	1.41	1.35
22	B	849	BCR	C17-C18	2.37	1.41	1.35
22	B	801	BCR	C17-C18	2.37	1.41	1.35
22	L	306	BCR	C14-C13	2.37	1.41	1.35
22	B	844	BCR	C10-C9	2.37	1.41	1.35
18	4	602	CLA	C3B-C4B	2.37	1.49	1.42
18	A	835	CLA	C3B-C4B	2.37	1.49	1.42
22	J	102	BCR	C21-C22	2.37	1.41	1.35
18	A	819	CLA	CHC-C1C	2.37	1.43	1.38
22	L	305	BCR	C14-C13	2.37	1.41	1.35
18	1	607	CLA	C3B-C4B	2.37	1.49	1.42
18	4	610	CLA	C3B-C4B	2.37	1.49	1.42
18	1	604	CLA	C3B-C4B	2.37	1.49	1.42
18	A	820	CLA	C3B-C4B	2.37	1.49	1.42
18	L	302	CLA	C3B-C4B	2.37	1.49	1.42
18	A	835	CLA	CHC-C1C	2.37	1.43	1.38
18	3	602	CLA	C3B-C4B	2.37	1.49	1.42
18	A	817	CLA	C3B-C4B	2.37	1.49	1.42
18	A	815	CLA	C3B-C4B	2.37	1.49	1.42
22	L	305	BCR	C17-C18	2.36	1.41	1.35
18	3	608	CLA	C3B-C4B	2.36	1.49	1.42
18	B	835	CLA	C3B-C4B	2.36	1.49	1.42
18	B	818	CLA	C3B-C4B	2.36	1.49	1.42
22	A	853	BCR	C21-C22	2.36	1.41	1.35
18	A	837	CLA	CHC-C1C	2.36	1.43	1.38
18	B	836	CLA	CHC-C1C	2.36	1.43	1.38
18	A	827	CLA	C3B-C4B	2.36	1.49	1.42
18	A	805	CLA	CHC-C1C	2.36	1.43	1.38
22	G	204	BCR	C21-C22	2.36	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	2	611	CLA	C3B-C4B	2.36	1.49	1.42
18	A	810	CLA	CHC-C1C	2.36	1.43	1.38
18	A	825	CLA	C3B-C4B	2.36	1.49	1.42
21	2	616	LUT	C28-C29	-2.36	1.40	1.46
18	A	844	CLA	C3B-C4B	2.36	1.49	1.42
18	L	303	CLA	C3B-C4B	2.36	1.49	1.42
22	L	301	BCR	C10-C9	2.36	1.41	1.35
18	B	825	CLA	C3B-C4B	2.36	1.49	1.42
22	A	853	BCR	C14-C13	2.36	1.41	1.35
18	4	601	CLA	C3B-C4B	2.35	1.49	1.42
18	A	838	CLA	C3B-C4B	2.35	1.49	1.42
22	4	618	BCR	C17-C18	2.35	1.41	1.35
22	B	846	BCR	C14-C13	2.35	1.41	1.35
22	L	305	BCR	C21-C22	2.35	1.41	1.35
18	A	816	CLA	C3B-C4B	2.35	1.49	1.42
22	I	101	BCR	C12-C13	-2.35	1.40	1.46
22	B	848	BCR	C19-C18	-2.35	1.40	1.46
22	B	846	BCR	C10-C9	2.35	1.41	1.35
22	L	305	BCR	C10-C9	2.35	1.41	1.35
18	2	609	CLA	C3B-C4B	2.35	1.49	1.42
18	B	826	CLA	C3B-C4B	2.35	1.49	1.42
21	1	616	LUT	C10-C9	2.35	1.41	1.35
18	A	805	CLA	C3B-C4B	2.35	1.49	1.42
22	B	801	BCR	C21-C22	2.35	1.41	1.35
22	A	849	BCR	C10-C9	2.34	1.41	1.35
18	A	824	CLA	CHC-C1C	2.34	1.43	1.38
18	4	613	CLA	C3B-C4B	2.34	1.49	1.42
18	B	829	CLA	C3B-C4B	2.34	1.49	1.42
21	2	616	LUT	C32-C33	-2.34	1.40	1.46
18	3	603	CLA	C3B-C4B	2.34	1.49	1.42
22	B	847	BCR	C14-C13	2.34	1.41	1.35
22	K	202	BCR	C14-C13	2.34	1.41	1.35
18	A	841	CLA	C3B-C4B	2.34	1.49	1.42
18	H	201	CLA	C3B-C4B	2.34	1.49	1.42
18	K	206	CLA	CHC-C1C	2.34	1.43	1.38
21	3	613	LUT	C28-C29	-2.34	1.40	1.46
22	B	845	BCR	C12-C13	-2.34	1.40	1.46
22	A	853	BCR	C17-C18	2.34	1.41	1.35
18	A	822	CLA	C3B-C4B	2.34	1.49	1.42
22	A	852	BCR	C21-C22	2.34	1.41	1.35
18	A	811	CLA	C3B-C4B	2.34	1.49	1.42
18	G	203	CLA	C3B-C4B	2.34	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	1	603	CLA	C3B-C4B	2.34	1.49	1.42
22	B	849	BCR	C10-C9	2.34	1.41	1.35
21	3	613	LUT	C32-C33	-2.34	1.40	1.46
18	B	804	CLA	CHC-C1C	2.34	1.43	1.38
18	A	831	CLA	C3B-C4B	2.34	1.49	1.42
18	2	602	CLA	C3B-C4B	2.34	1.49	1.42
18	A	812	CLA	C3B-C4B	2.34	1.49	1.42
22	A	852	BCR	C10-C9	2.34	1.41	1.35
22	A	852	BCR	C14-C13	2.34	1.41	1.35
22	A	850	BCR	C19-C18	-2.34	1.41	1.46
22	4	618	BCR	C14-C13	2.34	1.41	1.35
22	B	846	BCR	C17-C18	2.34	1.41	1.35
18	B	839	CLA	C3B-C4B	2.34	1.49	1.42
18	A	803	CLA	CHC-C1C	2.34	1.43	1.38
18	2	602	CLA	CHC-C1C	2.34	1.43	1.38
18	B	828	CLA	CHC-C1C	2.34	1.43	1.38
18	1	608	CLA	CHC-C1C	2.33	1.43	1.38
22	K	202	BCR	C17-C18	2.33	1.41	1.35
22	K	205	BCR	C14-C13	2.33	1.41	1.35
22	A	852	BCR	C17-C18	2.33	1.41	1.35
22	K	202	BCR	C21-C22	2.33	1.41	1.35
18	A	803	CLA	C3B-C4B	2.33	1.49	1.42
18	A	839	CLA	C3B-C4B	2.33	1.49	1.42
18	K	206	CLA	C3B-C4B	2.33	1.49	1.42
18	B	822	CLA	CHC-C1C	2.33	1.43	1.38
21	3	613	LUT	C12-C13	-2.33	1.41	1.46
22	3	614	BCR	C19-C18	-2.33	1.41	1.46
18	B	837	CLA	C3B-C4B	2.33	1.49	1.42
22	A	848	BCR	C21-C22	2.33	1.41	1.35
18	4	608	CLA	C3B-C4B	2.33	1.49	1.42
18	B	822	CLA	C3B-C4B	2.33	1.49	1.42
18	B	833	CLA	C3B-C4B	2.33	1.49	1.42
18	B	813	CLA	C3B-C4B	2.33	1.49	1.42
18	3	607	CLA	CHC-C1C	2.33	1.43	1.38
18	B	837	CLA	CHC-C1C	2.33	1.43	1.38
18	A	827	CLA	CHC-C1C	2.33	1.43	1.38
18	3	601	CLA	C3B-C4B	2.33	1.49	1.42
18	1	605	CLA	CHC-C1C	2.33	1.43	1.38
22	B	844	BCR	C14-C13	2.33	1.41	1.35
21	2	619	LUT	C30-C29	2.32	1.41	1.35
18	B	804	CLA	C3B-C4B	2.32	1.49	1.42
18	B	807	CLA	C3B-C4B	2.32	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	3	614	BCR	C17-C18	2.32	1.41	1.35
18	4	614	CLA	C3B-C4B	2.32	1.49	1.42
18	B	827	CLA	C3B-C4B	2.32	1.49	1.42
18	B	814	CLA	C3B-C4B	2.32	1.49	1.42
18	A	815	CLA	CHC-C1C	2.32	1.43	1.38
21	2	619	LUT	C34-C33	2.32	1.41	1.35
18	4	612	CLA	C3B-C4B	2.32	1.49	1.42
18	B	813	CLA	CHC-C1C	2.32	1.43	1.38
18	A	806	CLA	C3B-C4B	2.32	1.49	1.42
18	K	203	CLA	C3B-C4B	2.32	1.49	1.42
18	J	101	CLA	CHC-C1C	2.32	1.43	1.38
22	4	618	BCR	C21-C22	2.32	1.41	1.35
21	4	616	LUT	C32-C33	-2.32	1.41	1.46
18	B	803	CLA	C3B-C4B	2.32	1.49	1.42
18	1	605	CLA	C3B-C4B	2.32	1.49	1.42
18	B	809	CLA	C3B-C4B	2.32	1.49	1.42
18	B	821	CLA	C3B-C4B	2.32	1.49	1.42
18	B	816	CLA	C3B-C4B	2.32	1.49	1.42
18	B	831	CLA	C3B-C4B	2.32	1.49	1.42
22	L	301	BCR	C12-C13	-2.32	1.41	1.46
22	3	614	BCR	C10-C9	2.32	1.41	1.35
21	2	619	LUT	C14-C13	2.32	1.41	1.35
18	K	201	CLA	C3B-C4B	2.32	1.49	1.42
18	B	829	CLA	CHC-C1C	2.32	1.43	1.38
18	1	602	CLA	C3B-C4B	2.31	1.49	1.42
22	B	847	BCR	C10-C9	2.31	1.41	1.35
18	A	811	CLA	CHC-C1C	2.31	1.43	1.38
22	B	845	BCR	C10-C9	2.31	1.41	1.35
18	B	811	CLA	CHC-C1C	2.31	1.43	1.38
18	1	604	CLA	CHC-C1C	2.31	1.43	1.38
18	4	610	CLA	CHC-C1C	2.31	1.43	1.38
18	2	608	CLA	C3B-C4B	2.31	1.49	1.42
18	A	833	CLA	C3B-C4B	2.31	1.49	1.42
18	B	824	CLA	C3B-C4B	2.31	1.49	1.42
18	B	815	CLA	C3B-C4B	2.31	1.49	1.42
22	F	304	BCR	C23-C22	-2.31	1.41	1.46
18	B	841	CLA	C3B-C4B	2.31	1.49	1.42
18	B	824	CLA	CHC-C1C	2.31	1.43	1.38
18	A	830	CLA	C3B-C4B	2.31	1.49	1.42
22	G	204	BCR	C17-C18	2.31	1.41	1.35
18	2	612	CLA	C3B-C4B	2.31	1.49	1.42
18	K	204	CLA	C3B-C4B	2.31	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	2	609	CLA	CHC-C1C	2.31	1.43	1.38
21	2	619	LUT	C10-C9	2.31	1.41	1.35
22	B	849	BCR	C21-C22	2.31	1.41	1.35
18	B	817	CLA	C3B-C4B	2.31	1.49	1.42
18	B	805	CLA	CHC-C1C	2.31	1.43	1.38
22	B	844	BCR	C17-C18	2.31	1.41	1.35
18	A	808	CLA	CHC-C1C	2.31	1.43	1.38
18	A	833	CLA	CHC-C1C	2.31	1.43	1.38
18	A	836	CLA	CHC-C1C	2.31	1.43	1.38
19	1	614	XAT	O24-C25	-2.31	1.43	1.46
22	4	618	BCR	C10-C9	2.31	1.41	1.35
18	B	833	CLA	CHC-C1C	2.31	1.43	1.38
22	K	205	BCR	C17-C18	2.30	1.41	1.35
18	4	602	CLA	CHC-C1C	2.30	1.43	1.38
21	4	616	LUT	C12-C13	-2.30	1.41	1.46
18	4	611	CLA	CHC-C1C	2.30	1.43	1.38
18	A	809	CLA	CHC-C1C	2.30	1.43	1.38
22	B	847	BCR	C17-C18	2.30	1.41	1.35
22	3	614	BCR	C14-C13	2.30	1.41	1.35
18	2	612	CLA	CHC-C1C	2.30	1.43	1.38
18	B	818	CLA	CHC-C1C	2.30	1.43	1.38
22	I	101	BCR	C19-C18	-2.30	1.41	1.46
22	B	848	BCR	C12-C13	-2.30	1.41	1.46
18	3	608	CLA	CHC-C1C	2.30	1.43	1.38
18	A	841	CLA	CHC-C1C	2.30	1.43	1.38
18	F	302	CLA	C3B-C4B	2.30	1.49	1.42
18	1	613	CLA	CHC-C1C	2.30	1.43	1.38
18	2	608	CLA	CHC-C1C	2.30	1.43	1.38
22	G	204	BCR	C12-C13	-2.30	1.41	1.46
18	A	809	CLA	C3B-C4B	2.30	1.49	1.42
18	B	830	CLA	C3B-C4B	2.30	1.49	1.42
21	2	619	LUT	C32-C33	-2.29	1.41	1.46
18	B	814	CLA	CHC-C1C	2.29	1.43	1.38
18	B	823	CLA	C3B-C4B	2.29	1.49	1.42
18	A	832	CLA	C3B-C4B	2.29	1.49	1.42
18	A	802	CLA	CHC-C1C	2.29	1.43	1.38
18	B	816	CLA	CHC-C1C	2.29	1.43	1.38
18	B	810	CLA	CHC-C1C	2.29	1.43	1.38
21	4	616	LUT	C34-C33	2.29	1.41	1.35
22	A	848	BCR	C19-C18	-2.29	1.41	1.46
22	A	848	BCR	C10-C9	2.29	1.41	1.35
18	B	809	CLA	CHC-C1C	2.29	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	L	305	BCR	C12-C13	-2.29	1.41	1.46
18	K	203	CLA	CHC-C1C	2.29	1.43	1.38
18	3	601	CLA	CHC-C1C	2.29	1.43	1.38
18	A	834	CLA	C3B-C4B	2.29	1.49	1.42
18	B	831	CLA	CHC-C1C	2.29	1.43	1.38
18	A	826	CLA	C3B-C4B	2.29	1.49	1.42
22	I	101	BCR	C17-C18	2.29	1.41	1.35
18	B	820	CLA	C3B-C4B	2.29	1.49	1.42
18	4	613	CLA	CHC-C1C	2.29	1.43	1.38
18	A	812	CLA	CHC-C1C	2.29	1.43	1.38
18	L	304	CLA	C3B-C4B	2.29	1.49	1.42
21	2	619	LUT	C12-C13	-2.29	1.41	1.46
18	A	816	CLA	CHC-C1C	2.28	1.43	1.38
18	A	838	CLA	CHC-C1C	2.28	1.43	1.38
18	B	815	CLA	CHC-C1C	2.28	1.43	1.38
22	I	101	BCR	C10-C9	2.28	1.41	1.35
18	3	611	CLA	CHC-C1C	2.28	1.43	1.38
18	A	823	CLA	CHC-C1C	2.28	1.43	1.38
18	B	835	CLA	CHC-C1C	2.28	1.43	1.38
19	2	617	XAT	C28-C29	-2.28	1.41	1.46
18	B	808	CLA	C3B-C4B	2.28	1.49	1.42
18	B	821	CLA	CHC-C1C	2.28	1.43	1.38
21	4	616	LUT	C30-C29	2.28	1.41	1.35
18	3	610	CLA	CHC-C1C	2.28	1.43	1.38
22	G	204	BCR	C10-C9	2.28	1.41	1.35
18	A	842	CLA	C3B-C4B	2.28	1.49	1.42
18	F	302	CLA	CHC-C1C	2.28	1.43	1.38
18	A	822	CLA	CHC-C1C	2.28	1.43	1.38
18	B	803	CLA	CHC-C1C	2.28	1.43	1.38
22	B	848	BCR	C10-C9	2.28	1.41	1.35
18	A	845	CLA	CHC-C1C	2.28	1.43	1.38
18	A	831	CLA	CHC-C1C	2.28	1.43	1.38
18	B	807	CLA	CHC-C1C	2.28	1.43	1.38
18	1	610	CLA	CHC-C1C	2.27	1.43	1.38
18	2	613	CLA	C3B-C4B	2.27	1.49	1.42
22	A	848	BCR	C17-C18	2.27	1.41	1.35
18	B	827	CLA	CHC-C1C	2.27	1.43	1.38
18	G	203	CLA	CHC-C1C	2.27	1.43	1.38
18	A	843	CLA	C3B-C4B	2.27	1.49	1.42
22	B	848	BCR	C17-C18	2.27	1.41	1.35
18	1	603	CLA	CHC-C1C	2.27	1.43	1.38
18	L	304	CLA	CHC-C1C	2.27	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	832	CLA	CHC-C1C	2.27	1.43	1.38
18	B	812	CLA	CHC-C1C	2.27	1.43	1.38
22	A	848	BCR	C14-C13	2.27	1.41	1.35
18	A	845	CLA	C3B-C4B	2.27	1.49	1.42
18	A	807	CLA	CHC-C1C	2.27	1.43	1.38
18	A	840	CLA	CHC-C1C	2.27	1.43	1.38
22	B	848	BCR	C14-C13	2.27	1.41	1.35
18	2	613	CLA	CHC-C1C	2.27	1.43	1.38
18	4	601	CLA	CHC-C1C	2.27	1.43	1.38
22	B	847	BCR	C19-C18	-2.27	1.41	1.46
18	2	604	CLA	C3B-C4B	2.27	1.49	1.42
22	I	101	BCR	C14-C13	2.27	1.41	1.35
18	G	201	CLA	CHC-C1C	2.27	1.43	1.38
18	2	603	CLA	C3B-C4B	2.27	1.49	1.42
18	A	839	CLA	CHC-C1C	2.27	1.43	1.38
22	G	204	BCR	C19-C18	-2.27	1.41	1.46
21	2	616	LUT	C10-C9	2.27	1.41	1.35
18	3	605	CLA	CHC-C1C	2.27	1.43	1.38
18	4	604	CLA	CHC-C1C	2.27	1.43	1.38
18	B	834	CLA	CHC-C1C	2.27	1.43	1.38
18	L	303	CLA	CHC-C1C	2.26	1.43	1.38
18	3	609	CLA	CHC-C1C	2.26	1.43	1.38
18	A	806	CLA	CHC-C1C	2.26	1.43	1.38
18	B	841	CLA	CHC-C1C	2.26	1.43	1.38
22	3	614	BCR	C12-C13	-2.26	1.41	1.46
18	1	611	CLA	CHC-C1C	2.26	1.43	1.38
18	1	602	CLA	CHC-C1C	2.26	1.43	1.38
18	B	840	CLA	CHC-C1C	2.26	1.43	1.38
18	A	825	CLA	CHC-C1C	2.26	1.43	1.38
18	A	804	CLA	C3B-C4B	2.26	1.49	1.42
22	4	618	BCR	C12-C13	-2.26	1.41	1.46
22	B	847	BCR	C12-C13	-2.26	1.41	1.46
22	G	204	BCR	C14-C13	2.26	1.41	1.35
21	4	616	LUT	C14-C13	2.26	1.41	1.35
18	A	813	CLA	CHC-C1C	2.26	1.43	1.38
21	3	613	LUT	C14-C13	2.26	1.41	1.35
18	K	201	CLA	CHC-C1C	2.25	1.43	1.38
18	A	818	CLA	C3B-C4B	2.25	1.49	1.42
21	4	616	LUT	C10-C9	2.25	1.41	1.35
18	4	603	CLA	CHC-C1C	2.25	1.43	1.38
18	3	602	CLA	CHC-C1C	2.25	1.43	1.38
18	B	817	CLA	CHC-C1C	2.25	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	F	303	CLA	CHC-C1C	2.25	1.43	1.38
18	A	829	CLA	CHC-C1C	2.25	1.43	1.38
18	1	612	CLA	C3B-C4B	2.25	1.49	1.42
18	A	817	CLA	CHC-C1C	2.25	1.43	1.38
22	B	847	BCR	C21-C22	2.25	1.41	1.35
18	4	614	CLA	CHC-C1C	2.25	1.43	1.38
22	A	848	BCR	C12-C13	-2.25	1.41	1.46
18	A	804	CLA	CHC-C1C	2.25	1.43	1.38
18	B	832	CLA	CHC-C1C	2.25	1.43	1.38
18	A	842	CLA	CMB-C2B	-2.25	1.46	1.50
18	B	806	CLA	C3B-C4B	2.25	1.49	1.42
18	B	830	CLA	CHC-C1C	2.24	1.43	1.38
18	A	830	CLA	CHC-C1C	2.24	1.43	1.38
18	A	820	CLA	CHC-C1C	2.24	1.43	1.38
18	B	823	CLA	CHC-C1C	2.24	1.43	1.38
18	L	302	CLA	CHC-C1C	2.24	1.43	1.38
22	B	849	BCR	C12-C13	-2.24	1.41	1.46
18	4	608	CLA	CHC-C1C	2.24	1.43	1.38
18	A	826	CLA	CHC-C1C	2.24	1.43	1.38
21	4	616	LUT	C28-C29	-2.24	1.41	1.46
18	2	603	CLA	CHC-C1C	2.24	1.43	1.38
22	B	801	BCR	C12-C13	-2.24	1.41	1.46
24	A	801	CL0	MG-NB	2.24	2.10	2.05
18	2	610	CLA	CHC-C1C	2.24	1.43	1.38
18	1	607	CLA	CHC-C1C	2.24	1.43	1.38
18	3	604	CLA	CHC-C1C	2.24	1.43	1.38
18	B	826	CLA	CHC-C1C	2.23	1.43	1.38
18	3	612	CLA	C3B-C4B	2.23	1.49	1.42
22	B	845	BCR	C14-C13	2.23	1.41	1.35
18	B	808	CLA	CHC-C1C	2.23	1.43	1.38
22	3	614	BCR	C21-C22	2.23	1.41	1.35
18	4	612	CLA	CHC-C1C	2.23	1.43	1.38
17	3	606	CHL	CBD-CGD	-2.23	1.49	1.52
18	G	202	CLA	CHC-C1C	2.23	1.42	1.38
18	K	204	CLA	CHC-C1C	2.22	1.42	1.38
18	B	819	CLA	C3B-C4B	2.22	1.49	1.42
22	B	849	BCR	C19-C18	-2.22	1.41	1.46
18	B	838	CLA	CHC-C1C	2.22	1.42	1.38
22	B	848	BCR	C21-C22	2.22	1.40	1.35
22	A	853	BCR	C19-C18	-2.22	1.41	1.46
18	B	819	CLA	CHC-C1C	2.22	1.42	1.38
22	B	844	BCR	C12-C13	-2.22	1.41	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	821	CLA	CHC-C1C	2.22	1.42	1.38
22	A	849	BCR	C19-C18	-2.22	1.41	1.46
22	B	846	BCR	C19-C18	-2.22	1.41	1.46
22	A	852	BCR	C19-C18	-2.21	1.41	1.46
21	2	619	LUT	C28-C29	-2.21	1.41	1.46
18	2	611	CLA	CHC-C1C	2.21	1.42	1.38
18	A	834	CLA	CHC-C1C	2.21	1.42	1.38
18	B	820	CLA	CHC-C1C	2.21	1.42	1.38
22	A	850	BCR	C21-C22	2.21	1.40	1.35
22	B	801	BCR	C19-C18	-2.21	1.41	1.46
18	A	843	CLA	CHC-C1C	2.21	1.42	1.38
18	3	603	CLA	CHC-C1C	2.20	1.42	1.38
22	I	101	BCR	C21-C22	2.20	1.40	1.35
22	K	205	BCR	C19-C18	-2.20	1.41	1.46
18	B	839	CLA	CHC-C1C	2.20	1.42	1.38
18	B	808	CLA	CMD-C2D	-2.20	1.46	1.50
22	J	102	BCR	C19-C18	-2.20	1.41	1.46
18	A	842	CLA	CMD-C2D	-2.20	1.46	1.50
22	4	618	BCR	C19-C18	-2.20	1.41	1.46
21	3	613	LUT	C30-C29	2.20	1.40	1.35
22	A	853	BCR	C12-C13	-2.20	1.41	1.46
18	B	802	CLA	CHC-C1C	2.20	1.42	1.38
18	2	604	CLA	CHC-C1C	2.19	1.42	1.38
21	2	616	LUT	C12-C13	-2.19	1.41	1.46
18	B	806	CLA	CHC-C1C	2.19	1.42	1.38
18	H	201	CLA	CHC-C1C	2.19	1.42	1.38
18	A	829	CLA	C3B-C4B	2.19	1.49	1.42
22	L	305	BCR	C19-C18	-2.19	1.41	1.46
18	A	842	CLA	MG-NB	-2.18	2.01	2.05
18	B	802	CLA	CMD-C2D	-2.18	1.46	1.50
22	B	846	BCR	C12-C13	-2.18	1.41	1.46
18	A	818	CLA	CHC-C1C	2.18	1.42	1.38
19	4	617	XAT	C32-C33	-2.18	1.41	1.46
22	K	202	BCR	C19-C18	-2.17	1.41	1.46
22	A	850	BCR	C12-C13	-2.17	1.41	1.46
22	L	301	BCR	C20-C19	2.17	1.40	1.34
21	2	616	LUT	C30-C29	2.17	1.40	1.35
19	4	617	XAT	C8-C9	-2.17	1.41	1.46
19	4	617	XAT	C28-C29	-2.16	1.41	1.46
22	A	849	BCR	C12-C13	-2.16	1.41	1.46
18	L	302	CLA	CMB-C2B	-2.16	1.46	1.50
21	1	616	LUT	C12-C13	-2.15	1.41	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	844	CLA	MG-NB	-2.15	2.01	2.05
22	J	102	BCR	C12-C13	-2.15	1.41	1.46
18	A	803	CLA	MG-NB	-2.15	2.01	2.05
18	3	612	CLA	CHC-C1C	2.15	1.42	1.38
18	A	842	CLA	CHC-C1C	2.15	1.42	1.38
18	B	823	CLA	CMD-C2D	-2.14	1.46	1.50
18	B	828	CLA	CMD-C2D	-2.14	1.46	1.50
18	B	817	CLA	CMB-C2B	-2.13	1.46	1.50
18	B	839	CLA	CMD-C2D	-2.13	1.46	1.50
22	K	202	BCR	C12-C13	-2.13	1.41	1.46
18	K	201	CLA	CBD-CAD	2.13	1.56	1.51
18	B	829	CLA	CMD-C2D	-2.13	1.46	1.50
18	2	609	CLA	CMD-C2D	-2.13	1.46	1.50
18	3	612	CLA	CMD-C2D	-2.12	1.46	1.50
22	B	843	BCR	C19-C18	-2.12	1.41	1.46
18	4	613	CLA	CMD-C2D	-2.12	1.46	1.50
22	B	845	BCR	C19-C18	-2.12	1.41	1.46
17	4	607	CHL	CBD-CGD	-2.12	1.49	1.52
18	2	604	CLA	MG-NB	-2.12	2.01	2.05
18	4	611	CLA	CMD-C2D	-2.12	1.46	1.50
18	4	604	CLA	CMB-C2B	-2.12	1.46	1.50
18	B	808	CLA	MG-NB	-2.11	2.01	2.05
19	2	617	XAT	C32-C33	-2.11	1.41	1.46
18	4	603	CLA	CMD-C2D	-2.11	1.46	1.50
18	K	204	CLA	CMC-C2C	-2.11	1.46	1.50
19	4	617	XAT	C12-C13	-2.11	1.41	1.46
18	A	810	CLA	CMD-C2D	-2.11	1.46	1.50
18	1	609	CLA	CHC-C1C	2.11	1.42	1.38
18	3	612	CLA	MG-NB	-2.11	2.01	2.05
18	B	826	CLA	MG-NB	-2.11	2.01	2.05
18	4	604	CLA	MG-NB	-2.11	2.01	2.05
18	B	822	CLA	MG-NB	-2.11	2.01	2.05
22	L	306	BCR	C19-C18	-2.11	1.41	1.46
22	B	843	BCR	C12-C13	-2.11	1.41	1.46
18	B	819	CLA	CMB-C2B	-2.11	1.46	1.50
18	1	612	CLA	CHC-C1C	2.10	1.42	1.38
18	3	609	CLA	CMD-C2D	-2.10	1.46	1.50
18	B	807	CLA	CMD-C2D	-2.10	1.46	1.50
18	B	829	CLA	CMB-C2B	-2.10	1.46	1.50
18	2	612	CLA	MG-NB	-2.10	2.01	2.05
18	3	601	CLA	MG-NB	-2.10	2.01	2.05
18	3	603	CLA	MG-NB	-2.10	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	811	CLA	CMD-C2D	-2.10	1.46	1.50
18	1	613	CLA	CMD-C2D	-2.10	1.46	1.50
18	4	603	CLA	MG-NB	-2.10	2.01	2.05
21	1	616	LUT	C32-C33	-2.09	1.41	1.46
18	2	603	CLA	MG-NB	-2.09	2.01	2.05
18	1	608	CLA	CMD-C2D	-2.09	1.46	1.50
18	A	819	CLA	CMC-C2C	-2.09	1.46	1.50
18	B	803	CLA	CMC-C2C	-2.09	1.46	1.50
18	K	201	CLA	MG-NB	-2.09	2.01	2.05
18	B	822	CLA	CMB-C2B	-2.09	1.46	1.50
18	A	818	CLA	MG-NB	-2.09	2.01	2.05
18	2	612	CLA	CMD-C2D	-2.09	1.46	1.50
18	3	609	CLA	CMB-C2B	-2.08	1.46	1.50
18	B	836	CLA	CMD-C2D	-2.08	1.46	1.50
18	B	825	CLA	MG-NB	-2.08	2.01	2.05
18	4	608	CLA	CMD-C2D	-2.08	1.46	1.50
18	B	838	CLA	CMB-C2B	-2.08	1.46	1.50
19	2	617	XAT	C12-C13	-2.08	1.41	1.46
18	A	810	CLA	CMB-C2B	-2.08	1.46	1.50
18	L	302	CLA	MG-NB	-2.08	2.01	2.05
18	B	826	CLA	CMD-C2D	-2.08	1.46	1.50
18	1	608	CLA	MG-NB	-2.08	2.01	2.05
18	3	607	CLA	CMD-C2D	-2.08	1.46	1.50
18	4	603	CLA	CMB-C2B	-2.08	1.46	1.50
18	B	810	CLA	CMD-C2D	-2.08	1.46	1.50
18	A	813	CLA	CMD-C2D	-2.08	1.46	1.50
18	A	840	CLA	CMB-C2B	-2.08	1.46	1.50
18	2	609	CLA	MG-NB	-2.08	2.01	2.05
18	3	611	CLA	CBD-CAD	2.08	1.56	1.51
18	A	828	CLA	CMC-C2C	-2.07	1.46	1.50
22	F	304	BCR	C19-C18	-2.07	1.41	1.46
18	1	603	CLA	CMD-C2D	-2.07	1.46	1.50
18	A	839	CLA	MG-NB	-2.07	2.01	2.05
18	3	601	CLA	CMD-C2D	-2.07	1.46	1.50
18	B	815	CLA	CMD-C2D	-2.07	1.46	1.50
18	3	604	CLA	CMD-C2D	-2.07	1.46	1.50
17	2	607	CHL	CBD-CGD	-2.07	1.49	1.52
18	B	834	CLA	CMD-C2D	-2.07	1.46	1.50
18	B	809	CLA	MG-NB	-2.07	2.01	2.05
18	A	844	CLA	CMB-C2B	-2.07	1.46	1.50
18	1	610	CLA	MG-NB	-2.07	2.01	2.05
18	B	819	CLA	MG-NB	-2.07	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	4	612	CLA	MG-NB	-2.07	2.01	2.05
18	A	802	CLA	CMD-C2D	-2.07	1.46	1.50
18	G	202	CLA	CMD-C2D	-2.07	1.46	1.50
18	A	820	CLA	MG-NB	-2.07	2.01	2.05
18	B	830	CLA	CMB-C2B	-2.07	1.46	1.50
18	B	840	CLA	CMD-C2D	-2.07	1.46	1.50
18	A	824	CLA	CMD-C2D	-2.07	1.46	1.50
18	G	203	CLA	MG-NB	-2.07	2.01	2.05
18	4	614	CLA	MG-NB	-2.07	2.01	2.05
18	B	820	CLA	CMD-C2D	-2.07	1.46	1.50
18	4	610	CLA	MG-NB	-2.07	2.01	2.05
18	2	613	CLA	MG-NB	-2.07	2.01	2.05
18	4	609	CLA	CMD-C2D	-2.07	1.46	1.50
18	1	612	CLA	CMB-C2B	-2.07	1.46	1.50
18	A	830	CLA	CMD-C2D	-2.07	1.46	1.50
18	A	817	CLA	CMD-C2D	-2.07	1.46	1.50
18	2	611	CLA	CMD-C2D	-2.06	1.46	1.50
18	2	610	CLA	MG-NB	-2.06	2.01	2.05
18	B	813	CLA	MG-NB	-2.06	2.01	2.05
18	K	206	CLA	MG-NB	-2.06	2.01	2.05
18	3	605	CLA	CMD-C2D	-2.06	1.46	1.50
18	B	813	CLA	CMD-C2D	-2.06	1.46	1.50
18	2	613	CLA	CMB-C2B	-2.06	1.46	1.50
18	A	807	CLA	CMD-C2D	-2.06	1.46	1.50
18	A	812	CLA	CMB-C2B	-2.06	1.46	1.50
18	B	830	CLA	MG-NB	-2.06	2.01	2.05
18	B	839	CLA	MG-NB	-2.06	2.01	2.05
18	3	602	CLA	MG-NB	-2.06	2.01	2.05
18	A	838	CLA	MG-NB	-2.06	2.01	2.05
18	1	612	CLA	CMD-C2D	-2.06	1.46	1.50
18	B	805	CLA	CMD-C2D	-2.06	1.46	1.50
18	B	821	CLA	MG-NB	-2.06	2.01	2.05
18	2	602	CLA	CMD-C2D	-2.06	1.46	1.50
18	A	816	CLA	CMD-C2D	-2.06	1.46	1.50
18	K	204	CLA	CMB-C2B	-2.06	1.46	1.50
18	F	302	CLA	MG-NB	-2.06	2.01	2.05
22	L	306	BCR	C12-C13	-2.06	1.41	1.46
18	2	604	CLA	CMD-C2D	-2.06	1.46	1.50
18	B	838	CLA	CMD-C2D	-2.06	1.46	1.50
18	A	822	CLA	CMB-C2B	-2.06	1.46	1.50
18	B	835	CLA	CMD-C2D	-2.06	1.46	1.50
18	A	806	CLA	CMC-C2C	-2.06	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	F	303	CLA	CMB-C2B	-2.06	1.46	1.50
18	A	832	CLA	CMD-C2D	-2.06	1.46	1.50
18	3	605	CLA	MG-NB	-2.05	2.01	2.05
18	A	835	CLA	CMD-C2D	-2.05	1.46	1.50
18	B	817	CLA	CMC-C2C	-2.05	1.46	1.50
18	A	838	CLA	CMB-C2B	-2.05	1.46	1.50
18	A	812	CLA	MG-NB	-2.05	2.01	2.05
18	1	604	CLA	CMD-C2D	-2.05	1.46	1.50
18	B	841	CLA	CMD-C2D	-2.05	1.46	1.50
18	A	804	CLA	MG-NB	-2.05	2.01	2.05
18	A	821	CLA	CMD-C2D	-2.05	1.46	1.50
18	3	603	CLA	CMB-C2B	-2.05	1.46	1.50
18	A	820	CLA	CMD-C2D	-2.05	1.46	1.50
18	A	832	CLA	CMB-C2B	-2.05	1.46	1.50
18	J	101	CLA	CMB-C2B	-2.05	1.46	1.50
18	A	812	CLA	CMD-C2D	-2.05	1.46	1.50
18	4	602	CLA	MG-NB	-2.05	2.01	2.05
18	A	825	CLA	CMD-C2D	-2.05	1.46	1.50
18	A	804	CLA	CMD-C2D	-2.05	1.46	1.50
18	B	835	CLA	CMB-C2B	-2.05	1.46	1.50
18	F	302	CLA	CMD-C2D	-2.05	1.46	1.50
18	B	823	CLA	MG-NB	-2.05	2.01	2.05
18	B	827	CLA	CMD-C2D	-2.05	1.46	1.50
18	A	841	CLA	CMD-C2D	-2.05	1.46	1.50
18	A	802	CLA	MG-NB	-2.05	2.01	2.05
18	1	611	CLA	CMD-C2D	-2.05	1.46	1.50
18	4	602	CLA	CMD-C2D	-2.05	1.46	1.50
18	K	203	CLA	CMD-C2D	-2.05	1.46	1.50
18	A	810	CLA	MG-NB	-2.05	2.01	2.05
18	3	611	CLA	CMD-C2D	-2.05	1.46	1.50
18	B	819	CLA	CMD-C2D	-2.05	1.46	1.50
18	B	806	CLA	CMD-C2D	-2.05	1.46	1.50
18	K	204	CLA	CMD-C2D	-2.05	1.46	1.50
18	A	829	CLA	MG-NB	-2.05	2.01	2.05
18	B	827	CLA	MG-NB	-2.05	2.01	2.05
18	B	817	CLA	MG-NB	-2.05	2.01	2.05
18	A	829	CLA	CMD-C2D	-2.05	1.46	1.50
18	2	611	CLA	MG-NB	-2.04	2.01	2.05
18	B	839	CLA	CMB-C2B	-2.04	1.46	1.50
18	B	822	CLA	CMD-C2D	-2.04	1.46	1.50
18	4	609	CLA	CMC-C2C	-2.04	1.46	1.50
18	A	823	CLA	CMD-C2D	-2.04	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	4	604	CLA	CMD-C2D	-2.04	1.46	1.50
18	2	608	CLA	CMD-C2D	-2.04	1.46	1.50
18	B	829	CLA	MG-NB	-2.04	2.01	2.05
18	B	832	CLA	CMD-C2D	-2.04	1.46	1.50
18	1	607	CLA	CMD-C2D	-2.04	1.46	1.50
18	2	613	CLA	CMD-C2D	-2.04	1.46	1.50
18	A	809	CLA	CMD-C2D	-2.04	1.46	1.50
18	B	811	CLA	CMD-C2D	-2.04	1.46	1.50
18	L	302	CLA	CMD-C2D	-2.04	1.46	1.50
18	2	603	CLA	CMD-C2D	-2.04	1.46	1.50
18	4	609	CLA	CMB-C2B	-2.04	1.46	1.50
18	B	827	CLA	CMB-C2B	-2.04	1.46	1.50
18	B	828	CLA	CMB-C2B	-2.04	1.46	1.50
18	A	833	CLA	CMD-C2D	-2.04	1.46	1.50
18	A	836	CLA	CMD-C2D	-2.04	1.46	1.50
18	B	824	CLA	MG-NB	-2.04	2.01	2.05
18	A	831	CLA	CMD-C2D	-2.04	1.46	1.50
18	B	814	CLA	CMD-C2D	-2.04	1.46	1.50
18	F	301	CLA	MG-NB	-2.04	2.01	2.05
18	3	608	CLA	CMD-C2D	-2.04	1.46	1.50
18	1	603	CLA	CMB-C2B	-2.04	1.46	1.50
18	F	301	CLA	CMD-C2D	-2.04	1.46	1.50
18	1	613	CLA	MG-NB	-2.04	2.01	2.05
18	A	808	CLA	CMB-C2B	-2.04	1.46	1.50
18	B	824	CLA	CMD-C2D	-2.04	1.46	1.50
18	A	834	CLA	CMD-C2D	-2.04	1.46	1.50
18	A	816	CLA	MG-NB	-2.04	2.01	2.05
18	B	841	CLA	MG-NB	-2.04	2.01	2.05
18	3	611	CLA	CMB-C2B	-2.04	1.46	1.50
18	A	822	CLA	MG-NB	-2.04	2.01	2.05
18	4	608	CLA	CMB-C2B	-2.04	1.46	1.50
18	3	608	CLA	MG-NB	-2.04	2.01	2.05
18	A	815	CLA	MG-NB	-2.04	2.01	2.05
22	K	205	BCR	C11-C12	2.04	1.40	1.34
18	A	840	CLA	CMD-C2D	-2.04	1.46	1.50
18	1	613	CLA	CMB-C2B	-2.03	1.46	1.50
18	4	614	CLA	CMD-C2D	-2.03	1.46	1.50
19	1	614	XAT	O4-C5	-2.03	1.43	1.46
18	A	822	CLA	CMD-C2D	-2.03	1.46	1.50
18	A	806	CLA	CMD-C2D	-2.03	1.46	1.50
18	A	834	CLA	CMB-C2B	-2.03	1.46	1.50
18	A	827	CLA	CMD-C2D	-2.03	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	834	CLA	CMB-C2B	-2.03	1.46	1.50
18	2	604	CLA	CMB-C2B	-2.03	1.46	1.50
18	A	821	CLA	CMB-C2B	-2.03	1.46	1.50
18	4	612	CLA	CMD-C2D	-2.03	1.46	1.50
18	A	815	CLA	CMD-C2D	-2.03	1.46	1.50
18	B	830	CLA	CMD-C2D	-2.03	1.46	1.50
18	B	805	CLA	CMB-C2B	-2.03	1.46	1.50
18	B	816	CLA	CMD-C2D	-2.03	1.46	1.50
18	3	611	CLA	MG-NB	-2.03	2.01	2.05
18	3	603	CLA	CMD-C2D	-2.03	1.46	1.50
18	A	845	CLA	CMB-C2B	-2.03	1.46	1.50
18	B	833	CLA	CMC-C2C	-2.03	1.46	1.50
18	3	610	CLA	MG-NB	-2.03	2.01	2.05
18	A	831	CLA	CMB-C2B	-2.03	1.46	1.50
18	B	809	CLA	CMB-C2B	-2.03	1.46	1.50
18	2	602	CLA	MG-NB	-2.03	2.01	2.05
18	H	201	CLA	MG-NB	-2.03	2.01	2.05
18	K	204	CLA	MG-NB	-2.03	2.01	2.05
18	A	807	CLA	CMB-C2B	-2.03	1.46	1.50
18	A	818	CLA	CMD-C2D	-2.03	1.46	1.50
18	A	843	CLA	CMD-C2D	-2.03	1.46	1.50
18	H	201	CLA	CMD-C2D	-2.03	1.46	1.50
18	B	812	CLA	CMB-C2B	-2.03	1.46	1.50
18	B	802	CLA	CMB-C2B	-2.03	1.46	1.50
18	B	836	CLA	CMB-C2B	-2.03	1.46	1.50
18	K	206	CLA	CMD-C2D	-2.03	1.46	1.50
18	3	609	CLA	MG-NB	-2.03	2.01	2.05
18	A	841	CLA	MG-NB	-2.03	2.01	2.05
18	B	818	CLA	MG-NB	-2.03	2.01	2.05
18	1	607	CLA	CMB-C2B	-2.03	1.46	1.50
18	G	201	CLA	CMD-C2D	-2.03	1.46	1.50
18	3	604	CLA	CMB-C2B	-2.03	1.46	1.50
18	A	813	CLA	CMB-C2B	-2.03	1.46	1.50
18	A	814	CLA	CMB-C2B	-2.03	1.46	1.50
18	H	201	CLA	CMB-C2B	-2.03	1.46	1.50
22	A	852	BCR	C11-C12	2.03	1.40	1.34
18	3	605	CLA	CMB-C2B	-2.03	1.46	1.50
18	B	833	CLA	CMD-C2D	-2.03	1.46	1.50
18	B	815	CLA	CMB-C2B	-2.03	1.46	1.50
18	B	803	CLA	CMD-C2D	-2.03	1.46	1.50
18	A	839	CLA	CMD-C2D	-2.03	1.46	1.50
18	B	808	CLA	CMB-C2B	-2.03	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	836	CLA	MG-NB	-2.03	2.01	2.05
18	4	601	CLA	CMC-C2C	-2.03	1.46	1.50
18	A	814	CLA	CMD-C2D	-2.03	1.46	1.50
18	A	819	CLA	CMB-C2B	-2.03	1.46	1.50
18	1	611	CLA	MG-NB	-2.03	2.01	2.05
18	4	611	CLA	MG-NB	-2.03	2.01	2.05
18	A	802	CLA	CMB-C2B	-2.03	1.46	1.50
18	B	804	CLA	CMD-C2D	-2.03	1.46	1.50
18	1	605	CLA	CMB-C2B	-2.02	1.46	1.50
18	1	610	CLA	CMD-C2D	-2.02	1.46	1.50
18	2	610	CLA	CMD-C2D	-2.02	1.46	1.50
18	A	837	CLA	CMD-C2D	-2.02	1.46	1.50
18	3	602	CLA	CMD-C2D	-2.02	1.46	1.50
18	L	304	CLA	CMD-C2D	-2.02	1.46	1.50
18	4	601	CLA	CMB-C2B	-2.02	1.46	1.50
18	L	304	CLA	CMB-C2B	-2.02	1.46	1.50
18	1	609	CLA	MG-NB	-2.02	2.01	2.05
18	G	203	CLA	CMD-C2D	-2.02	1.46	1.50
18	4	601	CLA	CMD-C2D	-2.02	1.46	1.50
18	A	819	CLA	CMD-C2D	-2.02	1.46	1.50
18	L	303	CLA	CMD-C2D	-2.02	1.46	1.50
18	A	817	CLA	CMB-C2B	-2.02	1.46	1.50
18	3	602	CLA	CMB-C2B	-2.02	1.46	1.50
18	A	808	CLA	CMD-C2D	-2.02	1.46	1.50
18	A	828	CLA	CMD-C2D	-2.02	1.46	1.50
18	A	834	CLA	MG-NB	-2.02	2.01	2.05
18	B	804	CLA	MG-NB	-2.02	2.01	2.05
18	B	811	CLA	CMB-C2B	-2.02	1.46	1.50
18	B	831	CLA	CMD-C2D	-2.02	1.46	1.50
18	B	817	CLA	CMD-C2D	-2.02	1.46	1.50
18	1	603	CLA	MG-NB	-2.02	2.01	2.05
18	3	604	CLA	MG-NB	-2.02	2.01	2.05
18	B	811	CLA	MG-NB	-2.02	2.01	2.05
18	F	301	CLA	CMB-C2B	-2.02	1.46	1.50
18	A	811	CLA	MG-NB	-2.02	2.01	2.05
18	4	609	CLA	MG-NB	-2.02	2.01	2.05
18	A	805	CLA	MG-NB	-2.02	2.01	2.05
18	B	812	CLA	CMD-C2D	-2.02	1.46	1.50
18	K	203	CLA	MG-NB	-2.02	2.01	2.05
24	A	801	CL0	OBD-CAD	2.02	1.28	1.21
18	B	816	CLA	MG-NB	-2.02	2.01	2.05
18	B	806	CLA	MG-NB	-2.02	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	820	CLA	CMB-C2B	-2.02	1.46	1.50
18	4	608	CLA	MG-NB	-2.02	2.01	2.05
18	1	604	CLA	CMB-C2B	-2.01	1.46	1.50
18	A	845	CLA	CMD-C2D	-2.01	1.46	1.50
18	A	836	CLA	CMB-C2B	-2.01	1.46	1.50
18	1	604	CLA	MG-NB	-2.01	2.01	2.05
22	A	851	BCR	C12-C13	-2.01	1.41	1.46
22	B	844	BCR	C20-C19	2.01	1.39	1.34
18	A	806	CLA	MG-NB	-2.01	2.01	2.05
18	1	611	CLA	CMB-C2B	-2.01	1.46	1.50
18	1	605	CLA	MG-NB	-2.01	2.01	2.05
18	B	823	CLA	CMB-C2B	-2.01	1.46	1.50
18	G	201	CLA	CMB-C2B	-2.01	1.46	1.50
18	1	602	CLA	MG-NB	-2.01	2.01	2.05
18	A	816	CLA	CMB-C2B	-2.01	1.46	1.50
18	4	610	CLA	CMD-C2D	-2.01	1.46	1.50
18	B	835	CLA	MG-NB	-2.01	2.01	2.05
18	A	824	CLA	CMB-C2B	-2.01	1.46	1.50
18	A	814	CLA	CMC-C2C	-2.01	1.46	1.50
18	B	821	CLA	CMD-C2D	-2.01	1.46	1.50
18	4	614	CLA	CMB-C2B	-2.01	1.46	1.50
18	A	837	CLA	MG-NB	-2.01	2.01	2.05
18	1	605	CLA	CMC-C2C	-2.01	1.46	1.50
18	1	610	CLA	CMB-C2B	-2.01	1.46	1.50
18	4	610	CLA	CMC-C2C	-2.01	1.46	1.50
18	A	835	CLA	MG-NB	-2.01	2.01	2.05
18	B	803	CLA	MG-NB	-2.01	2.01	2.05
18	A	845	CLA	MG-NB	-2.01	2.01	2.05
18	F	302	CLA	CMC-C2C	-2.01	1.46	1.50
18	A	825	CLA	CMB-C2B	-2.01	1.46	1.50
18	B	813	CLA	CMC-C2C	-2.01	1.46	1.50
18	A	828	CLA	MG-NB	-2.01	2.01	2.05
18	A	826	CLA	CMD-C2D	-2.01	1.46	1.50
18	B	806	CLA	CMB-C2B	-2.01	1.46	1.50
18	3	607	CLA	CMB-C2B	-2.01	1.46	1.50
18	B	841	CLA	CMC-C2C	-2.01	1.46	1.50
18	1	609	CLA	CMB-C2B	-2.01	1.46	1.50
18	2	602	CLA	CMB-C2B	-2.01	1.46	1.50
18	2	610	CLA	CMB-C2B	-2.01	1.46	1.50
18	1	608	CLA	CMB-C2B	-2.01	1.46	1.50
18	A	804	CLA	CMB-C2B	-2.01	1.46	1.50
18	J	101	CLA	CMD-C2D	-2.01	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	G	202	CLA	MG-NB	-2.01	2.01	2.05
18	A	838	CLA	CMD-C2D	-2.01	1.46	1.50
18	4	611	CLA	CMB-C2B	-2.00	1.46	1.50
18	A	803	CLA	CMD-C2D	-2.00	1.46	1.50
18	A	802	CLA	CMC-C2C	-2.00	1.46	1.50
18	B	840	CLA	CMB-C2B	-2.00	1.46	1.50
18	3	610	CLA	CMB-C2B	-2.00	1.46	1.50
18	A	827	CLA	MG-NB	-2.00	2.01	2.05
18	A	833	CLA	MG-NB	-2.00	2.01	2.05
18	B	840	CLA	MG-NB	-2.00	2.01	2.05
18	1	602	CLA	CMC-C2C	-2.00	1.46	1.50
18	A	809	CLA	MG-NB	-2.00	2.01	2.05
18	2	603	CLA	CMB-C2B	-2.00	1.46	1.50
18	B	831	CLA	MG-NB	-2.00	2.01	2.05
18	K	201	CLA	CMB-C2B	-2.00	1.46	1.50
18	A	808	CLA	MG-NB	-2.00	2.01	2.05
18	1	612	CLA	MG-NB	-2.00	2.01	2.05
18	A	836	CLA	MG-NB	-2.00	2.01	2.05
18	2	609	CLA	CMC-C2C	-2.00	1.46	1.50
18	B	808	CLA	CMC-C2C	-2.00	1.46	1.50
18	4	613	CLA	MG-NB	-2.00	2.01	2.05
18	B	837	CLA	MG-NB	-2.00	2.01	2.05

All (1364) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	818	CLA	O2D-CGD-CBD	26.49	157.54	111.23
18	A	818	CLA	O2D-CGD-O1D	-25.34	74.53	123.85
18	A	818	CLA	O1D-CGD-CBD	-21.04	83.01	124.52
18	B	836	CLA	C5-C3-C4	-15.99	77.79	114.59
18	B	836	CLA	C4-C3-C2	-13.38	82.51	122.66
18	B	836	CLA	C5-C3-C2	12.55	160.30	122.66
24	A	801	CL0	C4D-CHA-C1A	-10.81	114.37	121.32
19	1	614	XAT	C38-C25-C26	-9.39	106.84	122.30
17	2	601	CHL	O2D-CGD-CBD	9.30	121.17	110.95
19	1	614	XAT	O4-C5-C4	9.21	122.12	113.49
17	2	615	CHL	O2D-CGD-CBD	8.28	120.05	110.95
17	2	606	CHL	O2D-CGD-CBD	8.25	120.01	110.95
17	2	605	CHL	O2D-CGD-CBD	8.02	119.76	110.95
19	1	614	XAT	C18-C5-C6	-7.87	109.34	122.30
17	2	607	CHL	O2D-CGD-CBD	7.87	119.59	110.95
22	B	843	BCR	C16-C15-C14	7.84	139.55	123.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	4	607	CHL	O2D-CGD-CBD	7.83	119.55	110.95
17	4	606	CHL	O2D-CGD-CBD	7.81	119.52	110.95
17	3	606	CHL	O2D-CGD-CBD	7.78	119.49	110.95
22	L	301	BCR	C16-C15-C14	7.43	138.73	123.52
22	L	301	BCR	C15-C16-C17	7.39	138.65	123.52
19	1	614	XAT	O24-C25-C24	7.24	120.27	113.49
18	1	609	CLA	C4A-NA-C1A	7.16	109.94	106.68
22	A	849	BCR	C15-C16-C17	7.07	137.98	123.52
18	2	611	CLA	C4A-NA-C1A	7.06	109.90	106.68
19	1	614	XAT	O24-C25-C38	7.05	122.93	115.05
21	2	616	LUT	C15-C35-C34	7.05	137.95	123.52
18	1	612	CLA	C4A-NA-C1A	7.00	109.87	106.68
18	4	614	CLA	C4A-NA-C1A	6.91	109.83	106.68
18	A	818	CLA	C4A-NA-C1A	6.91	109.83	106.68
18	A	830	CLA	C4A-NA-C1A	6.90	109.83	106.68
18	A	828	CLA	C4A-NA-C1A	6.89	109.82	106.68
18	A	819	CLA	C4A-NA-C1A	6.87	109.81	106.68
18	F	302	CLA	C4A-NA-C1A	6.85	109.81	106.68
18	A	813	CLA	C4A-NA-C1A	6.81	109.78	106.68
18	A	827	CLA	C4A-NA-C1A	6.80	109.78	106.68
21	3	613	LUT	C15-C35-C34	6.80	137.43	123.52
18	B	841	CLA	C4A-NA-C1A	6.79	109.78	106.68
18	1	604	CLA	C4A-NA-C1A	6.78	109.77	106.68
18	2	604	CLA	C4A-NA-C1A	6.78	109.77	106.68
18	A	843	CLA	C4A-NA-C1A	6.77	109.77	106.68
18	B	807	CLA	C4A-NA-C1A	6.77	109.77	106.68
18	B	804	CLA	C4A-NA-C1A	6.75	109.76	106.68
18	B	811	CLA	C4A-NA-C1A	6.73	109.75	106.68
18	B	840	CLA	C4A-NA-C1A	6.73	109.75	106.68
18	K	204	CLA	C4A-NA-C1A	6.73	109.75	106.68
18	B	826	CLA	C4A-NA-C1A	6.72	109.75	106.68
18	B	809	CLA	C4A-NA-C1A	6.72	109.74	106.68
18	3	605	CLA	C4A-NA-C1A	6.71	109.74	106.68
18	H	201	CLA	C4A-NA-C1A	6.71	109.74	106.68
18	A	831	CLA	C4A-NA-C1A	6.71	109.74	106.68
18	A	808	CLA	C4A-NA-C1A	6.70	109.74	106.68
18	B	808	CLA	C4A-NA-C1A	6.70	109.73	106.68
18	B	819	CLA	C4A-NA-C1A	6.70	109.73	106.68
18	G	202	CLA	C4A-NA-C1A	6.70	109.73	106.68
18	2	613	CLA	C4A-NA-C1A	6.69	109.73	106.68
18	A	812	CLA	C4A-NA-C1A	6.69	109.73	106.68
18	B	814	CLA	C4A-NA-C1A	6.69	109.73	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	817	CLA	C4A-NA-C1A	6.68	109.73	106.68
18	1	605	CLA	C4A-NA-C1A	6.68	109.72	106.68
18	4	602	CLA	C4A-NA-C1A	6.67	109.72	106.68
18	4	601	CLA	C4A-NA-C1A	6.67	109.72	106.68
18	A	839	CLA	C4A-NA-C1A	6.66	109.72	106.68
18	L	302	CLA	C4A-NA-C1A	6.66	109.72	106.68
18	2	608	CLA	C4A-NA-C1A	6.65	109.71	106.68
18	3	612	CLA	C4A-NA-C1A	6.65	109.71	106.68
18	4	613	CLA	C4A-NA-C1A	6.64	109.71	106.68
18	A	806	CLA	C4A-NA-C1A	6.64	109.71	106.68
18	B	818	CLA	C4A-NA-C1A	6.64	109.71	106.68
18	B	837	CLA	C4A-NA-C1A	6.64	109.71	106.68
18	B	815	CLA	C4A-NA-C1A	6.64	109.71	106.68
18	1	603	CLA	C4A-NA-C1A	6.63	109.71	106.68
18	A	826	CLA	C4A-NA-C1A	6.63	109.71	106.68
18	A	829	CLA	C4A-NA-C1A	6.63	109.71	106.68
18	4	612	CLA	C4A-NA-C1A	6.63	109.70	106.68
18	L	304	CLA	C4A-NA-C1A	6.63	109.70	106.68
18	3	601	CLA	C4A-NA-C1A	6.61	109.69	106.68
18	B	825	CLA	C4A-NA-C1A	6.61	109.69	106.68
18	1	611	CLA	C4A-NA-C1A	6.61	109.69	106.68
18	L	303	CLA	C4A-NA-C1A	6.60	109.69	106.68
18	G	203	CLA	C4A-NA-C1A	6.60	109.69	106.68
18	4	608	CLA	C4A-NA-C1A	6.60	109.69	106.68
18	B	813	CLA	C4A-NA-C1A	6.59	109.69	106.68
18	4	610	CLA	C4A-NA-C1A	6.59	109.69	106.68
18	B	827	CLA	C4A-NA-C1A	6.59	109.69	106.68
18	A	840	CLA	C4A-NA-C1A	6.59	109.68	106.68
18	3	609	CLA	C4A-NA-C1A	6.58	109.68	106.68
18	B	831	CLA	C4A-NA-C1A	6.58	109.68	106.68
18	J	101	CLA	C4A-NA-C1A	6.58	109.68	106.68
18	B	816	CLA	C4A-NA-C1A	6.58	109.68	106.68
18	1	607	CLA	C4A-NA-C1A	6.57	109.68	106.68
18	A	804	CLA	C4A-NA-C1A	6.56	109.67	106.68
18	A	842	CLA	C4A-NA-C1A	6.56	109.67	106.68
18	B	806	CLA	C4A-NA-C1A	6.56	109.67	106.68
18	A	805	CLA	C4A-NA-C1A	6.56	109.67	106.68
18	A	825	CLA	C4A-NA-C1A	6.55	109.67	106.68
18	4	603	CLA	C4A-NA-C1A	6.55	109.67	106.68
18	A	816	CLA	C4A-NA-C1A	6.55	109.67	106.68
22	A	851	BCR	C16-C15-C14	6.54	136.91	123.52
18	A	841	CLA	C4A-NA-C1A	6.54	109.66	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	B	834	CLA	C4A-NA-C1A	6.54	109.66	106.68
18	A	838	CLA	C4A-NA-C1A	6.54	109.66	106.68
18	A	833	CLA	C4A-NA-C1A	6.53	109.66	106.68
18	B	820	CLA	C4A-NA-C1A	6.53	109.66	106.68
18	A	845	CLA	C4A-NA-C1A	6.53	109.66	106.68
18	B	830	CLA	C4A-NA-C1A	6.53	109.66	106.68
18	B	829	CLA	C4A-NA-C1A	6.53	109.66	106.68
18	A	802	CLA	C4A-NA-C1A	6.52	109.66	106.68
18	A	832	CLA	C4A-NA-C1A	6.52	109.65	106.68
18	1	610	CLA	C4A-NA-C1A	6.50	109.65	106.68
18	B	824	CLA	C4A-NA-C1A	6.50	109.65	106.68
18	K	201	CLA	C4A-NA-C1A	6.50	109.64	106.68
18	A	836	CLA	C4A-NA-C1A	6.50	109.64	106.68
22	A	850	BCR	C15-C16-C17	6.50	136.81	123.52
18	3	608	CLA	C4A-NA-C1A	6.50	109.64	106.68
18	B	839	CLA	C4A-NA-C1A	6.49	109.64	106.68
18	2	609	CLA	C4A-NA-C1A	6.49	109.64	106.68
18	A	820	CLA	C4A-NA-C1A	6.48	109.64	106.68
18	B	823	CLA	C4A-NA-C1A	6.48	109.64	106.68
18	2	612	CLA	C4A-NA-C1A	6.48	109.63	106.68
18	B	803	CLA	C4A-NA-C1A	6.47	109.63	106.68
18	A	809	CLA	C4A-NA-C1A	6.47	109.63	106.68
18	B	817	CLA	C4A-NA-C1A	6.47	109.63	106.68
18	F	303	CLA	C4A-NA-C1A	6.47	109.63	106.68
18	B	821	CLA	C4A-NA-C1A	6.47	109.63	106.68
18	G	201	CLA	C4A-NA-C1A	6.47	109.63	106.68
18	B	838	CLA	C4A-NA-C1A	6.46	109.63	106.68
18	3	611	CLA	C4A-NA-C1A	6.46	109.63	106.68
18	2	603	CLA	C4A-NA-C1A	6.45	109.62	106.68
18	B	805	CLA	C4A-NA-C1A	6.45	109.62	106.68
18	4	604	CLA	C4A-NA-C1A	6.44	109.62	106.68
18	A	811	CLA	C4A-NA-C1A	6.44	109.62	106.68
18	3	610	CLA	C4A-NA-C1A	6.42	109.61	106.68
18	B	835	CLA	C4A-NA-C1A	6.42	109.61	106.68
18	B	812	CLA	C4A-NA-C1A	6.42	109.61	106.68
22	A	851	BCR	C8-C9-C10	6.42	129.11	119.01
18	1	602	CLA	C4A-NA-C1A	6.42	109.61	106.68
18	3	607	CLA	C4A-NA-C1A	6.42	109.61	106.68
18	A	834	CLA	C4A-NA-C1A	6.42	109.61	106.68
18	4	611	CLA	C4A-NA-C1A	6.41	109.60	106.68
18	A	823	CLA	C4A-NA-C1A	6.41	109.60	106.68
18	B	802	CLA	C4A-NA-C1A	6.40	109.60	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	824	CLA	C4A-NA-C1A	6.40	109.60	106.68
18	1	613	CLA	C4A-NA-C1A	6.39	109.60	106.68
18	A	821	CLA	C4A-NA-C1A	6.38	109.59	106.68
18	A	815	CLA	C4A-NA-C1A	6.36	109.58	106.68
18	A	835	CLA	C4A-NA-C1A	6.35	109.57	106.68
18	A	837	CLA	C4A-NA-C1A	6.35	109.57	106.68
18	B	833	CLA	C4A-NA-C1A	6.35	109.57	106.68
18	A	822	CLA	C4A-NA-C1A	6.34	109.57	106.68
18	B	810	CLA	C4A-NA-C1A	6.33	109.57	106.68
18	B	832	CLA	C4A-NA-C1A	6.33	109.57	106.68
18	3	602	CLA	C4A-NA-C1A	6.33	109.56	106.68
18	3	604	CLA	C4A-NA-C1A	6.32	109.56	106.68
18	F	301	CLA	C4A-NA-C1A	6.32	109.56	106.68
22	A	850	BCR	C16-C15-C14	6.30	136.41	123.52
18	B	828	CLA	C4A-NA-C1A	6.30	109.55	106.68
18	1	608	CLA	C4A-NA-C1A	6.29	109.55	106.68
18	3	603	CLA	C4A-NA-C1A	6.29	109.55	106.68
18	K	203	CLA	C4A-NA-C1A	6.29	109.55	106.68
18	2	602	CLA	C4A-NA-C1A	6.28	109.55	106.68
18	K	206	CLA	C4A-NA-C1A	6.28	109.54	106.68
18	A	810	CLA	C4A-NA-C1A	6.24	109.53	106.68
18	B	822	CLA	C4A-NA-C1A	6.20	109.51	106.68
18	A	807	CLA	C4A-NA-C1A	6.15	109.49	106.68
18	B	836	CLA	C4A-NA-C1A	6.13	109.47	106.68
17	4	607	CHL	C1B-CHB-C4A	6.13	125.26	121.32
18	A	814	CLA	C4A-NA-C1A	6.05	109.44	106.68
18	4	609	CLA	C4A-NA-C1A	6.05	109.44	106.68
19	2	617	XAT	C15-C35-C34	6.04	135.88	123.52
21	2	619	LUT	C15-C35-C34	5.83	135.44	123.52
19	2	617	XAT	C35-C15-C14	5.82	135.43	123.52
22	K	205	BCR	C15-C16-C17	5.77	135.32	123.52
18	A	803	CLA	C4A-NA-C1A	5.69	109.27	106.68
17	4	615	CHL	CHA-C1A-C2A	-5.67	119.99	133.31
17	4	605	CHL	CHA-C1A-C2A	-5.67	119.99	133.31
17	4	607	CHL	CHA-C1A-C2A	-5.66	120.03	133.31
17	4	615	CHL	C1B-CHB-C4A	5.61	124.93	121.32
18	A	844	CLA	C4A-NA-C1A	5.59	109.23	106.68
22	F	304	BCR	C24-C23-C22	5.55	134.45	126.23
22	F	304	BCR	C15-C16-C17	5.52	134.82	123.52
17	4	606	CHL	CHA-C1A-C2A	-5.47	120.46	133.31
17	3	606	CHL	CHA-C1A-C2A	-5.43	120.57	133.31
22	B	849	BCR	C30-C25-C26	-5.39	115.27	122.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	2	606	CHL	CHA-C1A-C2A	-5.39	120.66	133.31
17	2	607	CHL	CHA-C1A-C2A	-5.35	120.75	133.31
22	A	851	BCR	C23-C22-C21	5.32	127.38	119.01
17	2	601	CHL	CHA-C1A-C2A	-5.32	120.82	133.31
17	1	601	CHL	CHA-C1A-C2A	-5.26	120.95	133.31
22	B	846	BCR	C16-C15-C14	5.25	134.27	123.52
19	1	614	XAT	O4-C5-C18	5.22	120.89	115.05
21	1	616	LUT	C30-C31-C32	5.20	138.26	123.20
21	1	616	LUT	C27-C28-C29	5.13	137.37	126.32
22	K	202	BCR	C16-C15-C14	5.07	133.90	123.52
22	A	851	BCR	C7-C8-C9	-5.05	118.76	126.23
21	1	616	LUT	C15-C35-C34	5.01	133.76	123.52
22	J	102	BCR	C16-C15-C14	4.88	133.50	123.52
17	2	615	CHL	CHA-C1A-C2A	-4.81	122.01	133.31
19	1	614	XAT	C35-C34-C33	-4.81	120.54	127.28
21	2	616	LUT	C7-C8-C9	4.78	133.30	126.23
22	B	847	BCR	C16-C15-C14	4.76	133.25	123.52
17	2	605	CHL	CHA-C1A-C2A	-4.73	122.21	133.31
22	B	845	BCR	C19-C18-C17	4.71	126.42	119.01
17	4	605	CHL	C1B-CHB-C4A	4.71	124.35	121.32
22	F	304	BCR	C21-C20-C19	4.56	136.42	123.20
22	F	304	BCR	C16-C15-C14	4.53	132.79	123.52
22	A	851	BCR	C11-C10-C9	4.52	133.62	127.28
22	A	851	BCR	C34-C9-C10	-4.45	115.61	122.82
22	A	853	BCR	C16-C15-C14	4.44	132.61	123.52
22	L	306	BCR	C16-C15-C14	4.43	132.58	123.52
22	K	202	BCR	C15-C16-C17	4.42	132.56	123.52
17	3	606	CHL	C1B-CHB-C4A	4.40	124.16	121.32
22	G	204	BCR	C15-C16-C17	4.39	132.50	123.52
22	A	848	BCR	C15-C16-C17	4.37	132.46	123.52
22	4	618	BCR	C30-C25-C26	-4.34	116.71	122.64
21	1	616	LUT	C39-C29-C28	4.28	124.62	118.09
22	B	801	BCR	C16-C15-C14	4.28	132.27	123.52
17	4	606	CHL	C1B-CHB-C4A	4.26	124.07	121.32
21	1	616	LUT	C31-C30-C29	4.25	133.25	127.28
22	K	205	BCR	C19-C18-C17	4.25	125.70	119.01
22	A	852	BCR	C16-C15-C14	4.22	132.16	123.52
22	B	844	BCR	C21-C20-C19	4.21	135.41	123.20
22	B	848	BCR	C15-C16-C17	4.21	132.13	123.52
22	B	849	BCR	C16-C15-C14	4.21	132.13	123.52
22	B	844	BCR	C16-C15-C14	4.14	132.00	123.52
18	4	613	CLA	CAA-C2A-C3A	-4.14	101.81	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	852	BCR	C10-C11-C12	4.13	135.18	123.20
22	A	851	BCR	C37-C22-C21	-4.12	116.14	122.82
22	L	301	BCR	C12-C13-C14	4.12	125.49	119.01
22	A	851	BCR	C15-C16-C17	4.11	131.94	123.52
17	2	607	CHL	C1B-CHB-C4A	4.11	123.97	121.32
27	B	850	DGD	O2G-C1B-C2B	4.08	120.32	111.48
22	L	306	BCR	C8-C9-C10	4.07	125.41	119.01
22	A	849	BCR	C30-C25-C26	-4.06	117.09	122.64
22	A	849	BCR	C21-C20-C19	4.05	134.94	123.20
18	B	821	CLA	CAA-C2A-C3A	-4.03	102.11	113.00
22	L	301	BCR	C21-C20-C19	4.03	134.87	123.20
22	A	851	BCR	C12-C13-C14	3.97	125.26	119.01
22	B	845	BCR	C1-C6-C5	-3.97	117.21	122.64
21	1	616	LUT	C32-C33-C34	3.96	125.24	119.01
22	L	305	BCR	C16-C15-C14	3.96	131.62	123.52
22	I	101	BCR	C15-C16-C17	3.95	131.61	123.52
22	B	801	BCR	C10-C11-C12	3.95	134.64	123.20
22	3	614	BCR	C16-C15-C14	3.95	131.59	123.52
21	2	616	LUT	C19-C9-C10	-3.93	116.44	122.82
21	2	619	LUT	C8-C9-C10	3.91	125.16	119.01
22	F	304	BCR	C20-C21-C22	3.91	132.76	127.28
21	2	616	LUT	C39-C29-C30	-3.91	116.48	122.82
22	F	304	BCR	C12-C13-C14	3.91	125.16	119.01
22	4	618	BCR	C16-C15-C14	3.90	131.51	123.52
22	L	306	BCR	C34-C9-C10	-3.90	116.49	122.82
21	2	616	LUT	C28-C29-C30	3.90	125.14	119.01
22	K	205	BCR	C10-C11-C12	3.88	134.46	123.20
22	K	202	BCR	C12-C13-C14	3.87	125.10	119.01
22	A	853	BCR	C10-C11-C12	3.87	134.41	123.20
20	1	615	LHG	O7-C7-C8	3.87	119.85	111.48
24	A	801	CL0	C1-C2-C3	-3.83	119.92	126.20
21	3	613	LUT	C39-C29-C30	-3.82	116.62	122.82
19	4	617	XAT	C15-C35-C34	3.82	131.33	123.52
22	B	843	BCR	C34-C9-C10	-3.81	116.64	122.82
21	2	619	LUT	C19-C9-C10	-3.81	116.64	122.82
22	B	845	BCR	C20-C21-C22	3.81	132.62	127.28
22	B	843	BCR	C8-C9-C10	3.80	124.99	119.01
22	B	844	BCR	C15-C16-C17	3.79	131.28	123.52
21	3	613	LUT	C28-C29-C30	3.75	124.91	119.01
22	B	845	BCR	C36-C18-C17	-3.75	116.75	122.82
22	L	306	BCR	C37-C22-C21	-3.74	116.76	122.82
22	L	305	BCR	C15-C16-C17	3.73	131.14	123.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	K	202	BCR	C34-C9-C10	-3.72	116.80	122.82
22	K	202	BCR	C37-C22-C21	-3.71	116.80	122.82
22	B	844	BCR	C37-C22-C21	-3.71	116.80	122.82
22	K	205	BCR	C37-C22-C21	-3.69	116.83	122.82
19	2	617	XAT	C28-C29-C30	3.68	124.80	119.01
22	A	852	BCR	C37-C22-C21	-3.67	116.87	122.82
21	2	619	LUT	C32-C33-C34	3.67	124.78	119.01
19	2	617	XAT	C39-C29-C30	-3.66	116.88	122.82
19	4	617	XAT	C19-C9-C10	-3.66	116.89	122.82
22	J	102	BCR	C34-C9-C10	-3.66	116.89	122.82
22	B	846	BCR	C34-C9-C10	-3.65	116.90	122.82
22	B	845	BCR	C21-C20-C19	3.65	133.76	123.20
22	A	850	BCR	C34-C9-C10	-3.64	116.92	122.82
22	F	304	BCR	C34-C9-C10	-3.62	116.95	122.82
22	B	801	BCR	C8-C9-C10	3.61	124.69	119.01
22	L	306	BCR	C23-C22-C21	3.61	124.69	119.01
22	L	306	BCR	C12-C13-C14	3.60	124.68	119.01
21	2	619	LUT	C39-C29-C30	-3.60	116.98	122.82
22	L	305	BCR	C37-C22-C21	-3.60	116.98	122.82
19	2	617	XAT	C19-C9-C10	-3.60	116.98	122.82
21	1	616	LUT	C19-C9-C10	-3.60	116.98	122.82
22	L	301	BCR	C37-C22-C21	-3.60	116.98	122.82
18	A	804	CLA	CAA-C2A-C3A	-3.60	103.28	113.00
22	A	852	BCR	C19-C18-C17	3.60	124.67	119.01
18	B	813	CLA	O2D-CGD-O1D	-3.58	116.88	123.85
22	K	205	BCR	C34-C9-C10	-3.57	117.03	122.82
22	K	205	BCR	C36-C18-C17	-3.57	117.03	122.82
22	A	853	BCR	C11-C10-C9	3.57	132.28	127.28
17	1	601	CHL	C1-C2-C3	-3.55	120.38	126.20
21	4	616	LUT	C15-C35-C34	3.55	130.78	123.52
22	B	846	BCR	C12-C13-C14	3.55	124.59	119.01
22	B	844	BCR	C34-C9-C10	-3.54	117.09	122.82
22	G	204	BCR	C37-C22-C21	-3.53	117.09	122.82
21	1	616	LUT	C26-C27-C28	3.53	130.07	124.58
22	A	852	BCR	C23-C22-C21	3.53	124.56	119.01
22	J	102	BCR	C8-C9-C10	3.52	124.54	119.01
18	A	804	CLA	O2D-CGD-O1D	-3.52	117.00	123.85
22	L	306	BCR	C15-C16-C17	3.51	130.71	123.52
22	L	301	BCR	C36-C18-C17	-3.50	117.14	122.82
22	B	849	BCR	C37-C22-C21	-3.50	117.15	122.82
22	B	801	BCR	C37-C22-C21	-3.50	117.15	122.82
18	1	612	CLA	O2D-CGD-O1D	-3.49	117.05	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	848	BCR	C37-C22-C21	-3.49	117.16	122.82
22	3	614	BCR	C34-C9-C10	-3.48	117.17	122.82
22	J	102	BCR	C12-C13-C14	3.48	124.48	119.01
22	B	845	BCR	C34-C9-C10	-3.47	117.19	122.82
22	F	304	BCR	C10-C11-C12	3.46	133.23	123.20
18	A	813	CLA	O2D-CGD-O1D	-3.46	117.11	123.85
22	J	102	BCR	C37-C22-C21	-3.45	117.22	122.82
22	A	853	BCR	C37-C22-C21	-3.45	117.22	122.82
22	L	305	BCR	C34-C9-C10	-3.44	117.24	122.82
22	L	301	BCR	C34-C9-C10	-3.44	117.25	122.82
22	K	202	BCR	C8-C9-C10	3.44	124.41	119.01
22	L	301	BCR	C35-C13-C14	-3.44	117.25	122.82
19	4	617	XAT	C35-C15-C14	3.43	130.54	123.52
19	4	617	XAT	C39-C29-C30	-3.42	117.28	122.82
22	B	847	BCR	C34-C9-C10	-3.42	117.28	122.82
22	B	844	BCR	C23-C22-C21	3.42	124.39	119.01
22	A	849	BCR	C1-C6-C5	-3.41	117.97	122.64
17	2	606	CHL	C1B-CHB-C4A	3.41	123.52	121.32
22	A	848	BCR	C34-C9-C10	-3.40	117.30	122.82
21	1	616	LUT	C40-C33-C34	-3.40	117.30	122.82
24	A	801	CL0	C2C-C1C-NC	3.40	120.08	110.46
18	A	814	CLA	C3B-C4B-NB	-3.39	107.50	110.53
22	F	304	BCR	C1-C6-C5	-3.39	118.00	122.64
22	4	618	BCR	C34-C9-C10	-3.38	117.34	122.82
22	A	849	BCR	C34-C9-C10	-3.38	117.34	122.82
22	B	848	BCR	C37-C22-C21	-3.38	117.34	122.82
22	4	618	BCR	C37-C22-C21	-3.38	117.34	122.82
22	B	846	BCR	C37-C22-C21	-3.38	117.35	122.82
22	K	202	BCR	C35-C13-C14	-3.38	117.35	122.82
22	A	852	BCR	C34-C9-C10	-3.37	117.35	122.82
18	4	614	CLA	O2D-CGD-O1D	-3.36	117.30	123.85
18	A	803	CLA	C3B-C4B-NB	-3.36	107.53	110.53
22	A	849	BCR	C20-C21-C22	3.36	131.99	127.28
22	A	852	BCR	C15-C16-C17	3.35	130.38	123.52
22	4	618	BCR	C15-C16-C17	3.35	130.37	123.52
18	3	605	CLA	O2D-CGD-O1D	-3.34	117.34	123.85
22	K	205	BCR	C21-C20-C19	3.33	132.85	123.20
22	B	848	BCR	C34-C9-C10	-3.33	117.42	122.82
18	A	844	CLA	C3B-C4B-NB	-3.33	107.56	110.53
22	B	847	BCR	C37-C22-C21	-3.32	117.43	122.82
22	3	614	BCR	C37-C22-C21	-3.32	117.44	122.82
22	F	304	BCR	C35-C13-C14	-3.32	117.44	122.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	I	101	BCR	C37-C22-C21	-3.32	117.44	122.82
22	K	202	BCR	C19-C18-C17	3.32	124.22	119.01
22	K	205	BCR	C23-C22-C21	3.31	124.21	119.01
22	B	849	BCR	C15-C16-C17	3.30	130.28	123.52
18	A	810	CLA	CAA-C2A-C3A	-3.30	104.08	113.00
21	2	616	LUT	C35-C34-C33	3.30	131.91	127.28
22	B	843	BCR	C37-C22-C21	-3.29	117.49	122.82
22	G	204	BCR	C34-C9-C10	-3.29	117.49	122.82
22	A	850	BCR	C37-C22-C21	-3.28	117.49	122.82
22	I	101	BCR	C34-C9-C10	-3.28	117.50	122.82
18	B	822	CLA	CAA-C2A-C3A	-3.28	104.13	113.00
22	A	853	BCR	C12-C13-C14	3.28	124.16	119.01
22	B	849	BCR	C34-C9-C10	-3.27	117.52	122.82
22	B	843	BCR	C15-C14-C13	3.27	131.86	127.28
21	2	619	LUT	C40-C33-C34	-3.26	117.54	122.82
17	2	607	CHL	C1-C2-C3	-3.24	121.52	126.76
18	B	808	CLA	C3B-C4B-NB	-3.24	107.64	110.53
18	L	303	CLA	O2D-CGD-O1D	-3.24	117.55	123.85
21	4	616	LUT	C19-C9-C10	-3.24	117.57	122.82
18	A	835	CLA	O2D-CGD-O1D	-3.24	117.55	123.85
21	1	616	LUT	C35-C15-C14	3.23	130.13	123.52
22	A	850	BCR	C16-C17-C18	3.23	131.81	127.28
22	K	202	BCR	C23-C22-C21	3.22	124.07	119.01
21	4	616	LUT	C39-C29-C30	-3.22	117.61	122.82
18	B	832	CLA	C3B-C4B-NB	-3.21	107.66	110.53
18	F	301	CLA	C3B-C4B-NB	-3.21	107.66	110.53
18	B	828	CLA	C3B-C4B-NB	-3.21	107.67	110.53
18	4	609	CLA	C3B-C4B-NB	-3.20	107.67	110.53
22	L	306	BCR	C35-C13-C14	-3.19	117.64	122.82
24	A	801	CL0	O2A-CGA-CBA	3.19	121.57	111.83
21	2	616	LUT	C30-C31-C32	3.19	132.45	123.20
22	B	849	BCR	C12-C13-C14	3.19	124.02	119.01
17	1	601	CHL	C1B-CHB-C4A	3.18	123.37	121.32
19	2	617	XAT	C30-C31-C32	3.18	132.42	123.20
18	B	825	CLA	O2D-CGD-O1D	-3.18	117.66	123.85
22	L	306	BCR	C10-C11-C12	3.17	132.40	123.20
17	2	605	CHL	C4C-C3C-C2C	-3.17	101.11	108.42
22	B	846	BCR	C35-C13-C14	-3.17	117.68	122.82
22	B	801	BCR	C7-C8-C9	-3.17	121.55	126.23
18	B	827	CLA	O2D-CGD-O1D	-3.16	117.69	123.85
22	B	847	BCR	C12-C13-C14	3.16	123.98	119.01
22	B	801	BCR	C11-C10-C9	3.16	131.71	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	852	BCR	C35-C13-C14	-3.16	117.69	122.82
22	A	850	BCR	C15-C14-C13	3.16	131.71	127.28
22	3	614	BCR	C15-C16-C17	3.16	129.98	123.52
22	B	844	BCR	C12-C13-C14	3.16	123.97	119.01
21	1	616	LUT	C12-C13-C14	3.15	123.97	119.01
18	B	812	CLA	C3B-C4B-NB	-3.15	107.72	110.53
19	2	617	XAT	C32-C33-C34	3.15	123.97	119.01
18	B	814	CLA	O2D-CGD-O1D	-3.14	117.73	123.85
22	G	204	BCR	C19-C18-C17	3.14	123.95	119.01
18	A	838	CLA	C3B-C4B-NB	-3.14	107.73	110.53
22	L	306	BCR	C19-C18-C17	3.14	123.95	119.01
18	B	837	CLA	O2D-CGD-O1D	-3.14	117.74	123.85
22	L	305	BCR	C19-C18-C17	3.14	123.94	119.01
17	4	606	CHL	C4C-C3C-C2C	-3.13	101.00	113.37
22	J	102	BCR	C35-C13-C14	-3.13	117.74	122.82
22	L	301	BCR	C19-C18-C17	3.13	123.93	119.01
22	A	851	BCR	C20-C21-C22	3.13	131.67	127.28
18	B	822	CLA	O2D-CGD-O1D	-3.13	117.76	123.85
22	L	305	BCR	C12-C13-C14	3.13	123.93	119.01
22	A	848	BCR	C19-C18-C17	3.13	123.92	119.01
18	3	608	CLA	CAA-C2A-C3A	-3.12	109.09	116.23
18	3	607	CLA	C3B-C4B-NB	-3.11	107.75	110.53
18	1	608	CLA	CAA-C2A-C3A	-3.11	109.11	116.23
18	B	804	CLA	O2D-CGD-O1D	-3.10	117.81	123.85
18	B	836	CLA	C3B-C4B-NB	-3.10	107.76	110.53
18	B	805	CLA	C3B-C4B-NB	-3.10	107.76	110.53
22	A	852	BCR	C36-C18-C17	-3.10	117.80	122.82
18	A	810	CLA	C3B-C4B-NB	-3.10	107.77	110.53
17	4	605	CHL	C4C-C3C-C2C	-3.09	101.30	108.42
22	A	849	BCR	C16-C17-C18	3.09	131.62	127.28
18	4	601	CLA	O2D-CGD-O1D	-3.09	117.84	123.85
22	B	846	BCR	C8-C9-C10	3.09	123.86	119.01
17	3	606	CHL	CBC-CAC-C3C	-3.09	108.45	112.87
18	2	602	CLA	C3B-C4B-NB	-3.09	107.78	110.53
22	B	801	BCR	C12-C13-C14	3.08	123.85	119.01
18	B	819	CLA	O2D-CGD-O1D	-3.08	117.86	123.85
22	B	844	BCR	C36-C18-C17	-3.08	117.83	122.82
24	A	801	CL0	CMB-C2B-C3B	3.07	130.82	124.68
18	B	805	CLA	O2D-CGD-O1D	-3.06	117.89	123.85
18	A	809	CLA	O2D-CGD-O1D	-3.06	117.89	123.85
18	B	826	CLA	O2D-CGD-O1D	-3.06	117.89	123.85
22	A	852	BCR	C1-C6-C5	-3.06	118.46	122.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	840	CLA	O2D-CGD-O1D	-3.05	117.92	123.85
22	B	801	BCR	C15-C16-C17	3.05	129.75	123.52
18	B	841	CLA	O2D-CGD-O1D	-3.04	117.92	123.85
18	L	302	CLA	C3B-C4B-NB	-3.04	107.81	110.53
18	A	810	CLA	O2D-CGD-O1D	-3.04	117.94	123.85
18	B	818	CLA	O2D-CGD-O1D	-3.04	117.94	123.85
18	B	833	CLA	O2D-CGD-O1D	-3.04	117.94	123.85
18	4	601	CLA	C3B-C4B-NB	-3.03	107.82	110.53
18	A	807	CLA	C3B-C4B-NB	-3.03	107.83	110.53
18	2	604	CLA	C3B-C4B-NB	-3.02	107.83	110.53
22	A	853	BCR	C35-C13-C14	-3.02	117.92	122.82
18	A	802	CLA	CHB-C4A-NA	3.02	128.76	124.40
18	4	611	CLA	C3B-C4B-NB	-3.02	107.84	110.53
18	A	808	CLA	C3B-C4B-NB	-3.02	107.84	110.53
18	B	802	CLA	C3B-C4B-NB	-3.02	107.84	110.53
18	G	201	CLA	O2D-CGD-O1D	-3.01	117.98	123.85
18	3	604	CLA	C3B-C4B-NB	-3.01	107.84	110.53
18	4	610	CLA	C3B-C4B-NB	-3.00	107.85	110.53
18	H	201	CLA	O2D-CGD-O1D	-3.00	118.01	123.85
19	1	614	XAT	C15-C14-C13	-3.00	123.08	127.28
21	4	616	LUT	C35-C15-C14	3.00	129.65	123.52
18	A	840	CLA	C3B-C4B-NB	-3.00	107.86	110.53
18	B	807	CLA	O2D-CGD-O1D	-2.99	118.02	123.85
18	A	837	CLA	C3B-C4B-NB	-2.99	107.86	110.53
18	B	810	CLA	C3B-C4B-NB	-2.99	107.86	110.53
18	K	204	CLA	O2D-CGD-O1D	-2.99	118.03	123.85
18	B	832	CLA	O2D-CGD-O1D	-2.99	118.03	123.85
22	K	202	BCR	C36-C18-C17	-2.99	117.97	122.82
18	A	802	CLA	C3B-C4B-NB	-2.99	107.86	110.53
18	3	611	CLA	C3B-C4B-NB	-2.99	107.86	110.53
18	A	812	CLA	C3B-C4B-NB	-2.99	107.86	110.53
18	B	822	CLA	C1-C2-C3	-2.99	121.30	126.20
22	G	204	BCR	C36-C18-C17	-2.99	117.98	122.82
18	2	610	CLA	O2D-CGD-O1D	-2.99	118.03	123.85
18	B	838	CLA	O2D-CGD-O1D	-2.99	118.03	123.85
22	A	853	BCR	C15-C16-C17	2.99	129.63	123.52
18	B	817	CLA	C3B-C4B-NB	-2.99	107.86	110.53
18	A	826	CLA	O2D-CGD-O1D	-2.98	118.04	123.85
18	F	303	CLA	O2D-CGD-O1D	-2.98	118.04	123.85
22	F	304	BCR	C8-C9-C10	2.98	123.70	119.01
18	3	602	CLA	C3B-C4B-NB	-2.98	107.87	110.53
17	1	601	CHL	O2A-CGA-CBA	2.98	120.93	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	B	815	CLA	O2D-CGD-O1D	-2.98	118.04	123.85
18	3	608	CLA	CMA-C3A-C2A	-2.98	109.39	116.23
17	3	606	CHL	C4C-C3C-C2C	-2.98	101.60	113.37
18	B	803	CLA	CHB-C4A-NA	2.98	128.70	124.40
18	K	203	CLA	O2D-CGD-O1D	-2.98	118.05	123.85
18	A	810	CLA	C1-C2-C3	-2.98	121.94	126.76
18	1	609	CLA	C3B-C4B-NB	-2.98	107.87	110.53
18	A	835	CLA	C3B-C4B-NB	-2.98	107.87	110.53
22	B	844	BCR	C35-C13-C14	-2.98	117.99	122.82
18	A	825	CLA	C3B-C4B-NB	-2.98	107.87	110.53
18	A	834	CLA	O2D-CGD-O1D	-2.97	118.06	123.85
18	B	820	CLA	O2D-CGD-O1D	-2.97	118.06	123.85
18	A	813	CLA	C3B-C4B-NB	-2.97	107.88	110.53
18	A	815	CLA	O2D-CGD-O1D	-2.97	118.06	123.85
18	B	823	CLA	O2D-CGD-O1D	-2.97	118.06	123.85
18	A	819	CLA	C3B-C4B-NB	-2.97	107.88	110.53
18	A	844	CLA	O2D-CGD-O1D	-2.97	118.07	123.85
18	B	811	CLA	O2D-CGD-O1D	-2.97	118.07	123.85
18	4	613	CLA	O2D-CGD-O1D	-2.97	118.07	123.85
19	1	614	XAT	C27-C28-C29	-2.97	120.92	125.53
17	2	607	CHL	O2A-CGA-CBA	2.97	120.88	111.83
22	L	305	BCR	C36-C18-C17	-2.97	118.01	122.82
18	2	612	CLA	O2D-CGD-O1D	-2.97	118.07	123.85
18	A	830	CLA	CHB-C4A-NA	2.96	128.68	124.40
18	4	612	CLA	O2D-CGD-O1D	-2.96	118.08	123.85
22	L	306	BCR	C36-C18-C17	-2.96	118.02	122.82
18	J	101	CLA	C3B-C4B-NB	-2.96	107.89	110.53
24	A	801	CL0	C4C-C3C-C2C	-2.96	101.67	113.37
22	B	847	BCR	C35-C13-C14	-2.96	118.02	122.82
18	A	836	CLA	C3B-C4B-NB	-2.96	107.89	110.53
18	1	604	CLA	C3B-C4B-NB	-2.96	107.89	110.53
18	B	823	CLA	C3B-C4B-NB	-2.96	107.89	110.53
18	A	824	CLA	C3B-C4B-NB	-2.96	107.89	110.53
22	A	848	BCR	C36-C18-C17	-2.95	118.03	122.82
18	B	835	CLA	C3B-C4B-NB	-2.95	107.89	110.53
18	3	610	CLA	C3B-C4B-NB	-2.95	107.89	110.53
18	3	612	CLA	C3B-C4B-NB	-2.95	107.90	110.53
18	B	840	CLA	C3B-C4B-NB	-2.95	107.90	110.53
18	A	832	CLA	O2D-CGD-O1D	-2.95	118.11	123.85
18	A	821	CLA	O2D-CGD-O1D	-2.95	118.11	123.85
18	A	838	CLA	O2D-CGD-O1D	-2.95	118.11	123.85
18	A	833	CLA	O2D-CGD-O1D	-2.95	118.11	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	B	836	CLA	O2D-CGD-O1D	-2.95	118.11	123.85
17	2	601	CHL	O1D-CGD-CBD	-2.94	120.26	124.72
18	B	804	CLA	CAA-C2A-C3A	-2.94	109.48	116.23
22	B	845	BCR	C12-C13-C14	2.94	123.64	119.01
17	4	615	CHL	C1C-CHC-C4B	2.94	126.60	116.07
18	2	604	CLA	O2D-CGD-O1D	-2.94	118.12	123.85
18	B	827	CLA	C3B-C4B-NB	-2.94	107.91	110.53
22	A	850	BCR	C8-C9-C10	2.94	123.63	119.01
18	K	201	CLA	C3B-C4B-NB	-2.94	107.91	110.53
18	B	803	CLA	C3B-C4B-NB	-2.94	107.91	110.53
18	1	609	CLA	CHB-C4A-NA	2.94	128.64	124.40
18	A	820	CLA	O2D-CGD-O1D	-2.94	118.14	123.85
22	L	305	BCR	C35-C13-C14	-2.93	118.06	122.82
22	K	202	BCR	C10-C11-C12	2.93	131.70	123.20
18	L	302	CLA	O2D-CGD-O1D	-2.93	118.14	123.85
18	A	822	CLA	C3B-C4B-NB	-2.93	107.91	110.53
22	L	306	BCR	C7-C8-C9	2.93	130.57	126.23
22	B	801	BCR	C35-C13-C14	-2.93	118.07	122.82
19	4	617	XAT	C8-C9-C10	2.93	123.62	119.01
18	2	602	CLA	O2D-CGD-O1D	-2.93	118.15	123.85
17	4	605	CHL	C1C-CHC-C4B	2.93	126.54	116.07
18	A	823	CLA	O2D-CGD-O1D	-2.92	118.16	123.85
18	1	603	CLA	O2D-CGD-O1D	-2.92	118.16	123.85
18	B	824	CLA	C3B-C4B-NB	-2.92	107.92	110.53
18	1	611	CLA	O2D-CGD-O1D	-2.92	118.16	123.85
18	1	611	CLA	C3B-C4B-NB	-2.92	107.92	110.53
18	A	829	CLA	C3B-C4B-NB	-2.92	107.92	110.53
18	A	845	CLA	O2D-CGD-O1D	-2.92	118.16	123.85
18	3	601	CLA	O2D-CGD-O1D	-2.92	118.17	123.85
18	4	602	CLA	O2D-CGD-O1D	-2.92	118.17	123.85
21	1	616	LUT	C20-C13-C14	-2.92	118.09	122.82
18	1	607	CLA	C3B-C4B-NB	-2.92	107.93	110.53
18	B	834	CLA	C3B-C4B-NB	-2.92	107.93	110.53
18	A	842	CLA	O2D-CGD-O1D	-2.92	118.17	123.85
22	K	205	BCR	C35-C13-C14	-2.92	118.09	122.82
18	3	609	CLA	C3B-C4B-NB	-2.91	107.93	110.53
18	A	828	CLA	C3B-C4B-NB	-2.91	107.93	110.53
22	4	618	BCR	C12-C13-C14	2.91	123.59	119.01
18	1	604	CLA	O2D-CGD-O1D	-2.91	118.18	123.85
27	B	850	DGD	C2G-O2G-C1B	-2.91	110.83	117.80
18	B	813	CLA	O2D-CGD-CBD	2.91	116.32	111.23
22	B	849	BCR	C19-C18-C17	2.91	123.58	119.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	821	CLA	C3B-C4B-NB	-2.91	107.93	110.53
18	F	302	CLA	C3B-C4B-NB	-2.91	107.93	110.53
21	3	613	LUT	C35-C34-C33	2.91	131.36	127.28
18	B	840	CLA	O2D-CGD-O1D	-2.91	118.19	123.85
18	B	817	CLA	O2D-CGD-O1D	-2.91	118.19	123.85
22	B	849	BCR	C35-C13-C14	-2.91	118.11	122.82
18	A	827	CLA	O2D-CGD-O1D	-2.91	118.19	123.85
18	1	610	CLA	CAA-C2A-C3A	-2.90	109.58	116.23
18	B	830	CLA	O2D-CGD-O1D	-2.90	118.20	123.85
22	A	851	BCR	C24-C23-C22	-2.90	121.94	126.23
18	4	608	CLA	C3B-C4B-NB	-2.90	107.94	110.53
18	4	614	CLA	C3B-C4B-NB	-2.90	107.94	110.53
18	B	824	CLA	O2D-CGD-O1D	-2.90	118.21	123.85
18	2	610	CLA	CHA-C1A-NA	-2.90	123.49	126.67
18	A	834	CLA	C3B-C4B-NB	-2.90	107.94	110.53
18	F	303	CLA	C3B-C4B-NB	-2.90	107.94	110.53
18	B	816	CLA	O2D-CGD-O1D	-2.90	118.21	123.85
18	B	819	CLA	C3B-C4B-NB	-2.89	107.95	110.53
18	A	839	CLA	C3B-C4B-NB	-2.89	107.95	110.53
18	A	819	CLA	O2D-CGD-O1D	-2.89	118.22	123.85
18	A	837	CLA	O2D-CGD-O1D	-2.89	118.22	123.85
18	A	836	CLA	O2D-CGD-O1D	-2.89	118.22	123.85
18	B	839	CLA	C3B-C4B-NB	-2.89	107.95	110.53
18	K	204	CLA	C3B-C4B-NB	-2.88	107.95	110.53
18	F	303	CLA	CAA-C2A-C3A	-2.88	109.62	116.23
18	L	303	CLA	C3B-C4B-NB	-2.88	107.96	110.53
21	1	616	LUT	C39-C29-C30	-2.88	118.15	122.82
18	A	805	CLA	O2D-CGD-O1D	-2.88	118.24	123.85
18	1	602	CLA	O2D-CGD-O1D	-2.88	118.25	123.85
18	A	828	CLA	O2D-CGD-O1D	-2.88	118.25	123.85
18	B	810	CLA	O2D-CGD-O1D	-2.88	118.25	123.85
18	A	830	CLA	CAA-C2A-C3A	-2.88	105.23	113.00
17	2	615	CHL	C1C-CHC-C4B	2.88	126.36	116.07
24	A	801	CL0	CBC-CAC-C3C	-2.88	108.76	112.87
18	A	816	CLA	O2D-CGD-O1D	-2.87	118.25	123.85
18	A	806	CLA	O2D-CGD-O1D	-2.87	118.26	123.85
18	B	807	CLA	C3B-C4B-NB	-2.87	107.97	110.53
18	3	607	CLA	O2D-CGD-O1D	-2.87	118.26	123.85
21	3	613	LUT	C8-C9-C10	2.87	123.52	119.01
18	B	821	CLA	O2D-CGD-O1D	-2.87	118.27	123.85
18	B	802	CLA	O2D-CGD-O1D	-2.87	118.27	123.85
18	B	816	CLA	C3B-C4B-NB	-2.87	107.97	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	F	304	BCR	C37-C22-C23	2.87	122.47	118.09
18	A	839	CLA	O2D-CGD-O1D	-2.87	118.27	123.85
18	J	101	CLA	O2D-CGD-O1D	-2.87	118.27	123.85
18	2	613	CLA	C3B-C4B-NB	-2.87	107.97	110.53
18	A	816	CLA	C3B-C4B-NB	-2.87	107.97	110.53
22	B	844	BCR	C30-C25-C26	-2.86	118.72	122.64
21	3	613	LUT	C30-C31-C32	2.86	131.50	123.20
18	A	807	CLA	O2D-CGD-O1D	-2.86	118.27	123.85
18	A	811	CLA	O2D-CGD-O1D	-2.86	118.27	123.85
18	A	822	CLA	O2D-CGD-O1D	-2.86	118.27	123.85
18	A	831	CLA	O2D-CGD-O1D	-2.86	118.28	123.85
18	B	831	CLA	O2D-CGD-O1D	-2.86	118.28	123.85
21	2	619	LUT	C26-C27-C28	2.86	129.03	124.58
18	3	603	CLA	O2D-CGD-O1D	-2.86	118.28	123.85
18	B	838	CLA	C3B-C4B-NB	-2.86	107.98	110.53
22	A	852	BCR	C21-C20-C19	2.86	131.49	123.20
17	2	606	CHL	C1C-CHC-C4B	2.86	126.30	116.07
18	K	206	CLA	C3B-C4B-NB	-2.86	107.98	110.53
22	F	304	BCR	C19-C18-C17	2.86	123.50	119.01
18	B	834	CLA	O2D-CGD-O1D	-2.86	118.29	123.85
21	2	619	LUT	C28-C29-C30	2.86	123.50	119.01
22	B	848	BCR	C19-C18-C17	2.86	123.50	119.01
18	A	817	CLA	C3B-C4B-NB	-2.86	107.98	110.53
18	G	201	CLA	C3B-C4B-NB	-2.85	107.98	110.53
18	A	824	CLA	CAA-C2A-C3A	-2.85	109.69	116.23
18	1	602	CLA	C3B-C4B-NB	-2.85	107.99	110.53
18	B	808	CLA	O2D-CGD-O1D	-2.85	118.31	123.85
19	4	617	XAT	C12-C13-C14	2.85	123.48	119.01
18	B	812	CLA	O2D-CGD-O1D	-2.84	118.31	123.85
18	4	613	CLA	CHB-C4A-NA	2.84	128.50	124.40
18	G	202	CLA	C3B-C4B-NB	-2.84	107.99	110.53
18	4	608	CLA	O2D-CGD-O1D	-2.84	118.31	123.85
22	L	305	BCR	C23-C22-C21	2.84	123.48	119.01
22	A	848	BCR	C16-C15-C14	2.84	129.33	123.52
21	2	616	LUT	C19-C9-C8	2.84	122.43	118.09
18	2	613	CLA	O2D-CGD-O1D	-2.84	118.32	123.85
18	1	605	CLA	C3B-C4B-NB	-2.84	108.00	110.53
18	4	604	CLA	O2D-CGD-O1D	-2.84	118.32	123.85
18	G	203	CLA	O2D-CGD-O1D	-2.84	118.33	123.85
22	4	618	BCR	C35-C13-C14	-2.84	118.22	122.82
18	1	608	CLA	O2D-CGD-O1D	-2.84	118.33	123.85
18	G	202	CLA	O2D-CGD-O1D	-2.83	118.33	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	4	617	XAT	C20-C13-C14	-2.83	118.23	122.82
17	1	606	CHL	C1B-CHB-C4A	-2.83	119.50	121.32
18	A	814	CLA	O2D-CGD-O1D	-2.83	118.33	123.85
19	2	617	XAT	C12-C13-C14	2.83	123.46	119.01
18	B	803	CLA	O2D-CGD-O1D	-2.83	118.34	123.85
18	B	828	CLA	O2D-CGD-O1D	-2.83	118.34	123.85
18	4	610	CLA	O2D-CGD-O1D	-2.83	118.34	123.85
18	B	804	CLA	C3B-C4B-NB	-2.83	108.01	110.53
18	A	824	CLA	O2D-CGD-O1D	-2.82	118.35	123.85
18	3	612	CLA	CAA-C2A-C3A	-2.82	109.75	116.23
18	B	835	CLA	O2D-CGD-O1D	-2.82	118.35	123.85
18	A	845	CLA	C3B-C4B-NB	-2.82	108.01	110.53
18	4	603	CLA	O2D-CGD-O1D	-2.82	118.36	123.85
17	2	605	CHL	OMC-CMC-C2C	-2.82	120.22	125.12
22	A	851	BCR	C35-C13-C14	-2.82	118.25	122.82
17	4	607	CHL	C1C-CHC-C4B	2.82	126.15	116.07
18	A	841	CLA	O2D-CGD-O1D	-2.82	118.36	123.85
18	B	839	CLA	O2D-CGD-O1D	-2.82	118.37	123.85
18	B	822	CLA	C3B-C4B-NB	-2.82	108.02	110.53
18	A	817	CLA	O2D-CGD-O1D	-2.82	118.37	123.85
22	B	845	BCR	C35-C13-C14	-2.81	118.26	122.82
18	A	832	CLA	C3B-C4B-NB	-2.81	108.02	110.53
18	H	201	CLA	C3B-C4B-NB	-2.81	108.02	110.53
22	3	614	BCR	C12-C13-C14	2.81	123.43	119.01
18	B	833	CLA	CAA-C2A-C3A	-2.81	105.40	113.00
24	A	801	CL0	C4-C3-C5	2.81	120.11	115.23
19	1	614	XAT	C26-C27-C28	-2.81	120.05	125.99
18	A	802	CLA	O2D-CGD-O1D	-2.81	118.38	123.85
18	A	815	CLA	C3B-C4B-NB	-2.81	108.02	110.53
17	1	601	CHL	C1C-CHC-C4B	2.81	126.12	116.07
22	B	848	BCR	C36-C18-C17	-2.81	118.27	122.82
22	3	614	BCR	C35-C13-C14	-2.80	118.27	122.82
18	A	825	CLA	O2D-CGD-O1D	-2.80	118.39	123.85
18	3	602	CLA	O2D-CGD-O1D	-2.80	118.40	123.85
18	F	301	CLA	O2D-CGD-O1D	-2.80	118.40	123.85
22	A	851	BCR	C36-C18-C17	-2.80	118.28	122.82
22	G	204	BCR	C16-C15-C14	2.80	129.24	123.52
18	B	814	CLA	C3B-C4B-NB	-2.80	108.03	110.53
17	2	601	CHL	C1C-CHC-C4B	2.80	126.08	116.07
18	2	610	CLA	C1A-CHA-C4D	-2.79	121.83	125.69
18	B	841	CLA	C3B-C4B-NB	-2.79	108.04	110.53
18	1	613	CLA	CAA-C2A-C3A	-2.79	109.83	116.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	3	611	CLA	CAA-C2A-C3A	-2.79	109.83	116.23
22	I	101	BCR	C16-C15-C14	2.79	129.23	123.52
18	A	843	CLA	O2D-CGD-O1D	-2.79	118.42	123.85
18	1	605	CLA	O2D-CGD-O1D	-2.79	118.43	123.85
19	4	617	XAT	C32-C33-C34	2.78	123.39	119.01
21	1	616	LUT	C8-C9-C10	2.78	123.39	119.01
18	A	841	CLA	C3B-C4B-NB	-2.78	108.05	110.53
22	A	851	BCR	C19-C18-C17	2.78	123.38	119.01
19	4	617	XAT	C40-C33-C34	-2.78	118.32	122.82
18	B	815	CLA	C3B-C4B-NB	-2.78	108.05	110.53
18	B	829	CLA	O2D-CGD-O1D	-2.77	118.45	123.85
17	3	606	CHL	C1C-CHC-C4B	2.77	125.99	116.07
17	4	606	CHL	C1C-CHC-C4B	2.77	125.99	116.07
18	B	837	CLA	C3B-C4B-NB	-2.77	108.06	110.53
18	3	610	CLA	CAA-C2A-C3A	-2.77	109.88	116.23
18	K	203	CLA	C3B-C4B-NB	-2.77	108.06	110.53
21	2	619	LUT	C7-C8-C9	-2.77	122.14	126.23
22	F	304	BCR	C37-C22-C21	-2.77	118.33	122.82
18	A	829	CLA	O2D-CGD-O1D	-2.77	118.46	123.85
18	A	804	CLA	CHB-C4A-NA	2.76	128.39	124.40
18	B	833	CLA	C3B-C4B-NB	-2.76	108.06	110.53
22	B	849	BCR	C36-C18-C17	-2.76	118.34	122.82
18	A	802	CLA	O2A-CGA-O1A	-2.76	116.72	123.63
18	A	806	CLA	C3B-C4B-NB	-2.76	108.06	110.53
18	K	201	CLA	CAA-C2A-C3A	-2.76	109.90	116.23
18	4	609	CLA	O2D-CGD-O1D	-2.76	118.48	123.85
18	A	804	CLA	C3B-C4B-NB	-2.76	108.07	110.53
18	B	813	CLA	C3B-C4B-NB	-2.76	108.07	110.53
21	2	616	LUT	C12-C13-C14	2.76	123.34	119.01
18	A	814	CLA	CHB-C4A-NA	2.75	128.37	124.40
18	A	819	CLA	CHB-C4A-NA	2.75	128.37	124.40
18	A	830	CLA	O2D-CGD-O1D	-2.75	118.50	123.85
22	B	801	BCR	C36-C18-C17	-2.75	118.36	122.82
18	L	304	CLA	O2D-CGD-O1D	-2.75	118.50	123.85
18	F	302	CLA	CHB-C4A-NA	2.75	128.37	124.40
21	3	613	LUT	C35-C15-C14	2.75	129.14	123.52
22	J	102	BCR	C15-C16-C17	2.75	129.14	123.52
18	B	829	CLA	C3B-C4B-NB	-2.75	108.08	110.53
18	A	803	CLA	O2D-CGD-O1D	-2.74	118.51	123.85
18	B	806	CLA	O2D-CGD-O1D	-2.74	118.51	123.85
18	A	805	CLA	C3B-C4B-NB	-2.74	108.08	110.53
18	B	830	CLA	C3B-C4B-NB	-2.74	108.08	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	4	602	CLA	C3B-C4B-NB	-2.74	108.09	110.53
18	2	608	CLA	O2D-CGD-O1D	-2.74	118.52	123.85
18	3	608	CLA	O2D-CGD-O1D	-2.74	118.52	123.85
18	B	811	CLA	CHB-C4A-NA	2.74	128.35	124.40
22	I	101	BCR	C36-C18-C17	-2.74	118.38	122.82
18	B	809	CLA	O2D-CGD-O1D	-2.74	118.52	123.85
22	B	845	BCR	C16-C17-C18	2.74	131.11	127.28
18	A	833	CLA	C3B-C4B-NB	-2.73	108.09	110.53
18	2	603	CLA	C3B-C4B-NB	-2.73	108.09	110.53
18	1	604	CLA	CHB-C4A-NA	2.73	128.34	124.40
18	2	609	CLA	O2D-CGD-O1D	-2.73	118.53	123.85
18	4	614	CLA	CHB-C4A-NA	2.73	128.34	124.40
18	B	825	CLA	CHB-C4A-NA	2.73	128.34	124.40
18	1	603	CLA	C3B-C4B-NB	-2.73	108.09	110.53
18	3	603	CLA	C3B-C4B-NB	-2.73	108.09	110.53
18	1	612	CLA	O2D-CGD-CBD	2.73	116.00	111.23
18	3	601	CLA	C3B-C4B-NB	-2.73	108.10	110.53
18	B	821	CLA	C3B-C4B-NB	-2.72	108.10	110.53
18	2	604	CLA	CHB-C4A-NA	2.72	128.33	124.40
17	2	605	CHL	C1C-CHC-C4B	2.72	125.80	116.07
18	B	834	CLA	CHB-C4A-NA	2.72	128.32	124.40
17	2	601	CHL	O2D-CGD-O1D	-2.72	118.56	123.85
18	3	612	CLA	O2D-CGD-O1D	-2.72	117.92	124.08
18	A	812	CLA	O2D-CGD-O1D	-2.71	118.56	123.85
18	A	808	CLA	O2D-CGD-O1D	-2.71	118.57	123.85
18	2	609	CLA	C3B-C4B-NB	-2.71	108.11	110.53
18	B	831	CLA	C3B-C4B-NB	-2.71	108.11	110.53
18	A	842	CLA	CHB-C4A-NA	2.71	128.31	124.40
18	A	828	CLA	CHB-C4A-NA	2.71	128.31	124.40
18	3	608	CLA	C3B-C4B-NB	-2.71	108.11	110.53
18	A	827	CLA	C3B-C4B-NB	-2.71	108.11	110.53
17	1	606	CHL	O2D-CGD-CBD	2.71	120.55	113.90
22	L	301	BCR	C10-C11-C12	2.71	131.05	123.20
18	2	609	CLA	CHB-C4A-NA	2.71	128.31	124.40
18	A	809	CLA	C3B-C4B-NB	-2.71	108.11	110.53
18	A	811	CLA	C3B-C4B-NB	-2.71	108.11	110.53
18	K	206	CLA	C3A-C2A-C1A	-2.71	103.53	106.30
18	B	825	CLA	C3B-C4B-NB	-2.71	108.11	110.53
18	2	608	CLA	CHB-C4A-NA	2.71	128.30	124.40
21	3	613	LUT	C26-C27-C28	2.70	128.79	124.58
22	I	101	BCR	C19-C18-C17	2.70	123.26	119.01
18	4	613	CLA	C3B-C4B-NB	-2.70	108.12	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	820	CLA	C3B-C4B-NB	-2.70	108.12	110.53
18	B	826	CLA	C3B-C4B-NB	-2.70	108.12	110.53
17	2	615	CHL	O1D-CGD-CBD	-2.70	120.63	124.72
24	A	801	CL0	CMC-C2C-C1C	2.70	129.59	124.73
18	3	607	CLA	CHB-C4A-NA	2.70	128.29	124.40
18	L	303	CLA	CHB-C4A-NA	2.70	128.29	124.40
18	A	826	CLA	C3B-C4B-NB	-2.70	108.12	110.53
18	4	601	CLA	CHB-C4A-NA	2.69	128.29	124.40
22	B	801	BCR	C19-C18-C17	2.69	123.25	119.01
18	1	612	CLA	CHB-C4A-NA	2.69	128.29	124.40
18	A	813	CLA	O2D-CGD-CBD	2.69	115.93	111.23
18	B	822	CLA	CHB-C4A-NA	2.69	128.28	124.40
18	L	304	CLA	CHB-C4A-NA	2.69	128.28	124.40
17	2	606	CHL	CBC-CAC-C3C	-2.69	109.03	112.87
22	L	301	BCR	C23-C22-C21	2.69	123.23	119.01
18	B	821	CLA	CHB-C4A-NA	2.69	128.28	124.40
18	A	805	CLA	CHB-C4A-NA	2.68	128.27	124.40
18	B	809	CLA	CHB-C4A-NA	2.68	128.27	124.40
22	B	848	BCR	C16-C15-C14	2.68	129.01	123.52
21	3	613	LUT	C19-C9-C10	-2.68	118.47	122.82
17	2	607	CHL	C1C-CHC-C4B	2.68	125.65	116.07
18	A	835	CLA	CHB-C4A-NA	2.68	128.26	124.40
22	3	614	BCR	C36-C18-C17	-2.68	118.48	122.82
22	J	102	BCR	C36-C18-C17	-2.67	118.49	122.82
22	4	618	BCR	C36-C18-C17	-2.67	118.49	122.82
22	G	204	BCR	C35-C13-C14	-2.67	118.49	122.82
18	4	609	CLA	CHB-C4A-NA	2.67	128.25	124.40
18	2	611	CLA	CHB-C4A-NA	2.67	128.25	124.40
18	1	612	CLA	C3B-C4B-NB	-2.66	108.15	110.53
18	B	841	CLA	CHB-C4A-NA	2.66	128.24	124.40
18	1	609	CLA	O2D-CGD-O1D	-2.66	118.67	123.85
18	A	809	CLA	CHB-C4A-NA	2.66	128.24	124.40
18	B	816	CLA	C1-C2-C3	-2.66	121.84	126.20
18	A	843	CLA	CHB-C4A-NA	2.66	128.24	124.40
18	A	813	CLA	CHB-C4A-NA	2.66	128.23	124.40
22	A	853	BCR	C36-C18-C17	-2.66	118.51	122.82
18	2	608	CLA	C3B-C4B-NB	-2.66	108.16	110.53
18	3	612	CLA	CHB-C4A-NA	2.65	128.23	124.40
18	B	820	CLA	C1-C2-C3	-2.65	122.47	126.76
22	A	848	BCR	C35-C13-C14	-2.65	118.52	122.82
18	4	608	CLA	CHB-C4A-NA	2.65	128.22	124.40
18	B	813	CLA	CHB-C4A-NA	2.65	128.22	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	B	806	CLA	CHB-C4A-NA	2.65	128.22	124.40
18	B	804	CLA	CHB-C4A-NA	2.65	128.22	124.40
18	B	806	CLA	C3B-C4B-NB	-2.65	108.17	110.53
18	B	820	CLA	C3B-C4B-NB	-2.65	108.17	110.53
18	A	836	CLA	CHB-C4A-NA	2.65	128.22	124.40
17	2	601	CHL	C1B-CHB-C4A	2.64	123.02	121.32
18	A	832	CLA	CHB-C4A-NA	2.64	128.21	124.40
17	4	607	CHL	CBC-CAC-C3C	-2.64	109.09	112.87
18	A	829	CLA	CHB-C4A-NA	2.64	128.21	124.40
18	B	839	CLA	CHB-C4A-NA	2.64	128.21	124.40
17	4	605	CHL	O2D-CGD-CBD	2.64	120.37	113.90
18	2	602	CLA	CHB-C4A-NA	2.64	128.21	124.40
18	3	610	CLA	O2D-CGD-O1D	-2.64	118.09	124.08
21	4	616	LUT	C40-C33-C34	-2.64	118.54	122.82
18	B	818	CLA	C1-C2-C3	-2.64	121.88	126.20
18	A	808	CLA	CHB-C4A-NA	2.64	128.21	124.40
18	A	818	CLA	C3B-C4B-NB	-2.64	108.18	110.53
18	3	608	CLA	CHB-C4A-NA	2.63	128.20	124.40
18	G	203	CLA	C3B-C4B-NB	-2.63	108.18	110.53
18	A	833	CLA	CHB-C4A-NA	2.63	128.20	124.40
21	3	613	LUT	C10-C11-C12	2.63	130.82	123.20
18	A	844	CLA	CHB-C4A-NA	2.63	128.20	124.40
18	B	808	CLA	CHB-C4A-NA	2.63	128.20	124.40
18	A	818	CLA	CHB-C4A-NA	2.63	128.20	124.40
18	L	304	CLA	C3B-C4B-NB	-2.63	108.18	110.53
18	A	811	CLA	CHB-C4A-NA	2.63	128.19	124.40
18	A	823	CLA	C3B-C4B-NB	-2.63	108.18	110.53
21	2	616	LUT	C20-C13-C14	-2.63	118.56	122.82
18	1	603	CLA	CHB-C4A-NA	2.63	128.19	124.40
18	B	827	CLA	CHB-C4A-NA	2.63	128.19	124.40
18	B	840	CLA	CHB-C4A-NA	2.63	128.19	124.40
18	A	834	CLA	CHB-C4A-NA	2.62	128.19	124.40
18	A	812	CLA	CHB-C4A-NA	2.62	128.19	124.40
22	F	304	BCR	C16-C17-C18	2.62	130.96	127.28
18	4	610	CLA	CHB-C4A-NA	2.62	128.19	124.40
18	B	818	CLA	CHB-C4A-NA	2.62	128.19	124.40
18	B	810	CLA	CHB-C4A-NA	2.62	128.18	124.40
18	A	831	CLA	C3B-C4B-NB	-2.62	108.19	110.53
22	A	849	BCR	C35-C13-C14	-2.62	118.58	122.82
17	1	601	CHL	O2D-CGD-CBD	2.61	120.31	113.90
18	B	819	CLA	CHB-C4A-NA	2.61	128.17	124.40
22	A	849	BCR	C16-C15-C14	2.61	128.86	123.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	K	203	CLA	CAA-C2A-C3A	-2.61	105.94	113.00
18	A	831	CLA	CHB-C4A-NA	2.61	128.17	124.40
18	3	601	CLA	CHB-C4A-NA	2.61	128.17	124.40
22	B	846	BCR	C10-C11-C12	2.61	130.76	123.20
21	3	613	LUT	C11-C10-C9	2.61	130.94	127.28
18	G	202	CLA	CHB-C4A-NA	2.61	128.17	124.40
18	B	830	CLA	CHB-C4A-NA	2.61	128.16	124.40
18	4	602	CLA	CHB-C4A-NA	2.61	128.16	124.40
18	B	817	CLA	CHB-C4A-NA	2.61	128.16	124.40
17	2	606	CHL	O1D-CGD-CBD	-2.60	120.77	124.72
18	B	837	CLA	CHB-C4A-NA	2.60	128.16	124.40
18	A	842	CLA	CMB-C2B-C1B	-2.60	121.45	125.42
18	A	843	CLA	C3B-C4B-NB	-2.60	108.21	110.53
18	3	603	CLA	CHB-C4A-NA	2.60	128.16	124.40
18	B	824	CLA	CHB-C4A-NA	2.60	128.15	124.40
22	B	844	BCR	C8-C9-C10	2.60	123.09	119.01
18	A	840	CLA	CHB-C4A-NA	2.60	128.15	124.40
18	B	809	CLA	C3B-C4B-NB	-2.60	108.21	110.53
17	1	606	CHL	C1C-CHC-C4B	2.60	125.36	116.07
18	B	831	CLA	CHB-C4A-NA	2.60	128.15	124.40
18	1	602	CLA	CHB-C4A-NA	2.59	128.14	124.40
18	1	607	CLA	CHB-C4A-NA	2.59	128.14	124.40
18	B	808	CLA	O2A-CGA-O1A	-2.59	117.14	123.63
18	A	827	CLA	CHB-C4A-NA	2.59	128.14	124.40
18	B	828	CLA	CHB-C4A-NA	2.59	128.14	124.40
18	A	821	CLA	CHB-C4A-NA	2.59	128.14	124.40
18	4	604	CLA	CHB-C4A-NA	2.59	128.14	124.40
18	3	605	CLA	CHB-C4A-NA	2.59	128.13	124.40
18	2	612	CLA	C3B-C4B-NB	-2.59	108.22	110.53
18	B	820	CLA	CHB-C4A-NA	2.59	128.13	124.40
22	4	618	BCR	C19-C18-C17	2.58	123.07	119.01
22	B	849	BCR	C30-C25-C24	2.58	122.66	115.65
22	A	853	BCR	C19-C18-C17	2.58	123.07	119.01
18	A	825	CLA	CHB-C4A-NA	2.58	128.12	124.40
18	A	841	CLA	CHB-C4A-NA	2.58	128.12	124.40
17	2	605	CHL	O1D-CGD-CBD	-2.58	120.81	124.72
18	4	611	CLA	CHB-C4A-NA	2.58	128.12	124.40
22	A	849	BCR	C37-C22-C21	-2.58	118.64	122.82
22	B	844	BCR	C19-C18-C17	2.58	123.06	119.01
17	4	605	CHL	CAC-C3C-C4C	2.58	129.37	124.73
22	K	202	BCR	C30-C25-C24	2.58	122.64	115.65
18	B	836	CLA	C1-C2-C3	-2.58	122.59	126.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	G	203	CLA	CHB-C4A-NA	2.58	128.12	124.40
27	B	850	DGD	O1G-C1A-C2A	2.58	119.69	111.83
18	2	603	CLA	CHB-C4A-NA	2.57	128.12	124.40
18	B	814	CLA	CHB-C4A-NA	2.57	128.12	124.40
22	A	852	BCR	C12-C13-C14	2.57	123.06	119.01
22	B	801	BCR	C34-C9-C10	-2.57	118.64	122.82
18	B	812	CLA	CHB-C4A-NA	2.57	128.11	124.40
18	B	815	CLA	CHB-C4A-NA	2.57	128.11	124.40
18	G	201	CLA	CHB-C4A-NA	2.57	128.11	124.40
18	B	807	CLA	CHB-C4A-NA	2.57	128.11	124.40
18	2	610	CLA	CAB-C3B-C2B	2.57	130.36	123.53
18	1	610	CLA	CHB-C4A-NA	2.57	128.11	124.40
17	2	607	CHL	CBC-CAC-C3C	-2.57	109.19	112.87
19	2	617	XAT	C40-C33-C34	-2.57	118.66	122.82
18	B	838	CLA	CHB-C4A-NA	2.57	128.11	124.40
25	A	855	PQN	C11-C3-C2	-2.57	120.49	124.89
18	K	203	CLA	CHB-C4A-NA	2.57	128.10	124.40
17	2	605	CHL	CAC-C3C-C4C	2.57	129.35	124.73
18	1	613	CLA	CHB-C4A-NA	2.57	128.10	124.40
18	A	816	CLA	CHB-C4A-NA	2.57	128.10	124.40
19	2	617	XAT	C35-C34-C33	2.56	130.88	127.28
19	1	614	XAT	C6-C7-C8	-2.56	120.57	125.99
22	J	102	BCR	C19-C18-C17	2.56	123.04	119.01
18	K	206	CLA	O2D-CGD-O1D	-2.56	118.27	124.08
18	1	608	CLA	CHB-C4A-NA	2.56	128.10	124.40
18	B	826	CLA	CHB-C4A-NA	2.56	128.10	124.40
18	4	612	CLA	CHB-C4A-NA	2.56	128.09	124.40
18	4	612	CLA	C3B-C4B-NB	-2.56	108.25	110.53
21	4	616	LUT	C19-C9-C8	2.56	122.00	118.09
18	2	611	CLA	O2D-CGD-O1D	-2.56	118.87	123.85
18	1	613	CLA	O2D-CGD-O1D	-2.56	118.28	124.08
18	A	845	CLA	CHB-C4A-NA	2.55	128.09	124.40
18	B	816	CLA	CHB-C4A-NA	2.55	128.08	124.40
18	A	832	CLA	C1-C2-C3	-2.55	122.63	126.76
18	A	838	CLA	CHB-C4A-NA	2.55	128.08	124.40
22	B	843	BCR	C1-C6-C7	2.55	122.56	115.65
18	A	826	CLA	CHB-C4A-NA	2.55	128.08	124.40
22	A	849	BCR	C19-C18-C17	2.55	123.02	119.01
22	J	102	BCR	C10-C11-C12	2.55	130.58	123.20
18	2	611	CLA	C3B-C4B-NB	-2.55	108.26	110.53
21	3	613	LUT	C32-C33-C34	2.55	123.01	119.01
18	A	806	CLA	CHB-C4A-NA	2.55	128.07	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	K	201	CLA	CHB-C4A-NA	2.55	128.07	124.40
22	I	101	BCR	C35-C13-C14	-2.54	118.69	122.82
18	B	818	CLA	C3B-C4B-NB	-2.54	108.26	110.53
21	4	616	LUT	C39-C29-C28	2.54	121.97	118.09
18	B	832	CLA	CHB-C4A-NA	2.54	128.07	124.40
18	A	839	CLA	CHB-C4A-NA	2.54	128.07	124.40
18	B	833	CLA	CHB-C4A-NA	2.54	128.07	124.40
22	B	846	BCR	C36-C18-C17	-2.54	118.70	122.82
18	J	101	CLA	CHB-C4A-NA	2.54	128.06	124.40
18	2	612	CLA	CHB-C4A-NA	2.54	128.06	124.40
18	A	822	CLA	CHB-C4A-NA	2.54	128.06	124.40
18	F	303	CLA	CHB-C4A-NA	2.54	128.06	124.40
18	L	302	CLA	CHB-C4A-NA	2.54	128.06	124.40
18	A	815	CLA	CHB-C4A-NA	2.53	128.06	124.40
18	A	803	CLA	CHB-C4A-NA	2.53	128.05	124.40
21	2	616	LUT	C35-C15-C14	2.53	128.70	123.52
17	4	607	CHL	O1D-CGD-CBD	-2.53	120.88	124.72
18	A	837	CLA	CHB-C4A-NA	2.53	128.05	124.40
19	2	617	XAT	C20-C13-C14	-2.53	118.72	122.82
18	A	810	CLA	CHB-C4A-NA	2.53	128.05	124.40
18	H	201	CLA	CHB-C4A-NA	2.53	128.05	124.40
18	A	824	CLA	CHB-C4A-NA	2.53	128.05	124.40
18	2	603	CLA	O2D-CGD-O1D	-2.53	118.35	124.08
18	1	611	CLA	CHB-C4A-NA	2.53	128.04	124.40
22	B	848	BCR	C35-C13-C14	-2.52	118.73	122.82
22	B	843	BCR	C36-C18-C17	-2.52	118.73	122.82
22	A	848	BCR	C12-C13-C14	2.52	122.97	119.01
18	A	823	CLA	CHB-C4A-NA	2.52	128.03	124.40
18	B	829	CLA	CHB-C4A-NA	2.52	128.03	124.40
22	3	614	BCR	C19-C18-C17	2.52	122.97	119.01
18	B	835	CLA	CHB-C4A-NA	2.51	128.03	124.40
17	2	606	CHL	CMA-C3A-C4A	-2.51	109.20	114.61
18	2	613	CLA	CHB-C4A-NA	2.51	128.02	124.40
18	B	805	CLA	CHB-C4A-NA	2.51	128.02	124.40
18	A	820	CLA	CHB-C4A-NA	2.50	128.01	124.40
18	B	802	CLA	CHB-C4A-NA	2.50	128.01	124.40
21	4	616	LUT	C20-C13-C14	-2.50	118.76	122.82
18	1	607	CLA	O2D-CGD-O1D	-2.50	118.41	124.08
18	3	609	CLA	O2D-CGD-O1D	-2.50	118.41	124.08
18	4	611	CLA	O2D-CGD-O1D	-2.50	118.41	124.08
22	G	204	BCR	C30-C25-C26	-2.50	119.22	122.64
18	3	610	CLA	CHB-C4A-NA	2.50	128.01	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	2	605	CHL	CMB-C2B-C3B	2.50	129.67	124.68
18	3	604	CLA	O2D-CGD-O1D	-2.50	118.42	124.08
18	A	807	CLA	CHB-C4A-NA	2.50	128.00	124.40
22	A	853	BCR	C34-C9-C10	-2.49	118.77	122.82
22	B	847	BCR	C36-C18-C17	-2.49	118.77	122.82
22	B	846	BCR	C15-C16-C17	2.49	128.62	123.52
18	1	605	CLA	CHB-C4A-NA	2.49	128.00	124.40
18	3	609	CLA	CHB-C4A-NA	2.49	128.00	124.40
17	2	601	CHL	CMB-C2B-C3B	2.49	129.66	124.68
18	3	604	CLA	CHB-C4A-NA	2.49	128.00	124.40
18	1	610	CLA	O2D-CGD-O1D	-2.49	118.43	124.08
17	4	606	CHL	O1D-CGD-CBD	-2.49	120.95	124.72
17	2	615	CHL	OMC-CMC-C2C	-2.48	120.81	125.12
18	B	819	CLA	C1-C2-C3	-2.48	122.13	126.20
18	3	611	CLA	CHB-C4A-NA	2.48	127.98	124.40
21	3	613	LUT	C27-C28-C29	-2.48	121.00	126.32
18	3	602	CLA	CHB-C4A-NA	2.48	127.97	124.40
22	K	202	BCR	C30-C25-C26	-2.47	119.25	122.64
21	4	616	LUT	C32-C33-C34	2.47	122.90	119.01
18	A	817	CLA	CHB-C4A-NA	2.47	127.97	124.40
17	1	606	CHL	CMB-C2B-C3B	2.47	129.63	124.68
17	4	615	CHL	O2D-CGD-CBD	2.47	119.97	113.90
22	A	851	BCR	C15-C14-C13	2.47	130.75	127.28
22	A	851	BCR	C30-C25-C26	-2.47	119.26	122.64
18	A	830	CLA	C3B-C4B-NB	-2.47	108.32	110.53
22	J	102	BCR	C1-C6-C5	-2.47	119.26	122.64
21	2	616	LUT	C26-C27-C28	2.47	128.43	124.58
19	2	617	XAT	C15-C14-C13	2.47	130.74	127.28
21	3	613	LUT	C20-C13-C14	-2.47	118.82	122.82
22	B	849	BCR	C23-C22-C21	2.47	122.89	119.01
18	4	603	CLA	CHB-C4A-NA	2.46	127.95	124.40
18	K	204	CLA	CHB-C4A-NA	2.46	127.95	124.40
21	2	619	LUT	C30-C31-C32	2.46	130.32	123.20
18	F	301	CLA	CHB-C4A-NA	2.46	127.95	124.40
18	B	836	CLA	CHB-C4A-NA	2.46	127.95	124.40
17	2	607	CHL	O1D-CGD-CBD	-2.46	121.00	124.72
22	L	306	BCR	C1-C6-C5	-2.45	119.28	122.64
17	3	606	CHL	O1D-CGD-CBD	-2.45	121.01	124.72
18	4	609	CLA	C1-C2-C3	-2.45	122.18	126.20
22	A	851	BCR	C30-C25-C24	2.45	122.29	115.65
18	4	614	CLA	O2D-CGD-CBD	2.44	115.50	111.23
22	G	204	BCR	C12-C13-C14	2.44	122.85	119.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	K	205	BCR	C1-C6-C5	-2.44	119.30	122.64
17	2	615	CHL	CMB-C2B-C3B	2.44	129.56	124.68
18	B	821	CLA	CAA-CBA-CGA	-2.43	106.30	113.21
25	B	842	PQN	C11-C3-C2	-2.43	120.72	124.89
22	B	843	BCR	C1-C6-C5	-2.43	119.31	122.64
18	B	823	CLA	CHB-C4A-NA	2.43	127.90	124.40
18	4	603	CLA	CAB-C3B-C2B	2.43	129.98	123.53
22	A	849	BCR	C12-C13-C14	2.43	122.83	119.01
22	L	306	BCR	C21-C20-C19	2.43	130.23	123.20
18	1	613	CLA	CAB-C3B-C2B	2.43	129.98	123.53
17	3	606	CHL	CMB-C2B-C3B	2.42	129.53	124.68
18	1	610	CLA	CAB-C3B-C2B	2.42	129.95	123.53
18	F	302	CLA	O2D-CGD-O1D	-2.42	119.15	123.85
22	K	205	BCR	C30-C25-C26	-2.42	119.33	122.64
18	1	608	CLA	CAB-C3B-C2B	2.41	129.94	123.53
17	4	606	CHL	CBC-CAC-C3C	-2.41	109.42	112.87
22	A	853	BCR	C30-C25-C24	2.40	122.17	115.65
22	B	848	BCR	C30-C25-C24	2.40	122.16	115.65
18	B	811	CLA	CAB-C3B-C2B	2.40	129.91	123.53
22	F	304	BCR	C36-C18-C17	-2.40	118.93	122.82
22	L	305	BCR	C30-C25-C24	2.40	122.16	115.65
22	B	847	BCR	C15-C16-C17	2.39	128.42	123.52
22	L	305	BCR	C1-C6-C7	2.39	122.14	115.65
17	4	615	CHL	CMB-C2B-C3B	2.39	129.70	124.69
22	A	850	BCR	C12-C13-C14	2.39	122.77	119.01
18	3	605	CLA	CAB-C3B-C2B	2.39	129.88	123.53
18	1	608	CLA	CMB-C2B-C3B	2.39	129.88	123.53
17	1	601	CHL	C4-C3-C5	2.39	119.37	115.23
18	A	842	CLA	C3B-C4B-NB	-2.39	108.40	110.53
22	B	801	BCR	C23-C22-C21	2.38	122.76	119.01
17	2	606	CHL	O2D-CGD-O1D	-2.38	119.21	123.85
17	2	601	CHL	CBC-CAC-C3C	-2.38	109.47	112.87
22	J	102	BCR	C1-C6-C7	2.38	122.11	115.65
18	B	808	CLA	C1-C2-C3	-2.38	122.30	126.20
22	B	849	BCR	C34-C9-C8	2.38	121.72	118.09
17	4	606	CHL	CMB-C2B-C3B	2.37	129.66	124.69
22	A	851	BCR	C11-C12-C13	2.37	132.87	126.36
17	2	607	CHL	CMB-C2B-C3B	2.37	129.42	124.68
17	2	606	CHL	CMB-C2B-C3B	2.37	129.42	124.68
18	A	820	CLA	CMB-C2B-C1B	-2.37	121.81	125.42
18	1	613	CLA	CMB-C2B-C3B	2.37	129.82	123.53
22	A	848	BCR	C30-C25-C24	2.36	122.06	115.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	K	205	BCR	C30-C25-C24	2.36	122.06	115.65
18	A	844	CLA	O2A-CGA-O1A	-2.36	117.72	123.63
17	4	605	CHL	CMA-C3A-C4A	-2.36	109.52	114.61
18	B	811	CLA	CMB-C2B-C3B	2.36	129.81	123.53
17	1	606	CHL	CBC-CAC-C3C	-2.36	109.50	112.87
17	4	605	CHL	OMC-CMC-C2C	-2.36	121.03	125.12
22	K	205	BCR	C1-C6-C7	2.36	122.04	115.65
20	1	615	LHG	O8-C23-C24	2.35	119.00	111.83
22	G	204	BCR	C23-C22-C21	2.35	122.70	119.01
18	B	811	CLA	C3B-C4B-NB	-2.35	107.89	110.33
18	4	609	CLA	O2A-CGA-O1A	-2.35	117.75	123.63
18	1	613	CLA	C3B-C4B-NB	-2.35	107.89	110.33
21	2	619	LUT	C20-C13-C14	-2.35	119.02	122.82
22	I	101	BCR	C34-C9-C8	2.35	121.67	118.09
22	A	853	BCR	C30-C25-C26	-2.34	119.43	122.64
18	1	608	CLA	C3B-C4B-NB	-2.34	107.90	110.33
17	4	607	CHL	OMC-CMC-C2C	-2.34	121.06	125.12
22	K	205	BCR	C16-C15-C14	2.34	128.31	123.52
17	4	607	CHL	CMB-C2B-C3B	2.34	129.35	124.68
18	A	838	CLA	C1-C2-C3	-2.34	122.37	126.20
18	2	610	CLA	CMB-C2B-C3B	2.34	129.74	123.53
18	A	841	CLA	C1-C2-C3	-2.33	122.37	126.20
18	A	830	CLA	C1-C2-C3	2.33	130.02	126.20
19	2	617	XAT	C8-C9-C10	2.33	122.67	119.01
18	4	604	CLA	CAB-C3B-C2B	2.33	129.72	123.53
18	1	610	CLA	CMB-C2B-C3B	2.33	129.72	123.53
22	K	202	BCR	C21-C20-C19	2.33	129.94	123.20
17	2	615	CHL	O2D-CGD-O1D	-2.33	119.32	123.85
18	1	610	CLA	C3B-C4B-NB	-2.32	107.92	110.33
18	B	825	CLA	C1-C2-C3	-2.32	122.39	126.20
17	1	601	CHL	CMB-C2B-C3B	2.32	129.32	124.68
17	1	601	CHL	O2D-CGD-O1D	-2.32	118.82	124.08
18	A	828	CLA	CMB-C2B-C1B	-2.32	121.89	125.42
18	3	605	CLA	C3B-C4B-NB	-2.32	107.92	110.33
22	K	205	BCR	C8-C9-C10	2.31	122.65	119.01
18	4	604	CLA	C3B-C4B-NB	-2.31	107.93	110.33
18	3	601	CLA	C1-C2-C3	-2.31	122.41	126.20
18	A	808	CLA	C1-C2-C3	-2.31	123.02	126.76
19	2	617	XAT	C27-C28-C29	-2.31	121.95	125.53
17	2	607	CHL	C5-C3-C4	2.31	119.90	114.59
18	A	810	CLA	O2A-CGA-O1A	-2.31	117.86	123.63
18	3	605	CLA	CMB-C2B-C3B	2.30	129.65	123.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	1	606	CHL	OMC-CMC-C2C	-2.30	121.13	125.12
18	A	841	CLA	O2A-CGA-O1A	-2.30	117.88	123.63
18	B	810	CLA	C1-C2-C3	-2.30	122.43	126.20
21	2	619	LUT	C15-C14-C13	2.30	130.50	127.28
18	2	610	CLA	C3B-C4B-NB	-2.30	107.94	110.33
18	K	206	CLA	CHB-C4A-NA	2.30	127.71	124.40
18	A	825	CLA	C1-C2-C3	-2.29	122.44	126.20
22	A	850	BCR	C1-C6-C7	2.29	121.86	115.65
22	I	101	BCR	C12-C13-C14	2.29	122.61	119.01
17	2	607	CHL	OMC-CMC-C2C	-2.29	121.15	125.12
22	L	305	BCR	C1-C6-C5	-2.28	119.52	122.64
17	2	607	CHL	O2D-CGD-O1D	-2.28	119.41	123.85
18	B	841	CLA	O2D-CGD-CBD	2.28	115.21	111.23
18	A	835	CLA	O2D-CGD-CBD	2.28	115.21	111.23
18	4	602	CLA	CMB-C2B-C1B	-2.28	121.95	125.42
18	A	804	CLA	O2A-CGA-O1A	-2.27	117.94	123.63
17	2	607	CHL	CMA-C3A-C4A	-2.27	109.71	114.61
17	2	605	CHL	O2D-CGD-O1D	-2.27	119.43	123.85
18	B	818	CLA	CMB-C2B-C1B	-2.27	121.97	125.42
22	L	306	BCR	C1-C6-C7	2.27	121.80	115.65
20	1	615	LHG	C5-O7-C7	-2.27	112.37	117.80
21	2	619	LUT	C11-C10-C9	2.27	130.46	127.28
22	B	843	BCR	C16-C17-C18	2.26	130.45	127.28
22	B	846	BCR	C19-C18-C17	2.26	122.57	119.01
18	A	845	CLA	C1-C2-C3	-2.26	123.11	126.76
22	B	843	BCR	C10-C11-C12	2.26	129.75	123.20
18	B	821	CLA	O2A-CGA-O1A	-2.26	117.98	123.63
18	4	614	CLA	C1-C2-C3	-2.26	123.11	126.76
22	B	849	BCR	C7-C8-C9	2.25	129.57	126.23
19	4	617	XAT	O4-C6-C7	-2.25	110.42	116.88
18	4	603	CLA	CMB-C2B-C3B	2.25	129.51	123.53
22	3	614	BCR	C30-C25-C24	2.25	121.75	115.65
17	3	606	CHL	O2D-CGD-O1D	-2.24	119.48	123.85
22	A	849	BCR	C36-C18-C17	-2.24	119.18	122.82
18	A	814	CLA	O2A-CGA-O1A	-2.24	118.02	123.63
18	B	825	CLA	CMB-C2B-C1B	-2.24	122.01	125.42
22	J	102	BCR	C7-C8-C9	2.24	129.55	126.23
22	B	845	BCR	C37-C22-C21	-2.24	119.19	122.82
22	B	848	BCR	C12-C13-C14	2.23	122.52	119.01
18	4	604	CLA	CMB-C2B-C3B	2.23	129.47	123.53
18	4	603	CLA	C3B-C4B-NB	-2.23	108.01	110.33
17	2	606	CHL	OMC-CMC-C2C	-2.23	121.24	125.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	3	613	LUT	C12-C13-C14	2.23	122.52	119.01
22	G	204	BCR	C34-C9-C8	2.23	121.50	118.09
22	B	843	BCR	C12-C13-C14	2.23	122.52	119.01
22	B	843	BCR	C35-C13-C14	-2.23	119.20	122.82
22	A	848	BCR	C30-C25-C26	-2.23	119.59	122.64
22	A	852	BCR	C24-C23-C22	2.23	129.53	126.23
18	B	805	CLA	O2A-CGA-O1A	-2.23	118.06	123.63
17	2	601	CHL	OMC-CMC-C2C	-2.22	121.26	125.12
22	L	305	BCR	C30-C25-C26	-2.22	119.60	122.64
17	4	606	CHL	O2D-CGD-O1D	-2.22	119.53	123.85
18	A	827	CLA	O2A-CGA-O1A	-2.22	118.08	123.63
21	4	616	LUT	C12-C13-C14	2.22	122.50	119.01
22	B	848	BCR	C34-C9-C8	2.21	121.47	118.09
18	B	813	CLA	C1-C2-C3	-2.21	122.57	126.20
18	3	602	CLA	O2A-CGA-O1A	-2.21	118.09	123.63
21	2	616	LUT	C27-C28-C29	-2.21	121.57	126.32
18	B	839	CLA	O2A-CGA-O1A	-2.21	118.10	123.63
18	B	834	CLA	C1-C2-C3	-2.21	122.58	126.20
22	B	847	BCR	C19-C18-C17	2.21	122.48	119.01
17	1	601	CHL	OMC-CMC-C2C	-2.21	121.29	125.12
18	2	612	CLA	CMB-C2B-C1B	-2.21	122.06	125.42
24	A	801	CL0	CMA-C3A-C4A	-2.21	109.86	114.61
22	A	853	BCR	C1-C6-C5	-2.21	119.62	122.64
18	B	824	CLA	C1-C2-C3	-2.20	122.58	126.20
17	4	615	CHL	OMC-CMC-C2C	-2.20	121.30	125.12
18	B	816	CLA	O2A-CGA-O1A	-2.20	118.12	123.63
18	A	835	CLA	C1-C2-C3	-2.20	122.59	126.20
18	B	836	CLA	O2A-CGA-O1A	-2.20	118.12	123.63
17	4	607	CHL	O2D-CGD-O1D	-2.20	119.57	123.85
22	J	102	BCR	C23-C22-C21	2.20	122.47	119.01
18	A	804	CLA	O2D-CGD-CBD	2.20	115.07	111.23
17	4	607	CHL	CMA-C3A-C4A	-2.20	109.88	114.61
18	F	302	CLA	C1-C2-C3	-2.19	122.61	126.20
17	1	606	CHL	O2D-CGD-O1D	-2.19	119.11	124.08
22	I	101	BCR	C37-C22-C23	2.19	121.43	118.09
18	A	834	CLA	C1-C2-C3	-2.18	122.62	126.20
17	4	605	CHL	CMB-C2B-C3B	2.18	129.03	124.68
19	1	614	XAT	O24-C25-C26	-2.18	57.20	58.93
17	4	606	CHL	C4C-CHD-C1D	2.18	123.85	116.07
27	B	850	DGD	O2G-C1B-O1B	-2.17	118.62	123.70
19	1	614	XAT	C10-C11-C12	-2.17	116.90	123.20
18	B	813	CLA	O2A-CGA-O1A	-2.17	118.20	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	2	609	CLA	CMB-C2B-C1B	-2.17	122.12	125.42
21	4	616	LUT	C7-C8-C9	2.17	129.44	126.23
17	4	615	CHL	C4C-CHD-C1D	2.16	123.81	116.07
18	B	814	CLA	O2D-CGD-CBD	2.16	115.01	111.23
18	A	809	CLA	O2A-CGA-O1A	-2.16	118.22	123.63
22	B	843	BCR	C19-C18-C17	2.16	122.41	119.01
18	B	827	CLA	O2D-CGD-CBD	2.16	115.01	111.23
18	B	837	CLA	O2A-CGA-O1A	-2.16	118.22	123.63
18	A	808	CLA	O2A-CGA-O1A	-2.16	118.22	123.63
24	A	801	CL0	O2A-CGA-O1A	-2.16	118.22	123.63
18	A	844	CLA	C1-C2-C3	-2.16	122.66	126.20
19	4	617	XAT	C10-C11-C12	2.16	129.46	123.20
18	B	825	CLA	O2D-CGD-CBD	2.16	115.01	111.23
18	L	303	CLA	O2D-CGD-CBD	2.16	115.00	111.23
21	3	613	LUT	C40-C33-C34	-2.16	119.32	122.82
22	A	851	BCR	C10-C11-C12	-2.16	116.95	123.20
22	A	852	BCR	C30-C25-C24	2.15	121.50	115.65
18	B	820	CLA	O2A-CGA-O1A	-2.15	118.24	123.63
18	A	805	CLA	C1-C2-C3	-2.15	122.67	126.20
22	A	848	BCR	C23-C22-C21	2.15	122.39	119.01
18	B	834	CLA	O2A-CGA-O1A	-2.15	118.25	123.63
17	4	615	CHL	O2D-CGD-O1D	-2.15	119.20	124.08
18	A	806	CLA	C1-C2-C3	-2.15	122.67	126.20
18	2	611	CLA	CMB-C2B-C1B	-2.15	122.14	125.42
18	B	826	CLA	O2A-CGA-O1A	-2.15	118.26	123.63
18	A	829	CLA	O2A-CGA-O1A	-2.15	118.26	123.63
17	2	601	CHL	O2A-CGA-CBA	2.14	120.24	112.14
22	A	850	BCR	C35-C13-C14	-2.14	119.34	122.82
18	B	817	CLA	C1-C2-C3	-2.14	122.69	126.20
18	B	809	CLA	CMB-C2B-C1B	-2.14	122.16	125.42
22	3	614	BCR	C37-C22-C23	2.14	121.36	118.09
19	1	614	XAT	C35-C15-C14	-2.14	119.14	123.52
18	A	842	CLA	CAA-C2A-C3A	-2.14	107.22	113.00
22	L	305	BCR	C21-C20-C19	2.14	129.39	123.20
18	2	602	CLA	O2A-CGA-O1A	-2.14	118.28	123.63
18	B	822	CLA	CMB-C2B-C1B	-2.14	122.17	125.42
18	A	825	CLA	O2A-CGA-O1A	-2.13	118.30	123.63
17	2	601	CHL	C4C-CHD-C1D	2.13	123.69	116.07
22	B	845	BCR	C24-C23-C22	-2.13	123.08	126.23
18	B	819	CLA	O2A-CGA-O1A	-2.13	118.30	123.63
22	L	301	BCR	C8-C9-C10	2.13	122.36	119.01
17	3	606	CHL	CAC-C3C-C4C	2.13	129.50	124.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	853	BCR	C1-C6-C7	2.13	121.42	115.65
17	1	601	CHL	CBC-CAC-C3C	-2.13	109.83	112.87
18	B	824	CLA	O2A-CGA-O1A	-2.12	118.32	123.63
19	1	614	XAT	C31-C30-C29	-2.12	124.30	127.28
18	A	839	CLA	O2A-CGA-O1A	-2.12	118.32	123.63
18	B	803	CLA	O2A-CGA-O1A	-2.12	118.32	123.63
19	1	614	XAT	O4-C5-C6	-2.12	57.25	58.93
18	1	604	CLA	O2A-CGA-O1A	-2.12	118.33	123.63
17	3	606	CHL	C4C-CHD-C1D	2.11	123.63	116.07
18	A	840	CLA	C1-C2-C3	-2.11	122.74	126.20
18	A	807	CLA	C1-C2-C3	-2.11	122.74	126.20
18	A	810	CLA	CAA-CBA-CGA	-2.11	107.21	113.21
17	1	601	CHL	C4C-CHD-C1D	2.11	123.62	116.07
17	4	607	CHL	CAC-C3C-C4C	2.11	129.45	124.03
18	A	838	CLA	O2A-CGA-O1A	-2.11	118.35	123.63
22	B	845	BCR	C8-C9-C10	2.11	122.32	119.01
18	B	829	CLA	O2A-CGA-O1A	-2.10	118.36	123.63
18	B	826	CLA	CMB-C2B-C1B	-2.10	122.22	125.42
18	4	612	CLA	CMB-C2B-C1B	-2.10	122.22	125.42
22	A	850	BCR	C1-C6-C5	-2.10	119.76	122.64
18	B	822	CLA	O2A-CGA-O1A	-2.10	118.37	123.63
18	J	101	CLA	O2A-CGA-O1A	-2.10	118.37	123.63
17	2	605	CHL	C4C-CHD-C1D	2.10	123.58	116.07
18	A	828	CLA	CMB-C2B-C3B	2.10	131.49	126.55
18	4	602	CLA	CMB-C2B-C3B	2.10	131.48	126.55
22	3	614	BCR	C30-C25-C26	-2.10	119.77	122.64
18	A	831	CLA	CMB-C2B-C1B	-2.10	122.23	125.42
22	B	843	BCR	C7-C8-C9	-2.09	123.14	126.23
21	3	613	LUT	C1-C6-C7	2.09	121.33	115.65
18	A	811	CLA	C1-C2-C3	-2.09	122.77	126.20
18	A	812	CLA	C1-C2-C3	-2.09	122.77	126.20
17	4	607	CHL	C4C-CHD-C1D	2.09	123.55	116.07
17	4	605	CHL	O2D-CGD-O1D	-2.09	119.33	124.08
17	4	605	CHL	CMD-C2D-C3D	-2.09	120.50	124.68
18	1	602	CLA	O2A-CGA-O1A	-2.09	118.40	123.63
18	B	817	CLA	O2A-CGA-O1A	-2.09	118.40	123.63
17	2	607	CHL	C4C-CHD-C1D	2.09	123.54	116.07
18	B	828	CLA	O2A-CGA-O1A	-2.09	118.41	123.63
18	1	603	CLA	O2A-CGA-O1A	-2.09	118.41	123.63
18	A	818	CLA	O2A-CGA-O1A	-2.08	118.42	123.63
18	A	809	CLA	C1-C2-C3	-2.08	122.78	126.20
22	B	845	BCR	C30-C25-C26	-2.08	119.79	122.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	848	BCR	C37-C22-C23	2.08	121.27	118.09
18	B	837	CLA	O2D-CGD-CBD	2.08	114.87	111.23
18	3	601	CLA	O2A-CGA-O1A	-2.08	118.42	123.63
17	2	607	CHL	CAC-C3C-C4C	2.08	129.38	124.03
22	K	205	BCR	C12-C13-C14	2.08	122.28	119.01
18	B	807	CLA	O2A-CGA-O1A	-2.08	118.43	123.63
17	4	606	CHL	CAC-C3C-C4C	2.08	129.37	124.03
24	A	801	CL0	C3C-C4C-NC	2.08	119.73	114.65
18	F	301	CLA	O2A-CGA-O1A	-2.08	118.43	123.63
18	B	825	CLA	CMB-C2B-C3B	2.08	131.44	126.55
18	A	820	CLA	CMB-C2B-C3B	2.08	131.43	126.55
18	B	814	CLA	O2A-CGA-O1A	-2.08	118.44	123.63
18	A	834	CLA	O2A-CGA-O1A	-2.07	118.44	123.63
18	A	842	CLA	CMB-C2B-C3B	2.07	131.43	126.55
18	B	825	CLA	O2A-CGA-O1A	-2.07	118.44	123.63
22	L	306	BCR	C24-C23-C22	2.07	129.30	126.23
22	B	847	BCR	C37-C22-C23	2.07	121.25	118.09
18	A	840	CLA	O2A-CGA-O1A	-2.07	118.45	123.63
22	A	850	BCR	C19-C18-C17	2.07	122.26	119.01
18	B	838	CLA	O2A-CGA-O1A	-2.07	118.45	123.63
17	2	615	CHL	C4C-CHD-C1D	2.07	123.47	116.07
17	4	605	CHL	C4C-CHD-C1D	2.07	123.47	116.07
18	B	806	CLA	O2A-CGA-O1A	-2.07	118.46	123.63
20	2	618	LHG	O7-C7-C8	2.07	115.95	111.48
22	L	305	BCR	C8-C9-C10	2.07	122.26	119.01
18	B	802	CLA	O2A-CGA-O1A	-2.07	118.46	123.63
18	F	302	CLA	O2A-CGA-O1A	-2.07	118.46	123.63
18	A	813	CLA	O2A-CGA-O1A	-2.06	118.47	123.63
18	B	818	CLA	CMB-C2B-C3B	2.06	131.40	126.55
22	K	205	BCR	C11-C12-C13	2.06	132.02	126.36
18	A	832	CLA	O2A-CGA-O1A	-2.06	118.47	123.63
18	A	803	CLA	C1-C2-C3	-2.06	122.82	126.20
18	A	827	CLA	C1-C2-C3	-2.06	122.82	126.20
22	B	845	BCR	C16-C15-C14	2.06	127.73	123.52
19	1	614	XAT	C7-C8-C9	-2.06	122.34	125.53
18	2	609	CLA	CMB-C2B-C3B	2.06	131.39	126.55
18	B	809	CLA	O2A-CGA-O1A	-2.06	118.48	123.63
18	A	810	CLA	O2D-CGD-CBD	2.06	114.82	111.23
22	B	847	BCR	C8-C9-C10	2.05	122.23	119.01
22	A	849	BCR	C34-C9-C8	2.05	121.22	118.09
18	4	602	CLA	O2A-CGA-O1A	-2.05	118.50	123.63
17	4	615	CHL	CAC-C3C-C4C	2.05	129.30	124.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	3	609	CLA	O2A-CGA-O1A	-2.05	118.50	123.63
22	B	846	BCR	C1-C6-C7	2.05	121.21	115.65
18	A	831	CLA	O2A-CGA-O1A	-2.05	118.51	123.63
18	A	807	CLA	O2A-CGA-O1A	-2.05	118.51	123.63
18	L	303	CLA	O2A-CGA-O1A	-2.05	118.51	123.63
18	B	813	CLA	CMB-C2B-C1B	-2.04	122.31	125.42
18	4	612	CLA	O2A-CGA-O1A	-2.04	118.53	123.63
18	A	822	CLA	O2A-CGA-O1A	-2.04	118.53	123.63
18	A	830	CLA	C2A-C1A-CHA	2.04	127.40	123.87
18	A	823	CLA	CMB-C2B-C1B	-2.03	122.32	125.42
18	A	811	CLA	O2A-CGA-O1A	-2.03	118.54	123.63
18	G	203	CLA	CMB-C2B-C1B	-2.03	122.32	125.42
17	2	606	CHL	C4C-CHD-C1D	2.03	123.33	116.07
18	A	819	CLA	O2A-CGA-O1A	-2.03	118.56	123.63
21	1	616	LUT	C10-C11-C12	2.03	129.07	123.20
18	3	603	CLA	CMB-C2B-C1B	-2.03	122.33	125.42
18	B	833	CLA	O2A-CGA-O1A	-2.03	118.12	123.33
18	A	835	CLA	O2A-CGA-O1A	-2.03	118.56	123.63
18	2	612	CLA	O2A-CGA-O1A	-2.02	118.56	123.63
18	B	827	CLA	O2A-CGA-O1A	-2.02	118.56	123.63
22	A	850	BCR	C10-C11-C12	2.02	129.06	123.20
17	2	615	CHL	CAC-C3C-C4C	2.02	129.23	124.03
18	B	811	CLA	C1-C2-C3	-2.02	122.89	126.20
17	2	606	CHL	CAC-C3C-C4C	2.02	129.23	124.03
18	A	819	CLA	C1-C2-C3	-2.02	122.89	126.20
18	1	608	CLA	CMA-C3A-C2A	-2.02	111.60	116.23
19	4	617	XAT	C16-C1-C2	-2.02	105.42	108.97
18	A	839	CLA	C1-C2-C3	-2.02	122.89	126.20
22	B	847	BCR	C1-C6-C7	2.02	121.12	115.65
22	A	853	BCR	C23-C22-C21	2.01	122.18	119.01
22	A	852	BCR	C11-C12-C13	2.01	131.89	126.36
18	G	201	CLA	O2D-CGD-CBD	2.01	114.75	111.23
18	A	828	CLA	C1-C2-C3	-2.01	122.90	126.20
18	B	804	CLA	CMA-C3A-C2A	-2.01	111.62	116.23
22	G	204	BCR	C1-C6-C7	2.01	121.11	115.65
18	A	845	CLA	O2A-CGA-O1A	-2.01	118.60	123.63
17	1	606	CHL	CAC-C3C-C4C	2.01	129.20	124.03
18	B	818	CLA	O2A-CGA-O1A	-2.01	118.60	123.63
22	B	848	BCR	C30-C25-C26	-2.01	119.89	122.64
22	A	849	BCR	C27-C26-C25	-2.01	119.99	122.70
18	A	826	CLA	O2A-CGA-O1A	-2.01	118.61	123.63
17	1	601	CHL	CAC-C3C-C4C	2.00	129.18	124.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	2	615	CHL	CMA-C3A-C4A	-2.00	110.29	114.61
22	4	618	BCR	C1-C6-C7	2.00	121.09	115.65
17	1	606	CHL	C4C-CHD-C1D	2.00	123.23	116.07
18	2	612	CLA	CMB-C2B-C3B	2.00	131.26	126.55

All (179) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
17	1	601	CHL	ND
17	1	601	CHL	NC
17	1	601	CHL	NA
17	1	606	CHL	ND
17	1	606	CHL	NC
17	1	606	CHL	NA
17	2	605	CHL	ND
17	2	605	CHL	NC
17	2	605	CHL	NA
17	2	615	CHL	ND
17	2	615	CHL	NC
17	2	615	CHL	NA
17	2	601	CHL	ND
17	2	601	CHL	NC
17	2	601	CHL	NA
17	2	606	CHL	ND
17	2	606	CHL	NC
17	2	606	CHL	NA
17	2	607	CHL	ND
17	2	607	CHL	NC
17	2	607	CHL	NA
17	3	606	CHL	ND
17	3	606	CHL	NC
17	3	606	CHL	NA
17	4	606	CHL	ND
17	4	606	CHL	NC
17	4	606	CHL	NA
17	4	615	CHL	ND
17	4	615	CHL	NC
17	4	615	CHL	NA
17	4	605	CHL	ND
17	4	605	CHL	NC
17	4	605	CHL	NA
17	4	607	CHL	ND

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Mol	Chain	Res	Type	Atom
17	4	607	CHL	NC
17	4	607	CHL	NA
18	1	602	CLA	ND
18	1	603	CLA	ND
18	1	604	CLA	ND
18	1	605	CLA	ND
18	1	607	CLA	ND
18	1	608	CLA	ND
18	1	609	CLA	ND
18	1	610	CLA	ND
18	1	611	CLA	ND
18	1	612	CLA	ND
18	1	613	CLA	ND
18	2	611	CLA	ND
18	2	612	CLA	ND
18	2	609	CLA	ND
18	2	602	CLA	ND
18	2	604	CLA	ND
18	2	613	CLA	ND
18	2	610	CLA	ND
18	2	608	CLA	ND
18	2	603	CLA	ND
18	3	605	CLA	ND
18	3	611	CLA	ND
18	3	608	CLA	ND
18	3	609	CLA	ND
18	3	604	CLA	ND
18	3	603	CLA	ND
18	3	601	CLA	ND
18	3	612	CLA	ND
18	3	610	CLA	ND
18	3	607	CLA	ND
18	3	602	CLA	ND
18	4	602	CLA	ND
18	4	601	CLA	ND
18	4	608	CLA	ND
18	4	609	CLA	ND
18	4	613	CLA	ND
18	4	612	CLA	ND
18	4	611	CLA	ND
18	4	610	CLA	ND
18	4	604	CLA	ND

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Mol	Chain	Res	Type	Atom
18	4	614	CLA	ND
18	4	603	CLA	ND
18	A	819	CLA	ND
18	A	807	CLA	ND
18	A	805	CLA	ND
18	A	822	CLA	ND
18	A	821	CLA	ND
18	A	818	CLA	ND
18	A	825	CLA	ND
18	A	820	CLA	ND
18	A	806	CLA	ND
18	A	809	CLA	ND
18	A	804	CLA	ND
18	A	813	CLA	ND
18	A	808	CLA	ND
18	A	811	CLA	ND
18	A	810	CLA	ND
18	A	823	CLA	ND
18	A	824	CLA	ND
18	A	826	CLA	ND
18	A	803	CLA	ND
18	A	802	CLA	ND
18	A	830	CLA	ND
18	A	840	CLA	ND
18	A	845	CLA	ND
18	A	831	CLA	ND
18	A	835	CLA	ND
18	A	842	CLA	ND
18	A	834	CLA	ND
18	A	843	CLA	ND
18	A	844	CLA	ND
18	A	841	CLA	ND
18	A	839	CLA	ND
18	A	817	CLA	ND
18	A	815	CLA	ND
18	A	814	CLA	ND
18	A	816	CLA	ND
18	A	828	CLA	ND
18	A	827	CLA	ND
18	A	833	CLA	ND
18	A	812	CLA	ND
18	A	829	CLA	ND

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Mol	Chain	Res	Type	Atom
18	A	836	CLA	ND
18	A	838	CLA	ND
18	A	832	CLA	ND
18	A	837	CLA	ND
18	B	818	CLA	ND
18	B	830	CLA	ND
18	B	837	CLA	ND
18	B	821	CLA	ND
18	B	805	CLA	ND
18	B	826	CLA	ND
18	B	835	CLA	ND
18	B	834	CLA	ND
18	B	823	CLA	ND
18	B	833	CLA	ND
18	B	808	CLA	ND
18	B	819	CLA	ND
18	B	809	CLA	ND
18	B	810	CLA	ND
18	B	811	CLA	ND
18	B	816	CLA	ND
18	B	841	CLA	ND
18	B	831	CLA	ND
18	B	814	CLA	ND
18	B	827	CLA	ND
18	B	828	CLA	ND
18	B	813	CLA	ND
18	B	812	CLA	ND
18	B	806	CLA	ND
18	B	824	CLA	ND
18	B	825	CLA	ND
18	B	832	CLA	ND
18	B	839	CLA	ND
18	B	802	CLA	ND
18	B	807	CLA	ND
18	B	820	CLA	ND
18	B	815	CLA	ND
18	B	803	CLA	ND
18	B	829	CLA	ND
18	B	804	CLA	ND
18	B	817	CLA	ND
18	B	822	CLA	ND
18	B	836	CLA	ND

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Mol	Chain	Res	Type	Atom
18	B	840	CLA	ND
18	B	838	CLA	ND
18	F	303	CLA	ND
18	F	301	CLA	ND
18	F	302	CLA	ND
18	G	201	CLA	ND
18	G	202	CLA	ND
18	G	203	CLA	ND
18	H	201	CLA	ND
18	J	101	CLA	ND
18	K	206	CLA	ND
18	K	201	CLA	ND
18	K	204	CLA	ND
18	K	203	CLA	ND
18	L	304	CLA	ND
18	L	303	CLA	ND
18	L	302	CLA	ND
24	A	801	CL0	NC
24	A	801	CL0	NA

All (1473) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
17	2	605	CHL	C1C-C2C-CMC-OMC
17	2	605	CHL	C3C-C2C-CMC-OMC
17	2	601	CHL	C3A-C2A-CAA-CBA
17	2	607	CHL	CHA-CBD-CGD-O1D
17	3	606	CHL	CHA-CBD-CGD-O2D
17	3	606	CHL	CBD-CGD-O2D-CED
18	1	604	CLA	C1A-C2A-CAA-CBA
18	1	605	CLA	C1A-C2A-CAA-CBA
18	1	605	CLA	C3A-C2A-CAA-CBA
18	1	605	CLA	CBA-CGA-O2A-C1
18	1	607	CLA	C1A-C2A-CAA-CBA
18	1	607	CLA	C3A-C2A-CAA-CBA
18	1	608	CLA	CBD-CGD-O2D-CED
18	1	609	CLA	CBD-CGD-O2D-CED
18	1	611	CLA	CHA-CBD-CGD-O1D
18	1	611	CLA	CHA-CBD-CGD-O2D
18	1	612	CLA	CHA-CBD-CGD-O2D
18	2	612	CLA	C11-C12-C13-C14
18	2	602	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
18	2	602	CLA	CHA-CBD-CGD-O2D
18	2	604	CLA	CAA-CBA-CGA-O1A
18	2	604	CLA	CHA-CBD-CGD-O1D
18	2	604	CLA	CHA-CBD-CGD-O2D
18	2	613	CLA	C2B-C3B-CAB-CBB
18	2	613	CLA	C4B-C3B-CAB-CBB
18	2	613	CLA	CBD-CGD-O2D-CED
18	2	610	CLA	CMA-C3A-C4A-CHB
18	2	610	CLA	CMA-C3A-C4A-NA
18	2	608	CLA	C3A-C2A-CAA-CBA
18	3	605	CLA	C1A-C2A-CAA-CBA
18	3	605	CLA	C3A-C2A-CAA-CBA
18	3	605	CLA	CAD-CBD-CGD-O1D
18	3	605	CLA	CAD-CBD-CGD-O2D
18	3	603	CLA	C1A-C2A-CAA-CBA
18	3	603	CLA	C3A-C2A-CAA-CBA
18	3	603	CLA	CHA-CBD-CGD-O2D
18	3	601	CLA	CHA-CBD-CGD-O1D
18	3	601	CLA	CHA-CBD-CGD-O2D
18	4	608	CLA	C1A-C2A-CAA-CBA
18	4	608	CLA	C3A-C2A-CAA-CBA
18	4	609	CLA	CBD-CGD-O2D-CED
18	4	613	CLA	C1A-C2A-CAA-CBA
18	4	612	CLA	CBD-CGD-O2D-CED
18	4	612	CLA	C6-C7-C8-C9
18	4	604	CLA	CBD-CGD-O2D-CED
18	4	614	CLA	CHA-CBD-CGD-O1D
18	4	614	CLA	CHA-CBD-CGD-O2D
18	A	819	CLA	C1A-C2A-CAA-CBA
18	A	819	CLA	C3A-C2A-CAA-CBA
18	A	805	CLA	C3A-C2A-CAA-CBA
18	A	822	CLA	C1A-C2A-CAA-CBA
18	A	818	CLA	CBD-CGD-O2D-CED
18	A	825	CLA	C1A-C2A-CAA-CBA
18	A	825	CLA	C3A-C2A-CAA-CBA
18	A	820	CLA	C1A-C2A-CAA-CBA
18	A	820	CLA	C3A-C2A-CAA-CBA
18	A	806	CLA	C1A-C2A-CAA-CBA
18	A	806	CLA	C3A-C2A-CAA-CBA
18	A	806	CLA	CAD-CBD-CGD-O1D
18	A	806	CLA	CAD-CBD-CGD-O2D
18	A	809	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
18	A	809	CLA	CHA-CBD-CGD-O2D
18	A	804	CLA	C1A-C2A-CAA-CBA
18	A	804	CLA	CAD-CBD-CGD-O1D
18	A	804	CLA	CAD-CBD-CGD-O2D
18	A	804	CLA	C11-C10-C8-C9
18	A	813	CLA	CHA-CBD-CGD-O1D
18	A	813	CLA	CHA-CBD-CGD-O2D
18	A	811	CLA	CBD-CGD-O2D-CED
18	A	823	CLA	C1A-C2A-CAA-CBA
18	A	823	CLA	C3A-C2A-CAA-CBA
18	A	826	CLA	C11-C12-C13-C14
18	A	802	CLA	C1A-C2A-CAA-CBA
18	A	802	CLA	C3A-C2A-CAA-CBA
18	A	802	CLA	CBD-CGD-O2D-CED
18	A	830	CLA	C1A-C2A-CAA-CBA
18	A	830	CLA	O2A-C1-C2-C3
18	A	845	CLA	C3A-C2A-CAA-CBA
18	A	845	CLA	C2B-C3B-CAB-CBB
18	A	845	CLA	C4B-C3B-CAB-CBB
18	A	835	CLA	CHA-CBD-CGD-O1D
18	A	835	CLA	CHA-CBD-CGD-O2D
18	A	842	CLA	C1A-C2A-CAA-CBA
18	A	842	CLA	C3A-C2A-CAA-CBA
18	A	841	CLA	C1A-C2A-CAA-CBA
18	A	841	CLA	C3A-C2A-CAA-CBA
18	A	841	CLA	CBD-CGD-O2D-CED
18	A	817	CLA	C1A-C2A-CAA-CBA
18	A	817	CLA	C3A-C2A-CAA-CBA
18	A	814	CLA	C1A-C2A-CAA-CBA
18	A	814	CLA	C3A-C2A-CAA-CBA
18	A	827	CLA	C3A-C2A-CAA-CBA
18	A	812	CLA	C2B-C3B-CAB-CBB
18	A	812	CLA	C4B-C3B-CAB-CBB
18	A	836	CLA	C1A-C2A-CAA-CBA
18	B	818	CLA	C3A-C2A-CAA-CBA
18	B	830	CLA	CBD-CGD-O2D-CED
18	B	821	CLA	C1A-C2A-CAA-CBA
18	B	805	CLA	C1A-C2A-CAA-CBA
18	B	805	CLA	C3A-C2A-CAA-CBA
18	B	805	CLA	C6-C7-C8-C9
18	B	826	CLA	C1A-C2A-CAA-CBA
18	B	835	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
18	B	834	CLA	C1A-C2A-CAA-CBA
18	B	834	CLA	C3A-C2A-CAA-CBA
18	B	823	CLA	C1A-C2A-CAA-CBA
18	B	823	CLA	C3A-C2A-CAA-CBA
18	B	833	CLA	CHA-CBD-CGD-O1D
18	B	833	CLA	CHA-CBD-CGD-O2D
18	B	819	CLA	C1A-C2A-CAA-CBA
18	B	819	CLA	C3A-C2A-CAA-CBA
18	B	819	CLA	C2B-C3B-CAB-CBB
18	B	819	CLA	C4B-C3B-CAB-CBB
18	B	819	CLA	CHA-CBD-CGD-O1D
18	B	819	CLA	CHA-CBD-CGD-O2D
18	B	809	CLA	C1A-C2A-CAA-CBA
18	B	811	CLA	C1A-C2A-CAA-CBA
18	B	811	CLA	CHA-CBD-CGD-O1D
18	B	811	CLA	CHA-CBD-CGD-O2D
18	B	814	CLA	C11-C10-C8-C9
18	B	827	CLA	C1A-C2A-CAA-CBA
18	B	827	CLA	C3A-C2A-CAA-CBA
18	B	827	CLA	C11-C12-C13-C15
18	B	828	CLA	C1A-C2A-CAA-CBA
18	B	828	CLA	C3A-C2A-CAA-CBA
18	B	825	CLA	C1A-C2A-CAA-CBA
18	B	825	CLA	C3A-C2A-CAA-CBA
18	B	825	CLA	CHA-CBD-CGD-O1D
18	B	825	CLA	CHA-CBD-CGD-O2D
18	B	825	CLA	C11-C12-C13-C14
18	B	832	CLA	C1A-C2A-CAA-CBA
18	B	832	CLA	C3A-C2A-CAA-CBA
18	B	802	CLA	C3A-C2A-CAA-CBA
18	B	802	CLA	CBD-CGD-O2D-CED
18	B	820	CLA	C1A-C2A-CAA-CBA
18	B	820	CLA	C3A-C2A-CAA-CBA
18	B	803	CLA	CBD-CGD-O2D-CED
18	B	803	CLA	O1D-CGD-O2D-CED
18	B	804	CLA	CHA-CBD-CGD-O1D
18	B	804	CLA	CHA-CBD-CGD-O2D
18	B	817	CLA	C2B-C3B-CAB-CBB
18	B	817	CLA	C4B-C3B-CAB-CBB
18	B	822	CLA	C1A-C2A-CAA-CBA
18	B	836	CLA	CHA-CBD-CGD-O1D
18	B	836	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
18	B	840	CLA	C1A-C2A-CAA-CBA
18	B	840	CLA	C3A-C2A-CAA-CBA
18	B	840	CLA	C6-C7-C8-C9
18	F	303	CLA	CHA-CBD-CGD-O2D
18	F	301	CLA	CBD-CGD-O2D-CED
18	F	302	CLA	CBD-CGD-O2D-CED
18	G	201	CLA	CHA-CBD-CGD-O1D
18	G	201	CLA	CHA-CBD-CGD-O2D
18	G	202	CLA	C1A-C2A-CAA-CBA
18	G	202	CLA	C3A-C2A-CAA-CBA
18	H	201	CLA	CBD-CGD-O2D-CED
18	K	204	CLA	C1A-C2A-CAA-CBA
18	K	204	CLA	CHA-CBD-CGD-O1D
18	K	204	CLA	CHA-CBD-CGD-O2D
18	K	204	CLA	CBD-CGD-O2D-CED
18	K	203	CLA	C1A-C2A-CAA-CBA
18	L	304	CLA	C2B-C3B-CAB-CBB
18	L	304	CLA	C4B-C3B-CAB-CBB
19	1	614	XAT	C5-C6-C7-C8
19	1	614	XAT	O4-C6-C7-C8
19	1	614	XAT	C7-C8-C9-C10
19	1	614	XAT	C11-C12-C13-C14
19	1	614	XAT	O24-C26-C27-C28
19	2	617	XAT	O4-C6-C7-C8
19	2	617	XAT	C11-C10-C9-C19
19	2	617	XAT	C10-C11-C12-C13
19	2	617	XAT	C13-C14-C15-C35
19	2	617	XAT	O24-C26-C27-C28
19	2	617	XAT	C28-C29-C30-C31
19	2	617	XAT	C39-C29-C30-C31
19	2	617	XAT	C33-C34-C35-C15
20	1	615	LHG	C1-C2-C3-O3
20	1	615	LHG	C2-C3-O3-P
20	1	615	LHG	C3-O3-P-O4
20	1	615	LHG	C3-O3-P-O5
20	1	615	LHG	C3-O3-P-O6
20	1	615	LHG	C4-O6-P-O5
20	1	615	LHG	O7-C5-C6-O8
20	2	618	LHG	C3-O3-P-O5
20	2	618	LHG	O9-C7-O7-C5
20	2	618	LHG	C8-C7-O7-C5
20	2	618	LHG	O10-C23-O8-C6

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Mol	Chain	Res	Type	Atoms
20	2	618	LHG	C24-C23-O8-C6
20	A	846	LHG	O10-C23-O8-C6
20	A	846	LHG	C24-C23-O8-C6
20	B	851	LHG	C8-C7-O7-C5
20	B	852	LHG	C2-C3-O3-P
20	B	852	LHG	C3-O3-P-O5
20	B	852	LHG	C4-O6-P-O3
20	B	852	LHG	C4-O6-P-O4
21	2	619	LUT	C5-C6-C7-C8
21	2	619	LUT	C25-C26-C27-C28
21	3	613	LUT	C9-C10-C11-C12
21	3	613	LUT	C21-C26-C27-C28
21	3	613	LUT	C25-C26-C27-C28
22	3	614	BCR	C21-C22-C23-C24
22	4	618	BCR	C23-C24-C25-C26
22	A	849	BCR	C23-C24-C25-C26
22	A	849	BCR	C23-C24-C25-C30
22	A	852	BCR	C35-C13-C14-C15
22	A	852	BCR	C14-C15-C16-C17
22	A	852	BCR	C16-C17-C18-C19
22	A	852	BCR	C16-C17-C18-C36
22	B	846	BCR	C23-C24-C25-C26
22	B	846	BCR	C23-C24-C25-C30
22	B	844	BCR	C12-C13-C14-C15
22	B	844	BCR	C35-C13-C14-C15
22	B	844	BCR	C18-C19-C20-C21
22	B	801	BCR	C1-C6-C7-C8
22	B	801	BCR	C5-C6-C7-C8
22	B	849	BCR	C22-C23-C24-C25
22	F	304	BCR	C15-C16-C17-C18
27	B	850	DGD	O2G-C2G-C3G-O3G
18	2	609	CLA	O1D-CGD-O2D-CED
18	4	604	CLA	O1D-CGD-O2D-CED
18	B	802	CLA	O1D-CGD-O2D-CED
18	H	201	CLA	O1D-CGD-O2D-CED
18	1	608	CLA	O1D-CGD-O2D-CED
18	3	608	CLA	O1D-CGD-O2D-CED
18	4	609	CLA	O1D-CGD-O2D-CED
18	A	818	CLA	O1D-CGD-O2D-CED
18	A	802	CLA	O1D-CGD-O2D-CED
18	A	829	CLA	O1D-CGD-O2D-CED
18	K	204	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
18	1	605	CLA	CBD-CGD-O2D-CED
18	2	612	CLA	CBD-CGD-O2D-CED
18	2	609	CLA	CBD-CGD-O2D-CED
18	2	608	CLA	CBD-CGD-O2D-CED
18	3	608	CLA	CBD-CGD-O2D-CED
18	4	614	CLA	CBD-CGD-O2D-CED
18	A	813	CLA	CBD-CGD-O2D-CED
18	A	803	CLA	CBD-CGD-O2D-CED
18	A	829	CLA	CBD-CGD-O2D-CED
18	B	822	CLA	CBD-CGD-O2D-CED
18	G	201	CLA	CBD-CGD-O2D-CED
18	3	602	CLA	O1A-CGA-O2A-C1
18	A	803	CLA	O1A-CGA-O2A-C1
18	A	830	CLA	O1A-CGA-O2A-C1
18	A	835	CLA	O1A-CGA-O2A-C1
18	B	802	CLA	O1A-CGA-O2A-C1
18	B	836	CLA	O1A-CGA-O2A-C1
18	F	302	CLA	O1D-CGD-O2D-CED
18	B	822	CLA	O1D-CGD-O2D-CED
18	3	602	CLA	CBA-CGA-O2A-C1
18	A	803	CLA	CBA-CGA-O2A-C1
18	A	830	CLA	CBA-CGA-O2A-C1
18	A	835	CLA	CBA-CGA-O2A-C1
18	B	816	CLA	CBD-CGD-O2D-CED
18	1	603	CLA	O1A-CGA-O2A-C1
18	2	609	CLA	O1A-CGA-O2A-C1
18	B	814	CLA	O1A-CGA-O2A-C1
18	1	605	CLA	O1A-CGA-O2A-C1
18	2	613	CLA	O1D-CGD-O2D-CED
18	A	811	CLA	O1D-CGD-O2D-CED
18	B	830	CLA	O1D-CGD-O2D-CED
18	G	201	CLA	O1D-CGD-O2D-CED
18	1	609	CLA	O1D-CGD-O2D-CED
18	4	612	CLA	O1D-CGD-O2D-CED
18	A	841	CLA	O1D-CGD-O2D-CED
18	F	301	CLA	O1D-CGD-O2D-CED
18	3	605	CLA	CBD-CGD-O2D-CED
18	3	607	CLA	CBD-CGD-O2D-CED
18	B	827	CLA	O1A-CGA-O2A-C1
20	B	851	LHG	O9-C7-O7-C5
18	3	602	CLA	C3-C5-C6-C7
18	A	819	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
18	A	807	CLA	C3-C5-C6-C7
18	A	818	CLA	C3-C5-C6-C7
18	A	803	CLA	C3-C5-C6-C7
18	A	834	CLA	C3-C5-C6-C7
18	A	843	CLA	C3-C5-C6-C7
18	A	844	CLA	C3-C5-C6-C7
18	A	841	CLA	C3-C5-C6-C7
18	A	814	CLA	C3-C5-C6-C7
18	A	828	CLA	C3-C5-C6-C7
18	B	805	CLA	C3-C5-C6-C7
18	B	841	CLA	C3-C5-C6-C7
18	B	814	CLA	C3-C5-C6-C7
18	B	806	CLA	C3-C5-C6-C7
18	B	840	CLA	C3-C5-C6-C7
18	H	201	CLA	C3-C5-C6-C7
18	B	802	CLA	CBA-CGA-O2A-C1
18	B	836	CLA	CBA-CGA-O2A-C1
17	2	607	CHL	CBD-CGD-O2D-CED
17	4	607	CHL	CBD-CGD-O2D-CED
18	2	604	CLA	CBD-CGD-O2D-CED
18	A	834	CLA	CBD-CGD-O2D-CED
18	B	835	CLA	CBD-CGD-O2D-CED
18	B	819	CLA	CBD-CGD-O2D-CED
18	B	809	CLA	CBD-CGD-O2D-CED
18	B	827	CLA	CBD-CGD-O2D-CED
17	3	606	CHL	O1D-CGD-O2D-CED
18	2	602	CLA	C4-C3-C5-C6
18	A	820	CLA	C4-C3-C5-C6
18	A	839	CLA	C4-C3-C5-C6
18	B	809	CLA	C4-C3-C5-C6
18	B	814	CLA	C4-C3-C5-C6
18	B	824	CLA	C4-C3-C5-C6
18	F	301	CLA	C4-C3-C5-C6
18	2	602	CLA	C2-C3-C5-C6
18	A	820	CLA	C2-C3-C5-C6
18	A	839	CLA	C2-C3-C5-C6
18	B	814	CLA	C2-C3-C5-C6
18	B	824	CLA	C2-C3-C5-C6
18	F	301	CLA	C2-C3-C5-C6
18	A	806	CLA	CBD-CGD-O2D-CED
18	H	201	CLA	C2A-CAA-CBA-CGA
18	A	833	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
18	B	829	CLA	C3-C5-C6-C7
18	1	603	CLA	CBA-CGA-O2A-C1
18	2	609	CLA	CBA-CGA-O2A-C1
18	B	814	CLA	CBA-CGA-O2A-C1
18	B	827	CLA	CBA-CGA-O2A-C1
21	1	616	LUT	C29-C30-C31-C32
21	2	616	LUT	C33-C34-C35-C15
21	3	613	LUT	C33-C34-C35-C15
22	A	849	BCR	C15-C16-C17-C18
22	A	849	BCR	C19-C20-C21-C22
22	A	853	BCR	C9-C10-C11-C12
22	A	850	BCR	C13-C14-C15-C16
22	A	850	BCR	C15-C16-C17-C18
22	A	851	BCR	C13-C14-C15-C16
22	B	801	BCR	C9-C10-C11-C12
22	B	843	BCR	C13-C14-C15-C16
22	B	845	BCR	C19-C20-C21-C22
22	F	304	BCR	C19-C20-C21-C22
18	A	818	CLA	O1A-CGA-O2A-C1
18	A	820	CLA	O1A-CGA-O2A-C1
18	A	811	CLA	O1A-CGA-O2A-C1
18	A	839	CLA	O1A-CGA-O2A-C1
18	L	303	CLA	O1A-CGA-O2A-C1
18	B	827	CLA	C3-C5-C6-C7
18	L	303	CLA	C3-C5-C6-C7
24	A	801	CL0	C3-C5-C6-C7
17	2	601	CHL	CBD-CGD-O2D-CED
18	3	603	CLA	CBD-CGD-O2D-CED
18	B	840	CLA	CBD-CGD-O2D-CED
20	1	615	LHG	O2-C2-C3-O3
18	4	614	CLA	O1D-CGD-O2D-CED
18	A	818	CLA	CBA-CGA-O2A-C1
18	A	839	CLA	CBA-CGA-O2A-C1
18	L	303	CLA	CBA-CGA-O2A-C1
17	4	606	CHL	CBD-CGD-O2D-CED
18	3	602	CLA	CBD-CGD-O2D-CED
18	A	839	CLA	CBD-CGD-O2D-CED
18	A	813	CLA	O1D-CGD-O2D-CED
18	4	602	CLA	C3-C5-C6-C7
18	B	803	CLA	C3-C5-C6-C7
18	B	822	CLA	C3-C5-C6-C7
18	1	602	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
18	4	603	CLA	CBD-CGD-O2D-CED
18	B	813	CLA	CBD-CGD-O2D-CED
18	J	101	CLA	CBD-CGD-O2D-CED
18	1	605	CLA	O1D-CGD-O2D-CED
18	2	612	CLA	O1D-CGD-O2D-CED
18	A	803	CLA	O1D-CGD-O2D-CED
18	A	820	CLA	CBA-CGA-O2A-C1
18	A	811	CLA	CBA-CGA-O2A-C1
25	B	842	PQN	C14-C13-C15-C16
25	B	842	PQN	C12-C13-C15-C16
17	2	606	CHL	CBD-CGD-O2D-CED
17	3	606	CHL	C2A-CAA-CBA-CGA
18	2	608	CLA	O1D-CGD-O2D-CED
18	A	842	CLA	CBA-CGA-O2A-C1
18	A	838	CLA	CBA-CGA-O2A-C1
18	1	612	CLA	CBD-CGD-O2D-CED
18	2	610	CLA	CBD-CGD-O2D-CED
18	3	601	CLA	CBD-CGD-O2D-CED
18	B	834	CLA	CBD-CGD-O2D-CED
18	B	816	CLA	O1D-CGD-O2D-CED
18	A	842	CLA	O1A-CGA-O2A-C1
18	A	838	CLA	O1A-CGA-O2A-C1
18	3	605	CLA	O1D-CGD-O2D-CED
17	1	601	CHL	CBA-CGA-O2A-C1
18	A	825	CLA	CBA-CGA-O2A-C1
18	A	802	CLA	CBA-CGA-O2A-C1
18	A	845	CLA	CBA-CGA-O2A-C1
18	B	822	CLA	CBA-CGA-O2A-C1
18	F	301	CLA	CBA-CGA-O2A-C1
20	1	615	LHG	C26-C27-C28-C29
18	K	203	CLA	CBD-CGD-O2D-CED
18	3	607	CLA	O1D-CGD-O2D-CED
18	A	834	CLA	O1D-CGD-O2D-CED
18	A	833	CLA	C4-C3-C5-C6
18	A	833	CLA	C2-C3-C5-C6
18	B	809	CLA	C2-C3-C5-C6
18	3	601	CLA	C11-C10-C8-C9
18	4	612	CLA	C11-C10-C8-C9
18	A	819	CLA	C6-C7-C8-C9
18	A	807	CLA	C11-C10-C8-C9
18	A	820	CLA	C11-C10-C8-C9
18	A	806	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
18	A	811	CLA	C14-C13-C15-C16
18	A	826	CLA	C11-C10-C8-C9
18	A	802	CLA	C11-C12-C13-C14
18	A	835	CLA	C11-C10-C8-C9
18	A	841	CLA	C14-C13-C15-C16
18	A	812	CLA	C6-C7-C8-C9
18	B	805	CLA	C11-C10-C8-C9
18	B	808	CLA	C6-C7-C8-C9
18	B	808	CLA	C14-C13-C15-C16
18	B	809	CLA	C11-C10-C8-C9
18	B	828	CLA	C14-C13-C15-C16
18	B	825	CLA	C14-C13-C15-C16
18	B	802	CLA	C11-C12-C13-C14
18	B	803	CLA	C11-C10-C8-C9
18	B	840	CLA	C14-C13-C15-C16
18	F	301	CLA	C6-C7-C8-C9
18	H	201	CLA	C6-C7-C8-C9
17	4	607	CHL	O1D-CGD-O2D-CED
17	2	607	CHL	O1D-CGD-O2D-CED
18	B	822	CLA	O1A-CGA-O2A-C1
19	1	614	XAT	C7-C8-C9-C19
19	1	614	XAT	C11-C12-C13-C20
19	4	617	XAT	C7-C8-C9-C19
22	3	614	BCR	C37-C22-C23-C24
22	A	852	BCR	C37-C22-C23-C24
22	A	850	BCR	C7-C8-C9-C34
22	A	851	BCR	C11-C12-C13-C35
22	B	846	BCR	C7-C8-C9-C34
22	B	845	BCR	C36-C18-C19-C20
22	B	845	BCR	C37-C22-C23-C24
22	F	304	BCR	C11-C12-C13-C35
22	J	102	BCR	C7-C8-C9-C34
22	L	306	BCR	C7-C8-C9-C34
19	4	617	XAT	C7-C8-C9-C10
22	A	852	BCR	C21-C22-C23-C24
22	A	850	BCR	C7-C8-C9-C10
22	A	851	BCR	C11-C12-C13-C14
22	B	846	BCR	C7-C8-C9-C10
22	B	845	BCR	C17-C18-C19-C20
22	B	845	BCR	C21-C22-C23-C24
22	F	304	BCR	C11-C12-C13-C14
22	J	102	BCR	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
22	L	306	BCR	C7-C8-C9-C10
18	A	822	CLA	C2A-CAA-CBA-CGA
18	A	838	CLA	C2A-CAA-CBA-CGA
18	B	841	CLA	CBD-CGD-O2D-CED
18	A	832	CLA	CBA-CGA-O2A-C1
18	A	812	CLA	C5-C6-C7-C8
18	A	843	CLA	C2-C1-O2A-CGA
18	2	604	CLA	O1D-CGD-O2D-CED
18	B	809	CLA	O1D-CGD-O2D-CED
17	2	615	CHL	CBD-CGD-O2D-CED
18	A	809	CLA	CBD-CGD-O2D-CED
18	4	602	CLA	C5-C6-C7-C8
18	A	828	CLA	C15-C16-C17-C18
18	A	819	CLA	CBD-CGD-O2D-CED
18	B	808	CLA	CBD-CGD-O2D-CED
18	A	804	CLA	C6-C7-C8-C10
18	A	829	CLA	C11-C10-C8-C7
18	B	810	CLA	C6-C7-C8-C10
18	B	841	CLA	C12-C13-C15-C16
18	A	842	CLA	C13-C15-C16-C17
18	B	835	CLA	O1D-CGD-O2D-CED
18	2	612	CLA	C3-C5-C6-C7
18	B	802	CLA	C3-C5-C6-C7
17	1	601	CHL	O1A-CGA-O2A-C1
18	A	802	CLA	O1A-CGA-O2A-C1
18	A	845	CLA	O1A-CGA-O2A-C1
18	A	816	CLA	CBD-CGD-O2D-CED
18	A	822	CLA	C15-C16-C17-C18
18	A	806	CLA	C10-C11-C12-C13
18	A	806	CLA	C13-C15-C16-C17
18	A	835	CLA	C15-C16-C17-C18
18	A	812	CLA	C10-C11-C12-C13
20	1	615	LHG	C5-C4-O6-P
17	2	601	CHL	C2A-CAA-CBA-CGA
17	2	607	CHL	C2A-CAA-CBA-CGA
18	1	605	CLA	C2A-CAA-CBA-CGA
18	2	611	CLA	C2A-CAA-CBA-CGA
18	2	608	CLA	C2A-CAA-CBA-CGA
18	2	603	CLA	C2A-CAA-CBA-CGA
18	A	809	CLA	C2A-CAA-CBA-CGA
18	A	843	CLA	C2A-CAA-CBA-CGA
18	A	832	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
18	B	813	CLA	C2A-CAA-CBA-CGA
18	B	832	CLA	C2A-CAA-CBA-CGA
18	B	839	CLA	C2A-CAA-CBA-CGA
18	B	802	CLA	C2A-CAA-CBA-CGA
22	K	205	BCR	C10-C11-C12-C13
18	2	602	CLA	C5-C6-C7-C8
18	A	831	CLA	C13-C15-C16-C17
18	B	837	CLA	C5-C6-C7-C8
18	B	826	CLA	C8-C10-C11-C12
18	B	814	CLA	C5-C6-C7-C8
18	B	822	CLA	C13-C15-C16-C17
20	1	615	LHG	C7-C8-C9-C10
18	B	819	CLA	O1D-CGD-O2D-CED
18	F	301	CLA	O1A-CGA-O2A-C1
18	A	819	CLA	C5-C6-C7-C8
18	A	820	CLA	C5-C6-C7-C8
18	A	804	CLA	C8-C10-C11-C12
18	A	835	CLA	C8-C10-C11-C12
18	A	828	CLA	C8-C10-C11-C12
18	A	812	CLA	C8-C10-C11-C12
18	B	805	CLA	C10-C11-C12-C13
18	B	808	CLA	C13-C15-C16-C17
18	B	806	CLA	C10-C11-C12-C13
18	B	841	CLA	CBA-CGA-O2A-C1
18	A	825	CLA	O1A-CGA-O2A-C1
18	2	602	CLA	C15-C16-C17-C18
18	A	844	CLA	C5-C6-C7-C8
18	A	806	CLA	O1D-CGD-O2D-CED
18	B	827	CLA	O1D-CGD-O2D-CED
18	H	201	CLA	C8-C10-C11-C12
20	1	615	LHG	C34-C35-C36-C37
18	B	840	CLA	O1D-CGD-O2D-CED
18	A	828	CLA	C5-C6-C7-C8
18	H	201	CLA	C5-C6-C7-C8
18	A	813	CLA	CBA-CGA-O2A-C1
18	J	101	CLA	CBA-CGA-O2A-C1
18	A	832	CLA	O1A-CGA-O2A-C1
18	B	808	CLA	C3-C5-C6-C7
18	A	804	CLA	C5-C6-C7-C8
18	1	607	CLA	C2A-CAA-CBA-CGA
18	G	203	CLA	C2A-CAA-CBA-CGA
18	3	602	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
18	A	843	CLA	CBA-CGA-O2A-C1
18	B	811	CLA	CBA-CGA-O2A-C1
18	3	601	CLA	C8-C10-C11-C12
18	A	806	CLA	C8-C10-C11-C12
18	A	828	CLA	C13-C15-C16-C17
18	B	814	CLA	C8-C10-C11-C12
18	B	813	CLA	C13-C15-C16-C17
18	A	836	CLA	CBD-CGD-O2D-CED
18	3	603	CLA	O1D-CGD-O2D-CED
18	A	842	CLA	C8-C10-C11-C12
18	A	829	CLA	C15-C16-C17-C18
18	B	817	CLA	C5-C6-C7-C8
18	B	840	CLA	C5-C6-C7-C8
17	2	601	CHL	O1D-CGD-O2D-CED
18	A	839	CLA	O1D-CGD-O2D-CED
18	A	807	CLA	C5-C6-C7-C8
18	A	829	CLA	C8-C10-C11-C12
18	B	806	CLA	C5-C6-C7-C8
17	4	606	CHL	O1D-CGD-O2D-CED
18	B	813	CLA	CBA-CGA-O2A-C1
18	B	817	CLA	CBA-CGA-O2A-C1
18	A	840	CLA	C4-C3-C5-C6
18	A	830	CLA	C3-C5-C6-C7
18	B	832	CLA	C15-C16-C17-C18
18	1	602	CLA	O1D-CGD-O2D-CED
18	A	819	CLA	CBA-CGA-O2A-C1
18	A	839	CLA	C6-C7-C8-C10
19	2	617	XAT	C20-C13-C14-C15
21	3	613	LUT	C11-C10-C9-C19
22	A	849	BCR	C20-C21-C22-C37
22	B	844	BCR	C16-C17-C18-C36
22	B	849	BCR	C11-C10-C9-C34
22	F	304	BCR	C35-C13-C14-C15
22	K	205	BCR	C20-C21-C22-C37
18	J	101	CLA	O1D-CGD-O2D-CED
24	A	801	CL0	C10-C11-C12-C13
19	2	617	XAT	C31-C32-C33-C40
21	2	616	LUT	C31-C32-C33-C40
22	4	618	BCR	C7-C8-C9-C34
22	A	853	BCR	C11-C12-C13-C35
22	B	846	BCR	C37-C22-C23-C24
22	K	205	BCR	C7-C8-C9-C34

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Mol	Chain	Res	Type	Atoms
22	K	205	BCR	C36-C18-C19-C20
22	L	306	BCR	C37-C22-C23-C24
21	2	616	LUT	C31-C32-C33-C34
22	A	853	BCR	C11-C12-C13-C14
22	L	306	BCR	C21-C22-C23-C24
18	A	813	CLA	O1A-CGA-O2A-C1
18	A	843	CLA	O1A-CGA-O2A-C1
18	1	603	CLA	C2A-CAA-CBA-CGA
18	A	812	CLA	C2A-CAA-CBA-CGA
18	B	826	CLA	C2A-CAA-CBA-CGA
18	B	809	CLA	C2A-CAA-CBA-CGA
18	B	817	CLA	C2A-CAA-CBA-CGA
17	2	606	CHL	O1D-CGD-O2D-CED
18	4	603	CLA	O1D-CGD-O2D-CED
18	B	824	CLA	C16-C17-C18-C19
18	B	824	CLA	C16-C17-C18-C20
19	2	617	XAT	C11-C10-C9-C8
22	A	852	BCR	C12-C13-C14-C15
22	B	844	BCR	C16-C17-C18-C19
22	B	849	BCR	C11-C10-C9-C8
22	K	205	BCR	C20-C21-C22-C23
18	4	602	CLA	C10-C11-C12-C13
18	A	811	CLA	C8-C10-C11-C12
18	B	839	CLA	C13-C15-C16-C17
18	3	601	CLA	O1D-CGD-O2D-CED
23	4	620	LMG	C29-C28-O8-C9
18	2	612	CLA	C10-C11-C12-C13
18	A	812	CLA	C3-C5-C6-C7
18	B	813	CLA	O1D-CGD-O2D-CED
18	A	839	CLA	C6-C7-C8-C9
18	B	816	CLA	C6-C7-C8-C10
18	B	828	CLA	C16-C17-C18-C20
18	B	822	CLA	C16-C17-C18-C19
18	B	811	CLA	O1A-CGA-O2A-C1
18	B	841	CLA	O1A-CGA-O2A-C1
22	B	844	BCR	C14-C15-C16-C17
20	1	615	LHG	C13-C14-C15-C16
18	J	101	CLA	O1A-CGA-O2A-C1
18	A	834	CLA	CBA-CGA-O2A-C1
18	1	603	CLA	C5-C6-C7-C8
18	2	604	CLA	C4B-C3B-CAB-CBB
18	4	610	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
18	A	819	CLA	C4B-C3B-CAB-CBB
18	A	825	CLA	C4B-C3B-CAB-CBB
18	A	803	CLA	C4B-C3B-CAB-CBB
18	A	834	CLA	C4B-C3B-CAB-CBB
18	A	838	CLA	C4B-C3B-CAB-CBB
18	B	823	CLA	C4B-C3B-CAB-CBB
20	1	615	LHG	C23-C24-C25-C26
18	2	612	CLA	C16-C17-C18-C20
18	B	816	CLA	C6-C7-C8-C9
18	2	609	CLA	C2A-CAA-CBA-CGA
18	G	201	CLA	C2A-CAA-CBA-CGA
18	B	805	CLA	C5-C6-C7-C8
20	1	615	LHG	C15-C16-C17-C18
18	2	602	CLA	C6-C7-C8-C10
20	1	615	LHG	C25-C26-C27-C28
18	B	809	CLA	C8-C10-C11-C12
18	B	817	CLA	O1A-CGA-O2A-C1
18	2	602	CLA	C3-C5-C6-C7
18	A	829	CLA	C3-C5-C6-C7
18	1	604	CLA	C3A-C2A-CAA-CBA
18	1	612	CLA	C3A-C2A-CAA-CBA
18	2	611	CLA	C3A-C2A-CAA-CBA
18	A	810	CLA	C3A-C2A-CAA-CBA
18	A	830	CLA	C3A-C2A-CAA-CBA
18	A	815	CLA	C3A-C2A-CAA-CBA
18	B	826	CLA	C3A-C2A-CAA-CBA
18	B	833	CLA	C3A-C2A-CAA-CBA
18	B	809	CLA	C3A-C2A-CAA-CBA
18	B	810	CLA	C3A-C2A-CAA-CBA
18	B	811	CLA	C3A-C2A-CAA-CBA
18	B	824	CLA	C3A-C2A-CAA-CBA
18	B	815	CLA	C3A-C2A-CAA-CBA
18	G	201	CLA	C3A-C2A-CAA-CBA
18	K	203	CLA	C3A-C2A-CAA-CBA
18	2	610	CLA	O1D-CGD-O2D-CED
18	4	601	CLA	CBA-CGA-O2A-C1
18	B	837	CLA	C8-C10-C11-C12
20	1	615	LHG	C11-C10-C9-C8
27	B	850	DGD	C9A-CAA-CBA-CCA
18	B	827	CLA	C10-C11-C12-C13
18	B	840	CLA	CBA-CGA-O2A-C1
18	4	612	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
18	B	813	CLA	O1A-CGA-O2A-C1
18	B	834	CLA	O1D-CGD-O2D-CED
18	1	612	CLA	O1D-CGD-O2D-CED
20	1	615	LHG	C12-C13-C14-C15
18	A	812	CLA	C16-C17-C18-C20
18	A	819	CLA	O1A-CGA-O2A-C1
18	2	604	CLA	C2B-C3B-CAB-CBB
18	4	610	CLA	C2B-C3B-CAB-CBB
18	A	819	CLA	C2B-C3B-CAB-CBB
18	A	825	CLA	C2B-C3B-CAB-CBB
18	A	834	CLA	C2B-C3B-CAB-CBB
18	A	838	CLA	C2B-C3B-CAB-CBB
18	B	823	CLA	C2B-C3B-CAB-CBB
18	B	839	CLA	C2B-C3B-CAB-CBB
21	2	619	LUT	C1-C6-C7-C8
21	4	616	LUT	C1-C6-C7-C8
21	4	616	LUT	C5-C6-C7-C8
22	4	618	BCR	C23-C24-C25-C30
22	B	844	BCR	C23-C24-C25-C26
22	B	844	BCR	C23-C24-C25-C30
22	B	849	BCR	C23-C24-C25-C26
22	F	304	BCR	C1-C6-C7-C8
22	F	304	BCR	C5-C6-C7-C8
18	B	811	CLA	CBD-CGD-O2D-CED
18	L	303	CLA	C8-C10-C11-C12
25	A	855	PQN	C25-C26-C27-C28
20	1	615	LHG	C27-C28-C29-C30
18	3	602	CLA	C2A-CAA-CBA-CGA
18	4	604	CLA	C2A-CAA-CBA-CGA
18	A	819	CLA	C2A-CAA-CBA-CGA
18	A	830	CLA	C2A-CAA-CBA-CGA
18	A	829	CLA	C2A-CAA-CBA-CGA
20	1	615	LHG	C10-C11-C12-C13
18	A	834	CLA	O1A-CGA-O2A-C1
19	2	617	XAT	C30-C31-C32-C33
22	F	304	BCR	C10-C11-C12-C13
22	K	205	BCR	C18-C19-C20-C21
18	B	841	CLA	C13-C15-C16-C17
18	A	840	CLA	C2-C3-C5-C6
18	B	822	CLA	C16-C17-C18-C20
18	A	802	CLA	C3-C5-C6-C7
18	2	602	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
21	2	616	LUT	C6-C7-C8-C9
18	B	820	CLA	CBA-CGA-O2A-C1
18	B	828	CLA	C16-C17-C18-C19
27	B	850	DGD	C2B-C1B-O2G-C2G
18	2	613	CLA	C2A-CAA-CBA-CGA
20	B	851	LHG	C23-C24-C25-C26
18	2	612	CLA	C16-C17-C18-C19
18	A	830	CLA	C4-C3-C5-C6
18	A	834	CLA	C13-C15-C16-C17
18	B	805	CLA	C8-C10-C11-C12
18	B	840	CLA	O1A-CGA-O2A-C1
27	B	850	DGD	O1B-C1B-O2G-C2G
23	4	620	LMG	O10-C28-O8-C9
27	B	850	DGD	CCB-CDB-CEB-CFB
23	4	619	LMG	O6-C5-C6-O5
18	A	805	CLA	CBA-CGA-O2A-C1
18	4	609	CLA	C5-C6-C7-C8
18	B	818	CLA	C3-C5-C6-C7
18	3	609	CLA	C2A-CAA-CBA-CGA
18	A	818	CLA	C2A-CAA-CBA-CGA
18	A	802	CLA	C2A-CAA-CBA-CGA
18	B	823	CLA	CBD-CGD-O2D-CED
20	1	615	LHG	C18-C19-C20-C21
20	1	615	LHG	C17-C18-C19-C20
18	K	203	CLA	O1D-CGD-O2D-CED
18	1	609	CLA	C1A-C2A-CAA-CBA
18	1	612	CLA	C1A-C2A-CAA-CBA
18	2	611	CLA	C1A-C2A-CAA-CBA
18	2	604	CLA	C1A-C2A-CAA-CBA
18	2	608	CLA	C1A-C2A-CAA-CBA
18	A	805	CLA	C1A-C2A-CAA-CBA
18	A	810	CLA	C1A-C2A-CAA-CBA
18	A	845	CLA	C1A-C2A-CAA-CBA
18	A	815	CLA	C1A-C2A-CAA-CBA
18	A	827	CLA	C1A-C2A-CAA-CBA
18	A	833	CLA	C1A-C2A-CAA-CBA
18	A	812	CLA	C1A-C2A-CAA-CBA
18	B	818	CLA	C1A-C2A-CAA-CBA
18	B	833	CLA	C1A-C2A-CAA-CBA
18	B	810	CLA	C1A-C2A-CAA-CBA
18	B	824	CLA	C1A-C2A-CAA-CBA
18	B	802	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
18	B	815	CLA	C1A-C2A-CAA-CBA
18	F	302	CLA	C1A-C2A-CAA-CBA
18	G	201	CLA	C1A-C2A-CAA-CBA
18	2	612	CLA	C5-C6-C7-C8
18	B	832	CLA	C3-C5-C6-C7
18	3	601	CLA	C11-C10-C8-C7
18	A	809	CLA	C11-C10-C8-C7
18	A	804	CLA	C12-C13-C15-C16
18	A	811	CLA	C11-C12-C13-C15
18	A	811	CLA	C12-C13-C15-C16
18	A	802	CLA	C6-C7-C8-C10
18	A	802	CLA	C11-C12-C13-C15
18	A	802	CLA	C12-C13-C15-C16
18	A	831	CLA	C11-C10-C8-C7
18	A	842	CLA	C11-C10-C8-C7
18	A	844	CLA	C12-C13-C15-C16
18	A	828	CLA	C11-C12-C13-C15
18	B	808	CLA	C11-C12-C13-C15
18	B	809	CLA	C12-C13-C15-C16
18	B	827	CLA	C12-C13-C15-C16
18	B	828	CLA	C12-C13-C15-C16
18	B	806	CLA	C11-C10-C8-C7
18	B	806	CLA	C11-C12-C13-C15
18	H	201	CLA	C6-C7-C8-C10
18	H	201	CLA	C11-C10-C8-C7
18	B	840	CLA	C16-C17-C18-C20
18	A	803	CLA	C10-C11-C12-C13
18	4	611	CLA	C3A-C2A-CAA-CBA
18	B	802	CLA	C8-C10-C11-C12
18	B	828	CLA	C4-C3-C5-C6
18	3	601	CLA	C2-C3-C5-C6
17	2	615	CHL	O1D-CGD-O2D-CED
18	A	809	CLA	O1D-CGD-O2D-CED
18	A	806	CLA	C2A-CAA-CBA-CGA
18	A	813	CLA	C2A-CAA-CBA-CGA
18	A	803	CLA	C2A-CAA-CBA-CGA
18	A	818	CLA	C6-C7-C8-C9
18	A	806	CLA	C14-C13-C15-C16
18	A	802	CLA	C6-C7-C8-C9
18	A	831	CLA	C11-C10-C8-C9
18	A	843	CLA	C6-C7-C8-C9
18	A	828	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
18	A	812	CLA	C14-C13-C15-C16
18	A	829	CLA	C6-C7-C8-C9
18	B	806	CLA	C11-C12-C13-C14
18	B	824	CLA	C14-C13-C15-C16
18	B	817	CLA	C6-C7-C8-C9
18	B	828	CLA	CBA-CGA-O2A-C1
18	B	829	CLA	CBA-CGA-O2A-C1
18	B	820	CLA	O1A-CGA-O2A-C1
18	B	808	CLA	C5-C6-C7-C8
20	1	615	LHG	C4-C5-C6-O8
27	B	850	DGD	C1G-C2G-C3G-O3G
18	A	831	CLA	C5-C6-C7-C8
18	B	807	CLA	CBA-CGA-O2A-C1
17	2	601	CHL	CHA-CBD-CGD-O1D
17	2	601	CHL	CHA-CBD-CGD-O2D
17	2	607	CHL	CHA-CBD-CGD-O2D
17	3	606	CHL	CHA-CBD-CGD-O1D
21	2	619	LUT	C11-C10-C9-C19
22	F	304	BCR	C11-C10-C9-C34
18	A	805	CLA	O1A-CGA-O2A-C1
18	1	603	CLA	C4-C3-C5-C6
18	A	807	CLA	C2-C3-C5-C6
18	B	828	CLA	C2-C3-C5-C6
18	B	808	CLA	O1D-CGD-O2D-CED
22	K	205	BCR	C7-C8-C9-C10
18	A	835	CLA	C10-C11-C12-C13
18	L	303	CLA	C10-C11-C12-C13
18	B	841	CLA	O1D-CGD-O2D-CED
20	2	618	LHG	C6-C5-O7-C7
22	B	849	BCR	C10-C11-C12-C13
18	B	840	CLA	C16-C17-C18-C19
18	B	828	CLA	C13-C15-C16-C17
18	A	819	CLA	O1D-CGD-O2D-CED
18	A	816	CLA	O1D-CGD-O2D-CED
19	2	617	XAT	C12-C13-C14-C15
22	F	304	BCR	C12-C13-C14-C15
18	B	810	CLA	C5-C6-C7-C8
18	B	817	CLA	C11-C12-C13-C14
23	4	619	LMG	C30-C31-C32-C33
18	B	825	CLA	C10-C11-C12-C13
27	B	850	DGD	CCA-CDA-CEA-CFA
18	3	603	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
18	B	822	CLA	C2A-CAA-CBA-CGA
18	B	837	CLA	C3-C5-C6-C7
18	A	820	CLA	C13-C15-C16-C17
20	B	852	LHG	C8-C7-O7-C5
18	B	829	CLA	O1A-CGA-O2A-C1
18	A	812	CLA	C15-C16-C17-C18
18	A	807	CLA	C4-C3-C5-C6
18	A	803	CLA	C4-C3-C5-C6
18	B	827	CLA	C4-C3-C5-C6
18	B	813	CLA	C4-C3-C5-C6
18	A	807	CLA	C8-C10-C11-C12
18	B	841	CLA	C8-C10-C11-C12
18	A	809	CLA	C11-C10-C8-C9
18	A	804	CLA	C6-C7-C8-C9
18	A	804	CLA	C14-C13-C15-C16
18	A	811	CLA	C11-C12-C13-C14
18	A	803	CLA	C6-C7-C8-C9
18	A	802	CLA	C14-C13-C15-C16
18	A	835	CLA	C11-C12-C13-C14
18	A	842	CLA	C11-C10-C8-C9
18	A	844	CLA	C14-C13-C15-C16
18	A	814	CLA	C14-C13-C15-C16
18	B	808	CLA	C11-C12-C13-C14
18	B	809	CLA	C14-C13-C15-C16
18	B	814	CLA	C11-C12-C13-C14
18	B	827	CLA	C14-C13-C15-C16
18	B	806	CLA	C6-C7-C8-C9
18	H	201	CLA	C11-C10-C8-C9
18	A	812	CLA	C13-C15-C16-C17
18	B	828	CLA	O1A-CGA-O2A-C1
18	1	604	CLA	C4B-C3B-CAB-CBB
18	3	612	CLA	C4B-C3B-CAB-CBB
18	4	608	CLA	C4B-C3B-CAB-CBB
18	4	614	CLA	C4B-C3B-CAB-CBB
18	A	824	CLA	C4B-C3B-CAB-CBB
18	A	844	CLA	C4B-C3B-CAB-CBB
18	A	829	CLA	C4B-C3B-CAB-CBB
18	A	836	CLA	C4B-C3B-CAB-CBB
18	B	827	CLA	C4B-C3B-CAB-CBB
18	B	839	CLA	C4B-C3B-CAB-CBB
18	B	836	CLA	C4B-C3B-CAB-CBB
18	H	201	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
18	J	101	CLA	C4B-C3B-CAB-CBB
18	4	612	CLA	C5-C6-C7-C8
18	B	813	CLA	C15-C16-C17-C18
18	B	841	CLA	C16-C17-C18-C20
18	B	819	CLA	C2A-CAA-CBA-CGA
23	4	619	LMG	C2-C1-O1-C7
18	1	603	CLA	C3-C5-C6-C7
18	3	601	CLA	C3-C5-C6-C7
18	B	824	CLA	C3-C5-C6-C7
20	1	615	LHG	O6-C4-C5-C6
18	A	819	CLA	C11-C12-C13-C14
18	A	806	CLA	C12-C13-C15-C16
18	A	804	CLA	C11-C10-C8-C7
18	A	804	CLA	C11-C12-C13-C15
18	A	826	CLA	C11-C12-C13-C15
18	A	831	CLA	C12-C13-C15-C16
18	A	835	CLA	C11-C12-C13-C15
18	A	843	CLA	C6-C7-C8-C10
18	A	844	CLA	C6-C7-C8-C10
18	A	814	CLA	C12-C13-C15-C16
18	A	812	CLA	C12-C13-C15-C16
18	A	829	CLA	C6-C7-C8-C10
18	B	809	CLA	C11-C10-C8-C7
18	B	814	CLA	C11-C10-C8-C7
18	B	814	CLA	C11-C12-C13-C15
18	B	813	CLA	C11-C12-C13-C15
18	B	806	CLA	C6-C7-C8-C10
18	B	824	CLA	C12-C13-C15-C16
18	B	825	CLA	C12-C13-C15-C16
18	B	803	CLA	C11-C10-C8-C7
18	B	817	CLA	C6-C7-C8-C10
18	B	840	CLA	C6-C7-C8-C10
20	A	847	LHG	C5-C6-O8-C23
20	1	615	LHG	C19-C20-C21-C22
18	A	822	CLA	CBD-CGD-O2D-CED
18	2	604	CLA	C3A-C2A-CAA-CBA
18	3	601	CLA	C4-C3-C5-C6
18	A	822	CLA	C3A-C2A-CAA-CBA
18	A	833	CLA	C3A-C2A-CAA-CBA
18	A	836	CLA	C3A-C2A-CAA-CBA
18	B	822	CLA	C3A-C2A-CAA-CBA
18	K	204	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
20	A	846	LHG	C27-C28-C29-C30
18	A	807	CLA	C15-C16-C17-C18
18	A	841	CLA	C5-C6-C7-C8
18	1	603	CLA	C6-C7-C8-C9
18	B	807	CLA	O1A-CGA-O2A-C1
18	B	841	CLA	C2A-CAA-CBA-CGA
18	B	811	CLA	C5-C6-C7-C8
23	4	620	LMG	C7-C8-C9-O8
18	A	822	CLA	C4-C3-C5-C6
18	A	835	CLA	C4-C3-C5-C6
18	B	810	CLA	C4-C3-C5-C6
18	B	827	CLA	C2-C3-C5-C6
18	B	813	CLA	C2-C3-C5-C6
18	A	834	CLA	C5-C6-C7-C8
18	A	836	CLA	O1D-CGD-O2D-CED
18	A	812	CLA	C16-C17-C18-C19
20	1	615	LHG	O6-C4-C5-O7
18	1	604	CLA	C2B-C3B-CAB-CBB
18	3	612	CLA	C2B-C3B-CAB-CBB
18	4	608	CLA	C2B-C3B-CAB-CBB
18	4	614	CLA	C2B-C3B-CAB-CBB
18	A	824	CLA	C2B-C3B-CAB-CBB
18	A	836	CLA	C2B-C3B-CAB-CBB
18	B	836	CLA	C2B-C3B-CAB-CBB
18	H	201	CLA	C2B-C3B-CAB-CBB
18	J	101	CLA	C2B-C3B-CAB-CBB
22	B	845	BCR	C5-C6-C7-C8
18	B	827	CLA	C15-C16-C17-C18
18	B	803	CLA	C15-C16-C17-C18
20	2	618	LHG	C2-C3-O3-P
20	B	852	LHG	C5-C4-O6-P
18	A	831	CLA	C3-C5-C6-C7
18	B	832	CLA	C16-C17-C18-C19
18	A	814	CLA	CAA-CBA-CGA-O2A
18	B	820	CLA	C2A-CAA-CBA-CGA
20	1	615	LHG	C14-C15-C16-C17
18	B	809	CLA	C3-C5-C6-C7
18	3	609	CLA	C4-C3-C5-C6
18	3	609	CLA	C2-C3-C5-C6
18	B	841	CLA	C16-C17-C18-C19
18	2	602	CLA	C14-C13-C15-C16
18	B	827	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
22	B	849	BCR	C6-C7-C8-C9
22	K	205	BCR	C22-C23-C24-C25
22	F	304	BCR	C14-C15-C16-C17
18	B	811	CLA	O1D-CGD-O2D-CED
23	4	620	LMG	C2-C1-O1-C7
18	4	611	CLA	C1A-C2A-CAA-CBA
18	B	835	CLA	C1A-C2A-CAA-CBA
17	1	601	CHL	C3-C5-C6-C7
20	1	615	LHG	O1-C1-C2-O2
18	A	822	CLA	C2-C3-C5-C6
18	A	803	CLA	C2-C3-C5-C6
18	A	835	CLA	C2-C3-C5-C6
18	B	810	CLA	C2-C3-C5-C6
18	B	832	CLA	C16-C17-C18-C20
18	B	837	CLA	C15-C16-C17-C18
19	2	617	XAT	C40-C33-C34-C35
18	2	602	CLA	CBA-CGA-O2A-C1
18	4	612	CLA	CBA-CGA-O2A-C1
18	A	809	CLA	CBA-CGA-O2A-C1
18	B	837	CLA	CBA-CGA-O2A-C1
18	A	820	CLA	C8-C10-C11-C12
18	B	841	CLA	C15-C16-C17-C18
18	2	612	CLA	C12-C13-C15-C16
18	2	602	CLA	C12-C13-C15-C16
18	A	831	CLA	C11-C12-C13-C15
18	A	842	CLA	C11-C12-C13-C15
18	A	841	CLA	C12-C13-C15-C16
18	B	818	CLA	C11-C10-C8-C7
18	B	805	CLA	C11-C10-C8-C7
18	F	301	CLA	C6-C7-C8-C10
18	1	609	CLA	C2A-CAA-CBA-CGA
18	B	827	CLA	C8-C10-C11-C12
19	2	617	XAT	C31-C32-C33-C34
22	4	618	BCR	C7-C8-C9-C10
22	K	205	BCR	C17-C18-C19-C20
18	B	828	CLA	C2A-CAA-CBA-CGA
18	B	807	CLA	C2A-CAA-CBA-CGA
18	A	818	CLA	C5-C6-C7-C8
18	L	303	CLA	C15-C16-C17-C18
18	A	806	CLA	C15-C16-C17-C18
18	B	834	CLA	C3-C5-C6-C7
18	A	831	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
21	3	613	LUT	C11-C10-C9-C8
22	A	849	BCR	C20-C21-C22-C23
22	F	304	BCR	C11-C10-C9-C8
20	1	615	LHG	C35-C36-C37-C38
18	A	802	CLA	C15-C16-C17-C18
18	A	829	CLA	C13-C15-C16-C17
20	B	852	LHG	C4-C5-C6-O8
18	B	840	CLA	C15-C16-C17-C18
18	A	844	CLA	C16-C17-C18-C20
18	A	841	CLA	C2A-CAA-CBA-CGA
18	4	601	CLA	O1A-CGA-O2A-C1
18	F	301	CLA	C3-C5-C6-C7
18	B	818	CLA	C11-C10-C8-C9
18	B	809	CLA	C6-C7-C8-C9
18	A	826	CLA	C8-C10-C11-C12
18	A	833	CLA	CBD-CGD-O2D-CED
21	1	616	LUT	C26-C27-C28-C29
18	A	812	CLA	C2-C1-O2A-CGA
17	1	601	CHL	C4-C3-C5-C6
18	A	830	CLA	C2-C3-C5-C6
18	B	837	CLA	C10-C11-C12-C13
18	4	603	CLA	C2A-CAA-CBA-CGA
18	A	841	CLA	C8-C10-C11-C12
18	2	602	CLA	O1A-CGA-O2A-C1
18	4	612	CLA	O1A-CGA-O2A-C1
18	A	809	CLA	O1A-CGA-O2A-C1
18	1	607	CLA	C4B-C3B-CAB-CBB
18	1	611	CLA	C4B-C3B-CAB-CBB
18	1	612	CLA	C4B-C3B-CAB-CBB
18	3	611	CLA	C4B-C3B-CAB-CBB
18	3	609	CLA	C4B-C3B-CAB-CBB
18	3	604	CLA	C4B-C3B-CAB-CBB
18	3	610	CLA	C4B-C3B-CAB-CBB
18	3	602	CLA	C4B-C3B-CAB-CBB
18	4	601	CLA	C4B-C3B-CAB-CBB
18	4	611	CLA	C4B-C3B-CAB-CBB
18	A	813	CLA	C4B-C3B-CAB-CBB
18	A	808	CLA	C4B-C3B-CAB-CBB
18	A	810	CLA	C4B-C3B-CAB-CBB
18	A	840	CLA	C4B-C3B-CAB-CBB
18	A	817	CLA	C4B-C3B-CAB-CBB
18	A	837	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
18	B	835	CLA	C4B-C3B-CAB-CBB
18	B	834	CLA	C4B-C3B-CAB-CBB
18	B	808	CLA	C4B-C3B-CAB-CBB
18	B	840	CLA	C4B-C3B-CAB-CBB
18	F	303	CLA	C4B-C3B-CAB-CBB
18	F	301	CLA	C4B-C3B-CAB-CBB
18	G	201	CLA	C4B-C3B-CAB-CBB
18	G	202	CLA	C4B-C3B-CAB-CBB
18	K	201	CLA	C4B-C3B-CAB-CBB
18	K	204	CLA	C4B-C3B-CAB-CBB
18	L	302	CLA	C4B-C3B-CAB-CBB
18	B	823	CLA	O1D-CGD-O2D-CED
18	A	812	CLA	CBA-CGA-O2A-C1
18	B	839	CLA	CBA-CGA-O2A-C1
18	B	837	CLA	O1A-CGA-O2A-C1
17	1	601	CHL	C2A-CAA-CBA-CGA
18	A	812	CLA	C6-C7-C8-C10
18	B	808	CLA	C12-C13-C15-C16
18	B	814	CLA	C6-C7-C8-C10
18	F	301	CLA	C11-C10-C8-C7
25	B	842	PQN	C16-C17-C18-C20
25	B	842	PQN	C22-C23-C25-C26
18	B	819	CLA	C6-C7-C8-C10
18	A	824	CLA	CBD-CGD-O2D-CED
18	A	808	CLA	CBA-CGA-O2A-C1
18	B	826	CLA	C5-C6-C7-C8
20	2	618	LHG	C5-C4-O6-P
18	4	609	CLA	C4-C3-C5-C6
18	A	842	CLA	C2C-C3C-CAC-CBC
20	1	615	LHG	C8-C7-O7-C5
18	2	612	CLA	C14-C13-C15-C16
18	A	831	CLA	C11-C12-C13-C14
18	A	831	CLA	C14-C13-C15-C16
18	A	842	CLA	C11-C12-C13-C14
18	B	810	CLA	C6-C7-C8-C9
19	1	614	XAT	C33-C34-C35-C15
18	A	814	CLA	C13-C15-C16-C17
17	1	601	CHL	CAD-CBD-CGD-O1D
18	1	604	CLA	C1-C2-C3-C4
18	3	609	CLA	CAD-CBD-CGD-O1D
18	A	822	CLA	O1D-CGD-O2D-CED
18	A	812	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
23	4	620	LMG	O7-C8-C9-O8
18	B	839	CLA	O1A-CGA-O2A-C1
17	4	605	CHL	C1A-C2A-CAA-CBA
18	A	841	CLA	CAD-CBD-CGD-O2D
18	B	822	CLA	CAD-CBD-CGD-O2D
18	F	302	CLA	CAD-CBD-CGD-O2D
18	1	602	CLA	CBA-CGA-O2A-C1
18	B	822	CLA	C5-C6-C7-C8
18	A	835	CLA	C16-C17-C18-C20
18	A	844	CLA	C16-C17-C18-C19
18	B	808	CLA	C16-C17-C18-C20
18	4	614	CLA	C2A-CAA-CBA-CGA
24	A	801	CL0	C2A-CAA-CBA-CGA
18	2	612	CLA	C15-C16-C17-C18
18	1	602	CLA	O1A-CGA-O2A-C1
17	2	606	CHL	CHA-CBD-CGD-O1D
17	2	606	CHL	CHA-CBD-CGD-O2D
17	4	606	CHL	CHA-CBD-CGD-O1D
17	4	606	CHL	CHA-CBD-CGD-O2D
17	4	605	CHL	CHA-CBD-CGD-O2D
17	4	605	CHL	CAD-CBD-CGD-O2D
18	1	610	CLA	CHA-CBD-CGD-O2D
18	1	612	CLA	CHA-CBD-CGD-O1D
18	3	603	CLA	CHA-CBD-CGD-O1D
18	4	611	CLA	CHA-CBD-CGD-O2D
18	A	823	CLA	CHA-CBD-CGD-O1D
18	A	823	CLA	CHA-CBD-CGD-O2D
18	A	841	CLA	CAD-CBD-CGD-O1D
18	A	836	CLA	CHA-CBD-CGD-O1D
18	A	836	CLA	CHA-CBD-CGD-O2D
18	A	838	CLA	CHA-CBD-CGD-O1D
18	A	838	CLA	CHA-CBD-CGD-O2D
18	B	813	CLA	CAD-CBD-CGD-O1D
18	B	822	CLA	CAD-CBD-CGD-O1D
18	F	303	CLA	CHA-CBD-CGD-O1D
18	F	301	CLA	CHA-CBD-CGD-O1D
18	F	302	CLA	CAD-CBD-CGD-O1D
20	A	846	LHG	C3-O3-P-O5
18	A	818	CLA	C4-C3-C5-C6
18	1	607	CLA	C2B-C3B-CAB-CBB
18	1	611	CLA	C2B-C3B-CAB-CBB
18	1	612	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
18	3	611	CLA	C2B-C3B-CAB-CBB
18	3	604	CLA	C2B-C3B-CAB-CBB
18	3	610	CLA	C2B-C3B-CAB-CBB
18	3	602	CLA	C2B-C3B-CAB-CBB
18	4	611	CLA	C2B-C3B-CAB-CBB
18	A	808	CLA	C2B-C3B-CAB-CBB
18	A	810	CLA	C2B-C3B-CAB-CBB
18	A	803	CLA	C2B-C3B-CAB-CBB
18	A	837	CLA	C2B-C3B-CAB-CBB
18	B	835	CLA	C2B-C3B-CAB-CBB
18	B	834	CLA	C2B-C3B-CAB-CBB
18	B	808	CLA	C2B-C3B-CAB-CBB
18	B	840	CLA	C2B-C3B-CAB-CBB
18	F	301	CLA	C2B-C3B-CAB-CBB
18	G	201	CLA	C2B-C3B-CAB-CBB
18	K	201	CLA	C2B-C3B-CAB-CBB
18	K	204	CLA	C2B-C3B-CAB-CBB
18	L	302	CLA	C2B-C3B-CAB-CBB
22	B	845	BCR	C1-C6-C7-C8
18	1	603	CLA	C2-C3-C5-C6
27	B	850	DGD	CBB-CCB-CDB-CEB
18	A	808	CLA	O1A-CGA-O2A-C1
22	A	852	BCR	C10-C11-C12-C13
22	L	301	BCR	C18-C19-C20-C21
18	B	826	CLA	C10-C11-C12-C13
20	B	851	LHG	C26-C27-C28-C29
18	4	601	CLA	CAA-CBA-CGA-O2A
18	A	820	CLA	C6-C7-C8-C9
18	A	804	CLA	C11-C12-C13-C14
18	A	802	CLA	C11-C10-C8-C9
18	A	844	CLA	C6-C7-C8-C9
18	B	805	CLA	C14-C13-C15-C16
18	B	808	CLA	C11-C10-C8-C9
18	B	813	CLA	C11-C12-C13-C14
21	2	619	LUT	C11-C10-C9-C8
22	L	301	BCR	C11-C10-C9-C8
20	1	615	LHG	O9-C7-O7-C5
18	4	614	CLA	O1A-CGA-O2A-C1
18	B	819	CLA	C6-C7-C8-C9
27	B	850	DGD	C6B-C7B-C8B-C9B
20	B	852	LHG	O7-C5-C6-O8
18	A	822	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
18	A	841	CLA	CAA-CBA-CGA-O2A
18	A	829	CLA	C16-C17-C18-C20
18	L	303	CLA	C13-C15-C16-C17
18	B	832	CLA	C13-C15-C16-C17
24	A	801	CL0	CAA-CBA-CGA-O2A
18	K	204	CLA	CBA-CGA-O2A-C1
22	B	846	BCR	C21-C22-C23-C24
18	A	833	CLA	O1D-CGD-O2D-CED
18	4	614	CLA	CBA-CGA-O2A-C1
18	A	819	CLA	CAA-CBA-CGA-O2A
18	A	824	CLA	O1D-CGD-O2D-CED
18	3	601	CLA	C2A-CAA-CBA-CGA
18	4	612	CLA	C2A-CAA-CBA-CGA
18	B	808	CLA	C16-C17-C18-C19
18	B	841	CLA	C4-C3-C5-C6
23	4	620	LMG	O7-C10-C11-C12
18	A	822	CLA	O1A-CGA-O2A-C1
20	B	852	LHG	O9-C7-O7-C5
18	B	841	CLA	C14-C13-C15-C16
18	B	806	CLA	C14-C13-C15-C16
18	B	832	CLA	CBA-CGA-O2A-C1
18	4	609	CLA	C4B-C3B-CAB-CBB
18	A	835	CLA	C4B-C3B-CAB-CBB
18	A	814	CLA	C10-C11-C12-C13
18	B	824	CLA	CBA-CGA-O2A-C1
18	A	842	CLA	C4C-C3C-CAC-CBC
18	B	832	CLA	O1A-CGA-O2A-C1
18	A	835	CLA	C11-C10-C8-C7
18	B	841	CLA	C11-C10-C8-C7
18	B	802	CLA	C11-C12-C13-C15
24	A	801	CL0	C11-C12-C13-C15
17	2	605	CHL	O1D-CGD-O2D-CED
18	1	611	CLA	CAA-CBA-CGA-O2A
18	B	805	CLA	O1A-CGA-O2A-C1
18	B	824	CLA	O1A-CGA-O2A-C1
20	1	615	LHG	C31-C32-C33-C34
18	4	613	CLA	C3A-C2A-CAA-CBA
18	A	804	CLA	C3A-C2A-CAA-CBA
18	A	813	CLA	C3A-C2A-CAA-CBA
18	A	843	CLA	C3A-C2A-CAA-CBA
18	B	821	CLA	C3A-C2A-CAA-CBA
18	H	201	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
18	A	839	CLA	C2A-CAA-CBA-CGA
20	1	615	LHG	C32-C33-C34-C35
22	A	852	BCR	C11-C10-C9-C34
22	A	851	BCR	C11-C10-C9-C34
22	A	851	BCR	C20-C21-C22-C37
22	B	845	BCR	C16-C17-C18-C36
22	K	202	BCR	C16-C17-C18-C36
22	L	305	BCR	C16-C17-C18-C36
22	L	301	BCR	C11-C10-C9-C34
18	A	830	CLA	C2-C1-O2A-CGA
18	B	817	CLA	C2-C1-O2A-CGA
18	B	816	CLA	C5-C6-C7-C8
18	1	611	CLA	CAA-CBA-CGA-O1A
18	2	608	CLA	CAA-CBA-CGA-O1A
18	A	803	CLA	C11-C12-C13-C14
18	A	831	CLA	C6-C7-C8-C9
18	A	829	CLA	C11-C10-C8-C9
18	B	841	CLA	C11-C10-C8-C9
18	B	825	CLA	C11-C10-C8-C9
18	L	303	CLA	C11-C12-C13-C14
25	B	842	PQN	C24-C23-C25-C26
18	1	607	CLA	CAA-CBA-CGA-O2A
20	B	851	LHG	C4-C5-O7-C7
17	2	607	CHL	C1A-C2A-CAA-CBA
18	G	203	CLA	CAA-CBA-CGA-O1A
18	B	818	CLA	C4-C3-C5-C6
18	B	841	CLA	C2-C3-C5-C6
18	A	814	CLA	C2A-CAA-CBA-CGA
18	2	609	CLA	C1A-C2A-CAA-CBA
18	4	604	CLA	C1A-C2A-CAA-CBA
18	A	813	CLA	C1A-C2A-CAA-CBA
18	A	843	CLA	C1A-C2A-CAA-CBA
18	B	803	CLA	C1A-C2A-CAA-CBA
18	H	201	CLA	C1A-C2A-CAA-CBA
19	2	617	XAT	C32-C33-C34-C35
22	A	852	BCR	C11-C10-C9-C8
22	A	851	BCR	C11-C10-C9-C8
22	A	851	BCR	C20-C21-C22-C23
22	B	845	BCR	C16-C17-C18-C19
22	K	202	BCR	C16-C17-C18-C19
22	L	305	BCR	C16-C17-C18-C19
18	A	835	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
24	A	801	CL0	O1A-CGA-O2A-C1
18	3	609	CLA	C2B-C3B-CAB-CBB
18	4	601	CLA	C2B-C3B-CAB-CBB
18	4	609	CLA	C2B-C3B-CAB-CBB
18	A	813	CLA	C2B-C3B-CAB-CBB
18	A	840	CLA	C2B-C3B-CAB-CBB
18	A	835	CLA	C2B-C3B-CAB-CBB
18	A	817	CLA	C2B-C3B-CAB-CBB
18	F	303	CLA	C2B-C3B-CAB-CBB
18	G	202	CLA	C2B-C3B-CAB-CBB
18	2	608	CLA	CAA-CBA-CGA-O2A
18	B	805	CLA	CBA-CGA-O2A-C1
18	A	809	CLA	C16-C17-C18-C20
18	B	809	CLA	C5-C6-C7-C8
18	1	607	CLA	CAA-CBA-CGA-O1A
18	4	603	CLA	CAA-CBA-CGA-O1A
18	A	819	CLA	C4-C3-C5-C6
18	3	603	CLA	CAA-CBA-CGA-O2A
18	4	612	CLA	C11-C10-C8-C7
18	A	819	CLA	C6-C7-C8-C10
18	B	805	CLA	C6-C7-C8-C10
18	B	828	CLA	C6-C7-C8-C10
18	B	813	CLA	C11-C10-C8-C7
18	B	806	CLA	C12-C13-C15-C16
18	B	840	CLA	C11-C10-C8-C7
18	A	829	CLA	C16-C17-C18-C19
18	1	602	CLA	C2A-CAA-CBA-CGA
18	B	816	CLA	C2A-CAA-CBA-CGA
18	A	818	CLA	C8-C10-C11-C12
18	3	603	CLA	CAA-CBA-CGA-O1A
24	A	801	CL0	CBA-CGA-O2A-C1
18	A	818	CLA	C11-C12-C13-C14
17	1	601	CHL	C2-C3-C5-C6
18	L	303	CLA	C16-C17-C18-C20
18	A	830	CLA	O1D-CGD-O2D-CED
18	4	603	CLA	CAA-CBA-CGA-O2A
18	B	834	CLA	C6-C7-C8-C9
18	B	802	CLA	C11-C10-C8-C9
18	F	301	CLA	C11-C10-C8-C9
24	A	801	CL0	C4-C3-C5-C6
18	G	203	CLA	CAA-CBA-CGA-O2A
18	A	830	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
18	B	839	CLA	C15-C16-C17-C18
18	2	611	CLA	CAA-CBA-CGA-O1A
18	2	603	CLA	CAA-CBA-CGA-O2A
18	1	604	CLA	C2A-CAA-CBA-CGA
18	B	805	CLA	CAA-CBA-CGA-O2A
18	B	817	CLA	CAA-CBA-CGA-O2A
22	B	844	BCR	C15-C16-C17-C18
18	A	815	CLA	CAA-CBA-CGA-O2A
18	2	602	CLA	C4B-C3B-CAB-CBB
18	B	803	CLA	C4B-C3B-CAB-CBB
18	B	827	CLA	C16-C17-C18-C20
17	2	605	CHL	CBD-CGD-O2D-CED
22	3	614	BCR	C20-C21-C22-C37
22	B	844	BCR	C11-C10-C9-C34
18	A	843	CLA	C5-C6-C7-C8
18	K	203	CLA	CAA-CBA-CGA-O2A
18	3	601	CLA	C11-C12-C13-C14
18	A	820	CLA	C11-C10-C8-C7
18	A	803	CLA	C11-C10-C8-C7
18	A	803	CLA	C11-C12-C13-C15
18	B	834	CLA	C6-C7-C8-C10
18	K	203	CLA	CAA-CBA-CGA-O1A
18	B	821	CLA	CAA-CBA-CGA-O2A
17	4	607	CHL	CAA-CBA-CGA-O2A
18	B	805	CLA	C11-C12-C13-C14
18	B	810	CLA	C14-C13-C15-C16
18	B	839	CLA	C6-C7-C8-C9
18	2	612	CLA	C2A-CAA-CBA-CGA
18	A	836	CLA	C2A-CAA-CBA-CGA
18	K	204	CLA	C2A-CAA-CBA-CGA
17	1	601	CHL	C2-C1-O2A-CGA
18	A	822	CLA	C2-C1-O2A-CGA
18	A	809	CLA	C2-C1-O2A-CGA
18	A	802	CLA	C5-C6-C7-C8
18	3	607	CLA	C3A-C2A-CAA-CBA
18	A	803	CLA	C3A-C2A-CAA-CBA
18	B	837	CLA	C3A-C2A-CAA-CBA
18	B	803	CLA	C3A-C2A-CAA-CBA
18	F	302	CLA	C3A-C2A-CAA-CBA
18	4	604	CLA	CAA-CBA-CGA-O2A
18	4	609	CLA	C2-C3-C5-C6
17	1	601	CHL	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
18	2	611	CLA	CAA-CBA-CGA-O2A
18	2	603	CLA	CAA-CBA-CGA-O1A
18	A	815	CLA	CAA-CBA-CGA-O1A
18	B	828	CLA	C3-C5-C6-C7
18	A	835	CLA	CBD-CGD-O2D-CED
18	A	818	CLA	C2-C3-C5-C6
19	4	617	XAT	O4-C6-C7-C8
22	B	844	BCR	C11-C10-C9-C8
18	B	841	CLA	CAA-CBA-CGA-O2A
18	4	604	CLA	CAA-CBA-CGA-O1A
27	B	850	DGD	C1B-C2B-C3B-C4B
17	4	607	CHL	CAA-CBA-CGA-O1A
18	2	612	CLA	C8-C10-C11-C12
20	B	852	LHG	C30-C31-C32-C33
18	3	602	CLA	CAA-CBA-CGA-O2A
18	A	804	CLA	CAA-CBA-CGA-O2A
18	A	814	CLA	CAA-CBA-CGA-O1A
18	A	818	CLA	C11-C10-C8-C9
25	B	842	PQN	C16-C17-C18-C19
18	A	809	CLA	C16-C17-C18-C19
18	B	827	CLA	C16-C17-C18-C19
18	L	303	CLA	C16-C17-C18-C19
18	B	809	CLA	CAA-CBA-CGA-O2A
18	B	837	CLA	C16-C17-C18-C20
18	B	809	CLA	C16-C17-C18-C20
18	A	806	CLA	CBA-CGA-O2A-C1
18	4	612	CLA	C6-C7-C8-C10
18	A	807	CLA	C11-C10-C8-C7
18	B	808	CLA	C6-C7-C8-C10
18	B	839	CLA	C6-C7-C8-C10
18	B	802	CLA	C11-C10-C8-C7
18	B	840	CLA	C12-C13-C15-C16
18	B	828	CLA	C15-C16-C17-C18
18	4	608	CLA	CAA-CBA-CGA-O2A
18	A	844	CLA	C2B-C3B-CAB-CBB
18	A	816	CLA	C2B-C3B-CAB-CBB
18	A	829	CLA	C2B-C3B-CAB-CBB
18	B	827	CLA	C2B-C3B-CAB-CBB
18	B	807	CLA	C2B-C3B-CAB-CBB
22	4	618	BCR	C1-C6-C7-C8
22	4	618	BCR	C5-C6-C7-C8
22	A	852	BCR	C1-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
22	A	852	BCR	C5-C6-C7-C8
22	B	846	BCR	C1-C6-C7-C8
22	B	846	BCR	C5-C6-C7-C8
22	B	847	BCR	C1-C6-C7-C8
22	B	847	BCR	C5-C6-C7-C8
22	B	849	BCR	C23-C24-C25-C30
22	G	204	BCR	C1-C6-C7-C8
22	G	204	BCR	C5-C6-C7-C8
22	L	306	BCR	C5-C6-C7-C8
18	A	842	CLA	C2-C1-O2A-CGA
18	B	827	CLA	C2-C1-O2A-CGA
18	A	842	CLA	C16-C17-C18-C20
18	A	843	CLA	C8-C10-C11-C12
18	2	609	CLA	C2-C1-O2A-CGA
23	4	619	LMG	C8-C9-O8-C28
18	A	806	CLA	O1A-CGA-O2A-C1
17	2	607	CHL	CAA-CBA-CGA-O2A
18	A	807	CLA	CAA-CBA-CGA-O2A
18	A	826	CLA	CAA-CBA-CGA-O2A
18	A	825	CLA	C2A-CAA-CBA-CGA
18	J	101	CLA	C2A-CAA-CBA-CGA
18	3	609	CLA	CAA-CBA-CGA-O2A
18	B	832	CLA	CAA-CBA-CGA-O2A
18	K	204	CLA	O1A-CGA-O2A-C1
18	B	814	CLA	C6-C7-C8-C9
18	B	828	CLA	C6-C7-C8-C9
18	B	813	CLA	C11-C10-C8-C9
18	B	832	CLA	C11-C10-C8-C9
18	A	807	CLA	O1A-CGA-O2A-C1
18	A	803	CLA	C1A-C2A-CAA-CBA
18	A	816	CLA	C4B-C3B-CAB-CBB
18	B	810	CLA	C4B-C3B-CAB-CBB
18	B	807	CLA	C4B-C3B-CAB-CBB
18	A	840	CLA	CAA-CBA-CGA-O2A
18	B	811	CLA	CAA-CBA-CGA-O2A
22	A	852	BCR	C13-C14-C15-C16
20	B	852	LHG	C11-C12-C13-C14
18	A	807	CLA	CBA-CGA-O2A-C1
18	A	842	CLA	CAA-CBA-CGA-O2A
18	A	821	CLA	C2A-CAA-CBA-CGA
18	B	818	CLA	C2A-CAA-CBA-CGA
18	3	602	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
18	A	803	CLA	C2-C1-O2A-CGA
18	A	832	CLA	C2-C1-O2A-CGA
18	B	841	CLA	C2-C1-O2A-CGA
18	B	836	CLA	C2-C1-O2A-CGA
18	2	612	CLA	C11-C12-C13-C15
18	A	806	CLA	C6-C7-C8-C10
18	A	806	CLA	C11-C10-C8-C7
18	A	826	CLA	C11-C10-C8-C7
18	B	810	CLA	C12-C13-C15-C16
18	B	825	CLA	C11-C12-C13-C15
18	4	608	CLA	CAA-CBA-CGA-O1A
18	B	828	CLA	C5-C6-C7-C8
18	2	602	CLA	C2A-CAA-CBA-CGA
18	4	602	CLA	C2A-CAA-CBA-CGA
18	B	824	CLA	C2A-CAA-CBA-CGA
18	2	602	CLA	C16-C17-C18-C19
20	B	852	LHG	O7-C7-C8-C9
23	4	620	LMG	C8-C9-O8-C28
23	4	619	LMG	C29-C28-O8-C9
18	1	607	CLA	CHA-CBD-CGD-O1D
18	4	611	CLA	CHA-CBD-CGD-O1D
18	B	822	CLA	C8-C10-C11-C12
17	2	607	CHL	CAA-CBA-CGA-O1A
18	A	807	CLA	CAA-CBA-CGA-O1A
18	3	609	CLA	CAA-CBA-CGA-O1A
18	A	805	CLA	C3-C5-C6-C7
18	A	804	CLA	C2A-CAA-CBA-CGA
18	A	815	CLA	C2A-CAA-CBA-CGA
18	A	803	CLA	C11-C10-C8-C9
18	B	841	CLA	C6-C7-C8-C9
18	B	811	CLA	CAA-CBA-CGA-O1A
22	A	852	BCR	C15-C16-C17-C18
18	3	602	CLA	CAA-CBA-CGA-O1A
18	A	819	CLA	C2-C3-C5-C6
18	B	818	CLA	C2-C3-C5-C6
18	3	610	CLA	CAD-CBD-CGD-O1D
18	K	206	CLA	CAD-CBD-CGD-O1D
19	2	617	XAT	C1-C6-C7-C8
18	A	804	CLA	O1A-CGA-O2A-C1
18	B	809	CLA	CAA-CBA-CGA-O1A
18	B	814	CLA	C10-C11-C12-C13
18	B	802	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
18	A	830	CLA	C8-C10-C11-C12
18	A	840	CLA	CAA-CBA-CGA-O1A
20	B	852	LHG	O9-C7-C8-C9
18	B	806	CLA	CAA-CBA-CGA-O2A
18	A	809	CLA	C2C-C3C-CAC-CBC
18	K	204	CLA	CAA-CBA-CGA-O2A
18	B	832	CLA	CAA-CBA-CGA-O1A
18	A	809	CLA	C4C-C3C-CAC-CBC
18	2	610	CLA	CAD-CBD-CGD-O2D
18	A	844	CLA	CAD-CBD-CGD-O2D
18	B	813	CLA	CAD-CBD-CGD-O2D
18	L	304	CLA	CAD-CBD-CGD-O2D
22	B	801	BCR	C6-C7-C8-C9
18	B	837	CLA	C16-C17-C18-C19
18	A	844	CLA	C2A-CAA-CBA-CGA
27	B	850	DGD	CFB-CGB-CHB-CIB
18	A	826	CLA	CAA-CBA-CGA-O1A
18	B	805	CLA	C11-C12-C13-C15
18	4	614	CLA	CAA-CBA-CGA-O2A
18	A	814	CLA	C16-C17-C18-C20
20	1	615	LHG	C30-C31-C32-C33
18	3	601	CLA	CAA-CBA-CGA-O2A
18	4	602	CLA	CAA-CBA-CGA-O2A
20	2	618	LHG	O7-C7-C8-C9
18	A	837	CLA	CAA-CBA-CGA-O2A
18	A	842	CLA	CAA-CBA-CGA-O1A

There are no ring outliers.

164 monomers are involved in 464 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	B	806	CLA	3	0
18	1	603	CLA	1	0
18	B	836	CLA	2	0
18	A	829	CLA	6	0
18	B	823	CLA	2	0
18	A	844	CLA	4	0
18	B	840	CLA	6	0
18	B	833	CLA	1	0
22	A	849	BCR	2	0
18	4	613	CLA	2	0
22	3	614	BCR	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	B	834	CLA	1	0
18	B	838	CLA	2	0
18	A	821	CLA	2	0
18	3	612	CLA	1	0
18	A	826	CLA	2	0
20	B	852	LHG	3	0
18	A	845	CLA	1	0
22	A	851	BCR	8	0
23	4	620	LMG	1	0
18	J	101	CLA	2	0
18	B	825	CLA	2	0
25	B	842	PQN	2	0
18	A	814	CLA	2	0
18	3	601	CLA	4	0
21	2	616	LUT	4	0
18	A	810	CLA	1	0
18	B	821	CLA	1	0
18	A	842	CLA	5	0
21	1	616	LUT	3	0
18	4	610	CLA	1	0
18	A	813	CLA	4	0
18	B	822	CLA	8	0
18	A	817	CLA	1	0
21	2	619	LUT	6	0
18	B	818	CLA	4	0
18	A	827	CLA	1	0
18	2	604	CLA	5	0
18	A	811	CLA	3	0
22	B	843	BCR	4	0
18	A	819	CLA	4	0
27	B	850	DGD	5	0
17	2	601	CHL	1	0
18	4	608	CLA	2	0
19	2	617	XAT	7	0
18	B	832	CLA	6	0
18	1	608	CLA	1	0
18	2	602	CLA	8	0
18	B	812	CLA	1	0
18	A	804	CLA	6	0
22	J	102	BCR	6	0
22	A	848	BCR	3	0
20	1	615	LHG	13	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	A	853	BCR	7	0
18	1	612	CLA	1	0
18	A	830	CLA	4	0
18	B	819	CLA	1	0
18	A	807	CLA	3	0
22	A	850	BCR	5	0
18	4	603	CLA	1	0
17	4	615	CHL	1	0
18	F	301	CLA	1	0
18	2	612	CLA	4	0
18	3	607	CLA	3	0
18	A	835	CLA	5	0
18	B	804	CLA	1	0
22	B	801	BCR	10	0
18	A	828	CLA	1	0
18	A	822	CLA	4	0
22	B	846	BCR	7	0
18	B	830	CLA	1	0
19	1	614	XAT	18	0
18	K	201	CLA	1	0
22	B	844	BCR	2	0
18	1	604	CLA	3	0
18	A	815	CLA	1	0
17	4	605	CHL	1	0
22	B	849	BCR	4	0
18	A	820	CLA	4	0
22	F	304	BCR	2	0
18	A	831	CLA	1	0
18	4	609	CLA	4	0
18	A	808	CLA	2	0
18	4	602	CLA	5	0
21	3	613	LUT	6	0
17	2	607	CHL	2	0
18	B	826	CLA	3	0
18	A	840	CLA	1	0
18	1	609	CLA	7	0
18	A	833	CLA	3	0
22	L	306	BCR	5	0
18	A	803	CLA	3	0
18	B	814	CLA	3	0
18	B	820	CLA	2	0
18	L	303	CLA	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	I	101	BCR	1	0
17	3	606	CHL	1	0
18	B	808	CLA	5	0
18	A	825	CLA	3	0
18	2	609	CLA	5	0
18	B	837	CLA	2	0
19	4	617	XAT	5	0
22	B	845	BCR	8	0
18	4	612	CLA	2	0
25	A	855	PQN	3	0
18	A	809	CLA	9	0
18	B	817	CLA	3	0
18	A	841	CLA	6	0
17	1	601	CHL	10	0
18	B	803	CLA	4	0
18	A	843	CLA	2	0
22	B	847	BCR	4	0
18	B	827	CLA	5	0
18	1	605	CLA	1	0
18	G	201	CLA	1	0
18	B	802	CLA	4	0
22	K	205	BCR	4	0
18	3	602	CLA	2	0
18	B	809	CLA	4	0
18	3	605	CLA	1	0
18	A	818	CLA	1	0
18	H	201	CLA	2	0
18	B	841	CLA	2	0
17	2	605	CHL	3	0
18	B	824	CLA	6	0
18	A	805	CLA	3	0
22	L	305	BCR	9	0
17	4	607	CHL	2	0
20	B	851	LHG	2	0
18	3	609	CLA	1	0
22	B	848	BCR	5	0
18	1	602	CLA	8	0
20	2	618	LHG	3	0
24	A	801	CL0	5	0
22	G	204	BCR	2	0
18	A	832	CLA	1	0
20	A	846	LHG	6	0

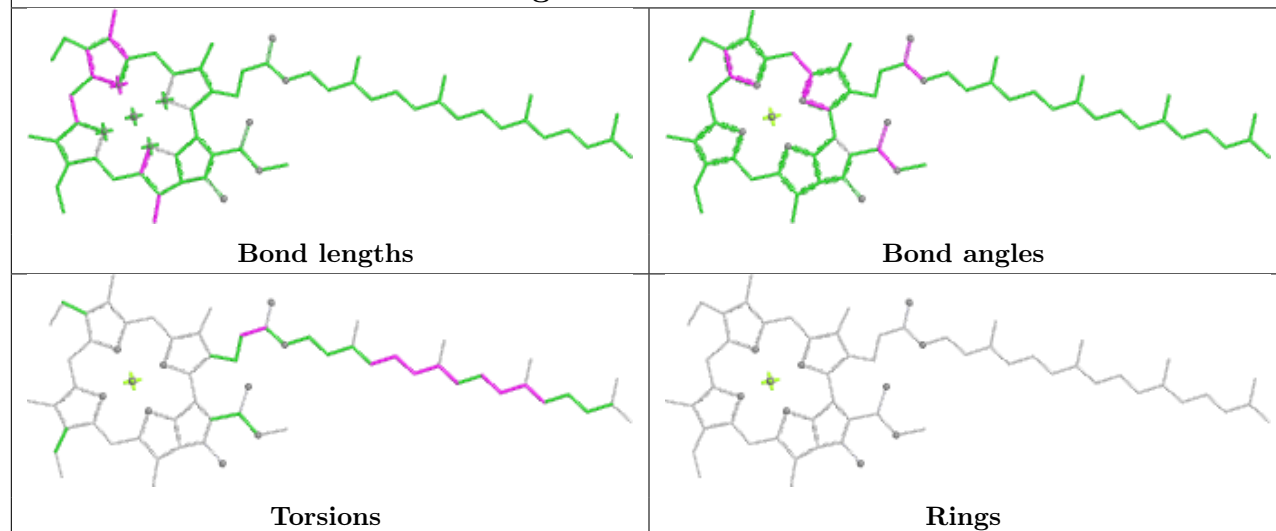
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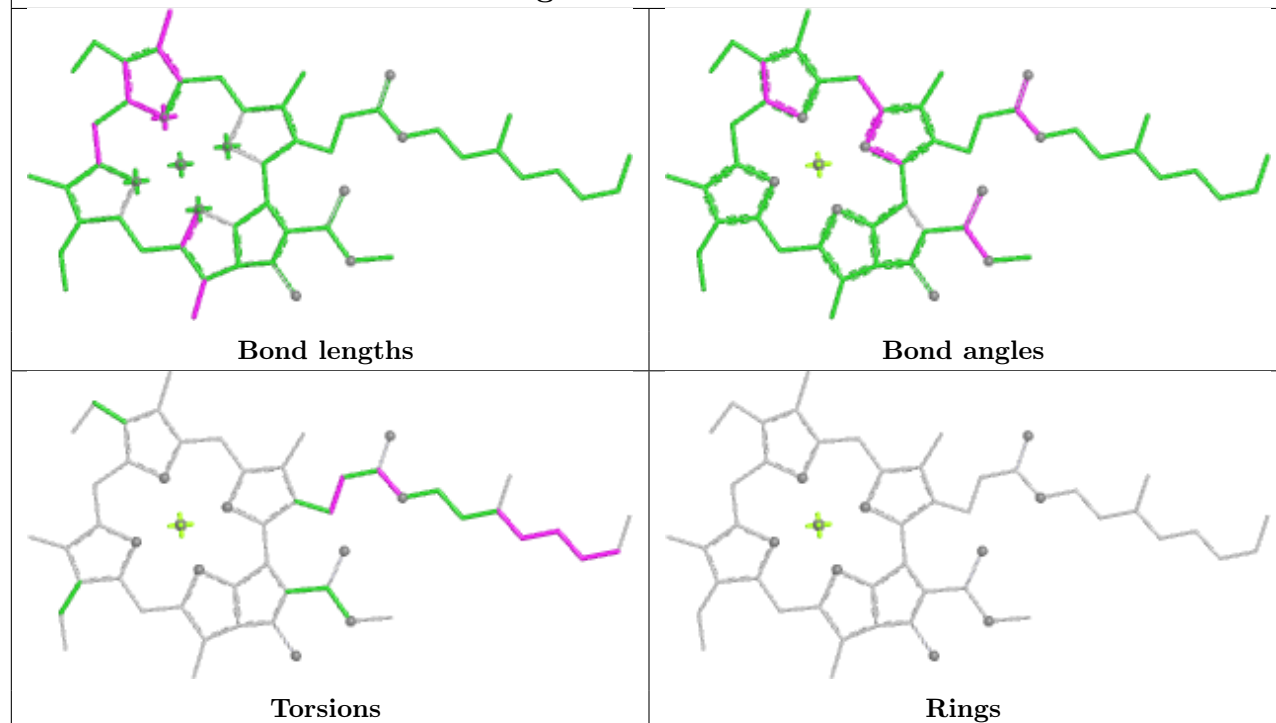
Mol	Chain	Res	Type	Clashes	Symm-Clashes
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22	A	852	BCR	2	0
18	2	608	CLA	2	0
18	A	812	CLA	6	0
18	B	805	CLA	6	0
22	4	618	BCR	4	0
22	K	202	BCR	3	0
18	2	613	CLA	1	0
18	F	302	CLA	5	0
18	A	823	CLA	1	0
18	B	828	CLA	6	0
17	2	615	CHL	5	0
18	1	611	CLA	1	0
18	1	607	CLA	1	0
22	L	301	BCR	4	0
18	3	603	CLA	2	0
18	A	806	CLA	3	0
18	A	802	CLA	3	0
18	A	836	CLA	1	0
18	L	302	CLA	2	0
18	B	813	CLA	4	0
18	K	204	CLA	1	0
18	A	839	CLA	1	0
18	A	834	CLA	3	0
18	4	614	CLA	2	0
21	4	616	LUT	4	0
18	B	831	CLA	1	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.

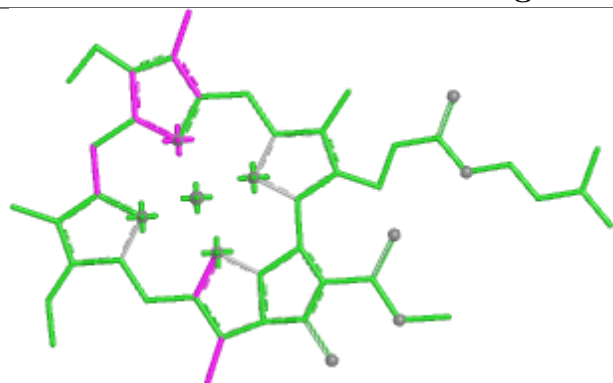
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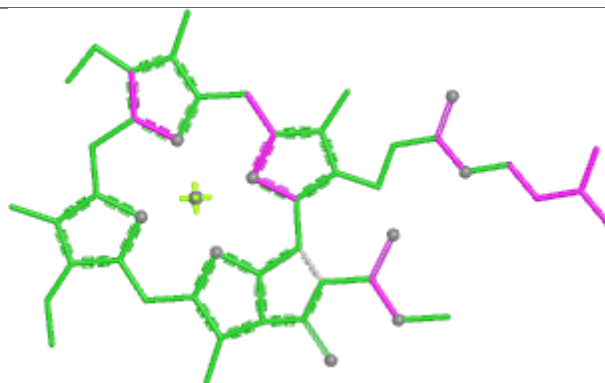
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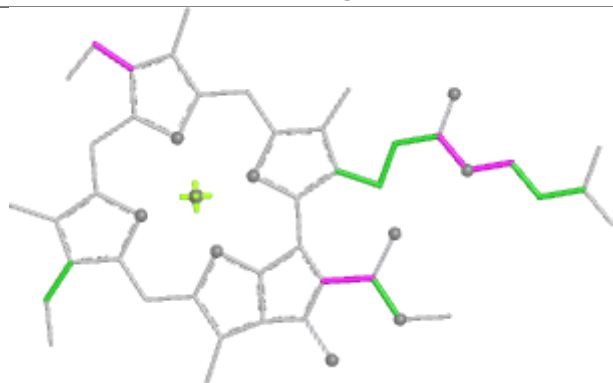
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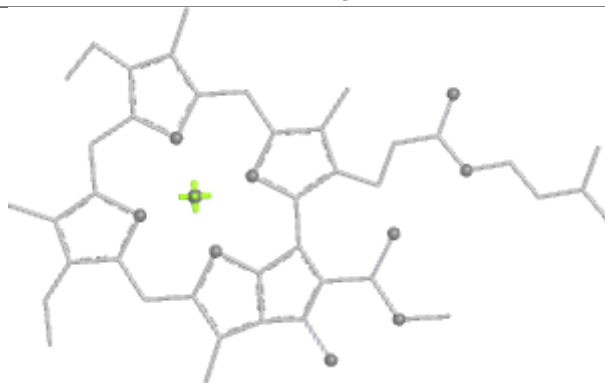
Bond lengths



Bond angles

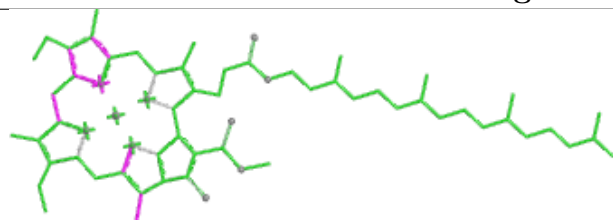


Torsions

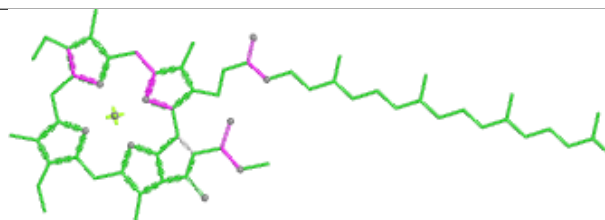


Rings

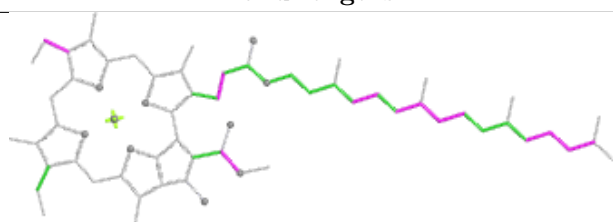
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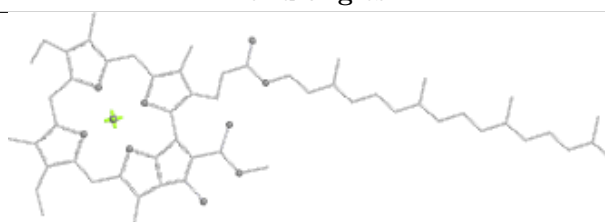
Bond lengths



Bond angles

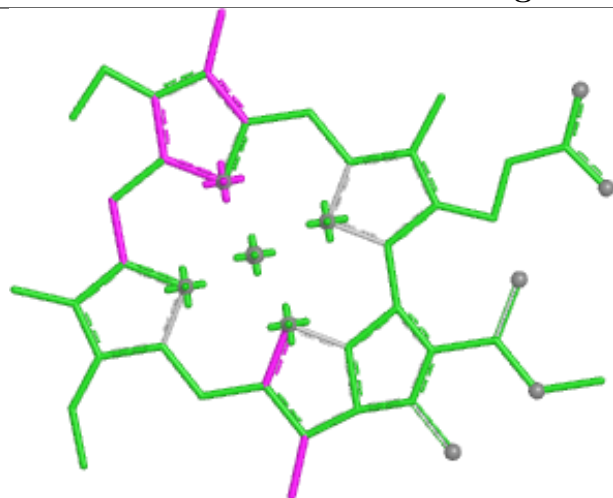


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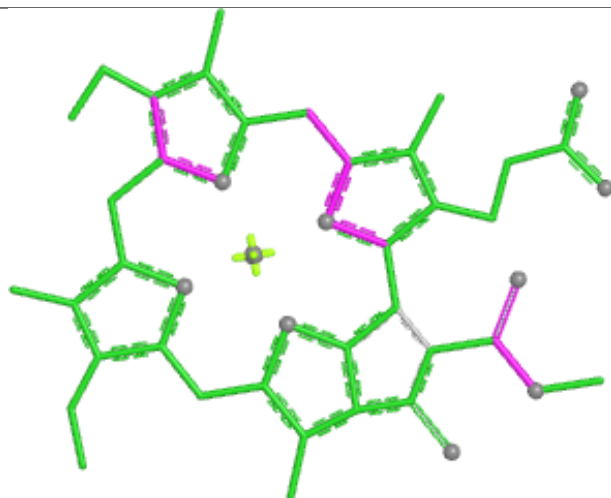


Rings

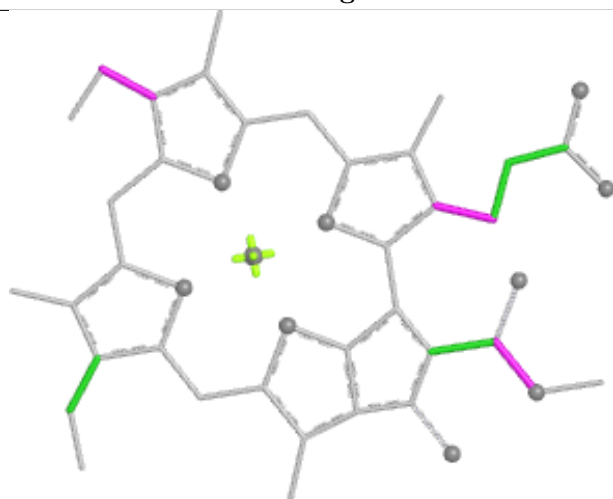
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Bond lengths



Bond angles

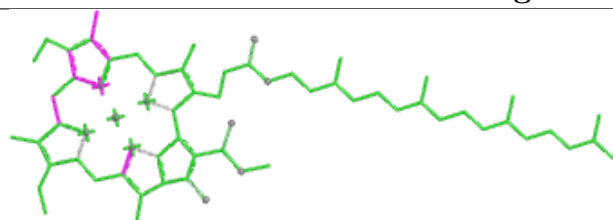


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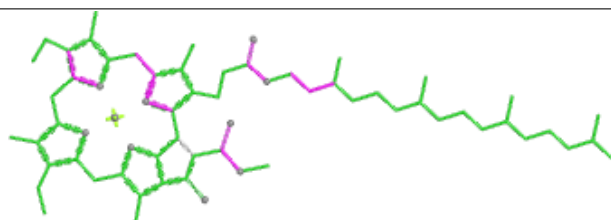


Rings

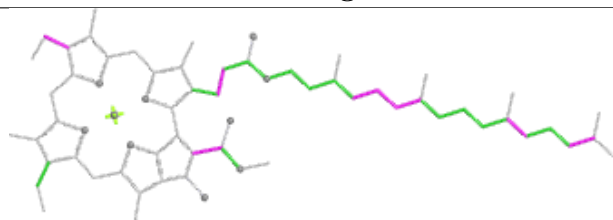
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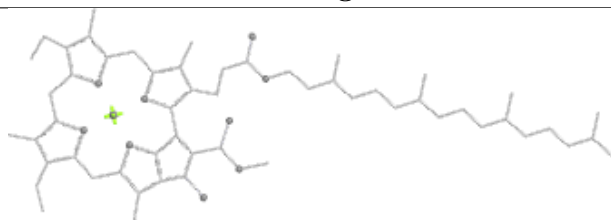
Bond lengths



Bond angles

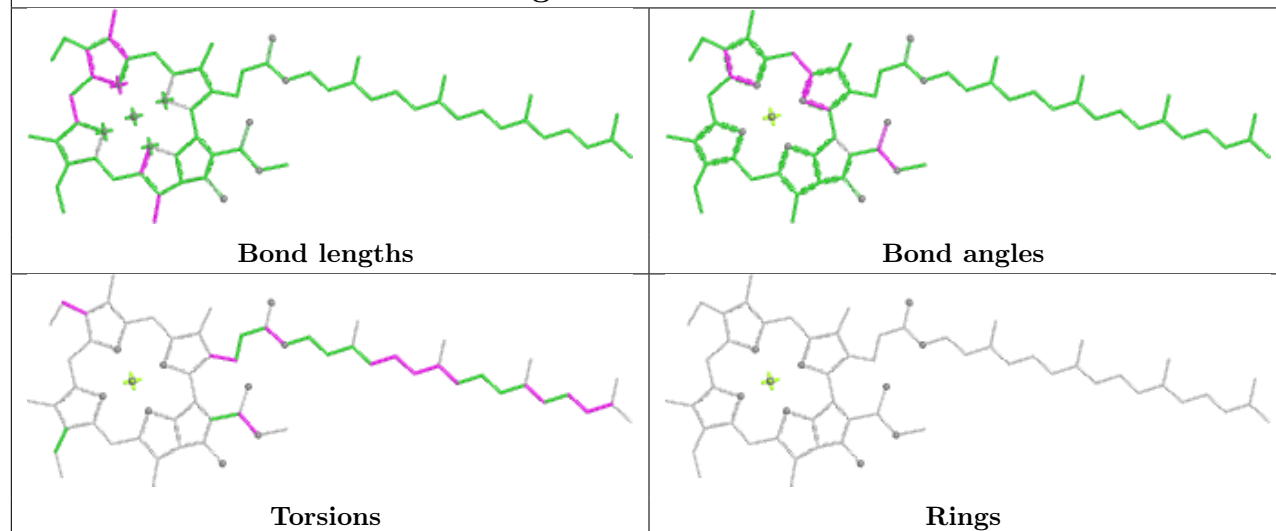


Torsions

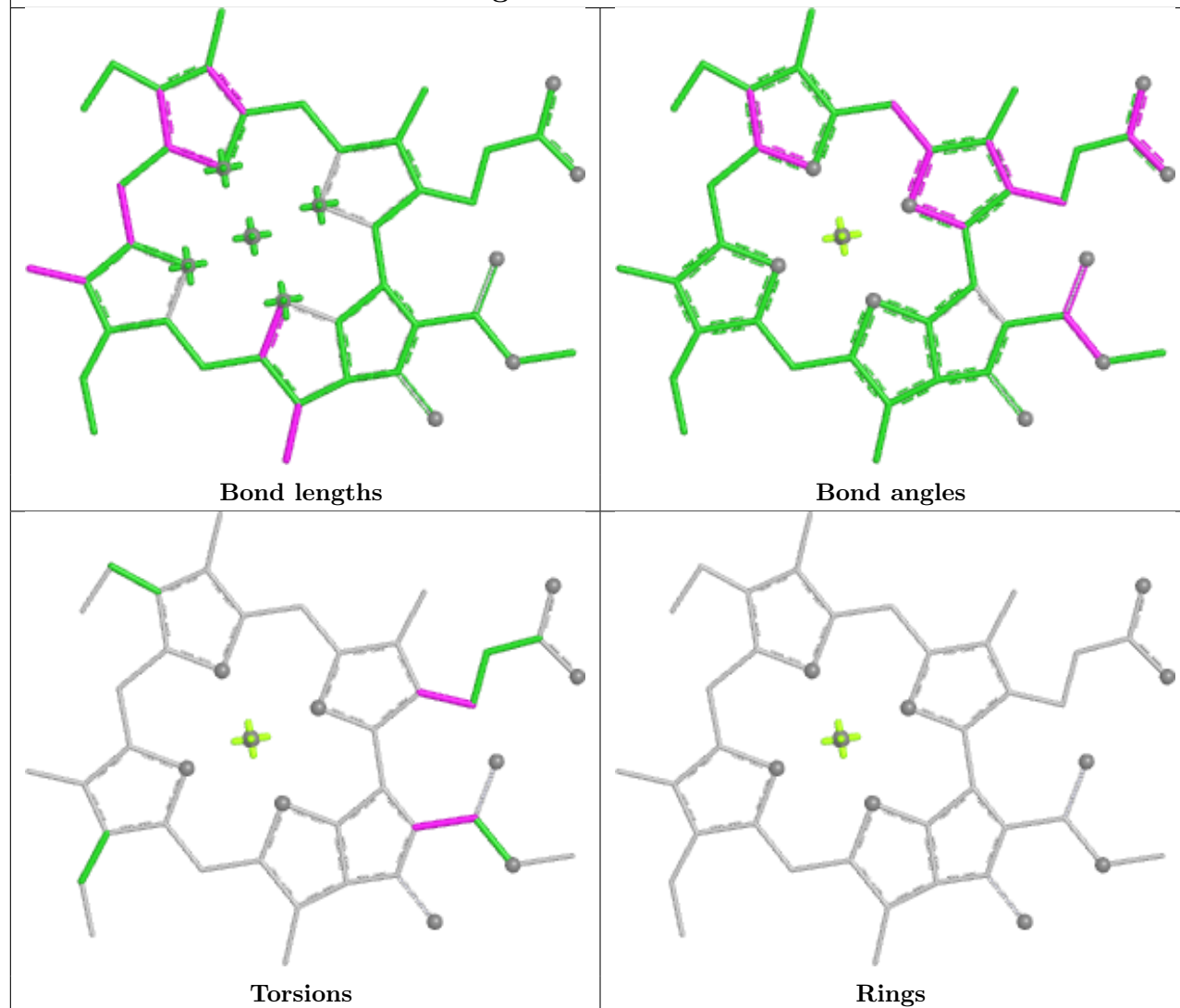


Rings

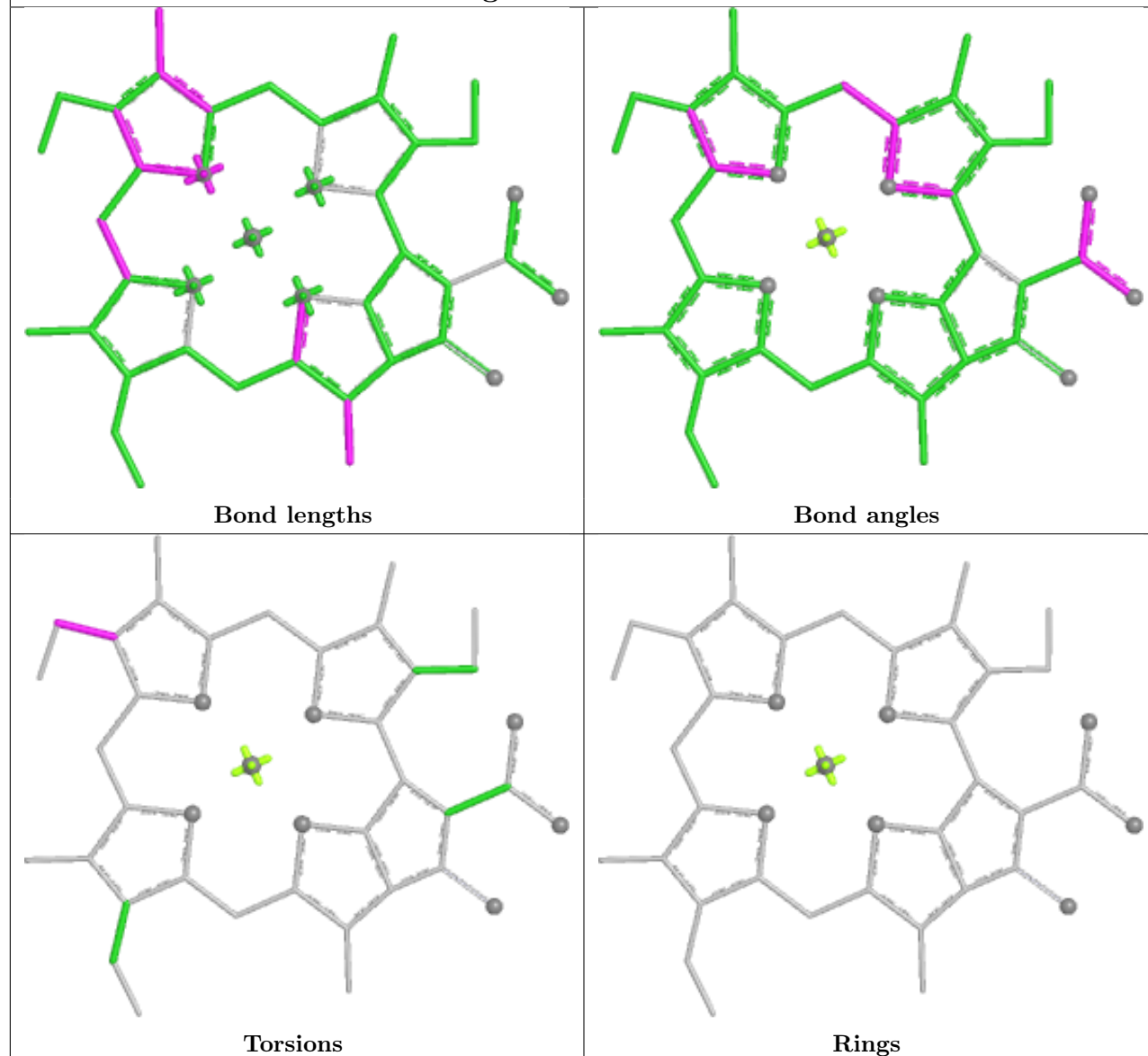
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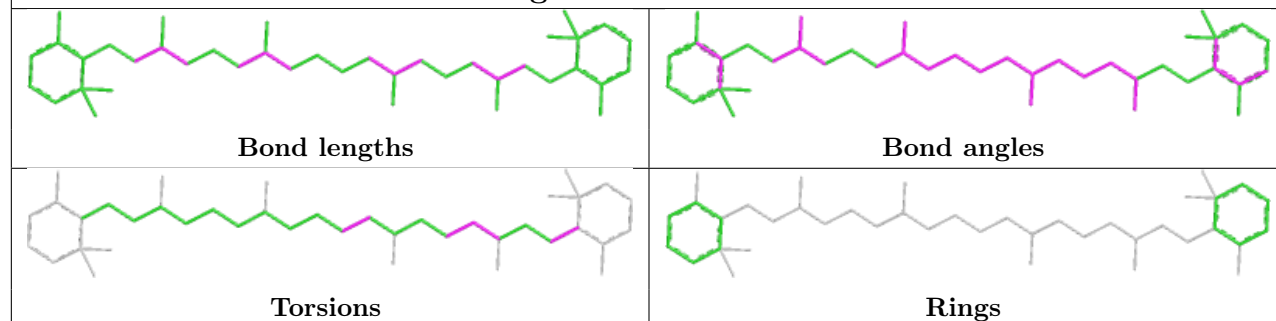
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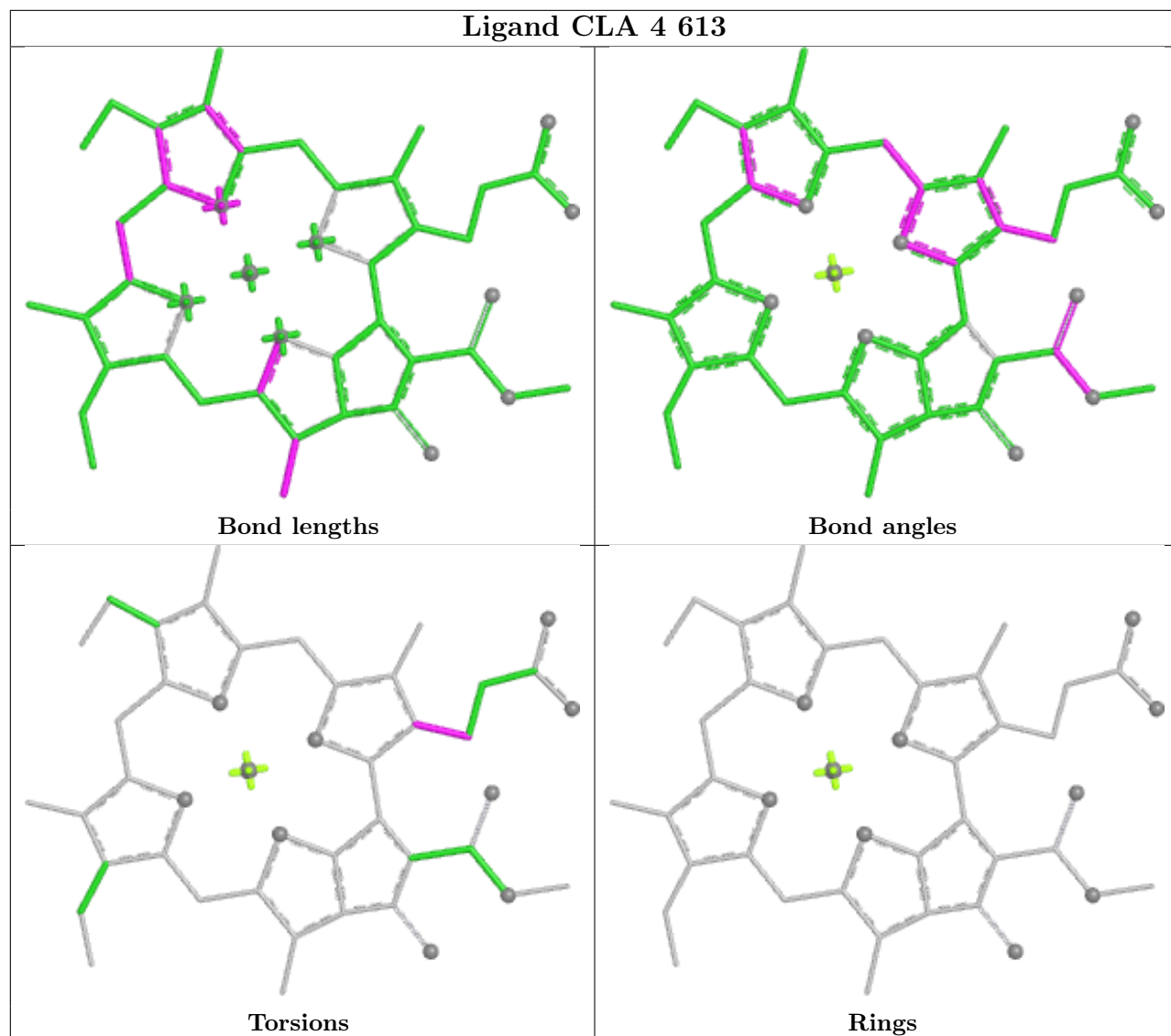
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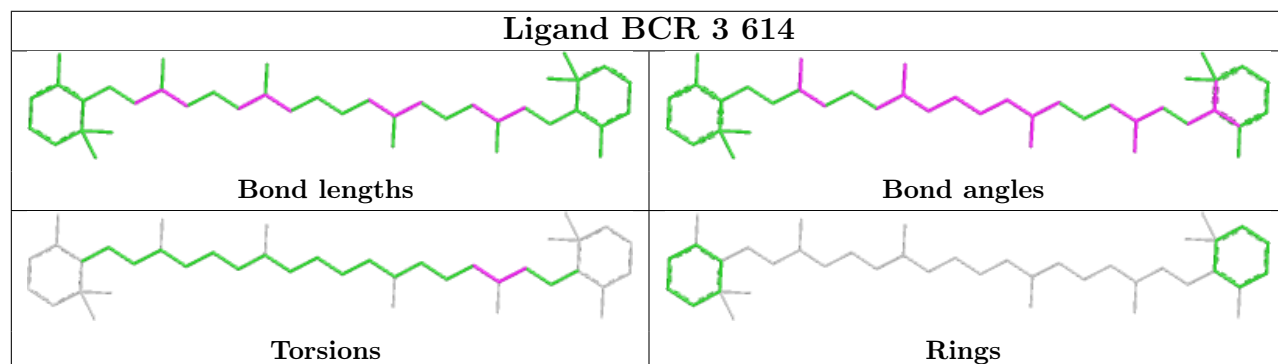
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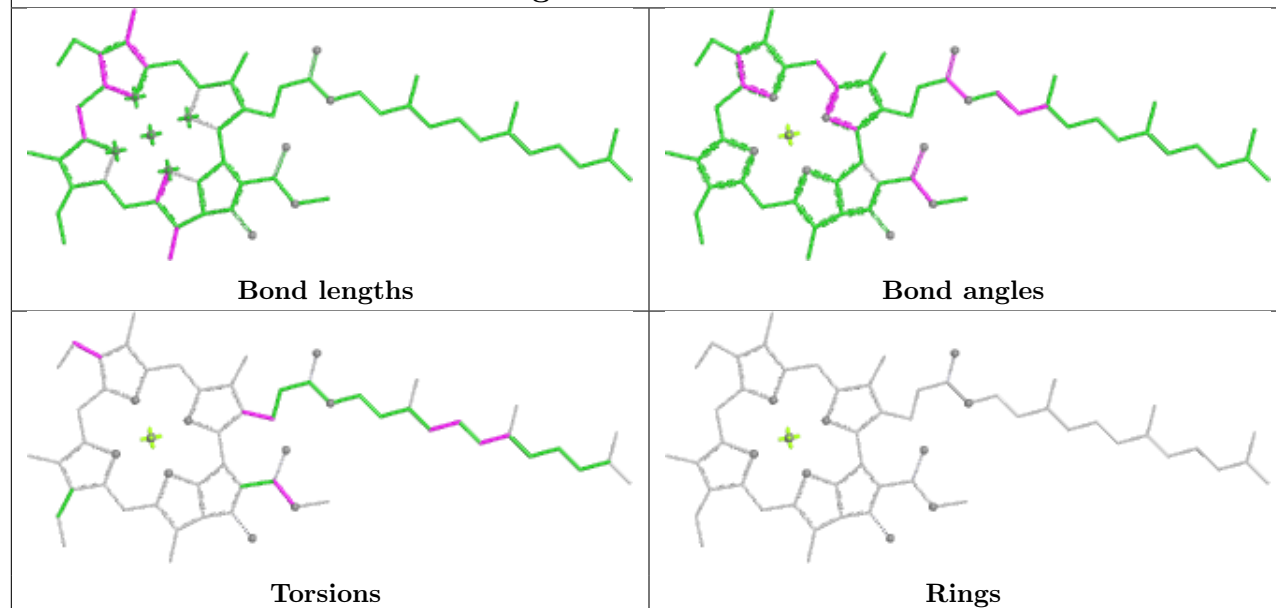
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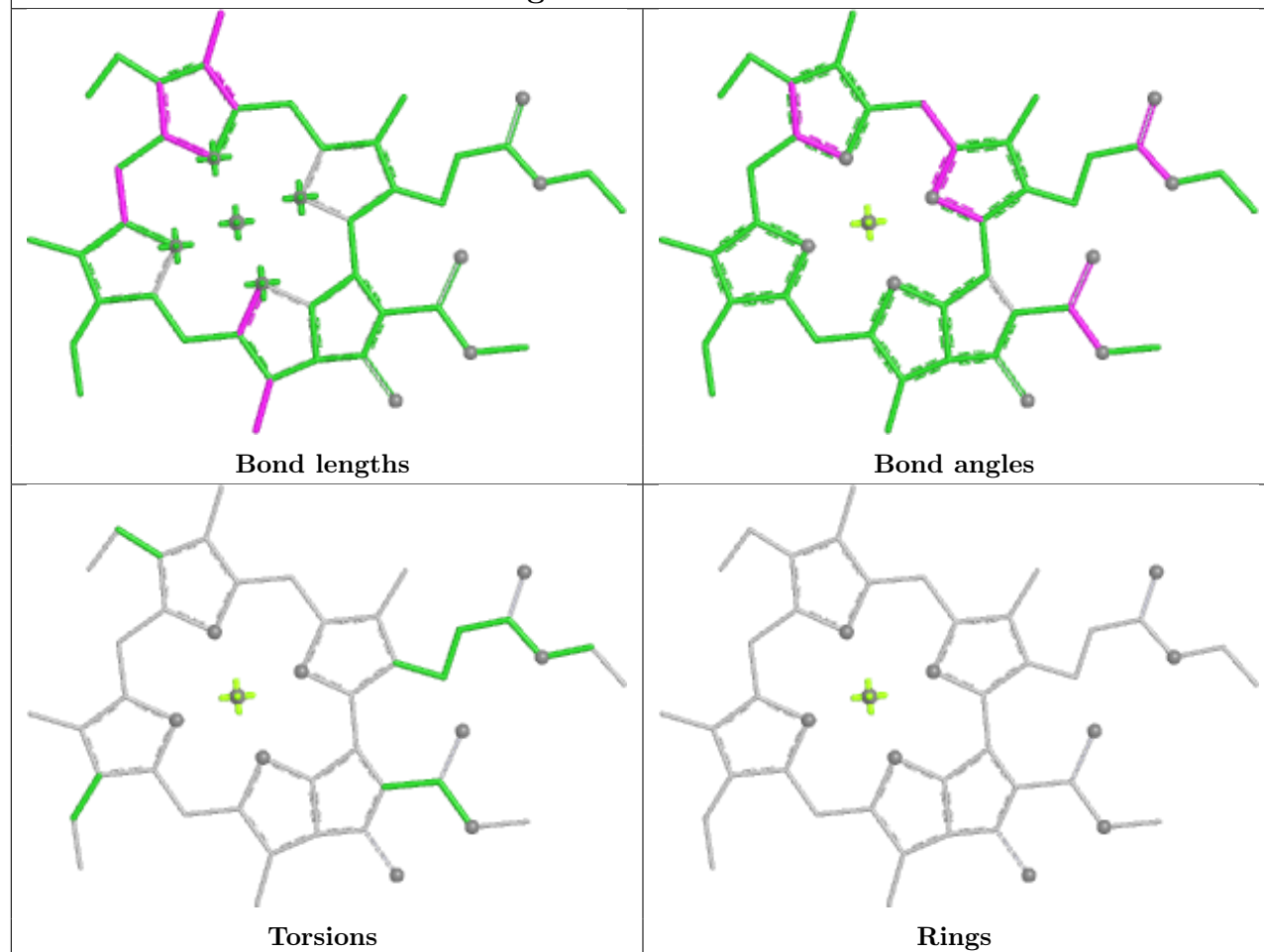
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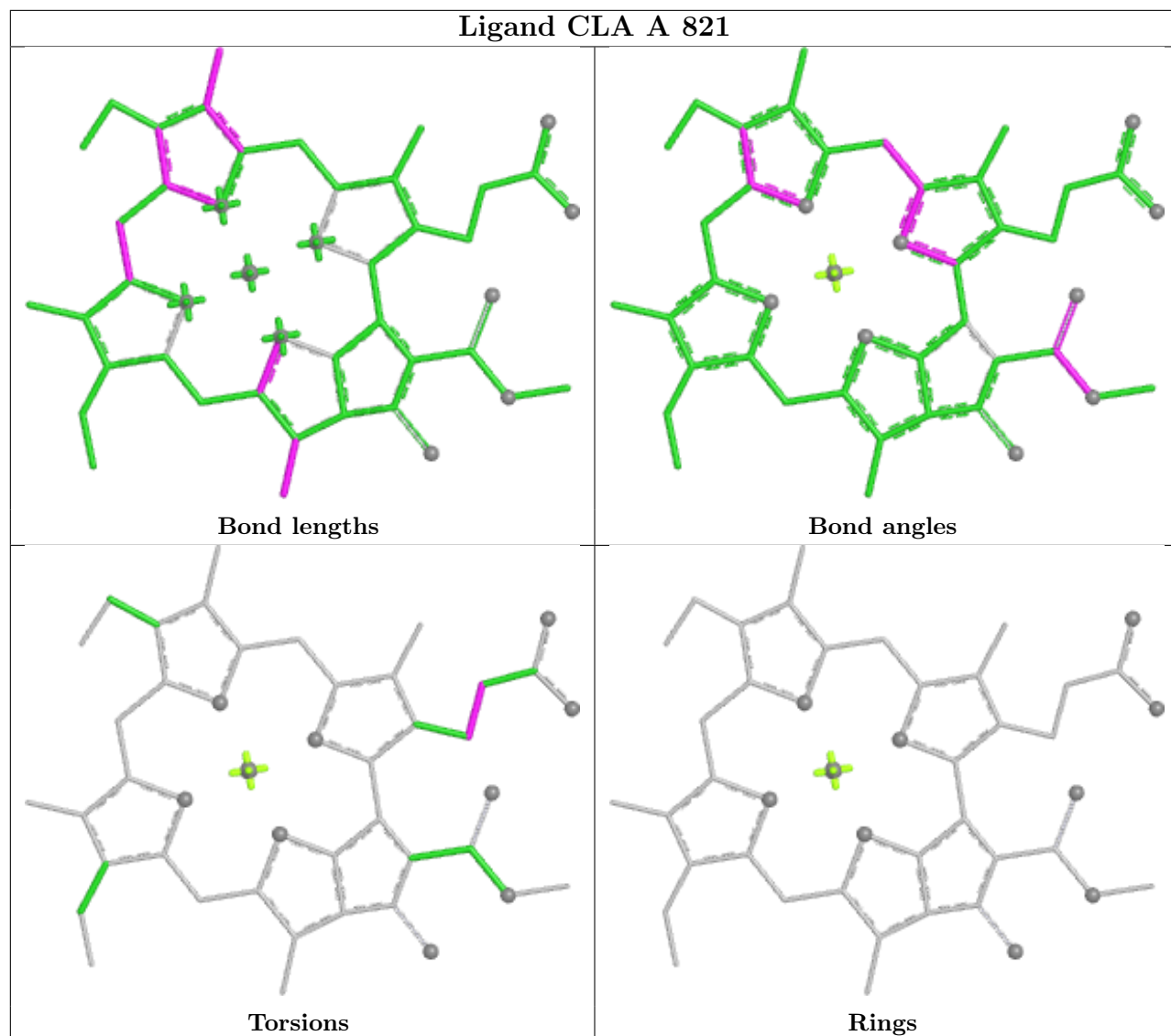


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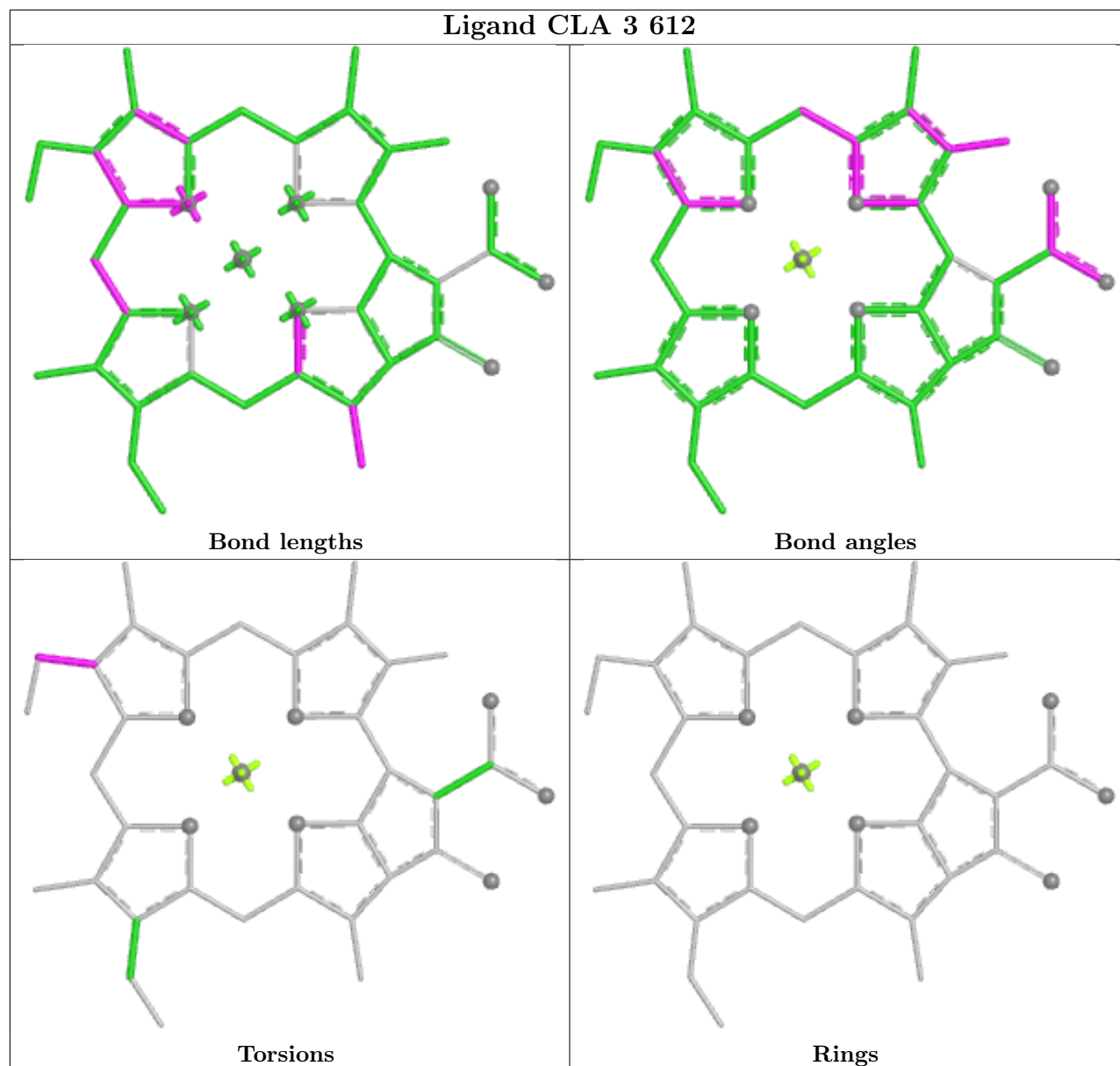


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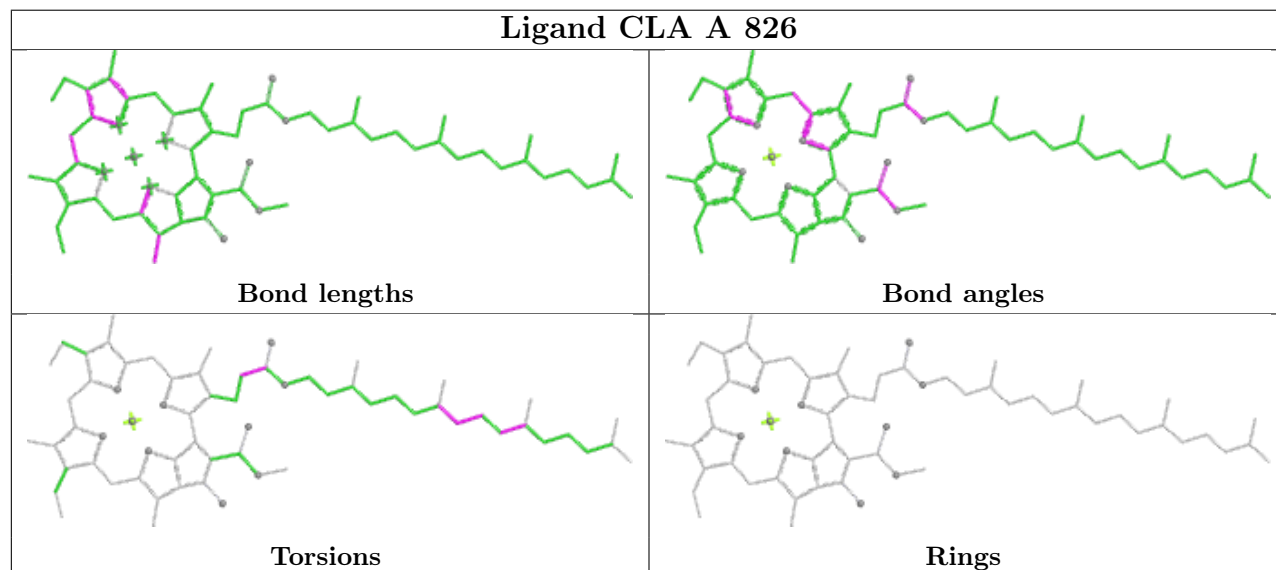


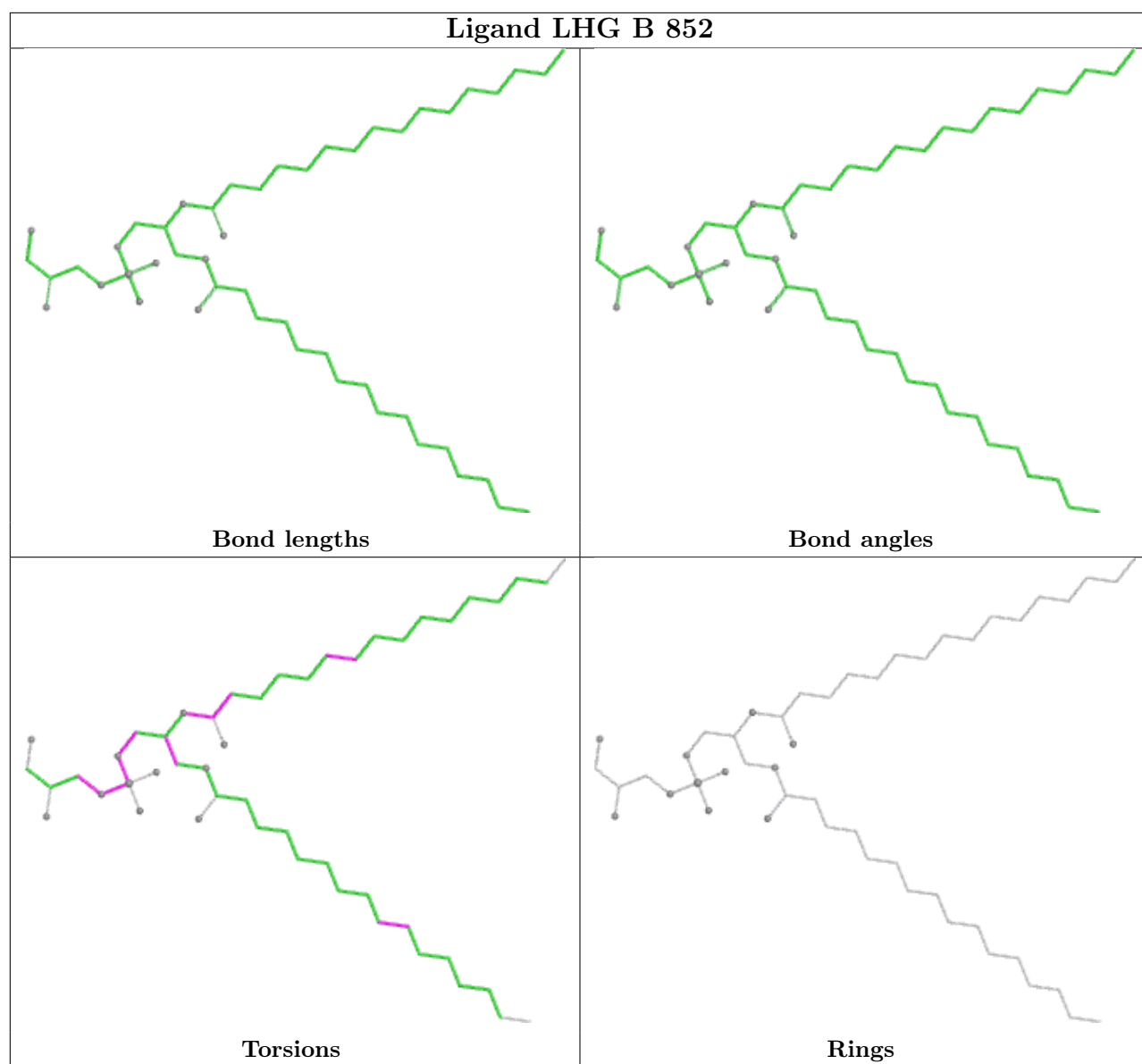


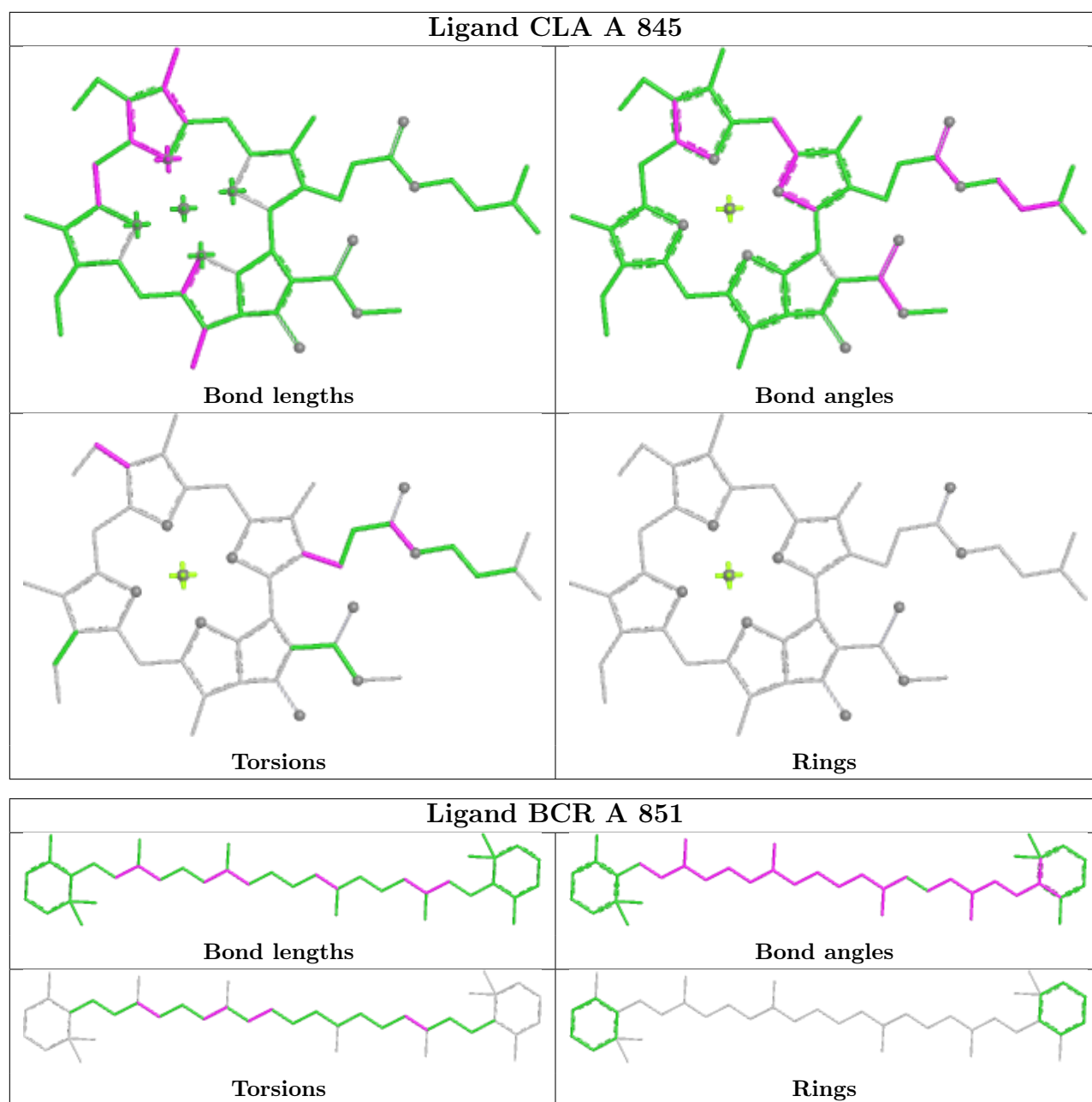
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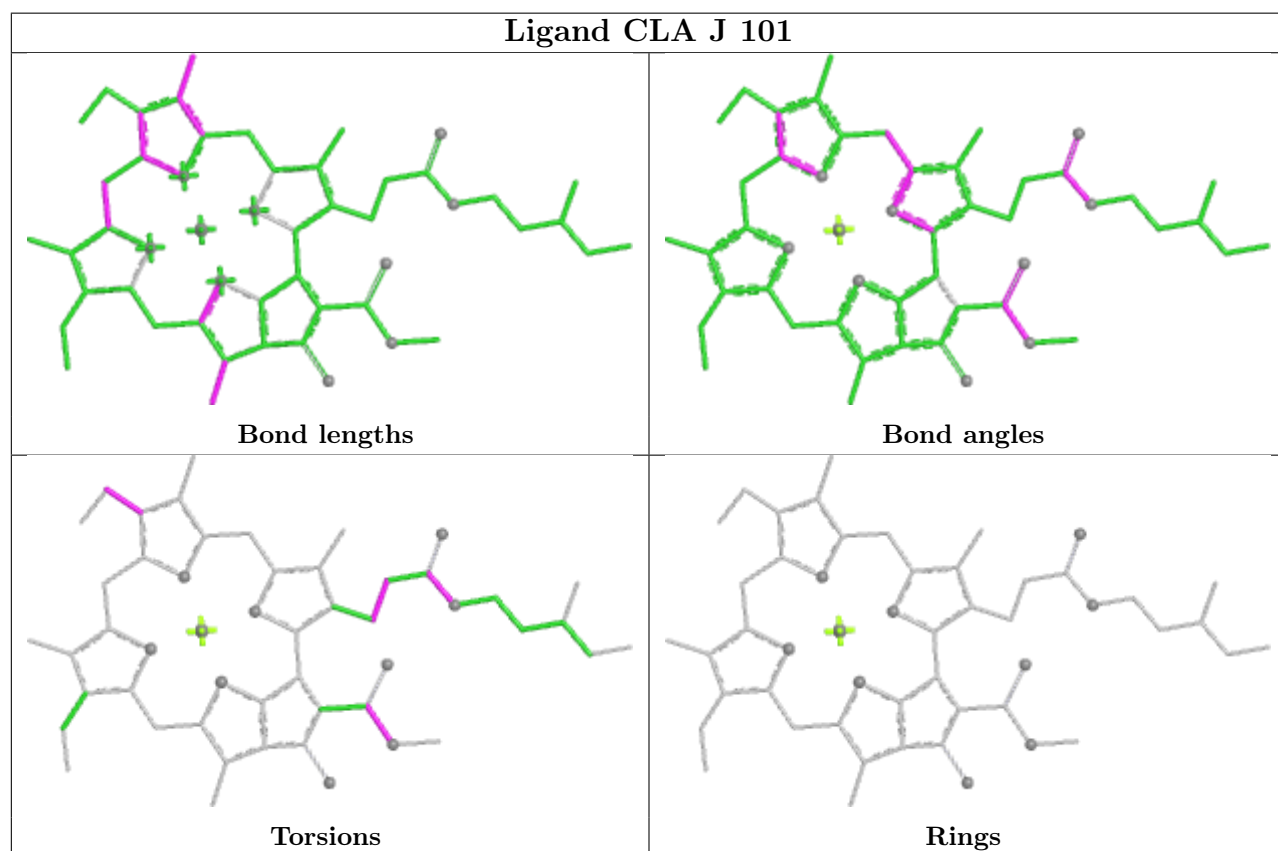
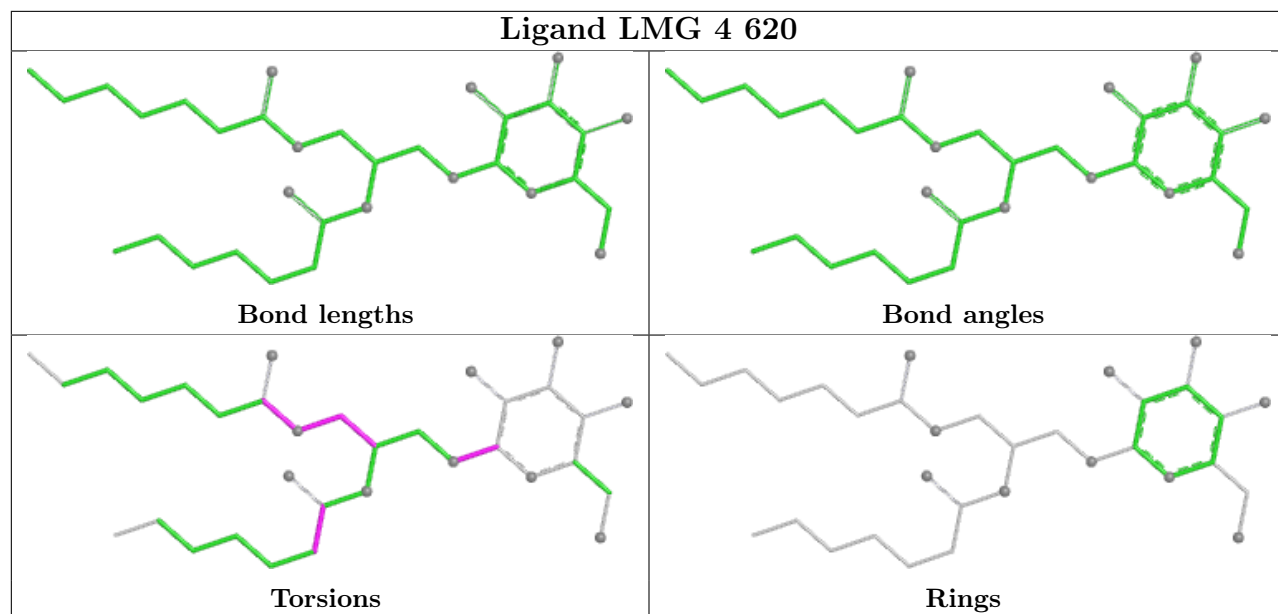


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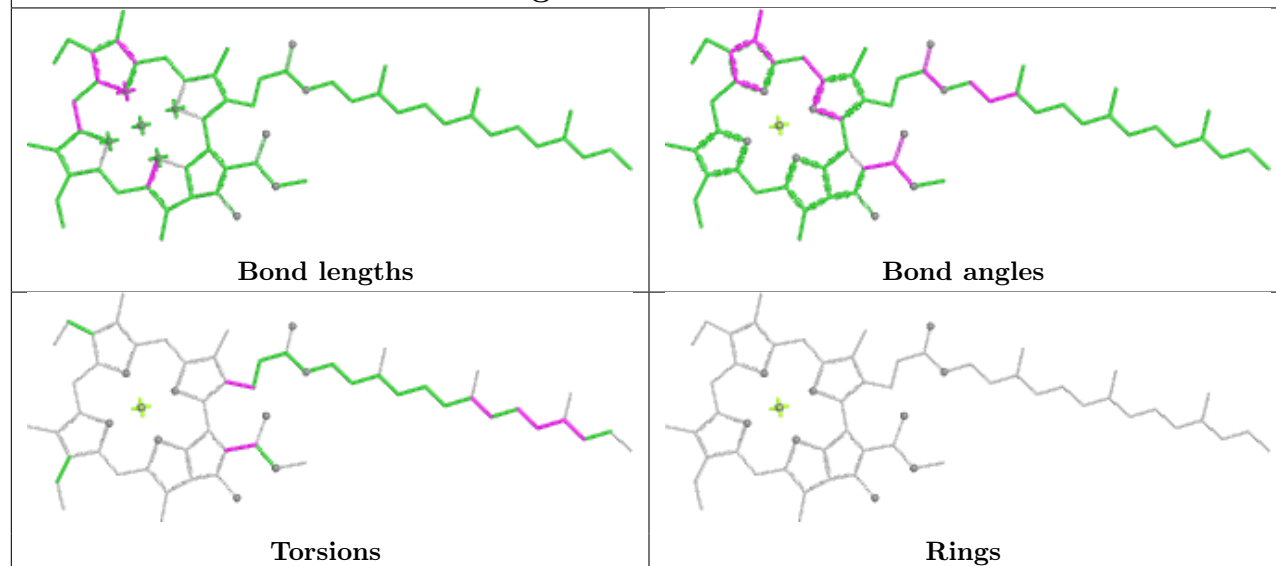




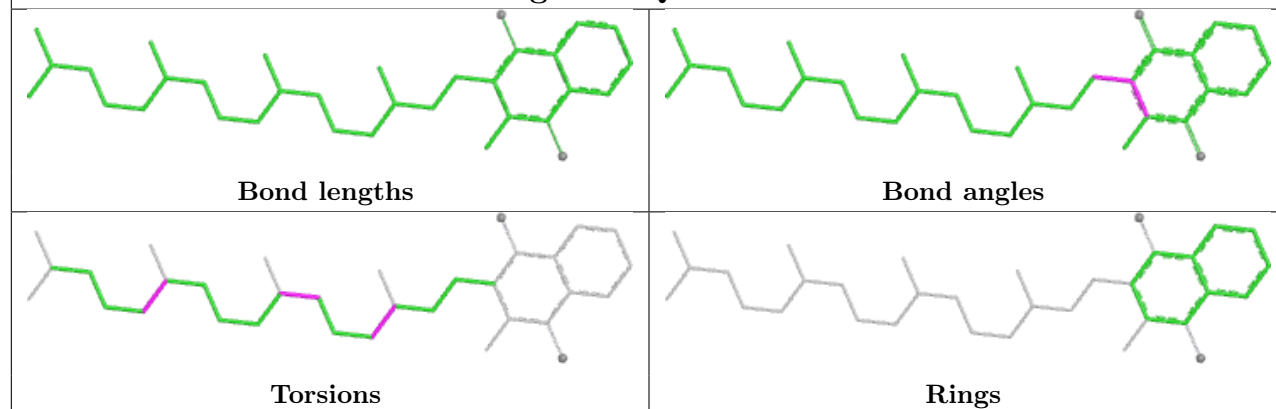




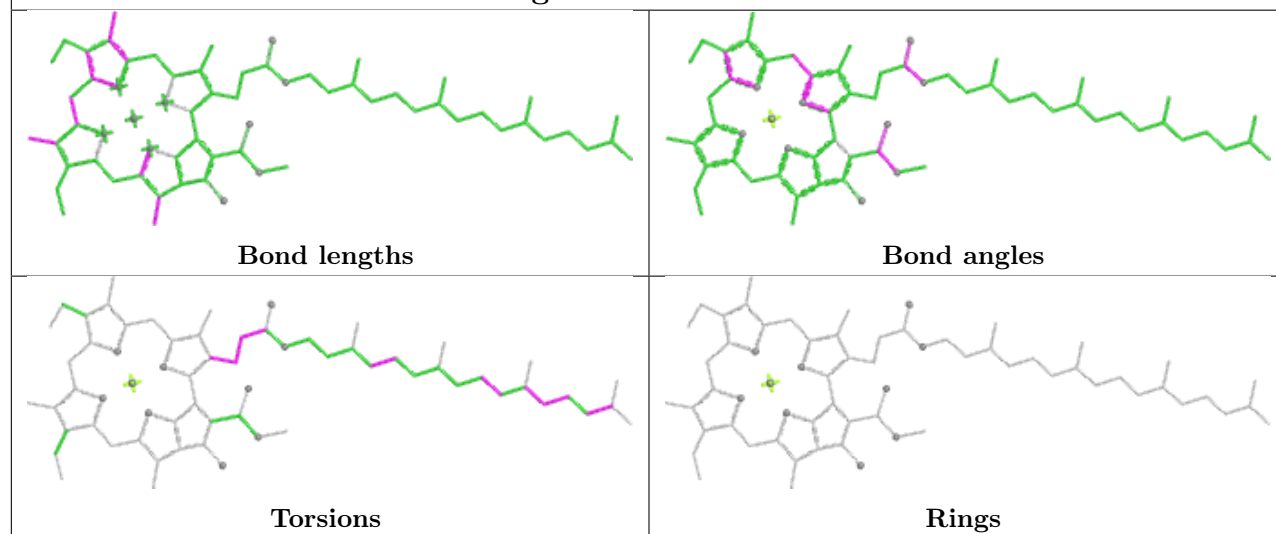
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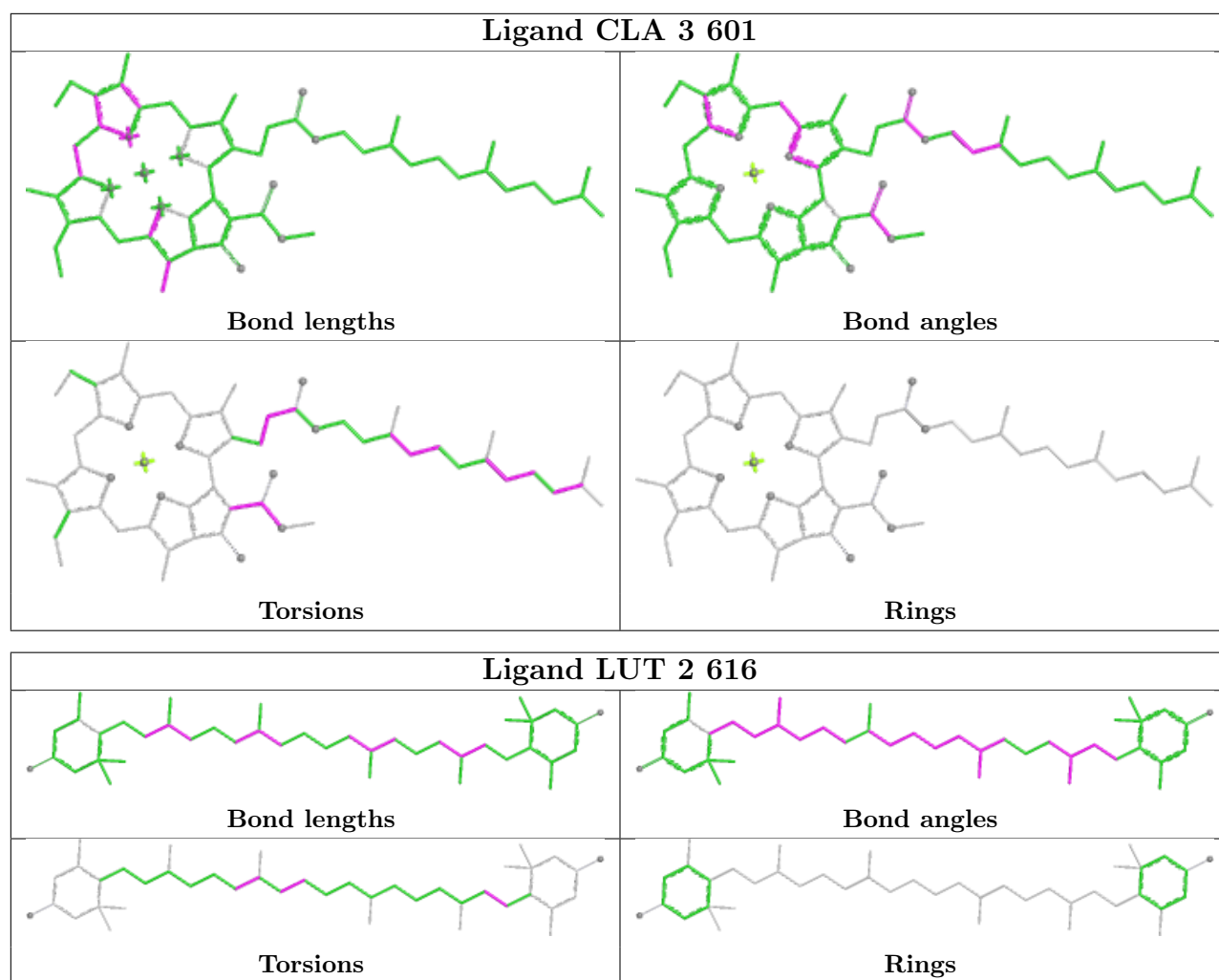


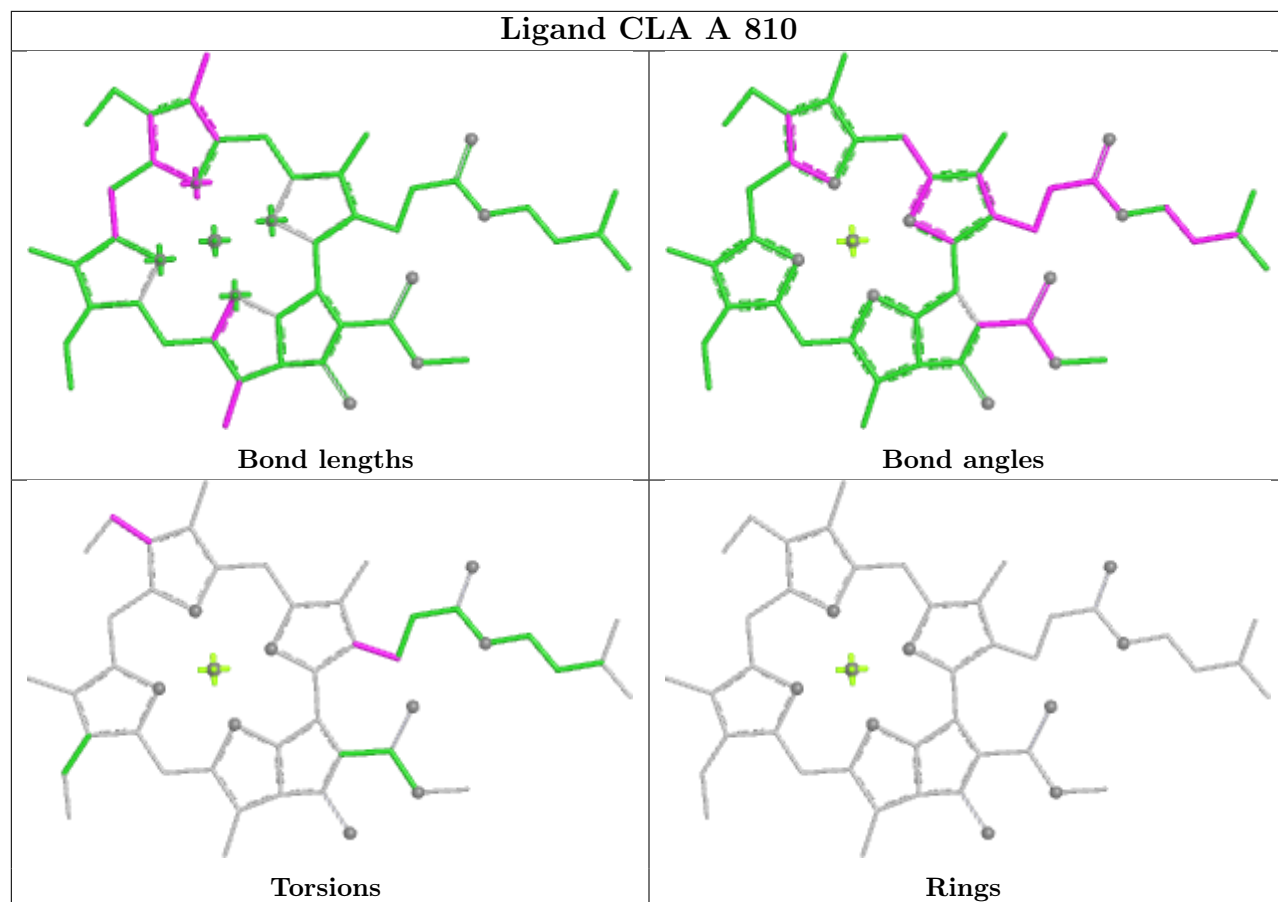
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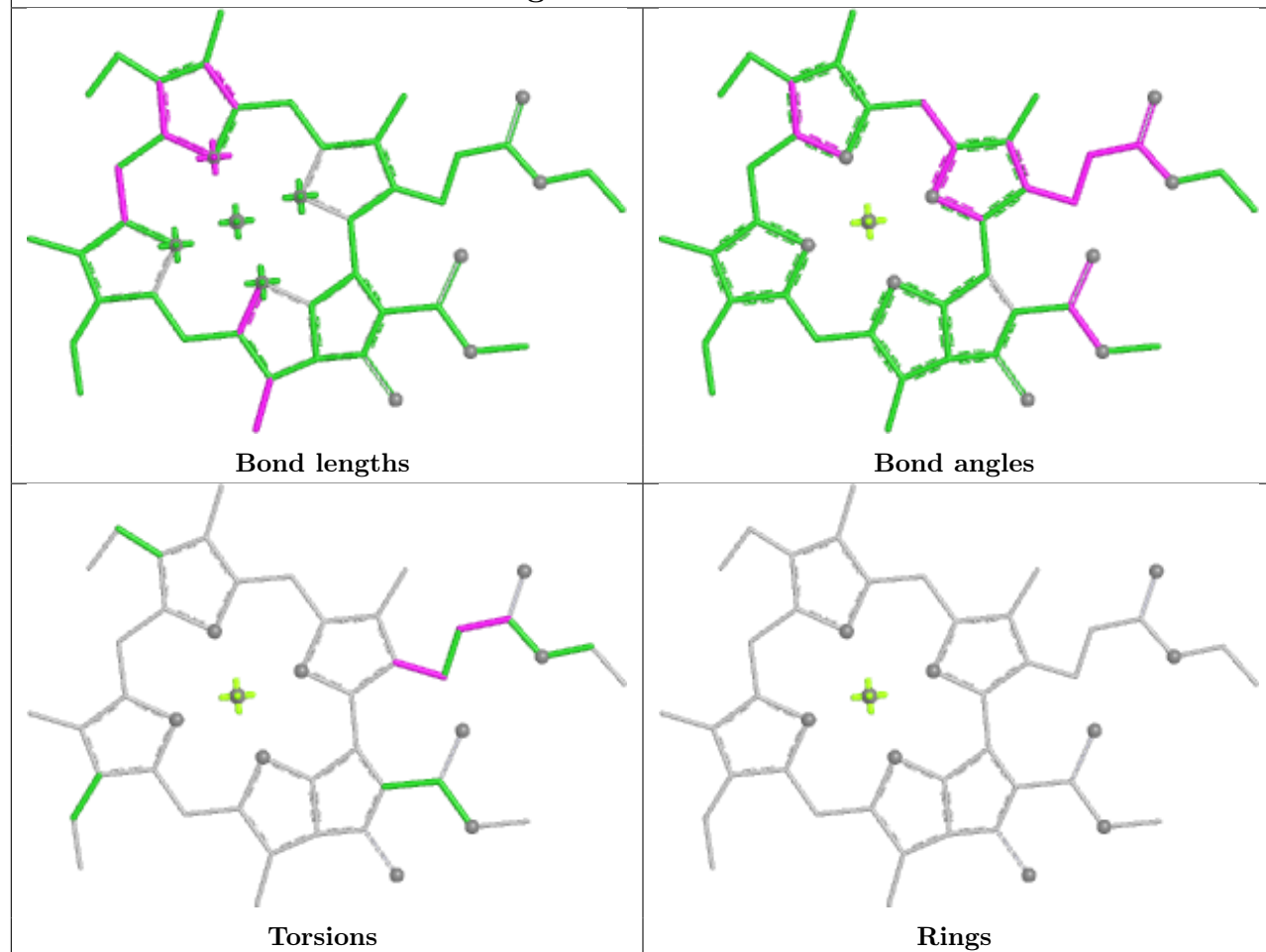
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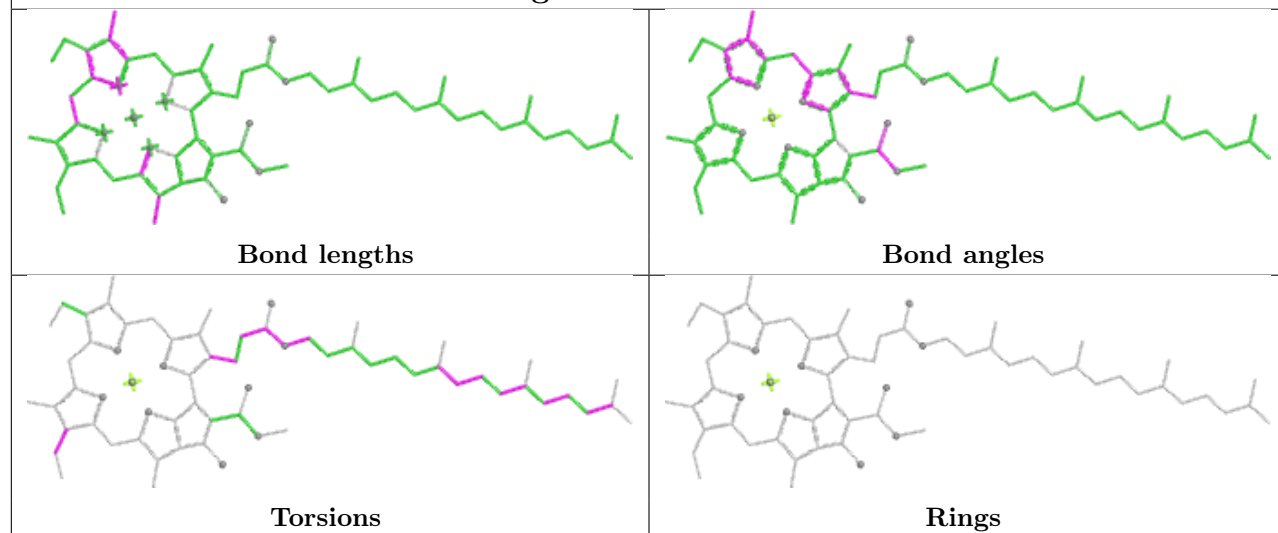




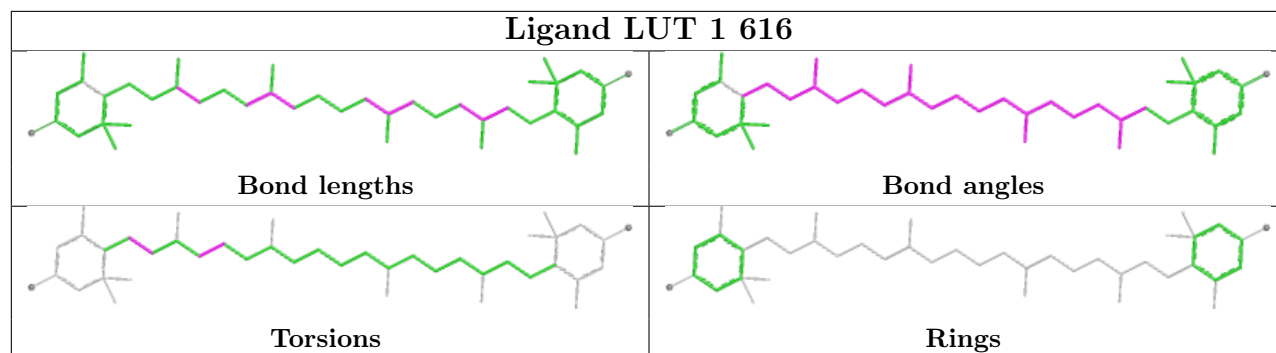
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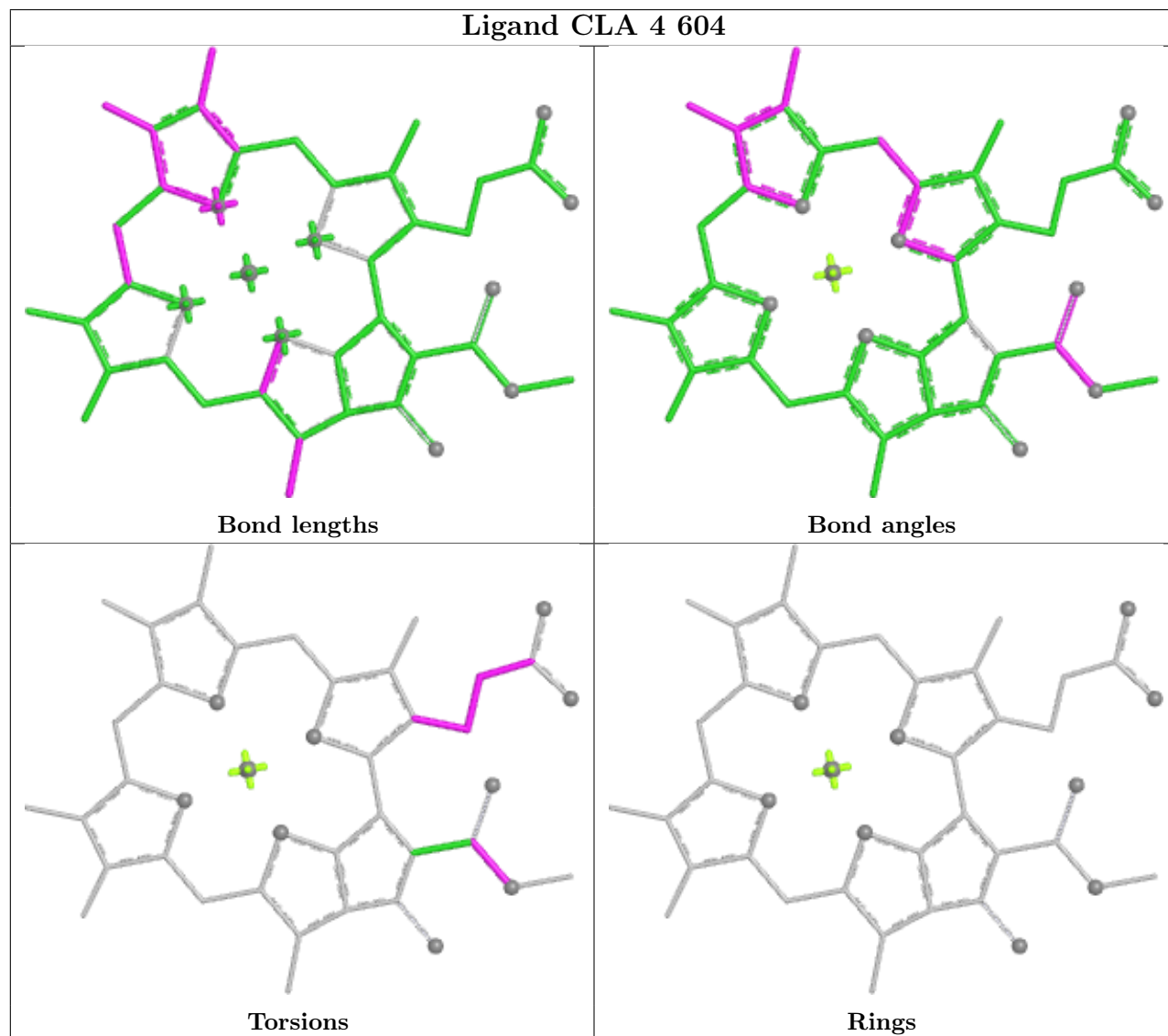
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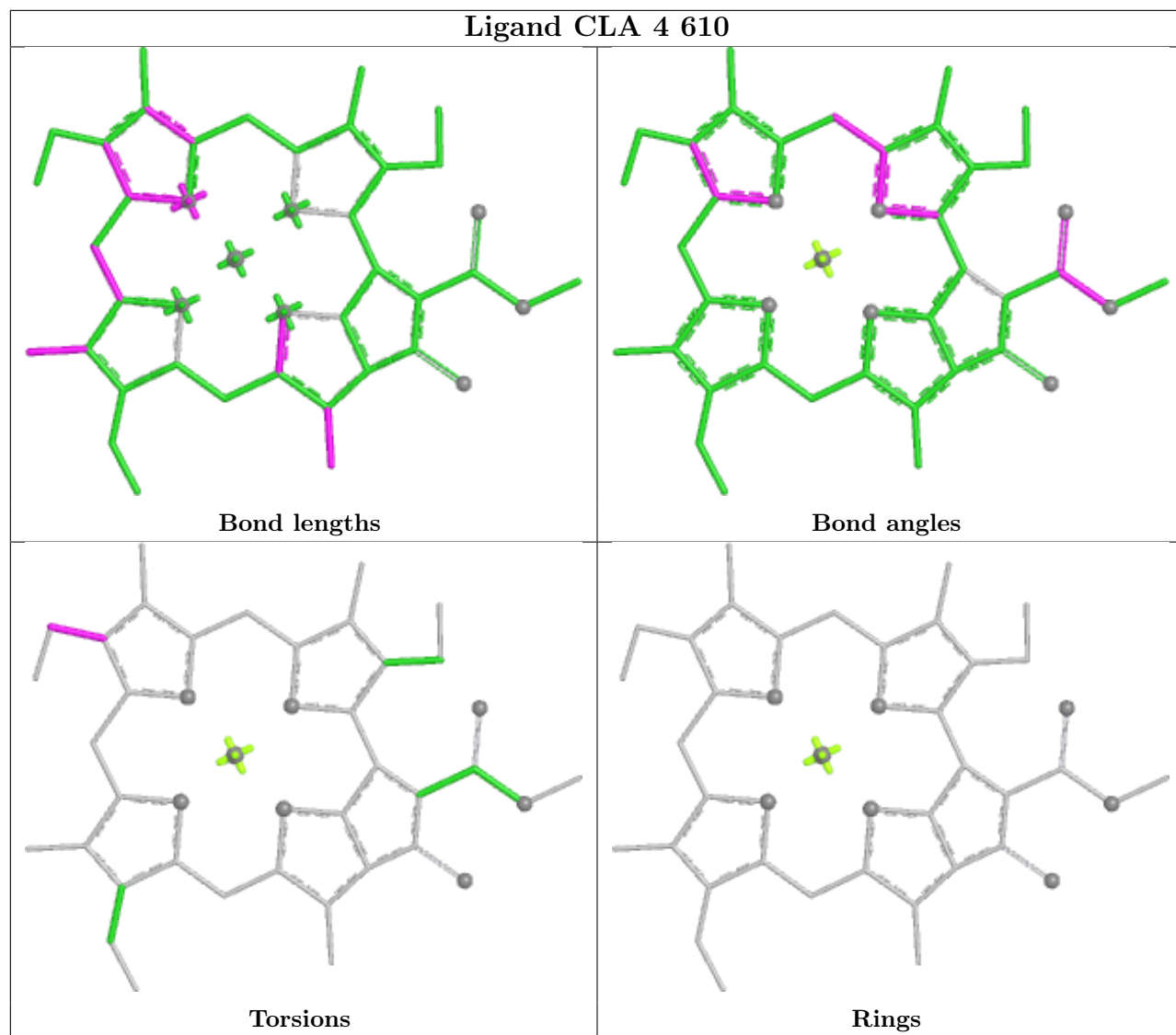


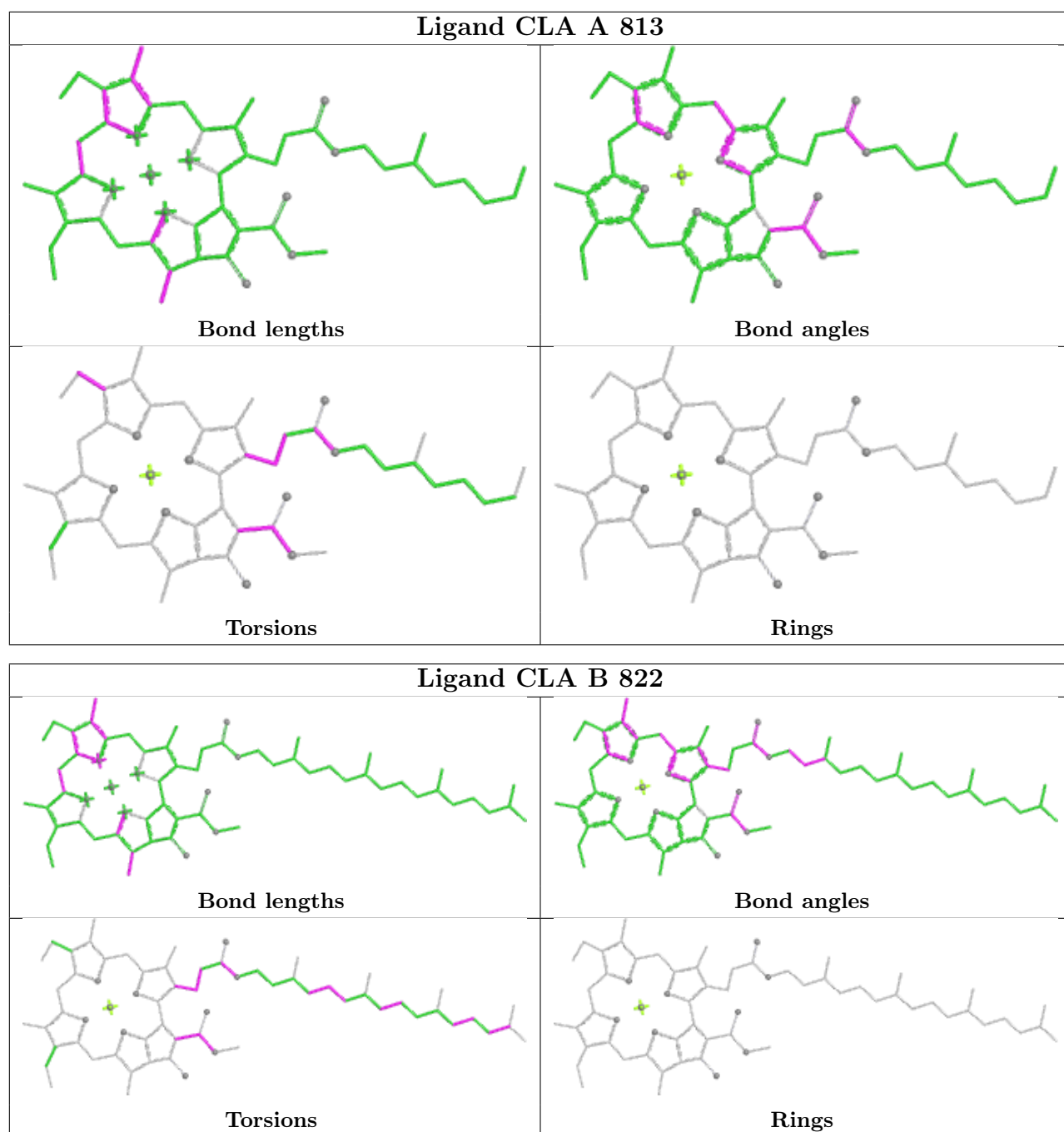
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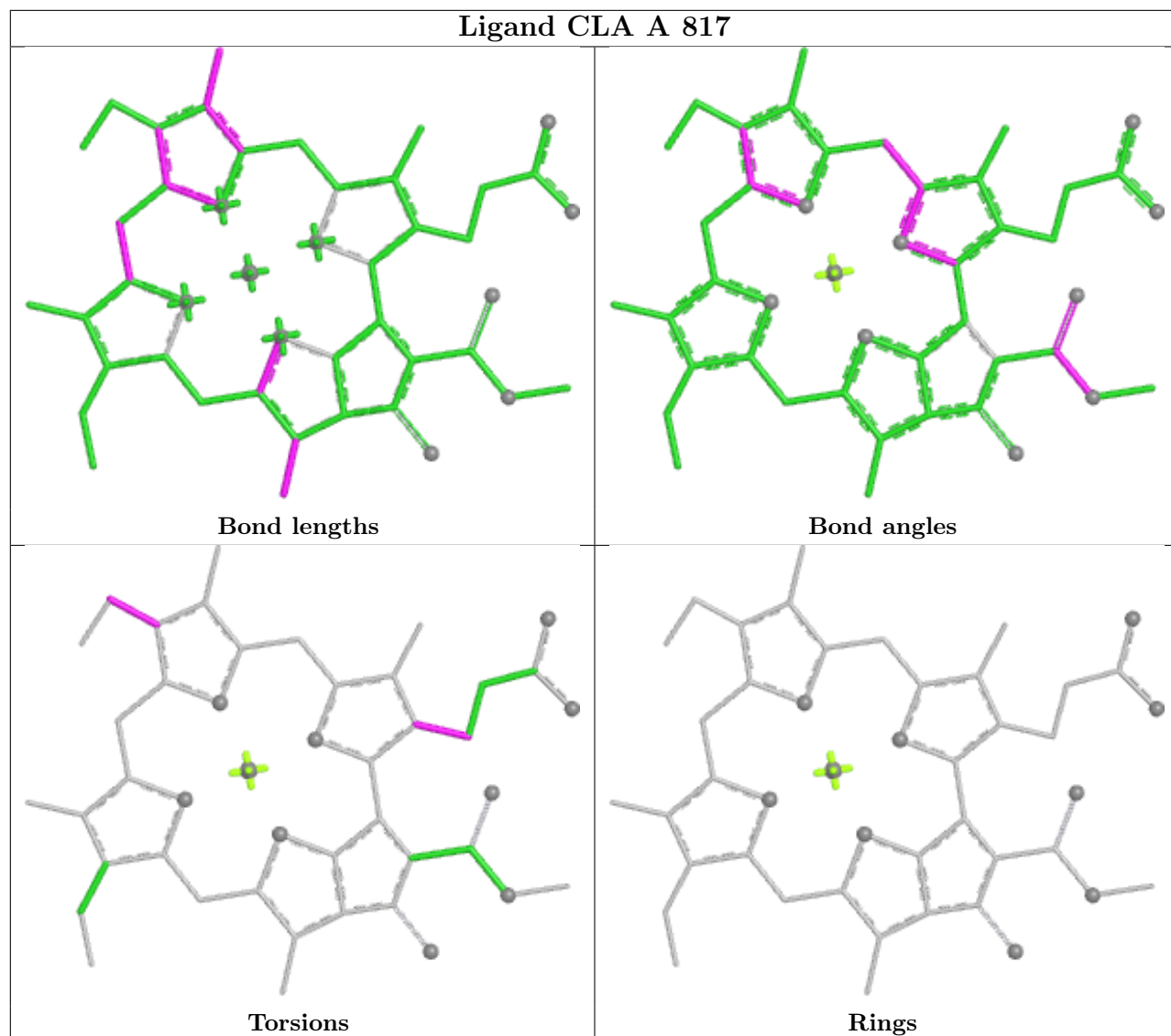


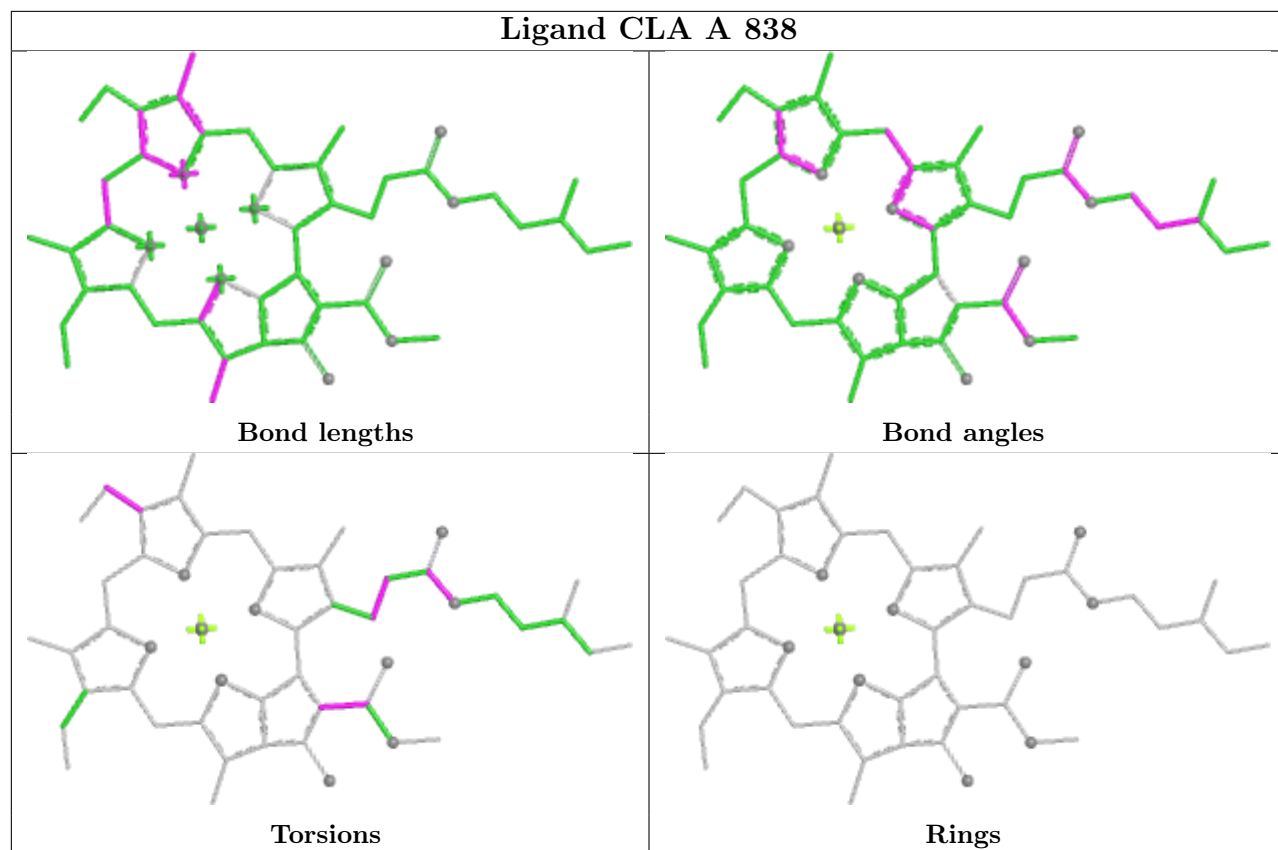
Ligand CLA 4 604



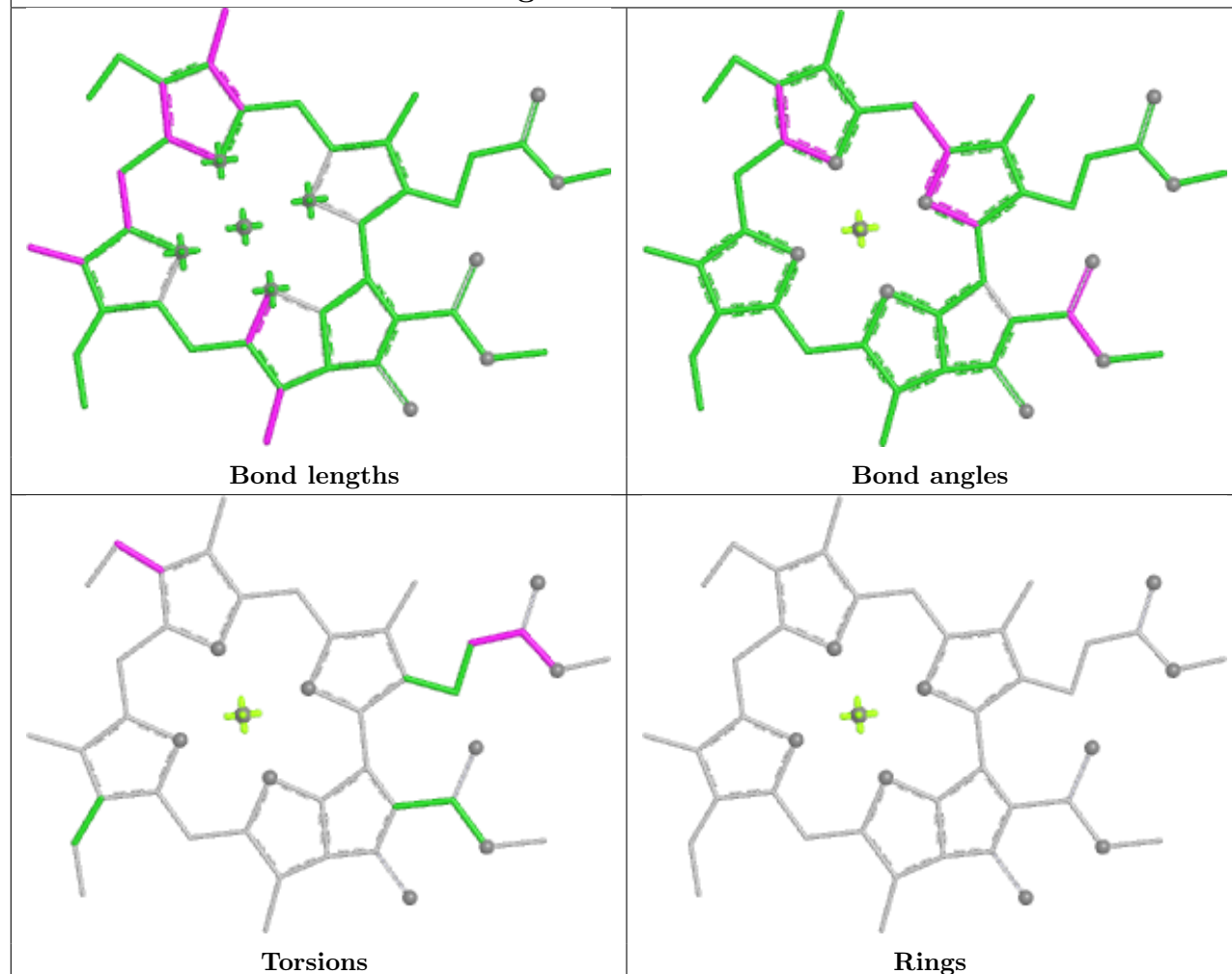




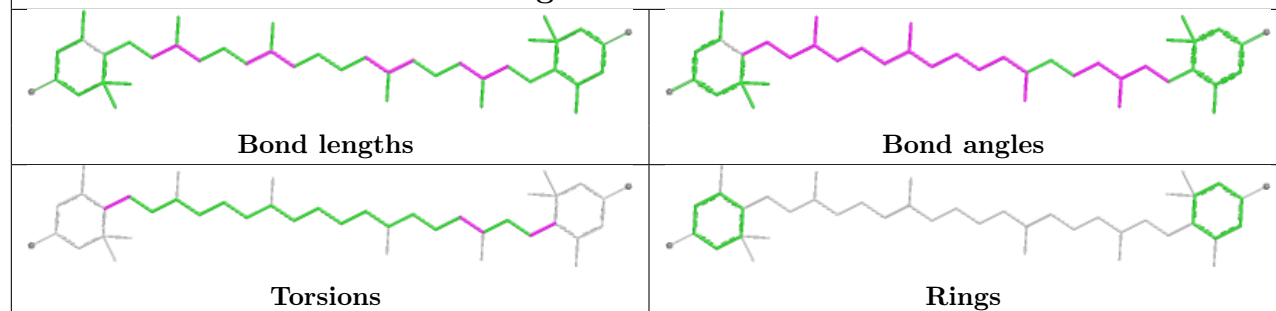


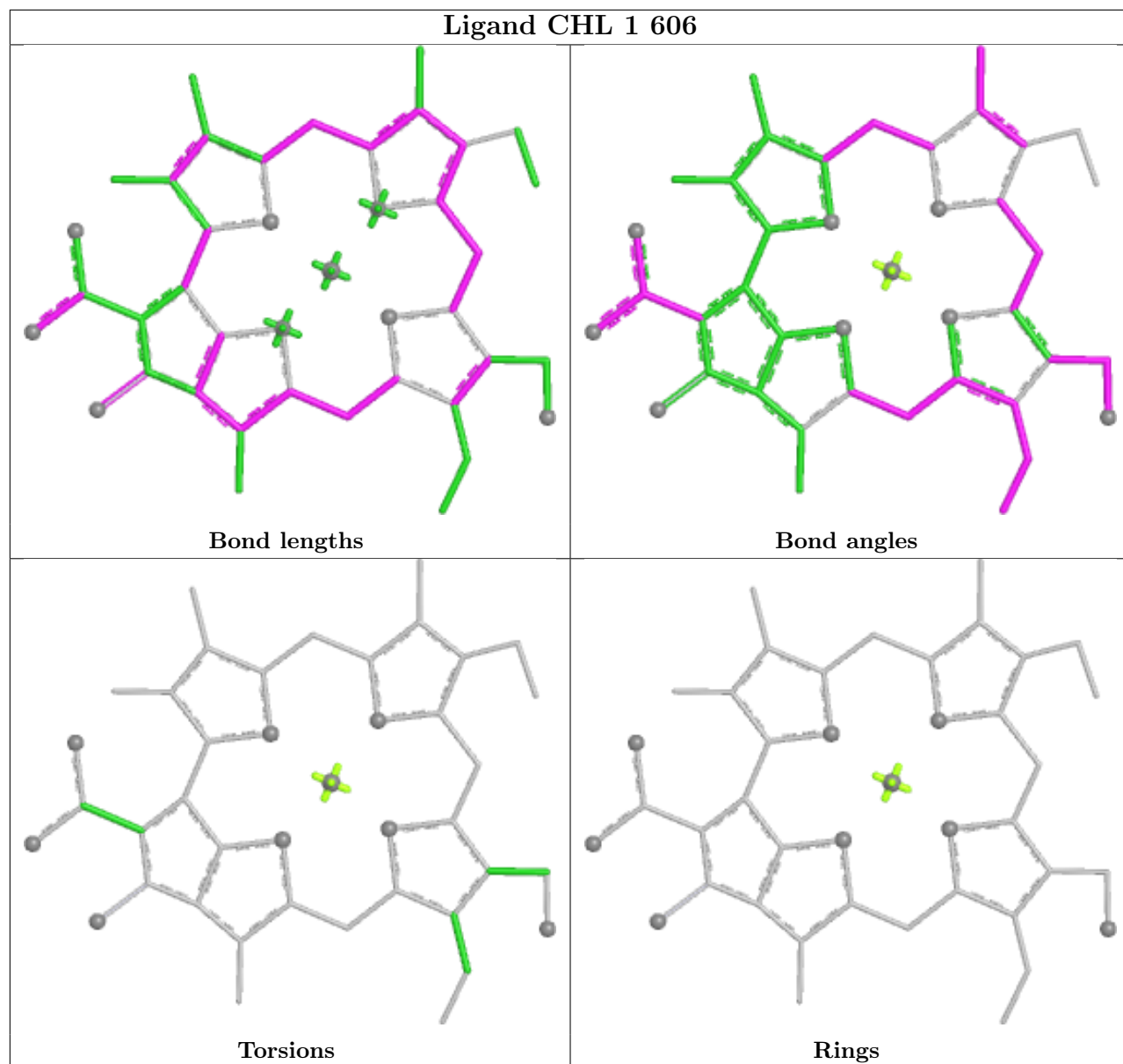


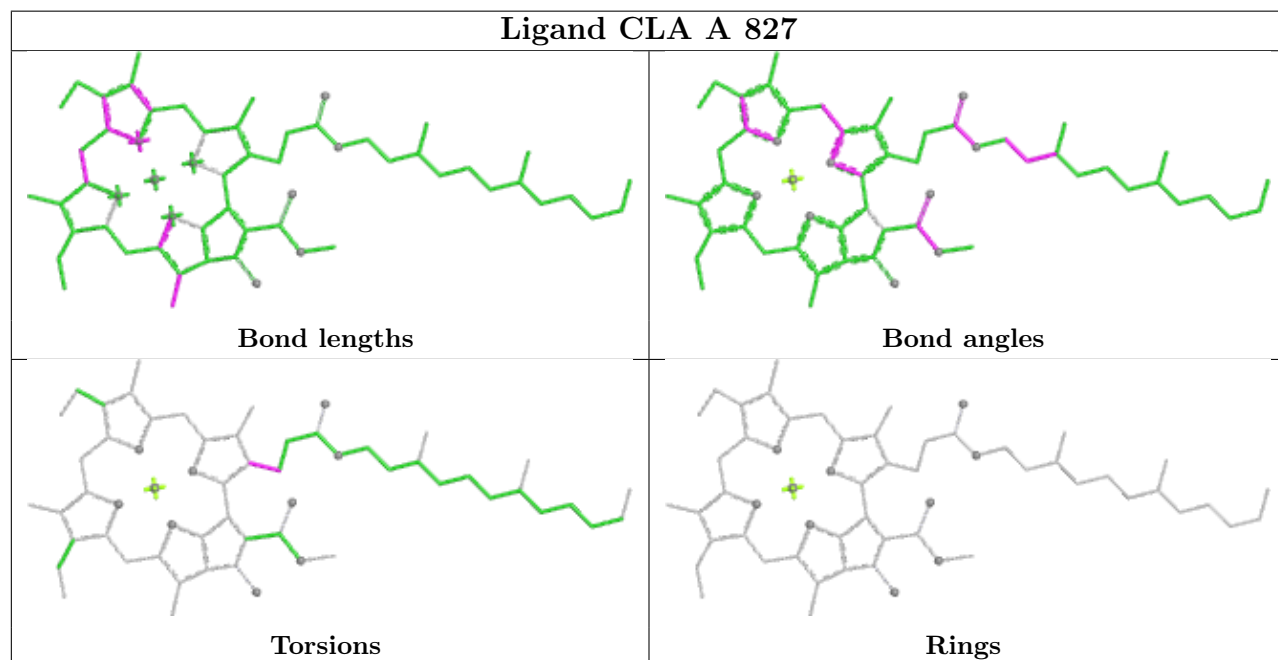
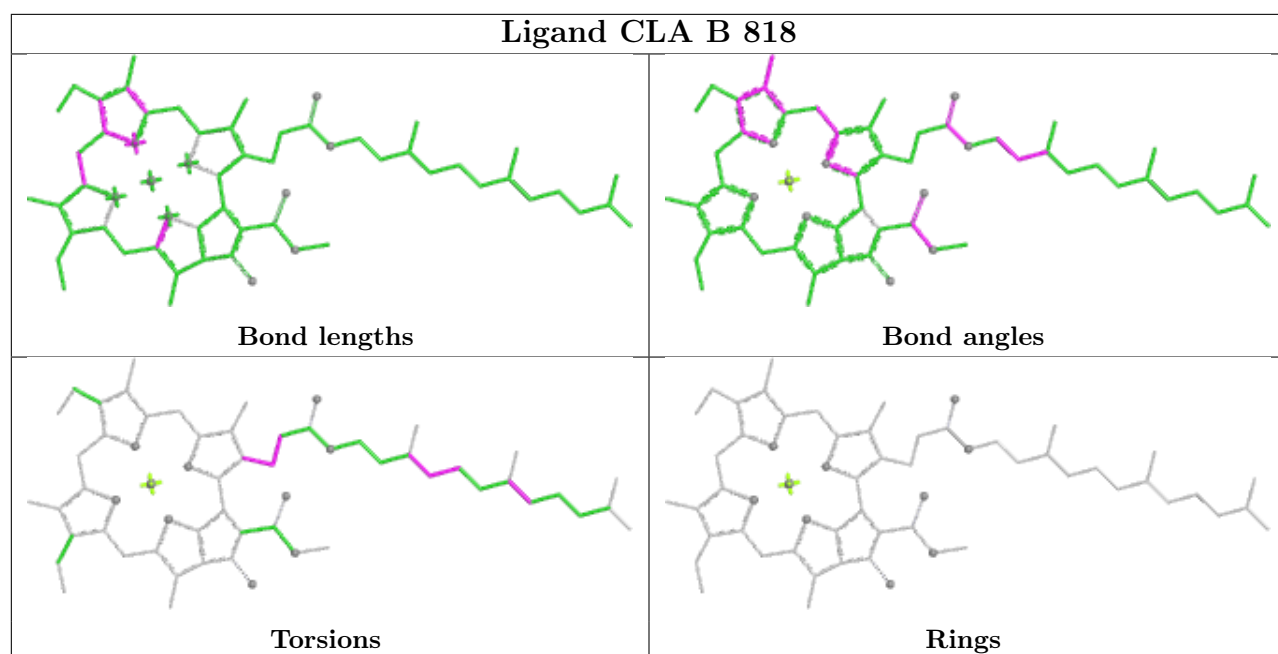
Ligand CLA 4 601

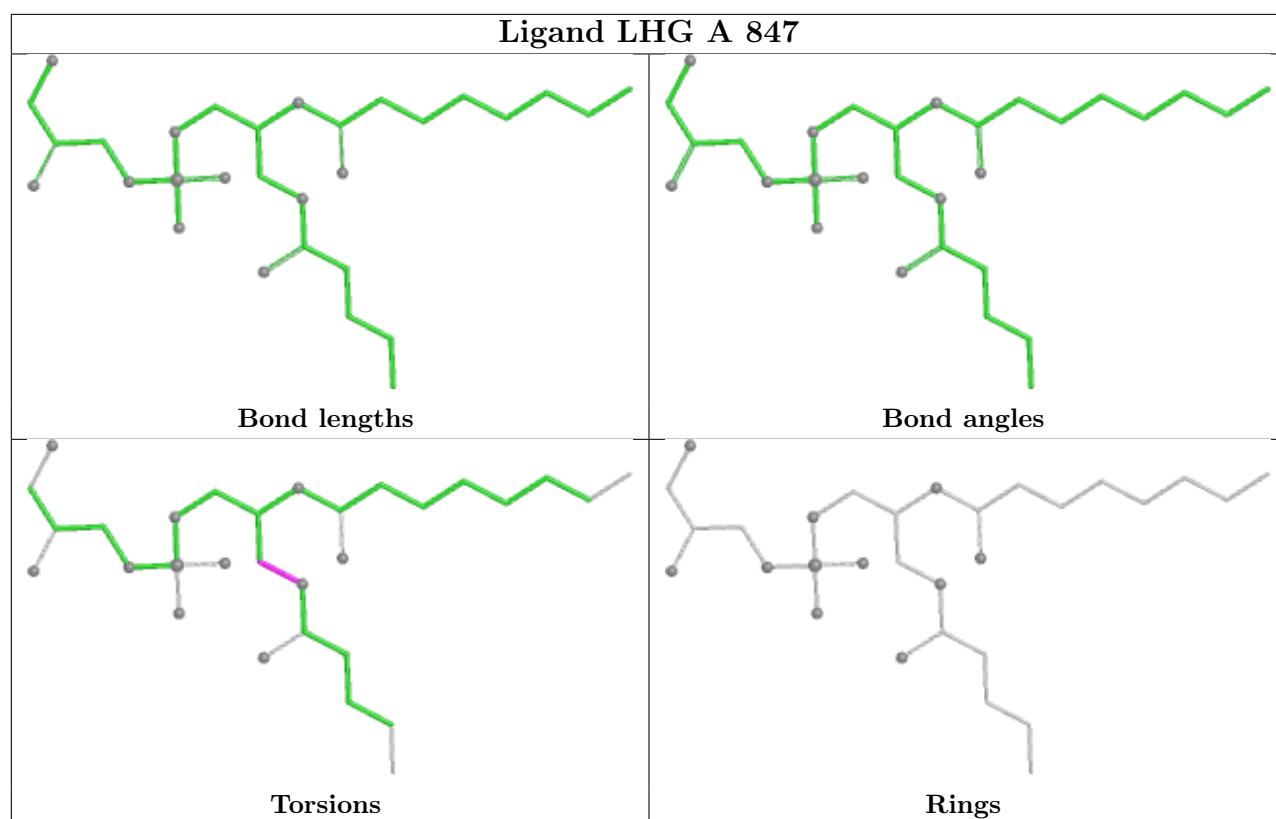


Ligand LUT 2 619

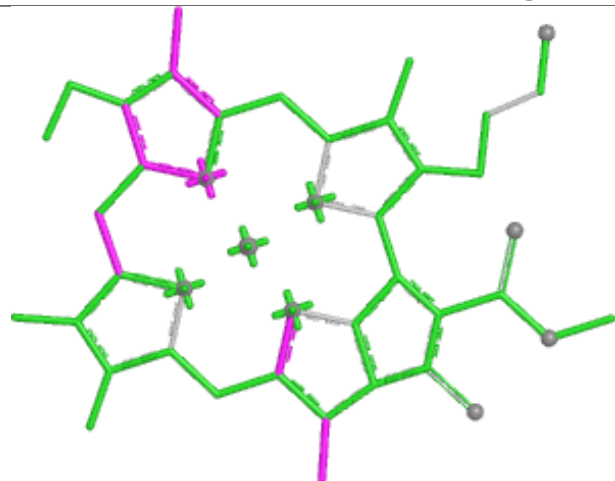




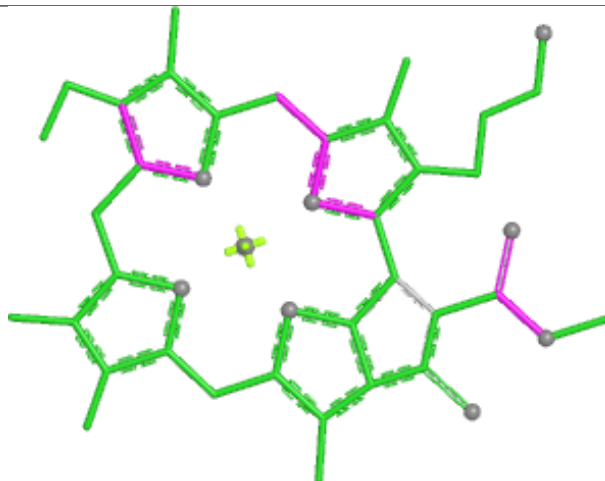




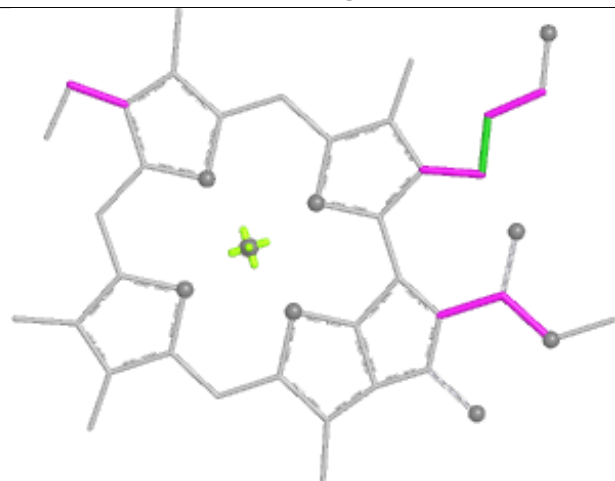
Ligand CLA 2 604



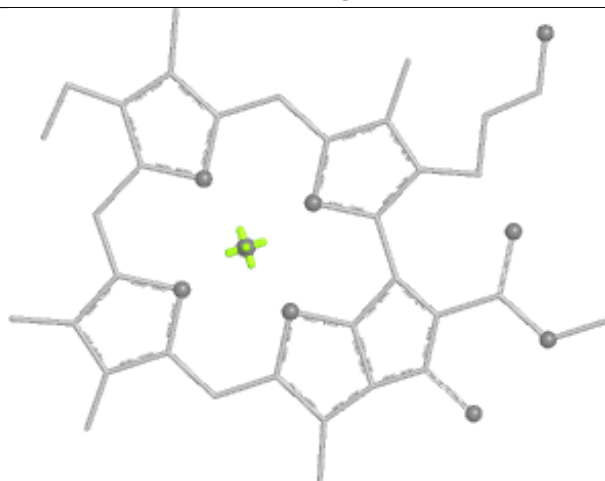
Bond lengths



Bond angles

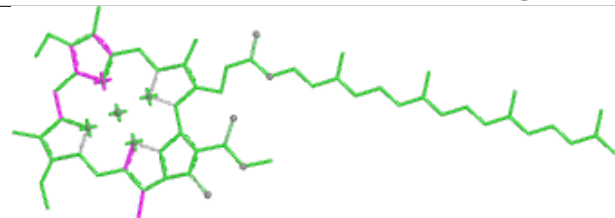


Torsions

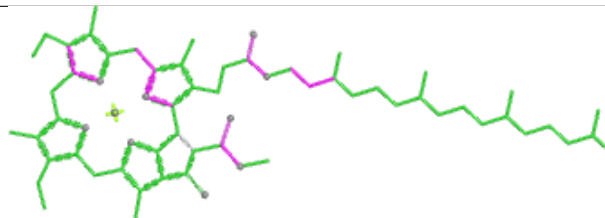


Rings

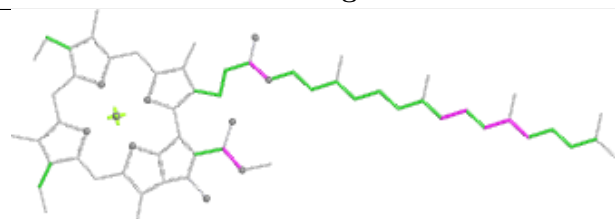
Ligand CLA A 811



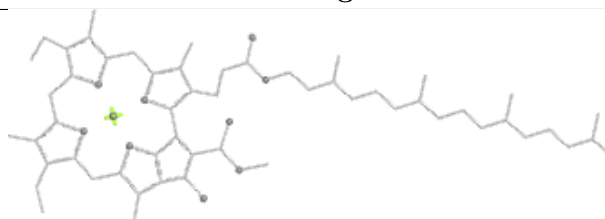
Bond lengths



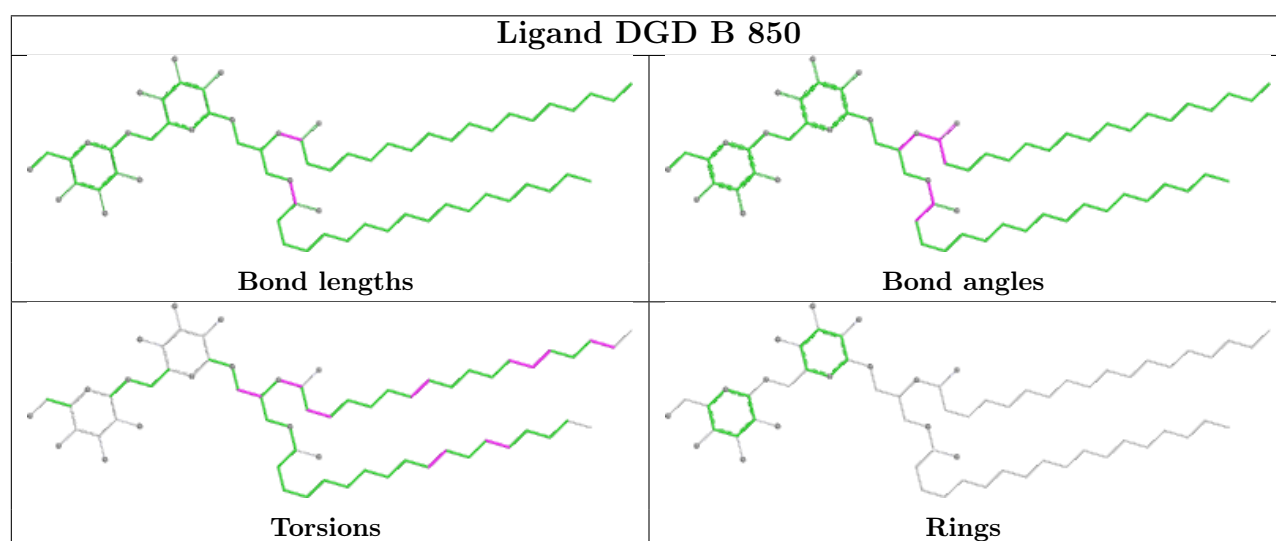
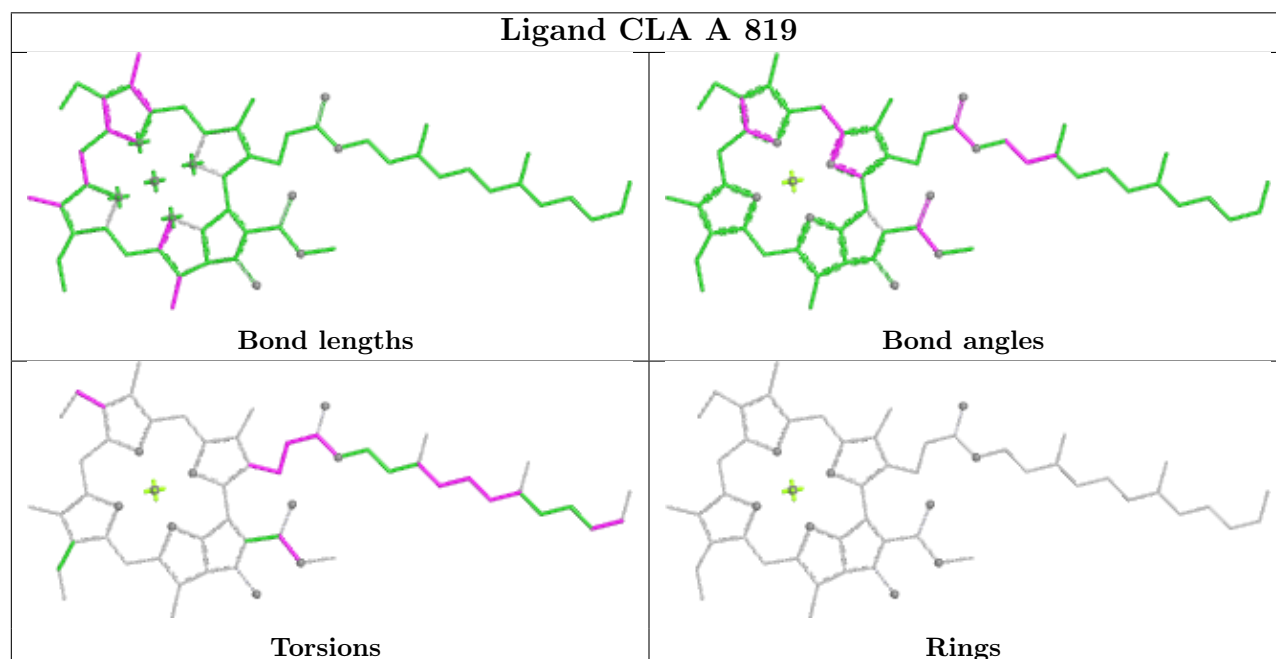
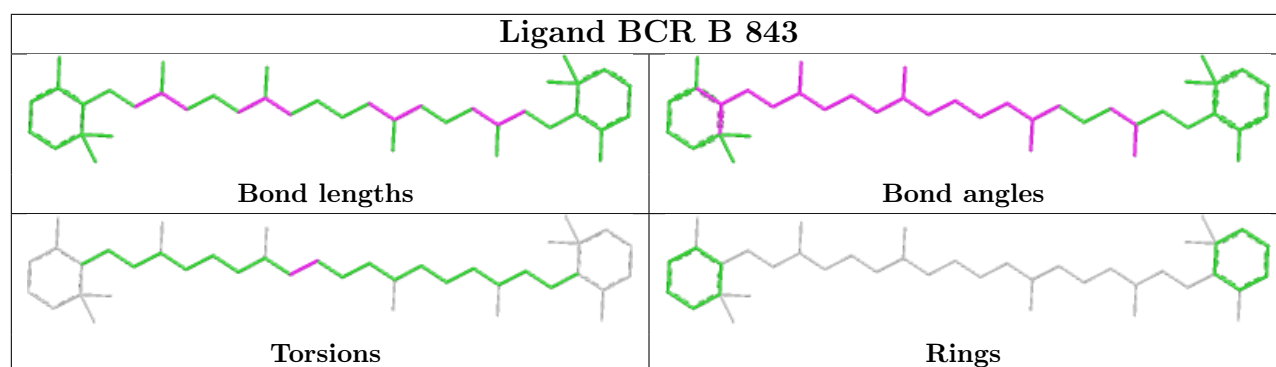
Bond angles

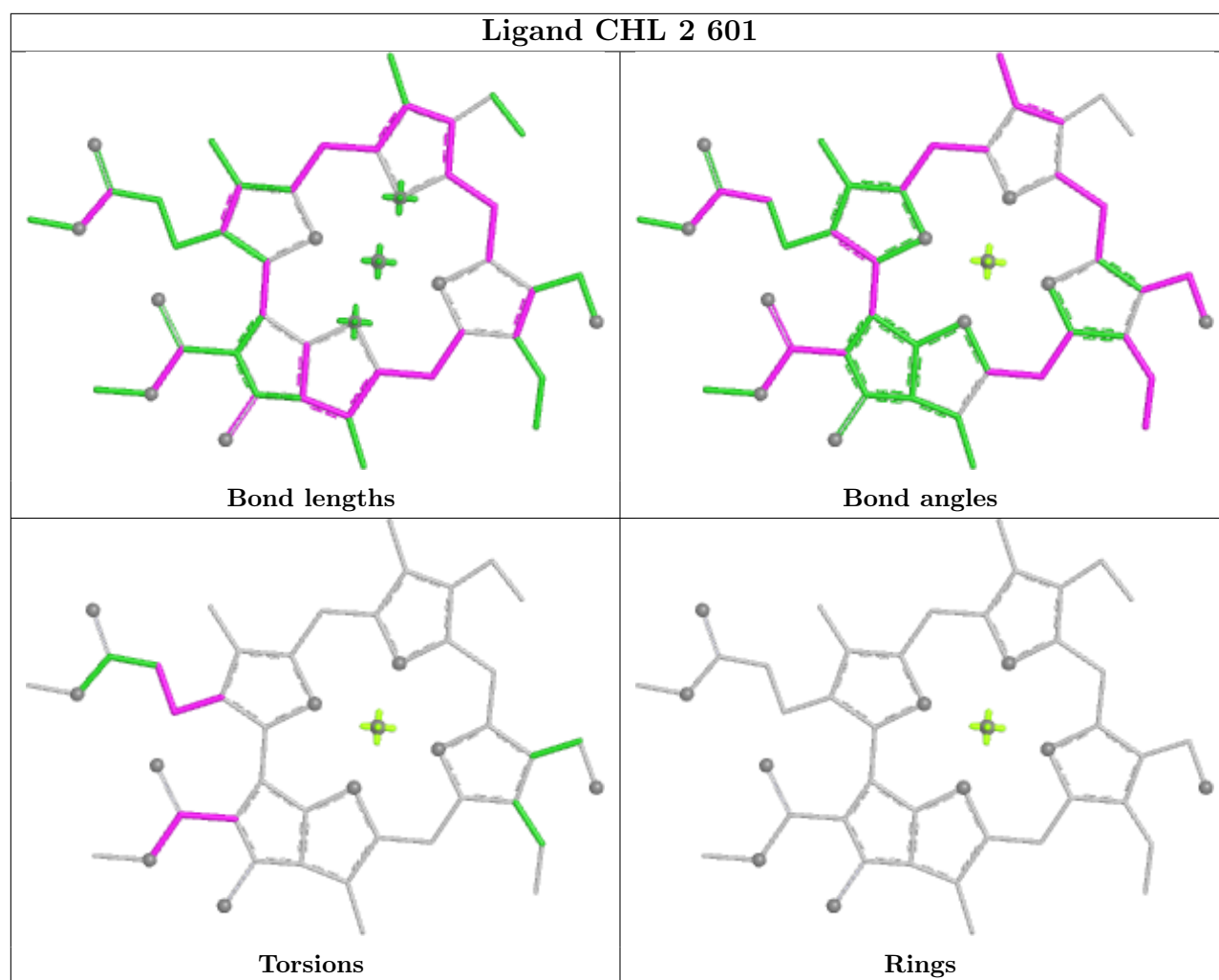


Torsions

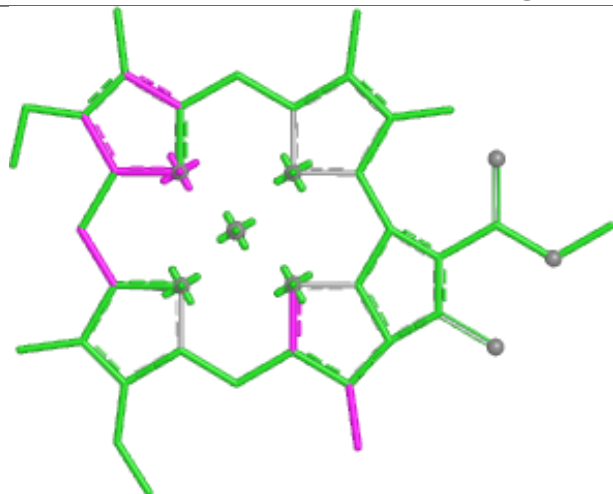


Rings

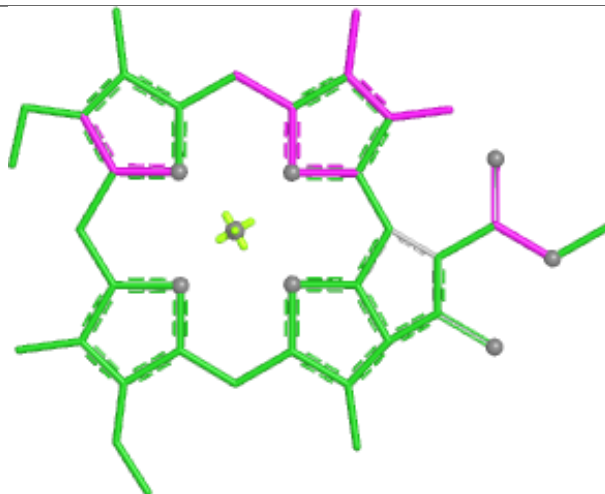




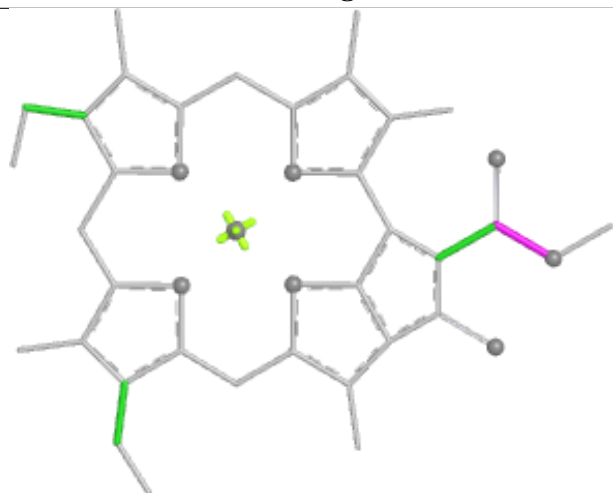
Ligand CLA 3 608



Bond lengths



Bond angles

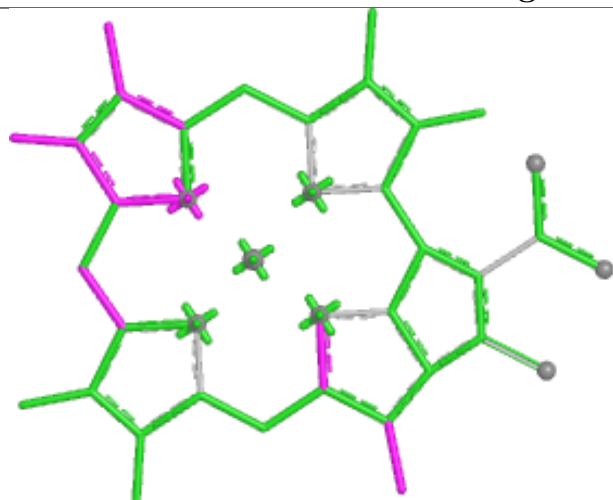


Torsions

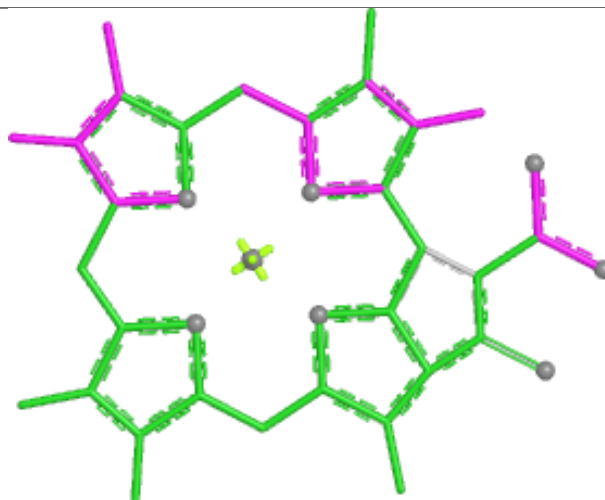


Rings

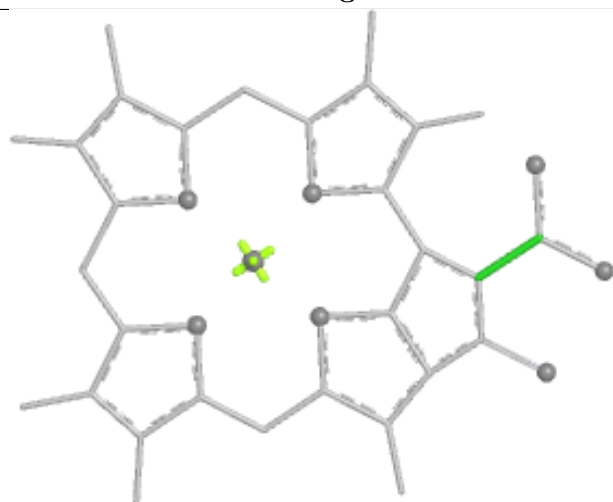
Ligand CLA 1 613



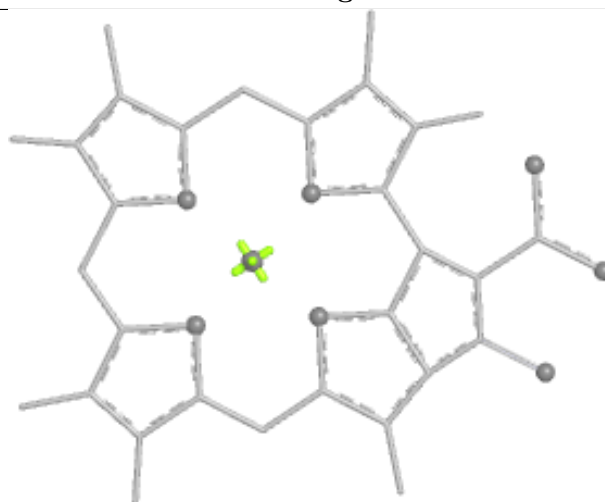
Bond lengths



Bond angles

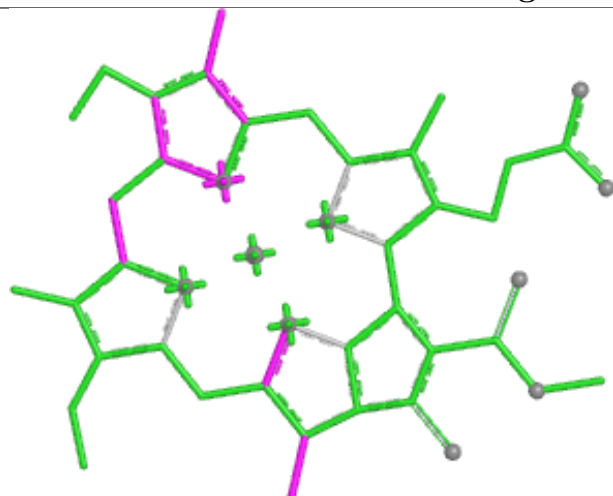


Torsions

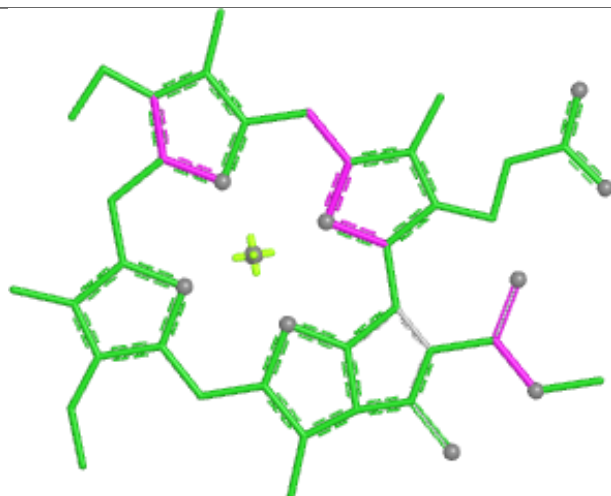


Rings

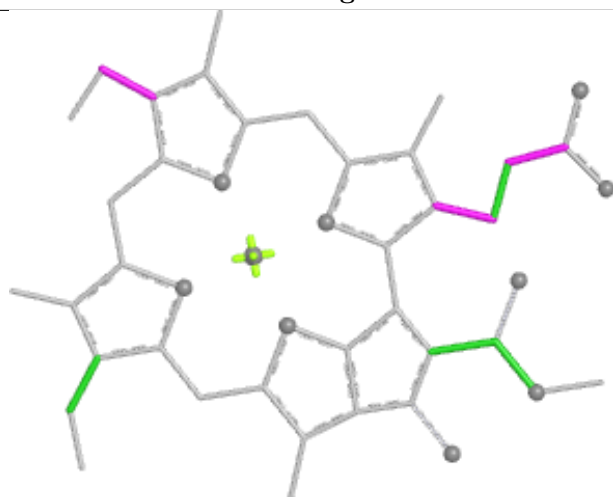
Ligand CLA 4 608



Bond lengths



Bond angles

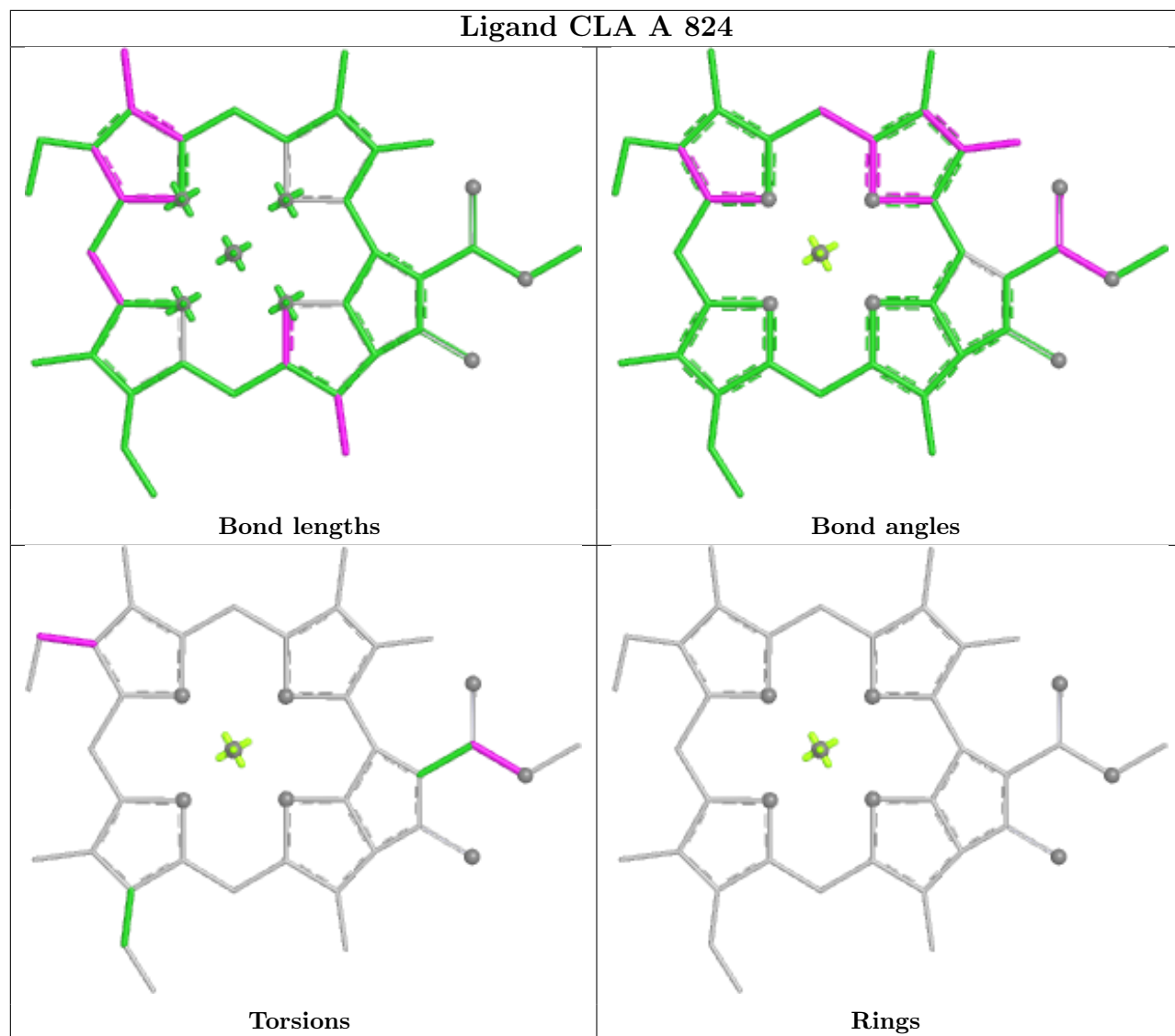


Torsions

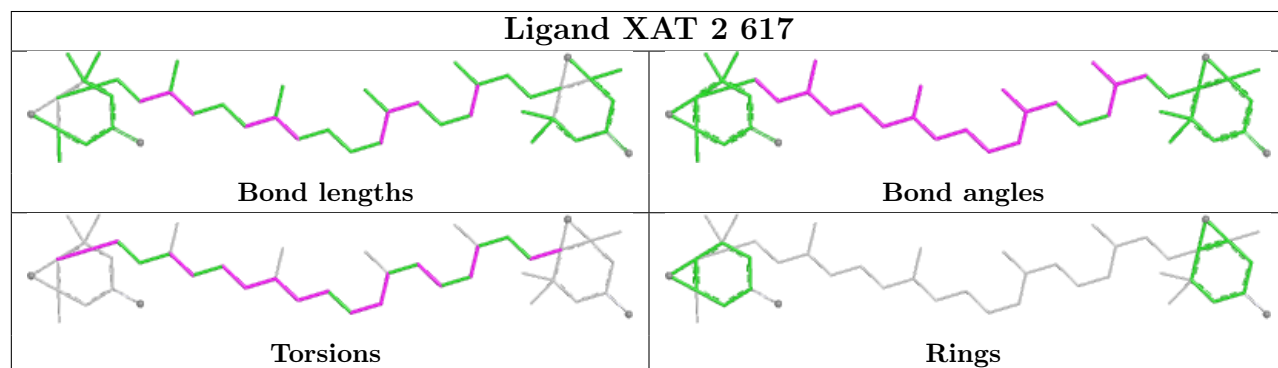


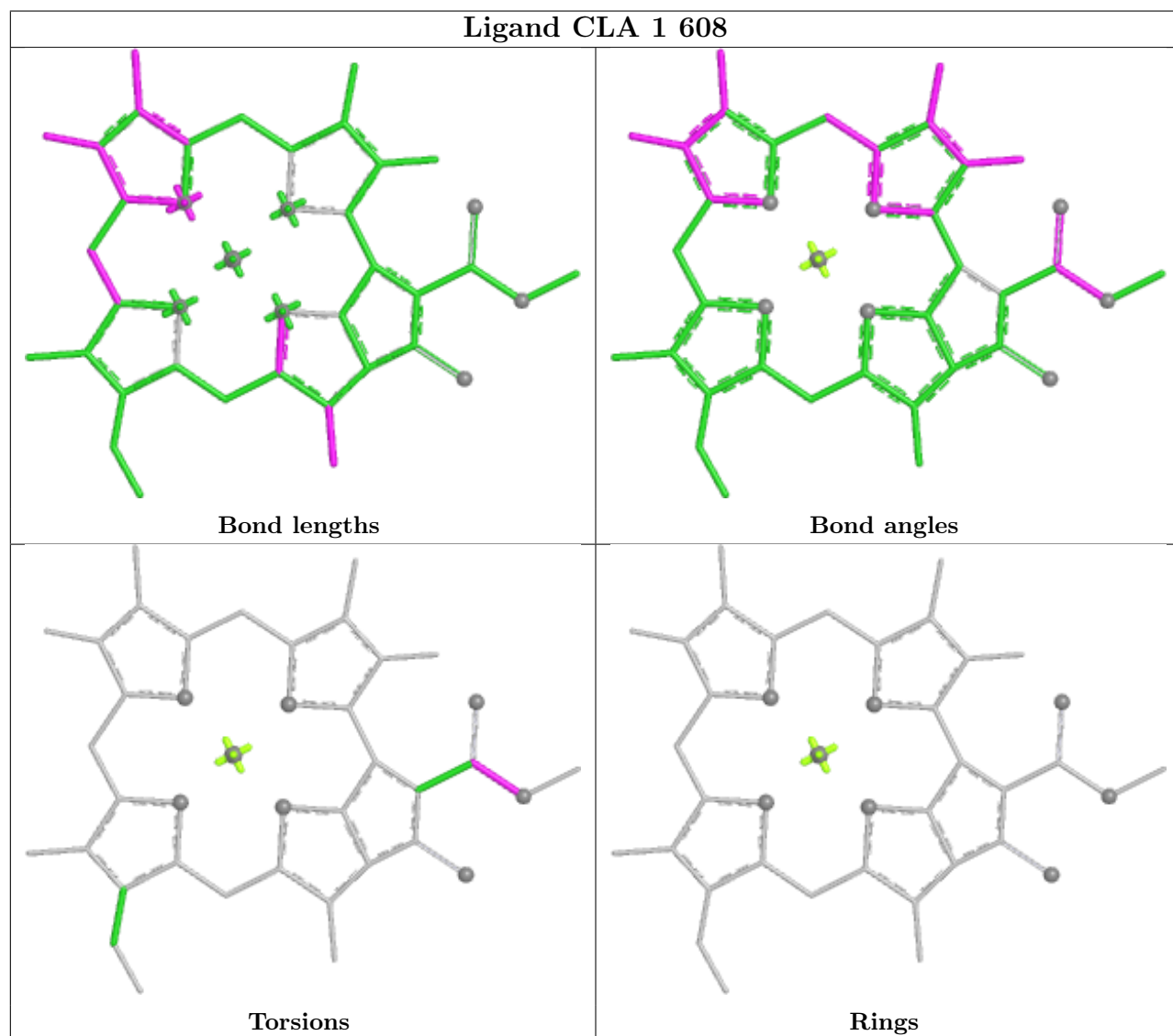
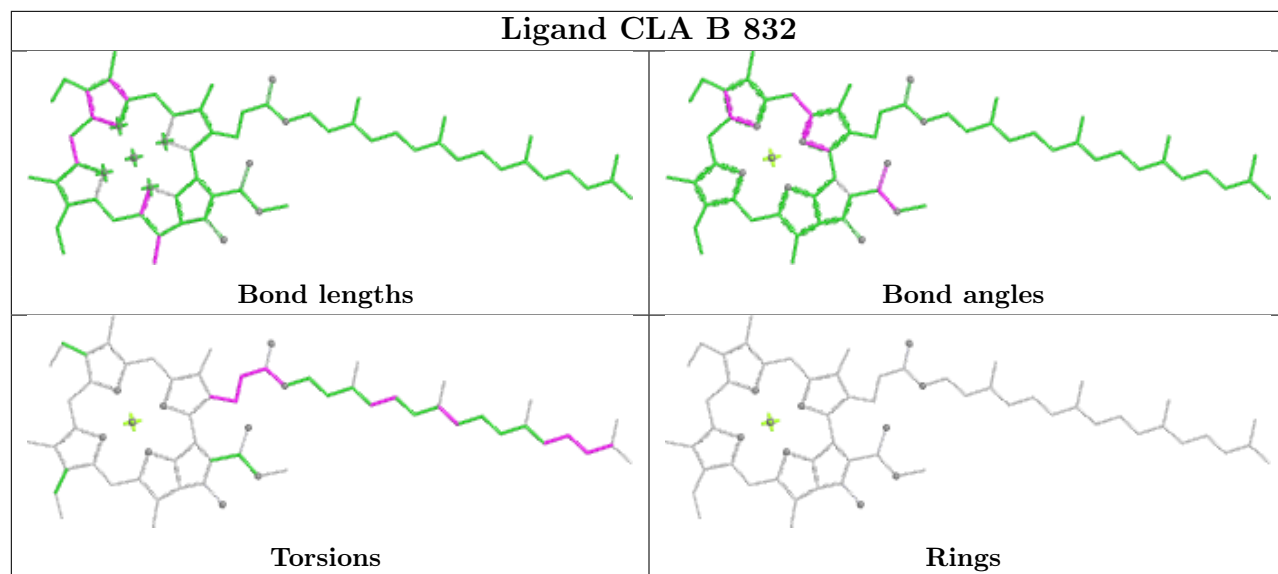
Rings

Ligand CLA A 824

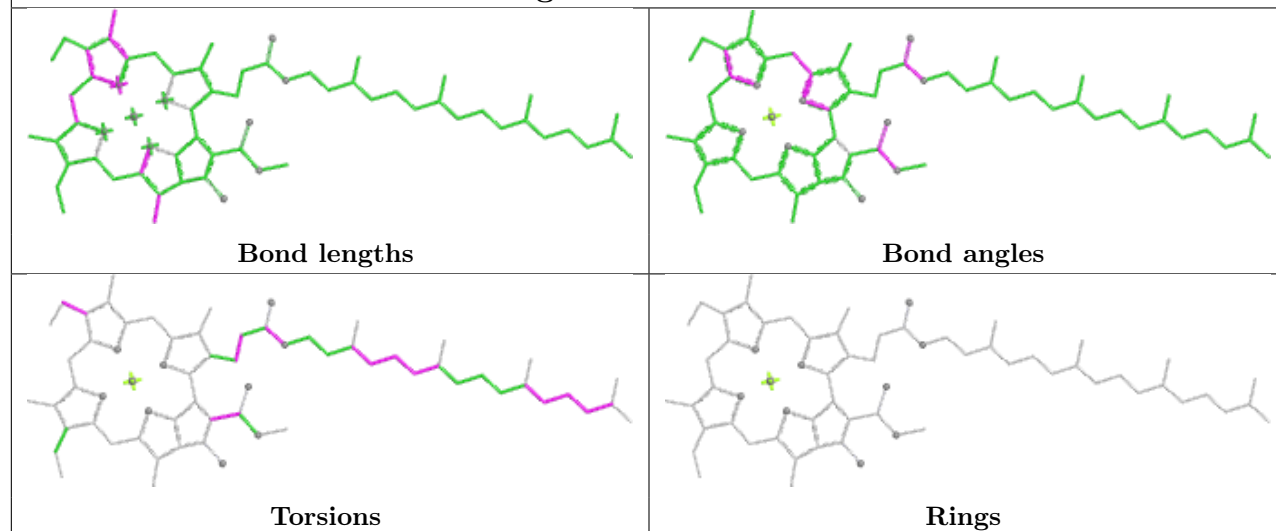


Ligand XAT 2 617

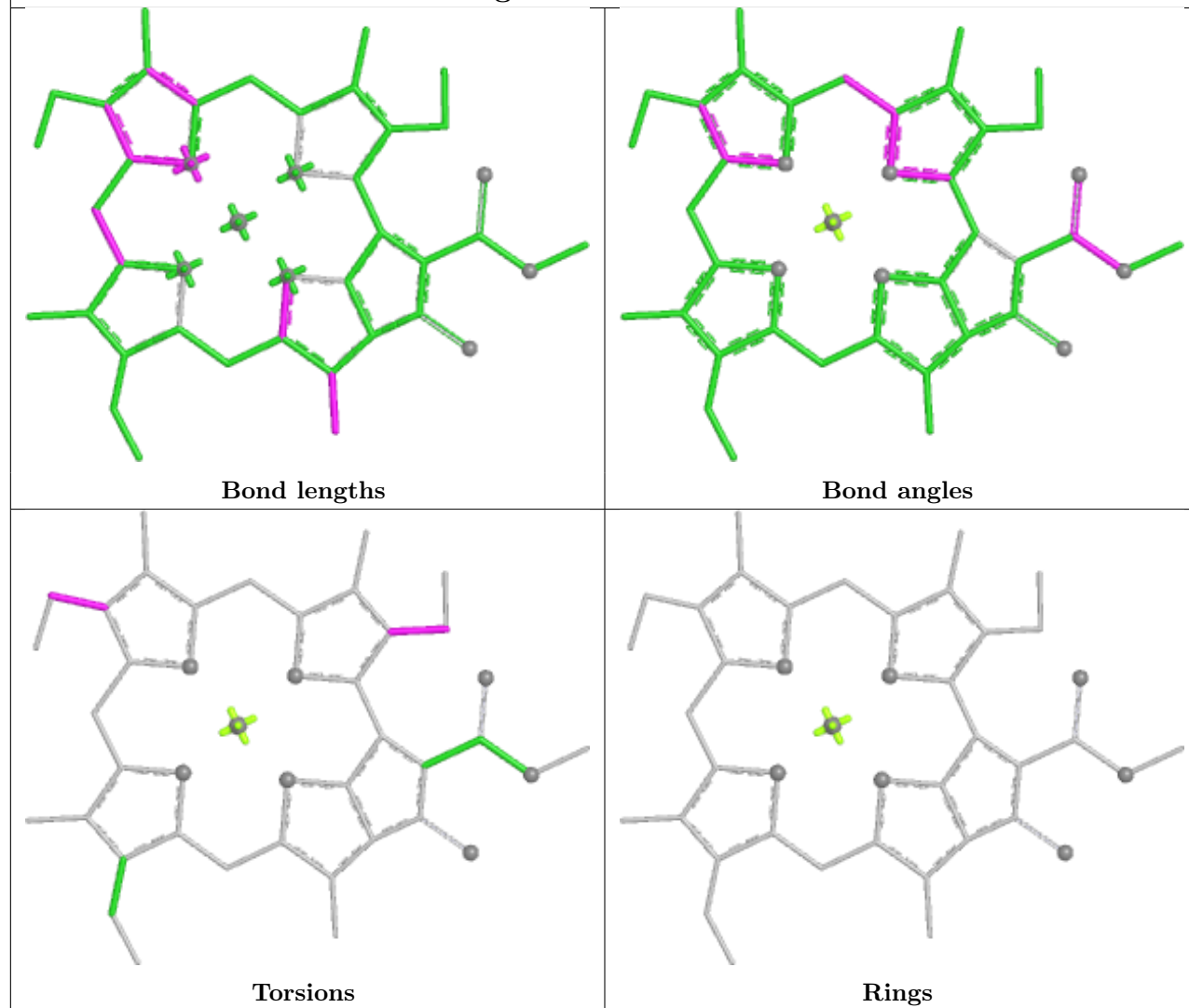




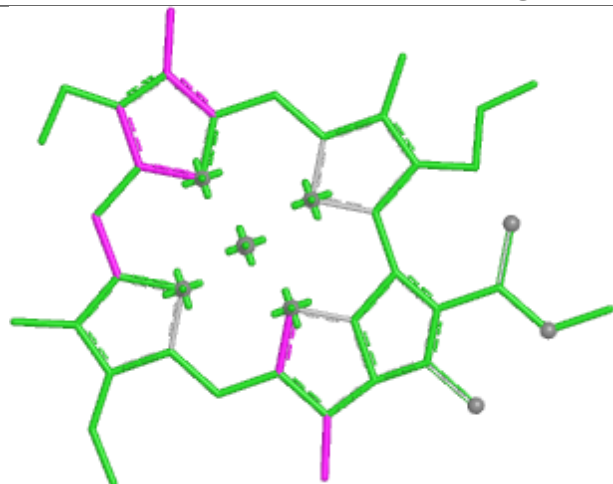
Ligand CLA 2 602



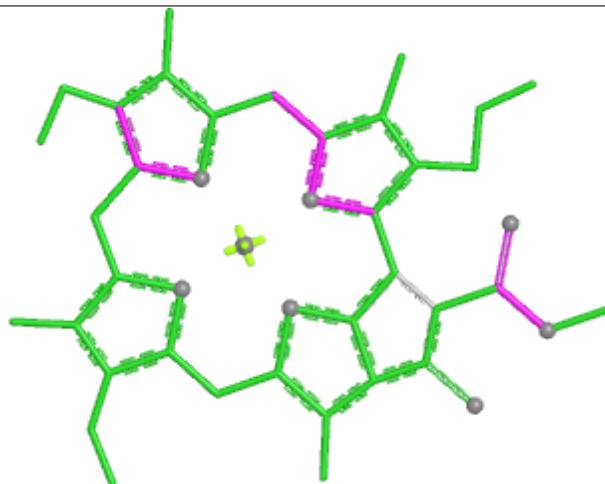
Ligand CLA G 202



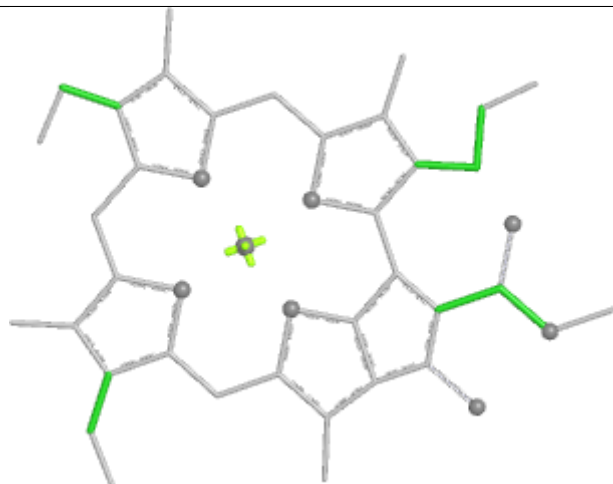
Ligand CLA B 812



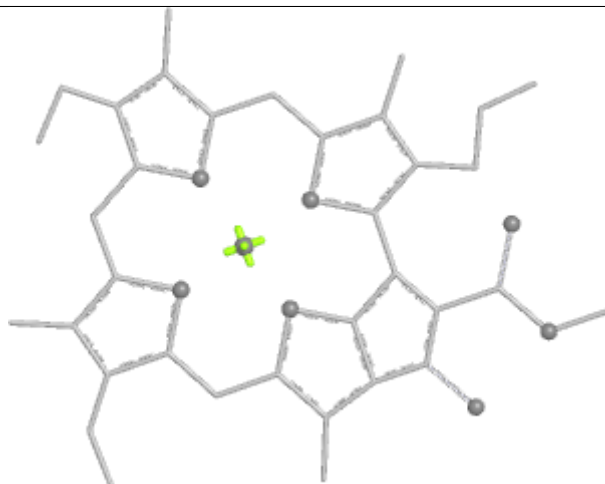
Bond lengths



Bond angles

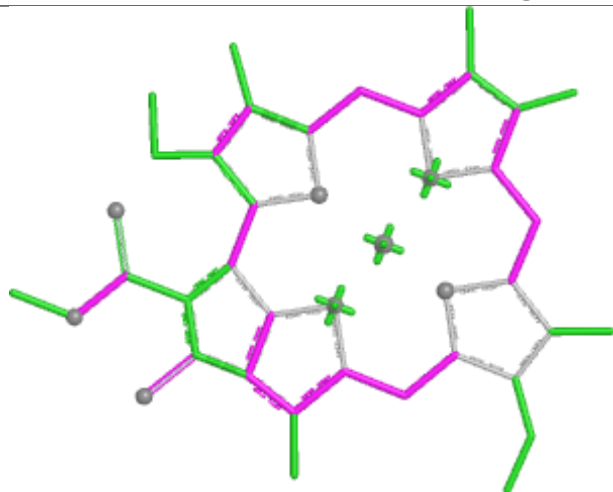


Torsions

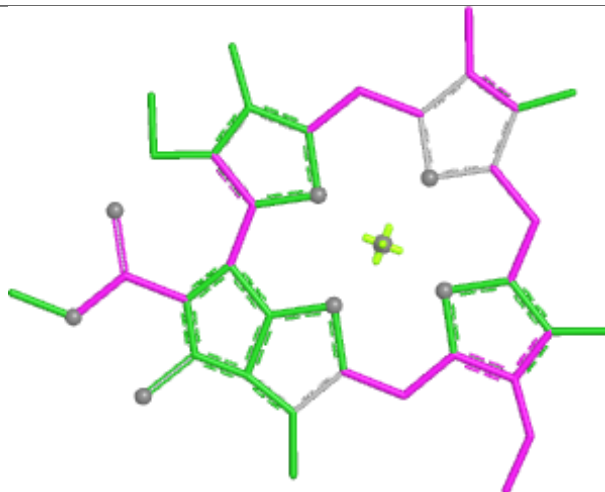


Rings

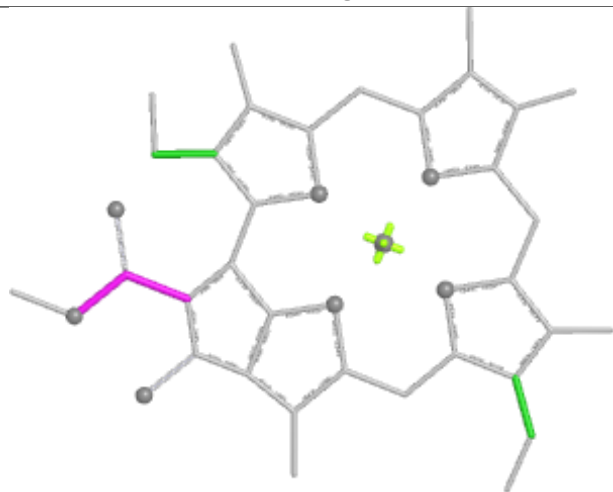
Ligand CHL 4 606



Bond lengths



Bond angles

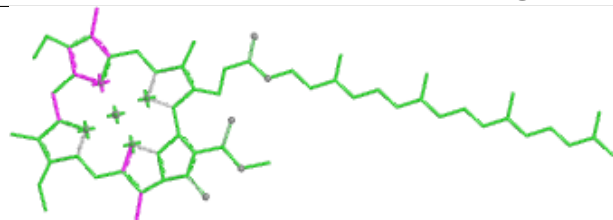


Torsions

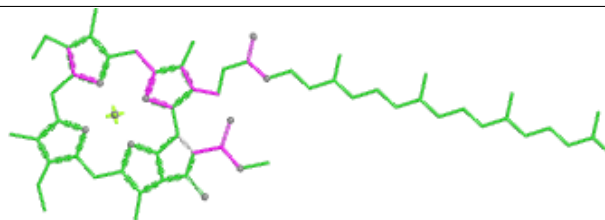


Rings

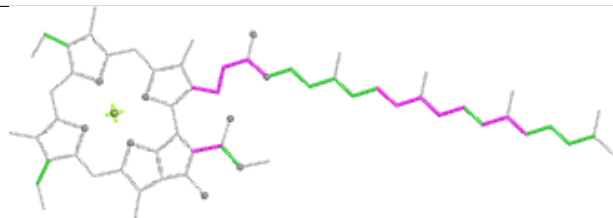
Ligand CLA A 804



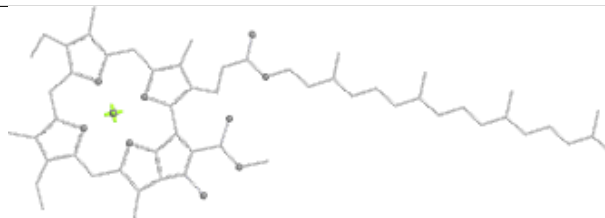
Bond lengths



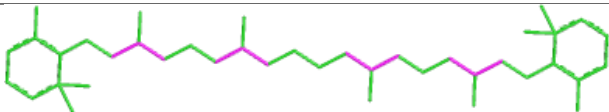
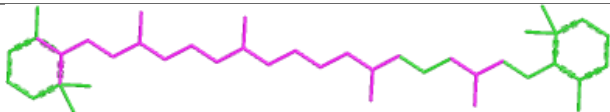
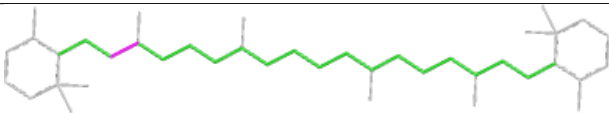
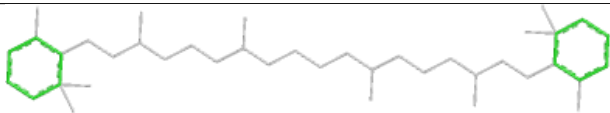
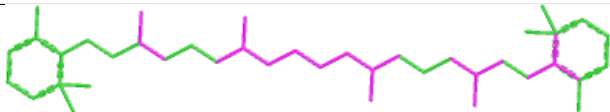
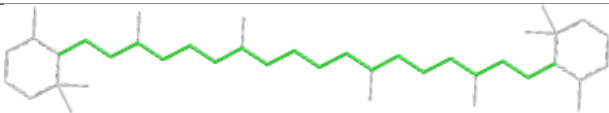
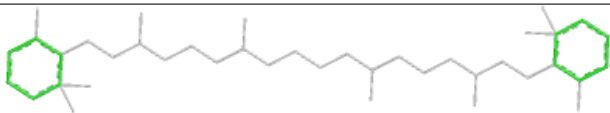
Bond angles



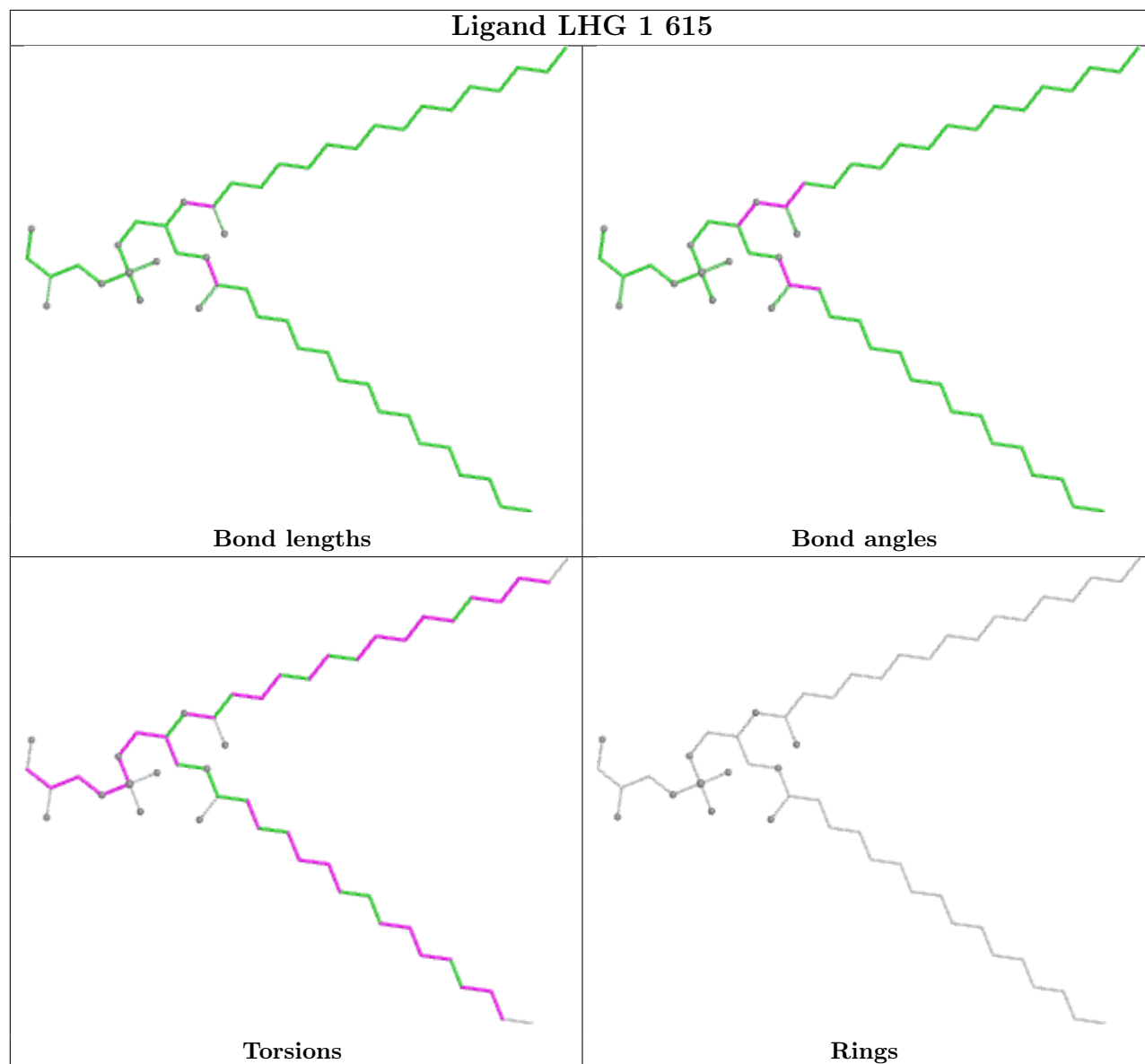
Torsions



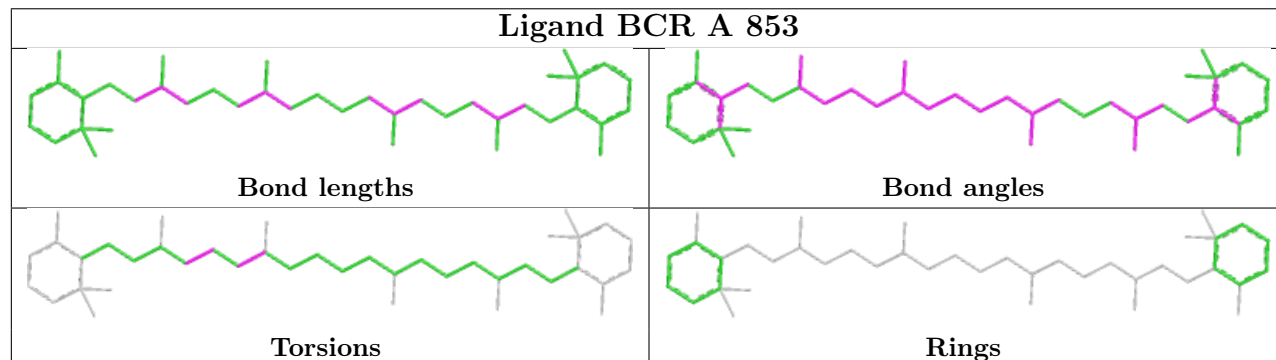
Rings

Ligand BCR J 102			
	Bond lengths		
	Torsions		
Ligand BCR A 848			
	Bond lengths		
	Torsions		

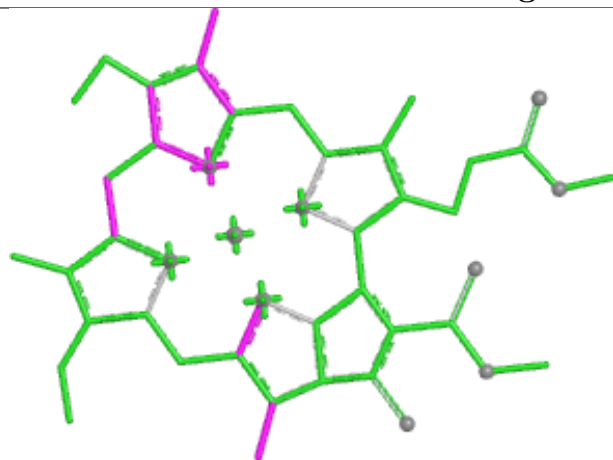
Ligand LHG 1 615



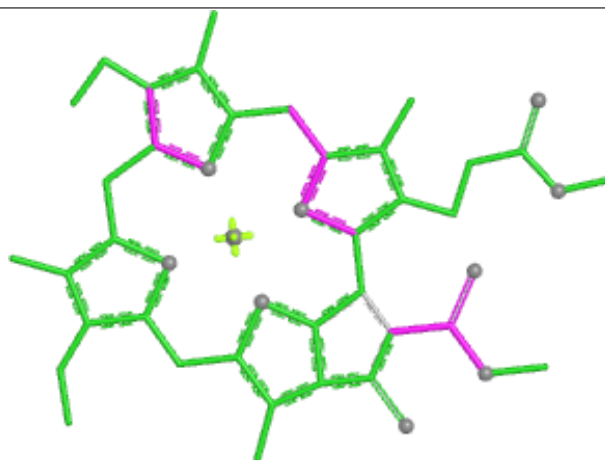
Ligand BCR A 853



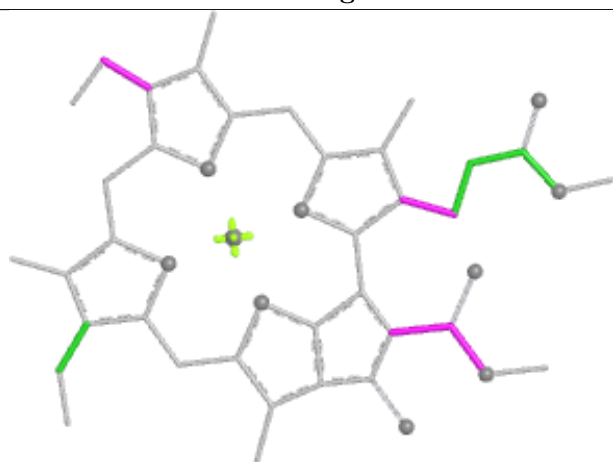
Ligand CLA 1 612



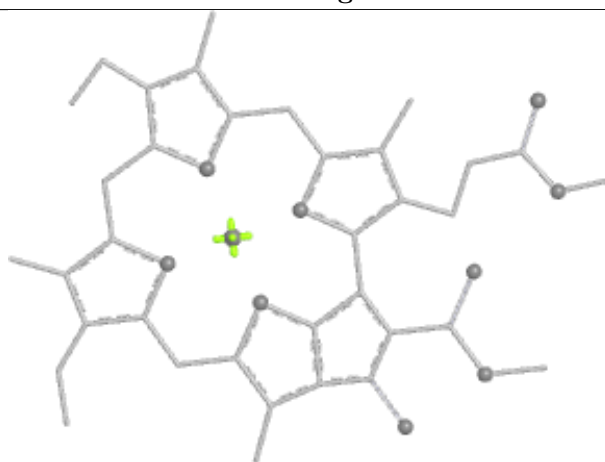
Bond lengths



Bond angles

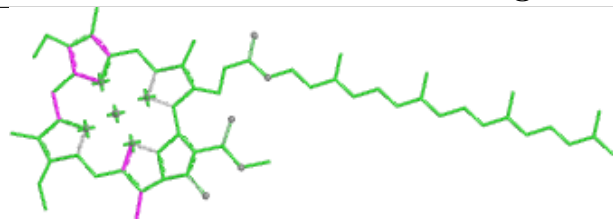


Torsions

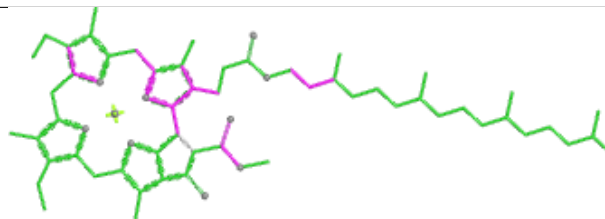


Rings

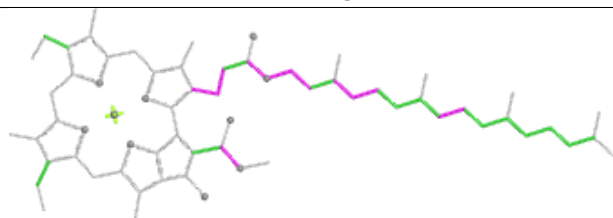
Ligand CLA A 830



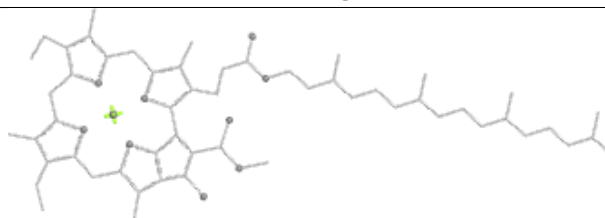
Bond lengths



Bond angles

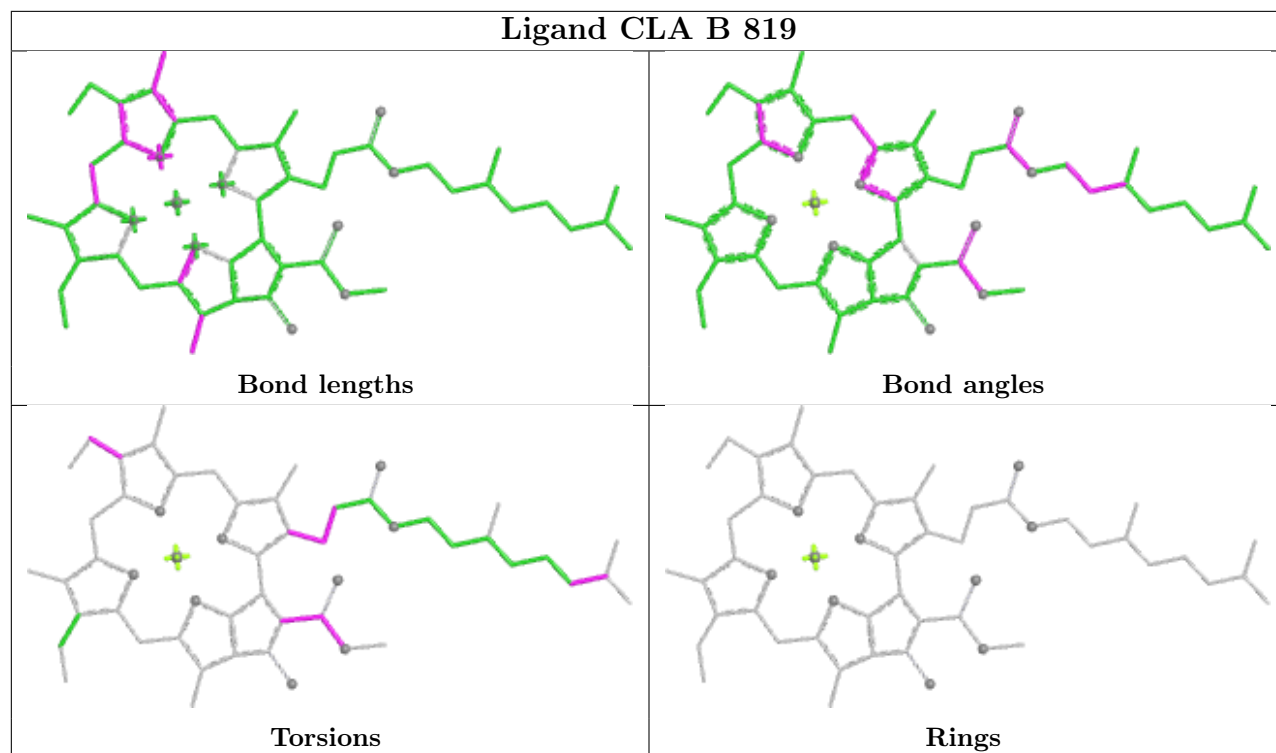


Torsions

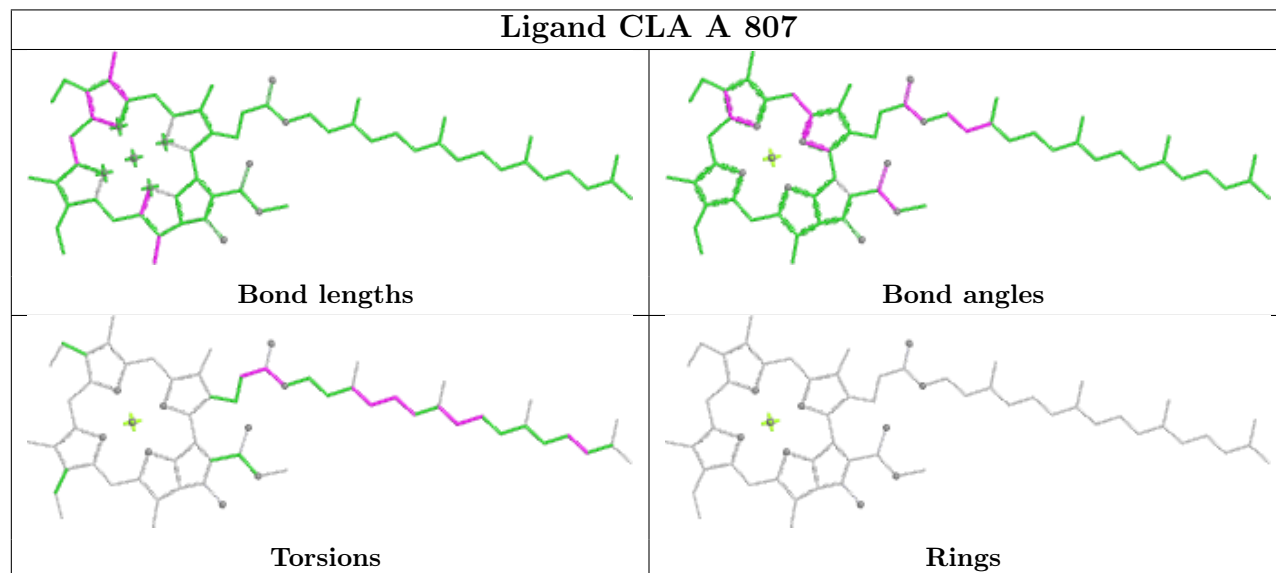


Rings

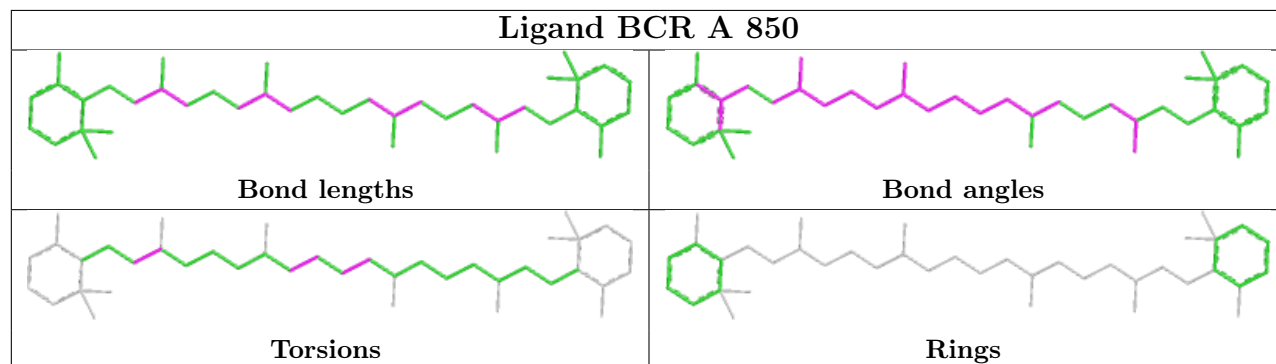
Ligand CLA B 819



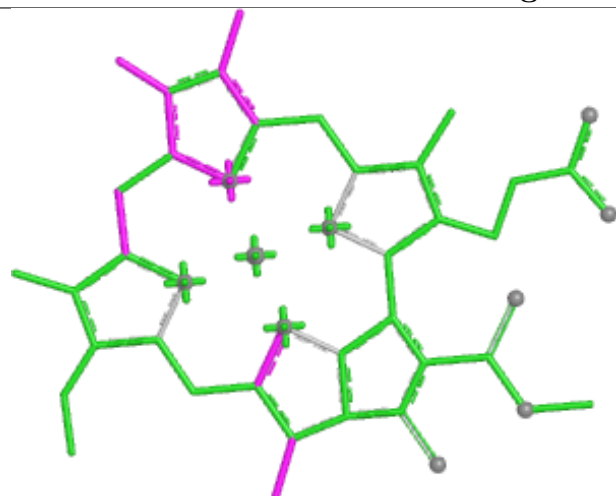
Ligand CLA A 807



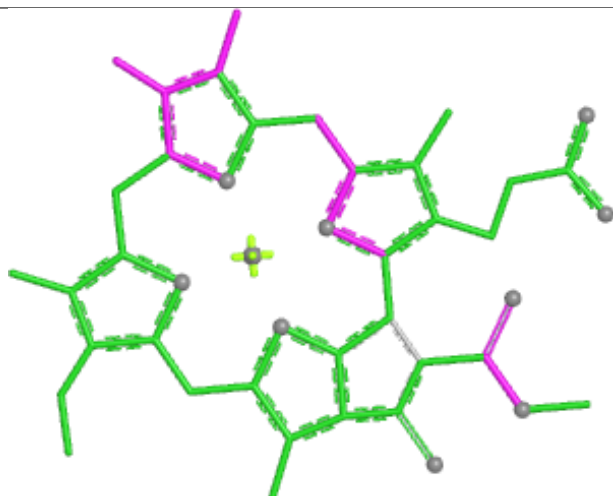
Ligand BCR A 850



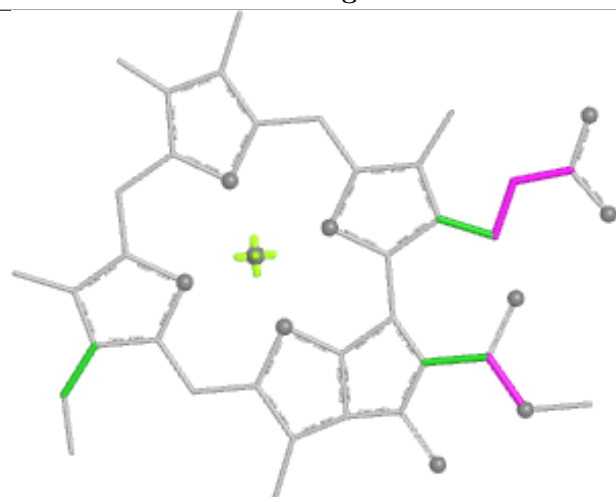
Ligand CLA 4 603



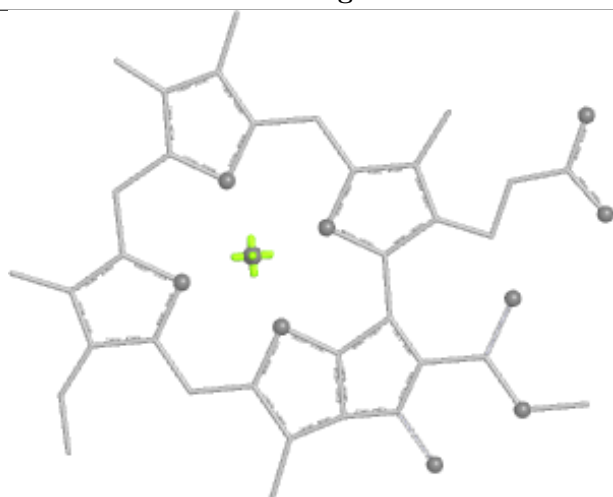
Bond lengths



Bond angles

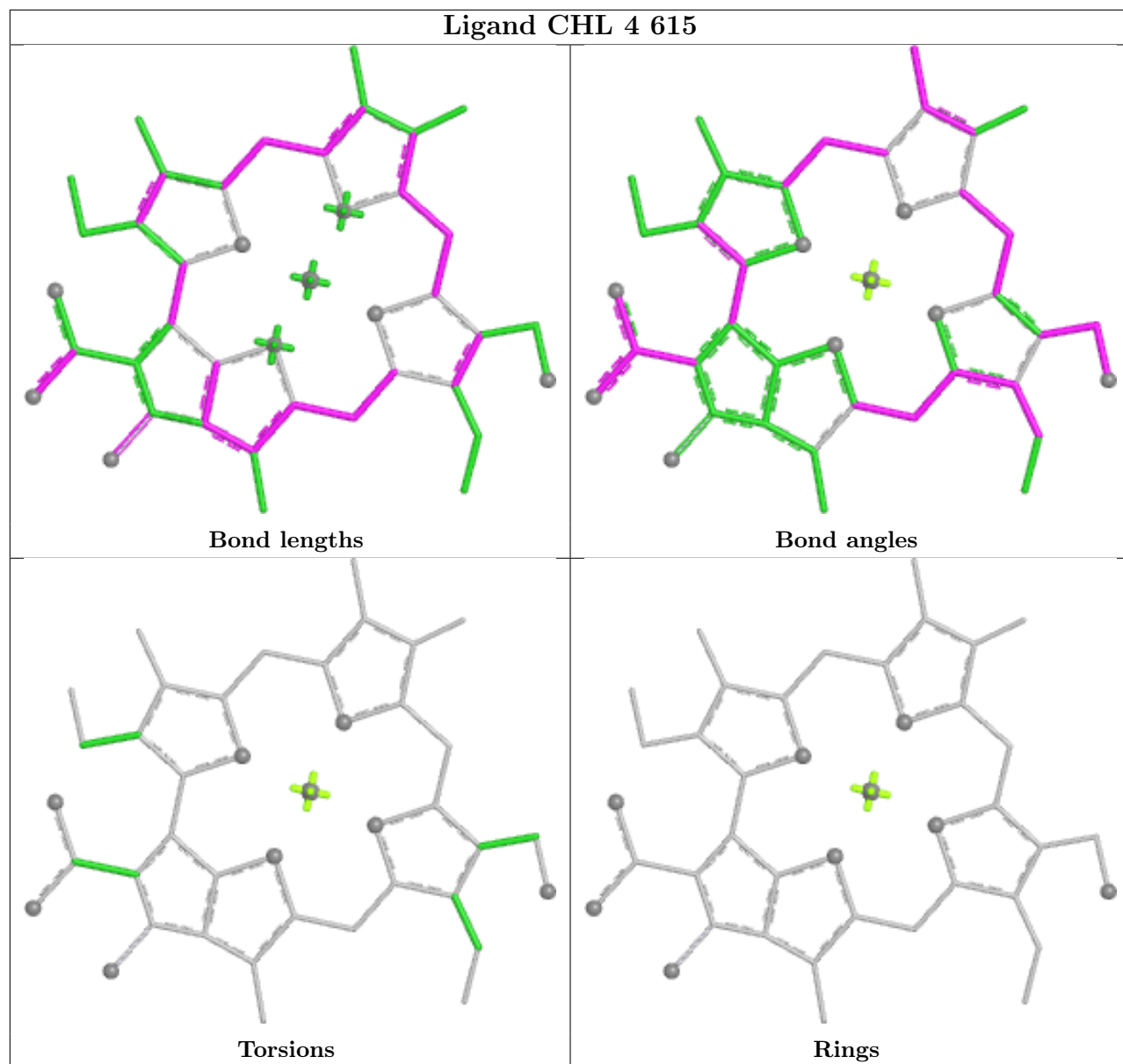


Torsions

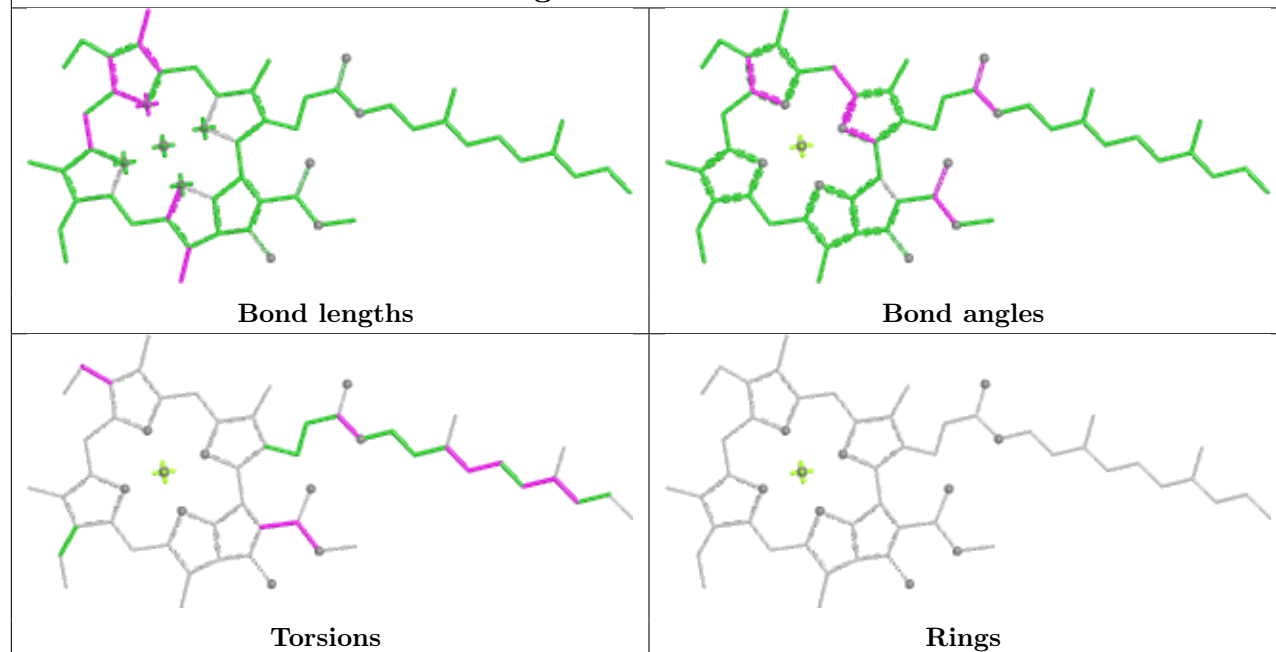


Rings

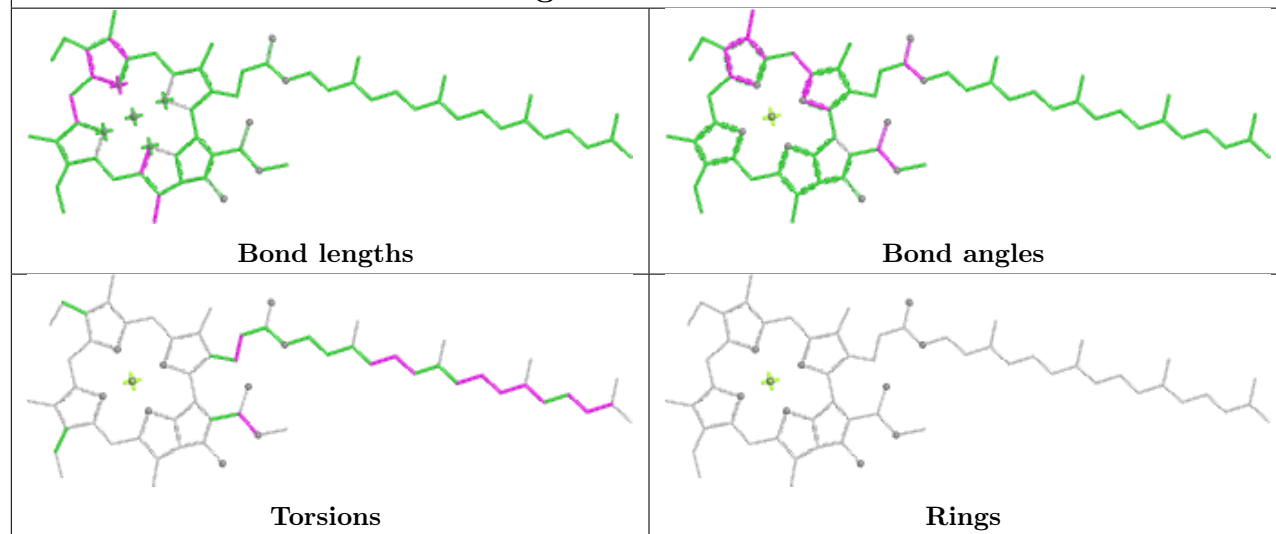
Ligand CHL 4 615



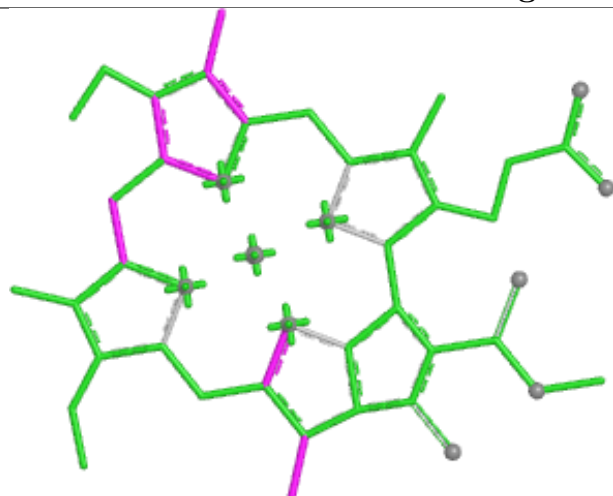
Ligand CLA F 301



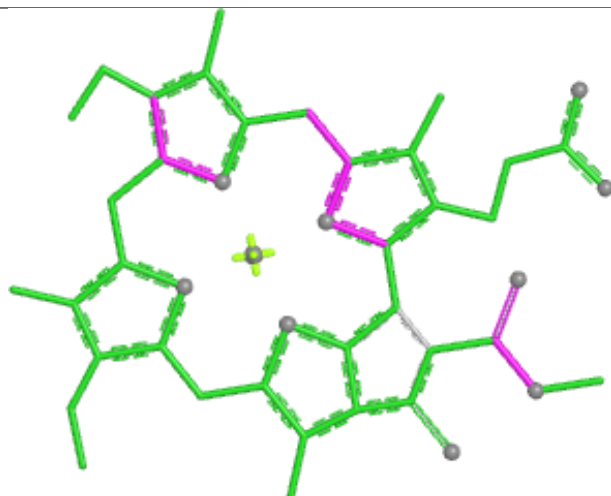
Ligand CLA 2 612



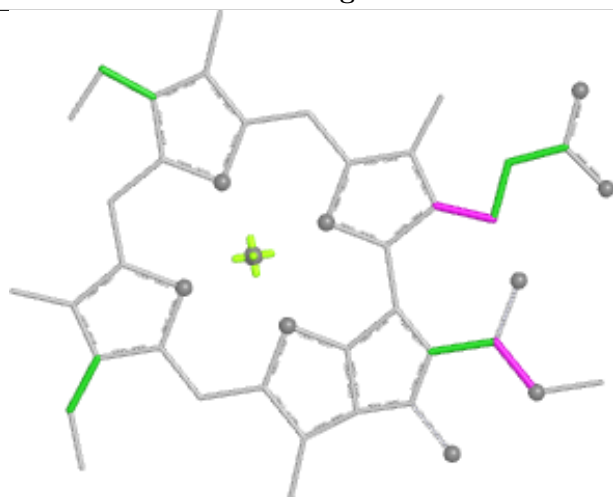
Ligand CLA 3 607



Bond lengths



Bond angles

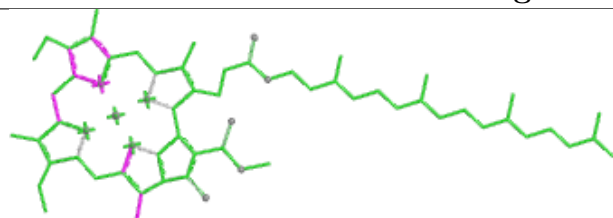


Torsions

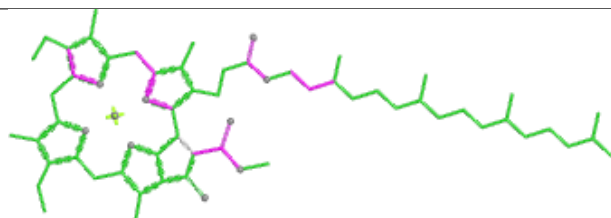


Rings

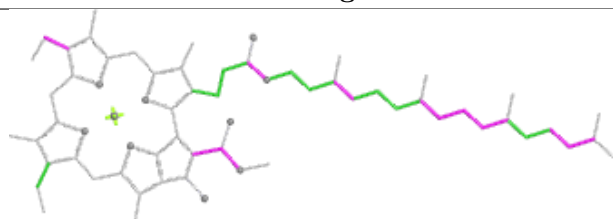
Ligand CLA A 835



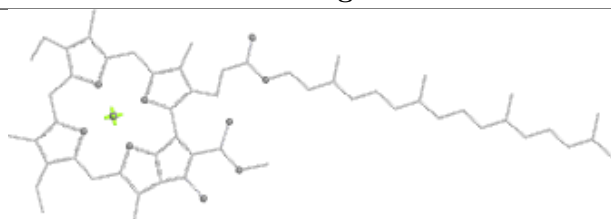
Bond lengths



Bond angles

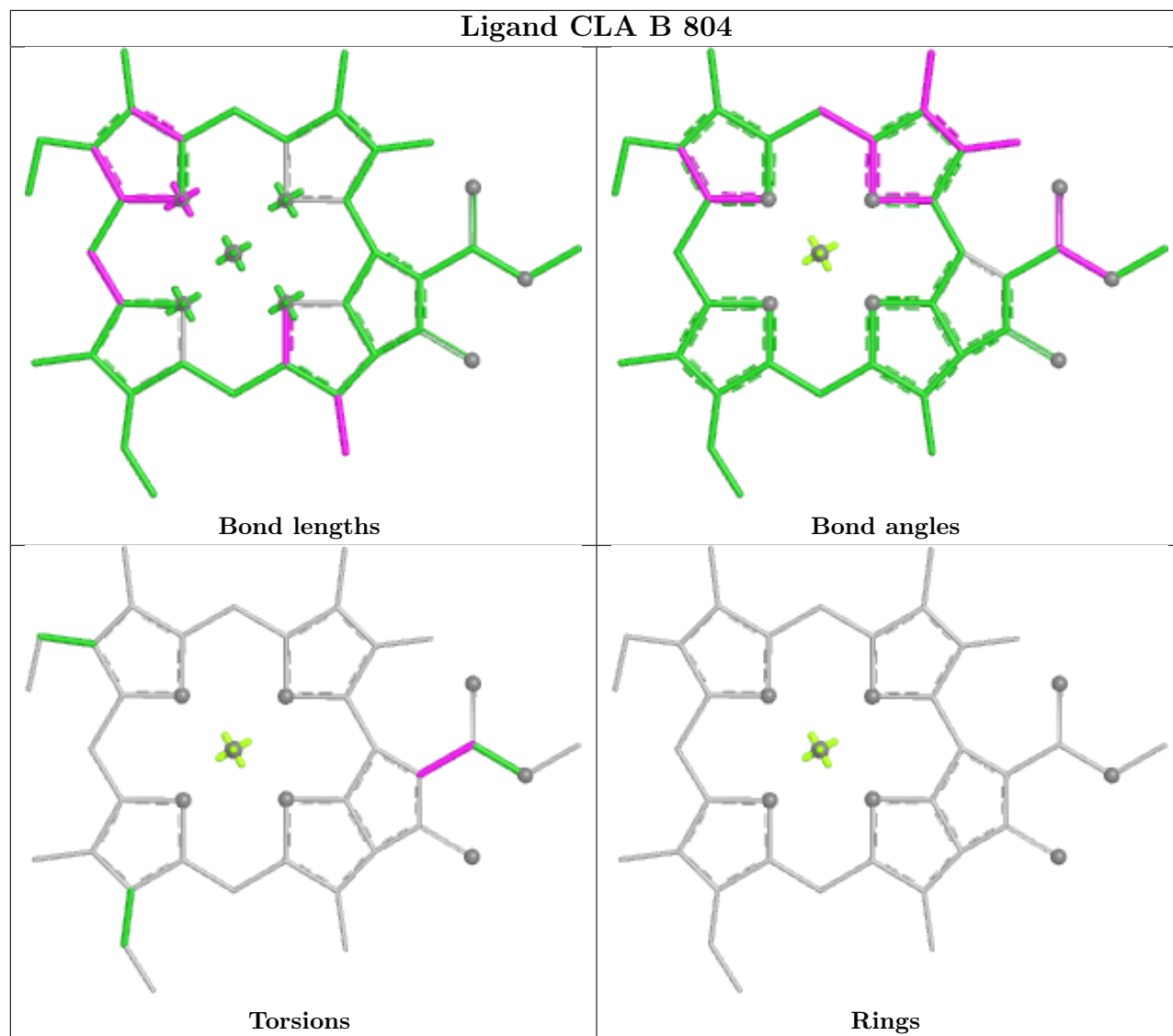


Torsions

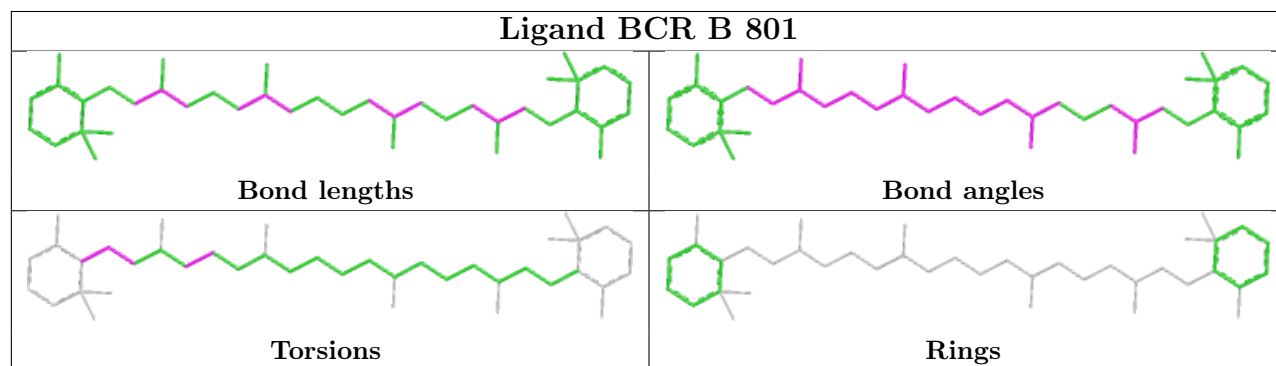


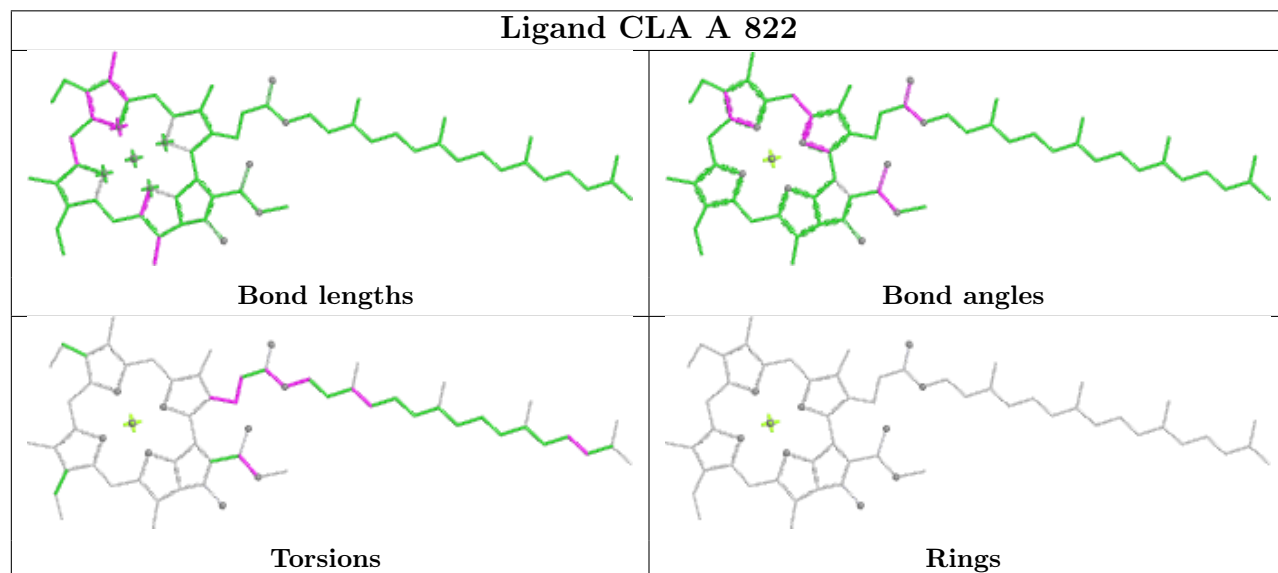
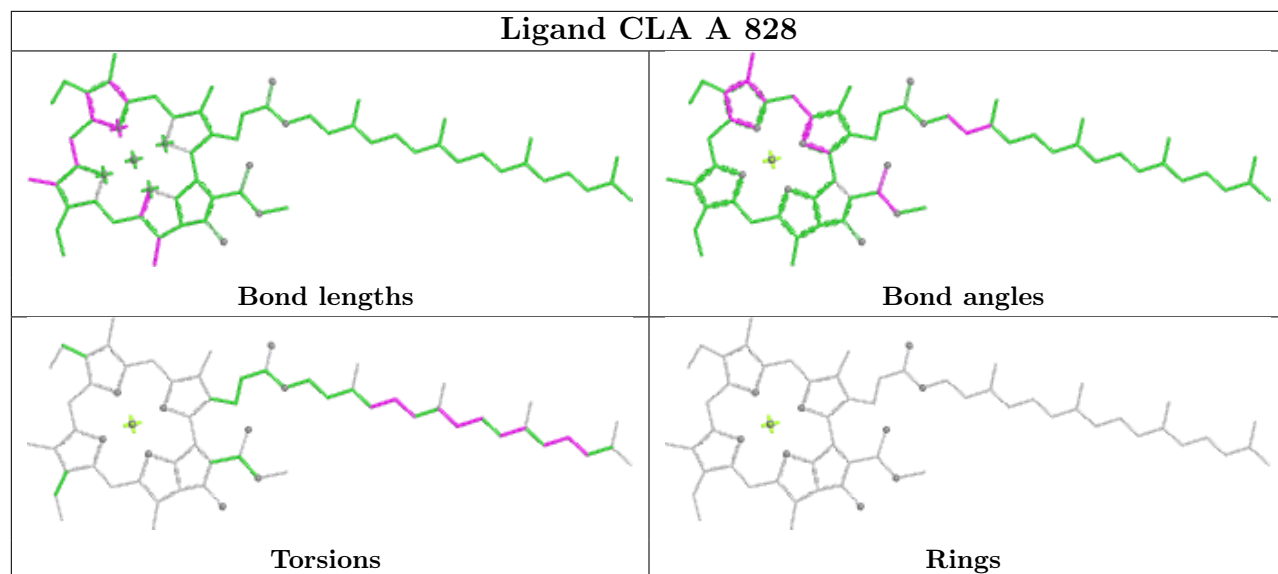
Rings

Ligand CLA B 804

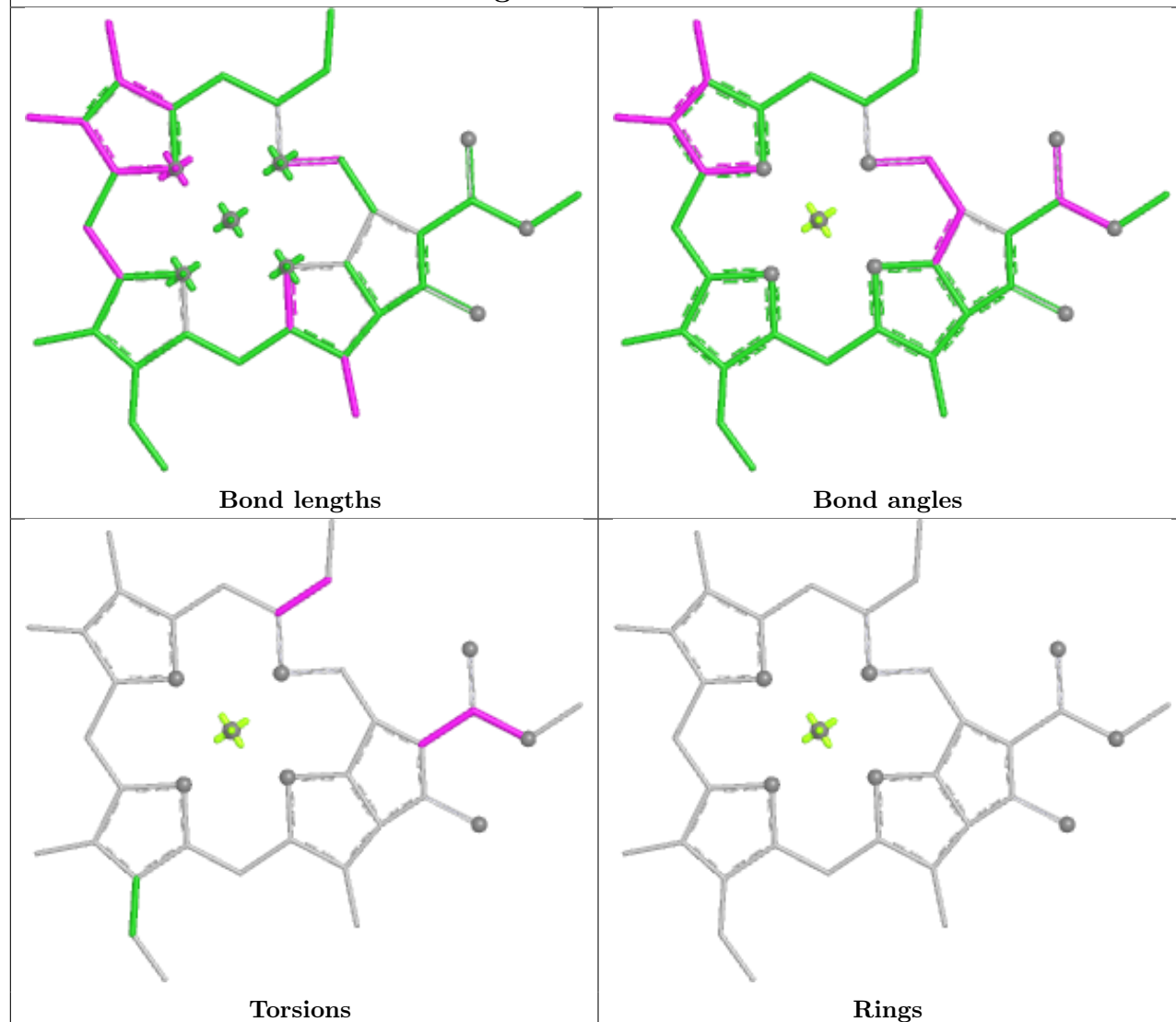


Ligand BCR B 801

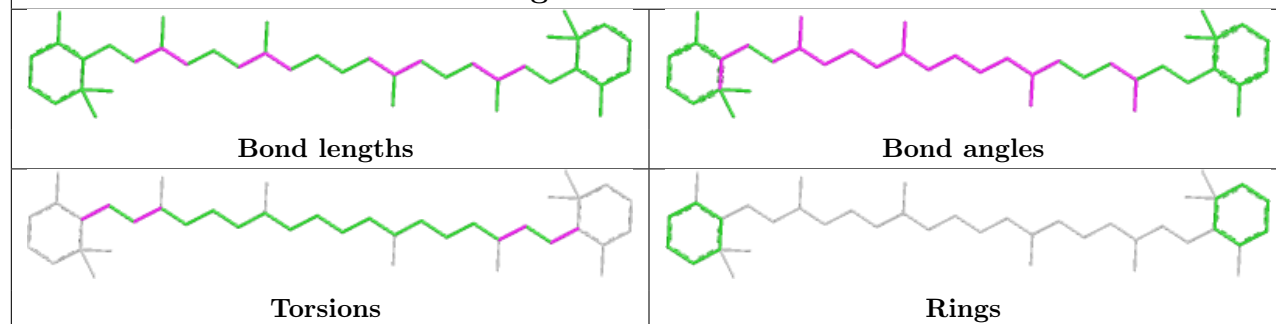




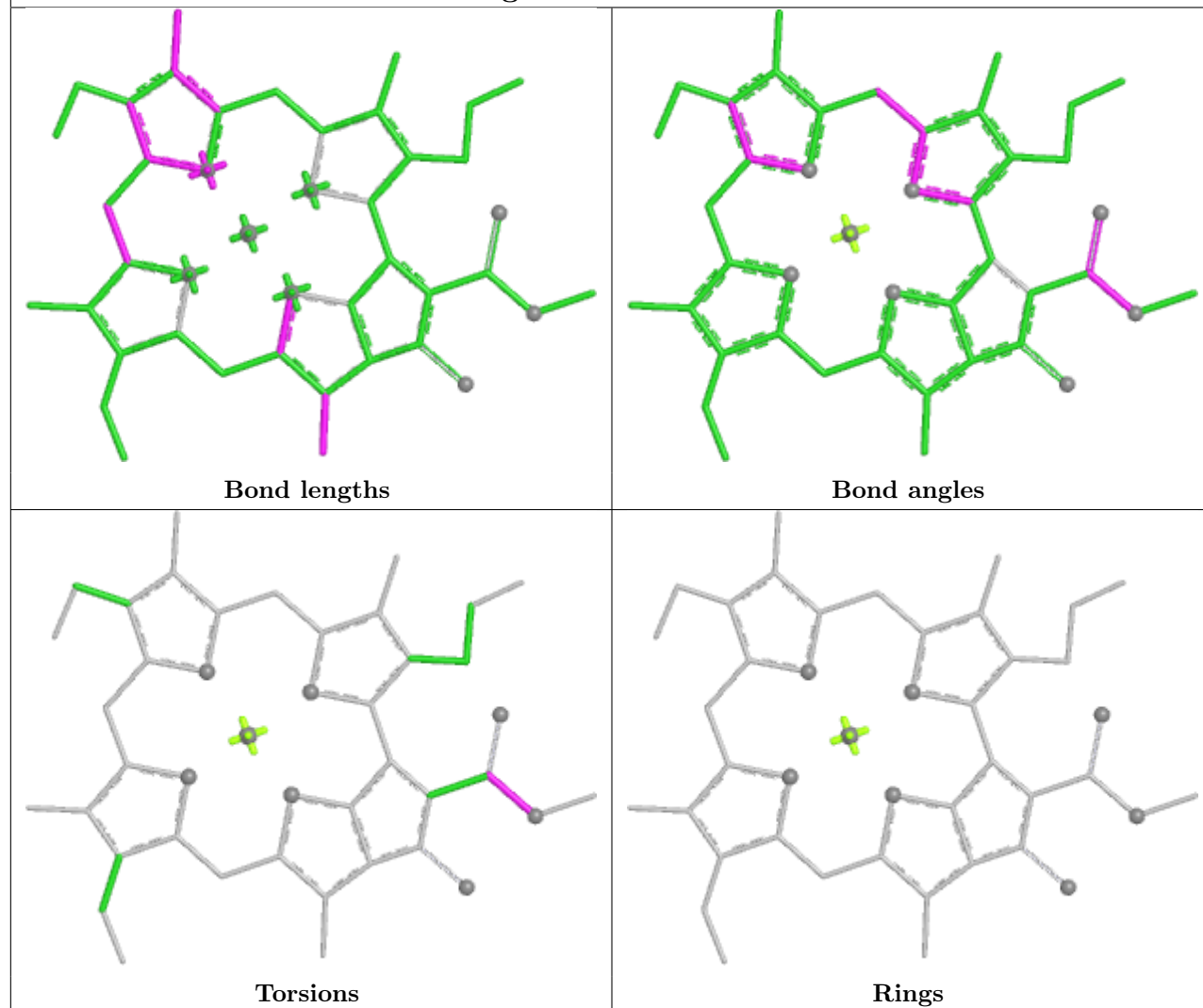
Ligand CLA 2 610



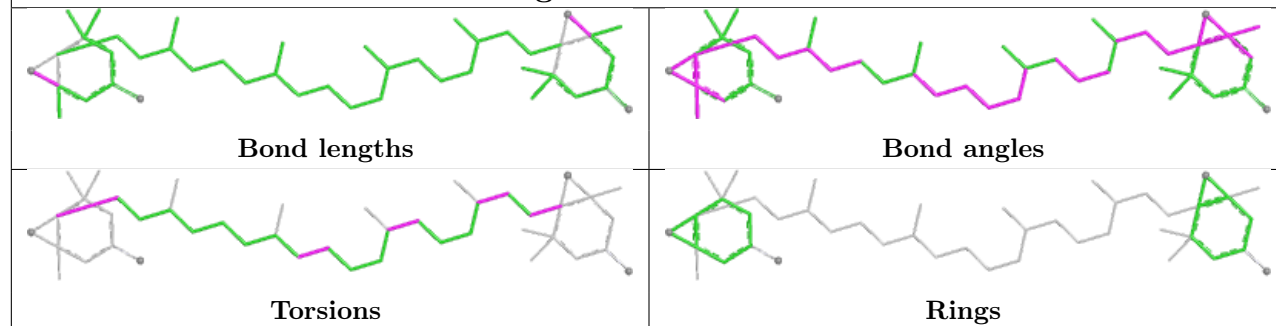
Ligand BCR B 846



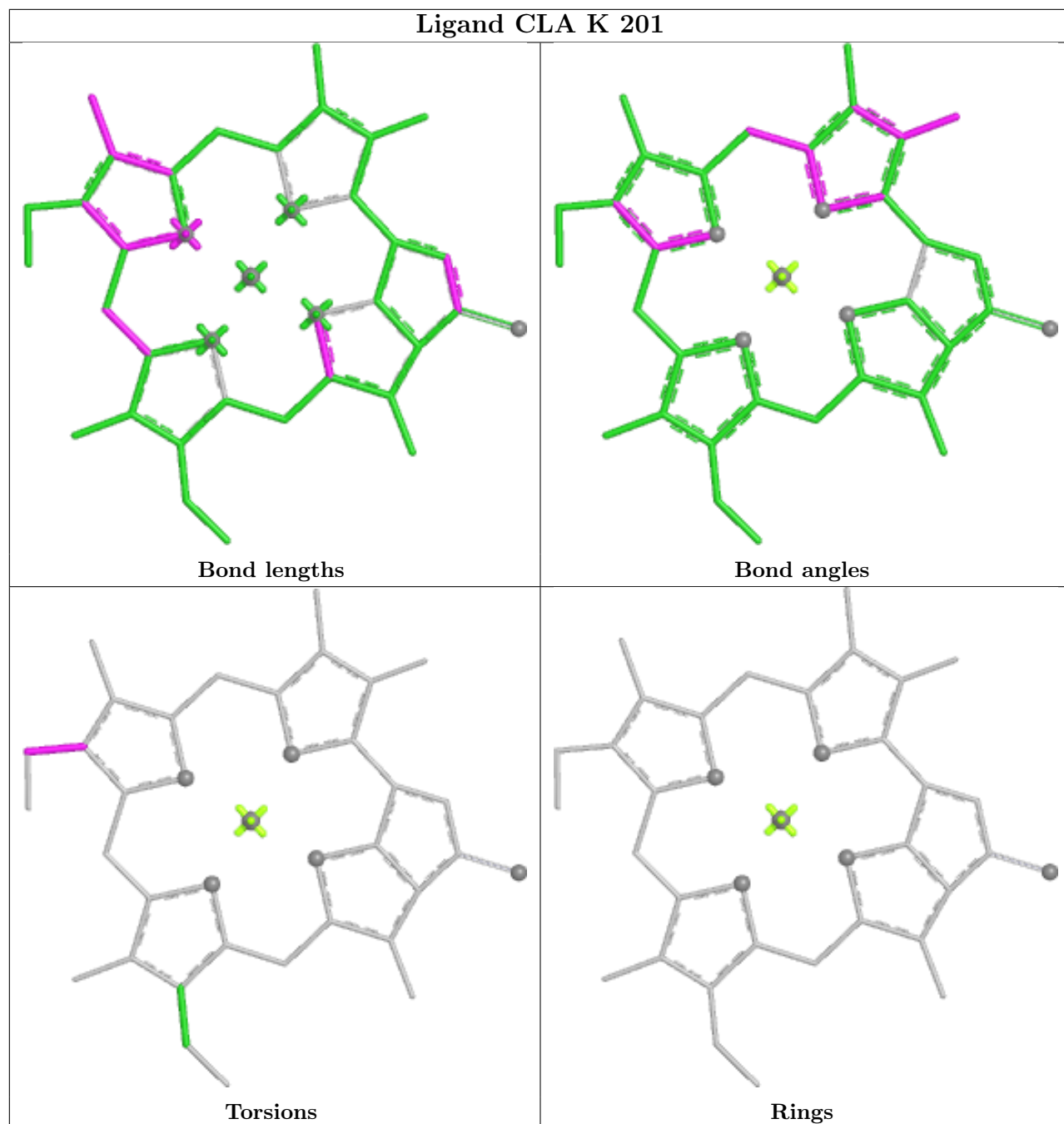
Ligand CLA B 830



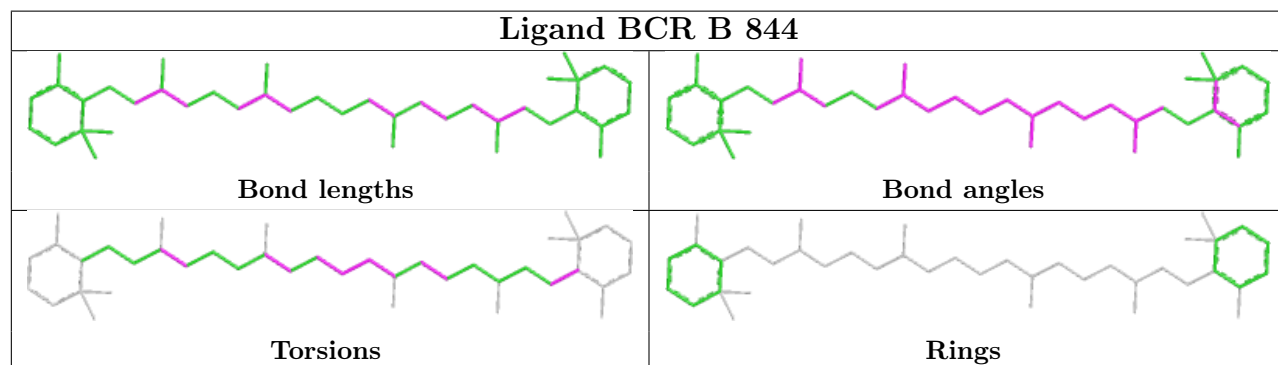
Ligand XAT 1 614

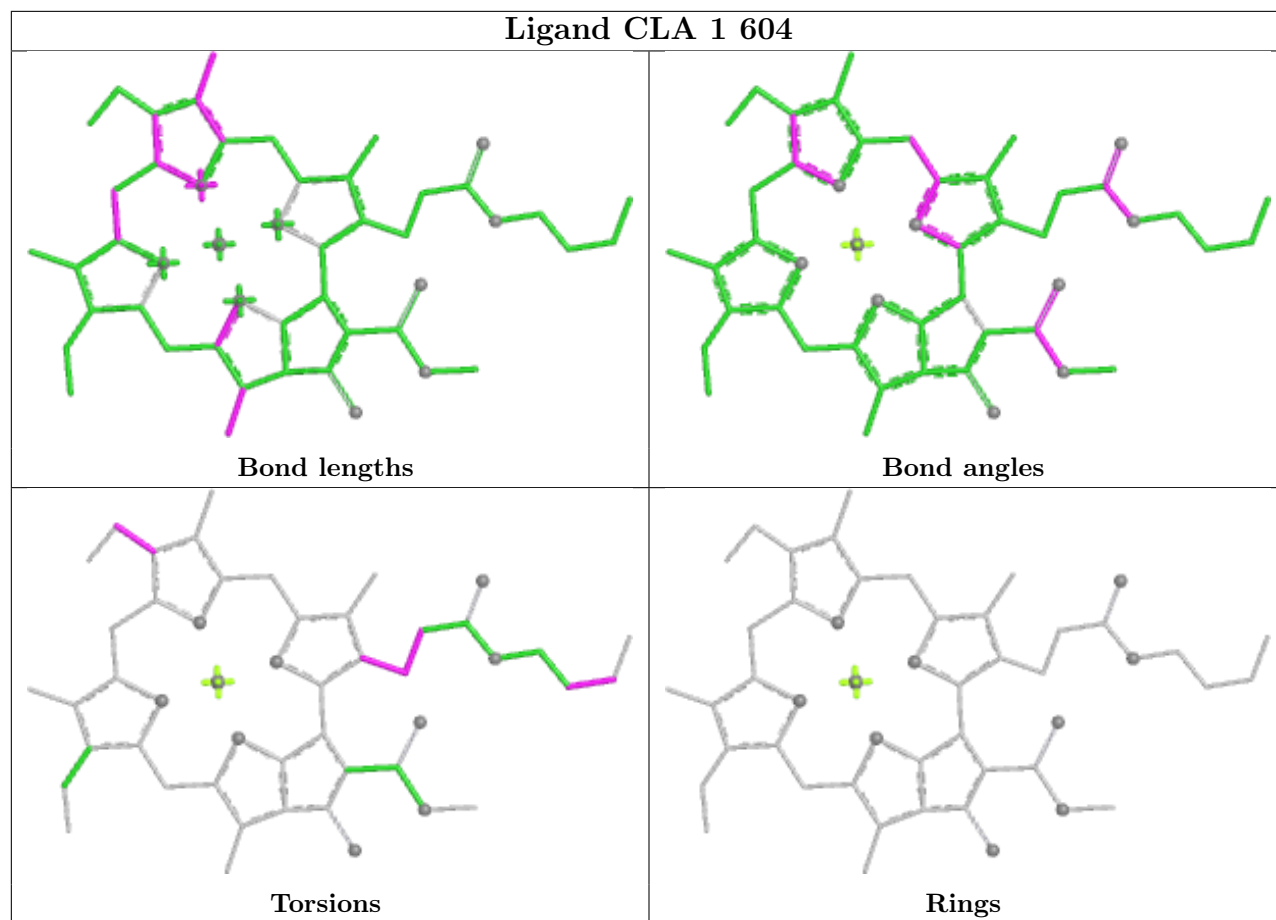


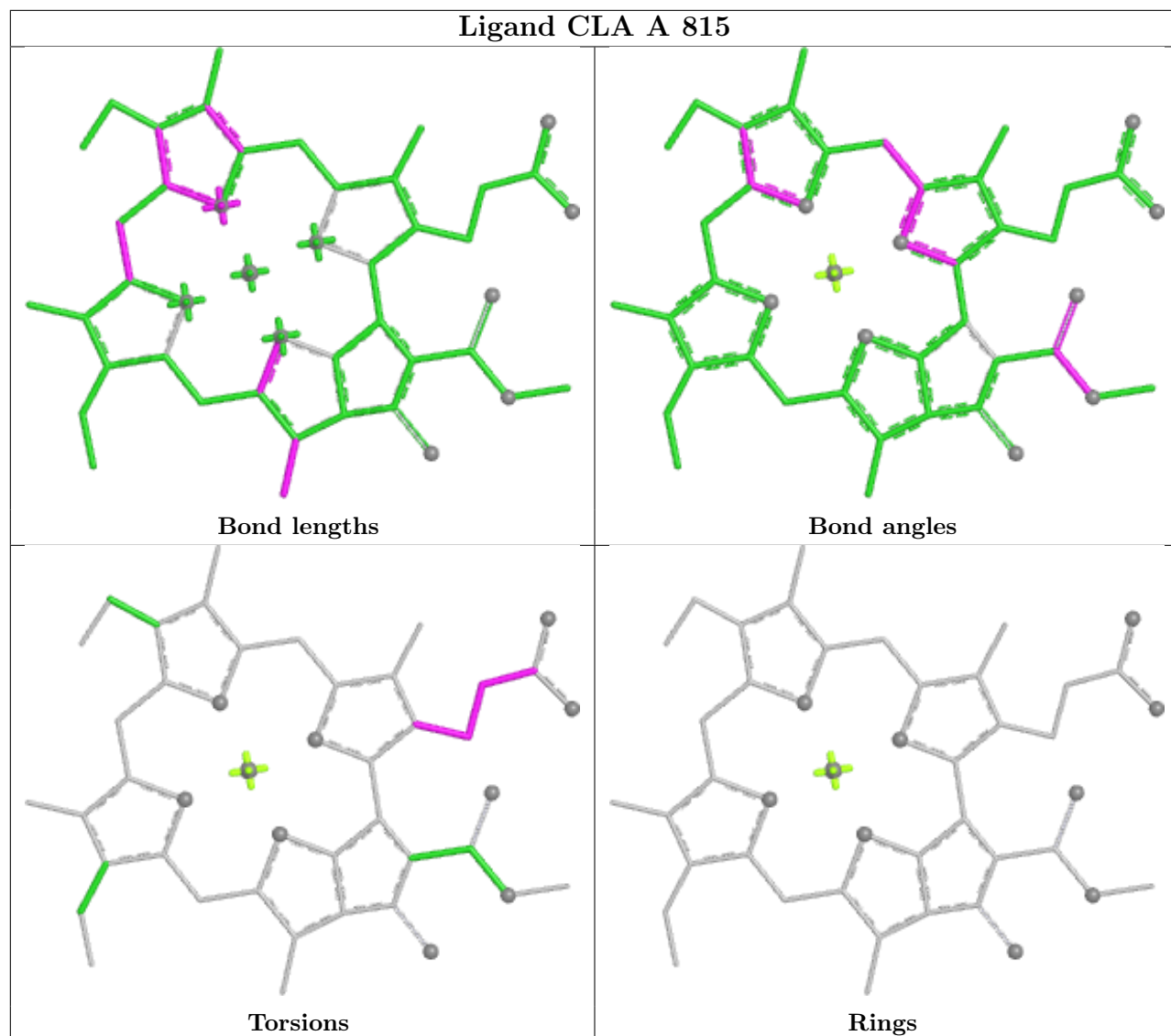
Ligand CLA K 201



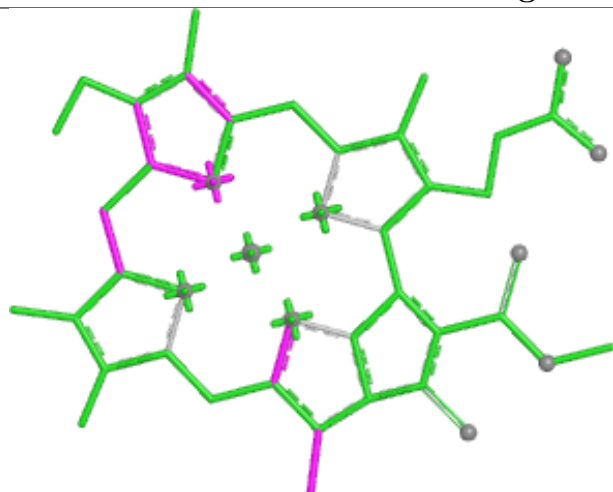
Ligand BCR B 844



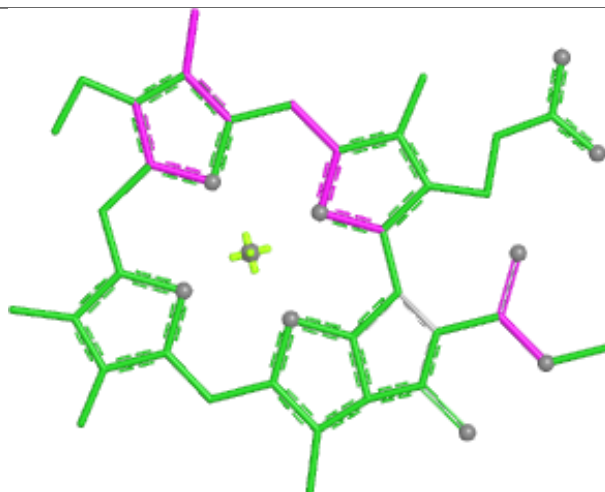




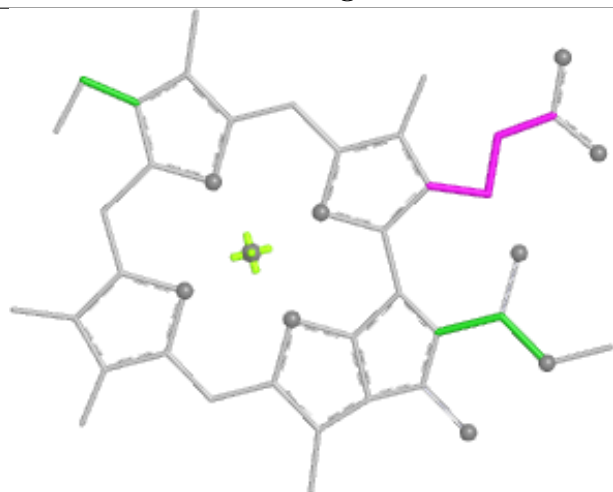
Ligand CLA 2 611



Bond lengths



Bond angles

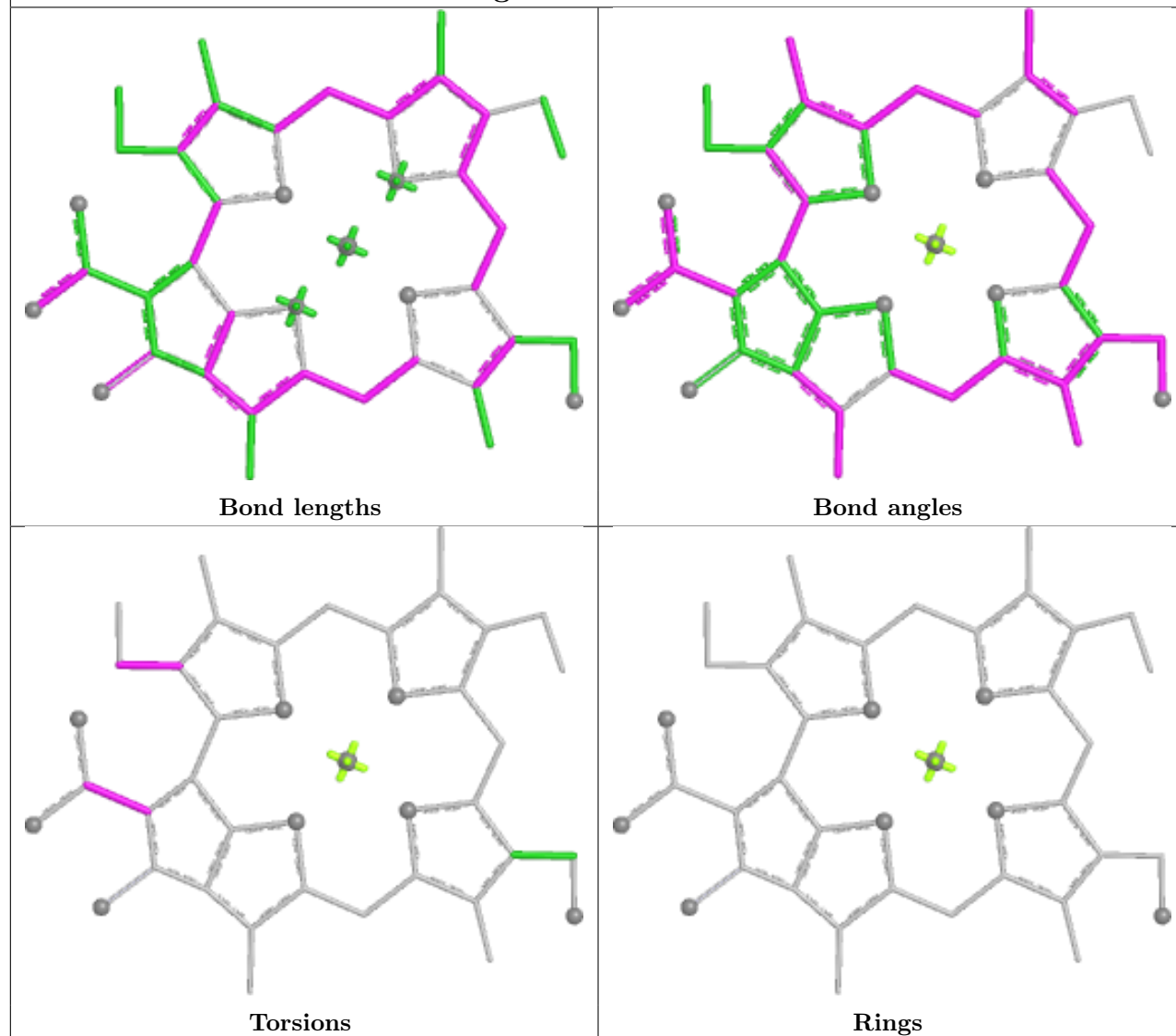


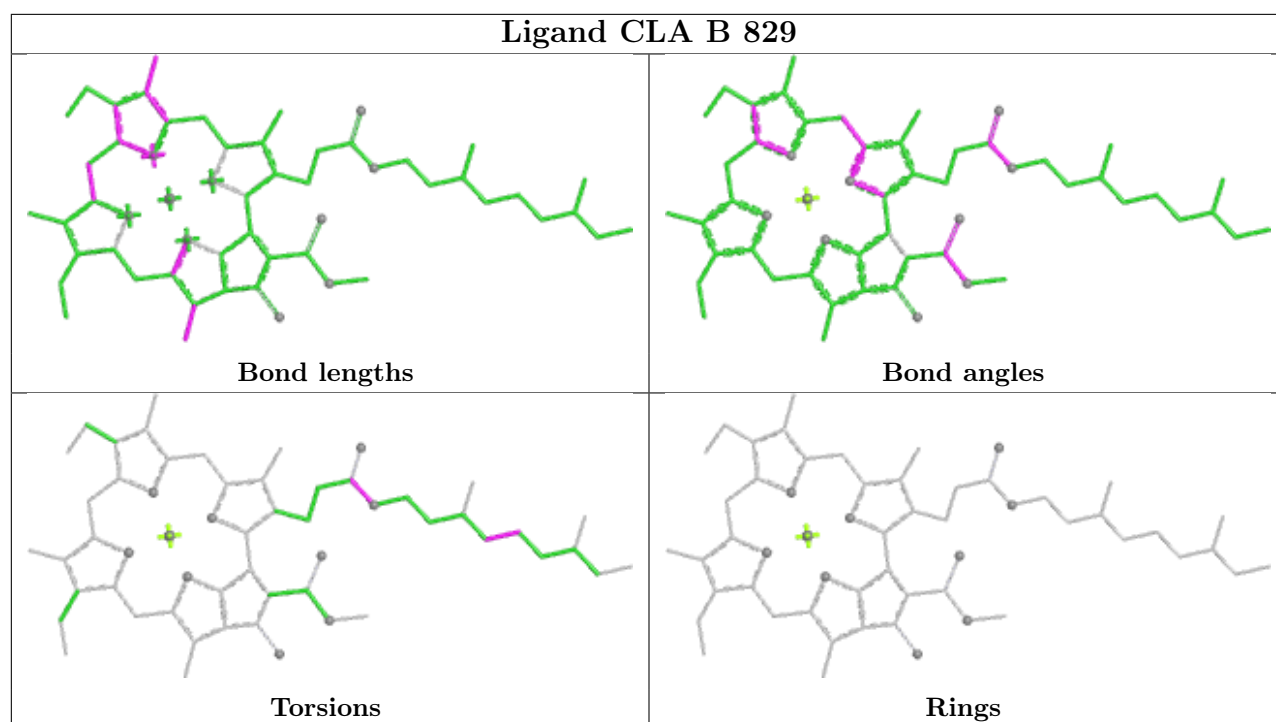
Torsions



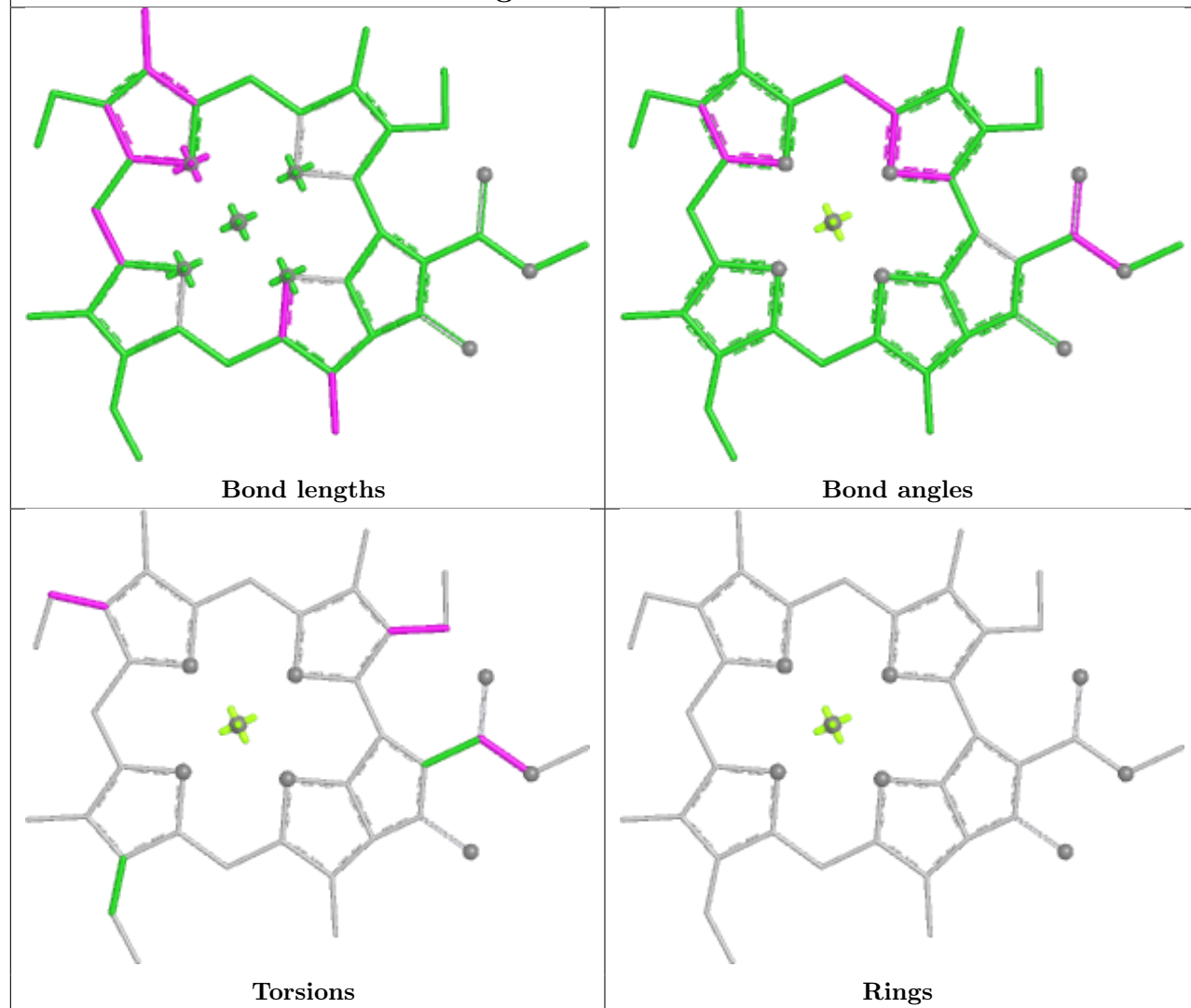
Rings

Ligand CHL 4 605

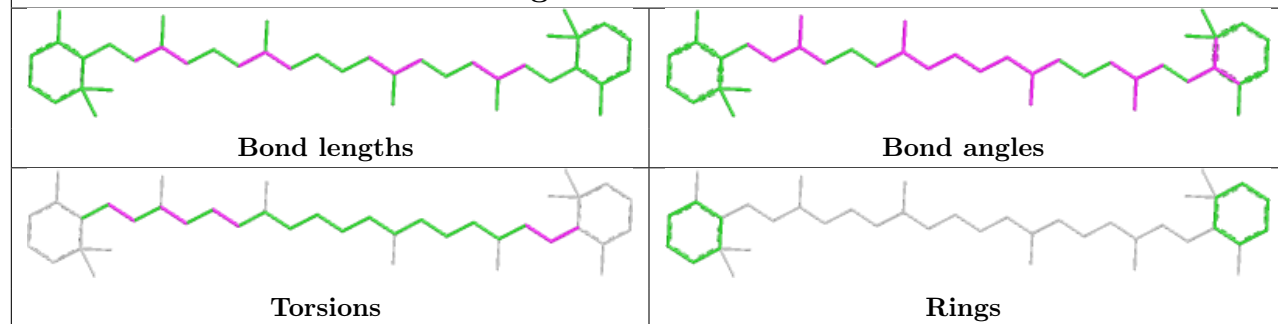


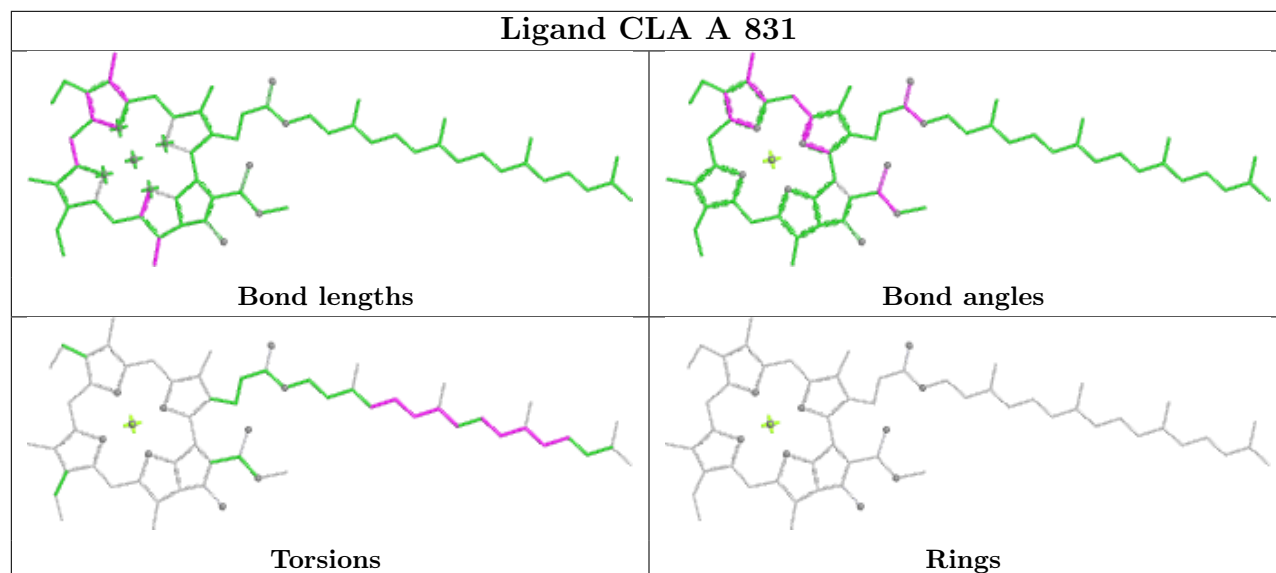
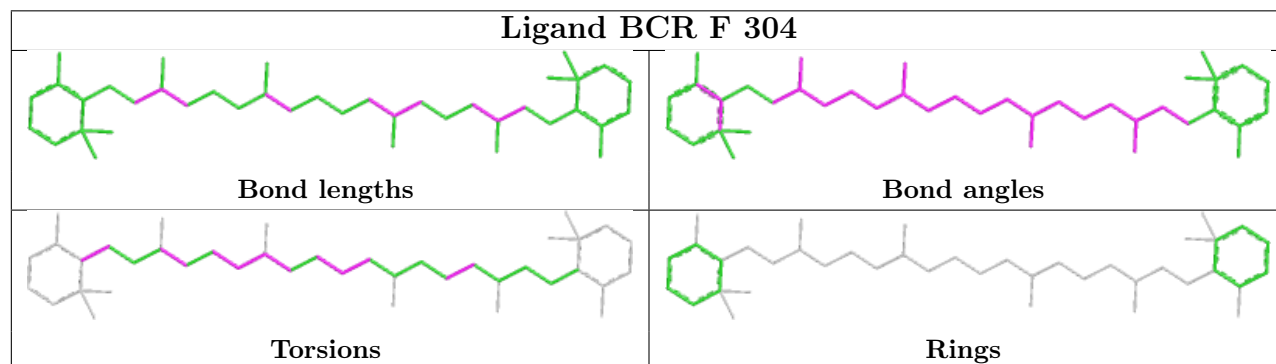
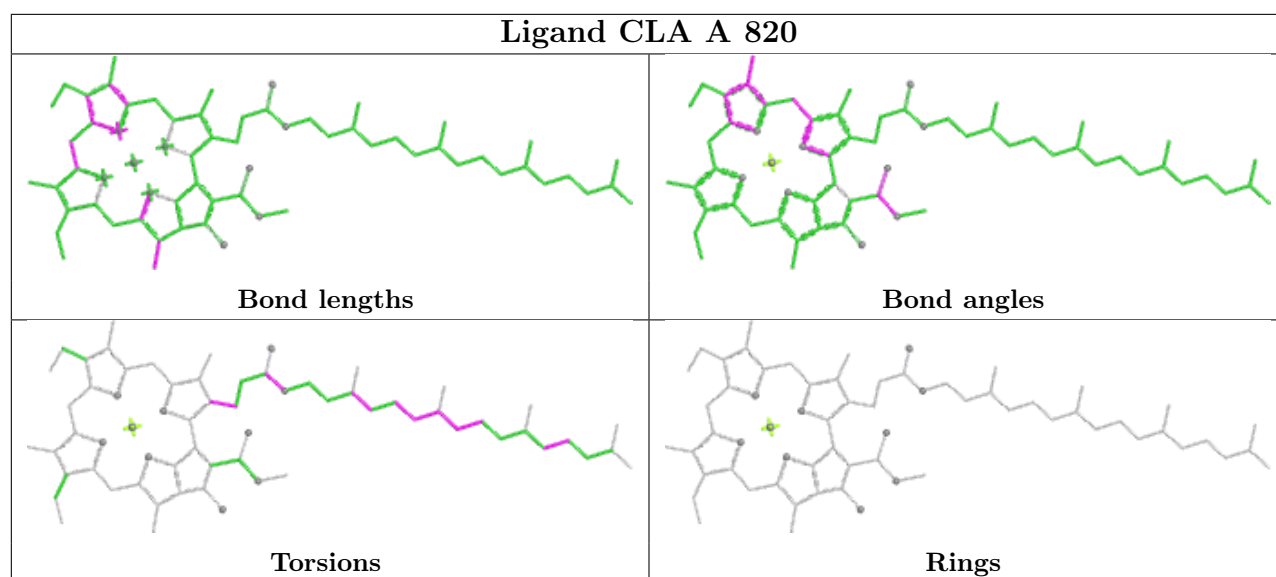


Ligand CLA B 835

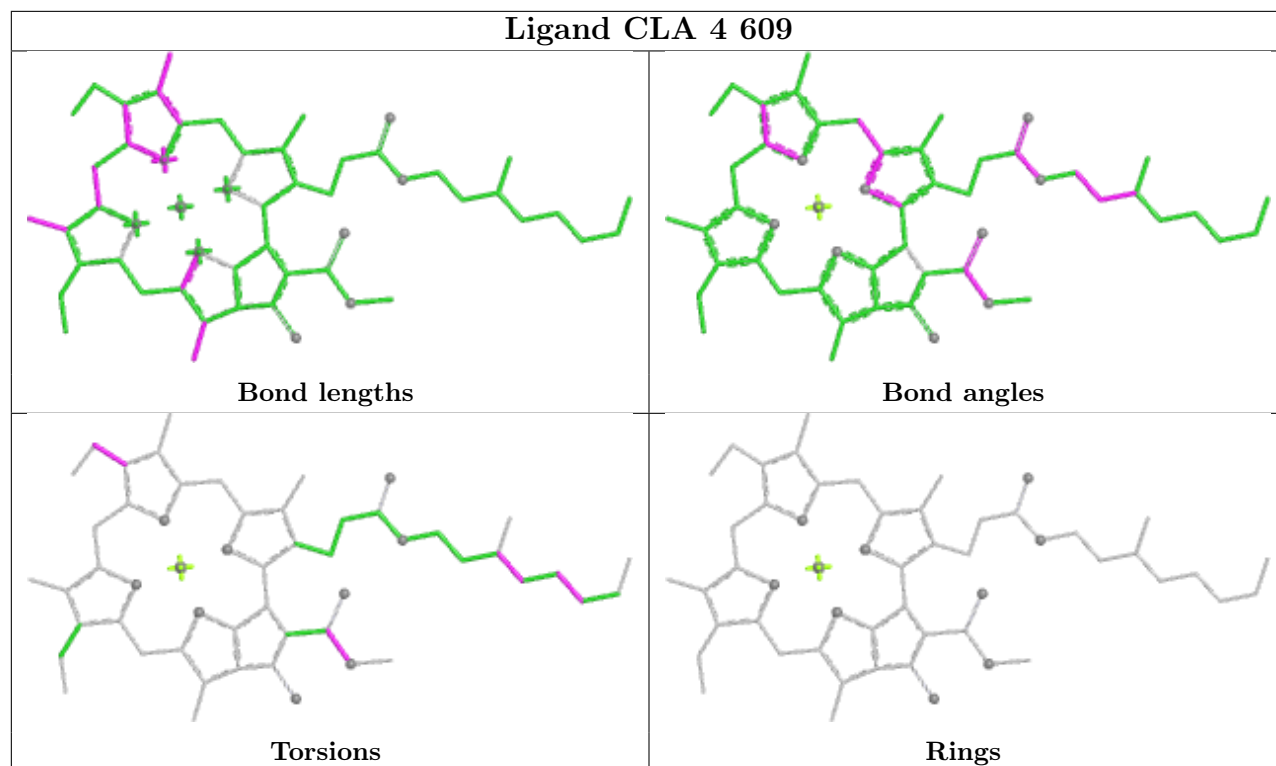


Ligand BCR B 849

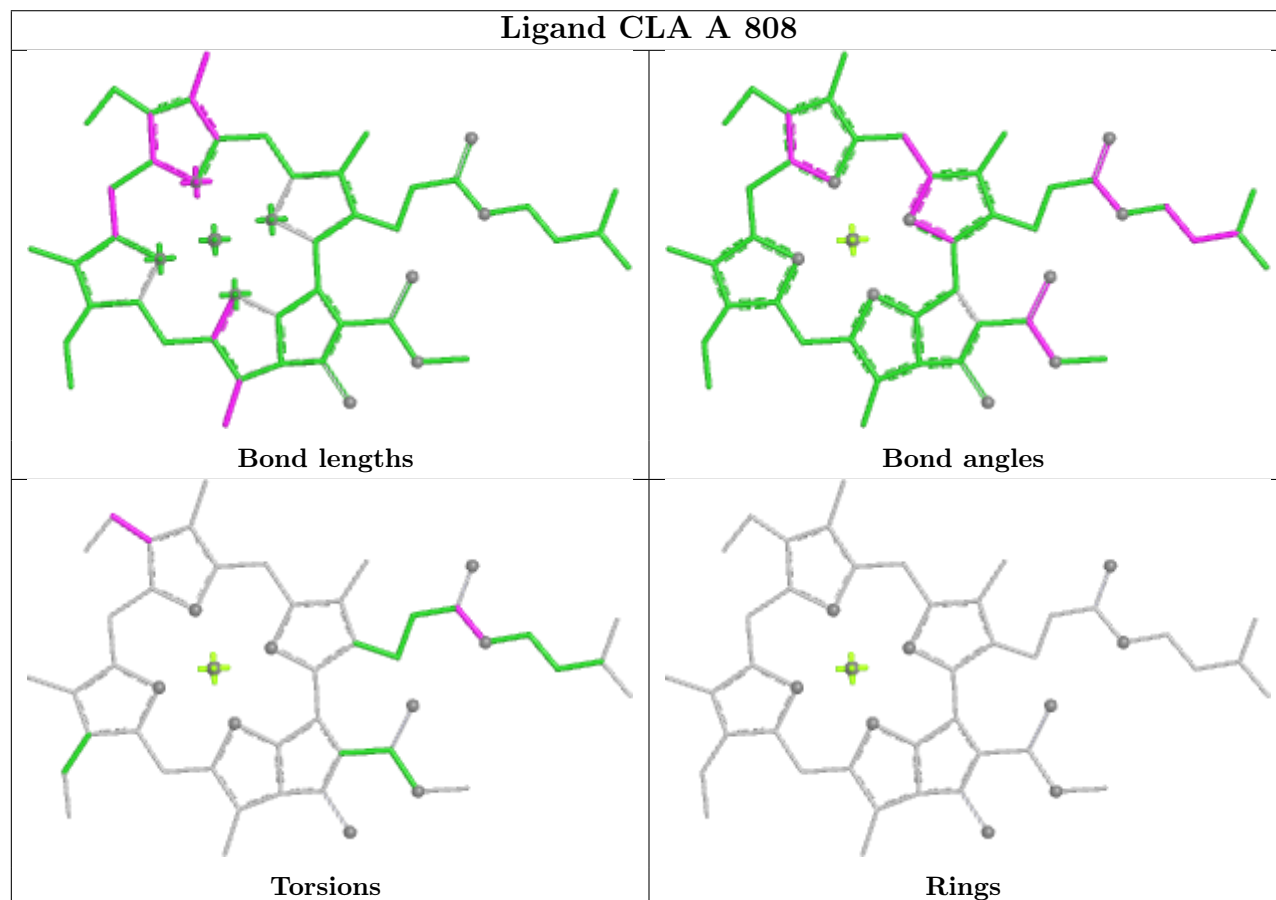




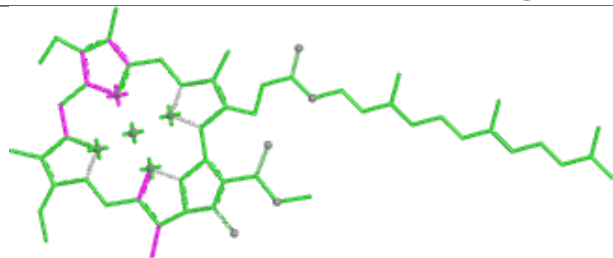
Ligand CLA 4 609



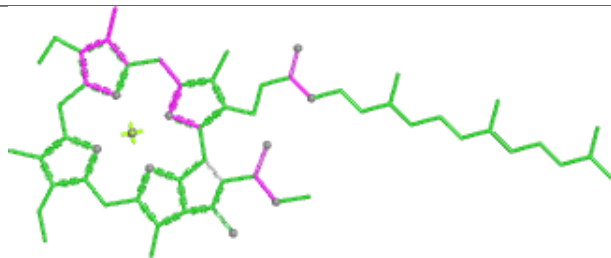
Ligand CLA A 808



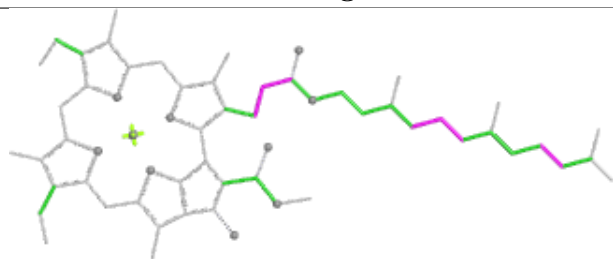
Ligand CLA 4 602



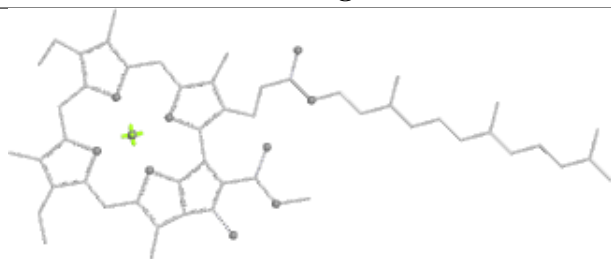
Bond lengths



Bond angles

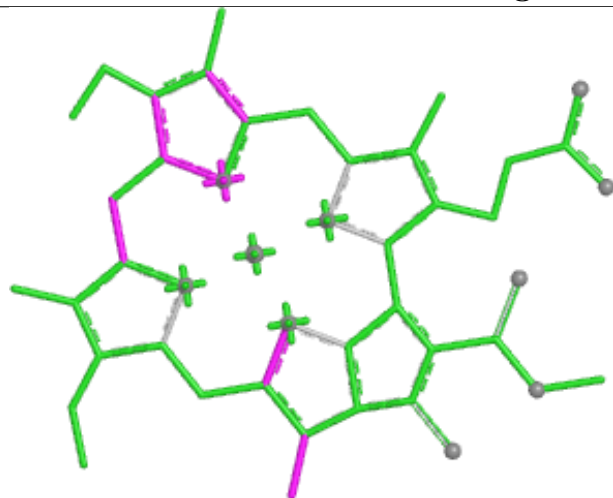


Torsions

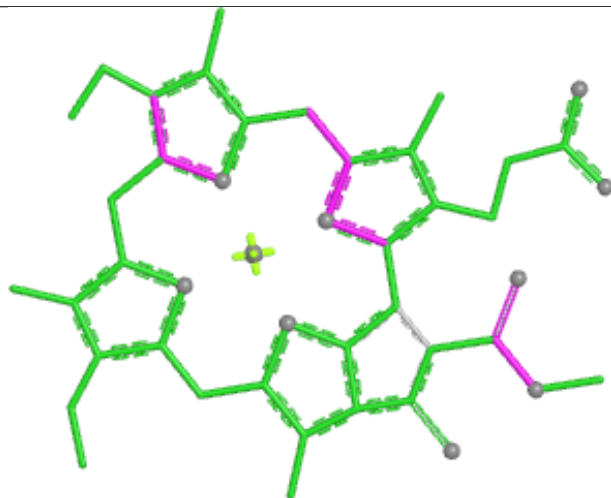


Rings

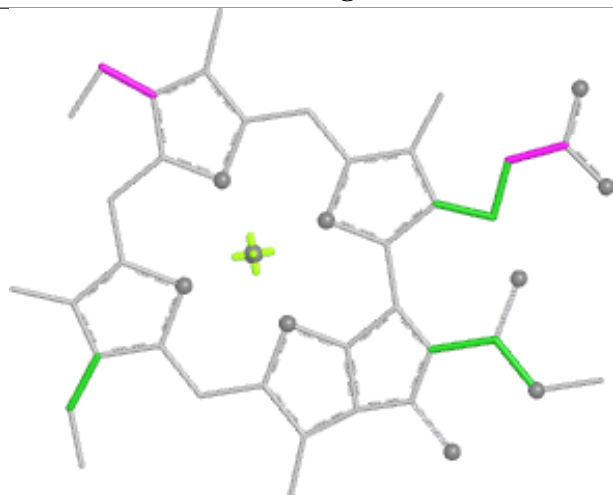
Ligand CLA A 837



Bond lengths



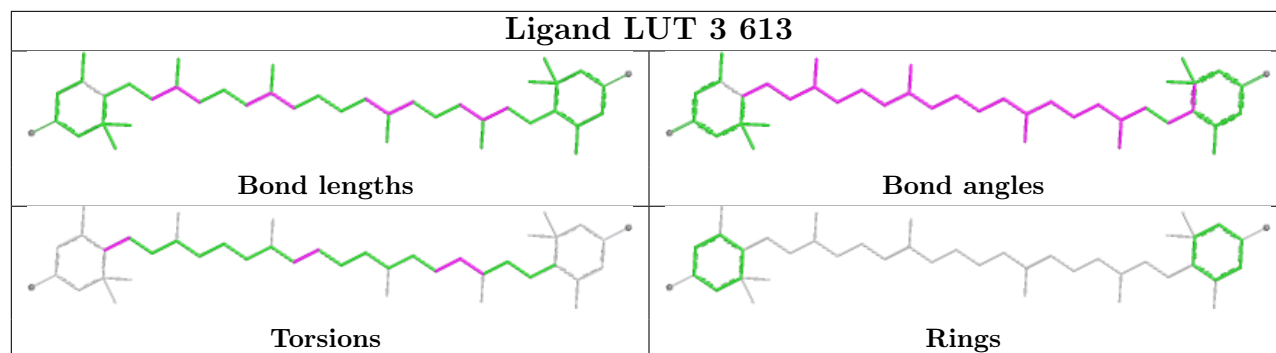
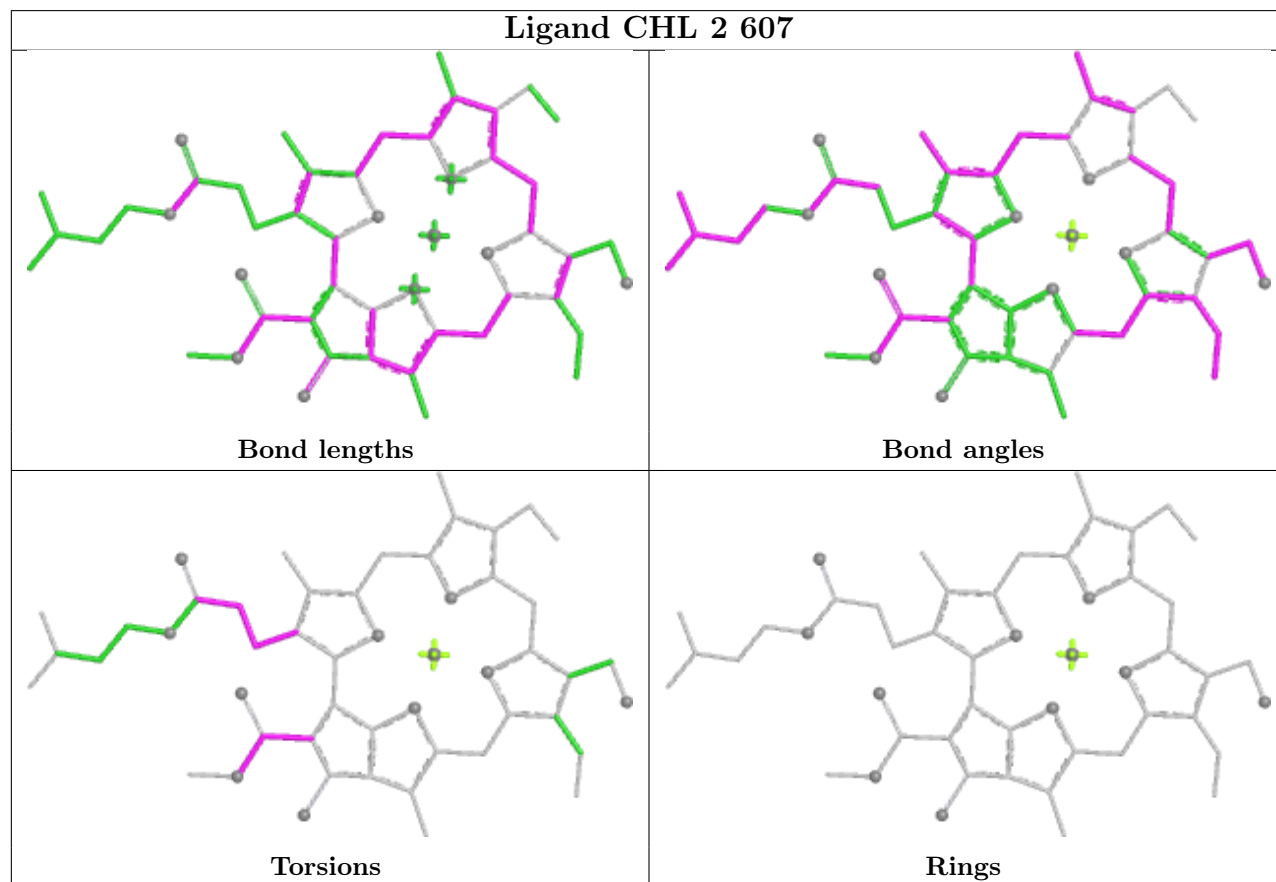
Bond angles



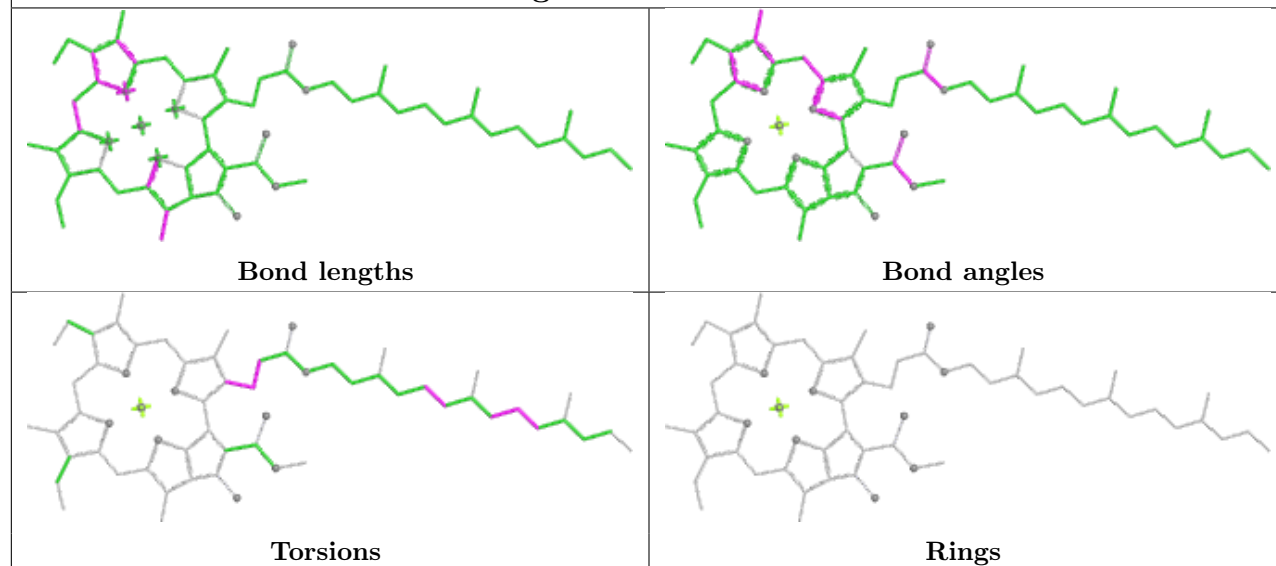
Torsions



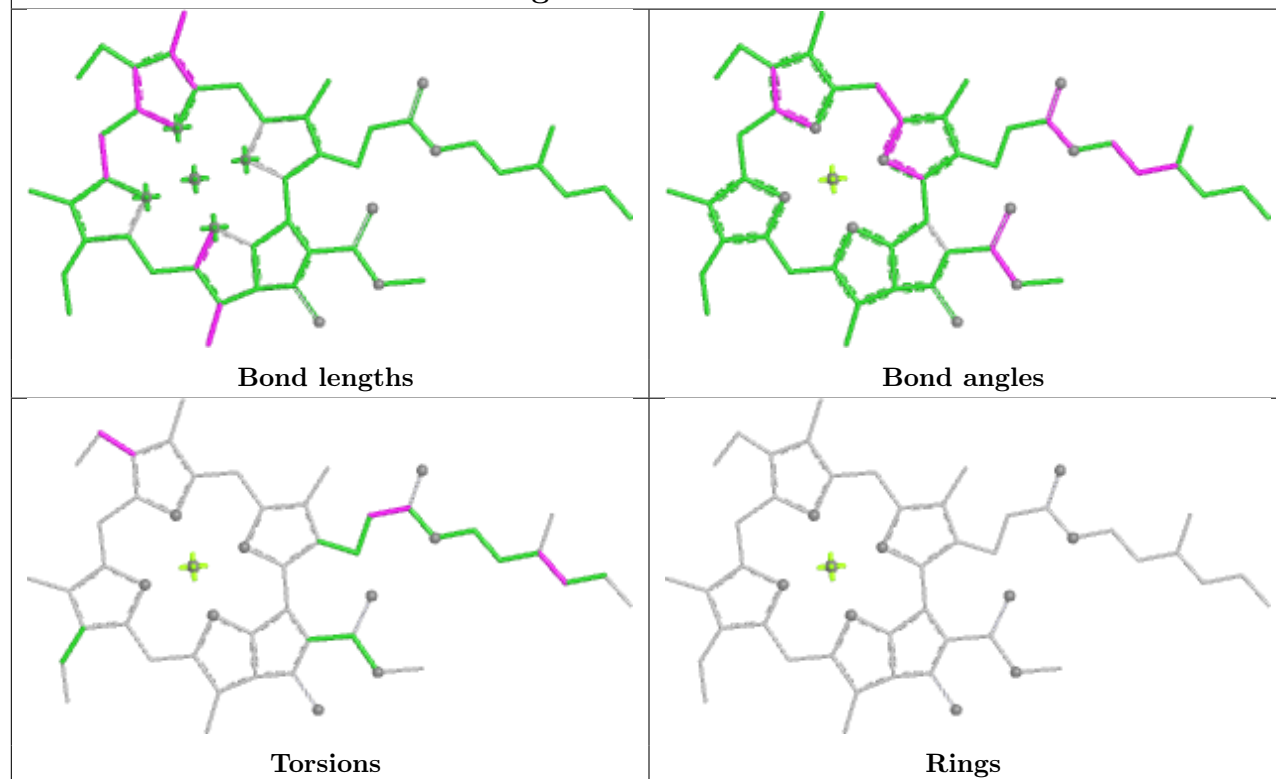
Rings

Ligand LUT 3 613**Ligand CHL 2 607**

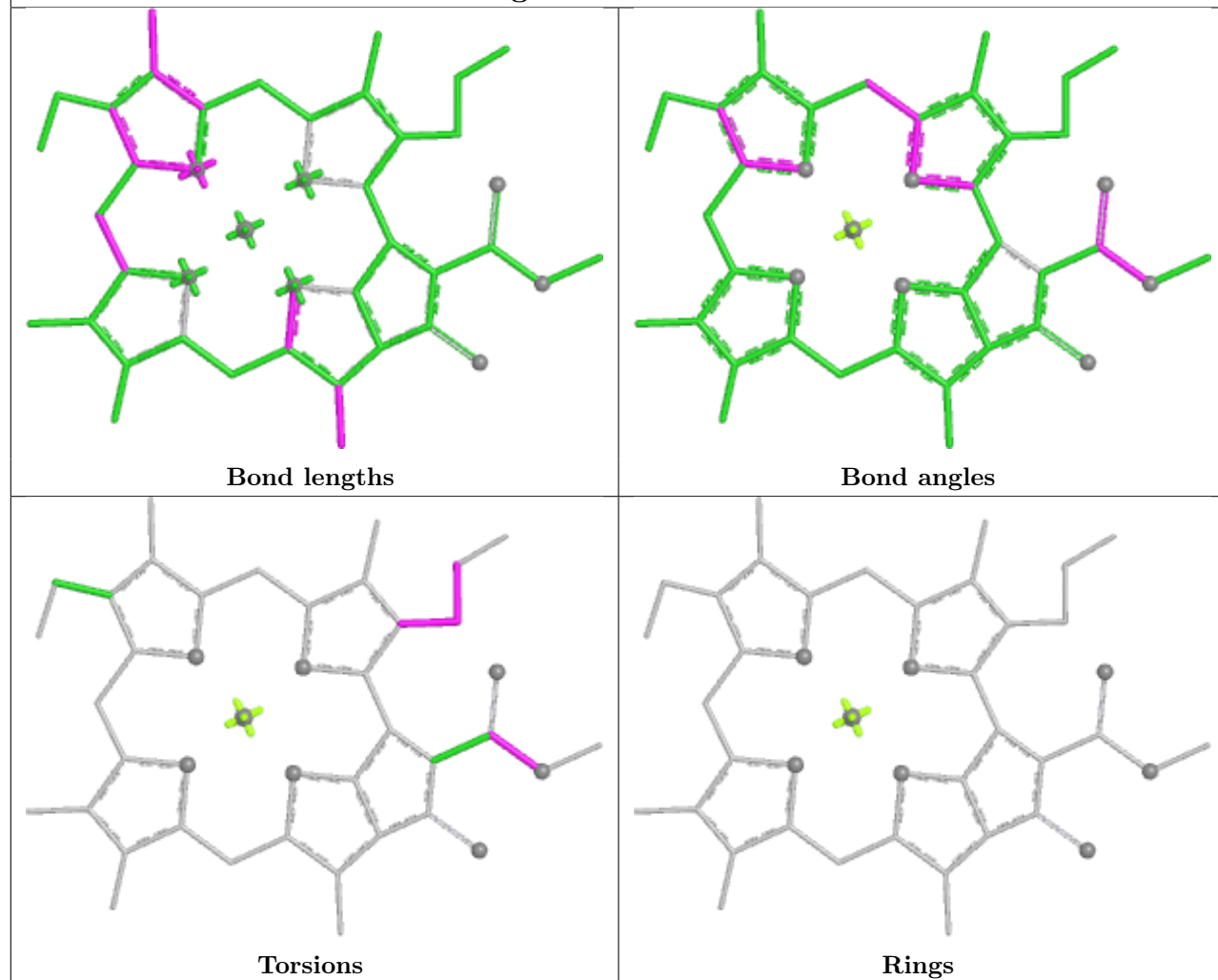
Ligand CLA B 826



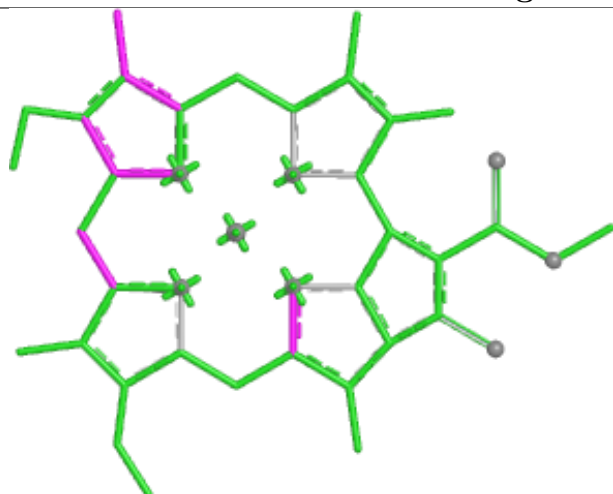
Ligand CLA A 840



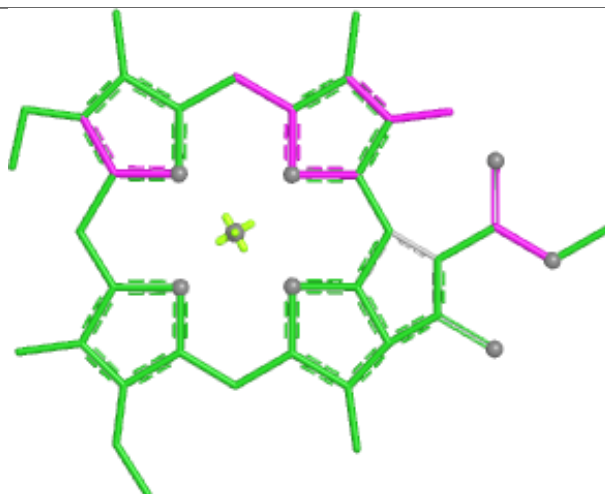
Ligand CLA 1 609



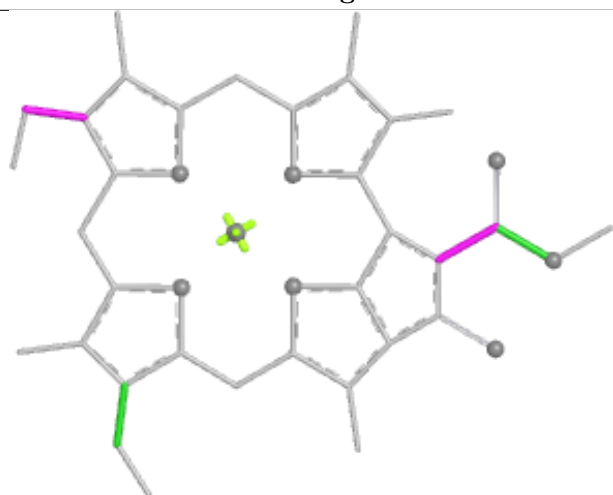
Ligand CLA F 303



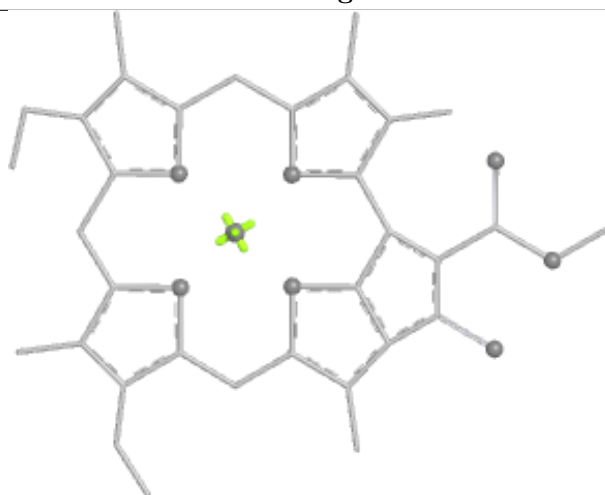
Bond lengths



Bond angles

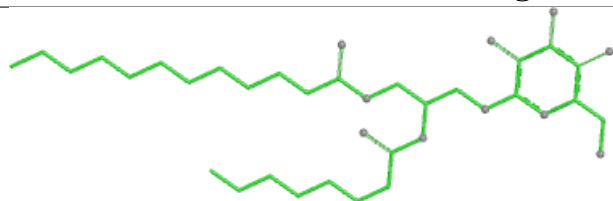


Torsions

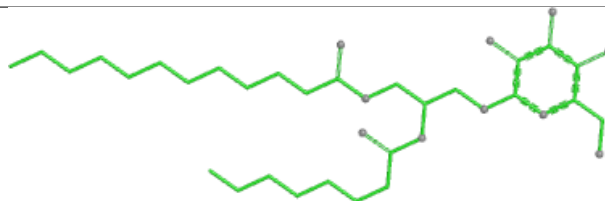


Rings

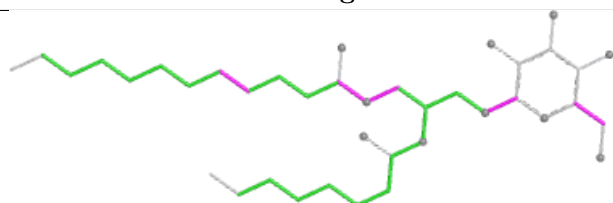
Ligand LMG 4 619



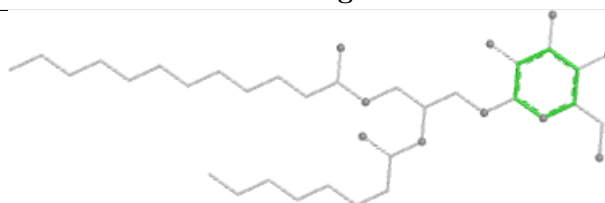
Bond lengths



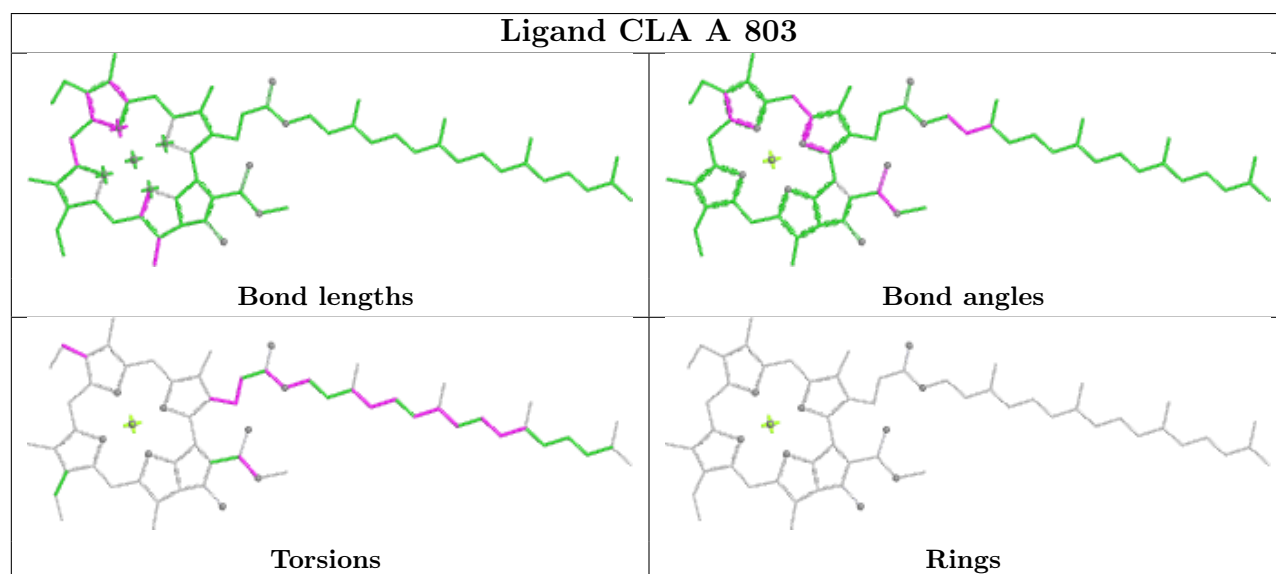
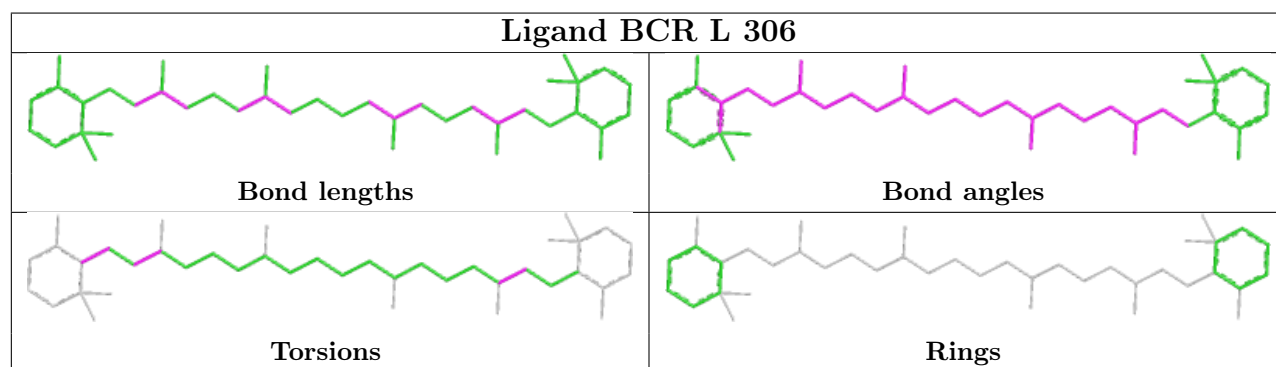
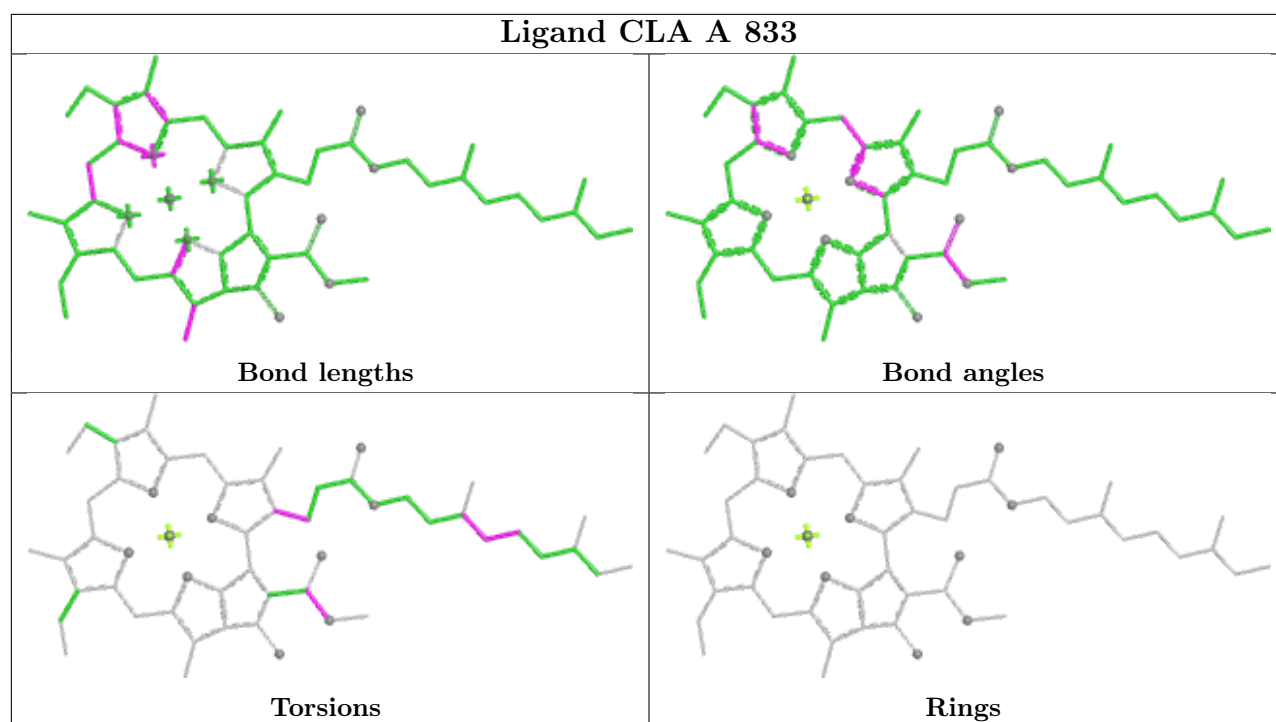
Bond angles



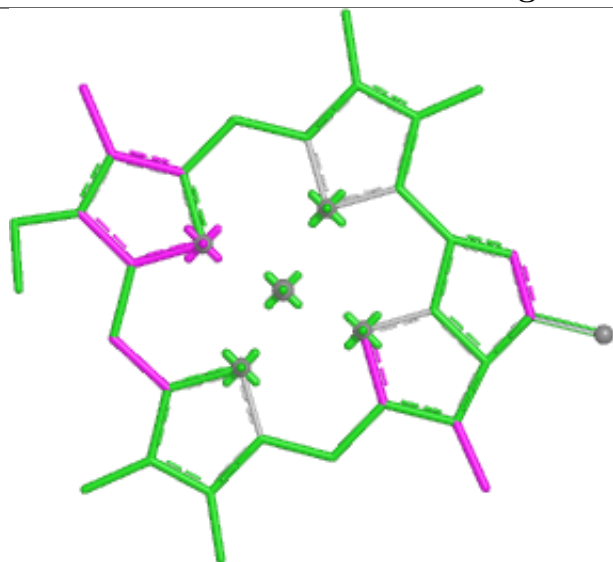
Torsions



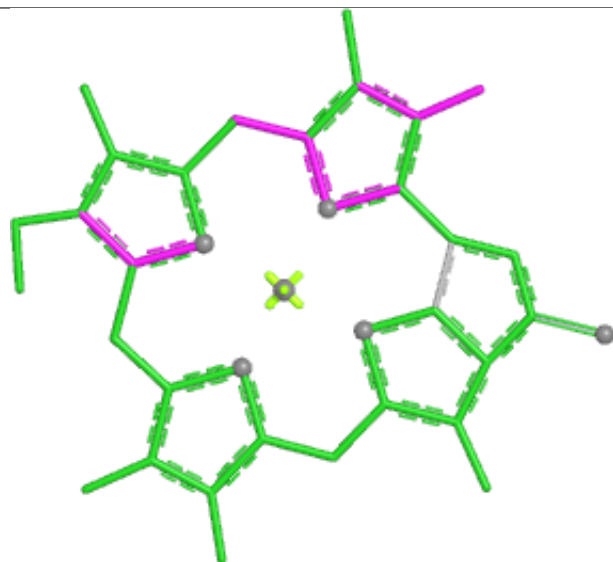
Rings



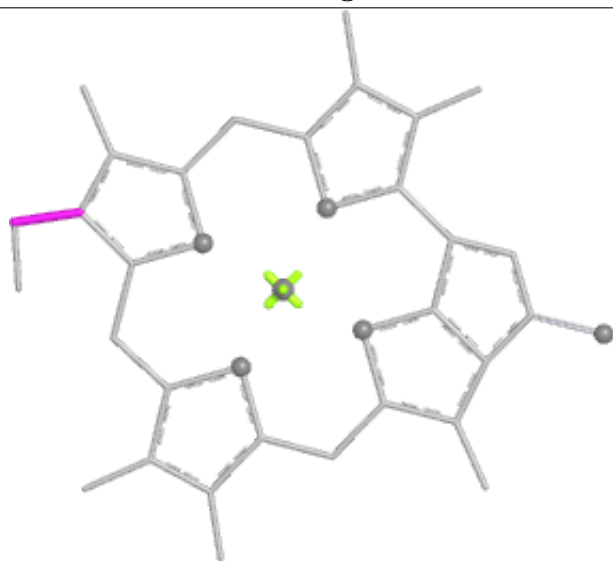
Ligand CLA 3 611



Bond lengths



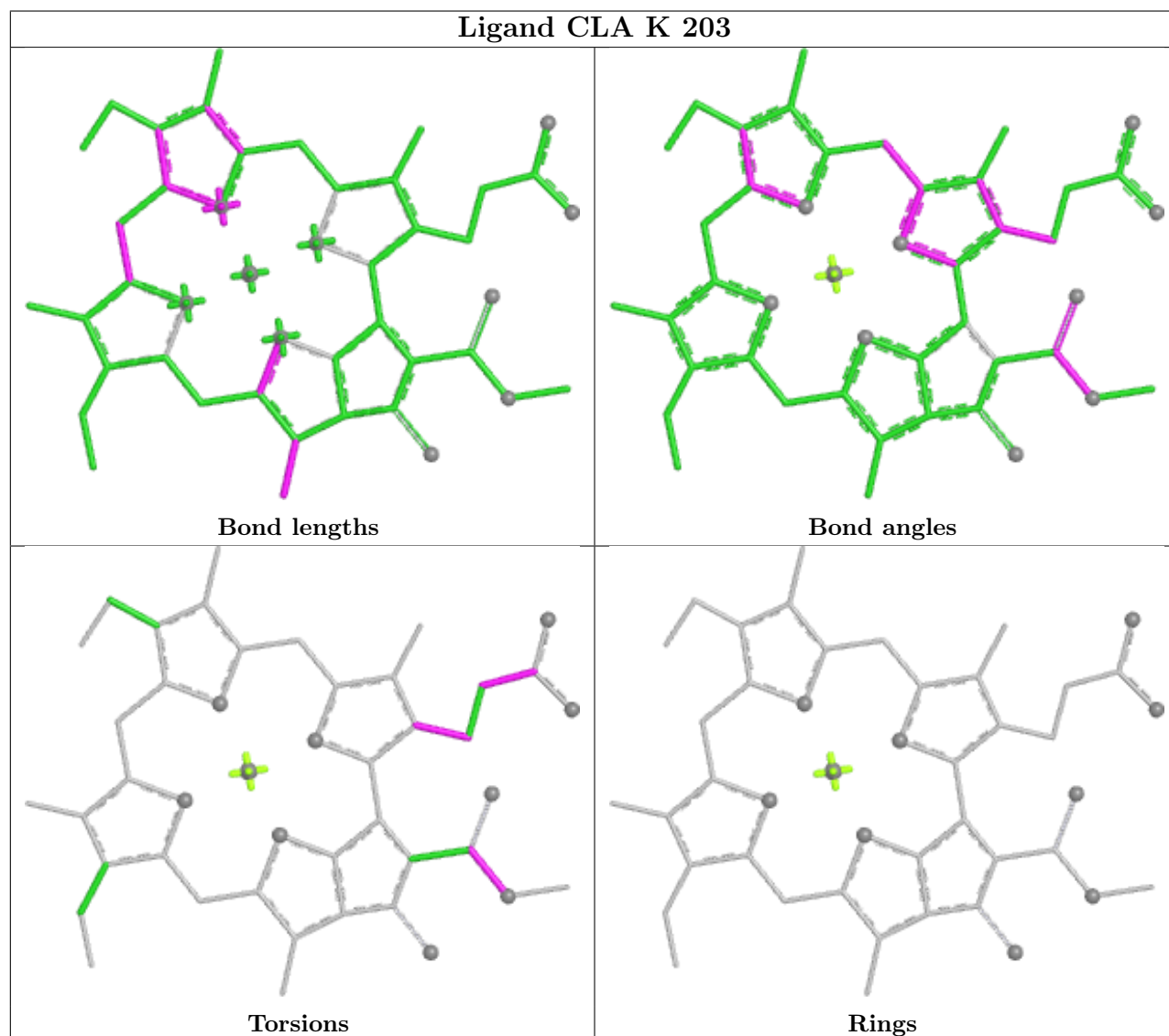
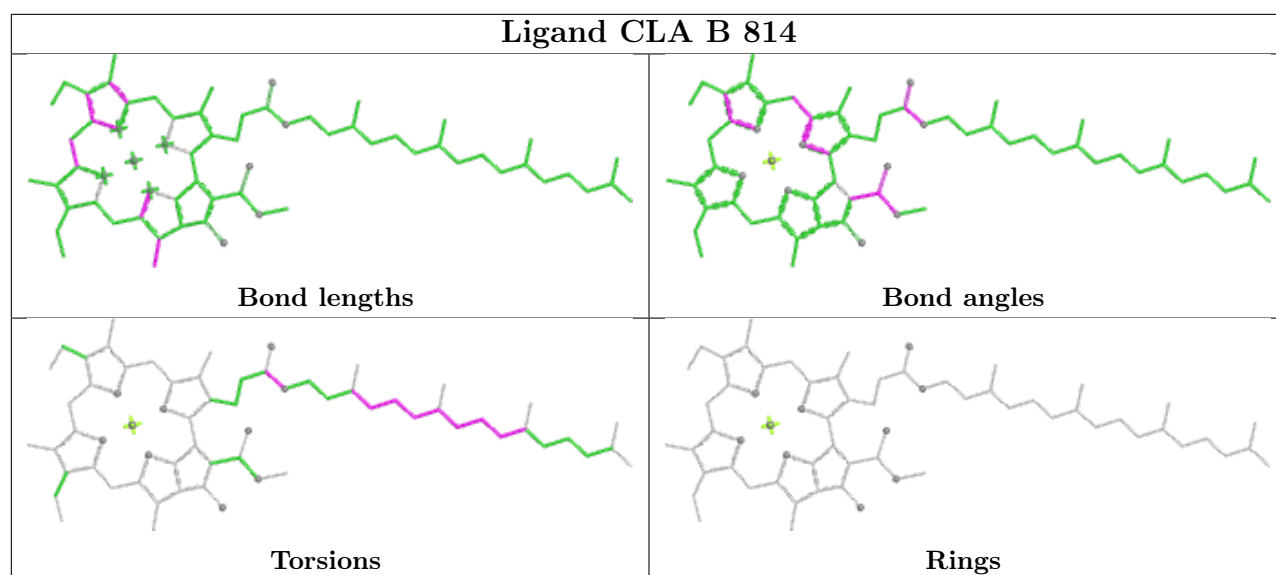
Bond angles

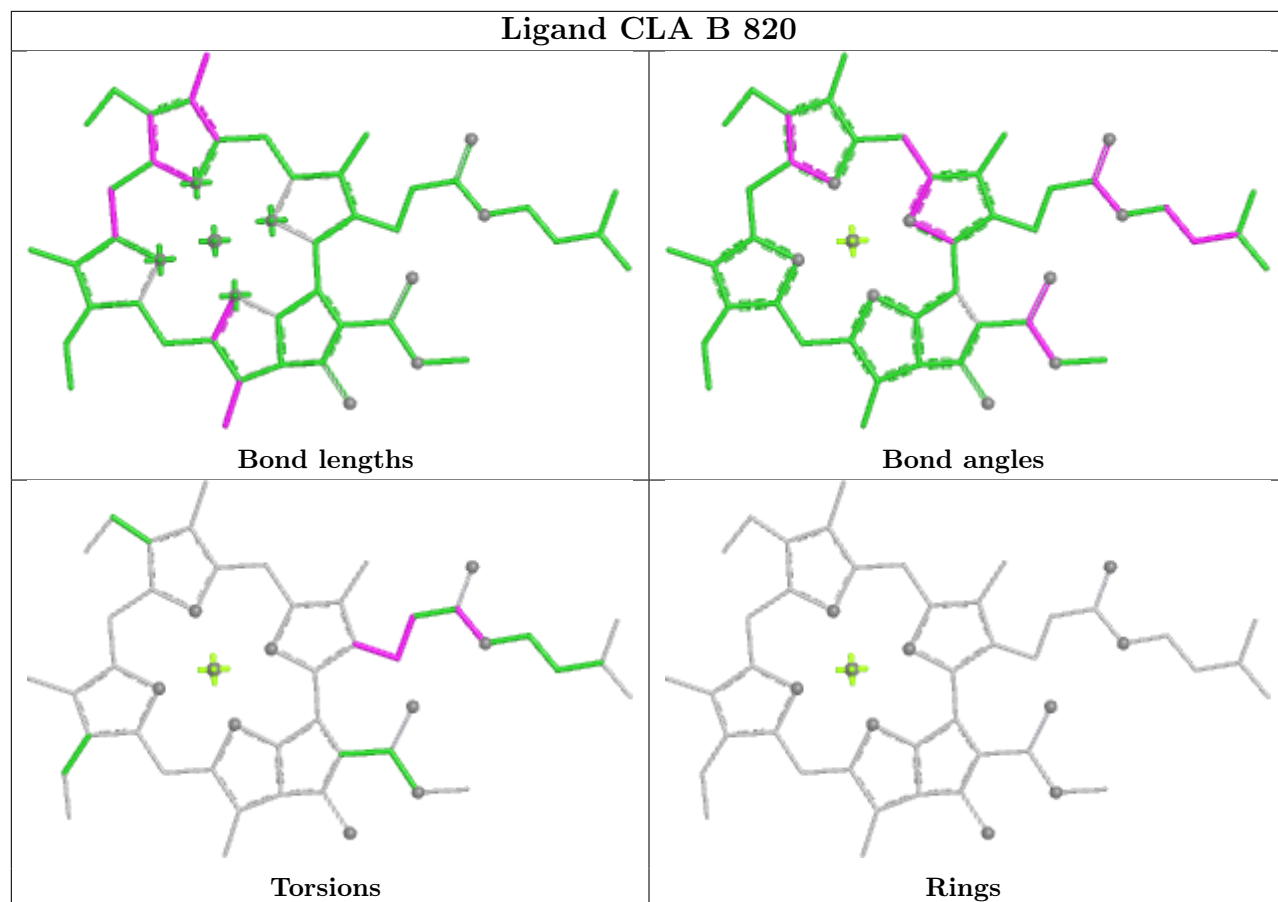


Torsions

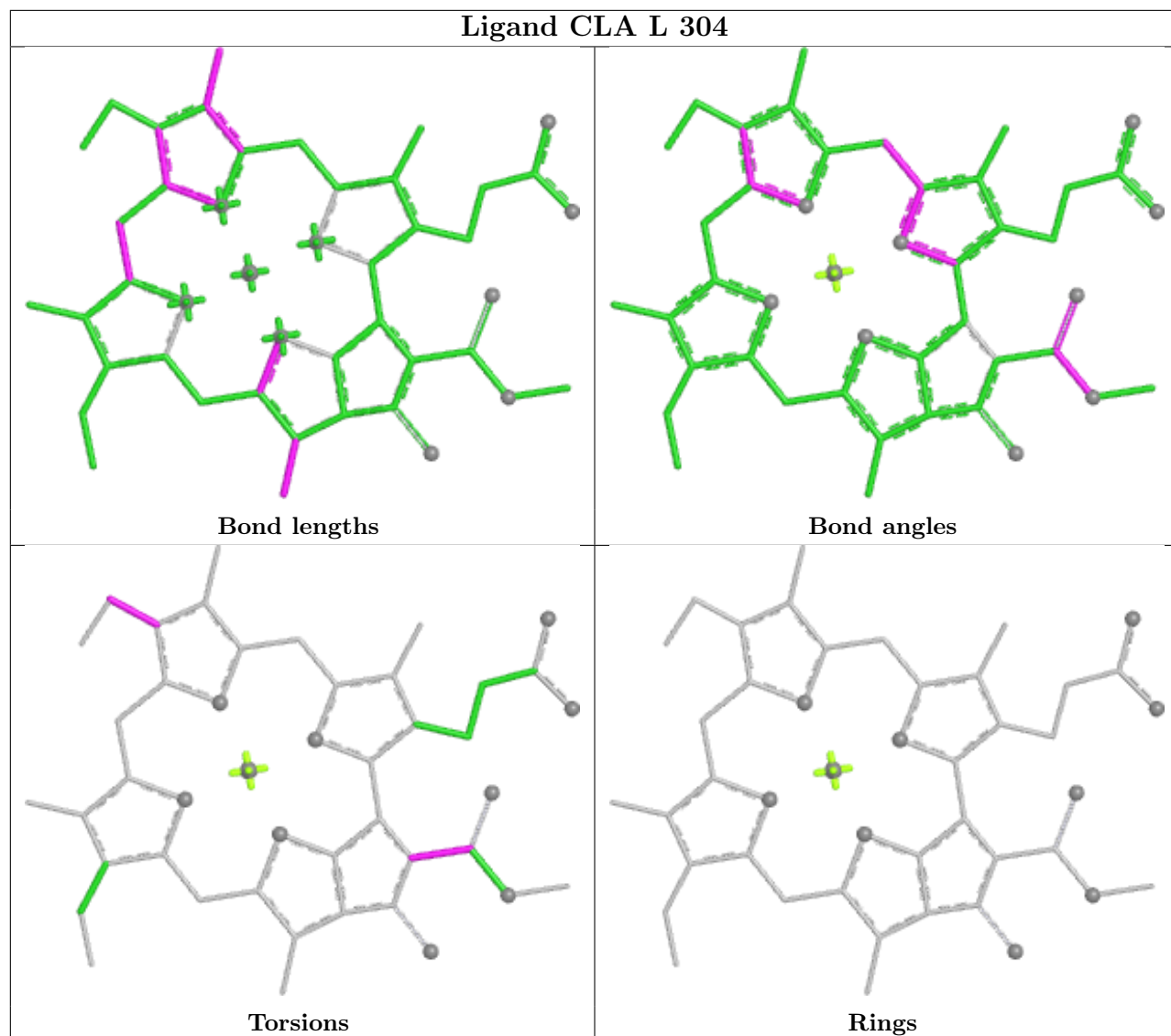


Rings

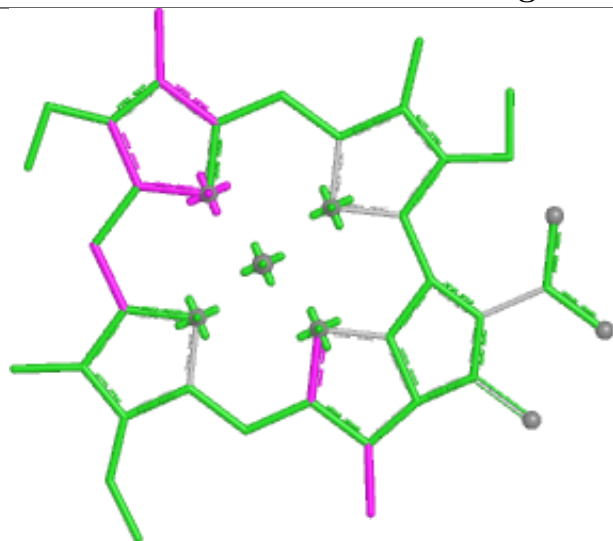




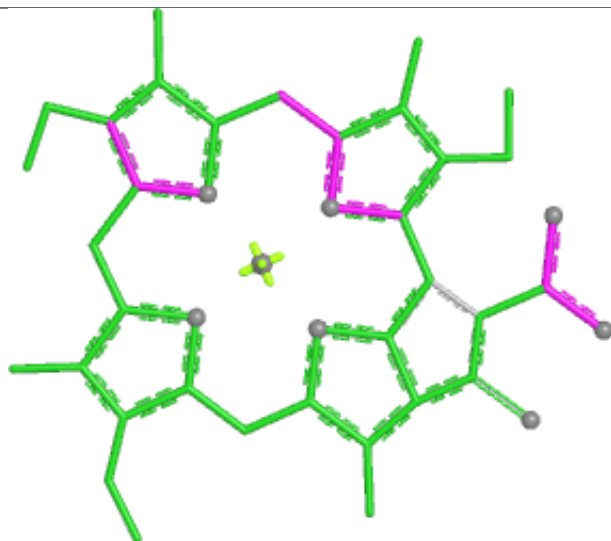
Ligand CLA L 304



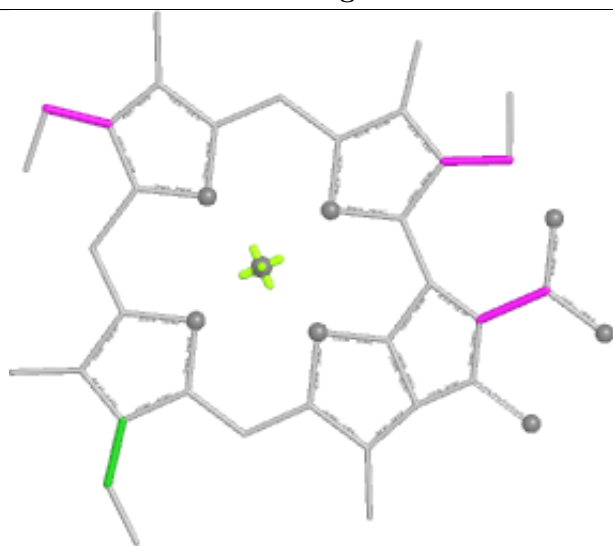
Ligand CLA 4 611



Bond lengths



Bond angles

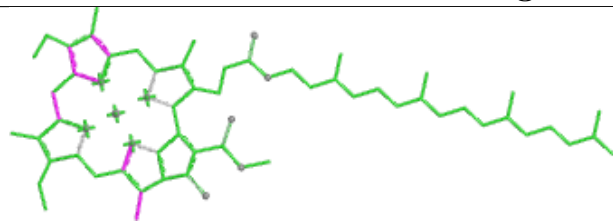


Torsions

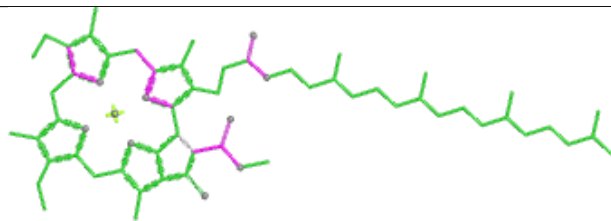


Rings

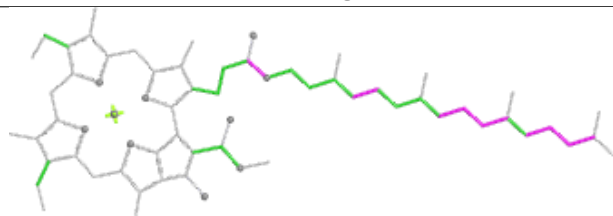
Ligand CLA L 303



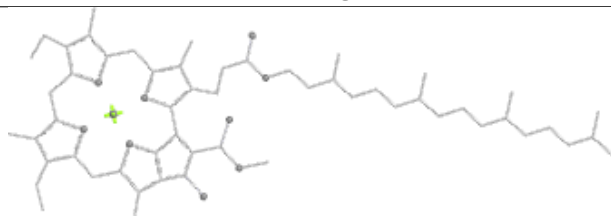
Bond lengths



Bond angles

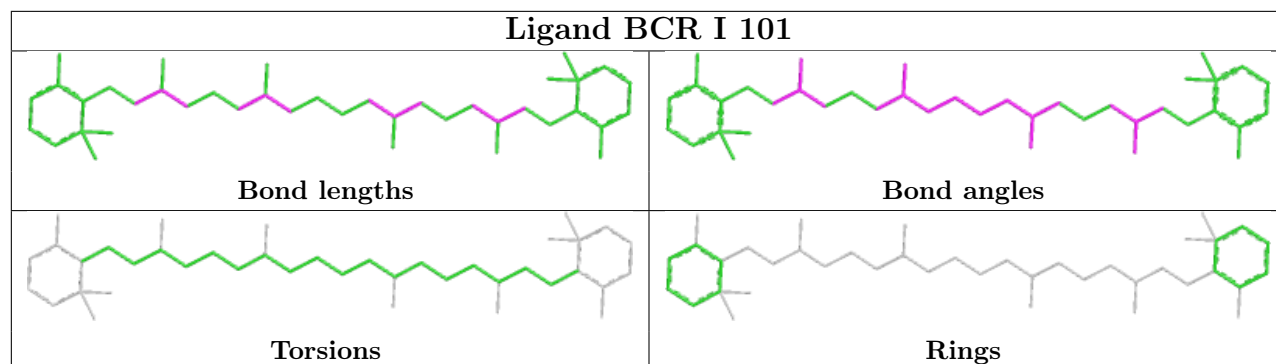


Torsions

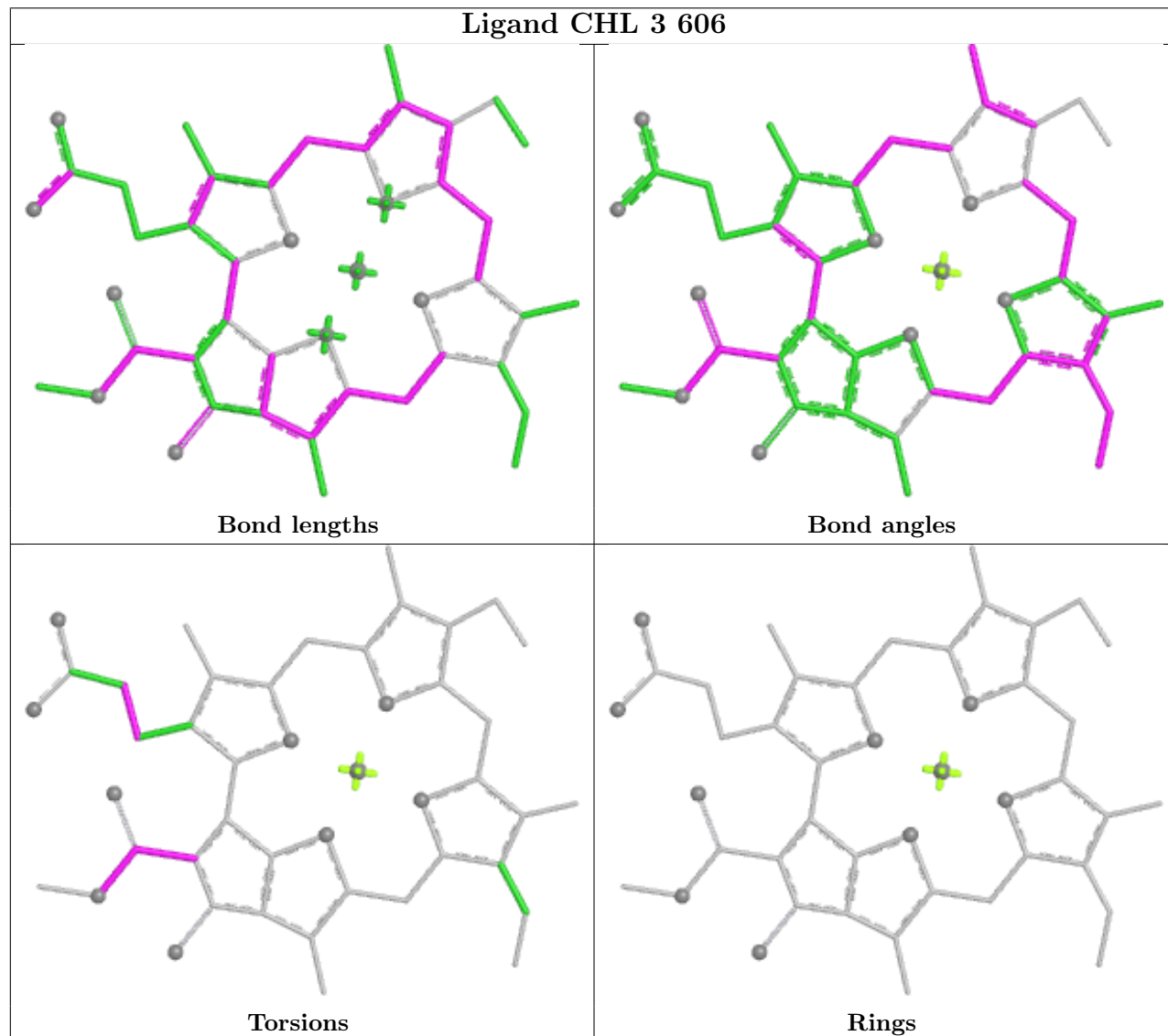


Rings

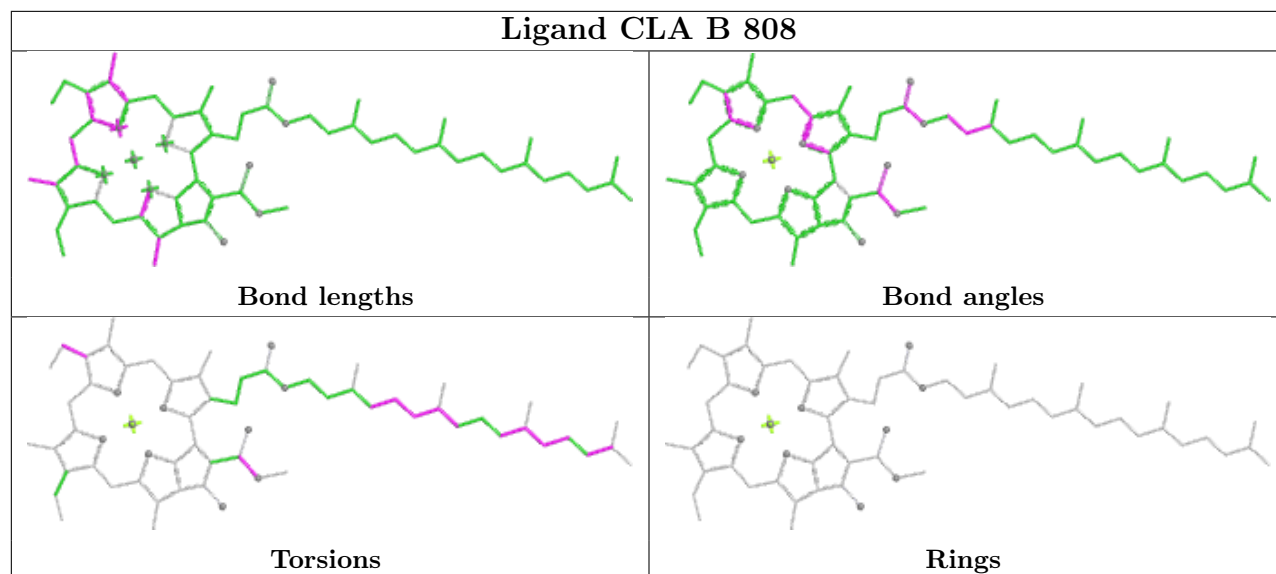
Ligand BCR I 101



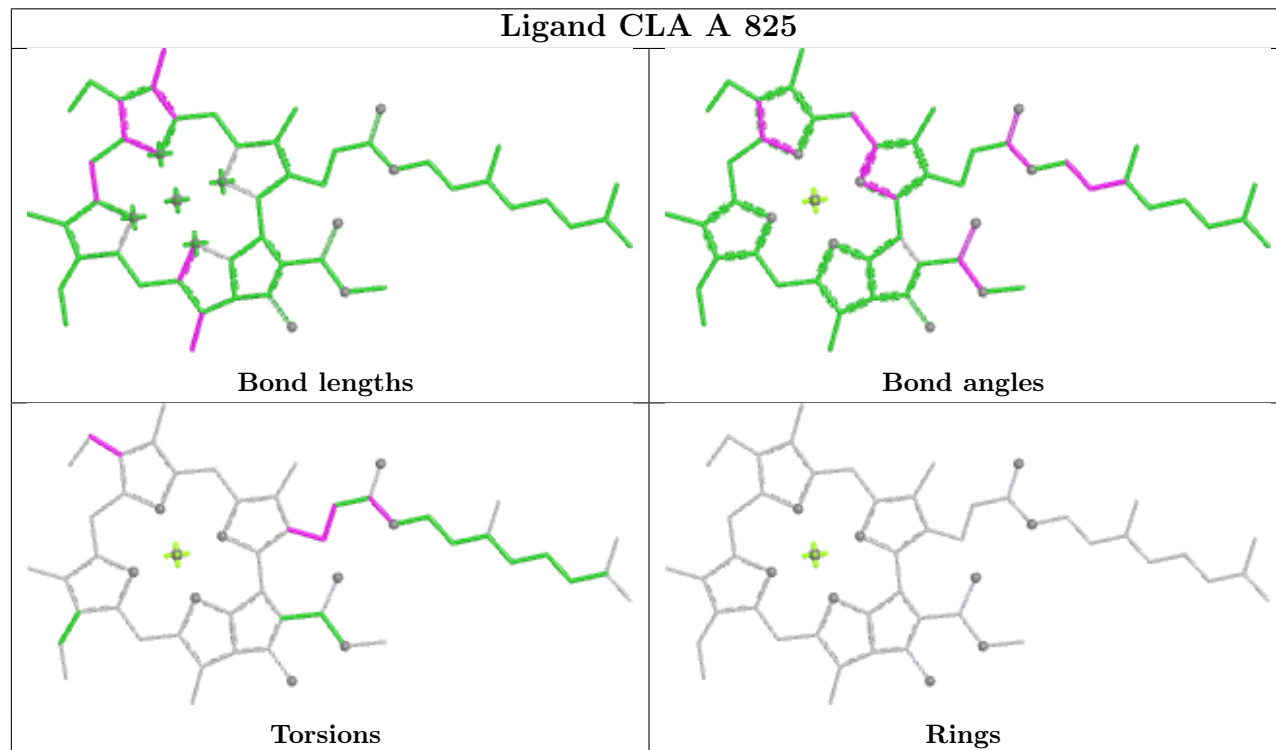
Ligand CHL 3 606



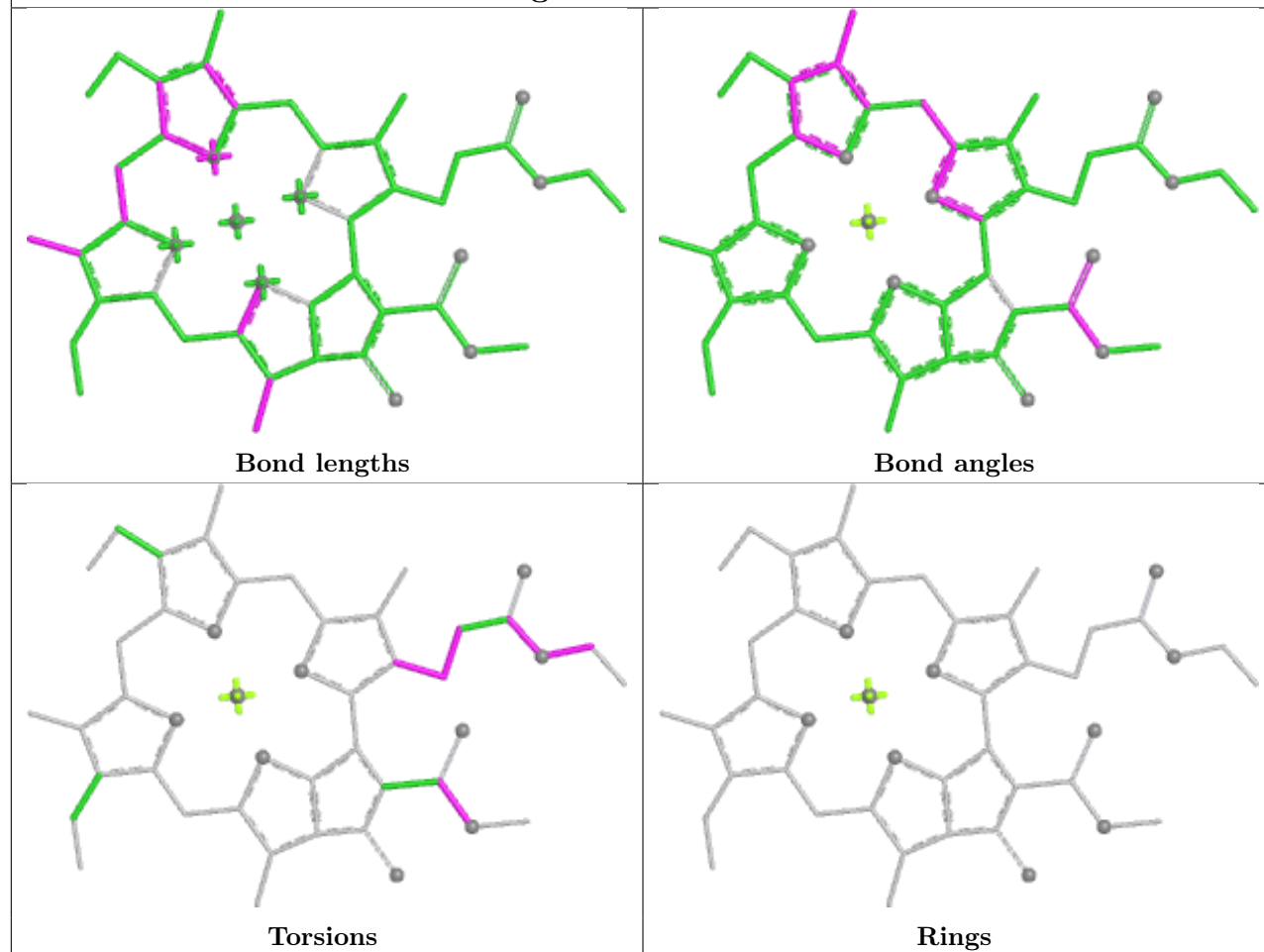
Ligand CLA B 808



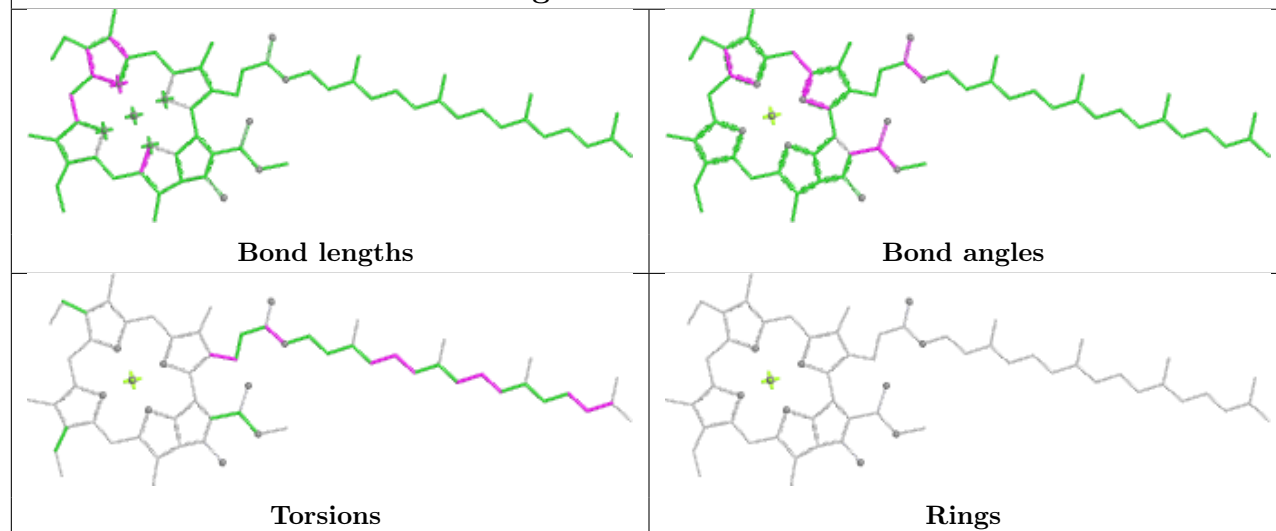
Ligand CLA A 825

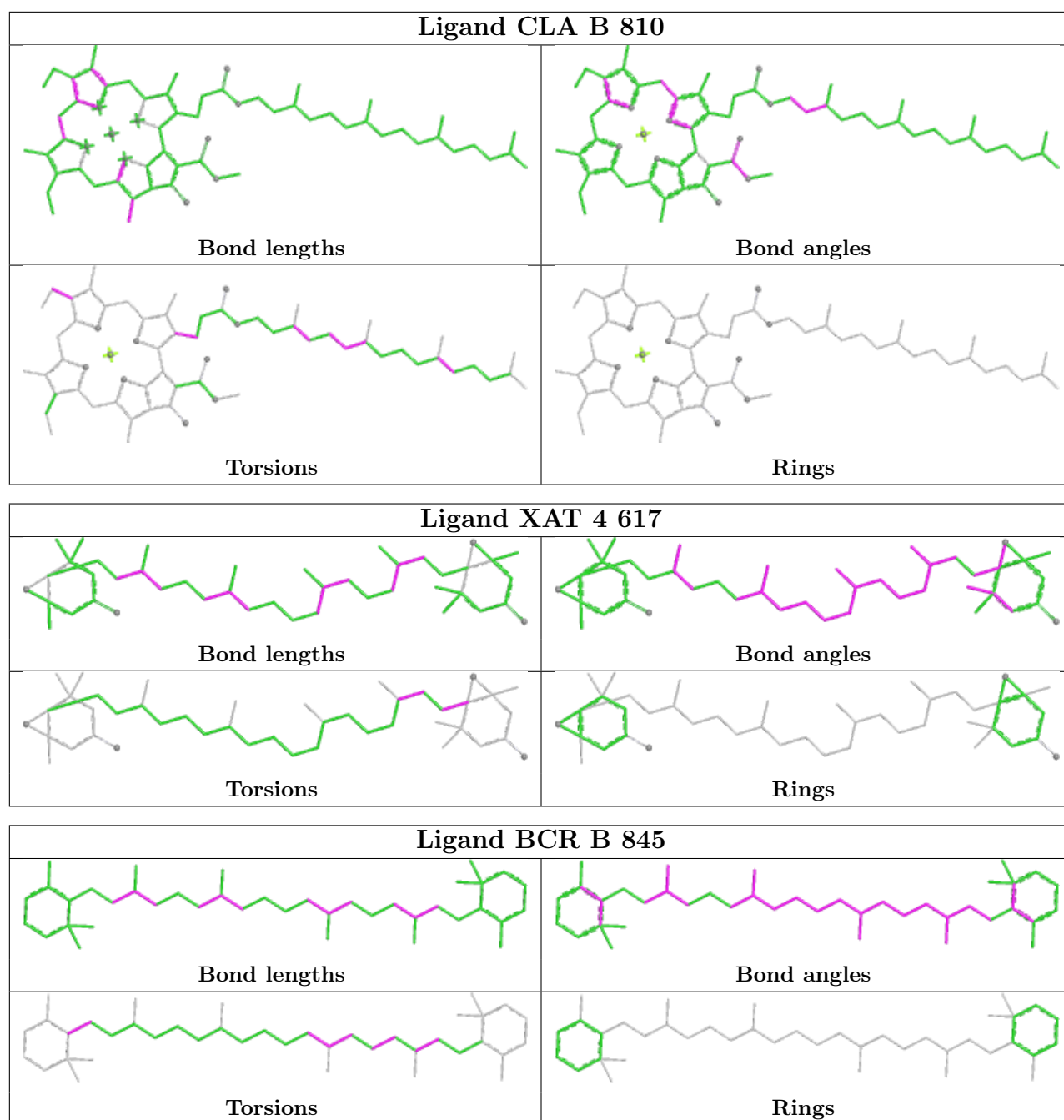


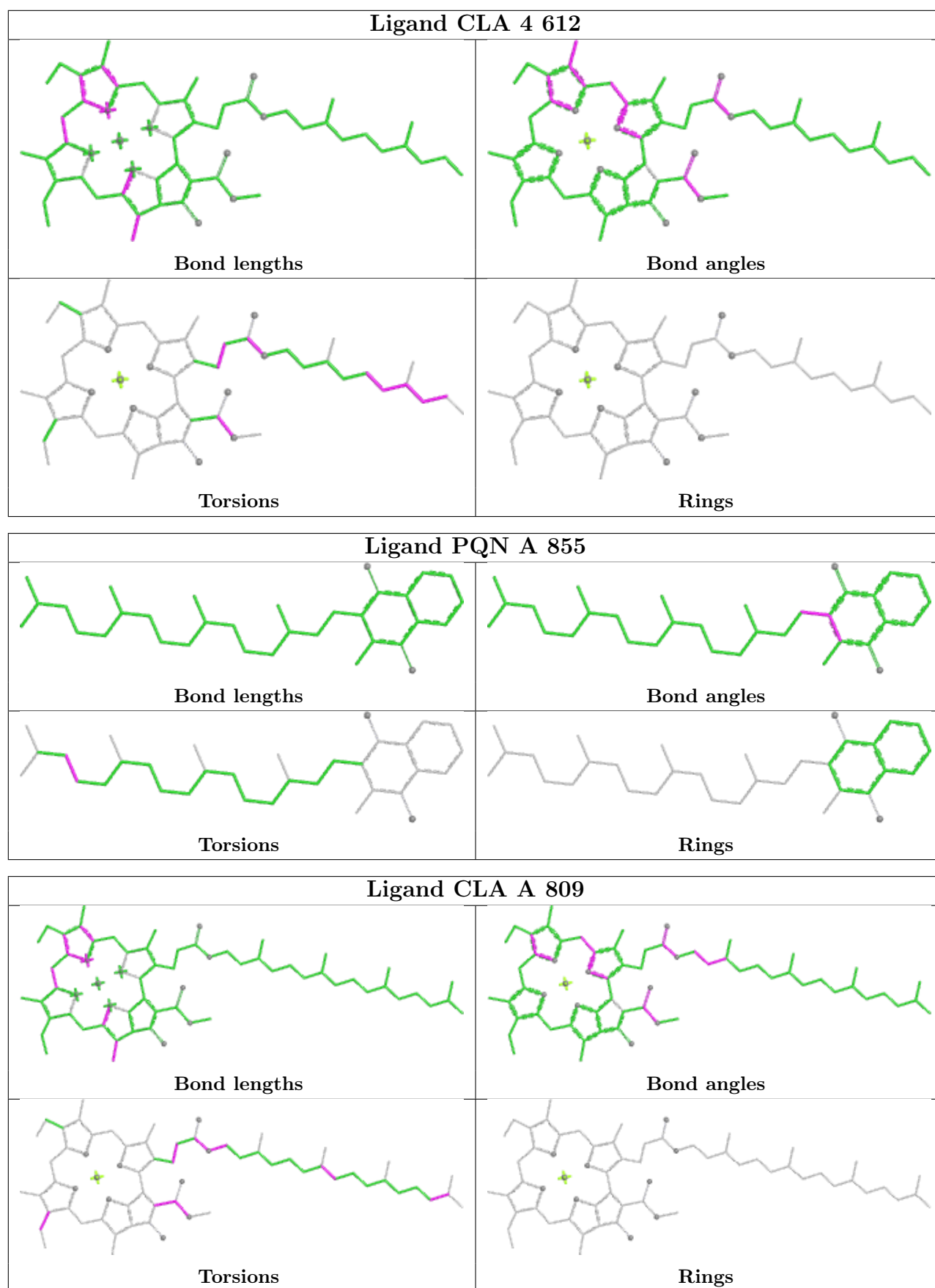
Ligand CLA 2 609

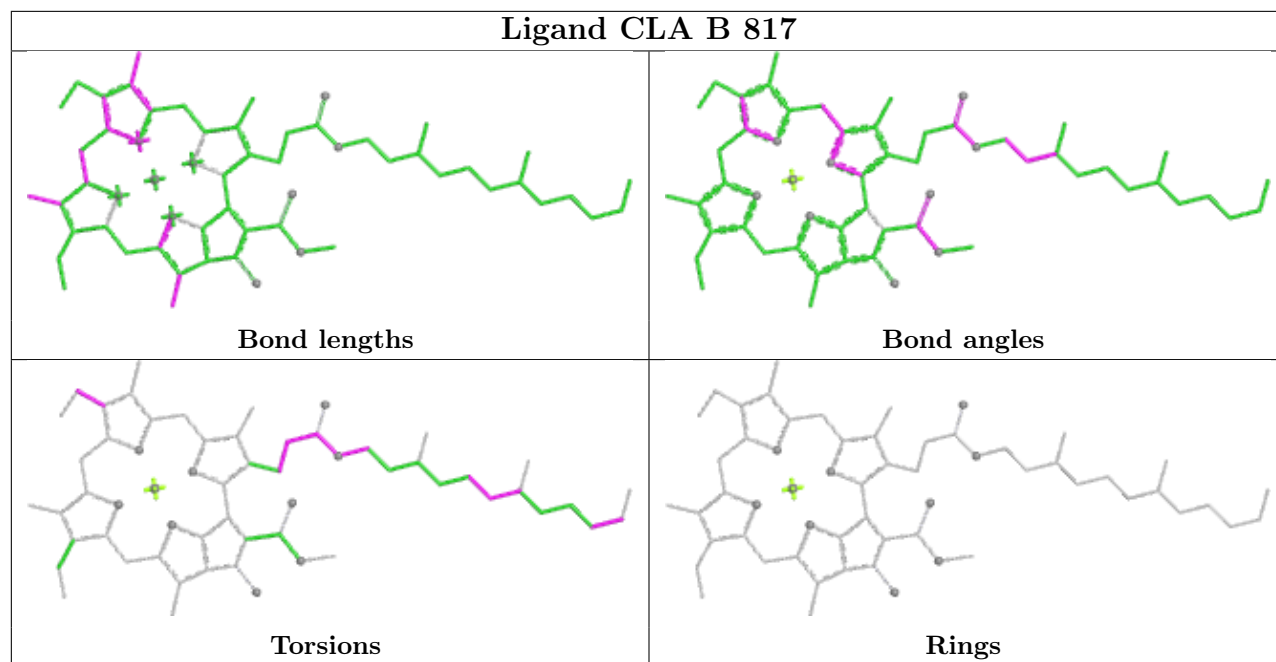


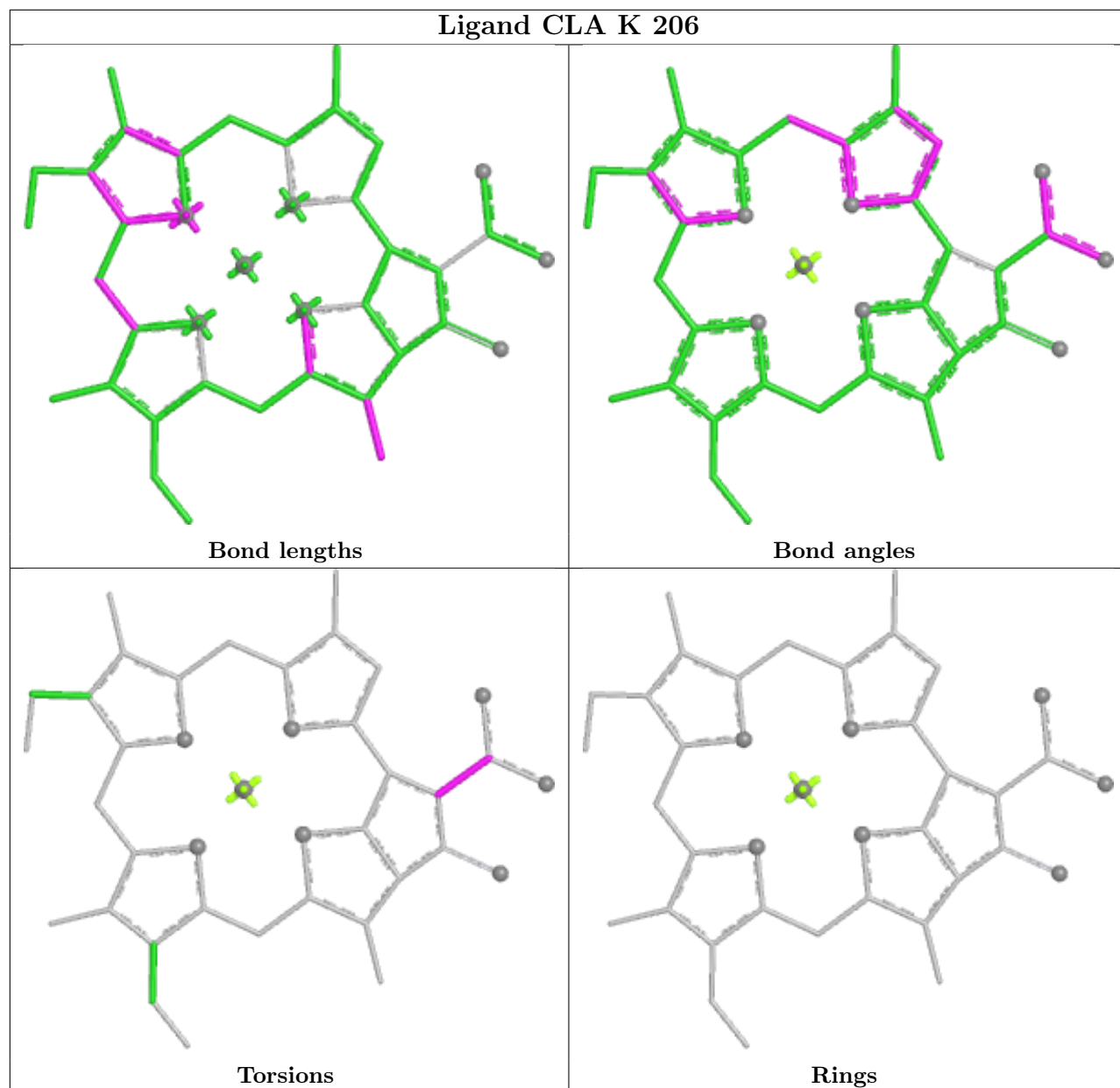
Ligand CLA B 837

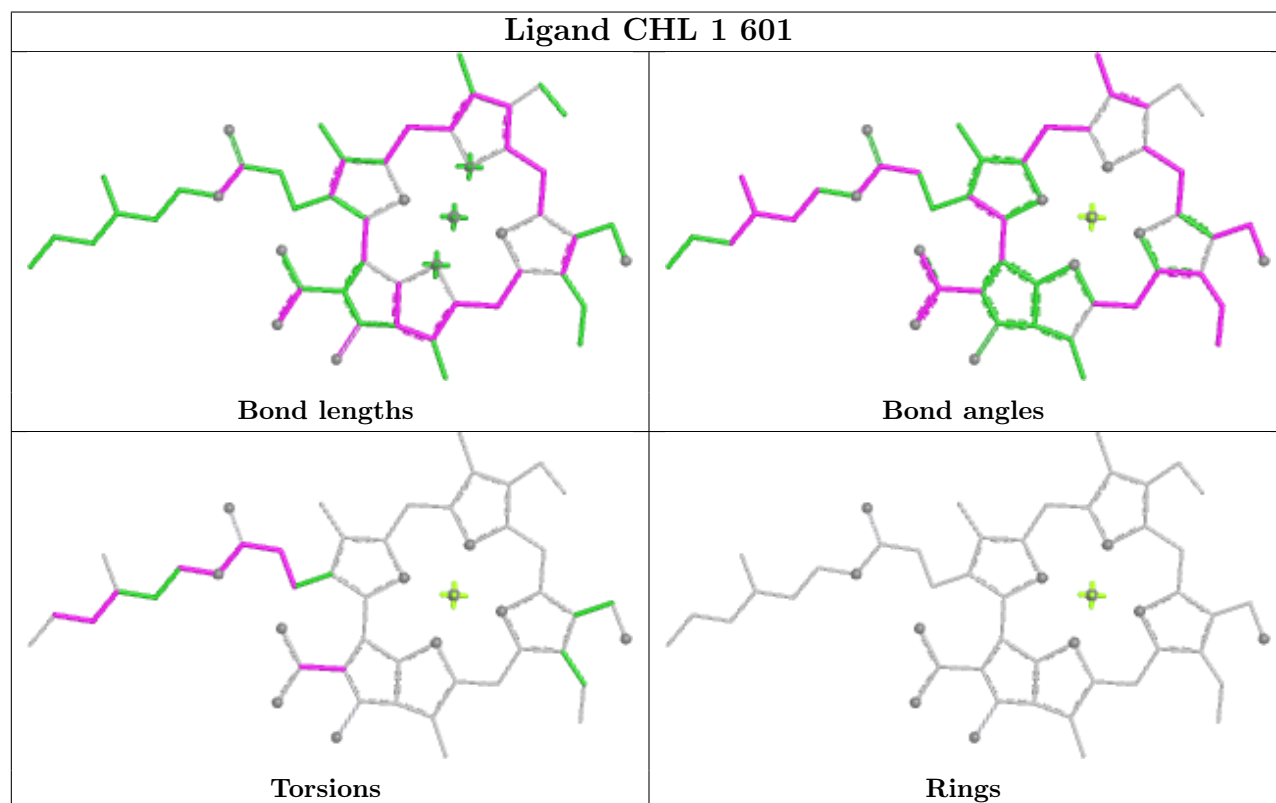
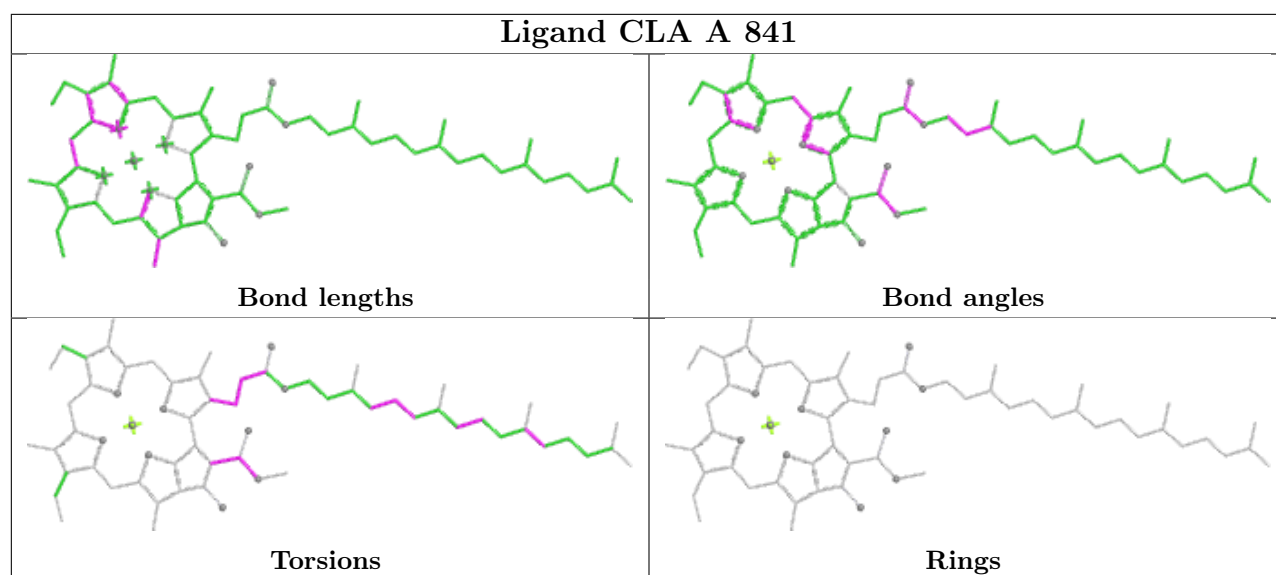


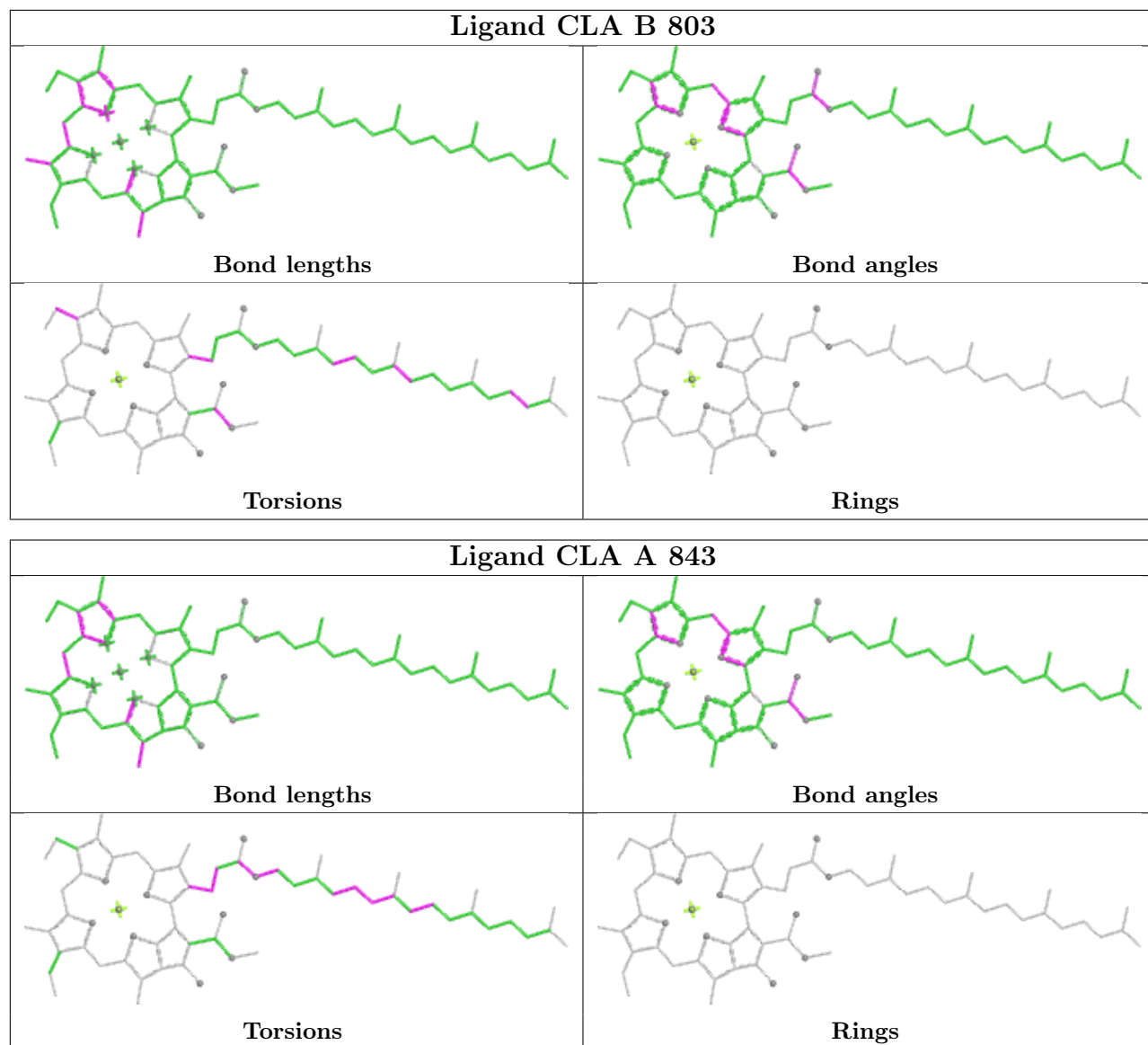




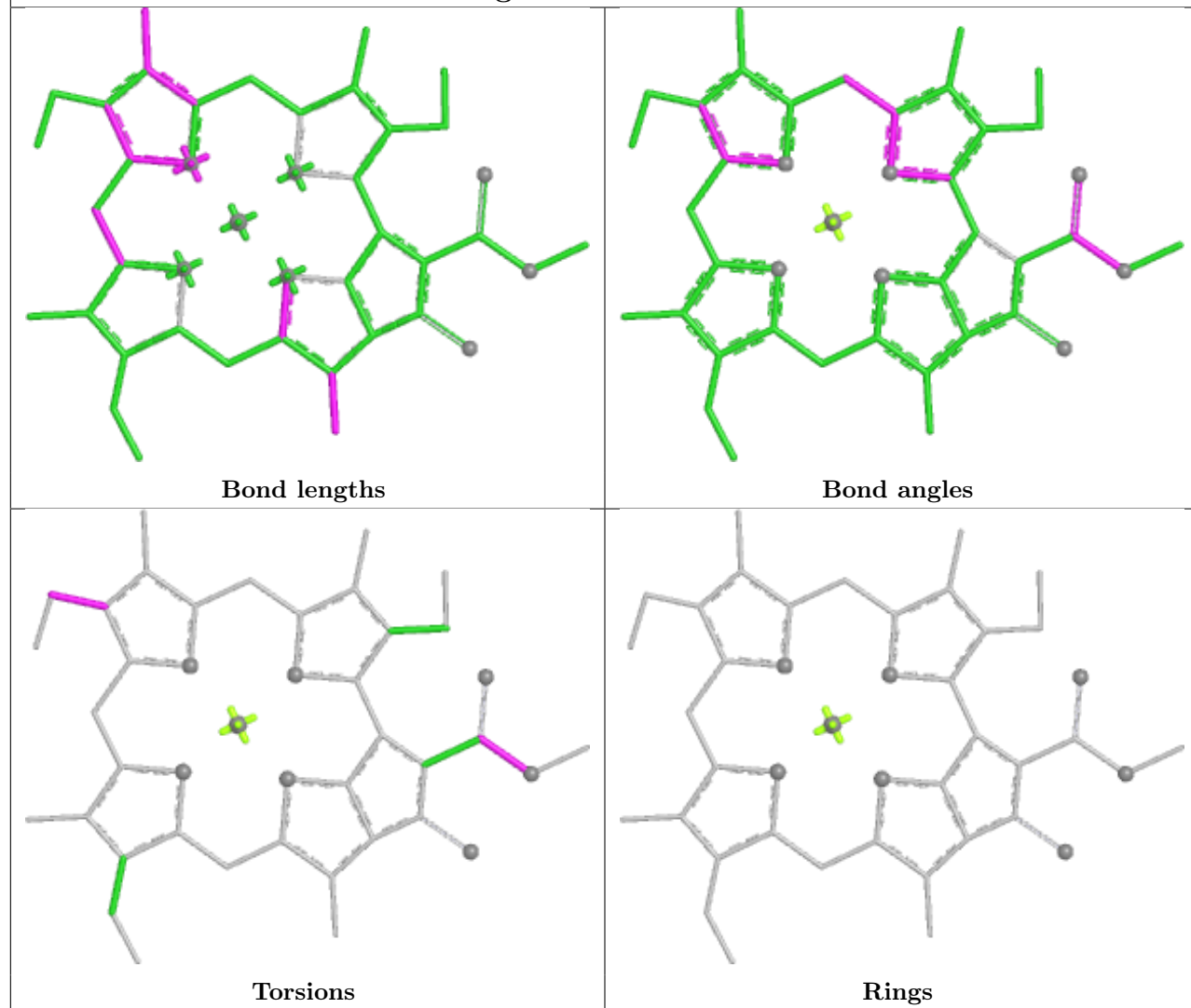




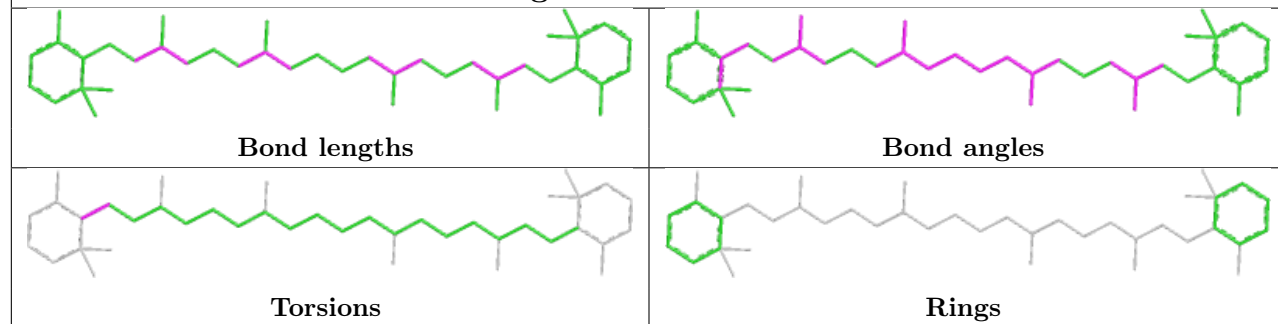




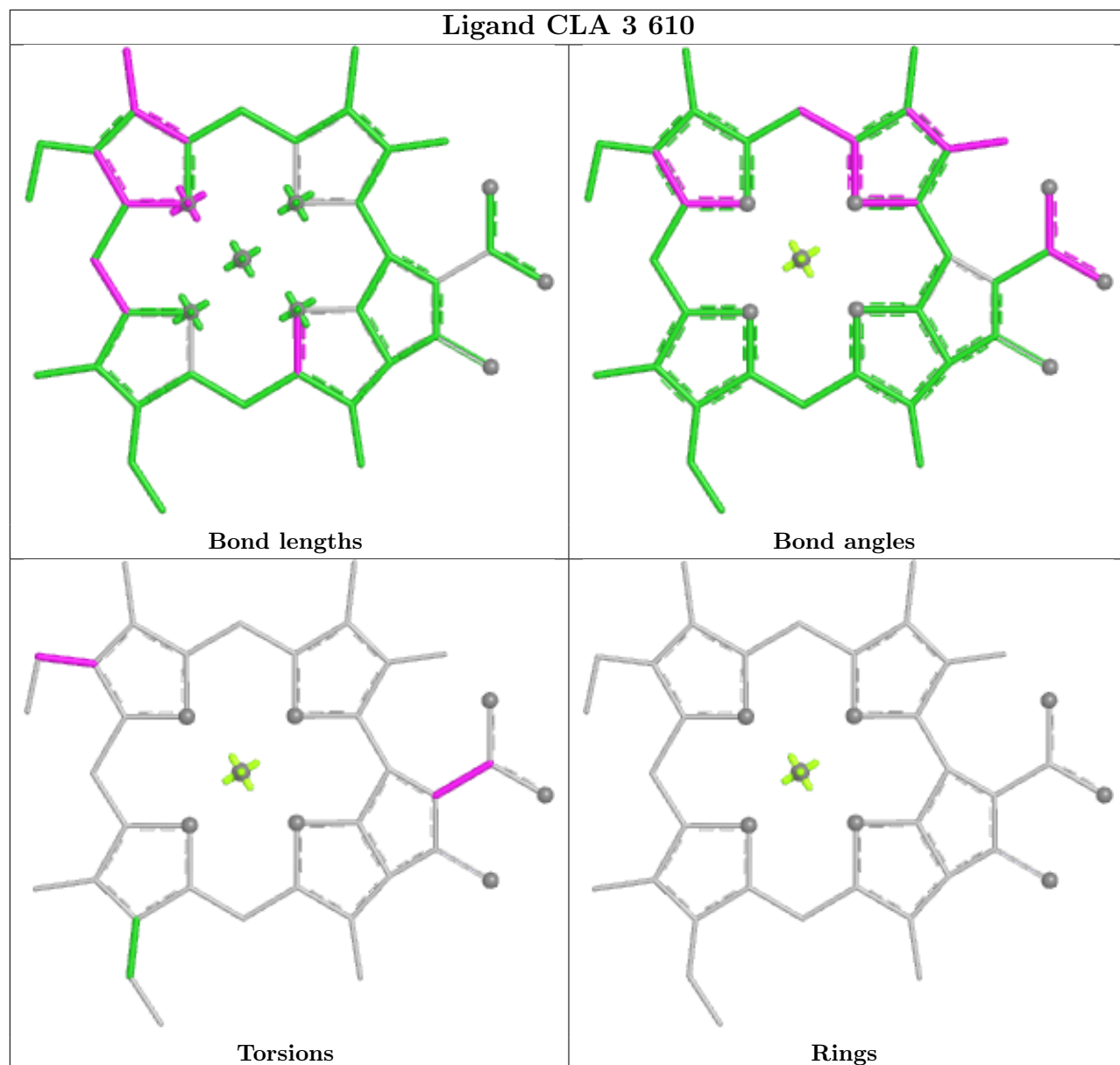
Ligand CLA A 816



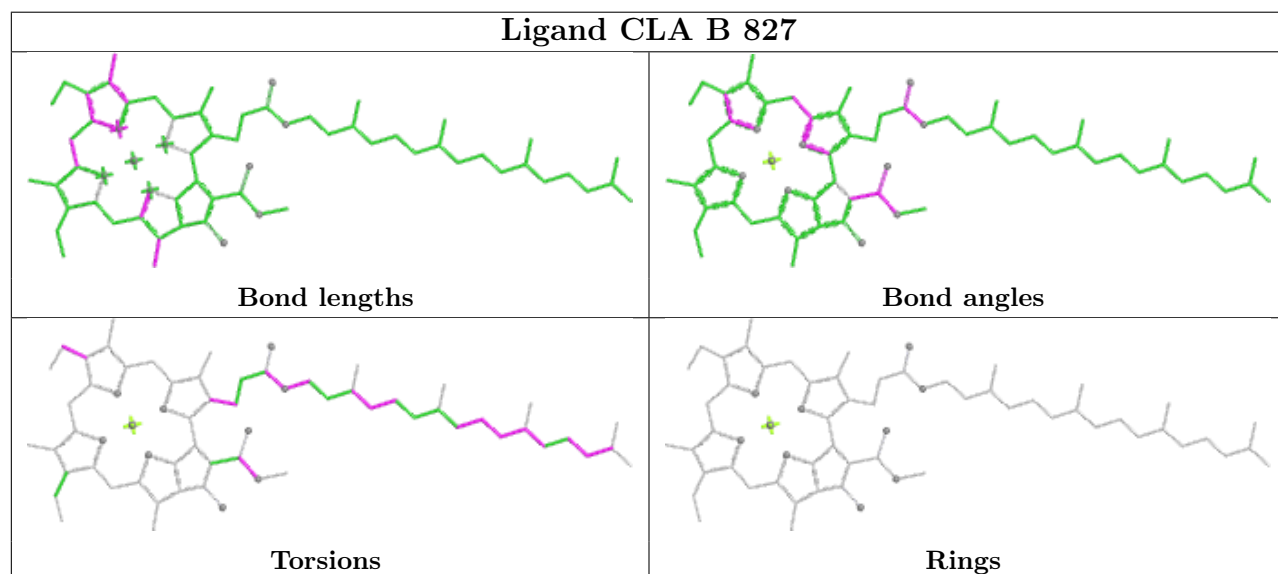
Ligand BCR B 847



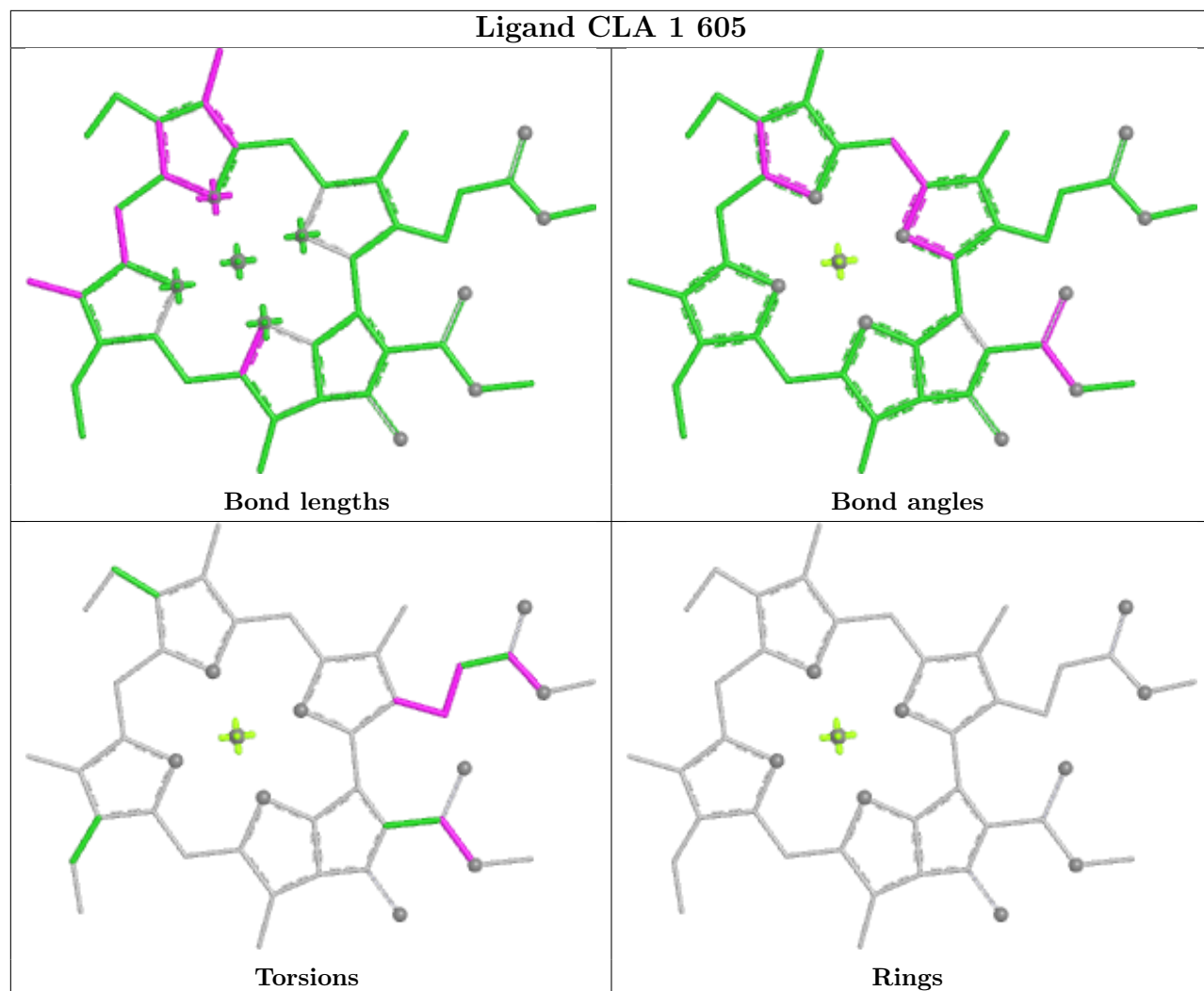
Ligand CLA 3 610

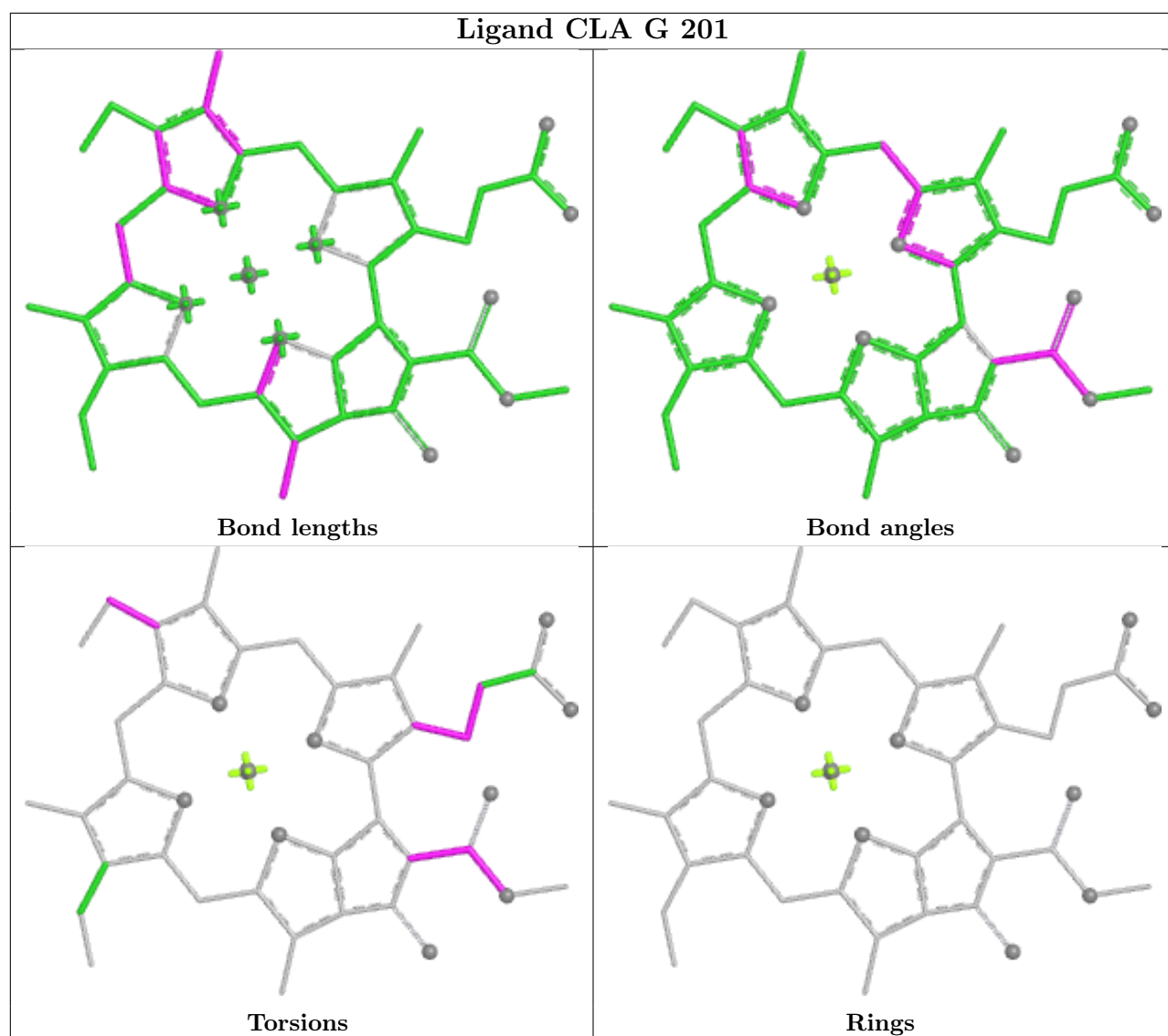


Ligand CLA B 827

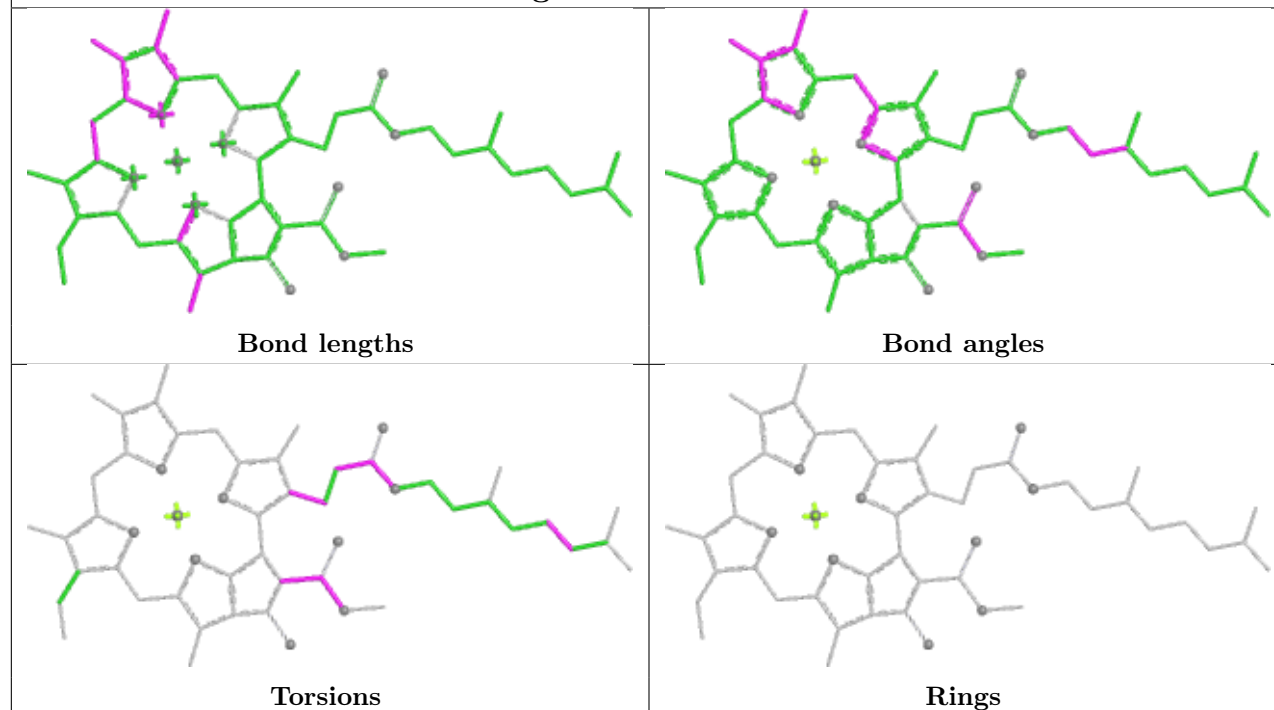


Ligand CLA 1 605

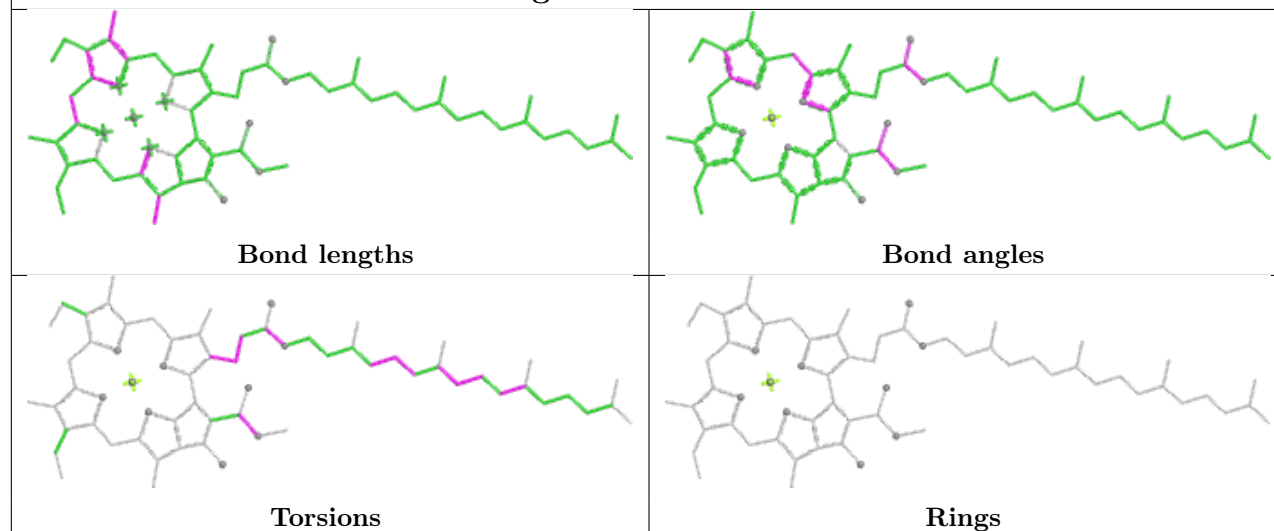




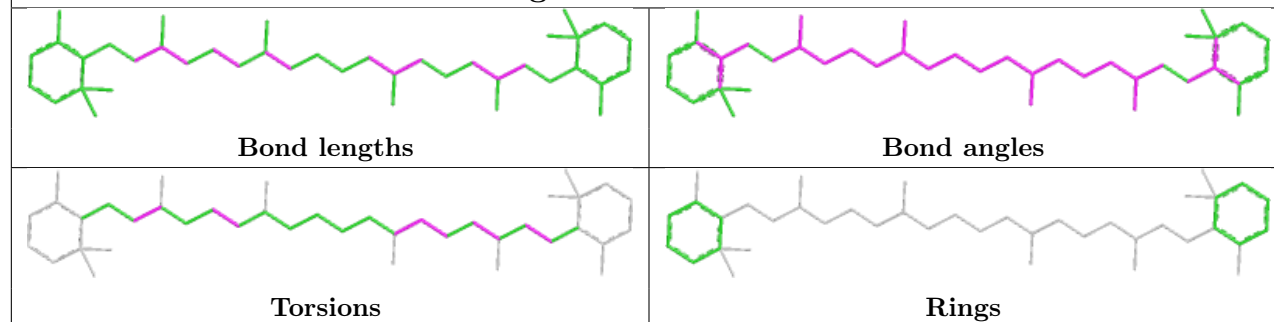
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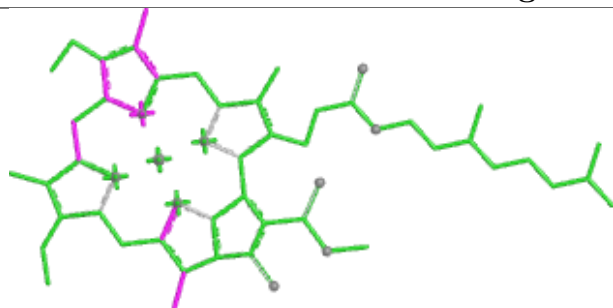


Ligand CLA B 802

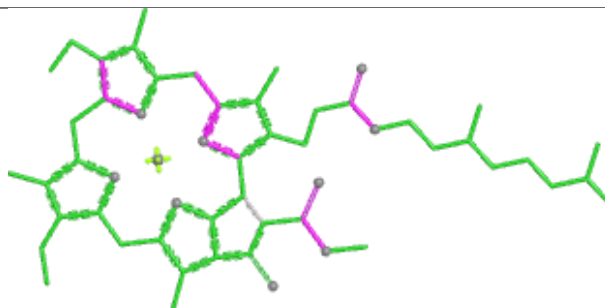


Ligand BCR K 205

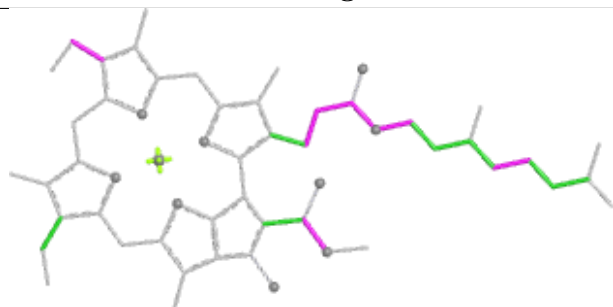


Ligand CLA 3 602

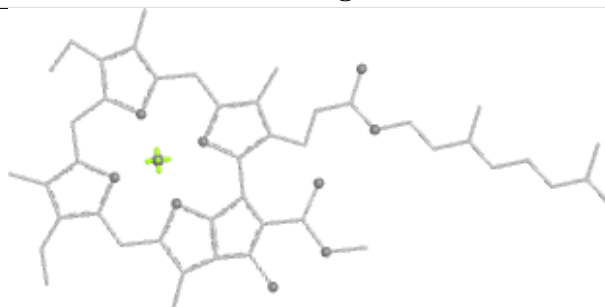
Bond lengths



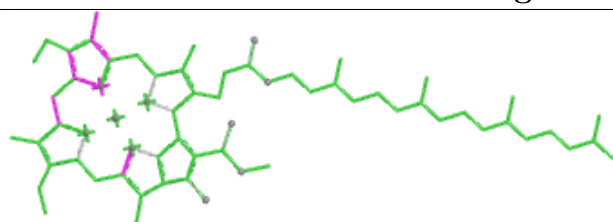
Bond angles



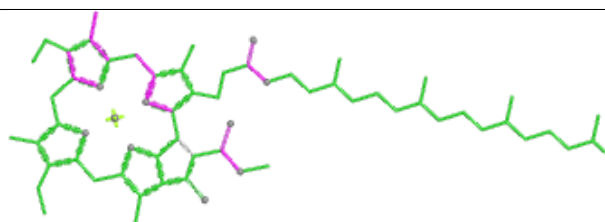
Torsions



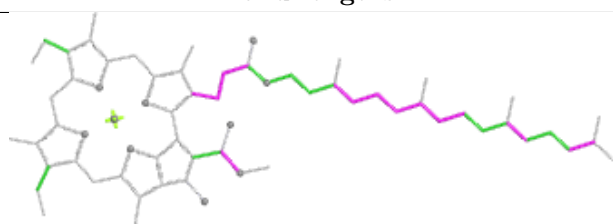
Rings

Ligand CLA B 809

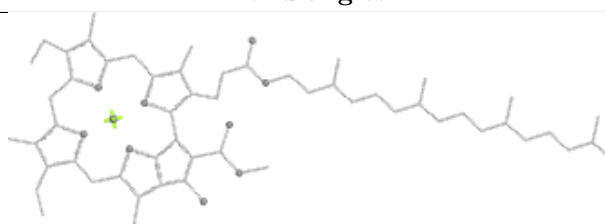
Bond lengths



Bond angles

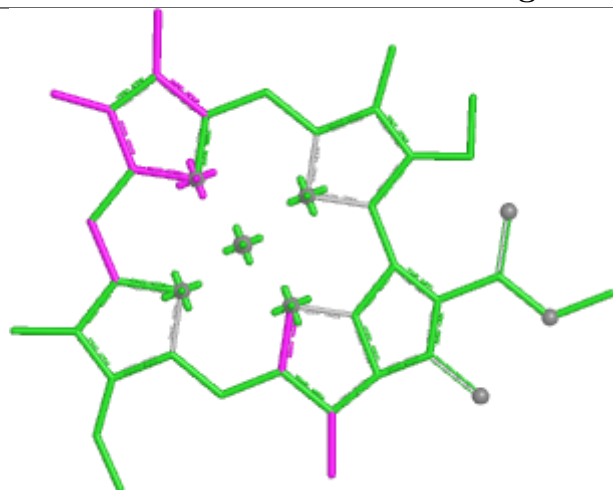


Torsions



Rings

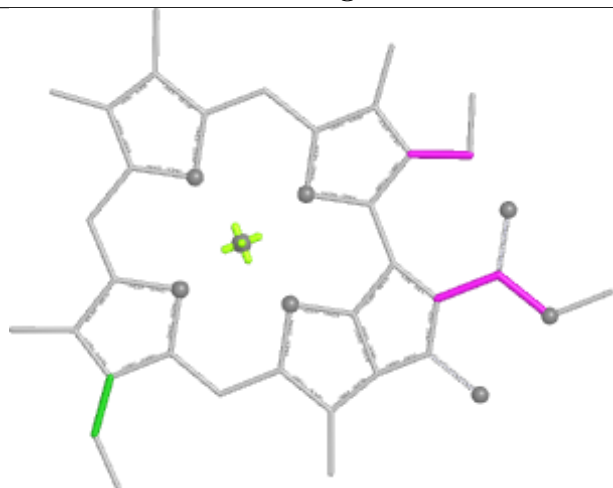
Ligand CLA 3 605



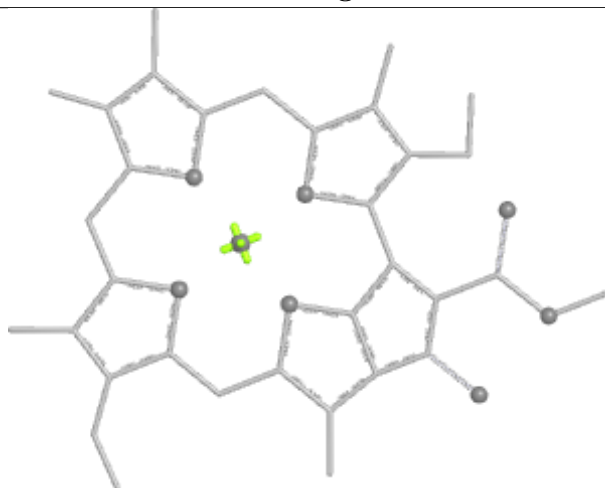
Bond lengths



Bond angles

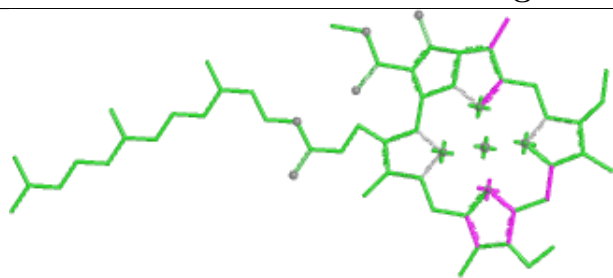


Torsions

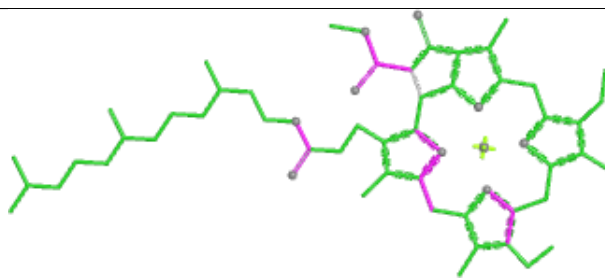


Rings

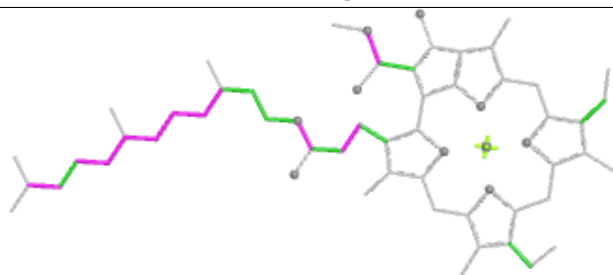
Ligand CLA A 818



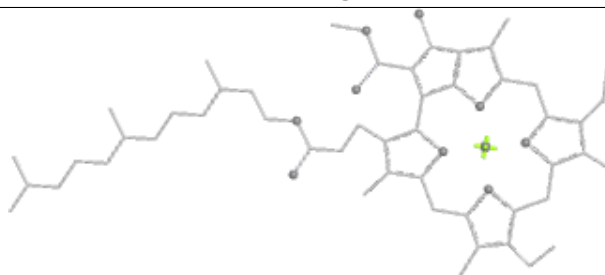
Bond lengths



Bond angles

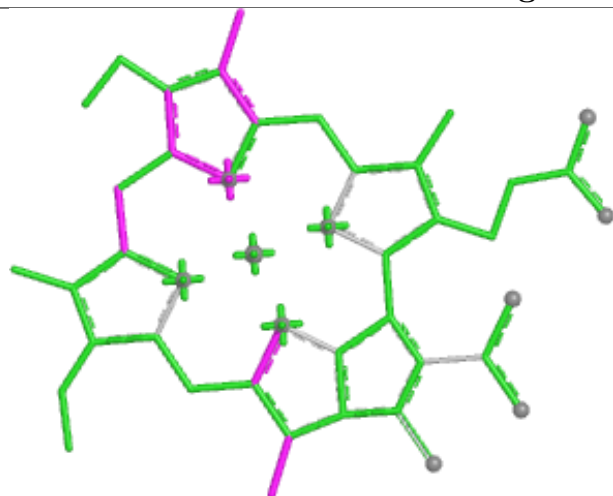


Torsions

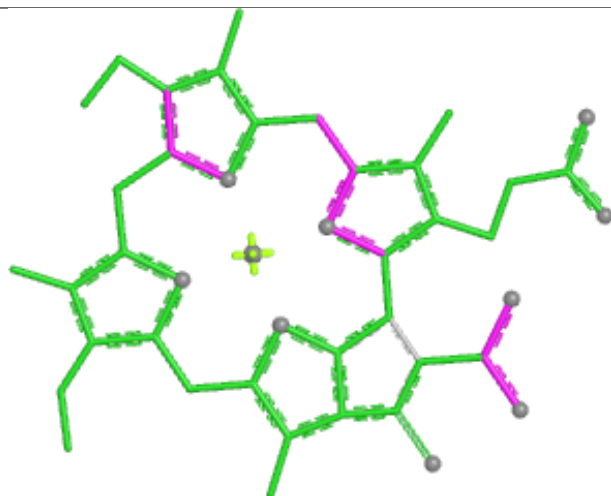


Rings

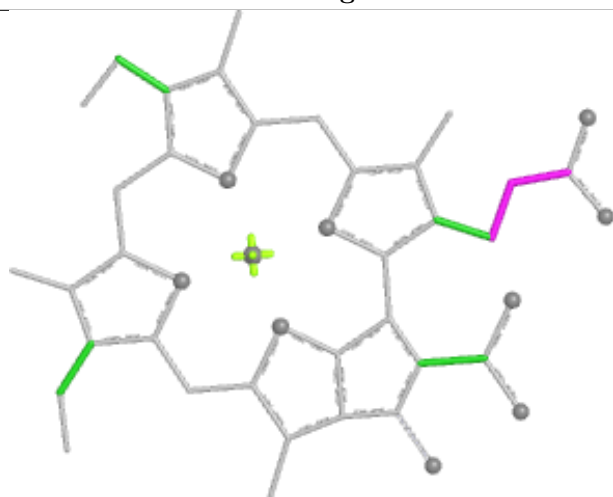
Ligand CLA 2 603



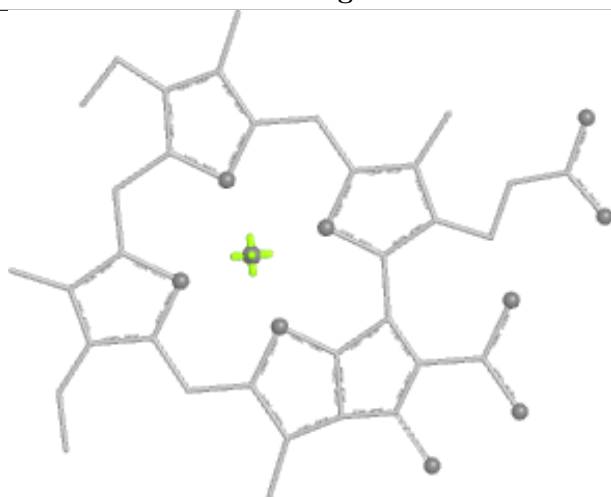
Bond lengths



Bond angles

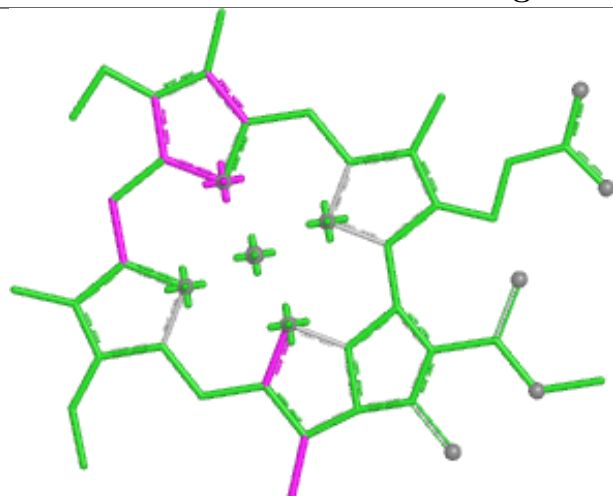


Torsions

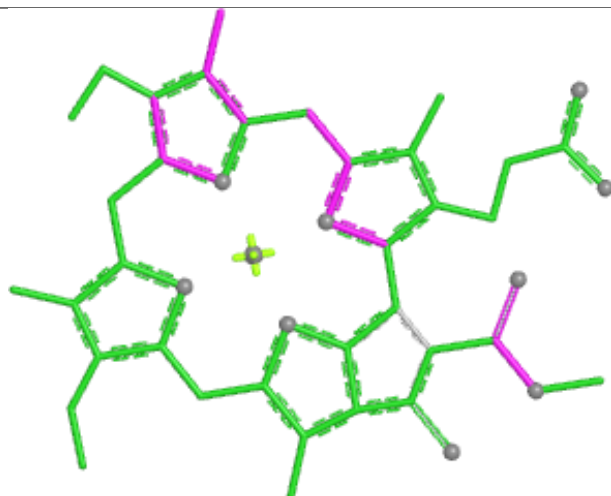


Rings

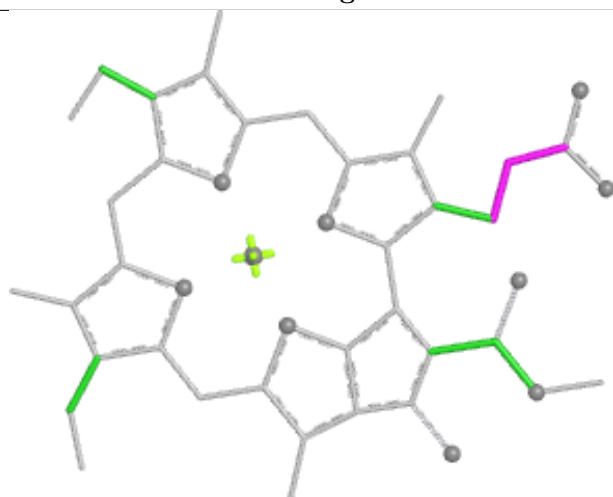
Ligand CLA G 203



Bond lengths



Bond angles

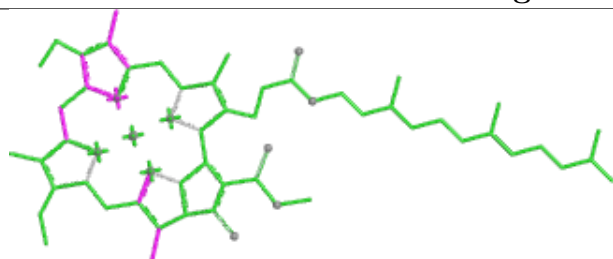


Torsions

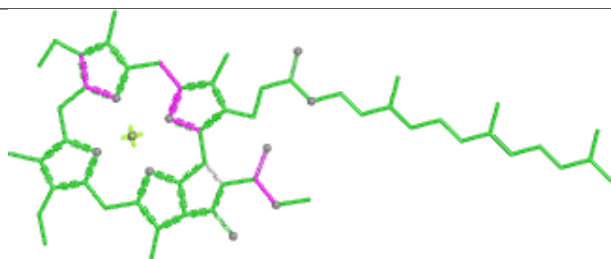


Rings

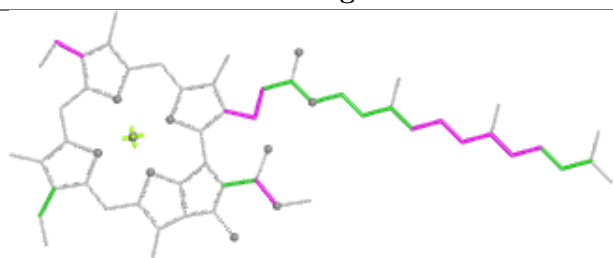
Ligand CLA H 201



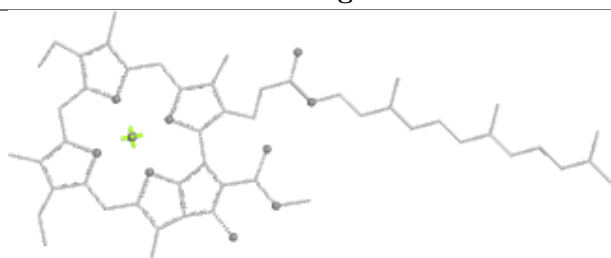
Bond lengths



Bond angles

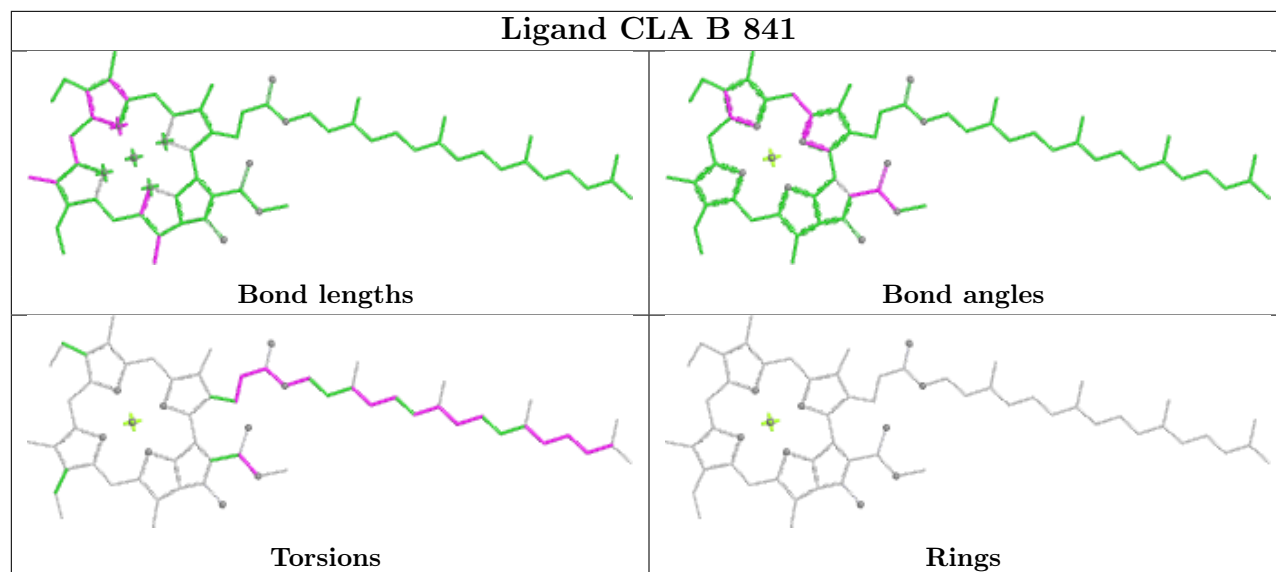


Torsions

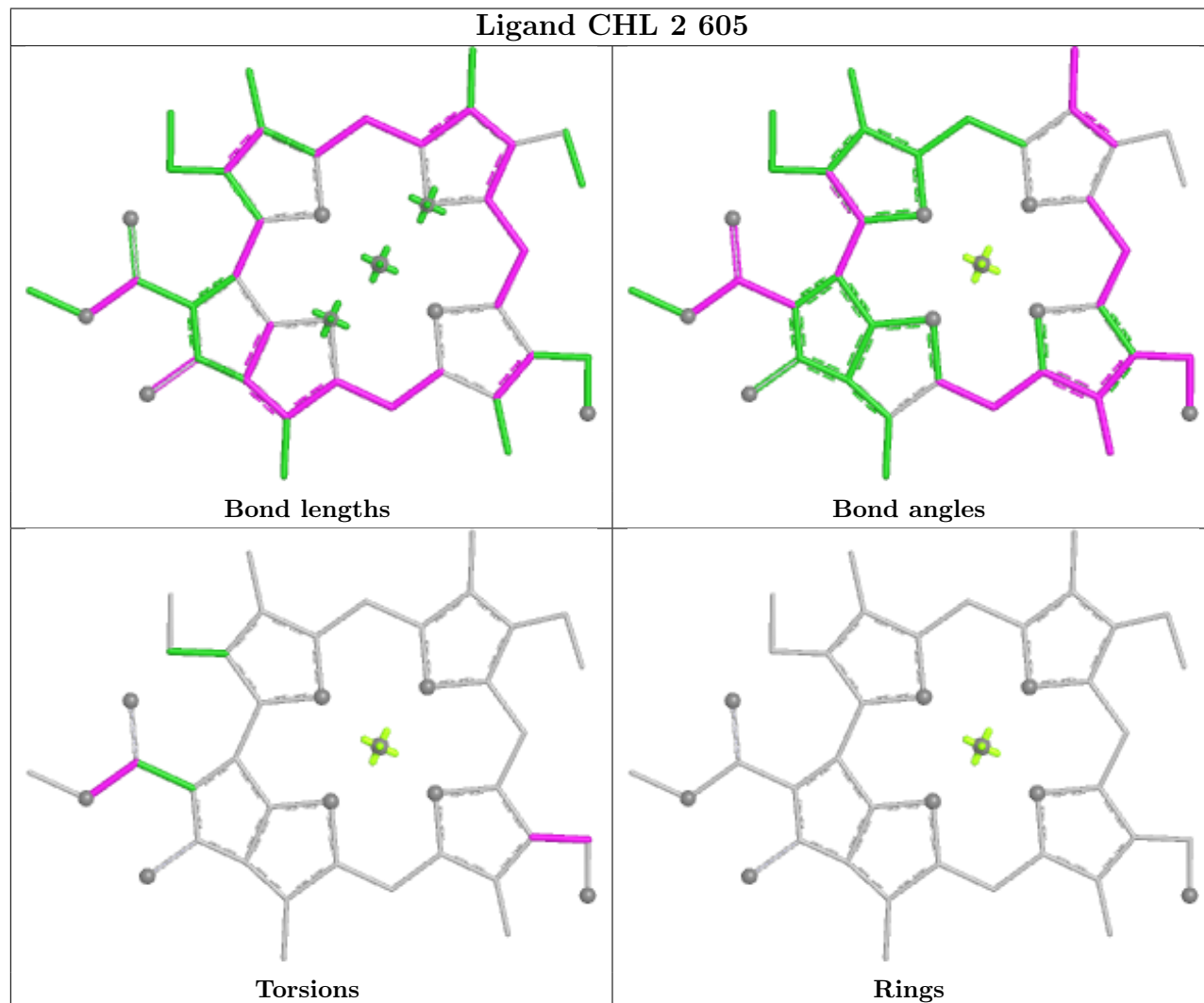


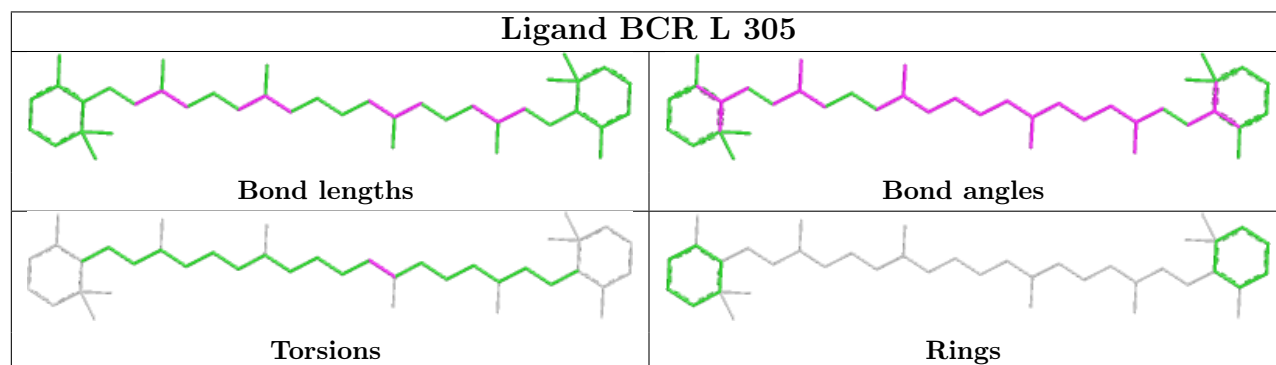
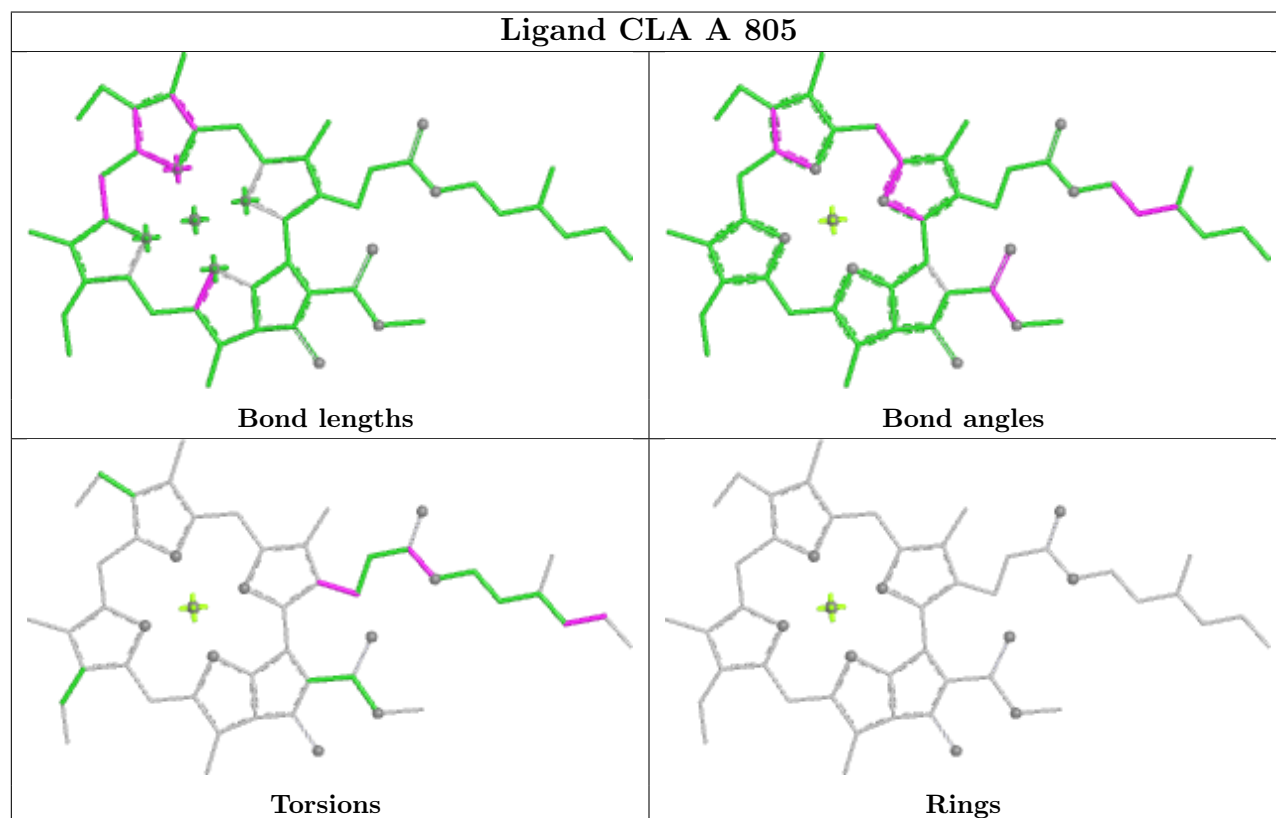
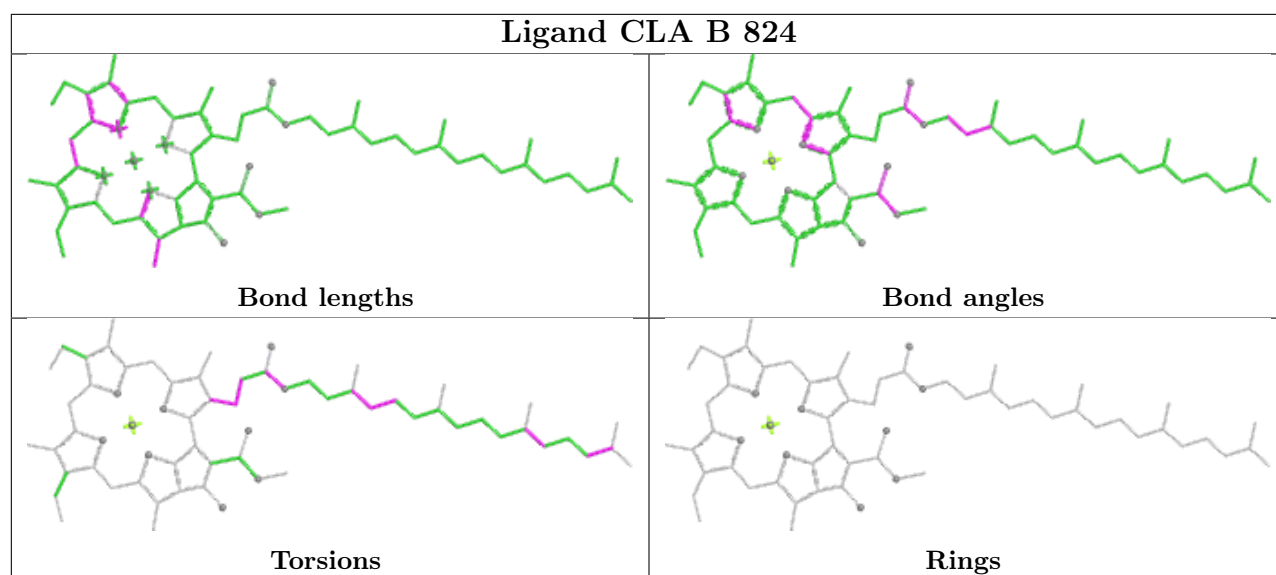
Rings

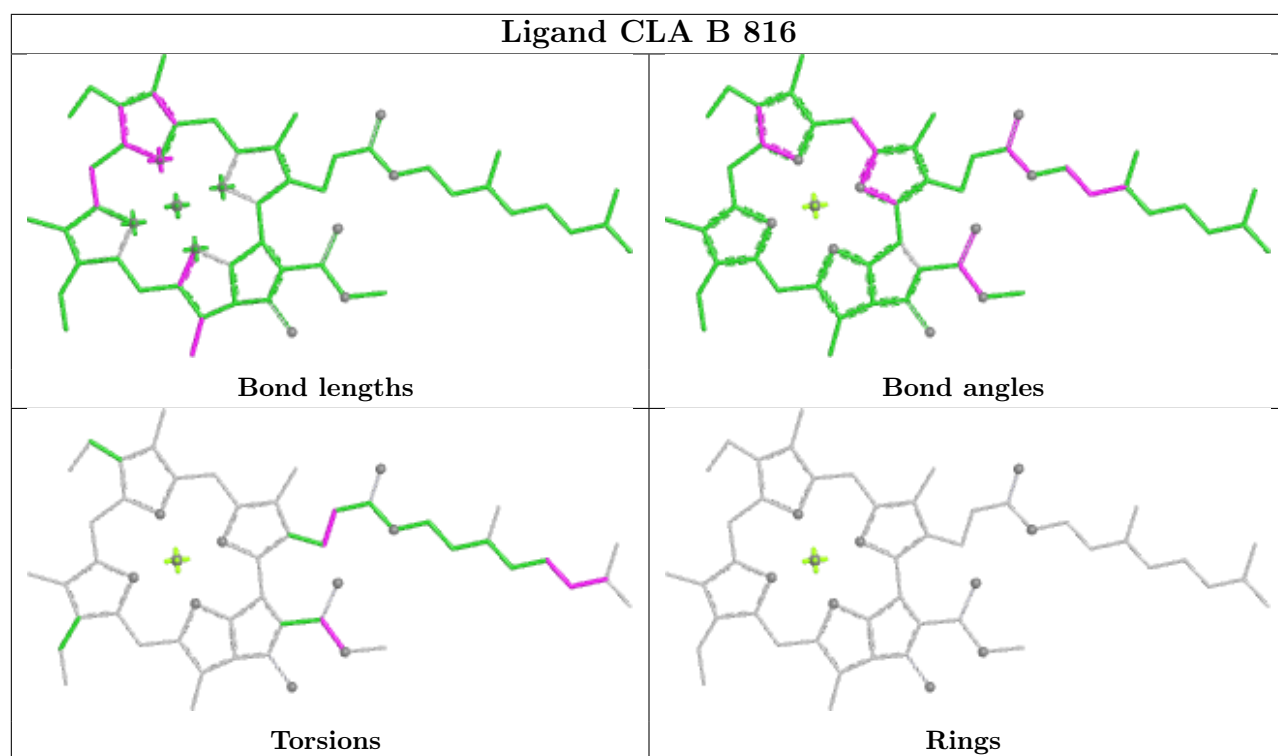
Ligand CLA B 841



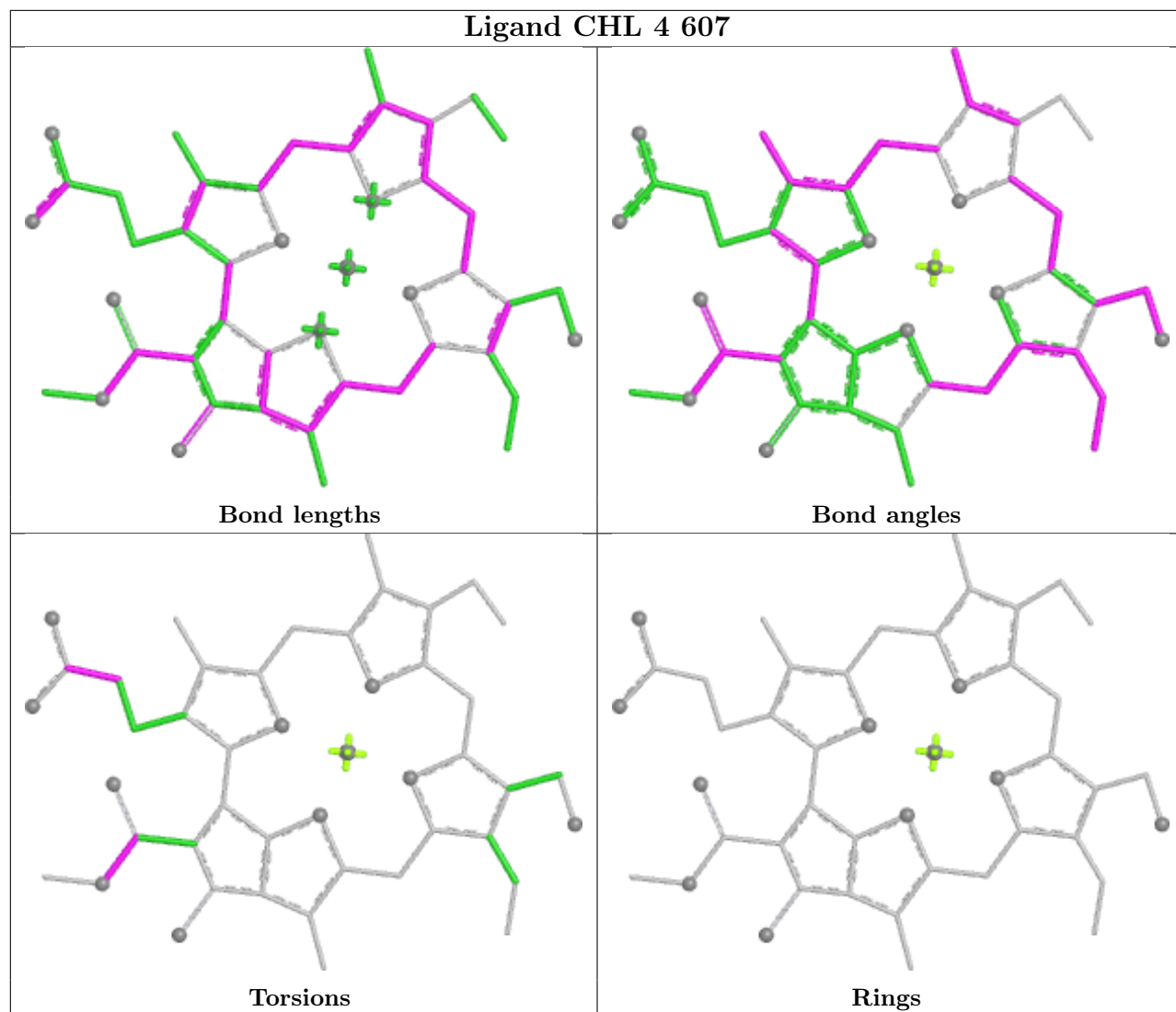
Ligand CHL 2 605

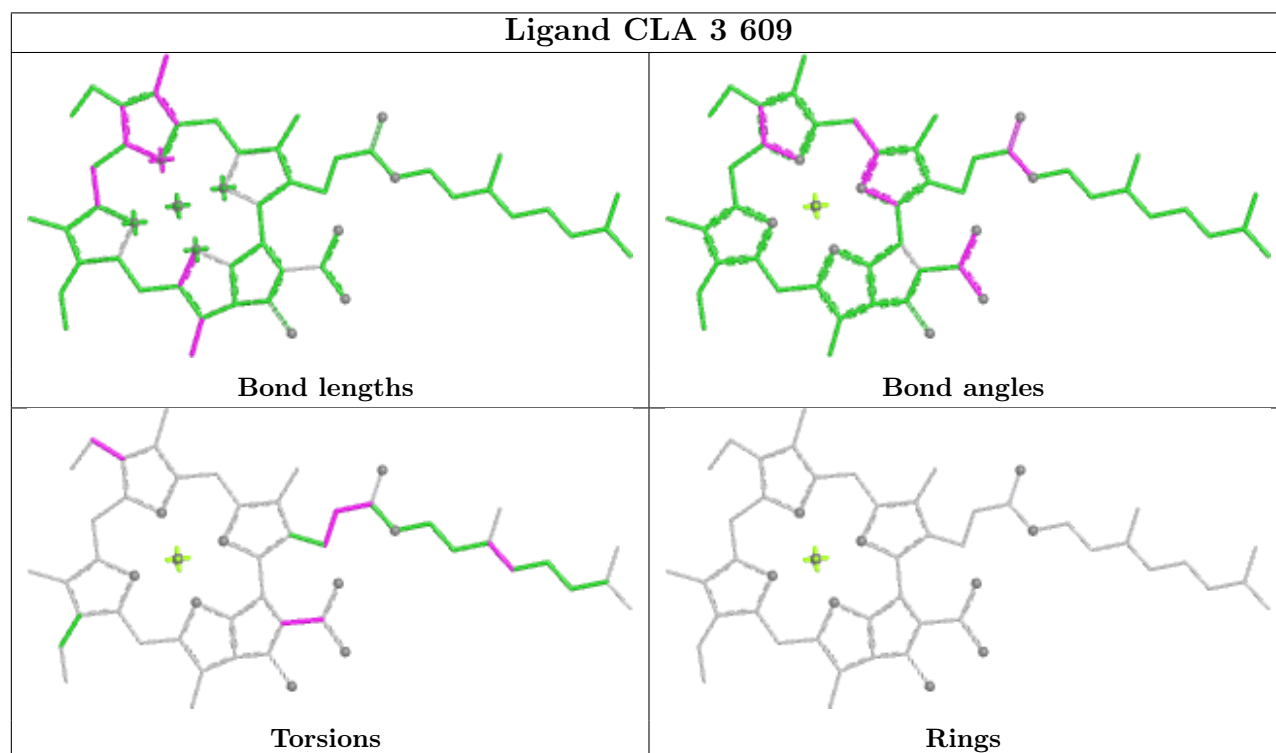
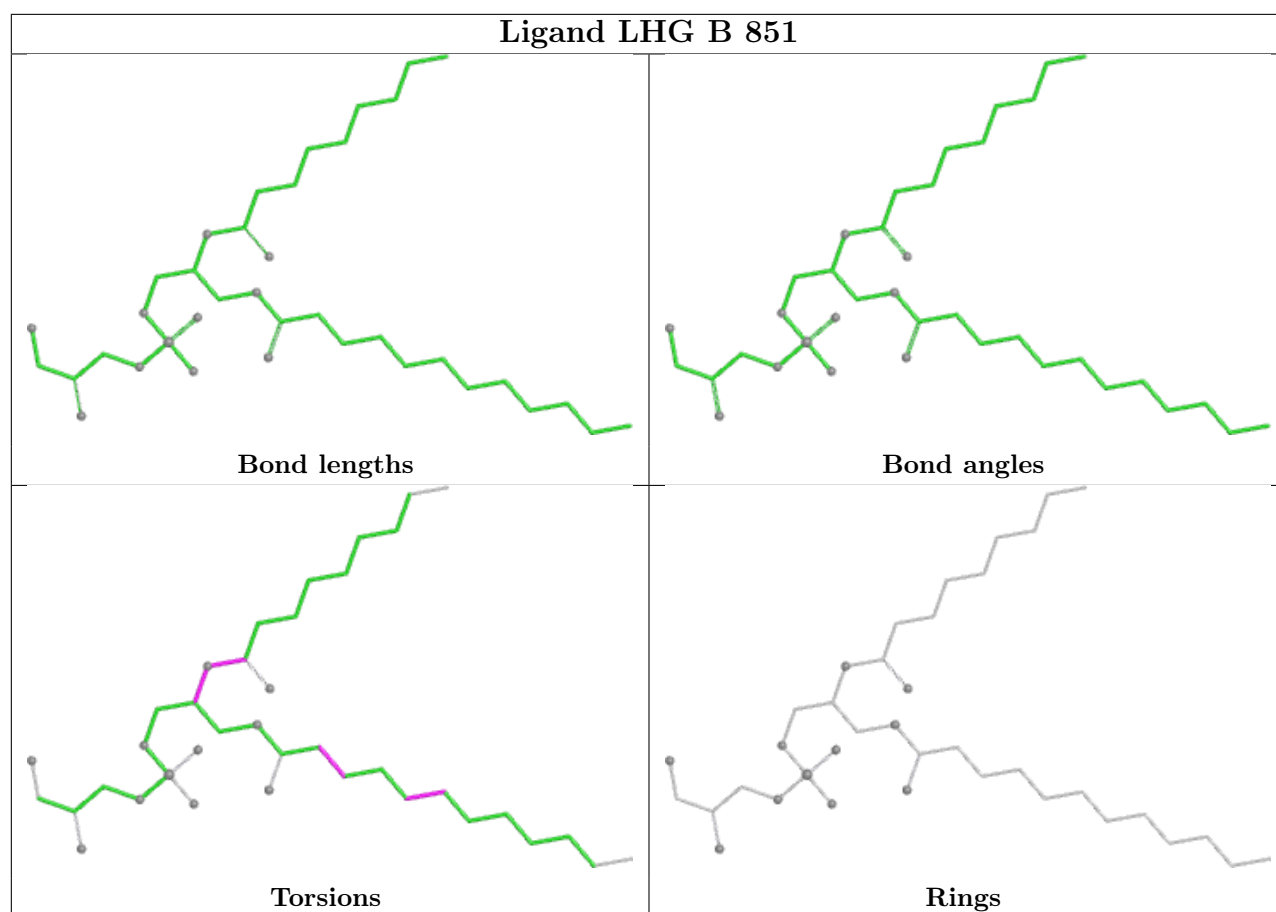


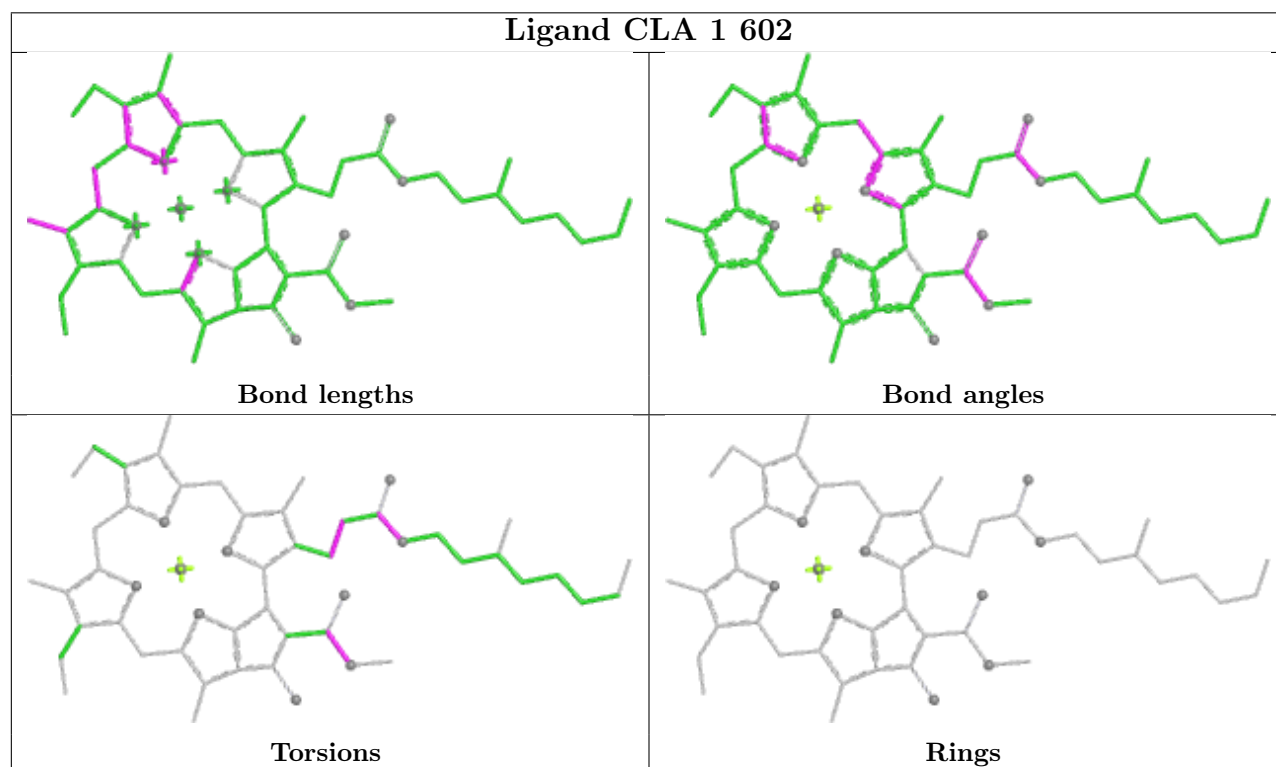
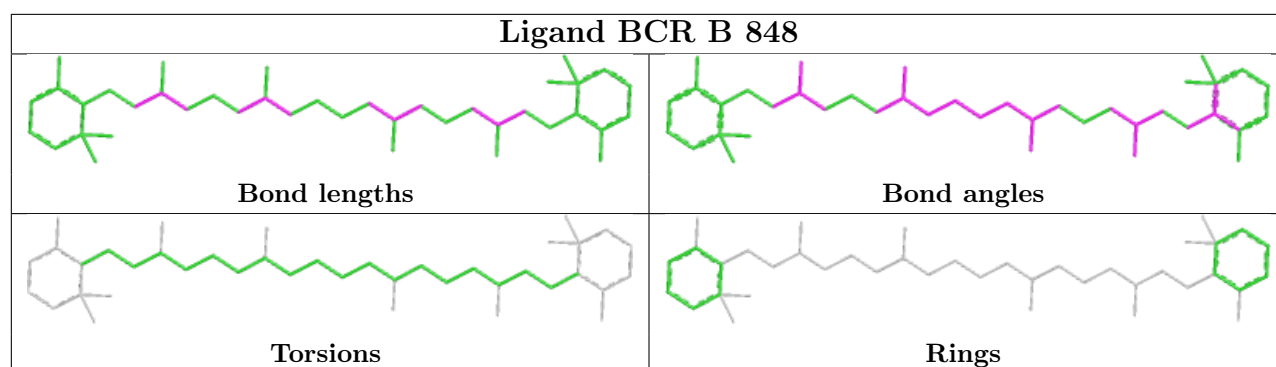


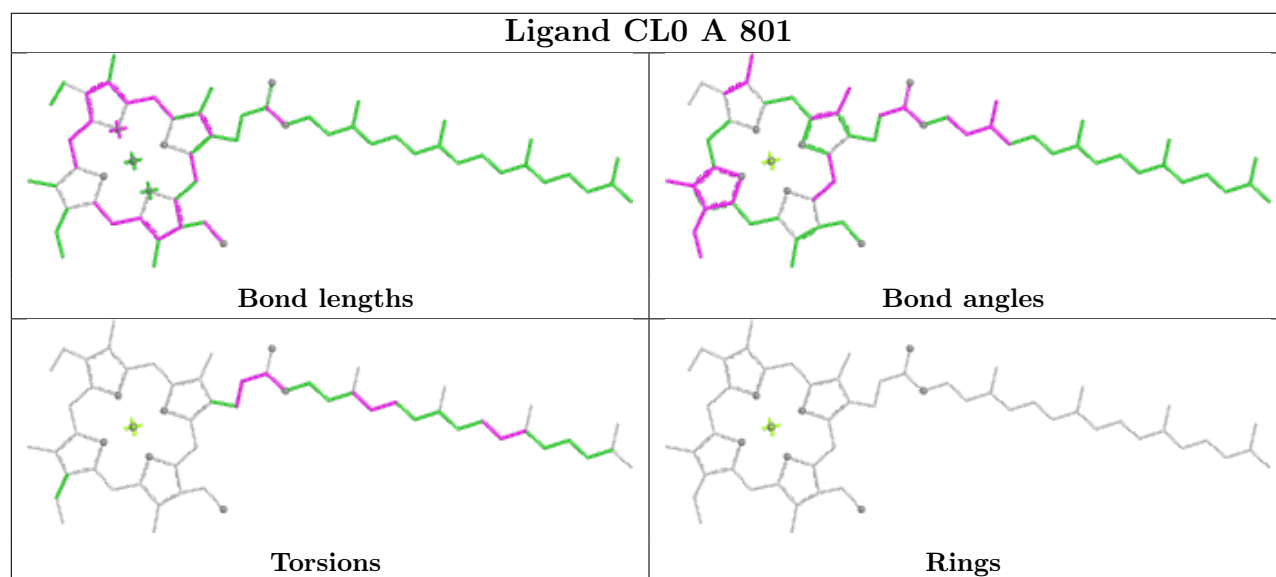
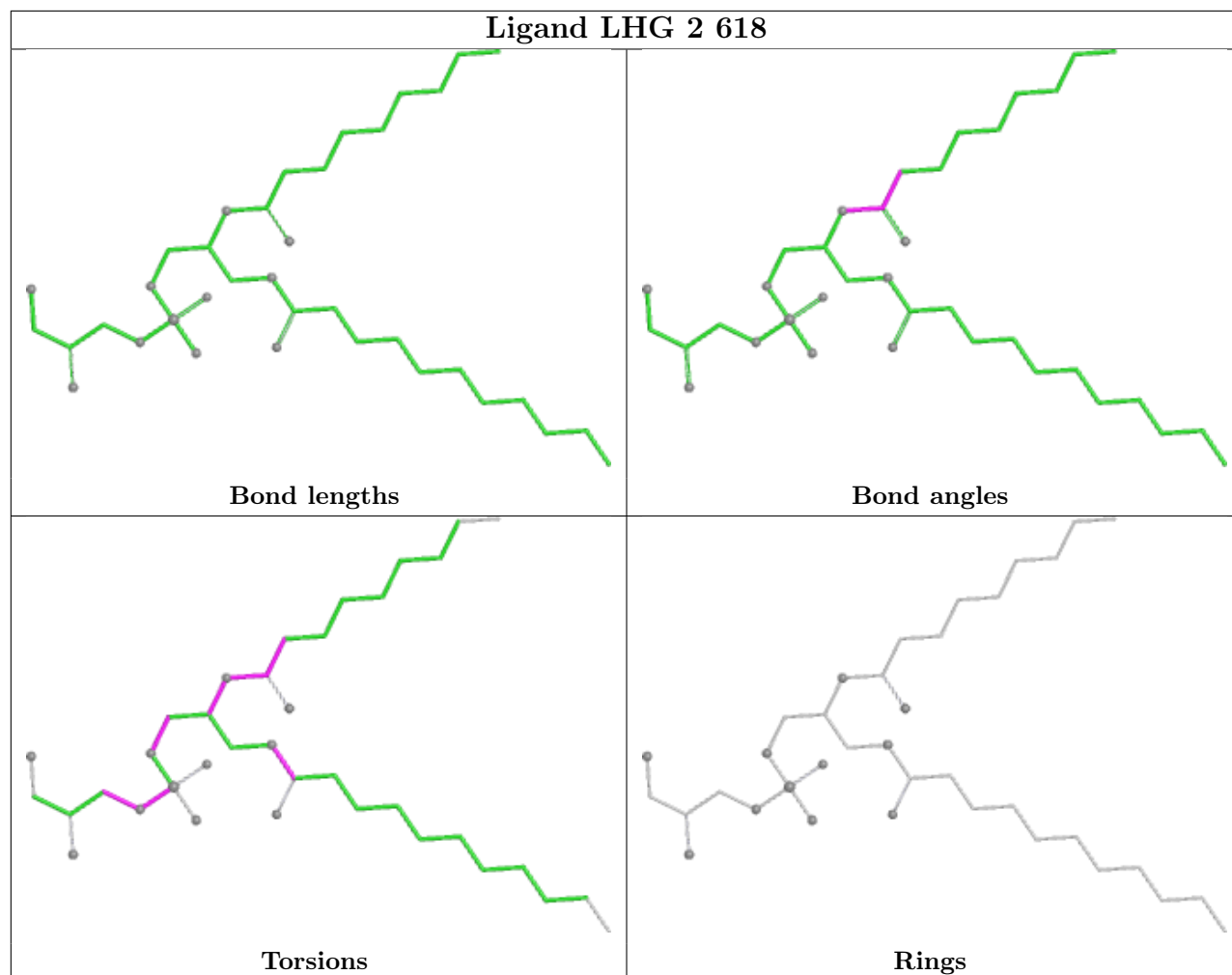


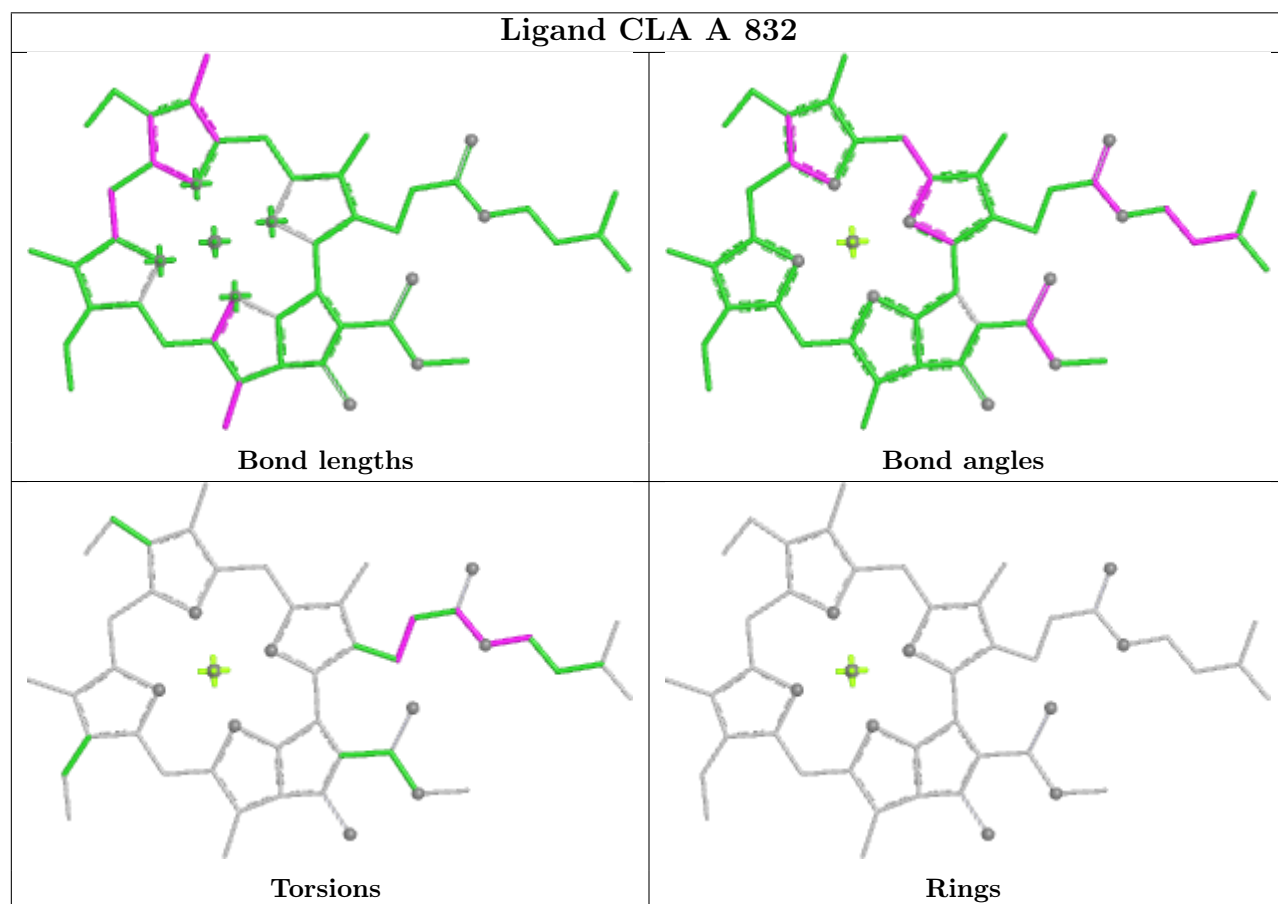
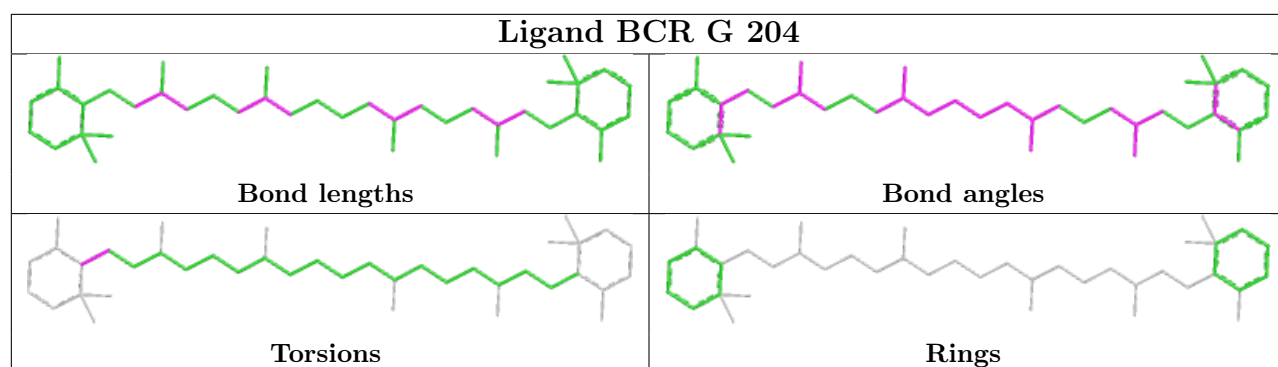
Ligand CHL 4 607

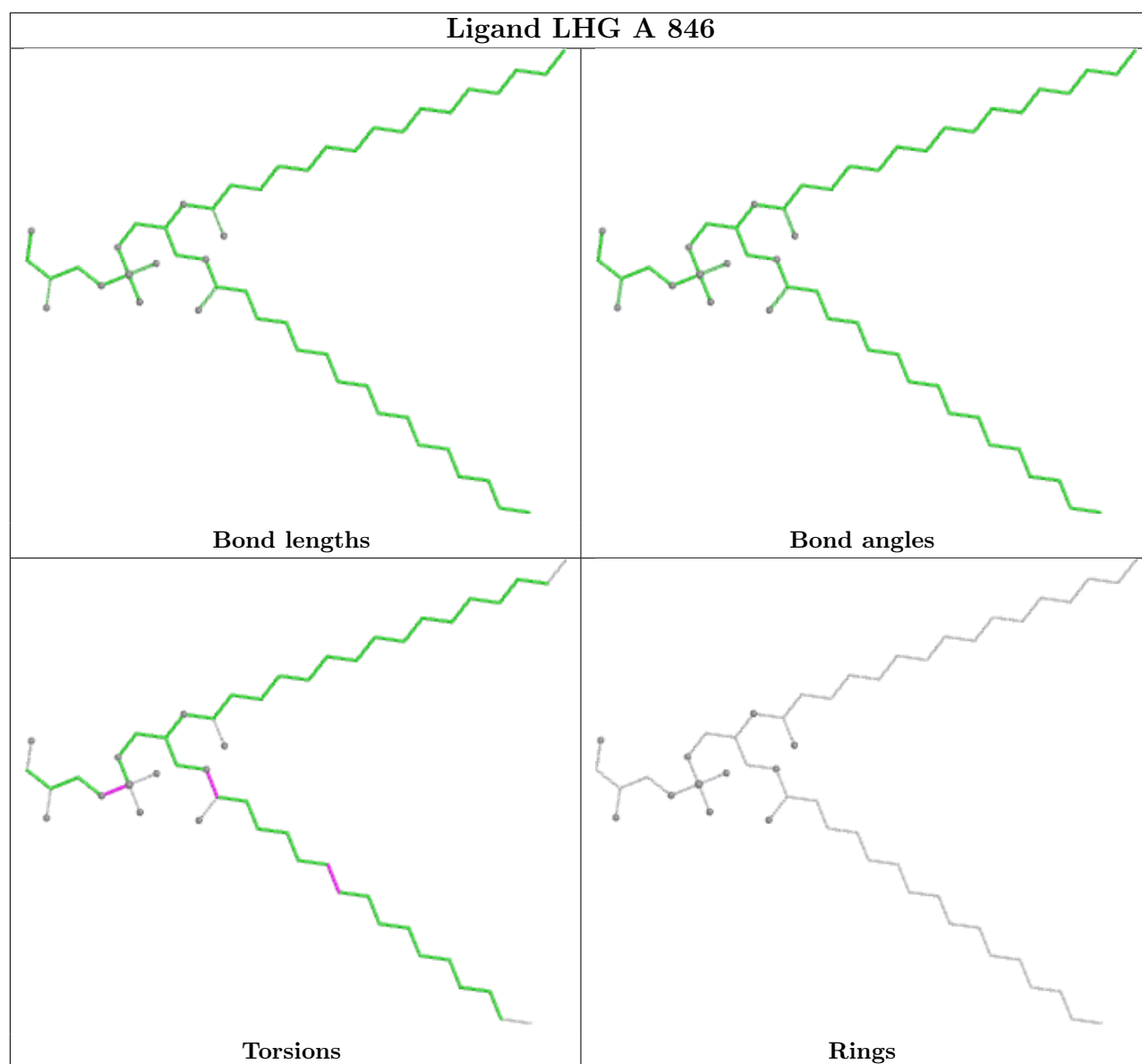




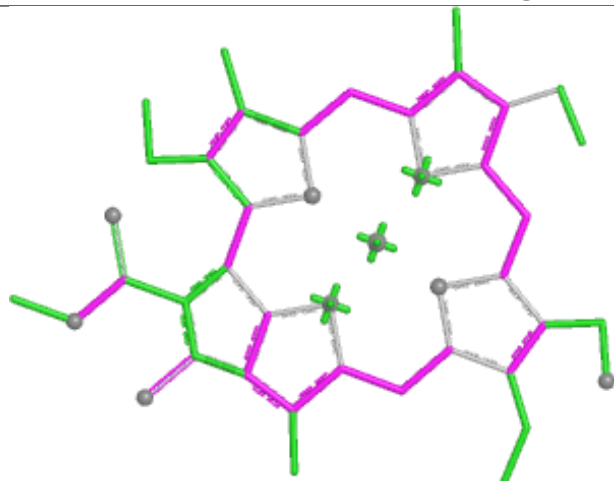




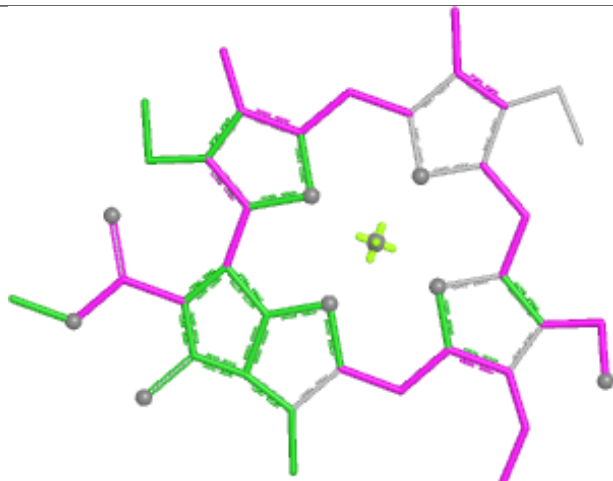




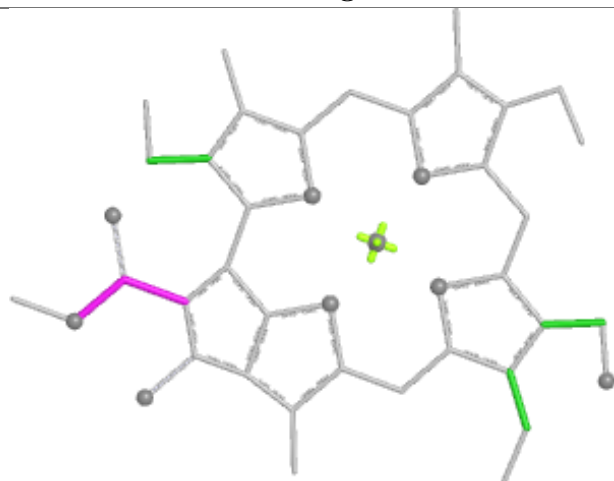
Ligand CHL 2 606



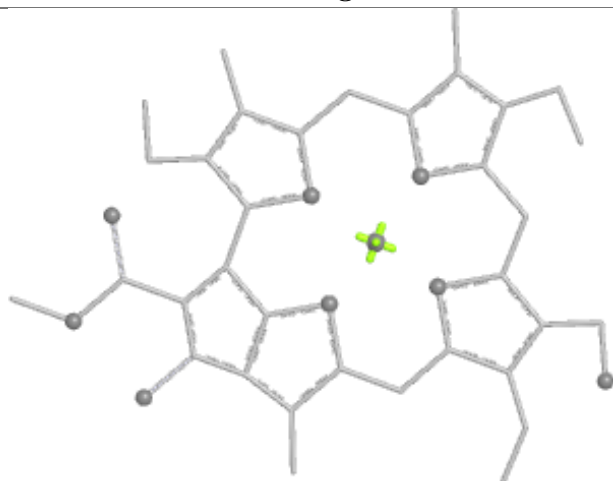
Bond lengths



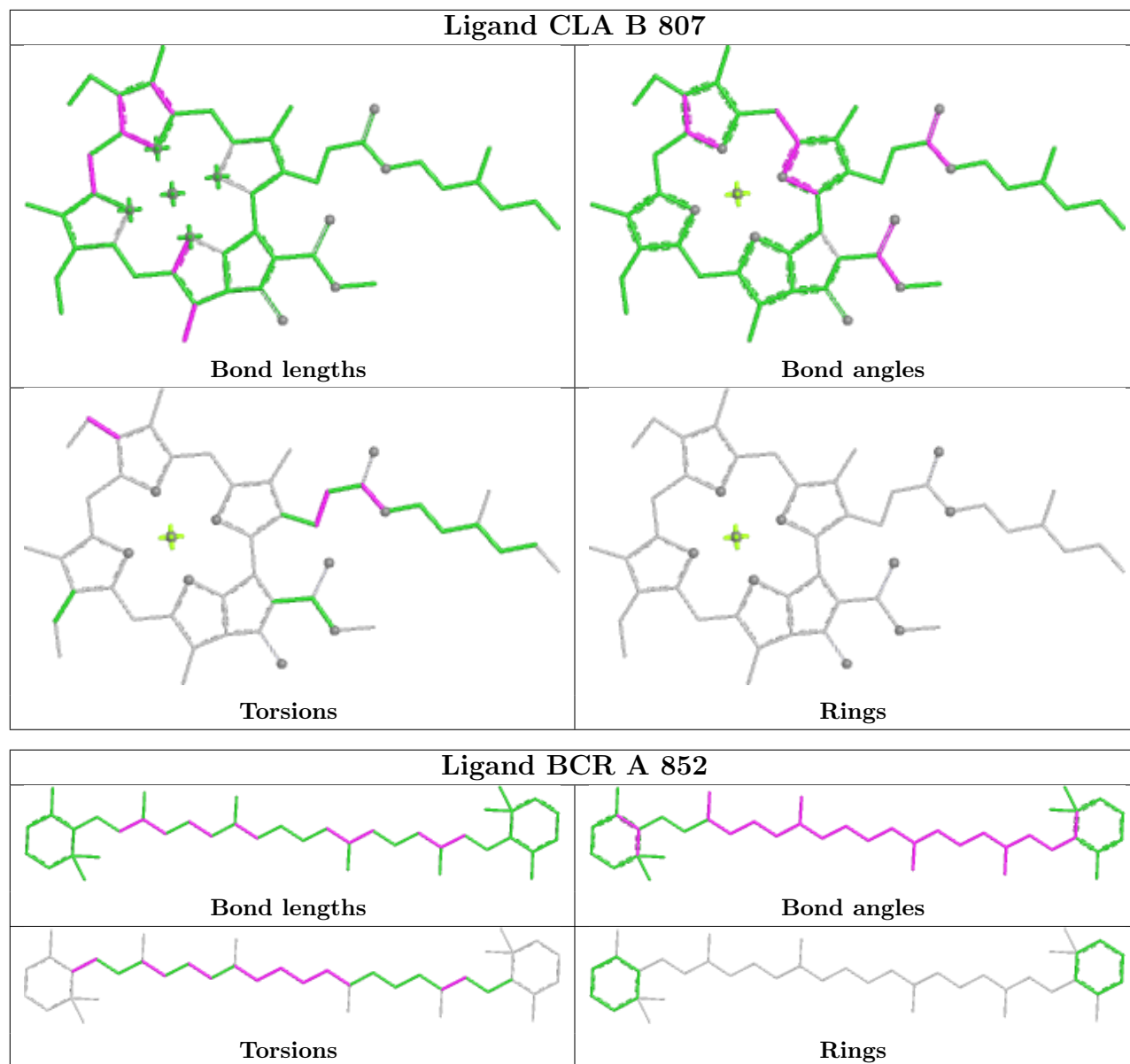
Bond angles



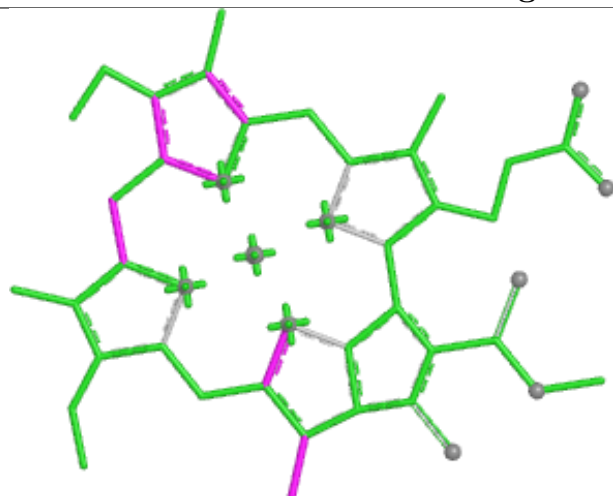
Torsions



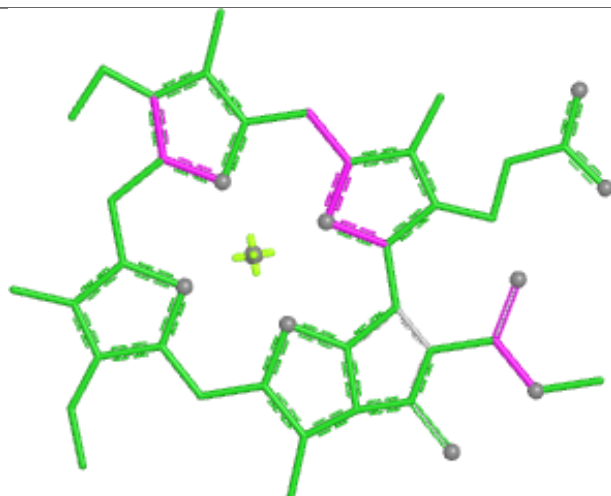
Rings



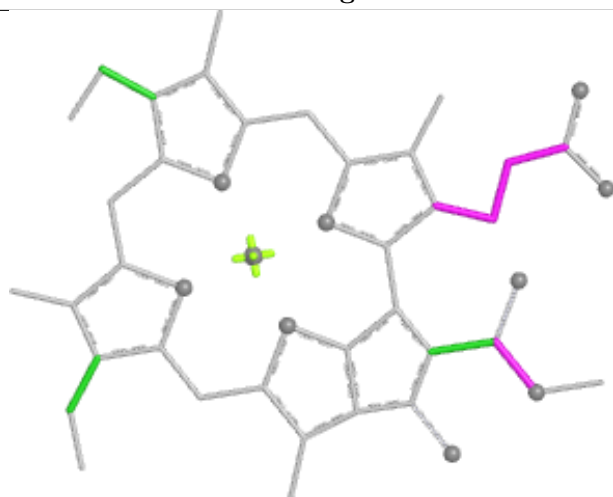
Ligand CLA 2 608



Bond lengths



Bond angles

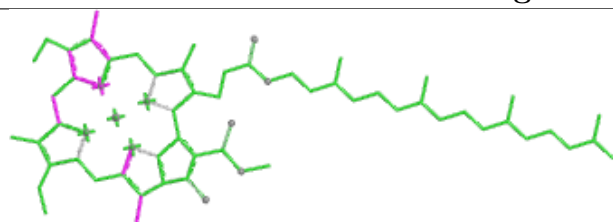


Torsions

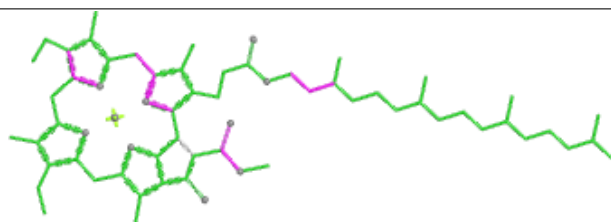


Rings

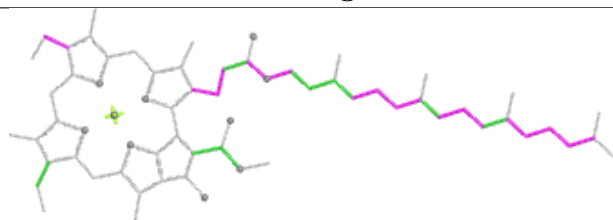
Ligand CLA A 812



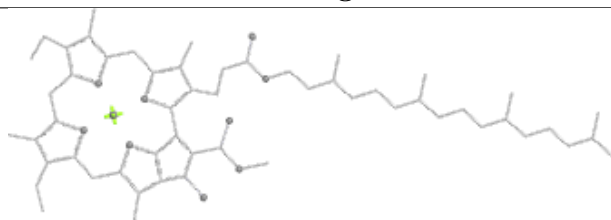
Bond lengths



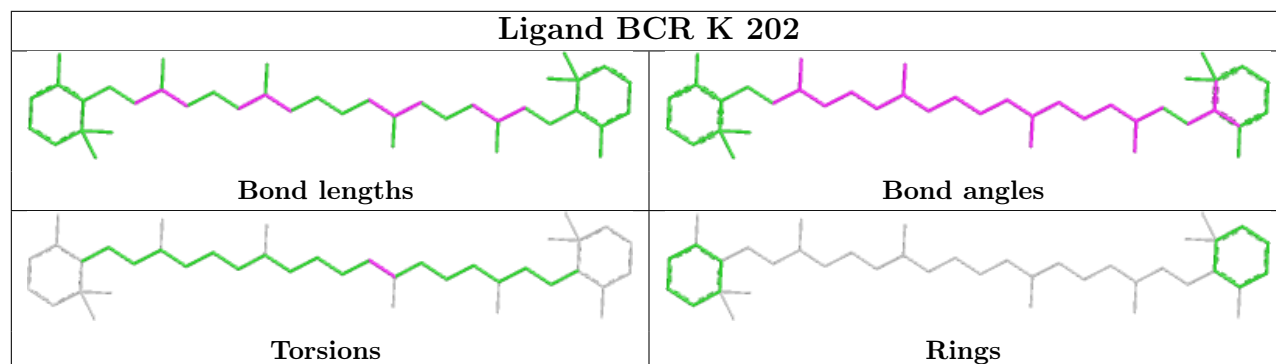
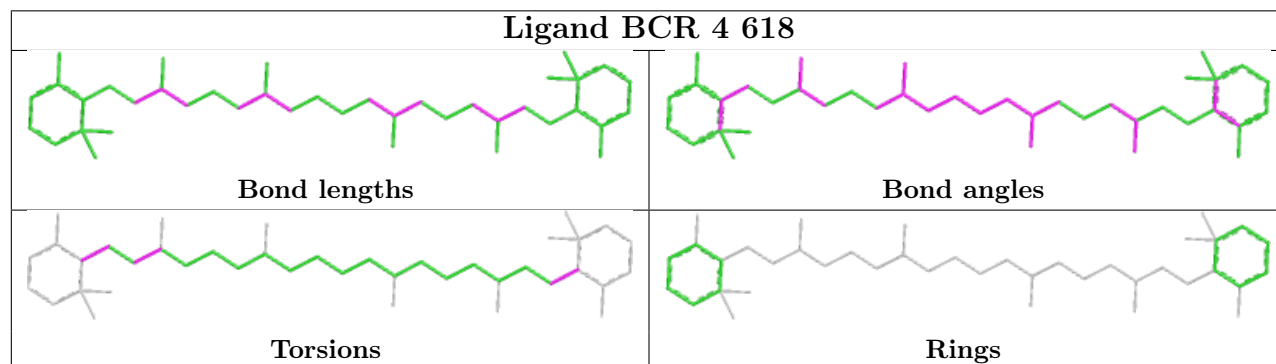
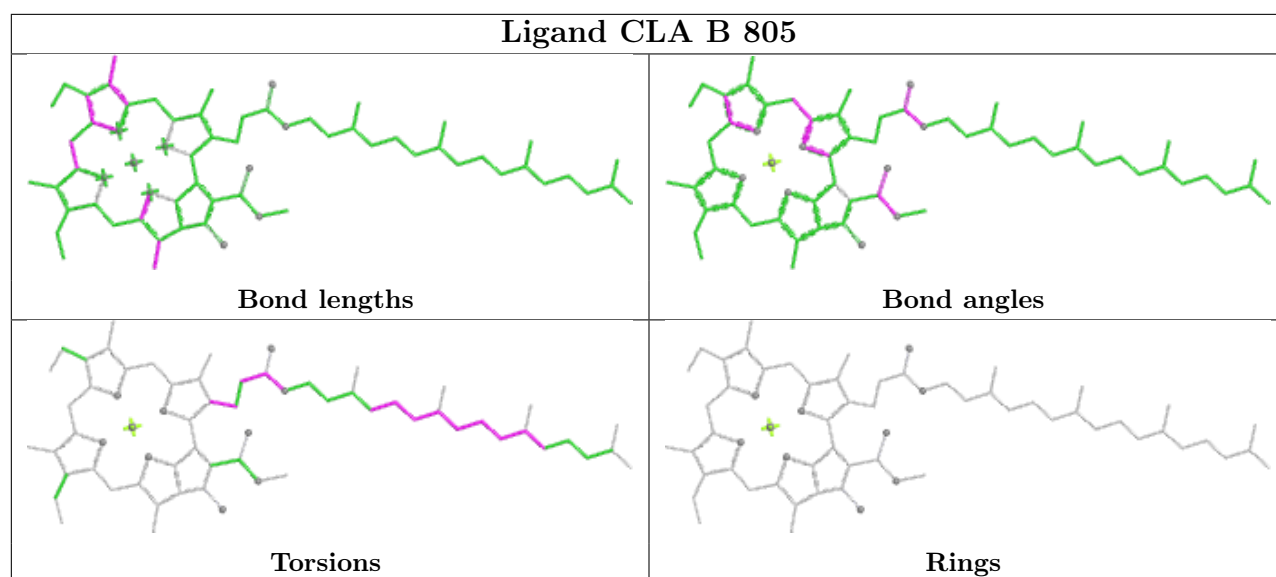
Bond angles



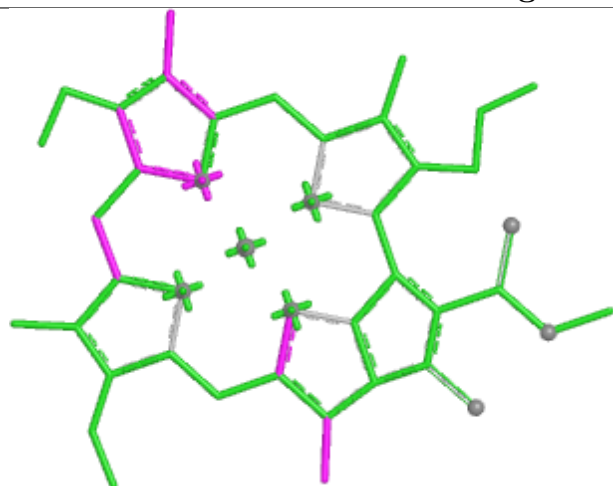
Torsions



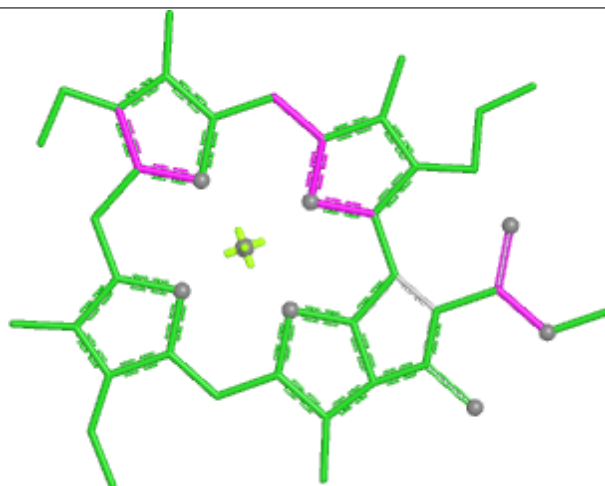
Rings



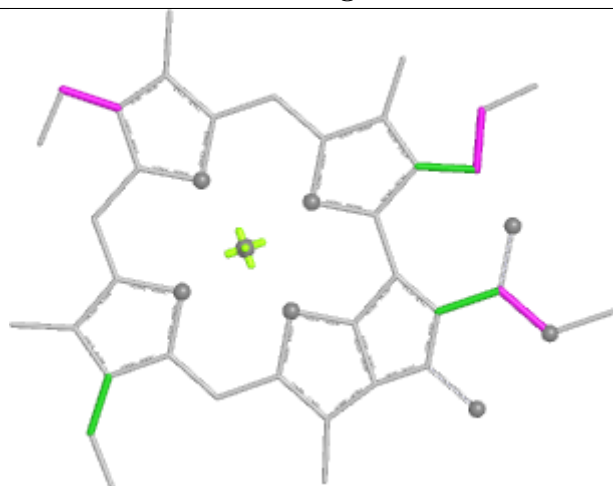
Ligand CLA 2 613



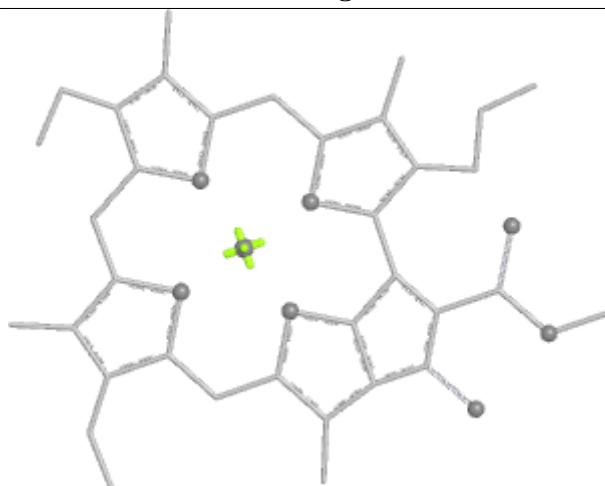
Bond lengths



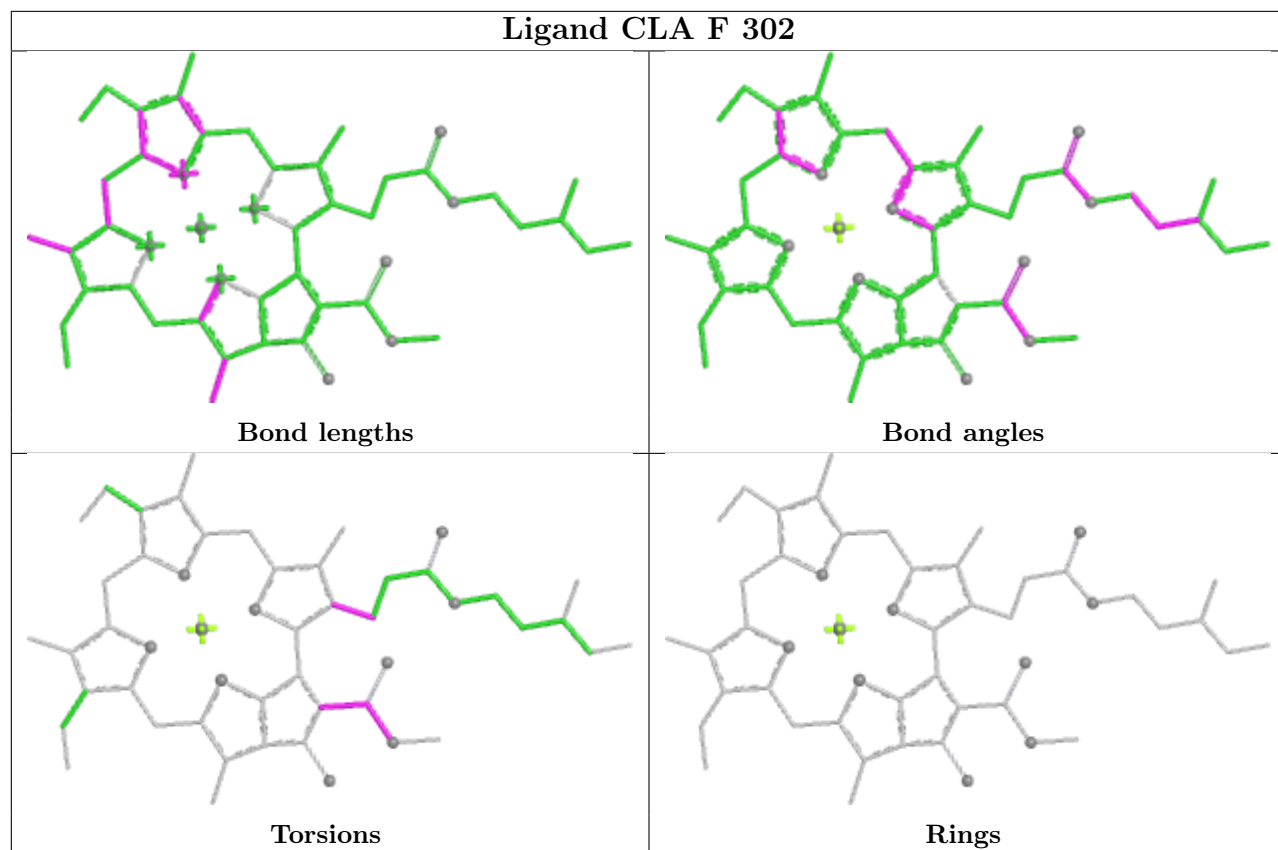
Bond angles



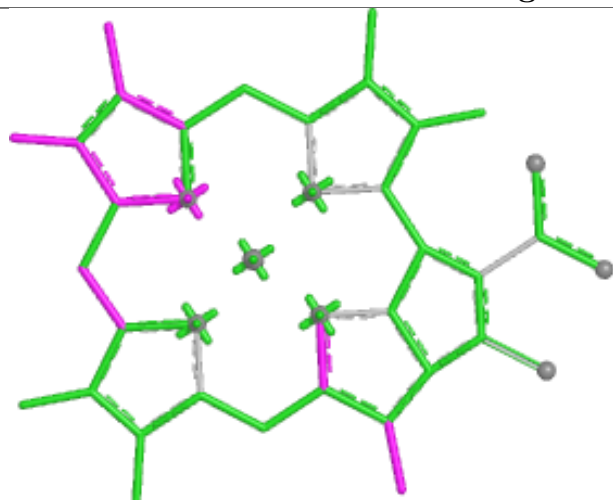
Torsions



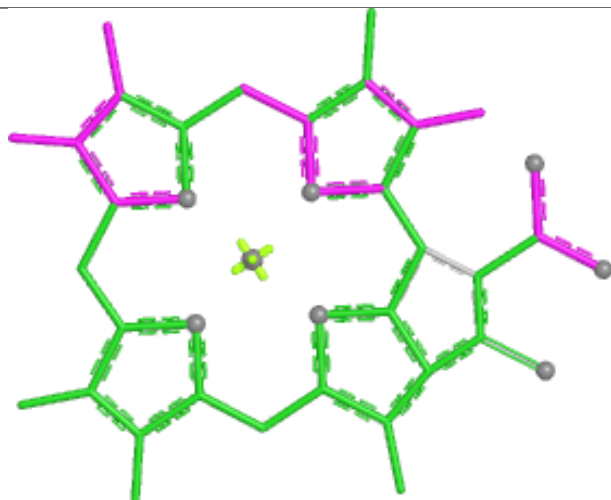
Rings



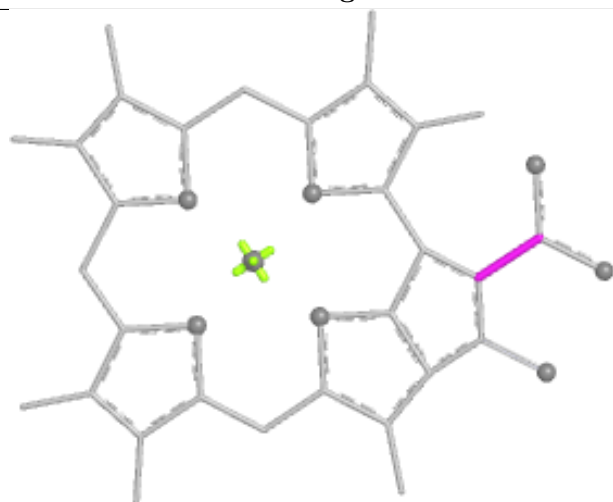
Ligand CLA 1 610



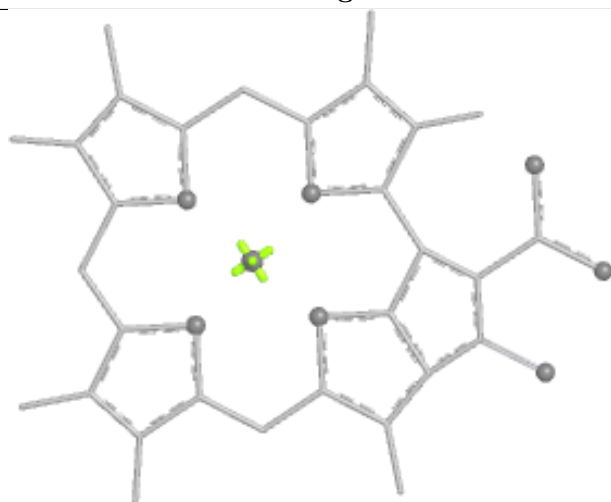
Bond lengths



Bond angles

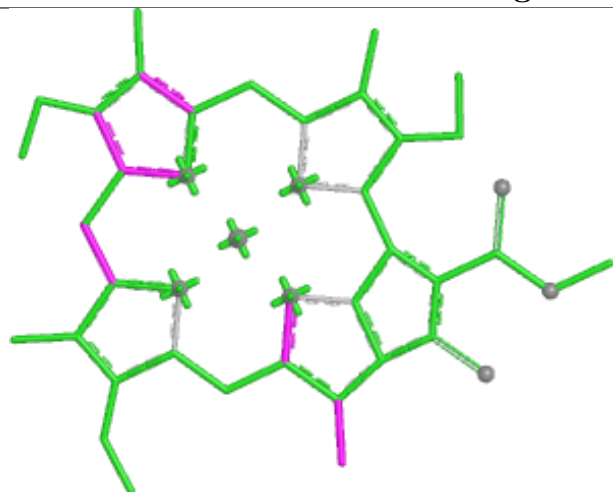


Torsions



Rings

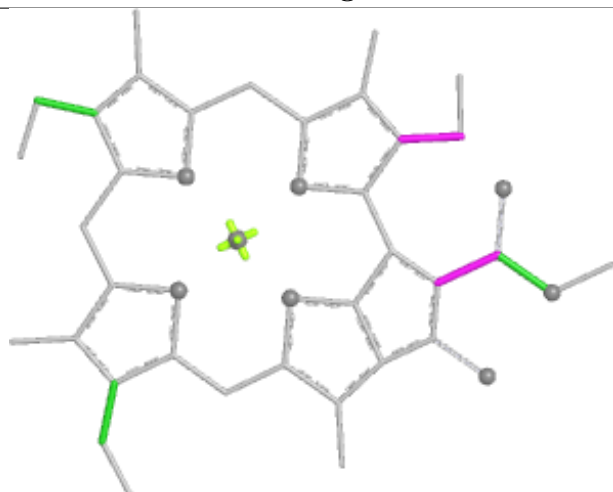
Ligand CLA A 823



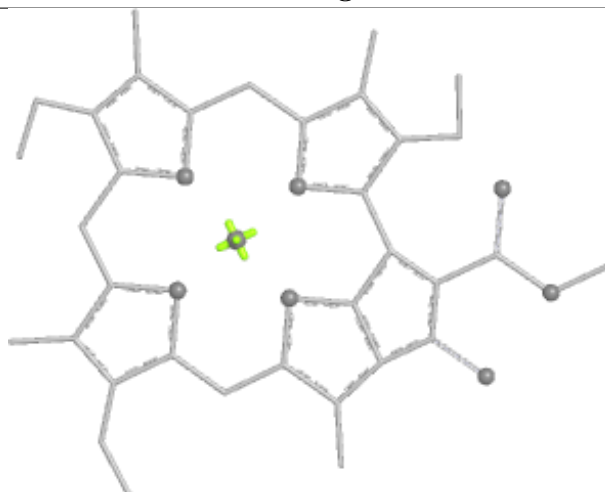
Bond lengths



Bond angles

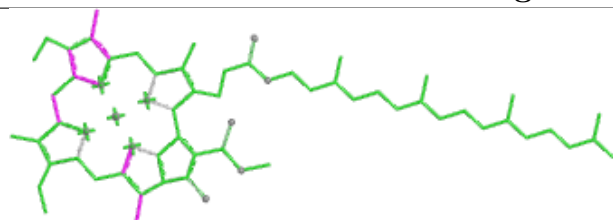


Torsions

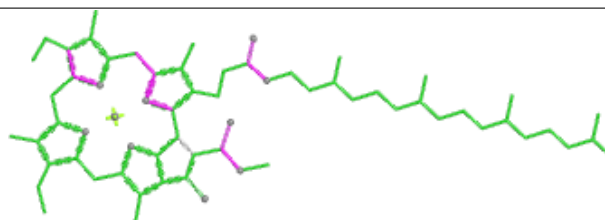


Rings

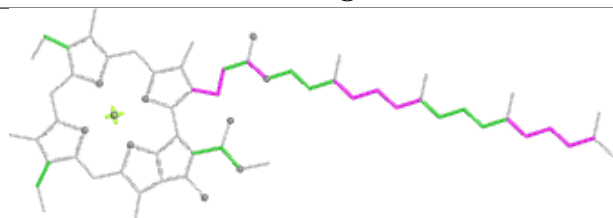
Ligand CLA B 828



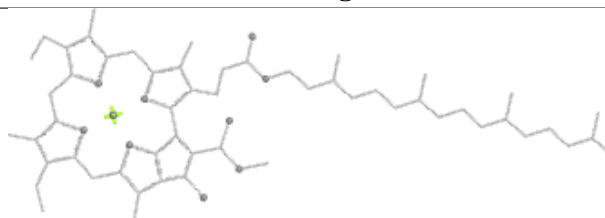
Bond lengths



Bond angles

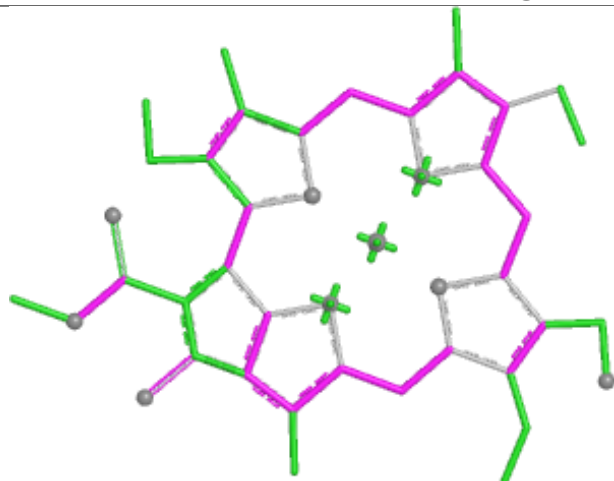


Torsions

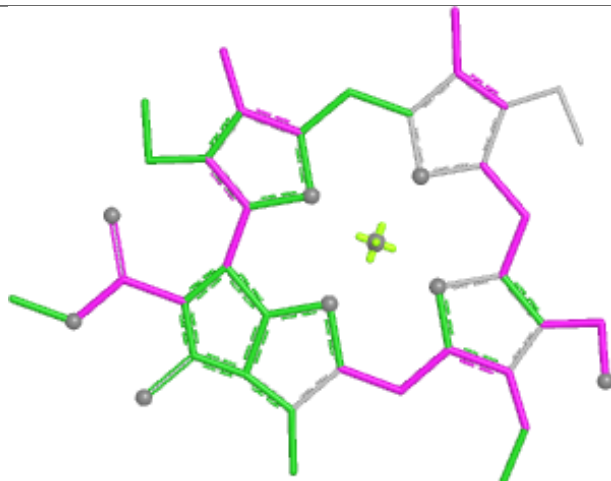


Rings

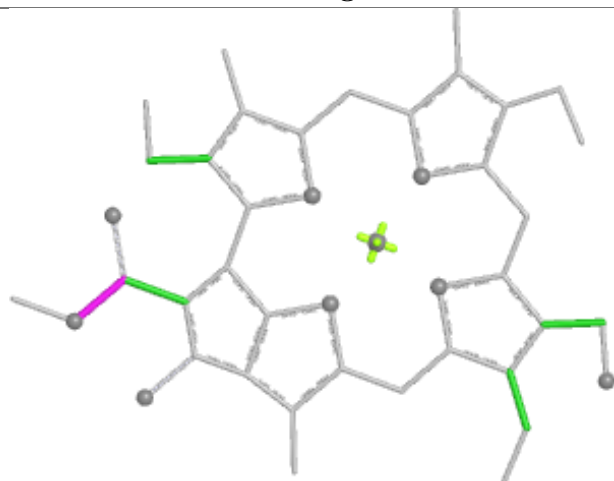
Ligand CHL 2 615



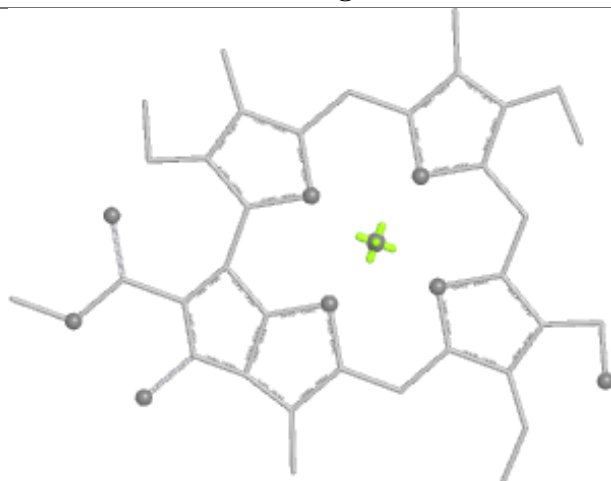
Bond lengths



Bond angles

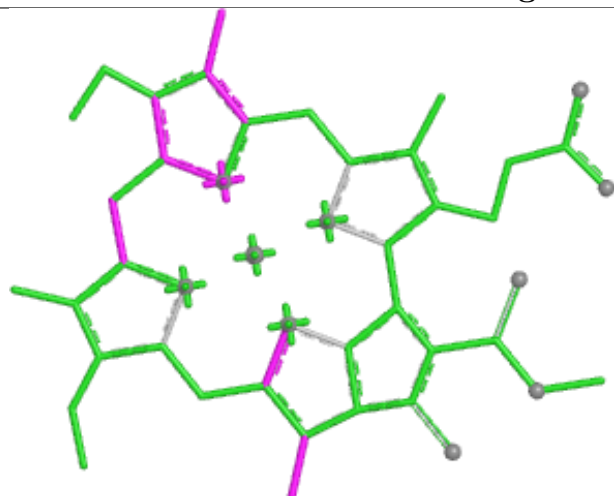


Torsions

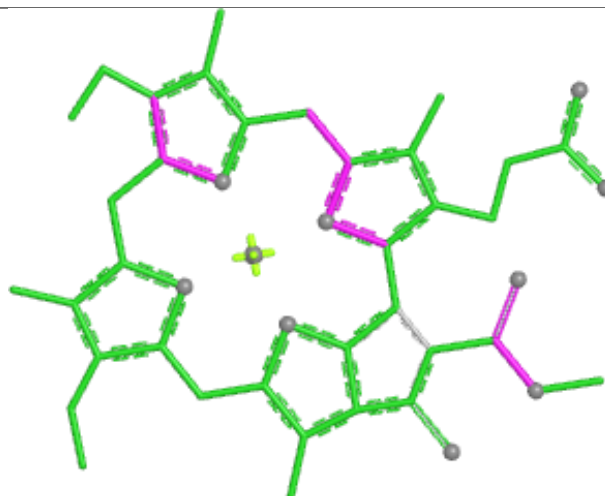


Rings

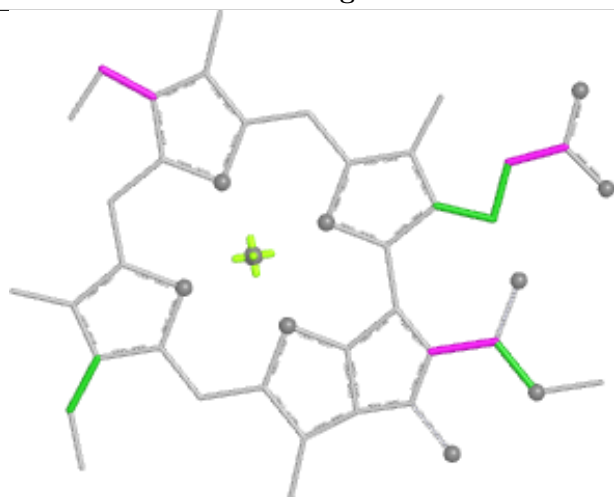
Ligand CLA 1 611



Bond lengths



Bond angles

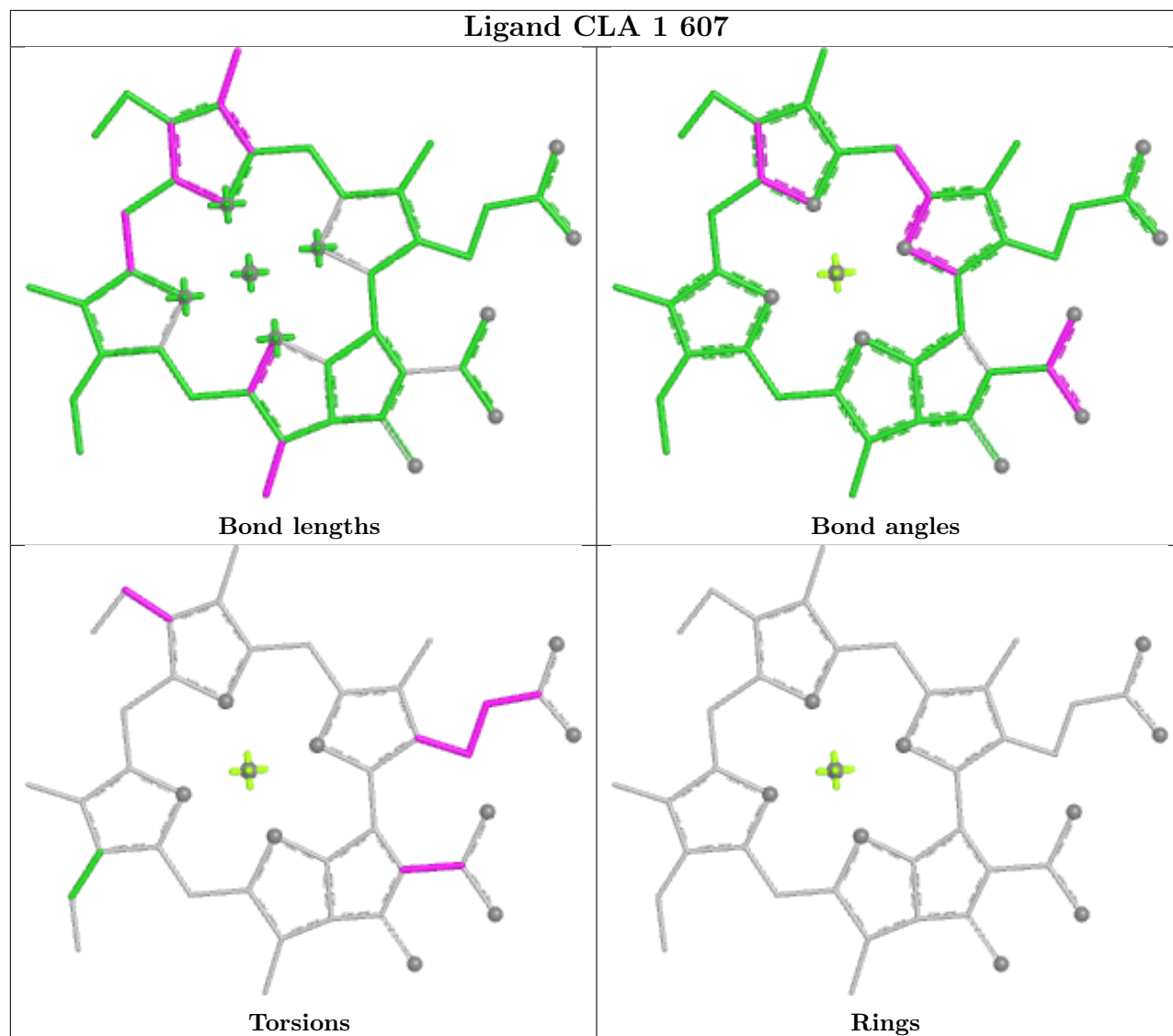


Torsions

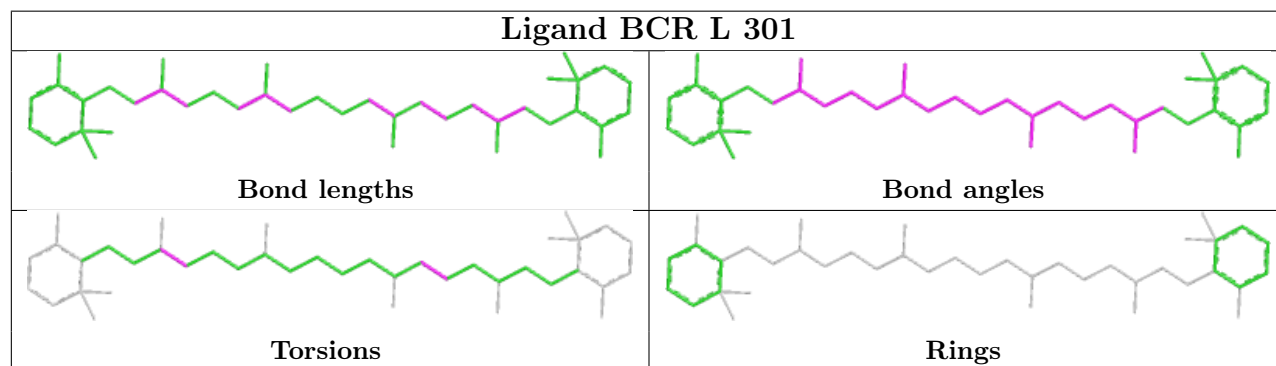


Rings

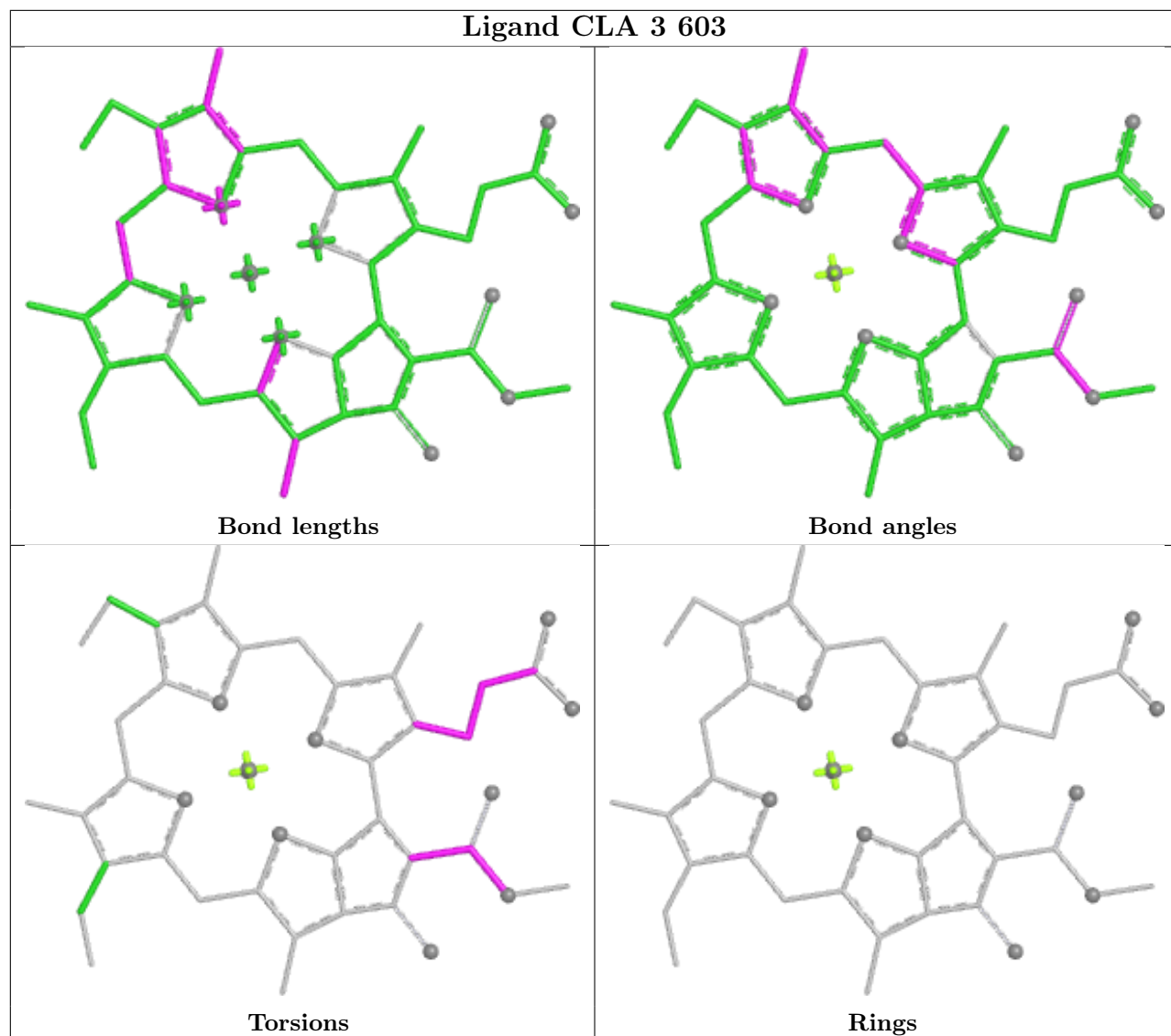
Ligand CLA 1 607



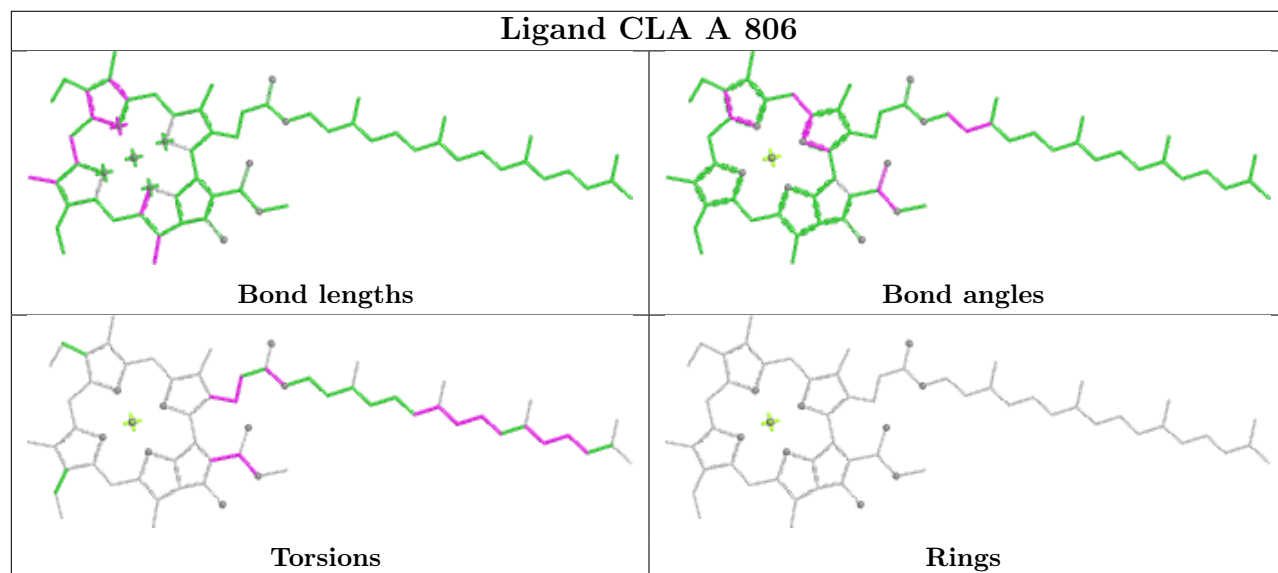
Ligand BCR L 301

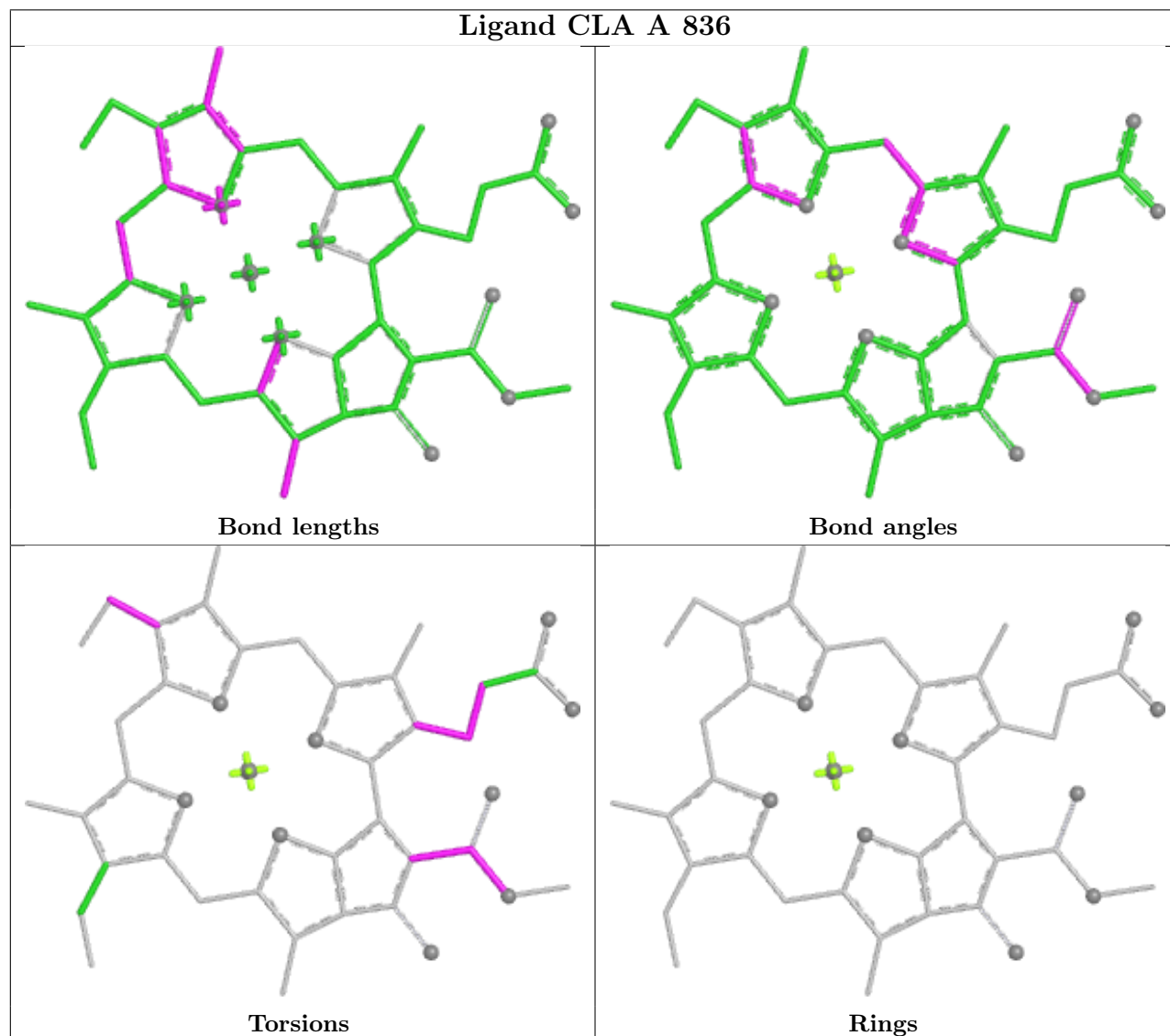
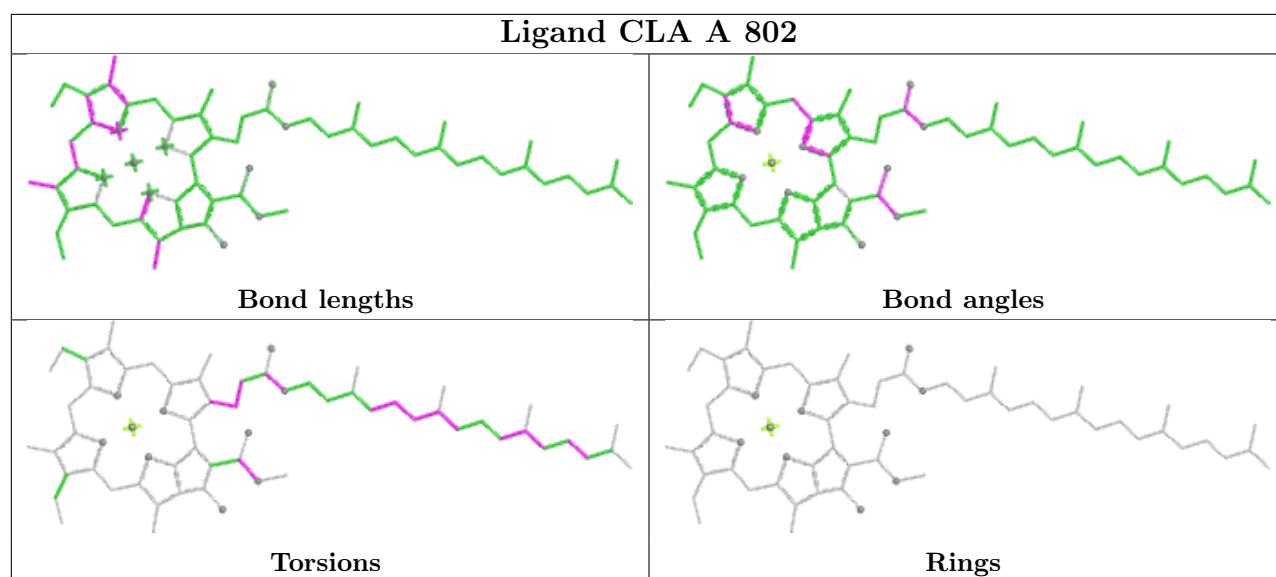


Ligand CLA 3 603

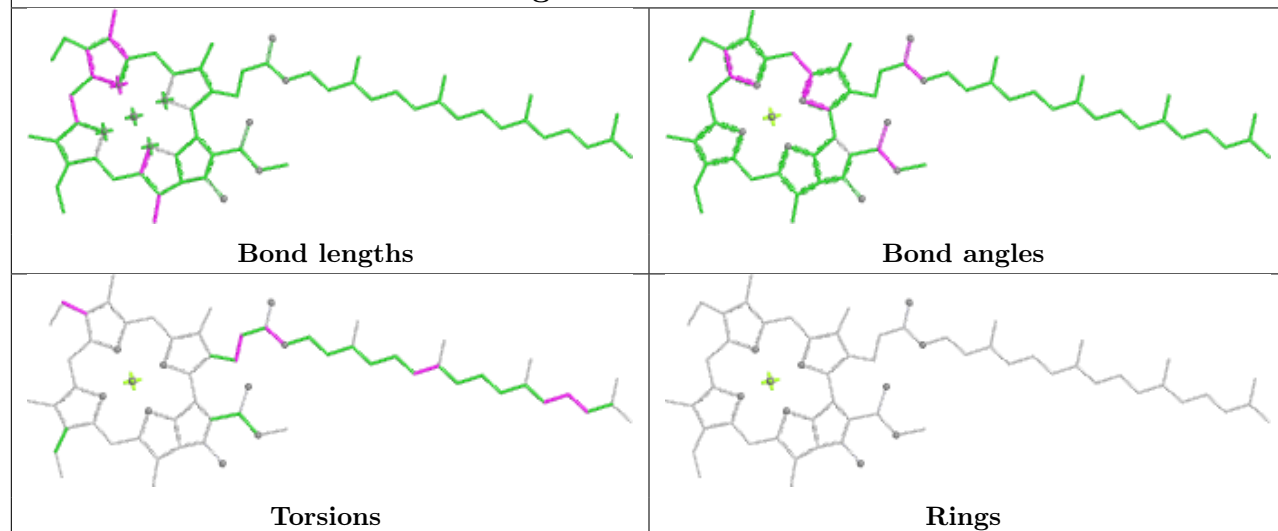


Ligand CLA A 806

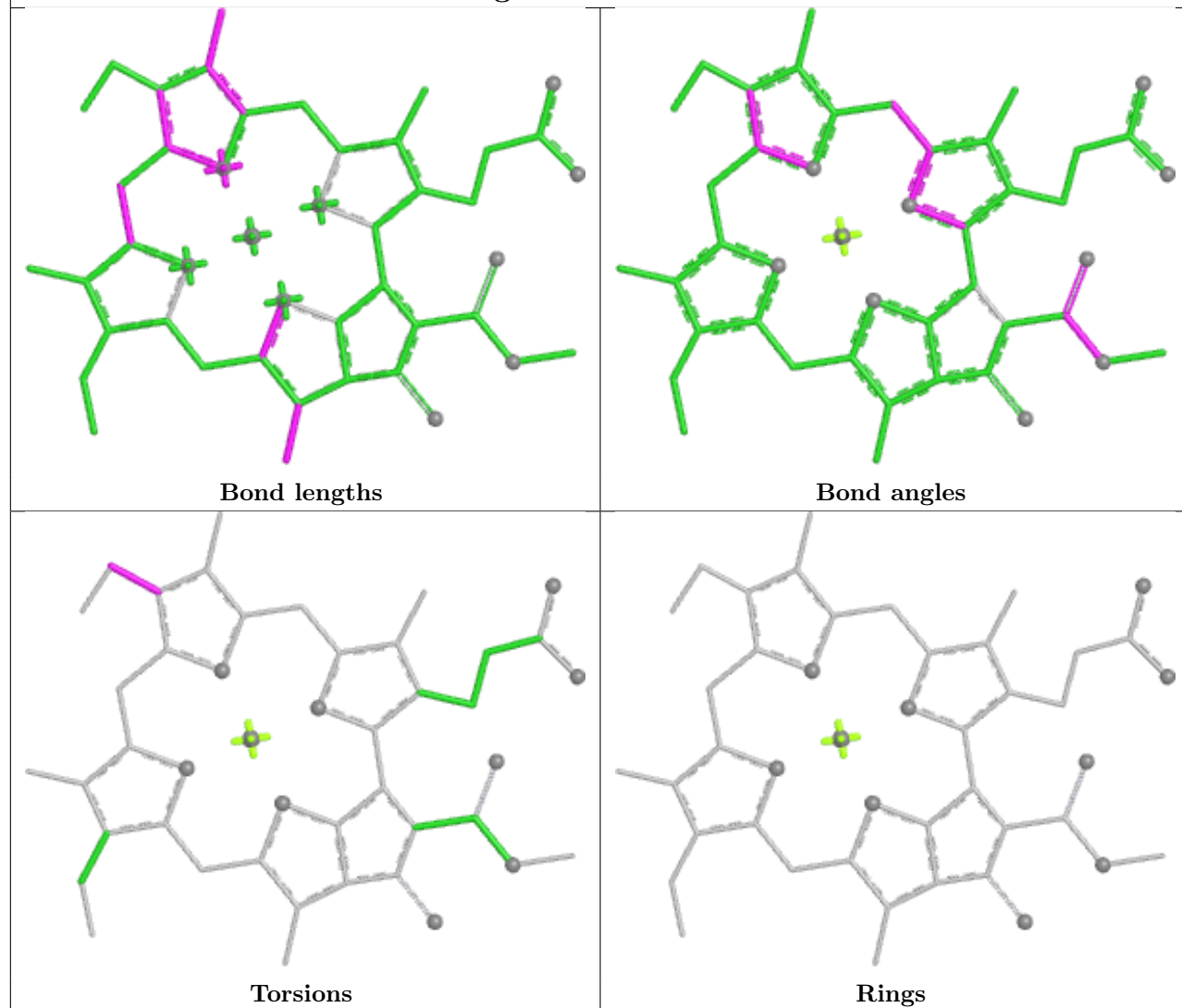


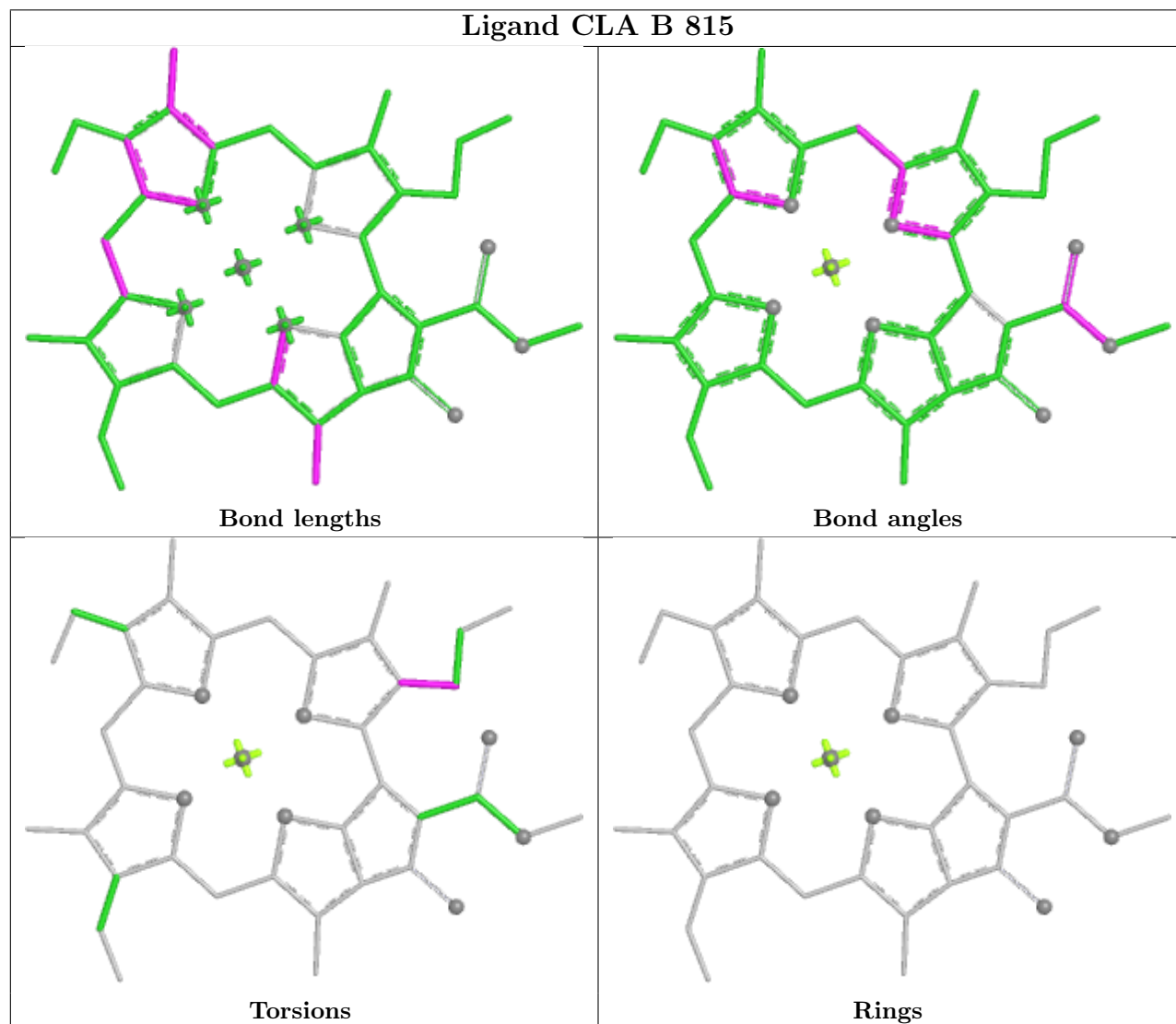
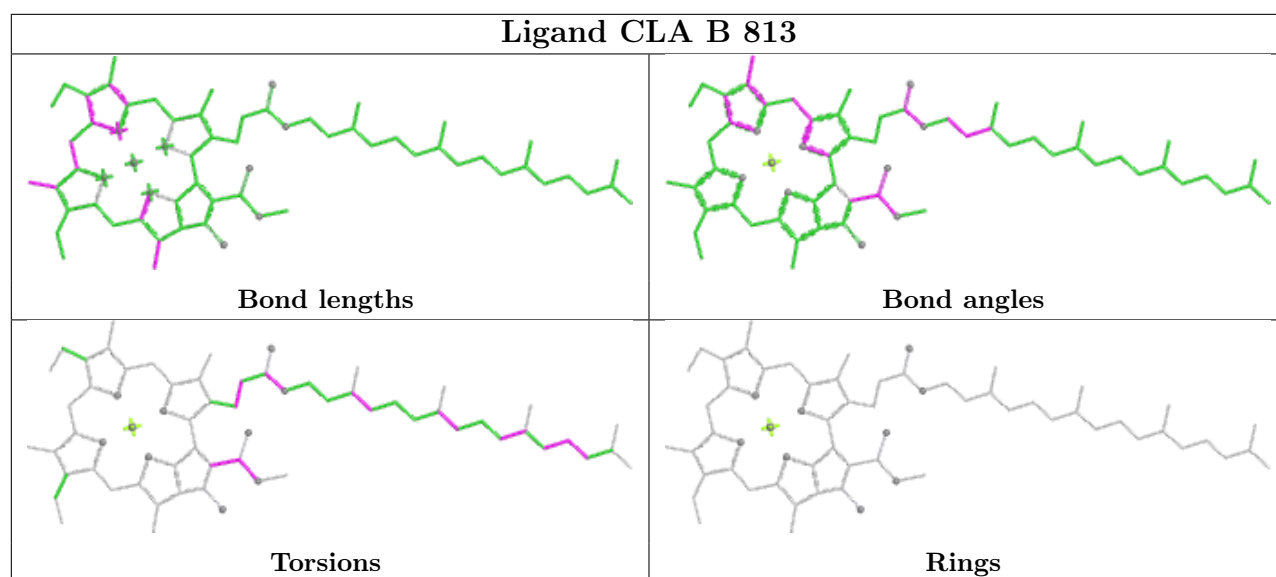


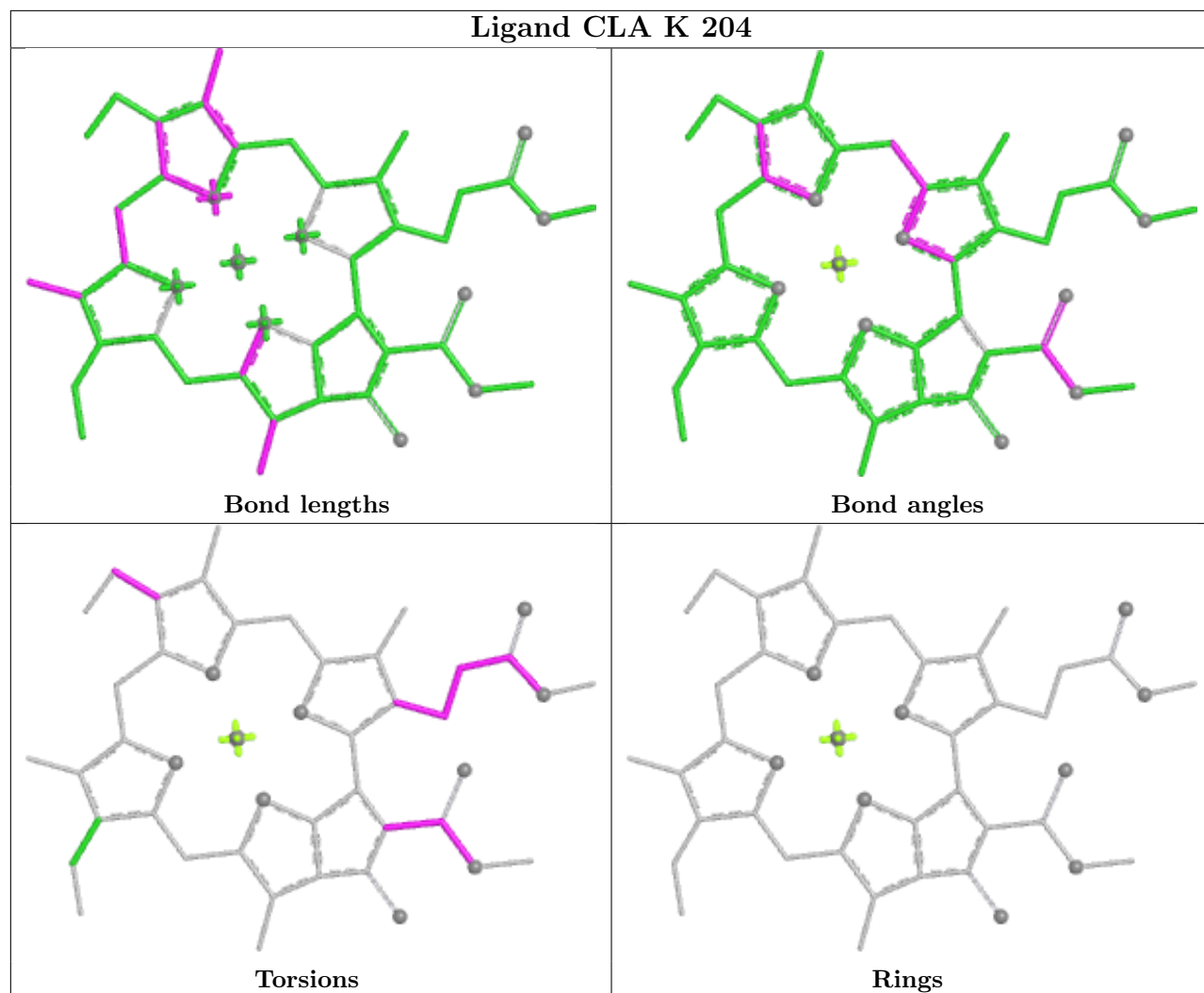
Ligand CLA B 839



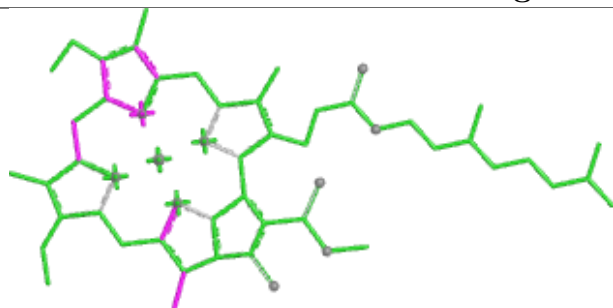
Ligand CLA L 302



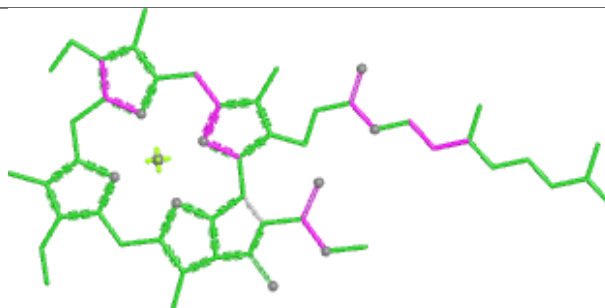




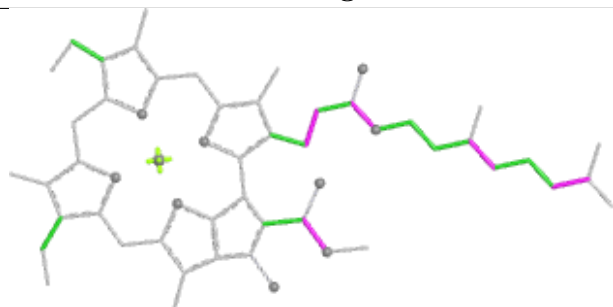
Ligand CLA A 839



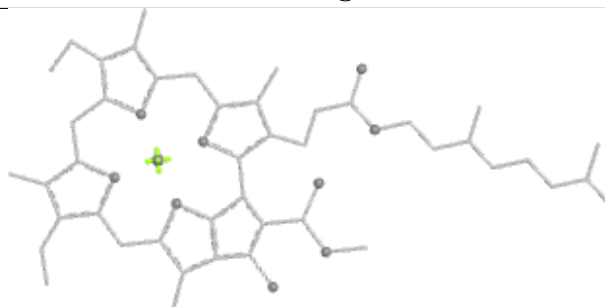
Bond lengths



Bond angles

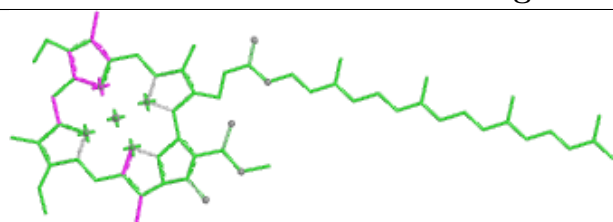


Torsions

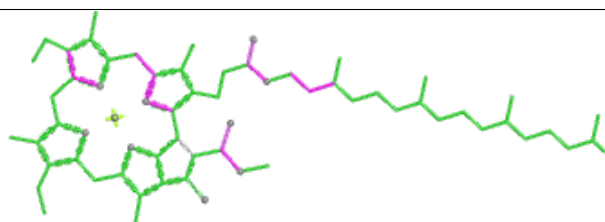


Rings

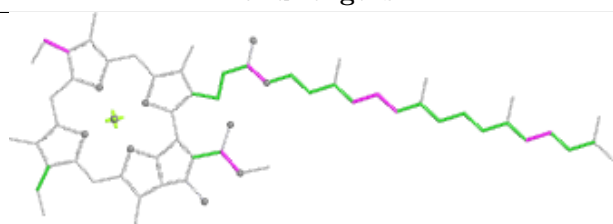
Ligand CLA A 834



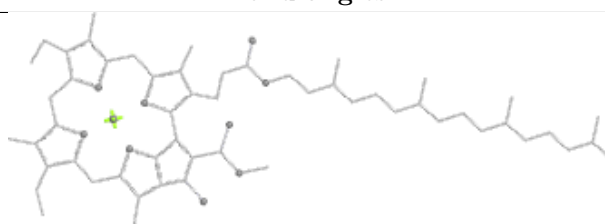
Bond lengths



Bond angles

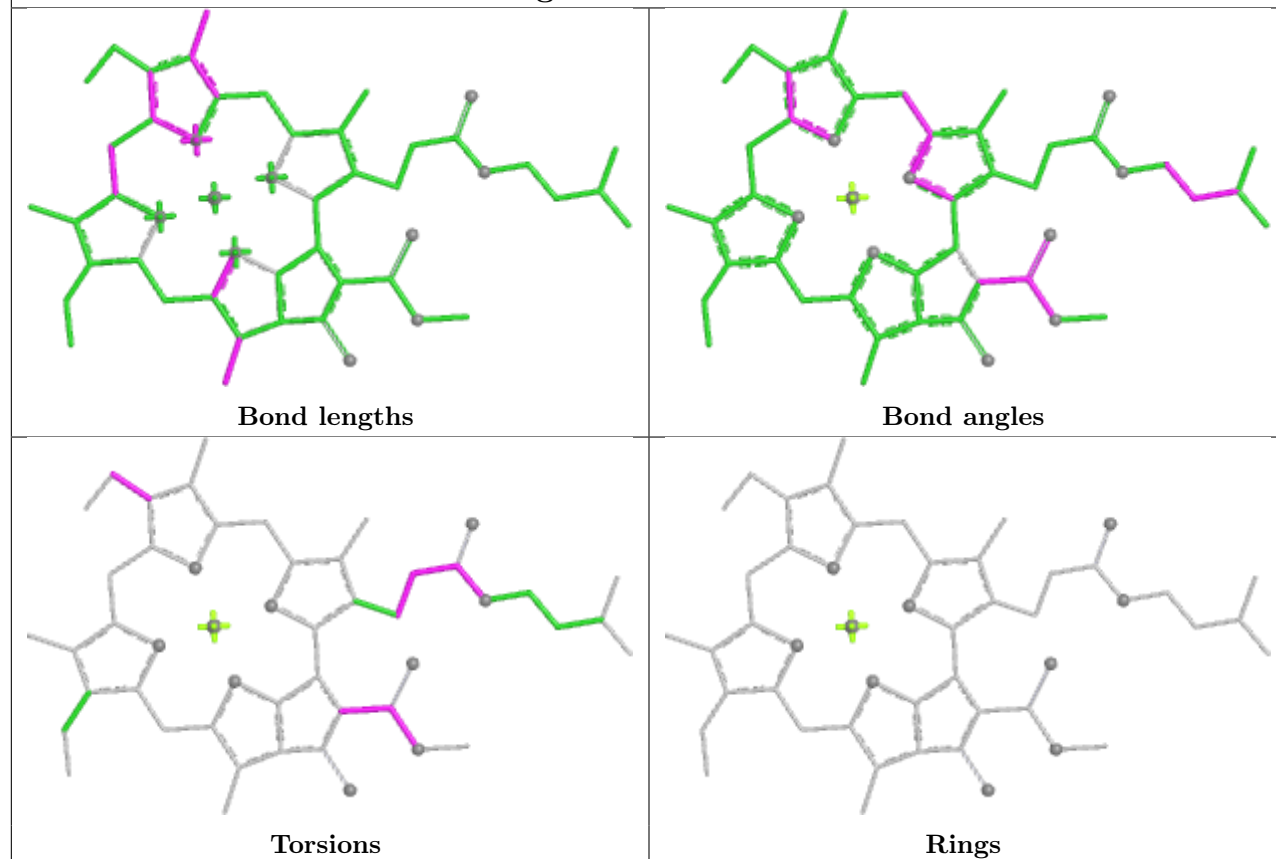


Torsions

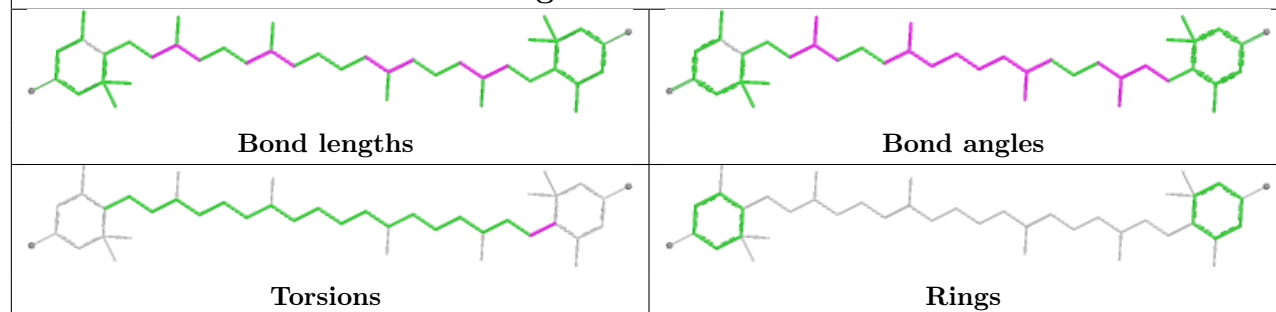


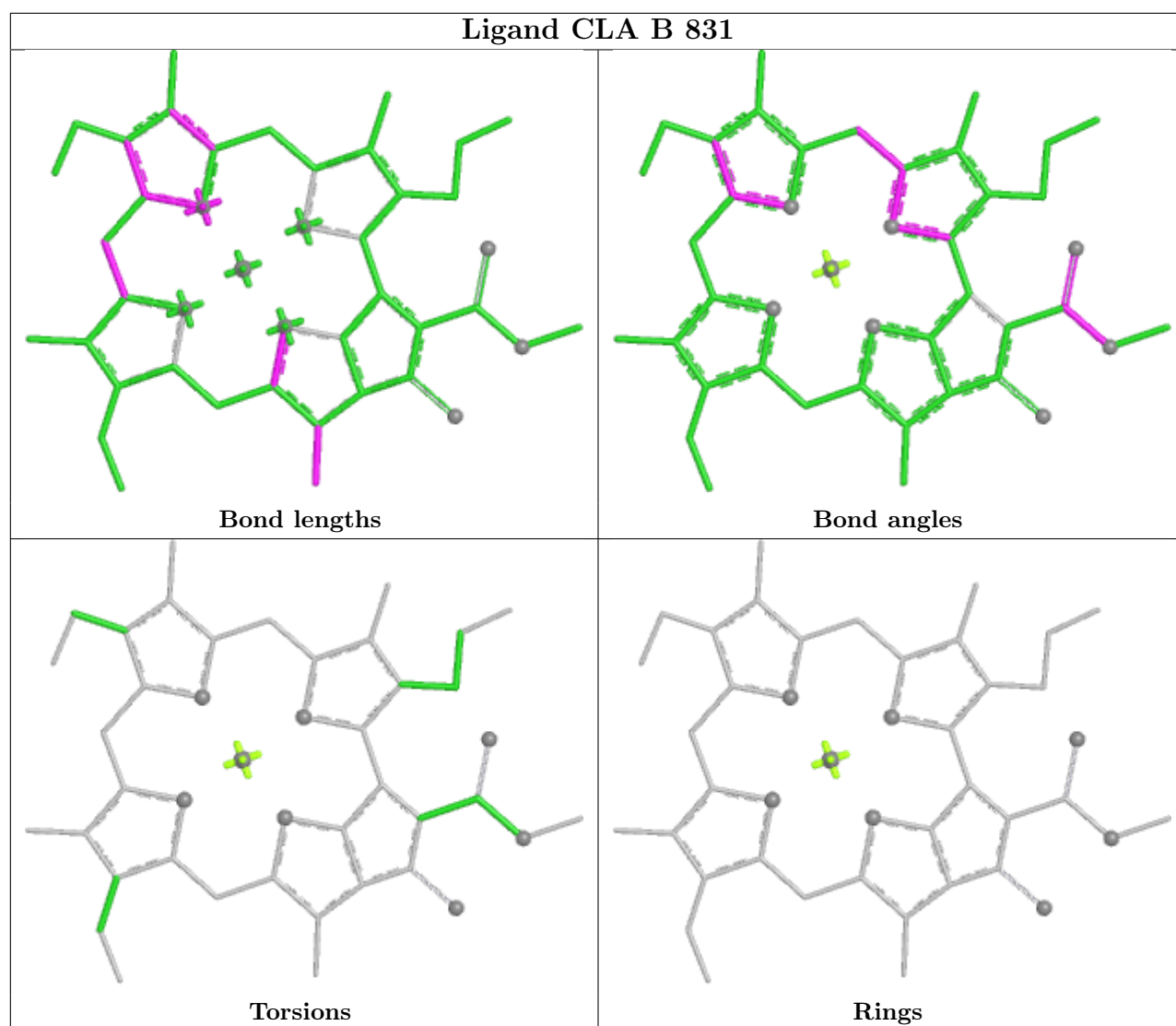
Rings

Ligand CLA 4 614



Ligand LUT 4 616





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.

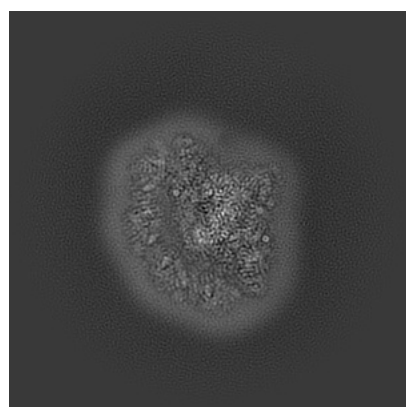
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-36037. These allow visual inspection of the internal detail of the map and identification of artifacts.

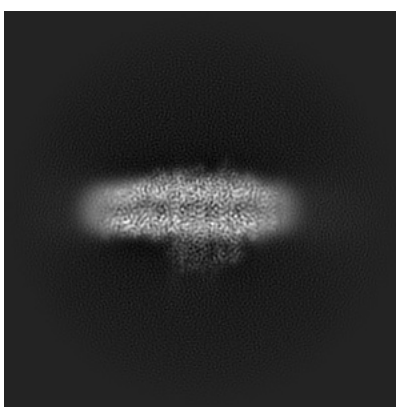
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

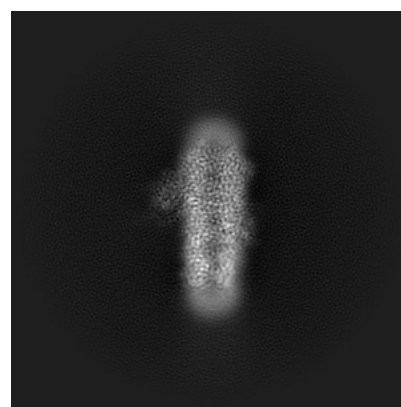
6.1.1 Primary map



X



Y

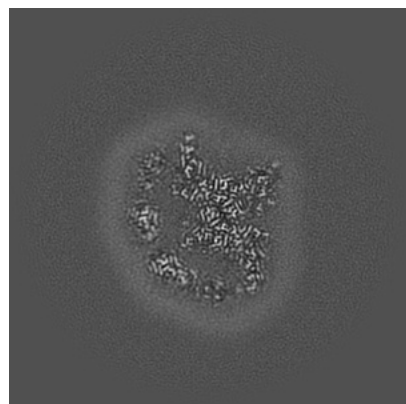


Z

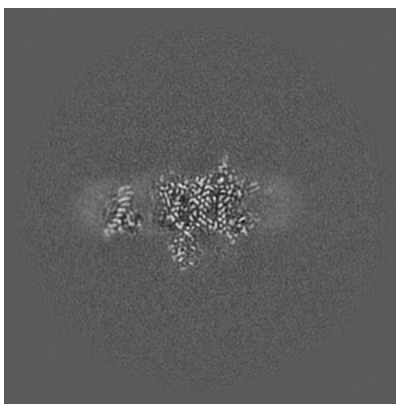
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

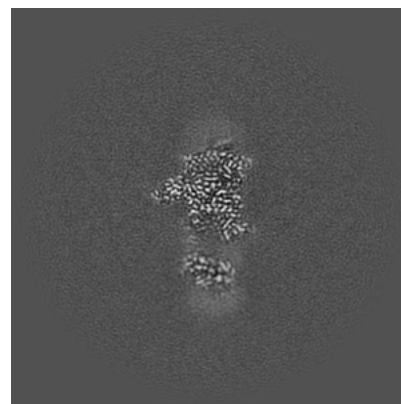
6.2.1 Primary map



X Index: 168



Y Index: 168

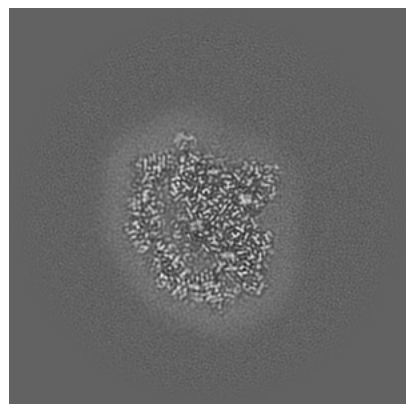


Z Index: 168

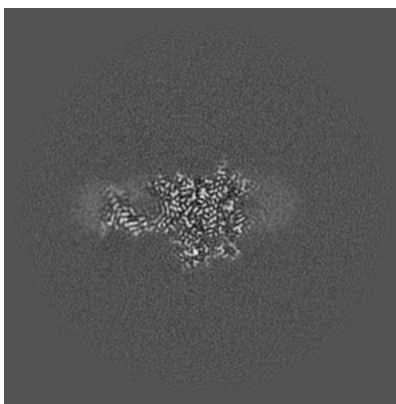
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

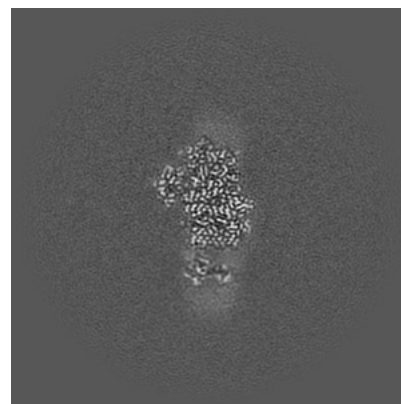
6.3.1 Primary map



X Index: 157



Y Index: 174

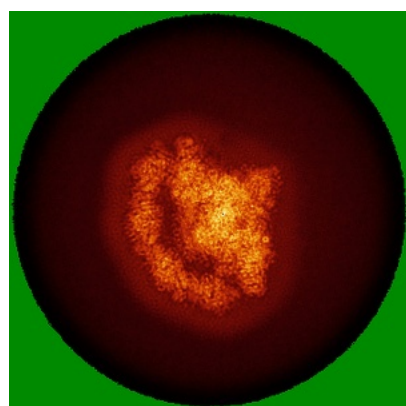


Z Index: 182

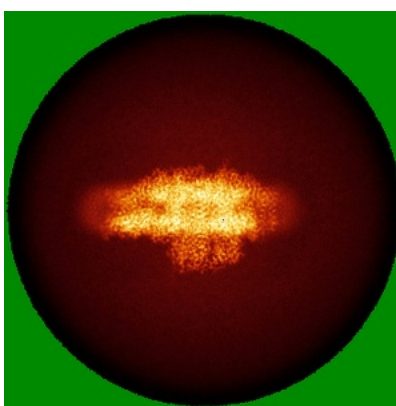
The images above show the largest variance slices of the map in three orthogonal directions.

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

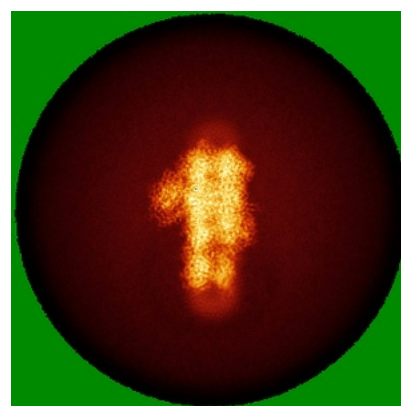
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views

This section was not generated.

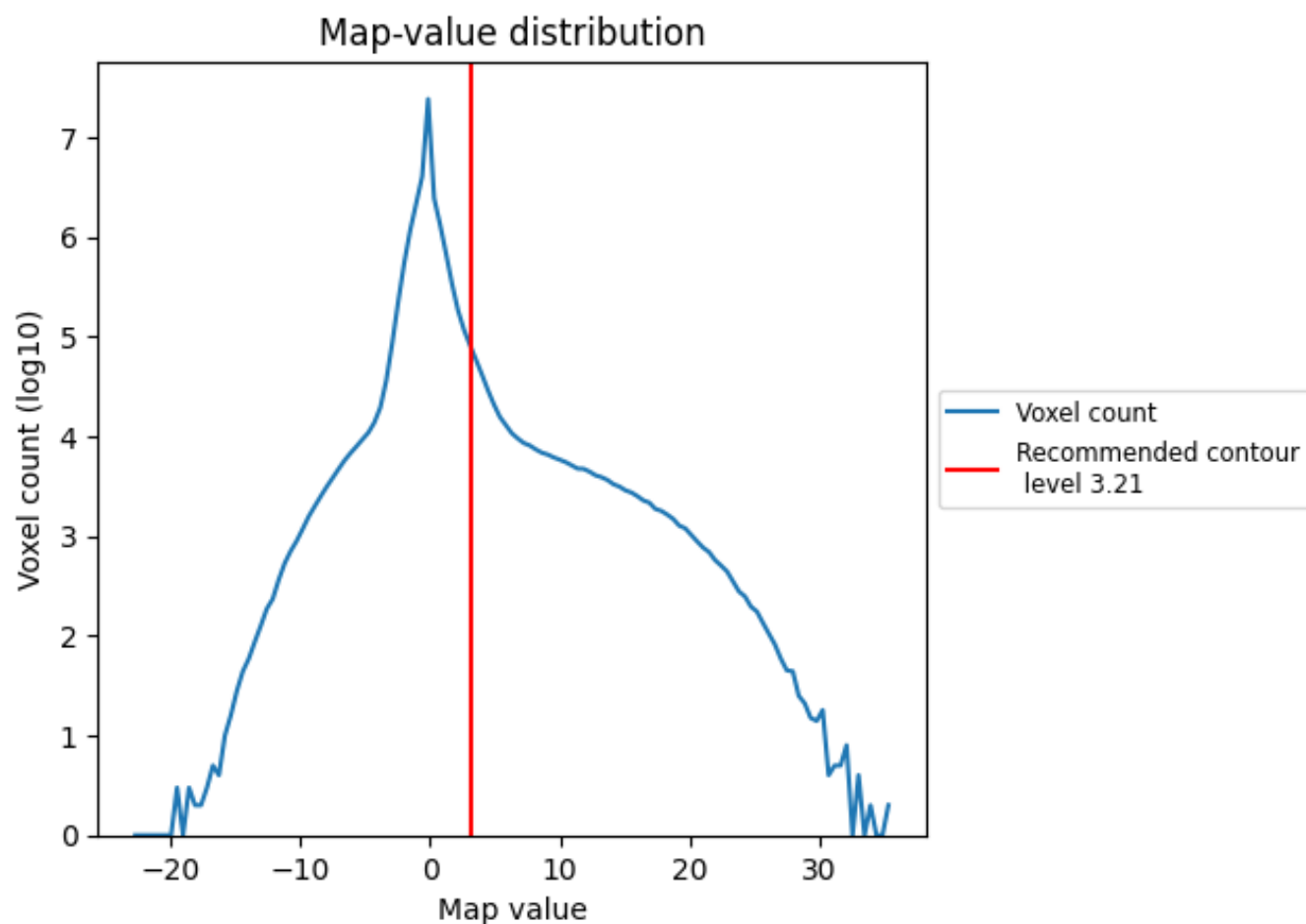
6.6 Mask visualisation

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

7 Map analysis [i](#)

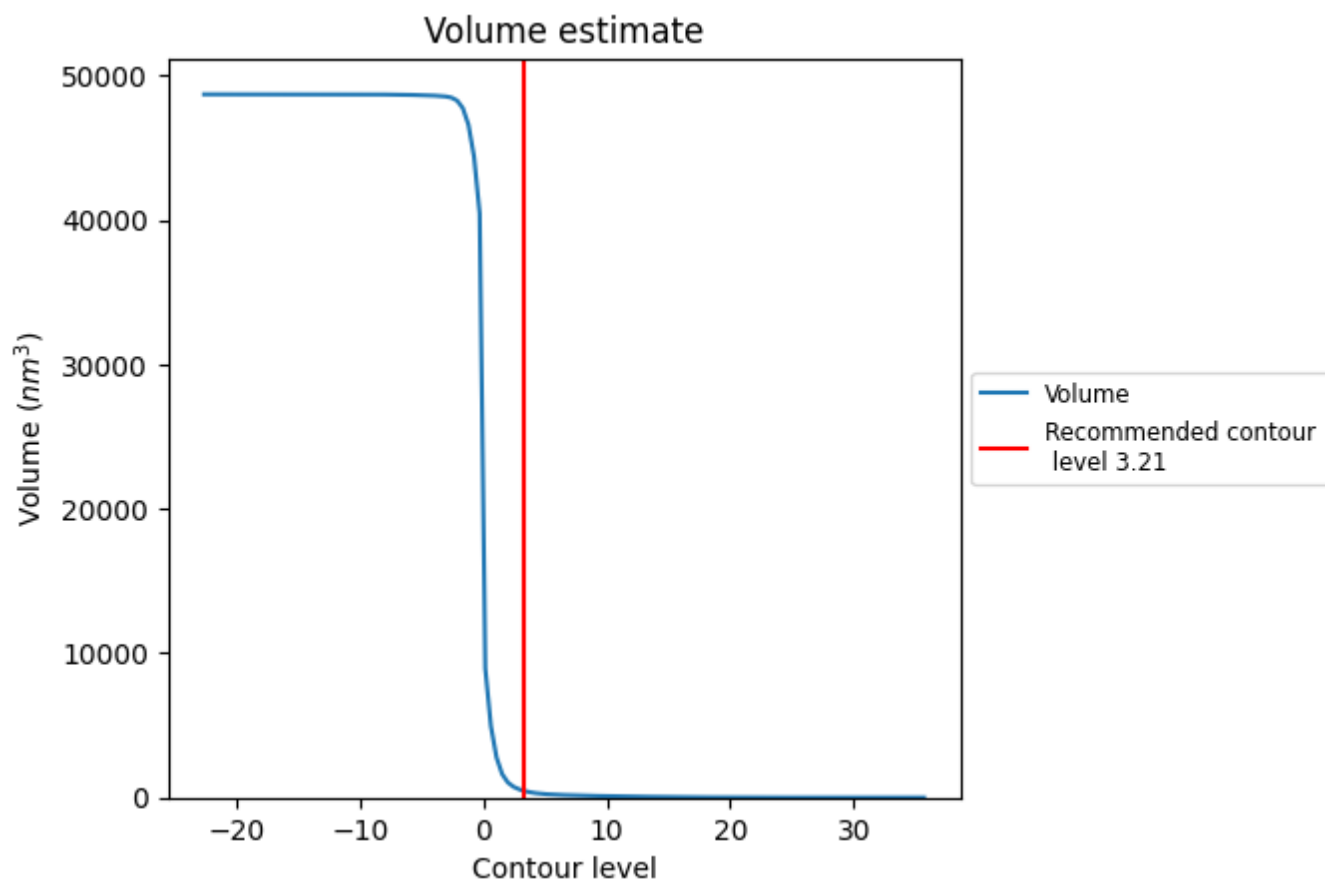
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

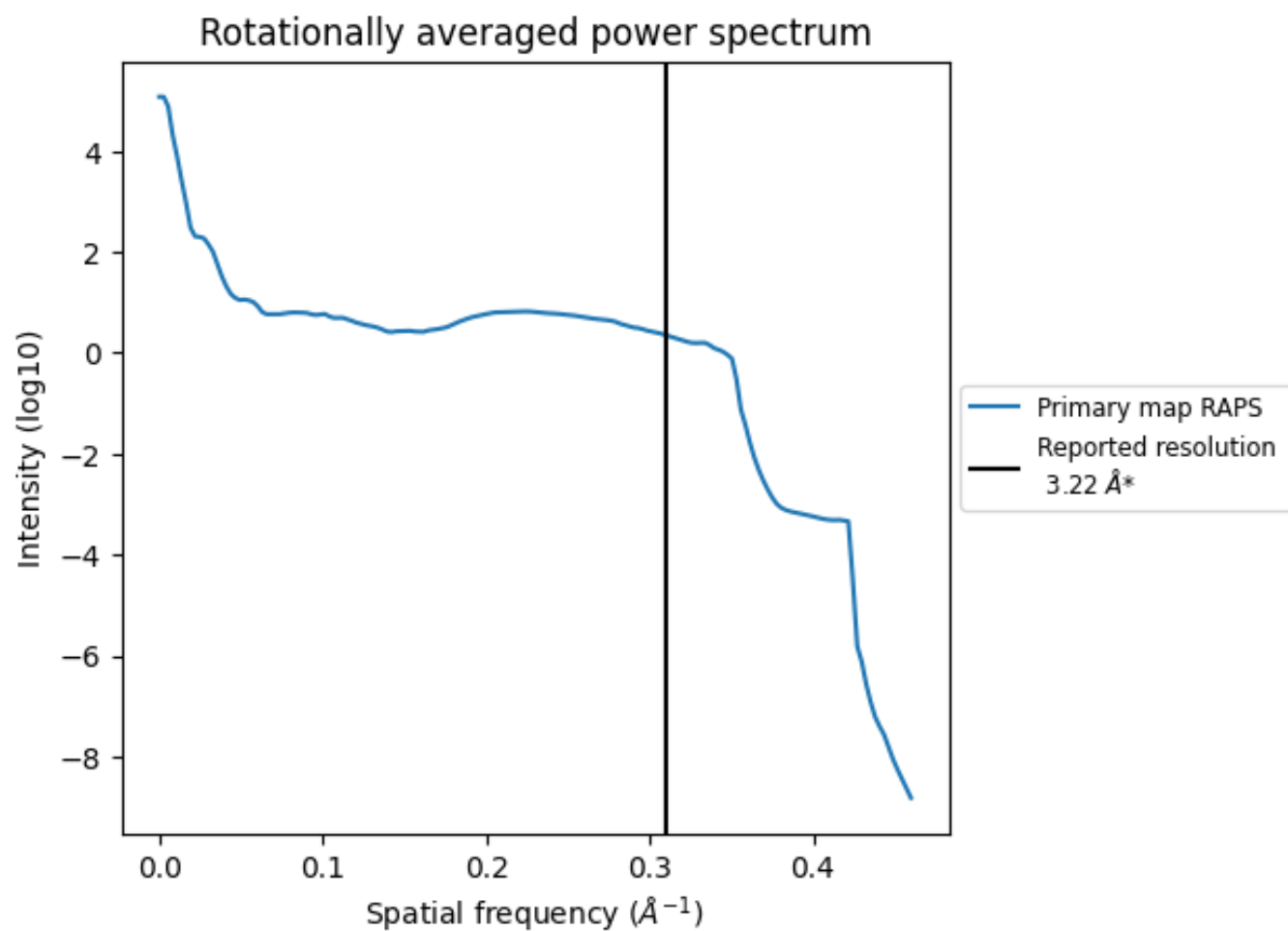
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 489 nm³; this corresponds to an approximate mass of 442 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 0.311 Å⁻¹

8 Fourier-Shell correlation

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

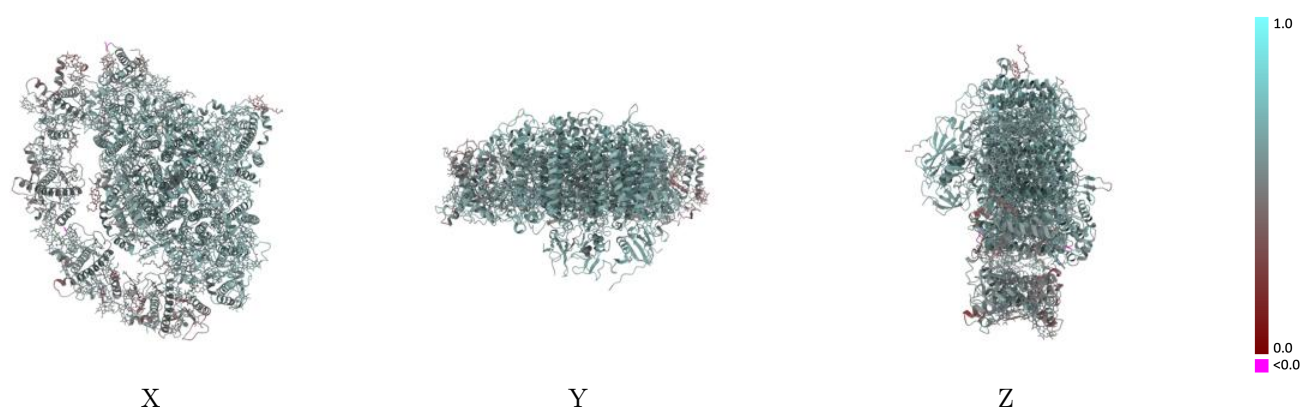
9 Map-model fit [i](#)

This section contains information regarding the fit between EMD map EMD-36037 and PDB model 8J7B. Per-residue inclusion information can be found in section 3 on page 26.

9.1 Map-model overlay [i](#)

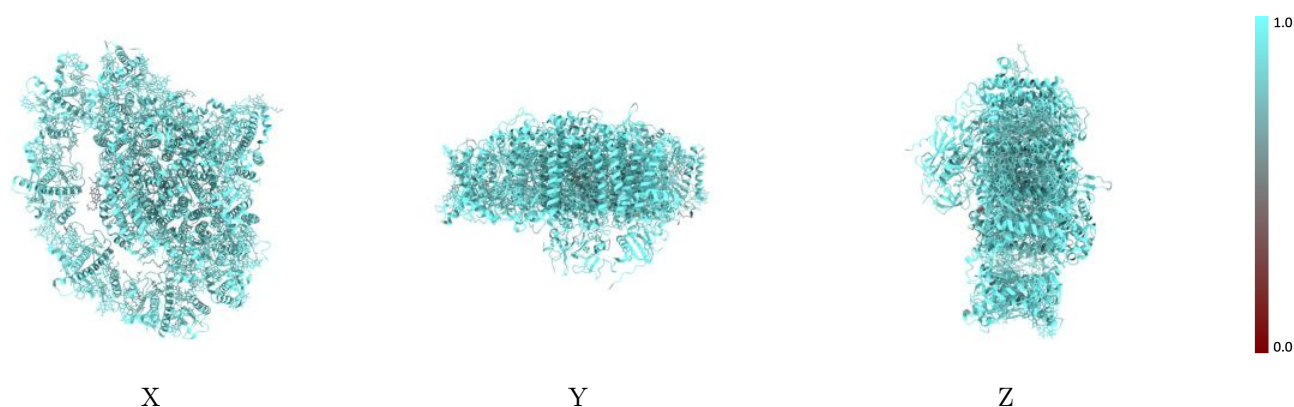
This section was not generated.

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



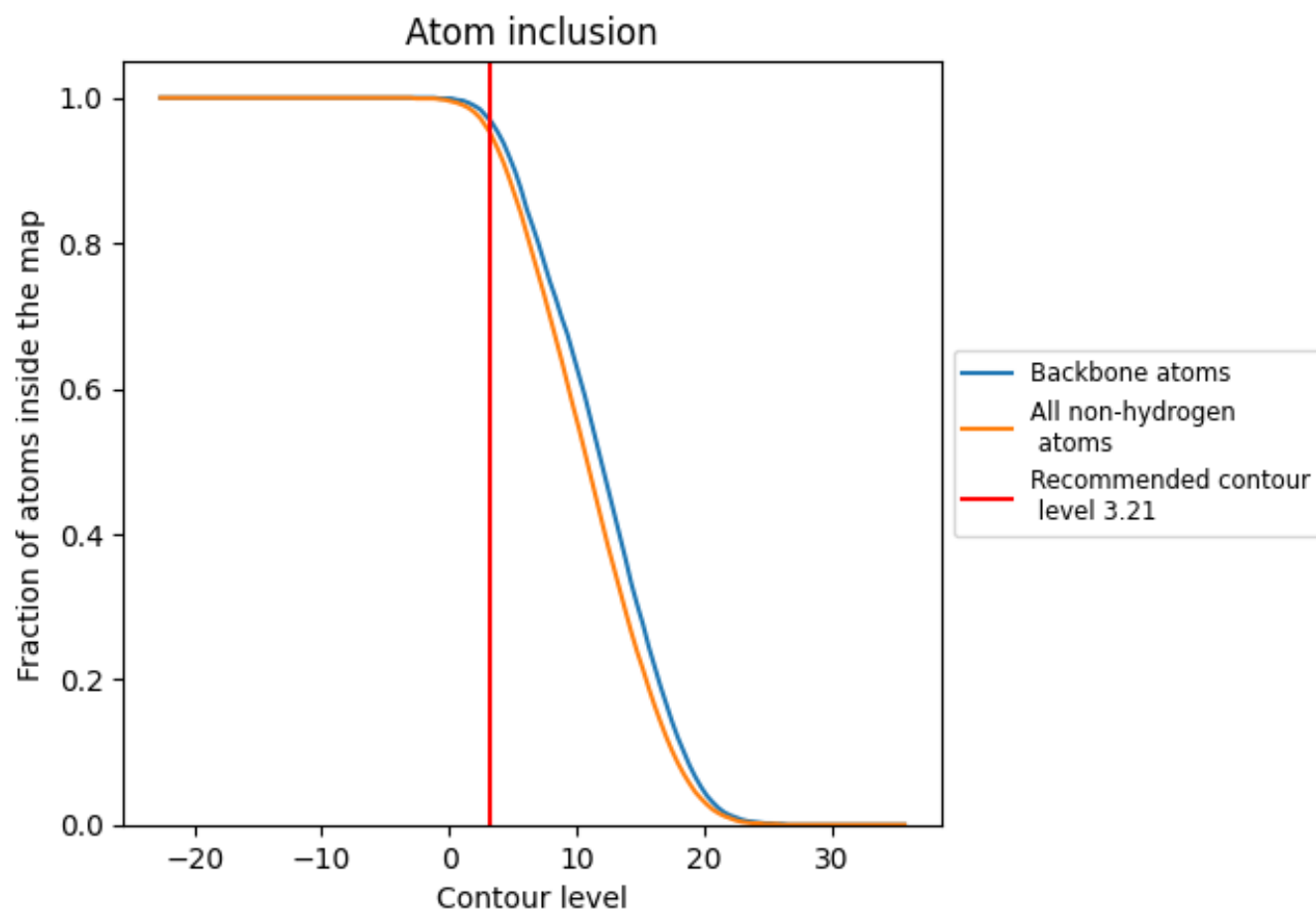
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (3.21).

9.4 Atom inclusion [i](#)



At the recommended contour level, 97% of all backbone atoms, 95% 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 (3.21) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9520	0.5760
1	0.9220	0.4980
2	0.9450	0.5180
3	0.9450	0.5120
4	0.9520	0.5350
A	0.9570	0.6050
B	0.9670	0.6150
C	0.9810	0.6130
D	0.9770	0.6080
E	0.9760	0.6050
F	0.9210	0.5690
G	0.9520	0.5730
H	0.9350	0.5650
I	0.9790	0.6000
J	0.8600	0.5340
K	0.8620	0.4680
L	0.9610	0.5960

1.0

0.0

<0.0