



Full wwPDB EM Validation Report ⓘ

May 22, 2024 – 04:35 PM JST

PDB ID : 8J7A
EMDB ID : EMD-36036
Title : Coordinates of Cryo-EM structure of the Arabidopsis thaliana PSI in state 1 (PSI-ST1)
Authors : Chen, S.J.B.; Wu, J.H.; Sui, S.F.; Zhang, L.X.
Deposited on : 2023-04-27
Resolution : 3.06 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.dev92
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36.2

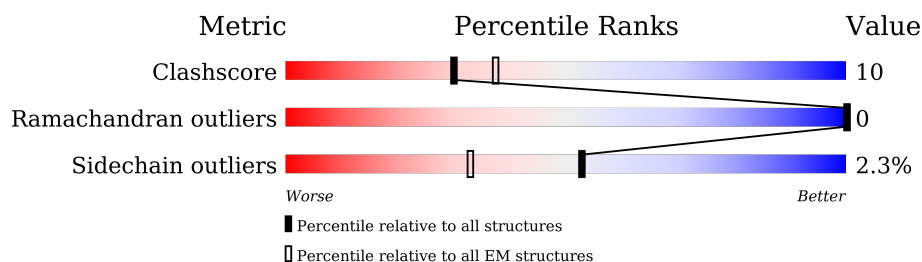
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.06 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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	
2	2	257	
3	3	273	
4	4	251	
5	A	750	
6	B	734	
7	C	81	
8	D	204	

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Mol	Chain	Length	Quality of chain
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	-	-	-
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	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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	-	-	-
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	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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	B	802	X	-	-	-
18	CLA	B	803	X	-	-	-
18	CLA	B	804	X	-	-	-
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	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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	-	-	-
18	CLA	G	203	X	-	-	-
18	CLA	H	201	X	-	-	-
18	CLA	K	201	X	-	-	-
18	CLA	K	203	X	-	-	-
18	CLA	K	204	X	-	-	-
18	CLA	L	302	X	-	-	-
18	CLA	L	303	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
18	CLA	L	304	X	-	-	-
24	CL0	A	801	X	-	-	-

2 Entry composition [i](#)

There are 27 unique types of molecules in this entry. The entry contains 34246 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	166	Total	C	N	O	S	0	0
			1296	844	215	232	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	217	Total	C	N	O	S	0	0
			1661	1085	269	302	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	709	Total	C	N	O	S	0	0
			5582	3662	946	956	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	149	Total	C	N	O	S	0	0
			1183	773	203	204	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	86	Total	C	N	O	0	0
			660	431	104	125		

- 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		

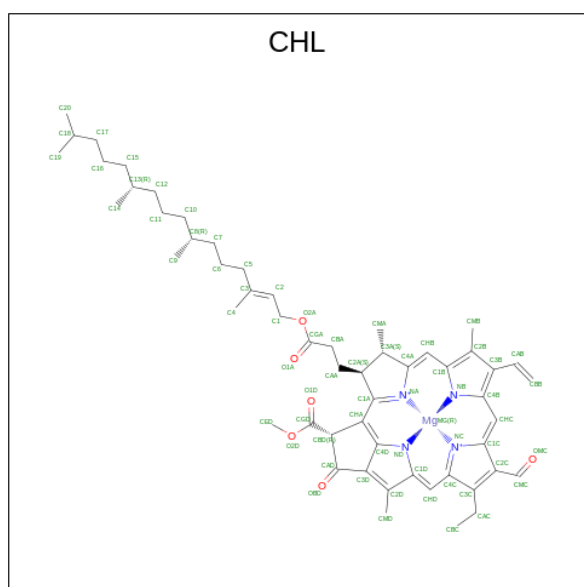
- Molecule 15 is a protein called Photosystem I reaction center subunit psaK, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	K	56	Total	C	N	O	S	0	0
			397	256	64	74	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	L	159	Total	C	N	O	S	0	0
			1200	795	190	213	2		

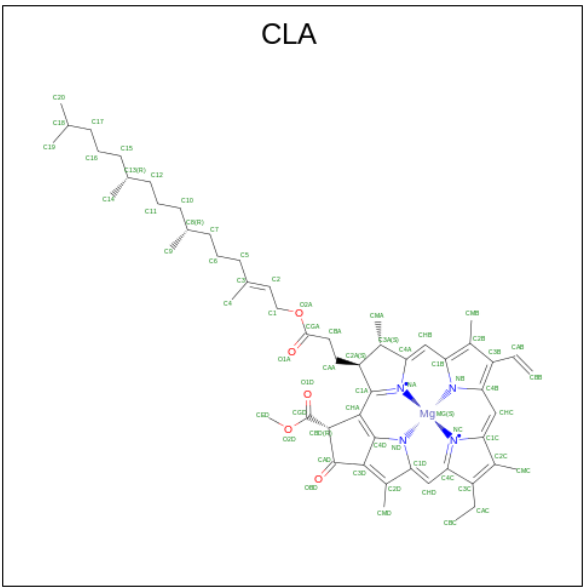
- Molecule 17 is CHLOROPHYLL B (three-letter code: CHL) (formula: $C_{55}H_{70}MgN_4O_6$) (labeled as "Ligand of Interest" by depositor).



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Mol	Chain	Residues	Atoms					AltConf
17	2	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
17	2	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
17	2	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
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 (three-letter code: CLA) (formula: C₅₅H₇₂MgN₄O₅) (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
			43	34	1	4	4	
18	2	1	Total	C	Mg	N	O	0
			65	55	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	35	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
			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
			47	37	1	4	5	
18	2	1	Total	C	Mg	N	O	0
			45	35	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
			54	44	1	4	5	
18	3	1	Total	C	Mg	N	O	0
			55	45	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
			45	35	1	4	5	
18	3	1	Total	C	Mg	N	O	0
			36	30	1	4	1	
18	3	1	Total	C	Mg	N	O	0
			60	50	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
			41	33	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
			45	35	1	4	5	
18	4	1	Total	C	Mg	N	O	0
			44	34	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
			60	50	1	4	5	
18	4	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
18	4	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
18	4	1	Total	C	Mg	N	O	0
			50	40	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
			57	47	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
			45	35	1	4	5	

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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
			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
			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
			50	40	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
			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
			52	42	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
			55	45	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
			55	45	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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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
			52	42	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
			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
			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
			60	50	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
			50	40	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
			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
			54	44	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
			41	33	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	

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Mol	Chain	Residues	Atoms					AltConf
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
			55	45	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
			62	52	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
			52	42	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
			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
			59	49	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
			43	35	1	4	3	
18	B	1	Total	C	Mg	N	O	0
			56	46	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
			43	35	1	4	3	

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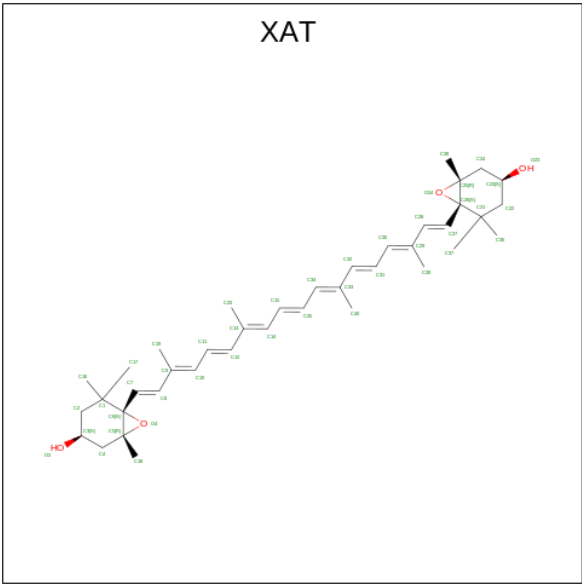
Mol	Chain	Residues	Atoms					AltConf
18	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			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
			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
			60	50	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
			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
			54	44	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
18	F	1	Total	C	Mg	N	O	0
			51	41	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	G	1	Total	C	Mg	N	O	0
			42	34	1	4	3	

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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
			45	35	1	4	5	
18	H	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
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	K	1	Total	C	Mg	N	O	0
			37	31	1	4	1	
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 (three-letter code: XAT) (formula: C₄₀H₅₆O₄).



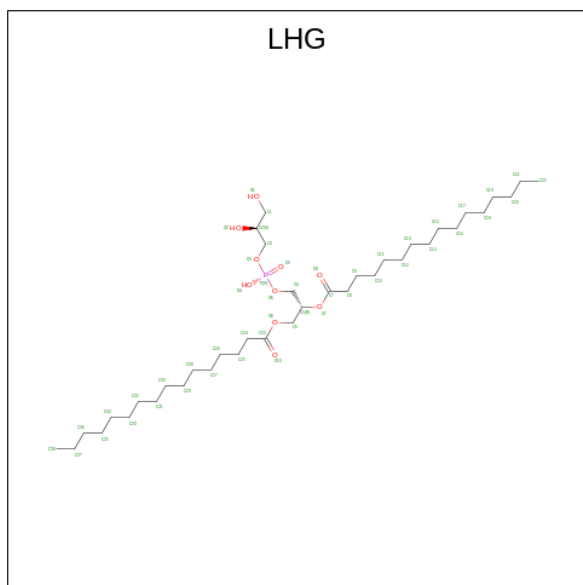
Mol	Chain	Residues	Atoms			AltConf
19	1	1	Total	C	O	0
			44	40	4	
19	2	1	Total	C	O	0
			44	40	4	

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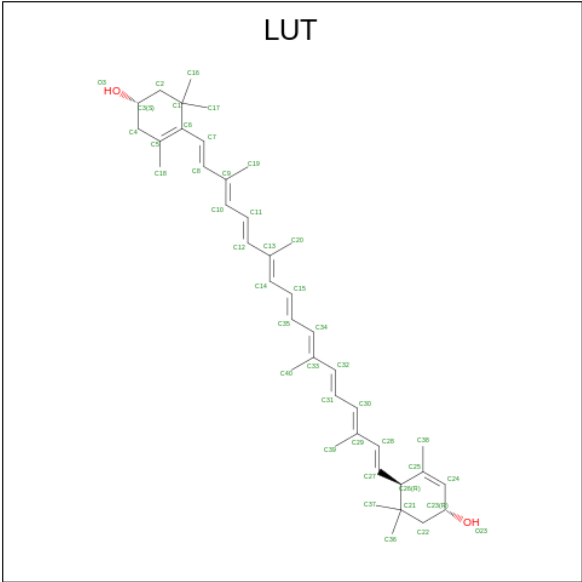
Mol	Chain	Residues	Atoms			AltConf
19	4	1	Total	C	O	0
			44	40	4	

- Molecule 20 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: $C_{38}H_{75}O_{10}P$).



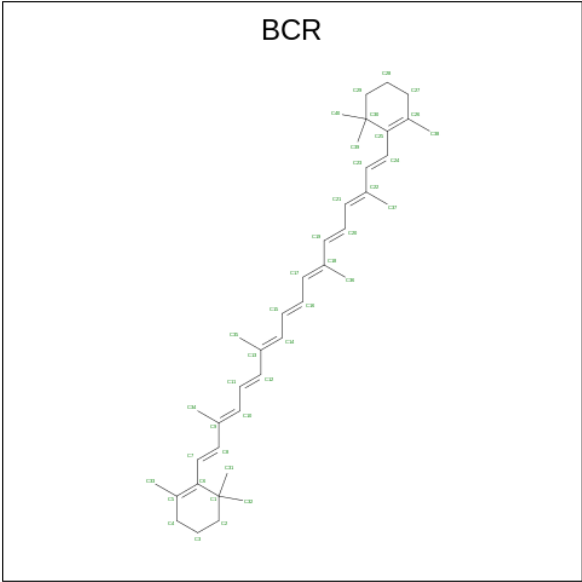
Mol	Chain	Residues	Atoms				AltConf
20	1	1	Total	C	O	P	0
			49	38	10	1	
20	2	1	Total	C	O	P	0
			37	26	10	1	
20	A	1	Total	C	O	P	0
			30	19	10	1	
20	A	1	Total	C	O	P	0
			49	38	10	1	
20	B	1	Total	C	O	P	0
			38	27	10	1	
20	B	1	Total	C	O	P	0
			49	38	10	1	

- Molecule 21 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (three-letter code: LUT) (formula: $C_{40}H_{56}O_2$).



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 (three-letter code: BCR) (formula: C₄₀H₅₆).



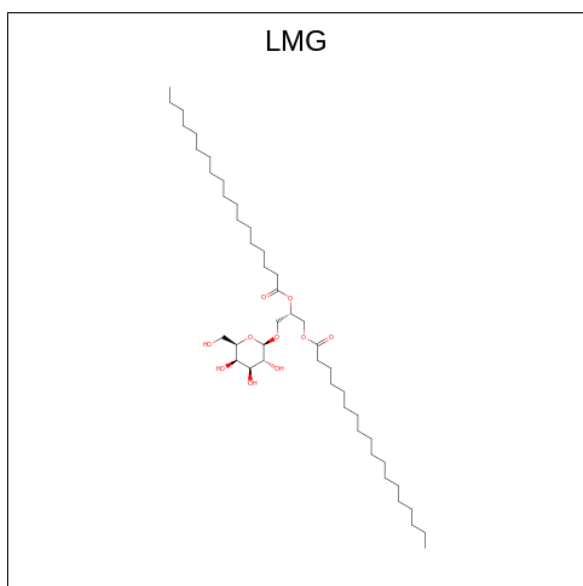
Mol	Chain	Residues	Atoms	AltConf
22	3	1	Total C 40 40	0
22	4	1	Total C 40 40	0
22	A	1	Total C 40 40	0
22	A	1	Total C 40 40	0
22	A	1	Total C 40 40	0
22	A	1	Total C 40 40	0
22	A	1	Total C 40 40	0
22	A	1	Total C 40 40	0
22	B	1	Total C 40 40	0
22	B	1	Total C 40 40	0
22	B	1	Total C 40 40	0
22	B	1	Total C 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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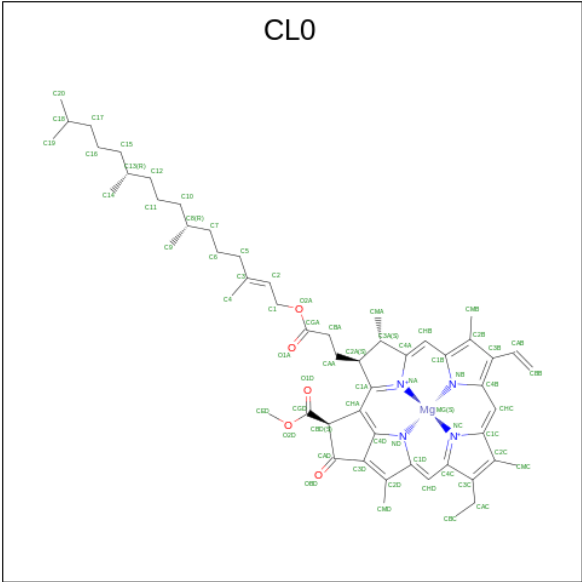
Mol	Chain	Residues	Atoms		AltConf
22	L	1	Total	C	0
			40	40	
22	L	1	Total	C	0
			40	40	
22	L	1	Total	C	0
			40	40	

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



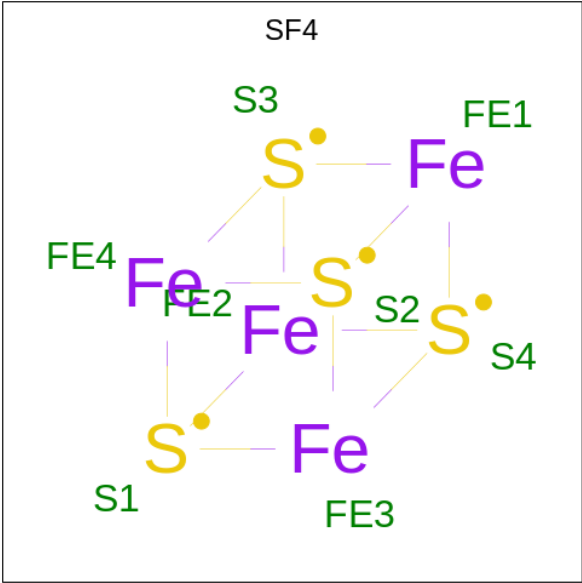
Mol	Chain	Residues	Atoms			AltConf
23	4	1	Total	C	O	0
			33	23	10	
23	4	1	Total	C	O	0
			39	29	10	

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



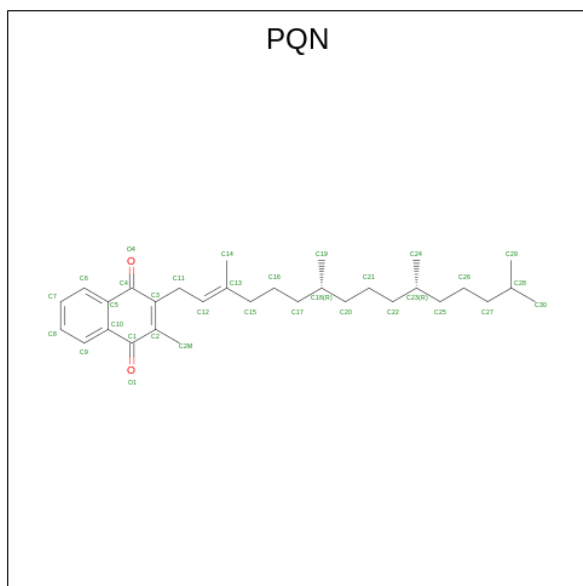
Mol	Chain	Residues	Atoms					AltConf
24	A	1	Total	C	Mg	N	O	0
			60	52	1	4	3	

- Molecule 25 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



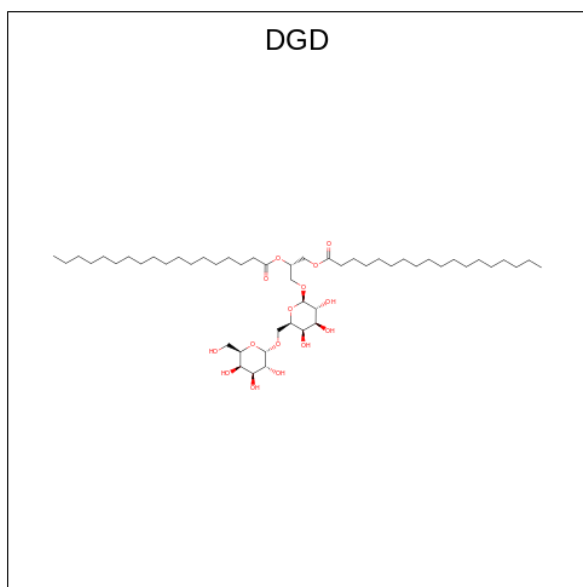
Mol	Chain	Residues	Atoms			AltConf
25	A	1	Total	Fe	S	0
			8	4	4	
25	C	1	Total	Fe	S	0
			8	4	4	
25	C	1	Total	Fe	S	0
			8	4	4	

- Molecule 26 is PHYLLOQUINONE (three-letter code: PQN) (formula: $C_{31}H_{46}O_2$).



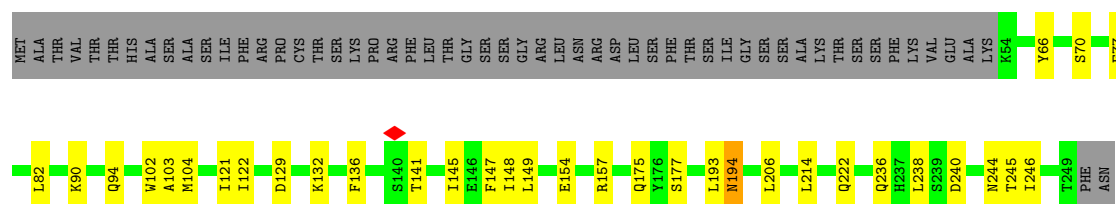
Mol	Chain	Residues	Atoms			AltConf
26	A	1	Total	C	O	0
			33	31	2	
26	B	1	Total	C	O	0
			33	31	2	

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




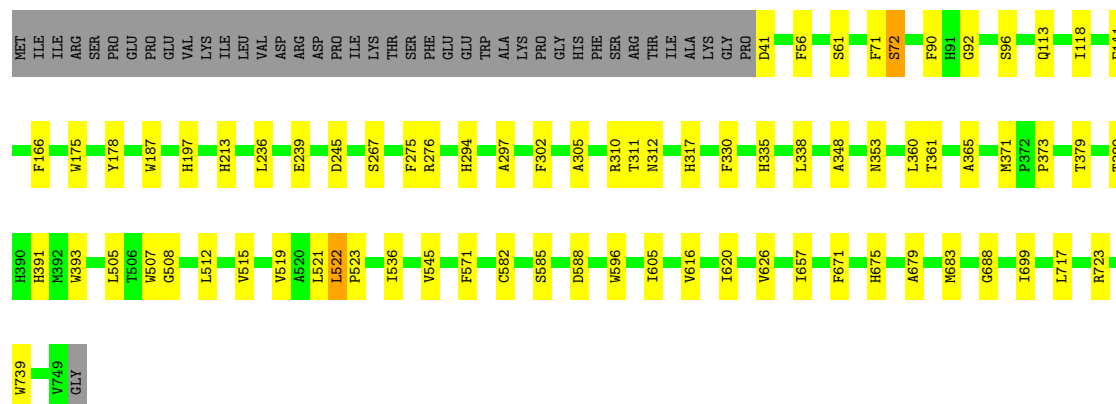
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
27	B	1	66	51	15	0

Chain 4:  65% 13% 22%



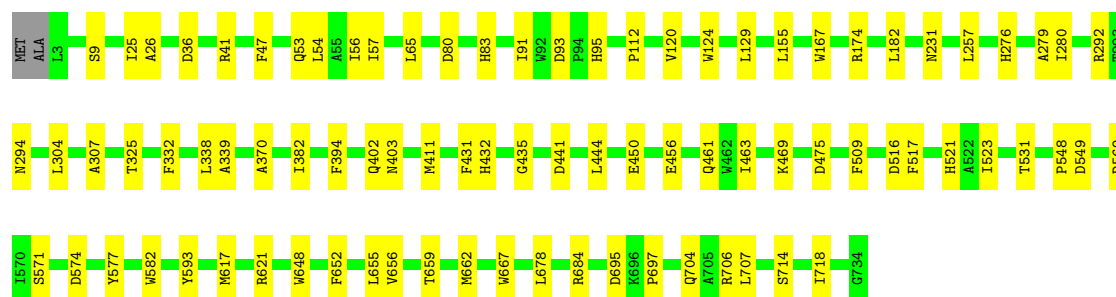
- Molecule 5: Photosystem I P700 chlorophyll a apoprotein A1

Chain A:  85% 10% 5%




- Molecule 6: Photosystem I P700 chlorophyll a apoprotein A2

Chain B:  88% 12%



- Molecule 7: Photosystem I iron-sulfur center

Chain C:  84% 15%



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

Chain D:  64% 6% 30%

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

Chain E: 41% . 55%

- Molecule 10: Photosystem I reaction center subunit III, chloroplastic

Chain F:  60% 8% 33%

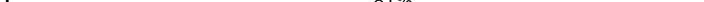
- Molecule 11: Photosystem I reaction center subunit V, chloroplastic

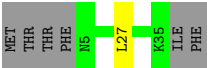
Chain G:  50% 5% • 43%

- Molecule 12: Photosystem I reaction center subunit VI-2, chloroplatic

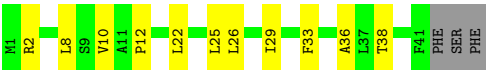
Chain H: 54% 5% • 41%

- Molecule 13: Photosystem I reaction center subunit VIII

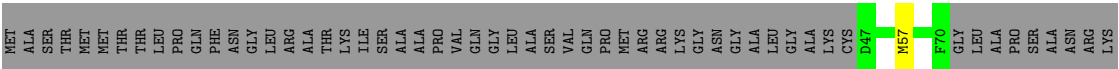
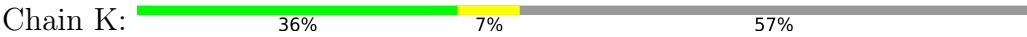
Chain I:  81% • 16%



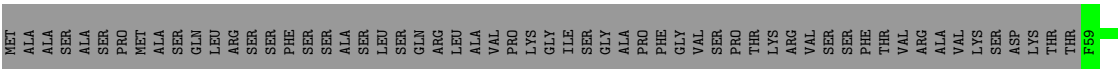
● Molecule 14: Photosystem I reaction center subunit IX



● 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	95588	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	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	48.607	Depositor
Minimum map value	-26.329	Depositor
Average map value	0.002	Depositor
Map value standard deviation	1.028	Depositor
Recommended contour level	2.57	Depositor
Map size (\AA)	410.88, 410.88, 410.88	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.07, 1.07, 1.07	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.28	0/1336	0.50	1/1816 (0.1%)
2	2	0.26	0/1622	0.47	0/2219
3	3	0.27	0/1712	0.46	0/2329
4	4	0.27	0/1599	0.43	0/2178
5	A	0.27	0/5772	0.44	0/7878
6	B	0.27	0/6065	0.45	0/8279
7	C	0.28	0/629	0.55	0/852
8	D	0.26	0/1157	0.49	0/1563
9	E	0.28	0/528	0.48	0/715
10	F	0.26	0/1213	0.46	0/1637
11	G	0.29	0/724	0.58	1/981 (0.1%)
12	H	0.26	0/680	0.43	0/927
13	I	0.26	0/245	0.39	0/333
14	J	0.26	0/336	0.50	0/458
15	K	0.25	0/401	0.43	0/542
16	L	0.27	0/1237	0.44	0/1690
All	All	0.27	0/25256	0.46	2/34397 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	G	64	PRO	CA-N-CD	-10.65	96.59	111.50
1	1	104	PRO	CA-N-CD	-8.76	99.23	111.50

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	1296	0	1277	38	0
2	2	1566	0	1519	23	0
3	3	1661	0	1625	27	0
4	4	1551	0	1508	39	0
5	A	5582	0	5436	56	0
6	B	5854	0	5646	70	0
7	C	616	0	600	10	0
8	D	1128	0	1134	6	0
9	E	517	0	526	3	0
10	F	1183	0	1215	9	0
11	G	708	0	700	9	0
12	H	660	0	650	5	0
13	I	239	0	258	1	0
14	J	327	0	342	12	0
15	K	397	0	409	5	0
16	L	1200	0	1202	13	0
17	1	93	0	62	7	0
17	2	226	0	150	5	0
17	3	45	0	30	1	0
17	4	169	0	100	5	0
18	1	496	0	354	28	0
18	2	434	0	352	27	0
18	3	498	0	377	19	0
18	4	527	0	412	28	0
18	A	2483	0	2456	130	0
18	B	2284	0	2242	100	0
18	F	149	0	123	10	0
18	G	132	0	97	1	0
18	H	60	0	59	2	0
18	K	128	0	91	1	0
18	L	155	0	138	8	0
19	1	44	0	56	9	0
19	2	44	0	56	6	0
19	4	44	0	52	20	0
20	1	49	0	74	20	0
20	2	37	0	44	0	0
20	A	79	0	104	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	B	87	0	120	1	0
21	1	42	0	56	9	0
21	2	84	0	112	13	0
21	3	42	0	56	7	0
21	4	42	0	56	3	0
22	3	40	0	56	2	0
22	4	40	0	56	8	0
22	A	240	0	336	31	0
22	B	320	0	448	51	0
22	F	40	0	56	2	0
22	G	40	0	56	3	0
22	I	40	0	56	3	0
22	J	40	0	56	4	0
22	K	80	0	112	9	0
22	L	120	0	168	14	0
23	4	72	0	84	1	0
24	A	60	0	68	7	0
25	A	8	0	0	0	0
25	C	16	0	0	0	0
26	A	33	0	46	6	0
26	B	33	0	46	2	0
27	B	66	0	96	8	0
All	All	34246	0	33616	675	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 10.

All (675) 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)
21:2:619:LUT:H8	21:2:619:LUT:H181	1.55	0.88
18:1:604:CLA:HMB3	19:1:614:XAT:H162	1.55	0.86
4:4:77:PHE:HE2	19:4:617:XAT:C38	1.88	0.85
6:B:54:LEU:HD12	18:B:813:CLA:HED1	1.65	0.79
2:2:143:VAL:HG22	18:4:613:CLA:HBA2	1.64	0.78
18:A:804:CLA:HBD	18:A:804:CLA:HBA2	1.64	0.77
18:A:809:CLA:HMC3	18:A:810:CLA:HMD2	1.66	0.77
22:4:618:BCR:H342	17:4:605:CHL:HHB	1.67	0.76
14:J:10:VAL:HG12	14:J:12:PRO:HD2	1.66	0.76
4:4:77:PHE:HE2	19:4:617:XAT:H383	1.50	0.76
18:A:829:CLA:H202	22:J:102:BCR:H19C	1.68	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:103:ALA:HB2	19:4:617:XAT:C20	2.15	0.75
6:B:25:ILE:HD11	22:L:305:BCR:H312	1.69	0.75
1:1:155:GLN:HG3	18:1:607:CLA:HMC3	1.69	0.75
14:J:25:LEU:O	14:J:29:ILE:HD12	1.87	0.75
18:B:814:CLA:H3A	22:B:845:BCR:H393	1.68	0.74
22:A:853:BCR:H12C	22:A:853:BCR:H341	1.67	0.74
22:B:801:BCR:H12C	22:B:801:BCR:H341	1.67	0.74
17:1:601:CHL:HAA1	20:1:615:LHG:H142	1.69	0.74
18:B:832:CLA:HHC	18:B:832:CLA:HBB1	1.71	0.72
22:A:850:BCR:H16C	22:A:850:BCR:H351	1.70	0.72
4:4:103:ALA:HB2	19:4:617:XAT:H202	1.71	0.72
22:L:306:BCR:H321	22:L:306:BCR:HC8	1.70	0.72
21:4:616:LUT:H8	21:4:616:LUT:H171	1.72	0.71
5:A:311:THR:HG22	5:A:312:ASN:H	1.55	0.71
20:1:615:LHG:HC32	20:1:615:LHG:HC91	1.70	0.71
1:1:156:ARG:NH2	18:1:608:CLA:O1D	2.23	0.71
22:B:848:BCR:H403	22:B:848:BCR:H23C	1.72	0.71
15:K:111:THR:O	15:K:115:ILE:HD12	1.92	0.70
22:K:205:BCR:H321	22:K:205:BCR:HC8	1.74	0.70
1:1:237:VAL:HG13	1:1:238:ILE:HG12	1.72	0.69
5:A:175:TRP:HB2	18:A:812:CLA:HMC3	1.72	0.69
22:3:614:BCR:H403	22:3:614:BCR:H23C	1.74	0.69
18:A:826:CLA:HMA3	18:A:822:CLA:HMB2	1.75	0.68
6:B:517:PHE:HA	18:B:837:CLA:HED1	1.75	0.68
22:J:102:BCR:HC8	22:J:102:BCR:H311	1.75	0.68
1:1:172:PHE:HB3	18:1:609:CLA:HMD2	1.74	0.68
18:A:803:CLA:HBA2	6:B:655:LEU:HB2	1.75	0.68
20:1:615:LHG:H132	20:1:615:LHG:H281	1.74	0.68
21:3:613:LUT:H401	21:3:613:LUT:H15	1.76	0.68
4:4:121:ILE:HG22	4:4:122:ILE:HG23	1.75	0.68
4:4:82:LEU:HD13	18:4:602:CLA:H42	1.75	0.67
22:B:849:BCR:H373	10:F:150:PHE:HE1	1.58	0.67
22:L:305:BCR:H321	22:L:305:BCR:HC8	1.75	0.67
18:A:804:CLA:H161	18:A:809:CLA:H143	1.76	0.67
2:2:104:GLY:HA3	19:2:617:XAT:H192	1.77	0.66
20:1:615:LHG:H342	20:1:615:LHG:H201	1.77	0.66
5:A:585:SER:OG	5:A:588:ASP:OD2	2.14	0.66
18:A:830:CLA:HBD	18:A:830:CLA:HBA1	1.78	0.66
16:L:209:LEU:HD13	18:L:304:CLA:HED3	1.78	0.65
5:A:393:TRP:CD1	18:A:829:CLA:HAB	2.31	0.65
4:4:77:PHE:CE2	19:4:617:XAT:H383	2.31	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:2:617:XAT:H401	19:2:617:XAT:H15	1.79	0.64
16:L:65:ILE:HA	16:L:75:GLU:HG3	1.77	0.64
15:K:102:THR:HG22	15:K:104:ALA:H	1.61	0.64
3:3:233:MET:HE3	18:3:601:CLA:HMC3	1.78	0.64
18:1:612:CLA:H3A	21:1:616:LUT:H383	1.80	0.64
18:3:612:CLA:HAB	18:3:607:CLA:HBA1	1.80	0.64
22:B:801:BCR:HC8	22:B:801:BCR:H331	1.80	0.64
22:B:847:BCR:HC8	22:B:847:BCR:H311	1.80	0.63
18:4:604:CLA:C2B	19:4:617:XAT:H182	2.28	0.63
18:A:805:CLA:HMA2	18:A:812:CLA:HMD2	1.79	0.63
11:G:119:LEU:HA	11:G:128:ASN:ND2	2.13	0.63
18:B:813:CLA:H2	18:B:805:CLA:H52	1.81	0.63
18:B:841:CLA:HED1	18:B:822:CLA:HAB	1.80	0.63
18:1:604:CLA:HBA1	18:1:604:CLA:HBD	1.80	0.63
18:B:805:CLA:H2	18:B:805:CLA:H92	1.81	0.63
22:A:851:BCR:H16C	22:A:851:BCR:H351	1.80	0.63
5:A:335:HIS:HB3	5:A:338:LEU:HD12	1.79	0.63
1:1:103:VAL:HG13	1:1:107:LEU:HD13	1.81	0.62
18:A:802:CLA:H202	18:A:842:CLA:H2	1.81	0.62
4:4:77:PHE:HE2	19:4:617:XAT:H382	1.61	0.62
18:A:842:CLA:HBA2	20:A:846:LHG:H162	1.81	0.62
22:A:849:BCR:H383	22:A:849:BCR:H23C	1.81	0.62
3:3:171:LEU:HD21	18:3:612:CLA:HMC3	1.79	0.62
6:B:53:GLN:HB2	18:B:805:CLA:HMB2	1.81	0.62
22:B:845:BCR:H16C	22:B:845:BCR:H20C	1.81	0.62
4:4:175:GLN:OE1	4:4:175:GLN:N	2.24	0.62
22:4:618:BCR:HC8	22:4:618:BCR:H321	1.81	0.62
18:A:843:CLA:HMC2	18:B:839:CLA:H11	1.82	0.61
6:B:656:VAL:HG22	18:B:840:CLA:HMB3	1.82	0.61
3:3:260:ASP:OD2	3:3:263:ASN:ND2	2.33	0.61
6:B:704:GLN:HG3	27:B:850:DGD:HA22	1.82	0.61
1:1:168:PRO:HG2	18:1:609:CLA:HMD3	1.82	0.61
4:4:141:THR:O	4:4:145:ILE:HG13	1.99	0.61
18:A:812:CLA:H141	18:A:812:CLA:H203	1.81	0.61
22:A:853:BCR:HC8	22:A:853:BCR:H311	1.82	0.61
6:B:707:LEU:HD23	27:B:850:DGD:HA21	1.82	0.61
4:4:77:PHE:CE2	19:4:617:XAT:C38	2.78	0.61
18:1:604:CLA:C4A	18:1:604:CLA:H12	2.31	0.61
20:1:615:LHG:H362	18:4:614:CLA:HAA2	1.83	0.61
5:A:505:LEU:HB2	5:A:521:LEU:HD23	1.83	0.61
7:C:24:ASP:OD2	8:D:161:HIS:ND1	2.33	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:97:ALA:HB1	19:1:614:XAT:H181	1.82	0.60
1:1:187:LEU:HD13	18:1:609:CLA:HAA2	1.83	0.60
22:A:851:BCR:H23C	22:A:851:BCR:H403	1.83	0.60
22:B:843:BCR:H16C	22:B:843:BCR:H351	1.83	0.60
22:A:850:BCR:H311	22:A:850:BCR:HC8	1.84	0.60
4:4:132:LYS:NZ	17:4:606:CHL:O1D	2.28	0.60
18:4:603:CLA:HMB2	19:4:617:XAT:C32	2.31	0.60
6:B:571:SER:OG	6:B:574:ASP:OD2	2.17	0.60
8:D:151:VAL:HG22	8:D:157:VAL:HG12	1.83	0.60
1:1:90:HIS:CD2	18:1:608:CLA:HMD1	2.36	0.60
22:K:205:BCR:H403	22:K:205:BCR:H23C	1.84	0.60
5:A:353:ASN:ND2	18:A:806:CLA:OBD	2.33	0.59
18:B:813:CLA:HMB1	18:B:813:CLA:HBB1	1.85	0.59
1:1:54:ARG:NH1	1:1:58:LEU:O	2.35	0.59
18:4:613:CLA:HBD	18:4:613:CLA:HBA1	1.83	0.59
22:A:848:BCR:H321	22:A:848:BCR:HC8	1.84	0.59
11:G:119:LEU:HA	11:G:128:ASN:HD21	1.67	0.59
18:A:828:CLA:HBB1	18:A:828:CLA:HMB1	1.84	0.59
22:B:846:BCR:HC8	22:B:846:BCR:H311	1.84	0.59
7:C:62:PHE:HD2	8:D:185:ILE:HG21	1.68	0.59
5:A:379:THR:HG21	5:A:515:VAL:HB	1.82	0.59
1:1:208:GLN:OE1	1:1:220:ASN:ND2	2.36	0.59
18:A:820:CLA:H91	18:A:820:CLA:H151	1.83	0.59
22:B:843:BCR:H311	22:B:843:BCR:HC8	1.85	0.58
18:1:603:CLA:HMD2	18:1:608:CLA:C1D	2.33	0.58
3:3:109:LEU:HD22	18:3:603:CLA:HBC1	1.84	0.58
5:A:739:TRP:HH2	18:A:809:CLA:HBC2	1.67	0.58
21:1:616:LUT:H391	21:1:616:LUT:H32	1.85	0.58
1:1:217:PRO:O	21:1:616:LUT:O23	2.22	0.58
20:A:846:LHG:H182	18:A:831:CLA:H203	1.86	0.58
18:F:302:CLA:HBA1	14:J:26:LEU:HD21	1.85	0.58
22:G:204:BCR:HC8	22:G:204:BCR:H311	1.86	0.58
5:A:338:LEU:HD13	18:A:825:CLA:HMD3	1.86	0.58
22:B:846:BCR:H323	20:B:852:LHG:H321	1.85	0.58
1:1:190:LYS:O	1:1:194:ASN:ND2	2.36	0.57
22:B:845:BCR:H362	18:B:828:CLA:H171	1.86	0.57
18:4:608:CLA:C1D	18:4:603:CLA:HMD2	2.34	0.57
20:1:615:LHG:H192	20:1:615:LHG:H361	1.87	0.57
6:B:36:ASP:O	6:B:41:ARG:NH1	2.37	0.57
6:B:155:LEU:HD11	18:B:811:CLA:HMD3	1.86	0.57
1:1:95:MET:SD	18:1:609:CLA:HAB	2.45	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:72:SER:OG	5:A:178:TYR:HB2	2.05	0.57
5:A:330:PHE:HD2	20:A:847:LHG:HC41	1.69	0.57
18:2:602:CLA:HMC2	19:2:617:XAT:H31	1.85	0.57
1:1:82:ARG:NH1	18:1:603:CLA:O1A	2.35	0.56
4:4:103:ALA:HB2	19:4:617:XAT:C13	2.35	0.56
18:A:820:CLA:HMB1	18:A:820:CLA:HBB1	1.87	0.56
6:B:523:ILE:HG21	18:B:836:CLA:HAB	1.87	0.56
2:2:155:ARG:NH2	18:2:608:CLA:O1D	2.35	0.56
16:L:170:THR:HG22	16:L:172:THR:H	1.71	0.56
18:2:604:CLA:HAB	17:2:605:CHL:C4C	2.35	0.56
18:A:804:CLA:H201	18:A:844:CLA:H203	1.87	0.56
6:B:469:LYS:NZ	6:B:509:PHE:O	2.36	0.56
22:B:849:BCR:H311	14:J:33:PHE:HD2	1.71	0.56
18:2:604:CLA:HBB2	17:2:605:CHL:C2C	2.37	0.55
6:B:307:ALA:HB3	18:B:822:CLA:HED3	1.87	0.55
22:L:305:BCR:H402	22:L:305:BCR:H23C	1.89	0.55
5:A:361:THR:HA	18:A:830:CLA:HBC2	1.88	0.55
18:A:821:CLA:HAB	22:K:205:BCR:H341	1.88	0.55
18:A:809:CLA:H201	20:A:846:LHG:H211	1.88	0.55
21:2:616:LUT:H391	18:2:611:CLA:HAB	1.88	0.55
6:B:659:THR:HA	18:B:803:CLA:HAB	1.88	0.55
18:B:809:CLA:HBB1	18:B:809:CLA:HMB1	1.88	0.55
18:B:820:CLA:HMB1	18:B:820:CLA:HBB1	1.89	0.55
20:1:615:LHG:H101	22:4:618:BCR:H393	1.89	0.55
18:B:840:CLA:HMD2	26:B:842:PQN:H172	1.89	0.55
18:A:841:CLA:H72	18:B:832:CLA:H42	1.89	0.55
18:A:811:CLA:HMB1	18:A:811:CLA:HBB1	1.90	0.54
5:A:699:ILE:HA	18:A:841:CLA:HED1	1.89	0.54
1:1:92:ARG:NH1	18:1:607:CLA:OBD	2.40	0.54
18:A:826:CLA:HBB1	18:A:822:CLA:H2	1.90	0.54
18:F:303:CLA:HMB2	22:F:304:BCR:H393	1.89	0.54
6:B:450:GLU:OE2	10:F:119:ARG:NH1	2.40	0.54
18:B:805:CLA:H43	22:B:844:BCR:H383	1.90	0.54
18:B:806:CLA:H2	18:B:806:CLA:HED3	1.88	0.54
22:K:202:BCR:H23C	22:K:202:BCR:H392	1.89	0.54
18:B:819:CLA:HMB2	18:B:824:CLA:HMA3	1.88	0.54
24:A:801:CL0:H14	18:B:802:CLA:C4A	2.37	0.54
18:2:602:CLA:CGA	18:2:602:CLA:H3A	2.38	0.54
3:3:79:LEU:HD13	18:A:813:CLA:H2	1.88	0.54
22:B:844:BCR:H361	22:B:844:BCR:H21C	1.90	0.54
1:1:230:HIS:NE2	4:4:145:ILE:HG12	2.23	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:233:ILE:HG13	18:1:612:CLA:HBC2	1.90	0.54
6:B:435:GLY:HA3	18:B:833:CLA:HAB	1.89	0.53
3:3:108:MET:HE1	18:3:608:CLA:HAB	1.90	0.53
18:A:842:CLA:HBD	18:A:842:CLA:HBA1	1.89	0.53
18:A:832:CLA:CGA	18:A:832:CLA:H3A	2.38	0.53
18:A:814:CLA:HHC	18:A:814:CLA:HBB1	1.89	0.53
1:1:207:VAL:HG11	18:1:612:CLA:HMD2	1.90	0.53
18:4:604:CLA:HMB3	19:4:617:XAT:H183	1.90	0.53
18:B:829:CLA:H102	27:B:850:DGD:HAG2	1.90	0.53
5:A:657:ILE:HD12	6:B:621:ARG:HG3	1.90	0.53
18:A:826:CLA:HBB1	18:A:826:CLA:HMB1	1.89	0.53
5:A:236:LEU:N	5:A:239:GLU:OE1	2.41	0.53
11:G:88:ARG:NH2	11:G:131:ASP:OD2	2.41	0.53
18:A:834:CLA:HMC2	18:L:304:CLA:HBB2	1.90	0.53
2:2:205:LEU:O	2:2:208:LYS:HG2	2.08	0.53
2:2:217:MET:HE1	18:2:602:CLA:HHC	1.90	0.53
17:1:601:CHL:HHC	17:1:601:CHL:HBB1	1.91	0.53
6:B:279:ALA:HA	18:B:816:CLA:HMC3	1.91	0.52
22:K:205:BCR:H343	22:K:202:BCR:H14C	1.90	0.52
2:2:205:LEU:HB3	18:2:609:CLA:HMA1	1.91	0.52
19:4:617:XAT:H242	19:4:617:XAT:H362	1.90	0.52
5:A:302:PHE:HE1	18:A:822:CLA:HAB	1.73	0.52
22:A:852:BCR:H403	22:A:852:BCR:H23C	1.91	0.52
17:2:607:CHL:H43	21:2:616:LUT:H173	1.91	0.52
18:B:825:CLA:HMB2	18:B:838:CLA:HBA1	1.92	0.52
2:2:81:SER:O	2:2:81:SER:OG	2.23	0.52
3:3:162:LEU:HB3	22:3:614:BCR:H363	1.91	0.52
12:H:80:SER:HB2	16:L:98:VAL:HG13	1.90	0.52
18:2:602:CLA:H42	18:2:602:CLA:C2B	2.39	0.52
22:A:848:BCR:H383	22:K:202:BCR:H10C	1.90	0.52
6:B:25:ILE:HG12	22:L:305:BCR:HC32	1.90	0.52
6:B:707:LEU:HD11	27:B:850:DGD:HB81	1.91	0.52
5:A:41:ASP:OD1	5:A:41:ASP:N	2.42	0.52
5:A:596:TRP:CH2	18:A:803:CLA:HAB	2.45	0.52
15:K:57:MET:HG2	15:K:117:GLY:HA3	1.91	0.52
17:2:615:CHL:HHC	17:2:615:CHL:HBB1	1.92	0.52
4:4:103:ALA:CB	19:4:617:XAT:H202	2.38	0.52
22:B:801:BCR:H341	22:B:801:BCR:C12	2.37	0.52
4:4:194:ASN:O	4:4:194:ASN:ND2	2.39	0.52
18:4:609:CLA:CGA	18:4:609:CLA:H3A	2.40	0.52
5:A:348:ALA:HB1	22:A:850:BCR:H393	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:1:615:LHG:H211	4:4:148:ILE:HD11	1.91	0.51
21:3:613:LUT:H161	21:3:613:LUT:H8	1.91	0.51
18:A:806:CLA:H192	22:A:849:BCR:H363	1.91	0.51
6:B:93:ASP:H	12:H:129:ILE:HD13	1.73	0.51
6:B:456:GLU:OE1	6:B:461:GLN:NE2	2.39	0.51
22:B:844:BCR:H352	18:B:828:CLA:H172	1.91	0.51
8:D:156:GLU:OE1	8:D:156:GLU:N	2.43	0.51
3:3:241:ILE:HG22	18:3:609:CLA:HMD3	1.92	0.51
5:A:512:LEU:HD11	5:A:519:VAL:HG13	1.91	0.51
6:B:695:ASP:OD1	6:B:695:ASP:N	2.42	0.51
19:2:617:XAT:H12	18:2:603:CLA:HMC2	1.92	0.51
12:H:83:ASN:ND2	18:H:201:CLA:HAC2	2.25	0.51
22:A:853:BCR:H23C	22:A:853:BCR:H393	1.93	0.51
6:B:25:ILE:HG21	27:B:850:DGD:HA72	1.92	0.51
17:1:601:CHL:C3B	20:1:615:LHG:H282	2.41	0.51
6:B:292:ARG:HD3	11:G:97:PRO:HD3	1.93	0.51
6:B:339:ALA:HB2	22:B:847:BCR:H372	1.92	0.51
10:F:70:SER:O	10:F:70:SER:OG	2.28	0.51
16:L:153:TYR:HB2	22:L:305:BCR:H361	1.93	0.51
2:2:66:ASP:OD1	2:2:66:ASP:N	2.34	0.50
18:A:830:CLA:HMB1	18:A:830:CLA:HBB1	1.93	0.50
6:B:120:VAL:HG21	18:B:808:CLA:HED1	1.91	0.50
18:B:838:CLA:HBB2	18:B:830:CLA:HAB	1.93	0.50
4:4:103:ALA:CA	19:4:617:XAT:H202	2.41	0.50
22:B:801:BCR:H312	18:B:832:CLA:CBB	2.41	0.50
18:A:825:CLA:H41	22:A:851:BCR:H15C	1.94	0.50
6:B:463:ILE:HD11	18:B:836:CLA:H11	1.93	0.50
5:A:545:VAL:HG11	18:A:840:CLA:HMB3	1.94	0.50
18:A:842:CLA:HMB1	18:A:842:CLA:HBB1	1.94	0.50
5:A:717:LEU:HD21	26:A:855:PQN:H151	1.93	0.50
18:A:844:CLA:HAB	6:B:582:TRP:CH2	2.47	0.50
18:B:806:CLA:HAB	18:B:828:CLA:HBB1	1.94	0.50
22:B:849:BCR:C10	14:J:36:ALA:HB1	2.41	0.50
3:3:167:GLU:OE1	3:3:170:ARG:NH2	2.40	0.50
3:3:223:LEU:HD11	3:3:227:LYS:HE3	1.94	0.50
5:A:522:LEU:HD21	5:A:616:VAL:HA	1.92	0.50
6:B:57:ILE:HA	18:B:806:CLA:HBC3	1.94	0.50
10:F:114:GLU:O	10:F:118:ARG:HG3	2.11	0.50
5:A:305:ALA:HB2	18:A:822:CLA:HBC2	1.94	0.49
18:A:835:CLA:HHB	18:A:834:CLA:HAB	1.93	0.49
26:A:855:PQN:H172	22:B:801:BCR:H382	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:103:ALA:N	19:4:617:XAT:H202	2.27	0.49
5:A:297:ALA:HB1	18:A:818:CLA:HBC2	1.93	0.49
5:A:389:THR:HG23	5:A:605:ILE:HG21	1.94	0.49
21:2:619:LUT:H172	18:4:610:CLA:HMC3	1.93	0.49
18:4:603:CLA:HMB2	19:4:617:XAT:H32	1.94	0.49
6:B:91:ILE:HB	6:B:112:PRO:HB2	1.94	0.49
22:B:801:BCR:HC31	22:B:849:BCR:H351	1.94	0.49
5:A:671:PHE:O	5:A:675:HIS:ND1	2.43	0.49
24:A:801:CL0:H59	24:A:801:CL0:H51	1.56	0.49
22:A:848:BCR:H323	18:A:806:CLA:H151	1.94	0.49
18:2:604:CLA:HED2	18:2:604:CLA:H2A	1.95	0.49
18:A:803:CLA:H2	6:B:655:LEU:HD22	1.93	0.49
6:B:9:SER:OG	27:B:850:DGD:O4E	2.24	0.49
21:2:616:LUT:H401	21:2:616:LUT:H15	1.95	0.49
3:3:151:ASP:OD1	3:3:151:ASP:N	2.46	0.49
6:B:370:ALA:HB1	18:B:827:CLA:HMA1	1.95	0.49
22:B:849:BCR:H311	14:J:33:PHE:CD2	2.47	0.49
18:4:602:CLA:CGA	18:4:602:CLA:H3A	2.43	0.48
24:A:801:CL0:H14	18:B:802:CLA:NA	2.28	0.48
16:L:107:VAL:HA	18:L:303:CLA:HED1	1.94	0.48
17:1:601:CHL:C4A	20:1:615:LHG:H131	2.43	0.48
18:2:603:CLA:HMD2	18:2:608:CLA:C1D	2.42	0.48
12:H:107:LEU:HD22	16:L:144:VAL:HG13	1.94	0.48
1:1:52:GLU:OE2	1:1:53:PRO:HD2	2.14	0.48
22:A:851:BCR:H351	22:A:851:BCR:C16	2.42	0.48
9:E:87:VAL:HB	9:E:138:VAL:HG13	1.94	0.48
15:K:115:ILE:HG22	18:K:203:CLA:HBC1	1.96	0.48
4:4:90:LYS:O	4:4:94:GLN:HG2	2.13	0.48
4:4:102:TRP:CE2	17:4:607:CHL:HED2	2.49	0.48
5:A:330:PHE:CD2	20:A:847:LHG:HC41	2.48	0.48
18:A:843:CLA:H93	18:A:843:CLA:HBB1	1.95	0.48
6:B:697:PRO:O	7:C:81:TYR:OH	2.24	0.48
18:A:832:CLA:HMA2	16:L:76:THR:HG21	1.94	0.48
1:1:221:LEU:HD22	21:1:616:LUT:H363	1.96	0.48
3:3:120:LEU:HD12	18:3:603:CLA:HMB1	1.96	0.48
5:A:294:HIS:HB2	18:A:819:CLA:C1B	2.44	0.48
22:4:618:BCR:H383	22:4:618:BCR:H23C	1.95	0.48
5:A:373:PRO:HG3	18:A:820:CLA:HBA1	1.95	0.48
18:A:841:CLA:H143	18:F:302:CLA:HBC1	1.96	0.48
5:A:739:TRP:CH2	18:A:809:CLA:HBC2	2.48	0.48
18:A:809:CLA:H203	18:A:812:CLA:H191	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:D:164:ASP:OD2	8:D:172:ASN:ND2	2.44	0.48
1:I:156:ARG:HG3	18:1:607:CLA:CHD	2.44	0.48
2:2:119:ILE:HG22	2:2:120:LEU:HD12	1.94	0.48
18:A:805:CLA:HMB1	18:A:805:CLA:HBB1	1.96	0.48
6:B:548:PRO:HD2	7:C:62:PHE:CZ	2.49	0.48
18:B:826:CLA:HMA3	22:B:847:BCR:H312	1.94	0.48
18:4:602:CLA:H93	19:4:617:XAT:H30	1.95	0.48
18:A:802:CLA:H3A	18:A:802:CLA:O2A	2.13	0.48
22:B:801:BCR:H383	22:B:801:BCR:H23C	1.95	0.48
21:2:619:LUT:H172	18:4:610:CLA:HHC	1.96	0.47
18:A:802:CLA:H143	18:A:844:CLA:H151	1.95	0.47
22:A:852:BCR:H323	18:A:829:CLA:H11	1.95	0.47
17:1:601:CHL:C4C	20:1:615:LHG:HC92	2.45	0.47
20:1:615:LHG:H251	20:1:615:LHG:HC81	1.97	0.47
18:A:834:CLA:H162	18:A:834:CLA:H141	1.69	0.47
18:B:825:CLA:H142	18:B:825:CLA:H111	1.73	0.47
18:4:604:CLA:HAA1	18:4:604:CLA:HED3	1.96	0.47
1:1:69:ASP:HA	19:1:614:XAT:O23	2.15	0.47
1:1:83:TYR:CD2	18:1:602:CLA:H11	2.50	0.47
3:3:221:LEU:HB3	18:3:608:CLA:HMA1	1.95	0.47
18:4:610:CLA:C1D	18:4:611:CLA:HMD2	2.45	0.47
18:B:808:CLA:O1A	18:B:827:CLA:HBD	2.15	0.47
12:H:63:ASP:OD2	12:H:66:ASN:ND2	2.33	0.47
18:2:608:CLA:H3A	18:2:608:CLA:HBA2	1.36	0.47
10:F:78:SER:HB3	10:F:81:PHE:HB2	1.97	0.47
1:1:68:PHE:CE2	19:1:614:XAT:H383	2.49	0.47
4:4:236:GLN:NE2	4:4:244:ASN:HD22	2.12	0.47
18:B:828:CLA:H112	18:B:828:CLA:H142	1.65	0.47
18:A:819:CLA:H62	18:A:819:CLA:H41	1.59	0.47
18:A:828:CLA:H93	18:A:828:CLA:H111	1.66	0.47
6:B:549:ASP:OD1	7:C:66:ARG:NH2	2.44	0.47
22:B:846:BCR:H403	22:B:846:BCR:H23C	1.96	0.47
18:B:840:CLA:H11	26:B:842:PQN:H272	1.96	0.47
21:1:616:LUT:H11	21:1:616:LUT:H191	1.82	0.46
5:A:360:LEU:HG	18:A:830:CLA:HBC1	1.97	0.46
18:A:806:CLA:H161	22:A:849:BCR:H353	1.97	0.46
18:A:842:CLA:HBC2	26:A:855:PQN:H192	1.96	0.46
22:A:852:BCR:H271	18:A:842:CLA:H141	1.95	0.46
18:A:830:CLA:HBA1	18:A:830:CLA:CHA	2.45	0.46
18:A:844:CLA:HMB3	18:B:802:CLA:H203	1.97	0.46
18:A:818:CLA:H92	18:A:818:CLA:H61	1.78	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:F:89:ILE:HD12	10:F:113:ILE:HG23	1.96	0.46
1:1:68:PHE:HE2	19:1:614:XAT:H383	1.80	0.46
2:2:170:VAL:HG23	2:2:171:PHE:CD2	2.51	0.46
5:A:620:ILE:HG12	5:A:626:VAL:HG22	1.96	0.46
22:F:304:BCR:H14C	22:F:304:BCR:H10C	1.97	0.46
18:1:607:CLA:H3A	18:1:607:CLA:HBA2	1.32	0.46
18:2:609:CLA:HMB1	18:2:609:CLA:HBB1	1.97	0.46
4:4:154:GLU:HG3	18:4:608:CLA:C4B	2.46	0.46
18:A:829:CLA:H72	18:A:829:CLA:H111	1.49	0.46
18:A:819:CLA:H91	18:A:819:CLA:H111	1.72	0.46
18:A:844:CLA:HMB3	18:B:802:CLA:H192	1.98	0.46
18:A:844:CLA:H3A	18:A:844:CLA:O1A	2.16	0.46
6:B:411:MET:HG3	22:B:846:BCR:H401	1.98	0.46
5:A:508:GLY:HA2	5:A:523:PRO:HB3	1.96	0.46
6:B:304:LEU:HA	18:B:822:CLA:HED1	1.96	0.46
3:3:171:LEU:HD13	18:3:607:CLA:HMA2	1.98	0.46
14:J:29:ILE:HD12	14:J:29:ILE:H	1.80	0.46
1:1:149:ILE:HG21	18:1:608:CLA:HMC3	1.97	0.46
4:4:136:PHE:HE1	17:4:605:CHL:HMD3	1.81	0.46
18:A:844:CLA:H202	18:A:829:CLA:H121	1.98	0.46
22:B:843:BCR:H11C	22:B:843:BCR:H341	1.81	0.46
1:1:95:MET:HG2	21:1:616:LUT:C14	2.46	0.46
17:1:601:CHL:C3C	20:1:615:LHG:HC92	2.46	0.46
18:1:604:CLA:O2A	18:1:605:CLA:HMA3	2.16	0.46
18:3:603:CLA:H3A	18:3:603:CLA:HBA1	1.38	0.46
22:A:848:BCR:H403	22:A:848:BCR:H23C	1.97	0.46
18:A:803:CLA:OBD	18:B:802:CLA:HMB3	2.15	0.46
18:B:814:CLA:H41	18:B:814:CLA:H62	1.45	0.46
18:A:804:CLA:H91	18:A:804:CLA:H111	1.70	0.45
18:A:839:CLA:HBB1	18:A:839:CLA:HMB1	1.98	0.45
6:B:517:PHE:HE1	22:B:849:BCR:H381	1.81	0.45
18:B:813:CLA:HMB3	22:B:844:BCR:H14C	1.98	0.45
22:I:101:BCR:H383	22:L:301:BCR:H363	1.98	0.45
20:1:615:LHG:H161	20:1:615:LHG:H301	1.96	0.45
18:B:809:CLA:H92	18:B:809:CLA:H62	1.71	0.45
7:C:60:THR:OG1	7:C:62:PHE:O	2.30	0.45
2:2:225:PHE:HA	2:2:228:ILE:HG22	1.98	0.45
21:2:616:LUT:H373	18:2:612:CLA:C2B	2.47	0.45
3:3:266:VAL:HG21	18:3:609:CLA:H11	1.98	0.45
5:A:582:CYS:HB2	6:B:667:TRP:HB3	1.99	0.45
6:B:124:TRP:HB3	6:B:129:LEU:HD12	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:221:LEU:O	1:1:225:LEU:HG	2.16	0.45
18:2:602:CLA:H3A	18:2:602:CLA:O1A	2.16	0.45
4:4:157:ARG:NH1	18:4:608:CLA:O1D	2.43	0.45
5:A:393:TRP:HD1	18:A:829:CLA:HAB	1.80	0.45
1:1:200:LEU:HD12	1:1:200:LEU:HA	1.79	0.45
20:1:615:LHG:H132	20:1:615:LHG:C28	2.43	0.45
18:4:614:CLA:O2D	18:4:614:CLA:H2A	2.17	0.45
18:A:830:CLA:HBA1	18:A:830:CLA:CB D	2.45	0.45
18:B:811:CLA:H41	18:B:811:CLA:H61	1.74	0.45
18:3:602:CLA:HMD2	18:3:607:CLA:C1D	2.47	0.45
18:A:806:CLA:H61	18:A:806:CLA:H2	1.69	0.45
6:B:26:ALA:O	18:B:829:CLA:H11	2.16	0.45
6:B:95:HIS:CE1	18:B:809:CLA:HMB3	2.52	0.45
22:B:844:BCR:H382	22:B:844:BCR:H23C	1.97	0.45
2:2:126:TYR:HB2	2:2:227:HIS:CD2	2.52	0.45
4:4:129:ASP:OD1	4:4:129:ASP:N	2.47	0.45
15:K:108:ALA:O	15:K:112:VAL:HG23	2.17	0.45
22:L:305:BCR:H361	22:L:305:BCR:H20C	1.87	0.45
18:3:609:CLA:C2B	21:3:613:LUT:H373	2.46	0.45
18:A:830:CLA:H41	18:A:830:CLA:H62	1.55	0.45
18:B:827:CLA:H152	18:B:827:CLA:H111	1.39	0.45
22:B:846:BCR:H11C	22:B:846:BCR:H341	1.81	0.45
22:J:102:BCR:H341	22:J:102:BCR:H11C	1.79	0.45
22:L:301:BCR:H15C	22:L:301:BCR:H351	1.76	0.45
22:A:851:BCR:H331	22:A:851:BCR:C8	2.45	0.44
6:B:167:TRP:CZ2	18:B:811:CLA:HMA1	2.52	0.44
6:B:718:ILE:HD13	18:B:827:CLA:HMC2	1.99	0.44
18:B:808:CLA:H141	18:B:808:CLA:H162	1.65	0.44
18:B:824:CLA:H62	18:B:824:CLA:H41	1.57	0.44
11:G:68:ILE:HG21	11:G:147:LEU:HD21	1.99	0.44
21:2:616:LUT:H22	18:2:609:CLA:C2	2.47	0.44
5:A:297:ALA:HA	18:A:818:CLA:HMC3	1.98	0.44
18:B:825:CLA:HAA2	18:B:826:CLA:OBD	2.17	0.44
11:G:68:ILE:HD11	11:G:146:ILE:HB	1.99	0.44
17:1:601:CHL:H61	17:1:601:CHL:H41	1.62	0.44
2:2:238:LEU:HB2	21:2:616:LUT:H24	1.99	0.44
4:4:193:LEU:HD12	21:4:616:LUT:H222	1.99	0.44
18:A:809:CLA:H202	18:A:809:CLA:H91	1.99	0.44
18:A:813:CLA:H3A	18:A:813:CLA:HBA2	1.65	0.44
18:B:809:CLA:H41	18:B:809:CLA:H61	1.56	0.44
18:B:818:CLA:O1A	18:B:828:CLA:HMD1	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:182:LEU:HD11	22:B:844:BCR:H363	1.99	0.44
6:B:652:PHE:O	6:B:656:VAL:HG23	2.17	0.44
18:B:802:CLA:H161	18:B:802:CLA:H121	1.72	0.44
22:B:801:BCR:H15C	22:B:801:BCR:H351	1.86	0.44
21:2:619:LUT:H181	21:2:619:LUT:C8	2.34	0.44
3:3:266:VAL:HG22	18:3:609:CLA:CAD	2.48	0.44
4:4:132:LYS:HZ2	17:4:606:CHL:CGD	2.26	0.44
5:A:213:HIS:HB2	18:A:815:CLA:CHC	2.48	0.44
18:A:802:CLA:H3A	18:A:802:CLA:HBA1	1.51	0.44
18:A:806:CLA:HBA1	18:A:806:CLA:H3A	1.33	0.44
18:B:826:CLA:H142	18:B:826:CLA:H111	1.83	0.44
18:L:303:CLA:H112	18:L:303:CLA:H71	1.74	0.44
5:A:588:ASP:OD1	5:A:723:ARG:NH1	2.51	0.44
22:A:848:BCR:H24C	22:A:848:BCR:H371	1.86	0.44
18:A:842:CLA:H62	18:A:842:CLA:H102	1.69	0.44
18:A:809:CLA:H101	18:A:809:CLA:H13	1.77	0.44
7:C:2:SER:OG	7:C:3:HIS:N	2.49	0.44
9:E:109:ASP:OD1	9:E:110:PRO:HD2	2.17	0.44
1:1:92:ARG:HH12	18:1:607:CLA:HMD1	1.81	0.44
1:1:164:LYS:HE3	1:1:164:LYS:HA	1.99	0.44
1:1:203:VAL:O	1:1:207:VAL:HG23	2.18	0.44
18:2:612:CLA:H141	18:2:612:CLA:H161	1.81	0.44
4:4:238:LEU:CD1	18:4:613:CLA:HAB	2.48	0.44
5:A:197:HIS:CG	18:A:814:CLA:HMC2	2.52	0.44
18:A:833:CLA:H41	18:A:833:CLA:H61	1.51	0.44
6:B:338:LEU:HD22	6:B:382:ILE:HG23	2.00	0.44
6:B:531:THR:HG21	18:B:838:CLA:HMB3	2.00	0.44
18:H:201:CLA:HMA1	18:L:302:CLA:HAA1	2.00	0.44
18:1:603:CLA:H41	18:1:603:CLA:H62	1.65	0.44
18:A:827:CLA:H62	18:A:827:CLA:H102	1.68	0.44
18:A:803:CLA:H142	6:B:648:TRP:HH2	1.83	0.44
18:B:822:CLA:HBA1	18:B:822:CLA:O1D	2.18	0.44
7:C:15:THR:HG22	7:C:28:MET:HG3	2.00	0.44
22:L:305:BCR:H331	22:L:305:BCR:HC7	1.80	0.44
18:2:602:CLA:H91	18:2:602:CLA:H111	1.79	0.44
18:2:609:CLA:CHA	18:2:609:CLA:HBA1	2.44	0.44
4:4:214:LEU:HD23	4:4:214:LEU:HA	1.87	0.44
22:4:618:BCR:H15C	22:4:618:BCR:H351	1.88	0.44
18:4:602:CLA:H93	18:4:602:CLA:H61	1.77	0.44
18:A:803:CLA:HBA1	18:A:803:CLA:H3A	1.57	0.44
21:3:613:LUT:H391	21:3:613:LUT:H31	1.78	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:A:809:CLA:H172	22:A:853:BCR:H372	2.01	0.43
22:A:851:BCR:H371	22:A:851:BCR:H24C	1.72	0.43
18:B:803:CLA:H202	18:B:803:CLA:H162	1.80	0.43
22:B:844:BCR:H371	22:B:844:BCR:H24C	1.72	0.43
8:D:72:THR:HG23	8:D:120:PRO:HB2	2.00	0.43
18:A:802:CLA:H92	18:A:802:CLA:H62	1.68	0.43
18:A:805:CLA:HBA2	18:A:805:CLA:H3A	1.59	0.43
6:B:174:ARG:HB2	18:B:813:CLA:HBC2	2.01	0.43
6:B:276:HIS:HB2	18:B:817:CLA:C1B	2.49	0.43
18:B:819:CLA:HBA1	18:B:819:CLA:H3A	1.80	0.43
18:B:825:CLA:H141	18:B:825:CLA:H162	1.73	0.43
18:B:832:CLA:CBB	18:B:833:CLA:HMB2	2.48	0.43
18:2:604:CLA:C2C	19:2:617:XAT:H183	2.48	0.43
18:A:826:CLA:H111	18:A:826:CLA:H93	1.66	0.43
22:A:850:BCR:H20C	22:A:850:BCR:H361	1.91	0.43
16:L:90:ASN:HB3	18:L:302:CLA:HAC1	2.00	0.43
22:L:301:BCR:H361	22:L:301:BCR:C21	2.48	0.43
18:B:822:CLA:H91	18:B:822:CLA:H111	1.73	0.43
20:1:615:LHG:C10	22:4:618:BCR:H281	2.49	0.43
4:4:240:ASP:HB2	4:4:244:ASN:OD1	2.17	0.43
18:A:834:CLA:HMA1	22:I:101:BCR:H272	2.01	0.43
18:A:841:CLA:H43	18:B:832:CLA:HAA2	1.99	0.43
22:B:847:BCR:H351	22:B:847:BCR:H15C	1.84	0.43
18:F:302:CLA:CAD	14:J:22:LEU:HD21	2.48	0.43
18:A:804:CLA:HBA2	18:A:804:CLA:CBD	2.40	0.43
6:B:444:LEU:HD12	6:B:444:LEU:O	2.19	0.43
18:B:828:CLA:H3A	18:B:828:CLA:HBA2	1.27	0.43
22:J:102:BCR:H351	22:J:102:BCR:H15C	1.81	0.43
2:2:242:LEU:HD11	18:2:613:CLA:HMC3	2.00	0.43
18:2:602:CLA:H162	18:2:602:CLA:H192	1.80	0.43
5:A:310:ARG:N	5:A:317:HIS:O	2.47	0.43
18:B:826:CLA:H13	22:B:847:BCR:H15C	2.00	0.43
10:F:203:TRP:CD1	10:F:204:PRO:HD3	2.54	0.43
18:A:812:CLA:H13	18:A:812:CLA:H172	1.71	0.43
18:A:812:CLA:H91	18:A:812:CLA:H111	1.65	0.43
4:4:149:LEU:HD11	22:4:618:BCR:C16	2.49	0.43
19:4:617:XAT:C28	19:4:617:XAT:H381	2.26	0.43
18:A:804:CLA:HBB2	18:A:812:CLA:H143	2.01	0.43
6:B:56:ILE:HG22	18:B:806:CLA:HBC2	2.01	0.43
22:B:849:BCR:H10C	14:J:38:THR:O	2.19	0.43
21:2:616:LUT:H202	18:2:611:CLA:H3A	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:238:LEU:HD13	4:4:238:LEU:HA	1.92	0.43
18:A:836:CLA:HBA1	18:A:836:CLA:H3A	1.92	0.43
6:B:684:ARG:HA	6:B:684:ARG:HD3	1.85	0.43
2:2:227:HIS:O	2:2:227:HIS:ND1	2.51	0.42
22:A:848:BCR:H20C	22:A:848:BCR:H361	1.90	0.42
26:A:855:PQN:H111	26:A:855:PQN:H2M1	1.83	0.42
18:B:837:CLA:H3A	18:B:837:CLA:HBA2	1.71	0.42
22:B:845:BCR:H11C	22:B:845:BCR:H341	1.89	0.42
11:G:64:PRO:O	11:G:68:ILE:HG22	2.19	0.42
14:J:2:ARG:HA	14:J:2:ARG:HD2	1.90	0.42
16:L:65:ILE:O	16:L:65:ILE:HG13	2.18	0.42
2:2:225:PHE:O	2:2:228:ILE:HG22	2.19	0.42
10:F:143:ASP:OD1	10:F:144:GLN:N	2.52	0.42
21:1:616:LUT:H401	21:1:616:LUT:H35	1.80	0.42
2:2:205:LEU:HA	2:2:208:LYS:HD2	2.01	0.42
5:A:56:PHE:CD2	18:A:806:CLA:HMC2	2.54	0.42
5:A:536:ILE:HG23	24:A:801:CL0:H70	2.01	0.42
18:A:825:CLA:HBA2	18:A:825:CLA:H3A	1.30	0.42
6:B:678:LEU:HD23	6:B:678:LEU:HA	1.87	0.42
18:B:825:CLA:H3A	18:B:825:CLA:HBA2	1.46	0.42
18:B:825:CLA:HMA1	22:B:847:BCR:H14C	2.02	0.42
22:B:847:BCR:H11C	22:B:847:BCR:H341	1.88	0.42
18:B:834:CLA:HBA1	18:B:834:CLA:H3A	1.66	0.42
11:G:64:PRO:O	11:G:64:PRO:HD2	2.18	0.42
18:A:804:CLA:H62	18:A:804:CLA:H2	1.81	0.42
22:B:846:BCR:H351	22:B:846:BCR:H15C	1.82	0.42
10:F:160:ILE:HG21	18:F:302:CLA:HMA3	2.02	0.42
20:1:615:LHG:H212	18:4:614:CLA:CMA	2.49	0.42
4:4:104:MET:SD	18:4:609:CLA:HAB	2.60	0.42
5:A:118:ILE:HD12	18:A:810:CLA:HMA3	2.01	0.42
18:B:806:CLA:H151	18:B:828:CLA:HBB2	2.01	0.42
18:F:302:CLA:HAA2	14:J:22:LEU:HD11	2.02	0.42
18:3:601:CLA:H2	18:3:601:CLA:H62	1.81	0.42
4:4:245:THR:HG22	4:4:246:ILE:H	1.84	0.42
5:A:596:TRP:HH2	18:A:803:CLA:HAB	1.83	0.42
6:B:325:THR:OG1	6:B:403:ASN:OD1	2.26	0.42
6:B:574:ASP:OD1	6:B:706:ARG:NH1	2.52	0.42
3:3:239:TYR:CE1	21:3:613:LUT:H363	2.54	0.42
4:4:77:PHE:CE2	19:4:617:XAT:H382	2.46	0.42
24:A:801:CL0:H51	24:A:801:CL0:H42	1.71	0.42
22:A:852:BCR:H20C	22:A:852:BCR:H361	1.79	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:B:828:CLA:H161	18:B:828:CLA:H141	1.77	0.42
18:F:301:CLA:H41	18:F:301:CLA:H62	1.55	0.42
22:K:202:BCR:H15C	22:K:202:BCR:H351	1.80	0.42
21:1:616:LUT:H15	21:1:616:LUT:H201	1.90	0.42
2:2:103:LEU:HD12	2:2:103:LEU:HA	1.90	0.42
5:A:571:PHE:CE1	5:A:585:SER:HB3	2.55	0.42
22:B:801:BCR:H312	18:B:832:CLA:HBB2	2.02	0.42
16:L:168:SER:O	16:L:168:SER:OG	2.34	0.42
3:3:119:ILE:HG22	3:3:120:LEU:HD23	2.01	0.42
4:4:206:LEU:HA	4:4:206:LEU:HD23	1.75	0.42
4:4:245:THR:HG22	4:4:246:ILE:N	2.35	0.42
6:B:432:HIS:HB2	22:B:849:BCR:H402	2.02	0.42
19:1:614:XAT:H31	19:1:614:XAT:H391	1.88	0.42
2:2:194:TRP:HB2	18:2:609:CLA:O2A	2.20	0.42
21:4:616:LUT:H35	21:4:616:LUT:H401	1.90	0.42
5:A:92:GLY:O	5:A:96:SER:OG	2.31	0.42
22:A:850:BCR:H331	22:A:850:BCR:HC7	1.77	0.42
6:B:280:ILE:HD13	6:B:280:ILE:HA	1.94	0.42
6:B:662:MET:HB2	18:B:803:CLA:C1C	2.50	0.42
18:B:805:CLA:H3A	18:B:805:CLA:HBA1	1.47	0.42
18:B:827:CLA:H72	18:B:827:CLA:H112	1.79	0.42
18:B:832:CLA:HHC	18:B:832:CLA:CBB	2.45	0.42
18:B:835:CLA:HMB3	18:B:834:CLA:HBA2	2.02	0.42
7:C:61:ASP:OD1	7:C:62:PHE:N	2.52	0.42
7:C:61:ASP:HB3	9:E:131:ASN:ND2	2.34	0.42
18:1:612:CLA:HED3	20:1:615:LHG:H322	2.02	0.41
5:A:365:ALA:HB2	5:A:391:HIS:HB2	2.02	0.41
22:A:848:BCR:H23C	22:A:848:BCR:H392	2.02	0.41
22:B:848:BCR:H15C	22:B:848:BCR:H351	1.95	0.41
22:L:306:BCR:H351	22:L:306:BCR:H15C	1.83	0.41
1:1:92:ARG:HD3	18:1:607:CLA:OBD	2.21	0.41
1:1:202:PHE:CZ	19:1:614:XAT:H10	2.55	0.41
3:3:119:ILE:HD13	3:3:119:ILE:HA	1.87	0.41
5:A:61:SER:O	5:A:61:SER:OG	2.32	0.41
22:B:846:BCR:H343	18:B:822:CLA:HBB2	2.01	0.41
22:B:845:BCR:H19C	22:B:845:BCR:C37	2.50	0.41
19:1:614:XAT:H242	19:1:614:XAT:H362	2.02	0.41
20:1:615:LHG:HC62	20:1:615:LHG:H242	1.82	0.41
4:4:147:PHE:CZ	18:4:614:CLA:HMB3	2.56	0.41
18:A:811:CLA:H2A	18:A:811:CLA:HED2	2.01	0.41
6:B:80:ASP:OD2	6:B:83:HIS:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:I:101:BCR:H11C	22:I:101:BCR:H341	1.93	0.41
2:2:145:LEU:HD12	2:2:145:LEU:HA	1.89	0.41
3:3:201:PRO:HD3	17:3:606:CHL:HMD2	2.03	0.41
18:A:833:CLA:HMB1	18:A:843:CLA:HAA2	2.03	0.41
18:B:818:CLA:HBB1	18:B:818:CLA:HMB1	2.02	0.41
1:1:161:ASP:OD2	1:1:164:LYS:HG2	2.20	0.41
20:1:615:LHG:H222	20:1:615:LHG:H372	2.02	0.41
3:3:108:MET:CE	18:3:608:CLA:HAB	2.49	0.41
5:A:187:TRP:CZ2	18:A:811:CLA:HMA1	2.55	0.41
18:A:841:CLA:H3A	18:A:841:CLA:HBA2	1.38	0.41
18:B:814:CLA:H162	18:B:814:CLA:H141	1.76	0.41
18:B:822:CLA:H112	18:B:822:CLA:H142	1.73	0.41
13:I:27:LEU:HD23	22:L:305:BCR:H323	2.02	0.41
3:3:120:LEU:HB3	3:3:125:LEU:HB2	2.01	0.41
24:A:801:CL0:H2	24:A:801:CL0:H15	2.02	0.41
18:A:807:CLA:H193	18:A:807:CLA:H161	1.73	0.41
18:B:825:CLA:H92	18:B:825:CLA:H61	1.80	0.41
22:K:202:BCR:H371	22:K:202:BCR:H24C	1.79	0.41
16:L:137:LEU:HD12	16:L:137:LEU:HA	1.91	0.41
18:L:303:CLA:H143	18:L:303:CLA:H111	1.82	0.41
18:1:609:CLA:CBB	18:1:609:CLA:HHC	2.51	0.41
19:2:617:XAT:H402	18:2:603:CLA:C2B	2.51	0.41
18:4:602:CLA:C9	19:4:617:XAT:H30	2.50	0.41
5:A:113:GLN:NE2	18:A:810:CLA:OBD	2.54	0.41
18:A:807:CLA:H143	18:A:807:CLA:H111	1.86	0.41
18:A:844:CLA:H43	6:B:441:ASP:HB3	2.03	0.41
26:A:855:PQN:H222	18:F:301:CLA:C1B	2.50	0.41
18:B:816:CLA:O1A	11:G:152:ASN:ND2	2.53	0.41
18:F:302:CLA:H52	18:F:302:CLA:H11	1.81	0.41
18:F:302:CLA:O1D	18:F:302:CLA:H2A	2.20	0.41
18:1:602:CLA:CBB	19:1:614:XAT:H32	2.50	0.41
21:2:619:LUT:H35	21:2:619:LUT:H401	1.83	0.41
18:A:821:CLA:HBA1	18:A:821:CLA:H3A	1.71	0.41
18:A:809:CLA:H62	18:A:809:CLA:H92	1.84	0.41
6:B:521:HIS:CD2	22:B:849:BCR:H281	2.55	0.41
6:B:714:SER:HB2	27:B:850:DGD:HBN1	2.02	0.41
16:L:152:ILE:HD13	16:L:152:ILE:HA	1.86	0.41
2:2:98:CYS:HB3	2:2:213:GLY:HA3	2.03	0.41
2:2:217:MET:HE1	18:2:602:CLA:CHC	2.50	0.41
3:3:106:PHE:CD2	18:3:607:CLA:HMD3	2.55	0.41
3:3:230:ARG:HA	3:3:233:MET:HE2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:3:613:LUT:H401	21:3:613:LUT:C15	2.43	0.41
18:4:602:CLA:HMB1	18:4:602:CLA:HBB1	2.02	0.41
5:A:90:PHE:CG	18:A:808:CLA:HBC3	2.55	0.41
5:A:596:TRP:HE1	18:B:803:CLA:C1D	2.34	0.41
18:A:806:CLA:H12	18:A:807:CLA:HBB1	2.01	0.41
18:A:827:CLA:H71	18:A:838:CLA:H43	2.03	0.41
22:A:850:BCR:H11C	22:A:850:BCR:H341	1.84	0.41
6:B:516:ASP:OD2	6:B:593:TYR:OH	2.35	0.41
18:B:814:CLA:H102	22:B:845:BCR:H363	2.03	0.41
22:B:843:BCR:H383	22:B:843:BCR:H23C	2.03	0.41
22:B:847:BCR:HC7	22:B:847:BCR:H331	1.81	0.41
18:G:201:CLA:CGA	18:G:201:CLA:H3A	2.50	0.41
14:J:26:LEU:HD23	14:J:26:LEU:HA	1.90	0.41
18:1:612:CLA:C3A	21:1:616:LUT:H383	2.50	0.41
18:4:612:CLA:H3A	18:4:612:CLA:HBA2	1.82	0.41
18:A:818:CLA:H11	18:A:818:CLA:H52	1.86	0.41
18:A:811:CLA:H141	18:A:811:CLA:H162	1.78	0.41
18:L:303:CLA:H141	18:L:303:CLA:H161	1.71	0.41
2:2:168:ASP:HB3	2:2:171:PHE:O	2.21	0.40
17:2:601:CHL:HBA1	17:2:601:CHL:H3A	1.40	0.40
18:A:804:CLA:H12	26:A:855:PQN:H243	2.03	0.40
18:A:802:CLA:H3A	18:A:802:CLA:CGA	2.41	0.40
18:A:820:CLA:H3A	18:A:820:CLA:HBA2	1.26	0.40
18:B:814:CLA:H93	18:B:814:CLA:H111	1.90	0.40
22:L:301:BCR:H361	22:L:301:BCR:H21C	2.02	0.40
1:1:149:ILE:O	1:1:152:VAL:HG12	2.20	0.40
1:1:192:ILE:O	1:1:196:ARG:HG3	2.21	0.40
21:2:616:LUT:H401	21:2:616:LUT:C15	2.52	0.40
23:4:619:LMG:HC71	23:4:619:LMG:HC2	1.88	0.40
22:A:851:BCR:H321	22:A:851:BCR:HC7	1.85	0.40
18:B:823:CLA:HBB1	18:B:830:CLA:HBC2	2.01	0.40
27:B:850:DGD:HBH1	27:B:850:DGD:HBT2	1.80	0.40
18:4:609:CLA:CGA	18:4:609:CLA:C3A	2.99	0.40
6:B:294:ASN:OD1	6:B:294:ASN:N	2.54	0.40
18:B:824:CLA:H141	18:B:824:CLA:H193	2.03	0.40
22:G:204:BCR:H15C	22:G:204:BCR:H351	1.94	0.40
3:3:106:PHE:HD2	18:3:607:CLA:HMD3	1.86	0.40
21:3:613:LUT:H181	21:3:613:LUT:H7	1.71	0.40
24:A:801:CL0:H35	24:A:801:CL0:H41	1.86	0.40
22:G:204:BCR:H20C	22:G:204:BCR:H361	1.91	0.40
22:K:202:BCR:H11C	22:K:202:BCR:H341	1.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:108:MET:HE1	18:3:608:CLA:HHC	2.03	0.40
3:3:186:LEU:HD23	3:3:186:LEU:HA	1.83	0.40
22:4:618:BCR:H24C	22:4:618:BCR:H371	1.96	0.40
5:A:679:ALA:O	18:A:802:CLA:HAB	2.22	0.40
5:A:688:GLY:HA3	6:B:569:ASP:HB2	2.03	0.40
18:A:819:CLA:H3A	18:A:819:CLA:HBA2	1.69	0.40
18:B:823:CLA:HBA1	18:B:823:CLA:H3A	1.77	0.40
18:B:841:CLA:H161	18:B:841:CLA:H121	1.46	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	162/241 (67%)	157 (97%)	5 (3%)	0	100	100
2	2	199/257 (77%)	195 (98%)	4 (2%)	0	100	100
3	3	215/273 (79%)	210 (98%)	5 (2%)	0	100	100
4	4	194/251 (77%)	189 (97%)	5 (3%)	0	100	100
5	A	707/750 (94%)	690 (98%)	17 (2%)	0	100	100
6	B	730/734 (100%)	712 (98%)	18 (2%)	0	100	100
7	C	78/81 (96%)	73 (94%)	5 (6%)	0	100	100
8	D	141/204 (69%)	135 (96%)	6 (4%)	0	100	100
9	E	62/143 (43%)	60 (97%)	2 (3%)	0	100	100
10	F	147/221 (66%)	146 (99%)	1 (1%)	0	100	100
11	G	89/160 (56%)	87 (98%)	2 (2%)	0	100	100
12	H	84/145 (58%)	84 (100%)	0	0	100	100
13	I	29/37 (78%)	28 (97%)	1 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	J	39/44 (89%)	39 (100%)	0	0	100	100
15	K	52/130 (40%)	51 (98%)	1 (2%)	0	100	100
16	L	157/219 (72%)	153 (98%)	4 (2%)	0	100	100
All	All	3085/3890 (79%)	3009 (98%)	76 (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	134/190 (70%)	130 (97%)	4 (3%)	41	69
2	2	163/205 (80%)	158 (97%)	5 (3%)	40	68
3	3	167/211 (79%)	165 (99%)	2 (1%)	71	87
4	4	163/210 (78%)	158 (97%)	5 (3%)	40	68
5	A	574/610 (94%)	562 (98%)	12 (2%)	53	77
6	B	599/600 (100%)	588 (98%)	11 (2%)	59	80
7	C	70/71 (99%)	68 (97%)	2 (3%)	42	70
8	D	121/170 (71%)	118 (98%)	3 (2%)	47	74
9	E	57/114 (50%)	56 (98%)	1 (2%)	59	80
10	F	122/185 (66%)	119 (98%)	3 (2%)	47	74
11	G	77/133 (58%)	74 (96%)	3 (4%)	32	63
12	H	72/113 (64%)	69 (96%)	3 (4%)	30	60
13	I	27/33 (82%)	27 (100%)	0	100	100
14	J	36/39 (92%)	35 (97%)	1 (3%)	43	71
15	K	43/95 (45%)	42 (98%)	1 (2%)	50	75
16	L	125/174 (72%)	123 (98%)	2 (2%)	62	83
All	All	2550/3153 (81%)	2492 (98%)	58 (2%)	53	75

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	69	ASP
1	1	172	PHE
1	1	210	SER
1	1	230	HIS
2	2	52	ARG
2	2	66	ASP
2	2	173	ASN
2	2	188	TRP
2	2	227	HIS
3	3	179	SER
3	3	265	ASN
4	4	66	TYR
4	4	70	SER
4	4	177	SER
4	4	194	ASN
4	4	222	GLN
5	A	71	PHE
5	A	72	SER
5	A	141	PHE
5	A	166	PHE
5	A	245	ASP
5	A	267	SER
5	A	275	PHE
5	A	276	ARG
5	A	371	MET
5	A	507	TRP
5	A	522	LEU
5	A	683	MET
6	B	47	PHE
6	B	65	LEU
6	B	231	ASN
6	B	257	LEU
6	B	332	PHE
6	B	394	PHE
6	B	402	GLN
6	B	431	PHE
6	B	475	ASP
6	B	577	TYR
6	B	617	MET
7	C	9	ASP
7	C	48	CYS
8	D	129	GLU

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Mol	Chain	Res	Type
8	D	140	SER
8	D	147	GLN
9	E	122	LYS
10	F	76	LYS
10	F	77	ASP
10	F	137	HIS
11	G	117	SER
11	G	131	ASP
11	G	152	ASN
12	H	77	ASP
12	H	80	SER
12	H	121	ASN
14	J	8	LEU
15	K	105	ASP
16	L	80	SER
16	L	175	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
4	4	236	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

198 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	802	-	65,73,73	1.49	7 (10%)	76,113,113	1.38	8 (10%)
18	CLA	G	202	-	42,50,73	1.83	6 (14%)	48,85,113	1.58	7 (14%)
18	CLA	B	836	-	50,58,73	1.68	7 (14%)	58,95,113	3.68	12 (20%)
18	CLA	A	806	-	65,73,73	1.48	7 (10%)	76,113,113	1.43	8 (10%)
17	CHL	1	606	-	40,49,74	2.59	16 (40%)	41,84,114	2.92	17 (41%)
18	CLA	B	813	-	65,73,73	1.45	7 (10%)	76,113,113	1.51	9 (11%)
18	CLA	B	821	-	47,55,73	1.71	6 (12%)	54,91,113	1.69	8 (14%)
22	BCR	B	801	-	41,41,41	1.81	8 (19%)	56,56,56	1.83	12 (21%)
18	CLA	B	810	-	65,73,73	1.48	7 (10%)	76,113,113	1.38	8 (10%)
18	CLA	4	603	-	44,52,73	1.83	7 (15%)	55,88,113	1.65	8 (14%)
20	LHG	B	852	-	48,48,48	0.27	0	51,54,54	0.32	0
18	CLA	2	602	-	65,73,73	1.47	7 (10%)	76,113,113	1.41	7 (9%)
18	CLA	3	610	-	39,48,73	1.90	5 (12%)	44,83,113	1.66	7 (15%)
18	CLA	A	827	-	59,67,73	1.54	7 (11%)	68,105,113	1.45	8 (11%)
18	CLA	B	827	-	65,73,73	1.48	6 (9%)	76,113,113	1.43	7 (9%)
18	CLA	2	603	-	43,52,73	1.81	7 (16%)	49,88,113	1.59	6 (12%)
18	CLA	A	843	-	65,73,73	1.46	7 (10%)	76,113,113	1.40	6 (7%)
18	CLA	2	613	-	43,51,73	1.82	6 (13%)	49,86,113	1.62	7 (14%)
18	CLA	B	833	-	45,53,73	1.76	7 (15%)	52,89,113	1.63	8 (15%)
22	BCR	4	618	-	41,41,41	1.74	8 (19%)	56,56,56	1.66	9 (16%)
18	CLA	4	608	4	45,53,73	1.81	6 (13%)	52,89,113	1.56	7 (13%)
18	CLA	A	814	-	65,73,73	1.48	8 (12%)	76,113,113	1.37	7 (9%)
18	CLA	F	303	10	41,49,73	1.84	6 (14%)	47,84,113	1.64	7 (14%)
18	CLA	B	822	-	65,73,73	1.48	6 (9%)	76,113,113	1.44	9 (11%)
18	CLA	1	603	-	54,62,73	1.63	6 (11%)	62,99,113	1.49	7 (11%)
22	BCR	B	847	-	41,41,41	1.71	8 (19%)	56,56,56	1.56	9 (16%)
18	CLA	4	602	4	60,68,73	1.53	7 (11%)	70,107,113	1.45	8 (11%)
18	CLA	B	826	-	62,70,73	1.51	7 (11%)	72,109,113	1.43	7 (9%)
18	CLA	K	204	-	46,54,73	1.78	6 (13%)	53,90,113	1.54	7 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	CLA	H	201	-	60,68,73	1.53	6 (10%)	70,107,113	1.39	8 (11%)
18	CLA	A	802	-	65,73,73	1.46	7 (10%)	76,113,113	1.47	7 (9%)
18	CLA	A	839	-	55,63,73	1.58	6 (10%)	64,101,113	1.55	8 (12%)
18	CLA	B	837	-	65,73,73	1.46	7 (10%)	76,113,113	1.45	8 (10%)
17	CHL	1	601	1	51,60,74	2.19	16 (31%)	54,97,114	2.66	23 (42%)
18	CLA	2	611	-	44,52,73	1.82	6 (13%)	51,88,113	1.64	8 (15%)
18	CLA	F	301	-	57,65,73	1.59	6 (10%)	66,103,113	1.45	7 (10%)
18	CLA	A	813	-	54,62,73	1.63	6 (11%)	62,99,113	1.53	8 (12%)
22	BCR	L	301	-	41,41,41	1.76	9 (21%)	56,56,56	2.22	12 (21%)
22	BCR	A	848	-	41,41,41	1.75	8 (19%)	56,56,56	1.66	11 (19%)
18	CLA	A	810	5	50,58,73	1.70	6 (12%)	58,95,113	1.59	10 (17%)
22	BCR	A	849	-	41,41,41	1.76	8 (19%)	56,56,56	2.00	13 (23%)
27	DGD	B	850	-	67,67,67	0.84	2 (2%)	81,81,81	0.98	3 (3%)
18	CLA	3	609	-	53,62,73	1.65	6 (11%)	61,100,113	1.47	9 (14%)
18	CLA	A	817	-	45,53,73	1.80	6 (13%)	52,89,113	1.58	6 (11%)
18	CLA	3	601	3	60,68,73	1.55	7 (11%)	70,107,113	1.44	8 (11%)
18	CLA	A	838	-	51,59,73	1.67	6 (11%)	59,96,113	1.50	7 (11%)
18	CLA	4	601	4	46,54,73	1.76	7 (15%)	53,90,113	1.58	7 (13%)
22	BCR	F	304	-	41,41,41	1.87	8 (19%)	56,56,56	2.15	16 (28%)
18	CLA	A	818	-	60,68,73	1.54	6 (10%)	70,107,113	5.15	10 (14%)
18	CLA	B	805	-	65,73,73	1.49	7 (10%)	76,113,113	1.40	7 (9%)
18	CLA	A	836	-	45,53,73	1.82	5 (11%)	52,89,113	1.59	7 (13%)
22	BCR	A	852	-	41,41,41	1.73	8 (19%)	56,56,56	2.02	15 (26%)
22	BCR	K	205	-	41,41,41	1.73	8 (19%)	56,56,56	1.90	16 (28%)
18	CLA	B	832	-	65,73,73	1.50	6 (9%)	76,113,113	1.33	6 (7%)
22	BCR	J	102	-	41,41,41	1.75	8 (19%)	56,56,56	1.81	14 (25%)
18	CLA	4	609	-	54,62,73	1.61	6 (11%)	62,99,113	1.52	8 (12%)
23	LMG	4	620	-	33,33,55	0.24	0	41,41,63	0.26	0
24	CL0	A	801	-	60,67,73	2.06	15 (25%)	68,102,113	3.72	29 (42%)
18	CLA	A	819	-	59,67,73	1.55	7 (11%)	68,105,113	1.44	8 (11%)
17	CHL	2	601	2	47,55,74	2.31	16 (34%)	50,91,114	2.76	19 (38%)
22	BCR	B	843	-	41,41,41	1.77	8 (19%)	56,56,56	1.92	13 (23%)
18	CLA	1	611	-	45,53,73	1.80	6 (13%)	52,89,113	1.58	6 (11%)
18	CLA	B	830	-	43,51,73	1.77	6 (13%)	49,86,113	1.62	7 (14%)
18	CLA	B	818	-	60,68,73	1.51	7 (11%)	70,107,113	1.55	9 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	LUT	3	613	-	42,43,43	1.70	8 (19%)	51,60,60	1.99	14 (27%)
18	CLA	A	825	-	55,63,73	1.58	5 (9%)	64,101,113	1.52	9 (14%)
18	CLA	F	302	-	51,59,73	1.68	5 (9%)	59,96,113	1.62	6 (10%)
20	LHG	A	847	-	29,29,48	0.35	0	32,35,54	0.43	0
21	LUT	2	616	-	42,43,43	1.65	8 (19%)	51,60,60	1.98	12 (23%)
18	CLA	A	841	-	65,73,73	1.45	7 (10%)	76,113,113	1.39	8 (10%)
22	BCR	L	306	-	41,41,41	1.71	8 (19%)	56,56,56	2.03	16 (28%)
18	CLA	1	609	-	42,50,73	1.82	6 (14%)	48,85,113	1.70	6 (12%)
18	CLA	K	201	15	38,45,73	1.91	6 (15%)	43,78,113	1.64	6 (13%)
18	CLA	1	602	1	54,62,73	1.60	6 (11%)	62,99,113	1.48	8 (12%)
21	LUT	1	616	-	42,43,43	1.68	7 (16%)	51,60,60	2.10	14 (27%)
17	CHL	4	615	4	40,49,74	2.24	13 (32%)	45,84,114	2.92	18 (40%)
18	CLA	B	814	-	65,73,73	1.47	6 (9%)	76,113,113	1.40	7 (9%)
18	CLA	B	819	-	55,63,73	1.62	8 (14%)	64,101,113	1.49	7 (10%)
18	CLA	B	840	-	65,73,73	1.48	6 (9%)	76,113,113	1.39	6 (7%)
22	BCR	B	849	-	41,41,41	1.77	8 (19%)	56,56,56	1.87	12 (21%)
25	SF4	C	101	-	0,12,12	-	-	-	-	-
22	BCR	I	101	-	41,41,41	1.71	8 (19%)	56,56,56	1.50	8 (14%)
18	CLA	A	834	-	65,73,73	1.48	6 (9%)	76,113,113	1.40	7 (9%)
18	CLA	B	803	-	65,73,73	1.46	8 (12%)	76,113,113	1.43	8 (10%)
18	CLA	2	612	-	65,73,73	1.46	6 (9%)	76,113,113	1.41	6 (7%)
20	LHG	1	615	18	48,48,48	0.93	2 (4%)	51,54,54	1.03	3 (5%)
18	CLA	A	832	-	50,58,73	1.68	6 (12%)	58,95,113	1.55	9 (15%)
18	CLA	B	812	-	43,51,73	1.80	6 (13%)	49,86,113	1.59	6 (12%)
18	CLA	B	823	-	45,53,73	1.78	7 (15%)	52,89,113	1.54	7 (13%)
18	CLA	B	809	6	65,73,73	1.46	7 (10%)	76,113,113	1.44	8 (10%)
18	CLA	1	607	-	43,52,73	1.83	7 (16%)	49,88,113	1.58	6 (12%)
18	CLA	1	605	-	46,54,73	1.77	5 (10%)	53,90,113	1.62	6 (11%)
18	CLA	1	613	-	37,46,73	2.01	7 (18%)	46,81,113	1.74	9 (19%)
18	CLA	A	816	-	42,50,73	1.82	6 (14%)	48,85,113	1.62	6 (12%)
22	BCR	B	846	-	41,41,41	1.74	8 (19%)	56,56,56	1.69	10 (17%)
18	CLA	K	203	-	45,53,73	1.78	5 (11%)	52,89,113	1.63	8 (15%)
18	CLA	B	839	-	65,73,73	1.48	6 (9%)	76,113,113	1.37	8 (10%)
18	CLA	G	201	-	45,53,73	1.80	6 (13%)	52,89,113	1.56	7 (13%)
18	CLA	3	611	-	37,44,73	1.93	7 (18%)	42,77,113	1.64	7 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	CLA	B	820	-	50,58,73	1.66	6 (12%)	58,95,113	1.63	9 (15%)
19	XAT	1	614	-	39,47,47	0.85	1 (2%)	54,74,74	3.17	23 (42%)
18	CLA	3	604	-	40,49,73	1.87	6 (15%)	45,84,113	1.59	6 (13%)
18	CLA	B	817	-	59,67,73	1.56	7 (11%)	68,105,113	1.47	9 (13%)
18	CLA	L	304	-	45,53,73	1.79	7 (15%)	52,89,113	1.59	6 (11%)
18	CLA	4	614	-	50,58,73	1.68	6 (12%)	58,95,113	1.58	8 (13%)
18	CLA	A	821	-	45,53,73	1.78	6 (13%)	52,89,113	1.60	6 (11%)
18	CLA	A	844	-	65,73,73	1.49	9 (13%)	76,113,113	1.38	8 (10%)
18	CLA	4	611	-	40,49,73	1.89	6 (15%)	45,84,113	1.61	6 (13%)
22	BCR	B	845	-	41,41,41	1.83	8 (19%)	56,56,56	1.94	14 (25%)
18	CLA	G	203	11	45,53,73	1.76	6 (13%)	52,89,113	1.60	6 (11%)
18	CLA	A	842	-	65,73,73	1.45	6 (9%)	76,113,113	1.53	7 (9%)
18	CLA	4	610	-	42,50,73	1.80	6 (14%)	48,85,113	1.59	6 (12%)
18	CLA	2	604	-	43,51,73	1.81	9 (20%)	48,86,113	1.63	6 (12%)
18	CLA	2	610	20	38,45,73	2.95	9 (23%)	41,76,113	1.48	7 (17%)
18	CLA	B	825	-	62,70,73	1.48	6 (9%)	72,109,113	1.49	9 (12%)
17	CHL	2	615	2	43,51,74	2.36	15 (34%)	45,86,114	2.88	19 (42%)
18	CLA	B	835	-	42,50,73	1.85	5 (11%)	48,85,113	1.57	7 (14%)
18	CLA	3	612	-	39,48,73	1.84	6 (15%)	44,83,113	1.72	7 (15%)
22	BCR	L	305	-	41,41,41	1.76	8 (19%)	56,56,56	1.78	13 (23%)
18	CLA	1	604	-	49,57,73	1.70	6 (12%)	55,93,113	1.72	8 (14%)
21	LUT	2	619	-	42,43,43	1.68	8 (19%)	51,60,60	1.82	11 (21%)
18	CLA	A	829	-	65,73,73	1.47	7 (10%)	76,113,113	1.38	7 (9%)
18	CLA	B	807	-	52,60,73	1.64	6 (11%)	60,97,113	1.52	8 (13%)
18	CLA	3	602	-	55,63,73	1.63	6 (10%)	64,101,113	1.42	7 (10%)
18	CLA	A	804	-	65,73,73	1.48	6 (9%)	76,113,113	1.55	10 (13%)
18	CLA	3	605	-	41,49,73	1.89	7 (17%)	51,84,113	1.69	9 (17%)
18	CLA	A	803	-	65,73,73	1.48	8 (12%)	76,113,113	1.32	7 (9%)
18	CLA	B	816	-	55,63,73	1.59	7 (12%)	64,101,113	1.50	9 (14%)
18	CLA	B	824	-	65,73,73	1.47	6 (9%)	76,113,113	1.42	7 (9%)
17	CHL	3	606	-	45,53,74	2.34	15 (33%)	52,89,114	2.62	17 (32%)
18	CLA	A	820	-	65,73,73	1.45	6 (9%)	76,113,113	1.46	6 (7%)
18	CLA	A	808	-	50,58,73	1.66	6 (12%)	58,95,113	1.60	8 (13%)
18	CLA	A	833	-	56,64,73	1.57	6 (10%)	65,102,113	1.51	7 (10%)
18	CLA	1	608	-	40,48,73	1.88	7 (17%)	50,83,113	1.72	9 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	CLA	B	806	-	65,73,73	1.46	6 (9%)	76,113,113	1.38	7 (9%)
18	CLA	B	829	-	56,64,73	1.59	6 (10%)	65,102,113	1.49	7 (10%)
17	CHL	2	607	-	51,59,74	2.19	16 (31%)	55,96,114	2.70	20 (36%)
18	CLA	A	826	-	65,73,73	1.46	6 (9%)	76,113,113	1.45	7 (9%)
18	CLA	A	809	5	65,73,73	1.47	6 (9%)	76,113,113	1.47	8 (10%)
25	SF4	A	854	-	0,12,12	-	-	-	-	-
18	CLA	B	834	-	60,68,73	1.56	6 (10%)	70,107,113	1.42	8 (11%)
17	CHL	2	605	-	42,50,74	2.35	15 (35%)	45,85,114	2.85	18 (40%)
18	CLA	1	612	-	46,54,73	1.74	5 (10%)	53,90,113	1.58	6 (11%)
18	CLA	2	609	-	47,55,73	1.69	7 (14%)	54,91,113	1.63	6 (11%)
20	LHG	A	846	-	48,48,48	0.28	0	51,54,54	0.33	0
22	BCR	G	204	-	41,41,41	1.71	8 (19%)	56,56,56	1.67	12 (21%)
23	LMG	4	619	-	39,39,55	0.23	0	47,47,63	0.23	0
18	CLA	1	610	20	37,46,73	1.98	7 (18%)	46,81,113	1.74	9 (19%)
18	CLA	4	613	-	45,53,73	1.78	6 (13%)	52,89,113	1.75	8 (15%)
18	CLA	3	608	-	41,49,73	1.82	7 (17%)	47,84,113	1.72	9 (19%)
18	CLA	L	302	16	45,53,73	1.78	6 (13%)	52,89,113	1.60	7 (13%)
18	CLA	A	835	-	65,73,73	1.47	6 (9%)	76,113,113	1.46	9 (11%)
18	CLA	B	831	-	43,51,73	1.78	6 (13%)	49,86,113	1.63	7 (14%)
26	PQN	B	842	-	34,34,34	0.40	0	42,45,45	0.41	0
18	CLA	A	823	-	42,50,73	1.82	5 (11%)	48,85,113	1.63	7 (14%)
22	BCR	B	848	-	41,41,41	1.73	8 (19%)	56,56,56	1.55	10 (17%)
22	BCR	3	614	-	41,41,41	1.72	8 (19%)	56,56,56	1.63	13 (23%)
18	CLA	B	808	-	65,73,73	1.45	8 (12%)	76,113,113	1.42	8 (10%)
18	CLA	A	830	-	65,73,73	1.45	6 (9%)	76,113,113	1.57	9 (11%)
18	CLA	B	838	-	47,55,73	1.74	6 (12%)	54,91,113	1.57	8 (14%)
18	CLA	B	815	-	43,51,73	1.79	7 (16%)	49,86,113	1.63	7 (14%)
22	BCR	B	844	-	41,41,41	1.76	8 (19%)	56,56,56	1.90	13 (23%)
26	PQN	A	855	-	34,34,34	0.38	0	42,45,45	0.42	0
17	CHL	4	606	-	41,49,74	2.43	14 (34%)	51,84,114	2.76	18 (35%)
22	BCR	A	853	-	41,41,41	1.82	8 (19%)	56,56,56	1.82	14 (25%)
18	CLA	A	811	-	65,73,73	1.45	6 (9%)	76,113,113	1.41	7 (9%)
20	LHG	2	618	18	36,36,48	0.31	0	39,42,54	0.48	0
18	CLA	A	828	-	65,73,73	1.46	7 (10%)	76,113,113	1.46	7 (9%)
18	CLA	A	840	-	52,60,73	1.66	6 (11%)	60,97,113	1.54	8 (13%)
18	CLA	4	604	-	43,51,73	1.88	6 (13%)	54,87,113	1.64	9 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	CLA	B	841	20	65,73,73	1.49	6 (9%)	76,113,113	1.38	8 (10%)
18	CLA	A	831	-	65,73,73	1.46	6 (9%)	76,113,113	1.43	8 (10%)
18	CLA	B	804	-	41,49,73	1.81	6 (14%)	47,84,113	1.76	8 (17%)
22	BCR	A	850	-	41,41,41	1.79	8 (19%)	56,56,56	1.89	13 (23%)
21	LUT	4	616	-	42,43,43	1.63	8 (19%)	51,60,60	1.60	10 (19%)
18	CLA	A	822	-	65,73,73	1.46	6 (9%)	76,113,113	1.41	8 (10%)
25	SF4	C	102	-	0,12,12	-	-	-	-	-
18	CLA	A	807	-	65,73,73	1.51	7 (10%)	76,113,113	1.36	8 (10%)
18	CLA	3	607	-	45,53,73	1.80	7 (15%)	52,89,113	1.55	6 (11%)
18	CLA	L	303	-	65,73,73	1.47	6 (9%)	76,113,113	1.43	7 (9%)
18	CLA	4	612	-	57,65,73	1.56	6 (10%)	66,103,113	1.50	8 (12%)
19	XAT	4	617	-	39,47,47	6.04	29 (74%)	54,74,74	5.93	34 (62%)
20	LHG	B	851	18	37,37,48	0.31	0	40,43,54	0.48	0
22	BCR	A	851	-	41,41,41	1.83	8 (19%)	56,56,56	2.47	20 (35%)
19	XAT	2	617	-	39,47,47	1.81	7 (17%)	54,74,74	2.10	15 (27%)
18	CLA	A	815	-	45,53,73	1.74	7 (15%)	52,89,113	1.72	9 (17%)
17	CHL	4	605	-	40,49,74	2.39	15 (37%)	42,84,114	2.78	18 (42%)
18	CLA	B	828	-	65,73,73	1.50	7 (10%)	76,113,113	1.37	7 (9%)
18	CLA	B	811	-	54,62,73	1.66	7 (12%)	67,100,113	1.53	10 (14%)
18	CLA	A	837	5	45,53,73	1.80	6 (13%)	52,89,113	1.58	7 (13%)
18	CLA	A	812	-	65,73,73	1.49	6 (9%)	76,113,113	1.42	8 (10%)
17	CHL	4	607	-	46,54,74	2.22	16 (34%)	49,90,114	2.84	20 (40%)
22	BCR	K	202	-	41,41,41	1.80	7 (17%)	56,56,56	1.95	14 (25%)
18	CLA	2	608	2	45,53,73	1.76	6 (13%)	52,89,113	1.62	6 (11%)
18	CLA	A	824	-	41,49,73	1.87	5 (12%)	47,84,113	1.67	8 (17%)
18	CLA	A	805	-	52,60,73	1.64	6 (11%)	60,97,113	1.57	8 (13%)
17	CHL	2	606	-	43,51,74	2.39	15 (34%)	45,86,114	2.86	21 (46%)
18	CLA	3	603	-	45,53,73	1.80	5 (11%)	52,89,113	1.60	8 (15%)

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	802	-	1/1/15/20	17/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	G	202	-	1/1/10/20	2/10/88/115	-
18	CLA	B	836	-	1/1/12/20	4/19/97/115	-
18	CLA	A	806	-	1/1/15/20	21/37/115/115	-
17	CHL	1	606	-	3/3/15/26	0/8/106/137	-
18	CLA	B	813	-	1/1/15/20	12/37/115/115	-
18	CLA	B	821	-	1/1/11/20	6/16/94/115	-
22	BCR	B	801	-	-	7/29/63/63	0/2/2/2
18	CLA	B	810	-	1/1/15/20	12/37/115/115	-
18	CLA	4	603	-	1/1/11/20	4/13/89/115	-
20	LHG	B	852	-	-	11/53/53/53	-
18	CLA	2	602	-	1/1/15/20	15/37/115/115	-
18	CLA	3	610	-	1/1/10/20	0/6/84/115	-
18	CLA	A	827	-	1/1/13/20	7/30/108/115	-
18	CLA	B	827	-	1/1/15/20	20/37/115/115	-
18	CLA	2	603	-	1/1/11/20	3/11/89/115	-
18	CLA	A	843	-	1/1/15/20	16/37/115/115	-
18	CLA	2	613	-	1/1/10/20	3/11/89/115	-
18	CLA	B	833	-	1/1/11/20	4/13/91/115	-
22	BCR	4	618	-	-	9/29/63/63	0/2/2/2
18	CLA	4	608	4	1/1/11/20	5/13/91/115	-
18	CLA	A	814	-	1/1/15/20	15/37/115/115	-
18	CLA	F	303	10	1/1/10/20	2/8/86/115	-
18	CLA	B	822	-	1/1/15/20	16/37/115/115	-
18	CLA	1	603	-	1/1/12/20	8/24/102/115	-
22	BCR	B	847	-	-	2/29/63/63	0/2/2/2
18	CLA	4	602	4	1/1/14/20	9/31/109/115	-
18	CLA	B	826	-	1/1/14/20	6/34/112/115	-
18	CLA	K	204	-	1/1/11/20	10/15/93/115	-
18	CLA	H	201	-	1/1/14/20	16/31/109/115	-
18	CLA	A	802	-	1/1/15/20	11/37/115/115	-
18	CLA	A	839	-	1/1/13/20	7/25/103/115	-
18	CLA	B	837	-	1/1/15/20	13/37/115/115	-
17	CHL	1	601	1	3/3/17/26	8/22/120/137	-
18	CLA	2	611	-	1/1/11/20	8/11/89/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	F	301	-	1/1/13/20	11/28/106/115	-
18	CLA	A	813	-	1/1/12/20	9/24/102/115	-
22	BCR	L	301	-	-	3/29/63/63	0/2/2/2
22	BCR	A	848	-	-	2/29/63/63	0/2/2/2
18	CLA	A	810	5	1/1/12/20	4/19/97/115	-
22	BCR	A	849	-	-	5/29/63/63	0/2/2/2
27	DGD	B	850	-	-	14/55/95/95	0/2/2/2
18	CLA	3	609	-	1/1/13/20	9/23/101/115	-
18	CLA	A	817	-	1/1/11/20	3/13/91/115	-
18	CLA	3	601	3	1/1/14/20	11/31/109/115	-
18	CLA	A	838	-	1/1/12/20	6/21/99/115	-
18	CLA	4	601	4	1/1/11/20	8/15/93/115	-
22	BCR	F	304	-	-	12/29/63/63	0/2/2/2
18	CLA	A	818	-	1/1/14/20	12/31/109/115	-
18	CLA	B	805	-	1/1/15/20	24/37/115/115	-
18	CLA	A	836	-	1/1/11/20	3/13/91/115	-
22	BCR	A	852	-	-	14/29/63/63	0/2/2/2
22	BCR	K	205	-	-	6/29/63/63	0/2/2/2
18	CLA	B	832	-	1/1/15/20	14/37/115/115	-
22	BCR	J	102	-	-	2/29/63/63	0/2/2/2
18	CLA	4	609	-	1/1/12/20	4/24/102/115	-
23	LMG	4	620	-	-	5/28/48/70	0/1/1/1
24	CL0	A	801	-	2/2/16/25	15/33/115/135	-
18	CLA	A	819	-	1/1/13/20	15/30/108/115	-
17	CHL	2	601	2	3/3/16/26	5/17/115/137	-
22	BCR	B	843	-	-	1/29/63/63	0/2/2/2
18	CLA	1	611	-	1/1/11/20	5/13/91/115	-
18	CLA	B	830	-	1/1/10/20	2/11/89/115	-
18	CLA	B	818	-	1/1/14/20	8/31/109/115	-
21	LUT	3	613	-	-	6/29/67/67	0/2/2/2
18	CLA	A	825	-	1/1/13/20	10/25/103/115	-
18	CLA	F	302	-	1/1/12/20	10/21/99/115	-
20	LHG	A	847	-	-	3/34/34/53	-
21	LUT	2	616	-	-	6/29/67/67	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	A	841	-	1/1/15/20	13/37/115/115	-
22	BCR	L	306	-	-	4/29/63/63	0/2/2/2
18	CLA	1	609	-	1/1/10/20	4/9/87/115	-
18	CLA	K	201	15	1/1/8/20	0/2/76/115	-
18	CLA	1	602	1	1/1/12/20	9/24/102/115	-
21	LUT	1	616	-	-	3/29/67/67	0/2/2/2
17	CHL	4	615	4	3/3/15/26	0/10/106/137	-
18	CLA	B	814	-	1/1/15/20	17/37/115/115	-
18	CLA	B	819	-	1/1/13/20	9/25/103/115	-
18	CLA	B	840	-	1/1/15/20	9/37/115/115	-
22	BCR	B	849	-	-	7/29/63/63	0/2/2/2
25	SF4	C	101	-	-	-	0/6/5/5
22	BCR	I	101	-	-	0/29/63/63	0/2/2/2
18	CLA	A	834	-	1/1/15/20	8/37/115/115	-
18	CLA	B	803	-	1/1/15/20	10/37/115/115	-
18	CLA	2	612	-	1/1/15/20	18/37/115/115	-
20	LHG	1	615	18	-	33/53/53/53	-
18	CLA	A	832	-	1/1/12/20	7/19/97/115	-
18	CLA	B	812	-	1/1/10/20	0/11/89/115	-
18	CLA	B	823	-	1/1/11/20	4/13/91/115	-
18	CLA	B	809	6	1/1/15/20	16/37/115/115	-
18	CLA	1	607	-	1/1/11/20	7/11/89/115	-
18	CLA	1	605	-	1/1/11/20	7/15/93/115	-
18	CLA	1	613	-	1/1/10/20	1/4/80/115	-
18	CLA	A	816	-	1/1/10/20	3/10/88/115	-
22	BCR	B	846	-	-	8/29/63/63	0/2/2/2
18	CLA	K	203	-	1/1/11/20	6/13/91/115	-
18	CLA	B	839	-	1/1/15/20	7/37/115/115	-
18	CLA	G	201	-	1/1/11/20	3/13/91/115	-
18	CLA	3	611	-	1/1/8/20	0/0/74/115	-
18	CLA	B	820	-	1/1/12/20	5/19/97/115	-
19	XAT	1	614	-	-	5/31/93/93	0/4/4/4
18	CLA	3	604	-	1/1/10/20	0/8/86/115	-
18	CLA	B	817	-	1/1/13/20	11/30/108/115	-
18	CLA	L	304	-	1/1/11/20	3/13/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	4	614	-	1/1/12/20	6/19/97/115	-
18	CLA	A	821	-	1/1/11/20	5/13/91/115	-
18	CLA	A	844	-	1/1/15/20	10/37/115/115	-
18	CLA	4	611	-	1/1/10/20	0/8/86/115	-
22	BCR	B	845	-	-	9/29/63/63	0/2/2/2
18	CLA	G	203	11	1/1/11/20	3/13/91/115	-
18	CLA	A	842	-	1/1/15/20	11/37/115/115	-
18	CLA	4	610	-	1/1/10/20	2/10/88/115	-
18	CLA	2	604	-	1/1/10/20	7/9/88/115	-
18	CLA	2	610	20	1/1/7/20	2/10/70/115	-
18	CLA	B	825	-	1/1/14/20	13/34/112/115	-
17	CHL	2	615	2	3/3/15/26	2/12/110/137	-
18	CLA	B	835	-	1/1/10/20	4/10/88/115	-
18	CLA	3	612	-	1/1/10/20	0/6/84/115	-
22	BCR	L	305	-	-	2/29/63/63	0/2/2/2
18	CLA	1	604	-	1/1/11/20	9/18/96/115	-
21	LUT	2	619	-	-	5/29/67/67	0/2/2/2
18	CLA	A	829	-	1/1/15/20	17/37/115/115	-
18	CLA	B	807	-	1/1/12/20	1/22/100/115	-
18	CLA	3	602	-	1/1/13/20	11/25/103/115	-
18	CLA	A	804	-	1/1/15/20	17/37/115/115	-
18	CLA	3	605	-	1/1/10/20	1/10/86/115	-
18	CLA	A	803	-	1/1/15/20	19/37/115/115	-
18	CLA	B	816	-	1/1/13/20	9/25/103/115	-
18	CLA	B	824	-	1/1/15/20	16/37/115/115	-
17	CHL	3	606	-	3/3/16/26	7/13/111/137	-
18	CLA	A	820	-	1/1/15/20	16/37/115/115	-
18	CLA	A	808	-	1/1/12/20	0/19/97/115	-
18	CLA	A	833	-	1/1/13/20	4/27/105/115	-
18	CLA	1	608	-	1/1/10/20	3/8/84/115	-
18	CLA	B	806	-	1/1/15/20	13/37/115/115	-
18	CLA	B	829	-	1/1/13/20	6/27/105/115	-
17	CHL	2	607	-	3/3/17/26	4/21/119/137	-
18	CLA	A	826	-	1/1/15/20	12/37/115/115	-
18	CLA	A	809	5	1/1/15/20	13/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	SF4	A	854	-	-	-	0/6/5/5
18	CLA	B	834	-	1/1/14/20	5/31/109/115	-
17	CHL	2	605	-	3/3/15/26	4/10/108/137	-
18	CLA	1	612	-	1/1/11/20	7/15/93/115	-
18	CLA	2	609	-	1/1/11/20	6/16/94/115	-
20	LHG	A	846	-	-	5/53/53/53	-
22	BCR	G	204	-	-	3/29/63/63	0/2/2/2
23	LMG	4	619	-	-	4/34/54/70	0/1/1/1
18	CLA	1	610	20	1/1/10/20	0/4/80/115	-
18	CLA	4	613	-	1/1/11/20	6/13/91/115	-
18	CLA	3	608	-	1/1/10/20	3/8/86/115	-
18	CLA	L	302	16	1/1/11/20	1/13/91/115	-
18	CLA	A	835	-	1/1/15/20	14/37/115/115	-
18	CLA	B	831	-	1/1/10/20	1/11/89/115	-
26	PQN	B	842	-	-	7/23/43/43	0/2/2/2
18	CLA	A	823	-	1/1/10/20	4/10/88/115	-
22	BCR	B	848	-	-	0/29/63/63	0/2/2/2
22	BCR	3	614	-	-	3/29/63/63	0/2/2/2
18	CLA	B	808	-	1/1/15/20	11/37/115/115	-
18	CLA	A	830	-	1/1/15/20	11/37/115/115	-
18	CLA	B	838	-	1/1/11/20	3/16/94/115	-
18	CLA	B	815	-	1/1/10/20	5/11/89/115	-
22	BCR	B	844	-	-	11/29/63/63	0/2/2/2
26	PQN	A	855	-	-	1/23/43/43	0/2/2/2
17	CHL	4	606	-	3/3/15/26	2/10/106/137	-
22	BCR	A	853	-	-	4/29/63/63	0/2/2/2
18	CLA	A	811	-	1/1/15/20	13/37/115/115	-
20	LHG	2	618	18	-	11/41/41/53	-
18	CLA	A	828	-	1/1/15/20	9/37/115/115	-
18	CLA	A	840	-	1/1/12/20	5/22/100/115	-
18	CLA	4	604	-	1/1/11/20	6/11/87/115	-
18	CLA	B	841	20	1/1/15/20	20/37/115/115	-
18	CLA	A	831	-	1/1/15/20	8/37/115/115	-
18	CLA	B	804	-	1/1/10/20	2/8/86/115	-
22	BCR	A	850	-	-	4/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	LUT	4	616	-	-	2/29/67/67	0/2/2/2
18	CLA	A	822	-	1/1/15/20	11/37/115/115	-
25	SF4	C	102	-	-	-	0/6/5/5
18	CLA	A	807	-	1/1/15/20	14/37/115/115	-
18	CLA	3	607	-	1/1/11/20	2/13/91/115	-
18	CLA	L	303	-	1/1/15/20	11/37/115/115	-
18	CLA	4	612	-	1/1/13/20	11/28/106/115	-
19	XAT	4	617	-	-	3/31/93/93	0/4/4/4
20	LHG	B	851	18	-	5/42/42/53	-
22	BCR	A	851	-	-	7/29/63/63	0/2/2/2
19	XAT	2	617	-	-	15/31/93/93	0/4/4/4
18	CLA	A	815	-	1/1/11/20	5/13/91/115	-
17	CHL	4	605	-	3/3/15/26	5/8/106/137	-
18	CLA	B	828	-	1/1/15/20	17/37/115/115	-
18	CLA	B	811	-	1/1/13/20	11/25/101/115	-
18	CLA	A	837	5	1/1/11/20	3/13/91/115	-
18	CLA	A	812	-	1/1/15/20	21/37/115/115	-
17	CHL	4	607	-	3/3/16/26	6/15/113/137	-
22	BCR	K	202	-	-	2/29/63/63	0/2/2/2
18	CLA	2	608	2	1/1/11/20	7/13/91/115	-
18	CLA	A	824	-	1/1/10/20	2/8/86/115	-
18	CLA	A	805	-	1/1/12/20	4/22/100/115	-
17	CHL	2	606	-	3/3/15/26	2/12/110/137	-
18	CLA	3	603	-	1/1/11/20	3/13/91/115	-

All (1355) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	4	617	XAT	O24-C25	-13.10	1.27	1.46
18	2	610	CLA	C1A-NA	12.61	1.40	1.29
19	4	617	XAT	C2-C3	-11.35	1.36	1.52
19	4	617	XAT	C2-C1	-10.99	1.37	1.54
19	4	617	XAT	O4-C5	-10.50	1.31	1.46
19	4	617	XAT	C24-C25	-10.18	1.37	1.52
19	4	617	XAT	C38-C25	-9.14	1.37	1.51
19	4	617	XAT	C4-C3	-8.48	1.40	1.52
19	4	617	XAT	C4-C5	-8.34	1.40	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	801	CL0	C1D-ND	8.20	1.47	1.37
19	4	617	XAT	C24-C23	-8.15	1.40	1.52
18	A	836	CLA	C4B-NB	7.77	1.42	1.35
19	4	617	XAT	C22-C23	-7.74	1.41	1.52
18	A	807	CLA	C4B-NB	7.68	1.42	1.35
18	A	837	CLA	C4B-NB	7.65	1.42	1.35
18	1	607	CLA	C4B-NB	7.63	1.42	1.35
18	B	832	CLA	C4B-NB	7.62	1.42	1.35
18	2	611	CLA	C4B-NB	7.61	1.42	1.35
18	G	201	CLA	C4B-NB	7.61	1.42	1.35
18	2	613	CLA	C4B-NB	7.59	1.42	1.35
18	4	611	CLA	C4B-NB	7.59	1.42	1.35
18	1	605	CLA	C4B-NB	7.58	1.42	1.35
18	A	817	CLA	C4B-NB	7.58	1.42	1.35
18	B	834	CLA	C4B-NB	7.57	1.42	1.35
18	B	828	CLA	C4B-NB	7.57	1.42	1.35
18	K	204	CLA	C4B-NB	7.54	1.41	1.35
18	1	611	CLA	C4B-NB	7.54	1.41	1.35
18	4	608	CLA	C4B-NB	7.54	1.41	1.35
18	A	813	CLA	C4B-NB	7.53	1.41	1.35
18	G	202	CLA	C4B-NB	7.53	1.41	1.35
18	B	805	CLA	C4B-NB	7.52	1.41	1.35
18	B	835	CLA	C4B-NB	7.52	1.41	1.35
18	A	824	CLA	C4B-NB	7.52	1.41	1.35
18	3	604	CLA	C4B-NB	7.51	1.41	1.35
18	3	610	CLA	C4B-NB	7.50	1.41	1.35
18	B	812	CLA	C4B-NB	7.50	1.41	1.35
18	A	810	CLA	C4B-NB	7.50	1.41	1.35
18	F	302	CLA	C4B-NB	7.50	1.41	1.35
18	4	601	CLA	C4B-NB	7.49	1.41	1.35
18	1	609	CLA	C4B-NB	7.49	1.41	1.35
18	B	838	CLA	C4B-NB	7.48	1.41	1.35
18	3	603	CLA	C4B-NB	7.47	1.41	1.35
18	K	201	CLA	C4B-NB	7.45	1.41	1.35
18	A	823	CLA	C4B-NB	7.45	1.41	1.35
18	F	303	CLA	C4B-NB	7.45	1.41	1.35
18	3	607	CLA	C4B-NB	7.45	1.41	1.35
18	B	802	CLA	C4B-NB	7.44	1.41	1.35
18	1	613	CLA	C4B-NB	7.44	1.41	1.35
19	4	617	XAT	C17-C1	-7.44	1.39	1.53
18	4	604	CLA	C4B-NB	7.43	1.41	1.35
18	4	614	CLA	C4B-NB	7.43	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	L	302	CLA	C4B-NB	7.43	1.41	1.35
18	A	812	CLA	C4B-NB	7.42	1.41	1.35
18	B	841	CLA	C4B-NB	7.42	1.41	1.35
18	3	611	CLA	C4B-NB	7.41	1.41	1.35
18	A	840	CLA	C4B-NB	7.40	1.41	1.35
18	3	609	CLA	C4B-NB	7.40	1.41	1.35
18	K	203	CLA	C4B-NB	7.39	1.41	1.35
18	3	602	CLA	C4B-NB	7.39	1.41	1.35
18	A	838	CLA	C4B-NB	7.38	1.41	1.35
18	3	605	CLA	C4B-NB	7.36	1.41	1.35
18	L	304	CLA	C4B-NB	7.36	1.41	1.35
18	H	201	CLA	C4B-NB	7.36	1.41	1.35
18	F	301	CLA	C4B-NB	7.35	1.41	1.35
18	B	840	CLA	C4B-NB	7.35	1.41	1.35
18	A	814	CLA	C4B-NB	7.34	1.41	1.35
18	A	816	CLA	C4B-NB	7.34	1.41	1.35
18	1	604	CLA	C4B-NB	7.34	1.41	1.35
18	A	821	CLA	C4B-NB	7.33	1.41	1.35
18	B	822	CLA	C4B-NB	7.33	1.41	1.35
18	B	823	CLA	C4B-NB	7.33	1.41	1.35
18	B	815	CLA	C4B-NB	7.33	1.41	1.35
18	B	811	CLA	C4B-NB	7.33	1.41	1.35
18	2	610	CLA	C4B-NB	7.32	1.41	1.35
18	A	834	CLA	C4B-NB	7.32	1.41	1.35
18	B	839	CLA	C4B-NB	7.32	1.41	1.35
18	1	603	CLA	C4B-NB	7.32	1.41	1.35
18	B	817	CLA	C4B-NB	7.31	1.41	1.35
18	B	810	CLA	C4B-NB	7.31	1.41	1.35
18	4	602	CLA	C4B-NB	7.31	1.41	1.35
18	B	831	CLA	C4B-NB	7.31	1.41	1.35
18	3	601	CLA	C4B-NB	7.31	1.41	1.35
18	B	819	CLA	C4B-NB	7.30	1.41	1.35
18	B	804	CLA	C4B-NB	7.30	1.41	1.35
18	B	837	CLA	C4B-NB	7.29	1.41	1.35
18	B	830	CLA	C4B-NB	7.29	1.41	1.35
19	4	617	XAT	C20-C13	-7.29	1.35	1.50
18	1	610	CLA	C4B-NB	7.29	1.41	1.35
18	A	804	CLA	C4B-NB	7.29	1.41	1.35
18	A	844	CLA	C4B-NB	7.29	1.41	1.35
18	B	829	CLA	C4B-NB	7.28	1.41	1.35
18	1	612	CLA	C4B-NB	7.28	1.41	1.35
18	2	603	CLA	C4B-NB	7.28	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	832	CLA	C4B-NB	7.28	1.41	1.35
18	G	203	CLA	C4B-NB	7.28	1.41	1.35
18	A	819	CLA	C4B-NB	7.28	1.41	1.35
18	A	806	CLA	C4B-NB	7.27	1.41	1.35
18	A	818	CLA	C4B-NB	7.26	1.41	1.35
18	4	613	CLA	C4B-NB	7.25	1.41	1.35
18	A	805	CLA	C4B-NB	7.25	1.41	1.35
18	4	610	CLA	C4B-NB	7.24	1.41	1.35
18	L	303	CLA	C4B-NB	7.24	1.41	1.35
18	B	836	CLA	C4B-NB	7.24	1.41	1.35
18	A	827	CLA	C4B-NB	7.24	1.41	1.35
18	B	820	CLA	C4B-NB	7.23	1.41	1.35
18	A	809	CLA	C4B-NB	7.23	1.41	1.35
18	B	824	CLA	C4B-NB	7.23	1.41	1.35
18	A	828	CLA	C4B-NB	7.22	1.41	1.35
18	4	612	CLA	C4B-NB	7.22	1.41	1.35
18	B	826	CLA	C4B-NB	7.22	1.41	1.35
18	B	827	CLA	C4B-NB	7.21	1.41	1.35
18	B	814	CLA	C4B-NB	7.20	1.41	1.35
18	B	809	CLA	C4B-NB	7.20	1.41	1.35
18	A	822	CLA	C4B-NB	7.20	1.41	1.35
18	B	825	CLA	C4B-NB	7.19	1.41	1.35
18	3	608	CLA	C4B-NB	7.18	1.41	1.35
18	A	831	CLA	C4B-NB	7.18	1.41	1.35
18	A	808	CLA	C4B-NB	7.17	1.41	1.35
18	2	608	CLA	C4B-NB	7.17	1.41	1.35
18	4	603	CLA	C4B-NB	7.17	1.41	1.35
18	2	612	CLA	C4B-NB	7.16	1.41	1.35
18	A	835	CLA	C4B-NB	7.16	1.41	1.35
18	A	811	CLA	C4B-NB	7.15	1.41	1.35
18	1	608	CLA	C4B-NB	7.15	1.41	1.35
18	2	609	CLA	C4B-NB	7.14	1.41	1.35
18	A	820	CLA	C4B-NB	7.14	1.41	1.35
18	A	825	CLA	C4B-NB	7.14	1.41	1.35
18	4	609	CLA	C4B-NB	7.13	1.41	1.35
18	B	803	CLA	C4B-NB	7.13	1.41	1.35
18	A	839	CLA	C4B-NB	7.13	1.41	1.35
18	B	806	CLA	C4B-NB	7.13	1.41	1.35
18	1	602	CLA	C4B-NB	7.12	1.41	1.35
18	3	612	CLA	C4B-NB	7.11	1.41	1.35
18	B	807	CLA	C4B-NB	7.11	1.41	1.35
18	A	841	CLA	C4B-NB	7.11	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	821	CLA	C4B-NB	7.11	1.41	1.35
18	A	802	CLA	C4B-NB	7.11	1.41	1.35
18	A	833	CLA	C4B-NB	7.10	1.41	1.35
18	A	842	CLA	C4B-NB	7.10	1.41	1.35
18	A	815	CLA	C4B-NB	7.10	1.41	1.35
18	B	833	CLA	C4B-NB	7.10	1.41	1.35
18	A	830	CLA	C4B-NB	7.09	1.41	1.35
18	A	829	CLA	C4B-NB	7.09	1.41	1.35
18	A	826	CLA	C4B-NB	7.09	1.41	1.35
18	A	843	CLA	C4B-NB	7.09	1.41	1.35
18	2	602	CLA	C4B-NB	7.08	1.41	1.35
18	B	813	CLA	C4B-NB	7.06	1.41	1.35
18	B	818	CLA	C4B-NB	7.02	1.41	1.35
18	B	816	CLA	C4B-NB	7.00	1.41	1.35
18	B	808	CLA	C4B-NB	6.99	1.41	1.35
18	2	604	CLA	C4B-NB	6.87	1.41	1.35
18	A	803	CLA	C4B-NB	6.81	1.41	1.35
19	4	617	XAT	C22-C21	-6.54	1.44	1.54
19	4	617	XAT	C19-C9	-6.48	1.37	1.50
24	A	801	CL0	C3D-C4D	-6.48	1.34	1.46
19	4	617	XAT	C37-C21	-5.55	1.43	1.53
19	4	617	XAT	C16-C1	-5.54	1.43	1.53
17	1	606	CHL	C3B-C2B	5.49	1.48	1.40
17	1	606	CHL	CHC-C1C	5.33	1.48	1.35
17	4	606	CHL	CHC-C1C	5.27	1.48	1.35
22	F	304	BCR	C21-C22	5.26	1.42	1.35
18	2	610	CLA	CHB-C4A	5.23	1.38	1.34
17	4	606	CHL	O2D-CGD	5.22	1.45	1.33
17	2	606	CHL	CHC-C1C	5.19	1.48	1.35
17	2	605	CHL	CHC-C1C	5.14	1.48	1.35
17	2	615	CHL	CHC-C1C	5.14	1.48	1.35
17	2	606	CHL	O2D-CGD	5.13	1.45	1.33
17	2	615	CHL	O2D-CGD	5.12	1.45	1.33
17	1	606	CHL	CHD-C1D	5.09	1.48	1.38
19	2	617	XAT	C34-C33	5.08	1.42	1.35
22	B	845	BCR	C21-C22	5.08	1.42	1.35
17	2	605	CHL	O2D-CGD	5.08	1.45	1.33
17	2	601	CHL	CHC-C1C	5.08	1.48	1.35
22	A	853	BCR	C10-C9	5.08	1.42	1.35
22	F	304	BCR	C17-C18	5.06	1.42	1.35
17	3	606	CHL	O2D-CGD	5.03	1.45	1.33
17	2	606	CHL	C3B-C2B	5.02	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	4	605	CHL	CHC-C1C	5.02	1.47	1.35
17	2	601	CHL	O2D-CGD	5.01	1.45	1.33
17	4	606	CHL	C3C-C2C	5.00	1.47	1.36
19	4	617	XAT	C39-C29	-5.00	1.40	1.50
17	1	601	CHL	CHC-C1C	5.00	1.47	1.35
17	2	607	CHL	O2D-CGD	4.98	1.45	1.33
17	1	606	CHL	C2C-C3C	4.97	1.47	1.36
17	4	615	CHL	CHC-C1C	4.96	1.47	1.35
17	4	606	CHL	CHD-C1D	4.95	1.48	1.38
17	2	607	CHL	CHC-C1C	4.95	1.47	1.35
17	3	606	CHL	CHC-C1C	4.94	1.47	1.35
17	4	605	CHL	C3B-C2B	4.93	1.47	1.40
19	4	617	XAT	C18-C5	-4.92	1.44	1.51
17	4	607	CHL	O2D-CGD	4.91	1.45	1.33
17	2	601	CHL	C3B-C2B	4.87	1.47	1.40
17	2	607	CHL	C3D-C4D	-4.86	1.33	1.44
17	2	615	CHL	C3B-C2B	4.81	1.47	1.40
17	2	601	CHL	C3D-C4D	-4.80	1.33	1.44
17	1	601	CHL	C3D-C4D	-4.79	1.33	1.44
17	2	605	CHL	C3B-C2B	4.77	1.47	1.40
22	B	801	BCR	C10-C9	4.76	1.42	1.35
17	4	607	CHL	C3D-C4D	-4.76	1.33	1.44
21	3	613	LUT	C10-C9	4.74	1.42	1.35
17	1	601	CHL	C3B-C2B	4.74	1.46	1.40
17	3	606	CHL	C3D-C4D	-4.72	1.33	1.44
17	2	606	CHL	C2C-C3C	4.72	1.46	1.36
17	4	606	CHL	C3D-C4D	-4.72	1.33	1.44
17	1	606	CHL	C3D-C4D	-4.72	1.33	1.44
17	2	615	CHL	C2C-C3C	4.69	1.46	1.36
22	A	850	BCR	C17-C18	4.69	1.42	1.35
17	2	605	CHL	C3D-C4D	-4.69	1.33	1.44
17	2	606	CHL	C3D-C4D	-4.68	1.33	1.44
17	4	605	CHL	C2C-C3C	4.68	1.46	1.37
17	2	615	CHL	C3D-C4D	-4.67	1.33	1.44
17	2	606	CHL	CHD-C1D	4.67	1.47	1.38
17	4	607	CHL	CHC-C1C	4.67	1.46	1.35
17	4	605	CHL	O2D-CGD	4.66	1.45	1.30
17	1	606	CHL	O2D-CGD	4.64	1.45	1.30
17	4	615	CHL	C3D-C4D	-4.64	1.33	1.44
17	2	615	CHL	CHD-C1D	4.64	1.47	1.38
19	4	617	XAT	C40-C33	-4.63	1.41	1.50
17	4	605	CHL	C3D-C4D	-4.63	1.33	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	4	615	CHL	O2D-CGD	4.63	1.45	1.30
22	A	850	BCR	C14-C13	4.62	1.41	1.35
17	3	606	CHL	C3B-C2B	4.61	1.46	1.40
19	4	617	XAT	C36-C21	-4.61	1.44	1.53
17	2	605	CHL	C2C-C3C	4.60	1.46	1.37
17	4	605	CHL	CHD-C1D	4.60	1.47	1.38
17	1	601	CHL	O2D-CGD	4.60	1.45	1.30
17	2	601	CHL	C2C-C3C	4.59	1.46	1.36
22	A	851	BCR	C21-C22	4.59	1.41	1.35
22	A	849	BCR	C21-C22	4.57	1.41	1.35
17	2	601	CHL	CHD-C1D	4.56	1.47	1.38
17	1	601	CHL	CHD-C1D	4.56	1.47	1.38
17	4	615	CHL	C2C-C3C	4.55	1.46	1.36
17	3	606	CHL	C3C-C2C	4.55	1.46	1.36
21	1	616	LUT	C30-C29	4.55	1.41	1.35
17	1	601	CHL	C2C-C3C	4.54	1.46	1.36
22	F	304	BCR	C10-C9	4.53	1.41	1.35
17	3	606	CHL	CHD-C1D	4.52	1.47	1.38
17	3	606	CHL	O2A-CGA	4.52	1.45	1.30
17	1	606	CHL	CHD-C4C	4.51	1.49	1.39
17	2	607	CHL	C2C-C3C	4.50	1.46	1.36
17	2	605	CHL	CHD-C1D	4.50	1.47	1.38
21	2	616	LUT	C34-C33	4.48	1.41	1.35
22	K	202	BCR	C10-C9	4.47	1.41	1.35
17	4	607	CHL	O2A-CGA	4.46	1.45	1.30
17	4	606	CHL	CHD-C4C	4.46	1.49	1.39
19	2	617	XAT	C14-C13	4.45	1.41	1.35
17	2	607	CHL	C3B-C2B	4.44	1.46	1.40
22	A	851	BCR	C14-C13	4.42	1.41	1.35
17	2	607	CHL	CHD-C1D	4.41	1.47	1.38
22	B	843	BCR	C14-C13	4.41	1.41	1.35
21	3	613	LUT	C34-C33	4.41	1.41	1.35
17	4	615	CHL	CHD-C1D	4.39	1.46	1.38
22	A	851	BCR	C17-C18	4.39	1.41	1.35
22	K	202	BCR	C17-C18	4.38	1.41	1.35
19	4	617	XAT	C10-C9	-4.37	1.30	1.35
22	B	844	BCR	C21-C22	4.37	1.41	1.35
22	K	202	BCR	C14-C13	4.37	1.41	1.35
19	2	617	XAT	C30-C29	4.36	1.41	1.35
22	B	849	BCR	C10-C9	4.35	1.41	1.35
22	K	202	BCR	C21-C22	4.35	1.41	1.35
22	B	849	BCR	C14-C13	4.31	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	845	BCR	C10-C9	4.31	1.41	1.35
22	A	851	BCR	C10-C9	4.28	1.41	1.35
19	2	617	XAT	C10-C9	4.27	1.41	1.35
24	A	801	CL0	C3D-C2D	4.27	1.45	1.37
22	A	849	BCR	C17-C18	4.27	1.41	1.35
22	A	853	BCR	C21-C22	4.26	1.41	1.35
22	B	845	BCR	C17-C18	4.26	1.41	1.35
17	4	607	CHL	C2C-C3C	4.26	1.45	1.36
20	1	615	LHG	O8-C23	4.26	1.45	1.33
22	A	853	BCR	C17-C18	4.25	1.41	1.35
17	2	607	CHL	O2A-CGA	4.25	1.45	1.33
21	1	616	LUT	C10-C9	4.23	1.41	1.35
27	B	850	DGD	O1G-C1A	4.23	1.45	1.33
17	4	607	CHL	CHD-C1D	4.22	1.46	1.38
22	K	205	BCR	C21-C22	4.21	1.41	1.35
22	A	853	BCR	C14-C13	4.21	1.41	1.35
22	L	301	BCR	C14-C13	4.20	1.41	1.35
21	1	616	LUT	C14-C13	4.20	1.41	1.35
22	B	849	BCR	C17-C18	4.20	1.41	1.35
22	J	102	BCR	C14-C13	4.20	1.41	1.35
22	B	843	BCR	C17-C18	4.19	1.41	1.35
17	2	606	CHL	CHD-C4C	4.19	1.48	1.39
17	4	607	CHL	C3B-C2B	4.18	1.46	1.40
22	B	843	BCR	C21-C22	4.18	1.41	1.35
17	1	601	CHL	O2A-CGA	4.18	1.45	1.33
22	B	801	BCR	C17-C18	4.17	1.41	1.35
22	L	301	BCR	C21-C22	4.17	1.41	1.35
22	F	304	BCR	C14-C13	4.17	1.41	1.35
21	2	619	LUT	C30-C29	4.16	1.41	1.35
22	J	102	BCR	C10-C9	4.15	1.41	1.35
22	B	845	BCR	C14-C13	4.15	1.41	1.35
17	4	605	CHL	CHD-C4C	4.14	1.48	1.39
22	A	852	BCR	C21-C22	4.14	1.41	1.35
22	A	848	BCR	C21-C22	4.14	1.41	1.35
24	A	801	CL0	C3C-C2C	4.13	1.45	1.36
21	2	619	LUT	C34-C33	4.13	1.41	1.35
22	4	618	BCR	C14-C13	4.13	1.41	1.35
22	A	849	BCR	C14-C13	4.13	1.41	1.35
22	J	102	BCR	C17-C18	4.12	1.41	1.35
22	A	848	BCR	C17-C18	4.12	1.41	1.35
17	1	601	CHL	CHD-C4C	4.11	1.48	1.39
22	L	301	BCR	C17-C18	4.11	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	2	619	LUT	C14-C13	4.11	1.41	1.35
22	B	844	BCR	C10-C9	4.10	1.41	1.35
22	4	618	BCR	C21-C22	4.10	1.41	1.35
17	2	615	CHL	CHD-C4C	4.10	1.48	1.39
22	B	843	BCR	C10-C9	4.10	1.41	1.35
22	B	849	BCR	C21-C22	4.10	1.41	1.35
22	B	801	BCR	C21-C22	4.09	1.41	1.35
22	J	102	BCR	C21-C22	4.09	1.41	1.35
22	L	305	BCR	C10-C9	4.09	1.41	1.35
21	2	619	LUT	C10-C9	4.09	1.41	1.35
22	L	306	BCR	C10-C9	4.09	1.41	1.35
22	B	801	BCR	C14-C13	4.08	1.41	1.35
17	2	601	CHL	CHD-C4C	4.08	1.48	1.39
17	3	606	CHL	CHD-C4C	4.07	1.48	1.39
27	B	850	DGD	O2G-C1B	4.07	1.45	1.34
21	3	613	LUT	C14-C13	4.06	1.41	1.35
22	L	305	BCR	C14-C13	4.06	1.41	1.35
22	4	618	BCR	C17-C18	4.05	1.41	1.35
22	A	848	BCR	C14-C13	4.04	1.41	1.35
17	2	607	CHL	CHD-C4C	4.04	1.48	1.39
21	1	616	LUT	C34-C33	4.04	1.41	1.35
24	A	801	CL0	O2A-CGA	4.04	1.45	1.33
17	2	605	CHL	CHD-C4C	4.04	1.48	1.39
20	1	615	LHG	O7-C7	4.03	1.45	1.34
22	A	849	BCR	C10-C9	4.03	1.41	1.35
22	B	848	BCR	C17-C18	4.03	1.41	1.35
22	B	846	BCR	C10-C9	4.03	1.41	1.35
22	L	305	BCR	C21-C22	4.03	1.41	1.35
22	B	846	BCR	C17-C18	4.03	1.41	1.35
22	B	846	BCR	C21-C22	4.02	1.41	1.35
22	A	852	BCR	C17-C18	4.02	1.41	1.35
22	B	844	BCR	C14-C13	4.01	1.41	1.35
22	K	205	BCR	C14-C13	4.00	1.41	1.35
18	3	603	CLA	C1D-ND	3.99	1.42	1.37
22	L	301	BCR	C10-C9	3.99	1.41	1.35
22	B	844	BCR	C17-C18	3.99	1.41	1.35
21	4	616	LUT	C30-C29	3.99	1.41	1.35
17	2	601	CHL	O2A-CGA	3.99	1.45	1.33
18	A	824	CLA	C1D-ND	3.99	1.42	1.37
18	1	605	CLA	C1D-ND	3.98	1.42	1.37
22	K	205	BCR	C17-C18	3.98	1.41	1.35
22	B	848	BCR	C14-C13	3.98	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	4	615	CHL	CHD-C4C	3.97	1.48	1.39
22	A	848	BCR	C10-C9	3.97	1.41	1.35
22	L	306	BCR	C14-C13	3.97	1.41	1.35
22	B	846	BCR	C14-C13	3.96	1.41	1.35
18	2	611	CLA	C1D-ND	3.96	1.42	1.37
22	I	101	BCR	C14-C13	3.96	1.41	1.35
22	G	204	BCR	C21-C22	3.95	1.41	1.35
22	L	305	BCR	C17-C18	3.95	1.41	1.35
18	B	835	CLA	C1D-ND	3.95	1.42	1.37
22	A	852	BCR	C10-C9	3.94	1.41	1.35
22	B	848	BCR	C10-C9	3.94	1.41	1.35
18	3	609	CLA	C1D-ND	3.94	1.42	1.37
21	4	616	LUT	C14-C13	3.93	1.41	1.35
22	A	850	BCR	C10-C9	3.93	1.41	1.35
18	K	201	CLA	C1D-ND	3.92	1.42	1.37
22	G	204	BCR	C17-C18	3.91	1.41	1.35
22	3	614	BCR	C21-C22	3.91	1.41	1.35
22	3	614	BCR	C17-C18	3.91	1.41	1.35
22	B	847	BCR	C14-C13	3.91	1.41	1.35
22	K	205	BCR	C10-C9	3.90	1.41	1.35
19	4	617	XAT	O3-C3	-3.90	1.31	1.43
22	3	614	BCR	C10-C9	3.89	1.40	1.35
22	I	101	BCR	C17-C18	3.89	1.40	1.35
22	4	618	BCR	C10-C9	3.89	1.40	1.35
22	G	204	BCR	C14-C13	3.89	1.40	1.35
22	L	306	BCR	C17-C18	3.89	1.40	1.35
21	4	616	LUT	C34-C33	3.88	1.40	1.35
18	A	817	CLA	C1D-ND	3.88	1.42	1.37
18	3	610	CLA	C1D-ND	3.87	1.42	1.37
22	A	852	BCR	C14-C13	3.87	1.40	1.35
18	3	605	CLA	C1D-ND	3.87	1.42	1.37
18	A	837	CLA	C1D-ND	3.87	1.42	1.37
18	2	604	CLA	C1D-ND	3.87	1.42	1.37
22	3	614	BCR	C14-C13	3.86	1.40	1.35
21	2	616	LUT	C10-C9	3.85	1.40	1.35
21	4	616	LUT	C10-C9	3.84	1.40	1.35
21	2	616	LUT	C14-C13	3.84	1.40	1.35
22	L	306	BCR	C21-C22	3.84	1.40	1.35
18	G	201	CLA	C1D-ND	3.84	1.42	1.37
18	A	808	CLA	C1D-ND	3.83	1.42	1.37
18	A	812	CLA	C1D-ND	3.83	1.42	1.37
18	2	613	CLA	C1D-ND	3.83	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	F	302	CLA	C1D-ND	3.83	1.42	1.37
18	F	301	CLA	C1D-ND	3.83	1.42	1.37
17	4	607	CHL	CHD-C4C	3.83	1.48	1.39
18	L	304	CLA	C1D-ND	3.83	1.42	1.37
18	A	826	CLA	C1D-ND	3.82	1.42	1.37
18	B	820	CLA	C1D-ND	3.82	1.42	1.37
24	A	801	CL0	C3B-C2B	3.82	1.45	1.40
18	1	604	CLA	C1D-ND	3.82	1.42	1.37
18	A	828	CLA	C1D-ND	3.81	1.42	1.37
18	3	602	CLA	C1D-ND	3.81	1.42	1.37
18	A	836	CLA	C1D-ND	3.81	1.42	1.37
22	I	101	BCR	C10-C9	3.81	1.40	1.35
18	B	827	CLA	C1D-ND	3.81	1.42	1.37
21	3	613	LUT	C30-C29	3.81	1.40	1.35
18	1	611	CLA	C1D-ND	3.80	1.42	1.37
18	4	608	CLA	C1D-ND	3.80	1.42	1.37
21	2	616	LUT	C30-C29	3.80	1.40	1.35
22	B	848	BCR	C21-C22	3.80	1.40	1.35
18	3	608	CLA	C1D-ND	3.80	1.42	1.37
18	F	303	CLA	C1D-ND	3.80	1.42	1.37
18	A	835	CLA	C1D-ND	3.80	1.42	1.37
18	B	810	CLA	C1D-ND	3.79	1.42	1.37
18	2	610	CLA	C1D-ND	3.79	1.42	1.37
18	A	839	CLA	C1D-ND	3.79	1.42	1.37
18	B	832	CLA	C1D-ND	3.79	1.42	1.37
18	1	612	CLA	C1D-ND	3.78	1.42	1.37
18	G	202	CLA	C1D-ND	3.78	1.42	1.37
18	K	203	CLA	C1D-ND	3.78	1.42	1.37
22	B	847	BCR	C17-C18	3.78	1.40	1.35
18	1	613	CLA	C1D-ND	3.77	1.42	1.37
18	A	804	CLA	C1D-ND	3.77	1.42	1.37
18	B	841	CLA	C1D-ND	3.77	1.42	1.37
18	K	204	CLA	C1D-ND	3.77	1.42	1.37
22	B	847	BCR	C21-C22	3.77	1.40	1.35
17	4	605	CHL	OBD-CAD	3.77	1.29	1.22
22	B	847	BCR	C10-C9	3.77	1.40	1.35
18	4	601	CLA	C1D-ND	3.77	1.42	1.37
18	B	834	CLA	C1D-ND	3.76	1.42	1.37
18	H	201	CLA	C1D-ND	3.75	1.42	1.37
18	A	823	CLA	C1D-ND	3.75	1.42	1.37
18	B	805	CLA	C1D-ND	3.75	1.42	1.37
18	G	203	CLA	C1D-ND	3.75	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	818	CLA	C1D-ND	3.75	1.42	1.37
17	4	615	CHL	OBD-CAD	3.75	1.28	1.22
18	A	809	CLA	C1D-ND	3.74	1.42	1.37
19	4	617	XAT	O23-C23	-3.74	1.32	1.43
18	1	610	CLA	C1D-ND	3.74	1.42	1.37
18	4	604	CLA	C1D-ND	3.74	1.42	1.37
18	A	820	CLA	C1D-ND	3.74	1.42	1.37
18	B	839	CLA	C1D-ND	3.74	1.42	1.37
18	1	602	CLA	C1D-ND	3.74	1.42	1.37
18	1	607	CLA	C1D-ND	3.74	1.42	1.37
18	B	818	CLA	C1D-ND	3.74	1.42	1.37
18	B	833	CLA	C1D-ND	3.74	1.42	1.37
18	A	807	CLA	C1D-ND	3.73	1.42	1.37
18	A	834	CLA	C1D-ND	3.73	1.42	1.37
24	A	801	CL0	CHC-C1C	3.73	1.44	1.35
18	2	602	CLA	C1D-ND	3.73	1.42	1.37
18	A	821	CLA	C1D-ND	3.73	1.42	1.37
18	A	816	CLA	C1D-ND	3.73	1.42	1.37
18	1	603	CLA	C1D-ND	3.73	1.42	1.37
18	4	611	CLA	C1D-ND	3.73	1.42	1.37
18	A	833	CLA	C1D-ND	3.73	1.42	1.37
18	B	840	CLA	C1D-ND	3.73	1.42	1.37
17	4	606	CHL	OBD-CAD	3.72	1.28	1.22
18	3	601	CLA	C1D-ND	3.72	1.42	1.37
18	B	824	CLA	C1D-ND	3.72	1.42	1.37
18	A	805	CLA	C1D-ND	3.72	1.42	1.37
18	A	814	CLA	C1D-ND	3.72	1.42	1.37
17	2	606	CHL	OBD-CAD	3.72	1.28	1.22
18	B	807	CLA	C1D-ND	3.72	1.42	1.37
18	B	819	CLA	C1D-ND	3.72	1.42	1.37
18	3	607	CLA	C1D-ND	3.71	1.42	1.37
18	B	817	CLA	C1D-ND	3.71	1.42	1.37
18	L	302	CLA	C1D-ND	3.71	1.42	1.37
22	A	850	BCR	C21-C22	3.70	1.40	1.35
18	2	603	CLA	C1D-ND	3.70	1.42	1.37
18	3	611	CLA	C1D-ND	3.70	1.42	1.37
18	A	832	CLA	C1D-ND	3.70	1.42	1.37
18	B	814	CLA	C1D-ND	3.70	1.42	1.37
18	B	815	CLA	C1D-ND	3.70	1.42	1.37
18	B	804	CLA	C1D-ND	3.70	1.42	1.37
18	4	613	CLA	C1D-ND	3.70	1.42	1.37
18	A	806	CLA	C1D-ND	3.70	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	I	101	BCR	C21-C22	3.70	1.40	1.35
18	A	827	CLA	C1D-ND	3.69	1.42	1.37
18	A	840	CLA	C1D-ND	3.69	1.42	1.37
18	4	602	CLA	C1D-ND	3.69	1.42	1.37
18	2	612	CLA	C1D-ND	3.69	1.42	1.37
18	A	813	CLA	C1D-ND	3.68	1.42	1.37
18	4	614	CLA	C1D-ND	3.68	1.42	1.37
18	L	303	CLA	C1D-ND	3.68	1.42	1.37
17	4	607	CHL	OBD-CAD	3.68	1.28	1.22
18	B	822	CLA	C1D-ND	3.68	1.42	1.37
18	B	837	CLA	C1D-ND	3.67	1.42	1.37
18	B	809	CLA	C1D-ND	3.67	1.42	1.37
18	B	816	CLA	C1D-ND	3.67	1.42	1.37
18	A	811	CLA	C1D-ND	3.67	1.42	1.37
18	A	838	CLA	C1D-ND	3.66	1.42	1.37
18	B	806	CLA	C1D-ND	3.66	1.42	1.37
18	B	838	CLA	C1D-ND	3.66	1.42	1.37
18	B	811	CLA	C1D-ND	3.65	1.42	1.37
18	B	821	CLA	C1D-ND	3.65	1.42	1.37
18	B	825	CLA	C1D-ND	3.65	1.42	1.37
18	3	612	CLA	C1D-ND	3.65	1.42	1.37
17	1	606	CHL	OBD-CAD	3.65	1.28	1.22
17	2	615	CHL	OBD-CAD	3.65	1.28	1.22
18	A	842	CLA	C1D-ND	3.65	1.42	1.37
18	4	604	CLA	CAB-C3B	-3.65	1.44	1.51
17	1	601	CHL	OBD-CAD	3.64	1.28	1.22
18	A	843	CLA	C1D-ND	3.64	1.42	1.37
18	B	812	CLA	C1D-ND	3.64	1.42	1.37
18	A	829	CLA	C1D-ND	3.64	1.42	1.37
18	B	836	CLA	C1D-ND	3.63	1.42	1.37
18	4	609	CLA	C1D-ND	3.63	1.42	1.37
18	B	823	CLA	C1D-ND	3.63	1.42	1.37
17	2	601	CHL	OBD-CAD	3.63	1.28	1.22
22	G	204	BCR	C10-C9	3.63	1.40	1.35
18	B	826	CLA	C1D-ND	3.63	1.42	1.37
18	1	608	CLA	C1D-ND	3.63	1.42	1.37
18	B	831	CLA	C1D-ND	3.63	1.42	1.37
18	A	825	CLA	C1D-ND	3.63	1.42	1.37
18	A	831	CLA	C1D-ND	3.62	1.42	1.37
18	B	813	CLA	C1D-ND	3.62	1.42	1.37
18	A	844	CLA	C1D-ND	3.62	1.42	1.37
18	A	841	CLA	C1D-ND	3.62	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	4	603	CLA	C1D-ND	3.61	1.42	1.37
18	4	612	CLA	C1D-ND	3.61	1.42	1.37
18	1	608	CLA	CAB-C3B	-3.61	1.44	1.51
18	A	810	CLA	C1D-ND	3.61	1.42	1.37
18	A	815	CLA	C1D-ND	3.60	1.42	1.37
18	A	802	CLA	C1D-ND	3.60	1.42	1.37
17	2	605	CHL	OBD-CAD	3.59	1.28	1.22
18	B	829	CLA	C1D-ND	3.59	1.42	1.37
18	3	604	CLA	C1D-ND	3.59	1.42	1.37
18	A	803	CLA	C1D-ND	3.59	1.42	1.37
18	4	610	CLA	C1D-ND	3.58	1.42	1.37
18	2	609	CLA	C1D-ND	3.58	1.42	1.37
18	2	610	CLA	CAB-C3B	-3.58	1.44	1.51
18	1	610	CLA	CAB-C3B	-3.57	1.44	1.51
17	3	606	CHL	OBD-CAD	3.57	1.28	1.22
18	A	822	CLA	C1D-ND	3.57	1.42	1.37
18	A	819	CLA	C1D-ND	3.56	1.42	1.37
18	2	608	CLA	C1D-ND	3.56	1.42	1.37
18	B	811	CLA	CAB-C3B	-3.56	1.44	1.51
18	4	603	CLA	CAB-C3B	-3.55	1.44	1.51
18	B	828	CLA	C1D-ND	3.54	1.42	1.37
18	1	613	CLA	CAB-C3B	-3.54	1.44	1.51
18	A	830	CLA	C1D-ND	3.53	1.42	1.37
18	3	605	CLA	CAB-C3B	-3.53	1.44	1.51
18	B	808	CLA	C1D-ND	3.53	1.42	1.37
18	B	803	CLA	C1D-ND	3.51	1.42	1.37
17	2	607	CHL	OBD-CAD	3.50	1.28	1.22
18	B	802	CLA	C1D-ND	3.43	1.42	1.37
18	1	609	CLA	C1D-ND	3.43	1.42	1.37
18	B	830	CLA	C1D-ND	3.40	1.42	1.37
17	4	606	CHL	C3D-C2D	3.33	1.48	1.39
17	1	606	CHL	C3D-C2D	3.31	1.48	1.39
19	4	617	XAT	C11-C10	3.29	1.53	1.43
17	1	606	CHL	C1D-C2D	3.28	1.51	1.45
18	A	823	CLA	CHC-C1C	3.25	1.43	1.35
18	B	826	CLA	C4D-ND	-3.23	1.33	1.37
17	4	606	CHL	C1D-C2D	3.23	1.51	1.45
18	1	604	CLA	CHC-C1C	3.21	1.43	1.35
18	A	818	CLA	CHC-C1C	3.20	1.43	1.35
18	B	841	CLA	CHC-C1C	3.20	1.43	1.35
18	A	807	CLA	CHC-C1C	3.19	1.43	1.35
18	A	844	CLA	CHC-C1C	3.19	1.43	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	805	CLA	CHC-C1C	3.19	1.43	1.35
18	B	837	CLA	CHC-C1C	3.19	1.43	1.35
17	2	606	CHL	C3D-C2D	3.18	1.47	1.39
18	A	803	CLA	CHC-C1C	3.18	1.43	1.35
18	B	822	CLA	CHC-C1C	3.18	1.43	1.35
18	A	812	CLA	CHC-C1C	3.18	1.43	1.35
18	B	834	CLA	CHC-C1C	3.18	1.43	1.35
18	1	611	CLA	CHC-C1C	3.18	1.43	1.35
18	A	802	CLA	CHC-C1C	3.17	1.43	1.35
18	A	832	CLA	CHC-C1C	3.17	1.43	1.35
18	B	802	CLA	CHC-C1C	3.17	1.43	1.35
18	A	806	CLA	CHC-C1C	3.17	1.43	1.35
18	A	819	CLA	CHC-C1C	3.16	1.43	1.35
18	4	611	CLA	CHC-C1C	3.16	1.43	1.35
18	A	836	CLA	CHC-C1C	3.16	1.43	1.35
18	B	831	CLA	CHC-C1C	3.16	1.43	1.35
18	4	608	CLA	CHC-C1C	3.16	1.43	1.35
18	K	203	CLA	CHC-C1C	3.16	1.43	1.35
18	4	609	CLA	CHC-C1C	3.16	1.43	1.35
18	B	804	CLA	CHC-C1C	3.16	1.43	1.35
18	1	610	CLA	CHC-C1C	3.16	1.43	1.35
18	K	201	CLA	CHC-C1C	3.16	1.43	1.35
18	A	828	CLA	CHC-C1C	3.15	1.43	1.35
18	2	602	CLA	CHC-C1C	3.15	1.43	1.35
18	B	817	CLA	CHC-C1C	3.15	1.43	1.35
18	1	603	CLA	CHC-C1C	3.15	1.43	1.35
18	A	837	CLA	CHC-C1C	3.15	1.43	1.35
18	4	610	CLA	CHC-C1C	3.15	1.43	1.35
18	B	828	CLA	CHC-C1C	3.15	1.43	1.35
18	A	814	CLA	CHC-C1C	3.15	1.43	1.35
18	A	838	CLA	CHC-C1C	3.14	1.43	1.35
18	3	605	CLA	CHC-C1C	3.14	1.43	1.35
18	A	810	CLA	CHC-C1C	3.14	1.43	1.35
18	B	829	CLA	CHC-C1C	3.14	1.43	1.35
18	B	838	CLA	CHC-C1C	3.14	1.43	1.35
18	G	202	CLA	CHC-C1C	3.14	1.43	1.35
18	A	824	CLA	CHC-C1C	3.14	1.43	1.35
18	3	609	CLA	CHC-C1C	3.14	1.43	1.35
18	A	809	CLA	CHC-C1C	3.14	1.43	1.35
18	4	602	CLA	CHC-C1C	3.14	1.43	1.35
18	B	814	CLA	CHC-C1C	3.13	1.43	1.35
18	B	835	CLA	CHC-C1C	3.13	1.43	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	821	CLA	CHC-C1C	3.13	1.43	1.35
18	A	833	CLA	CHC-C1C	3.13	1.43	1.35
18	B	826	CLA	CHC-C1C	3.13	1.43	1.35
18	3	607	CLA	CHC-C1C	3.13	1.43	1.35
18	B	839	CLA	CHC-C1C	3.13	1.43	1.35
18	B	836	CLA	CHC-C1C	3.13	1.43	1.35
18	B	825	CLA	CHC-C1C	3.13	1.43	1.35
18	G	201	CLA	CHC-C1C	3.13	1.43	1.35
18	B	811	CLA	CHC-C1C	3.13	1.43	1.35
18	G	203	CLA	CHC-C1C	3.13	1.43	1.35
18	1	613	CLA	CHC-C1C	3.13	1.43	1.35
18	4	601	CLA	CHC-C1C	3.13	1.43	1.35
18	F	302	CLA	CHC-C1C	3.12	1.43	1.35
18	A	840	CLA	CHC-C1C	3.12	1.43	1.35
18	A	831	CLA	CHC-C1C	3.12	1.43	1.35
18	A	815	CLA	CHC-C1C	3.12	1.43	1.35
18	1	609	CLA	C4D-ND	-3.12	1.33	1.37
18	B	816	CLA	CHC-C1C	3.12	1.43	1.35
18	4	613	CLA	CHC-C1C	3.12	1.43	1.35
18	K	204	CLA	CHC-C1C	3.12	1.43	1.35
18	B	820	CLA	CHC-C1C	3.12	1.43	1.35
18	A	803	CLA	C4D-ND	-3.12	1.33	1.37
18	3	608	CLA	CHC-C1C	3.12	1.43	1.35
18	B	815	CLA	CHC-C1C	3.11	1.43	1.35
18	F	301	CLA	CHC-C1C	3.11	1.42	1.35
18	L	302	CLA	CHC-C1C	3.11	1.42	1.35
18	B	803	CLA	CHC-C1C	3.11	1.42	1.35
18	2	610	CLA	CHC-C1C	3.11	1.42	1.35
18	B	807	CLA	CHC-C1C	3.10	1.42	1.35
18	B	819	CLA	CHC-C1C	3.10	1.42	1.35
18	B	823	CLA	CHC-C1C	3.10	1.42	1.35
18	2	608	CLA	CHC-C1C	3.10	1.42	1.35
18	A	822	CLA	CHC-C1C	3.10	1.42	1.35
18	3	602	CLA	CHC-C1C	3.10	1.42	1.35
18	3	611	CLA	CHC-C1C	3.10	1.42	1.35
18	B	827	CLA	CHC-C1C	3.10	1.42	1.35
18	1	602	CLA	CHC-C1C	3.10	1.42	1.35
18	A	826	CLA	CHC-C1C	3.10	1.42	1.35
18	3	601	CLA	CHC-C1C	3.10	1.42	1.35
18	L	303	CLA	CHC-C1C	3.10	1.42	1.35
18	1	612	CLA	CHC-C1C	3.10	1.42	1.35
18	2	611	CLA	CHC-C1C	3.10	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	F	303	CLA	CHC-C1C	3.10	1.42	1.35
18	1	605	CLA	CHC-C1C	3.10	1.42	1.35
18	B	810	CLA	CHC-C1C	3.10	1.42	1.35
17	2	615	CHL	C3D-C2D	3.10	1.47	1.39
18	A	829	CLA	CHC-C1C	3.10	1.42	1.35
18	B	833	CLA	CHC-C1C	3.09	1.42	1.35
18	3	610	CLA	CHC-C1C	3.09	1.42	1.35
18	A	817	CLA	CHC-C1C	3.09	1.42	1.35
18	A	816	CLA	CHC-C1C	3.09	1.42	1.35
18	2	613	CLA	CHC-C1C	3.09	1.42	1.35
18	2	609	CLA	CHC-C1C	3.09	1.42	1.35
18	A	835	CLA	CHC-C1C	3.09	1.42	1.35
18	B	818	CLA	CHC-C1C	3.09	1.42	1.35
18	B	832	CLA	C4D-ND	-3.09	1.33	1.37
18	A	821	CLA	CHC-C1C	3.09	1.42	1.35
18	2	603	CLA	CHC-C1C	3.08	1.42	1.35
18	B	805	CLA	CHC-C1C	3.08	1.42	1.35
18	1	607	CLA	CHC-C1C	3.08	1.42	1.35
18	4	614	CLA	CHC-C1C	3.08	1.42	1.35
18	A	808	CLA	CHC-C1C	3.08	1.42	1.35
18	4	604	CLA	CHC-C1C	3.08	1.42	1.35
18	K	204	CLA	C4D-ND	-3.08	1.33	1.37
17	2	606	CHL	C1D-C2D	3.08	1.51	1.45
18	A	841	CLA	CHC-C1C	3.07	1.42	1.35
18	B	824	CLA	CHC-C1C	3.07	1.42	1.35
18	3	603	CLA	CHC-C1C	3.07	1.42	1.35
18	A	806	CLA	C4D-ND	-3.07	1.33	1.37
17	1	606	CHL	MG-NA	-3.07	1.99	2.06
18	3	604	CLA	CHC-C1C	3.07	1.42	1.35
18	2	612	CLA	CHC-C1C	3.07	1.42	1.35
18	A	820	CLA	CHC-C1C	3.06	1.42	1.35
18	2	604	CLA	CHC-C1C	3.06	1.42	1.35
18	B	813	CLA	C4D-ND	-3.06	1.33	1.37
18	B	830	CLA	CHC-C1C	3.06	1.42	1.35
18	A	811	CLA	CHC-C1C	3.06	1.42	1.35
18	4	603	CLA	CHC-C1C	3.06	1.42	1.35
18	B	812	CLA	CHC-C1C	3.05	1.42	1.35
18	B	836	CLA	C4D-ND	-3.05	1.33	1.37
18	A	827	CLA	CHC-C1C	3.05	1.42	1.35
18	4	612	CLA	CHC-C1C	3.05	1.42	1.35
18	B	838	CLA	C4D-ND	-3.05	1.33	1.37
18	A	843	CLA	CHC-C1C	3.05	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	808	CLA	CHC-C1C	3.05	1.42	1.35
22	B	845	BCR	C23-C22	-3.05	1.39	1.45
18	L	304	CLA	CHC-C1C	3.05	1.42	1.35
18	A	813	CLA	CHC-C1C	3.04	1.42	1.35
18	B	832	CLA	CHC-C1C	3.04	1.42	1.35
18	A	825	CLA	CHC-C1C	3.04	1.42	1.35
22	B	849	BCR	C23-C22	-3.04	1.39	1.45
18	A	830	CLA	CHC-C1C	3.04	1.42	1.35
18	1	612	CLA	C4D-ND	-3.03	1.33	1.37
18	B	816	CLA	C4D-ND	-3.03	1.33	1.37
18	3	603	CLA	C4D-ND	-3.03	1.33	1.37
18	1	608	CLA	CHC-C1C	3.03	1.42	1.35
18	B	809	CLA	CHC-C1C	3.02	1.42	1.35
18	B	824	CLA	C4D-ND	-3.02	1.33	1.37
18	B	807	CLA	C4D-ND	-3.02	1.33	1.37
18	A	827	CLA	C4D-ND	-3.02	1.33	1.37
18	A	804	CLA	CHC-C1C	3.02	1.42	1.35
18	H	201	CLA	CHC-C1C	3.02	1.42	1.35
18	A	834	CLA	CHC-C1C	3.02	1.42	1.35
18	A	842	CLA	C4D-ND	-3.02	1.33	1.37
18	1	613	CLA	C4D-ND	-3.02	1.33	1.37
18	3	601	CLA	C4D-ND	-3.02	1.33	1.37
18	A	814	CLA	C4D-ND	-3.02	1.33	1.37
18	B	840	CLA	C4D-ND	-3.01	1.33	1.37
18	B	813	CLA	CHC-C1C	3.01	1.42	1.35
18	A	839	CLA	C4D-ND	-3.01	1.33	1.37
18	2	609	CLA	C4D-ND	-3.01	1.33	1.37
18	A	816	CLA	C4D-ND	-3.01	1.33	1.37
17	4	605	CHL	C3D-C2D	3.01	1.47	1.39
17	2	615	CHL	C1D-C2D	3.01	1.51	1.45
18	B	831	CLA	C4D-ND	-3.01	1.33	1.37
18	4	613	CLA	C4D-ND	-3.01	1.33	1.37
17	4	606	CHL	MG-NA	-3.01	1.99	2.06
18	A	839	CLA	CHC-C1C	3.00	1.42	1.35
18	B	840	CLA	CHC-C1C	3.00	1.42	1.35
18	1	602	CLA	C4D-ND	-3.00	1.33	1.37
18	2	612	CLA	C4D-ND	-3.00	1.33	1.37
18	A	841	CLA	C4D-ND	-3.00	1.33	1.37
18	2	604	CLA	C4D-ND	-3.00	1.33	1.37
18	A	828	CLA	C4D-ND	-2.99	1.33	1.37
18	B	818	CLA	C4D-ND	-2.99	1.33	1.37
18	B	806	CLA	CHC-C1C	2.99	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	810	CLA	C4D-ND	-2.99	1.33	1.37
18	A	830	CLA	C4D-ND	-2.99	1.33	1.37
17	1	601	CHL	C1D-C2D	2.99	1.51	1.45
18	A	840	CLA	C4D-ND	-2.99	1.33	1.37
18	1	609	CLA	CHC-C1C	2.99	1.42	1.35
18	2	602	CLA	C4D-ND	-2.98	1.33	1.37
18	2	608	CLA	C4D-ND	-2.98	1.33	1.37
18	A	819	CLA	C4D-ND	-2.98	1.33	1.37
18	B	821	CLA	C4D-ND	-2.98	1.33	1.37
18	B	806	CLA	C4D-ND	-2.98	1.33	1.37
18	3	607	CLA	C4D-ND	-2.98	1.33	1.37
17	2	601	CHL	C3D-C2D	2.97	1.47	1.39
18	B	829	CLA	C4D-ND	-2.97	1.33	1.37
18	A	807	CLA	C4D-ND	-2.97	1.33	1.37
17	2	605	CHL	C3D-C2D	2.97	1.47	1.39
18	4	603	CLA	C4D-ND	-2.97	1.33	1.37
18	B	802	CLA	C4D-ND	-2.97	1.33	1.37
17	2	601	CHL	C1D-C2D	2.96	1.51	1.45
18	1	603	CLA	C4D-ND	-2.96	1.33	1.37
18	4	611	CLA	C4D-ND	-2.96	1.33	1.37
18	2	610	CLA	C4D-ND	-2.96	1.33	1.37
18	A	831	CLA	C4D-ND	-2.96	1.33	1.37
18	G	203	CLA	C4D-ND	-2.96	1.33	1.37
18	4	602	CLA	C4D-ND	-2.96	1.33	1.37
18	A	829	CLA	C4D-ND	-2.96	1.33	1.37
18	L	303	CLA	C4D-ND	-2.96	1.33	1.37
18	B	815	CLA	C4D-ND	-2.96	1.33	1.37
22	I	101	BCR	C23-C22	-2.96	1.39	1.45
18	B	833	CLA	C4D-ND	-2.96	1.33	1.37
19	4	617	XAT	C15-C14	2.96	1.52	1.43
22	4	618	BCR	C8-C9	-2.95	1.39	1.45
18	B	823	CLA	C4D-ND	-2.95	1.33	1.37
17	1	601	CHL	C3D-C2D	2.95	1.47	1.39
17	4	615	CHL	C3D-C2D	2.95	1.47	1.39
18	3	605	CLA	C4D-ND	-2.95	1.33	1.37
18	B	827	CLA	C4D-ND	-2.95	1.33	1.37
18	A	826	CLA	C4D-ND	-2.95	1.33	1.37
18	G	202	CLA	C4D-ND	-2.95	1.33	1.37
18	B	839	CLA	C4D-ND	-2.95	1.33	1.37
18	F	301	CLA	C4D-ND	-2.95	1.33	1.37
18	3	608	CLA	C4D-ND	-2.94	1.33	1.37
18	4	608	CLA	C4D-ND	-2.94	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	830	CLA	C4D-ND	-2.94	1.33	1.37
18	B	809	CLA	C4D-ND	-2.94	1.33	1.37
18	3	604	CLA	C4D-ND	-2.94	1.33	1.37
18	B	810	CLA	C4D-ND	-2.94	1.33	1.37
18	2	603	CLA	C4D-ND	-2.94	1.33	1.37
18	4	601	CLA	C4D-ND	-2.94	1.33	1.37
18	A	842	CLA	CHC-C1C	2.94	1.42	1.35
18	1	604	CLA	C4D-ND	-2.94	1.33	1.37
18	B	812	CLA	C4D-ND	-2.94	1.33	1.37
18	B	808	CLA	C4D-ND	-2.94	1.33	1.37
18	B	841	CLA	C4D-ND	-2.94	1.33	1.37
18	A	818	CLA	C4D-ND	-2.94	1.33	1.37
18	B	828	CLA	C4D-ND	-2.94	1.33	1.37
18	1	611	CLA	C4D-ND	-2.94	1.33	1.37
18	A	833	CLA	C4D-ND	-2.94	1.33	1.37
18	A	811	CLA	C4D-ND	-2.93	1.33	1.37
18	B	814	CLA	C4D-ND	-2.93	1.33	1.37
18	A	821	CLA	C4D-ND	-2.93	1.33	1.37
22	A	850	BCR	C23-C22	-2.93	1.39	1.45
18	4	604	CLA	C4D-ND	-2.93	1.33	1.37
18	3	609	CLA	C4D-ND	-2.93	1.33	1.37
18	A	820	CLA	C4D-ND	-2.93	1.33	1.37
22	A	852	BCR	C8-C9	-2.93	1.39	1.45
18	B	805	CLA	C4D-ND	-2.93	1.33	1.37
18	A	844	CLA	C4D-ND	-2.92	1.33	1.37
22	B	847	BCR	C23-C22	-2.92	1.39	1.45
18	3	612	CLA	CHC-C1C	2.92	1.42	1.35
18	B	817	CLA	C4D-ND	-2.92	1.33	1.37
18	A	843	CLA	C4D-ND	-2.92	1.33	1.37
18	A	825	CLA	C4D-ND	-2.92	1.33	1.37
18	B	820	CLA	C4D-ND	-2.92	1.33	1.37
18	4	610	CLA	C4D-ND	-2.92	1.33	1.37
18	A	805	CLA	C4D-ND	-2.91	1.33	1.37
18	A	815	CLA	C4D-ND	-2.91	1.33	1.37
18	A	832	CLA	C4D-ND	-2.91	1.33	1.37
18	2	613	CLA	C4D-ND	-2.91	1.33	1.37
18	4	609	CLA	C4D-ND	-2.91	1.33	1.37
18	B	804	CLA	C4D-ND	-2.91	1.33	1.37
18	L	304	CLA	C4D-ND	-2.91	1.33	1.37
22	B	848	BCR	C23-C22	-2.91	1.39	1.45
17	2	607	CHL	C1D-C2D	2.91	1.51	1.45
18	1	608	CLA	C4D-ND	-2.91	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	4	615	CHL	C1D-C2D	2.91	1.51	1.45
18	1	610	CLA	C4D-ND	-2.90	1.33	1.37
18	A	834	CLA	C4D-ND	-2.90	1.33	1.37
17	4	605	CHL	C1D-C2D	2.90	1.51	1.45
18	B	837	CLA	C4D-ND	-2.90	1.33	1.37
18	B	811	CLA	C4D-ND	-2.90	1.33	1.37
18	A	812	CLA	C4D-ND	-2.90	1.33	1.37
18	A	804	CLA	C4D-ND	-2.90	1.33	1.37
17	3	606	CHL	C3D-C2D	2.90	1.47	1.39
18	K	203	CLA	C4D-ND	-2.90	1.33	1.37
18	L	302	CLA	C4D-ND	-2.89	1.33	1.37
18	1	607	CLA	C4D-ND	-2.89	1.33	1.37
17	2	607	CHL	C3D-C2D	2.89	1.47	1.39
18	F	303	CLA	C4D-ND	-2.88	1.33	1.37
22	G	204	BCR	C8-C9	-2.88	1.39	1.45
18	A	808	CLA	C4D-ND	-2.88	1.33	1.37
18	A	822	CLA	C4D-ND	-2.88	1.33	1.37
18	K	201	CLA	C4D-ND	-2.88	1.33	1.37
18	A	809	CLA	C4D-ND	-2.87	1.33	1.37
18	B	819	CLA	C4D-ND	-2.87	1.33	1.37
18	B	834	CLA	C4D-ND	-2.87	1.33	1.37
22	3	614	BCR	C23-C22	-2.87	1.39	1.45
17	2	605	CHL	C1D-C2D	2.87	1.51	1.45
18	4	612	CLA	C4D-ND	-2.87	1.33	1.37
18	A	835	CLA	C4D-ND	-2.87	1.33	1.37
18	B	822	CLA	C4D-ND	-2.87	1.33	1.37
22	B	847	BCR	C8-C9	-2.87	1.39	1.45
18	3	610	CLA	C4D-ND	-2.86	1.33	1.37
18	4	614	CLA	C4D-ND	-2.85	1.33	1.37
18	A	817	CLA	C4D-ND	-2.85	1.33	1.37
18	2	611	CLA	C4D-ND	-2.85	1.33	1.37
22	B	846	BCR	C23-C22	-2.85	1.39	1.45
18	3	602	CLA	C4D-ND	-2.84	1.33	1.37
18	H	201	CLA	C4D-ND	-2.84	1.33	1.37
17	3	606	CHL	C1D-C2D	2.83	1.50	1.45
22	3	614	BCR	C8-C9	-2.83	1.39	1.45
22	L	305	BCR	C8-C9	-2.82	1.39	1.45
18	3	611	CLA	C4D-ND	-2.82	1.33	1.37
22	B	801	BCR	C8-C9	-2.82	1.39	1.45
18	A	802	CLA	C4D-ND	-2.82	1.33	1.37
22	B	848	BCR	C8-C9	-2.82	1.39	1.45
18	A	824	CLA	C4D-ND	-2.81	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	836	CLA	C4D-ND	-2.81	1.33	1.37
22	G	204	BCR	C23-C22	-2.81	1.39	1.45
18	3	612	CLA	C4D-ND	-2.80	1.33	1.37
18	A	838	CLA	C4D-ND	-2.80	1.33	1.37
22	I	101	BCR	C8-C9	-2.80	1.39	1.45
18	B	803	CLA	C4D-ND	-2.80	1.33	1.37
22	L	301	BCR	C8-C9	-2.80	1.39	1.45
22	B	844	BCR	C8-C9	-2.79	1.39	1.45
18	B	835	CLA	C4D-ND	-2.79	1.33	1.37
18	B	825	CLA	C4D-ND	-2.78	1.33	1.37
21	3	613	LUT	C8-C9	-2.78	1.40	1.45
18	G	201	CLA	C4D-ND	-2.77	1.33	1.37
22	A	852	BCR	C23-C22	-2.77	1.40	1.45
22	A	849	BCR	C23-C22	-2.77	1.40	1.45
17	4	607	CHL	C3D-C2D	2.77	1.46	1.39
24	A	801	CL0	OBD-CAD	2.77	1.28	1.22
18	A	823	CLA	C4D-ND	-2.77	1.33	1.37
22	L	305	BCR	C23-C22	-2.76	1.40	1.45
17	4	607	CHL	C1D-C2D	2.76	1.50	1.45
22	K	205	BCR	C8-C9	-2.76	1.40	1.45
18	F	302	CLA	C4D-ND	-2.75	1.33	1.37
21	4	616	LUT	C8-C9	-2.75	1.40	1.45
18	A	842	CLA	CMB-C2B	-2.75	1.45	1.51
22	A	850	BCR	C8-C9	-2.75	1.40	1.45
22	K	205	BCR	C23-C22	-2.74	1.40	1.45
22	A	848	BCR	C23-C22	-2.73	1.40	1.45
18	A	837	CLA	C4D-ND	-2.73	1.33	1.37
22	4	618	BCR	C23-C22	-2.72	1.40	1.45
22	B	845	BCR	C8-C9	-2.72	1.40	1.45
18	A	813	CLA	C4D-ND	-2.72	1.34	1.37
22	B	846	BCR	C8-C9	-2.72	1.40	1.45
22	B	844	BCR	C23-C22	-2.72	1.40	1.45
22	B	801	BCR	C23-C22	-2.71	1.40	1.45
22	L	306	BCR	C23-C22	-2.71	1.40	1.45
22	A	849	BCR	C8-C9	-2.71	1.40	1.45
22	A	848	BCR	C8-C9	-2.70	1.40	1.45
22	L	306	BCR	C8-C9	-2.70	1.40	1.45
22	A	853	BCR	C8-C9	-2.70	1.40	1.45
18	1	605	CLA	C4D-ND	-2.70	1.34	1.37
18	B	819	CLA	CMB-C2B	-2.70	1.46	1.51
18	B	828	CLA	CMB-C2B	-2.70	1.46	1.51
22	B	843	BCR	C8-C9	-2.69	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	829	CLA	CMB-C2B	-2.68	1.46	1.51
24	A	801	CL0	CHD-C1D	2.68	1.43	1.38
21	2	619	LUT	C8-C9	-2.67	1.40	1.45
22	J	102	BCR	C8-C9	-2.66	1.40	1.45
22	A	853	BCR	C23-C22	-2.66	1.40	1.45
17	2	615	CHL	MG-NA	-2.66	2.00	2.06
17	1	606	CHL	C4B-CHC	2.65	1.48	1.41
21	1	616	LUT	C8-C9	-2.65	1.40	1.45
22	J	102	BCR	C23-C22	-2.65	1.40	1.45
18	B	809	CLA	CMB-C2B	-2.64	1.46	1.51
22	B	843	BCR	C23-C22	-2.64	1.40	1.45
22	A	851	BCR	C8-C9	-2.63	1.40	1.45
18	A	822	CLA	CMB-C2B	-2.63	1.46	1.51
22	L	301	BCR	C23-C22	-2.63	1.40	1.45
17	1	606	CHL	C4C-C3C	2.62	1.49	1.45
18	4	603	CLA	CMB-C2B	-2.61	1.46	1.51
18	A	844	CLA	CMB-C2B	-2.60	1.46	1.51
18	B	836	CLA	CMB-C2B	-2.60	1.46	1.51
18	B	840	CLA	CMB-C2B	-2.59	1.46	1.51
22	F	304	BCR	C8-C9	-2.59	1.40	1.45
18	B	811	CLA	CMB-C2B	-2.59	1.46	1.51
17	4	606	CHL	C4C-C3C	2.59	1.49	1.45
18	B	813	CLA	CMB-C2B	-2.58	1.46	1.51
22	A	851	BCR	C23-C22	-2.58	1.40	1.45
18	A	803	CLA	CMB-C2B	-2.58	1.46	1.51
18	A	836	CLA	CMB-C2B	-2.58	1.46	1.51
18	B	818	CLA	CMB-C2B	-2.57	1.46	1.51
18	3	604	CLA	CMB-C2B	-2.57	1.46	1.51
18	A	831	CLA	CMB-C2B	-2.57	1.46	1.51
18	A	820	CLA	CMB-C2B	-2.57	1.46	1.51
18	3	607	CLA	CMB-C2B	-2.56	1.46	1.51
18	B	815	CLA	CMB-C2B	-2.56	1.46	1.51
17	2	606	CHL	MG-NA	-2.56	2.00	2.06
18	B	835	CLA	CMB-C2B	-2.56	1.46	1.51
18	B	817	CLA	CMB-C2B	-2.55	1.46	1.51
17	4	605	CHL	MG-NA	-2.55	2.00	2.06
22	B	849	BCR	C8-C9	-2.55	1.40	1.45
24	A	801	CL0	CHD-C4C	2.55	1.45	1.39
18	A	825	CLA	CMB-C2B	-2.55	1.46	1.51
18	L	304	CLA	CMB-C2B	-2.55	1.46	1.51
18	B	838	CLA	CMB-C2B	-2.55	1.46	1.51
17	4	606	CHL	C4B-CHC	2.55	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	L	302	CLA	CMB-C2B	-2.55	1.46	1.51
18	A	813	CLA	CMB-C2B	-2.55	1.46	1.51
17	1	606	CHL	C1B-CHB	2.54	1.48	1.41
18	4	609	CLA	CMB-C2B	-2.54	1.46	1.51
18	B	812	CLA	CMB-C2B	-2.54	1.46	1.51
18	4	608	CLA	CMB-C2B	-2.54	1.46	1.51
21	2	616	LUT	C8-C9	-2.54	1.40	1.45
22	K	202	BCR	C8-C9	-2.54	1.40	1.45
18	A	832	CLA	CMB-C2B	-2.54	1.46	1.51
18	A	819	CLA	CMB-C2B	-2.54	1.46	1.51
17	1	601	CHL	MG-NA	-2.53	2.00	2.06
18	B	839	CLA	CMB-C2B	-2.53	1.46	1.51
18	A	834	CLA	CMB-C2B	-2.53	1.46	1.51
18	2	604	CLA	CMB-C2B	-2.53	1.46	1.51
18	B	833	CLA	CMB-C2B	-2.53	1.46	1.51
18	A	817	CLA	CMB-C2B	-2.53	1.46	1.51
18	3	602	CLA	CMB-C2B	-2.53	1.46	1.51
18	B	834	CLA	CMB-C2B	-2.53	1.46	1.51
18	A	838	CLA	CMB-C2B	-2.52	1.46	1.51
18	A	840	CLA	CMB-C2B	-2.52	1.46	1.51
18	A	835	CLA	CMB-C2B	-2.52	1.46	1.51
18	A	807	CLA	CMB-C2B	-2.52	1.46	1.51
18	B	822	CLA	CMB-C2B	-2.51	1.46	1.51
18	A	826	CLA	CMB-C2B	-2.51	1.46	1.51
18	A	816	CLA	CMB-C2B	-2.51	1.46	1.51
17	4	606	CHL	C1B-CHB	2.51	1.48	1.41
18	B	805	CLA	CMB-C2B	-2.51	1.46	1.51
18	1	607	CLA	CMB-C2B	-2.51	1.46	1.51
18	A	802	CLA	CMB-C2B	-2.51	1.46	1.51
18	B	808	CLA	CMB-C2B	-2.51	1.46	1.51
22	B	847	BCR	C12-C13	-2.51	1.40	1.45
18	A	810	CLA	CMB-C2B	-2.50	1.46	1.51
18	B	831	CLA	CMB-C2B	-2.50	1.46	1.51
18	2	608	CLA	CMB-C2B	-2.50	1.46	1.51
22	K	202	BCR	C23-C22	-2.50	1.40	1.45
18	4	610	CLA	CMB-C2B	-2.50	1.46	1.51
18	B	807	CLA	CMB-C2B	-2.50	1.46	1.51
18	B	827	CLA	CMB-C2B	-2.50	1.46	1.51
18	4	613	CLA	CMB-C2B	-2.50	1.46	1.51
18	2	612	CLA	CMB-C2B	-2.50	1.46	1.51
18	1	609	CLA	CMD-C2D	-2.49	1.45	1.50
18	A	814	CLA	CMB-C2B	-2.49	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	806	CLA	CMB-C2B	-2.49	1.46	1.51
18	A	815	CLA	CMB-C2B	-2.49	1.46	1.51
18	F	301	CLA	CMB-C2B	-2.49	1.46	1.51
17	2	615	CHL	C4B-CHC	2.49	1.47	1.41
18	3	611	CLA	CMB-C2B	-2.48	1.46	1.51
18	B	814	CLA	CMB-C2B	-2.48	1.46	1.51
18	B	810	CLA	CMB-C2B	-2.48	1.46	1.51
18	A	821	CLA	CMB-C2B	-2.48	1.46	1.51
18	B	830	CLA	CMB-C2B	-2.48	1.46	1.51
18	4	611	CLA	CMB-C2B	-2.48	1.46	1.51
18	A	804	CLA	CMB-C2B	-2.48	1.46	1.51
18	A	809	CLA	CMB-C2B	-2.48	1.46	1.51
17	2	606	CHL	C4B-CHC	2.47	1.47	1.41
18	1	602	CLA	CMB-C2B	-2.47	1.46	1.51
18	3	605	CLA	CMB-C2B	-2.47	1.46	1.51
18	4	602	CLA	CMB-C2B	-2.47	1.46	1.51
18	3	609	CLA	CMB-C2B	-2.47	1.46	1.51
18	A	811	CLA	CMB-C2B	-2.47	1.46	1.51
18	B	802	CLA	CMB-C2B	-2.47	1.46	1.51
18	3	601	CLA	CMB-C2B	-2.47	1.46	1.51
18	4	604	CLA	CMB-C2B	-2.47	1.46	1.51
18	G	202	CLA	CMB-C2B	-2.47	1.46	1.51
18	1	603	CLA	CMB-C2B	-2.47	1.46	1.51
22	A	850	BCR	C19-C18	-2.47	1.40	1.45
18	3	603	CLA	CMB-C2B	-2.47	1.46	1.51
18	2	602	CLA	CMB-C2B	-2.46	1.46	1.51
18	B	824	CLA	CMB-C2B	-2.46	1.46	1.51
18	G	201	CLA	CMB-C2B	-2.46	1.46	1.51
17	2	605	CHL	C4B-CHC	2.46	1.47	1.41
18	4	601	CLA	CMB-C2B	-2.46	1.46	1.51
18	1	613	CLA	CMB-C2B	-2.46	1.46	1.51
18	A	812	CLA	CMB-C2B	-2.46	1.46	1.51
18	B	825	CLA	CMB-C2B	-2.46	1.46	1.51
18	1	612	CLA	CMB-C2B	-2.46	1.46	1.51
18	A	829	CLA	CMB-C2B	-2.46	1.46	1.51
18	B	820	CLA	CMB-C2B	-2.46	1.46	1.51
18	L	303	CLA	CMB-C2B	-2.46	1.46	1.51
18	3	608	CLA	CMB-C2B	-2.46	1.46	1.51
18	A	830	CLA	CMB-C2B	-2.46	1.46	1.51
18	A	805	CLA	CMB-C2B	-2.46	1.46	1.51
18	A	828	CLA	CMB-C2B	-2.46	1.46	1.51
17	1	606	CHL	C3A-C2A	-2.46	1.52	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	2	613	CLA	CMB-C2B	-2.45	1.46	1.51
18	3	612	CLA	CMB-C2B	-2.45	1.46	1.51
18	B	826	CLA	CMB-C2B	-2.45	1.46	1.51
18	B	823	CLA	CMB-C2B	-2.45	1.46	1.51
18	F	303	CLA	CMB-C2B	-2.45	1.46	1.51
18	2	610	CLA	CMB-C2B	-2.45	1.46	1.51
18	A	818	CLA	CMB-C2B	-2.45	1.46	1.51
18	B	832	CLA	CMB-C2B	-2.44	1.46	1.51
18	B	837	CLA	CMB-C2B	-2.44	1.46	1.51
18	A	808	CLA	CMB-C2B	-2.44	1.46	1.51
18	B	806	CLA	CMB-C2B	-2.44	1.46	1.51
18	4	612	CLA	CMB-C2B	-2.44	1.46	1.51
18	B	803	CLA	CMB-C2B	-2.44	1.46	1.51
18	H	201	CLA	CMB-C2B	-2.44	1.46	1.51
18	1	611	CLA	CMB-C2B	-2.44	1.46	1.51
18	1	608	CLA	CMB-C2B	-2.43	1.46	1.51
18	A	839	CLA	CMB-C2B	-2.43	1.46	1.51
18	B	816	CLA	CMB-C2B	-2.43	1.46	1.51
18	A	833	CLA	CMB-C2B	-2.43	1.46	1.51
18	K	204	CLA	CMB-C2B	-2.43	1.46	1.51
18	4	614	CLA	CMB-C2B	-2.43	1.46	1.51
18	B	804	CLA	CMB-C2B	-2.43	1.46	1.51
18	A	841	CLA	CMB-C2B	-2.43	1.46	1.51
18	2	611	CLA	CMB-C2B	-2.43	1.46	1.51
18	G	203	CLA	CMB-C2B	-2.43	1.46	1.51
18	2	603	CLA	CMB-C2B	-2.42	1.46	1.51
18	A	843	CLA	CMB-C2B	-2.42	1.46	1.51
18	A	837	CLA	CMB-C2B	-2.41	1.46	1.51
18	1	604	CLA	CMB-C2B	-2.41	1.46	1.51
18	K	201	CLA	CMB-C2B	-2.41	1.46	1.51
18	B	821	CLA	CMB-C2B	-2.41	1.46	1.51
22	B	848	BCR	C19-C18	-2.41	1.40	1.45
18	F	302	CLA	CMB-C2B	-2.41	1.46	1.51
18	A	827	CLA	CMB-C2B	-2.40	1.46	1.51
18	K	203	CLA	CMB-C2B	-2.40	1.46	1.51
21	2	616	LUT	C12-C13	-2.40	1.40	1.45
17	2	606	CHL	C4C-C3C	2.40	1.49	1.45
18	2	609	CLA	CMB-C2B	-2.39	1.46	1.51
18	A	824	CLA	CMB-C2B	-2.39	1.46	1.51
17	2	601	CHL	MG-NA	-2.39	2.00	2.06
17	4	605	CHL	C4B-CHC	2.39	1.47	1.41
18	B	841	CLA	CMB-C2B	-2.39	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	1	605	CLA	CMB-C2B	-2.39	1.46	1.51
18	1	610	CLA	CMB-C2B	-2.39	1.46	1.51
17	2	601	CHL	C4C-C3C	2.39	1.49	1.45
22	4	618	BCR	C12-C13	-2.39	1.40	1.45
21	4	616	LUT	C12-C13	-2.38	1.40	1.45
17	2	605	CHL	MG-NA	-2.38	2.00	2.06
22	L	301	BCR	C12-C13	-2.38	1.40	1.45
22	B	847	BCR	C19-C18	-2.38	1.40	1.45
22	G	204	BCR	C19-C18	-2.38	1.40	1.45
18	1	609	CLA	CMB-C2B	-2.37	1.46	1.51
18	3	610	CLA	CMB-C2B	-2.36	1.46	1.51
24	A	801	CL0	CHA-C1A	2.36	1.45	1.39
22	3	614	BCR	C19-C18	-2.36	1.40	1.45
22	I	101	BCR	C12-C13	-2.35	1.40	1.45
22	F	304	BCR	C23-C22	-2.35	1.40	1.45
22	G	204	BCR	C12-C13	-2.35	1.40	1.45
17	1	601	CHL	C4B-CHC	2.35	1.47	1.41
17	2	601	CHL	C4B-CHC	2.35	1.47	1.41
22	I	101	BCR	C19-C18	-2.35	1.40	1.45
17	4	605	CHL	C4C-C3C	2.34	1.49	1.44
17	3	606	CHL	C4C-C3C	2.34	1.49	1.45
17	2	605	CHL	C4C-C3C	2.33	1.49	1.44
21	3	613	LUT	C32-C33	-2.33	1.40	1.45
22	3	614	BCR	C12-C13	-2.33	1.40	1.45
18	A	823	CLA	CMB-C2B	-2.33	1.46	1.51
17	3	606	CHL	MG-NA	-2.32	2.00	2.06
18	2	604	CLA	C3B-CAB	-2.32	1.43	1.47
22	B	846	BCR	C19-C18	-2.32	1.41	1.45
17	2	607	CHL	C4B-CHC	2.32	1.47	1.41
17	2	601	CHL	C1B-CHB	2.32	1.47	1.41
21	4	616	LUT	C32-C33	-2.31	1.41	1.45
22	4	618	BCR	C19-C18	-2.31	1.41	1.45
22	A	848	BCR	C19-C18	-2.31	1.41	1.45
22	L	305	BCR	C12-C13	-2.31	1.41	1.45
17	2	607	CHL	C4C-C3C	2.31	1.49	1.45
21	2	616	LUT	C28-C29	-2.31	1.41	1.45
17	3	606	CHL	C4B-CHC	2.31	1.47	1.41
22	B	844	BCR	C12-C13	-2.30	1.41	1.45
22	B	845	BCR	C19-C18	-2.29	1.41	1.45
22	B	848	BCR	C12-C13	-2.29	1.41	1.45
21	2	616	LUT	C32-C33	-2.28	1.41	1.45
21	3	613	LUT	C28-C29	-2.28	1.41	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	4	615	CHL	MG-NA	-2.28	2.00	2.06
18	A	803	CLA	C3B-C2B	-2.27	1.37	1.40
21	3	613	LUT	C12-C13	-2.27	1.41	1.45
18	4	603	CLA	CMD-C2D	-2.27	1.46	1.50
22	L	305	BCR	C19-C18	-2.27	1.41	1.45
24	A	801	CL0	C1D-C2D	2.27	1.49	1.45
22	A	850	BCR	C12-C13	-2.27	1.41	1.45
18	1	613	CLA	CMD-C2D	-2.26	1.46	1.50
17	4	615	CHL	C4B-CHC	2.26	1.47	1.41
22	A	848	BCR	C12-C13	-2.25	1.41	1.45
18	B	828	CLA	CMD-C2D	-2.25	1.46	1.50
22	B	801	BCR	C19-C18	-2.25	1.41	1.45
21	2	619	LUT	C12-C13	-2.25	1.41	1.45
17	2	615	CHL	C4C-C3C	2.24	1.48	1.45
19	2	617	XAT	C28-C29	-2.24	1.41	1.45
21	2	619	LUT	C32-C33	-2.24	1.41	1.45
19	1	614	XAT	O24-C25	-2.24	1.43	1.46
22	B	846	BCR	C12-C13	-2.23	1.41	1.45
22	B	845	BCR	C12-C13	-2.23	1.41	1.45
18	A	810	CLA	CMD-C2D	-2.23	1.46	1.50
22	B	801	BCR	C12-C13	-2.23	1.41	1.45
18	A	843	CLA	CMD-C2D	-2.23	1.46	1.50
21	2	619	LUT	C28-C29	-2.23	1.41	1.45
17	2	606	CHL	C1B-CHB	2.22	1.47	1.41
18	1	603	CLA	CMD-C2D	-2.22	1.46	1.50
18	2	609	CLA	CMC-C2C	-2.22	1.46	1.50
18	A	803	CLA	C3B-CAB	-2.21	1.43	1.47
17	2	607	CHL	MG-NA	-2.21	2.01	2.06
22	B	849	BCR	C19-C18	-2.21	1.41	1.45
18	A	806	CLA	CMC-C2C	-2.21	1.46	1.50
18	4	611	CLA	CMD-C2D	-2.20	1.46	1.50
17	2	607	CHL	C1B-CHB	2.20	1.47	1.41
22	J	102	BCR	C19-C18	-2.20	1.41	1.45
17	2	615	CHL	C1B-CHB	2.20	1.47	1.41
17	4	605	CHL	C1B-CHB	2.20	1.47	1.41
17	4	615	CHL	C4C-C3C	2.20	1.48	1.45
17	2	605	CHL	C1B-CHB	2.19	1.47	1.41
21	4	616	LUT	C28-C29	-2.19	1.41	1.45
22	K	205	BCR	C19-C18	-2.19	1.41	1.45
17	1	601	CHL	C1B-CHB	2.19	1.47	1.41
17	3	606	CHL	C1B-CHB	2.19	1.47	1.41
22	A	849	BCR	C19-C18	-2.19	1.41	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	4	606	CHL	C1D-ND	-2.18	1.35	1.37
17	1	601	CHL	C4C-C3C	2.18	1.48	1.45
22	A	852	BCR	C19-C18	-2.18	1.41	1.45
18	B	802	CLA	CMD-C2D	-2.18	1.46	1.50
18	B	808	CLA	CMD-C2D	-2.17	1.46	1.50
22	B	844	BCR	C20-C19	2.17	1.40	1.34
22	L	301	BCR	C20-C19	2.17	1.40	1.34
19	4	617	XAT	C12-C13	-2.17	1.41	1.45
22	L	306	BCR	C19-C18	-2.17	1.41	1.45
18	A	826	CLA	CMD-C2D	-2.16	1.46	1.50
22	A	849	BCR	C12-C13	-2.16	1.41	1.45
21	1	616	LUT	C32-C33	-2.16	1.41	1.45
24	A	801	CL0	MG-NC	2.16	2.11	2.06
22	B	843	BCR	C12-C13	-2.16	1.41	1.45
18	A	830	CLA	CMD-C2D	-2.15	1.46	1.50
18	B	823	CLA	CMD-C2D	-2.15	1.46	1.50
22	B	843	BCR	C19-C18	-2.15	1.41	1.45
18	A	804	CLA	CMD-C2D	-2.15	1.46	1.50
18	2	604	CLA	C3B-C2B	-2.15	1.37	1.40
18	A	814	CLA	CMC-C2C	-2.14	1.46	1.50
22	L	306	BCR	C12-C13	-2.14	1.41	1.45
17	2	615	CHL	C1D-ND	-2.14	1.35	1.37
17	4	607	CHL	C4B-CHC	2.14	1.46	1.41
17	1	606	CHL	C1D-ND	-2.13	1.35	1.37
24	A	801	CL0	CHA-C4D	2.13	1.42	1.38
19	4	617	XAT	C14-C13	-2.13	1.33	1.35
18	A	834	CLA	CMD-C2D	-2.13	1.46	1.50
18	B	821	CLA	CMD-C2D	-2.13	1.46	1.50
22	A	853	BCR	C12-C13	-2.13	1.41	1.45
18	B	805	CLA	CMD-C2D	-2.13	1.46	1.50
18	B	823	CLA	CMC-C2C	-2.13	1.46	1.50
17	2	607	CHL	C1D-ND	-2.12	1.35	1.37
18	1	608	CLA	CMD-C2D	-2.12	1.46	1.50
18	A	806	CLA	CMD-C2D	-2.12	1.46	1.50
18	A	814	CLA	CMD-C2D	-2.12	1.46	1.50
18	B	830	CLA	CMD-C2D	-2.12	1.46	1.50
18	B	810	CLA	CMD-C2D	-2.12	1.46	1.50
18	A	803	CLA	CMD-C2D	-2.12	1.46	1.50
18	A	816	CLA	CMD-C2D	-2.12	1.46	1.50
18	A	820	CLA	CMD-C2D	-2.12	1.46	1.50
18	A	832	CLA	CMD-C2D	-2.12	1.46	1.50
18	A	807	CLA	CMD-C2D	-2.12	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	836	CLA	CMD-C2D	-2.12	1.46	1.50
18	2	608	CLA	CMD-C2D	-2.12	1.46	1.50
18	3	601	CLA	CMD-C2D	-2.12	1.46	1.50
18	2	603	CLA	CMD-C2D	-2.11	1.46	1.50
18	3	602	CLA	CMD-C2D	-2.11	1.46	1.50
17	2	601	CHL	C1D-ND	-2.11	1.35	1.37
22	A	851	BCR	C12-C13	-2.11	1.41	1.45
18	3	612	CLA	CMD-C2D	-2.11	1.46	1.50
18	B	829	CLA	CMD-C2D	-2.11	1.46	1.50
18	L	302	CLA	CMD-C2D	-2.11	1.46	1.50
18	A	819	CLA	CMD-C2D	-2.10	1.46	1.50
18	B	820	CLA	CMD-C2D	-2.10	1.46	1.50
21	1	616	LUT	C12-C13	-2.10	1.41	1.45
18	K	201	CLA	CBD-CAD	2.10	1.56	1.51
18	2	613	CLA	CMD-C2D	-2.10	1.46	1.50
18	A	838	CLA	CMD-C2D	-2.10	1.46	1.50
18	4	608	CLA	CMD-C2D	-2.10	1.46	1.50
18	B	804	CLA	CMD-C2D	-2.10	1.46	1.50
18	A	821	CLA	CMD-C2D	-2.10	1.46	1.50
22	K	202	BCR	C19-C18	-2.10	1.41	1.45
18	4	609	CLA	CMD-C2D	-2.10	1.46	1.50
18	A	802	CLA	CMD-C2D	-2.10	1.46	1.50
22	A	853	BCR	C19-C18	-2.09	1.41	1.45
18	3	608	CLA	CMD-C2D	-2.09	1.46	1.50
22	F	304	BCR	C19-C18	-2.09	1.41	1.45
18	1	610	CLA	CMD-C2D	-2.09	1.46	1.50
18	4	613	CLA	CMD-C2D	-2.09	1.46	1.50
18	B	817	CLA	CMD-C2D	-2.09	1.46	1.50
18	B	840	CLA	CMD-C2D	-2.09	1.46	1.50
22	J	102	BCR	C12-C13	-2.09	1.41	1.45
18	2	604	CLA	CMD-C2D	-2.09	1.46	1.50
22	A	851	BCR	C19-C18	-2.09	1.41	1.45
17	2	606	CHL	C1D-ND	-2.09	1.35	1.37
18	B	822	CLA	CMD-C2D	-2.09	1.46	1.50
18	B	833	CLA	CMD-C2D	-2.09	1.46	1.50
17	2	605	CHL	C1D-ND	-2.09	1.35	1.37
18	B	803	CLA	CMD-C2D	-2.09	1.46	1.50
18	F	301	CLA	CMD-C2D	-2.09	1.46	1.50
24	A	801	CL0	C1C-C2C	2.09	1.48	1.44
18	A	844	CLA	C3B-CAB	-2.09	1.43	1.47
18	A	841	CLA	CMD-C2D	-2.09	1.46	1.50
18	B	818	CLA	CMD-C2D	-2.09	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	826	CLA	CMD-C2D	-2.09	1.46	1.50
18	2	602	CLA	CMD-C2D	-2.09	1.46	1.50
17	1	601	CHL	C1D-ND	-2.08	1.35	1.37
18	A	840	CLA	CMD-C2D	-2.08	1.46	1.50
18	B	813	CLA	CMD-C2D	-2.08	1.46	1.50
18	A	833	CLA	CMD-C2D	-2.08	1.46	1.50
18	G	202	CLA	CMD-C2D	-2.08	1.46	1.50
18	B	815	CLA	CMD-C2D	-2.08	1.46	1.50
17	4	607	CHL	C4C-C3C	2.08	1.48	1.45
18	B	808	CLA	CMC-C2C	-2.08	1.46	1.50
18	L	303	CLA	CMD-C2D	-2.08	1.46	1.50
18	A	839	CLA	CMD-C2D	-2.07	1.46	1.50
18	2	609	CLA	CMD-C2D	-2.07	1.46	1.50
18	B	838	CLA	CMD-C2D	-2.07	1.46	1.50
18	H	201	CLA	CMD-C2D	-2.07	1.46	1.50
19	2	617	XAT	C12-C13	-2.07	1.41	1.45
18	B	817	CLA	CMC-C2C	-2.07	1.46	1.50
22	B	849	BCR	C12-C13	-2.07	1.41	1.45
18	3	604	CLA	CMD-C2D	-2.07	1.46	1.50
18	A	828	CLA	CMD-C2D	-2.07	1.46	1.50
18	L	304	CLA	CMD-C2D	-2.07	1.46	1.50
18	A	818	CLA	CMD-C2D	-2.07	1.46	1.50
18	1	607	CLA	CMD-C2D	-2.07	1.46	1.50
18	A	811	CLA	CMD-C2D	-2.07	1.46	1.50
18	4	614	CLA	CMD-C2D	-2.07	1.46	1.50
18	B	816	CLA	CMD-C2D	-2.07	1.46	1.50
18	3	611	CLA	CBD-CAD	2.07	1.56	1.51
18	B	837	CLA	CMD-C2D	-2.07	1.46	1.50
17	4	615	CHL	C1B-CHB	2.07	1.46	1.41
18	A	817	CLA	CMD-C2D	-2.07	1.46	1.50
18	4	612	CLA	CMD-C2D	-2.07	1.46	1.50
22	A	852	BCR	C11-C12	2.06	1.39	1.34
18	2	610	CLA	CMD-C2D	-2.06	1.46	1.50
18	A	828	CLA	CMC-C2C	-2.06	1.46	1.50
18	B	806	CLA	CMD-C2D	-2.06	1.46	1.50
18	A	814	CLA	C3B-C2B	-2.06	1.37	1.40
18	3	607	CLA	CMD-C2D	-2.06	1.46	1.50
18	A	843	CLA	CMC-C2C	-2.06	1.46	1.50
18	A	844	CLA	C3B-C2B	-2.06	1.37	1.40
18	B	807	CLA	CMD-C2D	-2.06	1.46	1.50
18	1	602	CLA	CMD-C2D	-2.06	1.46	1.50
18	A	802	CLA	CMC-C2C	-2.06	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	4	607	CHL	MG-NA	-2.06	2.01	2.06
18	B	827	CLA	CMD-C2D	-2.06	1.46	1.50
18	B	824	CLA	CMD-C2D	-2.06	1.46	1.50
18	B	834	CLA	CMD-C2D	-2.06	1.46	1.50
18	B	825	CLA	CMD-C2D	-2.06	1.46	1.50
18	A	831	CLA	CMD-C2D	-2.06	1.46	1.50
22	F	304	BCR	C11-C12	2.06	1.39	1.34
18	B	831	CLA	CMD-C2D	-2.06	1.46	1.50
18	B	839	CLA	CMD-C2D	-2.06	1.46	1.50
18	A	813	CLA	CMD-C2D	-2.05	1.46	1.50
19	2	617	XAT	C32-C33	-2.05	1.41	1.45
18	A	842	CLA	CMD-C2D	-2.05	1.46	1.50
18	B	813	CLA	CMC-C2C	-2.05	1.46	1.50
18	A	827	CLA	CMD-C2D	-2.05	1.46	1.50
18	A	809	CLA	CMD-C2D	-2.05	1.46	1.50
18	A	829	CLA	CMD-C2D	-2.05	1.46	1.50
18	3	609	CLA	CMD-C2D	-2.05	1.46	1.50
18	A	815	CLA	CMC-C2C	-2.05	1.46	1.50
18	4	602	CLA	CMD-C2D	-2.05	1.46	1.50
18	A	808	CLA	CMD-C2D	-2.05	1.46	1.50
18	3	607	CLA	C3B-C2B	-2.05	1.37	1.40
18	B	814	CLA	CMD-C2D	-2.04	1.46	1.50
18	2	602	CLA	CMC-C2C	-2.04	1.46	1.50
18	B	812	CLA	CMD-C2D	-2.04	1.46	1.50
18	A	819	CLA	CMC-C2C	-2.04	1.46	1.50
18	B	826	CLA	CMC-C2C	-2.04	1.46	1.50
18	B	828	CLA	C3B-C2B	-2.04	1.37	1.40
17	4	605	CHL	C1D-ND	-2.04	1.35	1.37
18	B	802	CLA	CMC-C2C	-2.04	1.46	1.50
18	3	605	CLA	CMD-C2D	-2.04	1.46	1.50
18	B	832	CLA	CMD-C2D	-2.04	1.46	1.50
18	B	836	CLA	CMC-C2C	-2.04	1.46	1.50
18	4	601	CLA	CMD-C2D	-2.04	1.46	1.50
18	B	815	CLA	CMC-C2C	-2.04	1.46	1.50
18	A	807	CLA	CMC-C2C	-2.03	1.46	1.50
18	A	805	CLA	CMD-C2D	-2.03	1.46	1.50
18	B	837	CLA	CMC-C2C	-2.03	1.46	1.50
18	A	837	CLA	CMD-C2D	-2.03	1.46	1.50
18	3	611	CLA	CMD-C2D	-2.03	1.46	1.50
18	A	844	CLA	CMD-C2D	-2.03	1.46	1.50
18	A	815	CLA	CMD-C2D	-2.03	1.46	1.50
18	A	835	CLA	C3B-CAB	-2.02	1.43	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	819	CLA	CMD-C2D	-2.02	1.46	1.50
18	B	819	CLA	CMC-C2C	-2.02	1.46	1.50
18	K	204	CLA	CMD-C2D	-2.02	1.46	1.50
18	2	612	CLA	CMD-C2D	-2.02	1.46	1.50
18	B	809	CLA	CMD-C2D	-2.02	1.46	1.50
18	B	808	CLA	C3B-CAB	-2.02	1.43	1.47
18	1	607	CLA	CMC-C2C	-2.02	1.46	1.50
18	A	827	CLA	CMC-C2C	-2.02	1.46	1.50
18	B	803	CLA	CMC-C2C	-2.02	1.46	1.50
18	B	841	CLA	CMD-C2D	-2.02	1.46	1.50
18	A	844	CLA	CMC-C2C	-2.02	1.46	1.50
18	1	611	CLA	CMD-C2D	-2.02	1.46	1.50
17	4	607	CHL	C1B-CHB	2.02	1.46	1.41
18	A	822	CLA	CMD-C2D	-2.02	1.46	1.50
18	4	610	CLA	CMD-C2D	-2.01	1.46	1.50
18	A	812	CLA	CMD-C2D	-2.01	1.46	1.50
17	4	607	CHL	C1D-ND	-2.01	1.35	1.37
18	4	602	CLA	CMC-C2C	-2.01	1.46	1.50
18	B	810	CLA	CMC-C2C	-2.01	1.46	1.50
18	B	818	CLA	CMC-C2C	-2.01	1.46	1.50
19	4	617	XAT	C8-C9	-2.01	1.41	1.45
18	G	201	CLA	CMD-C2D	-2.01	1.46	1.50
18	B	809	CLA	CMC-C2C	-2.01	1.46	1.50
18	B	819	CLA	C3B-C2B	-2.01	1.37	1.40
18	B	803	CLA	C3B-CAB	-2.01	1.43	1.47
18	3	608	CLA	CMC-C2C	-2.01	1.46	1.50
18	G	203	CLA	CMD-C2D	-2.01	1.46	1.50
18	F	303	CLA	CMD-C2D	-2.01	1.46	1.50
18	4	601	CLA	CMC-C2C	-2.01	1.46	1.50
18	2	611	CLA	CMD-C2D	-2.01	1.46	1.50
18	B	805	CLA	CMC-C2C	-2.01	1.46	1.50
18	B	811	CLA	CMD-C2D	-2.01	1.46	1.50
19	4	617	XAT	C31-C32	-2.01	1.29	1.34
18	2	603	CLA	CMC-C2C	-2.01	1.46	1.50
18	2	604	CLA	CMC-C2C	-2.01	1.46	1.50
22	L	301	BCR	C19-C18	-2.00	1.41	1.45
18	L	304	CLA	C3B-C2B	-2.00	1.37	1.40
18	A	841	CLA	CMC-C2C	-2.00	1.46	1.50
22	K	205	BCR	C11-C12	2.00	1.39	1.34
18	1	604	CLA	CMD-C2D	-2.00	1.46	1.50
18	3	601	CLA	CMC-C2C	-2.00	1.46	1.50
18	B	833	CLA	CMC-C2C	-2.00	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	829	CLA	C3B-CAB	-2.00	1.43	1.47
18	B	816	CLA	C3B-CAB	-2.00	1.43	1.47

All (1756) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	818	CLA	O2D-CGD-CBD	26.07	157.59	111.27
18	A	818	CLA	O2D-CGD-O1D	-25.32	74.34	123.84
18	A	818	CLA	O1D-CGD-CBD	-20.15	83.25	124.48
19	4	617	XAT	C4-C3-C2	-19.33	73.45	110.77
18	B	836	CLA	C5-C3-C4	-16.75	77.61	114.60
19	4	617	XAT	C38-C25-C26	-15.95	95.53	122.26
18	B	836	CLA	C4-C3-C2	-13.80	82.76	122.65
19	4	617	XAT	C18-C5-C6	-13.43	99.75	122.26
18	B	836	CLA	C5-C3-C2	13.05	160.37	122.65
24	A	801	CL0	C2C-C1C-NC	10.50	119.81	109.97
19	4	617	XAT	C28-C29-C30	10.20	134.59	118.94
24	A	801	CL0	C4A-NA-C1A	-9.99	102.21	106.71
24	A	801	CL0	CHA-C4D-C3D	-9.54	108.95	125.26
24	A	801	CL0	C3D-C2D-C1D	-8.57	98.89	107.08
19	1	614	XAT	O4-C5-C4	8.50	119.77	113.38
19	4	617	XAT	C18-C5-C4	8.40	123.73	114.28
17	2	607	CHL	CMD-C2D-C1D	8.37	139.47	124.71
19	4	617	XAT	O3-C3-C2	-8.31	93.29	109.80
17	4	607	CHL	CMD-C2D-C1D	8.27	139.29	124.71
19	4	617	XAT	C25-C24-C23	-8.25	96.42	112.75
17	3	606	CHL	CMD-C2D-C1D	8.24	139.23	124.71
17	4	605	CHL	CMD-C2D-C1D	8.20	139.17	124.71
17	1	601	CHL	CMD-C2D-C1D	8.18	139.13	124.71
17	2	601	CHL	CMD-C2D-C1D	8.16	139.10	124.71
19	1	614	XAT	C38-C25-C26	-8.16	108.59	122.26
17	2	615	CHL	CMD-C2D-C1D	8.15	139.08	124.71
17	2	605	CHL	CMD-C2D-C1D	8.13	139.04	124.71
17	4	615	CHL	CMD-C2D-C1D	8.12	139.03	124.71
24	A	801	CL0	C3C-C4C-NC	8.12	119.67	110.57
24	A	801	CL0	CMD-C2D-C1D	8.02	138.84	124.71
17	4	606	CHL	CMD-C2D-C1D	8.00	138.82	124.71
17	1	606	CHL	CMD-C2D-C1D	7.97	138.77	124.71
17	1	606	CHL	CHD-C1D-ND	-7.91	117.19	124.45
22	B	843	BCR	C16-C15-C14	7.91	139.67	123.47
17	2	606	CHL	CMD-C2D-C1D	7.88	138.61	124.71
19	4	617	XAT	C39-C29-C28	-7.86	105.69	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	4	617	XAT	C26-C27-C28	-7.77	109.56	125.99
19	1	614	XAT	O24-C25-C24	7.74	119.19	113.38
22	A	849	BCR	C15-C16-C17	7.73	139.31	123.47
17	4	606	CHL	CHD-C1D-ND	-7.70	117.38	124.45
22	L	301	BCR	C15-C16-C17	7.67	139.19	123.47
22	L	301	BCR	C16-C15-C14	7.65	139.13	123.47
19	1	614	XAT	C18-C5-C6	-7.64	109.45	122.26
19	4	617	XAT	O24-C25-C38	7.58	124.14	115.06
17	2	601	CHL	C2C-C3C-C4C	-7.37	101.24	106.49
18	F	302	CLA	C4A-NA-C1A	7.36	110.02	106.71
19	4	617	XAT	C5-C4-C3	-7.34	98.23	112.75
17	4	615	CHL	C2C-C3C-C4C	-7.33	101.26	106.49
18	1	609	CLA	C4A-NA-C1A	7.30	109.99	106.71
17	2	605	CHL	C2C-C3C-C4C	-7.29	101.08	106.49
17	2	607	CHL	C2C-C3C-C4C	-7.25	101.32	106.49
17	2	606	CHL	C2C-C3C-C4C	-7.19	101.36	106.49
22	A	851	BCR	C16-C15-C14	7.19	138.20	123.47
18	4	614	CLA	C4A-NA-C1A	7.19	109.94	106.71
17	2	615	CHL	C2C-C3C-C4C	-7.15	101.39	106.49
17	2	606	CHL	CHD-C1D-ND	-7.14	117.90	124.45
17	4	607	CHL	C2C-C3C-C4C	-7.11	101.42	106.49
18	A	839	CLA	C4A-NA-C1A	7.10	109.90	106.71
18	B	805	CLA	C4A-NA-C1A	7.05	109.88	106.71
18	A	830	CLA	C4A-NA-C1A	7.05	109.87	106.71
19	4	617	XAT	C11-C10-C9	7.05	137.37	127.31
22	A	851	BCR	C8-C9-C10	7.03	129.73	118.94
18	1	605	CLA	C4A-NA-C1A	7.02	109.86	106.71
18	A	813	CLA	C4A-NA-C1A	7.01	109.86	106.71
24	A	801	CL0	C2D-C1D-ND	7.01	115.27	110.10
18	A	804	CLA	C4A-NA-C1A	6.98	109.84	106.71
19	4	617	XAT	O4-C5-C18	6.97	123.40	115.06
21	2	616	LUT	C15-C35-C34	6.95	137.71	123.47
18	2	609	CLA	C4A-NA-C1A	6.95	109.83	106.71
17	1	606	CHL	C2C-C3C-C4C	-6.91	101.56	106.49
18	4	612	CLA	C4A-NA-C1A	6.91	109.81	106.71
18	2	613	CLA	C4A-NA-C1A	6.90	109.81	106.71
18	A	828	CLA	C4A-NA-C1A	6.89	109.81	106.71
17	1	601	CHL	C2C-C3C-C4C	-6.89	101.58	106.49
17	4	615	CHL	C1B-C2B-C3B	-6.88	100.52	106.92
18	B	840	CLA	C4A-NA-C1A	6.87	109.79	106.71
21	3	613	LUT	C15-C35-C34	6.85	137.51	123.47
17	2	615	CHL	CHD-C1D-ND	-6.85	118.16	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	B	811	CLA	C4A-NA-C1A	6.83	109.78	106.71
18	L	304	CLA	C4A-NA-C1A	6.83	109.78	106.71
18	A	842	CLA	C4A-NA-C1A	6.82	109.77	106.71
18	B	824	CLA	C4A-NA-C1A	6.82	109.77	106.71
18	B	814	CLA	C4A-NA-C1A	6.80	109.76	106.71
18	A	809	CLA	C4A-NA-C1A	6.80	109.76	106.71
18	A	834	CLA	C4A-NA-C1A	6.80	109.76	106.71
18	A	821	CLA	C4A-NA-C1A	6.79	109.76	106.71
17	2	601	CHL	CHD-C1D-ND	-6.79	118.21	124.45
18	A	808	CLA	C4A-NA-C1A	6.78	109.76	106.71
18	A	835	CLA	C4A-NA-C1A	6.78	109.76	106.71
18	1	604	CLA	C4A-NA-C1A	6.78	109.75	106.71
18	1	612	CLA	C4A-NA-C1A	6.77	109.75	106.71
17	4	606	CHL	C1B-C2B-C3B	-6.76	100.64	106.92
18	1	607	CLA	C4A-NA-C1A	6.76	109.74	106.71
18	B	812	CLA	C4A-NA-C1A	6.76	109.74	106.71
24	A	801	CL0	CHA-C4D-ND	6.75	130.66	124.45
18	B	827	CLA	C4A-NA-C1A	6.74	109.74	106.71
18	B	829	CLA	C4A-NA-C1A	6.74	109.74	106.71
18	1	611	CLA	C4A-NA-C1A	6.73	109.73	106.71
18	A	840	CLA	C4A-NA-C1A	6.72	109.73	106.71
18	A	807	CLA	C4A-NA-C1A	6.72	109.73	106.71
18	B	821	CLA	C4A-NA-C1A	6.72	109.73	106.71
18	4	601	CLA	C4A-NA-C1A	6.71	109.72	106.71
17	4	605	CHL	C2C-C3C-C4C	-6.71	101.51	106.49
18	A	831	CLA	C4A-NA-C1A	6.70	109.72	106.71
18	K	204	CLA	C4A-NA-C1A	6.70	109.72	106.71
18	4	603	CLA	C4A-NA-C1A	6.69	109.72	106.71
18	B	803	CLA	C4A-NA-C1A	6.69	109.71	106.71
17	1	601	CHL	CHD-C1D-ND	-6.68	118.31	124.45
17	2	607	CHL	CHD-C1D-ND	-6.67	118.32	124.45
18	2	608	CLA	C4A-NA-C1A	6.67	109.71	106.71
18	B	831	CLA	C4A-NA-C1A	6.67	109.70	106.71
17	4	605	CHL	CHD-C1D-ND	-6.67	118.33	124.45
18	3	601	CLA	C4A-NA-C1A	6.67	109.70	106.71
18	B	834	CLA	C4A-NA-C1A	6.66	109.70	106.71
18	B	825	CLA	C4A-NA-C1A	6.66	109.70	106.71
18	A	817	CLA	C4A-NA-C1A	6.66	109.70	106.71
18	4	604	CLA	C4A-NA-C1A	6.65	109.70	106.71
18	B	837	CLA	C4A-NA-C1A	6.65	109.69	106.71
18	B	830	CLA	C4A-NA-C1A	6.65	109.69	106.71
19	4	617	XAT	O24-C25-C26	-6.64	53.46	58.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	4	617	XAT	O23-C23-C24	-6.64	96.61	109.80
18	A	812	CLA	C4A-NA-C1A	6.63	109.69	106.71
18	B	817	CLA	C4A-NA-C1A	6.63	109.69	106.71
18	3	612	CLA	C4A-NA-C1A	6.63	109.69	106.71
18	A	826	CLA	C4A-NA-C1A	6.63	109.69	106.71
18	G	202	CLA	C4A-NA-C1A	6.63	109.69	106.71
18	B	804	CLA	C4A-NA-C1A	6.63	109.69	106.71
18	1	613	CLA	C4A-NA-C1A	6.62	109.68	106.71
18	B	808	CLA	C4A-NA-C1A	6.62	109.68	106.71
18	B	806	CLA	C4A-NA-C1A	6.62	109.68	106.71
18	B	832	CLA	C4A-NA-C1A	6.62	109.68	106.71
18	3	609	CLA	C4A-NA-C1A	6.61	109.68	106.71
18	A	818	CLA	C4A-NA-C1A	6.61	109.68	106.71
18	H	201	CLA	C4A-NA-C1A	6.61	109.68	106.71
22	A	850	BCR	C16-C15-C14	6.60	137.00	123.47
18	B	819	CLA	C4A-NA-C1A	6.60	109.67	106.71
18	B	807	CLA	C4A-NA-C1A	6.59	109.67	106.71
18	B	820	CLA	C4A-NA-C1A	6.59	109.67	106.71
18	A	837	CLA	C4A-NA-C1A	6.58	109.67	106.71
18	B	809	CLA	C4A-NA-C1A	6.58	109.67	106.71
18	2	611	CLA	C4A-NA-C1A	6.58	109.66	106.71
18	B	813	CLA	C4A-NA-C1A	6.58	109.66	106.71
18	B	815	CLA	C4A-NA-C1A	6.58	109.66	106.71
18	K	203	CLA	C4A-NA-C1A	6.58	109.66	106.71
18	B	828	CLA	C4A-NA-C1A	6.57	109.66	106.71
18	3	602	CLA	C4A-NA-C1A	6.56	109.66	106.71
18	3	605	CLA	C4A-NA-C1A	6.56	109.66	106.71
18	A	843	CLA	C4A-NA-C1A	6.55	109.65	106.71
18	A	824	CLA	C4A-NA-C1A	6.55	109.65	106.71
18	B	838	CLA	C4A-NA-C1A	6.55	109.65	106.71
18	A	816	CLA	C4A-NA-C1A	6.53	109.64	106.71
18	K	201	CLA	C4A-NA-C1A	6.53	109.64	106.71
18	B	818	CLA	C4A-NA-C1A	6.52	109.64	106.71
18	A	820	CLA	C4A-NA-C1A	6.52	109.64	106.71
18	F	301	CLA	C4A-NA-C1A	6.52	109.64	106.71
18	G	201	CLA	C4A-NA-C1A	6.52	109.64	106.71
18	3	604	CLA	C4A-NA-C1A	6.51	109.63	106.71
18	A	805	CLA	C4A-NA-C1A	6.51	109.63	106.71
18	A	811	CLA	C4A-NA-C1A	6.51	109.63	106.71
18	A	827	CLA	C4A-NA-C1A	6.50	109.63	106.71
18	2	603	CLA	C4A-NA-C1A	6.50	109.63	106.71
18	A	833	CLA	C4A-NA-C1A	6.50	109.63	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	2	612	CLA	C4A-NA-C1A	6.50	109.63	106.71
18	G	203	CLA	C4A-NA-C1A	6.49	109.63	106.71
18	1	608	CLA	C4A-NA-C1A	6.48	109.62	106.71
18	F	303	CLA	C4A-NA-C1A	6.48	109.62	106.71
18	4	611	CLA	C4A-NA-C1A	6.48	109.62	106.71
18	A	806	CLA	C4A-NA-C1A	6.48	109.62	106.71
18	L	303	CLA	C4A-NA-C1A	6.48	109.62	106.71
18	B	826	CLA	C4A-NA-C1A	6.47	109.62	106.71
18	A	822	CLA	C4A-NA-C1A	6.47	109.61	106.71
18	4	610	CLA	C4A-NA-C1A	6.46	109.61	106.71
18	A	819	CLA	C4A-NA-C1A	6.46	109.61	106.71
17	2	605	CHL	CHD-C1D-ND	-6.45	118.53	124.45
18	A	815	CLA	C4A-NA-C1A	6.44	109.60	106.71
18	1	603	CLA	C4A-NA-C1A	6.44	109.60	106.71
18	L	302	CLA	C4A-NA-C1A	6.43	109.60	106.71
18	B	833	CLA	C4A-NA-C1A	6.43	109.60	106.71
18	B	835	CLA	C4A-NA-C1A	6.42	109.59	106.71
17	4	615	CHL	CHD-C1D-ND	-6.41	118.56	124.45
18	A	836	CLA	C4A-NA-C1A	6.41	109.59	106.71
17	3	606	CHL	CHD-C1D-ND	-6.41	118.56	124.45
18	4	609	CLA	C4A-NA-C1A	6.40	109.58	106.71
18	A	823	CLA	C4A-NA-C1A	6.39	109.58	106.71
18	2	602	CLA	C4A-NA-C1A	6.39	109.58	106.71
18	B	810	CLA	C4A-NA-C1A	6.38	109.58	106.71
18	1	610	CLA	C4A-NA-C1A	6.38	109.58	106.71
18	A	841	CLA	C4A-NA-C1A	6.37	109.57	106.71
18	2	604	CLA	C4A-NA-C1A	6.36	109.56	106.71
18	3	611	CLA	C4A-NA-C1A	6.36	109.56	106.71
18	A	838	CLA	C4A-NA-C1A	6.35	109.56	106.71
18	3	610	CLA	C4A-NA-C1A	6.34	109.56	106.71
18	A	832	CLA	C4A-NA-C1A	6.34	109.56	106.71
19	4	617	XAT	C15-C14-C13	6.34	136.36	127.31
18	B	836	CLA	C4A-NA-C1A	6.33	109.55	106.71
18	4	602	CLA	C4A-NA-C1A	6.32	109.55	106.71
19	2	617	XAT	C35-C15-C14	6.32	136.41	123.47
18	A	829	CLA	C4A-NA-C1A	6.32	109.55	106.71
18	A	802	CLA	C4A-NA-C1A	6.29	109.53	106.71
18	A	825	CLA	C4A-NA-C1A	6.28	109.53	106.71
18	4	613	CLA	C4A-NA-C1A	6.27	109.53	106.71
18	B	822	CLA	C4A-NA-C1A	6.27	109.52	106.71
18	B	841	CLA	C4A-NA-C1A	6.27	109.52	106.71
18	B	816	CLA	C4A-NA-C1A	6.26	109.52	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	4	617	XAT	C37-C21-C36	-6.26	98.14	107.37
18	4	608	CLA	C4A-NA-C1A	6.26	109.52	106.71
18	B	839	CLA	C4A-NA-C1A	6.25	109.51	106.71
18	3	607	CLA	C4A-NA-C1A	6.24	109.51	106.71
18	B	823	CLA	C4A-NA-C1A	6.20	109.49	106.71
17	4	607	CHL	CHD-C1D-ND	-6.18	118.77	124.45
18	A	810	CLA	C4A-NA-C1A	6.17	109.48	106.71
22	A	850	BCR	C15-C16-C17	6.15	136.07	123.47
19	1	614	XAT	O4-C5-C18	6.15	122.42	115.06
22	F	304	BCR	C24-C23-C22	6.14	135.52	126.23
18	A	814	CLA	C4A-NA-C1A	6.13	109.46	106.71
18	A	844	CLA	C4A-NA-C1A	6.13	109.46	106.71
24	A	801	CL0	CHD-C4C-C3C	-6.06	115.93	124.84
19	4	617	XAT	O23-C23-C22	-6.05	97.77	109.80
18	1	602	CLA	C4A-NA-C1A	6.05	109.43	106.71
18	3	608	CLA	C4A-NA-C1A	6.03	109.42	106.71
18	3	603	CLA	C4A-NA-C1A	6.02	109.41	106.71
24	A	801	CL0	C3B-C4B-NB	5.99	116.95	109.21
19	4	617	XAT	O3-C3-C4	-5.95	97.97	109.80
18	B	802	CLA	C4A-NA-C1A	5.87	109.35	106.71
22	F	304	BCR	C15-C16-C17	5.87	135.50	123.47
19	2	617	XAT	C15-C35-C34	5.83	135.42	123.47
19	1	614	XAT	C35-C34-C33	-5.76	119.09	127.31
21	2	619	LUT	C15-C35-C34	5.74	135.24	123.47
24	A	801	CL0	CHD-C1D-ND	-5.64	119.27	124.45
22	B	845	BCR	C19-C18-C17	5.49	127.36	118.94
19	4	617	XAT	C40-C33-C34	-5.44	115.31	122.92
17	1	606	CHL	C1B-CHB-C4A	-5.43	119.37	130.12
22	K	202	BCR	C16-C15-C14	5.38	134.49	123.47
22	A	851	BCR	C34-C9-C10	-5.37	115.40	122.92
17	2	606	CHL	O2D-CGD-CBD	5.26	120.62	111.27
21	1	616	LUT	C15-C35-C34	5.18	134.07	123.47
18	A	803	CLA	C4A-NA-C1A	5.14	109.02	106.71
22	J	102	BCR	C16-C15-C14	5.14	134.00	123.47
22	A	851	BCR	C7-C8-C9	-5.10	118.53	126.23
19	1	614	XAT	O24-C25-C38	5.09	121.15	115.06
17	4	606	CHL	C1B-CHB-C4A	-5.09	120.05	130.12
17	2	601	CHL	O2D-CGD-CBD	5.09	120.30	111.27
22	K	205	BCR	C15-C16-C17	5.07	133.85	123.47
17	2	605	CHL	O2D-CGD-CBD	5.04	120.23	111.27
17	2	615	CHL	C1B-CHB-C4A	-5.01	120.20	130.12
22	B	849	BCR	C30-C25-C26	-5.01	115.56	122.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	801	CL0	C1C-C2C-C3C	-4.99	101.71	106.96
24	A	801	CL0	C4D-CHA-C1A	-4.97	114.64	126.62
17	2	615	CHL	O2D-CGD-CBD	4.97	120.10	111.27
22	A	853	BCR	C16-C15-C14	4.94	133.59	123.47
17	4	607	CHL	C3C-C4C-NC	4.92	116.09	110.57
22	A	851	BCR	C23-C22-C21	4.92	126.49	118.94
22	B	846	BCR	C16-C15-C14	4.91	133.53	123.47
17	3	606	CHL	O2D-CGD-CBD	4.91	119.99	111.27
19	1	614	XAT	C26-C27-C28	-4.89	115.66	125.99
24	A	801	CL0	C1D-CHD-C4C	-4.88	115.53	126.06
17	4	615	CHL	C3C-C4C-NC	4.85	116.01	110.57
17	2	605	CHL	C3C-C4C-NC	4.84	115.86	110.57
17	1	606	CHL	C4A-NA-C1A	4.80	108.86	106.71
22	L	306	BCR	C8-C9-C10	4.78	126.27	118.94
22	B	847	BCR	C16-C15-C14	4.77	133.24	123.47
21	1	616	LUT	C30-C31-C32	4.77	138.09	123.22
22	4	618	BCR	C16-C15-C14	4.76	133.22	123.47
17	2	607	CHL	C3C-C4C-NC	4.75	115.89	110.57
17	4	606	CHL	O2D-CGD-CBD	4.74	119.69	111.27
18	A	842	CLA	CMB-C2B-C1B	-4.72	121.21	128.46
19	1	614	XAT	C6-C7-C8	-4.70	116.05	125.99
22	L	306	BCR	C34-C9-C10	-4.67	116.38	122.92
19	4	617	XAT	C38-C25-C24	4.67	119.53	114.28
22	K	202	BCR	C15-C16-C17	4.67	133.04	123.47
17	3	606	CHL	C3C-C4C-NC	4.66	115.79	110.57
17	4	607	CHL	C3D-C2D-C1D	-4.66	99.48	105.83
22	L	306	BCR	C37-C22-C21	-4.65	116.41	122.92
22	B	845	BCR	C36-C18-C17	-4.65	116.42	122.92
22	A	851	BCR	C37-C22-C21	-4.64	116.42	122.92
21	3	613	LUT	C39-C29-C30	-4.63	116.44	122.92
19	4	617	XAT	C32-C33-C34	4.62	126.03	118.94
17	2	601	CHL	C3C-C4C-NC	4.62	115.75	110.57
17	2	607	CHL	C3D-C2D-C1D	-4.62	99.53	105.83
22	A	851	BCR	C11-C10-C9	4.60	133.87	127.31
18	A	820	CLA	CMB-C2B-C1B	-4.56	121.45	128.46
17	2	607	CHL	O2D-CGD-CBD	4.55	119.36	111.27
21	2	616	LUT	C7-C8-C9	4.55	133.12	126.23
22	A	852	BCR	C23-C22-C21	4.53	125.89	118.94
21	2	616	LUT	C39-C29-C30	-4.53	116.58	122.92
22	A	852	BCR	C37-C22-C21	-4.53	116.58	122.92
22	B	801	BCR	C16-C15-C14	4.53	132.75	123.47
19	4	617	XAT	C35-C34-C33	4.52	133.77	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	826	CLA	CMB-C2B-C1B	-4.52	121.52	128.46
17	4	605	CHL	C3C-C4C-NC	4.51	115.50	110.57
18	A	804	CLA	CAA-C2A-C3A	-4.51	100.42	112.78
17	4	606	CHL	C4A-NA-C1A	4.51	108.73	106.71
17	2	605	CHL	C3D-C2D-C1D	-4.50	99.68	105.83
17	2	606	CHL	C1B-CHB-C4A	-4.50	121.20	130.12
18	4	613	CLA	CAA-C2A-C3A	-4.49	100.49	112.78
17	4	615	CHL	C3D-C2D-C1D	-4.48	99.72	105.83
17	4	607	CHL	O2D-CGD-CBD	4.48	119.22	111.27
21	2	619	LUT	C19-C9-C10	-4.46	116.67	122.92
17	2	601	CHL	C3D-C2D-C1D	-4.45	99.76	105.83
22	J	102	BCR	C34-C9-C10	-4.45	116.69	122.92
22	A	852	BCR	C16-C15-C14	4.45	132.59	123.47
22	L	301	BCR	C37-C22-C21	-4.44	116.70	122.92
18	B	809	CLA	CMB-C2B-C1B	-4.44	121.64	128.46
24	A	801	CL0	C1B-CHB-C4A	-4.43	121.35	130.12
17	3	606	CHL	C2C-C1C-NC	4.42	114.11	109.97
22	K	202	BCR	C37-C22-C21	-4.40	116.76	122.92
18	B	820	CLA	CMB-C2B-C1B	-4.40	121.70	128.46
18	B	818	CLA	CMB-C2B-C1B	-4.40	121.70	128.46
17	3	606	CHL	C3D-C2D-C1D	-4.40	99.83	105.83
17	1	601	CHL	C3D-C2D-C1D	-4.40	99.83	105.83
17	2	615	CHL	C3C-C4C-NC	4.38	115.49	110.57
22	B	844	BCR	C37-C22-C21	-4.38	116.79	122.92
21	2	616	LUT	C19-C9-C10	-4.37	116.80	122.92
22	B	843	BCR	C34-C9-C10	-4.37	116.81	122.92
17	2	615	CHL	C3D-C2D-C1D	-4.36	99.87	105.83
17	4	605	CHL	C3D-C2D-C1D	-4.36	99.88	105.83
18	B	813	CLA	CMB-C2B-C1B	-4.35	121.78	128.46
17	2	606	CHL	C3C-C4C-NC	4.34	115.44	110.57
22	K	205	BCR	C37-C22-C21	-4.33	116.85	122.92
17	1	601	CHL	C3C-C4C-NC	4.33	115.43	110.57
22	B	844	BCR	C21-C20-C19	4.33	136.72	123.22
22	B	801	BCR	C8-C9-C10	4.32	125.57	118.94
19	2	617	XAT	C39-C29-C30	-4.32	116.87	122.92
22	B	846	BCR	C34-C9-C10	-4.32	116.88	122.92
22	G	204	BCR	C15-C16-C17	4.32	132.31	123.47
17	2	606	CHL	C3D-C2D-C1D	-4.31	99.95	105.83
22	K	205	BCR	C34-C9-C10	-4.30	116.90	122.92
21	1	616	LUT	C19-C9-C10	-4.30	116.90	122.92
18	A	805	CLA	CMB-C2B-C1B	-4.29	121.87	128.46
18	A	828	CLA	CMB-C2B-C1B	-4.29	121.88	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	849	BCR	C30-C25-C26	-4.28	116.58	122.61
22	L	306	BCR	C23-C22-C21	4.26	125.48	118.94
22	B	844	BCR	C15-C16-C17	4.26	132.20	123.47
19	4	617	XAT	O4-C5-C6	-4.26	55.43	58.96
22	F	304	BCR	C34-C9-C10	-4.26	116.96	122.92
18	A	825	CLA	CMB-C2B-C1B	-4.25	121.93	128.46
17	4	605	CHL	C1B-CHB-C4A	-4.24	121.72	130.12
27	B	850	DGD	O2G-C1B-C2B	4.24	120.64	111.50
21	1	616	LUT	C32-C33-C34	4.24	125.45	118.94
22	A	850	BCR	C34-C9-C10	-4.24	116.99	122.92
21	1	616	LUT	C39-C29-C28	4.23	124.75	118.08
18	B	804	CLA	CMB-C2B-C1B	-4.22	121.98	128.46
17	4	606	CHL	C3D-C2D-C1D	-4.21	100.08	105.83
18	A	830	CLA	CMB-C2B-C1B	-4.21	121.99	128.46
19	2	617	XAT	C28-C29-C30	4.21	125.40	118.94
22	L	305	BCR	C37-C22-C21	-4.21	117.03	122.92
22	B	844	BCR	C23-C22-C21	4.21	125.40	118.94
17	1	606	CHL	C3D-C2D-C1D	-4.21	100.09	105.83
22	A	848	BCR	C15-C16-C17	4.21	132.09	123.47
17	4	607	CHL	CHD-C4C-C3C	-4.21	118.66	124.84
22	B	844	BCR	C34-C9-C10	-4.20	117.03	122.92
18	B	826	CLA	CMB-C2B-C1B	-4.20	122.02	128.46
22	G	204	BCR	C37-C22-C21	-4.19	117.06	122.92
22	3	614	BCR	C34-C9-C10	-4.18	117.07	122.92
18	A	815	CLA	CMB-C2B-C1B	-4.18	122.04	128.46
18	A	802	CLA	CMB-C2B-C1B	-4.17	122.05	128.46
21	3	613	LUT	C28-C29-C30	4.17	125.35	118.94
22	K	202	BCR	C34-C9-C10	-4.17	117.08	122.92
17	2	605	CHL	C1B-CHB-C4A	-4.17	121.87	130.12
18	A	839	CLA	CMB-C2B-C1B	-4.16	122.07	128.46
22	L	301	BCR	C12-C13-C14	4.16	125.32	118.94
21	2	619	LUT	C39-C29-C30	-4.15	117.10	122.92
18	A	811	CLA	CMB-C2B-C1B	-4.15	122.08	128.46
18	B	825	CLA	CMB-C2B-C1B	-4.13	122.11	128.46
22	L	305	BCR	C16-C15-C14	4.13	131.94	123.47
18	A	831	CLA	CMB-C2B-C1B	-4.13	122.11	128.46
22	G	204	BCR	C34-C9-C10	-4.13	117.14	122.92
19	2	617	XAT	C19-C9-C10	-4.12	117.15	122.92
18	A	806	CLA	CMB-C2B-C1B	-4.12	122.13	128.46
22	J	102	BCR	C37-C22-C21	-4.12	117.15	122.92
22	L	301	BCR	C36-C18-C17	-4.12	117.15	122.92
22	4	618	BCR	C37-C22-C21	-4.11	117.17	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	L	306	BCR	C16-C15-C14	4.10	131.87	123.47
22	B	845	BCR	C1-C6-C5	-4.09	116.85	122.61
18	4	602	CLA	CMB-C2B-C1B	-4.09	122.18	128.46
22	A	848	BCR	C37-C22-C21	-4.08	117.20	122.92
22	L	301	BCR	C34-C9-C10	-4.08	117.20	122.92
17	4	607	CHL	C2D-C1D-ND	4.08	113.11	110.10
22	A	848	BCR	C34-C9-C10	-4.08	117.21	122.92
22	B	847	BCR	C34-C9-C10	-4.08	117.21	122.92
22	K	205	BCR	C19-C18-C17	4.07	125.19	118.94
22	B	849	BCR	C1-C6-C5	-4.06	116.89	122.61
22	B	844	BCR	C16-C15-C14	4.06	131.80	123.47
22	A	853	BCR	C37-C22-C21	-4.06	117.23	122.92
22	I	101	BCR	C34-C9-C10	-4.06	117.24	122.92
18	B	837	CLA	CMB-C2B-C1B	-4.06	122.23	128.46
18	B	824	CLA	CMB-C2B-C1B	-4.05	122.24	128.46
22	I	101	BCR	C15-C16-C17	4.05	131.77	123.47
18	2	602	CLA	CMB-C2B-C1B	-4.05	122.24	128.46
18	2	609	CLA	CMB-C2B-C1B	-4.05	122.24	128.46
18	A	809	CLA	CMB-C2B-C1B	-4.05	122.24	128.46
18	A	833	CLA	CMB-C2B-C1B	-4.04	122.25	128.46
22	F	304	BCR	C16-C15-C14	4.04	131.75	123.47
22	B	845	BCR	C34-C9-C10	-4.04	117.26	122.92
22	B	801	BCR	C37-C22-C21	-4.03	117.28	122.92
22	K	202	BCR	C12-C13-C14	4.02	125.12	118.94
21	1	616	LUT	C40-C33-C34	-4.02	117.29	122.92
18	A	822	CLA	CMB-C2B-C1B	-4.01	122.29	128.46
22	F	304	BCR	C12-C13-C14	4.01	125.09	118.94
22	A	849	BCR	C21-C20-C19	4.00	135.72	123.22
19	1	614	XAT	C38-C25-C24	3.99	118.77	114.28
22	L	301	BCR	C35-C13-C14	-3.98	117.34	122.92
21	4	616	LUT	C15-C35-C34	3.98	131.63	123.47
22	B	848	BCR	C15-C16-C17	3.98	131.63	123.47
21	2	616	LUT	C28-C29-C30	3.98	125.05	118.94
22	A	849	BCR	C34-C9-C10	-3.98	117.35	122.92
18	A	823	CLA	CMB-C2B-C1B	-3.98	122.35	128.46
22	K	205	BCR	C36-C18-C17	-3.97	117.36	122.92
22	I	101	BCR	C37-C22-C21	-3.97	117.36	122.92
18	A	827	CLA	CMB-C2B-C1B	-3.97	122.36	128.46
22	L	305	BCR	C34-C9-C10	-3.97	117.36	122.92
22	B	843	BCR	C37-C22-C21	-3.96	117.38	122.92
22	A	852	BCR	C19-C18-C17	3.95	125.00	118.94
18	2	612	CLA	CMB-C2B-C1B	-3.95	122.40	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	844	BCR	C36-C18-C17	-3.94	117.40	122.92
22	B	849	BCR	C34-C9-C10	-3.94	117.40	122.92
18	B	822	CLA	CMB-C2B-C1B	-3.93	122.42	128.46
18	A	808	CLA	CMB-C2B-C1B	-3.93	122.42	128.46
22	A	850	BCR	C37-C22-C21	-3.93	117.42	122.92
22	A	851	BCR	C12-C13-C14	3.93	124.97	118.94
21	1	616	LUT	C31-C30-C29	3.93	132.91	127.31
18	A	812	CLA	CMB-C2B-C1B	-3.93	122.43	128.46
17	4	607	CHL	CAC-C3C-C4C	3.93	129.90	124.81
22	B	849	BCR	C16-C15-C14	3.92	131.51	123.47
21	4	616	LUT	C19-C9-C10	-3.92	117.43	122.92
22	B	847	BCR	C37-C22-C21	-3.92	117.43	122.92
18	B	831	CLA	CMB-C2B-C1B	-3.92	122.44	128.46
22	A	852	BCR	C35-C13-C14	-3.92	117.44	122.92
21	1	616	LUT	C1-C6-C5	-3.91	117.10	122.61
18	2	611	CLA	CMB-C2B-C1B	-3.91	122.45	128.46
22	B	845	BCR	C20-C21-C22	3.91	132.89	127.31
22	4	618	BCR	C34-C9-C10	-3.90	117.45	122.92
22	K	202	BCR	C35-C13-C14	-3.90	117.45	122.92
18	1	603	CLA	CMB-C2B-C1B	-3.90	122.47	128.46
22	B	848	BCR	C34-C9-C10	-3.90	117.46	122.92
22	3	614	BCR	C37-C22-C21	-3.89	117.47	122.92
22	B	848	BCR	C37-C22-C21	-3.89	117.48	122.92
18	A	830	CLA	CAA-C2A-C3A	-3.88	102.16	112.78
17	3	606	CHL	C4C-C3C-C2C	-3.87	101.25	106.90
21	2	619	LUT	C32-C33-C34	3.87	124.88	118.94
22	B	846	BCR	C37-C22-C21	-3.87	117.50	122.92
20	1	615	LHG	O7-C7-C8	3.87	119.84	111.50
17	4	615	CHL	CHD-C4C-C3C	-3.87	119.15	124.84
21	4	616	LUT	C39-C29-C30	-3.87	117.51	122.92
22	J	102	BCR	C8-C9-C10	3.86	124.86	118.94
18	1	604	CLA	CMB-C2B-C1B	-3.86	122.53	128.46
22	B	843	BCR	C8-C9-C10	3.85	124.85	118.94
22	F	304	BCR	C35-C13-C14	-3.85	117.53	122.92
22	L	306	BCR	C12-C13-C14	3.85	124.85	118.94
17	4	606	CHL	C4C-C3C-C2C	-3.85	101.29	106.90
18	B	829	CLA	CMB-C2B-C1B	-3.85	122.55	128.46
21	2	619	LUT	C40-C33-C34	-3.84	117.54	122.92
18	2	610	CLA	CAB-C3B-C4B	-3.84	122.56	128.46
22	L	306	BCR	C35-C13-C14	-3.84	117.55	122.92
22	A	852	BCR	C36-C18-C17	-3.84	117.55	122.92
22	A	852	BCR	C34-C9-C10	-3.83	117.55	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	L	306	BCR	C15-C16-C17	3.83	131.32	123.47
17	4	607	CHL	C1D-ND-C4D	-3.83	103.61	106.33
17	4	607	CHL	C3B-C4B-NB	3.83	114.16	109.21
18	1	613	CLA	CAB-C3B-C4B	-3.82	122.60	128.46
18	F	302	CLA	CMB-C2B-C1B	-3.82	122.60	128.46
18	B	815	CLA	CMB-C2B-C1B	-3.82	122.60	128.46
18	2	608	CLA	CMB-C2B-C1B	-3.81	122.61	128.46
18	1	608	CLA	CAB-C3B-C4B	-3.81	122.61	128.46
22	A	852	BCR	C10-C11-C12	3.81	135.09	123.22
18	B	841	CLA	CMB-C2B-C1B	-3.80	122.63	128.46
19	4	617	XAT	C12-C13-C14	3.80	124.77	118.94
18	B	814	CLA	CMB-C2B-C1B	-3.79	122.63	128.46
22	J	102	BCR	C35-C13-C14	-3.79	117.61	122.92
18	3	603	CLA	CMB-C2B-C1B	-3.79	122.64	128.46
22	F	304	BCR	C20-C21-C22	3.79	132.72	127.31
22	J	102	BCR	C12-C13-C14	3.78	124.75	118.94
22	B	849	BCR	C37-C22-C21	-3.78	117.62	122.92
22	B	845	BCR	C12-C13-C14	3.77	124.72	118.94
22	B	849	BCR	C15-C16-C17	3.77	131.19	123.47
18	A	842	CLA	CMB-C2B-C3B	3.77	131.72	124.68
22	L	301	BCR	C21-C20-C19	3.76	134.97	123.22
17	4	606	CHL	C3C-C4C-NC	3.75	114.77	110.57
18	B	827	CLA	CMB-C2B-C1B	-3.75	122.71	128.46
22	A	853	BCR	C35-C13-C14	-3.74	117.68	122.92
18	A	841	CLA	CMB-C2B-C1B	-3.74	122.72	128.46
17	2	607	CHL	CHD-C4C-C3C	-3.74	119.35	124.84
18	B	821	CLA	CMB-C2B-C1B	-3.73	122.73	128.46
18	3	612	CLA	CMB-C2B-C1B	-3.72	122.75	128.46
22	A	853	BCR	C12-C13-C14	3.72	124.65	118.94
22	B	844	BCR	C30-C25-C26	-3.71	117.38	122.61
17	1	606	CHL	CAC-C3C-C4C	3.71	129.62	124.81
18	A	826	CLA	CMB-C2B-C3B	3.71	131.61	124.68
18	1	609	CLA	CMB-C2B-C1B	-3.70	122.77	128.46
22	B	801	BCR	C7-C8-C9	-3.70	120.64	126.23
22	4	618	BCR	C30-C25-C26	-3.69	117.41	122.61
22	3	614	BCR	C16-C15-C14	3.69	131.04	123.47
18	G	203	CLA	CMB-C2B-C1B	-3.69	122.79	128.46
22	K	202	BCR	C19-C18-C17	3.69	124.61	118.94
22	B	801	BCR	C10-C11-C12	3.69	134.74	123.22
18	A	820	CLA	CMB-C2B-C3B	3.69	131.58	124.68
22	L	305	BCR	C36-C18-C17	-3.69	117.76	122.92
18	A	816	CLA	CMB-C2B-C1B	-3.68	122.81	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	K	202	BCR	C36-C18-C17	-3.68	117.77	122.92
17	2	601	CHL	CAC-C3C-C4C	3.67	129.58	124.81
18	K	203	CLA	CMB-C2B-C1B	-3.67	122.82	128.46
18	B	820	CLA	CMB-C2B-C3B	3.67	131.54	124.68
17	4	606	CHL	CAC-C3C-C4C	3.67	129.57	124.81
22	L	305	BCR	C15-C16-C17	3.66	130.98	123.47
18	B	813	CLA	O2D-CGD-O1D	-3.66	116.68	123.84
18	4	612	CLA	CMB-C2B-C1B	-3.66	122.84	128.46
18	L	303	CLA	O2D-CGD-O1D	-3.66	116.69	123.84
22	B	845	BCR	C35-C13-C14	-3.66	117.80	122.92
18	4	603	CLA	CAB-C3B-C4B	-3.66	122.84	128.46
22	B	846	BCR	C35-C13-C14	-3.66	117.80	122.92
18	3	608	CLA	CMB-C2B-C1B	-3.65	122.86	128.46
22	F	304	BCR	C10-C11-C12	3.64	134.57	123.22
18	1	610	CLA	CAB-C3B-C4B	-3.64	122.88	128.46
17	3	606	CHL	CAC-C3C-C4C	3.63	129.53	124.81
24	A	801	CL0	C4C-C3C-C2C	-3.63	101.61	106.90
18	1	612	CLA	CMB-C2B-C1B	-3.63	122.88	128.46
17	1	601	CHL	C1B-CHB-C4A	-3.63	122.93	130.12
18	B	818	CLA	CMB-C2B-C3B	3.63	131.47	124.68
22	A	853	BCR	C11-C10-C9	3.62	132.48	127.31
18	3	601	CLA	CMB-C2B-C1B	-3.62	122.90	128.46
18	A	836	CLA	CMB-C2B-C1B	-3.62	122.90	128.46
18	B	816	CLA	CMB-C2B-C1B	-3.62	122.90	128.46
22	A	853	BCR	C10-C11-C12	3.61	134.48	123.22
22	L	306	BCR	C7-C8-C9	3.61	131.68	126.23
17	4	615	CHL	C2D-C1D-ND	3.61	112.76	110.10
17	1	606	CHL	C3C-C4C-NC	3.61	114.61	110.57
22	F	304	BCR	C21-C20-C19	3.60	134.46	123.22
18	1	605	CLA	CMB-C2B-C1B	-3.60	122.93	128.46
18	2	603	CLA	CMB-C2B-C1B	-3.60	122.93	128.46
18	4	609	CLA	CMB-C2B-C1B	-3.59	122.94	128.46
18	A	828	CLA	CMB-C2B-C3B	3.59	131.39	124.68
18	L	303	CLA	CMB-C2B-C1B	-3.59	122.95	128.46
18	B	839	CLA	CMB-C2B-C1B	-3.58	122.95	128.46
18	B	828	CLA	CMB-C2B-C1B	-3.58	122.96	128.46
22	B	846	BCR	C12-C13-C14	3.58	124.43	118.94
18	A	843	CLA	CMB-C2B-C1B	-3.57	122.97	128.46
21	1	616	LUT	C20-C13-C14	-3.57	117.92	122.92
18	B	803	CLA	CMB-C2B-C1B	-3.57	122.98	128.46
18	A	805	CLA	CMB-C2B-C3B	3.57	131.35	124.68
18	A	802	CLA	CMB-C2B-C3B	3.57	131.35	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	801	BCR	C35-C13-C14	-3.57	117.93	122.92
18	B	806	CLA	CMB-C2B-C1B	-3.56	122.98	128.46
18	1	602	CLA	CMB-C2B-C1B	-3.56	123.00	128.46
22	L	301	BCR	C19-C18-C17	3.56	124.40	118.94
17	3	606	CHL	CHD-C4C-C3C	-3.55	119.61	124.84
18	1	607	CLA	CMB-C2B-C1B	-3.55	123.00	128.46
18	B	833	CLA	CMB-C2B-C1B	-3.55	123.01	128.46
22	L	305	BCR	C19-C18-C17	3.55	124.38	118.94
18	A	810	CLA	CMB-C2B-C1B	-3.54	123.02	128.46
18	B	830	CLA	CMB-C2B-C1B	-3.54	123.02	128.46
18	1	611	CLA	CMB-C2B-C1B	-3.54	123.02	128.46
17	3	606	CHL	C3B-C4B-NB	3.54	113.78	109.21
18	A	830	CLA	CMB-C2B-C3B	3.54	131.30	124.68
17	1	601	CHL	C1-C2-C3	-3.54	119.93	126.04
18	B	809	CLA	CMB-C2B-C3B	3.54	131.29	124.68
18	3	605	CLA	CAB-C3B-C4B	-3.54	123.03	128.46
22	L	306	BCR	C36-C18-C17	-3.53	117.97	122.92
18	A	844	CLA	CMB-C2B-C1B	-3.53	123.04	128.46
17	2	606	CHL	CAC-C3C-C4C	3.53	129.39	124.81
18	B	819	CLA	CMB-C2B-C1B	-3.53	123.04	128.46
18	3	609	CLA	CMB-C2B-C1B	-3.52	123.05	128.46
18	4	610	CLA	CMB-C2B-C1B	-3.52	123.05	128.46
18	A	818	CLA	CMB-C2B-C1B	-3.52	123.05	128.46
18	A	840	CLA	CMB-C2B-C1B	-3.52	123.05	128.46
17	2	607	CHL	CAC-C3C-C4C	3.52	129.38	124.81
18	B	804	CLA	CMB-C2B-C3B	3.52	131.26	124.68
18	B	817	CLA	CMB-C2B-C1B	-3.52	123.06	128.46
18	1	604	CLA	CAA-C2A-C3A	-3.52	103.15	112.78
21	2	619	LUT	C8-C9-C10	3.52	124.33	118.94
18	A	832	CLA	CMB-C2B-C1B	-3.51	123.07	128.46
19	2	617	XAT	C32-C33-C34	3.51	124.33	118.94
19	1	614	XAT	C31-C30-C29	-3.51	122.30	127.31
17	1	601	CHL	CAC-C3C-C4C	3.51	129.37	124.81
18	4	611	CLA	CMB-C2B-C1B	-3.51	123.07	128.46
18	A	811	CLA	CMB-C2B-C3B	3.51	131.25	124.68
22	L	305	BCR	C35-C13-C14	-3.51	118.01	122.92
18	B	813	CLA	CMB-C2B-C3B	3.51	131.24	124.68
17	2	605	CHL	CHD-C4C-C3C	-3.51	119.50	124.98
22	L	301	BCR	C23-C22-C21	3.51	124.32	118.94
21	1	616	LUT	C39-C29-C30	-3.50	118.02	122.92
18	B	836	CLA	O2D-CGD-O1D	-3.50	116.99	123.84
18	B	807	CLA	CMB-C2B-C1B	-3.50	123.09	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	F	301	CLA	CMB-C2B-C1B	-3.49	123.09	128.46
18	4	603	CLA	CMB-C2B-C1B	-3.49	123.09	128.46
18	A	814	CLA	CMB-C2B-C1B	-3.49	123.10	128.46
18	A	815	CLA	CMB-C2B-C3B	3.49	131.21	124.68
18	A	813	CLA	O2D-CGD-O1D	-3.49	117.02	123.84
18	3	604	CLA	CMB-C2B-C1B	-3.49	123.11	128.46
18	B	836	CLA	CMB-C2B-C1B	-3.49	123.11	128.46
21	1	616	LUT	C12-C13-C14	3.48	124.29	118.94
22	B	847	BCR	C35-C13-C14	-3.48	118.04	122.92
18	4	613	CLA	CMB-C2B-C1B	-3.48	123.11	128.46
18	4	608	CLA	CMB-C2B-C1B	-3.48	123.11	128.46
18	A	838	CLA	CMB-C2B-C1B	-3.48	123.12	128.46
18	B	826	CLA	CMB-C2B-C3B	3.48	131.18	124.68
18	A	839	CLA	CMB-C2B-C3B	3.47	131.17	124.68
17	3	606	CHL	C1B-CHB-C4A	-3.46	123.26	130.12
17	2	601	CHL	CHD-C4C-C3C	-3.46	119.75	124.84
21	3	613	LUT	C19-C9-C10	-3.46	118.08	122.92
24	A	801	CL0	CHC-C1C-C2C	-3.46	117.15	126.72
19	4	617	XAT	O24-C25-C24	3.46	115.98	113.38
18	A	825	CLA	CMB-C2B-C3B	3.46	131.15	124.68
18	B	825	CLA	CMB-C2B-C3B	3.46	131.15	124.68
18	4	604	CLA	CAB-C3B-C4B	-3.46	123.15	128.46
18	B	805	CLA	O2D-CGD-O1D	-3.46	117.08	123.84
18	A	835	CLA	O2D-CGD-O1D	-3.45	117.09	123.84
22	G	204	BCR	C30-C25-C26	-3.45	117.75	122.61
22	4	618	BCR	C35-C13-C14	-3.44	118.10	122.92
18	A	806	CLA	CMB-C2B-C3B	3.44	131.12	124.68
22	B	849	BCR	C36-C18-C17	-3.44	118.11	122.92
18	3	610	CLA	CMB-C2B-C1B	-3.43	123.19	128.46
18	2	602	CLA	CMB-C2B-C3B	3.43	131.10	124.68
18	L	302	CLA	CMB-C2B-C1B	-3.43	123.19	128.46
18	B	838	CLA	CMB-C2B-C1B	-3.42	123.20	128.46
18	A	819	CLA	CMB-C2B-C1B	-3.42	123.20	128.46
17	4	606	CHL	C2C-C1C-NC	3.42	113.18	109.97
18	B	802	CLA	CMB-C2B-C1B	-3.42	123.21	128.46
17	4	607	CHL	C3D-C4D-ND	3.42	115.76	110.24
18	4	601	CLA	CMB-C2B-C1B	-3.42	123.22	128.46
22	A	848	BCR	C36-C18-C17	-3.41	118.14	122.92
18	K	201	CLA	CMB-C2B-C1B	-3.41	123.22	128.46
18	A	804	CLA	O2D-CGD-O1D	-3.41	117.16	123.84
17	1	601	CHL	CHD-C4C-C3C	-3.41	119.82	124.84
18	2	609	CLA	CMB-C2B-C3B	3.41	131.06	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	849	BCR	C35-C13-C14	-3.41	118.15	122.92
22	K	205	BCR	C10-C11-C12	3.41	133.85	123.22
22	A	849	BCR	C20-C21-C22	3.41	132.17	127.31
18	A	804	CLA	CMB-C2B-C1B	-3.41	123.23	128.46
18	A	829	CLA	CMB-C2B-C1B	-3.41	123.23	128.46
18	B	837	CLA	O2D-CGD-O1D	-3.40	117.18	123.84
18	A	809	CLA	CMB-C2B-C3B	3.40	131.04	124.68
18	A	835	CLA	CMB-C2B-C1B	-3.40	123.24	128.46
17	1	601	CHL	C6-C5-C3	-3.40	109.06	114.62
18	B	811	CLA	CAB-C3B-C4B	-3.40	123.24	128.46
22	L	306	BCR	C10-C11-C12	3.40	133.82	123.22
22	B	801	BCR	C12-C13-C14	3.40	124.15	118.94
17	2	601	CHL	C1B-CHB-C4A	-3.40	123.39	130.12
18	1	613	CLA	CMB-C2B-C1B	-3.39	123.25	128.46
19	1	614	XAT	C35-C15-C14	-3.39	116.53	123.47
18	F	303	CLA	CMB-C2B-C1B	-3.39	123.25	128.46
18	A	803	CLA	CMB-C2B-C1B	-3.39	123.25	128.46
22	K	205	BCR	C35-C13-C14	-3.39	118.17	122.92
18	4	602	CLA	CMB-C2B-C3B	3.39	131.02	124.68
22	G	204	BCR	C36-C18-C17	-3.39	118.18	122.92
18	B	834	CLA	CMB-C2B-C1B	-3.39	123.26	128.46
22	B	846	BCR	C8-C9-C10	3.39	124.14	118.94
18	B	840	CLA	CMB-C2B-C1B	-3.38	123.27	128.46
18	A	817	CLA	CMB-C2B-C1B	-3.38	123.27	128.46
22	B	844	BCR	C35-C13-C14	-3.37	118.20	122.92
18	A	813	CLA	CMB-C2B-C1B	-3.37	123.29	128.46
18	G	201	CLA	CMB-C2B-C1B	-3.37	123.29	128.46
18	2	613	CLA	CMB-C2B-C1B	-3.37	123.29	128.46
18	B	824	CLA	CMB-C2B-C3B	3.36	130.97	124.68
18	K	204	CLA	CMB-C2B-C1B	-3.36	123.30	128.46
18	A	833	CLA	CMB-C2B-C3B	3.36	130.97	124.68
22	B	845	BCR	C16-C17-C18	3.36	132.10	127.31
22	L	306	BCR	C19-C18-C17	3.36	124.10	118.94
18	B	811	CLA	CMB-C2B-C1B	-3.36	123.30	128.46
17	2	607	CHL	C2D-C1D-ND	3.36	112.58	110.10
18	B	825	CLA	O2D-CGD-O1D	-3.36	117.28	123.84
18	A	824	CLA	CMB-C2B-C1B	-3.35	123.31	128.46
18	A	834	CLA	CMB-C2B-C1B	-3.35	123.31	128.46
18	B	837	CLA	CMB-C2B-C3B	3.35	130.95	124.68
17	1	601	CHL	C3D-C4D-ND	3.35	115.66	110.24
18	3	607	CLA	CMB-C2B-C1B	-3.35	123.32	128.46
18	A	837	CLA	CMB-C2B-C1B	-3.35	123.32	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	809	CLA	O2D-CGD-O1D	-3.35	117.29	123.84
18	A	828	CLA	O2D-CGD-O1D	-3.34	117.30	123.84
17	2	605	CHL	C2D-C1D-ND	3.34	112.57	110.10
18	2	604	CLA	CMB-C2B-C1B	-3.34	123.33	128.46
18	4	614	CLA	O2D-CGD-O1D	-3.34	117.31	123.84
18	A	831	CLA	CMB-C2B-C3B	3.34	130.92	124.68
18	3	605	CLA	CMB-C2B-C1B	-3.33	123.34	128.46
17	2	615	CHL	CAC-C3C-C4C	3.33	129.13	124.81
17	4	615	CHL	C3D-C4D-ND	3.33	115.63	110.24
24	A	801	CL0	CMB-C2B-C3B	3.33	130.91	124.68
18	A	821	CLA	CMB-C2B-C1B	-3.33	123.35	128.46
18	1	610	CLA	CMB-C2B-C1B	-3.32	123.35	128.46
18	L	302	CLA	O2D-CGD-O1D	-3.32	117.34	123.84
17	4	605	CHL	CHD-C4C-C3C	-3.32	119.79	124.98
18	A	807	CLA	CMB-C2B-C1B	-3.32	123.36	128.46
22	3	614	BCR	C35-C13-C14	-3.32	118.27	122.92
22	3	614	BCR	C15-C16-C17	3.32	130.28	123.47
18	A	815	CLA	O2D-CGD-O1D	-3.32	117.35	123.84
22	L	305	BCR	C12-C13-C14	3.32	124.03	118.94
18	B	818	CLA	O2D-CGD-O1D	-3.32	117.35	123.84
22	B	847	BCR	C12-C13-C14	3.31	124.03	118.94
18	A	819	CLA	O2D-CGD-O1D	-3.31	117.36	123.84
18	B	820	CLA	O2D-CGD-O1D	-3.31	117.36	123.84
18	B	838	CLA	O2D-CGD-O1D	-3.31	117.36	123.84
18	A	823	CLA	CMB-C2B-C3B	3.31	130.87	124.68
18	A	827	CLA	CMB-C2B-C3B	3.31	130.87	124.68
18	B	812	CLA	CMB-C2B-C1B	-3.31	123.38	128.46
22	F	304	BCR	C8-C9-C10	3.30	124.01	118.94
22	K	202	BCR	C23-C22-C21	3.30	124.01	118.94
18	G	202	CLA	CMB-C2B-C1B	-3.30	123.39	128.46
18	3	611	CLA	CMB-C2B-C1B	-3.30	123.39	128.46
17	2	601	CHL	C3D-C4D-ND	3.30	115.58	110.24
22	B	801	BCR	C34-C9-C10	-3.30	118.30	122.92
18	4	604	CLA	CMB-C2B-C1B	-3.29	123.41	128.46
18	A	808	CLA	CMB-C2B-C3B	3.29	130.83	124.68
18	B	835	CLA	CMB-C2B-C1B	-3.29	123.41	128.46
18	B	810	CLA	CMB-C2B-C1B	-3.29	123.41	128.46
22	A	853	BCR	C36-C18-C17	-3.29	118.32	122.92
18	1	608	CLA	CMB-C2B-C1B	-3.28	123.42	128.46
18	A	831	CLA	O2D-CGD-O1D	-3.28	117.42	123.84
18	A	840	CLA	O2D-CGD-O1D	-3.28	117.42	123.84
17	3	606	CHL	C2D-C1D-ND	3.28	112.52	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	2	601	CHL	C3B-C4B-NB	3.28	113.45	109.21
18	B	805	CLA	CMB-C2B-C1B	-3.28	123.42	128.46
22	A	851	BCR	C36-C18-C17	-3.28	118.33	122.92
22	A	851	BCR	C35-C13-C14	-3.27	118.34	122.92
18	3	605	CLA	O2D-CGD-O1D	-3.27	117.44	123.84
18	2	610	CLA	CMB-C2B-C1B	-3.27	123.44	128.46
21	4	616	LUT	C40-C33-C34	-3.27	118.34	122.92
22	A	852	BCR	C21-C20-C19	3.26	133.40	123.22
17	2	607	CHL	C1-C2-C3	-3.26	121.47	126.75
18	B	808	CLA	CMB-C2B-C1B	-3.26	123.45	128.46
18	1	604	CLA	CMB-C2B-C3B	3.26	130.78	124.68
22	4	618	BCR	C12-C13-C14	3.26	123.94	118.94
22	I	101	BCR	C36-C18-C17	-3.26	118.36	122.92
18	H	201	CLA	CMB-C2B-C1B	-3.26	123.46	128.46
18	F	302	CLA	CMB-C2B-C3B	3.26	130.77	124.68
18	A	832	CLA	O2D-CGD-O1D	-3.25	117.48	123.84
22	B	849	BCR	C19-C18-C17	3.25	123.93	118.94
22	F	304	BCR	C37-C22-C21	-3.25	118.37	122.92
22	K	205	BCR	C23-C22-C21	3.25	123.93	118.94
22	A	852	BCR	C1-C6-C5	-3.25	118.04	122.61
22	3	614	BCR	C36-C18-C17	-3.25	118.37	122.92
18	L	304	CLA	CMB-C2B-C1B	-3.25	123.47	128.46
21	2	616	LUT	C35-C34-C33	3.25	131.94	127.31
18	A	812	CLA	CMB-C2B-C3B	3.25	130.75	124.68
18	B	831	CLA	CMB-C2B-C3B	3.25	130.75	124.68
18	B	833	CLA	O2D-CGD-O1D	-3.24	117.50	123.84
18	A	820	CLA	O2D-CGD-O1D	-3.24	117.50	123.84
17	4	615	CHL	C1D-ND-C4D	-3.24	104.03	106.33
18	2	612	CLA	CMB-C2B-C3B	3.24	130.74	124.68
18	B	807	CLA	O2D-CGD-O1D	-3.24	117.51	123.84
18	B	832	CLA	CMB-C2B-C1B	-3.23	123.49	128.46
18	B	827	CLA	O2D-CGD-O1D	-3.23	117.52	123.84
18	4	601	CLA	O2D-CGD-O1D	-3.23	117.53	123.84
18	B	821	CLA	CAA-C2A-C3A	-3.23	103.95	112.78
17	2	607	CHL	C3D-C4D-ND	3.23	115.45	110.24
18	B	808	CLA	O2D-CGD-O1D	-3.22	117.54	123.84
18	B	841	CLA	O2D-CGD-O1D	-3.22	117.54	123.84
17	4	605	CHL	C2D-C1D-ND	3.22	112.48	110.10
21	2	616	LUT	C20-C13-C14	-3.22	118.42	122.92
18	B	814	CLA	CMB-C2B-C3B	3.22	130.69	124.68
17	2	606	CHL	C3D-C4D-ND	3.21	115.44	110.24
18	B	823	CLA	CMB-C2B-C1B	-3.21	123.53	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	852	BCR	C15-C16-C17	3.21	130.05	123.47
22	A	851	BCR	C15-C16-C17	3.21	130.05	123.47
18	2	611	CLA	CMB-C2B-C3B	3.21	130.68	124.68
22	B	843	BCR	C15-C14-C13	3.21	131.89	127.31
18	1	603	CLA	CMB-C2B-C3B	3.21	130.68	124.68
22	B	844	BCR	C8-C9-C10	3.21	123.86	118.94
24	A	801	CL0	C1-C2-C3	-3.20	120.50	126.04
22	B	848	BCR	C36-C18-C17	-3.20	118.44	122.92
18	A	822	CLA	CMB-C2B-C3B	3.20	130.67	124.68
18	4	602	CLA	O2D-CGD-O1D	-3.20	117.58	123.84
17	2	607	CHL	C3B-C4B-NB	3.20	113.34	109.21
21	1	616	LUT	C8-C9-C10	3.19	123.84	118.94
17	4	605	CHL	C3B-C4B-NB	3.19	113.34	109.21
18	B	822	CLA	CMB-C2B-C3B	3.19	130.65	124.68
18	4	614	CLA	CMB-C2B-C1B	-3.19	123.56	128.46
17	2	615	CHL	CHD-C4C-C3C	-3.19	120.16	124.84
22	A	850	BCR	C15-C14-C13	3.18	131.85	127.31
22	A	848	BCR	C35-C13-C14	-3.18	118.47	122.92
22	B	801	BCR	C36-C18-C17	-3.18	118.47	122.92
17	4	615	CHL	CAC-C3C-C4C	3.18	128.93	124.81
17	4	615	CHL	C1B-CHB-C4A	-3.18	123.83	130.12
18	1	612	CLA	O2D-CGD-O1D	-3.17	117.63	123.84
18	B	819	CLA	O2D-CGD-O1D	-3.17	117.63	123.84
17	1	601	CHL	C3B-C4B-NB	3.17	113.31	109.21
21	1	616	LUT	C35-C15-C14	3.17	129.97	123.47
18	A	841	CLA	CMB-C2B-C3B	3.17	130.61	124.68
21	2	616	LUT	C30-C31-C32	3.17	133.11	123.22
18	A	806	CLA	O2D-CGD-O1D	-3.17	117.64	123.84
18	4	613	CLA	O2D-CGD-O1D	-3.17	117.65	123.84
22	K	202	BCR	C8-C9-C10	3.17	123.80	118.94
17	4	605	CHL	C3D-C4D-ND	3.16	115.36	110.24
18	2	608	CLA	CMB-C2B-C3B	3.16	130.59	124.68
18	B	818	CLA	C1-C2-C3	-3.16	120.58	126.04
21	2	616	LUT	C19-C9-C8	3.16	123.06	118.08
22	A	848	BCR	C19-C18-C17	3.16	123.79	118.94
22	A	849	BCR	C37-C22-C21	-3.16	118.50	122.92
17	3	606	CHL	C3D-C4D-ND	3.15	115.33	110.24
18	B	822	CLA	O2D-CGD-O1D	-3.15	117.68	123.84
18	B	821	CLA	CMB-C2B-C3B	3.15	130.56	124.68
18	B	816	CLA	CMB-C2B-C3B	3.14	130.56	124.68
22	A	848	BCR	C16-C15-C14	3.14	129.91	123.47
22	4	618	BCR	C36-C18-C17	-3.14	118.53	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	G	204	BCR	C19-C18-C17	3.14	123.75	118.94
18	A	826	CLA	O2D-CGD-O1D	-3.14	117.71	123.84
18	A	814	CLA	O2D-CGD-O1D	-3.14	117.71	123.84
18	3	602	CLA	CMB-C2B-C1B	-3.14	123.64	128.46
22	B	849	BCR	C12-C13-C14	3.13	123.75	118.94
18	B	841	CLA	CMB-C2B-C3B	3.13	130.54	124.68
18	3	612	CLA	CMB-C2B-C3B	3.13	130.54	124.68
18	2	613	CLA	O2D-CGD-O1D	-3.13	117.72	123.84
17	1	601	CHL	C2D-C1D-ND	3.12	112.41	110.10
22	A	850	BCR	C16-C17-C18	3.12	131.77	127.31
18	A	837	CLA	O2D-CGD-O1D	-3.12	117.74	123.84
17	2	601	CHL	C2D-C1D-ND	3.12	112.40	110.10
18	B	829	CLA	O2D-CGD-O1D	-3.12	117.75	123.84
18	B	815	CLA	CMB-C2B-C3B	3.11	130.50	124.68
18	B	812	CLA	O2D-CGD-O1D	-3.11	117.76	123.84
18	3	603	CLA	CMB-C2B-C3B	3.11	130.49	124.68
18	B	803	CLA	CMB-C2B-C3B	3.11	130.49	124.68
18	A	811	CLA	O2D-CGD-O1D	-3.10	117.77	123.84
19	1	614	XAT	C15-C14-C13	-3.10	122.89	127.31
18	B	840	CLA	O2D-CGD-O1D	-3.10	117.78	123.84
18	A	842	CLA	O2D-CGD-O1D	-3.10	117.78	123.84
18	4	612	CLA	O2D-CGD-O1D	-3.09	117.79	123.84
18	2	604	CLA	CMB-C2B-C3B	3.09	130.46	124.68
18	A	833	CLA	O2D-CGD-O1D	-3.09	117.80	123.84
18	K	203	CLA	CMB-C2B-C3B	3.09	130.46	124.68
18	A	817	CLA	O2D-CGD-O1D	-3.09	117.80	123.84
18	B	816	CLA	O2D-CGD-O1D	-3.09	117.80	123.84
18	4	609	CLA	CMB-C2B-C3B	3.09	130.46	124.68
18	B	827	CLA	CMB-C2B-C3B	3.09	130.46	124.68
18	G	203	CLA	CMB-C2B-C3B	3.09	130.46	124.68
22	J	102	BCR	C36-C18-C17	-3.09	118.60	122.92
18	A	816	CLA	CMB-C2B-C3B	3.09	130.45	124.68
18	B	810	CLA	O2D-CGD-O1D	-3.08	117.81	123.84
24	A	801	CL0	O2A-CGA-CBA	3.08	121.58	111.91
21	3	613	LUT	C20-C13-C14	-3.08	118.61	122.92
18	A	805	CLA	O2D-CGD-O1D	-3.08	117.81	123.84
17	4	606	CHL	C3D-C4D-ND	3.08	115.22	110.24
19	2	617	XAT	C40-C33-C34	-3.08	118.61	122.92
18	3	608	CLA	CMB-C2B-C3B	3.08	130.44	124.68
18	B	811	CLA	O2D-CGD-O1D	-3.08	117.82	123.84
17	2	605	CHL	C3D-C4D-ND	3.07	115.20	110.24
22	G	204	BCR	C35-C13-C14	-3.07	118.62	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	808	CLA	O2D-CGD-O1D	-3.07	117.84	123.84
18	3	608	CLA	CAA-C2A-C3A	-3.06	108.95	116.10
18	B	839	CLA	O2D-CGD-O1D	-3.06	117.85	123.84
21	3	613	LUT	C8-C9-C10	3.06	123.64	118.94
18	4	612	CLA	CMB-C2B-C3B	3.06	130.40	124.68
18	A	834	CLA	O2D-CGD-O1D	-3.06	117.86	123.84
17	2	606	CHL	CHD-C4C-C3C	-3.05	120.36	124.84
17	2	615	CHL	C3D-C4D-ND	3.05	115.17	110.24
19	2	617	XAT	C20-C13-C14	-3.05	118.65	122.92
18	A	821	CLA	O2D-CGD-O1D	-3.05	117.88	123.84
22	B	844	BCR	C12-C13-C14	3.05	123.62	118.94
22	B	846	BCR	C36-C18-C17	-3.04	118.66	122.92
18	A	802	CLA	CHB-C4A-NA	3.04	128.72	124.51
18	B	829	CLA	CMB-C2B-C3B	3.04	130.37	124.68
17	2	607	CHL	C1B-CHB-C4A	-3.04	124.09	130.12
22	I	101	BCR	C35-C13-C14	-3.04	118.67	122.92
18	A	804	CLA	CHB-C4A-NA	3.04	128.72	124.51
22	A	852	BCR	C12-C13-C14	3.04	123.60	118.94
18	2	603	CLA	CMB-C2B-C3B	3.04	130.36	124.68
18	B	815	CLA	O2D-CGD-O1D	-3.03	117.91	123.84
18	B	802	CLA	O2D-CGD-O1D	-3.03	117.91	123.84
18	B	814	CLA	O2D-CGD-O1D	-3.03	117.92	123.84
24	A	801	CL0	CAC-C3C-C4C	3.03	128.74	124.81
18	L	303	CLA	CMB-C2B-C3B	3.03	130.34	124.68
18	1	605	CLA	CMB-C2B-C3B	3.02	130.33	124.68
18	A	843	CLA	CMB-C2B-C3B	3.02	130.33	124.68
17	2	615	CHL	C3B-C4B-NB	3.02	113.11	109.21
18	B	821	CLA	O2D-CGD-O1D	-3.02	117.93	123.84
18	3	601	CLA	CMB-C2B-C3B	3.02	130.33	124.68
18	A	825	CLA	O2D-CGD-O1D	-3.02	117.93	123.84
17	2	606	CHL	C3B-C4B-NB	3.02	113.11	109.21
22	A	849	BCR	C16-C17-C18	3.02	131.62	127.31
18	B	803	CLA	O2D-CGD-O1D	-3.02	117.94	123.84
17	2	605	CHL	C3B-C4B-NB	3.01	113.11	109.21
18	A	818	CLA	CMB-C2B-C3B	3.01	130.31	124.68
18	B	830	CLA	O2D-CGD-O1D	-3.01	117.95	123.84
18	A	838	CLA	O2D-CGD-O1D	-3.01	117.96	123.84
18	B	813	CLA	O2D-CGD-CBD	3.01	116.61	111.27
18	1	609	CLA	CMB-C2B-C3B	3.01	130.30	124.68
18	B	826	CLA	O2D-CGD-O1D	-3.01	117.96	123.84
18	B	804	CLA	O2D-CGD-O1D	-3.00	117.97	123.84
18	A	830	CLA	CHB-C4A-NA	3.00	128.66	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	1	602	CLA	CMB-C2B-C3B	3.00	130.28	124.68
21	3	613	LUT	C30-C31-C32	2.99	132.56	123.22
18	1	602	CLA	O2D-CGD-O1D	-2.99	117.98	123.84
21	4	616	LUT	C20-C13-C14	-2.99	118.73	122.92
22	A	849	BCR	C35-C13-C14	-2.99	118.74	122.92
18	B	832	CLA	O2D-CGD-O1D	-2.99	118.00	123.84
18	G	203	CLA	O2D-CGD-O1D	-2.98	118.01	123.84
18	1	604	CLA	O2D-CGD-O1D	-2.98	118.01	123.84
22	B	848	BCR	C35-C13-C14	-2.98	118.75	122.92
18	2	612	CLA	O2D-CGD-O1D	-2.98	118.02	123.84
22	B	844	BCR	C19-C18-C17	2.98	123.51	118.94
18	1	605	CLA	O2D-CGD-O1D	-2.98	118.02	123.84
18	B	817	CLA	CMB-C2B-C3B	2.98	130.25	124.68
22	A	853	BCR	C19-C18-C17	2.97	123.50	118.94
18	2	602	CLA	O2D-CGD-O1D	-2.97	118.03	123.84
18	K	203	CLA	O2D-CGD-O1D	-2.97	118.04	123.84
22	B	847	BCR	C36-C18-C17	-2.97	118.77	122.92
18	B	809	CLA	O2D-CGD-O1D	-2.96	118.04	123.84
17	1	606	CHL	C3D-C4D-ND	2.96	115.03	110.24
18	A	823	CLA	O2D-CGD-O1D	-2.96	118.05	123.84
18	B	824	CLA	O2D-CGD-O1D	-2.96	118.06	123.84
22	A	853	BCR	C34-C9-C10	-2.96	118.78	122.92
18	A	830	CLA	O2D-CGD-O1D	-2.96	118.06	123.84
18	A	841	CLA	O2D-CGD-O1D	-2.96	118.06	123.84
18	B	839	CLA	CMB-C2B-C3B	2.96	130.21	124.68
21	4	616	LUT	C35-C15-C14	2.95	129.53	123.47
18	A	810	CLA	O2D-CGD-O1D	-2.95	118.07	123.84
18	A	803	CLA	CMB-C2B-C3B	2.95	130.19	124.68
18	A	827	CLA	O2D-CGD-O1D	-2.94	118.08	123.84
27	B	850	DGD	C2G-O2G-C1B	-2.94	110.55	117.79
18	1	609	CLA	CHB-C4A-NA	2.94	128.58	124.51
18	B	833	CLA	CMB-C2B-C3B	2.94	130.18	124.68
18	4	613	CLA	CMB-C2B-C3B	2.94	130.18	124.68
18	B	806	CLA	CMB-C2B-C3B	2.94	130.18	124.68
18	A	844	CLA	CMB-C2B-C3B	2.94	130.17	124.68
22	F	304	BCR	C16-C17-C18	2.93	131.50	127.31
18	1	612	CLA	CMB-C2B-C3B	2.93	130.16	124.68
17	2	607	CHL	O2A-CGA-CBA	2.93	121.10	111.91
17	2	605	CHL	CAC-C3C-C4C	2.93	129.50	125.04
18	A	829	CLA	CMB-C2B-C3B	2.93	130.16	124.68
18	B	804	CLA	CAA-C2A-C3A	-2.93	109.27	116.10
18	A	836	CLA	O2D-CGD-O1D	-2.92	118.12	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	801	BCR	C15-C16-C17	2.92	129.46	123.47
18	F	302	CLA	CHB-C4A-NA	2.92	128.55	124.51
22	A	853	BCR	C15-C16-C17	2.92	129.46	123.47
18	B	807	CLA	CMB-C2B-C3B	2.91	130.13	124.68
18	L	304	CLA	O2D-CGD-O1D	-2.91	118.14	123.84
18	3	601	CLA	O2D-CGD-O1D	-2.91	118.14	123.84
18	A	836	CLA	CMB-C2B-C3B	2.91	130.12	124.68
17	1	601	CHL	O2A-CGA-CBA	2.91	121.03	111.91
18	A	804	CLA	CMB-C2B-C3B	2.90	130.11	124.68
18	A	816	CLA	O2D-CGD-O1D	-2.90	118.16	123.84
22	3	614	BCR	C12-C13-C14	2.90	123.40	118.94
17	3	606	CHL	CMD-C2D-C3D	-2.90	120.94	127.61
18	G	201	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
24	A	801	CL0	C4-C3-C5	2.90	120.15	115.27
17	4	605	CHL	CMD-C2D-C3D	-2.90	120.94	127.61
18	B	830	CLA	CMB-C2B-C3B	2.90	130.10	124.68
18	A	802	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
18	A	807	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
18	F	301	CLA	CMB-C2B-C3B	2.89	130.09	124.68
18	B	803	CLA	CHB-C4A-NA	2.89	128.51	124.51
22	K	205	BCR	C16-C15-C14	2.89	129.40	123.47
18	3	609	CLA	CMB-C2B-C3B	2.89	130.08	124.68
18	4	610	CLA	CMB-C2B-C3B	2.89	130.08	124.68
18	3	608	CLA	O2D-CGD-O1D	-2.89	118.19	123.84
18	A	835	CLA	CMB-C2B-C3B	2.88	130.07	124.68
22	A	852	BCR	C24-C23-C22	2.88	130.59	126.23
21	3	613	LUT	C35-C15-C14	2.88	129.38	123.47
22	B	843	BCR	C36-C18-C17	-2.88	118.89	122.92
18	3	603	CLA	O2D-CGD-O1D	-2.88	118.21	123.84
18	1	611	CLA	CMB-C2B-C3B	2.88	130.06	124.68
18	A	832	CLA	CMB-C2B-C3B	2.88	130.06	124.68
17	2	607	CHL	CMD-C2D-C3D	-2.88	121.00	127.61
18	4	610	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
21	3	613	LUT	C32-C33-C34	2.87	123.35	118.94
18	A	810	CLA	CMB-C2B-C3B	2.87	130.05	124.68
17	2	607	CHL	C1D-ND-C4D	-2.87	104.30	106.33
17	3	606	CHL	C1D-ND-C4D	-2.87	104.30	106.33
18	B	828	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
18	A	812	CLA	O2D-CGD-O1D	-2.86	118.24	123.84
18	2	610	CLA	CAB-C3B-C2B	2.86	130.30	124.69
18	B	831	CLA	O2D-CGD-O1D	-2.86	118.24	123.84
18	B	808	CLA	CMB-C2B-C3B	2.86	130.03	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	1	601	CHL	CMD-C2D-C3D	-2.86	121.03	127.61
21	2	616	LUT	C12-C13-C14	2.86	123.33	118.94
18	4	611	CLA	CMB-C2B-C3B	2.86	130.03	124.68
18	2	604	CLA	CHB-C4A-NA	2.86	128.47	124.51
18	3	610	CLA	CMB-C2B-C3B	2.86	130.02	124.68
18	H	201	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
17	2	615	CHL	CMD-C2D-C3D	-2.86	121.05	127.61
18	A	822	CLA	O2D-CGD-O1D	-2.86	118.26	123.84
18	K	201	CLA	CMB-C2B-C3B	2.85	130.02	124.68
18	F	303	CLA	O2D-CGD-O1D	-2.85	118.26	123.84
18	A	843	CLA	O2D-CGD-O1D	-2.85	118.26	123.84
18	B	834	CLA	O2D-CGD-O1D	-2.85	118.26	123.84
18	1	613	CLA	CAB-C3B-C2B	2.85	130.27	124.69
17	1	601	CHL	C1D-ND-C4D	-2.85	104.31	106.33
17	2	615	CHL	C2D-C1D-ND	2.85	112.20	110.10
18	2	604	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
18	2	610	CLA	O2D-CGD-O1D	-2.85	118.28	123.84
18	L	303	CLA	O2D-CGD-CBD	2.84	116.31	111.27
18	1	608	CLA	CAB-C3B-C2B	2.84	130.25	124.69
22	B	801	BCR	C11-C10-C9	2.84	131.36	127.31
18	A	813	CLA	CHB-C4A-NA	2.84	128.44	124.51
22	K	205	BCR	C21-C20-C19	2.84	132.07	123.22
22	F	304	BCR	C1-C6-C5	-2.84	118.62	122.61
18	1	608	CLA	CAA-C2A-C3A	-2.84	109.48	116.10
18	4	603	CLA	CAB-C3B-C2B	2.83	130.24	124.69
18	B	836	CLA	CMB-C2B-C3B	2.83	129.98	124.68
18	A	829	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
17	4	606	CHL	CMD-C2D-C3D	-2.83	121.10	127.61
18	4	608	CLA	CMB-C2B-C3B	2.83	129.98	124.68
22	J	102	BCR	C10-C11-C12	2.83	132.06	123.22
24	A	801	CL0	C2A-C1A-CHA	-2.83	117.34	123.39
22	A	849	BCR	C36-C18-C17	-2.83	118.96	122.92
18	A	844	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
18	A	839	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
22	A	851	BCR	C19-C18-C17	2.82	123.28	118.94
18	3	608	CLA	CMA-C3A-C2A	-2.82	109.52	116.10
18	A	819	CLA	CMB-C2B-C3B	2.82	129.95	124.68
19	4	617	XAT	C20-C13-C14	-2.82	118.97	122.92
24	A	801	CL0	CMC-C2C-C1C	2.82	129.33	125.04
18	4	614	CLA	CHB-C4A-NA	2.82	128.41	124.51
17	1	606	CHL	CMD-C2D-C3D	-2.81	121.14	127.61
18	B	817	CLA	O2D-CGD-O1D	-2.81	118.34	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	1	607	CLA	CMB-C2B-C3B	2.81	129.94	124.68
18	2	608	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
17	2	601	CHL	CMD-C2D-C3D	-2.81	121.15	127.61
18	1	608	CLA	O2D-CGD-O1D	-2.81	118.35	123.84
18	2	610	CLA	C1A-CHA-C4D	-2.80	121.79	125.72
18	B	835	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
18	K	204	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
18	B	802	CLA	CMB-C2B-C3B	2.80	129.92	124.68
21	4	616	LUT	C32-C33-C34	2.80	123.24	118.94
18	4	604	CLA	O2D-CGD-O1D	-2.80	118.37	123.84
18	B	836	CLA	C1-C2-C3	-2.80	122.23	126.75
18	B	823	CLA	O2D-CGD-O1D	-2.80	118.37	123.84
22	I	101	BCR	C19-C18-C17	2.79	123.23	118.94
18	2	611	CLA	CHB-C4A-NA	2.79	128.37	124.51
18	A	803	CLA	O2D-CGD-O1D	-2.79	118.39	123.84
17	1	606	CHL	CHD-C1D-C2D	2.78	131.32	125.48
18	A	802	CLA	O2A-CGA-O1A	-2.78	116.57	123.59
18	F	303	CLA	CMB-C2B-C3B	2.78	129.88	124.68
22	B	848	BCR	C19-C18-C17	2.78	123.21	118.94
18	A	824	CLA	CAA-C2A-C3A	-2.78	109.61	116.10
18	A	838	CLA	CMB-C2B-C3B	2.78	129.88	124.68
18	F	301	CLA	O2D-CGD-O1D	-2.78	118.41	123.84
18	1	604	CLA	CBA-CAA-C2A	2.78	122.06	113.86
18	A	824	CLA	CMB-C2B-C3B	2.78	129.87	124.68
17	4	607	CHL	CMD-C2D-C3D	-2.78	121.23	127.61
19	1	614	XAT	O24-C25-C26	-2.78	56.66	58.96
18	B	819	CLA	CMB-C2B-C3B	2.77	129.87	124.68
17	2	606	CHL	C2D-C1D-ND	2.77	112.15	110.10
18	4	613	CLA	CHB-C4A-NA	2.77	128.34	124.51
17	4	615	CHL	CMD-C2D-C3D	-2.77	121.25	127.61
18	B	805	CLA	CHB-C4A-NA	2.76	128.33	124.51
22	3	614	BCR	C19-C18-C17	2.76	123.18	118.94
18	1	604	CLA	CHB-C4A-NA	2.76	128.33	124.51
18	1	603	CLA	O2D-CGD-O1D	-2.76	118.44	123.84
22	A	851	BCR	C20-C21-C22	2.76	131.25	127.31
18	A	813	CLA	O2D-CGD-CBD	2.76	116.17	111.27
21	2	619	LUT	C20-C13-C14	-2.76	119.06	122.92
21	3	613	LUT	C35-C34-C33	2.76	131.25	127.31
17	2	605	CHL	CMD-C2D-C3D	-2.76	121.27	127.61
18	G	202	CLA	O2D-CGD-O1D	-2.75	118.45	123.84
18	B	827	CLA	CHB-C4A-NA	2.75	128.32	124.51
18	3	604	CLA	CMB-C2B-C3B	2.75	129.83	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	B	806	CLA	O2D-CGD-O1D	-2.75	118.46	123.84
22	I	101	BCR	C16-C15-C14	2.75	129.10	123.47
22	A	848	BCR	C12-C13-C14	2.74	123.15	118.94
18	A	840	CLA	CMB-C2B-C3B	2.74	129.81	124.68
22	B	845	BCR	C21-C20-C19	2.74	131.78	123.22
22	A	850	BCR	C8-C9-C10	2.74	123.15	118.94
18	4	603	CLA	O2D-CGD-O1D	-2.74	118.48	123.84
18	4	601	CLA	CMB-C2B-C3B	2.74	129.80	124.68
17	1	601	CHL	CMB-C2B-C3B	2.74	129.80	124.68
19	2	617	XAT	C35-C34-C33	2.74	131.22	127.31
21	3	613	LUT	C40-C33-C34	-2.74	119.09	122.92
18	B	838	CLA	CMB-C2B-C3B	2.74	129.80	124.68
18	A	821	CLA	CMB-C2B-C3B	2.74	129.80	124.68
18	A	834	CLA	CMB-C2B-C3B	2.74	129.80	124.68
18	2	611	CLA	O2D-CGD-O1D	-2.74	118.49	123.84
21	2	619	LUT	C28-C29-C30	2.74	123.14	118.94
18	1	611	CLA	O2D-CGD-O1D	-2.73	118.50	123.84
18	B	818	CLA	CHB-C4A-NA	2.73	128.29	124.51
22	B	845	BCR	C16-C15-C14	2.73	129.07	123.47
18	2	609	CLA	CHB-C4A-NA	2.73	128.29	124.51
18	4	609	CLA	CHB-C4A-NA	2.73	128.29	124.51
18	A	814	CLA	CMB-C2B-C3B	2.73	129.78	124.68
18	3	602	CLA	O2D-CGD-O1D	-2.72	118.51	123.84
18	3	612	CLA	CAA-C2A-C3A	-2.72	109.74	116.10
18	3	610	CLA	CAA-C2A-C3A	-2.72	109.74	116.10
18	L	302	CLA	CMB-C2B-C3B	2.72	129.77	124.68
22	B	801	BCR	C19-C18-C17	2.72	123.12	118.94
18	3	611	CLA	CAA-C2A-C3A	-2.72	109.75	116.10
18	A	844	CLA	CHB-C4A-NA	2.72	128.27	124.51
22	B	843	BCR	C35-C13-C14	-2.72	119.11	122.92
18	B	817	CLA	CHB-C4A-NA	2.72	128.27	124.51
17	2	601	CHL	C1D-ND-C4D	-2.72	104.40	106.33
19	4	617	XAT	C30-C31-C32	-2.72	114.74	123.22
18	A	809	CLA	CHB-C4A-NA	2.71	128.26	124.51
18	K	204	CLA	CMB-C2B-C3B	2.71	129.75	124.68
19	2	617	XAT	C30-C31-C32	2.71	131.68	123.22
22	A	849	BCR	C19-C18-C17	2.71	123.10	118.94
18	2	609	CLA	O2D-CGD-O1D	-2.71	118.54	123.84
22	L	305	BCR	C23-C22-C21	2.71	123.09	118.94
17	4	607	CHL	CHB-C4A-NA	2.70	128.25	124.51
18	B	823	CLA	CMB-C2B-C3B	2.70	129.74	124.68
18	A	834	CLA	CHB-C4A-NA	2.70	128.25	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	810	CLA	CAA-C2A-C3A	-2.70	105.38	112.78
18	A	837	CLA	CMB-C2B-C3B	2.70	129.73	124.68
18	3	611	CLA	CMB-C2B-C3B	2.70	129.73	124.68
18	B	828	CLA	CHB-C4A-NA	2.70	128.25	124.51
18	3	612	CLA	O2D-CGD-O1D	-2.70	117.97	124.09
18	G	201	CLA	CMB-C2B-C3B	2.69	129.72	124.68
19	1	614	XAT	C5-C4-C3	-2.69	107.42	112.75
18	G	202	CLA	CMB-C2B-C3B	2.69	129.71	124.68
18	A	824	CLA	O2D-CGD-O1D	-2.68	118.59	123.84
17	4	605	CHL	C1D-ND-C4D	-2.68	104.43	106.33
17	2	606	CHL	CMD-C2D-C3D	-2.68	121.44	127.61
18	3	607	CLA	CMB-C2B-C3B	2.68	129.70	124.68
18	B	834	CLA	CMB-C2B-C3B	2.68	129.70	124.68
18	A	828	CLA	CHB-C4A-NA	2.68	128.22	124.51
19	2	617	XAT	C12-C13-C14	2.68	123.05	118.94
18	A	832	CLA	CHB-C4A-NA	2.68	128.22	124.51
18	A	835	CLA	CHB-C4A-NA	2.68	128.22	124.51
18	4	608	CLA	O2D-CGD-O1D	-2.68	118.60	123.84
18	2	613	CLA	CHB-C4A-NA	2.67	128.21	124.51
18	B	834	CLA	CHB-C4A-NA	2.67	128.21	124.51
18	A	807	CLA	CHB-C4A-NA	2.67	128.21	124.51
18	A	809	CLA	O2D-CGD-CBD	2.67	116.02	111.27
18	1	610	CLA	CAB-C3B-C2B	2.67	129.92	124.69
17	1	606	CHL	CMB-C2B-C3B	2.67	129.68	124.68
18	A	842	CLA	CHB-C4A-NA	2.67	128.21	124.51
22	L	306	BCR	C21-C20-C19	2.67	131.55	123.22
17	2	606	CHL	CMB-C2B-C3B	2.67	129.67	124.68
18	B	804	CLA	CHB-C4A-NA	2.67	128.20	124.51
18	3	612	CLA	CHB-C4A-NA	2.66	128.20	124.51
18	B	828	CLA	CMB-C2B-C3B	2.66	129.66	124.68
18	B	814	CLA	CHB-C4A-NA	2.66	128.19	124.51
22	B	848	BCR	C16-C15-C14	2.66	128.93	123.47
22	4	618	BCR	C19-C18-C17	2.66	123.02	118.94
18	4	614	CLA	CMB-C2B-C3B	2.66	129.66	124.68
18	1	605	CLA	CHB-C4A-NA	2.66	128.19	124.51
17	2	605	CHL	C1D-ND-C4D	-2.65	104.45	106.33
18	A	821	CLA	CHB-C4A-NA	2.65	128.18	124.51
18	B	825	CLA	CHB-C4A-NA	2.65	128.18	124.51
18	2	602	CLA	CHB-C4A-NA	2.65	128.18	124.51
18	B	840	CLA	CHB-C4A-NA	2.65	128.18	124.51
18	A	807	CLA	CMB-C2B-C3B	2.65	129.64	124.68
18	1	610	CLA	CMB-C2B-C3B	2.65	129.88	124.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	3	605	CLA	CAB-C3B-C2B	2.65	129.87	124.69
18	A	805	CLA	CHB-C4A-NA	2.65	128.17	124.51
22	F	304	BCR	C36-C18-C17	-2.64	119.22	122.92
17	4	605	CHL	CAC-C3C-C4C	2.64	129.07	125.04
18	A	824	CLA	CHB-C4A-NA	2.64	128.17	124.51
18	3	605	CLA	CMB-C2B-C3B	2.64	129.86	124.69
18	4	601	CLA	CHB-C4A-NA	2.64	128.16	124.51
17	2	601	CHL	O2D-CGD-O1D	-2.63	118.69	123.84
18	2	608	CLA	CHB-C4A-NA	2.63	128.15	124.51
18	A	836	CLA	CHB-C4A-NA	2.63	128.15	124.51
18	A	835	CLA	O2D-CGD-CBD	2.63	115.94	111.27
18	B	820	CLA	CHB-C4A-NA	2.63	128.15	124.51
18	2	613	CLA	CMB-C2B-C3B	2.63	129.60	124.68
18	B	810	CLA	CHB-C4A-NA	2.63	128.15	124.51
18	2	604	CLA	C1B-CHB-C4A	-2.63	124.91	130.12
17	4	606	CHL	CHD-C1D-C2D	2.63	130.99	125.48
18	A	840	CLA	CHB-C4A-NA	2.63	128.15	124.51
18	B	808	CLA	O2A-CGA-O1A	-2.63	116.96	123.59
18	F	303	CLA	CAA-C2A-C3A	-2.62	109.97	116.10
18	B	809	CLA	CHB-C4A-NA	2.62	128.14	124.51
18	A	829	CLA	CHB-C4A-NA	2.62	128.14	124.51
18	F	302	CLA	O2D-CGD-O1D	-2.62	118.71	123.84
18	4	603	CLA	CMB-C2B-C3B	2.62	129.82	124.69
18	1	608	CLA	CMB-C2B-C3B	2.62	129.82	124.69
18	B	819	CLA	CHB-C4A-NA	2.62	128.13	124.51
18	B	821	CLA	CHB-C4A-NA	2.62	128.13	124.51
18	B	810	CLA	CMB-C2B-C3B	2.62	129.57	124.68
17	4	605	CHL	CMB-C2B-C3B	2.61	129.57	124.68
18	K	201	CLA	CAA-C2A-C3A	-2.61	110.00	116.10
22	3	614	BCR	C1-C6-C5	-2.61	118.94	122.61
18	1	613	CLA	CAA-C2A-C3A	-2.61	110.01	116.10
18	A	817	CLA	CMB-C2B-C3B	2.61	129.56	124.68
18	B	840	CLA	CMB-C2B-C3B	2.61	129.56	124.68
18	A	814	CLA	CHB-C4A-NA	2.61	128.12	124.51
24	A	801	CL0	C4D-C3D-C2D	2.61	108.89	106.75
18	B	805	CLA	CMB-C2B-C3B	2.61	129.56	124.68
18	B	802	CLA	CGD-CBD-CAD	2.61	119.17	110.73
18	1	613	CLA	CMB-C2B-C3B	2.60	129.79	124.69
19	2	617	XAT	C15-C14-C13	2.60	131.03	127.31
18	A	818	CLA	CHB-C4A-NA	2.60	128.11	124.51
18	A	813	CLA	CMB-C2B-C3B	2.60	129.55	124.68
18	3	607	CLA	O2D-CGD-O1D	-2.60	118.75	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	815	CLA	CHB-C4A-NA	2.60	128.11	124.51
18	4	612	CLA	CHB-C4A-NA	2.60	128.10	124.51
17	4	615	CHL	CMB-C2B-C3B	2.60	129.78	124.69
18	1	611	CLA	CHB-C4A-NA	2.60	128.10	124.51
18	B	825	CLA	O2D-CGD-CBD	2.59	115.88	111.27
18	A	833	CLA	CHB-C4A-NA	2.59	128.10	124.51
18	A	812	CLA	CHB-C4A-NA	2.59	128.09	124.51
22	A	848	BCR	C23-C22-C21	2.59	122.92	118.94
18	3	609	CLA	CHB-C4A-NA	2.59	128.09	124.51
18	A	811	CLA	CHB-C4A-NA	2.59	128.09	124.51
18	2	603	CLA	O2D-CGD-O1D	-2.59	118.22	124.09
17	1	601	CHL	C4-C3-C5	2.58	119.62	115.27
17	2	605	CHL	CMB-C2B-C3B	2.58	129.51	124.68
18	B	812	CLA	CMB-C2B-C3B	2.58	129.51	124.68
18	B	811	CLA	CHB-C4A-NA	2.58	128.08	124.51
19	1	614	XAT	C25-C24-C23	-2.58	107.65	112.75
18	B	811	CLA	CMB-C2B-C3B	2.58	129.73	124.69
18	B	837	CLA	CHB-C4A-NA	2.58	128.07	124.51
18	3	607	CLA	CHB-C4A-NA	2.57	128.07	124.51
18	K	203	CLA	CHB-C4A-NA	2.57	128.07	124.51
18	H	201	CLA	CMB-C2B-C3B	2.57	129.49	124.68
18	B	835	CLA	CMB-C2B-C3B	2.57	129.49	124.68
19	1	614	XAT	O4-C5-C6	-2.57	56.83	58.96
18	A	822	CLA	CHB-C4A-NA	2.57	128.06	124.51
18	3	604	CLA	O2D-CGD-O1D	-2.57	118.26	124.09
18	4	604	CLA	CMB-C2B-C3B	2.57	129.71	124.69
18	A	838	CLA	CHB-C4A-NA	2.57	128.06	124.51
18	B	831	CLA	CHB-C4A-NA	2.57	128.06	124.51
18	3	602	CLA	CMB-C2B-C3B	2.56	129.48	124.68
19	4	617	XAT	C16-C1-C6	-2.56	103.12	110.05
22	G	204	BCR	C16-C15-C14	2.56	128.72	123.47
18	3	601	CLA	C1-C2-C3	-2.56	121.61	126.04
18	A	839	CLA	CHB-C4A-NA	2.56	128.05	124.51
18	A	808	CLA	CHB-C4A-NA	2.56	128.05	124.51
18	B	830	CLA	CHB-C4A-NA	2.56	128.05	124.51
22	L	301	BCR	C8-C9-C10	2.56	122.87	118.94
18	A	843	CLA	CHB-C4A-NA	2.56	128.05	124.51
21	3	613	LUT	C12-C13-C14	2.56	122.86	118.94
22	J	102	BCR	C15-C16-C17	2.55	128.71	123.47
18	1	607	CLA	CHB-C4A-NA	2.55	128.04	124.51
18	F	303	CLA	CHB-C4A-NA	2.55	128.04	124.51
18	3	602	CLA	CHB-C4A-NA	2.55	128.04	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	816	CLA	CHB-C4A-NA	2.55	128.04	124.51
18	B	816	CLA	C1-C2-C3	-2.55	121.63	126.04
22	B	846	BCR	C15-C16-C17	2.55	128.70	123.47
22	F	304	BCR	C37-C22-C23	2.55	122.10	118.08
18	3	610	CLA	O2D-CGD-O1D	-2.55	118.30	124.09
18	B	811	CLA	CAB-C3B-C2B	2.55	129.68	124.69
17	4	607	CHL	C2A-C1A-CHA	-2.55	119.40	123.86
18	4	604	CLA	CHB-C4A-NA	2.55	128.04	124.51
18	F	301	CLA	CHB-C4A-NA	2.55	128.04	124.51
18	G	203	CLA	CHB-C4A-NA	2.55	128.04	124.51
18	B	838	CLA	CHB-C4A-NA	2.55	128.03	124.51
18	4	611	CLA	CHB-C4A-NA	2.55	128.03	124.51
21	3	613	LUT	C10-C11-C12	2.54	131.16	123.22
18	4	611	CLA	O2D-CGD-O1D	-2.54	118.32	124.09
18	1	610	CLA	CHB-C4A-NA	2.54	128.03	124.51
18	L	304	CLA	CHB-C4A-NA	2.54	128.03	124.51
18	2	610	CLA	CMB-C2B-C3B	2.54	129.66	124.69
18	4	604	CLA	CAB-C3B-C2B	2.54	129.66	124.69
21	4	616	LUT	C19-C9-C8	2.54	122.08	118.08
22	J	102	BCR	C19-C18-C17	2.54	122.84	118.94
18	B	802	CLA	CHB-C4A-NA	2.54	128.02	124.51
18	B	832	CLA	CMB-C2B-C3B	2.54	129.42	124.68
18	B	812	CLA	CHB-C4A-NA	2.53	128.02	124.51
18	A	817	CLA	CHB-C4A-NA	2.53	128.01	124.51
17	4	607	CHL	C1C-C2C-C3C	-2.53	105.10	107.11
18	4	602	CLA	CHB-C4A-NA	2.53	128.01	124.51
18	L	303	CLA	CHB-C4A-NA	2.53	128.01	124.51
18	B	822	CLA	CHB-C4A-NA	2.53	128.01	124.51
18	3	605	CLA	CHB-C4A-NA	2.53	128.01	124.51
18	1	610	CLA	CAA-C2A-C3A	-2.53	110.19	116.10
18	A	823	CLA	CHB-C4A-NA	2.53	128.01	124.51
17	2	601	CHL	CMB-C2B-C3B	2.53	129.41	124.68
17	2	606	CHL	C4A-NA-C1A	2.53	107.84	106.71
18	A	806	CLA	CHB-C4A-NA	2.53	128.01	124.51
18	1	607	CLA	O2D-CGD-O1D	-2.53	118.35	124.09
18	3	601	CLA	CHB-C4A-NA	2.52	128.00	124.51
18	3	610	CLA	CHB-C4A-NA	2.52	128.00	124.51
18	4	609	CLA	O2D-CGD-O1D	-2.52	118.91	123.84
22	J	102	BCR	C7-C8-C9	2.52	130.04	126.23
19	2	617	XAT	C27-C28-C29	-2.52	121.62	125.53
18	1	608	CLA	CHB-C4A-NA	2.52	127.99	124.51
22	L	306	BCR	C24-C23-C22	2.52	130.04	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	B	808	CLA	CHB-C4A-NA	2.52	127.99	124.51
18	B	816	CLA	CHB-C4A-NA	2.52	127.99	124.51
17	2	615	CHL	CMB-C2B-C3B	2.52	129.39	124.68
17	2	615	CHL	C4A-NA-C1A	2.52	107.84	106.71
18	B	813	CLA	CHB-C4A-NA	2.51	127.99	124.51
18	K	201	CLA	CHB-C4A-NA	2.51	127.99	124.51
17	1	606	CHL	C3B-C4B-NB	2.51	112.46	109.21
18	L	304	CLA	CMB-C2B-C3B	2.51	129.38	124.68
18	A	810	CLA	CHB-C4A-NA	2.51	127.98	124.51
18	B	835	CLA	CHB-C4A-NA	2.51	127.98	124.51
18	3	609	CLA	O2D-CGD-O1D	-2.51	118.39	124.09
18	2	603	CLA	CHB-C4A-NA	2.51	127.98	124.51
18	A	831	CLA	CHB-C4A-NA	2.51	127.98	124.51
18	4	610	CLA	CHB-C4A-NA	2.51	127.98	124.51
18	B	806	CLA	CHB-C4A-NA	2.51	127.98	124.51
18	B	829	CLA	CHB-C4A-NA	2.51	127.98	124.51
18	B	836	CLA	CHB-C4A-NA	2.51	127.98	124.51
17	4	606	CHL	CMB-C2B-C3B	2.51	129.60	124.69
18	A	820	CLA	CHB-C4A-NA	2.51	127.98	124.51
18	G	202	CLA	CHB-C4A-NA	2.50	127.97	124.51
18	2	612	CLA	CHB-C4A-NA	2.50	127.97	124.51
18	A	825	CLA	CHB-C4A-NA	2.50	127.97	124.51
18	B	807	CLA	CHB-C4A-NA	2.50	127.97	124.51
18	3	608	CLA	CHB-C4A-NA	2.50	127.97	124.51
18	A	837	CLA	CHB-C4A-NA	2.50	127.97	124.51
18	3	611	CLA	CHB-C4A-NA	2.50	127.97	124.51
18	B	824	CLA	CHB-C4A-NA	2.49	127.96	124.51
20	1	615	LHG	O8-C23-C24	2.49	119.73	111.91
17	3	606	CHL	CMB-C2B-C3B	2.49	129.34	124.68
22	G	204	BCR	C23-C22-C21	2.49	122.76	118.94
18	B	830	CLA	CHD-C1D-ND	-2.49	122.17	124.45
18	B	815	CLA	CHB-C4A-NA	2.49	127.95	124.51
18	4	603	CLA	CHB-C4A-NA	2.49	127.95	124.51
18	G	201	CLA	CHB-C4A-NA	2.49	127.95	124.51
22	A	851	BCR	C15-C14-C13	2.49	130.86	127.31
18	A	826	CLA	CHB-C4A-NA	2.48	127.95	124.51
17	4	607	CHL	CBC-CAC-C3C	-2.48	105.58	112.43
22	K	205	BCR	C8-C9-C10	2.48	122.75	118.94
19	1	614	XAT	C27-C28-C29	-2.48	121.68	125.53
18	L	302	CLA	CHB-C4A-NA	2.48	127.94	124.51
22	L	306	BCR	C1-C6-C5	-2.48	119.13	122.61
18	A	819	CLA	CHB-C4A-NA	2.47	127.93	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	K	202	BCR	C30-C25-C24	2.47	122.78	115.78
22	K	202	BCR	C10-C11-C12	2.47	130.94	123.22
17	2	607	CHL	CMB-C2B-C3B	2.47	129.30	124.68
17	4	605	CHL	C1C-C2C-C3C	-2.47	105.15	107.11
24	A	801	CL0	CMD-C2D-C3D	-2.47	122.26	128.30
22	F	304	BCR	C19-C18-C17	2.47	122.73	118.94
18	A	841	CLA	CHB-C4A-NA	2.47	127.92	124.51
18	1	610	CLA	O2D-CGD-O1D	-2.46	118.49	124.09
19	4	617	XAT	C15-C35-C34	2.46	128.52	123.47
18	4	609	CLA	C1B-CHB-C4A	-2.46	125.24	130.12
18	1	603	CLA	CHB-C4A-NA	2.46	127.91	124.51
22	B	843	BCR	C12-C13-C14	2.46	122.71	118.94
18	4	608	CLA	CHB-C4A-NA	2.46	127.91	124.51
20	1	615	LHG	C5-O7-C7	-2.46	111.74	117.79
17	1	601	CHL	O2D-CGD-O1D	-2.46	118.51	124.09
17	2	607	CHL	C5-C3-C4	2.45	120.02	114.60
22	A	849	BCR	C1-C6-C5	-2.45	119.16	122.61
22	B	849	BCR	C30-C25-C24	2.45	122.72	115.78
22	I	101	BCR	C12-C13-C14	2.45	122.70	118.94
18	3	603	CLA	C1B-CHB-C4A	-2.45	125.26	130.12
22	B	845	BCR	C37-C22-C21	-2.45	119.49	122.92
18	1	609	CLA	O2D-CGD-O1D	-2.45	119.05	123.84
22	G	204	BCR	C12-C13-C14	2.45	122.70	118.94
18	3	603	CLA	CHB-C4A-NA	2.45	127.90	124.51
17	1	601	CHL	C1C-C2C-C3C	-2.44	105.17	107.11
18	B	832	CLA	CHB-C4A-NA	2.44	127.89	124.51
18	B	826	CLA	CHB-C4A-NA	2.44	127.89	124.51
18	A	815	CLA	CAA-C2A-C3A	-2.44	106.09	112.78
18	3	604	CLA	CHB-C4A-NA	2.44	127.88	124.51
18	A	803	CLA	CHB-C4A-NA	2.44	127.88	124.51
18	4	614	CLA	O2D-CGD-CBD	2.44	115.60	111.27
18	A	818	CLA	C1B-CHB-C4A	-2.43	125.30	130.12
18	B	839	CLA	CHB-C4A-NA	2.43	127.88	124.51
22	B	846	BCR	C19-C18-C17	2.43	122.67	118.94
17	4	607	CHL	CMB-C2B-C3B	2.43	129.23	124.68
21	4	616	LUT	C39-C29-C28	2.43	121.90	118.08
22	A	850	BCR	C35-C13-C14	-2.43	119.52	122.92
22	3	614	BCR	C8-C9-C10	2.43	122.66	118.94
18	B	816	CLA	C1B-CHB-C4A	-2.42	125.32	130.12
22	J	102	BCR	C23-C22-C21	2.42	122.65	118.94
18	B	841	CLA	CHB-C4A-NA	2.42	127.85	124.51
18	H	201	CLA	CHB-C4A-NA	2.41	127.85	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	1	609	CLA	C1B-CHB-C4A	-2.41	125.35	130.12
19	1	614	XAT	C10-C11-C12	-2.41	115.70	123.22
18	1	602	CLA	CHB-C4A-NA	2.41	127.84	124.51
19	1	614	XAT	C11-C10-C9	-2.40	123.88	127.31
17	2	606	CHL	O2D-CGD-O1D	-2.40	119.14	123.84
18	B	819	CLA	C1B-CHB-C4A	-2.40	125.36	130.12
18	B	833	CLA	CHB-C4A-NA	2.40	127.83	124.51
18	K	204	CLA	CHB-C4A-NA	2.40	127.83	124.51
18	B	822	CLA	CAA-C2A-C3A	-2.40	106.21	112.78
22	K	205	BCR	C12-C13-C14	2.40	122.62	118.94
18	3	607	CLA	C1B-CHB-C4A	-2.40	125.37	130.12
18	B	821	CLA	C1B-CHB-C4A	-2.39	125.38	130.12
18	A	831	CLA	C1B-CHB-C4A	-2.39	125.38	130.12
18	A	835	CLA	C1B-CHB-C4A	-2.39	125.39	130.12
18	B	808	CLA	C1B-CHB-C4A	-2.38	125.40	130.12
18	B	818	CLA	C1B-CHB-C4A	-2.38	125.40	130.12
27	B	850	DGD	O1G-C1A-C2A	2.38	119.38	111.91
18	B	821	CLA	O2A-CGA-O1A	-2.38	117.59	123.59
18	A	822	CLA	C1B-CHB-C4A	-2.37	125.41	130.12
18	A	803	CLA	C1B-CHB-C4A	-2.37	125.41	130.12
18	A	814	CLA	C1B-CHB-C4A	-2.37	125.42	130.12
18	A	832	CLA	C1-C2-C3	-2.37	122.91	126.75
18	A	804	CLA	O2D-CGD-CBD	2.37	115.48	111.27
18	A	827	CLA	CHB-C4A-NA	2.37	127.79	124.51
18	A	802	CLA	C1B-CHB-C4A	-2.37	125.43	130.12
18	A	820	CLA	C1B-CHB-C4A	-2.37	125.43	130.12
18	A	816	CLA	C1B-CHB-C4A	-2.36	125.44	130.12
18	1	612	CLA	CHB-C4A-NA	2.36	127.78	124.51
17	4	615	CHL	C1C-C2C-C3C	-2.36	105.24	107.11
18	4	613	CLA	C1B-CHB-C4A	-2.36	125.44	130.12
17	2	605	CHL	O2D-CGD-O1D	-2.36	119.23	123.84
18	A	844	CLA	O2A-CGA-O1A	-2.35	117.65	123.59
22	A	849	BCR	C12-C13-C14	2.35	122.55	118.94
18	3	612	CLA	C1B-CHB-C4A	-2.35	125.46	130.12
22	4	618	BCR	C15-C16-C17	2.35	128.29	123.47
18	A	824	CLA	C1B-CHB-C4A	-2.35	125.46	130.12
21	3	613	LUT	C11-C10-C9	2.35	130.66	127.31
21	2	616	LUT	C35-C15-C14	2.35	128.28	123.47
18	A	810	CLA	C1-C2-C3	-2.35	122.95	126.75
18	B	814	CLA	C1B-CHB-C4A	-2.34	125.48	130.12
18	B	834	CLA	C1B-CHB-C4A	-2.34	125.48	130.12
18	B	841	CLA	O2D-CGD-CBD	2.34	115.43	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	810	CLA	C1B-CHB-C4A	-2.34	125.48	130.12
22	A	851	BCR	C30-C25-C26	-2.34	119.32	122.61
18	1	604	CLA	C1B-CHB-C4A	-2.34	125.49	130.12
18	2	602	CLA	C1B-CHB-C4A	-2.34	125.49	130.12
18	A	825	CLA	C1B-CHB-C4A	-2.34	125.49	130.12
18	B	829	CLA	C1B-CHB-C4A	-2.34	125.49	130.12
18	A	841	CLA	C1B-CHB-C4A	-2.34	125.49	130.12
18	A	815	CLA	C1B-CHB-C4A	-2.33	125.49	130.12
22	B	843	BCR	C1-C6-C7	2.33	122.38	115.78
18	K	203	CLA	C1B-CHB-C4A	-2.33	125.50	130.12
18	A	829	CLA	C1B-CHB-C4A	-2.33	125.50	130.12
19	4	617	XAT	C37-C21-C26	2.33	116.34	110.05
18	L	304	CLA	C1B-CHB-C4A	-2.33	125.50	130.12
18	B	827	CLA	C1B-CHB-C4A	-2.33	125.51	130.12
22	B	847	BCR	C19-C18-C17	2.33	122.51	118.94
18	B	823	CLA	CHB-C4A-NA	2.32	127.72	124.51
17	2	607	CHL	C1C-C2C-C3C	-2.32	105.27	107.11
18	A	804	CLA	C1B-CHB-C4A	-2.32	125.52	130.12
18	A	844	CLA	C1B-CHB-C4A	-2.32	125.52	130.12
18	F	301	CLA	C1B-CHB-C4A	-2.32	125.53	130.12
18	3	609	CLA	C1B-CHB-C4A	-2.32	125.53	130.12
21	2	616	LUT	C40-C33-C34	-2.31	119.68	122.92
18	B	813	CLA	O2A-CGA-O1A	-2.31	117.75	123.59
18	1	613	CLA	CHB-C4A-NA	2.31	127.71	124.51
21	4	616	LUT	C12-C13-C14	2.31	122.49	118.94
18	A	829	CLA	O2A-CGA-O1A	-2.31	117.76	123.59
18	B	803	CLA	C1-C2-C3	-2.31	122.05	126.04
17	3	606	CHL	O2D-CGD-O1D	-2.31	119.32	123.84
18	A	832	CLA	C1B-CHB-C4A	-2.31	125.54	130.12
18	B	833	CLA	C1B-CHB-C4A	-2.31	125.54	130.12
18	K	201	CLA	C1B-CHB-C4A	-2.31	125.55	130.12
18	2	611	CLA	C1B-CHB-C4A	-2.31	125.55	130.12
18	A	811	CLA	C1B-CHB-C4A	-2.31	125.55	130.12
18	A	841	CLA	O2A-CGA-O1A	-2.31	117.77	123.59
18	A	835	CLA	C1-C2-C3	-2.31	122.05	126.04
22	B	846	BCR	C10-C11-C12	2.31	130.42	123.22
18	A	812	CLA	C1B-CHB-C4A	-2.31	125.55	130.12
18	A	808	CLA	C1B-CHB-C4A	-2.31	125.55	130.12
18	A	833	CLA	C1B-CHB-C4A	-2.31	125.55	130.12
22	K	202	BCR	C30-C25-C26	-2.30	119.37	122.61
18	2	609	CLA	C1B-CHB-C4A	-2.30	125.55	130.12
18	B	839	CLA	C1B-CHB-C4A	-2.30	125.56	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	B	817	CLA	C1B-CHB-C4A	-2.30	125.56	130.12
18	2	608	CLA	C1B-CHB-C4A	-2.30	125.56	130.12
18	B	807	CLA	C1B-CHB-C4A	-2.30	125.56	130.12
18	B	838	CLA	C1B-CHB-C4A	-2.30	125.56	130.12
18	B	836	CLA	C1B-CHB-C4A	-2.30	125.56	130.12
18	B	810	CLA	C1B-CHB-C4A	-2.30	125.56	130.12
18	A	809	CLA	C1B-CHB-C4A	-2.30	125.56	130.12
18	A	806	CLA	C1B-CHB-C4A	-2.30	125.57	130.12
17	2	615	CHL	O2D-CGD-O1D	-2.30	119.35	123.84
18	B	840	CLA	C1B-CHB-C4A	-2.30	125.57	130.12
19	4	617	XAT	C7-C8-C9	2.30	129.09	125.53
18	3	610	CLA	C1B-CHB-C4A	-2.29	125.57	130.12
18	B	825	CLA	C1B-CHB-C4A	-2.29	125.58	130.12
21	1	616	LUT	C10-C11-C12	2.29	130.37	123.22
18	B	804	CLA	C1B-CHB-C4A	-2.29	125.58	130.12
18	B	820	CLA	C1B-CHB-C4A	-2.29	125.58	130.12
19	4	617	XAT	C39-C29-C30	-2.29	119.71	122.92
22	K	202	BCR	C21-C20-C19	2.29	130.37	123.22
18	B	822	CLA	C1B-CHB-C4A	-2.29	125.58	130.12
18	B	828	CLA	C1B-CHB-C4A	-2.29	125.58	130.12
18	1	610	CLA	C1B-CHB-C4A	-2.29	125.59	130.12
18	B	809	CLA	C1B-CHB-C4A	-2.29	125.59	130.12
22	B	848	BCR	C12-C13-C14	2.29	122.45	118.94
22	K	205	BCR	C1-C6-C5	-2.29	119.39	122.61
18	B	839	CLA	O2A-CGA-O1A	-2.28	117.83	123.59
18	3	608	CLA	C1B-CHB-C4A	-2.28	125.59	130.12
18	3	609	CLA	C1-C2-C3	-2.28	122.10	126.04
18	4	611	CLA	C1B-CHB-C4A	-2.28	125.60	130.12
22	A	848	BCR	C30-C25-C24	2.28	122.23	115.78
18	L	303	CLA	C1B-CHB-C4A	-2.28	125.60	130.12
18	2	612	CLA	C1B-CHB-C4A	-2.28	125.60	130.12
18	3	601	CLA	C1B-CHB-C4A	-2.28	125.61	130.12
18	B	831	CLA	C1B-CHB-C4A	-2.28	125.61	130.12
18	L	302	CLA	C1B-CHB-C4A	-2.28	125.61	130.12
18	B	835	CLA	C1B-CHB-C4A	-2.28	125.61	130.12
18	A	805	CLA	C1B-CHB-C4A	-2.27	125.61	130.12
18	F	302	CLA	C1B-CHB-C4A	-2.27	125.61	130.12
18	4	614	CLA	C1-C2-C3	-2.27	123.07	126.75
18	A	823	CLA	C1B-CHB-C4A	-2.27	125.62	130.12
22	3	614	BCR	C37-C22-C23	2.27	121.65	118.08
18	B	841	CLA	C1B-CHB-C4A	-2.27	125.63	130.12
19	2	617	XAT	C8-C9-C10	2.27	122.42	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	4	603	CLA	C1B-CHB-C4A	-2.27	125.63	130.12
18	B	826	CLA	C1B-CHB-C4A	-2.27	125.63	130.12
18	2	613	CLA	C1B-CHB-C4A	-2.26	125.63	130.12
18	3	603	CLA	CHD-C1D-ND	-2.26	122.37	124.45
18	1	612	CLA	C1B-CHB-C4A	-2.26	125.63	130.12
18	A	804	CLA	O2A-CGA-O1A	-2.26	117.88	123.59
18	B	803	CLA	O2A-CGA-O1A	-2.26	117.88	123.59
18	A	819	CLA	C1B-CHB-C4A	-2.26	125.64	130.12
18	A	826	CLA	C1B-CHB-C4A	-2.26	125.64	130.12
18	A	842	CLA	C1B-CHB-C4A	-2.26	125.64	130.12
18	B	817	CLA	O2A-CGA-O1A	-2.26	117.89	123.59
17	2	607	CHL	O2D-CGD-O1D	-2.26	119.43	123.84
22	A	850	BCR	C36-C18-C17	-2.26	119.76	122.92
18	A	843	CLA	C1B-CHB-C4A	-2.26	125.65	130.12
18	3	608	CLA	CHD-C1D-ND	-2.26	122.38	124.45
18	B	825	CLA	O2A-CGA-O1A	-2.26	117.90	123.59
18	A	821	CLA	C1B-CHB-C4A	-2.26	125.65	130.12
17	2	605	CHL	OMC-CMC-C2C	-2.25	120.59	125.69
18	1	611	CLA	C1B-CHB-C4A	-2.25	125.65	130.12
22	B	849	BCR	C24-C23-C22	2.25	129.64	126.23
18	4	609	CLA	O2A-CGA-O1A	-2.25	117.90	123.59
18	A	836	CLA	C1B-CHB-C4A	-2.25	125.65	130.12
18	F	301	CLA	CHD-C1D-ND	-2.25	122.38	124.45
18	4	612	CLA	C1-C2-C3	-2.25	122.15	126.04
22	K	205	BCR	C30-C25-C24	2.25	122.15	115.78
18	G	203	CLA	C1B-CHB-C4A	-2.25	125.66	130.12
18	A	840	CLA	O2D-CGD-CBD	2.25	115.27	111.27
18	4	601	CLA	C1B-CHB-C4A	-2.25	125.66	130.12
17	2	601	CHL	C1C-C2C-C3C	-2.25	105.33	107.11
18	A	840	CLA	C1B-CHB-C4A	-2.25	125.67	130.12
22	A	848	BCR	C30-C25-C26	-2.25	119.45	122.61
18	3	605	CLA	C1B-CHB-C4A	-2.25	125.67	130.12
19	1	614	XAT	C18-C5-C4	2.25	116.81	114.28
18	2	603	CLA	C1B-CHB-C4A	-2.25	125.67	130.12
18	B	837	CLA	C1B-CHB-C4A	-2.25	125.67	130.12
18	4	614	CLA	C1B-CHB-C4A	-2.25	125.67	130.12
22	A	851	BCR	C30-C25-C24	2.25	122.13	115.78
17	4	605	CHL	OMC-CMC-C2C	-2.24	120.61	125.69
18	F	303	CLA	C1B-CHB-C4A	-2.24	125.67	130.12
17	1	606	CHL	O2D-CGD-O1D	-2.24	119.00	124.09
18	A	819	CLA	O2D-CGD-CBD	2.24	115.25	111.27
18	A	828	CLA	C1B-CHB-C4A	-2.24	125.69	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	1	614	XAT	C30-C31-C32	-2.24	116.24	123.22
18	B	813	CLA	C1B-CHB-C4A	-2.24	125.69	130.12
22	A	853	BCR	C23-C22-C21	2.23	122.37	118.94
18	A	835	CLA	O2A-CGA-O1A	-2.23	117.95	123.59
18	4	604	CLA	C1B-CHB-C4A	-2.23	125.69	130.12
18	B	803	CLA	C1B-CHB-C4A	-2.23	125.70	130.12
22	B	845	BCR	C30-C25-C26	-2.23	119.47	122.61
18	L	302	CLA	O2D-CGD-CBD	2.23	115.23	111.27
17	2	615	CHL	C1C-C2C-C3C	-2.23	105.34	107.11
18	2	613	CLA	O2D-CGD-CBD	2.23	115.23	111.27
18	3	602	CLA	C1B-CHB-C4A	-2.22	125.71	130.12
18	A	828	CLA	O2D-CGD-CBD	2.22	115.22	111.27
18	A	831	CLA	O2A-CGA-O1A	-2.22	117.99	123.59
18	1	603	CLA	C1B-CHB-C4A	-2.22	125.72	130.12
18	B	837	CLA	O2D-CGD-CBD	2.22	115.21	111.27
18	A	839	CLA	C1B-CHB-C4A	-2.22	125.72	130.12
18	B	805	CLA	C1B-CHB-C4A	-2.22	125.72	130.12
17	4	607	CHL	O2D-CGD-O1D	-2.22	119.50	123.84
18	B	828	CLA	O2A-CGA-O1A	-2.22	118.00	123.59
18	4	610	CLA	C1B-CHB-C4A	-2.22	125.72	130.12
22	L	305	BCR	C1-C6-C7	2.22	122.05	115.78
18	B	833	CLA	O2D-CGD-CBD	2.22	115.21	111.27
18	1	602	CLA	C1B-CHB-C4A	-2.22	125.73	130.12
18	3	611	CLA	C1B-CHB-C4A	-2.22	125.73	130.12
18	B	817	CLA	C1-C2-C3	-2.22	122.21	126.04
18	1	607	CLA	C1B-CHB-C4A	-2.21	125.73	130.12
18	A	827	CLA	O2A-CGA-O1A	-2.21	118.00	123.59
18	A	832	CLA	O2D-CGD-CBD	2.21	115.20	111.27
18	A	815	CLA	CHD-C1D-ND	-2.21	122.42	124.45
18	B	838	CLA	O2D-CGD-CBD	2.21	115.20	111.27
22	A	851	BCR	C11-C12-C13	2.21	132.63	126.42
17	2	605	CHL	CAA-C2A-C3A	-2.21	108.73	114.26
18	B	810	CLA	C1-C2-C3	-2.21	122.22	126.04
22	B	843	BCR	C10-C11-C12	2.21	130.11	123.22
22	B	843	BCR	C19-C18-C17	2.21	122.33	118.94
21	2	619	LUT	C15-C14-C13	2.21	130.46	127.31
18	A	827	CLA	C1B-CHB-C4A	-2.20	125.75	130.12
18	A	837	CLA	C1B-CHB-C4A	-2.20	125.76	130.12
17	2	606	CHL	C1D-ND-C4D	-2.20	104.77	106.33
18	B	805	CLA	O2A-CGA-O1A	-2.20	118.04	123.59
22	A	850	BCR	C12-C13-C14	2.20	122.32	118.94
18	A	839	CLA	O2A-CGA-O1A	-2.20	118.04	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	807	CLA	C1B-CHB-C4A	-2.20	125.77	130.12
22	J	102	BCR	C1-C6-C7	2.20	121.99	115.78
18	B	824	CLA	C1B-CHB-C4A	-2.20	125.77	130.12
18	B	811	CLA	C1B-CHB-C4A	-2.19	125.77	130.12
18	4	612	CLA	C1B-CHB-C4A	-2.19	125.77	130.12
18	B	815	CLA	C1B-CHB-C4A	-2.19	125.77	130.12
18	A	830	CLA	C1B-CHB-C4A	-2.19	125.77	130.12
17	4	615	CHL	O2D-CGD-O1D	-2.19	119.11	124.09
22	K	205	BCR	C30-C25-C26	-2.19	119.53	122.61
22	A	851	BCR	C24-C23-C22	-2.19	122.92	126.23
18	K	204	CLA	C1B-CHB-C4A	-2.19	125.78	130.12
18	1	613	CLA	C1B-CHB-C4A	-2.19	125.78	130.12
18	B	832	CLA	C1B-CHB-C4A	-2.19	125.78	130.12
18	B	820	CLA	O2D-CGD-CBD	2.19	115.16	111.27
22	A	853	BCR	C30-C25-C24	2.19	121.97	115.78
24	A	801	CL0	CHB-C4A-NA	2.19	127.54	124.51
18	A	808	CLA	C1-C2-C3	-2.19	123.21	126.75
18	B	836	CLA	O2A-CGA-O1A	-2.19	118.08	123.59
18	A	834	CLA	C1B-CHB-C4A	-2.19	125.79	130.12
22	B	843	BCR	C16-C17-C18	2.19	130.43	127.31
22	B	845	BCR	C24-C23-C22	-2.18	122.93	126.23
18	A	817	CLA	C1B-CHB-C4A	-2.18	125.79	130.12
18	B	823	CLA	C1B-CHB-C4A	-2.18	125.79	130.12
18	B	816	CLA	CHD-C1D-ND	-2.18	122.45	124.45
18	3	602	CLA	O2A-CGA-O1A	-2.18	118.08	123.59
18	A	838	CLA	C1B-CHB-C4A	-2.18	125.80	130.12
22	L	305	BCR	C30-C25-C24	2.18	121.95	115.78
22	L	306	BCR	C1-C6-C7	2.18	121.95	115.78
18	G	202	CLA	C1B-CHB-C4A	-2.18	125.80	130.12
22	K	205	BCR	C1-C6-C7	2.18	121.94	115.78
18	4	602	CLA	C1B-CHB-C4A	-2.18	125.81	130.12
18	B	807	CLA	O2A-CGA-O1A	-2.18	118.10	123.59
18	A	807	CLA	CHD-C1D-ND	-2.18	122.45	124.45
18	A	813	CLA	C1B-CHB-C4A	-2.17	125.81	130.12
17	1	601	CHL	C4D-CHA-C1A	-2.17	118.60	121.25
18	B	834	CLA	CHD-C1D-ND	-2.17	122.46	124.45
22	J	102	BCR	C1-C6-C5	-2.17	119.56	122.61
18	1	605	CLA	C1B-CHB-C4A	-2.17	125.82	130.12
18	1	608	CLA	C1B-CHB-C4A	-2.17	125.82	130.12
18	3	604	CLA	C1B-CHB-C4A	-2.17	125.82	130.12
22	B	845	BCR	C8-C9-C10	2.17	122.27	118.94
18	4	608	CLA	C1B-CHB-C4A	-2.16	125.83	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	810	CLA	O2A-CGA-O1A	-2.16	118.13	123.59
18	A	825	CLA	O2A-CGA-O1A	-2.16	118.14	123.59
22	A	850	BCR	C19-C18-C17	2.16	122.26	118.94
18	B	830	CLA	C1B-CHB-C4A	-2.16	125.84	130.12
18	B	818	CLA	O2A-CGA-O1A	-2.16	118.14	123.59
22	B	843	BCR	C1-C6-C5	-2.16	119.58	122.61
22	B	848	BCR	C30-C25-C24	2.16	121.88	115.78
18	2	610	CLA	C1B-CHB-C4A	-2.16	125.85	130.12
18	B	816	CLA	O2A-CGA-O1A	-2.16	118.15	123.59
19	4	617	XAT	C35-C15-C14	2.15	127.89	123.47
18	1	602	CLA	CHD-C1D-ND	-2.15	122.47	124.45
19	1	614	XAT	C20-C13-C12	2.15	121.47	118.08
18	H	201	CLA	C1B-CHB-C4A	-2.15	125.85	130.12
18	G	201	CLA	C1B-CHB-C4A	-2.15	125.86	130.12
18	A	842	CLA	CAA-C2A-C3A	-2.15	106.89	112.78
18	A	808	CLA	O2A-CGA-O1A	-2.15	118.17	123.59
18	B	812	CLA	C1B-CHB-C4A	-2.15	125.86	130.12
18	A	812	CLA	C1-C2-C3	-2.15	122.33	126.04
18	B	813	CLA	C1-C2-C3	-2.15	122.33	126.04
18	2	611	CLA	O2A-CGA-O1A	-2.14	117.95	123.30
18	K	203	CLA	CAA-C2A-C3A	-2.14	106.91	112.78
18	B	836	CLA	O2D-CGD-CBD	2.14	115.07	111.27
18	B	822	CLA	C1-C2-C3	-2.14	122.34	126.04
17	2	615	CHL	CAA-C2A-C3A	-2.14	108.91	114.26
17	4	606	CHL	CHD-C4C-C3C	-2.14	121.70	124.84
17	4	606	CHL	O2D-CGD-O1D	-2.13	119.66	123.84
18	A	840	CLA	O2A-CGA-O1A	-2.13	118.21	123.59
22	A	853	BCR	C30-C25-C26	-2.13	119.61	122.61
22	A	852	BCR	C30-C25-C24	2.13	121.81	115.78
17	2	606	CHL	CHD-C1D-C2D	2.13	129.95	125.48
18	A	832	CLA	O2A-CGA-O1A	-2.13	118.22	123.59
24	A	801	CL0	O2A-CGA-O1A	-2.13	118.22	123.59
22	B	848	BCR	C37-C22-C23	2.12	121.42	118.08
17	2	615	CHL	C1D-ND-C4D	-2.12	104.83	106.33
22	B	847	BCR	C8-C9-C10	2.12	122.20	118.94
22	A	849	BCR	C15-C14-C13	2.12	130.34	127.31
18	A	825	CLA	C1-C2-C3	-2.12	122.37	126.04
18	A	844	CLA	C1-C2-C3	-2.12	122.37	126.04
18	B	827	CLA	O2D-CGD-CBD	2.12	115.04	111.27
22	A	850	BCR	C37-C22-C23	2.12	121.42	118.08
18	A	839	CLA	C1-C2-C3	-2.12	122.37	126.04
18	B	810	CLA	CAA-C2A-C3A	-2.12	106.97	112.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	K	204	CLA	CHD-C1D-ND	-2.12	122.50	124.45
18	1	613	CLA	O2D-CGD-O1D	-2.12	119.27	124.09
22	G	204	BCR	C8-C9-C10	2.12	122.19	118.94
22	A	852	BCR	C34-C9-C8	2.12	121.42	118.08
18	4	613	CLA	O2A-CGA-O1A	-2.12	118.02	123.30
18	A	834	CLA	O2A-CGA-O1A	-2.12	118.25	123.59
18	A	815	CLA	O2D-CGD-CBD	2.12	115.03	111.27
18	A	812	CLA	CHD-C1D-ND	-2.12	122.51	124.45
18	B	806	CLA	C1B-CHB-C4A	-2.12	125.93	130.12
18	B	829	CLA	O2A-CGA-O1A	-2.12	118.25	123.59
17	2	606	CHL	C1C-C2C-C3C	-2.11	105.44	107.11
18	A	831	CLA	CHD-C1D-ND	-2.11	122.52	124.45
18	4	601	CLA	O2D-CGD-CBD	2.11	115.02	111.27
21	2	619	LUT	C11-C10-C9	2.11	130.32	127.31
18	B	839	CLA	CHD-C1D-ND	-2.11	122.52	124.45
18	B	818	CLA	O2D-CGD-CBD	2.11	115.01	111.27
18	B	820	CLA	C1-C2-C3	-2.11	123.34	126.75
22	B	847	BCR	C15-C16-C17	2.11	127.79	123.47
18	A	806	CLA	CHD-C1D-ND	-2.10	122.52	124.45
18	B	808	CLA	C1-C2-C3	-2.10	122.41	126.04
18	A	822	CLA	O2A-CGA-O1A	-2.10	118.29	123.59
18	4	609	CLA	CHD-C1D-ND	-2.10	122.52	124.45
17	4	607	CHL	OMC-CMC-C2C	-2.10	120.94	125.69
18	1	602	CLA	O2A-CGA-O1A	-2.10	118.29	123.59
18	K	203	CLA	CHD-C1D-ND	-2.10	122.52	124.45
18	H	201	CLA	O2A-CGA-O1A	-2.10	118.30	123.59
18	B	802	CLA	C1B-CHB-C4A	-2.09	125.97	130.12
18	A	818	CLA	O2A-CGA-O1A	-2.09	118.31	123.59
18	4	612	CLA	O2A-CGA-O1A	-2.09	118.32	123.59
18	3	605	CLA	CHD-C1D-ND	-2.09	122.54	124.45
18	B	826	CLA	O2A-CGA-O1A	-2.09	118.33	123.59
18	A	830	CLA	C2A-C1A-CHA	2.09	127.51	123.86
18	2	611	CLA	CHD-C1D-ND	-2.08	122.54	124.45
21	2	619	LUT	C30-C31-C32	2.08	129.72	123.22
22	3	614	BCR	C30-C25-C24	2.08	121.67	115.78
18	B	817	CLA	CHD-C1D-ND	-2.08	122.54	124.45
18	3	601	CLA	O2A-CGA-O1A	-2.08	118.34	123.59
17	4	605	CHL	O2D-CGD-O1D	-2.08	119.36	124.09
18	A	827	CLA	CHD-C1D-ND	-2.08	122.55	124.45
18	B	815	CLA	CHD-C1D-ND	-2.08	122.55	124.45
18	B	835	CLA	CHD-C1D-ND	-2.08	122.55	124.45
18	4	602	CLA	O2A-CGA-O1A	-2.08	118.35	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	1	601	CHL	OMC-CMC-C2C	-2.08	121.00	125.69
17	2	606	CHL	O1D-CGD-CBD	-2.07	120.24	124.48
18	A	824	CLA	CHD-C1D-ND	-2.07	122.55	124.45
18	H	201	CLA	C1-C2-C3	-2.07	122.46	126.04
18	B	824	CLA	O2A-CGA-O1A	-2.07	118.36	123.59
18	A	810	CLA	CHD-C1D-ND	-2.07	122.55	124.45
18	B	819	CLA	O2A-CGA-O1A	-2.07	118.36	123.59
22	A	850	BCR	C1-C6-C7	2.07	121.64	115.78
18	B	825	CLA	CHD-C1D-ND	-2.07	122.55	124.45
18	2	602	CLA	O2A-CGA-O1A	-2.07	118.37	123.59
18	A	833	CLA	CHD-C1D-ND	-2.06	122.56	124.45
18	A	825	CLA	CHD-C1D-ND	-2.06	122.56	124.45
18	B	837	CLA	O2A-CGA-O1A	-2.06	118.39	123.59
17	4	606	CHL	C2D-C1D-ND	2.06	111.62	110.10
18	B	831	CLA	CHD-C1D-ND	-2.06	122.56	124.45
18	3	611	CLA	CHD-C1D-ND	-2.06	122.56	124.45
18	A	805	CLA	CHD-C1D-ND	-2.06	122.56	124.45
18	B	838	CLA	CHD-C1D-ND	-2.05	122.57	124.45
18	A	814	CLA	O2A-CGA-O1A	-2.05	118.41	123.59
22	L	305	BCR	C30-C25-C26	-2.05	119.72	122.61
17	1	606	CHL	OMC-CMC-C2C	-2.05	121.05	125.69
22	A	851	BCR	C10-C11-C12	-2.05	116.82	123.22
18	3	609	CLA	CHD-C1D-ND	-2.05	122.57	124.45
18	A	836	CLA	CHD-C1D-ND	-2.05	122.57	124.45
18	B	806	CLA	O2A-CGA-O1A	-2.05	118.42	123.59
18	B	807	CLA	CHD-C1D-ND	-2.05	122.57	124.45
18	4	602	CLA	O2D-CGD-CBD	2.05	114.90	111.27
18	B	822	CLA	O2A-CGA-O1A	-2.04	118.43	123.59
18	A	837	CLA	O2D-CGD-CBD	2.04	114.90	111.27
18	B	814	CLA	O2A-CGA-O1A	-2.04	118.43	123.59
18	A	811	CLA	O2D-CGD-CBD	2.04	114.90	111.27
22	G	204	BCR	C1-C6-C7	2.04	121.56	115.78
18	B	809	CLA	O2A-CGA-O1A	-2.04	118.44	123.59
17	2	606	CHL	OMC-CMC-C2C	-2.04	121.07	125.69
18	A	809	CLA	O2A-CGA-O1A	-2.04	118.45	123.59
18	B	811	CLA	O2D-CGD-CBD	2.04	114.89	111.27
18	A	807	CLA	O2A-CGA-O1A	-2.04	118.45	123.59
22	A	851	BCR	C34-C9-C8	-2.04	114.87	118.08
18	3	603	CLA	O2A-CGA-O1A	-2.03	118.23	123.30
18	3	609	CLA	O2A-CGA-O1A	-2.03	118.46	123.59
18	B	811	CLA	O2A-CGA-O1A	-2.03	118.47	123.59
18	A	819	CLA	CHD-C1D-ND	-2.03	122.59	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	L	305	BCR	C21-C20-C19	2.03	129.55	123.22
18	A	826	CLA	O2A-CGA-O1A	-2.03	118.47	123.59
18	B	841	CLA	CHD-C1D-ND	-2.03	122.59	124.45
18	4	608	CLA	O2A-CGA-O1A	-2.03	118.25	123.30
19	2	617	XAT	C17-C1-C2	-2.03	105.46	108.98
22	A	853	BCR	C1-C6-C7	2.03	121.51	115.78
17	1	606	CHL	C1C-C2C-C3C	-2.03	105.51	107.11
17	2	601	CHL	OMC-CMC-C2C	-2.02	121.11	125.69
22	L	301	BCR	C10-C11-C12	2.02	129.53	123.22
18	1	603	CLA	O2A-CGA-O1A	-2.02	118.49	123.59
18	B	809	CLA	C1-C2-C3	-2.02	122.55	126.04
18	A	838	CLA	O2A-CGA-O1A	-2.02	118.49	123.59
17	4	605	CHL	C4D-CHA-C1A	-2.02	118.79	121.25
18	B	823	CLA	O2A-CGA-O1A	-2.02	118.27	123.30
18	B	834	CLA	O2A-CGA-O1A	-2.02	118.50	123.59
18	A	841	CLA	C1-C2-C3	-2.02	122.55	126.04
18	A	823	CLA	CHD-C1D-ND	-2.02	122.60	124.45
18	A	804	CLA	C2A-C1A-CHA	2.02	127.38	123.86
18	A	806	CLA	O2A-CGA-O1A	-2.02	118.51	123.59
18	B	804	CLA	O2D-CGD-CBD	2.01	114.85	111.27
17	1	606	CHL	CHD-C4C-C3C	-2.01	121.88	124.84
22	3	614	BCR	C30-C25-C26	-2.01	119.78	122.61
18	A	805	CLA	O2A-CGA-O1A	-2.01	118.52	123.59
18	G	202	CLA	CHD-C1D-ND	-2.01	122.61	124.45
18	A	830	CLA	O2A-CGA-O1A	-2.01	118.52	123.59
22	B	844	BCR	C20-C19-C18	2.01	132.06	126.42
18	G	201	CLA	O2A-CGA-O1A	-2.01	118.29	123.30
17	4	615	CHL	C4B-C3B-C2B	-2.01	105.05	106.92
18	B	820	CLA	O2A-CGA-O1A	-2.01	118.52	123.59
18	A	803	CLA	O2A-CGA-O1A	-2.01	118.52	123.59
17	2	601	CHL	O2A-CGA-CBA	2.01	120.17	112.23
17	1	601	CHL	O2A-CGA-O1A	-2.01	118.53	123.59
17	4	615	CHL	C2A-C1A-CHA	-2.01	120.35	123.86
18	4	604	CLA	CHD-C1D-ND	-2.01	122.61	124.45
18	A	822	CLA	CHD-C1D-ND	-2.01	122.61	124.45
18	A	813	CLA	O2A-CGA-O1A	-2.01	118.53	123.59
18	B	833	CLA	O2A-CGA-O1A	-2.00	118.31	123.30
18	A	818	CLA	CHD-C1D-ND	-2.00	122.61	124.45
24	A	801	CL0	C2A-C3A-C4A	-2.00	98.64	101.87
18	B	802	CLA	O2A-CGA-O1A	-2.00	118.54	123.59

All (176) chirality outliers are listed below:

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

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Mol	Chain	Res	Type	Atom
18	1	610	CLA	ND
18	1	611	CLA	ND
18	1	612	CLA	ND
18	1	613	CLA	ND
18	2	604	CLA	ND
18	2	602	CLA	ND
18	2	612	CLA	ND
18	2	613	CLA	ND
18	2	603	CLA	ND
18	2	610	CLA	ND
18	2	611	CLA	ND
18	2	609	CLA	ND
18	2	608	CLA	ND
18	3	612	CLA	ND
18	3	610	CLA	ND
18	3	609	CLA	ND
18	3	602	CLA	ND
18	3	604	CLA	ND
18	3	607	CLA	ND
18	3	603	CLA	ND
18	3	611	CLA	ND
18	3	601	CLA	ND
18	3	608	CLA	ND
18	3	605	CLA	ND
18	4	604	CLA	ND
18	4	608	CLA	ND
18	4	603	CLA	ND
18	4	609	CLA	ND
18	4	602	CLA	ND
18	4	610	CLA	ND
18	4	611	CLA	ND
18	4	614	CLA	ND
18	4	601	CLA	ND
18	4	613	CLA	ND
18	4	612	CLA	ND
18	A	804	CLA	ND
18	A	817	CLA	ND
18	A	821	CLA	ND
18	A	802	CLA	ND
18	A	819	CLA	ND
18	A	826	CLA	ND
18	A	833	CLA	ND

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Mol	Chain	Res	Type	Atom
18	A	828	CLA	ND
18	A	808	CLA	ND
18	A	806	CLA	ND
18	A	835	CLA	ND
18	A	822	CLA	ND
18	A	830	CLA	ND
18	A	807	CLA	ND
18	A	842	CLA	ND
18	A	827	CLA	ND
18	A	805	CLA	ND
18	A	809	CLA	ND
18	A	803	CLA	ND
18	A	837	CLA	ND
18	A	825	CLA	ND
18	A	838	CLA	ND
18	A	839	CLA	ND
18	A	834	CLA	ND
18	A	812	CLA	ND
18	A	840	CLA	ND
18	A	816	CLA	ND
18	A	815	CLA	ND
18	A	844	CLA	ND
18	A	820	CLA	ND
18	A	823	CLA	ND
18	A	818	CLA	ND
18	A	843	CLA	ND
18	A	829	CLA	ND
18	A	810	CLA	ND
18	A	832	CLA	ND
18	A	814	CLA	ND
18	A	811	CLA	ND
18	A	841	CLA	ND
18	A	813	CLA	ND
18	A	836	CLA	ND
18	A	831	CLA	ND
18	A	824	CLA	ND
18	B	802	CLA	ND
18	B	821	CLA	ND
18	B	808	CLA	ND
18	B	814	CLA	ND
18	B	803	CLA	ND
18	B	816	CLA	ND

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Mol	Chain	Res	Type	Atom
18	B	819	CLA	ND
18	B	825	CLA	ND
18	B	804	CLA	ND
18	B	807	CLA	ND
18	B	813	CLA	ND
18	B	820	CLA	ND
18	B	824	CLA	ND
18	B	805	CLA	ND
18	B	806	CLA	ND
18	B	827	CLA	ND
18	B	817	CLA	ND
18	B	838	CLA	ND
18	B	815	CLA	ND
18	B	829	CLA	ND
18	B	839	CLA	ND
18	B	832	CLA	ND
18	B	831	CLA	ND
18	B	836	CLA	ND
18	B	840	CLA	ND
18	B	837	CLA	ND
18	B	833	CLA	ND
18	B	823	CLA	ND
18	B	841	CLA	ND
18	B	822	CLA	ND
18	B	830	CLA	ND
18	B	826	CLA	ND
18	B	809	CLA	ND
18	B	810	CLA	ND
18	B	818	CLA	ND
18	B	835	CLA	ND
18	B	812	CLA	ND
18	B	828	CLA	ND
18	B	811	CLA	ND
18	B	834	CLA	ND
18	F	302	CLA	ND
18	F	303	CLA	ND
18	F	301	CLA	ND
18	G	202	CLA	ND
18	G	203	CLA	ND
18	G	201	CLA	ND
18	H	201	CLA	ND
18	K	204	CLA	ND

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Mol	Chain	Res	Type	Atom
18	K	203	CLA	ND
18	K	201	CLA	ND
18	L	304	CLA	ND
18	L	303	CLA	ND
18	L	302	CLA	ND
24	A	801	CL0	NA
24	A	801	CL0	NC

All (1440) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
17	1	601	CHL	CAD-CBD-CGD-O1D
17	1	601	CHL	CAD-CBD-CGD-O2D
17	2	601	CHL	C1A-C2A-CAA-CBA
17	2	601	CHL	C3A-C2A-CAA-CBA
17	3	606	CHL	C2A-CAA-CBA-CGA
17	3	606	CHL	CHA-CBD-CGD-O1D
17	3	606	CHL	CHA-CBD-CGD-O2D
17	4	605	CHL	C1A-C2A-CAA-CBA
17	4	605	CHL	C3C-C2C-CMC-OMC
17	4	607	CHL	CBD-CGD-O2D-CED
18	1	602	CLA	CBD-CGD-O2D-CED
18	1	604	CLA	C1A-C2A-CAA-CBA
18	1	607	CLA	C1A-C2A-CAA-CBA
18	1	607	CLA	C3A-C2A-CAA-CBA
18	1	609	CLA	CBD-CGD-O2D-CED
18	1	611	CLA	CBD-CGD-O2D-CED
18	1	612	CLA	CHA-CBD-CGD-O2D
18	2	604	CLA	C1A-C2A-CAA-CBA
18	2	604	CLA	C3A-C2A-CAA-CBA
18	2	612	CLA	CHA-CBD-CGD-O1D
18	2	612	CLA	CHA-CBD-CGD-O2D
18	2	612	CLA	CBD-CGD-O2D-CED
18	2	613	CLA	CHA-CBD-CGD-O1D
18	2	613	CLA	CHA-CBD-CGD-O2D
18	2	610	CLA	CMA-C3A-C4A-CHB
18	2	611	CLA	CBD-CGD-O2D-CED
18	2	609	CLA	CBD-CGD-O2D-CED
18	2	608	CLA	C1A-C2A-CAA-CBA
18	2	608	CLA	C3A-C2A-CAA-CBA
18	3	603	CLA	C1A-C2A-CAA-CBA
18	3	603	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
18	4	604	CLA	CBD-CGD-O2D-CED
18	4	608	CLA	C1A-C2A-CAA-CBA
18	4	608	CLA	C3A-C2A-CAA-CBA
18	4	610	CLA	CHA-CBD-CGD-O1D
18	4	610	CLA	CHA-CBD-CGD-O2D
18	4	614	CLA	CBD-CGD-O2D-CED
18	4	613	CLA	C1A-C2A-CAA-CBA
18	A	804	CLA	CAD-CBD-CGD-O1D
18	A	804	CLA	CAD-CBD-CGD-O2D
18	A	802	CLA	C1A-C2A-CAA-CBA
18	A	802	CLA	C3A-C2A-CAA-CBA
18	A	819	CLA	C1A-C2A-CAA-CBA
18	A	819	CLA	C3A-C2A-CAA-CBA
18	A	819	CLA	C6-C7-C8-C9
18	A	833	CLA	C4-C3-C5-C6
18	A	828	CLA	CHA-CBD-CGD-O1D
18	A	806	CLA	C1A-C2A-CAA-CBA
18	A	806	CLA	C3A-C2A-CAA-CBA
18	A	806	CLA	CHA-CBD-CGD-O1D
18	A	806	CLA	CHA-CBD-CGD-O2D
18	A	806	CLA	CAD-CBD-CGD-O1D
18	A	830	CLA	C1A-C2A-CAA-CBA
18	A	830	CLA	C3A-C2A-CAA-CBA
18	A	830	CLA	CBA-CGA-O2A-C1
18	A	830	CLA	O1A-CGA-O2A-C1
18	A	830	CLA	O2A-C1-C2-C3
18	A	830	CLA	C2-C3-C5-C6
18	A	830	CLA	C4-C3-C5-C6
18	A	842	CLA	C1A-C2A-CAA-CBA
18	A	842	CLA	C3A-C2A-CAA-CBA
18	A	827	CLA	C1A-C2A-CAA-CBA
18	A	827	CLA	C3A-C2A-CAA-CBA
18	A	805	CLA	C3A-C2A-CAA-CBA
18	A	809	CLA	CHA-CBD-CGD-O1D
18	A	809	CLA	CHA-CBD-CGD-O2D
18	A	837	CLA	CHA-CBD-CGD-O1D
18	A	837	CLA	CHA-CBD-CGD-O2D
18	A	825	CLA	C1A-C2A-CAA-CBA
18	A	825	CLA	C3A-C2A-CAA-CBA
18	A	825	CLA	CHA-CBD-CGD-O1D
18	A	839	CLA	C2-C3-C5-C6
18	A	839	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
18	A	816	CLA	C3A-C2A-CAA-CBA
18	A	816	CLA	CHA-CBD-CGD-O1D
18	A	816	CLA	CHA-CBD-CGD-O2D
18	A	820	CLA	C3A-C2A-CAA-CBA
18	A	818	CLA	CBD-CGD-O2D-CED
18	A	843	CLA	C1A-C2A-CAA-CBA
18	A	843	CLA	C3A-C2A-CAA-CBA
18	A	843	CLA	C2-C1-O2A-CGA
18	A	829	CLA	CHA-CBD-CGD-O1D
18	A	829	CLA	CHA-CBD-CGD-O2D
18	A	829	CLA	CBD-CGD-O2D-CED
18	A	832	CLA	CHA-CBD-CGD-O1D
18	A	832	CLA	CHA-CBD-CGD-O2D
18	A	841	CLA	C1A-C2A-CAA-CBA
18	A	841	CLA	C3A-C2A-CAA-CBA
18	A	841	CLA	CHA-CBD-CGD-O1D
18	A	841	CLA	CHA-CBD-CGD-O2D
18	A	841	CLA	CBD-CGD-O2D-CED
18	A	813	CLA	CHA-CBD-CGD-O2D
18	B	802	CLA	C3A-C2A-CAA-CBA
18	B	808	CLA	C6-C7-C8-C9
18	B	814	CLA	C2-C3-C5-C6
18	B	814	CLA	C4-C3-C5-C6
18	B	814	CLA	C11-C10-C8-C9
18	B	803	CLA	CHA-CBD-CGD-O1D
18	B	803	CLA	CHA-CBD-CGD-O2D
18	B	803	CLA	CBD-CGD-O2D-CED
18	B	825	CLA	C1A-C2A-CAA-CBA
18	B	820	CLA	C3A-C2A-CAA-CBA
18	B	824	CLA	C2-C3-C5-C6
18	B	824	CLA	C4-C3-C5-C6
18	B	805	CLA	C3A-C2A-CAA-CBA
18	B	805	CLA	C11-C10-C8-C9
18	B	827	CLA	C1A-C2A-CAA-CBA
18	B	827	CLA	C3A-C2A-CAA-CBA
18	B	838	CLA	C1A-C2A-CAA-CBA
18	B	832	CLA	C1A-C2A-CAA-CBA
18	B	832	CLA	C3A-C2A-CAA-CBA
18	B	836	CLA	CHA-CBD-CGD-O2D
18	B	833	CLA	CHA-CBD-CGD-O1D
18	B	833	CLA	CHA-CBD-CGD-O2D
18	B	823	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
18	B	823	CLA	C3A-C2A-CAA-CBA
18	B	822	CLA	CBD-CGD-O2D-CED
18	B	809	CLA	C1A-C2A-CAA-CBA
18	B	809	CLA	C2-C3-C5-C6
18	B	809	CLA	C4-C3-C5-C6
18	B	810	CLA	C6-C7-C8-C10
18	B	818	CLA	C3A-C2A-CAA-CBA
18	B	818	CLA	C2-C3-C5-C6
18	B	818	CLA	C4-C3-C5-C6
18	B	828	CLA	C1A-C2A-CAA-CBA
18	B	828	CLA	C3A-C2A-CAA-CBA
18	B	828	CLA	CHA-CBD-CGD-O1D
18	B	828	CLA	CHA-CBD-CGD-O2D
18	F	302	CLA	CBD-CGD-O2D-CED
18	F	301	CLA	C2-C3-C5-C6
18	F	301	CLA	C4-C3-C5-C6
18	G	202	CLA	C1A-C2A-CAA-CBA
18	G	202	CLA	C3A-C2A-CAA-CBA
18	G	201	CLA	CBD-CGD-O2D-CED
18	H	201	CLA	CBD-CGD-O2D-CED
18	K	204	CLA	C1A-C2A-CAA-CBA
18	K	204	CLA	CBD-CGD-O2D-CED
18	K	203	CLA	C3A-C2A-CAA-CBA
18	L	304	CLA	C1A-C2A-CAA-CBA
18	L	304	CLA	C3A-C2A-CAA-CBA
18	L	303	CLA	C11-C12-C13-C14
19	1	614	XAT	C11-C12-C13-C20
19	1	614	XAT	O24-C26-C27-C28
19	2	617	XAT	O4-C6-C7-C8
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	C30-C31-C32-C33
19	2	617	XAT	C31-C32-C33-C34
19	2	617	XAT	C31-C32-C33-C40
19	2	617	XAT	C33-C34-C35-C15
19	4	617	XAT	O4-C6-C7-C8
19	4	617	XAT	C11-C12-C13-C14
19	4	617	XAT	C11-C12-C13-C20
20	1	615	LHG	O1-C1-C2-O2
20	1	615	LHG	C2-C3-O3-P

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Mol	Chain	Res	Type	Atoms
20	1	615	LHG	C4-O6-P-O5
20	1	615	LHG	O10-C23-O8-C6
20	1	615	LHG	C24-C23-O8-C6
20	2	618	LHG	C3-O3-P-O5
20	2	618	LHG	C3-O3-P-O6
20	2	618	LHG	C8-C7-O7-C5
20	2	618	LHG	O10-C23-O8-C6
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	852	LHG	C2-C3-O3-P
20	B	852	LHG	C3-O3-P-O5
20	B	852	LHG	C4-O6-P-O3
21	2	616	LUT	C21-C26-C27-C28
21	2	616	LUT	C25-C26-C27-C28
21	2	619	LUT	C1-C6-C7-C8
21	2	619	LUT	C5-C6-C7-C8
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	3	614	BCR	C37-C22-C23-C24
22	A	848	BCR	C5-C6-C7-C8
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	A	852	BCR	C21-C22-C23-C24
22	A	852	BCR	C37-C22-C23-C24
22	A	850	BCR	C7-C8-C9-C10
22	A	850	BCR	C7-C8-C9-C34
22	A	849	BCR	C23-C24-C25-C26
22	A	849	BCR	C23-C24-C25-C30
22	A	851	BCR	C11-C12-C13-C14
22	A	851	BCR	C11-C12-C13-C35
22	B	801	BCR	C1-C6-C7-C8
22	B	801	BCR	C5-C6-C7-C8
22	B	801	BCR	C7-C8-C9-C34
22	B	846	BCR	C37-C22-C23-C24
22	B	846	BCR	C23-C24-C25-C26
22	B	846	BCR	C23-C24-C25-C30
22	B	849	BCR	C20-C21-C22-C23
22	B	849	BCR	C20-C21-C22-C37

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Mol	Chain	Res	Type	Atoms
22	B	844	BCR	C12-C13-C14-C15
22	B	844	BCR	C35-C13-C14-C15
22	F	304	BCR	C15-C16-C17-C18
22	J	102	BCR	C7-C8-C9-C10
22	J	102	BCR	C7-C8-C9-C34
22	K	205	BCR	C10-C11-C12-C13
27	B	850	DGD	O2G-C2G-C3G-O3G
18	1	608	CLA	O1D-CGD-O2D-CED
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	B	822	CLA	O1D-CGD-O2D-CED
18	B	835	CLA	O1D-CGD-O2D-CED
18	H	201	CLA	O1D-CGD-O2D-CED
18	3	607	CLA	O1D-CGD-O2D-CED
18	4	609	CLA	O1D-CGD-O2D-CED
18	A	802	CLA	O1D-CGD-O2D-CED
18	A	818	CLA	O1D-CGD-O2D-CED
18	A	841	CLA	O1D-CGD-O2D-CED
18	B	803	CLA	O1D-CGD-O2D-CED
18	F	301	CLA	O1D-CGD-O2D-CED
18	K	204	CLA	O1D-CGD-O2D-CED
17	2	607	CHL	CBD-CGD-O2D-CED
17	3	606	CHL	CBD-CGD-O2D-CED
17	4	606	CHL	CBD-CGD-O2D-CED
18	1	605	CLA	CBD-CGD-O2D-CED
18	1	608	CLA	CBD-CGD-O2D-CED
18	2	608	CLA	CBD-CGD-O2D-CED
18	3	607	CLA	CBD-CGD-O2D-CED
18	3	608	CLA	CBD-CGD-O2D-CED
18	4	609	CLA	CBD-CGD-O2D-CED
18	4	612	CLA	CBD-CGD-O2D-CED
18	A	802	CLA	CBD-CGD-O2D-CED
18	A	824	CLA	CBD-CGD-O2D-CED
18	B	802	CLA	CBD-CGD-O2D-CED
18	B	830	CLA	CBD-CGD-O2D-CED
18	B	810	CLA	CBD-CGD-O2D-CED
18	B	835	CLA	CBD-CGD-O2D-CED
18	F	301	CLA	CBD-CGD-O2D-CED
18	3	602	CLA	O1A-CGA-O2A-C1
18	A	803	CLA	O1A-CGA-O2A-C1
18	1	602	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
18	1	605	CLA	O1D-CGD-O2D-CED
18	2	611	CLA	O1D-CGD-O2D-CED
18	3	608	CLA	O1D-CGD-O2D-CED
18	A	824	CLA	O1D-CGD-O2D-CED
18	F	302	CLA	O1D-CGD-O2D-CED
18	1	611	CLA	O1D-CGD-O2D-CED
18	2	612	CLA	O1D-CGD-O2D-CED
18	4	614	CLA	O1D-CGD-O2D-CED
18	A	829	CLA	O1D-CGD-O2D-CED
18	G	201	CLA	O1D-CGD-O2D-CED
18	3	602	CLA	CBA-CGA-O2A-C1
18	A	803	CLA	CBA-CGA-O2A-C1
17	2	615	CHL	CBD-CGD-O2D-CED
18	2	604	CLA	CBD-CGD-O2D-CED
18	A	832	CLA	CBD-CGD-O2D-CED
18	A	814	CLA	CBD-CGD-O2D-CED
18	A	811	CLA	CBD-CGD-O2D-CED
18	B	816	CLA	CBD-CGD-O2D-CED
18	A	839	CLA	O1A-CGA-O2A-C1
18	A	820	CLA	O1A-CGA-O2A-C1
18	B	802	CLA	O1A-CGA-O2A-C1
18	1	609	CLA	O1D-CGD-O2D-CED
17	4	607	CHL	O1D-CGD-O2D-CED
18	B	814	CLA	CBD-CGD-O2D-CED
20	2	618	LHG	O9-C7-O7-C5
18	4	602	CLA	C3-C5-C6-C7
18	A	828	CLA	C3-C5-C6-C7
18	A	830	CLA	C3-C5-C6-C7
18	A	807	CLA	C3-C5-C6-C7
18	A	803	CLA	C3-C5-C6-C7
18	A	844	CLA	C3-C5-C6-C7
18	A	843	CLA	C3-C5-C6-C7
18	A	829	CLA	C3-C5-C6-C7
18	A	814	CLA	C3-C5-C6-C7
18	B	808	CLA	C3-C5-C6-C7
18	B	814	CLA	C3-C5-C6-C7
18	B	840	CLA	C3-C5-C6-C7
18	B	822	CLA	C3-C5-C6-C7
18	H	201	CLA	C3-C5-C6-C7
18	A	839	CLA	CBA-CGA-O2A-C1
18	B	802	CLA	CBA-CGA-O2A-C1
20	B	851	LHG	C8-C7-O7-C5

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Mol	Chain	Res	Type	Atoms
17	3	606	CHL	O1D-CGD-O2D-CED
18	A	813	CLA	CBD-CGD-O2D-CED
18	B	836	CLA	O1A-CGA-O2A-C1
17	1	601	CHL	C4-C3-C5-C6
18	2	602	CLA	C4-C3-C5-C6
18	A	833	CLA	C2-C3-C5-C6
18	B	815	CLA	CBD-CGD-O2D-CED
17	2	607	CHL	C2A-CAA-CBA-CGA
17	2	601	CHL	C2A-CAA-CBA-CGA
18	2	603	CLA	C2A-CAA-CBA-CGA
18	A	830	CLA	C2A-CAA-CBA-CGA
18	A	838	CLA	C2A-CAA-CBA-CGA
18	B	802	CLA	C2A-CAA-CBA-CGA
18	B	813	CLA	C2A-CAA-CBA-CGA
18	B	817	CLA	C2A-CAA-CBA-CGA
18	B	839	CLA	C2A-CAA-CBA-CGA
18	H	201	CLA	C2A-CAA-CBA-CGA
24	A	801	CL0	C2A-CAA-CBA-CGA
18	2	609	CLA	O1A-CGA-O2A-C1
18	L	303	CLA	O1A-CGA-O2A-C1
18	B	827	CLA	C3-C5-C6-C7
18	2	609	CLA	CBA-CGA-O2A-C1
18	A	820	CLA	CBA-CGA-O2A-C1
18	B	827	CLA	CBA-CGA-O2A-C1
18	L	303	CLA	CBA-CGA-O2A-C1
18	1	604	CLA	CBD-CGD-O2D-CED
18	K	203	CLA	CBD-CGD-O2D-CED
18	2	608	CLA	O1D-CGD-O2D-CED
20	B	851	LHG	O9-C7-O7-C5
18	A	818	CLA	O1A-CGA-O2A-C1
18	A	843	CLA	O1A-CGA-O2A-C1
18	A	811	CLA	O1A-CGA-O2A-C1
18	B	827	CLA	O1A-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	850	BCR	C13-C14-C15-C16
22	A	850	BCR	C15-C16-C17-C18
22	A	853	BCR	C9-C10-C11-C12
22	A	849	BCR	C15-C16-C17-C18
22	A	849	BCR	C19-C20-C21-C22
22	A	851	BCR	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
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
17	2	601	CHL	CBD-CGD-O2D-CED
18	A	803	CLA	CBD-CGD-O2D-CED
18	B	823	CLA	CBD-CGD-O2D-CED
18	A	818	CLA	C3-C5-C6-C7
18	1	603	CLA	CBA-CGA-O2A-C1
18	A	818	CLA	CBA-CGA-O2A-C1
18	B	836	CLA	CBA-CGA-O2A-C1
18	4	612	CLA	O1D-CGD-O2D-CED
18	B	827	CLA	CBD-CGD-O2D-CED
17	4	606	CHL	O1D-CGD-O2D-CED
18	B	830	CLA	O1D-CGD-O2D-CED
18	B	810	CLA	O1D-CGD-O2D-CED
18	A	819	CLA	C3-C5-C6-C7
18	B	806	CLA	C3-C5-C6-C7
18	1	604	CLA	CBA-CGA-O2A-C1
18	A	843	CLA	CBA-CGA-O2A-C1
18	A	811	CLA	CBA-CGA-O2A-C1
17	2	607	CHL	O1D-CGD-O2D-CED
20	1	615	LHG	C5-C4-O6-P
18	A	819	CLA	C4-C3-C5-C6
26	B	842	PQN	C14-C13-C15-C16
18	2	602	CLA	C2-C3-C5-C6
18	A	819	CLA	C2-C3-C5-C6
26	B	842	PQN	C12-C13-C15-C16
18	A	838	CLA	CBD-CGD-O2D-CED
18	A	809	CLA	C2A-CAA-CBA-CGA
18	A	843	CLA	C2A-CAA-CBA-CGA
18	1	603	CLA	O1A-CGA-O2A-C1
18	B	822	CLA	CBA-CGA-O2A-C1
18	A	814	CLA	O1D-CGD-O2D-CED
18	1	604	CLA	O1A-CGA-O2A-C1
20	1	615	LHG	C1-C2-C3-O3
18	2	612	CLA	C3-C5-C6-C7
18	A	841	CLA	C3-C5-C6-C7
18	L	303	CLA	C3-C5-C6-C7
18	A	832	CLA	O1D-CGD-O2D-CED
18	1	602	CLA	CBA-CGA-O2A-C1
18	A	802	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
18	A	835	CLA	CBA-CGA-O2A-C1
18	A	842	CLA	CBA-CGA-O2A-C1
18	A	825	CLA	CBA-CGA-O2A-C1
18	A	814	CLA	CBA-CGA-O2A-C1
18	B	814	CLA	CBA-CGA-O2A-C1
18	B	840	CLA	CBA-CGA-O2A-C1
18	B	811	CLA	CBA-CGA-O2A-C1
18	F	301	CLA	CBA-CGA-O2A-C1
18	A	835	CLA	C8-C10-C11-C12
18	A	822	CLA	C15-C16-C17-C18
18	B	802	CLA	C15-C16-C17-C18
18	B	814	CLA	O1A-CGA-O2A-C1
18	B	811	CLA	O1A-CGA-O2A-C1
18	F	301	CLA	O1A-CGA-O2A-C1
17	1	601	CHL	C2-C3-C5-C6
18	3	601	CLA	C11-C10-C8-C9
18	4	612	CLA	C6-C7-C8-C9
18	A	826	CLA	C11-C10-C8-C9
18	A	835	CLA	C11-C10-C8-C9
18	A	807	CLA	C11-C10-C8-C9
18	A	803	CLA	C6-C7-C8-C9
18	A	812	CLA	C6-C7-C8-C9
18	A	820	CLA	C11-C10-C8-C9
18	A	841	CLA	C14-C13-C15-C16
18	B	802	CLA	C11-C12-C13-C14
18	B	808	CLA	C14-C13-C15-C16
18	B	825	CLA	C11-C10-C8-C9
18	B	825	CLA	C11-C12-C13-C14
18	B	805	CLA	C6-C7-C8-C9
18	B	805	CLA	C14-C13-C15-C16
18	B	840	CLA	C6-C7-C8-C9
18	B	809	CLA	C6-C7-C8-C9
18	H	201	CLA	C6-C7-C8-C9
18	A	812	CLA	CBD-CGD-O2D-CED
18	4	602	CLA	C5-C6-C7-C8
18	A	802	CLA	C13-C15-C16-C17
18	A	812	CLA	C10-C11-C12-C13
18	A	839	CLA	C2A-CAA-CBA-CGA
18	A	829	CLA	C2A-CAA-CBA-CGA
18	A	814	CLA	C2A-CAA-CBA-CGA
18	B	820	CLA	C2A-CAA-CBA-CGA
19	1	614	XAT	C31-C32-C33-C40

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Mol	Chain	Res	Type	Atoms
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	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	L	306	BCR	C7-C8-C9-C34
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	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	L	306	BCR	C7-C8-C9-C10
22	L	306	BCR	C21-C22-C23-C24
18	B	840	CLA	O1A-CGA-O2A-C1
18	B	808	CLA	C13-C15-C16-C17
18	B	837	CLA	C15-C16-C17-C18
18	B	841	CLA	C8-C10-C11-C12
18	4	601	CLA	CBA-CGA-O2A-C1
18	B	841	CLA	CBD-CGD-O2D-CED
18	A	819	CLA	CBA-CGA-O2A-C1
18	A	822	CLA	CBA-CGA-O2A-C1
18	B	813	CLA	CBA-CGA-O2A-C1
18	A	820	CLA	C5-C6-C7-C8
18	B	822	CLA	C13-C15-C16-C17
18	B	826	CLA	C5-C6-C7-C8
18	B	809	CLA	C5-C6-C7-C8
18	A	825	CLA	O1A-CGA-O2A-C1
18	A	826	CLA	C8-C10-C11-C12
18	A	828	CLA	C5-C6-C7-C8
18	A	806	CLA	C10-C11-C12-C13
18	A	806	CLA	C13-C15-C16-C17
18	B	805	CLA	C5-C6-C7-C8
18	B	837	CLA	C5-C6-C7-C8
18	L	303	CLA	C10-C11-C12-C13
17	2	615	CHL	O1D-CGD-O2D-CED
20	1	615	LHG	C7-C8-C9-C10
20	B	851	LHG	C23-C24-C25-C26
18	2	612	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
18	A	807	CLA	C5-C6-C7-C8
18	B	824	CLA	C8-C10-C11-C12
18	B	826	CLA	C8-C10-C11-C12
18	A	832	CLA	CBA-CGA-O2A-C1
18	A	811	CLA	O1D-CGD-O2D-CED
17	2	606	CHL	CBD-CGD-O2D-CED
18	2	602	CLA	CBD-CGD-O2D-CED
18	B	809	CLA	CBD-CGD-O2D-CED
18	B	831	CLA	C2A-CAA-CBA-CGA
20	1	615	LHG	C11-C10-C9-C8
18	A	803	CLA	C8-C10-C11-C12
18	B	832	CLA	C15-C16-C17-C18
18	2	604	CLA	O1D-CGD-O2D-CED
18	2	602	CLA	C6-C7-C8-C10
18	A	804	CLA	C6-C7-C8-C10
18	B	802	CLA	C11-C10-C8-C7
18	B	827	CLA	C11-C12-C13-C15
18	1	602	CLA	O1A-CGA-O2A-C1
18	A	835	CLA	O1A-CGA-O2A-C1
18	A	814	CLA	O1A-CGA-O2A-C1
17	1	601	CHL	C2A-CAA-CBA-CGA
18	A	818	CLA	C2A-CAA-CBA-CGA
18	B	832	CLA	C2A-CAA-CBA-CGA
18	B	816	CLA	O1D-CGD-O2D-CED
18	2	602	CLA	C15-C16-C17-C18
18	A	812	CLA	C5-C6-C7-C8
18	B	813	CLA	C13-C15-C16-C17
18	B	827	CLA	C8-C10-C11-C12
18	B	828	CLA	C5-C6-C7-C8
18	B	828	CLA	C10-C11-C12-C13
18	B	828	CLA	C13-C15-C16-C17
18	H	201	CLA	C8-C10-C11-C12
18	A	823	CLA	CBD-CGD-O2D-CED
19	2	617	XAT	C10-C11-C12-C13
18	B	814	CLA	O1D-CGD-O2D-CED
20	1	615	LHG	O2-C2-C3-O3
18	1	602	CLA	C3-C5-C6-C7
18	A	828	CLA	C8-C10-C11-C12
18	A	841	CLA	C5-C6-C7-C8
18	B	814	CLA	C8-C10-C11-C12
18	A	842	CLA	O1A-CGA-O2A-C1
18	B	822	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
18	A	819	CLA	C5-C6-C7-C8
18	A	835	CLA	C10-C11-C12-C13
18	A	812	CLA	C8-C10-C11-C12
18	A	829	CLA	C15-C16-C17-C18
18	B	814	CLA	C5-C6-C7-C8
18	B	805	CLA	C13-C15-C16-C17
18	B	840	CLA	C5-C6-C7-C8
18	B	811	CLA	C5-C6-C7-C8
18	A	802	CLA	O1A-CGA-O2A-C1
18	A	819	CLA	O1A-CGA-O2A-C1
18	A	822	CLA	O1A-CGA-O2A-C1
18	B	813	CLA	O1A-CGA-O2A-C1
18	A	806	CLA	C15-C16-C17-C18
18	A	842	CLA	C8-C10-C11-C12
18	B	813	CLA	C15-C16-C17-C18
18	B	841	CLA	C13-C15-C16-C17
20	1	615	LHG	C3-O3-P-O6
18	B	837	CLA	C3-C5-C6-C7
17	1	601	CHL	CBA-CGA-O2A-C1
18	B	805	CLA	C8-C10-C11-C12
18	A	813	CLA	O1D-CGD-O2D-CED
18	1	603	CLA	C4-C3-C5-C6
18	B	822	CLA	C10-C11-C12-C13
18	3	609	CLA	C2A-CAA-CBA-CGA
18	A	819	CLA	C2A-CAA-CBA-CGA
18	B	809	CLA	C2A-CAA-CBA-CGA
18	B	828	CLA	C2A-CAA-CBA-CGA
18	G	203	CLA	C2A-CAA-CBA-CGA
18	G	201	CLA	C2A-CAA-CBA-CGA
18	A	838	CLA	CBA-CGA-O2A-C1
24	A	801	CL0	C10-C11-C12-C13
20	1	615	LHG	C33-C34-C35-C36
18	4	608	CLA	CBD-CGD-O2D-CED
18	B	839	CLA	C5-C6-C7-C8
19	2	617	XAT	C11-C10-C9-C19
19	2	617	XAT	C20-C13-C14-C15
21	3	613	LUT	C11-C10-C9-C19
22	A	852	BCR	C35-C13-C14-C15
22	B	844	BCR	C16-C17-C18-C36
22	F	304	BCR	C11-C10-C9-C34
22	F	304	BCR	C35-C13-C14-C15
18	B	802	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
18	B	815	CLA	O1D-CGD-O2D-CED
18	A	839	CLA	C6-C7-C8-C10
18	B	824	CLA	C16-C17-C18-C20
18	B	840	CLA	C16-C17-C18-C20
18	B	841	CLA	CBA-CGA-O2A-C1
18	1	604	CLA	O1D-CGD-O2D-CED
26	A	855	PQN	C25-C26-C27-C28
20	1	615	LHG	C28-C29-C30-C31
18	K	203	CLA	O1D-CGD-O2D-CED
18	A	832	CLA	O1A-CGA-O2A-C1
20	1	615	LHG	C24-C25-C26-C27
19	2	617	XAT	C11-C10-C9-C8
19	2	617	XAT	C12-C13-C14-C15
21	3	613	LUT	C11-C10-C9-C8
22	A	852	BCR	C12-C13-C14-C15
22	B	844	BCR	C16-C17-C18-C19
22	F	304	BCR	C11-C10-C9-C8
22	F	304	BCR	C12-C13-C14-C15
23	4	620	LMG	C2-C1-O1-C7
18	L	303	CLA	C8-C10-C11-C12
18	A	822	CLA	C2-C3-C5-C6
18	A	809	CLA	C11-C12-C13-C14
18	A	820	CLA	C11-C12-C13-C14
18	B	806	CLA	C6-C7-C8-C9
18	B	810	CLA	C14-C13-C15-C16
18	B	803	CLA	C13-C15-C16-C17
18	4	603	CLA	C2A-CAA-CBA-CGA
18	B	841	CLA	C2A-CAA-CBA-CGA
17	1	601	CHL	O1A-CGA-O2A-C1
20	1	615	LHG	O1-C1-C2-C3
19	1	614	XAT	C11-C12-C13-C14
18	2	602	CLA	C3-C5-C6-C7
18	A	834	CLA	C3-C5-C6-C7
18	A	814	CLA	C13-C15-C16-C17
18	B	805	CLA	C10-C11-C12-C13
27	B	850	DGD	C2B-C1B-O2G-C2G
20	1	615	LHG	C11-C12-C13-C14
18	2	612	CLA	C16-C17-C18-C19
18	A	839	CLA	C6-C7-C8-C9
18	B	824	CLA	C16-C17-C18-C19
18	B	840	CLA	C16-C17-C18-C19
18	A	820	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
20	1	615	LHG	C27-C28-C29-C30
27	B	850	DGD	C9A-CAA-CBA-CCA
18	A	804	CLA	C10-C11-C12-C13
18	A	838	CLA	O1A-CGA-O2A-C1
18	B	819	CLA	CBD-CGD-O2D-CED
18	1	604	CLA	C3A-C2A-CAA-CBA
18	1	605	CLA	C3A-C2A-CAA-CBA
18	1	612	CLA	C3A-C2A-CAA-CBA
18	2	611	CLA	C3A-C2A-CAA-CBA
18	A	815	CLA	C3A-C2A-CAA-CBA
18	A	810	CLA	C3A-C2A-CAA-CBA
18	B	821	CLA	C3A-C2A-CAA-CBA
18	B	825	CLA	C3A-C2A-CAA-CBA
18	B	824	CLA	C3A-C2A-CAA-CBA
18	B	838	CLA	C3A-C2A-CAA-CBA
18	B	815	CLA	C3A-C2A-CAA-CBA
18	B	822	CLA	C3A-C2A-CAA-CBA
18	B	809	CLA	C3A-C2A-CAA-CBA
18	B	810	CLA	C3A-C2A-CAA-CBA
18	A	843	CLA	C5-C6-C7-C8
17	2	601	CHL	O1D-CGD-O2D-CED
18	2	612	CLA	C16-C17-C18-C20
18	A	812	CLA	C16-C17-C18-C20
20	1	615	LHG	C25-C26-C27-C28
18	B	823	CLA	O1D-CGD-O2D-CED
27	B	850	DGD	O1B-C1B-O2G-C2G
18	3	602	CLA	CBD-CGD-O2D-CED
18	A	820	CLA	CBD-CGD-O2D-CED
22	B	844	BCR	C14-C15-C16-C17
18	3	602	CLA	C4-C3-C5-C6
18	3	601	CLA	C4-C3-C5-C6
18	A	804	CLA	C4-C3-C5-C6
18	A	822	CLA	C4-C3-C5-C6
18	3	601	CLA	C2-C3-C5-C6
18	A	804	CLA	C2-C3-C5-C6
18	A	803	CLA	O1D-CGD-O2D-CED
18	1	611	CLA	C2A-CAA-CBA-CGA
18	B	841	CLA	C16-C17-C18-C20
18	B	805	CLA	C3-C5-C6-C7
18	B	841	CLA	O1A-CGA-O2A-C1
20	1	615	LHG	C14-C15-C16-C17
18	A	812	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
18	L	303	CLA	C15-C16-C17-C18
18	B	832	CLA	C3-C5-C6-C7
21	1	616	LUT	C5-C6-C7-C8
21	4	616	LUT	C5-C6-C7-C8
22	4	618	BCR	C1-C6-C7-C8
22	4	618	BCR	C5-C6-C7-C8
22	4	618	BCR	C23-C24-C25-C26
22	A	848	BCR	C1-C6-C7-C8
22	A	852	BCR	C5-C6-C7-C8
22	B	849	BCR	C23-C24-C25-C26
22	B	845	BCR	C5-C6-C7-C8
22	B	844	BCR	C23-C24-C25-C26
22	B	844	BCR	C23-C24-C25-C30
22	G	204	BCR	C23-C24-C25-C26
22	G	204	BCR	C23-C24-C25-C30
18	B	806	CLA	C5-C6-C7-C8
20	1	615	LHG	C26-C27-C28-C29
18	3	601	CLA	C11-C10-C8-C7
18	A	826	CLA	C11-C10-C8-C7
18	A	807	CLA	C11-C10-C8-C7
18	A	809	CLA	C11-C12-C13-C15
18	A	803	CLA	C6-C7-C8-C10
18	A	829	CLA	C11-C10-C8-C7
18	A	831	CLA	C11-C10-C8-C7
18	A	831	CLA	C12-C13-C15-C16
18	B	805	CLA	C11-C12-C13-C15
18	B	806	CLA	C6-C7-C8-C10
18	B	806	CLA	C11-C12-C13-C15
18	B	827	CLA	C12-C13-C15-C16
18	B	810	CLA	C12-C13-C15-C16
18	4	601	CLA	O1A-CGA-O2A-C1
18	A	834	CLA	CBA-CGA-O2A-C1
18	A	813	CLA	CBA-CGA-O2A-C1
18	B	829	CLA	CBA-CGA-O2A-C1
18	1	602	CLA	C2A-CAA-CBA-CGA
18	A	802	CLA	C2A-CAA-CBA-CGA
18	A	806	CLA	C2A-CAA-CBA-CGA
18	A	832	CLA	C2A-CAA-CBA-CGA
18	B	811	CLA	C2A-CAA-CBA-CGA
18	H	201	CLA	C5-C6-C7-C8
18	A	806	CLA	C8-C10-C11-C12
18	1	603	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
22	B	801	BCR	C6-C7-C8-C9
17	2	605	CHL	CBD-CGD-O2D-CED
18	A	811	CLA	C16-C17-C18-C19
18	A	838	CLA	O1D-CGD-O2D-CED
22	L	301	BCR	C18-C19-C20-C21
18	A	812	CLA	C13-C15-C16-C17
18	B	827	CLA	O1D-CGD-O2D-CED
23	4	619	LMG	C2-C1-O1-C7
18	B	828	CLA	C15-C16-C17-C18
23	4	619	LMG	O6-C5-C6-O5
18	B	811	CLA	C4-C3-C5-C6
18	1	603	CLA	C2-C3-C5-C6
18	B	827	CLA	C2-C3-C5-C6
18	2	602	CLA	C6-C7-C8-C9
18	A	806	CLA	C11-C10-C8-C9
18	A	831	CLA	C14-C13-C15-C16
18	B	802	CLA	C11-C10-C8-C9
18	B	814	CLA	C11-C12-C13-C14
18	B	805	CLA	C11-C12-C13-C14
18	B	806	CLA	C11-C12-C13-C14
18	A	826	CLA	C3-C5-C6-C7
18	B	803	CLA	C3-C5-C6-C7
18	B	816	CLA	C3-C5-C6-C7
18	4	604	CLA	C2A-CAA-CBA-CGA
18	A	813	CLA	C2A-CAA-CBA-CGA
18	B	818	CLA	C2A-CAA-CBA-CGA
20	1	615	LHG	C13-C14-C15-C16
18	B	841	CLA	C10-C11-C12-C13
20	1	615	LHG	C16-C17-C18-C19
17	4	607	CHL	C1A-C2A-CAA-CBA
18	1	605	CLA	C1A-C2A-CAA-CBA
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	609	CLA	C1A-C2A-CAA-CBA
18	4	604	CLA	C1A-C2A-CAA-CBA
18	A	805	CLA	C1A-C2A-CAA-CBA
18	A	812	CLA	C1A-C2A-CAA-CBA
18	A	815	CLA	C1A-C2A-CAA-CBA
18	A	820	CLA	C1A-C2A-CAA-CBA
18	A	810	CLA	C1A-C2A-CAA-CBA
18	B	802	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
18	B	821	CLA	C1A-C2A-CAA-CBA
18	B	820	CLA	C1A-C2A-CAA-CBA
18	B	824	CLA	C1A-C2A-CAA-CBA
18	B	805	CLA	C1A-C2A-CAA-CBA
18	B	815	CLA	C1A-C2A-CAA-CBA
18	B	822	CLA	C1A-C2A-CAA-CBA
18	B	810	CLA	C1A-C2A-CAA-CBA
18	B	818	CLA	C1A-C2A-CAA-CBA
18	F	302	CLA	C1A-C2A-CAA-CBA
18	H	201	CLA	C1A-C2A-CAA-CBA
18	K	203	CLA	C1A-C2A-CAA-CBA
18	B	816	CLA	C6-C7-C8-C10
18	B	841	CLA	C16-C17-C18-C19
20	1	615	LHG	C29-C30-C31-C32
18	3	601	CLA	C8-C10-C11-C12
18	A	818	CLA	C5-C6-C7-C8
18	A	814	CLA	C10-C11-C12-C13
24	A	801	CL0	C3-C5-C6-C7
18	A	813	CLA	O1A-CGA-O2A-C1
18	B	825	CLA	CBA-CGA-O2A-C1
18	B	827	CLA	C10-C11-C12-C13
18	B	827	CLA	C4-C3-C5-C6
18	A	835	CLA	C2-C3-C5-C6
18	B	835	CLA	C3A-C2A-CAA-CBA
18	A	830	CLA	C8-C10-C11-C12
18	A	834	CLA	O1A-CGA-O2A-C1
18	B	816	CLA	C2A-CAA-CBA-CGA
18	A	809	CLA	C16-C17-C18-C20
18	H	201	CLA	C11-C12-C13-C14
18	3	601	CLA	C3-C5-C6-C7
20	B	852	LHG	C4-C5-C6-O8
18	A	809	CLA	CBA-CGA-O2A-C1
18	B	810	CLA	C5-C6-C7-C8
18	B	829	CLA	O1A-CGA-O2A-C1
27	B	850	DGD	CCA-CDA-CEA-CFA
18	B	825	CLA	C10-C11-C12-C13
18	B	829	CLA	C11-C10-C8-C9
27	B	850	DGD	O6D-C1D-O3G-C3G
20	1	615	LHG	C35-C36-C37-C38
18	B	817	CLA	CBA-CGA-O2A-C1
24	A	801	CL0	CAA-CBA-CGA-O2A
18	A	807	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
18	B	817	CLA	C5-C6-C7-C8
18	A	835	CLA	C4-C3-C5-C6
18	A	803	CLA	C4-C3-C5-C6
18	B	813	CLA	C4-C3-C5-C6
18	A	803	CLA	C2-C3-C5-C6
18	B	813	CLA	C2-C3-C5-C6
18	B	816	CLA	C6-C7-C8-C9
18	B	827	CLA	C16-C17-C18-C20
18	A	812	CLA	CBA-CGA-O2A-C1
20	B	851	LHG	C26-C27-C28-C29
20	2	618	LHG	C6-C5-O7-C7
18	2	612	CLA	C13-C15-C16-C17
18	A	807	CLA	C2-C1-O2A-CGA
18	A	820	CLA	C2-C1-O2A-CGA
18	A	814	CLA	C2-C1-O2A-CGA
18	B	827	CLA	C2-C1-O2A-CGA
18	B	809	CLA	O1D-CGD-O2D-CED
18	A	819	CLA	C11-C12-C13-C14
18	2	602	CLA	O1D-CGD-O2D-CED
18	A	812	CLA	O1D-CGD-O2D-CED
18	B	824	CLA	CBA-CGA-O2A-C1
18	B	805	CLA	CBA-CGA-O2A-C1
24	A	801	CL0	CBA-CGA-O2A-C1
18	1	609	CLA	C2A-CAA-CBA-CGA
18	A	812	CLA	C15-C16-C17-C18
17	2	606	CHL	O1D-CGD-O2D-CED
18	B	825	CLA	O1A-CGA-O2A-C1
18	3	602	CLA	C3-C5-C6-C7
18	A	835	CLA	C15-C16-C17-C18
18	A	844	CLA	C5-C6-C7-C8
17	1	601	CHL	C3-C5-C6-C7
18	A	840	CLA	C3-C5-C6-C7
18	4	601	CLA	CAA-CBA-CGA-O2A
18	B	827	CLA	C15-C16-C17-C18
23	4	619	LMG	C30-C31-C32-C33
18	2	602	CLA	C12-C13-C15-C16
18	A	804	CLA	C12-C13-C15-C16
18	A	835	CLA	C11-C10-C8-C7
18	A	835	CLA	C11-C12-C13-C15
18	A	842	CLA	C11-C10-C8-C7
18	A	803	CLA	C11-C12-C13-C15
18	A	812	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
18	A	844	CLA	C12-C13-C15-C16
18	B	802	CLA	C11-C12-C13-C15
18	B	808	CLA	C12-C13-C15-C16
18	B	814	CLA	C11-C10-C8-C7
18	B	814	CLA	C11-C12-C13-C15
18	B	824	CLA	C12-C13-C15-C16
18	B	817	CLA	C6-C7-C8-C10
18	B	841	CLA	C6-C7-C8-C10
18	B	841	CLA	C12-C13-C15-C16
18	B	809	CLA	C12-C13-C15-C16
18	H	201	CLA	C6-C7-C8-C10
18	L	303	CLA	C11-C12-C13-C15
24	A	801	CL0	C11-C12-C13-C15
23	4	620	LMG	O7-C10-C11-C12
18	A	804	CLA	C14-C13-C15-C16
18	A	806	CLA	C14-C13-C15-C16
18	A	835	CLA	C11-C12-C13-C14
18	A	842	CLA	C11-C10-C8-C9
18	A	803	CLA	C11-C12-C13-C14
18	A	803	CLA	C14-C13-C15-C16
18	A	812	CLA	C14-C13-C15-C16
18	A	844	CLA	C14-C13-C15-C16
18	A	818	CLA	C6-C7-C8-C9
18	A	818	CLA	C11-C10-C8-C9
18	A	814	CLA	C14-C13-C15-C16
18	A	831	CLA	C11-C10-C8-C9
18	B	808	CLA	C11-C12-C13-C14
18	B	824	CLA	C14-C13-C15-C16
18	B	827	CLA	C14-C13-C15-C16
18	B	841	CLA	C6-C7-C8-C9
18	B	841	CLA	C11-C12-C13-C14
18	B	809	CLA	C14-C13-C15-C16
18	B	834	CLA	C6-C7-C8-C9
18	2	611	CLA	C2A-CAA-CBA-CGA
18	A	823	CLA	O1D-CGD-O2D-CED
18	B	841	CLA	O1D-CGD-O2D-CED
22	K	205	BCR	C7-C8-C9-C34
18	B	827	CLA	C16-C17-C18-C19
22	B	846	BCR	C21-C22-C23-C24
18	A	811	CLA	C8-C10-C11-C12
18	B	817	CLA	O1A-CGA-O2A-C1
18	A	829	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
20	1	615	LHG	O6-C4-C5-C6
18	B	816	CLA	C5-C6-C7-C8
18	B	821	CLA	CAA-CBA-CGA-O2A
18	A	844	CLA	C4-C3-C5-C6
18	3	602	CLA	C2-C3-C5-C6
20	1	615	LHG	C18-C19-C20-C21
20	A	846	LHG	C27-C28-C29-C30
18	B	802	CLA	C8-C10-C11-C12
18	A	809	CLA	O1A-CGA-O2A-C1
18	1	605	CLA	CBA-CGA-O2A-C1
18	4	612	CLA	CBA-CGA-O2A-C1
18	A	806	CLA	CBA-CGA-O2A-C1
18	B	826	CLA	CBA-CGA-O2A-C1
27	B	850	DGD	C5B-C6B-C7B-C8B
20	2	618	LHG	C5-C4-O6-P
20	B	852	LHG	C5-C4-O6-P
18	A	813	CLA	C3A-C2A-CAA-CBA
18	B	819	CLA	C3A-C2A-CAA-CBA
18	H	201	CLA	C3A-C2A-CAA-CBA
18	K	204	CLA	C3A-C2A-CAA-CBA
18	4	608	CLA	O1D-CGD-O2D-CED
18	A	804	CLA	C8-C10-C11-C12
18	A	809	CLA	C16-C17-C18-C19
18	H	201	CLA	C11-C12-C13-C15
18	A	826	CLA	CBA-CGA-O2A-C1
18	A	814	CLA	C15-C16-C17-C18
18	2	604	CLA	C2A-CAA-CBA-CGA
27	B	850	DGD	C1G-C2G-C3G-O3G
24	A	801	CL0	O1A-CGA-O2A-C1
18	A	828	CLA	C15-C16-C17-C18
18	B	817	CLA	CAA-CBA-CGA-O2A
17	2	605	CHL	C3C-C2C-CMC-OMC
18	B	805	CLA	O1A-CGA-O2A-C1
18	A	833	CLA	C3-C5-C6-C7
18	1	612	CLA	C2A-CAA-CBA-CGA
18	2	612	CLA	C5-C6-C7-C8
18	2	602	CLA	CBA-CGA-O2A-C1
18	A	812	CLA	O1A-CGA-O2A-C1
18	B	824	CLA	O1A-CGA-O2A-C1
18	A	812	CLA	C16-C17-C18-C19
18	A	819	CLA	C8-C10-C11-C12
18	L	303	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
17	2	605	CHL	O1D-CGD-O2D-CED
18	1	603	CLA	C6-C7-C8-C9
18	A	811	CLA	C16-C17-C18-C20
18	4	612	CLA	C5-C6-C7-C8
18	A	804	CLA	C5-C6-C7-C8
18	A	806	CLA	CBD-CGD-O2D-CED
18	A	819	CLA	C11-C10-C8-C9
18	A	826	CLA	C11-C12-C13-C14
18	A	828	CLA	C11-C10-C8-C9
18	A	809	CLA	C11-C10-C8-C9
18	A	843	CLA	C6-C7-C8-C9
18	B	806	CLA	C14-C13-C15-C16
24	A	801	CL0	C6-C7-C8-C9
20	2	618	LHG	C2-C3-O3-P
18	3	602	CLA	C2A-CAA-CBA-CGA
18	4	612	CLA	C2A-CAA-CBA-CGA
18	A	820	CLA	O1D-CGD-O2D-CED
21	1	616	LUT	C1-C6-C7-C8
21	4	616	LUT	C1-C6-C7-C8
22	4	618	BCR	C23-C24-C25-C30
22	A	852	BCR	C1-C6-C7-C8
22	F	304	BCR	C1-C6-C7-C8
22	F	304	BCR	C5-C6-C7-C8
18	3	602	CLA	O1D-CGD-O2D-CED
19	1	614	XAT	C31-C32-C33-C34
22	4	618	BCR	C7-C8-C9-C10
22	B	801	BCR	C7-C8-C9-C10
18	B	819	CLA	O1D-CGD-O2D-CED
22	F	304	BCR	C14-C15-C16-C17
18	A	819	CLA	C6-C7-C8-C10
18	A	806	CLA	C12-C13-C15-C16
18	A	809	CLA	C11-C10-C8-C7
18	A	812	CLA	C12-C13-C15-C16
18	A	820	CLA	C11-C12-C13-C15
18	A	843	CLA	C6-C7-C8-C10
18	A	829	CLA	C6-C7-C8-C10
18	A	814	CLA	C12-C13-C15-C16
18	A	841	CLA	C12-C13-C15-C16
18	B	808	CLA	C6-C7-C8-C10
18	B	808	CLA	C11-C12-C13-C15
18	B	825	CLA	C11-C10-C8-C7
18	B	825	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
18	B	805	CLA	C6-C7-C8-C10
18	B	805	CLA	C11-C10-C8-C7
18	B	840	CLA	C6-C7-C8-C10
18	B	828	CLA	C6-C7-C8-C10
18	B	834	CLA	C6-C7-C8-C10
18	H	201	CLA	C11-C10-C8-C7
18	1	607	CLA	C2A-CAA-CBA-CGA
22	4	618	BCR	C11-C10-C9-C34
22	A	849	BCR	C20-C21-C22-C37
22	K	205	BCR	C20-C21-C22-C37
18	A	843	CLA	CBD-CGD-O2D-CED
18	B	839	CLA	CBA-CGA-O2A-C1
18	B	837	CLA	CBA-CGA-O2A-C1
18	B	806	CLA	C8-C10-C11-C12
18	1	608	CLA	CAD-CBD-CGD-O2D
18	4	603	CLA	CAD-CBD-CGD-O2D
18	4	609	CLA	CAD-CBD-CGD-O2D
18	4	614	CLA	CAD-CBD-CGD-O2D
18	A	806	CLA	CAD-CBD-CGD-O2D
18	A	803	CLA	CAD-CBD-CGD-O2D
18	A	810	CLA	CAD-CBD-CGD-O2D
18	A	836	CLA	CAD-CBD-CGD-O2D
18	B	815	CLA	CAD-CBD-CGD-O2D
18	B	839	CLA	CAD-CBD-CGD-O2D
18	B	841	CLA	CAD-CBD-CGD-O2D
18	B	810	CLA	CAD-CBD-CGD-O2D
18	B	835	CLA	CAD-CBD-CGD-O2D
18	B	834	CLA	CAD-CBD-CGD-O2D
18	F	301	CLA	CAD-CBD-CGD-O2D
18	L	304	CLA	CAD-CBD-CGD-O2D
18	L	302	CLA	CAD-CBD-CGD-O2D
18	B	828	CLA	CBA-CGA-O2A-C1
18	F	302	CLA	CBA-CGA-O2A-C1
18	B	805	CLA	C4-C3-C5-C6
20	1	615	LHG	O6-C4-C5-O7
18	A	825	CLA	C2A-CAA-CBA-CGA
18	A	812	CLA	C2A-CAA-CBA-CGA
18	A	820	CLA	C2A-CAA-CBA-CGA
18	K	204	CLA	C2A-CAA-CBA-CGA
18	1	602	CLA	CHA-CBD-CGD-O1D
18	1	602	CLA	CHA-CBD-CGD-O2D
18	1	604	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
18	1	604	CLA	CHA-CBD-CGD-O2D
18	1	612	CLA	CHA-CBD-CGD-O1D
18	2	604	CLA	CHA-CBD-CGD-O1D
18	2	604	CLA	CHA-CBD-CGD-O2D
18	4	601	CLA	CHA-CBD-CGD-O1D
18	4	601	CLA	CHA-CBD-CGD-O2D
18	4	612	CLA	CHA-CBD-CGD-O1D
18	4	612	CLA	CHA-CBD-CGD-O2D
18	A	828	CLA	CHA-CBD-CGD-O2D
18	A	835	CLA	CHA-CBD-CGD-O1D
18	A	835	CLA	CHA-CBD-CGD-O2D
18	A	822	CLA	CHA-CBD-CGD-O1D
18	A	825	CLA	CHA-CBD-CGD-O2D
18	A	840	CLA	CHA-CBD-CGD-O1D
18	A	840	CLA	CHA-CBD-CGD-O2D
18	A	823	CLA	CHA-CBD-CGD-O1D
18	A	823	CLA	CHA-CBD-CGD-O2D
18	A	813	CLA	CHA-CBD-CGD-O1D
18	B	821	CLA	CHA-CBD-CGD-O1D
18	B	821	CLA	CHA-CBD-CGD-O2D
18	B	819	CLA	CHA-CBD-CGD-O1D
18	B	819	CLA	CHA-CBD-CGD-O2D
18	B	813	CLA	CHA-CBD-CGD-O1D
18	B	836	CLA	CHA-CBD-CGD-O1D
18	B	822	CLA	CHA-CBD-CGD-O1D
18	B	822	CLA	CHA-CBD-CGD-O2D
18	B	811	CLA	CHA-CBD-CGD-O1D
18	B	811	CLA	CHA-CBD-CGD-O2D
18	F	303	CLA	CHA-CBD-CGD-O1D
18	F	303	CLA	CHA-CBD-CGD-O2D
18	H	201	CLA	CHA-CBD-CGD-O1D
18	H	201	CLA	CHA-CBD-CGD-O2D
18	4	612	CLA	O1A-CGA-O2A-C1
18	2	602	CLA	O1A-CGA-O2A-C1
18	A	826	CLA	O1A-CGA-O2A-C1
18	A	806	CLA	O1A-CGA-O2A-C1
18	B	805	CLA	CAA-CBA-CGA-O2A
18	A	843	CLA	C16-C17-C18-C20
18	B	824	CLA	C3-C5-C6-C7
18	B	809	CLA	C3-C5-C6-C7
18	B	841	CLA	C4-C3-C5-C6
18	A	830	CLA	C2C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
18	B	826	CLA	O1A-CGA-O2A-C1
18	B	841	CLA	C2-C3-C5-C6
18	B	810	CLA	C6-C7-C8-C9
18	B	828	CLA	C6-C7-C8-C9
18	H	201	CLA	C11-C10-C8-C9
18	F	302	CLA	O1A-CGA-O2A-C1
18	K	204	CLA	C2C-C3C-CAC-CBC
18	F	301	CLA	C3-C5-C6-C7
17	4	605	CHL	CHA-CBD-CGD-O2D
18	A	813	CLA	C1A-C2A-CAA-CBA
18	4	602	CLA	CBD-CGD-O2D-CED
18	A	819	CLA	CAA-CBA-CGA-O2A
18	B	811	CLA	C2-C3-C5-C6
18	B	839	CLA	O1A-CGA-O2A-C1
18	B	837	CLA	O1A-CGA-O2A-C1
20	1	615	LHG	C3-O3-P-O4
20	B	852	LHG	C4-O6-P-O4
18	B	826	CLA	C13-C15-C16-C17
18	A	829	CLA	C16-C17-C18-C20
18	1	602	CLA	CAD-CBD-CGD-O1D
18	1	605	CLA	CAD-CBD-CGD-O1D
18	4	613	CLA	CAD-CBD-CGD-O1D
18	A	841	CLA	CAD-CBD-CGD-O1D
18	B	822	CLA	CAD-CBD-CGD-O1D
18	F	302	CLA	CAD-CBD-CGD-O1D
18	F	302	CLA	C2-C3-C5-C6
18	2	613	CLA	C2A-CAA-CBA-CGA
18	A	828	CLA	C11-C12-C13-C15
18	A	820	CLA	C11-C10-C8-C7
18	A	811	CLA	C11-C12-C13-C15
18	A	836	CLA	C3A-C2A-CAA-CBA
18	B	814	CLA	C6-C7-C8-C10
18	B	805	CLA	C12-C13-C15-C16
18	B	809	CLA	C6-C7-C8-C10
26	B	842	PQN	C16-C17-C18-C20
26	B	842	PQN	C22-C23-C25-C26
18	B	817	CLA	C11-C12-C13-C14
18	B	828	CLA	O1A-CGA-O2A-C1
27	B	850	DGD	C3B-C4B-C5B-C6B
18	3	601	CLA	C2A-CAA-CBA-CGA
18	A	822	CLA	C2A-CAA-CBA-CGA
18	A	803	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
18	B	828	CLA	C16-C17-C18-C20
23	4	619	LMG	C28-C29-C30-C31
27	B	850	DGD	C1B-C2B-C3B-C4B
17	2	605	CHL	C1C-C2C-CMC-OMC
17	4	605	CHL	C1C-C2C-CMC-OMC
18	3	609	CLA	CAD-CBD-CGD-O1D
18	A	844	CLA	C8-C10-C11-C12
18	B	805	CLA	C2-C3-C5-C6
18	2	602	CLA	C14-C13-C15-C16
18	A	804	CLA	C6-C7-C8-C9
18	A	829	CLA	C6-C7-C8-C9
18	B	827	CLA	C11-C12-C13-C14
18	B	832	CLA	C11-C10-C8-C9
21	2	616	LUT	C6-C7-C8-C9
18	A	812	CLA	C3-C5-C6-C7
20	1	615	LHG	C32-C33-C34-C35
22	A	852	BCR	C10-C11-C12-C13
22	B	844	BCR	C18-C19-C20-C21
22	F	304	BCR	C10-C11-C12-C13
18	B	839	CLA	C16-C17-C18-C19
22	3	614	BCR	C20-C21-C22-C37
18	A	814	CLA	C16-C17-C18-C20
18	B	840	CLA	C15-C16-C17-C18
18	1	604	CLA	C1-C2-C3-C4
18	A	804	CLA	CAA-CBA-CGA-O2A
18	A	841	CLA	CAA-CBA-CGA-O2A
18	4	602	CLA	C2A-CAA-CBA-CGA
18	A	815	CLA	C2A-CAA-CBA-CGA
18	B	807	CLA	C2A-CAA-CBA-CGA
18	A	803	CLA	C2-C1-O2A-CGA
18	A	829	CLA	C16-C17-C18-C19
18	A	802	CLA	C5-C6-C7-C8
27	B	850	DGD	C6B-C7B-C8B-C9B
18	A	806	CLA	O1D-CGD-O2D-CED
18	L	303	CLA	C16-C17-C18-C20
22	B	845	BCR	C1-C6-C7-C8
18	B	828	CLA	C16-C17-C18-C19
21	2	619	LUT	C11-C10-C9-C8
22	A	851	BCR	C11-C10-C9-C8
20	B	852	LHG	O7-C5-C6-O8
20	2	618	LHG	C4-O6-P-O3
20	A	847	LHG	C4-O6-P-O3

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Mol	Chain	Res	Type	Atoms
20	A	846	LHG	C3-O3-P-O6
20	B	852	LHG	C3-O3-P-O6
18	A	804	CLA	C16-C17-C18-C20
18	A	843	CLA	O1D-CGD-O2D-CED
23	4	620	LMG	C7-C8-C9-O8
18	A	825	CLA	O1D-CGD-O2D-CED
18	A	818	CLA	C11-C10-C8-C7
18	B	806	CLA	C12-C13-C15-C16
18	A	834	CLA	C11-C10-C8-C9
18	B	817	CLA	C6-C7-C8-C9
18	B	802	CLA	C10-C11-C12-C13
18	B	822	CLA	C8-C10-C11-C12
22	A	852	BCR	C13-C14-C15-C16
18	A	806	CLA	C16-C17-C18-C20
22	B	849	BCR	C36-C18-C19-C20
18	A	820	CLA	C8-C10-C11-C12
18	B	829	CLA	C11-C10-C8-C7
18	A	844	CLA	C2-C3-C5-C6
18	A	802	CLA	C16-C17-C18-C20
18	4	602	CLA	O1D-CGD-O2D-CED
18	1	607	CLA	CAA-CBA-CGA-O1A
18	A	825	CLA	CBD-CGD-O2D-CED
18	A	834	CLA	CBD-CGD-O2D-CED
18	2	612	CLA	C2A-CAA-CBA-CGA
18	B	825	CLA	C5-C6-C7-C8
22	B	844	BCR	C15-C16-C17-C18
18	B	819	CLA	C3-C5-C6-C7
18	B	816	CLA	C4-C3-C5-C6
18	1	612	CLA	CBA-CGA-O2A-C1
18	B	816	CLA	C2-C3-C5-C6
18	G	203	CLA	CAA-CBA-CGA-O2A
18	B	841	CLA	C2-C1-O2A-CGA
18	2	602	CLA	C2A-CAA-CBA-CGA
18	2	608	CLA	C2A-CAA-CBA-CGA
18	4	614	CLA	C2A-CAA-CBA-CGA
20	A	847	LHG	O7-C7-C8-C9
18	4	613	CLA	C3A-C2A-CAA-CBA
18	A	803	CLA	C3A-C2A-CAA-CBA
18	B	834	CLA	C3A-C2A-CAA-CBA
24	A	801	CL0	C3A-C2A-CAA-CBA
18	A	826	CLA	C6-C7-C8-C9
18	B	803	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
18	B	825	CLA	C14-C13-C15-C16
18	B	818	CLA	C6-C7-C8-C9
18	B	828	CLA	C14-C13-C15-C16
18	A	806	CLA	C16-C17-C18-C19
18	L	303	CLA	C16-C17-C18-C19
21	2	619	LUT	C11-C10-C9-C19
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	K	202	BCR	C16-C17-C18-C36
22	L	305	BCR	C16-C17-C18-C36
18	1	605	CLA	O1A-CGA-O2A-C1
18	1	607	CLA	CAA-CBA-CGA-O2A
18	A	826	CLA	C5-C6-C7-C8
18	B	826	CLA	C10-C11-C12-C13
24	A	801	CL0	CAA-CBA-CGA-O1A
18	A	804	CLA	C1A-C2A-CAA-CBA
18	A	803	CLA	C1A-C2A-CAA-CBA
18	A	836	CLA	C1A-C2A-CAA-CBA
18	B	819	CLA	C1A-C2A-CAA-CBA
18	B	811	CLA	C1A-C2A-CAA-CBA
18	A	844	CLA	CBA-CGA-O2A-C1
18	A	806	CLA	C11-C10-C8-C7
18	A	807	CLA	C6-C7-C8-C10
18	A	811	CLA	C11-C10-C8-C7
18	B	806	CLA	C11-C10-C8-C7
18	B	837	CLA	C11-C12-C13-C15
18	4	603	CLA	CAA-CBA-CGA-O1A
18	4	601	CLA	CAA-CBA-CGA-O1A
18	2	609	CLA	C2A-CAA-CBA-CGA
18	B	805	CLA	C16-C17-C18-C20
18	B	822	CLA	C5-C6-C7-C8
18	B	806	CLA	C4-C3-C5-C6
18	A	807	CLA	C15-C16-C17-C18
18	A	834	CLA	C13-C15-C16-C17
22	A	852	BCR	C11-C10-C9-C8
22	A	851	BCR	C20-C21-C22-C23
22	B	845	BCR	C16-C17-C18-C19
22	K	205	BCR	C20-C21-C22-C23
22	K	202	BCR	C16-C17-C18-C19
22	L	305	BCR	C16-C17-C18-C19
18	A	807	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
18	A	834	CLA	O1D-CGD-O2D-CED
22	B	849	BCR	C22-C23-C24-C25
18	B	809	CLA	C16-C17-C18-C20
18	A	807	CLA	O1A-CGA-O2A-C1
18	B	808	CLA	C4-C3-C5-C6
18	A	809	CLA	C2-C1-O2A-CGA
18	B	817	CLA	C2-C1-O2A-CGA
18	G	203	CLA	CAA-CBA-CGA-O1A
18	2	612	CLA	C6-C7-C8-C9
18	B	818	CLA	C11-C10-C8-C9
18	A	844	CLA	O1A-CGA-O2A-C1
18	F	302	CLA	C4-C3-C5-C6
18	A	826	CLA	C15-C16-C17-C18
22	B	801	BCR	C23-C24-C25-C26
22	B	849	BCR	C23-C24-C25-C30
22	G	204	BCR	C5-C6-C7-C8
18	B	822	CLA	CAA-CBA-CGA-O2A
18	4	603	CLA	CAA-CBA-CGA-O2A
18	2	602	CLA	C5-C6-C7-C8
22	A	852	BCR	C15-C16-C17-C18
22	K	205	BCR	C7-C8-C9-C10
18	A	807	CLA	C16-C17-C18-C19
18	B	802	CLA	C5-C6-C7-C8
18	2	603	CLA	CAA-CBA-CGA-O2A
17	4	607	CHL	C2A-CAA-CBA-CGA
18	2	612	CLA	C15-C16-C17-C18
18	A	829	CLA	C13-C15-C16-C17
18	2	608	CLA	CAA-CBA-CGA-O2A
18	4	601	CLA	O1D-CGD-O2D-CED
18	B	814	CLA	C10-C11-C12-C13
18	A	825	CLA	C4-C3-C5-C6
18	B	821	CLA	CAA-CBA-CGA-O1A
18	3	609	CLA	C2-C3-C5-C6
18	A	828	CLA	C11-C10-C8-C7
18	A	831	CLA	C11-C12-C13-C15
18	B	813	CLA	C11-C12-C13-C15
24	A	801	CL0	C11-C10-C8-C7
18	A	817	CLA	CAA-CBA-CGA-O2A
18	K	203	CLA	CAA-CBA-CGA-O1A
19	2	617	XAT	C29-C30-C31-C32
22	4	618	BCR	C15-C16-C17-C18
18	A	835	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
18	K	203	CLA	CAA-CBA-CGA-O2A
23	4	620	LMG	O7-C8-C9-O8
18	A	805	CLA	CBA-CGA-O2A-C1
22	B	845	BCR	C16-C17-C18-C36
22	B	844	BCR	C11-C10-C9-C34
22	L	301	BCR	C11-C10-C9-C34
18	A	807	CLA	C4-C3-C5-C6
18	B	829	CLA	C4-C3-C5-C6
18	B	810	CLA	C4-C3-C5-C6
18	B	808	CLA	C2-C3-C5-C6
18	B	819	CLA	CBA-CGA-O2A-C1
18	4	602	CLA	C6-C7-C8-C9
18	A	802	CLA	C6-C7-C8-C9
18	A	811	CLA	C11-C10-C8-C9
18	A	811	CLA	C11-C12-C13-C14
18	B	814	CLA	C6-C7-C8-C9
18	B	813	CLA	C11-C12-C13-C14
18	B	837	CLA	C11-C12-C13-C14
26	B	842	PQN	C24-C23-C25-C26
18	A	805	CLA	O1A-CGA-O2A-C1
18	2	608	CLA	CAA-CBA-CGA-O1A
27	B	850	DGD	CEB-CFB-CGB-CHB
18	3	609	CLA	C3A-C2A-CAA-CBA
18	A	821	CLA	C3A-C2A-CAA-CBA
18	A	833	CLA	C3A-C2A-CAA-CBA
18	A	822	CLA	C3A-C2A-CAA-CBA
18	A	829	CLA	C3A-C2A-CAA-CBA
18	B	837	CLA	C3A-C2A-CAA-CBA
18	F	302	CLA	C3A-C2A-CAA-CBA
18	1	611	CLA	CAA-CBA-CGA-O2A
18	A	815	CLA	CAA-CBA-CGA-O2A
18	2	611	CLA	CAD-CBD-CGD-O2D
18	3	608	CLA	CAD-CBD-CGD-O2D
18	3	605	CLA	CAD-CBD-CGD-O2D
18	A	817	CLA	CAD-CBD-CGD-O2D
18	A	821	CLA	CAD-CBD-CGD-O2D
18	A	826	CLA	CAD-CBD-CGD-O2D
18	A	827	CLA	CAD-CBD-CGD-O2D
18	A	838	CLA	CAD-CBD-CGD-O2D
18	A	812	CLA	CAD-CBD-CGD-O2D
18	A	814	CLA	CAD-CBD-CGD-O2D
18	A	831	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
18	B	802	CLA	CAD-CBD-CGD-O2D
18	B	808	CLA	CAD-CBD-CGD-O2D
18	B	813	CLA	CAD-CBD-CGD-O2D
18	B	805	CLA	CAD-CBD-CGD-O2D
18	B	838	CLA	CAD-CBD-CGD-O2D
18	B	832	CLA	CAD-CBD-CGD-O2D
18	B	837	CLA	CAD-CBD-CGD-O2D
18	A	818	CLA	C8-C10-C11-C12
18	F	302	CLA	C2-C1-O2A-CGA
17	4	607	CHL	CAA-CBA-CGA-O2A
18	A	840	CLA	CAA-CBA-CGA-O2A
18	B	832	CLA	CAA-CBA-CGA-O2A
23	4	620	LMG	O9-C10-C11-C12
18	A	843	CLA	C16-C17-C18-C19
18	B	809	CLA	CAA-CBA-CGA-O2A
18	A	827	CLA	O1A-CGA-O2A-C1
18	4	613	CLA	CAA-CBA-CGA-O2A
18	A	827	CLA	CBA-CGA-O2A-C1
18	B	820	CLA	CAA-CBA-CGA-O2A
20	1	615	LHG	O7-C7-C8-C9
18	B	817	CLA	CAA-CBA-CGA-O1A
18	A	817	CLA	CAA-CBA-CGA-O1A
18	3	602	CLA	O2A-C1-C2-C3
18	4	614	CLA	O2A-C1-C2-C3
18	B	829	CLA	O2A-C1-C2-C3
18	F	301	CLA	O2A-C1-C2-C3
18	4	613	CLA	C2A-CAA-CBA-CGA
18	B	824	CLA	C2A-CAA-CBA-CGA
18	2	612	CLA	C10-C11-C12-C13
17	4	607	CHL	CAA-CBA-CGA-O1A
18	2	603	CLA	CAA-CBA-CGA-O1A
18	B	805	CLA	C16-C17-C18-C19
18	2	602	CLA	CHA-CBD-CGD-O1D
18	2	610	CLA	CHA-CBD-CGD-O1D
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	602	CLA	CHA-CBD-CGD-O1D
18	4	602	CLA	CHA-CBD-CGD-O2D
18	A	804	CLA	CHA-CBD-CGD-O1D
18	A	804	CLA	CHA-CBD-CGD-O2D
18	A	822	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
18	A	818	CLA	CHA-CBD-CGD-O2D
18	A	843	CLA	CHA-CBD-CGD-O1D
18	A	843	CLA	CHA-CBD-CGD-O2D
18	A	811	CLA	CHA-CBD-CGD-O1D
18	A	811	CLA	CHA-CBD-CGD-O2D
18	B	825	CLA	CHA-CBD-CGD-O1D
18	B	825	CLA	CHA-CBD-CGD-O2D
18	B	804	CLA	CHA-CBD-CGD-O1D
18	B	804	CLA	CHA-CBD-CGD-O2D
18	B	813	CLA	CHA-CBD-CGD-O2D
18	B	824	CLA	CHA-CBD-CGD-O1D
18	B	824	CLA	CHA-CBD-CGD-O2D
18	B	837	CLA	CHA-CBD-CGD-O1D
18	K	204	CLA	CHA-CBD-CGD-O1D
18	K	204	CLA	CHA-CBD-CGD-O2D
18	1	611	CLA	CAA-CBA-CGA-O1A
18	4	604	CLA	CAA-CBA-CGA-O2A
18	A	815	CLA	CAA-CBA-CGA-O1A
18	3	609	CLA	CAA-CBA-CGA-O2A
18	A	820	CLA	C10-C11-C12-C13
22	4	618	BCR	C11-C10-C9-C8
22	B	844	BCR	C11-C10-C9-C8
22	L	301	BCR	C11-C10-C9-C8
18	B	819	CLA	O1A-CGA-O2A-C1
18	1	603	CLA	CAA-CBA-CGA-O2A
18	F	301	CLA	CAA-CBA-CGA-O2A
20	B	852	LHG	O7-C7-C8-C9
17	3	606	CHL	CAA-CBA-CGA-O2A
18	A	827	CLA	C11-C12-C13-C14
18	A	831	CLA	C3-C5-C6-C7
18	A	826	CLA	C11-C12-C13-C15
18	A	807	CLA	C2-C3-C5-C6
18	B	803	CLA	C11-C12-C13-C15
18	K	204	CLA	CAA-CBA-CGA-O2A
18	A	807	CLA	C6-C7-C8-C9
18	A	831	CLA	C11-C12-C13-C14
18	B	832	CLA	C6-C7-C8-C9
26	B	842	PQN	C16-C17-C18-C19
20	A	847	LHG	C5-C6-O8-C23
27	B	850	DGD	CAA-CBA-CCA-CDA
18	B	832	CLA	CBA-CGA-O2A-C1
18	B	841	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
18	B	832	CLA	O1A-CGA-O2A-C1
18	B	814	CLA	C2A-CAA-CBA-CGA
18	A	821	CLA	CAA-CBA-CGA-O2A
18	B	832	CLA	CAA-CBA-CGA-O1A
18	B	810	CLA	C2-C3-C5-C6
18	A	840	CLA	CAA-CBA-CGA-O1A
18	B	809	CLA	CAA-CBA-CGA-O1A
18	1	607	CLA	CHA-CBD-CGD-O2D
18	3	609	CLA	C1A-C2A-CAA-CBA
18	A	821	CLA	C1A-C2A-CAA-CBA
18	A	822	CLA	C1A-C2A-CAA-CBA
18	B	803	CLA	C1A-C2A-CAA-CBA
18	B	817	CLA	C1A-C2A-CAA-CBA
18	B	837	CLA	C1A-C2A-CAA-CBA
18	B	834	CLA	C1A-C2A-CAA-CBA
24	A	801	CL0	C1A-C2A-CAA-CBA
18	A	842	CLA	C4C-C3C-CAC-CBC
20	1	615	LHG	O9-C7-C8-C9
18	4	613	CLA	CAA-CBA-CGA-O1A
18	A	844	CLA	C2A-CAA-CBA-CGA
18	B	837	CLA	C2A-CAA-CBA-CGA
20	1	615	LHG	C4-O6-P-O3
17	3	606	CHL	CAA-CBA-CGA-O1A
18	3	609	CLA	C4-C3-C5-C6
18	1	612	CLA	O1A-CGA-O2A-C1
20	1	615	LHG	C4-O6-P-O4
20	A	846	LHG	C3-O3-P-O5
18	K	204	CLA	CAA-CBA-CGA-O1A
17	2	607	CHL	CAA-CBA-CGA-O2A
22	A	853	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
18	3	609	CLA	CAA-CBA-CGA-O1A
20	B	852	LHG	O9-C7-C8-C9
18	4	612	CLA	C8-C10-C11-C12
20	2	618	LHG	O7-C7-C8-C9
18	2	611	CLA	CAA-CBA-CGA-O2A
22	K	205	BCR	C18-C19-C20-C21
18	B	820	CLA	CAA-CBA-CGA-O1A
18	2	612	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
18	4	604	CLA	CAA-CBA-CGA-O1A
18	B	811	CLA	CAA-CBA-CGA-O2A
18	A	841	CLA	C4-C3-C5-C6
18	4	614	CLA	CAD-CBD-CGD-O1D
18	A	822	CLA	CAD-CBD-CGD-O1D
18	A	842	CLA	CAD-CBD-CGD-O1D
18	A	834	CLA	CAD-CBD-CGD-O1D
18	B	827	CLA	CAD-CBD-CGD-O1D
20	B	851	LHG	C4-C5-O7-C7
18	4	601	CLA	CBD-CGD-O2D-CED
18	1	603	CLA	CAA-CBA-CGA-O1A
18	F	301	CLA	CAA-CBA-CGA-O1A
18	B	806	CLA	CAA-CBA-CGA-O2A
18	A	829	CLA	C11-C10-C8-C9
18	B	839	CLA	C6-C7-C8-C9
18	B	841	CLA	C14-C13-C15-C16
18	B	822	CLA	C11-C10-C8-C9
18	B	828	CLA	C11-C12-C13-C14
24	A	801	CL0	C14-C13-C15-C16
18	A	804	CLA	C13-C15-C16-C17
18	2	612	CLA	CAA-CBA-CGA-O2A
18	A	842	CLA	CAA-CBA-CGA-O2A
18	A	821	CLA	CAA-CBA-CGA-O1A
20	B	852	LHG	C30-C31-C32-C33
18	4	602	CLA	CAA-CBA-CGA-O2A
18	A	803	CLA	C10-C11-C12-C13
24	A	801	CL0	C4-C3-C5-C6
17	4	605	CHL	CHA-CBD-CGD-O1D
18	1	607	CLA	CHA-CBD-CGD-O1D
18	1	613	CLA	CHA-CBD-CGD-O1D
18	3	609	CLA	CAD-CBD-CGD-O2D
18	4	612	CLA	C6-C7-C8-C10
18	A	827	CLA	C6-C7-C8-C10
18	A	829	CLA	C12-C13-C15-C16
18	B	803	CLA	C3A-C2A-CAA-CBA
18	B	806	CLA	C2-C3-C5-C6
18	B	832	CLA	C6-C7-C8-C10
18	B	832	CLA	C11-C12-C13-C15
18	B	837	CLA	C12-C13-C15-C16
18	B	818	CLA	C11-C10-C8-C7
21	2	619	LUT	C25-C26-C27-C28
24	A	801	CL0	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
18	2	612	CLA	CAA-CBA-CGA-O1A
18	3	602	CLA	CAA-CBA-CGA-O1A
18	2	611	CLA	CAA-CBA-CGA-O1A
18	3	602	CLA	CAA-CBA-CGA-O2A
18	3	601	CLA	CAA-CBA-CGA-O2A
18	A	812	CLA	CAA-CBA-CGA-O2A
22	B	849	BCR	C17-C18-C19-C20
18	A	837	CLA	CAA-CBA-CGA-O2A
27	B	850	DGD	CDA-CEA-CFA-CGA
18	3	601	CLA	CAA-CBA-CGA-O1A
18	B	805	CLA	CAA-CBA-CGA-O1A
18	4	608	CLA	CAA-CBA-CGA-O2A
18	B	833	CLA	CAA-CBA-CGA-O2A
26	B	842	PQN	C15-C16-C17-C18
18	A	842	CLA	C2C-C3C-CAC-CBC
18	A	810	CLA	CAA-CBA-CGA-O2A
18	B	811	CLA	CAA-CBA-CGA-O1A
18	B	833	CLA	CAA-CBA-CGA-O1A
18	A	809	CLA	C4C-C3C-CAC-CBC
18	B	824	CLA	C13-C15-C16-C17
18	2	612	CLA	CBA-CGA-O2A-C1
18	4	609	CLA	C4-C3-C5-C6
18	A	814	CLA	CAA-CBA-CGA-O2A

There are no ring outliers.

164 monomers are involved in 534 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	B	802	CLA	6	0
18	B	836	CLA	2	0
18	A	806	CLA	8	0
18	B	813	CLA	5	0
22	B	801	BCR	9	0
18	4	603	CLA	3	0
20	B	852	LHG	1	0
18	2	602	CLA	8	0
18	A	827	CLA	2	0
18	B	827	CLA	5	0
18	2	603	CLA	3	0
18	A	843	CLA	3	0
18	2	613	CLA	1	0
18	B	833	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	4	618	BCR	8	0
18	4	608	CLA	3	0
18	A	814	CLA	2	0
18	F	303	CLA	1	0
18	B	822	CLA	7	0
18	1	603	CLA	3	0
22	B	847	BCR	8	0
18	4	602	CLA	6	0
18	B	826	CLA	4	0
18	H	201	CLA	2	0
18	A	802	CLA	7	0
18	A	839	CLA	1	0
18	B	837	CLA	2	0
17	1	601	CHL	7	0
18	2	611	CLA	2	0
18	F	301	CLA	2	0
18	A	813	CLA	2	0
22	L	301	BCR	4	0
22	A	848	BCR	7	0
18	A	810	CLA	3	0
22	A	849	BCR	3	0
27	B	850	DGD	8	0
18	3	609	CLA	4	0
18	3	601	CLA	2	0
18	A	838	CLA	1	0
22	F	304	BCR	2	0
18	A	818	CLA	4	0
18	B	805	CLA	5	0
18	A	836	CLA	1	0
22	A	852	BCR	4	0
22	K	205	BCR	4	0
18	B	832	CLA	7	0
22	J	102	BCR	4	0
18	4	609	CLA	3	0
24	A	801	CL0	7	0
18	A	819	CLA	4	0
17	2	601	CHL	1	0
22	B	843	BCR	4	0
18	B	830	CLA	2	0
18	B	818	CLA	2	0
21	3	613	LUT	7	0
18	A	825	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	F	302	CLA	7	0
20	A	847	LHG	2	0
21	2	616	LUT	8	0
18	A	841	CLA	5	0
22	L	306	BCR	2	0
18	1	609	CLA	5	0
18	1	602	CLA	2	0
21	1	616	LUT	9	0
18	B	814	CLA	5	0
18	B	819	CLA	2	0
18	B	840	CLA	3	0
22	B	849	BCR	9	0
22	I	101	BCR	3	0
18	A	834	CLA	4	0
18	B	803	CLA	4	0
18	2	612	CLA	2	0
20	1	615	LHG	20	0
18	A	832	CLA	2	0
18	B	823	CLA	2	0
18	B	809	CLA	4	0
18	1	607	CLA	6	0
18	1	605	CLA	1	0
22	B	846	BCR	7	0
18	K	203	CLA	1	0
18	B	839	CLA	1	0
18	G	201	CLA	1	0
18	B	820	CLA	1	0
19	1	614	XAT	9	0
18	B	817	CLA	1	0
18	L	304	CLA	2	0
18	4	614	CLA	4	0
18	A	821	CLA	2	0
18	A	844	CLA	8	0
18	4	611	CLA	1	0
22	B	845	BCR	6	0
18	A	842	CLA	7	0
18	4	610	CLA	3	0
18	2	604	CLA	4	0
18	B	825	CLA	7	0
17	2	615	CHL	1	0
18	B	835	CLA	1	0
18	3	612	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	L	305	BCR	8	0
18	1	604	CLA	4	0
21	2	619	LUT	5	0
18	A	829	CLA	6	0
18	3	602	CLA	1	0
18	A	804	CLA	8	0
18	A	803	CLA	7	0
18	B	816	CLA	2	0
18	B	824	CLA	3	0
17	3	606	CHL	1	0
18	A	820	CLA	4	0
18	A	808	CLA	1	0
18	A	833	CLA	2	0
18	1	608	CLA	4	0
18	B	806	CLA	5	0
18	B	829	CLA	2	0
17	2	607	CHL	1	0
18	A	826	CLA	4	0
18	A	809	CLA	10	0
18	B	834	CLA	2	0
17	2	605	CHL	2	0
18	1	612	CLA	5	0
18	2	609	CLA	5	0
20	A	846	LHG	3	0
22	G	204	BCR	3	0
23	4	619	LMG	1	0
18	4	613	CLA	3	0
18	3	608	CLA	4	0
18	L	302	CLA	2	0
18	A	835	CLA	1	0
26	B	842	PQN	2	0
22	B	848	BCR	2	0
22	3	614	BCR	2	0
18	B	808	CLA	3	0
18	A	830	CLA	7	0
18	B	838	CLA	3	0
22	B	844	BCR	7	0
26	A	855	PQN	6	0
17	4	606	CHL	2	0
22	A	853	BCR	4	0
18	A	811	CLA	4	0
18	A	828	CLA	2	0

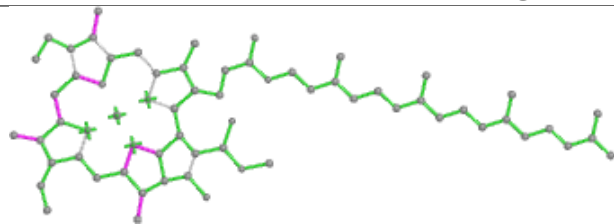
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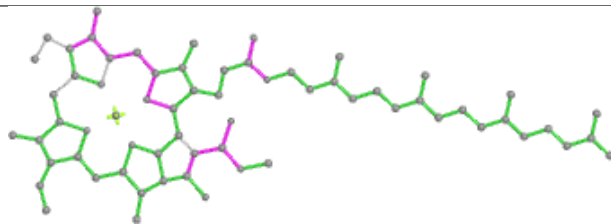
Mol	Chain	Res	Type	Clashes	Symm-Clashes
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18	4	604	CLA	3	0
18	B	841	CLA	2	0
18	A	831	CLA	1	0
22	A	850	BCR	6	0
21	4	616	LUT	3	0
18	A	822	CLA	4	0
18	A	807	CLA	3	0
18	3	607	CLA	5	0
18	L	303	CLA	4	0
18	4	612	CLA	1	0
19	4	617	XAT	20	0
22	A	851	BCR	7	0
19	2	617	XAT	6	0
18	A	815	CLA	1	0
17	4	605	CHL	2	0
18	B	828	CLA	8	0
18	B	811	CLA	3	0
18	A	812	CLA	7	0
17	4	607	CHL	1	0
22	K	202	BCR	6	0
18	2	608	CLA	3	0
18	A	805	CLA	3	0
18	3	603	CLA	3	0

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

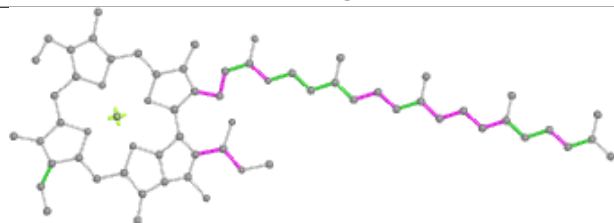
Ligand CLA B 802



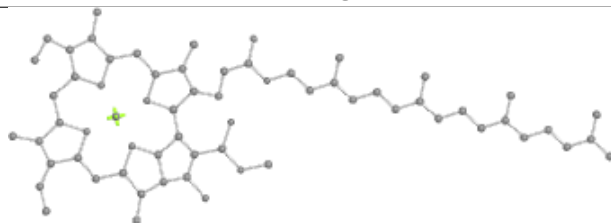
Bond lengths



Bond angles

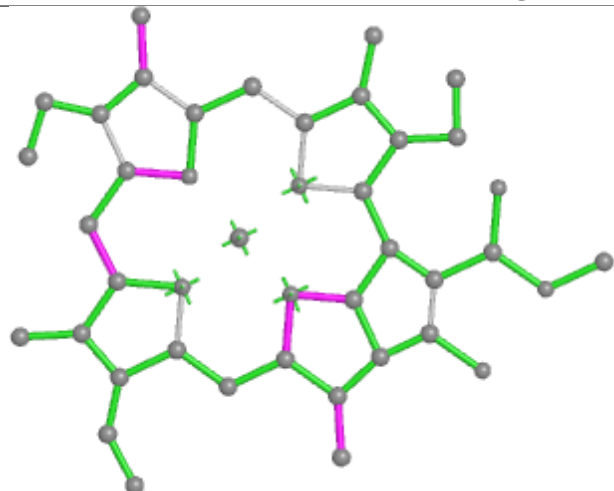


Torsions

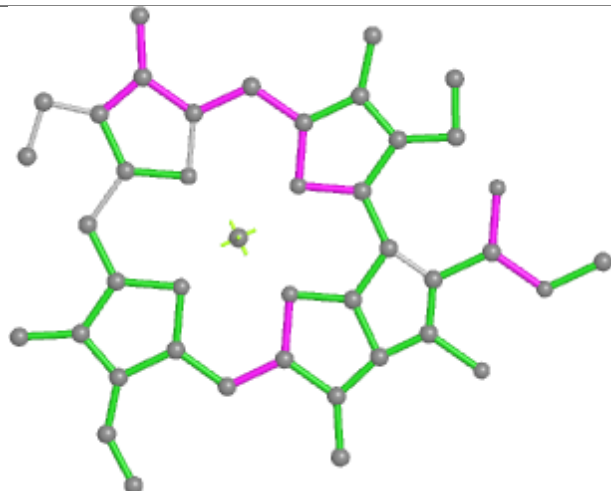


Rings

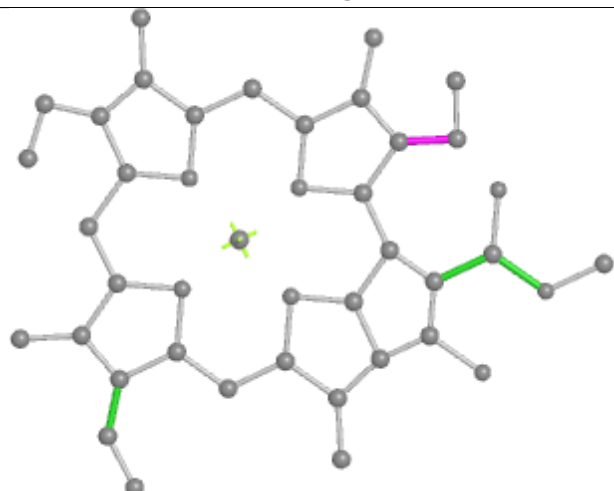
Ligand CLA G 202



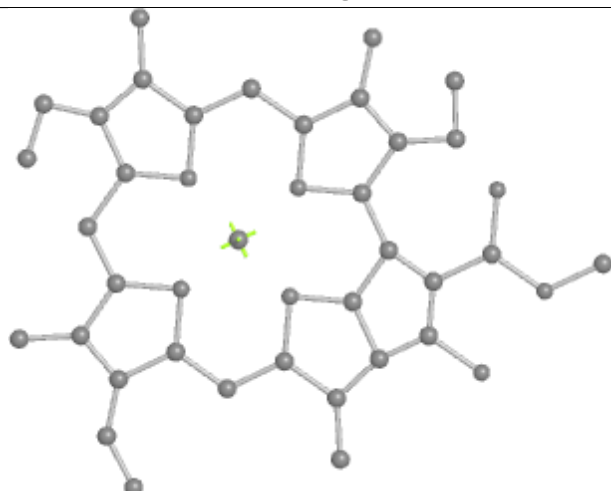
Bond lengths



Bond angles

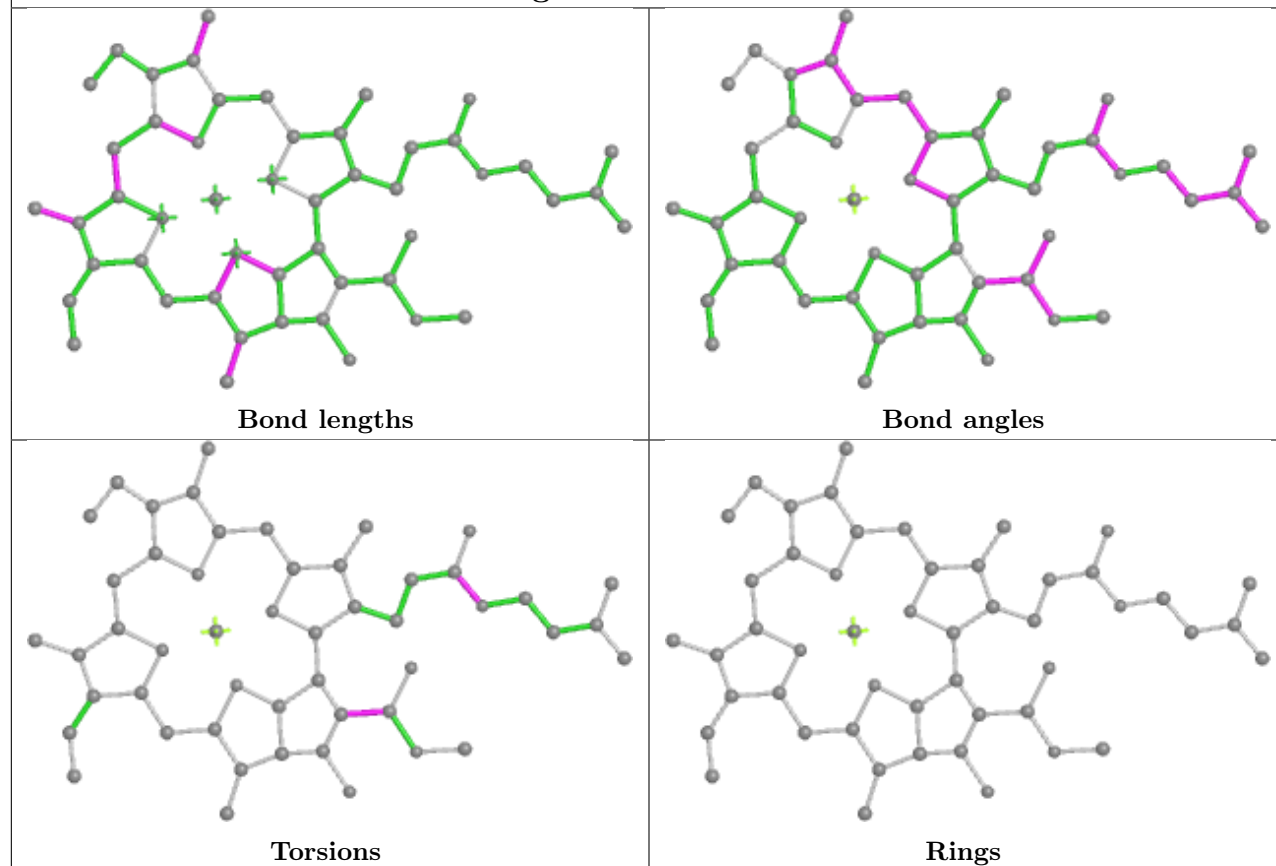


Torsions

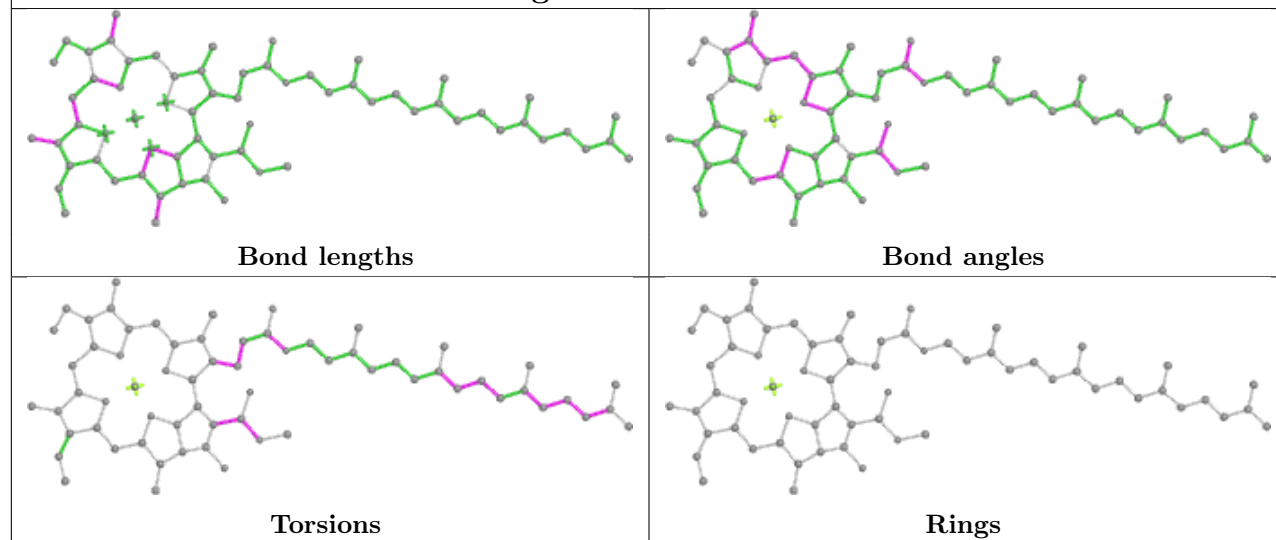


Rings

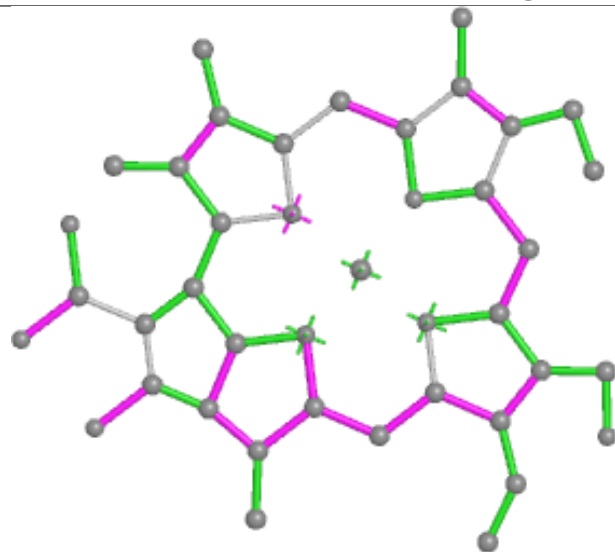
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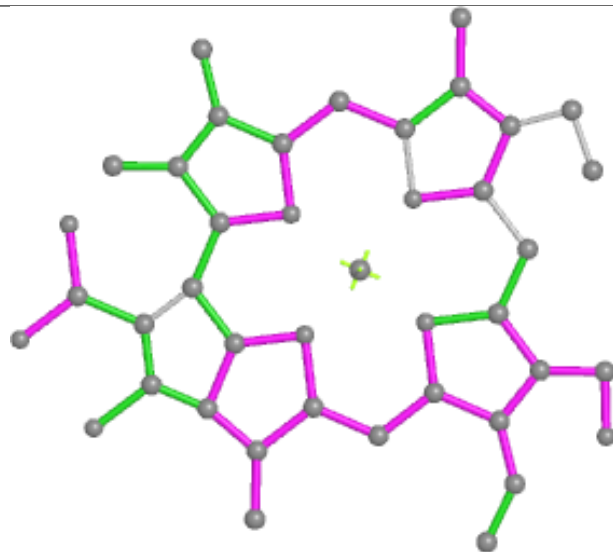
Ligand CLA A 806



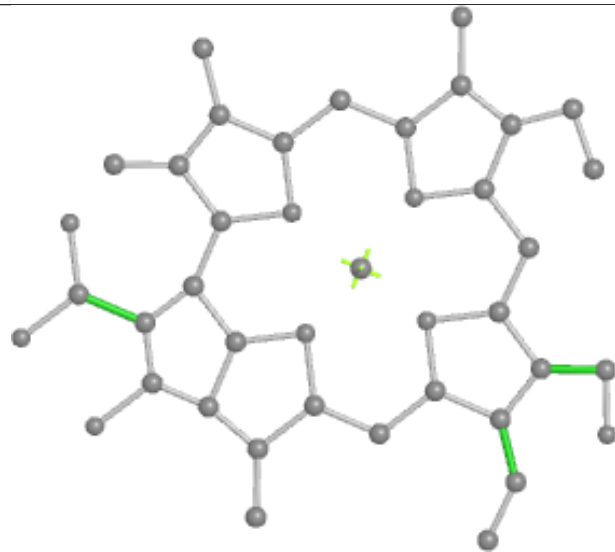
Ligand CHL 1 606



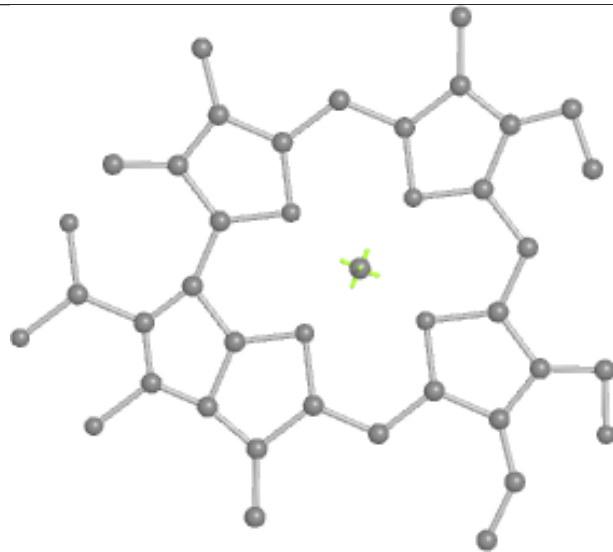
Bond lengths



Bond angles

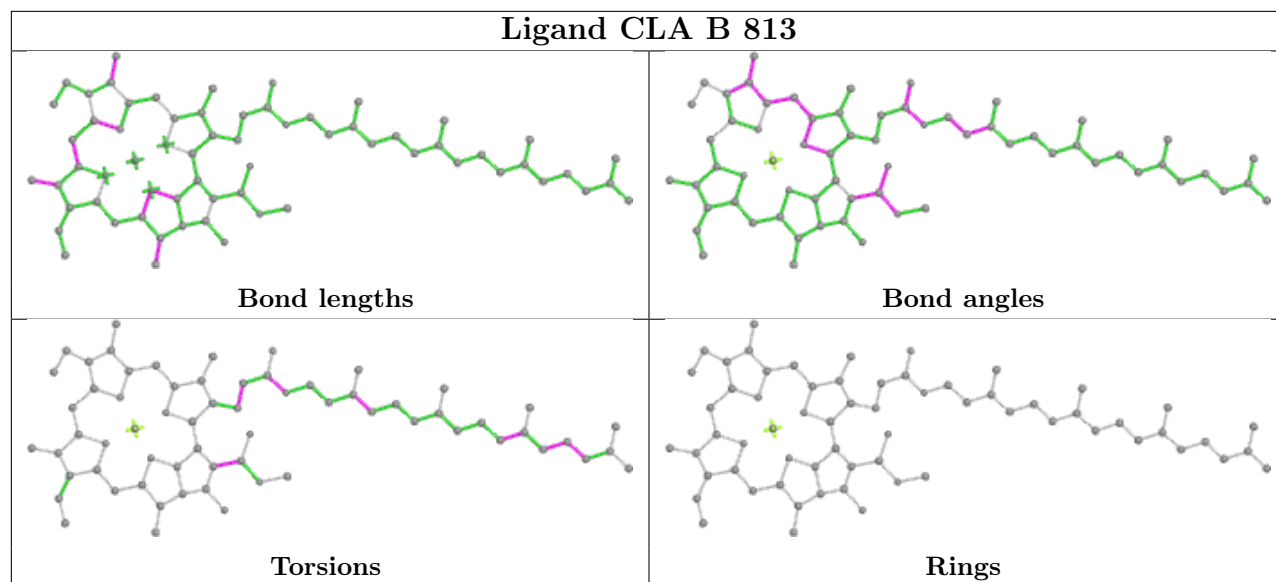


Torsions

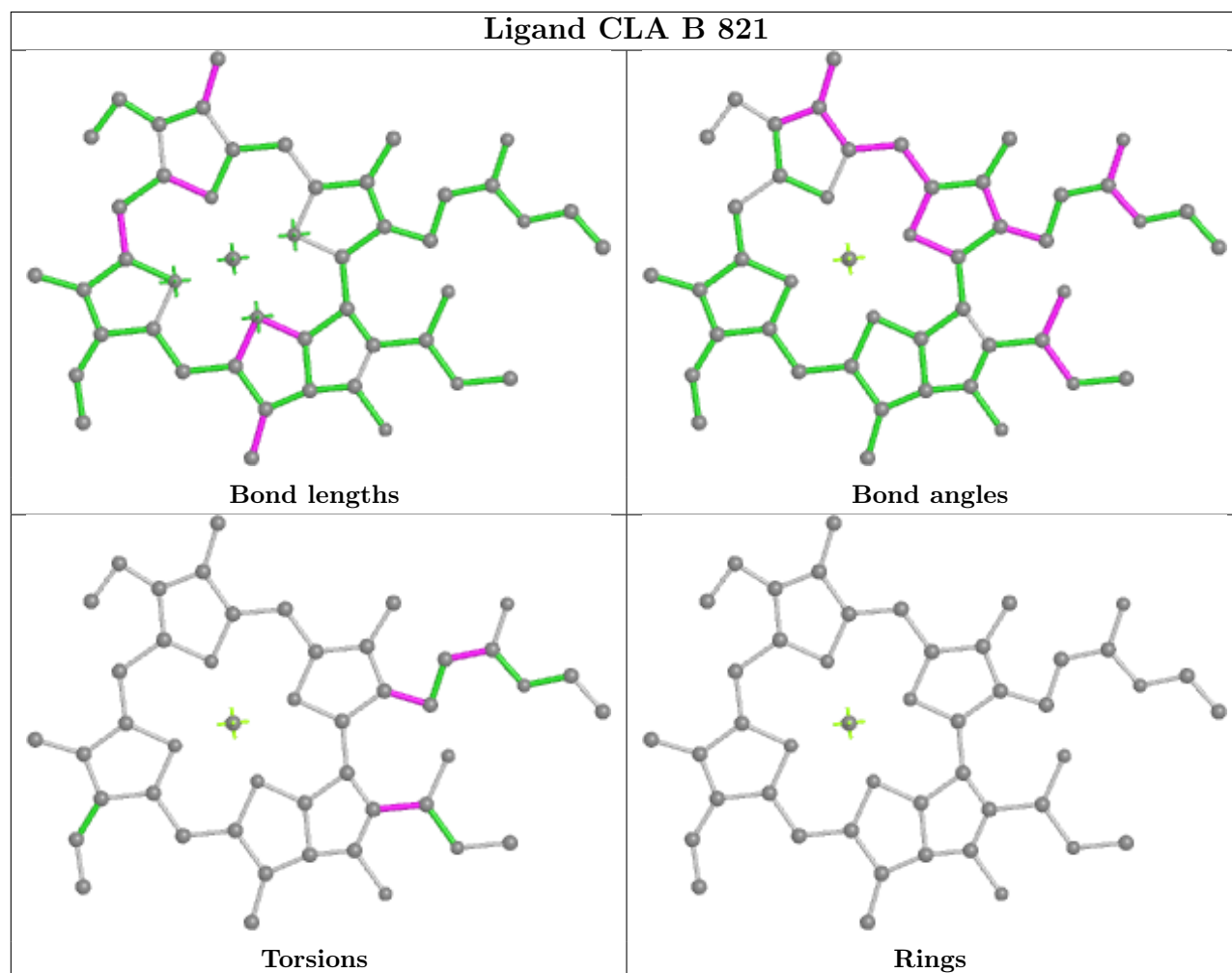


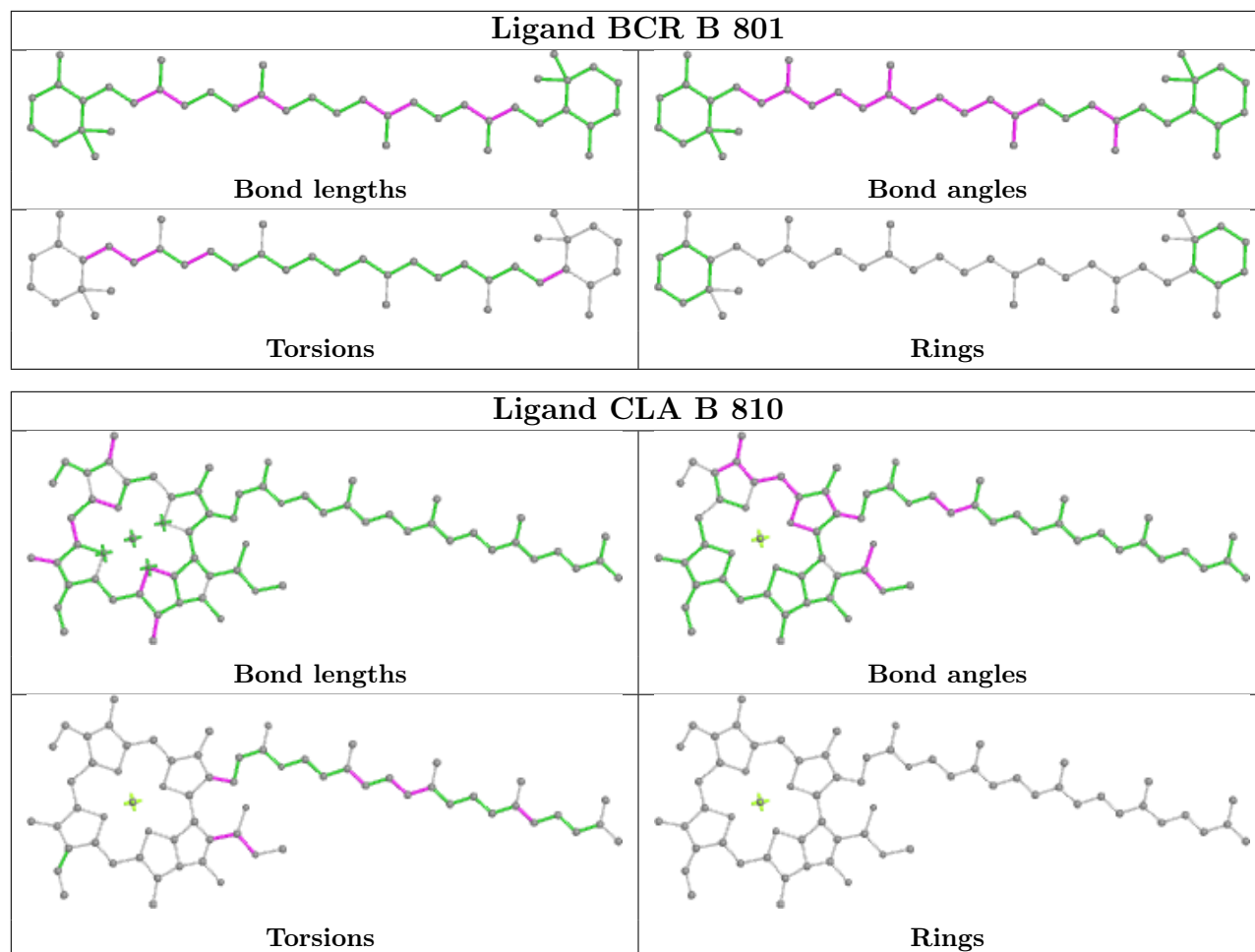
Rings

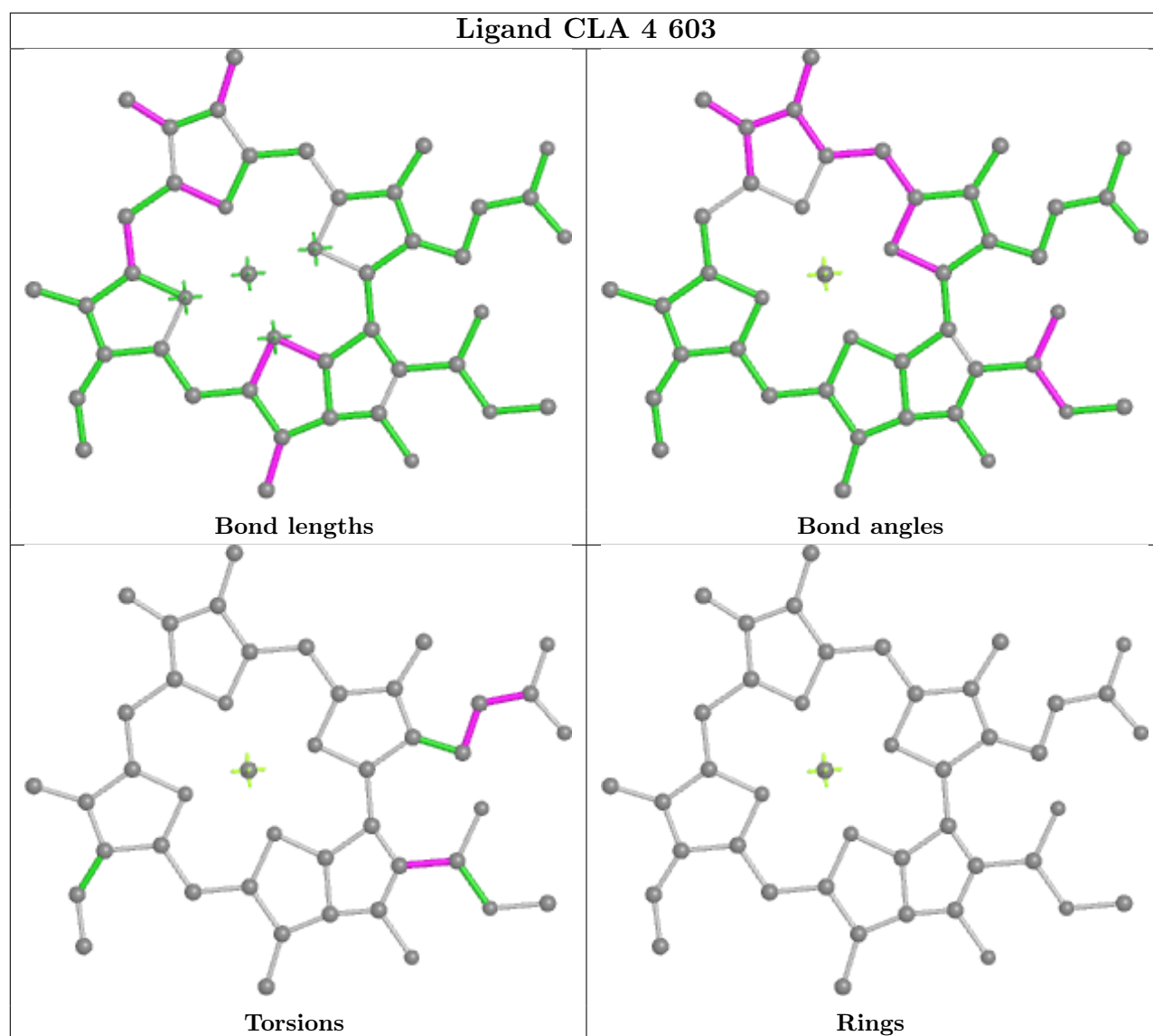
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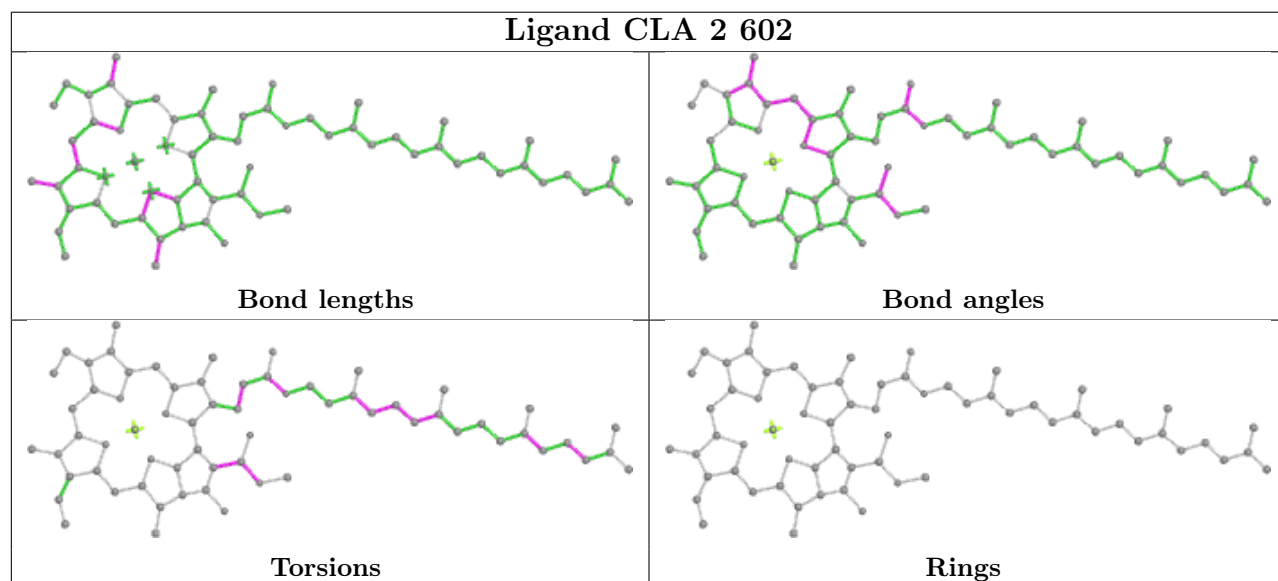
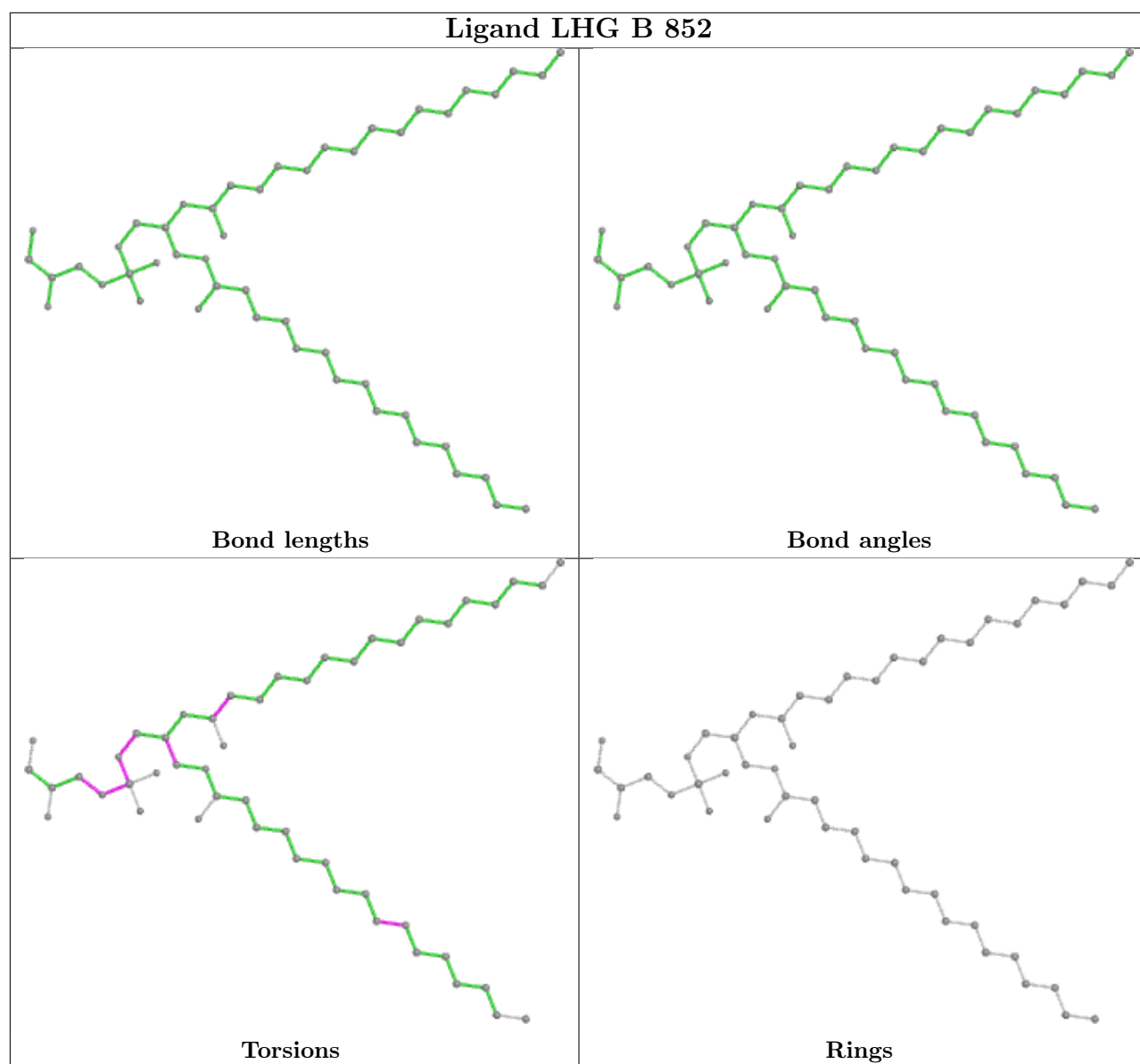


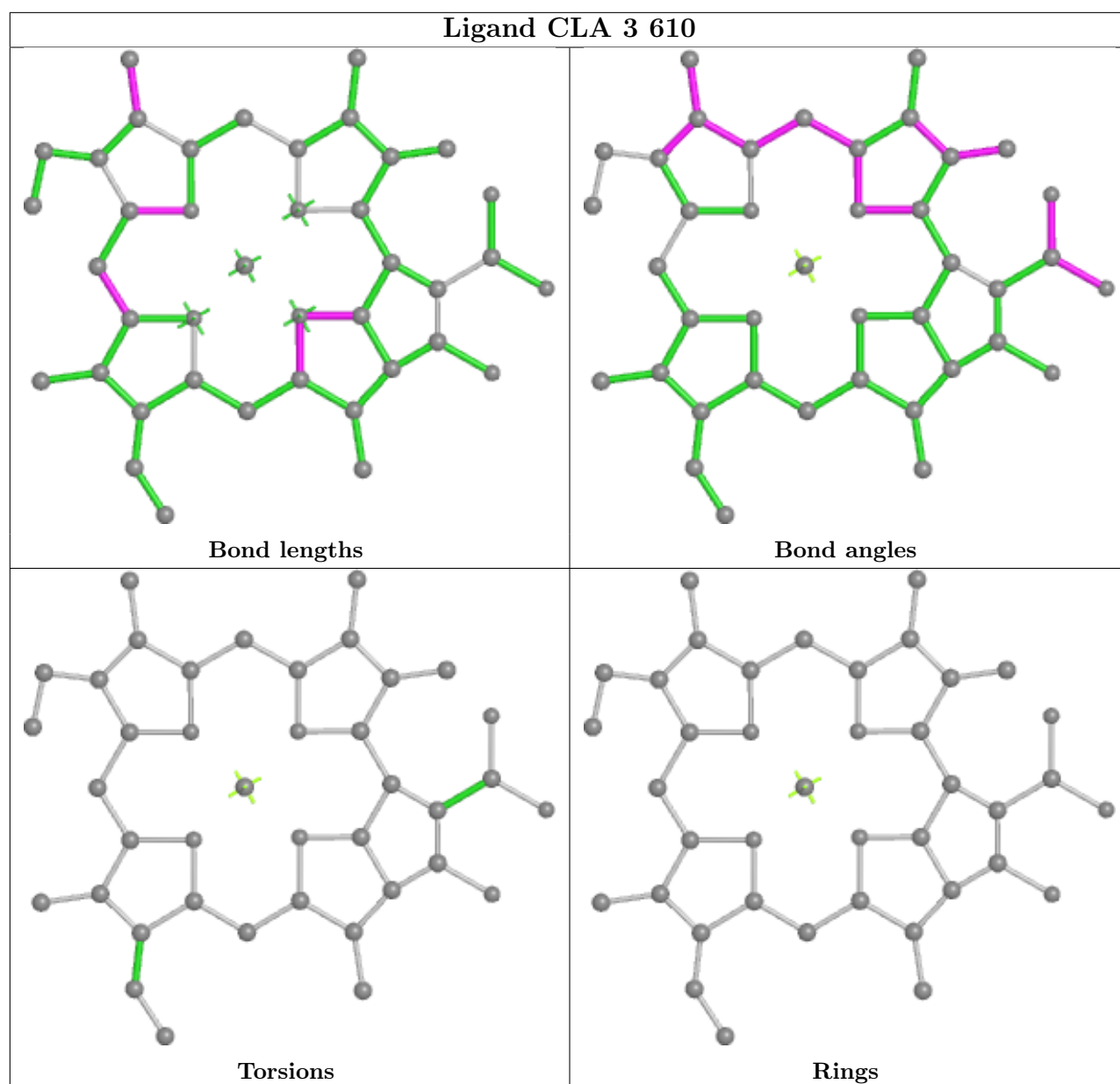
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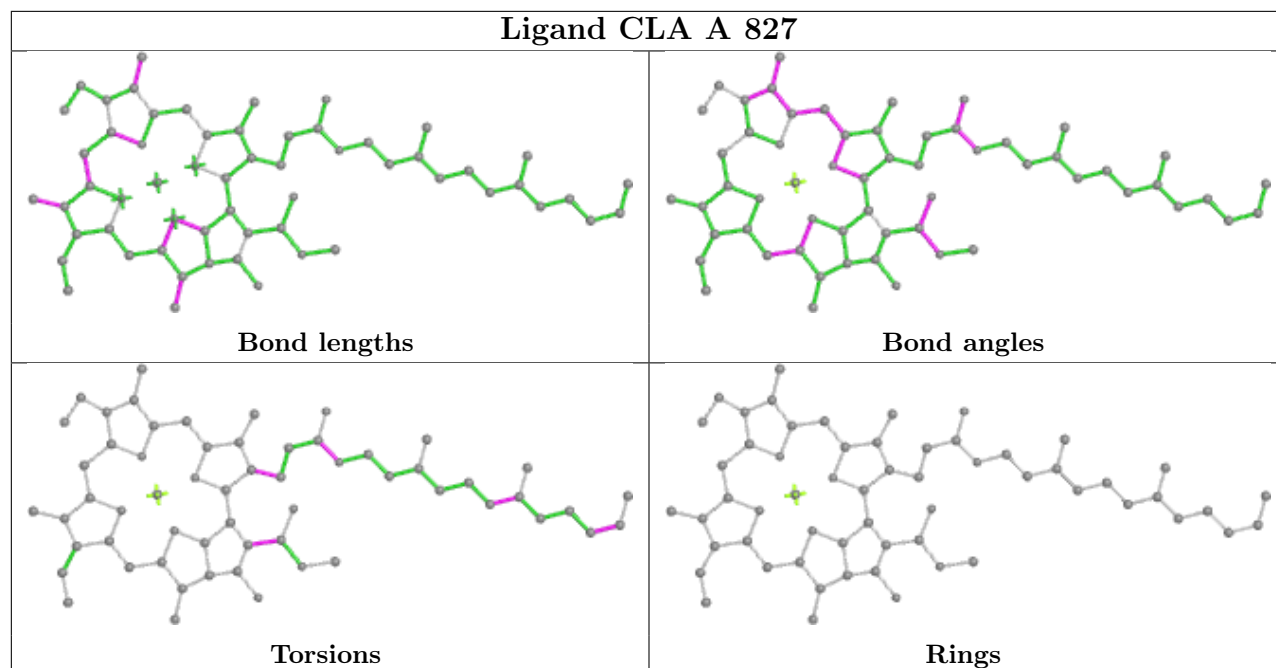




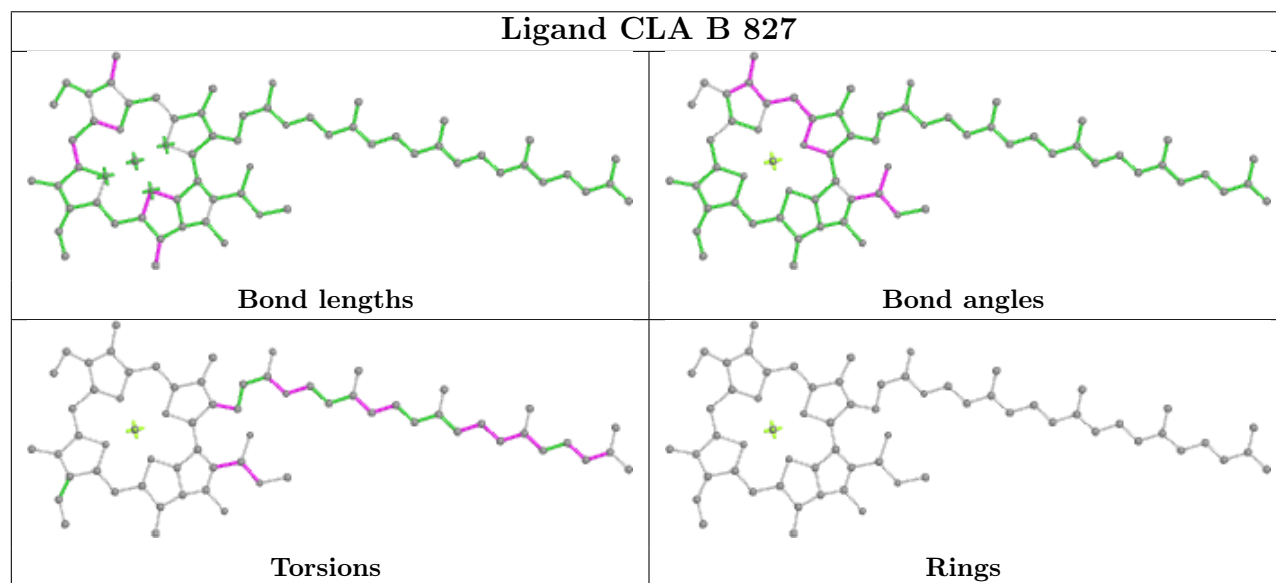




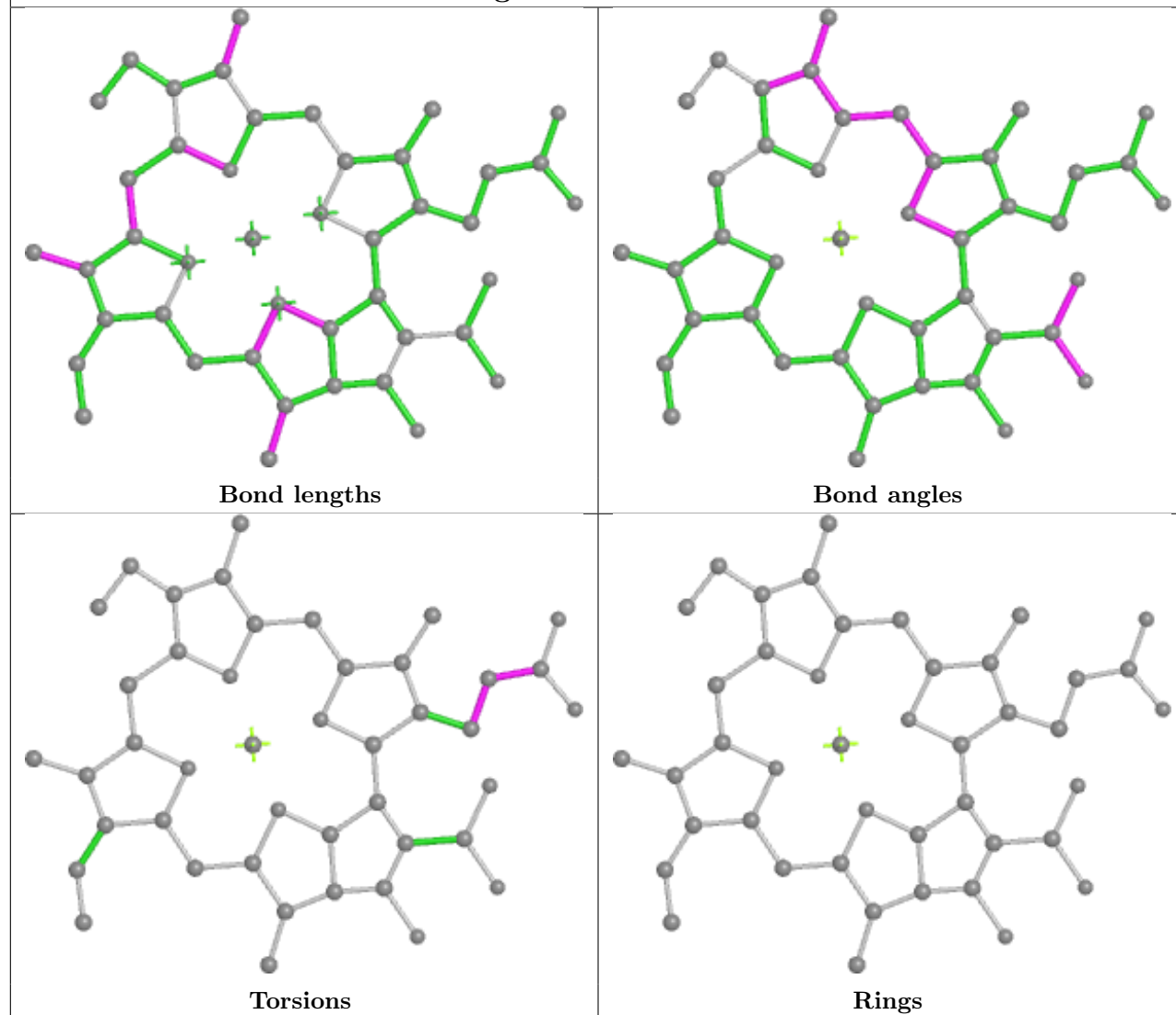
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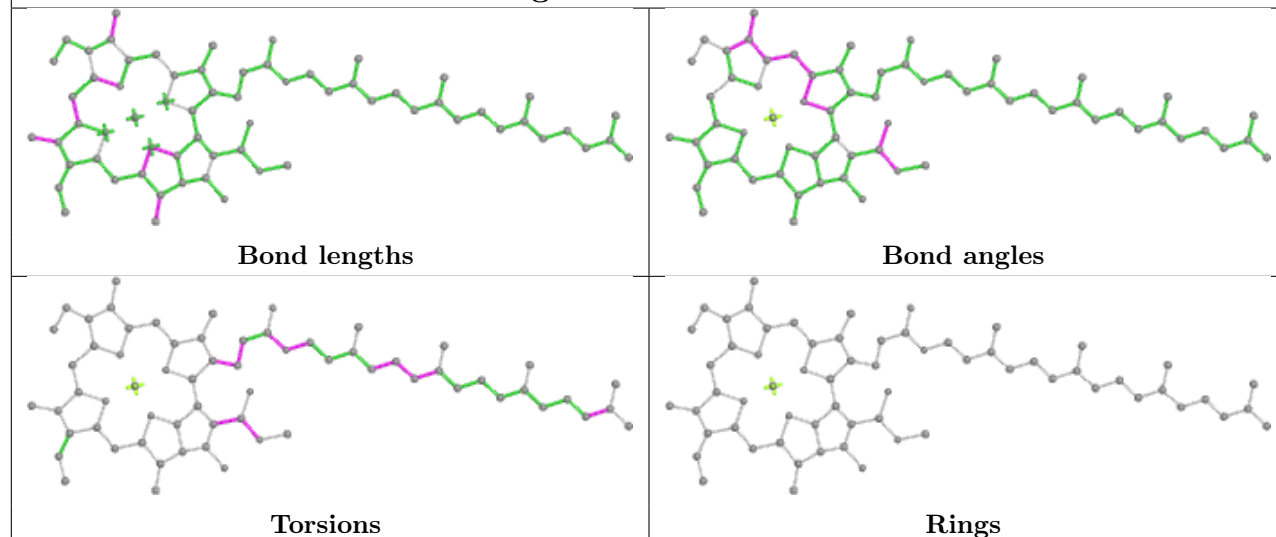
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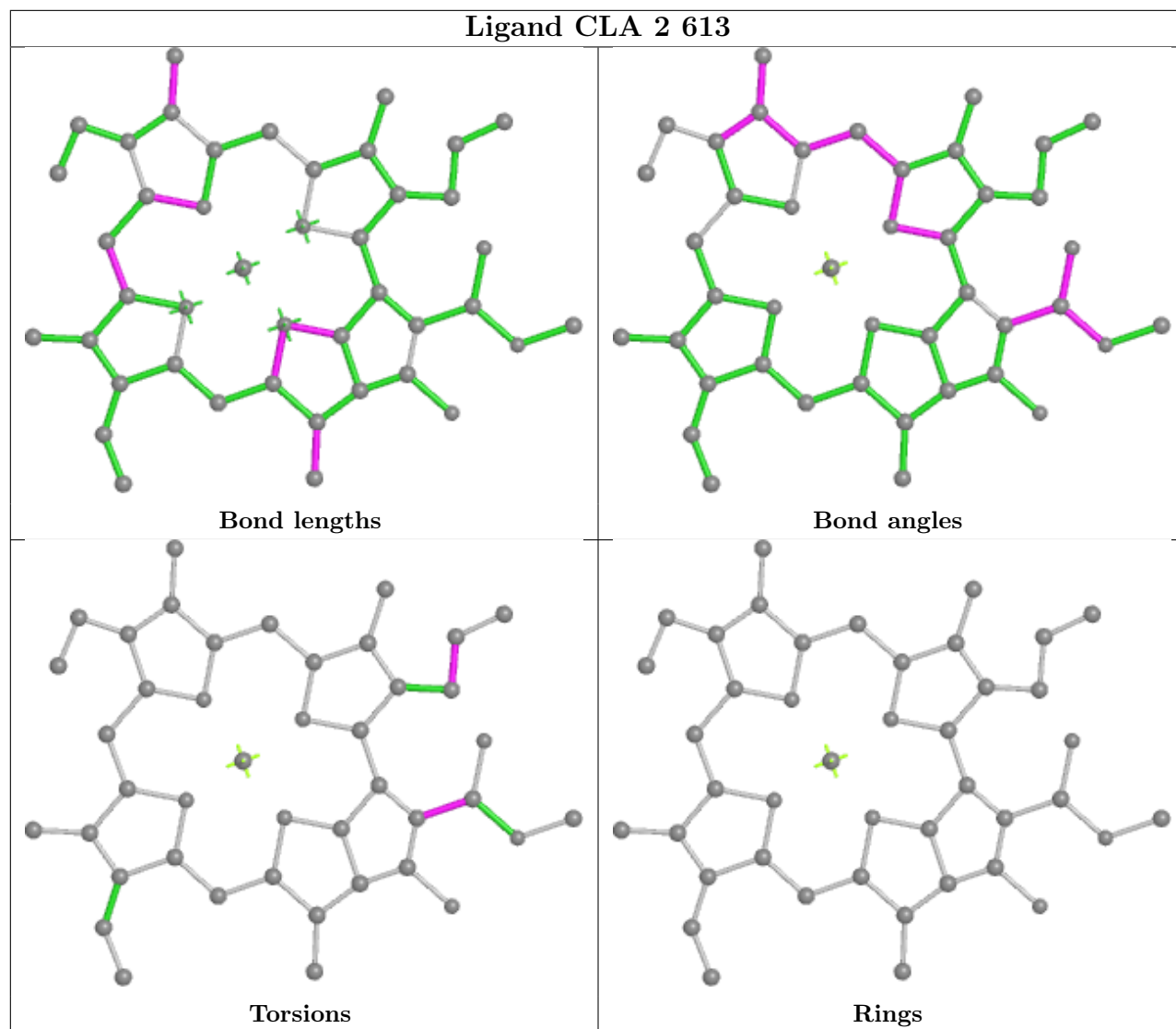
Ligand CLA 2 603



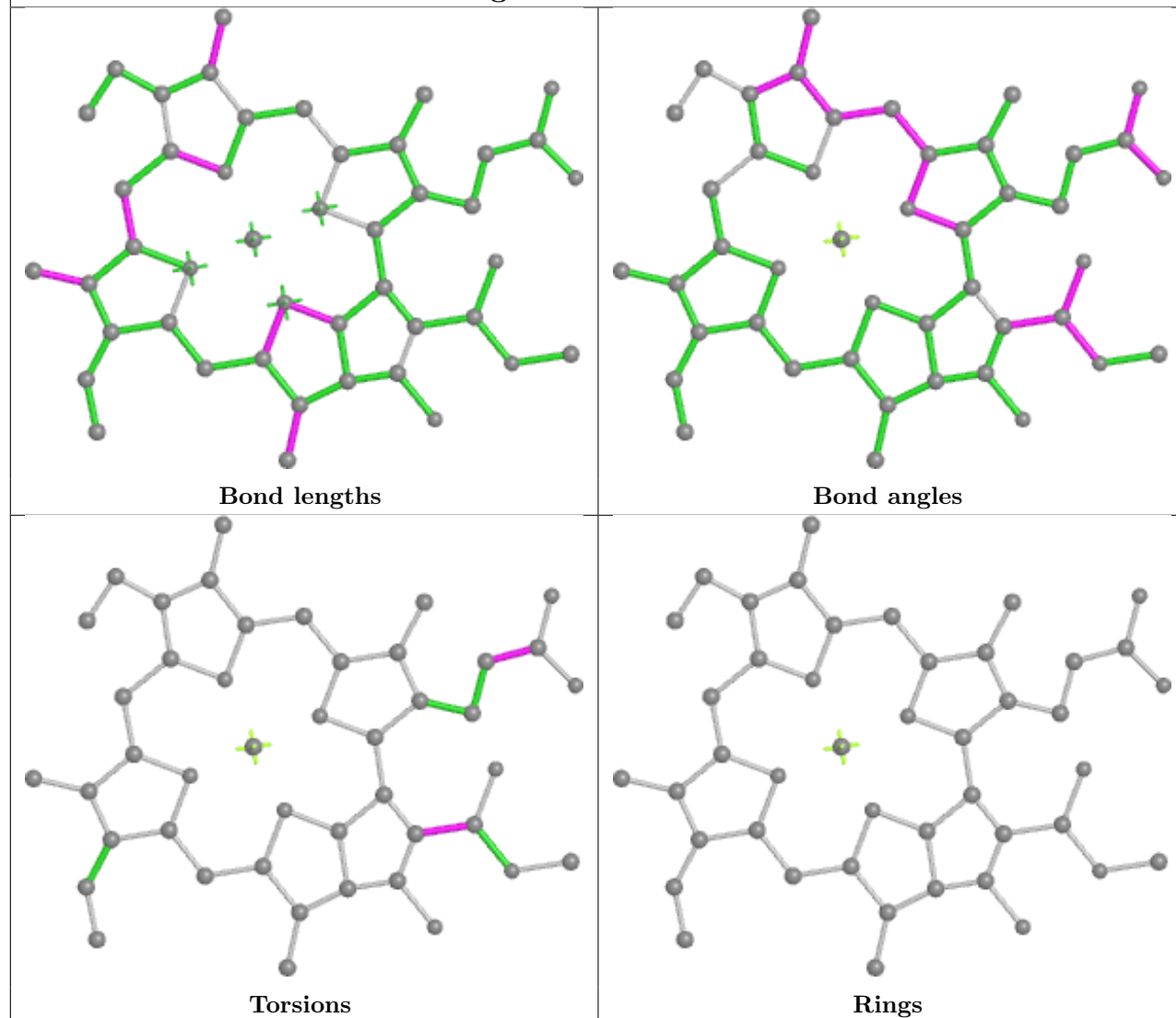
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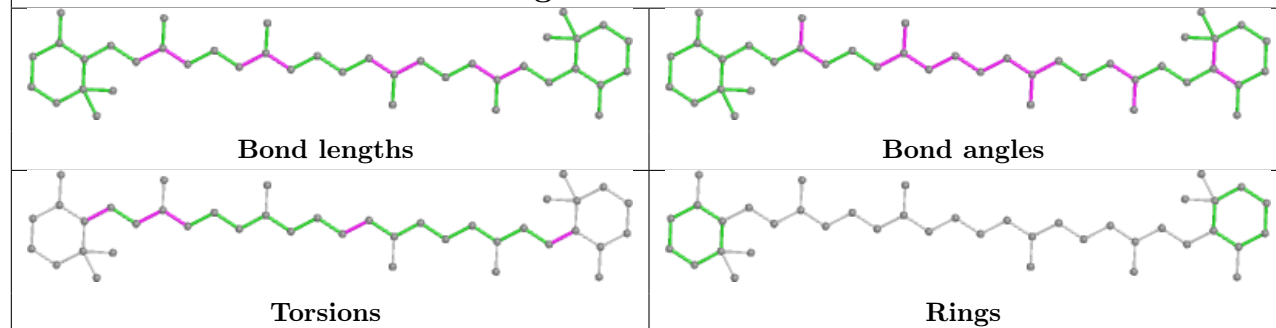
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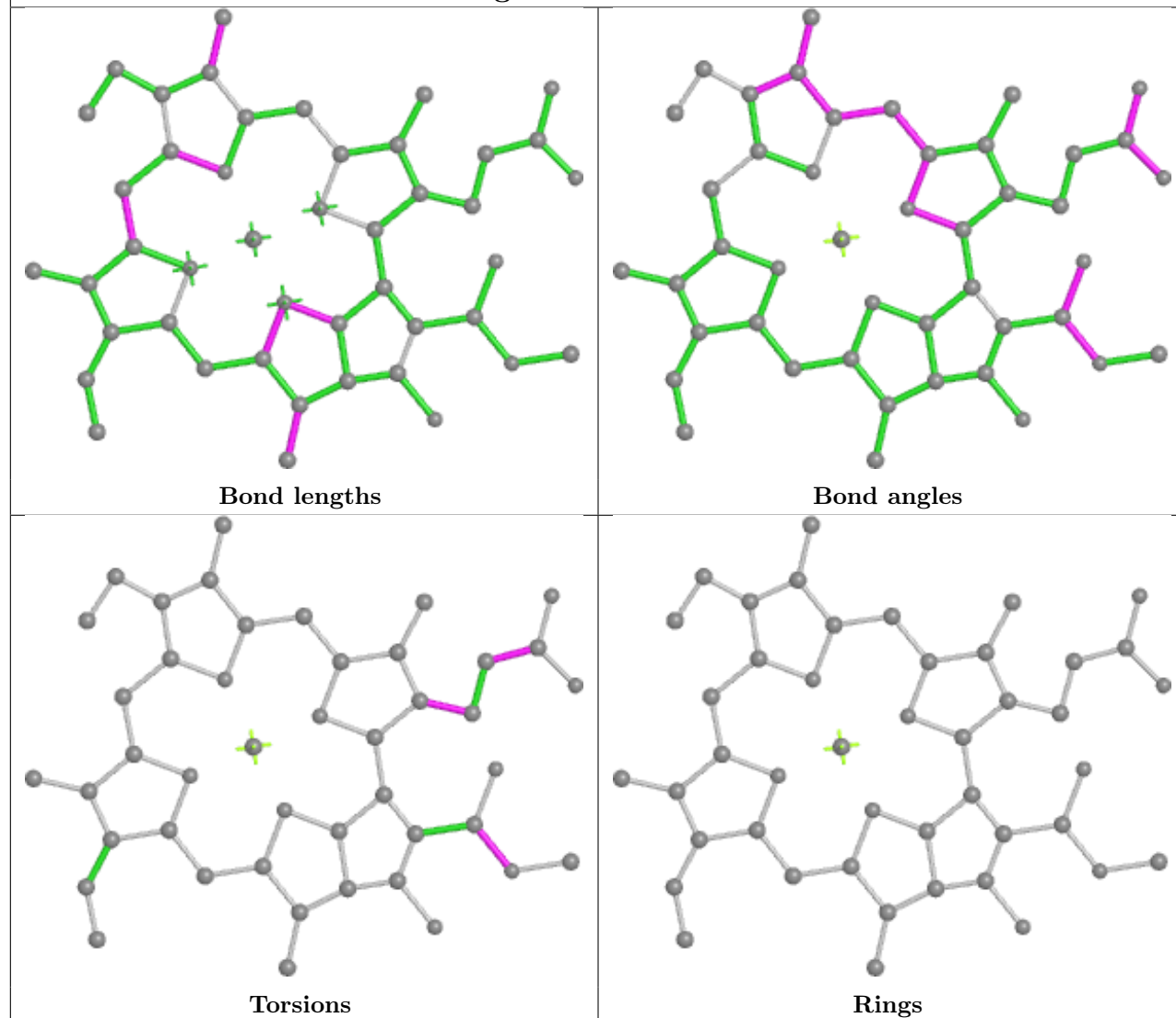
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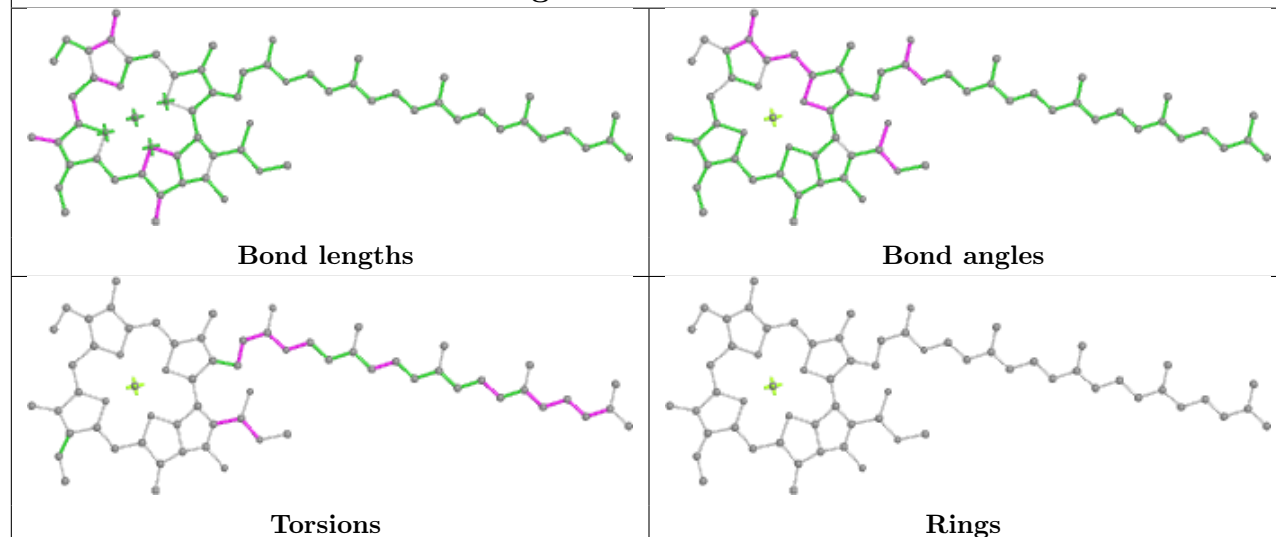
Ligand BCR 4 618



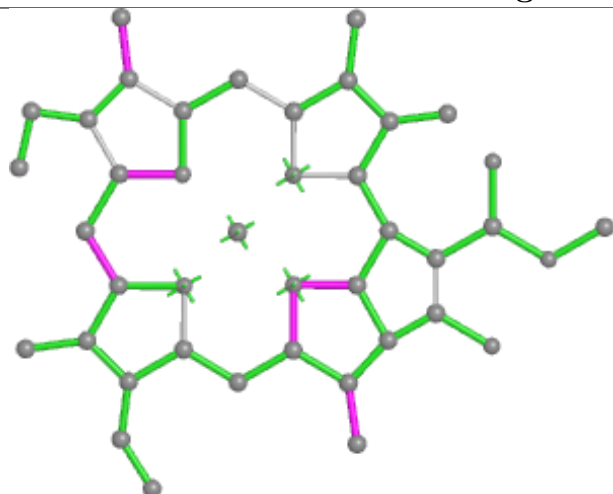
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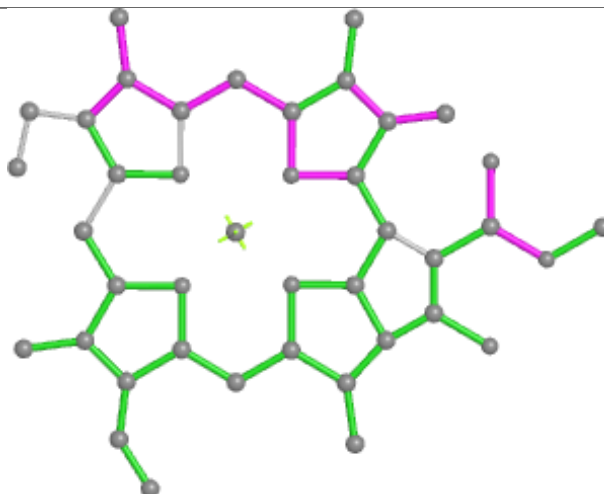
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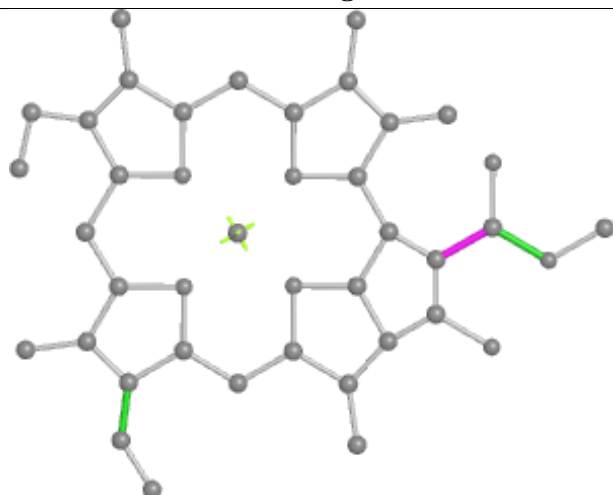
Ligand CLA F 303



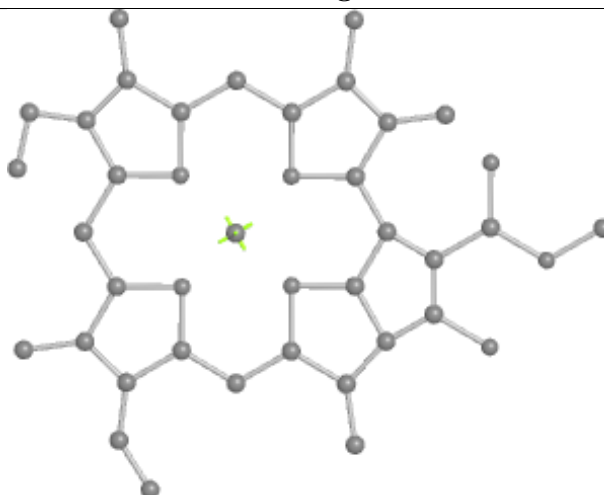
Bond lengths



Bond angles

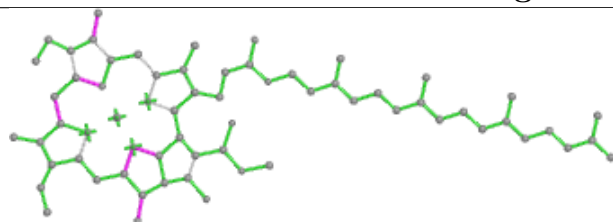


Torsions

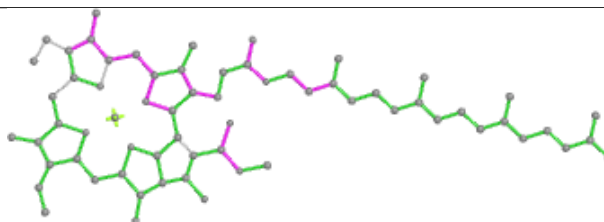


Rings

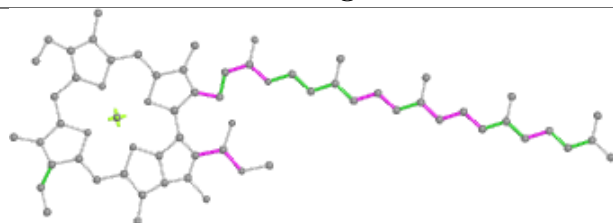
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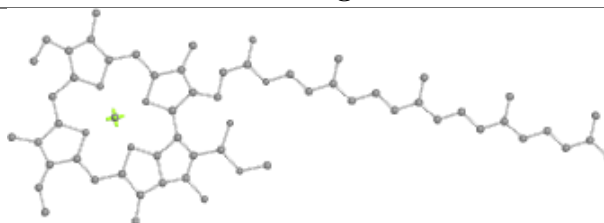
Bond lengths



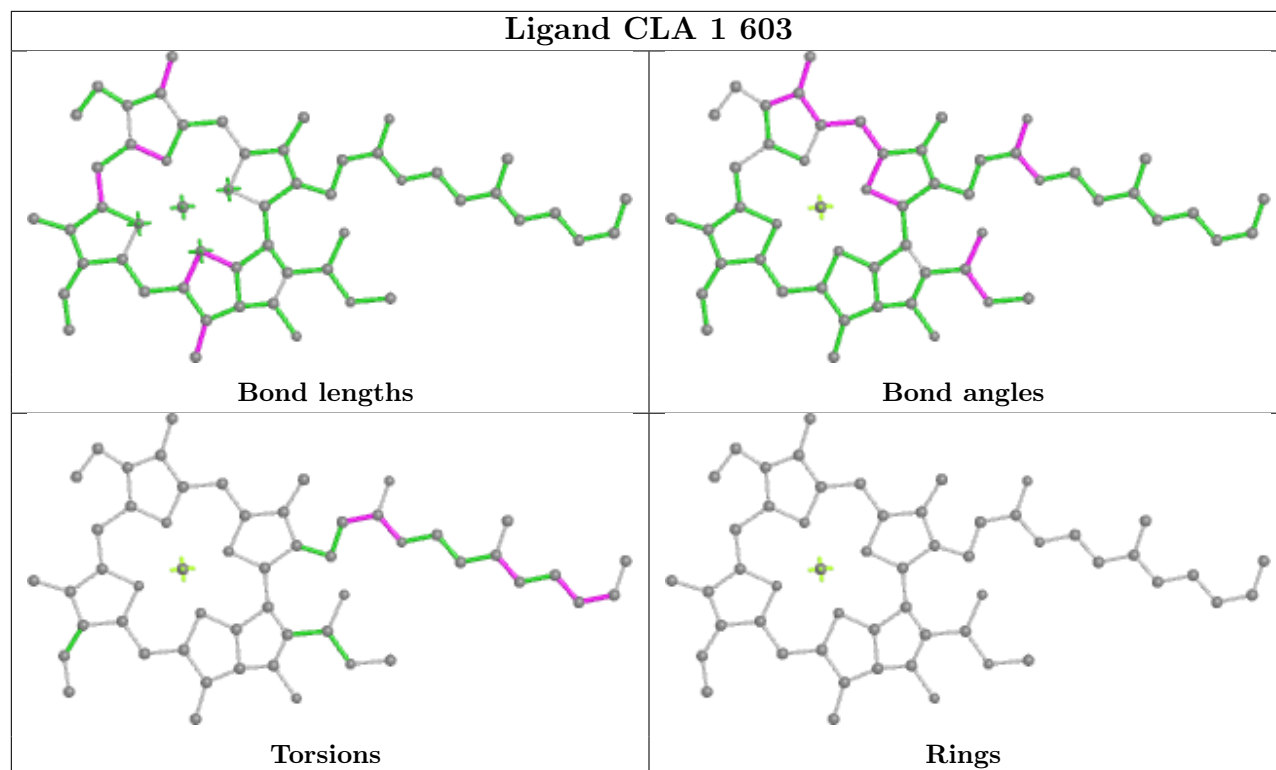
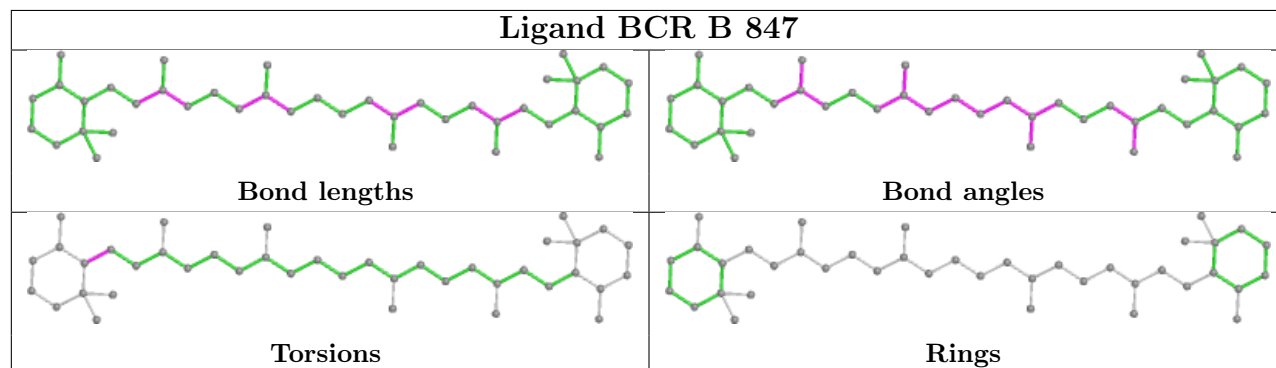
Bond angles

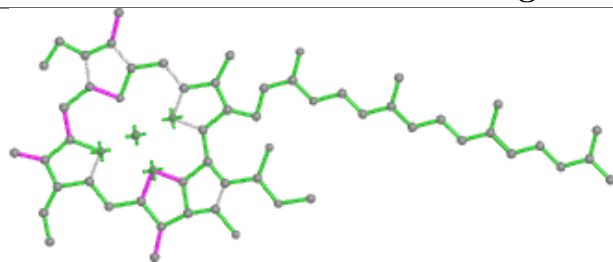


Torsions

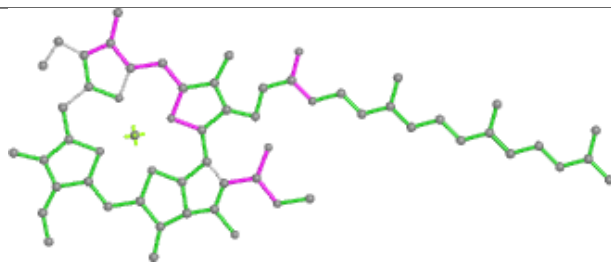


Rings

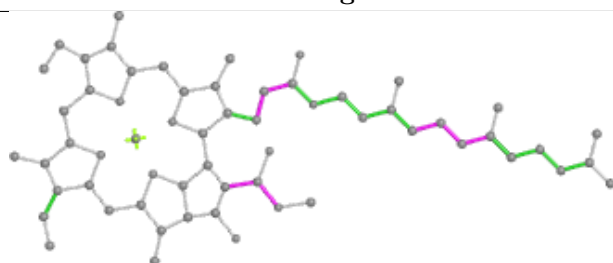
Ligand CLA 1 603**Ligand BCR B 847**

Ligand CLA 4 602

Bond lengths



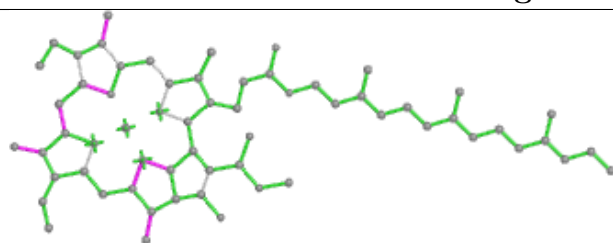
Bond angles



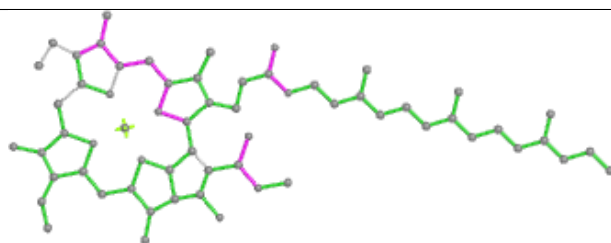
Torsions



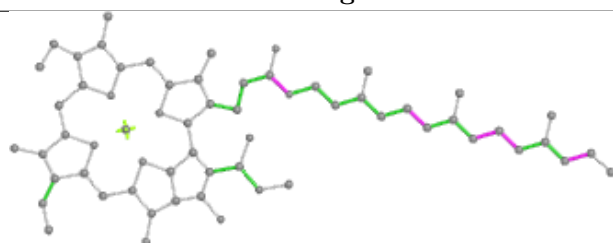
Rings

Ligand CLA B 826

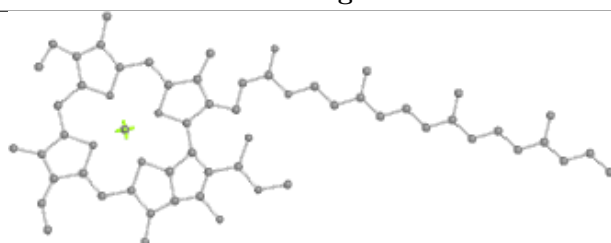
Bond lengths



Bond angles

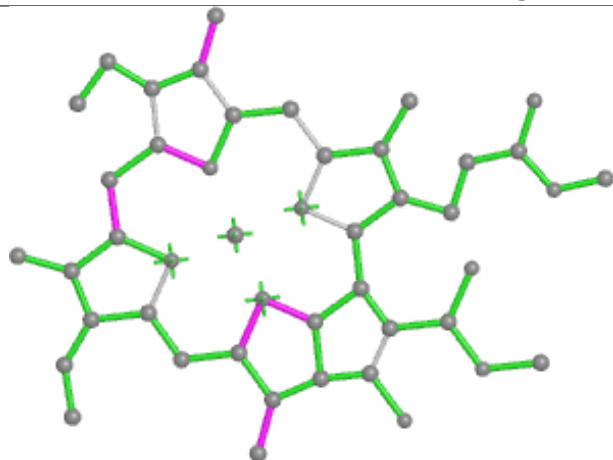


Torsions

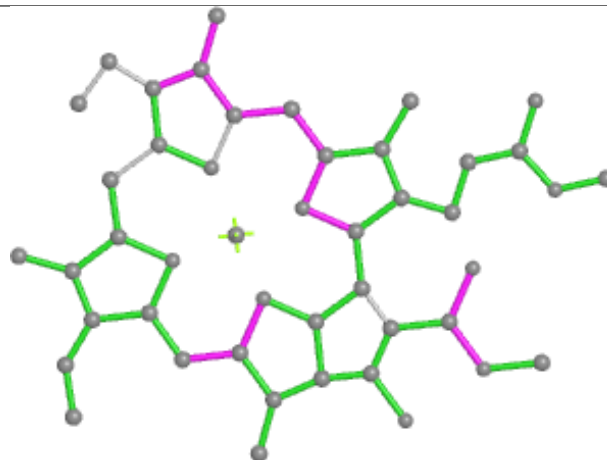


Rings

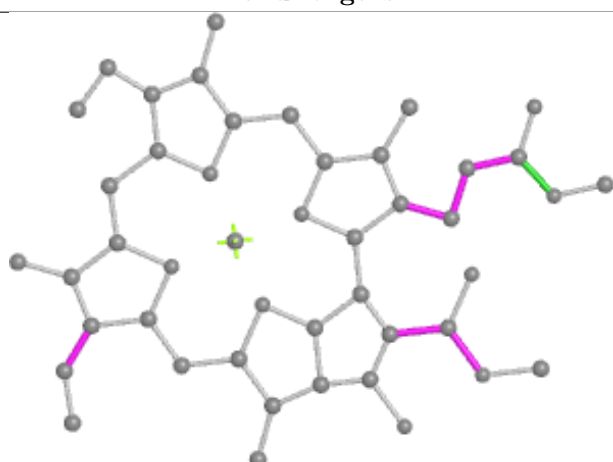
Ligand CLA K 204



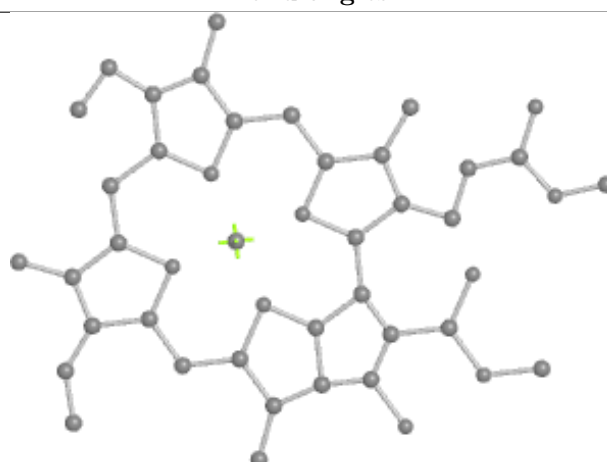
Bond lengths



Bond angles

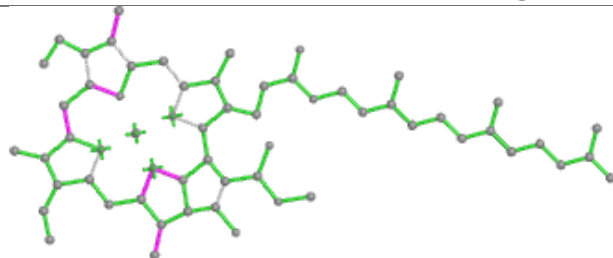


Torsions

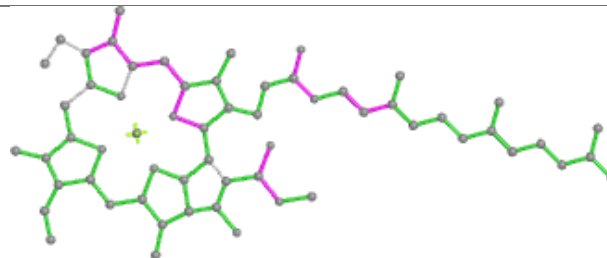


Rings

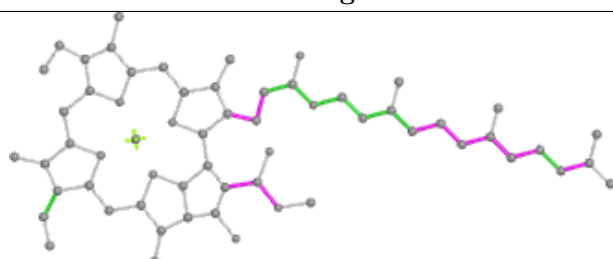
Ligand CLA H 201



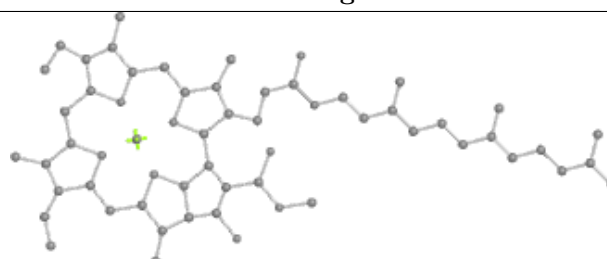
Bond lengths



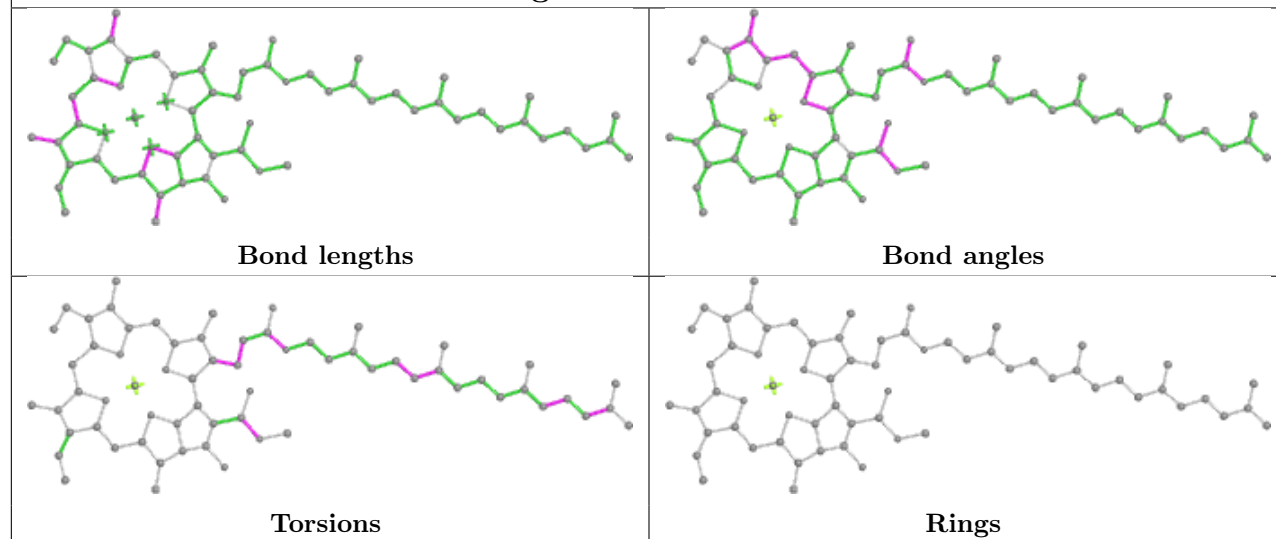
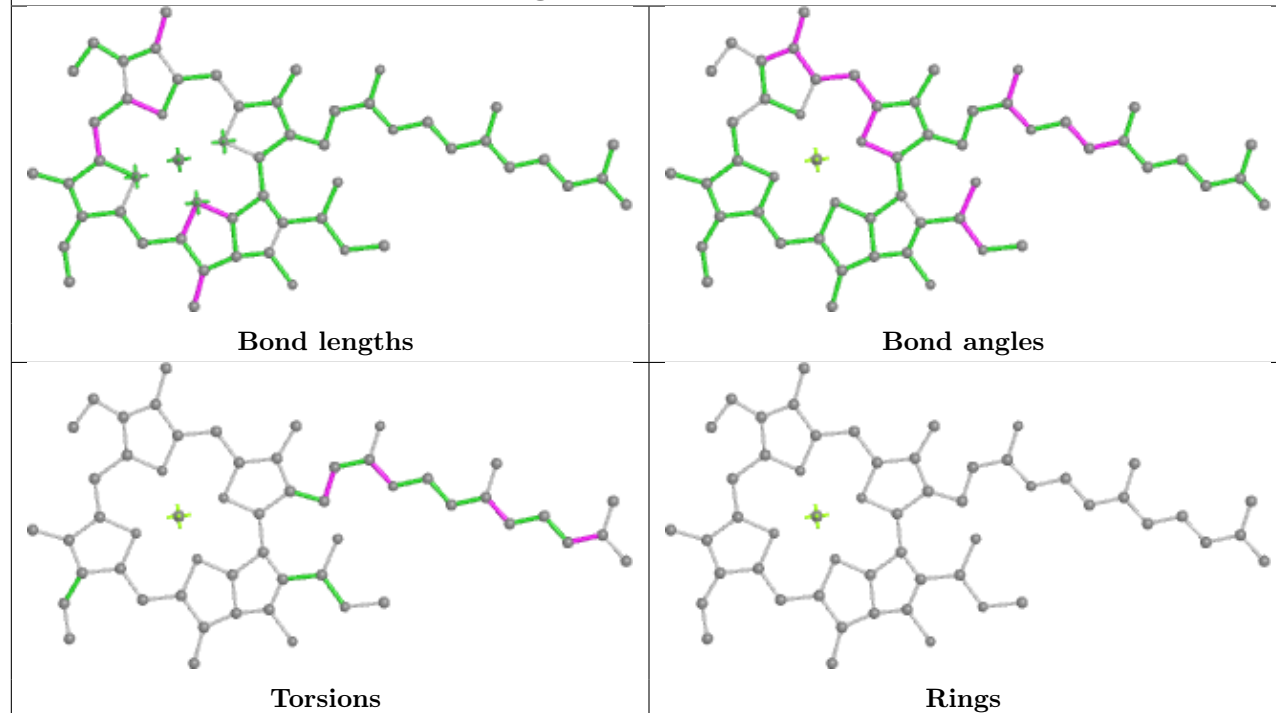
Bond angles



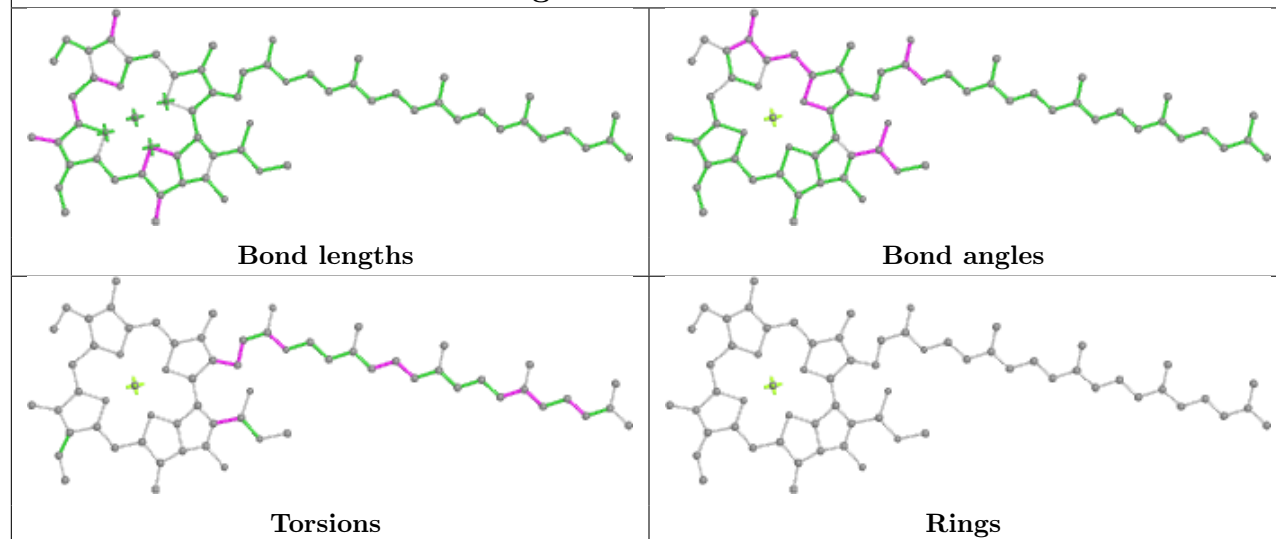
Torsions



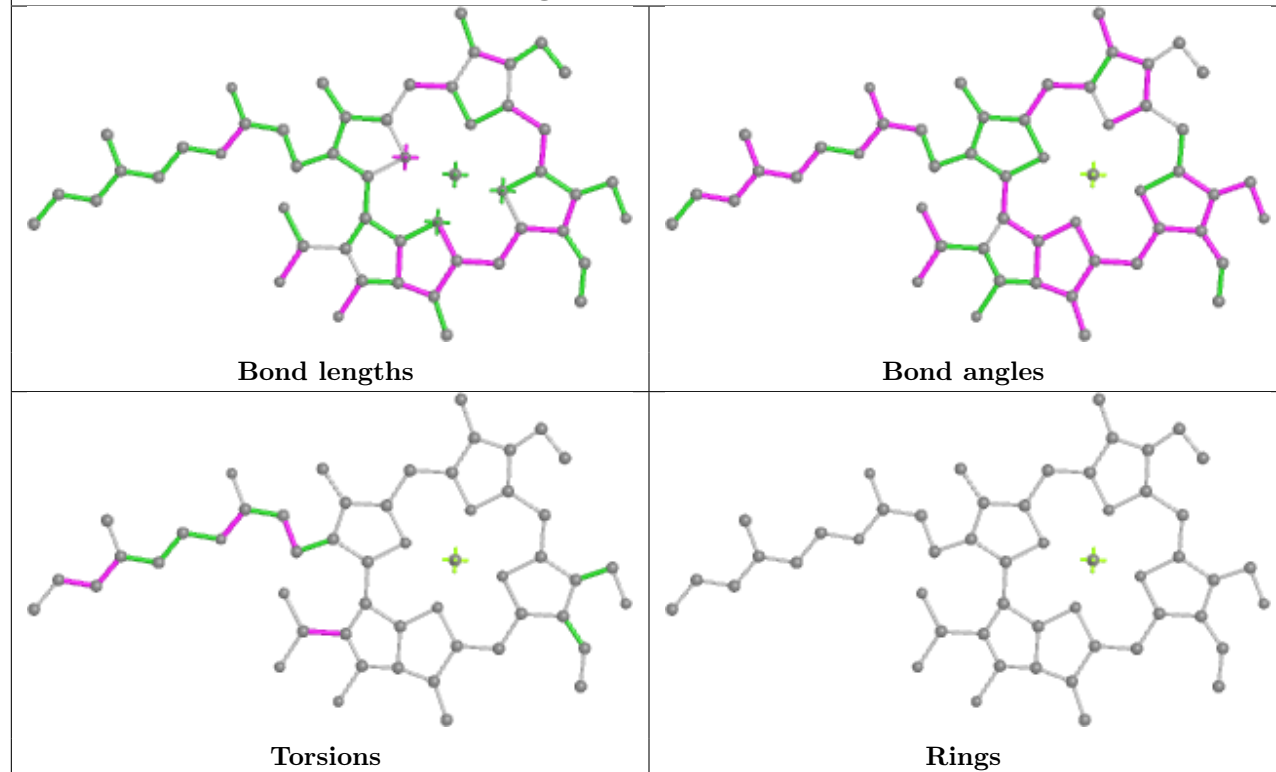
Rings

Ligand CLA A 802**Ligand CLA A 839**

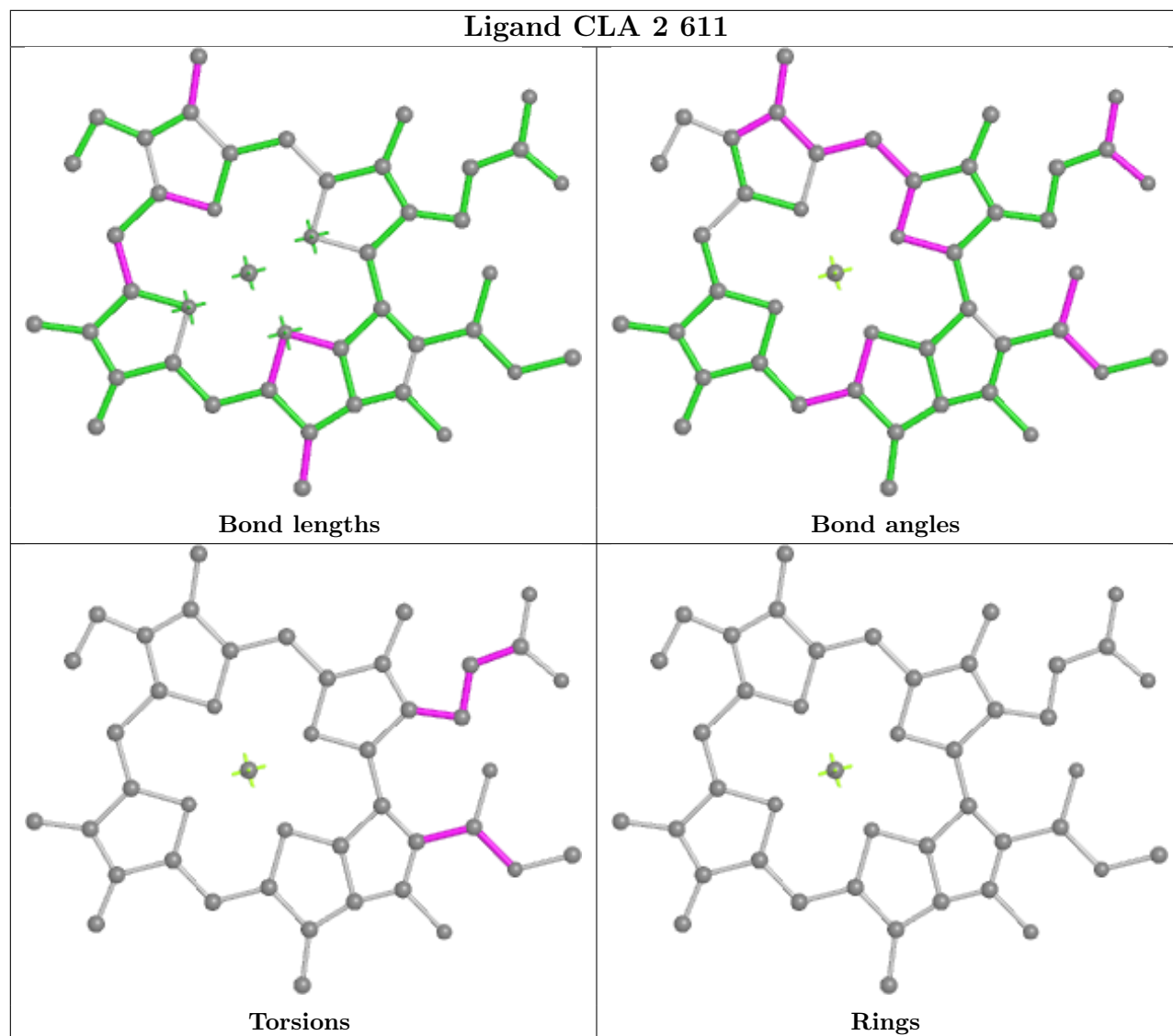
Ligand CLA B 837



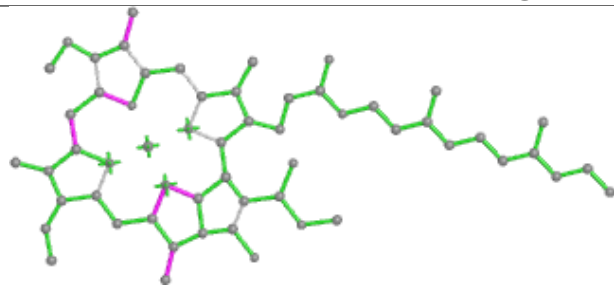
Ligand CHL 1 601



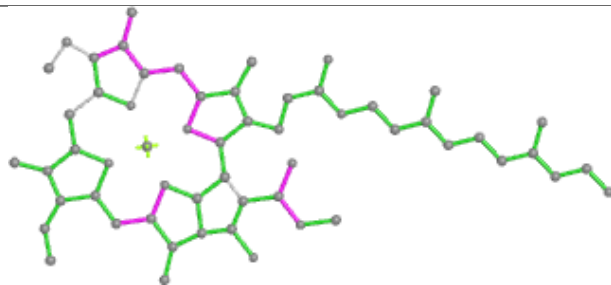
Ligand CLA 2 611



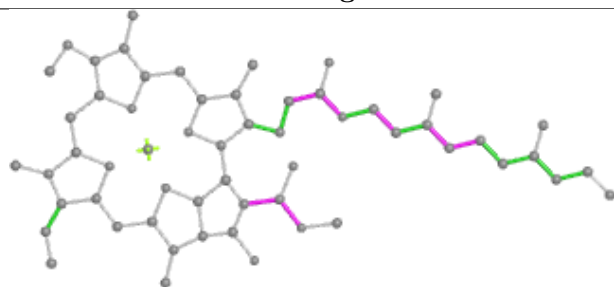
Ligand CLA F 301



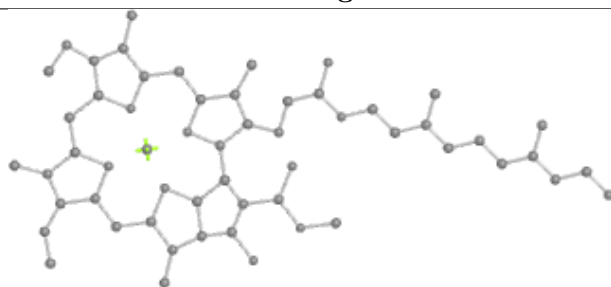
Bond lengths



Bond angles

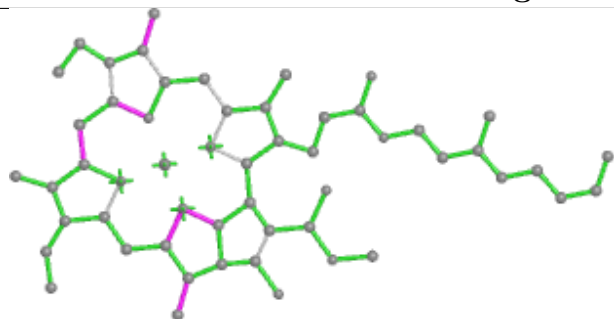


Torsions

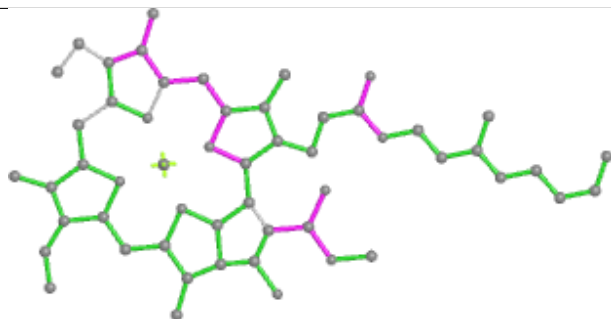


Rings

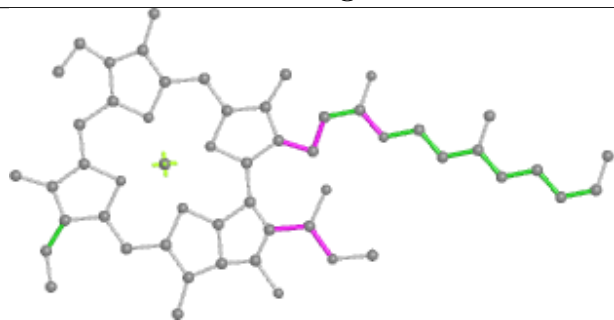
Ligand CLA A 813



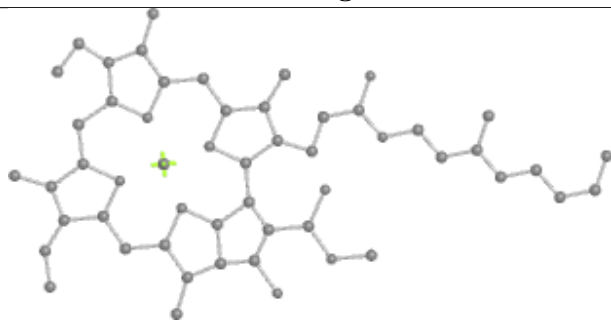
Bond lengths



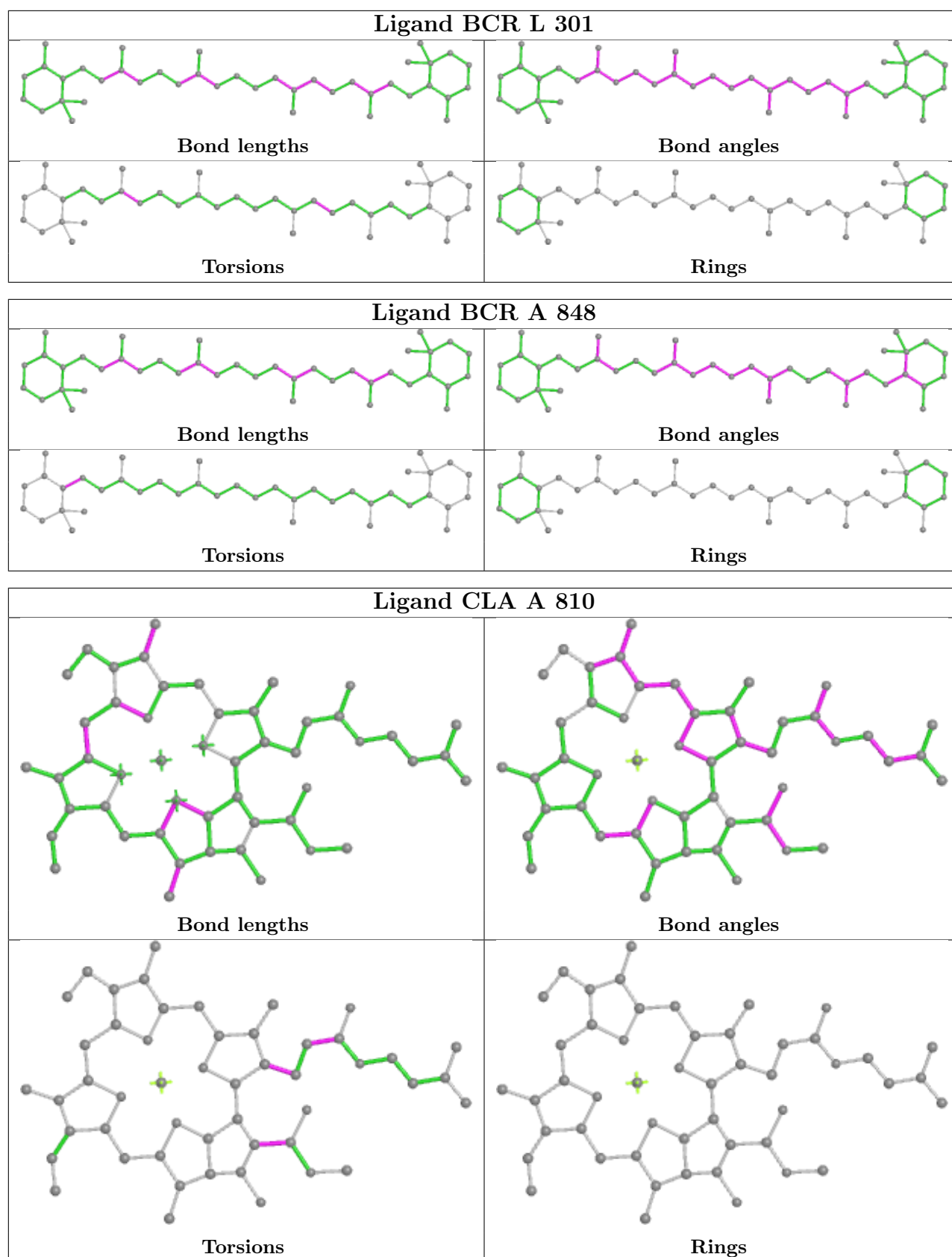
Bond angles

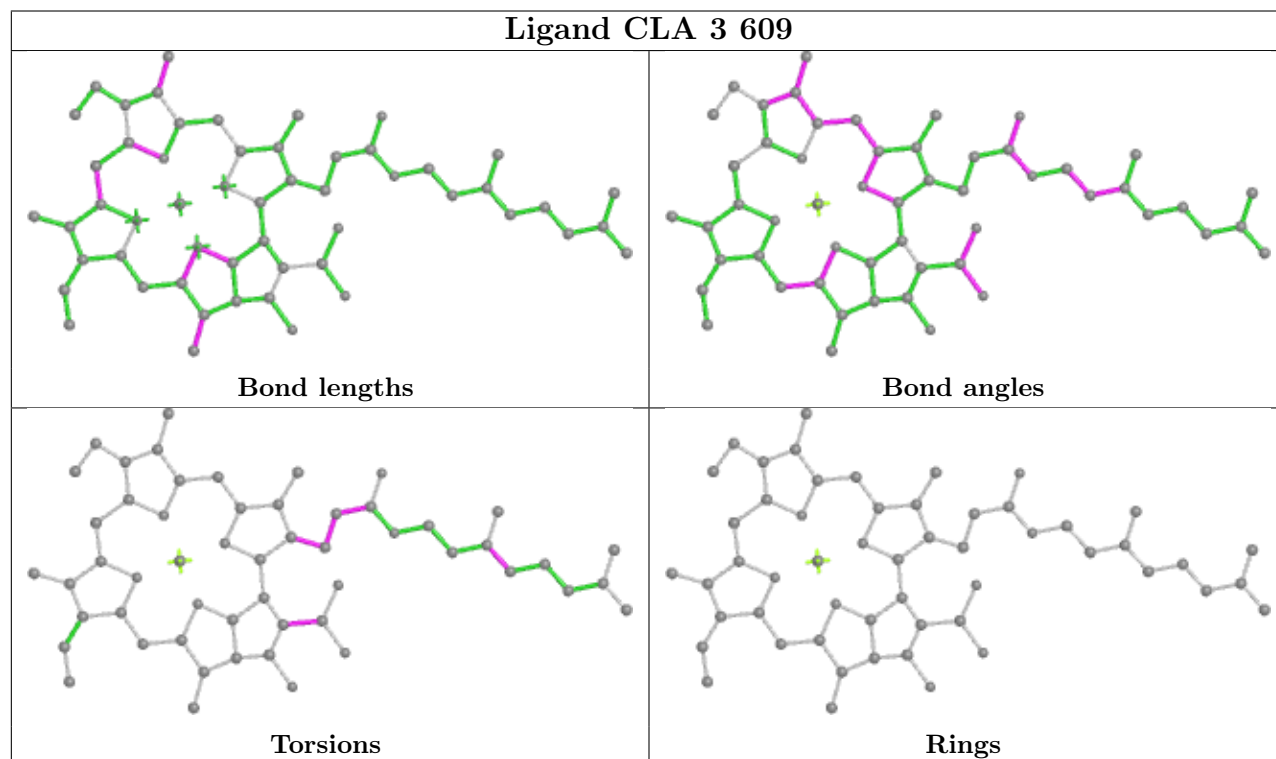
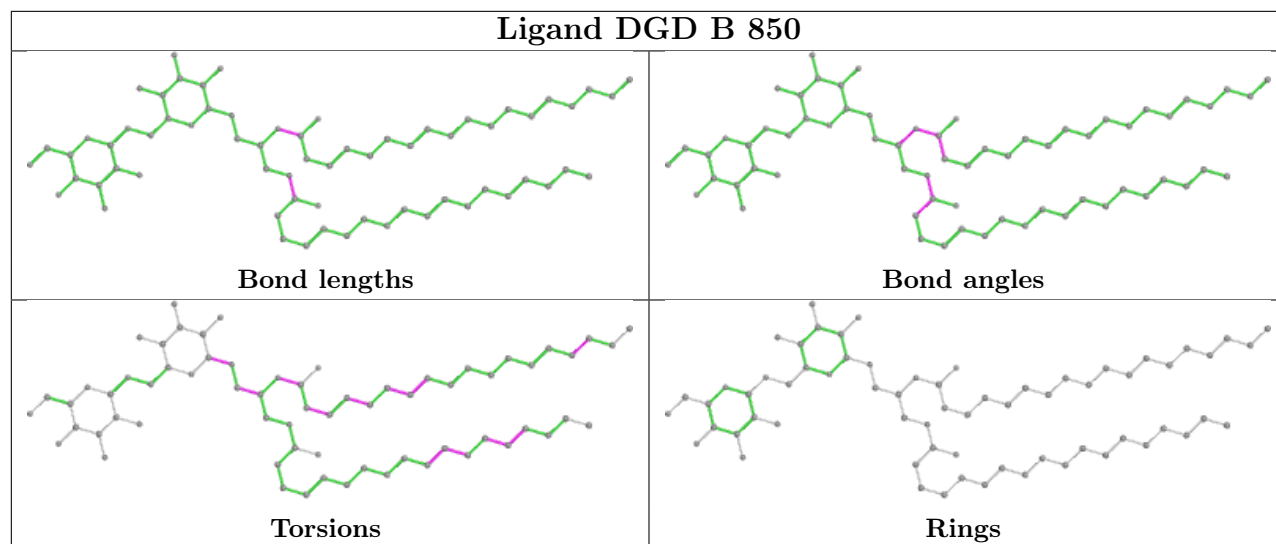
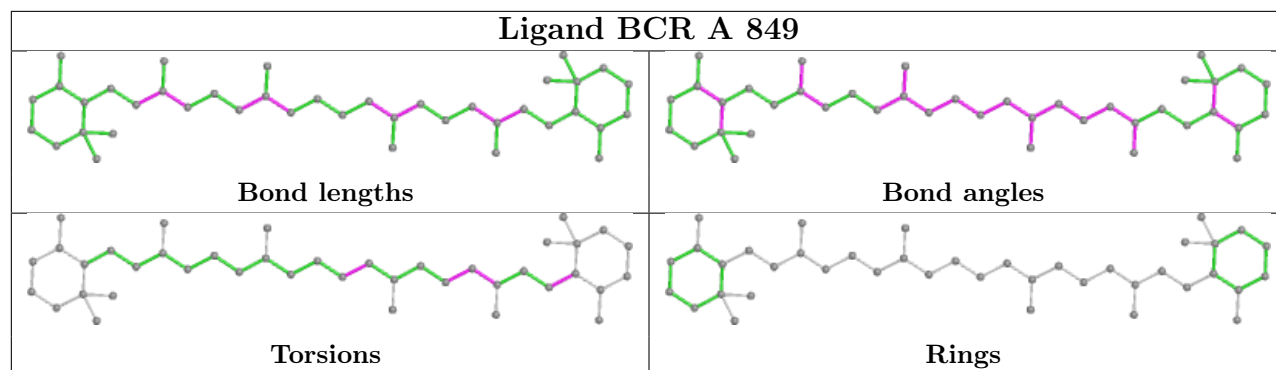


Torsions

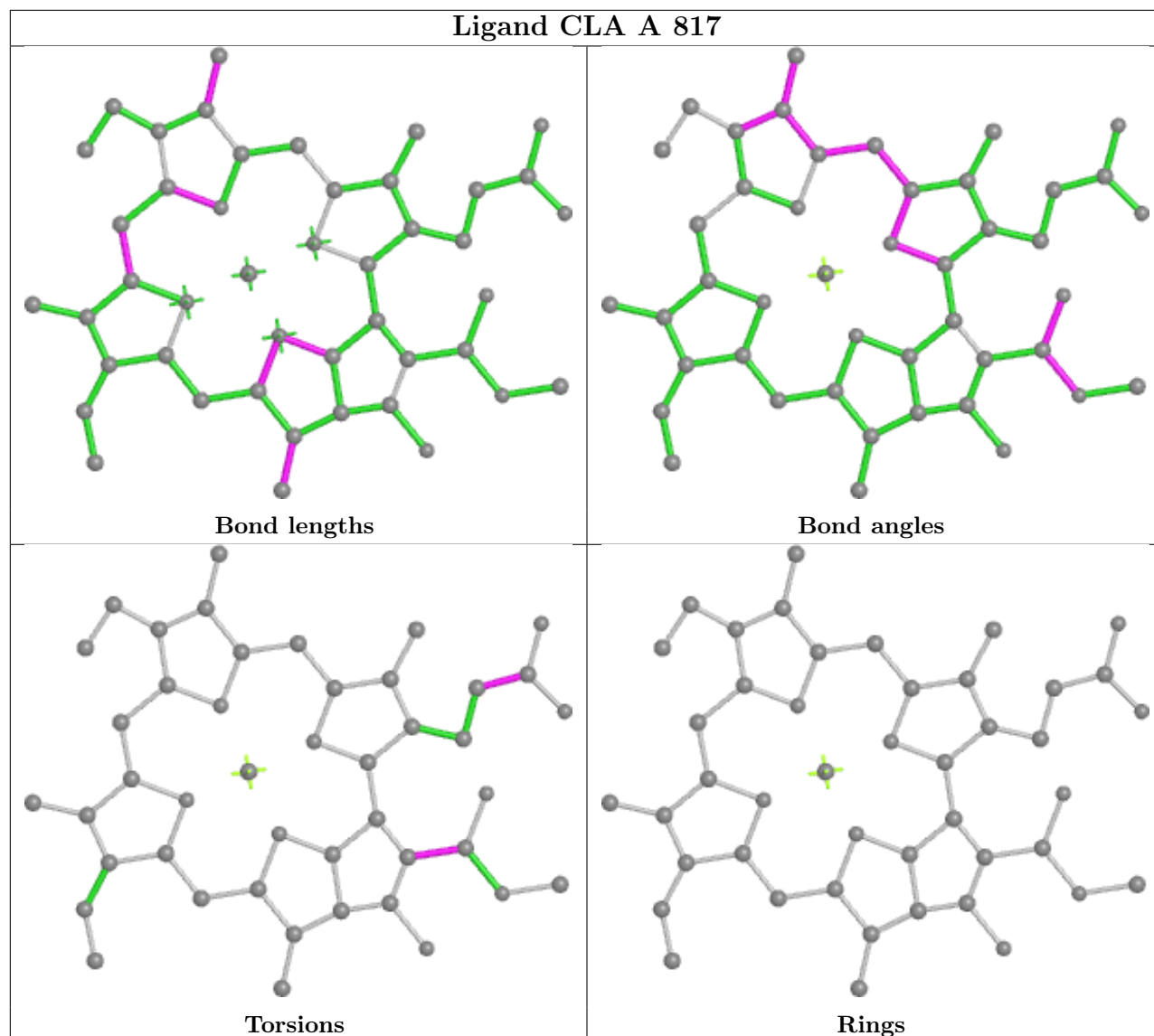


Rings

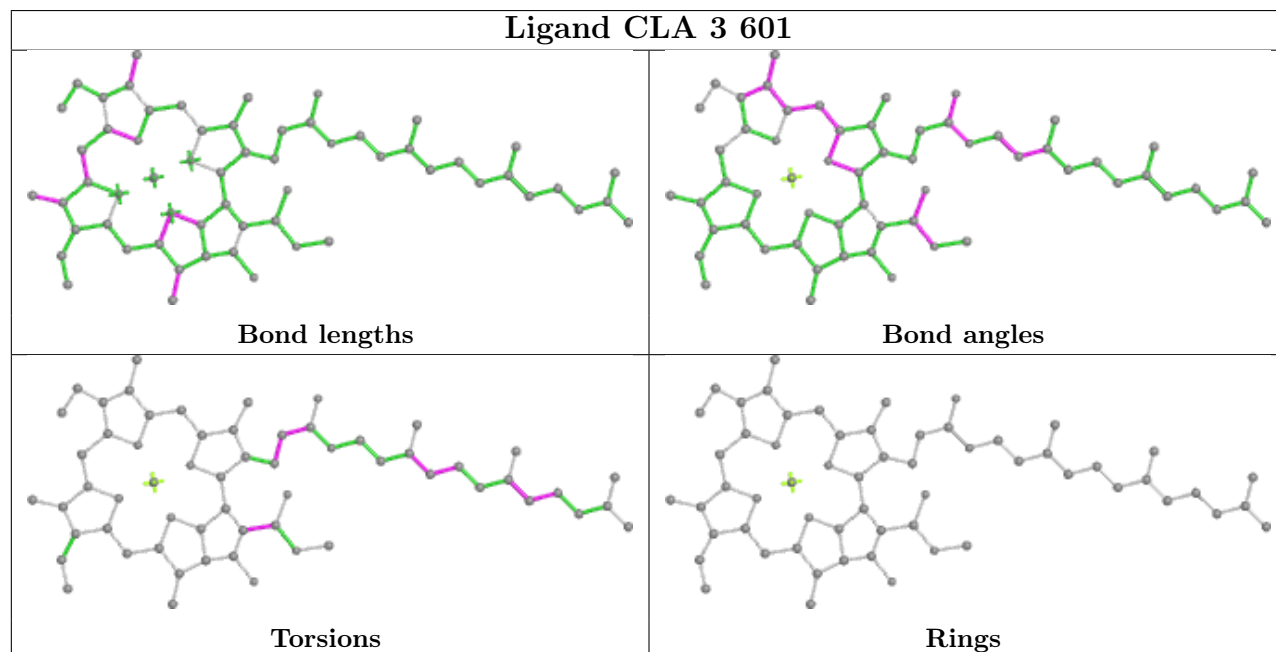


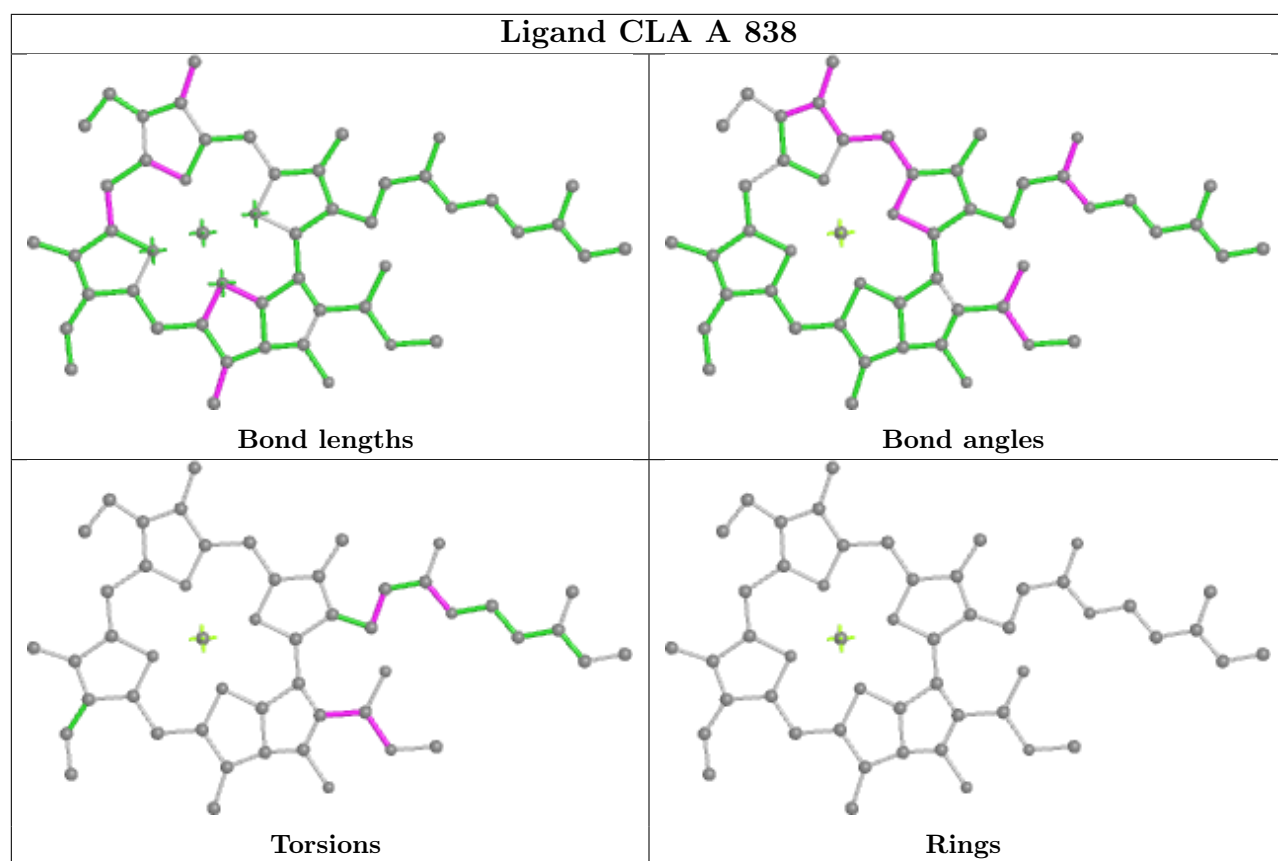


Ligand CLA A 817

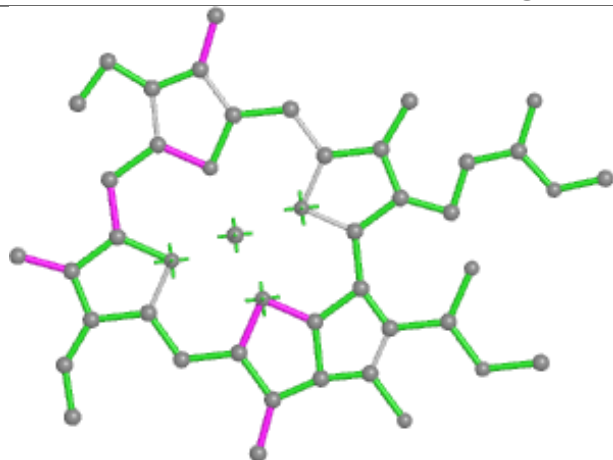


Ligand CLA 3 601

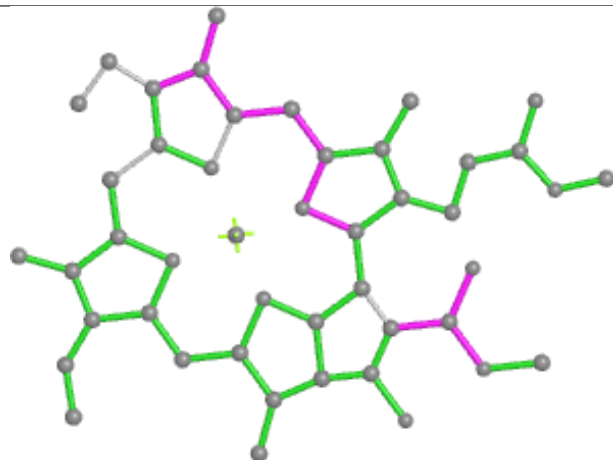




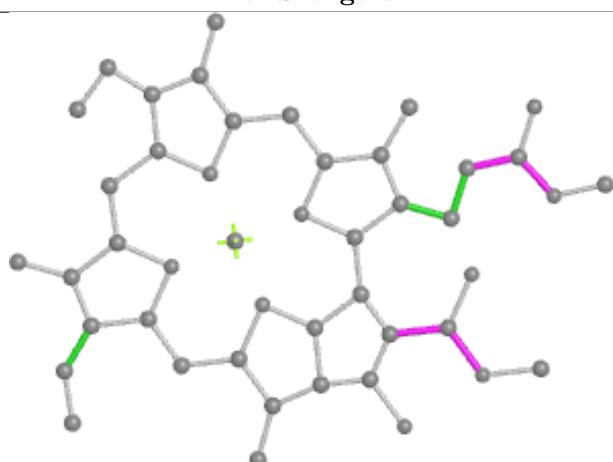
Ligand CLA 4 601



Bond lengths



Bond angles

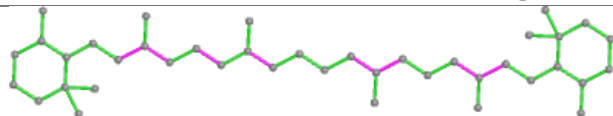


Torsions

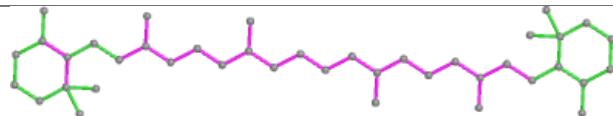


Rings

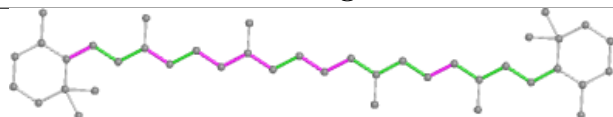
Ligand BCR F 304



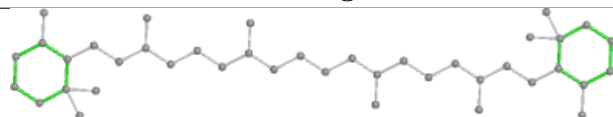
Bond lengths



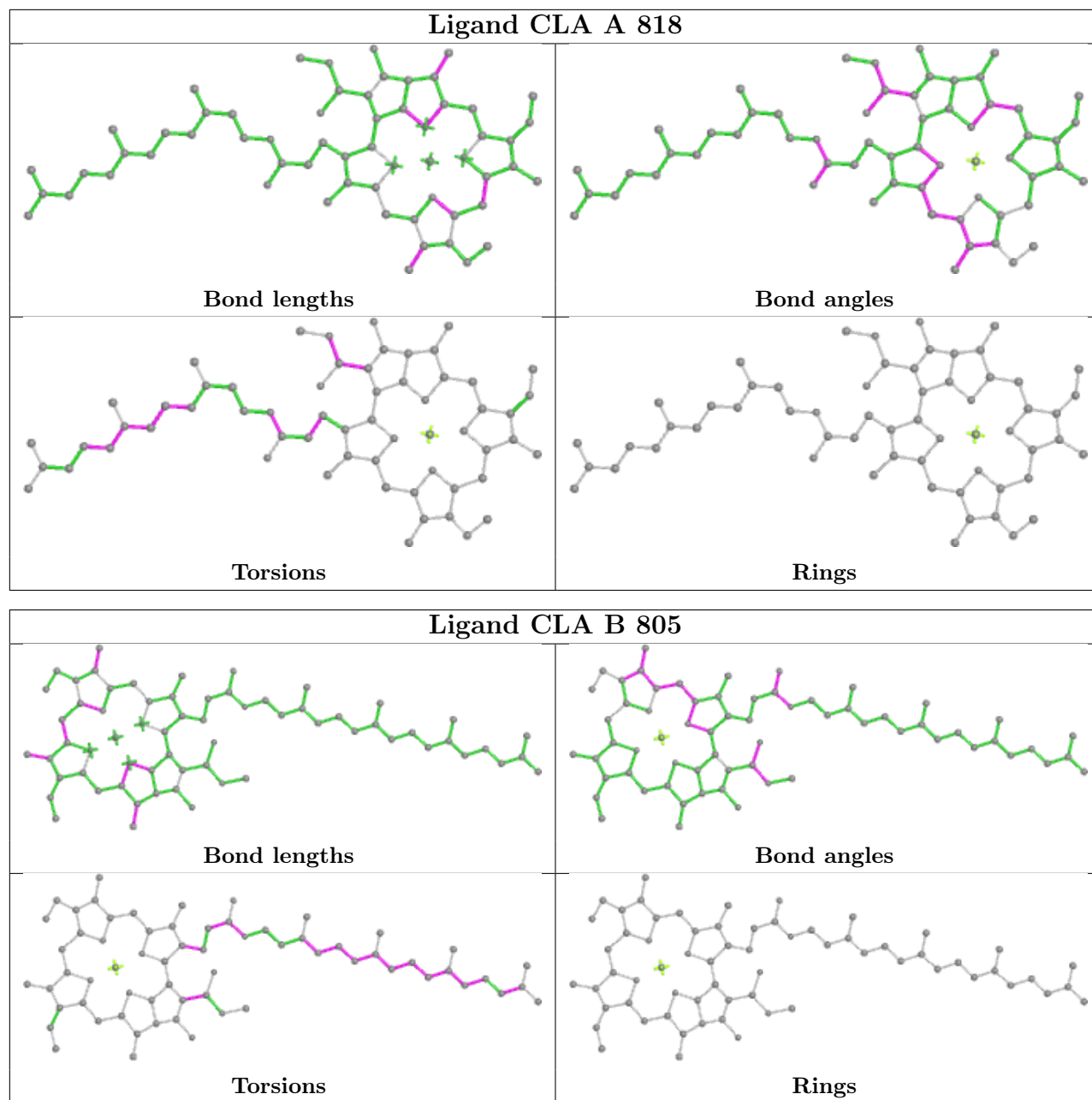
Bond angles



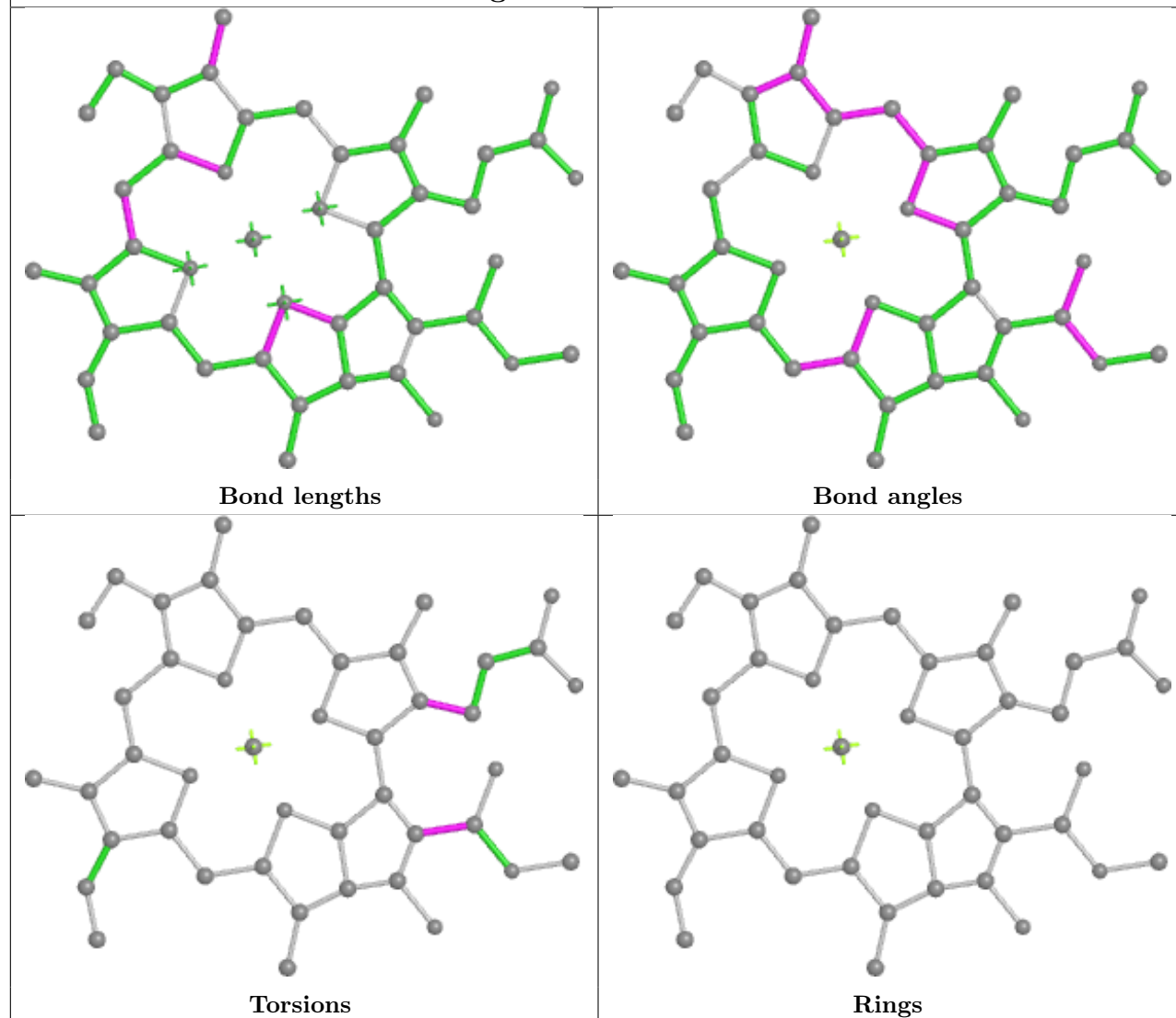
Torsions



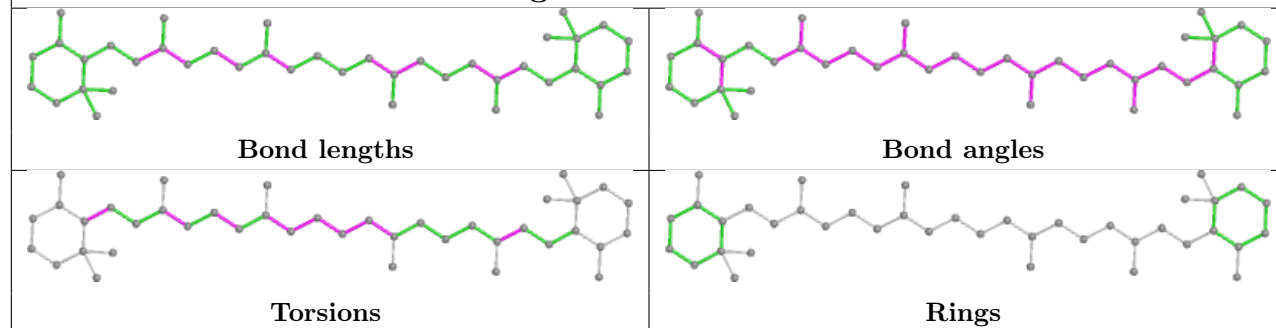
Rings

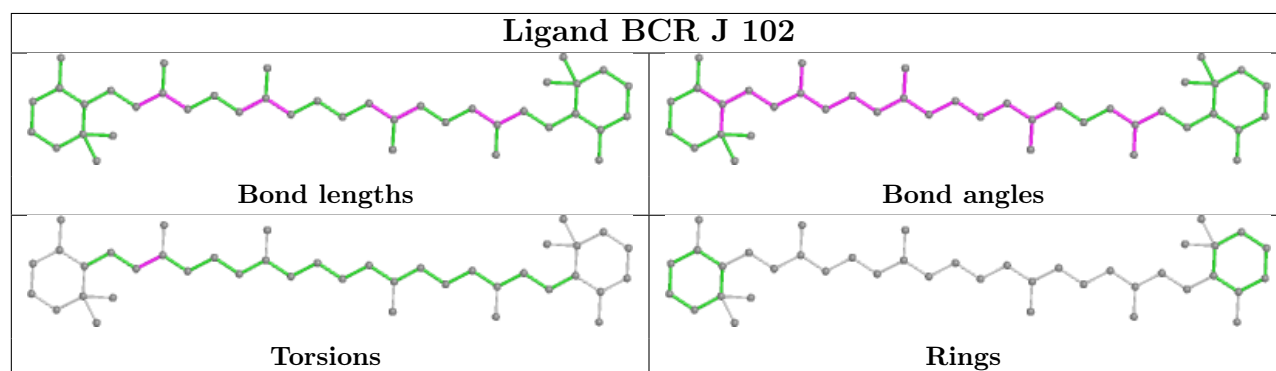
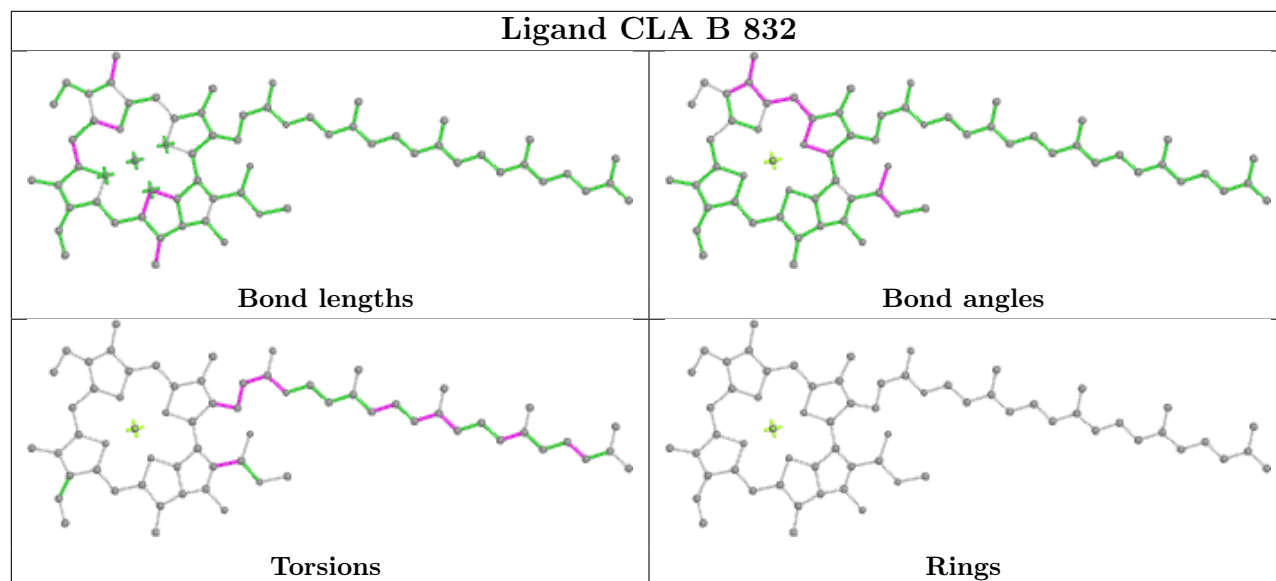
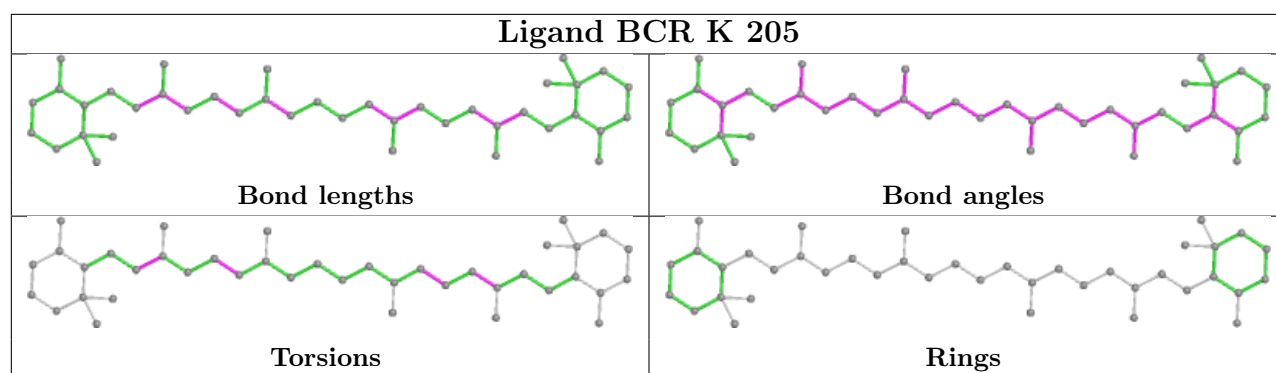


Ligand CLA A 836

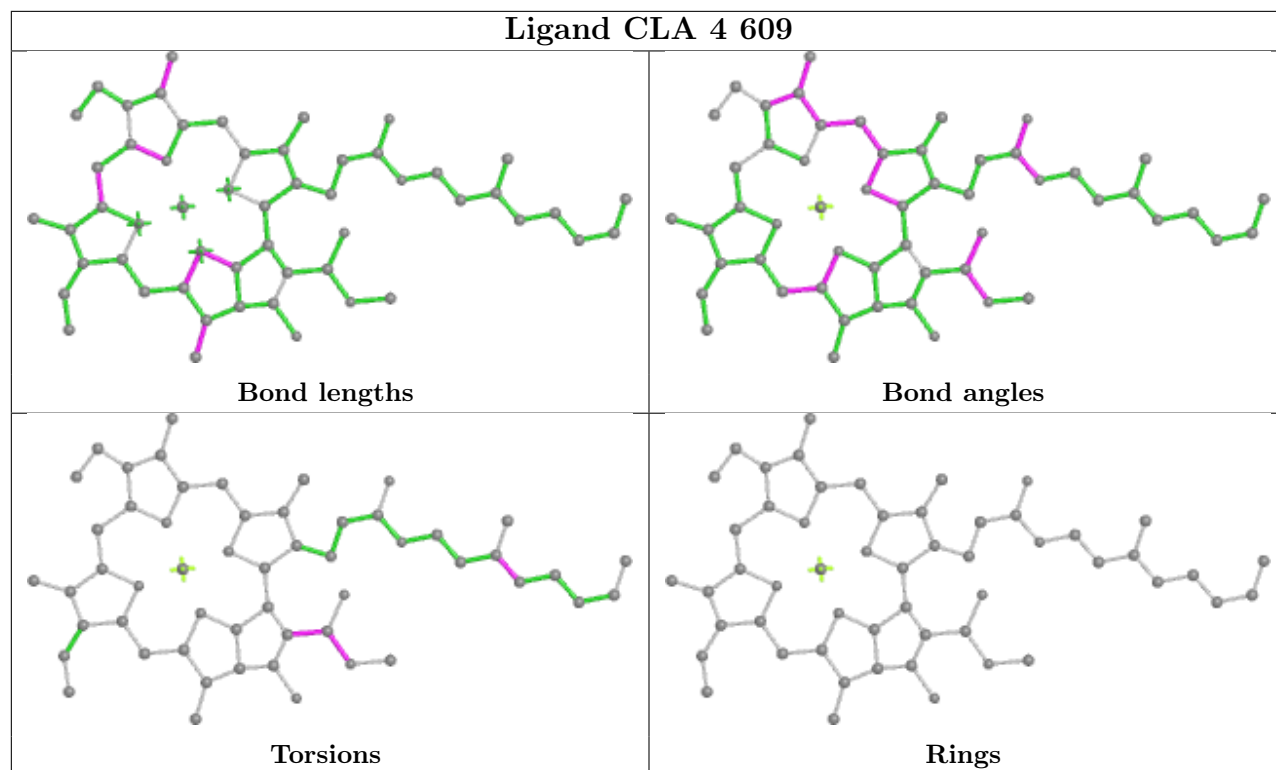


Ligand BCR A 852

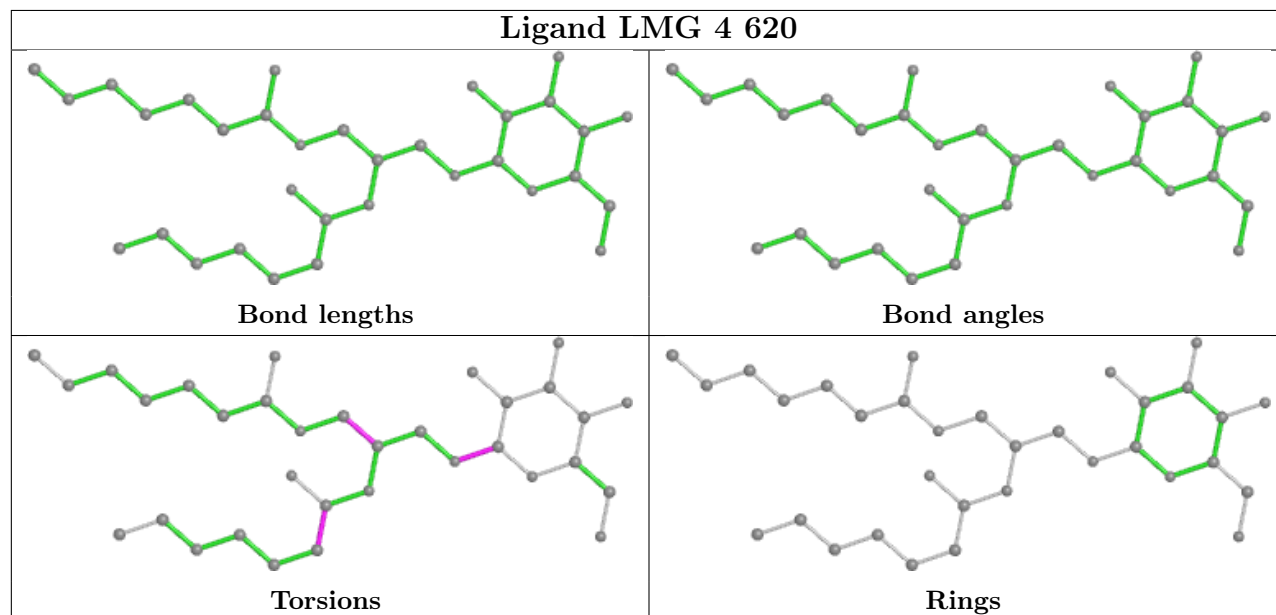




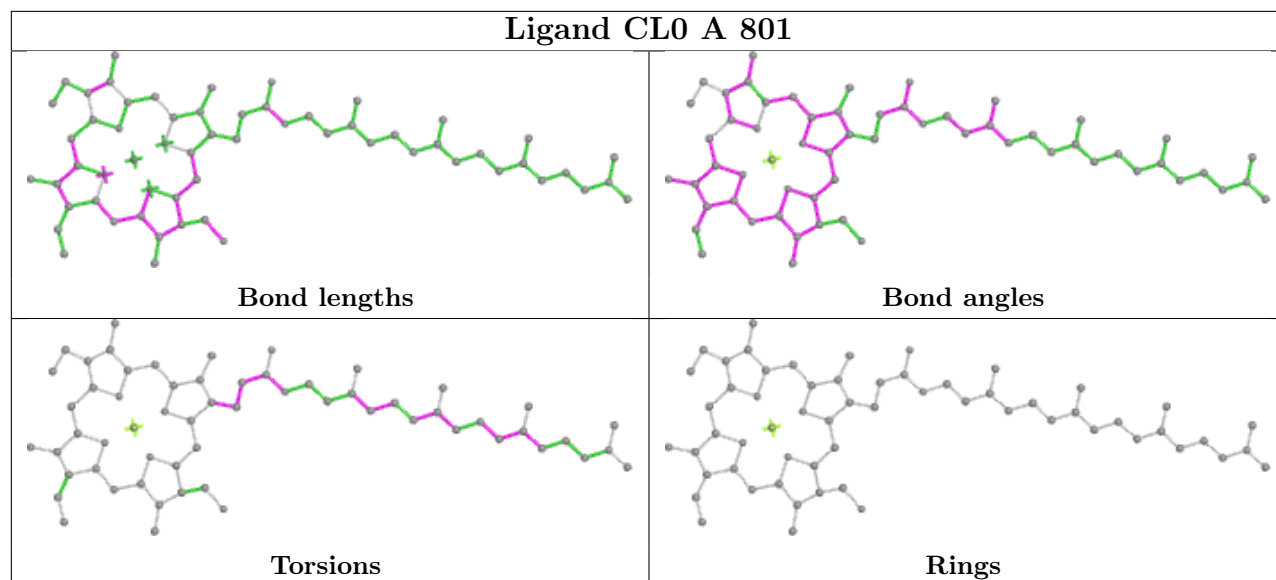
Ligand CLA 4 609



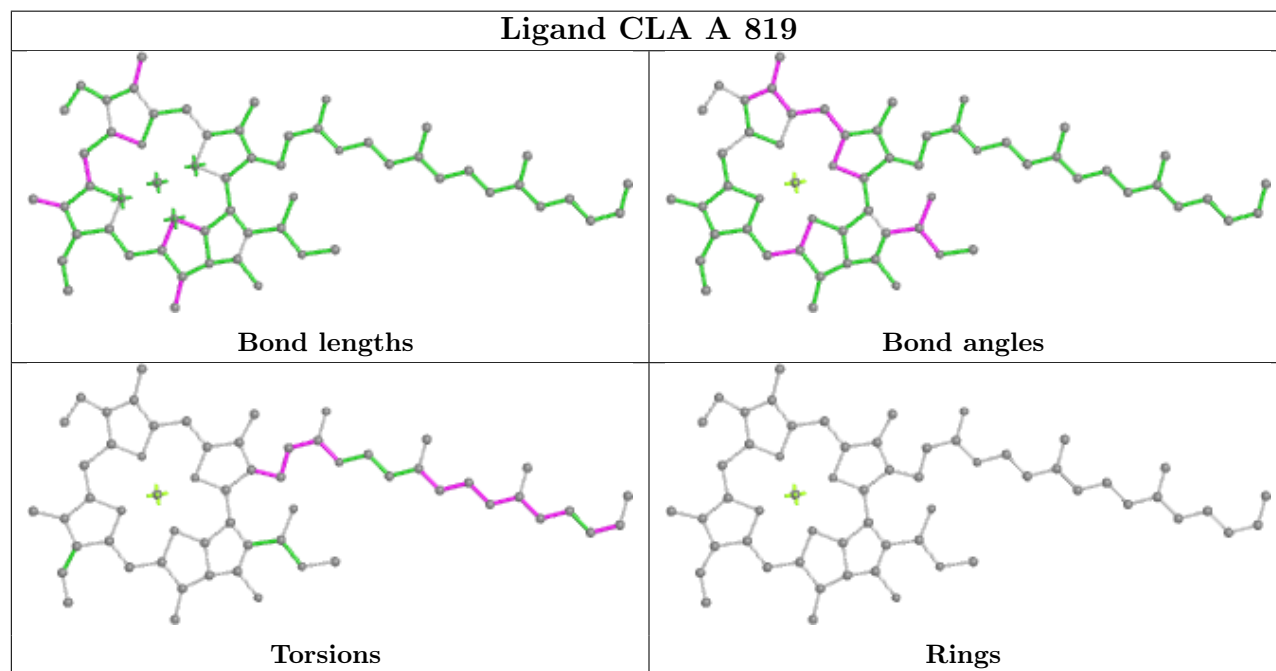
Ligand LMG 4 620

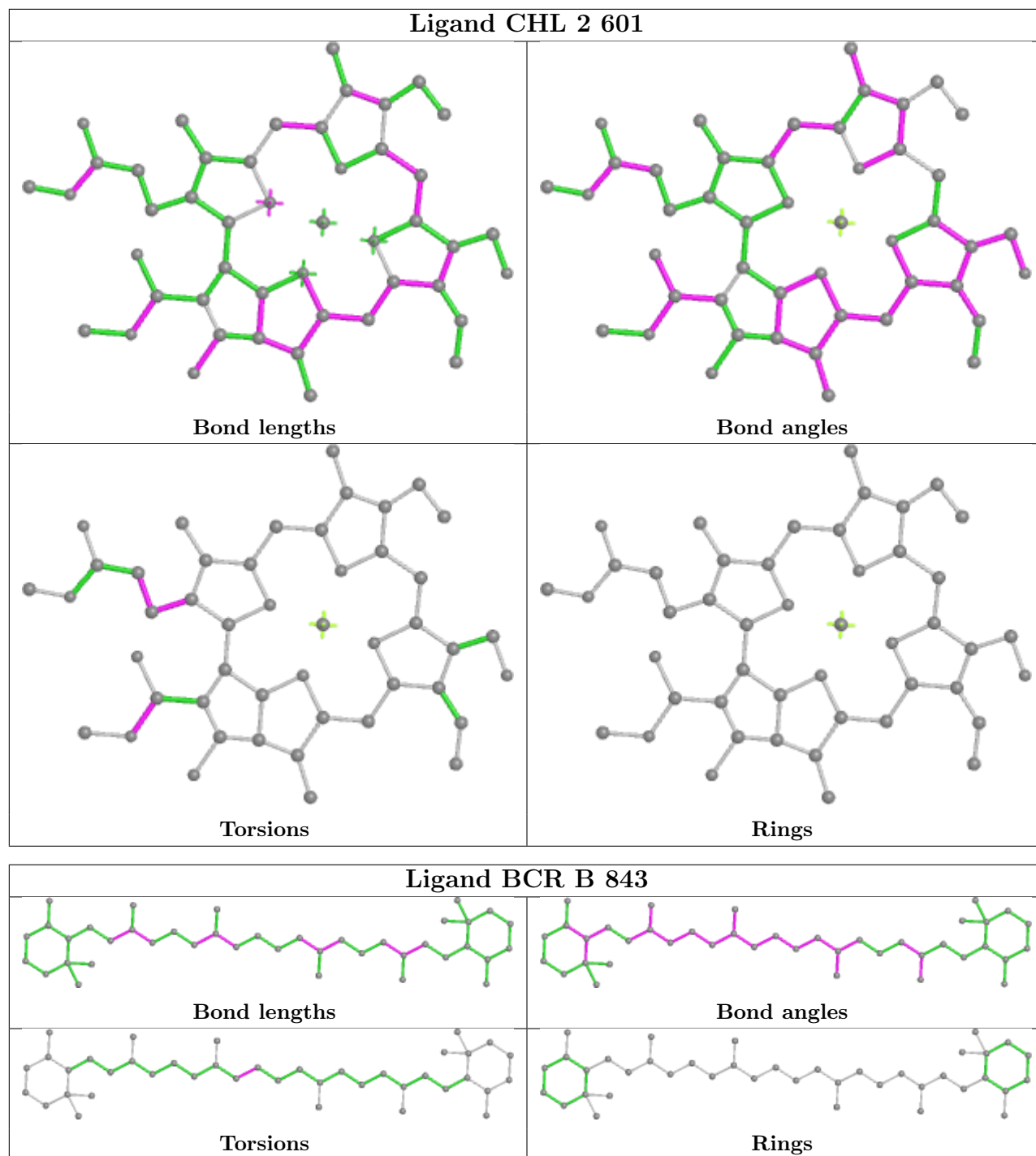


Ligand CL0 A 801

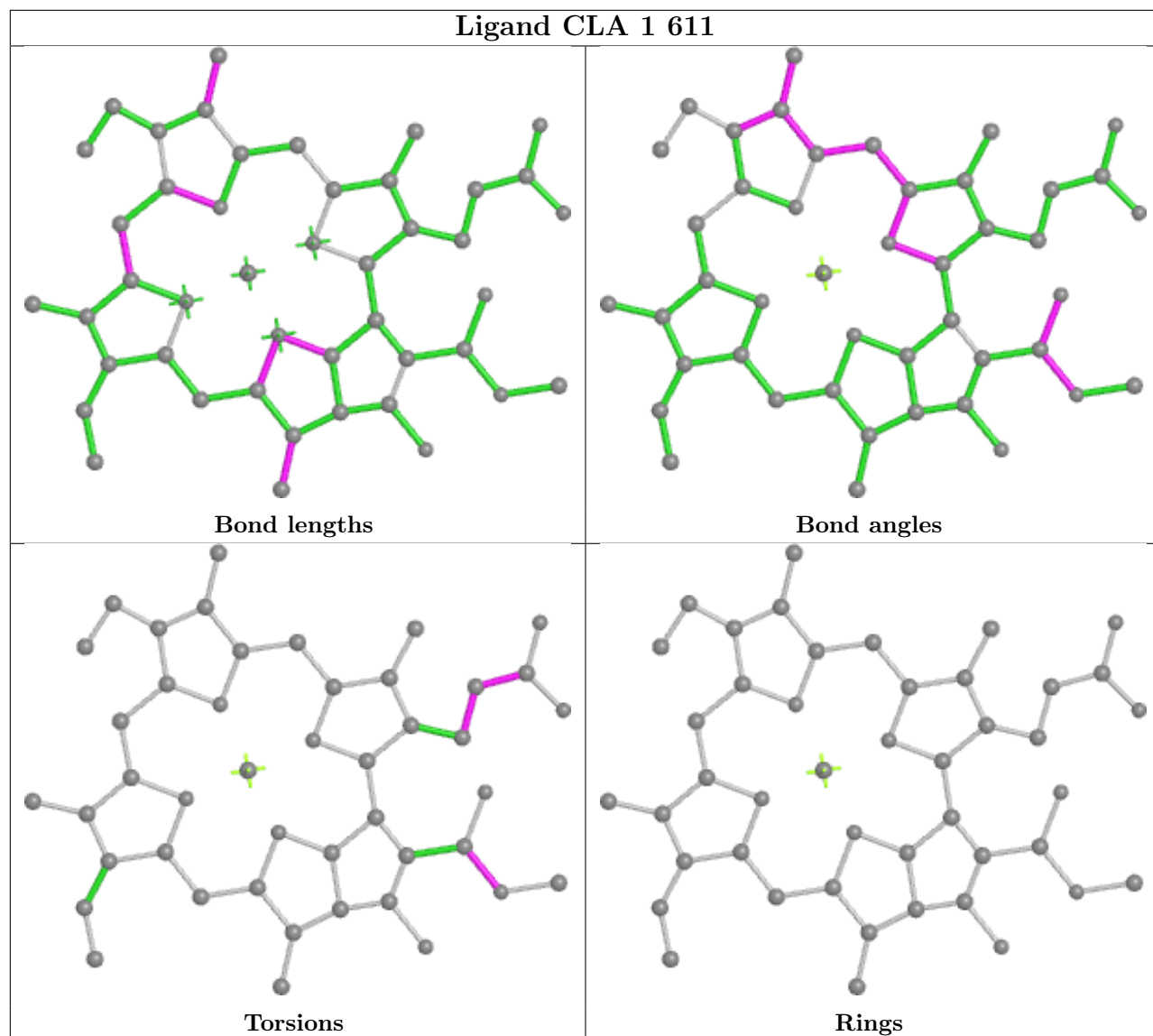


Ligand CLA A 819

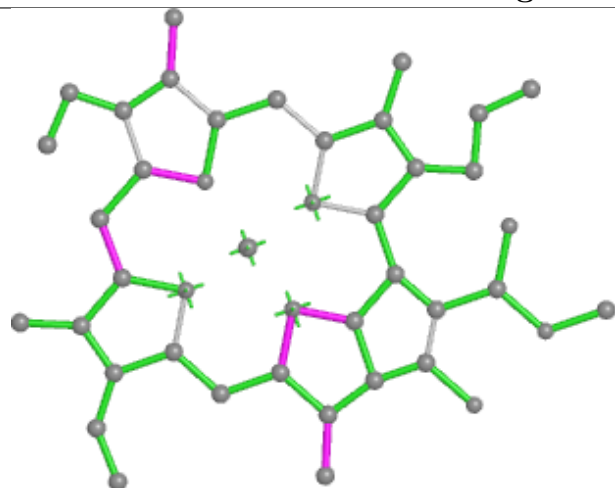




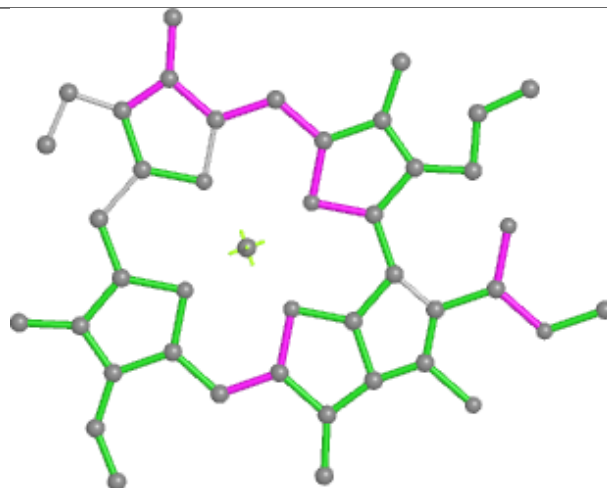
Ligand CLA 1 611



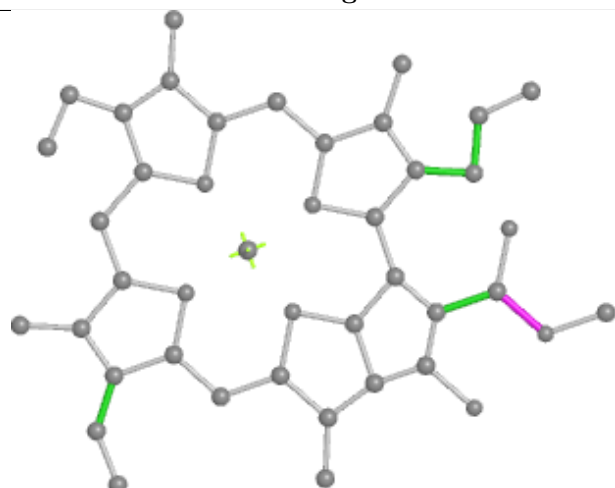
Ligand CLA B 830



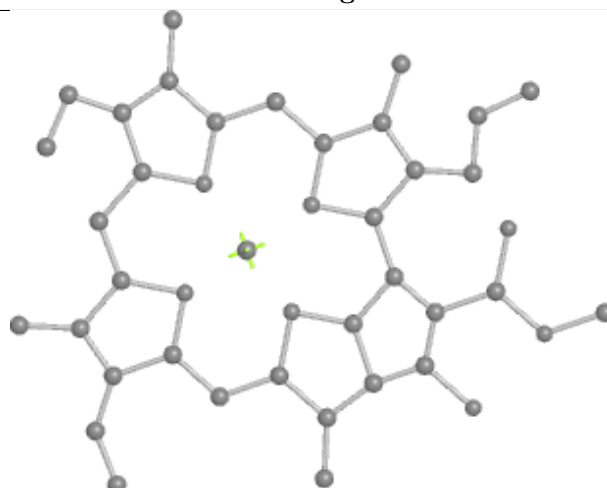
Bond lengths



Bond angles

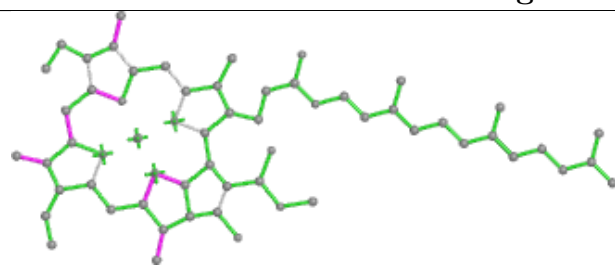


Torsions

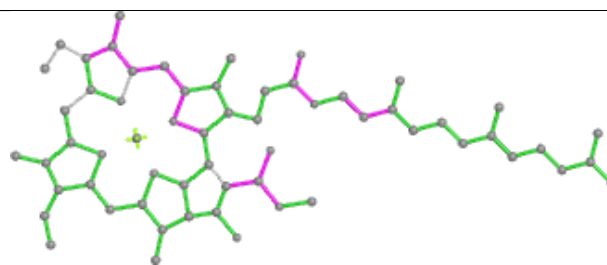


Rings

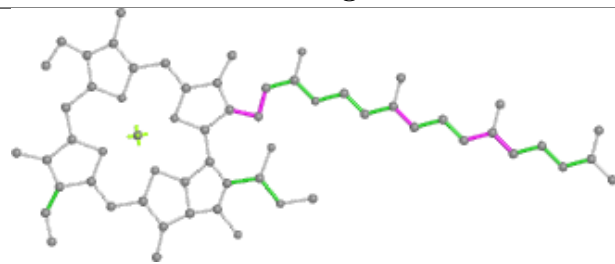
Ligand CLA B 818



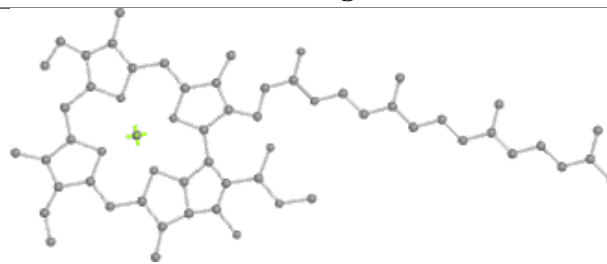
Bond lengths



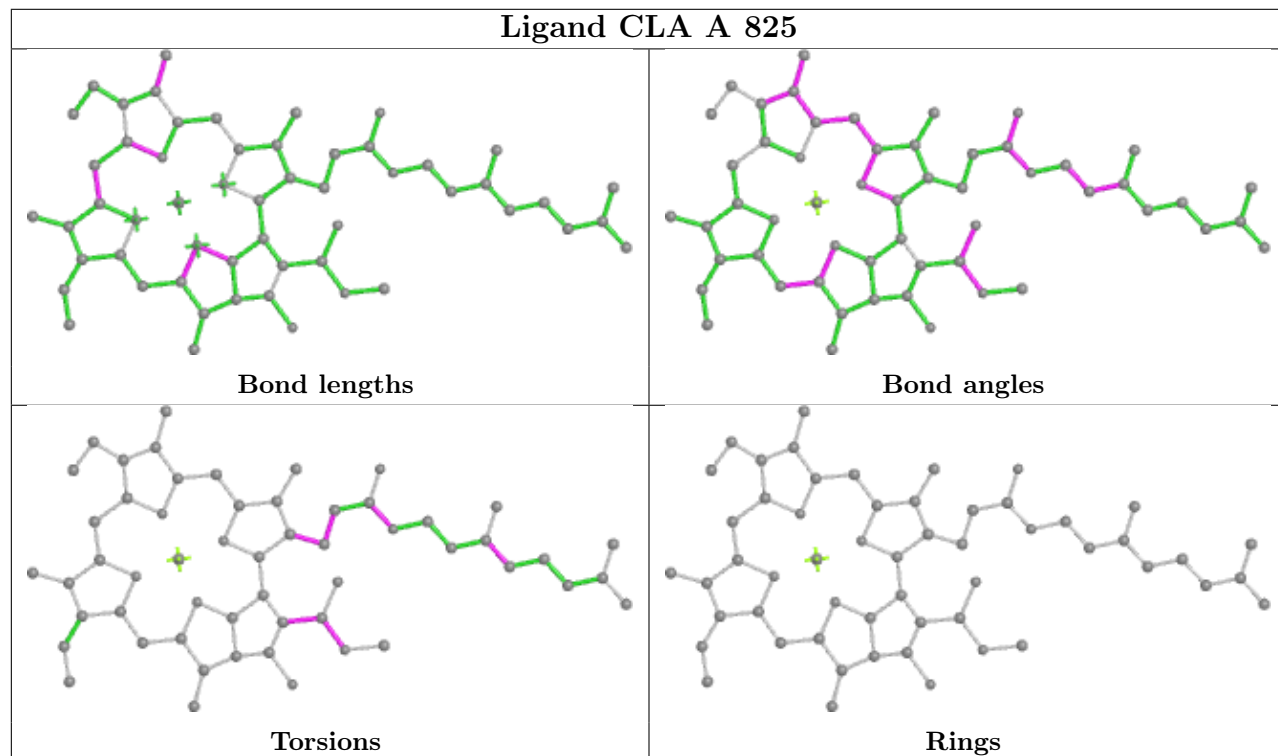
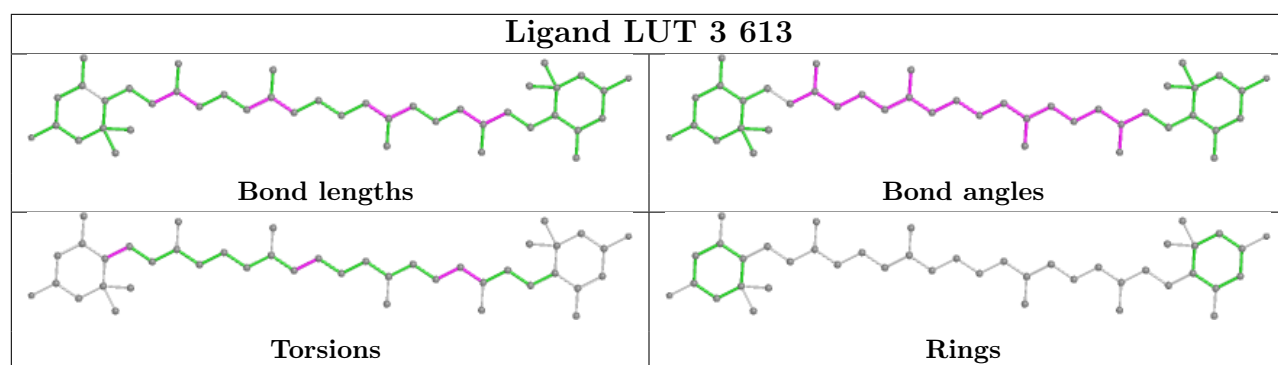
Bond angles



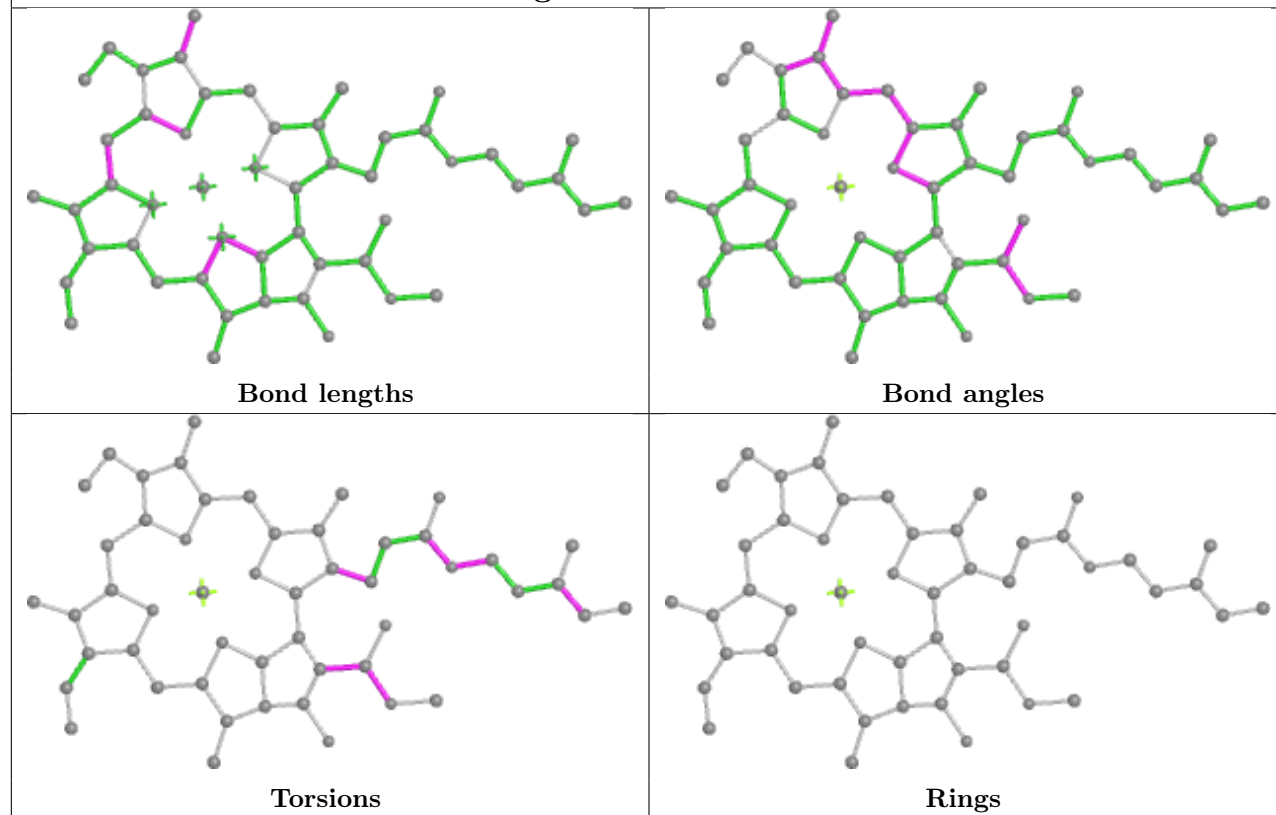
Torsions



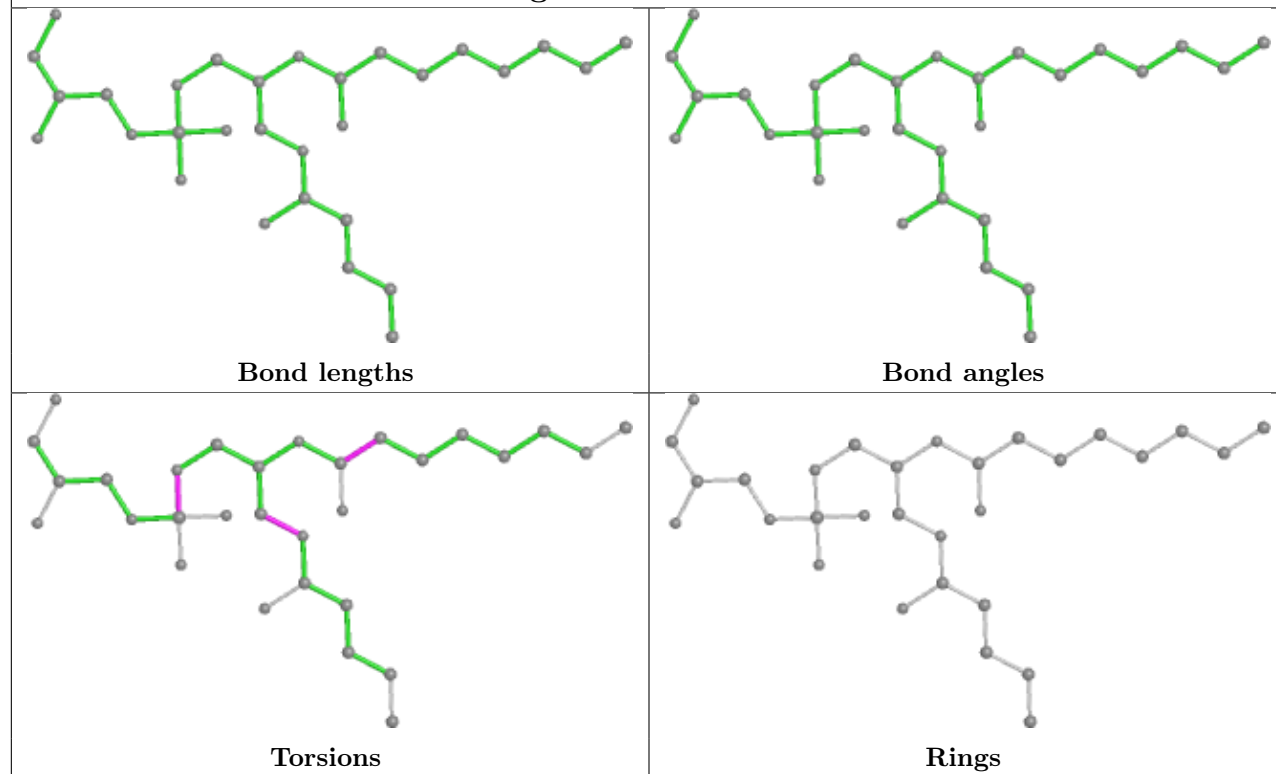
Rings

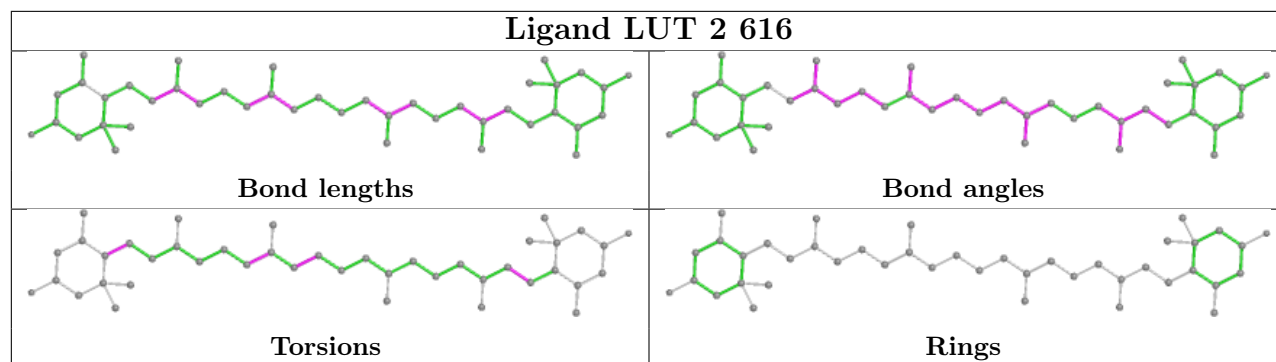
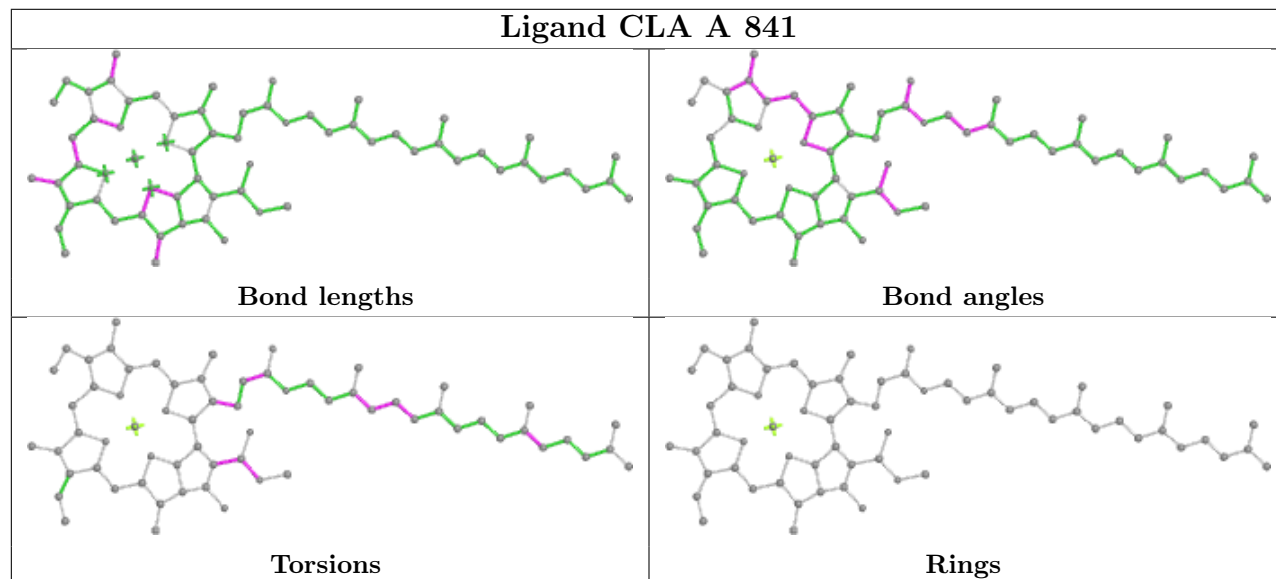
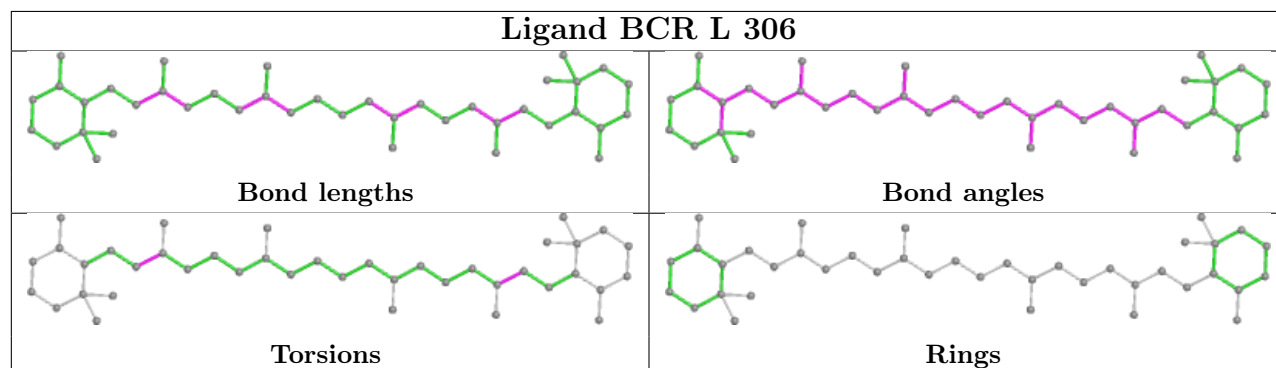


Ligand CLA F 302

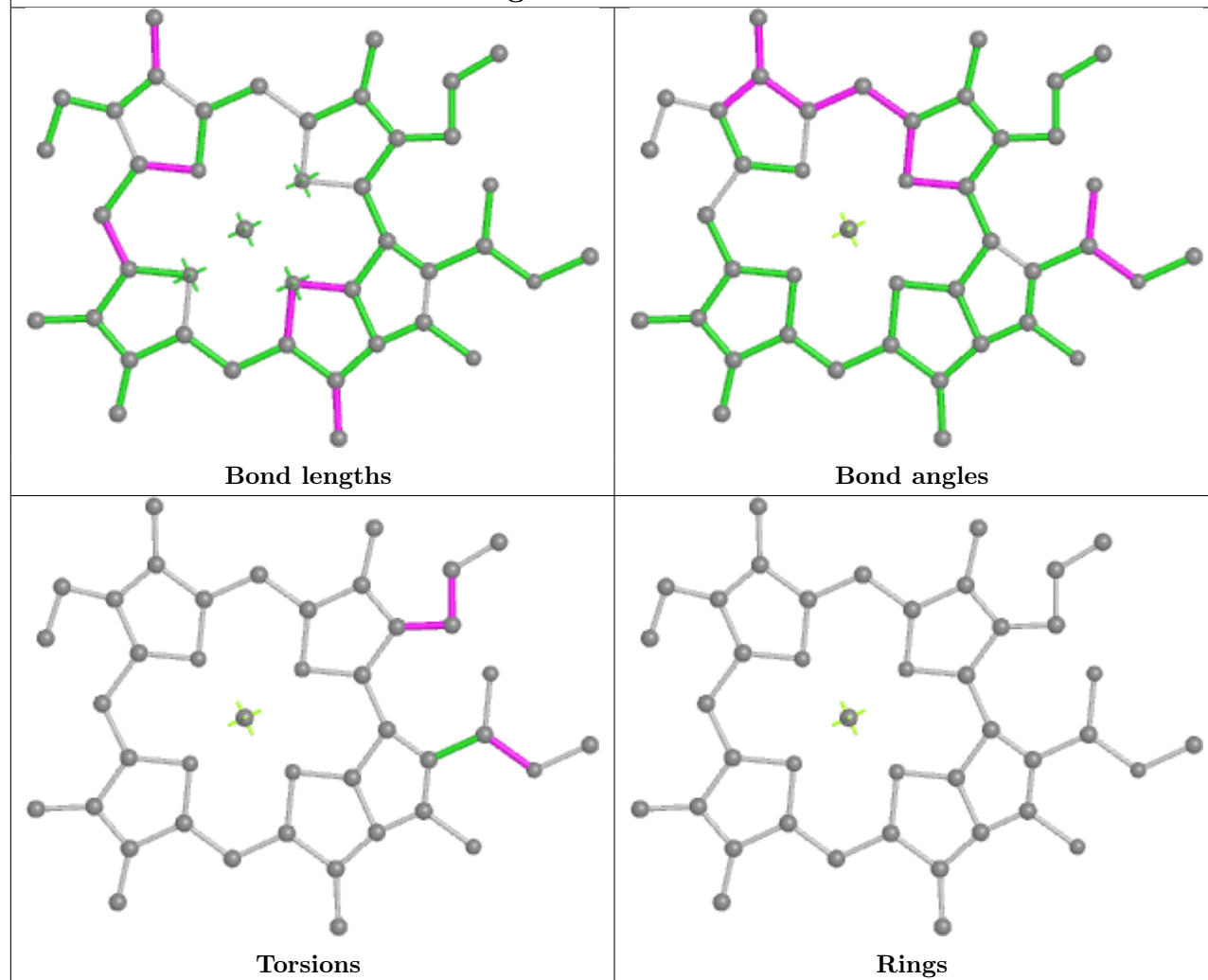


Ligand LHG A 847

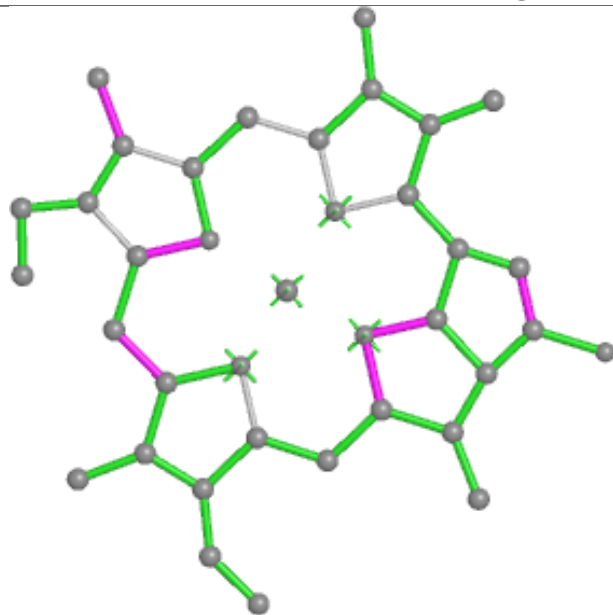


Ligand LUT 2 616**Ligand CLA A 841****Ligand BCR L 306**

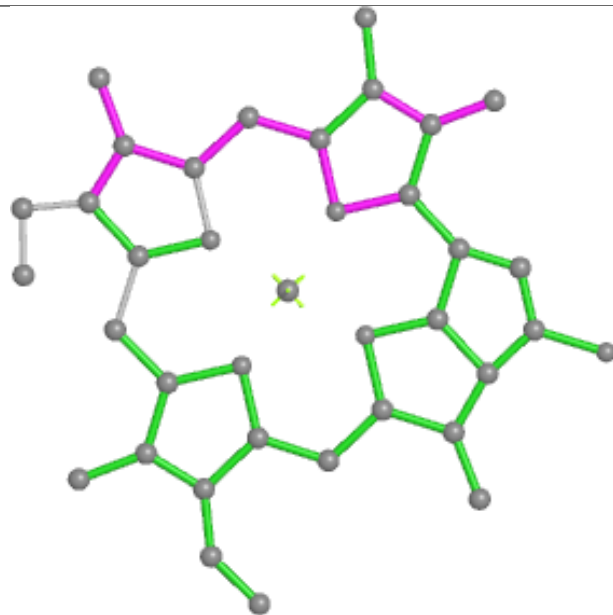
Ligand CLA 1 609



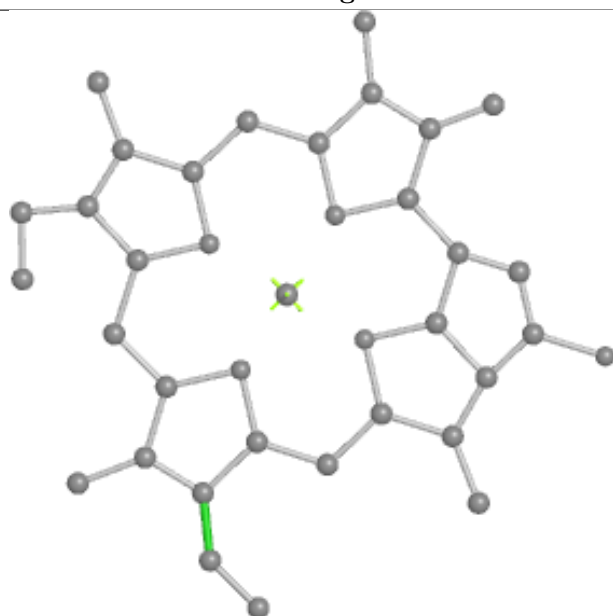
Ligand CLA K 201



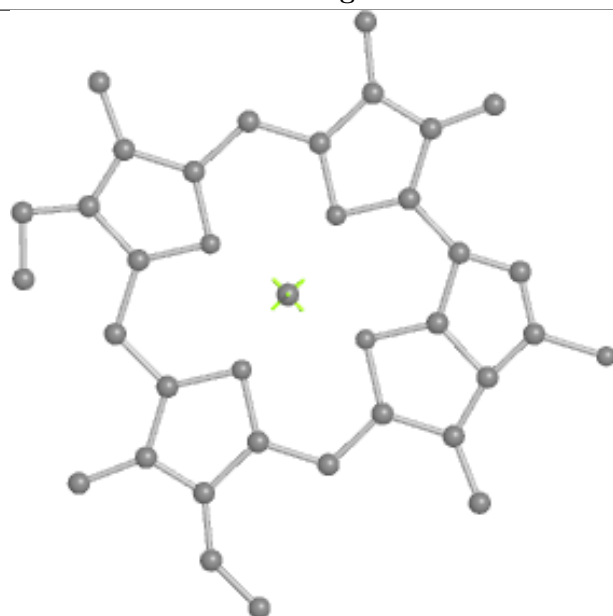
Bond lengths



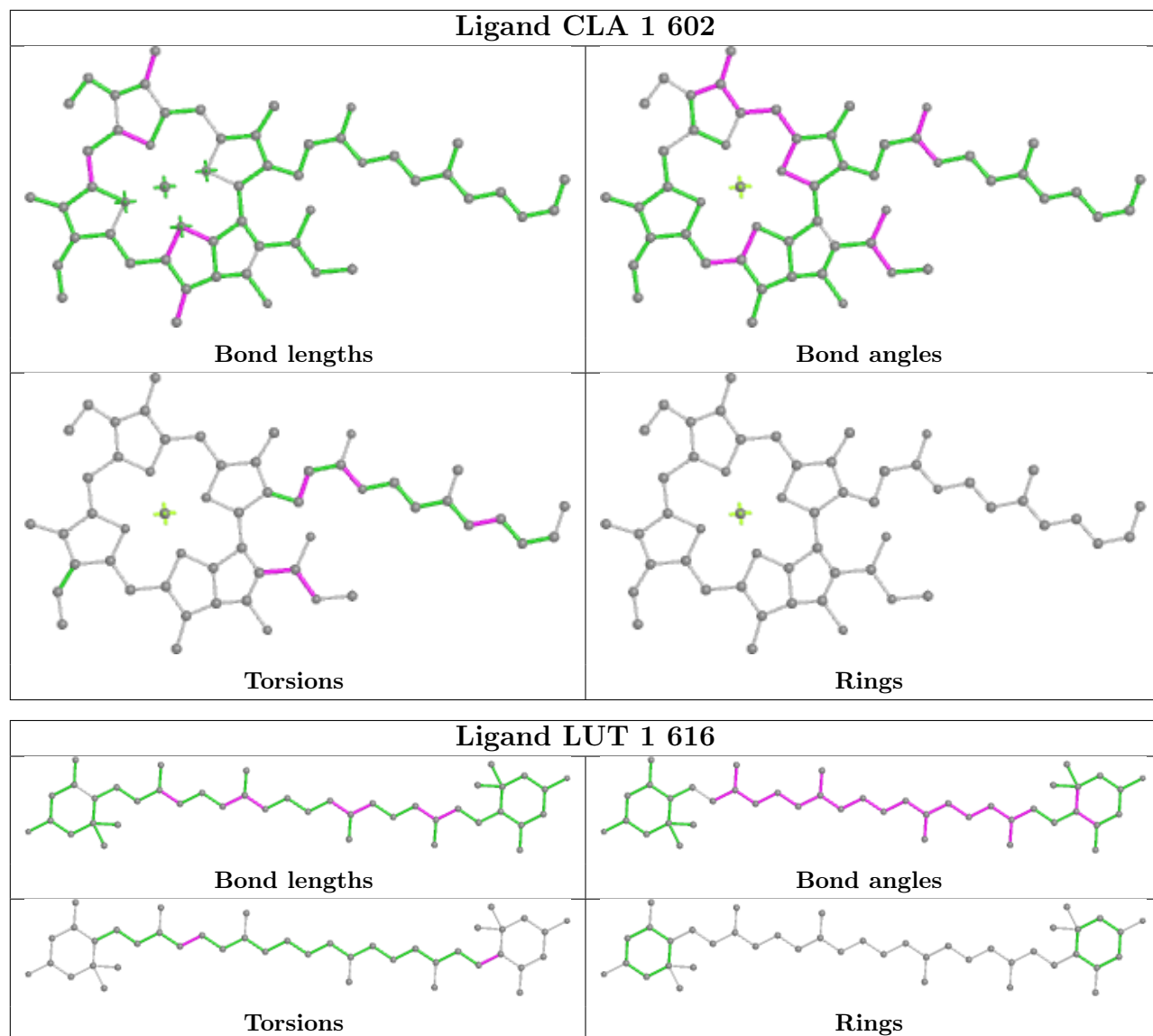
Bond angles



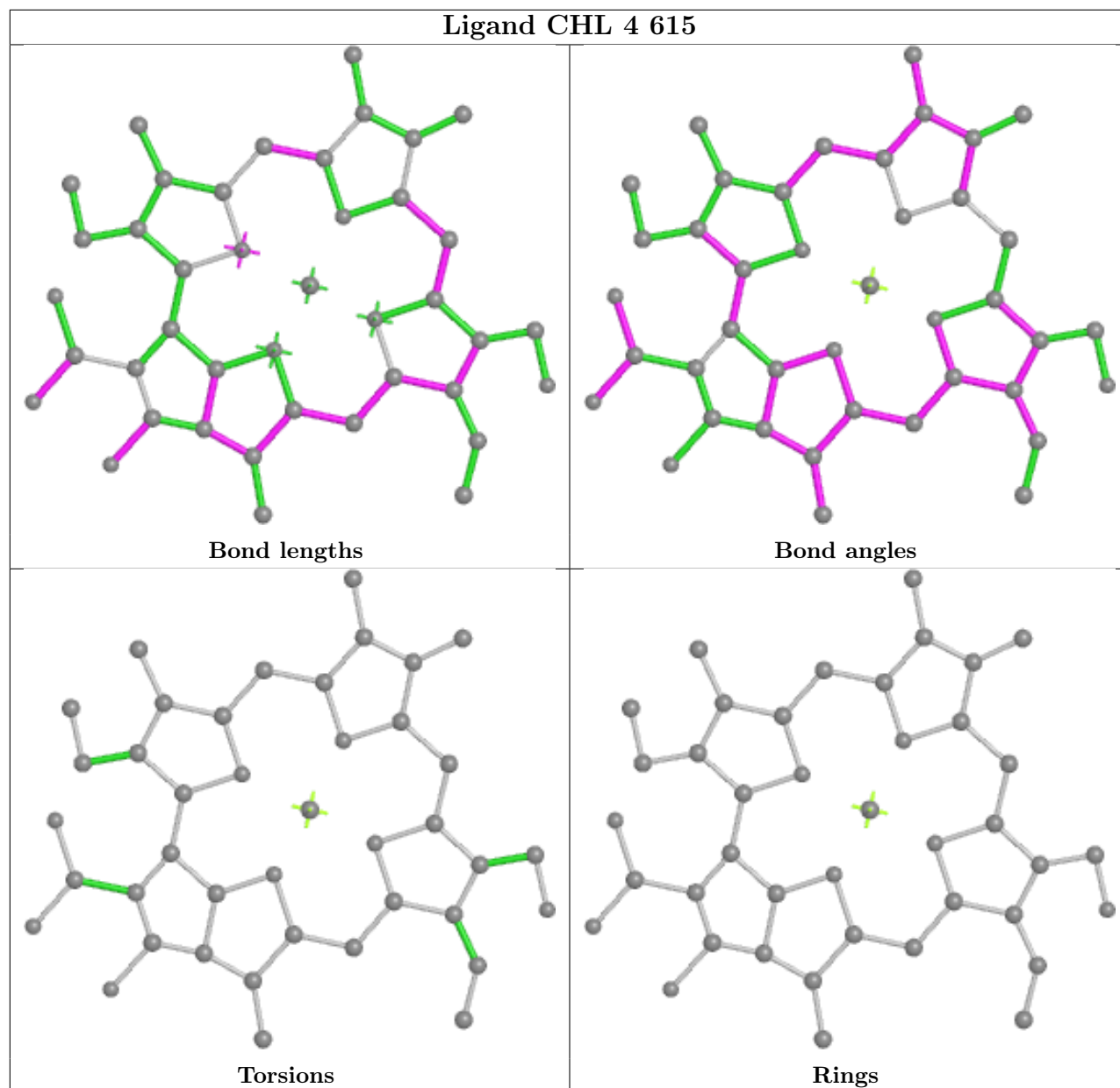
Torsions



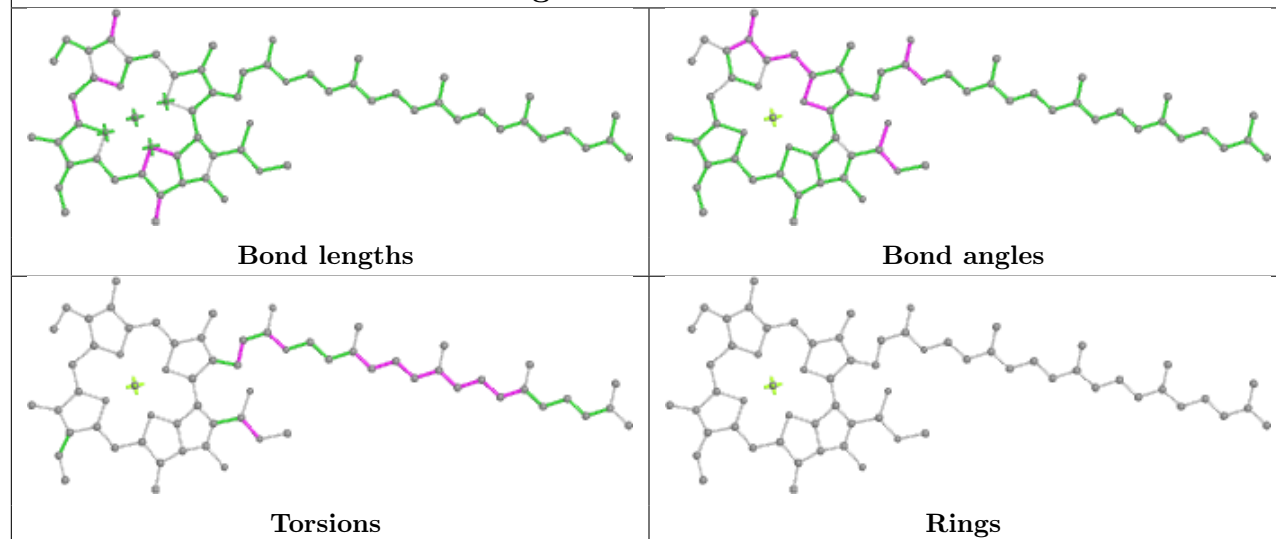
Rings



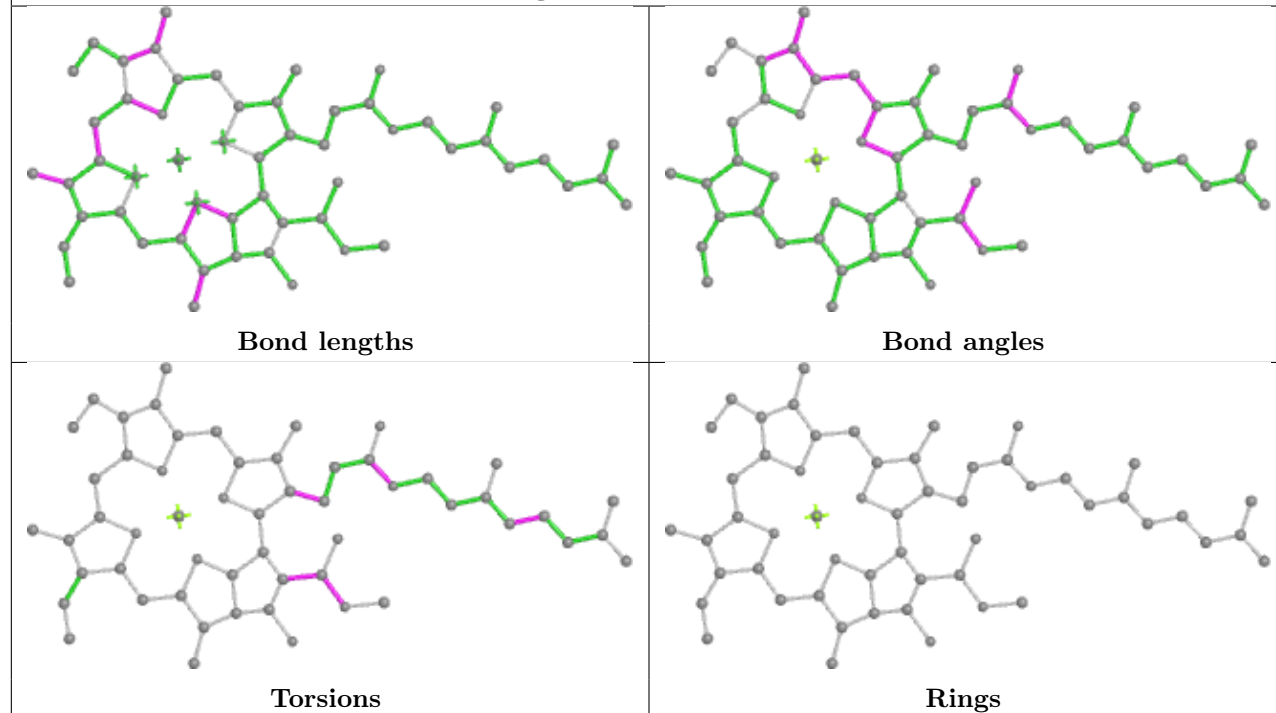
Ligand CHL 4 615

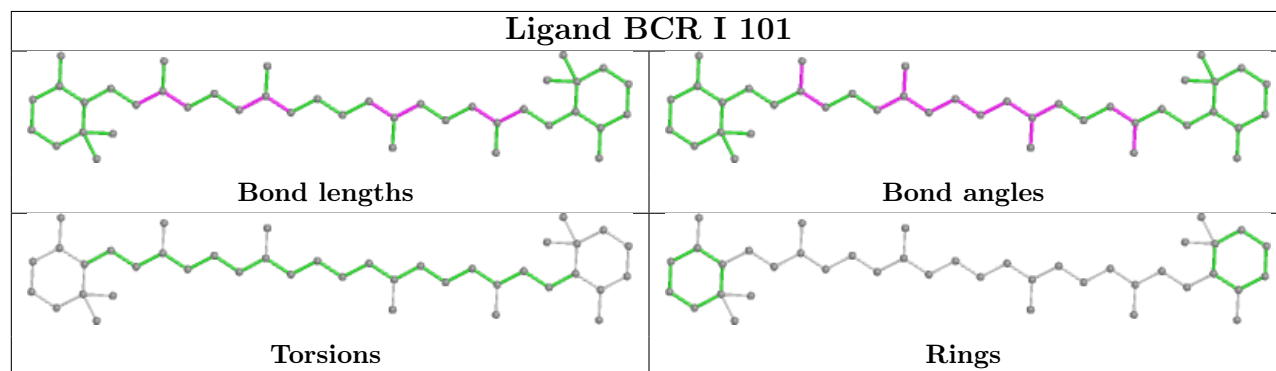
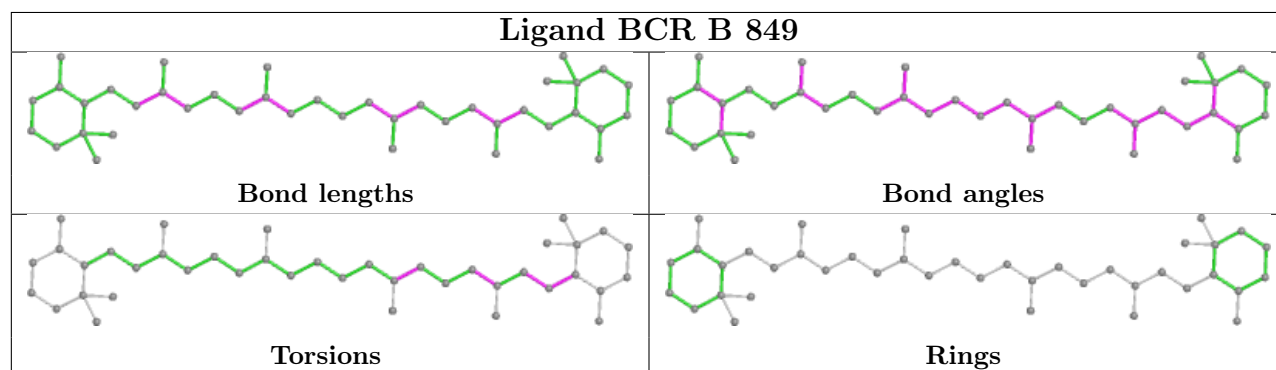
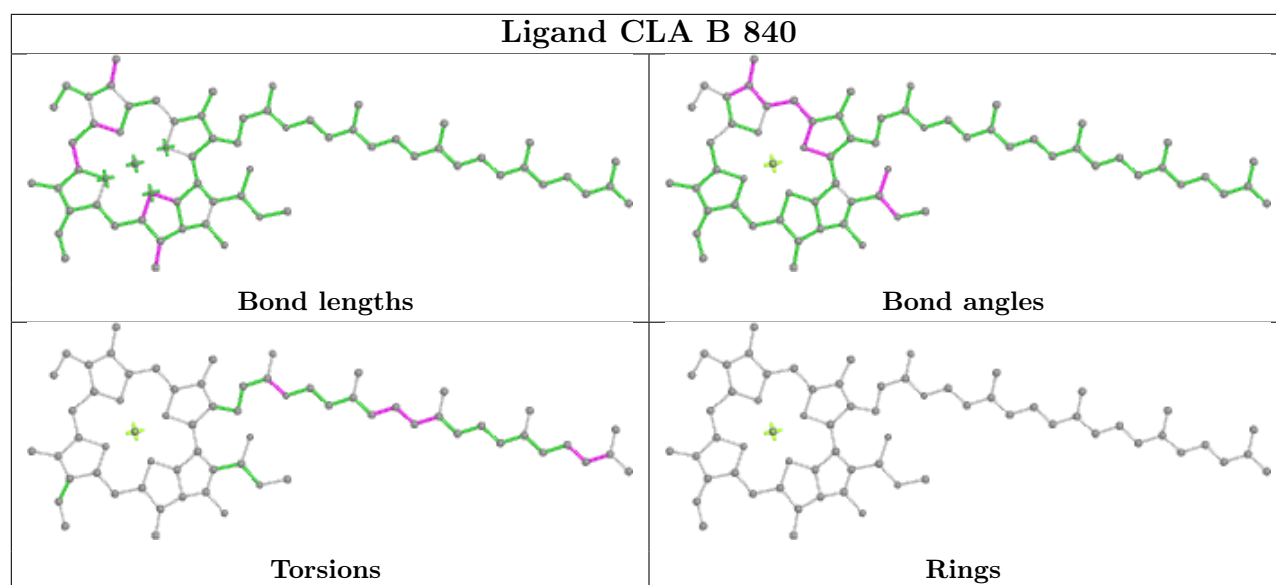


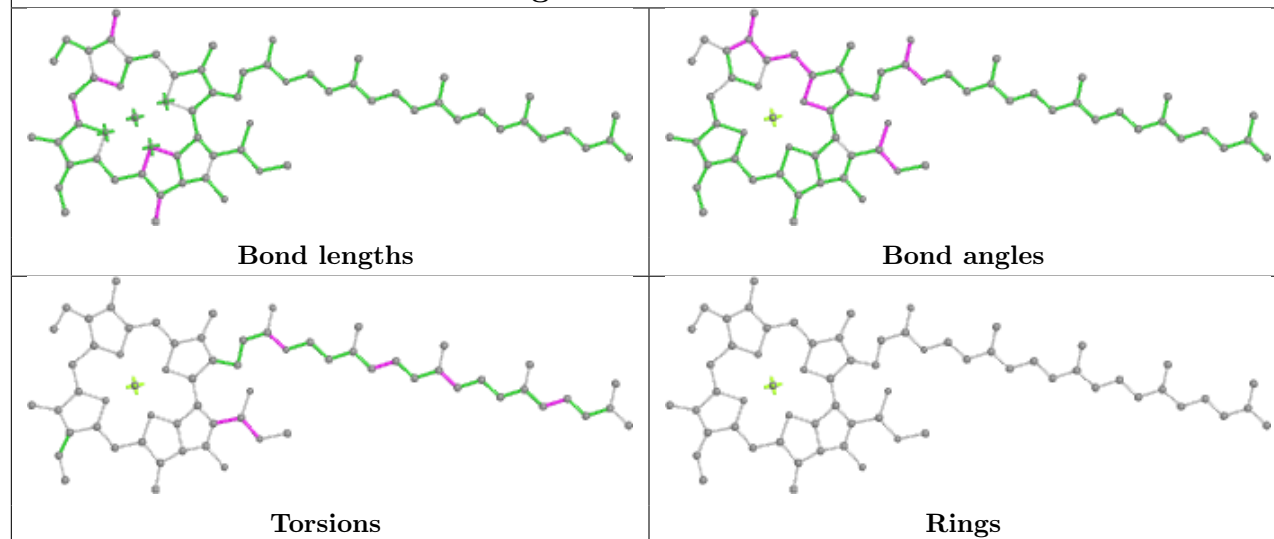
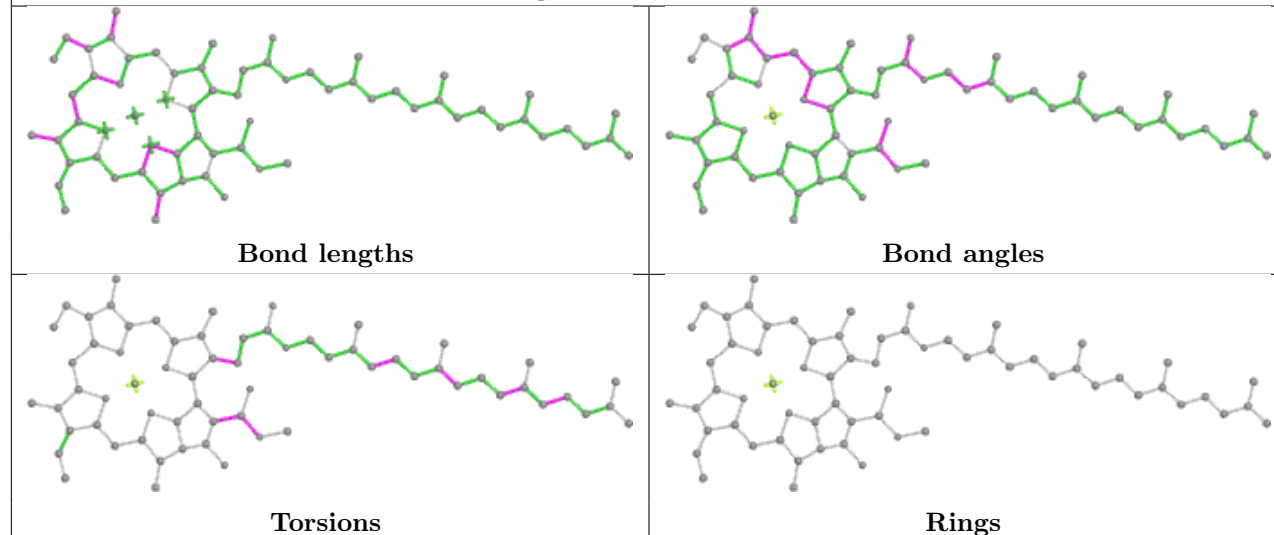
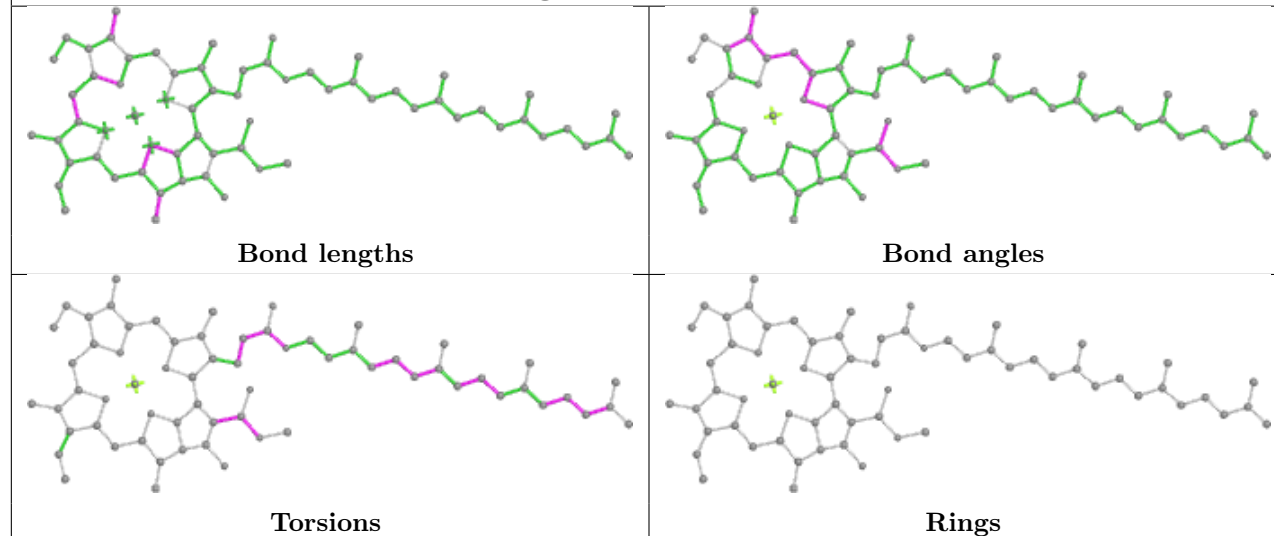
Ligand CLA B 814

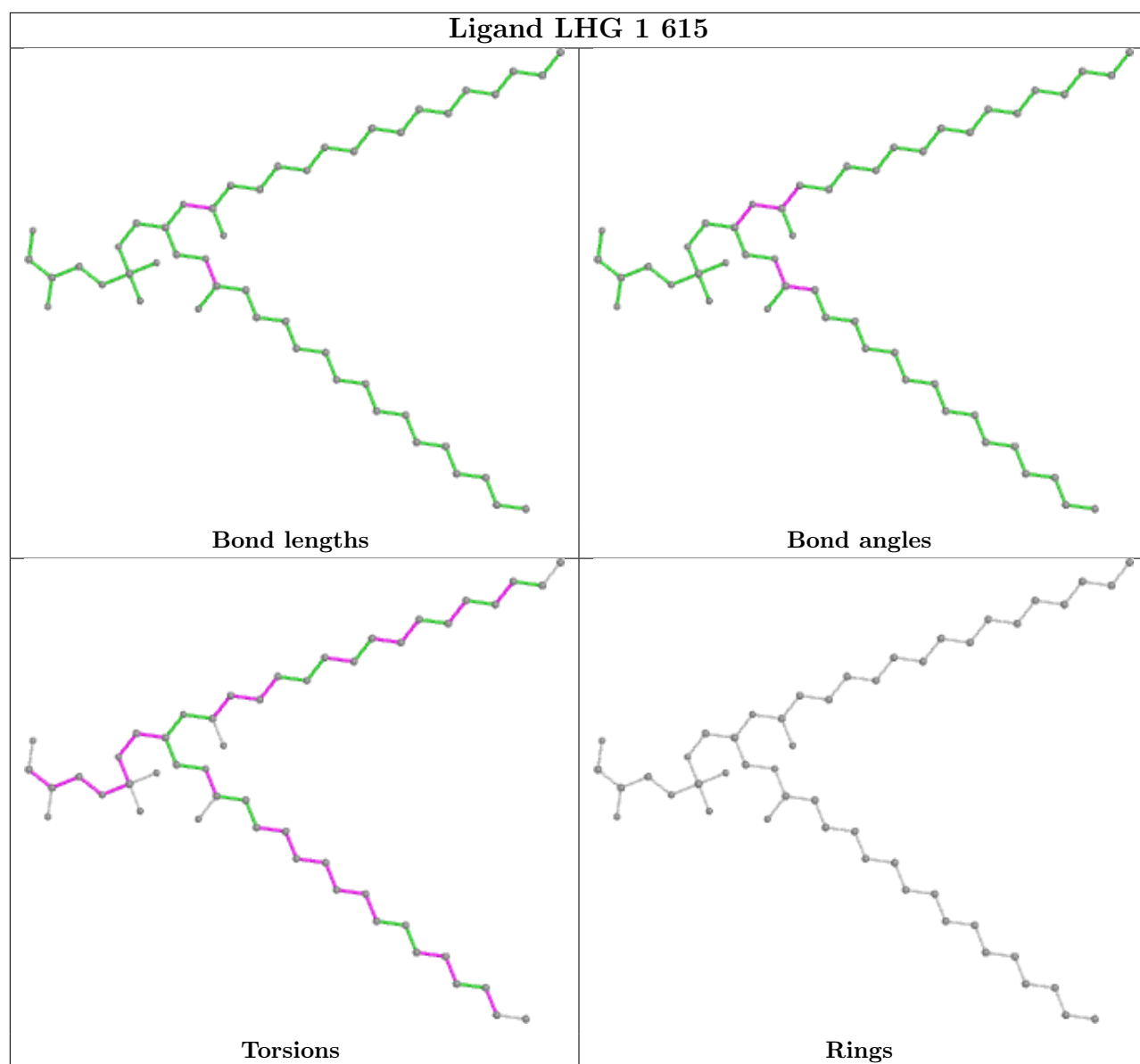


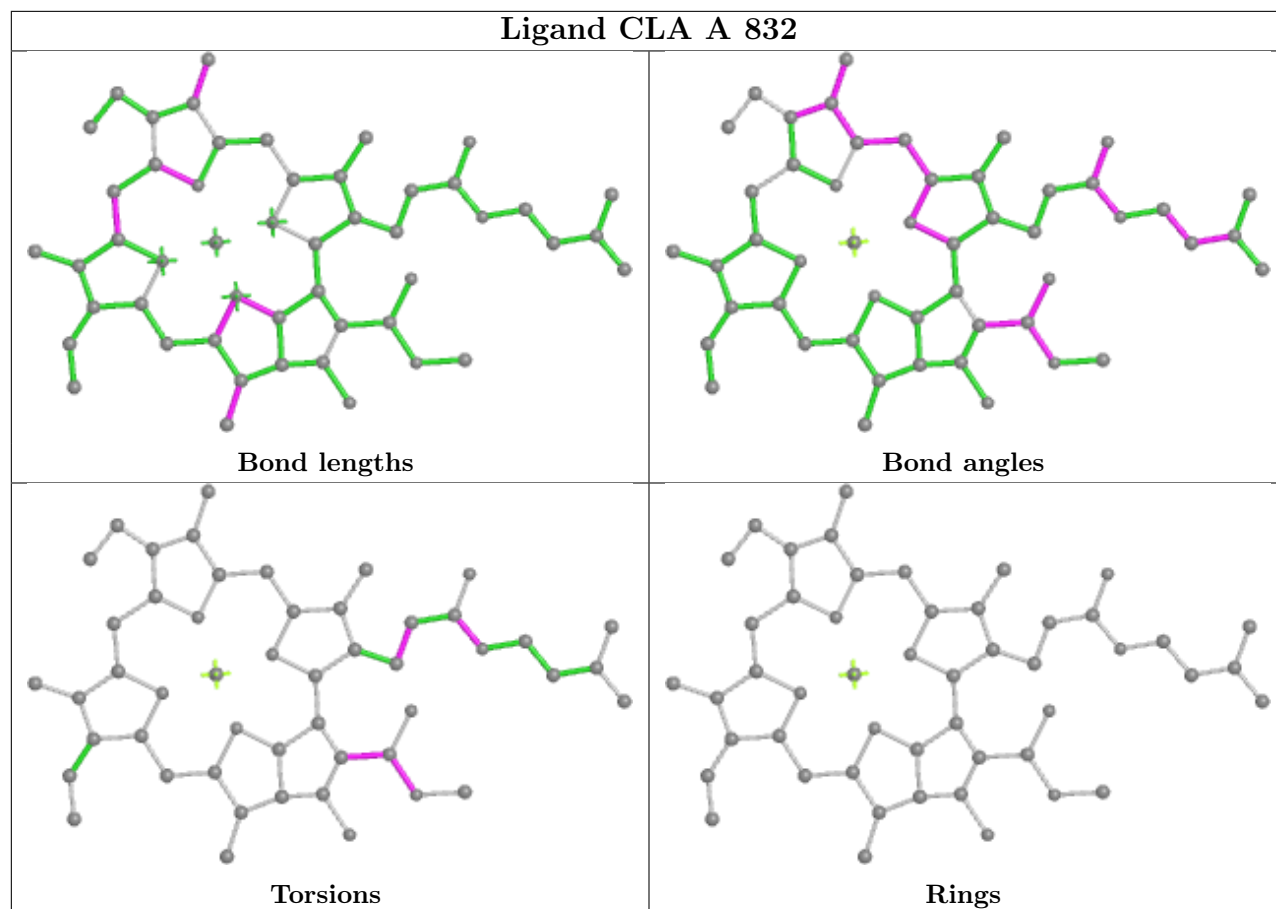
Ligand CLA B 819



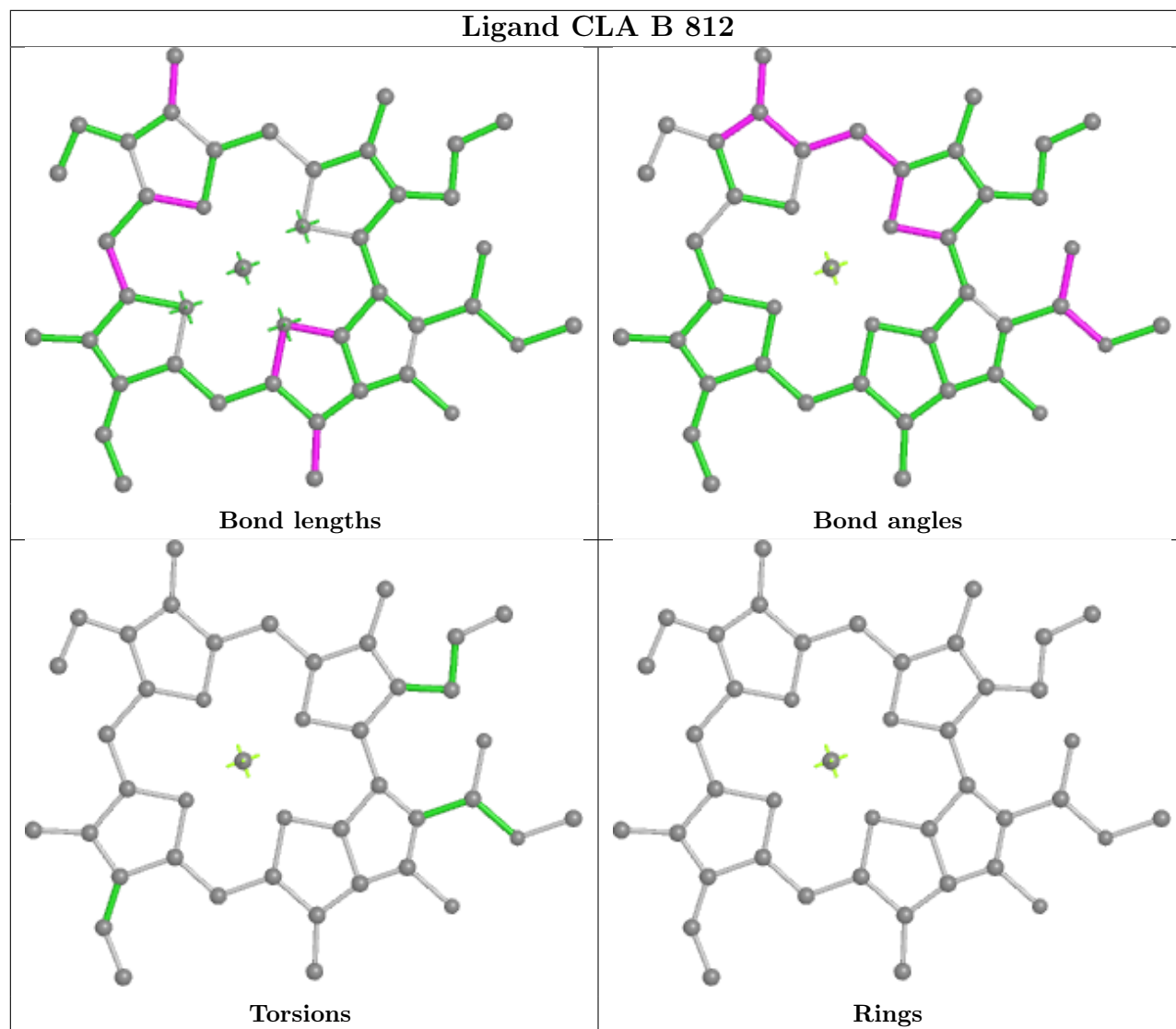


Ligand CLA A 834**Ligand CLA B 803****Ligand CLA 2 612**

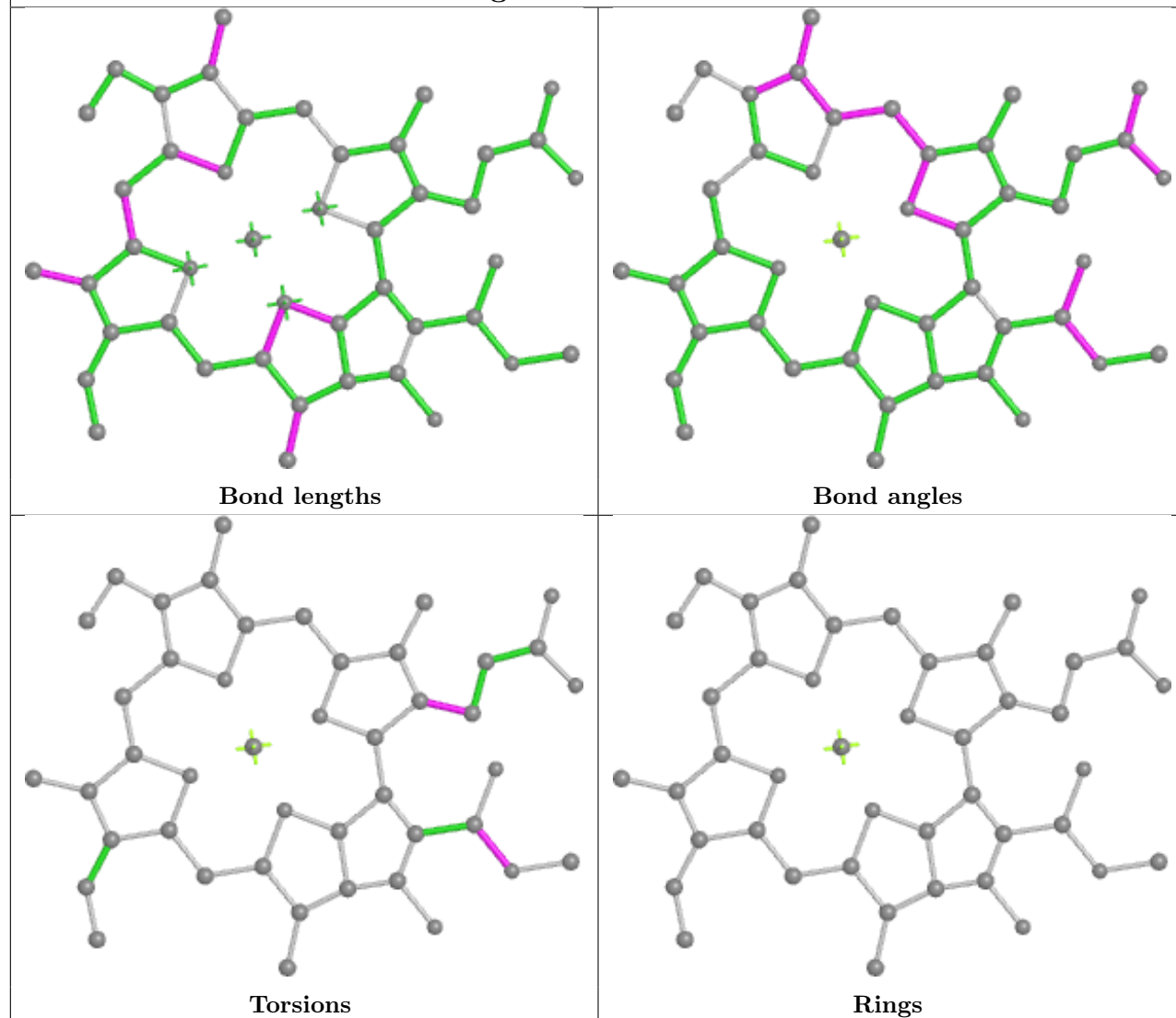




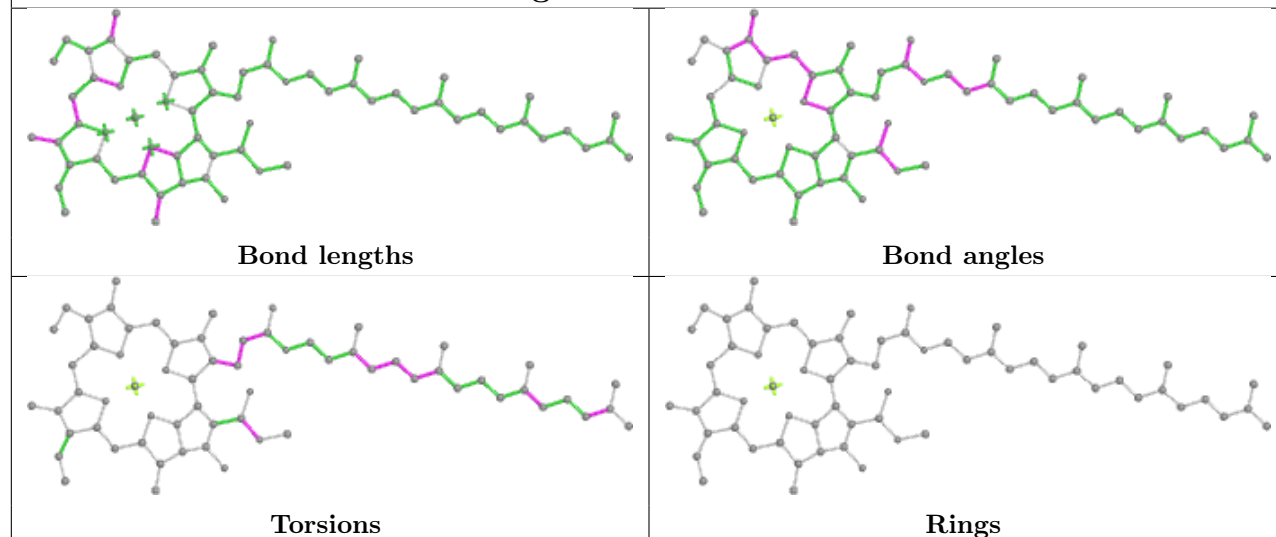
Ligand CLA B 812



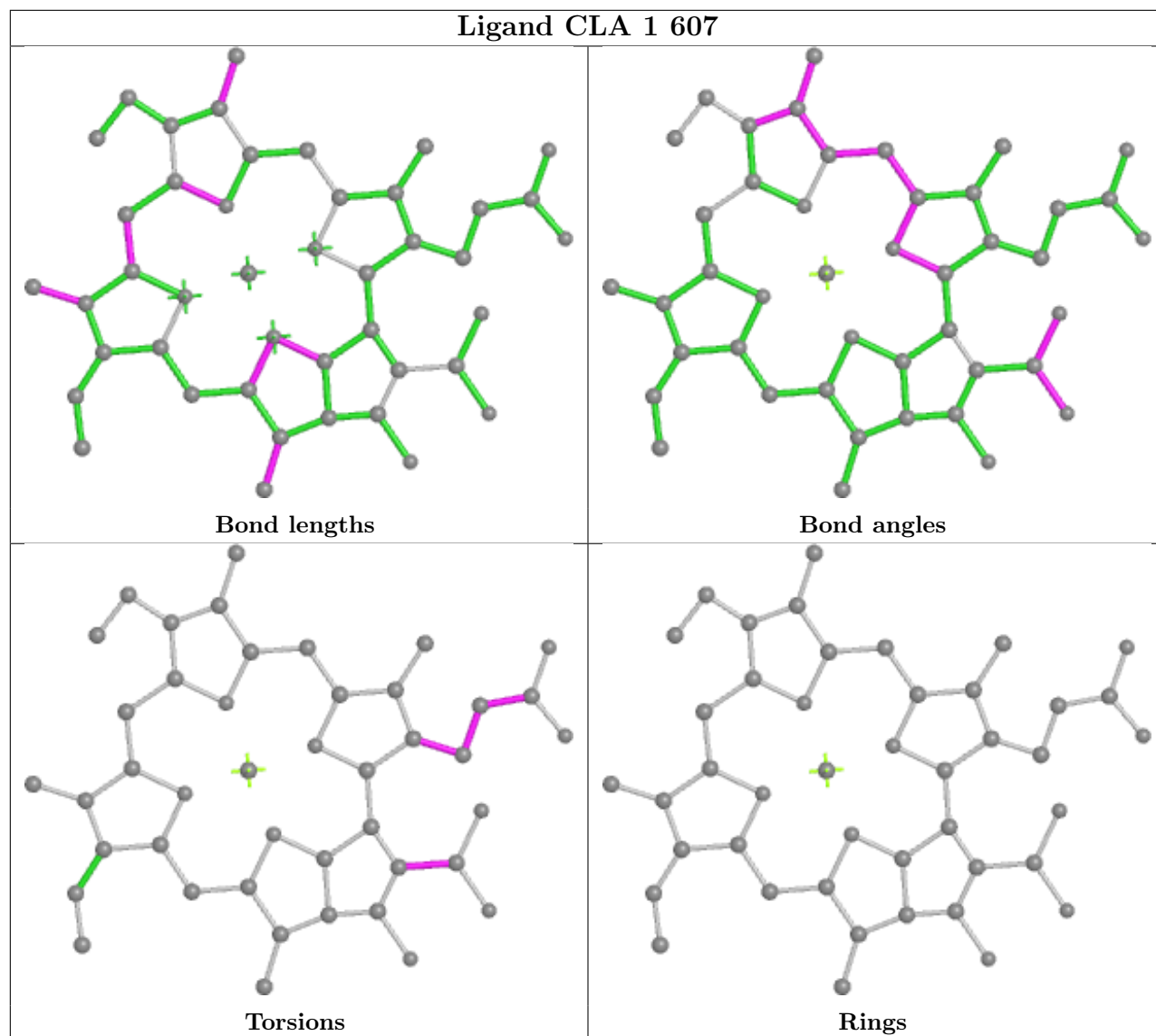
Ligand CLA B 823



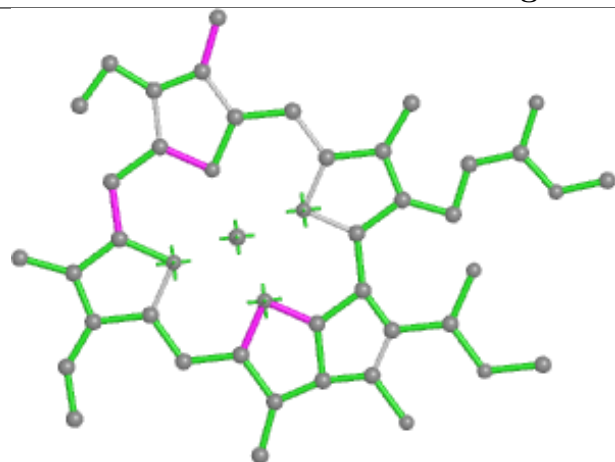
Ligand CLA B 809



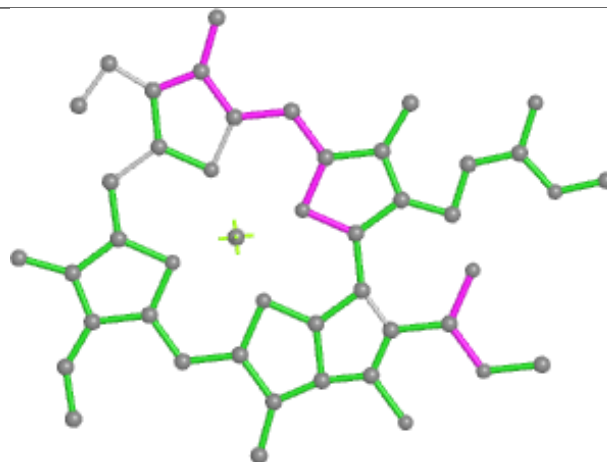
Ligand CLA 1 607



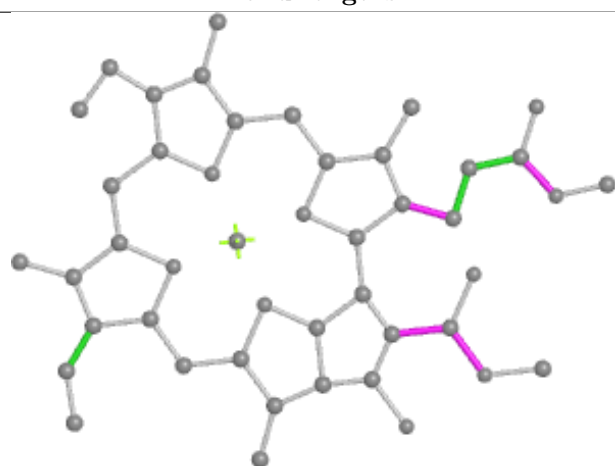
Ligand CLA 1 605



Bond lengths



Bond angles

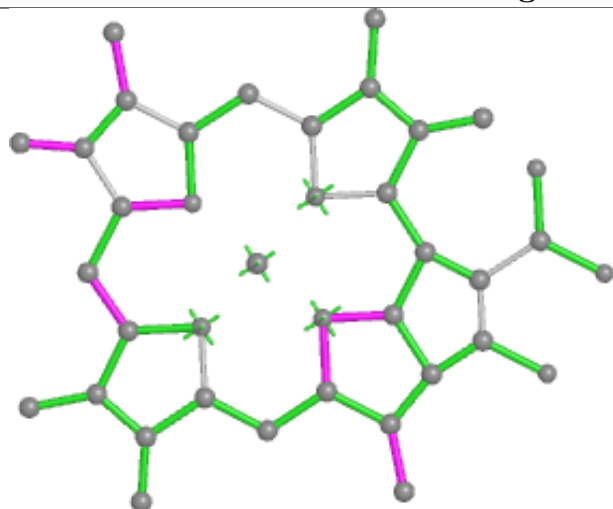


Torsions

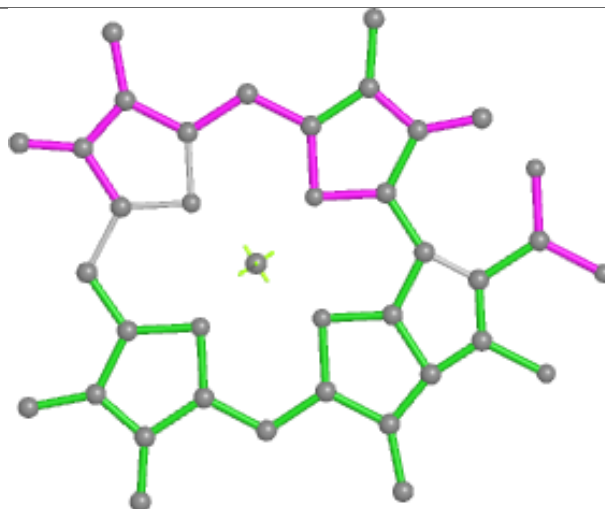


Rings

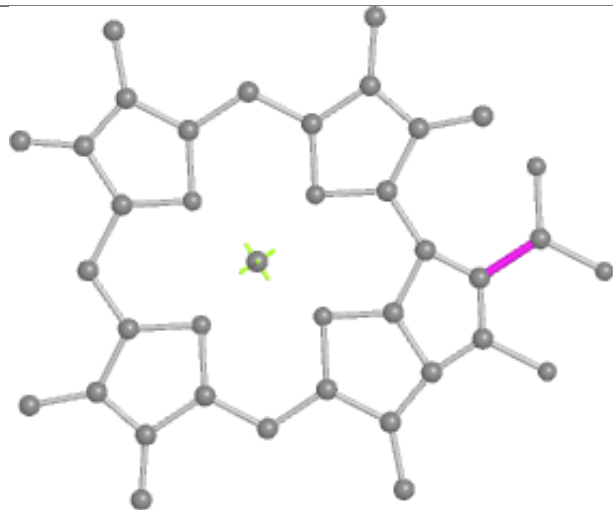
Ligand CLA 1 613



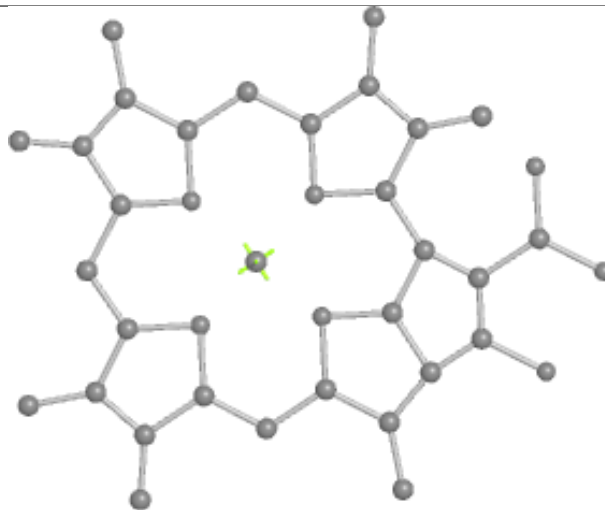
Bond lengths



Bond angles

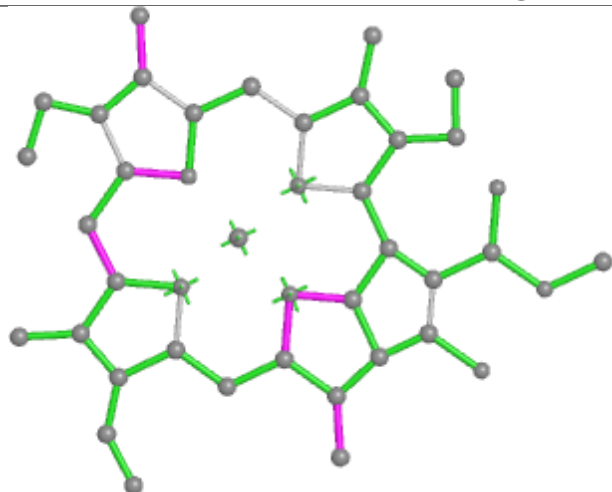


Torsions

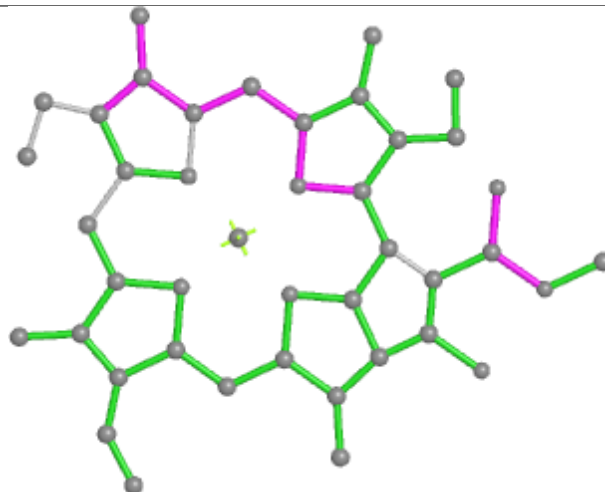


Rings

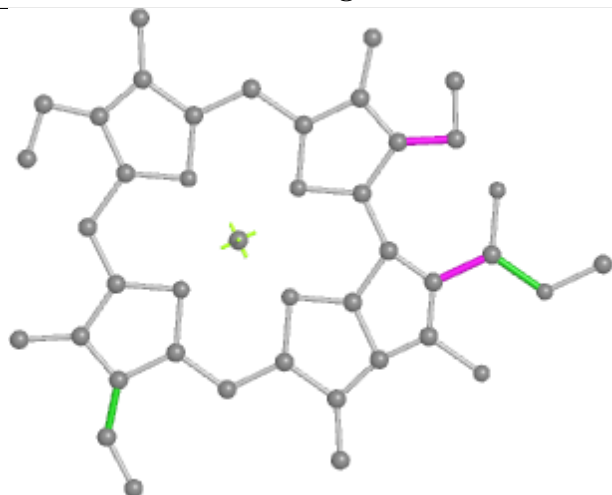
Ligand CLA A 816



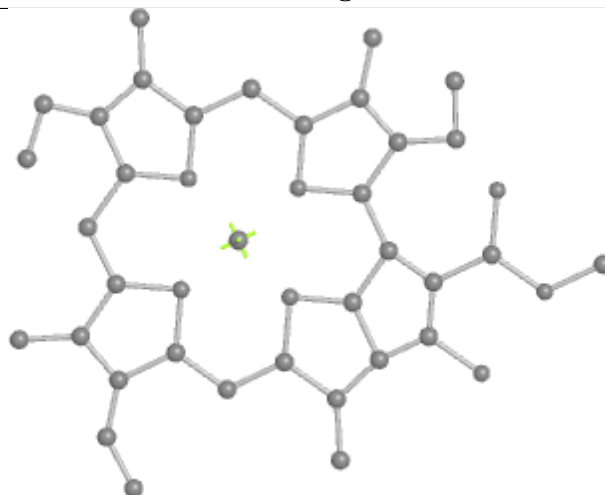
Bond lengths



Bond angles

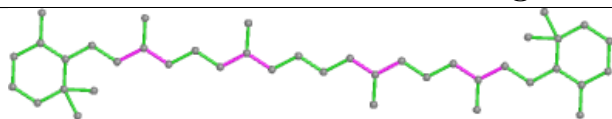


Torsions

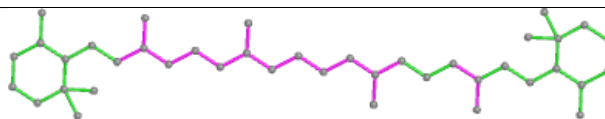


Rings

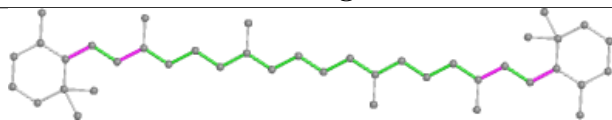
Ligand BCR B 846



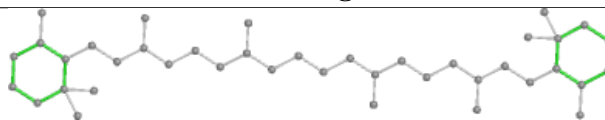
Bond lengths



Bond angles

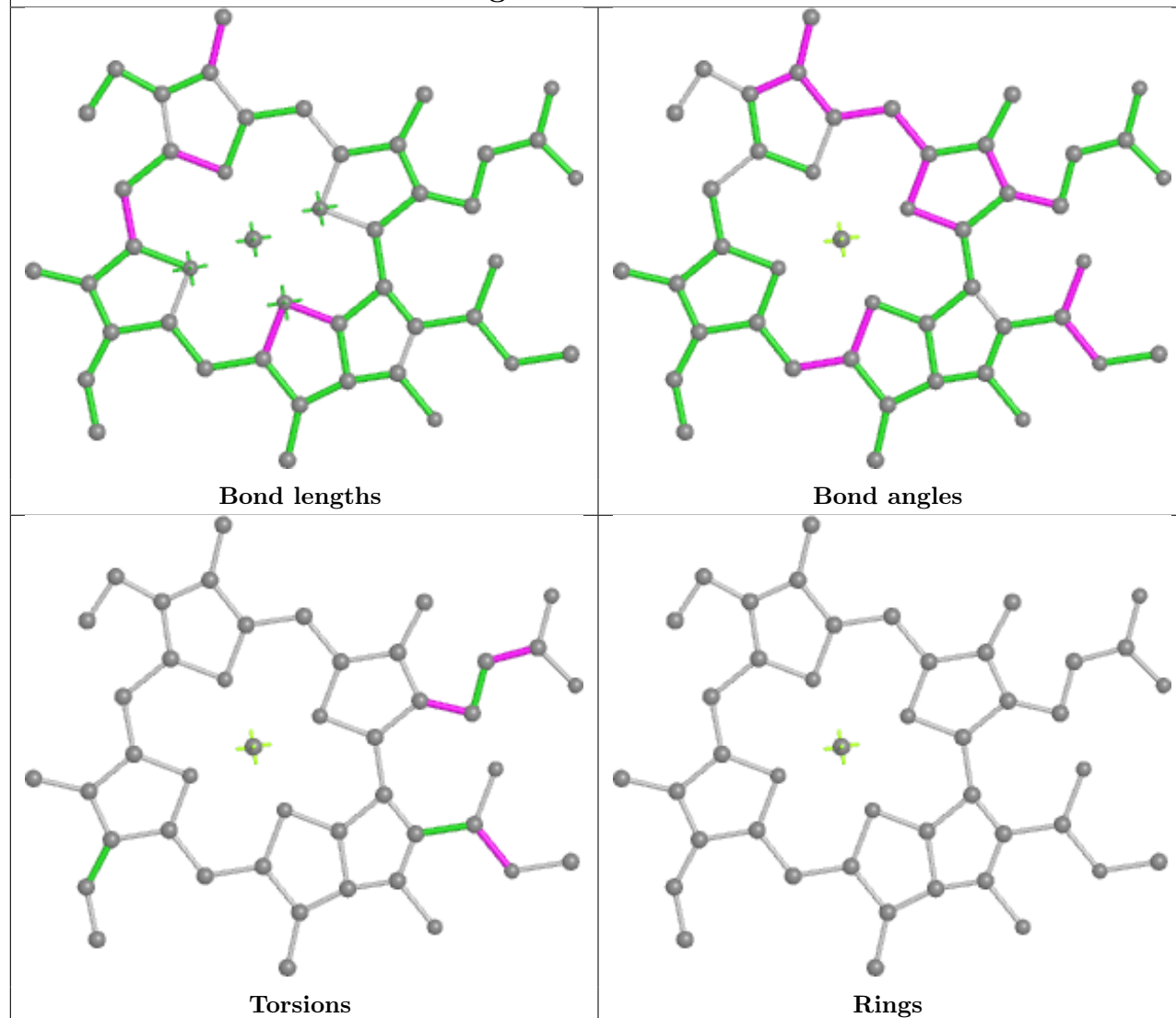


Torsions

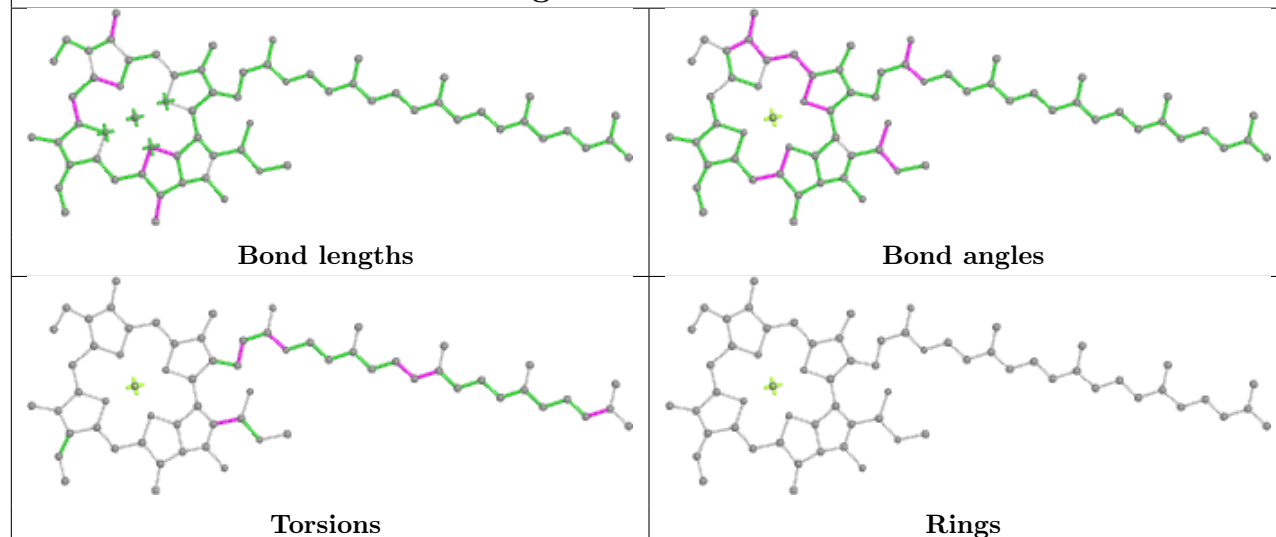


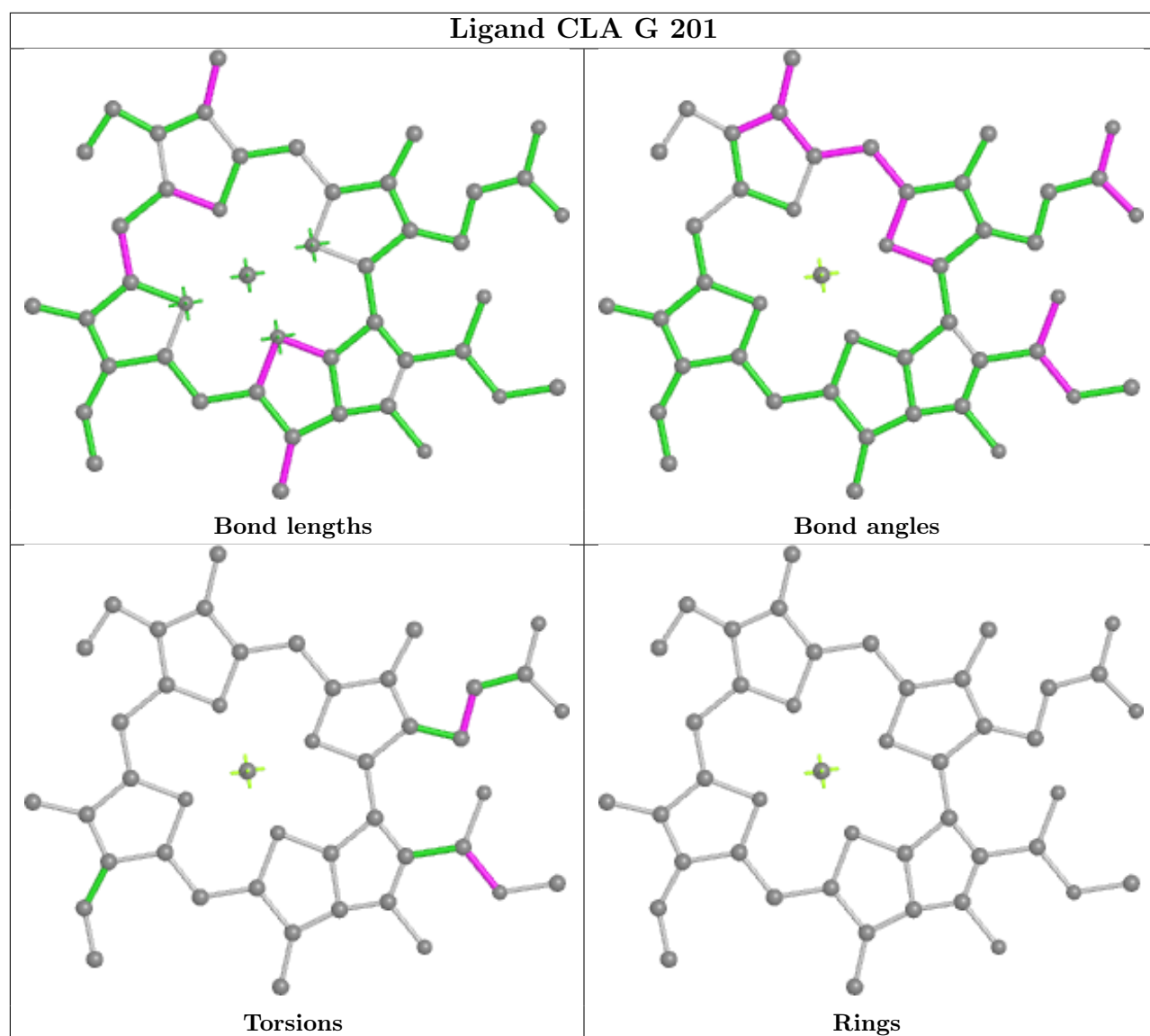
Rings

Ligand CLA K 203

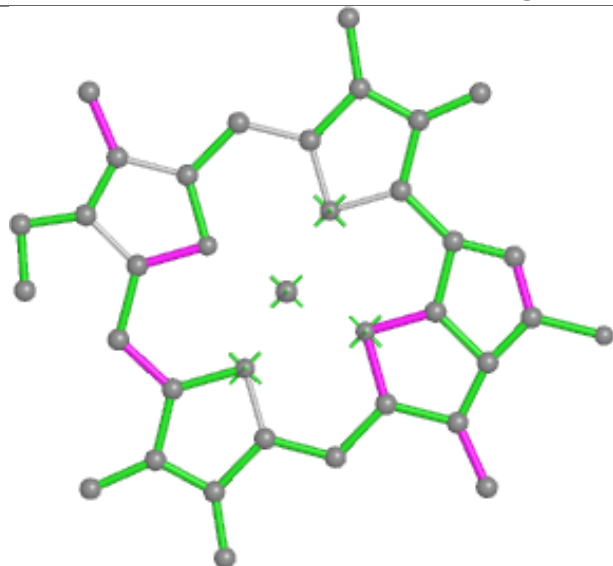


Ligand CLA B 839

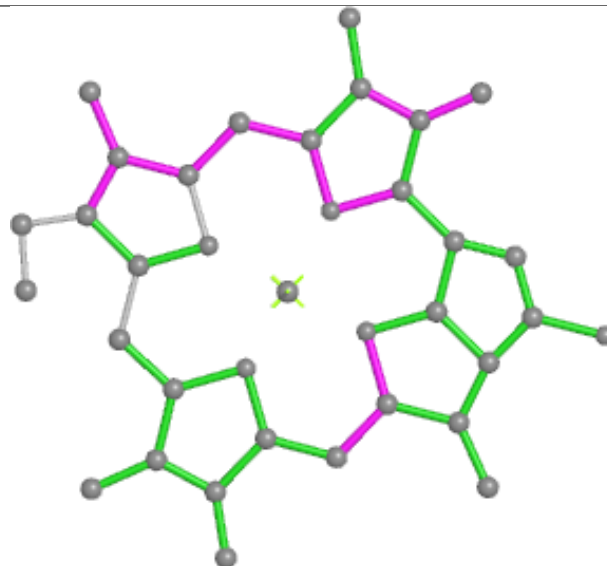




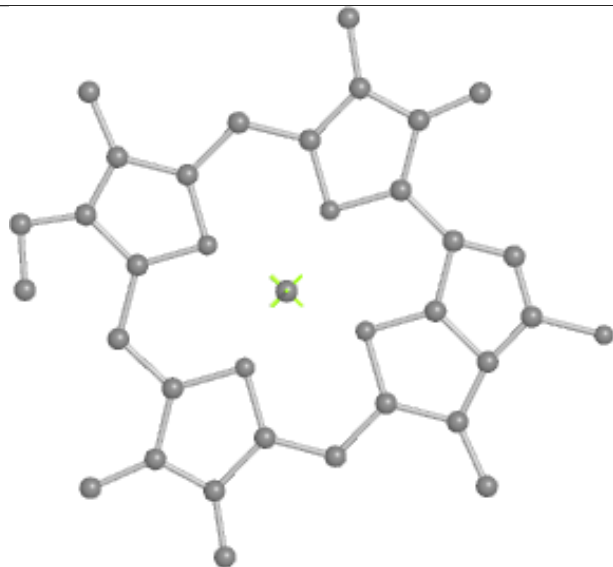
Ligand CLA 3 611



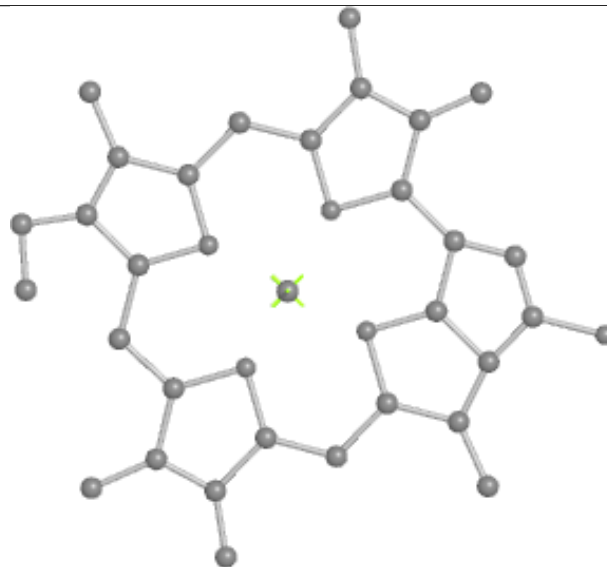
Bond lengths



Bond angles

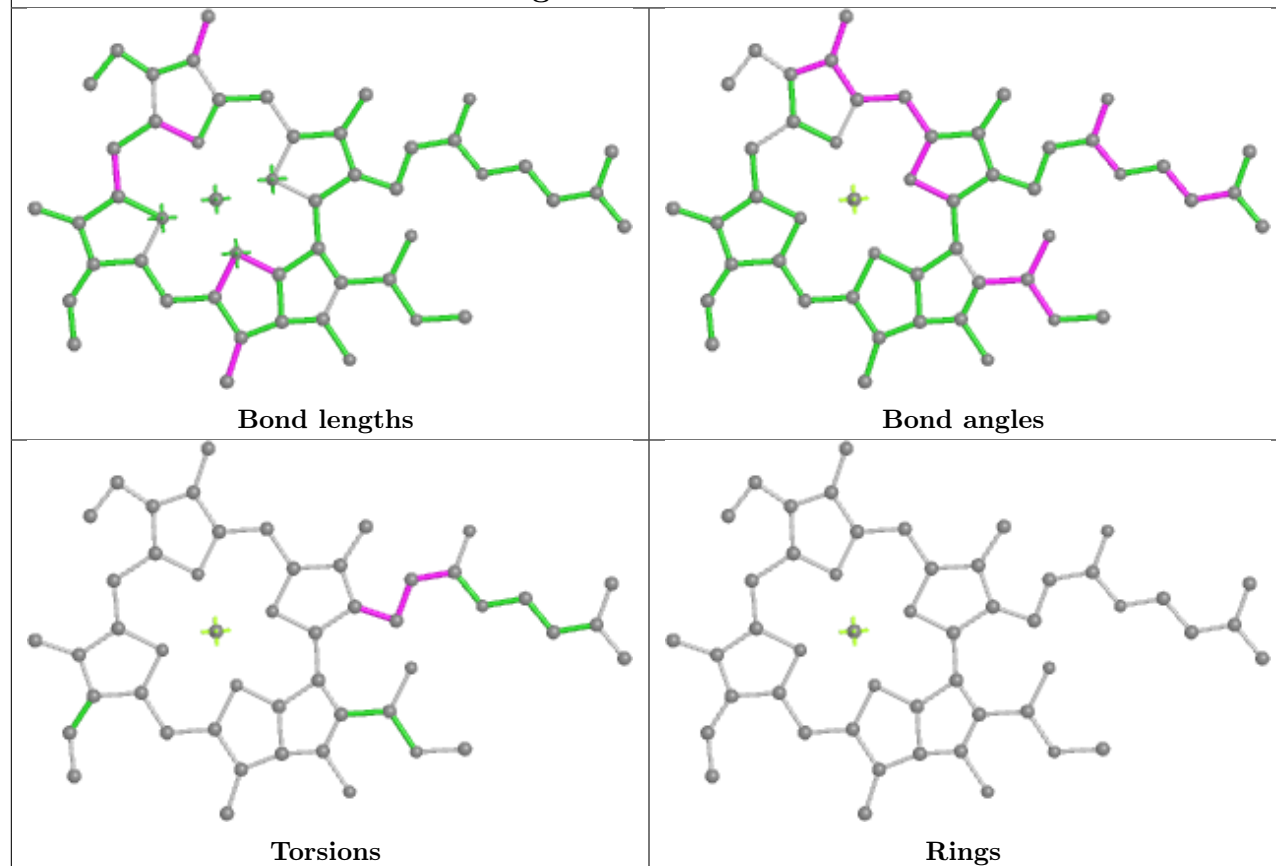


Torsions

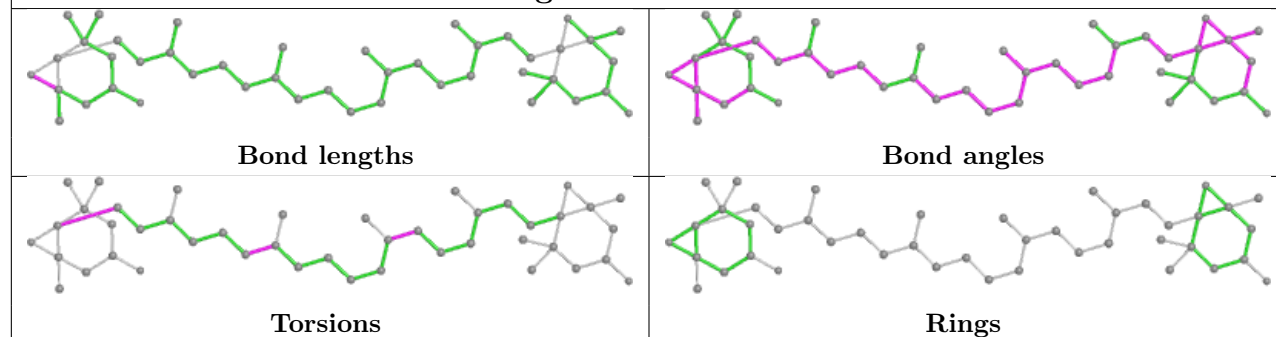


Rings

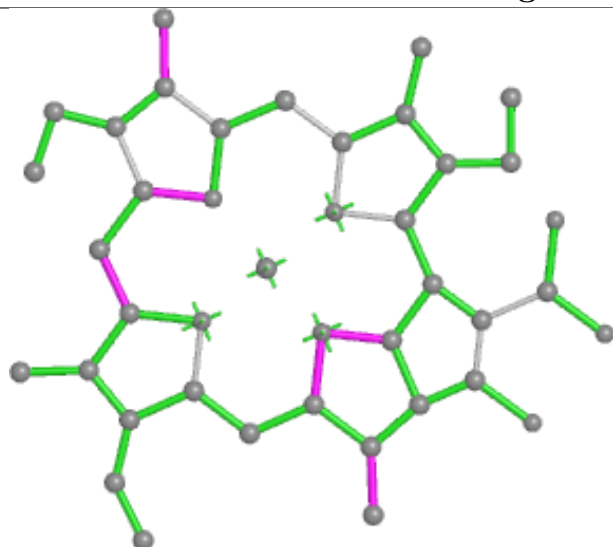
Ligand CLA B 820



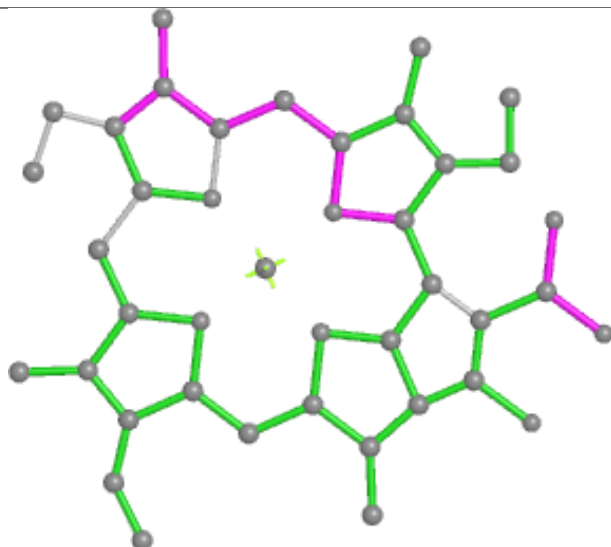
Ligand XAT 1 614



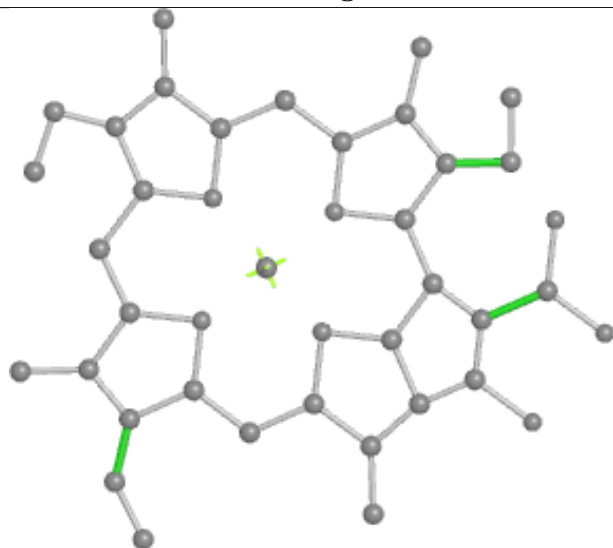
Ligand CLA 3 604



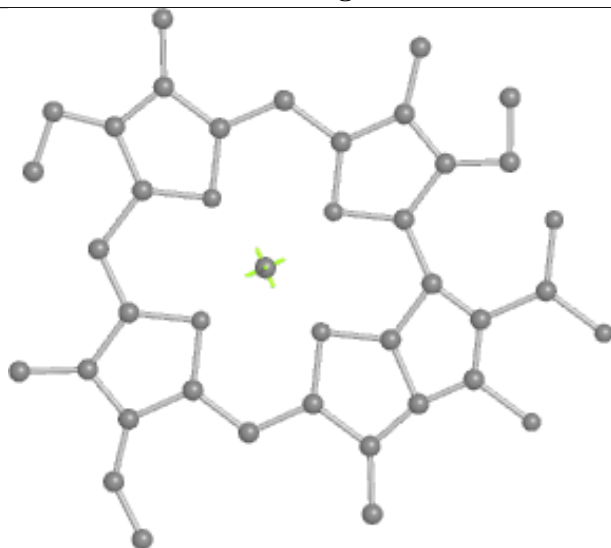
Bond lengths



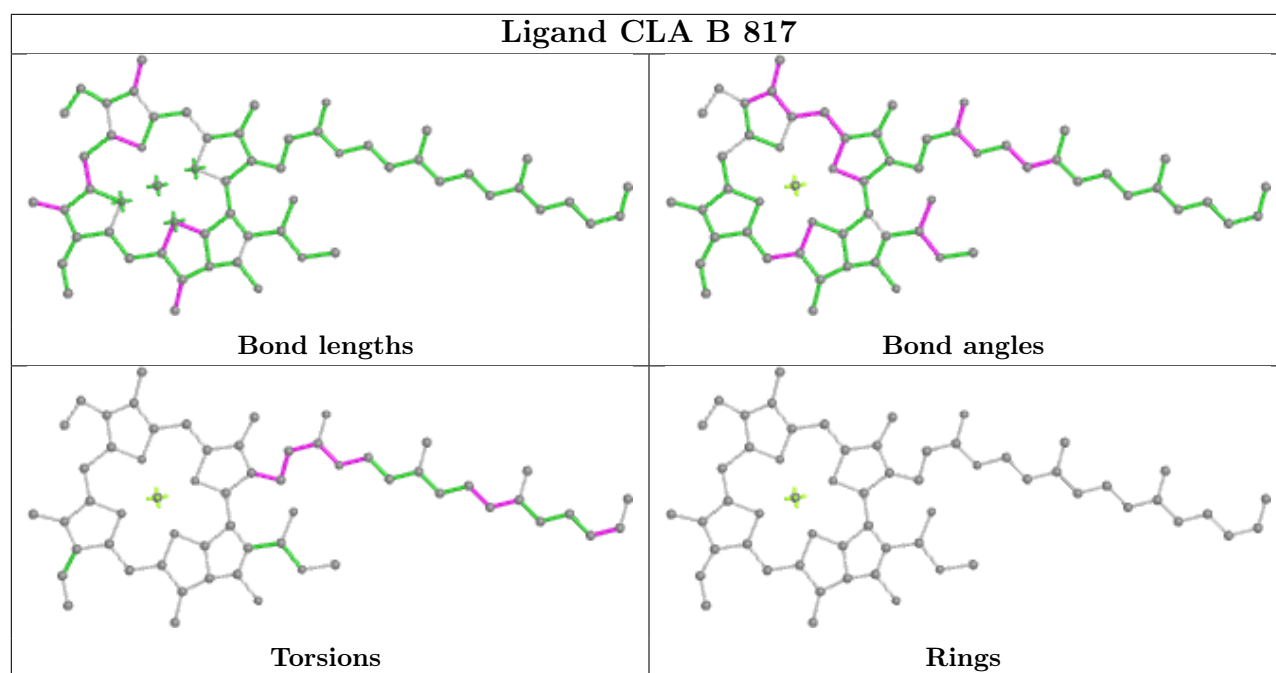
Bond angles



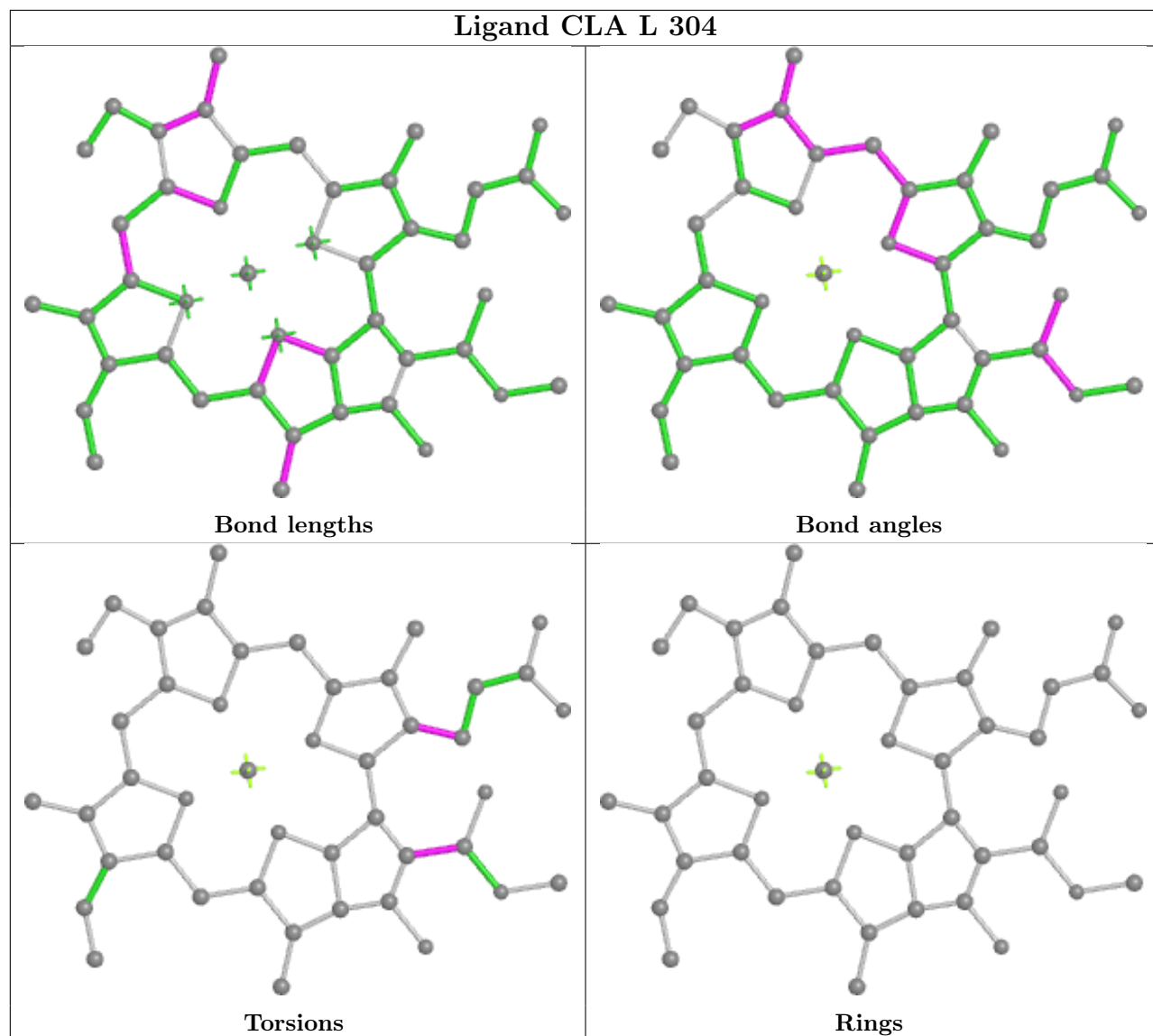
Torsions

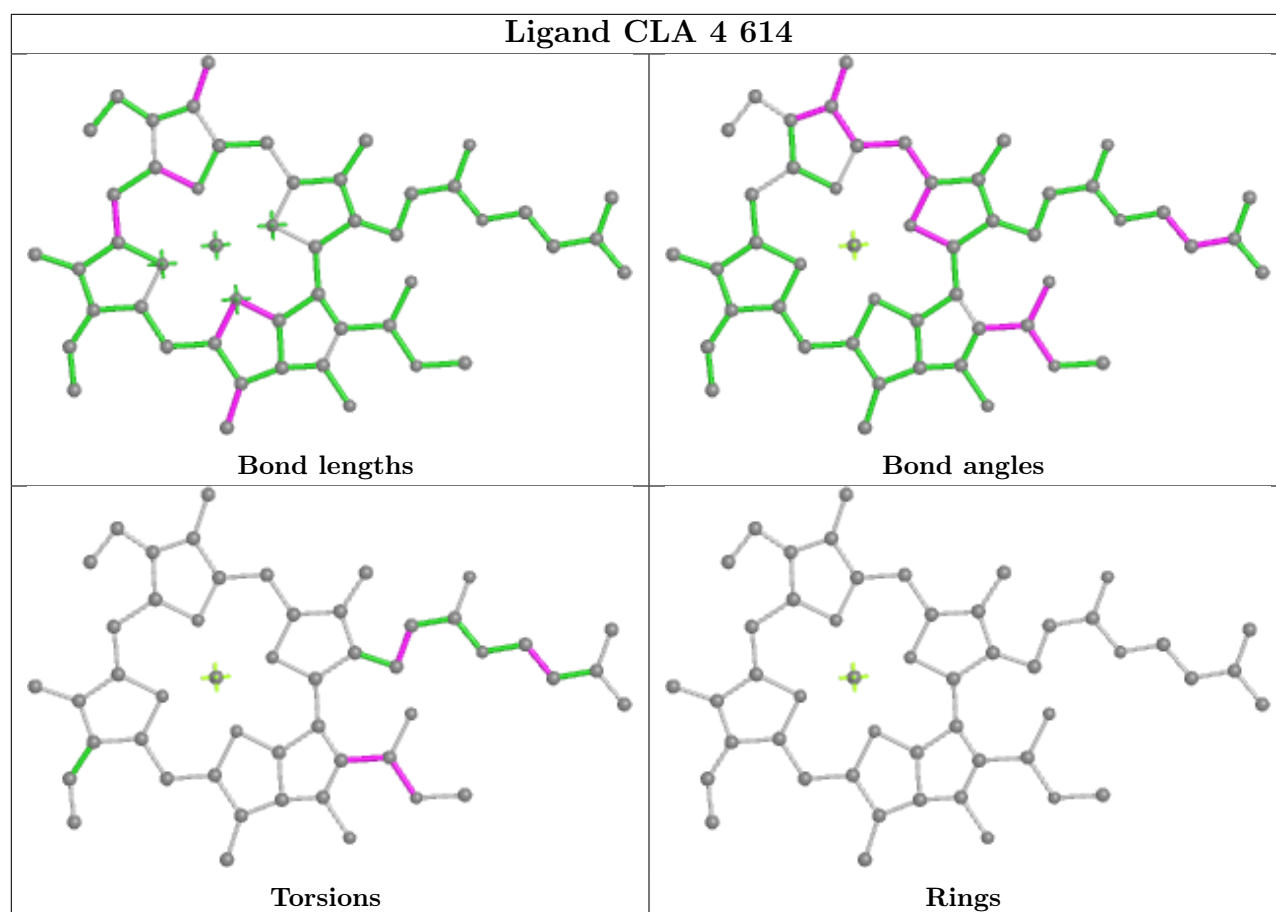


Rings

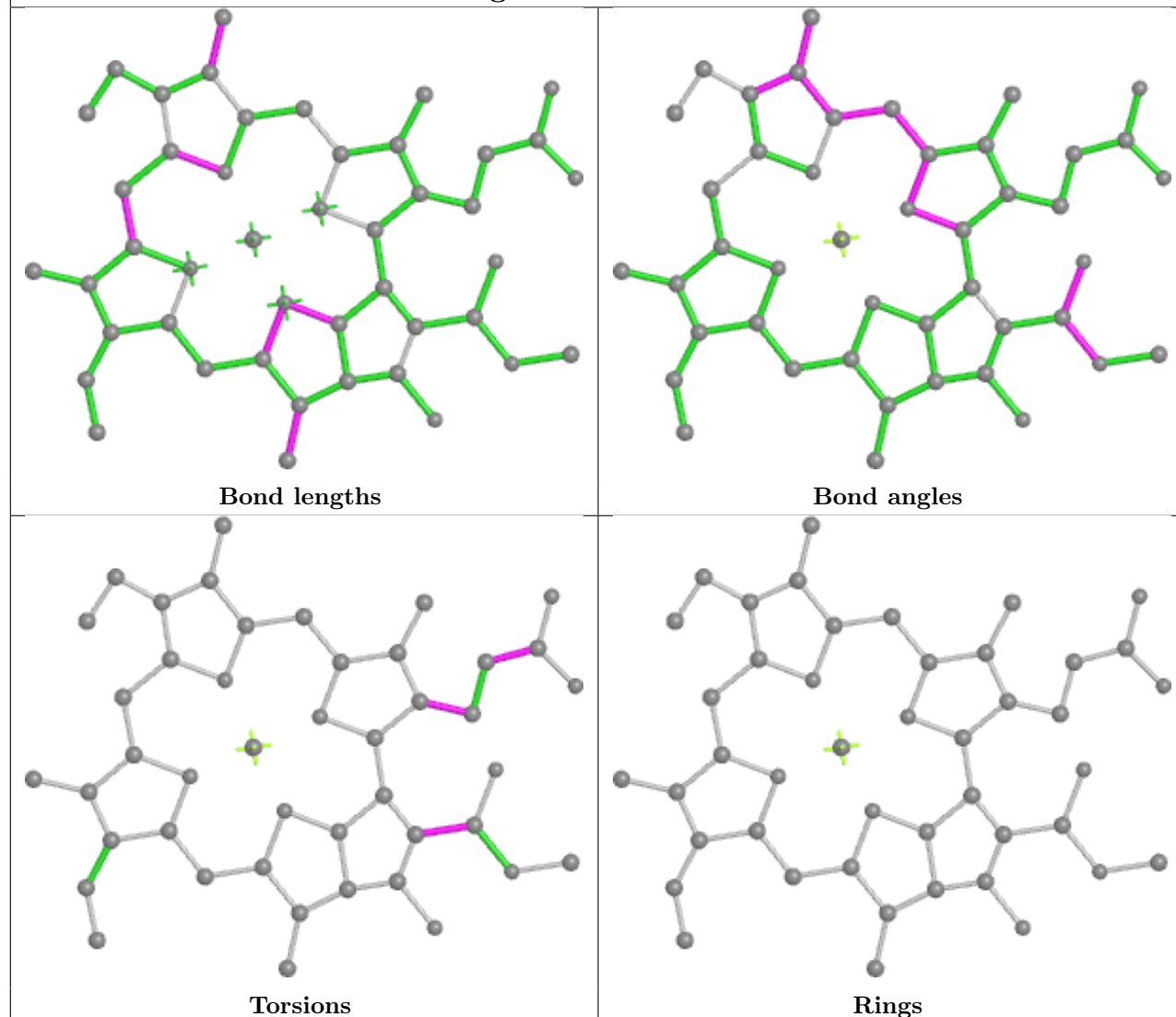


Ligand CLA L 304

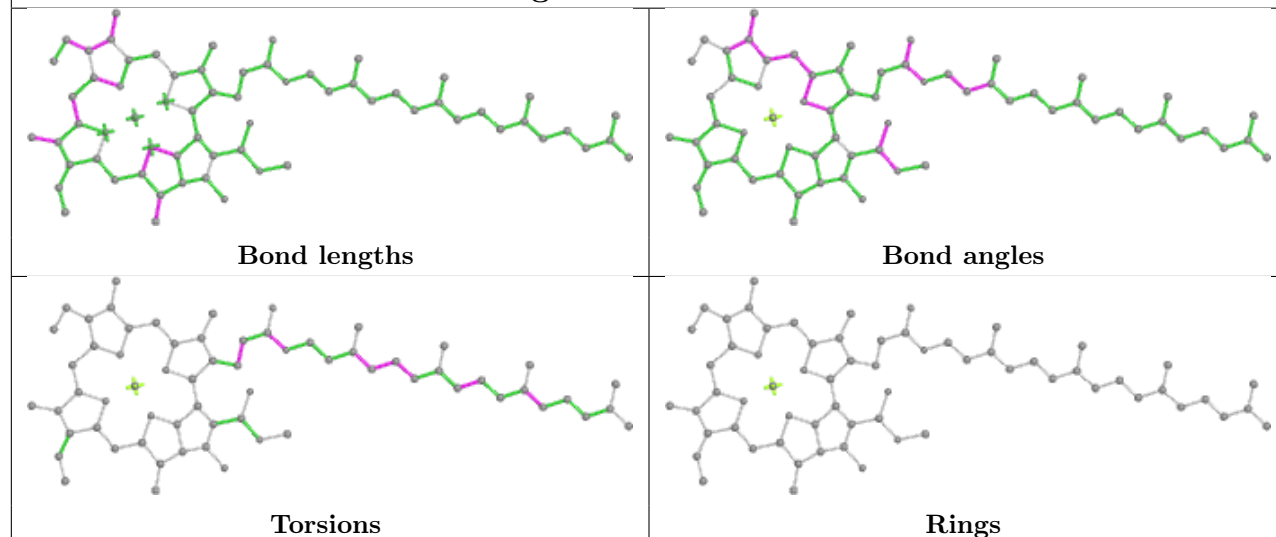




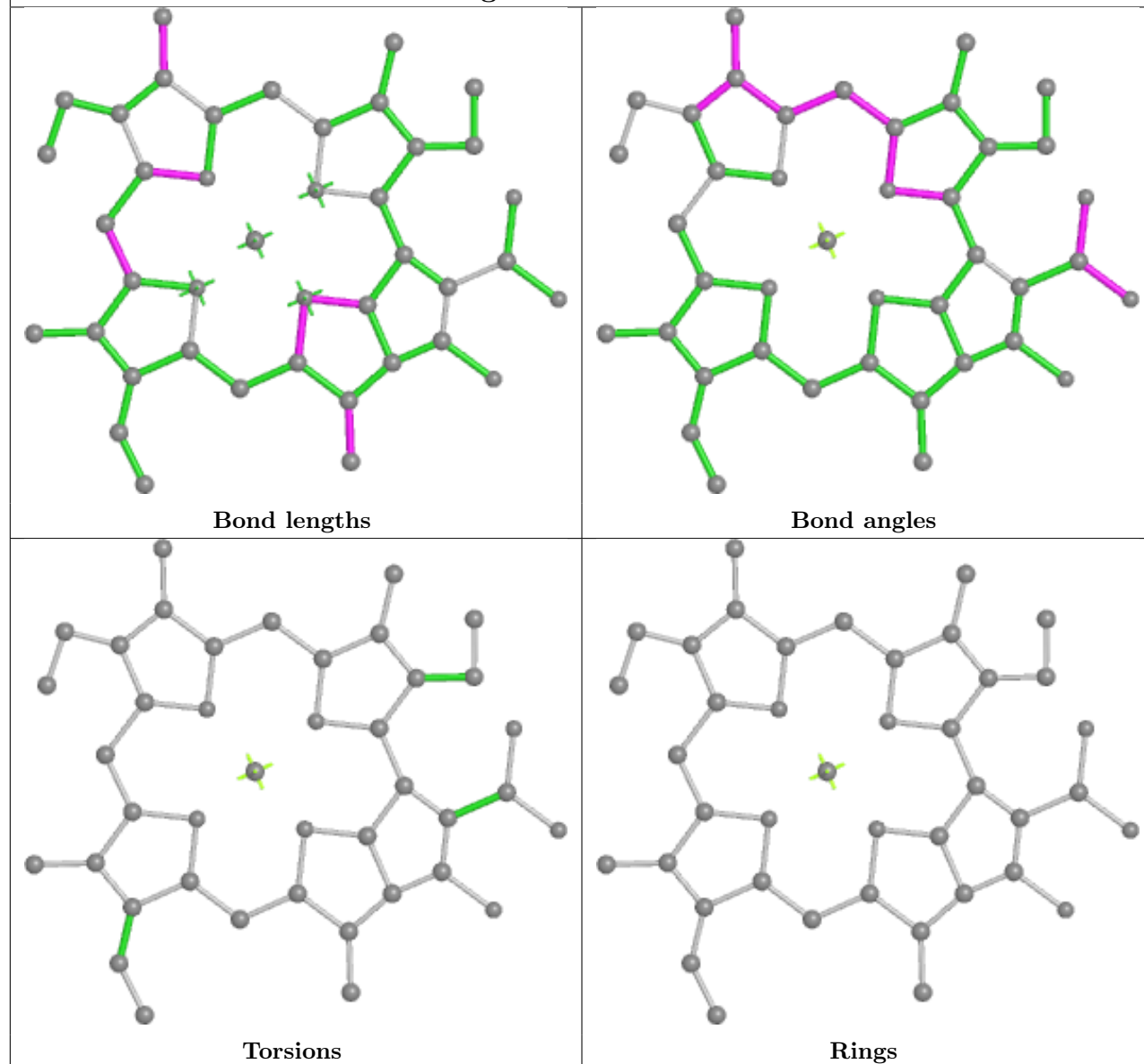
Ligand CLA A 821



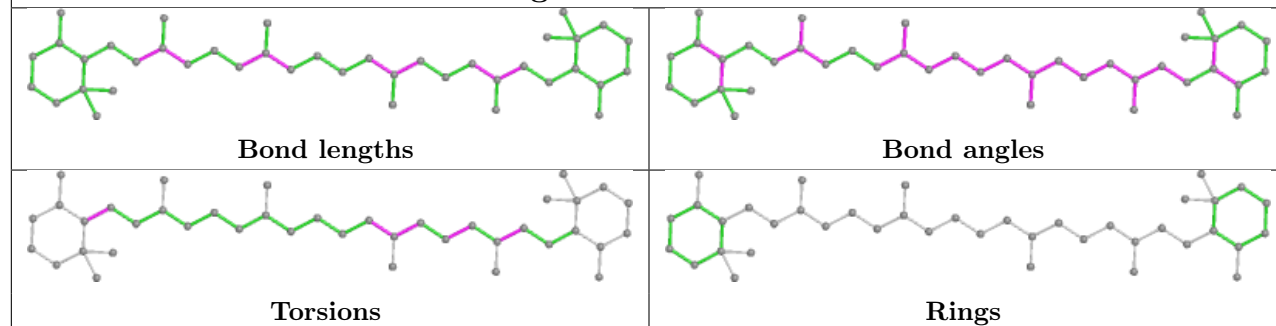
Ligand CLA A 844



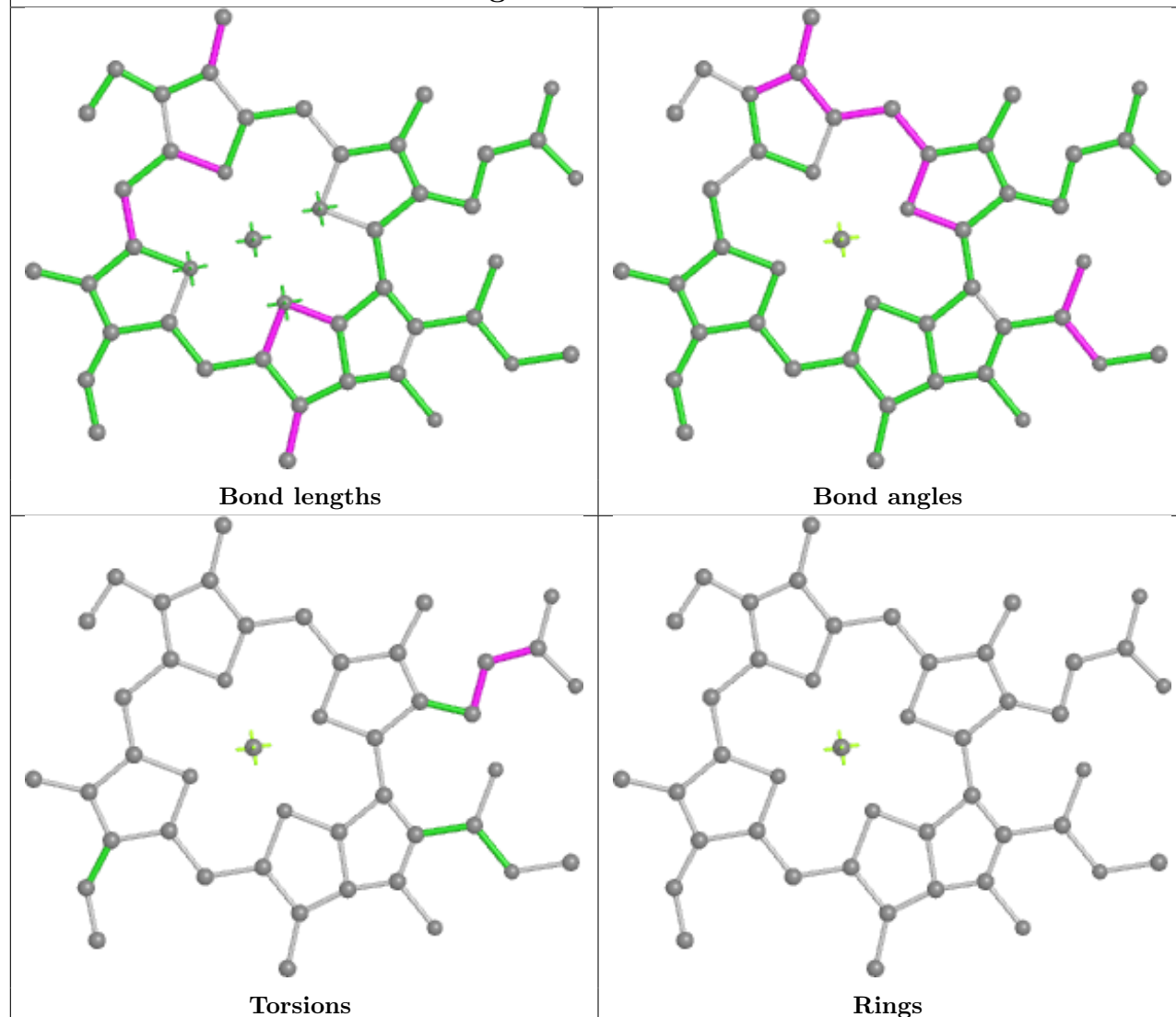
Ligand CLA 4 611



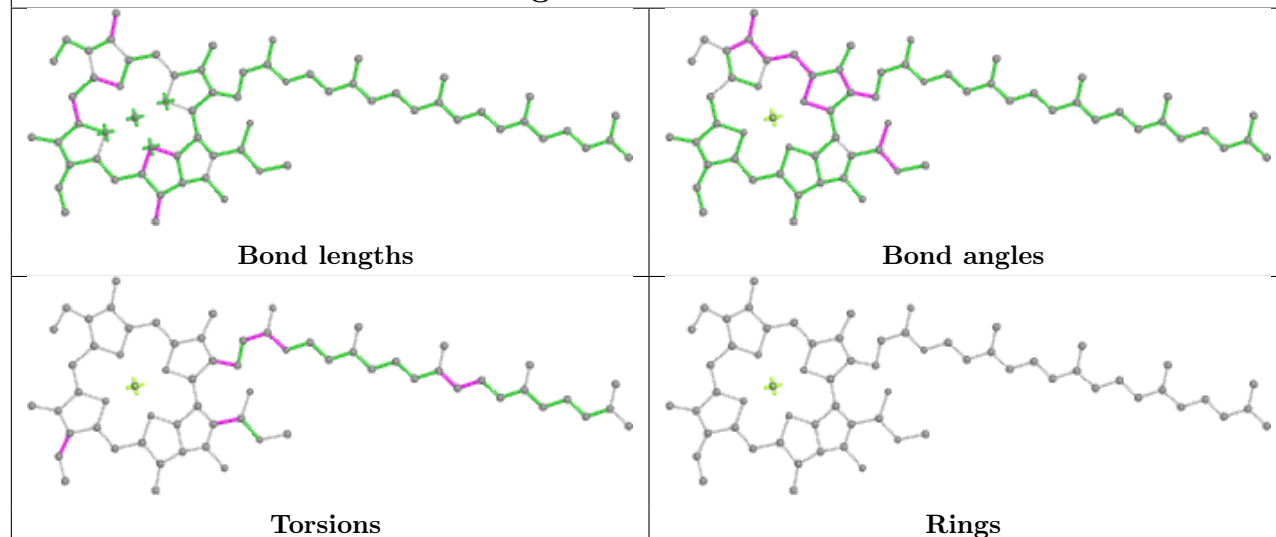
Ligand BCR B 845



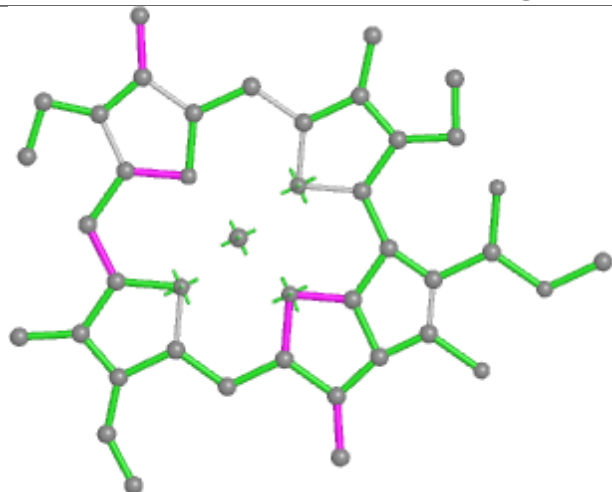
Ligand CLA G 203



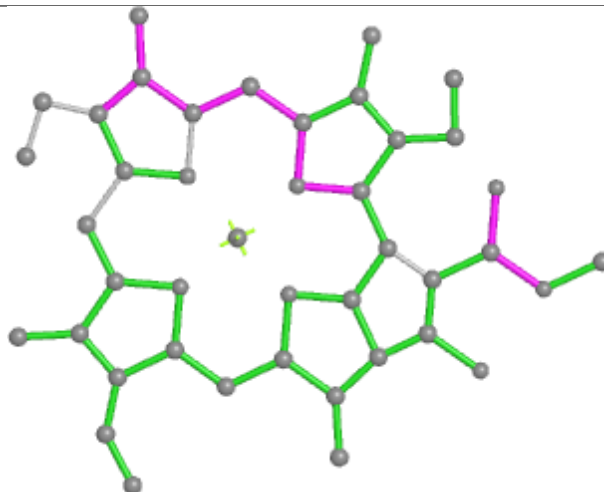
Ligand CLA A 842



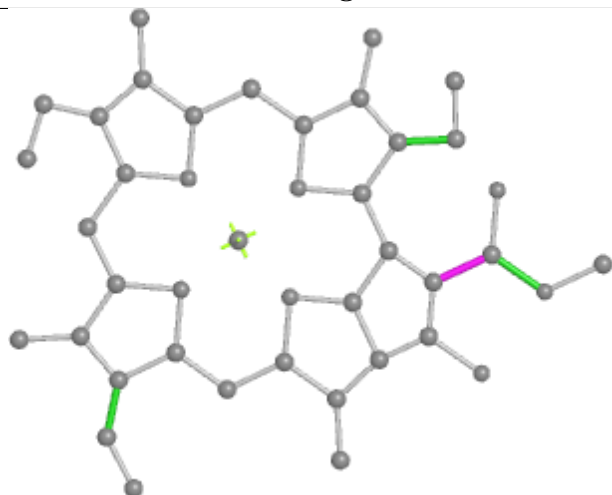
Ligand CLA 4 610



Bond lengths



Bond angles

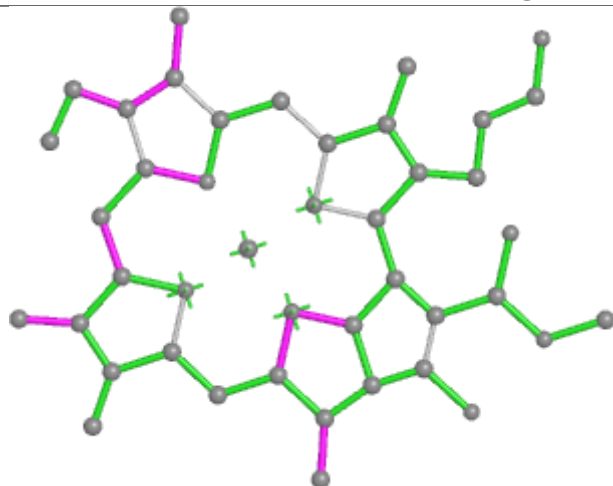


Torsions

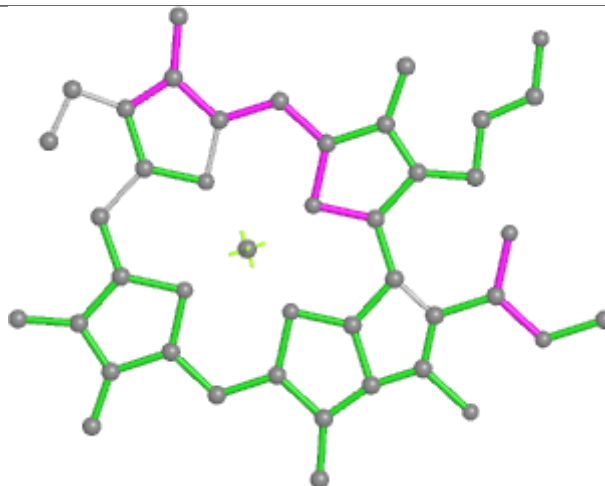


Rings

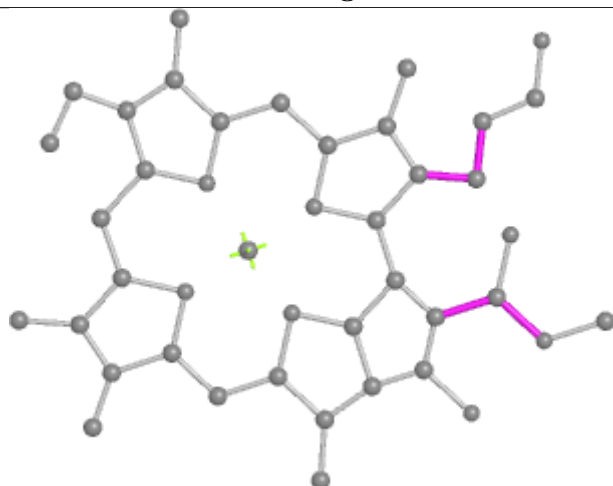
Ligand CLA 2 604



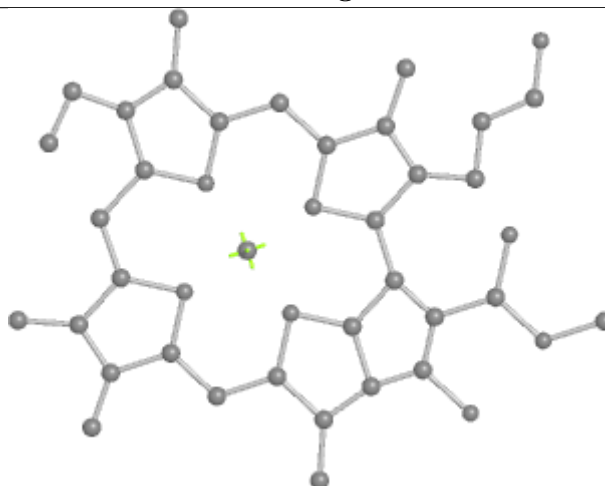
Bond lengths



Bond angles

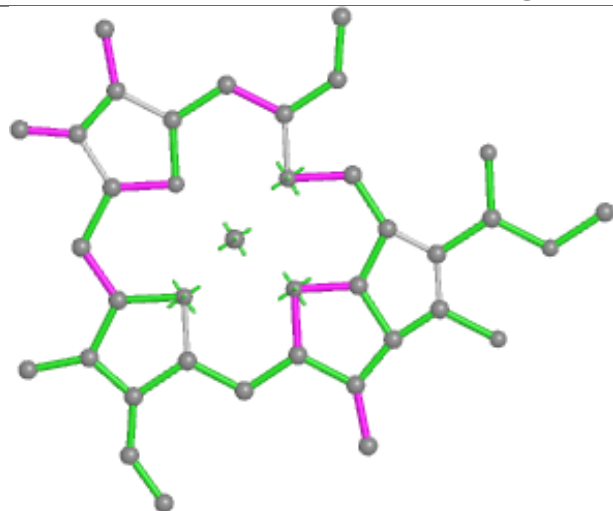


Torsions

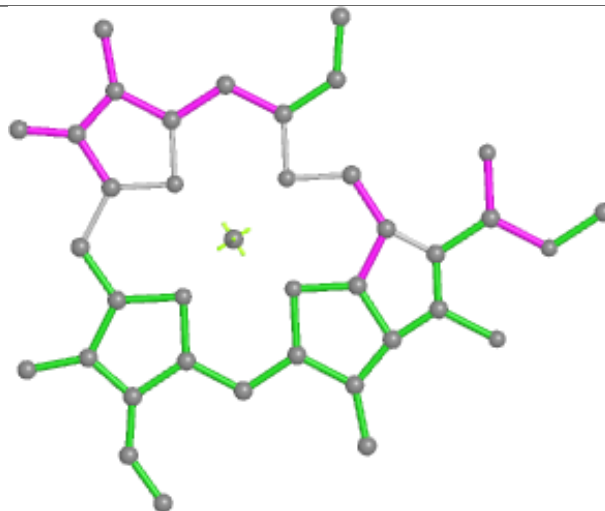


Rings

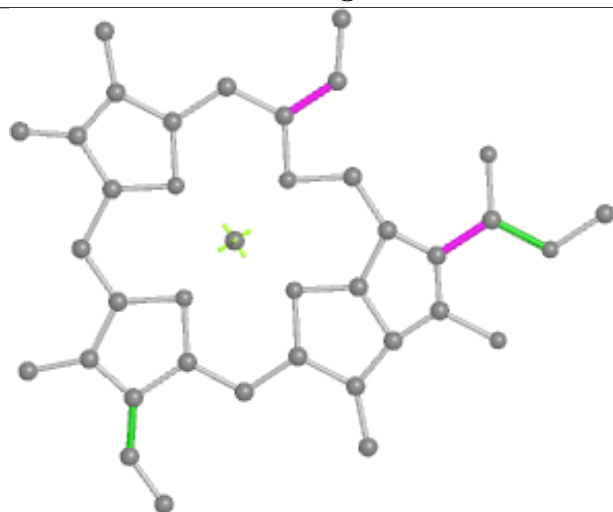
Ligand CLA 2 610



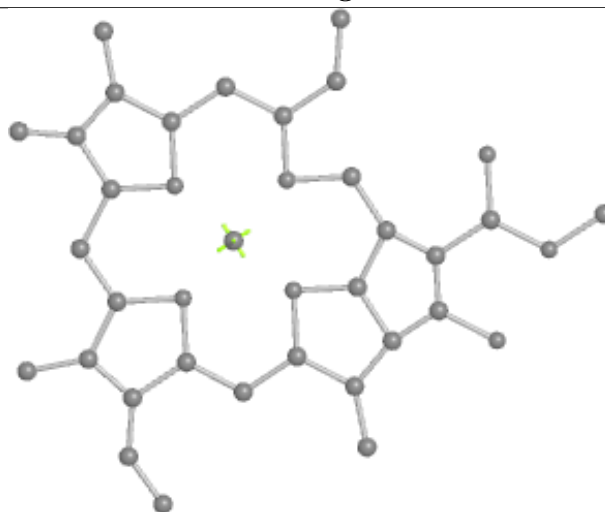
Bond lengths



Bond angles

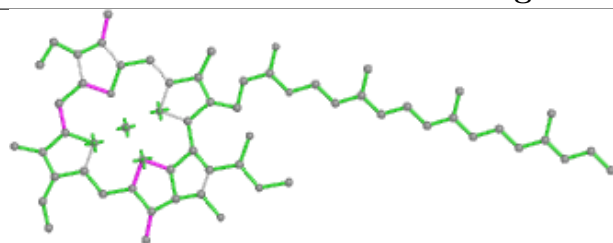


Torsions

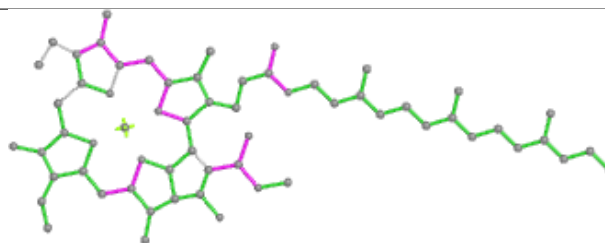


Rings

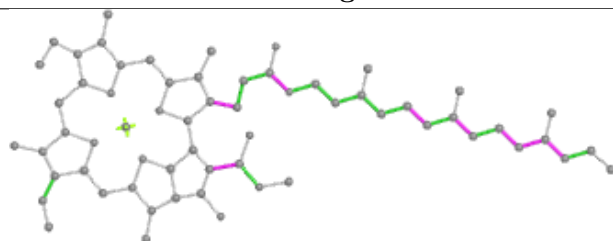
Ligand CLA B 825



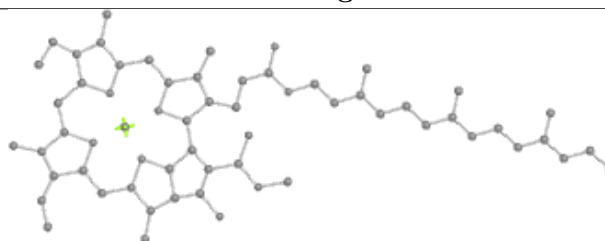
Bond lengths



Bond angles

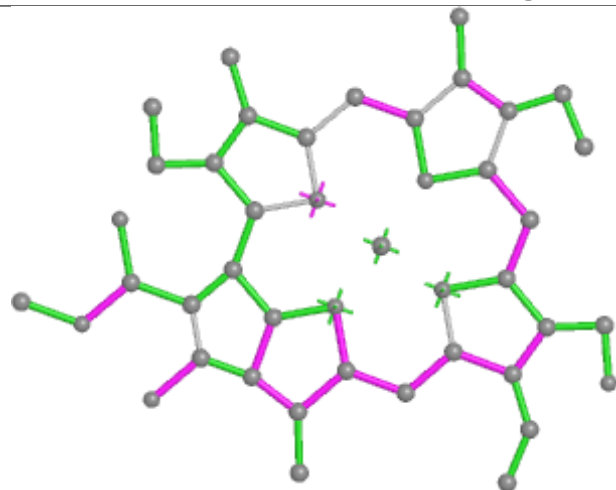


Torsions

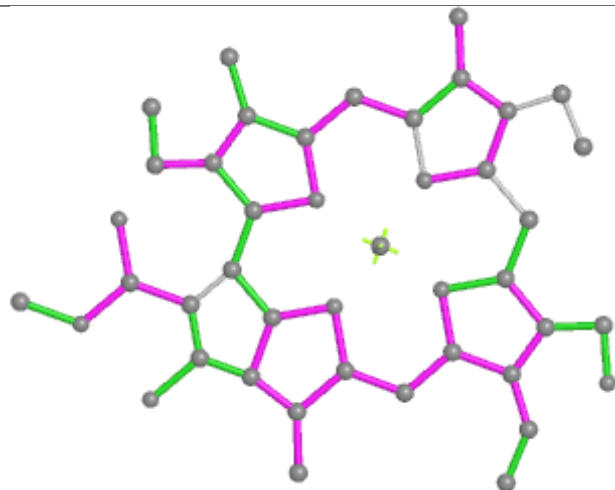


Rings

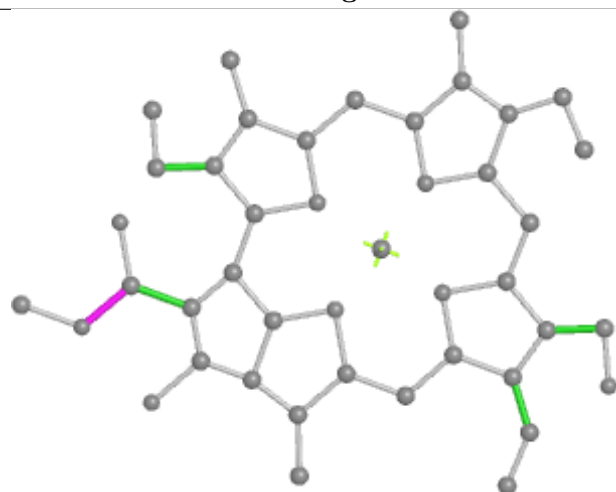
Ligand CHL 2 615



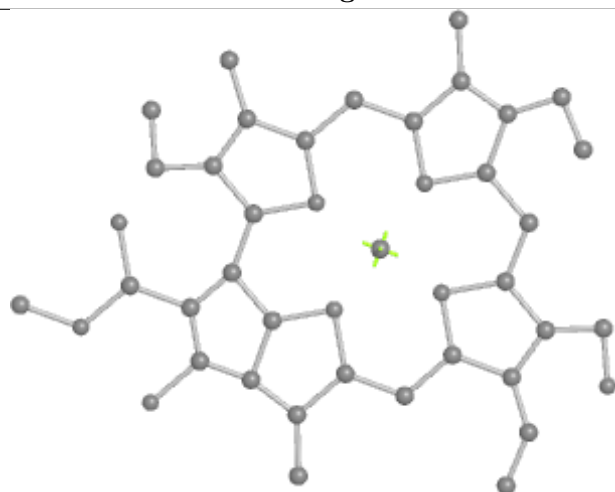
Bond lengths



Bond angles

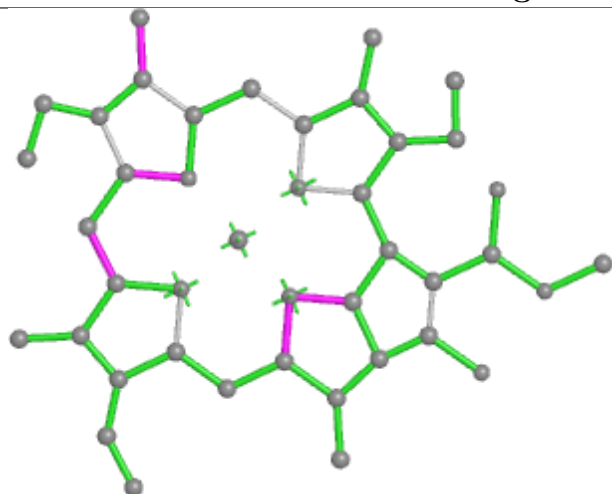


Torsions

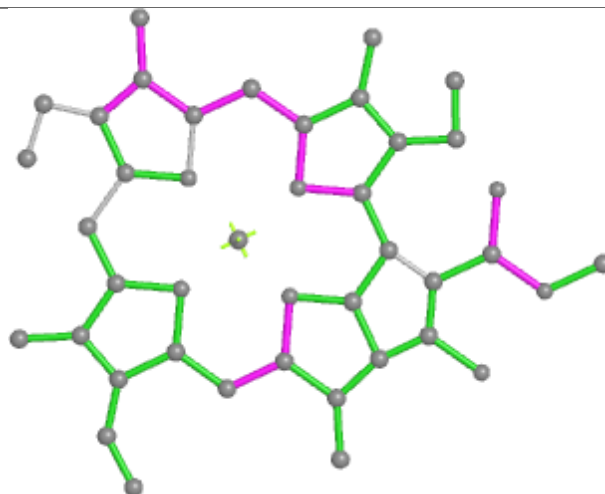


Rings

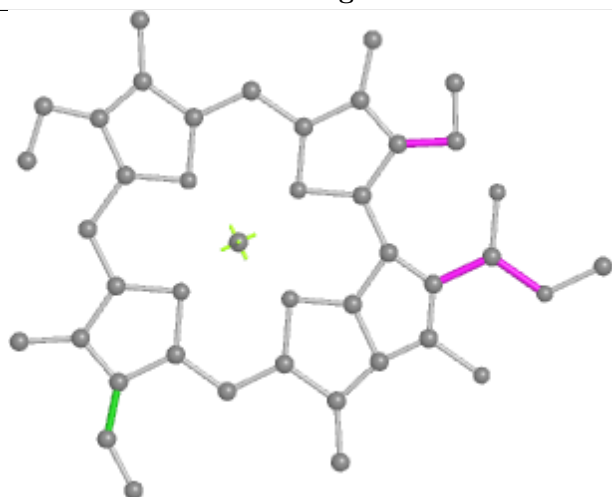
Ligand CLA B 835



Bond lengths



Bond angles

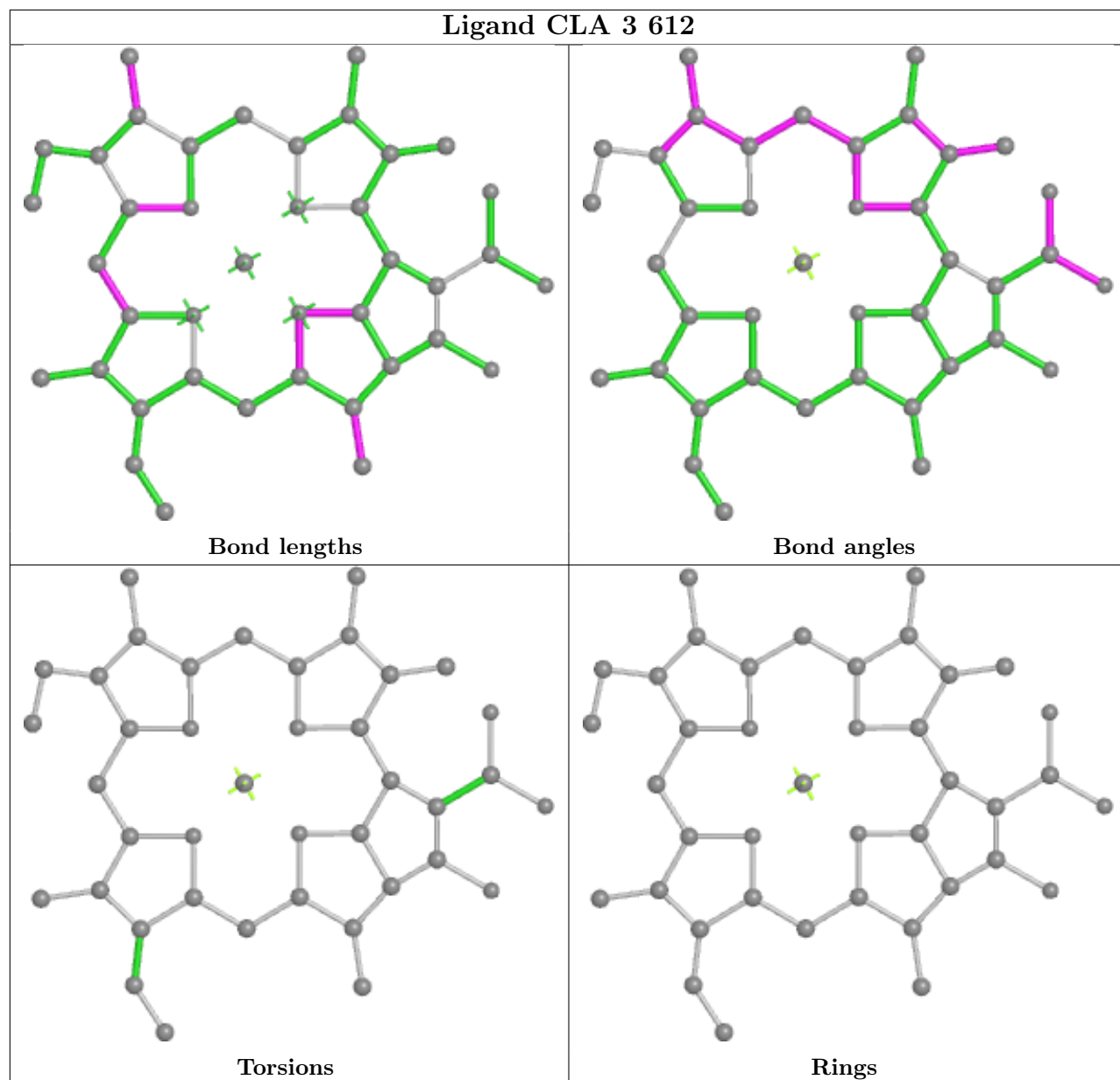


Torsions

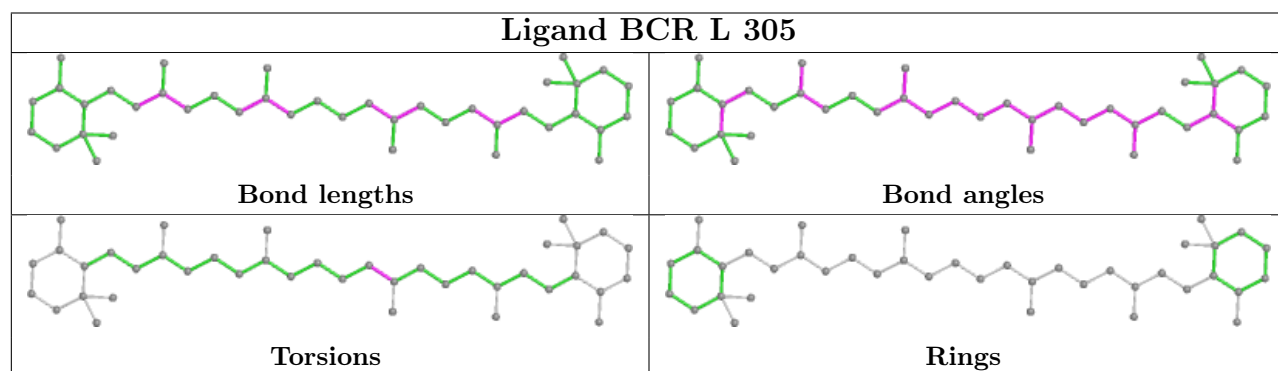


Rings

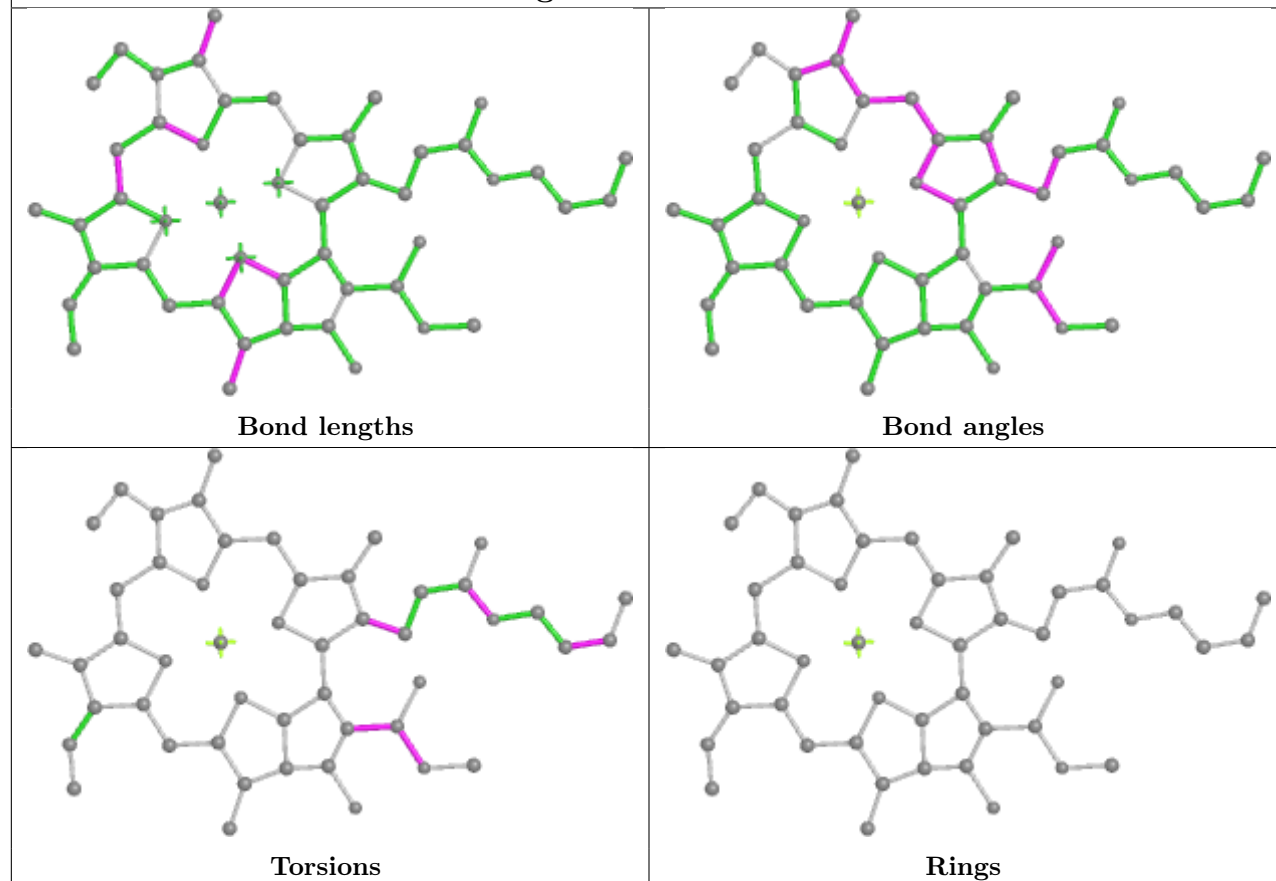
Ligand CLA 3 612



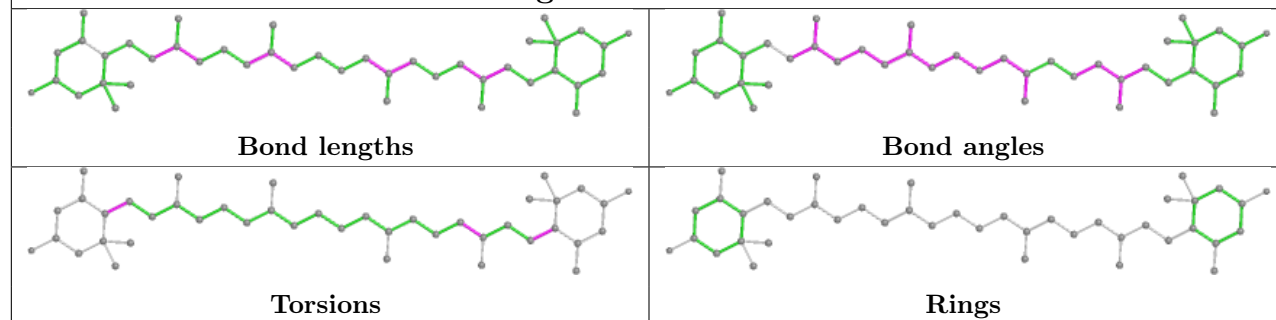
Ligand BCR L 305



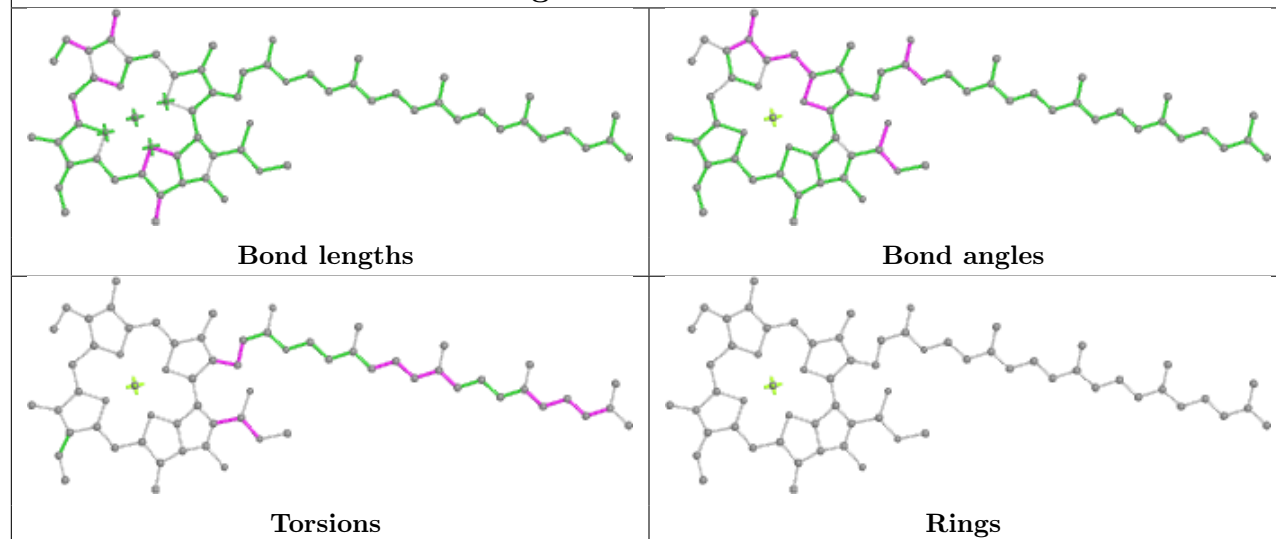
Ligand CLA 1 604



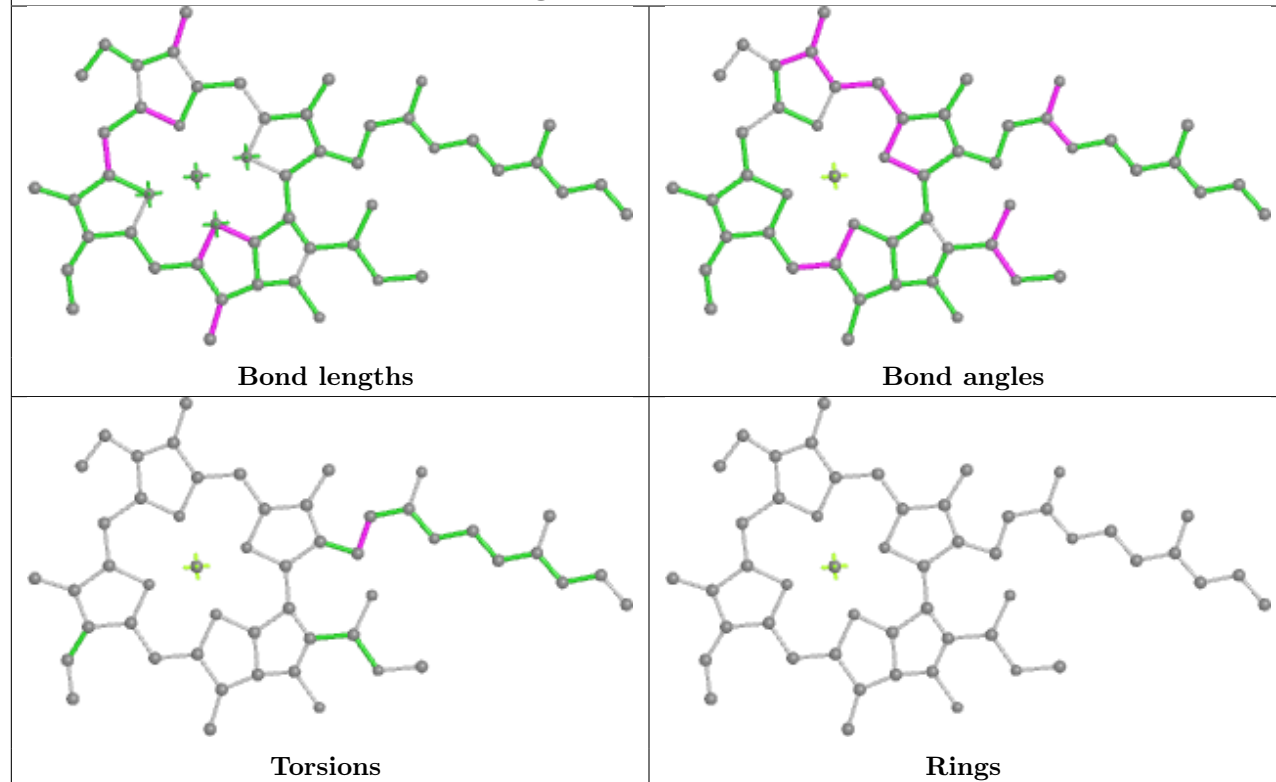
Ligand LUT 2 619

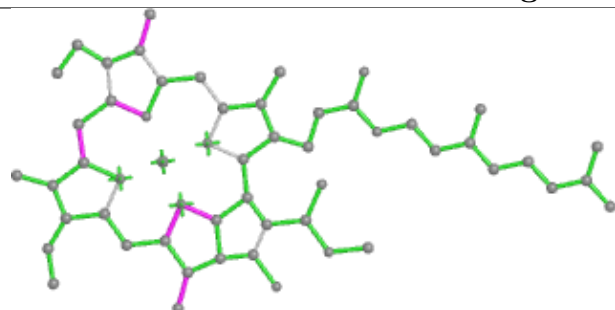


Ligand CLA A 829

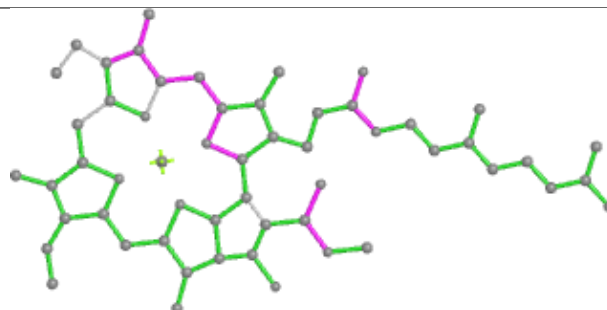


Ligand CLA B 807

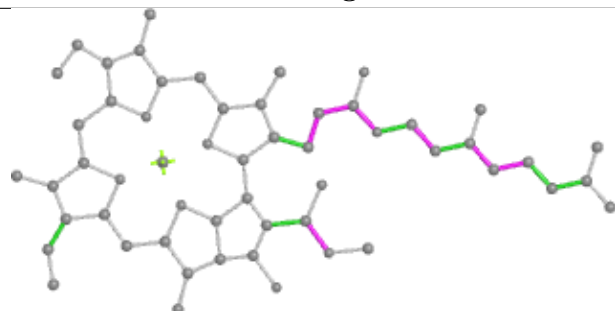


Ligand CLA 3 602

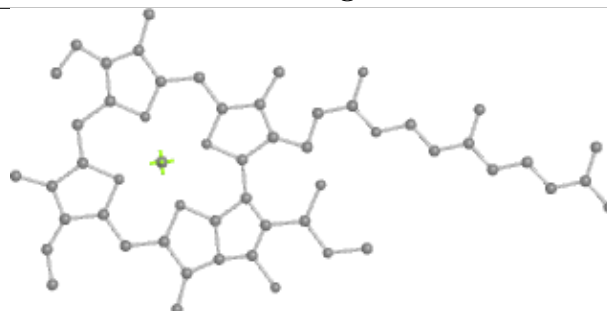
Bond lengths



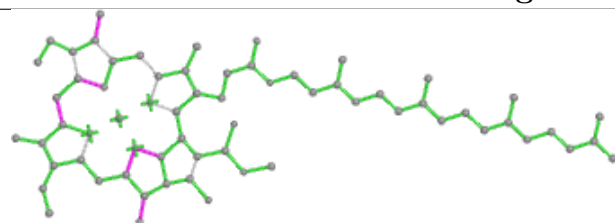
Bond angles



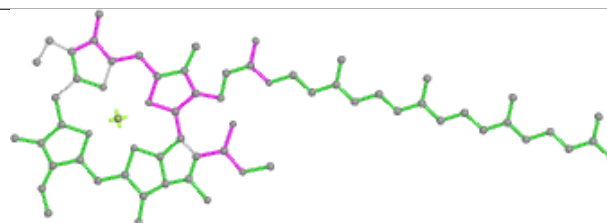
Torsions



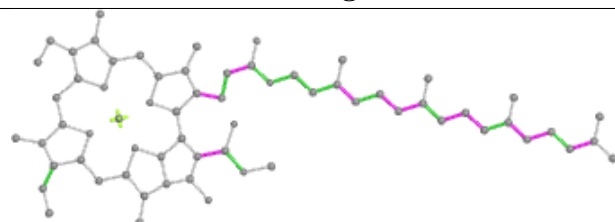
Rings

Ligand CLA A 804

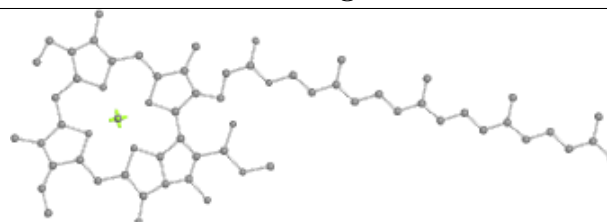
Bond lengths



Bond angles

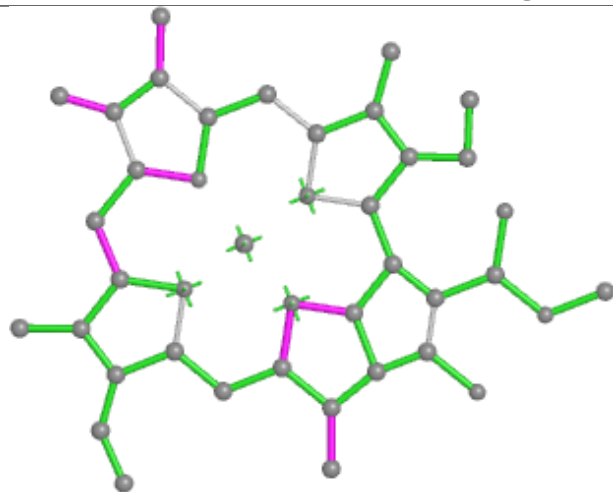


Torsions

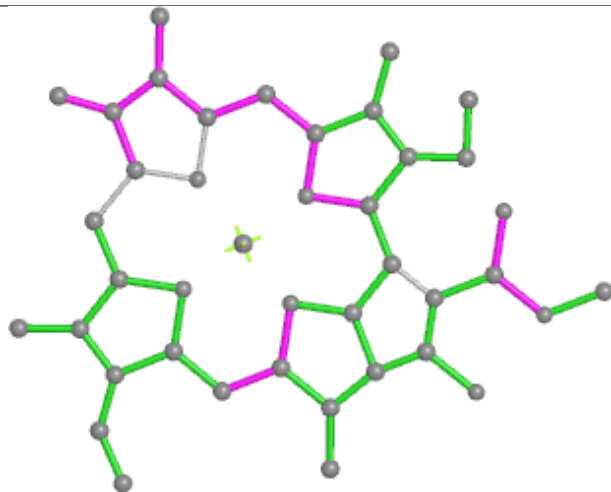


Rings

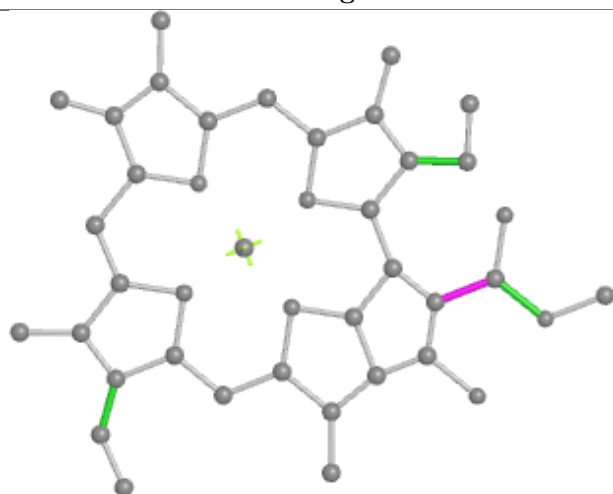
Ligand CLA 3 605



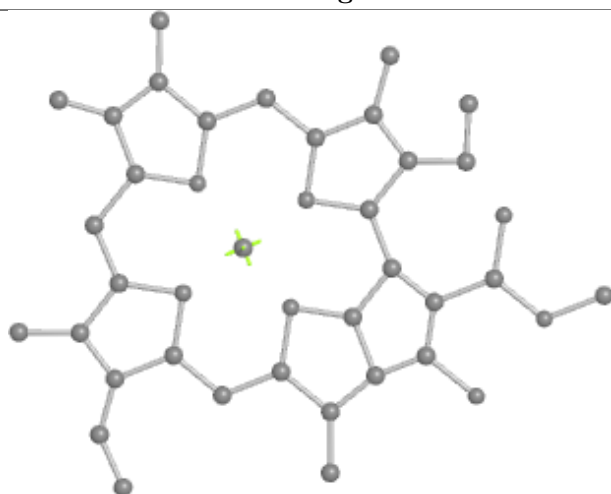
Bond lengths



Bond angles

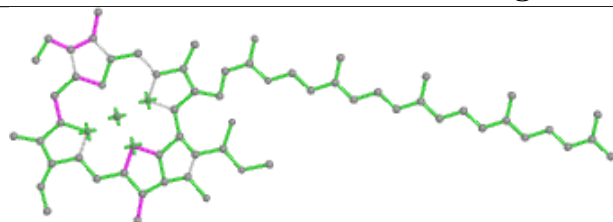


Torsions

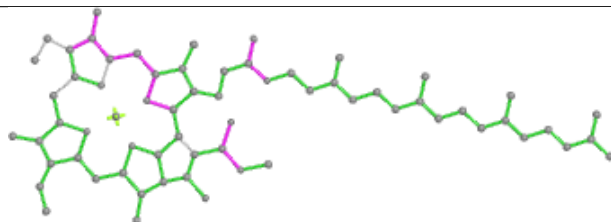


Rings

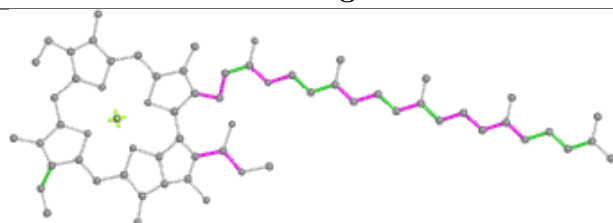
Ligand CLA A 803



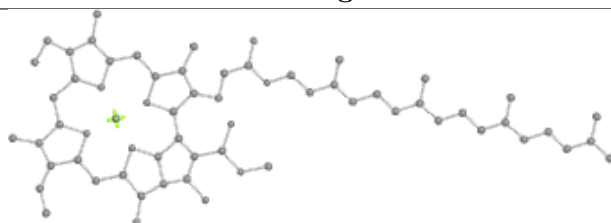
Bond lengths



Bond angles

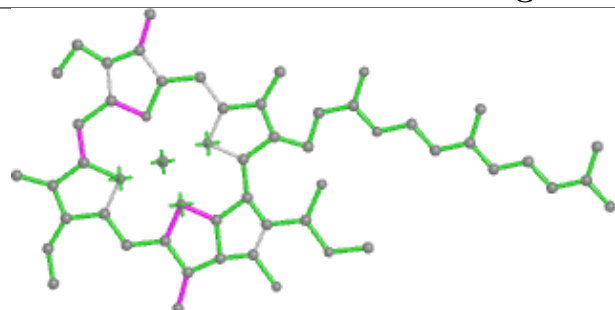


Torsions

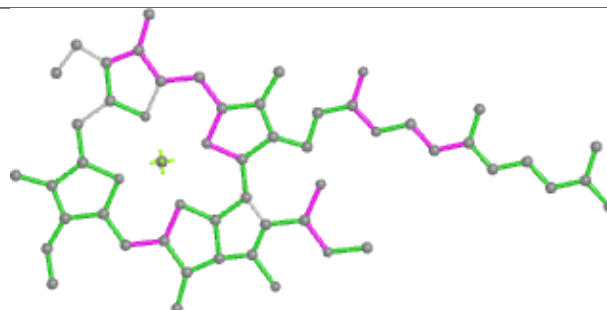


Rings

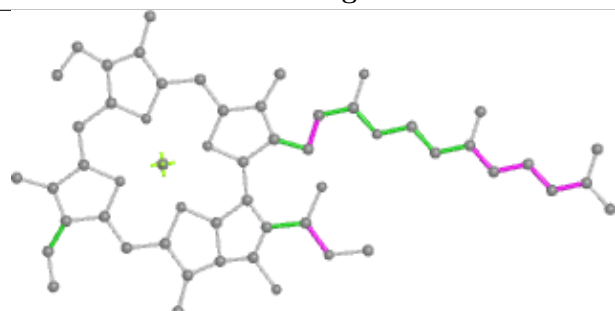
Ligand CLA B 816



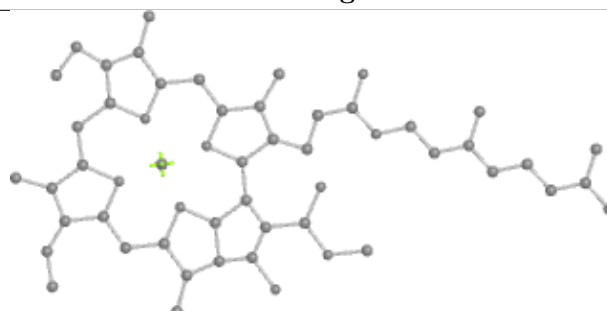
Bond lengths



Bond angles

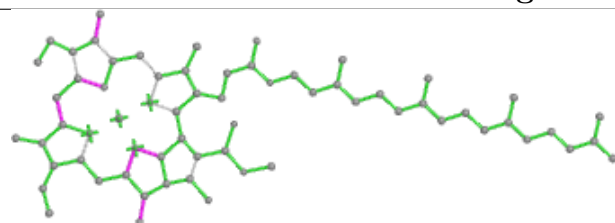


Torsions

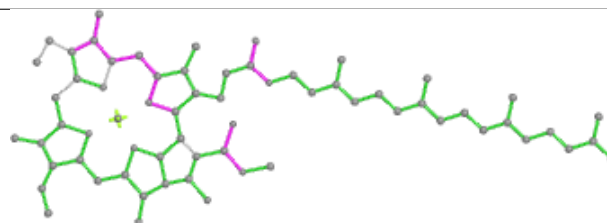


Rings

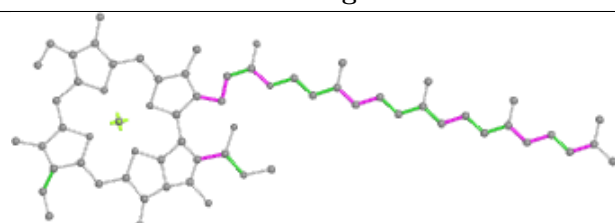
Ligand CLA B 824



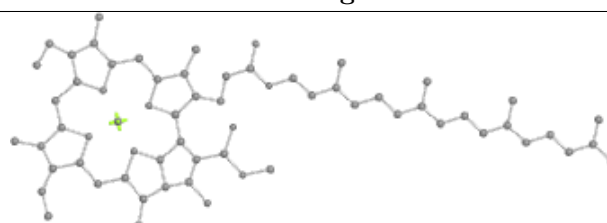
Bond lengths



Bond angles

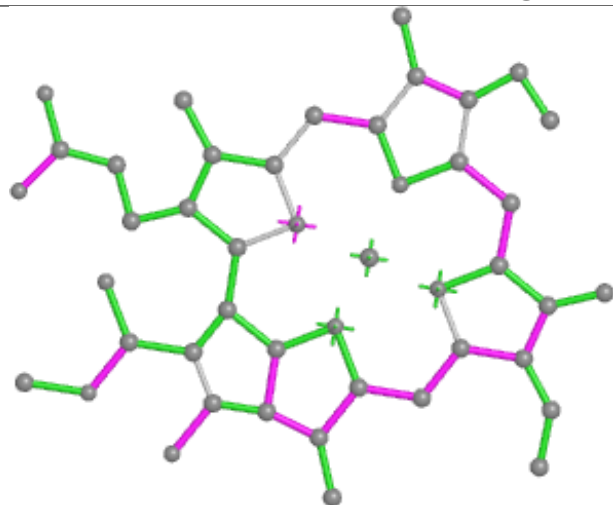


Torsions

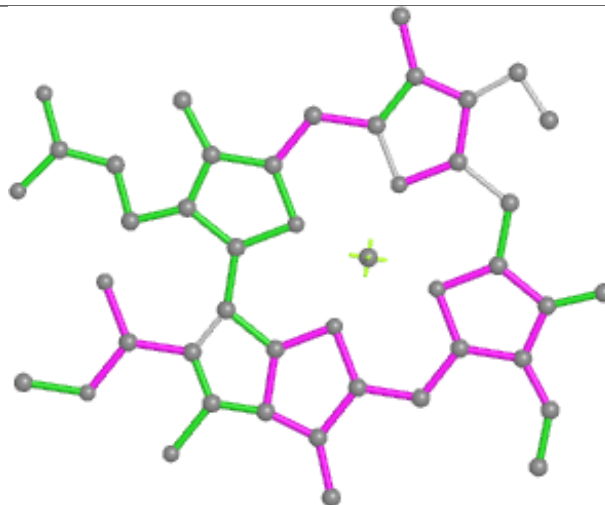


Rings

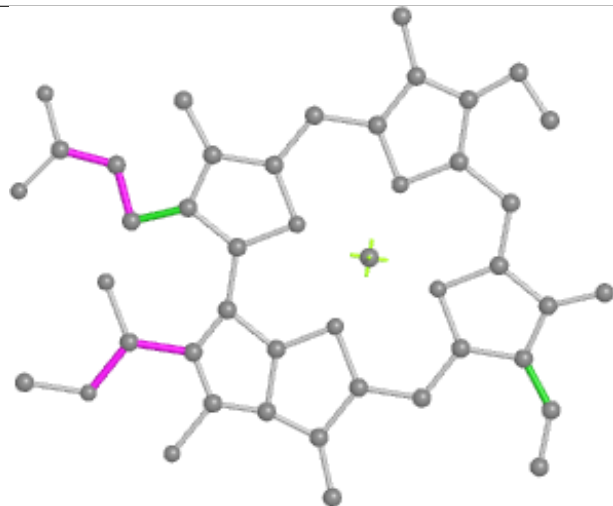
Ligand CHL 3 606



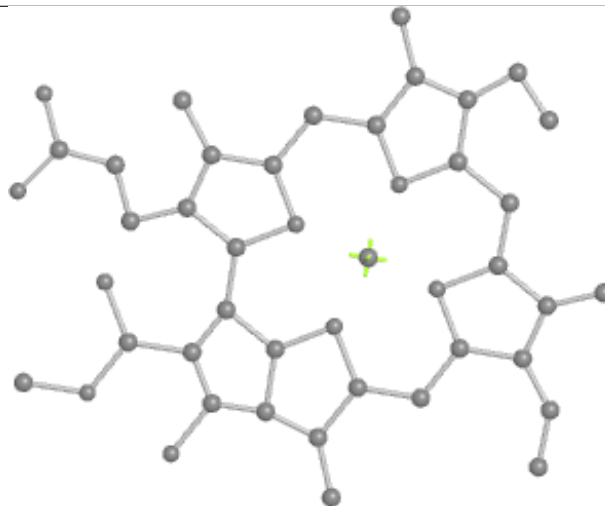
Bond lengths



Bond angles

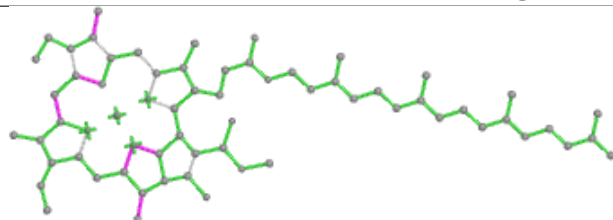


Torsions

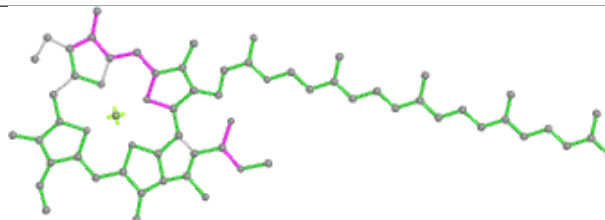


Rings

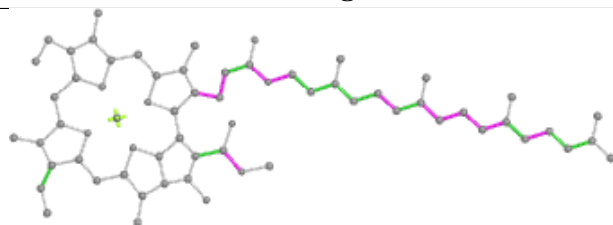
Ligand CLA A 820



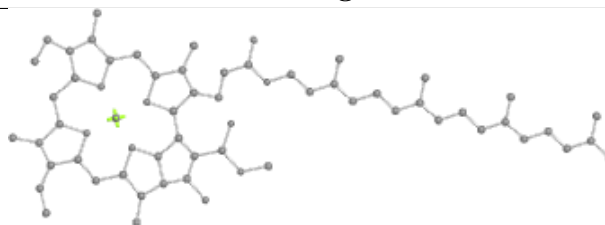
Bond lengths



Bond angles

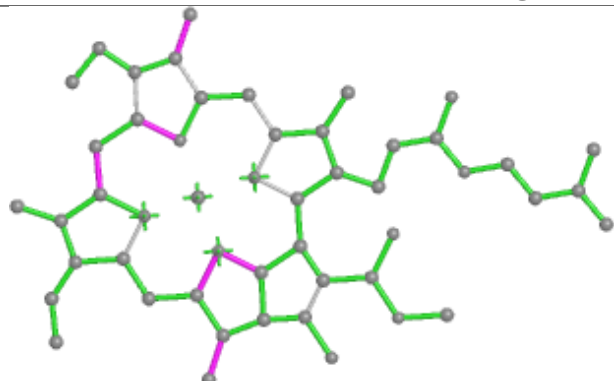


Torsions

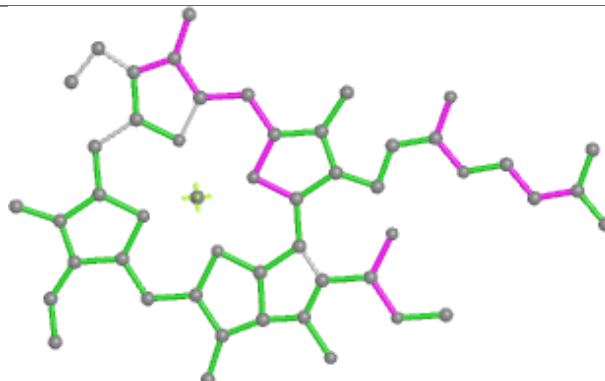


Rings

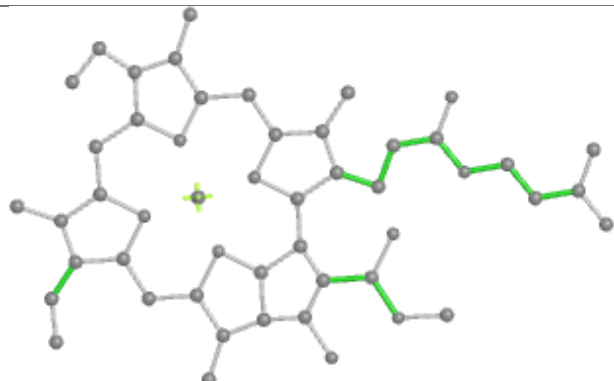
Ligand CLA A 808



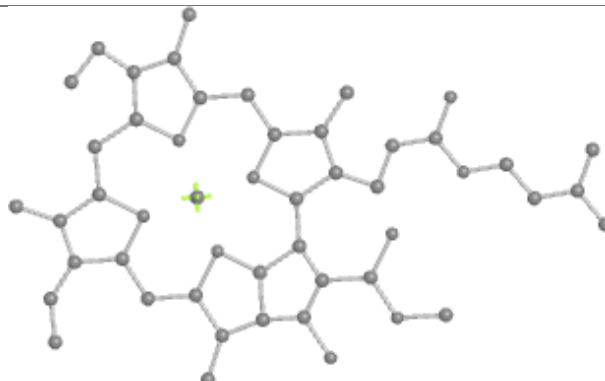
Bond lengths



Bond angles

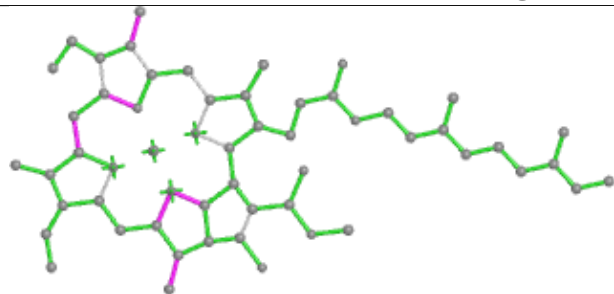


Torsions

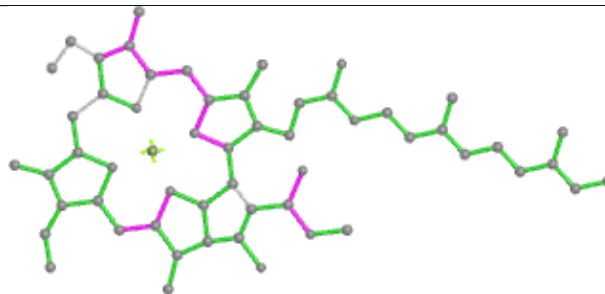


Rings

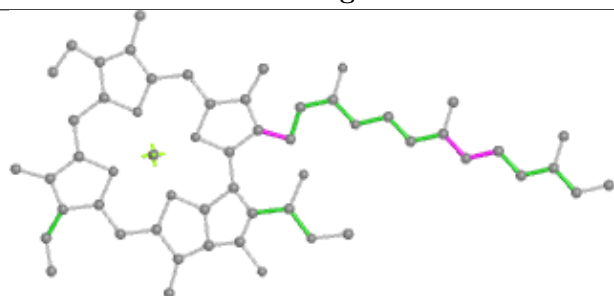
Ligand CLA A 833



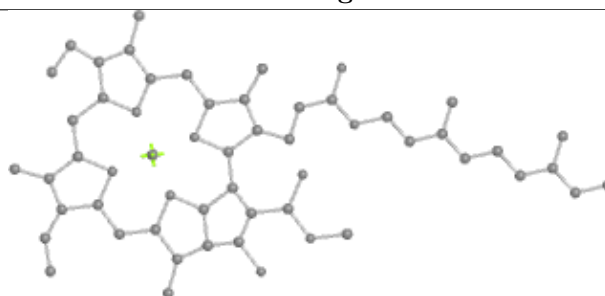
Bond lengths



Bond angles

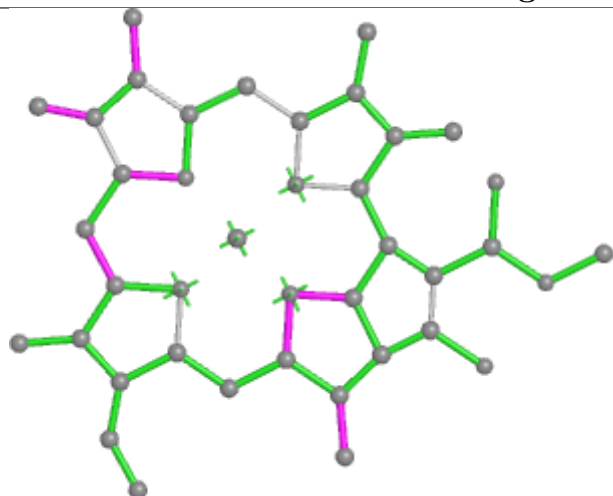


Torsions

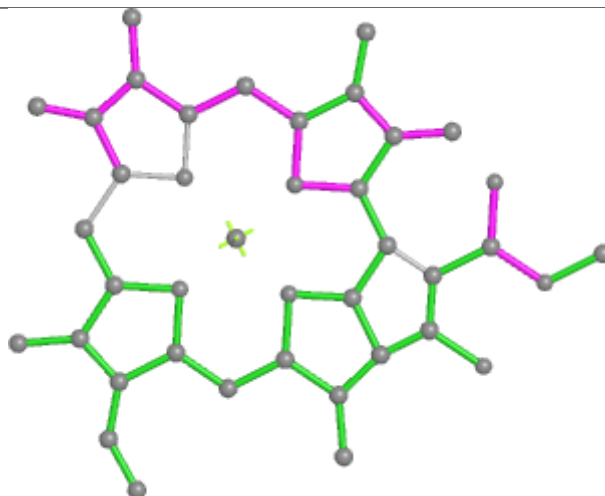


Rings

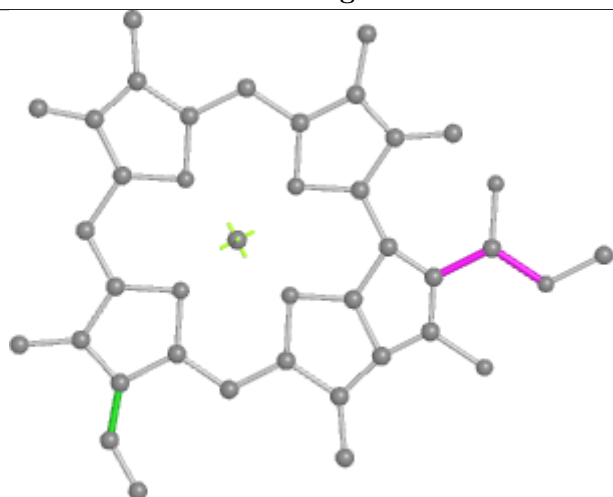
Ligand CLA 1 608



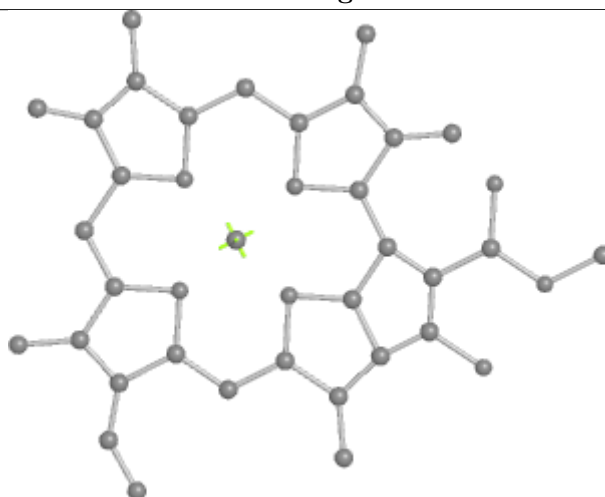
Bond lengths



Bond angles

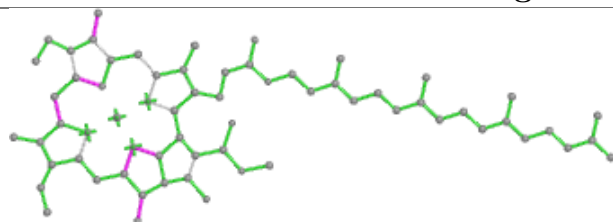


Torsions

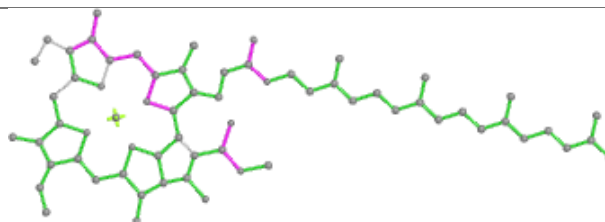


Rings

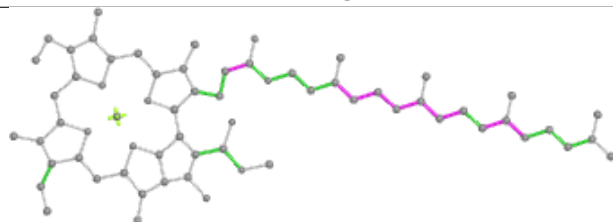
Ligand CLA B 806



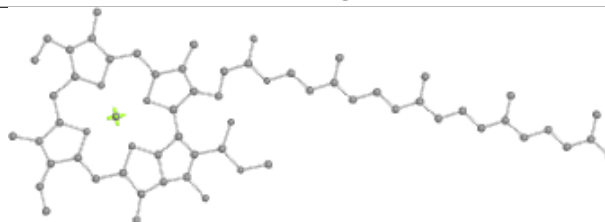
Bond lengths



Bond angles

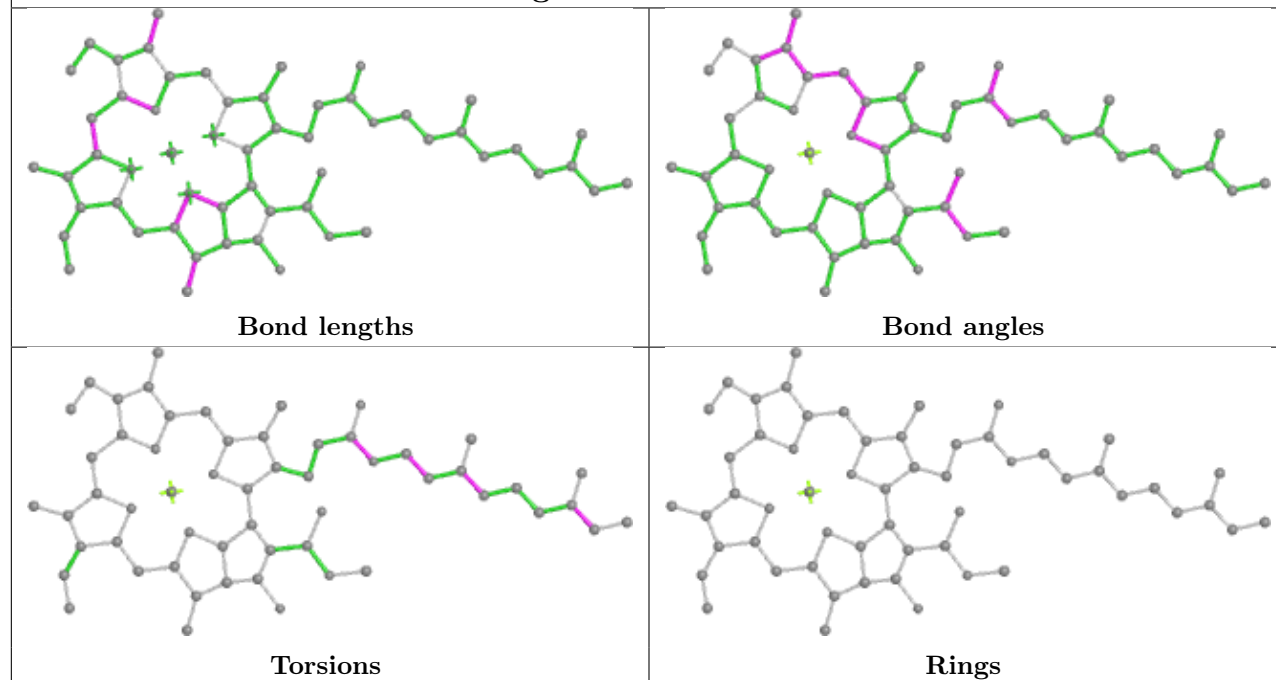


Torsions

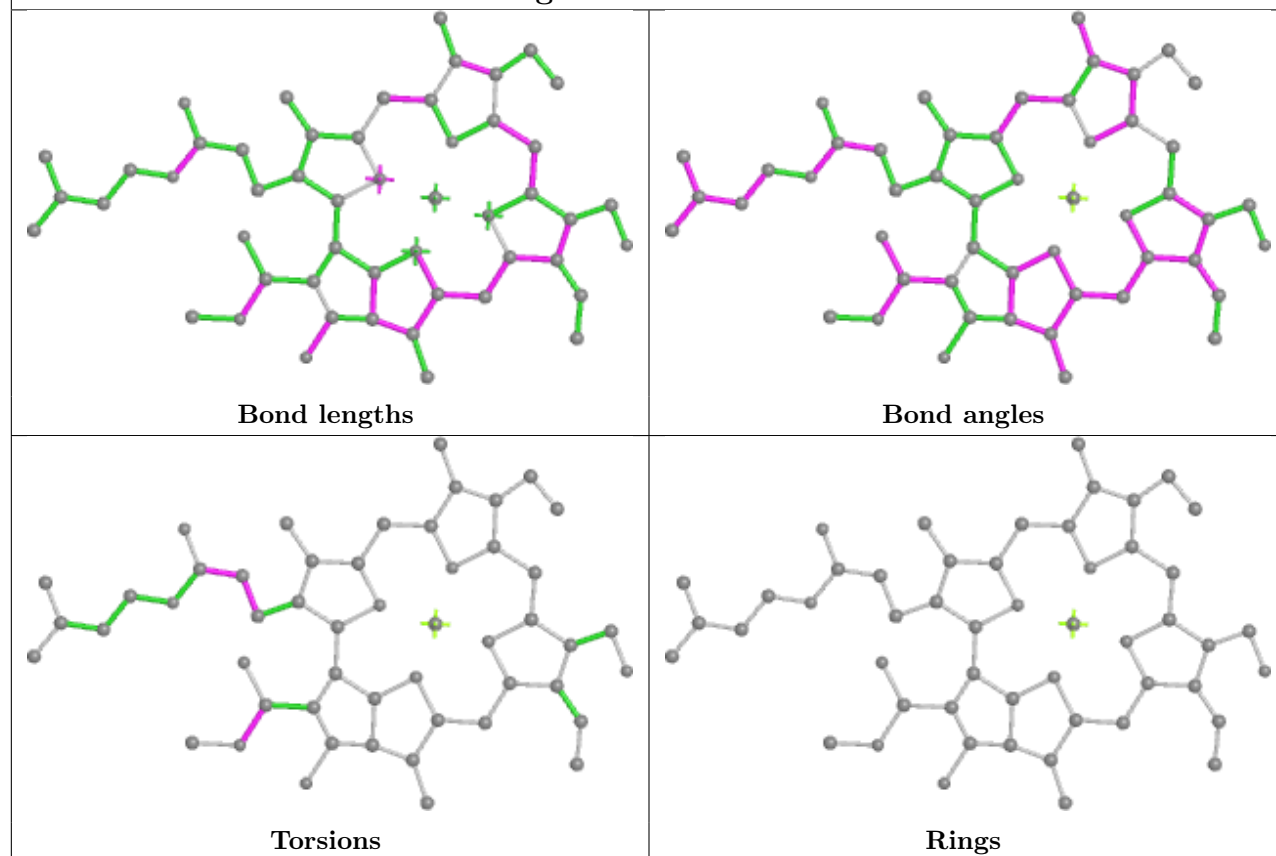


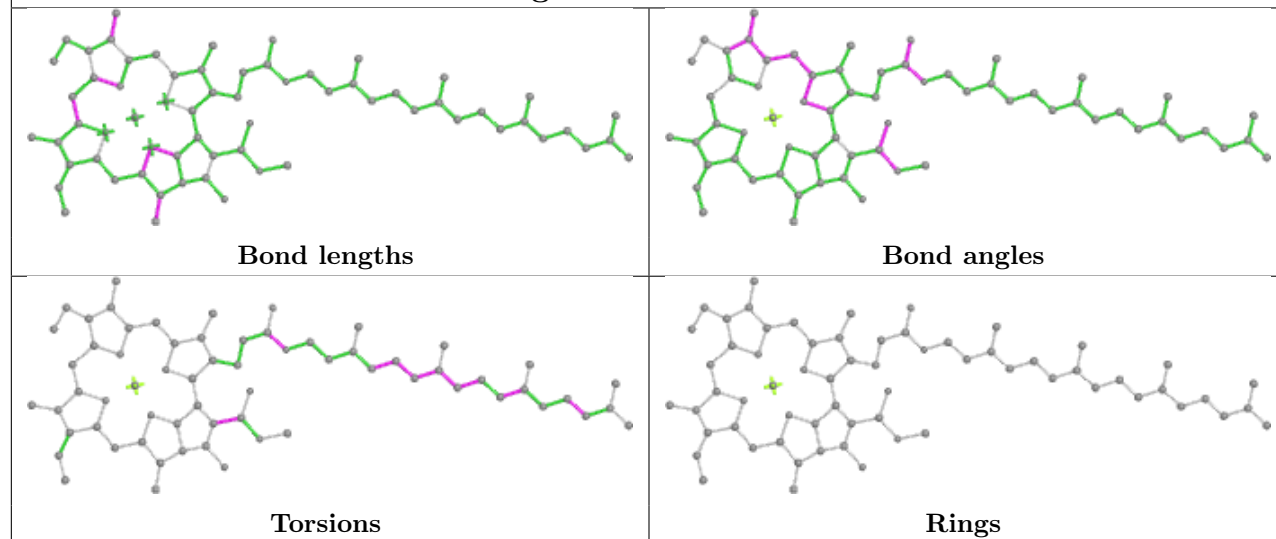
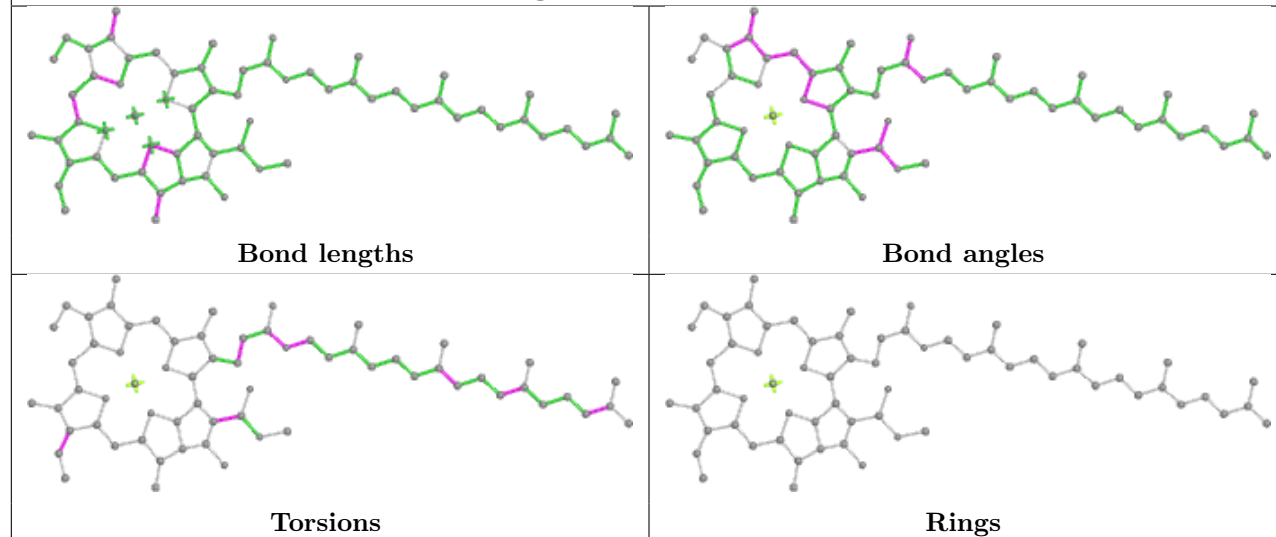
Rings

Ligand CLA B 829

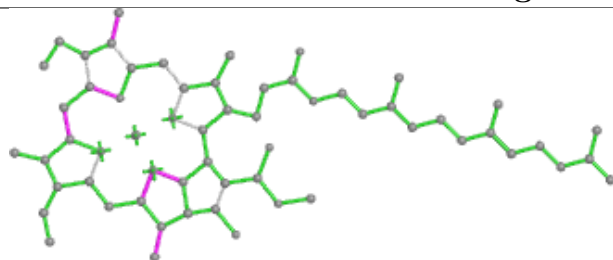


Ligand CHL 2 607

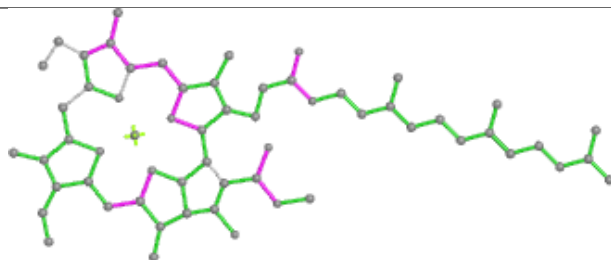


Ligand CLA A 826**Ligand CLA A 809**

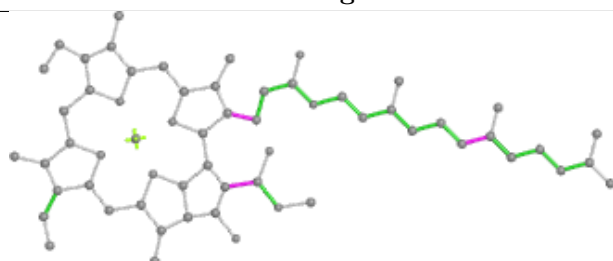
Ligand CLA B 834



Bond lengths



Bond angles

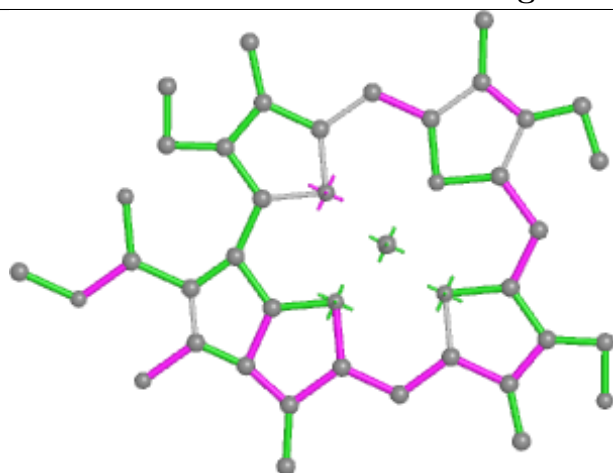


Torsions

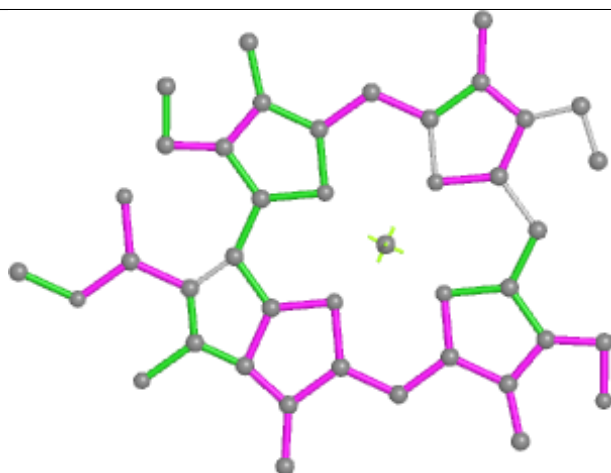


Rings

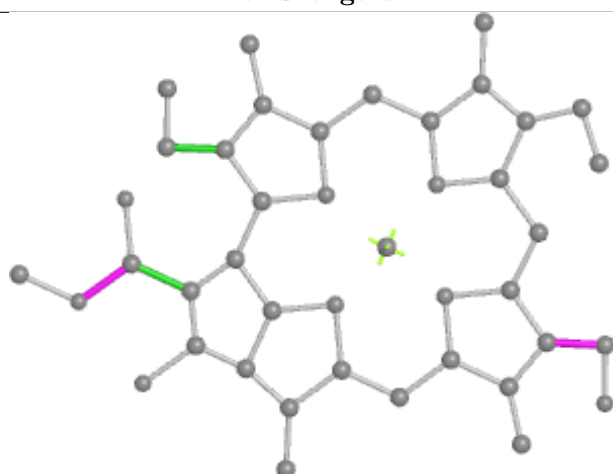
Ligand CHL 2 605



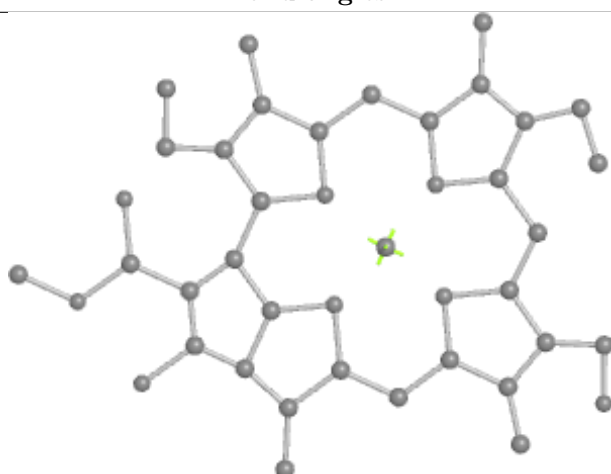
Bond lengths



Bond angles

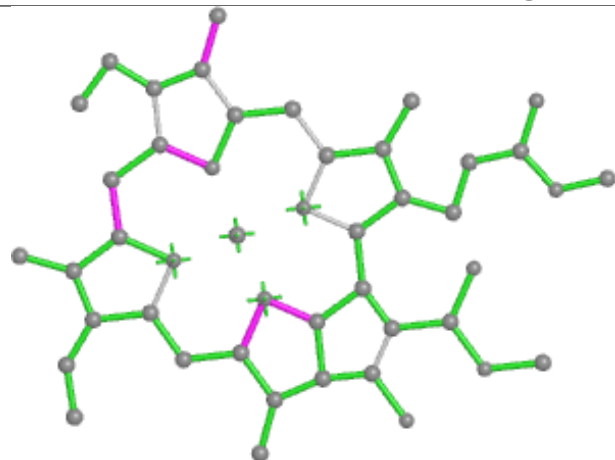


Torsions

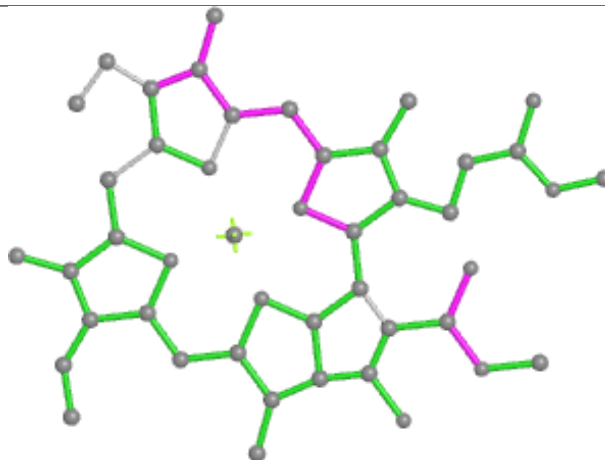


Rings

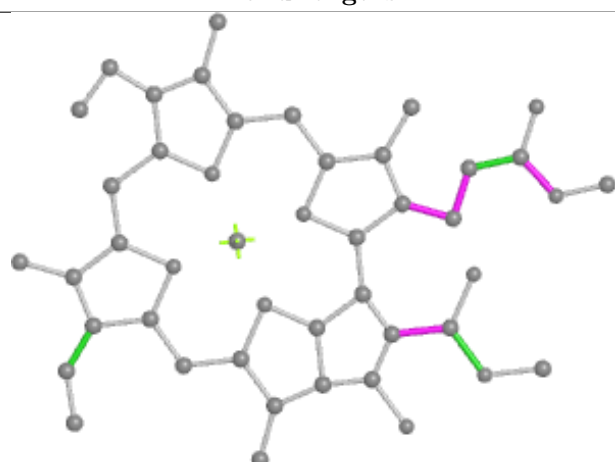
Ligand CLA 1 612



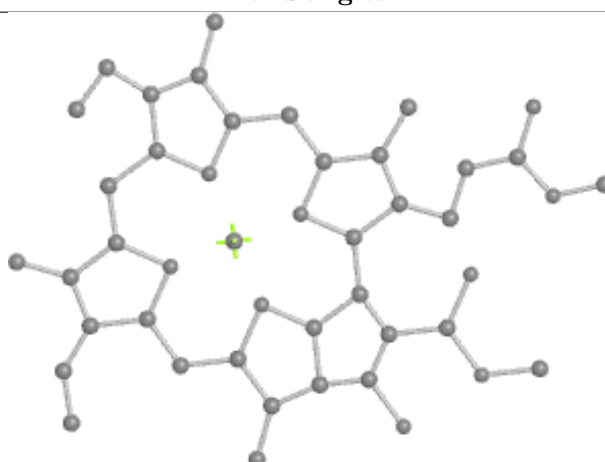
Bond lengths



Bond angles

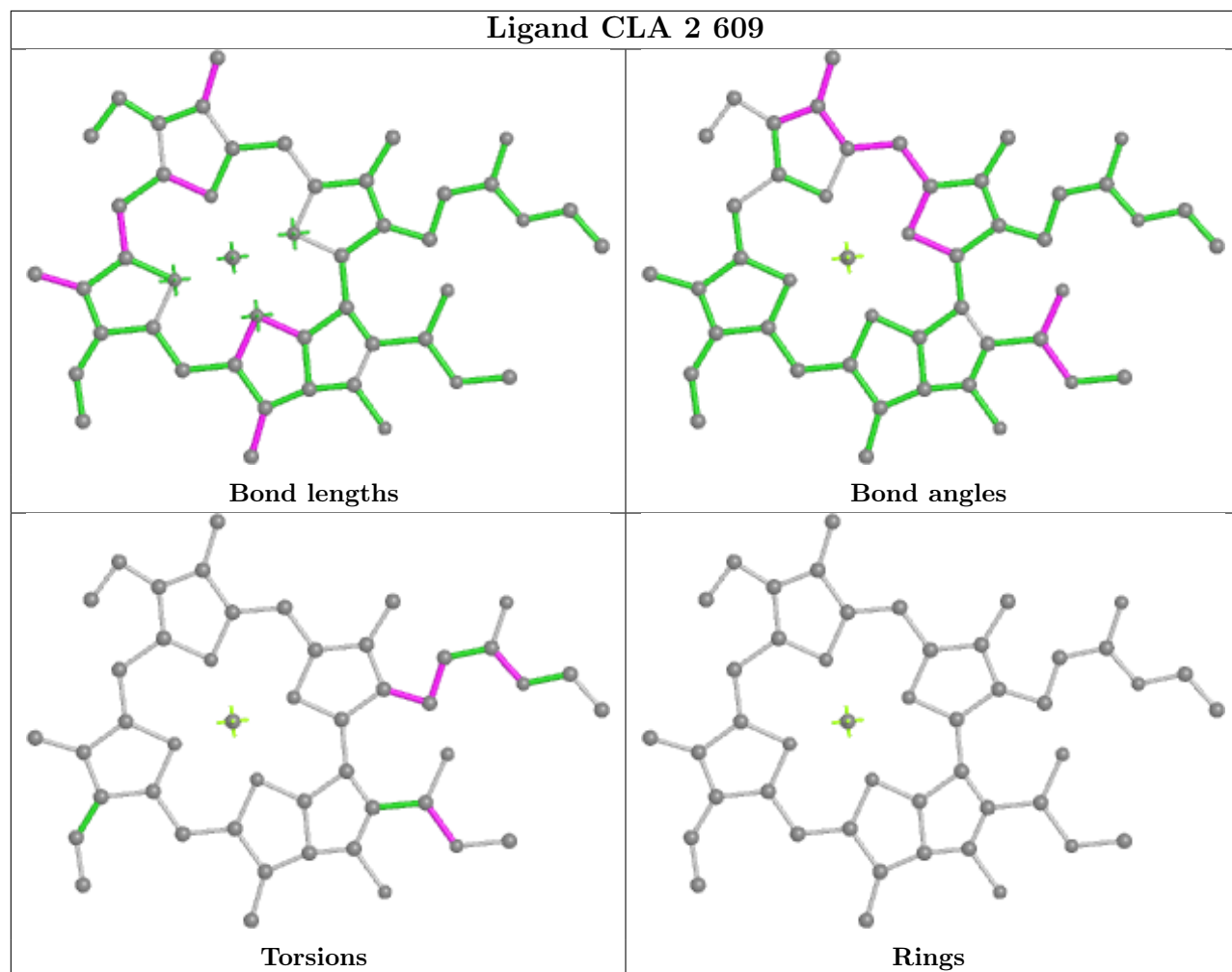


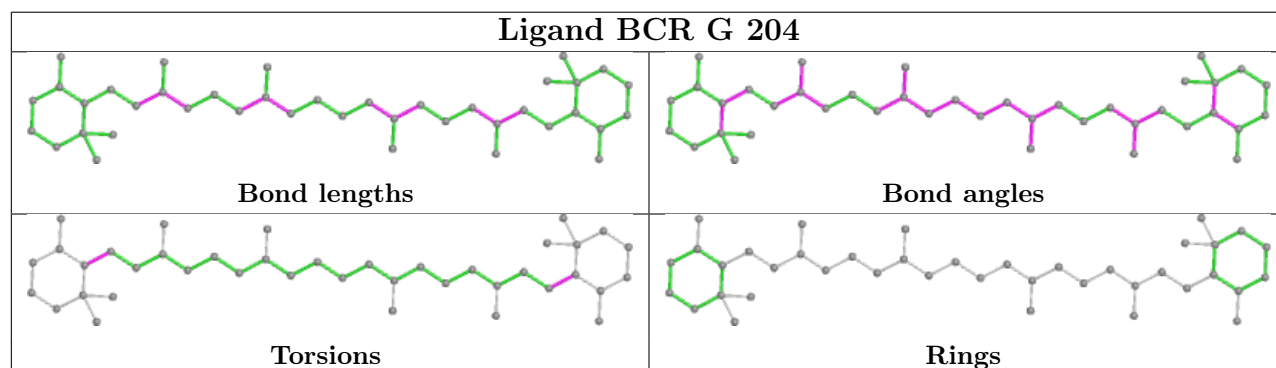
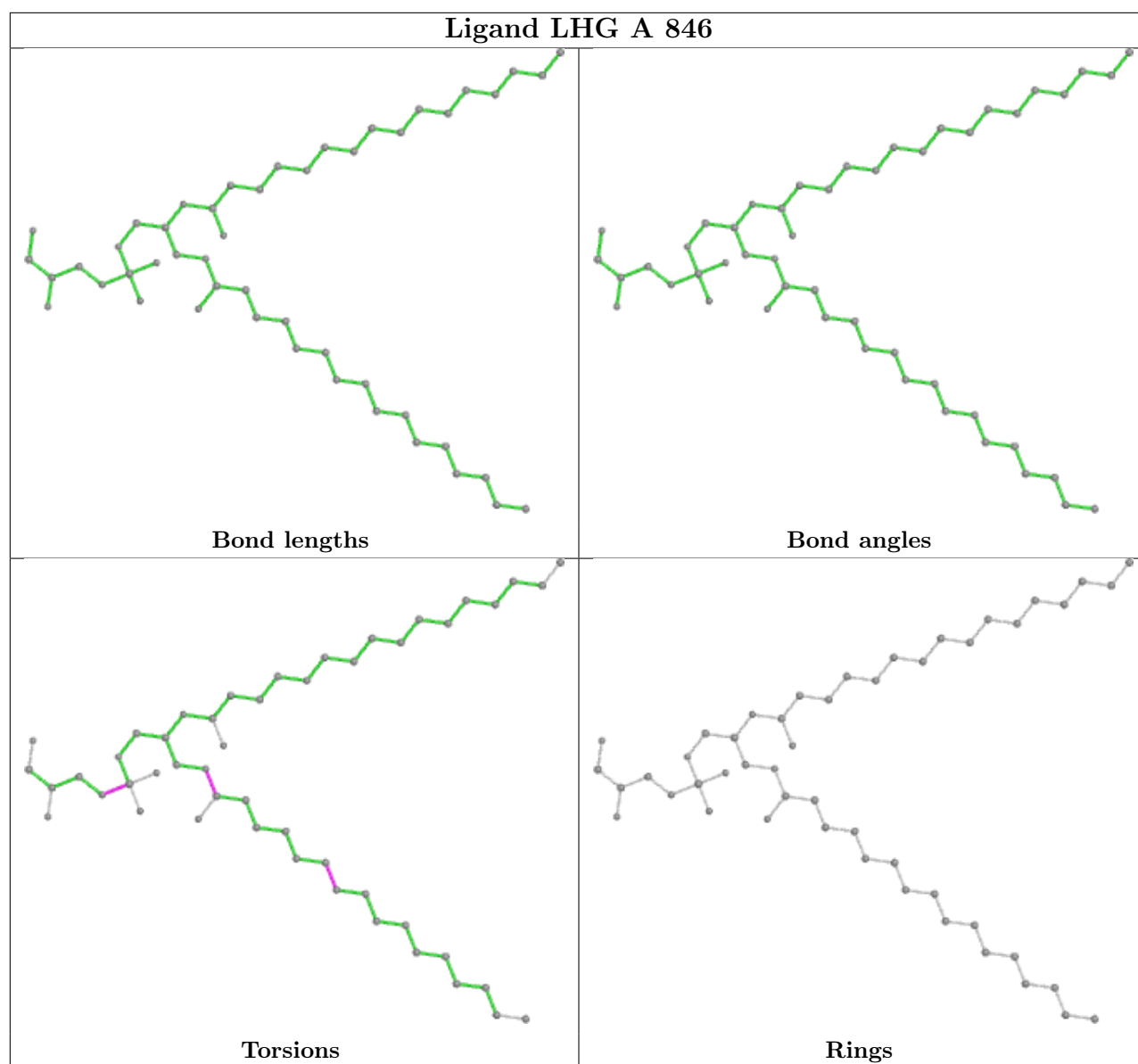
Torsions

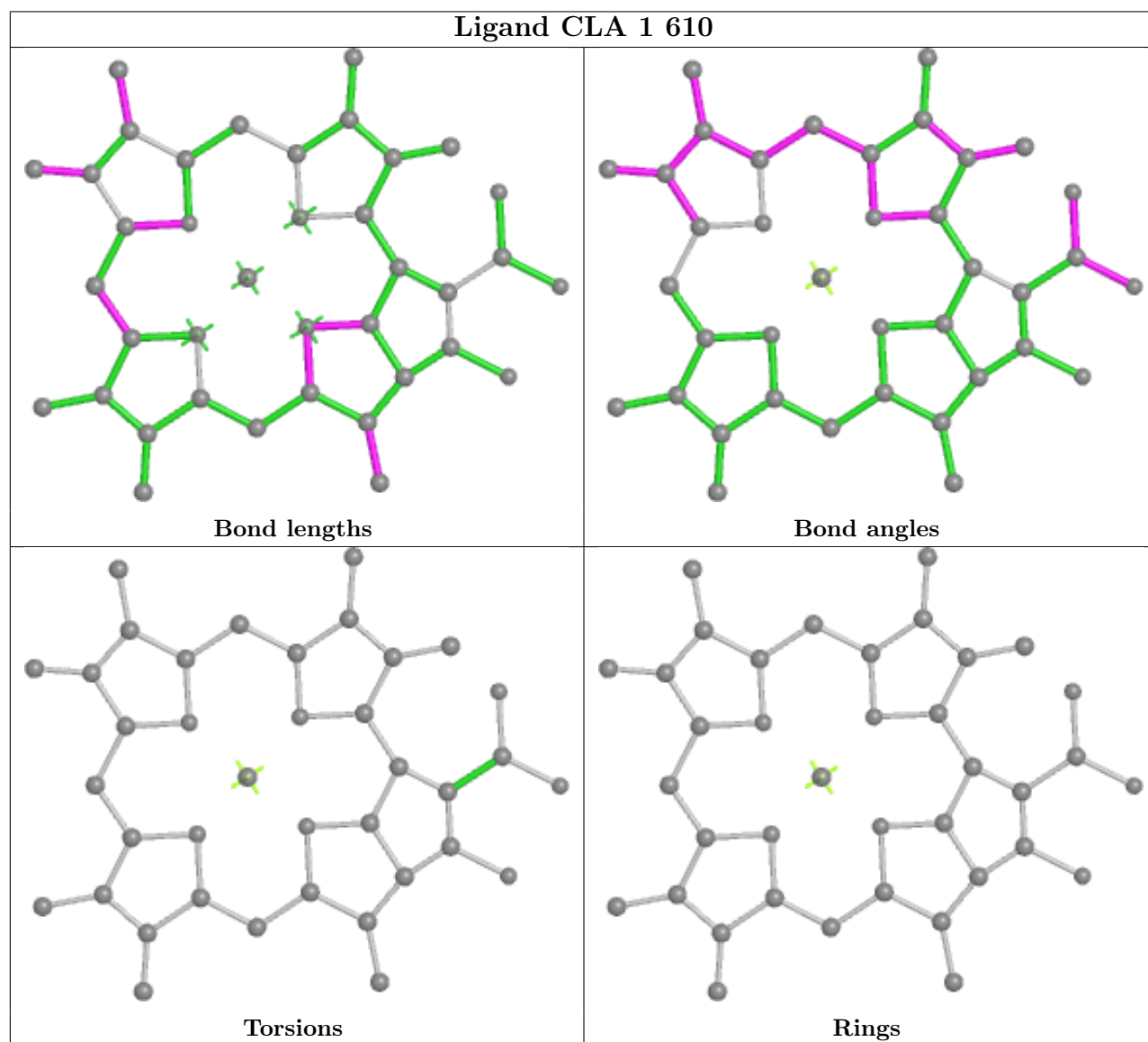
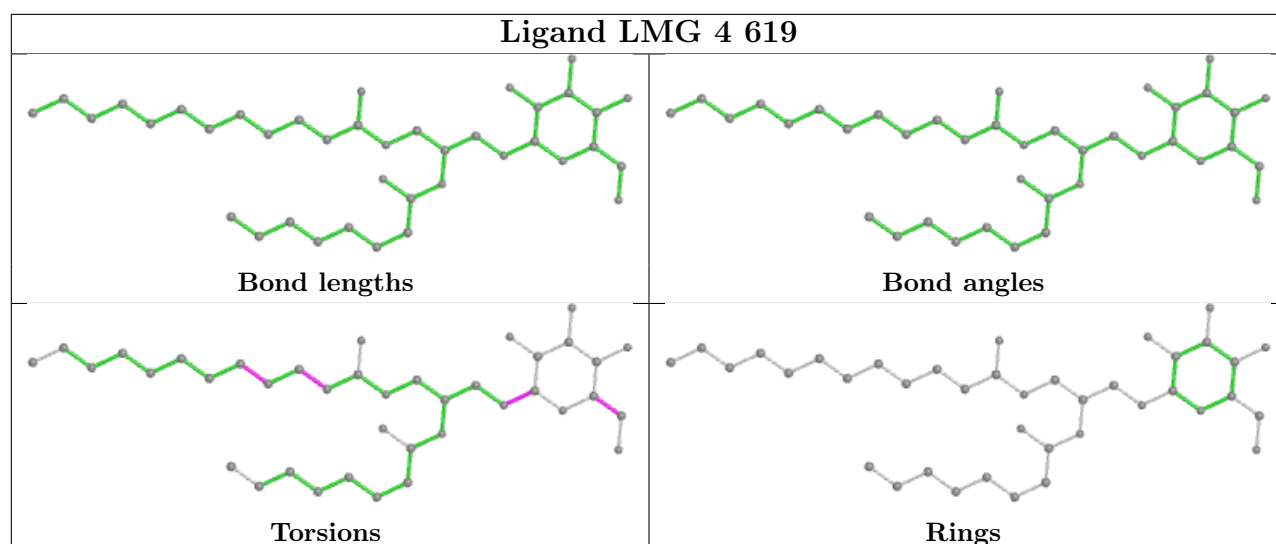


Rings

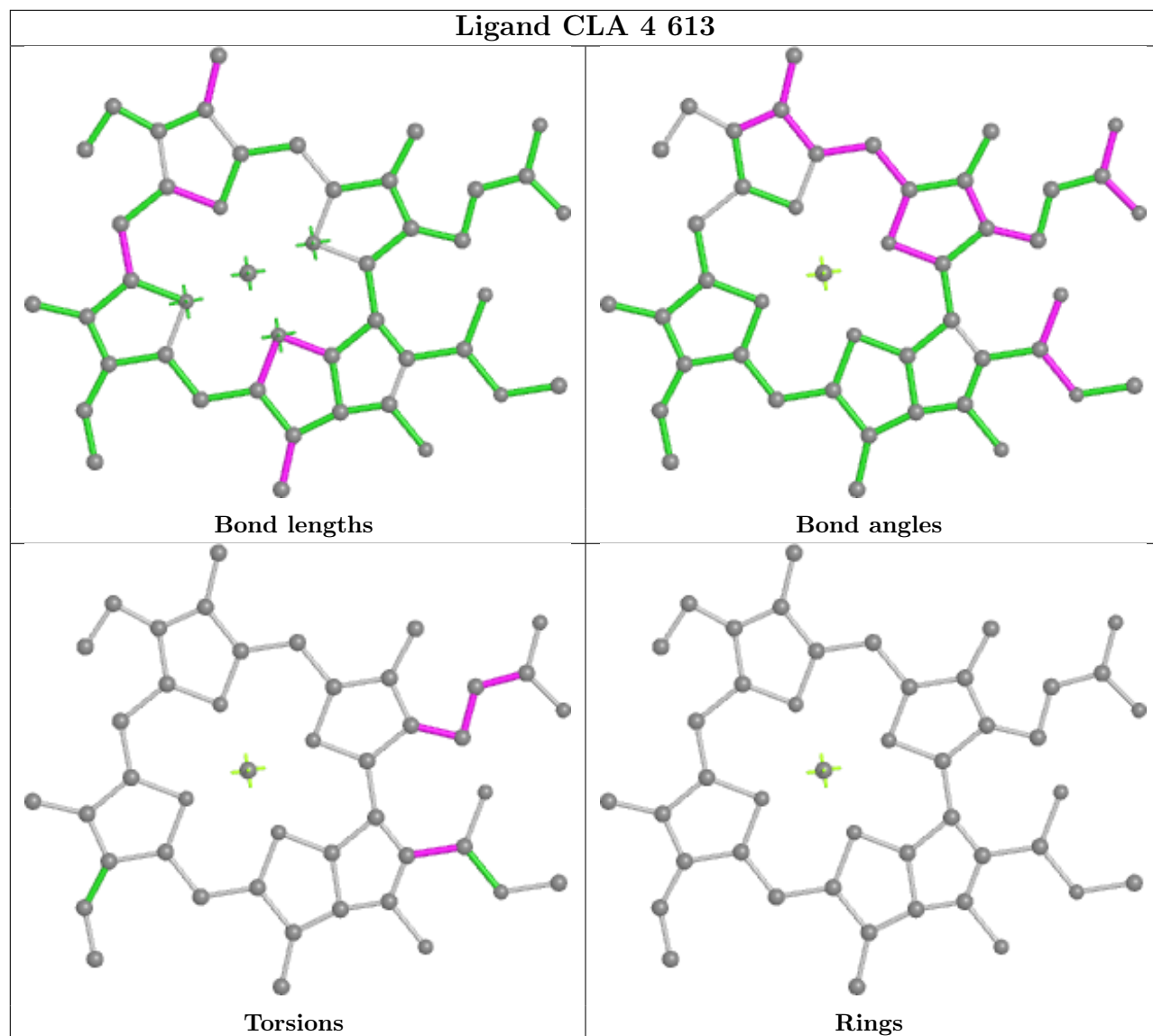
Ligand CLA 2 609



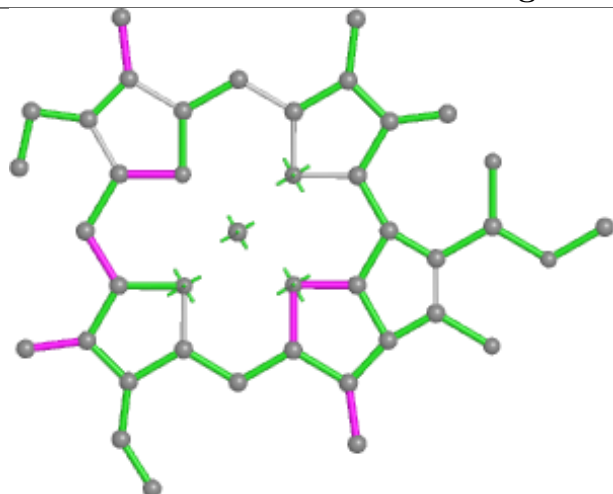




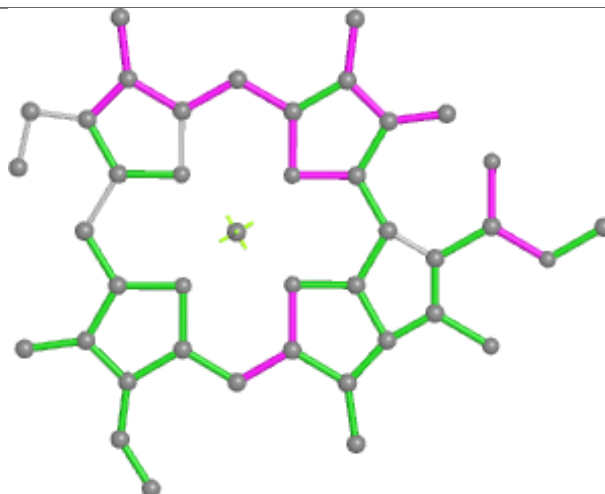
Ligand CLA 4 613



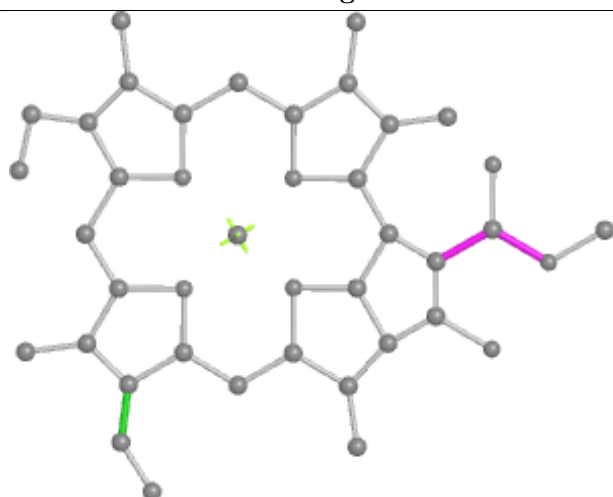
Ligand CLA 3 608



Bond lengths



Bond angles

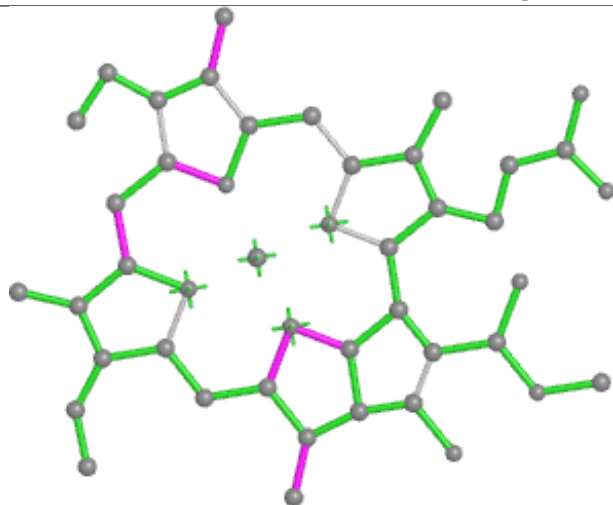


Torsions

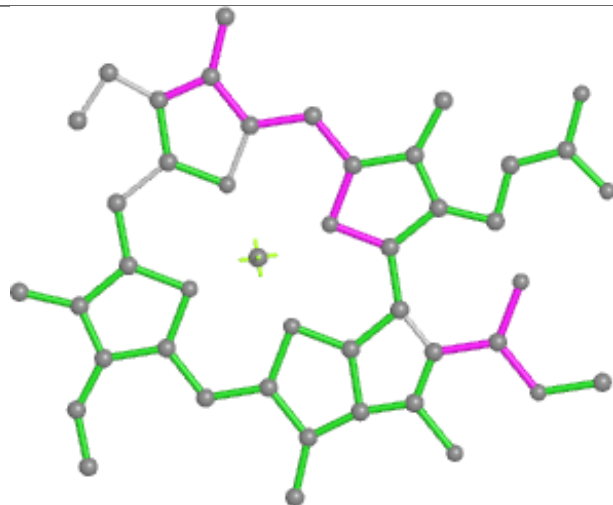


Rings

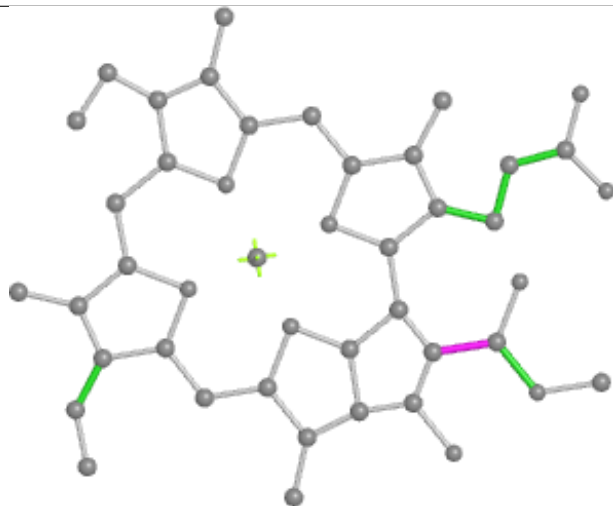
Ligand CLA L 302



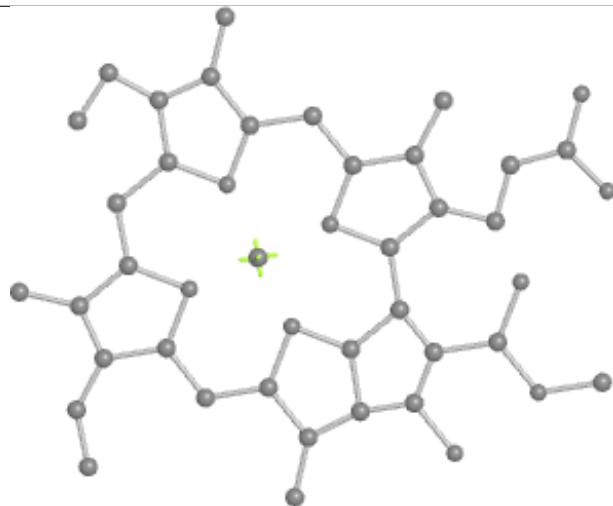
Bond lengths



Bond angles

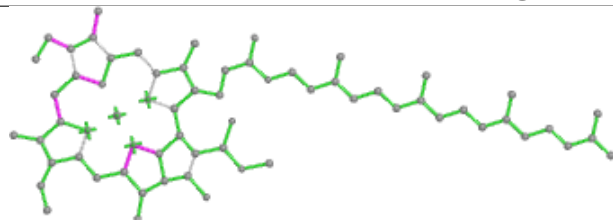


Torsions

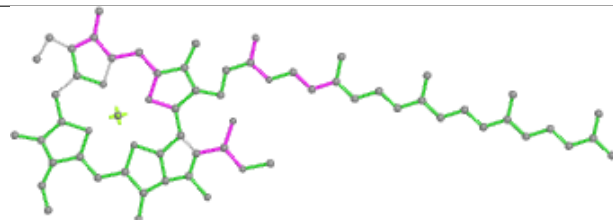


Rings

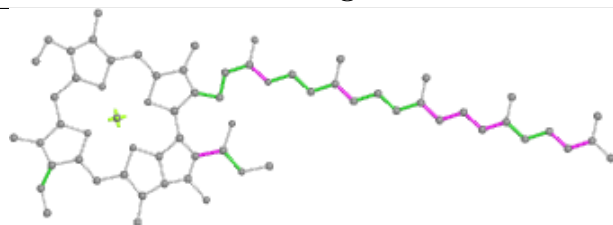
Ligand CLA A 835



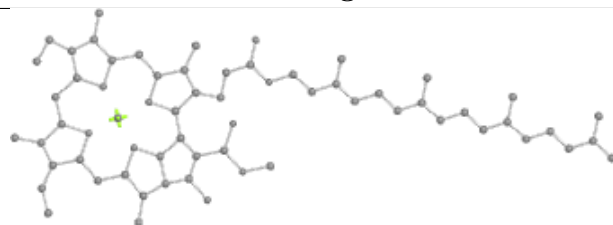
Bond lengths



Bond angles

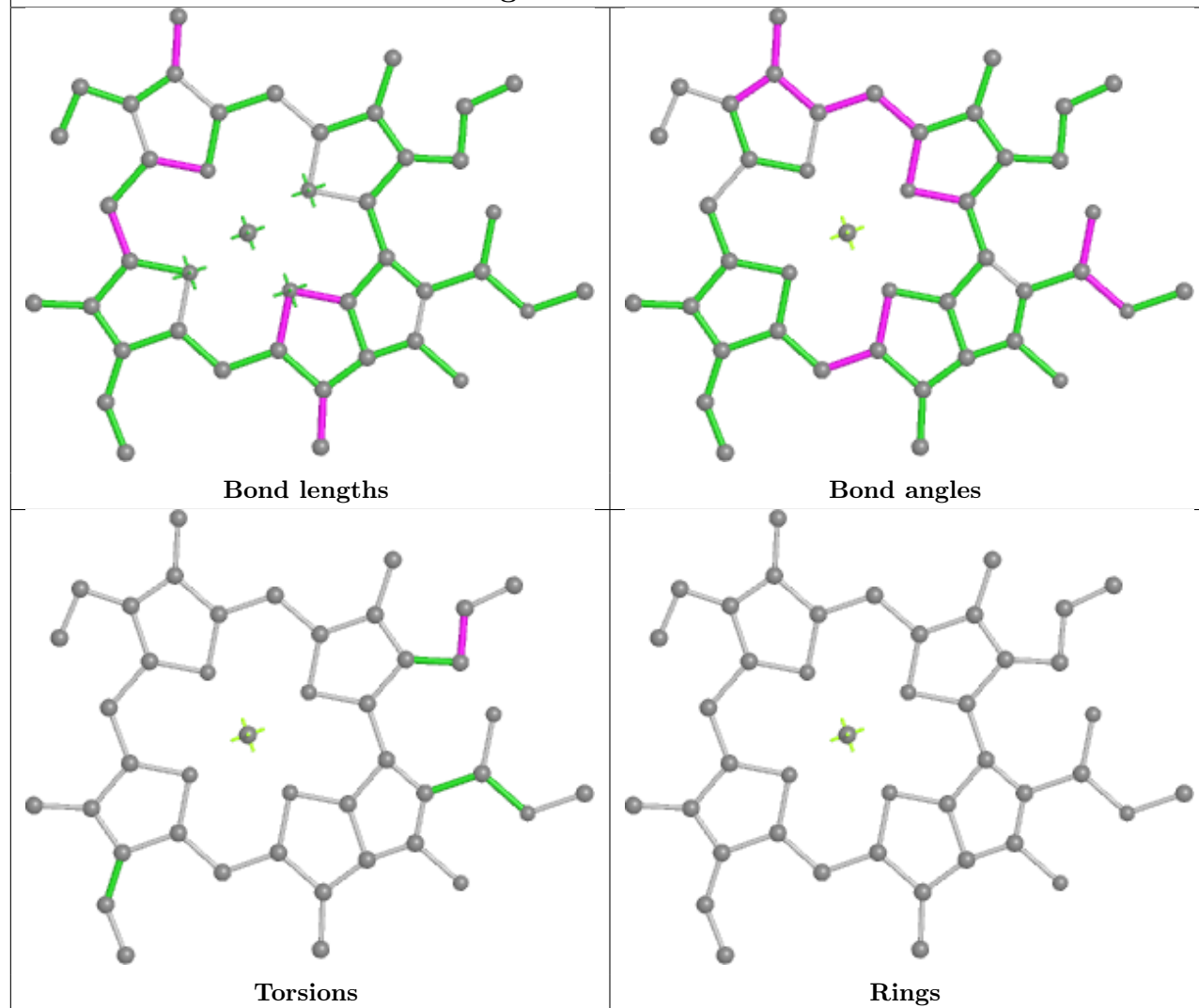


Torsions

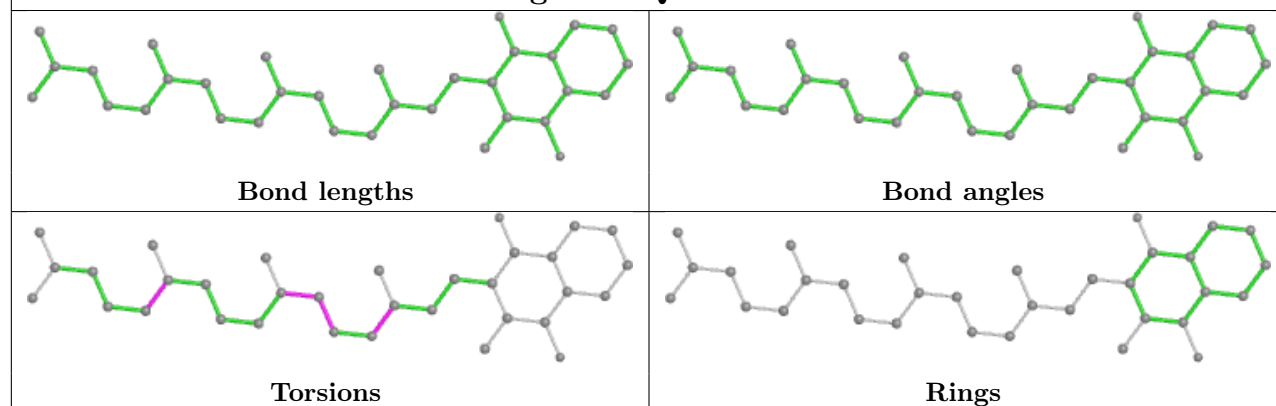


Rings

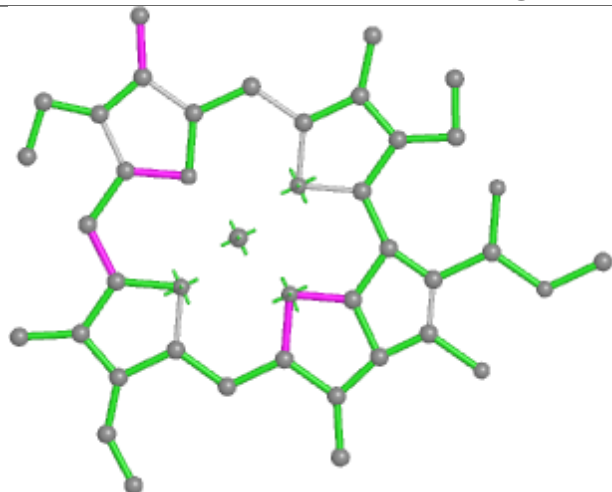
Ligand CLA B 831



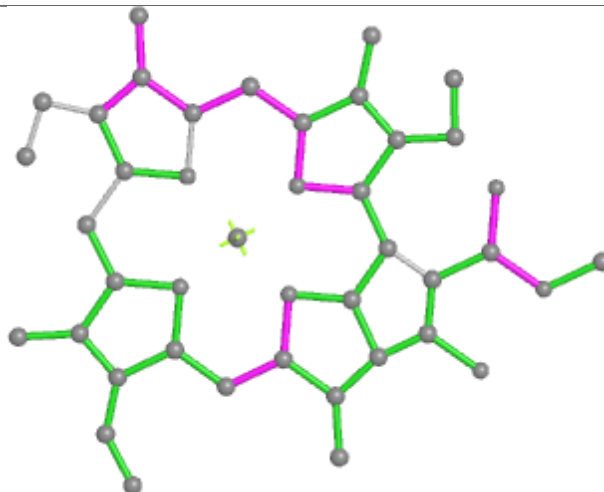
Ligand PQN B 842



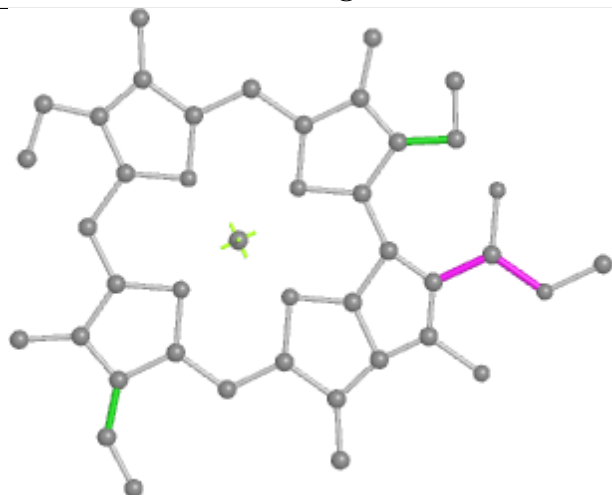
Ligand CLA A 823



Bond lengths



Bond angles

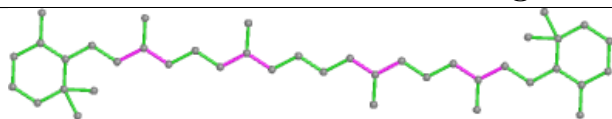


Torsions

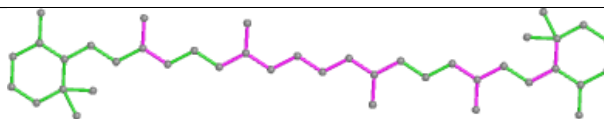


Rings

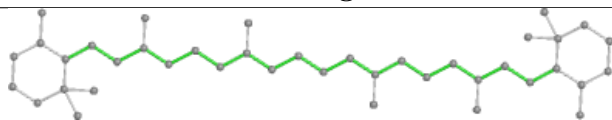
Ligand BCR B 848



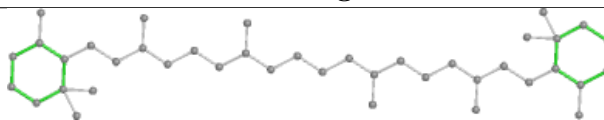
Bond lengths



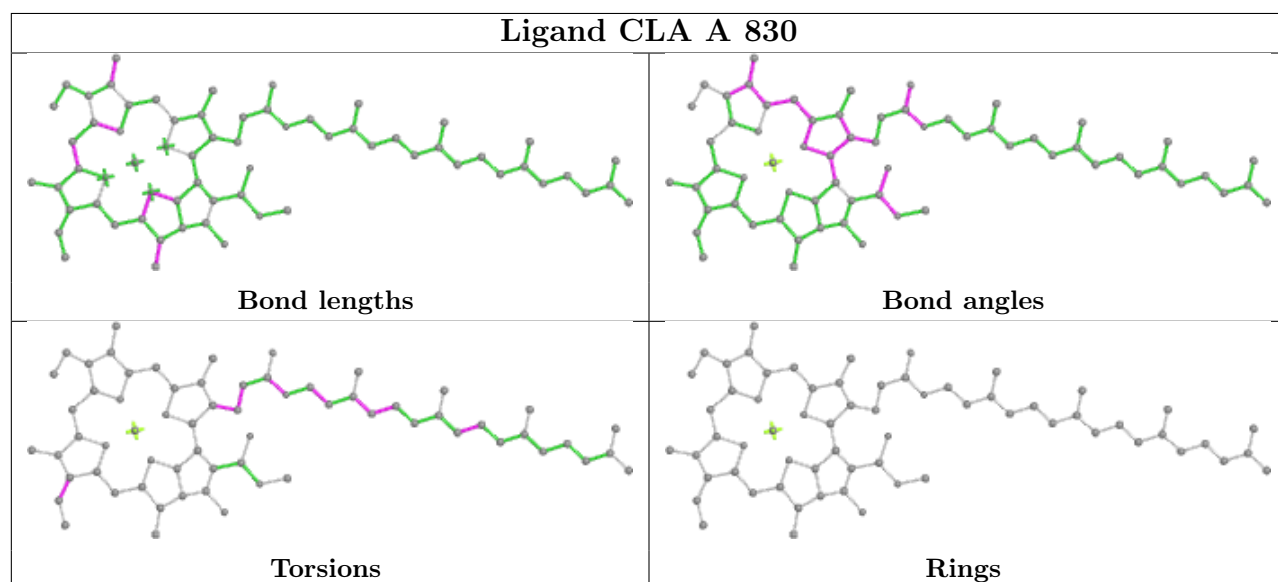
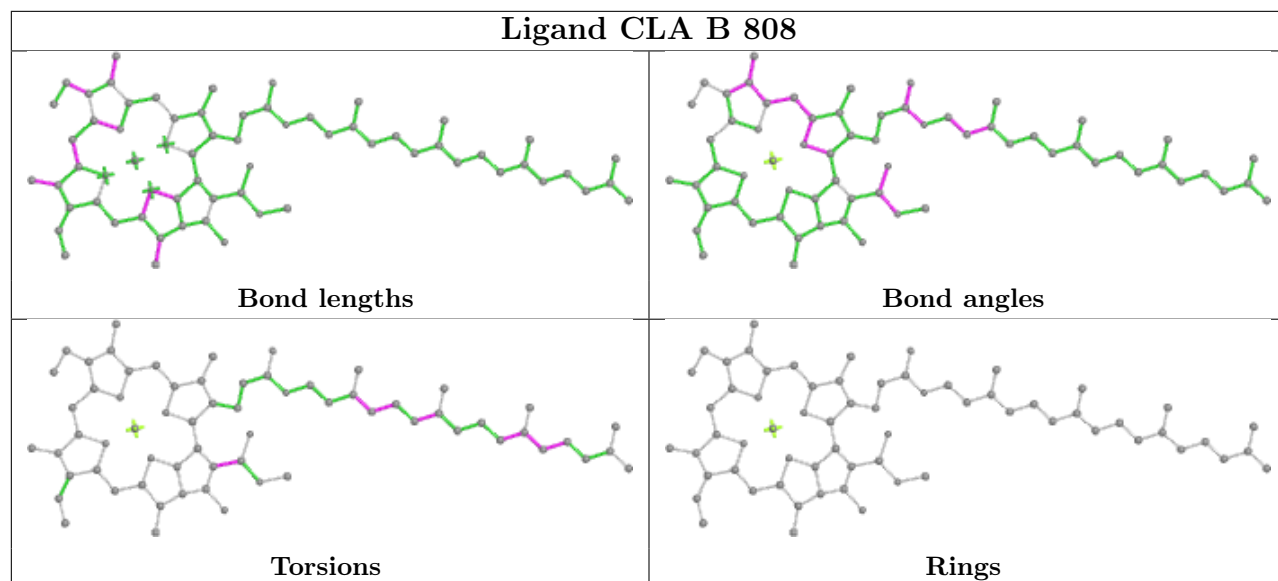
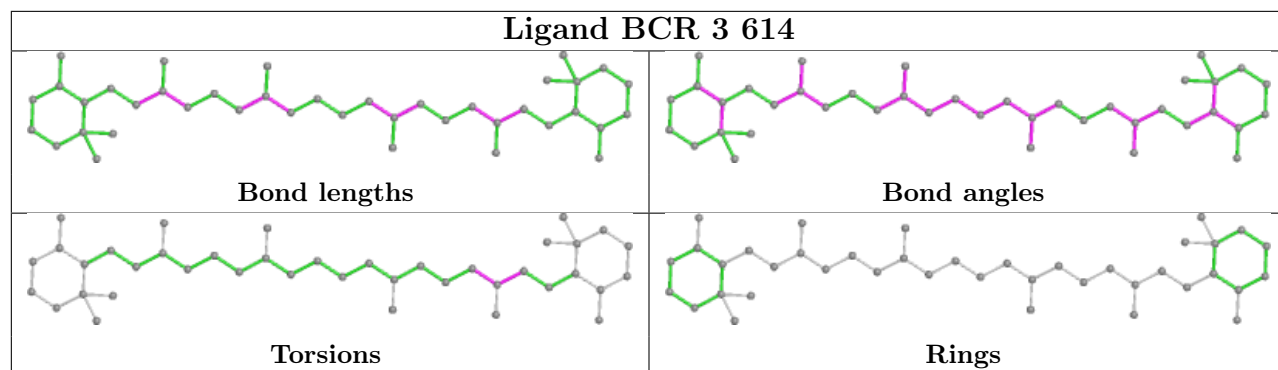
Bond angles



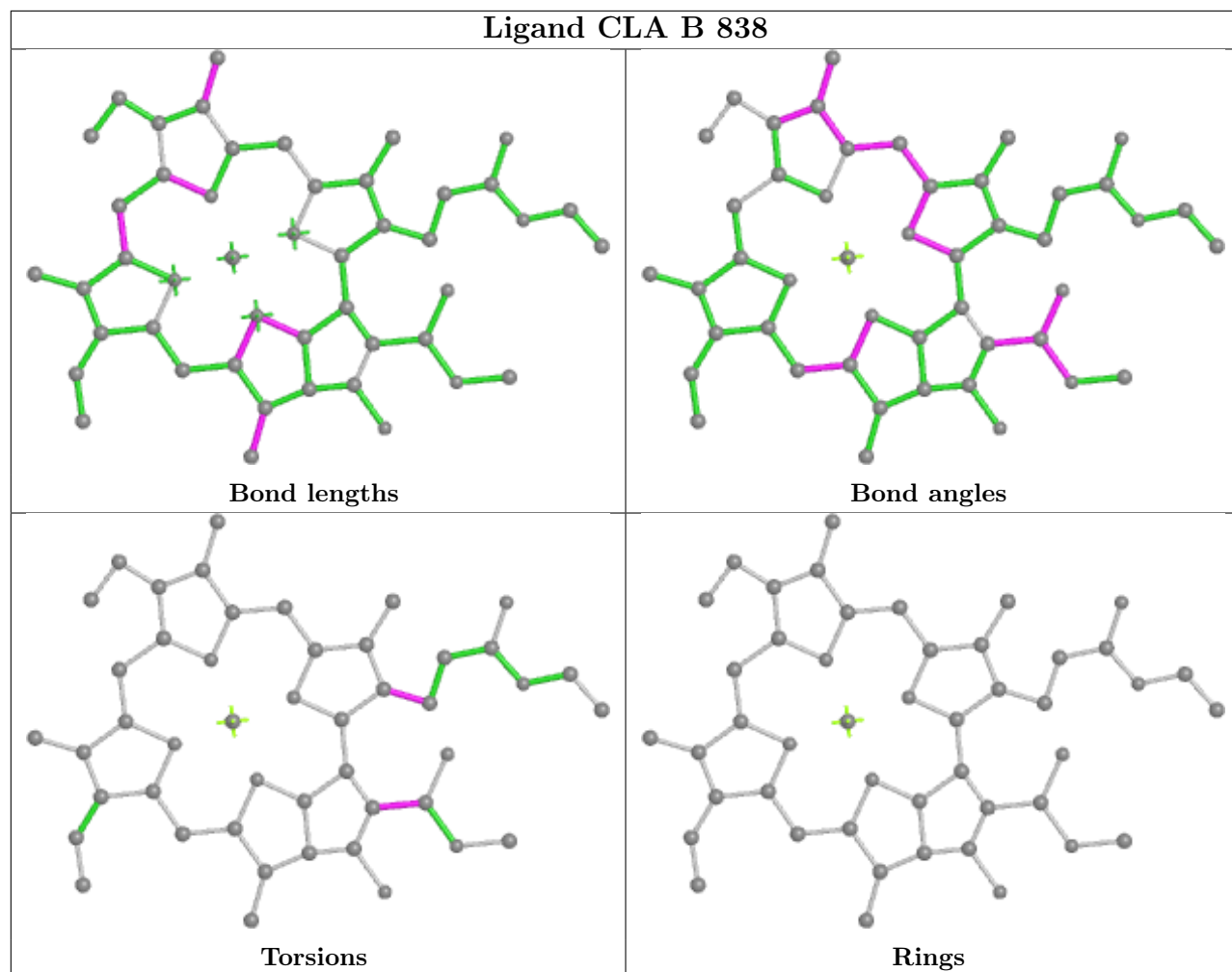
Torsions



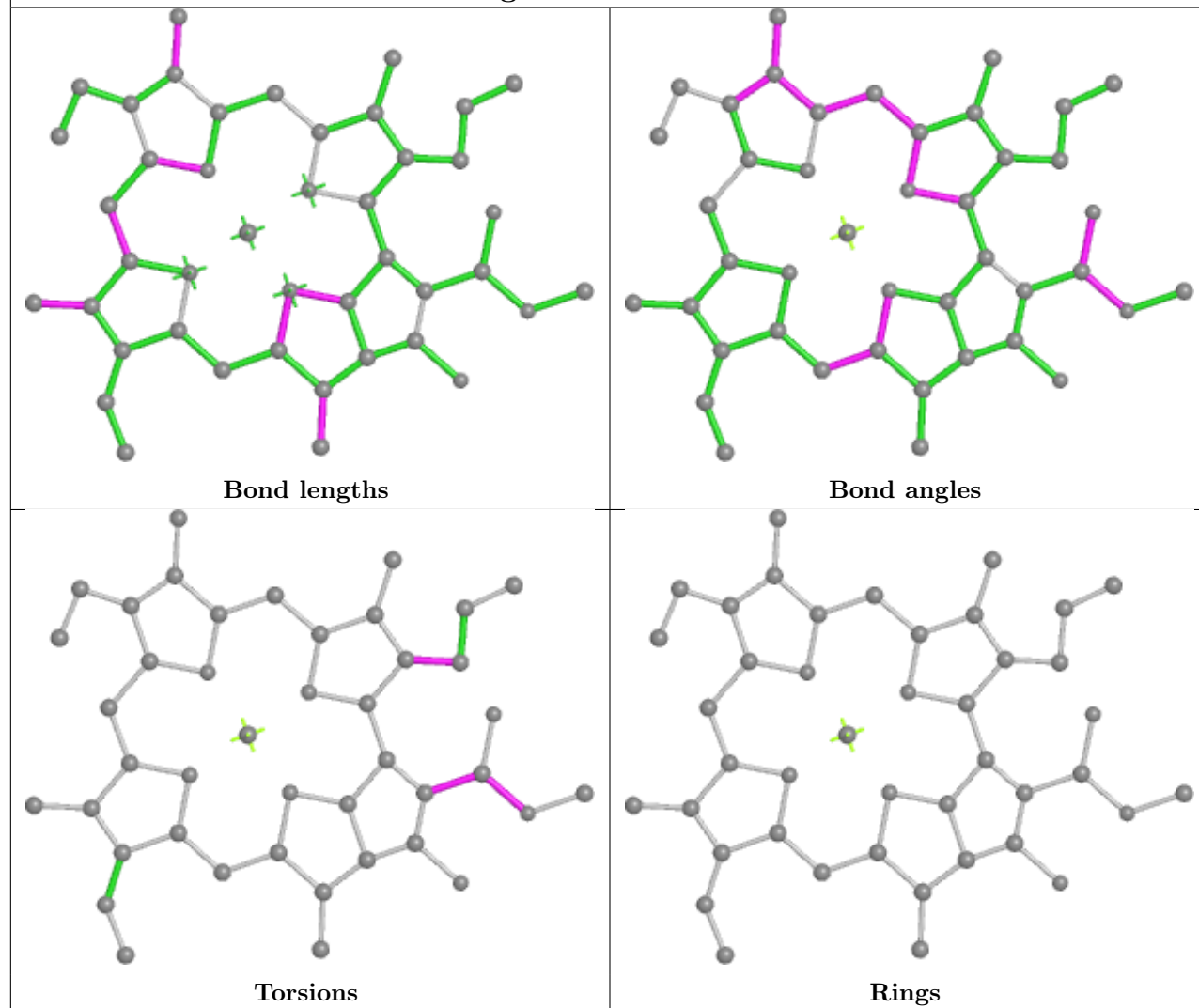
Rings



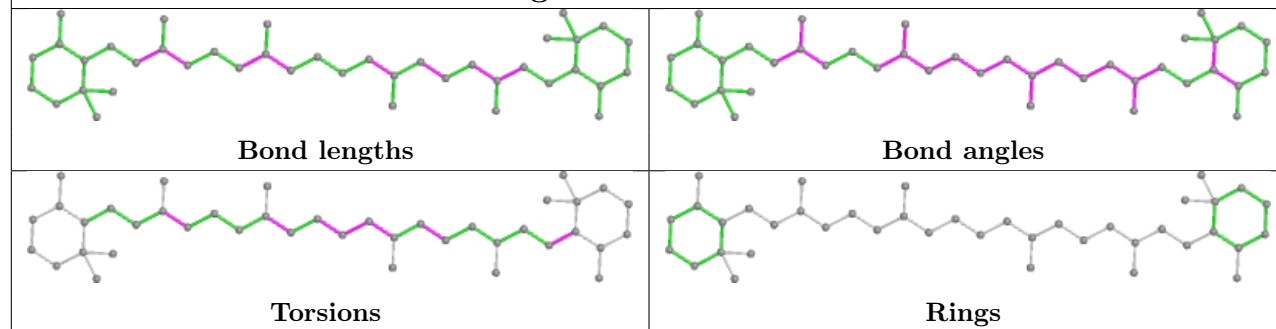
Ligand CLA B 838

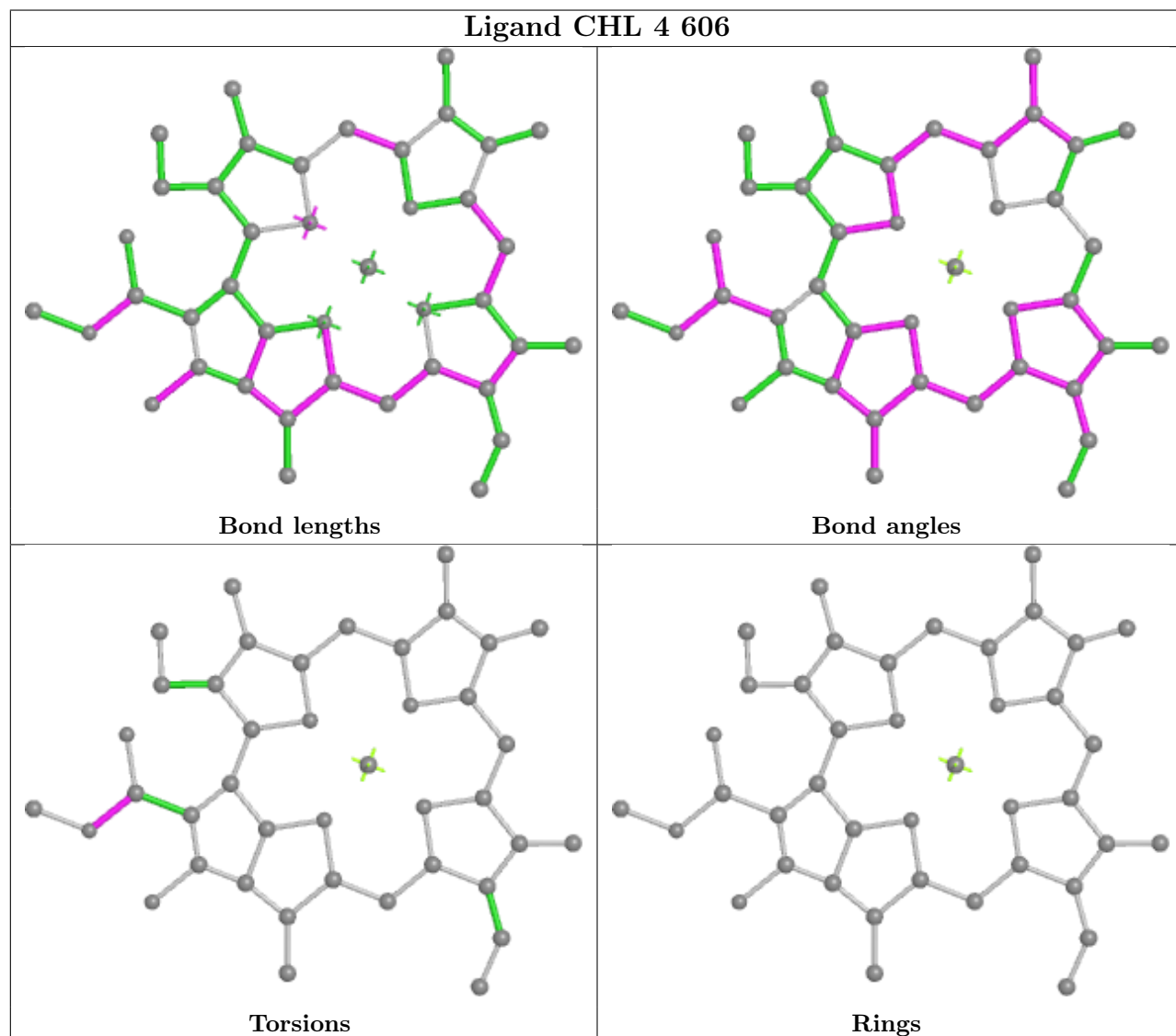
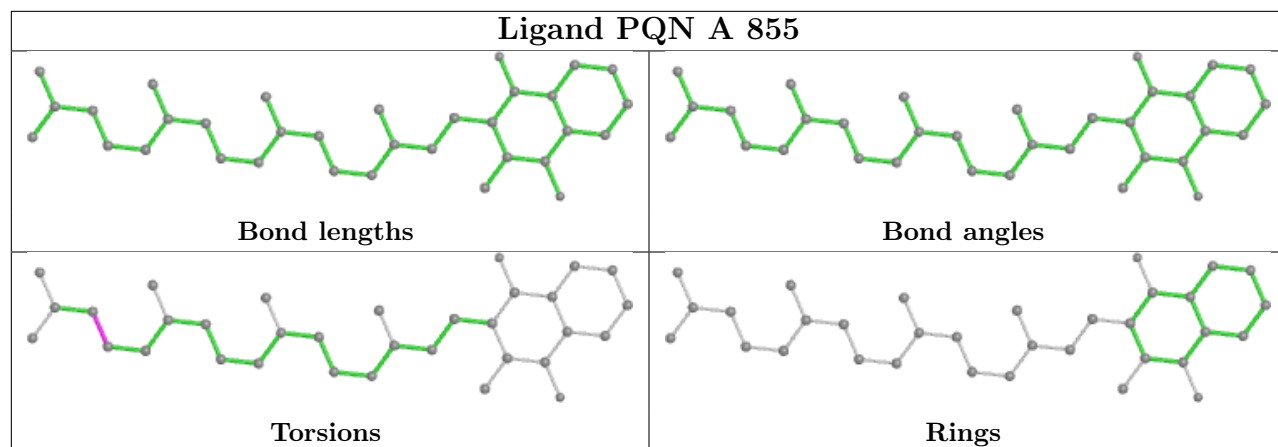


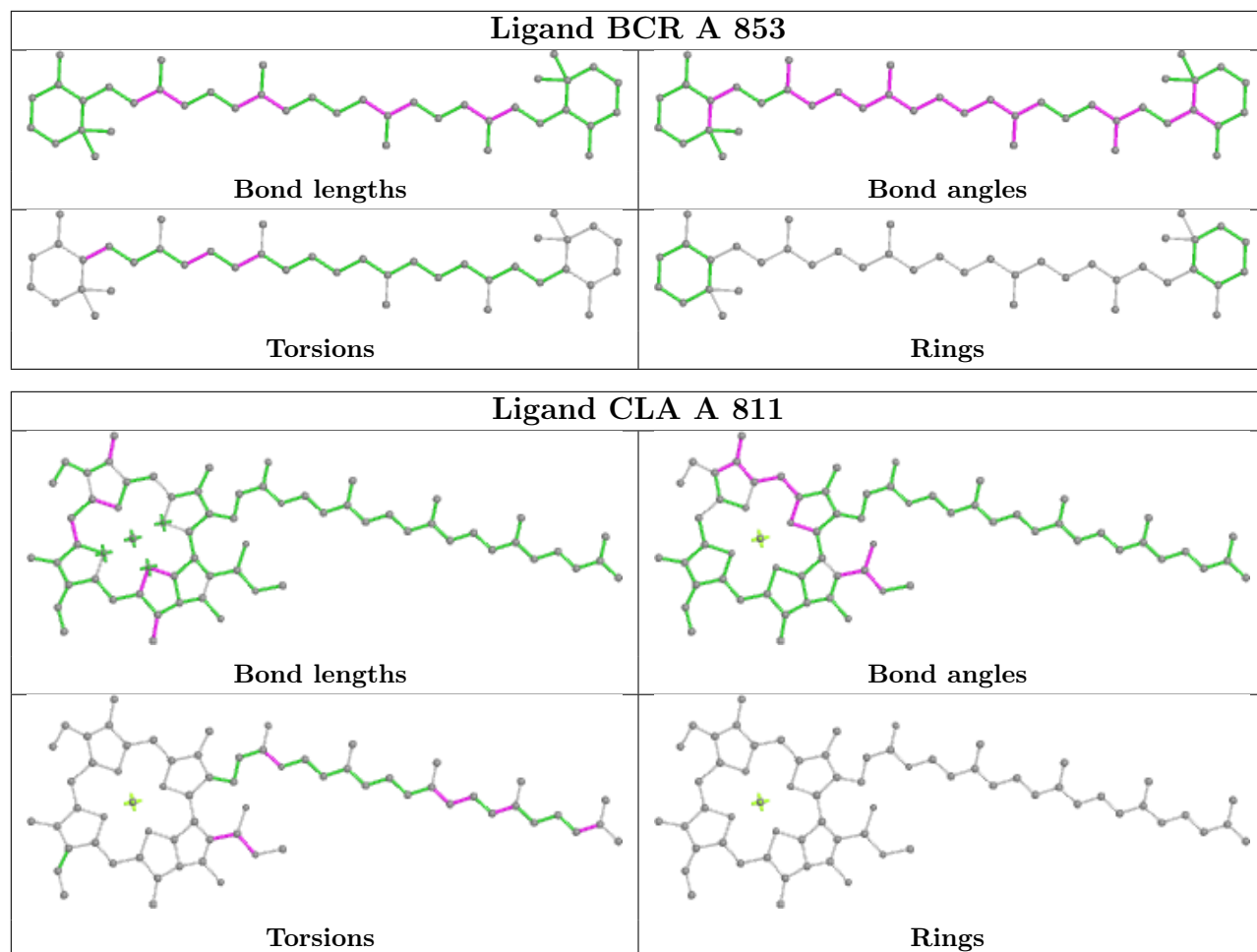
Ligand CLA B 815



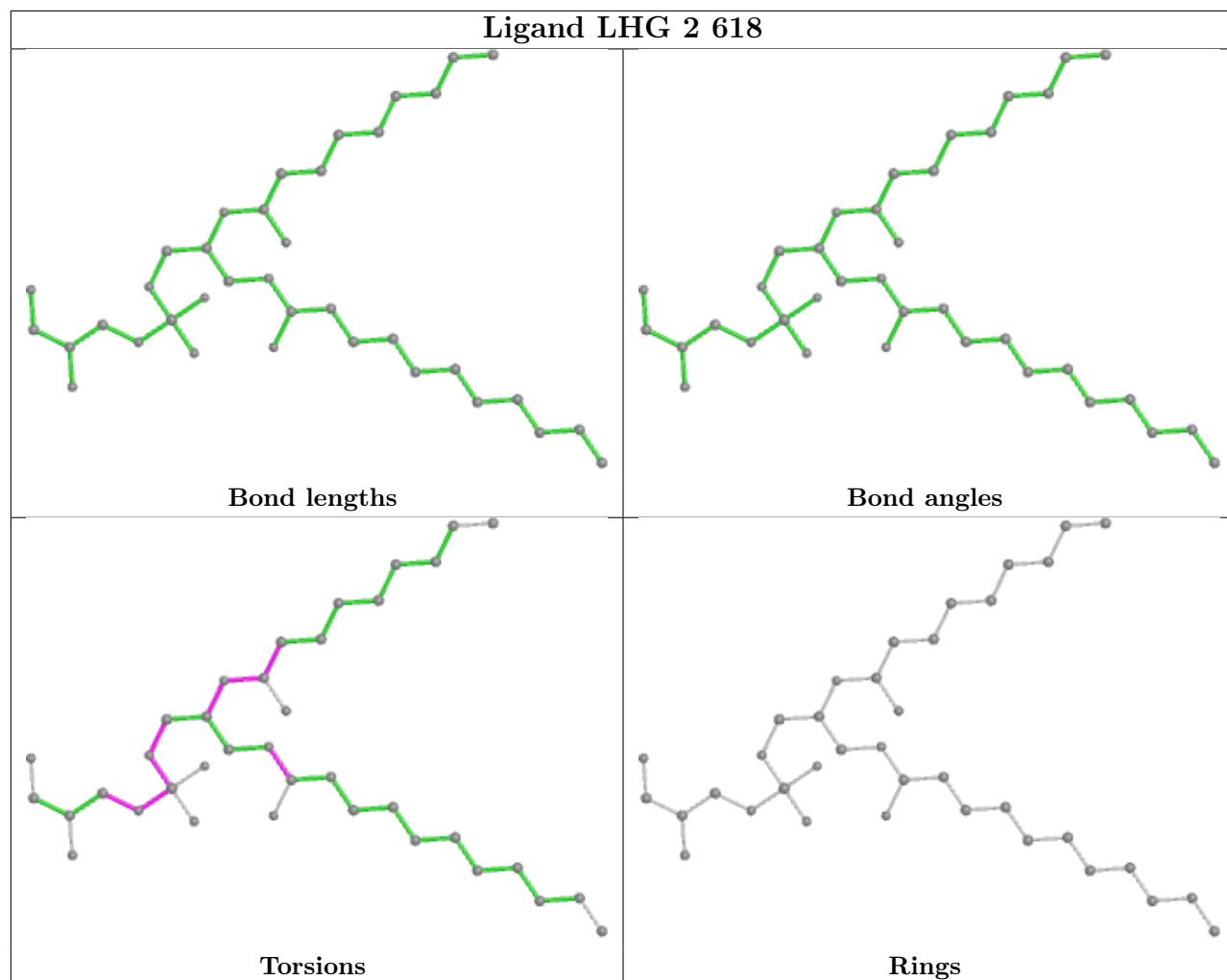
Ligand BCR B 844



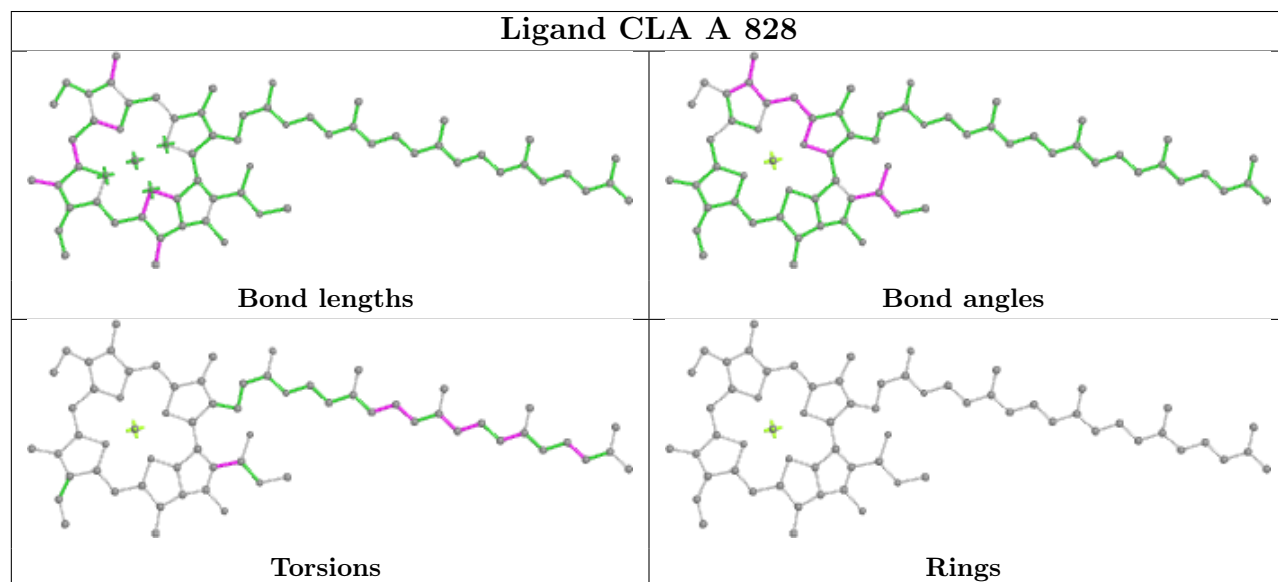


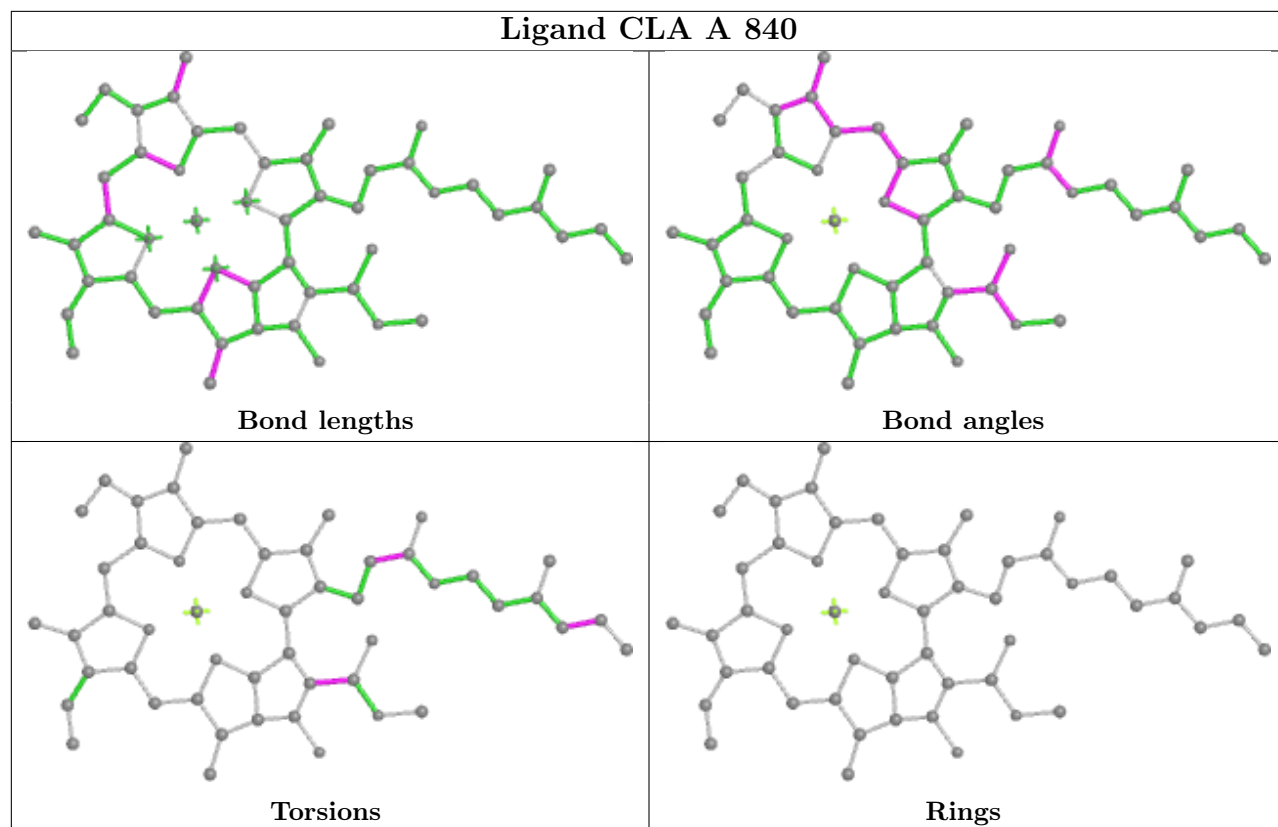


Ligand LHG 2 618

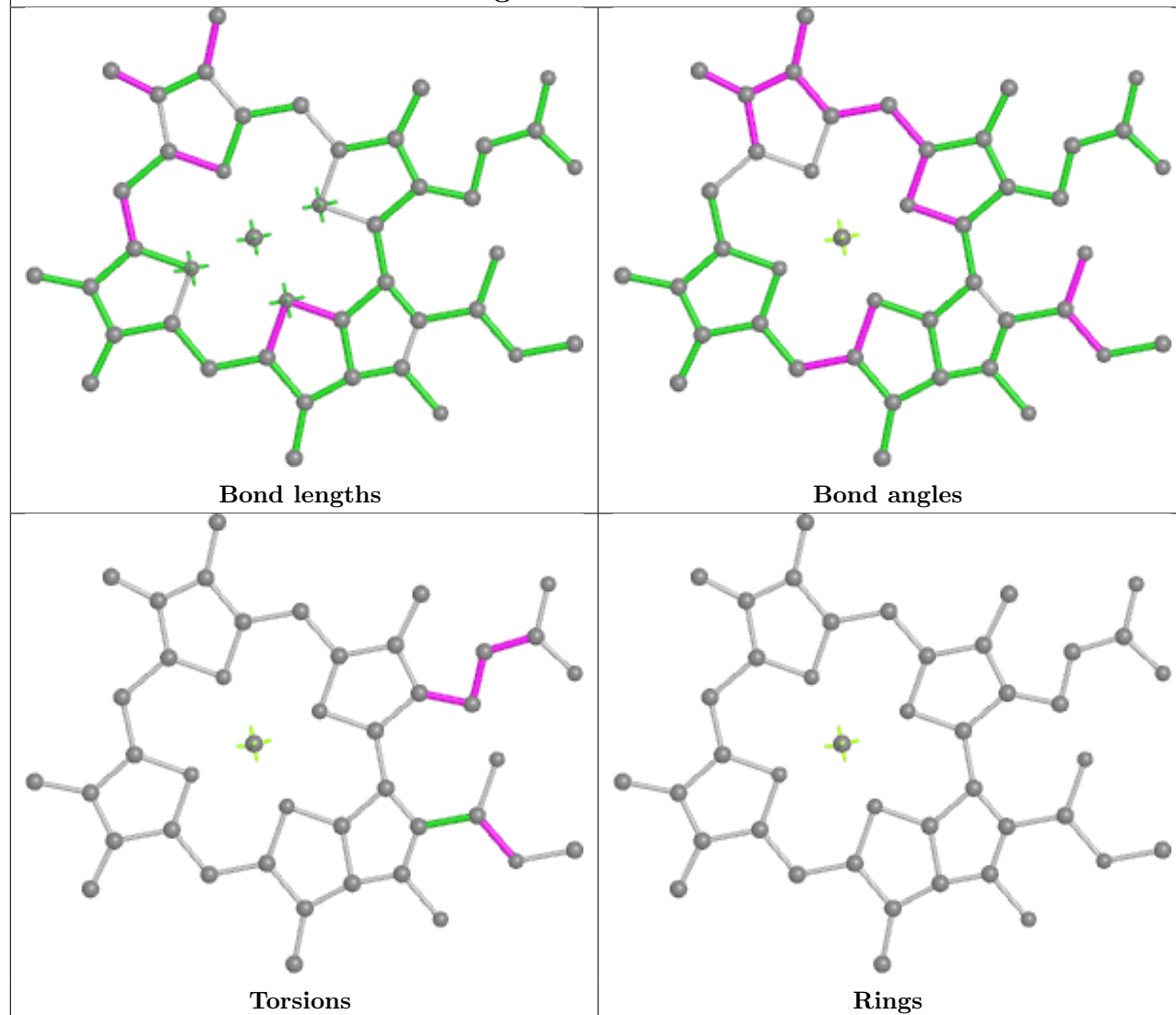


Ligand CLA A 828

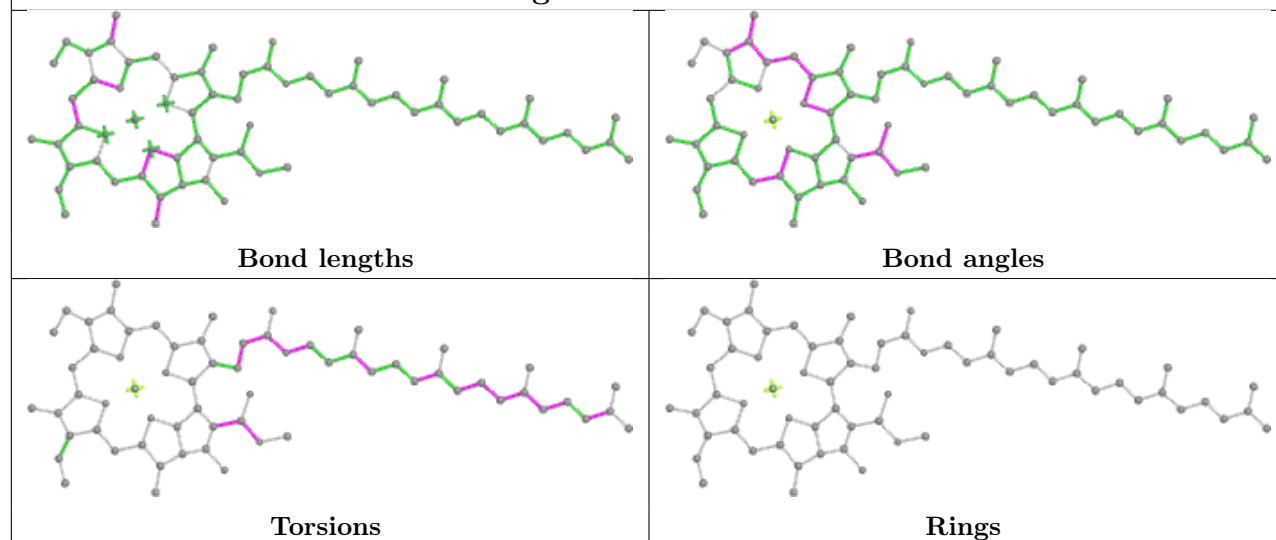




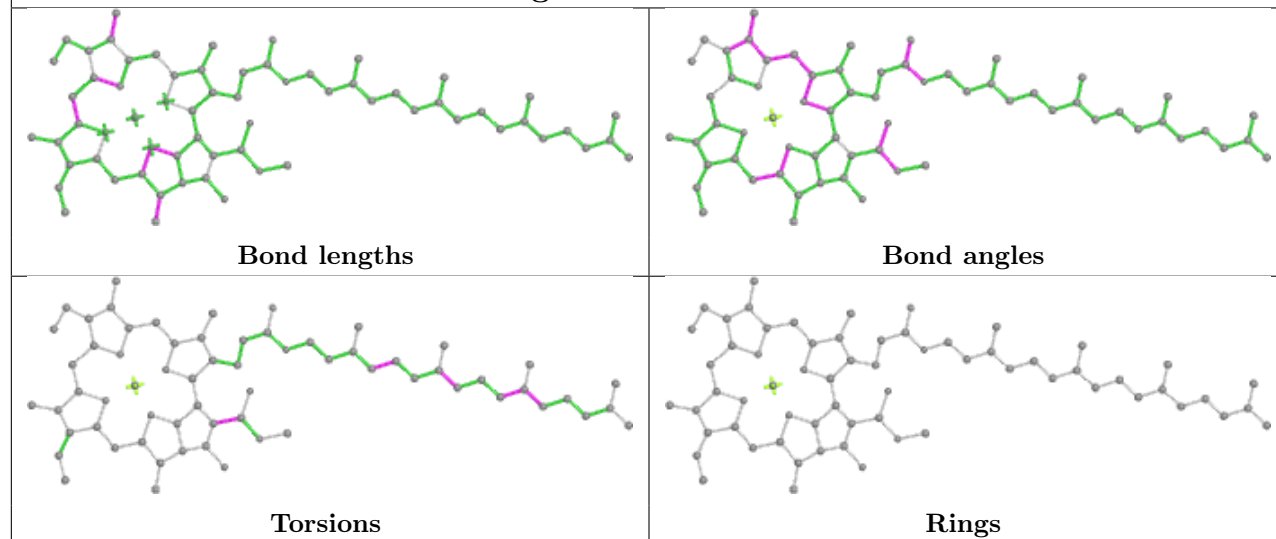
Ligand CLA 4 604



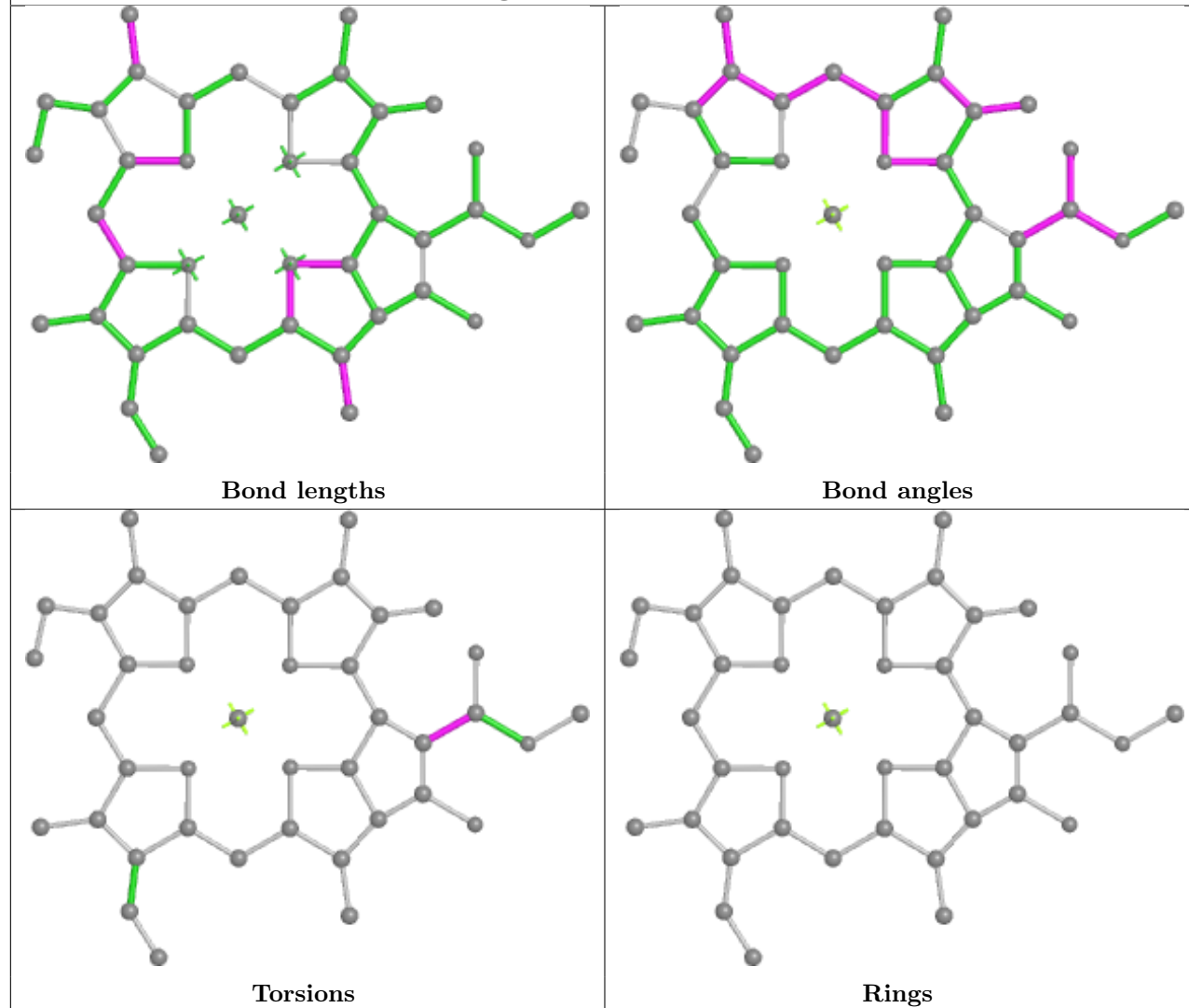
Ligand CLA B 841

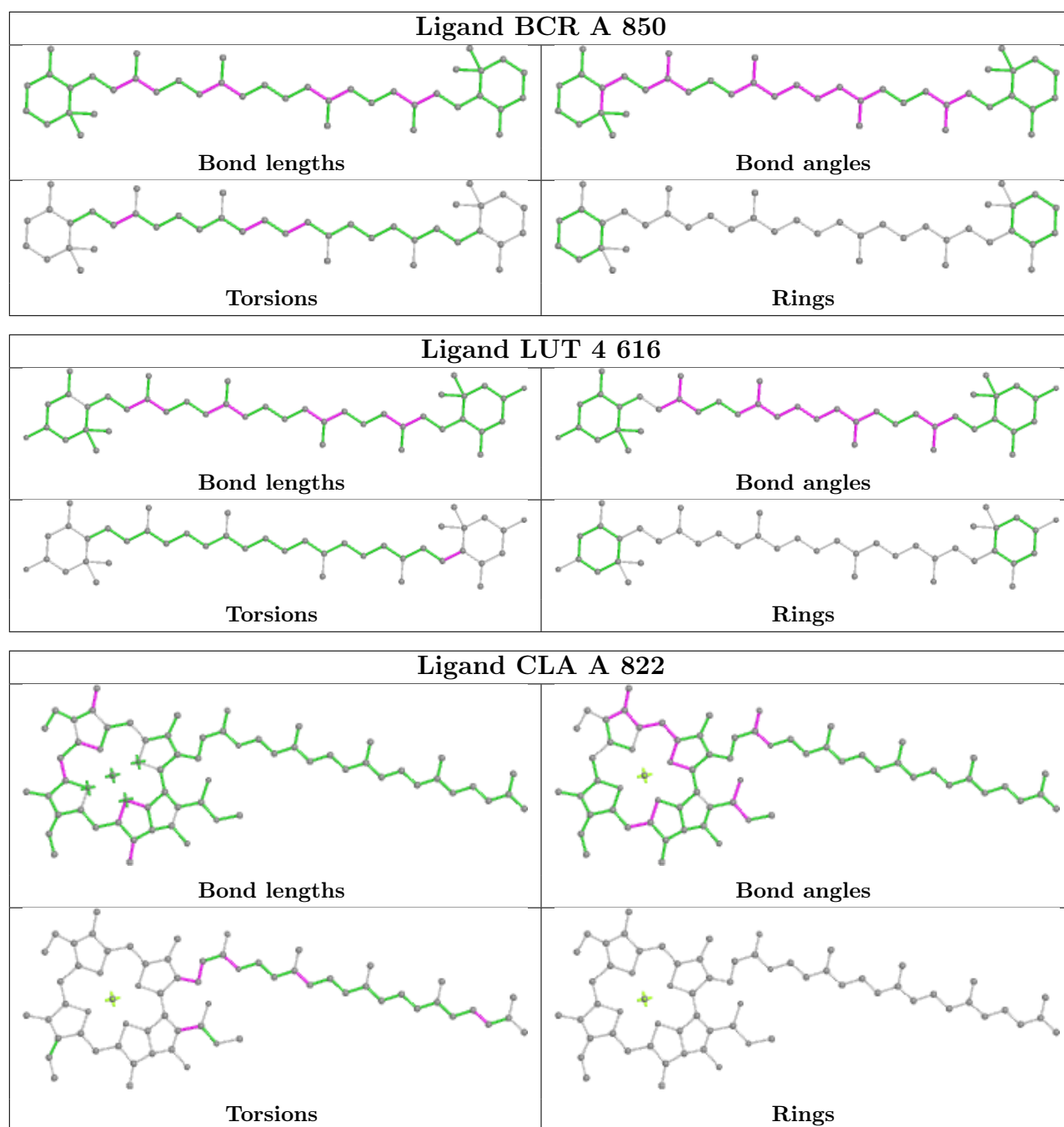


Ligand CLA A 831

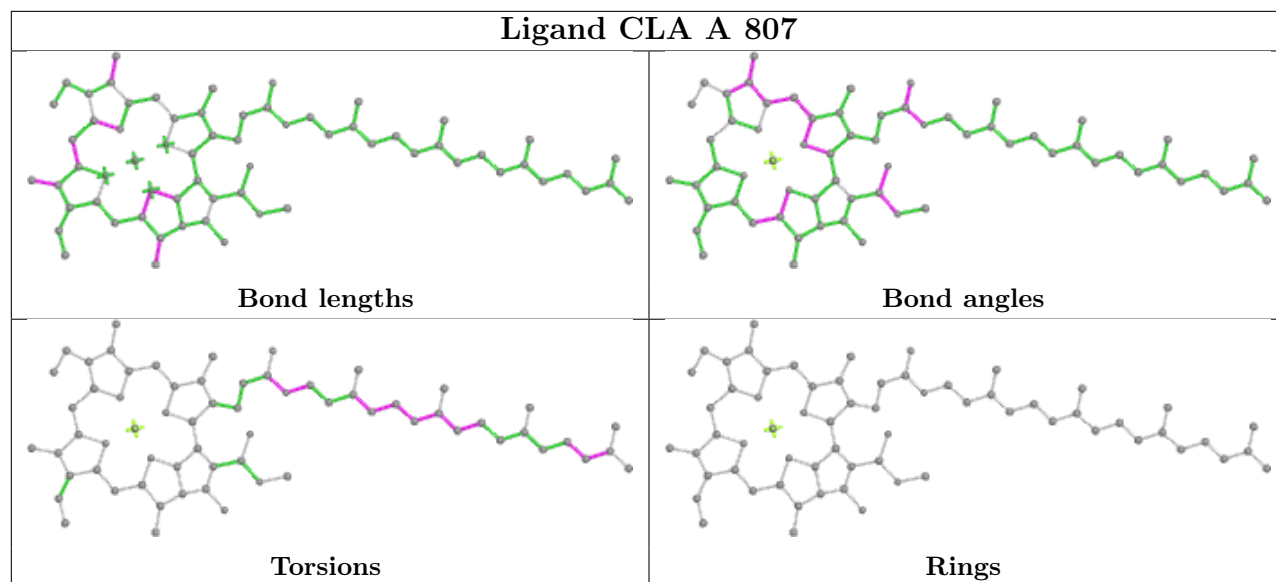


Ligand CLA B 804

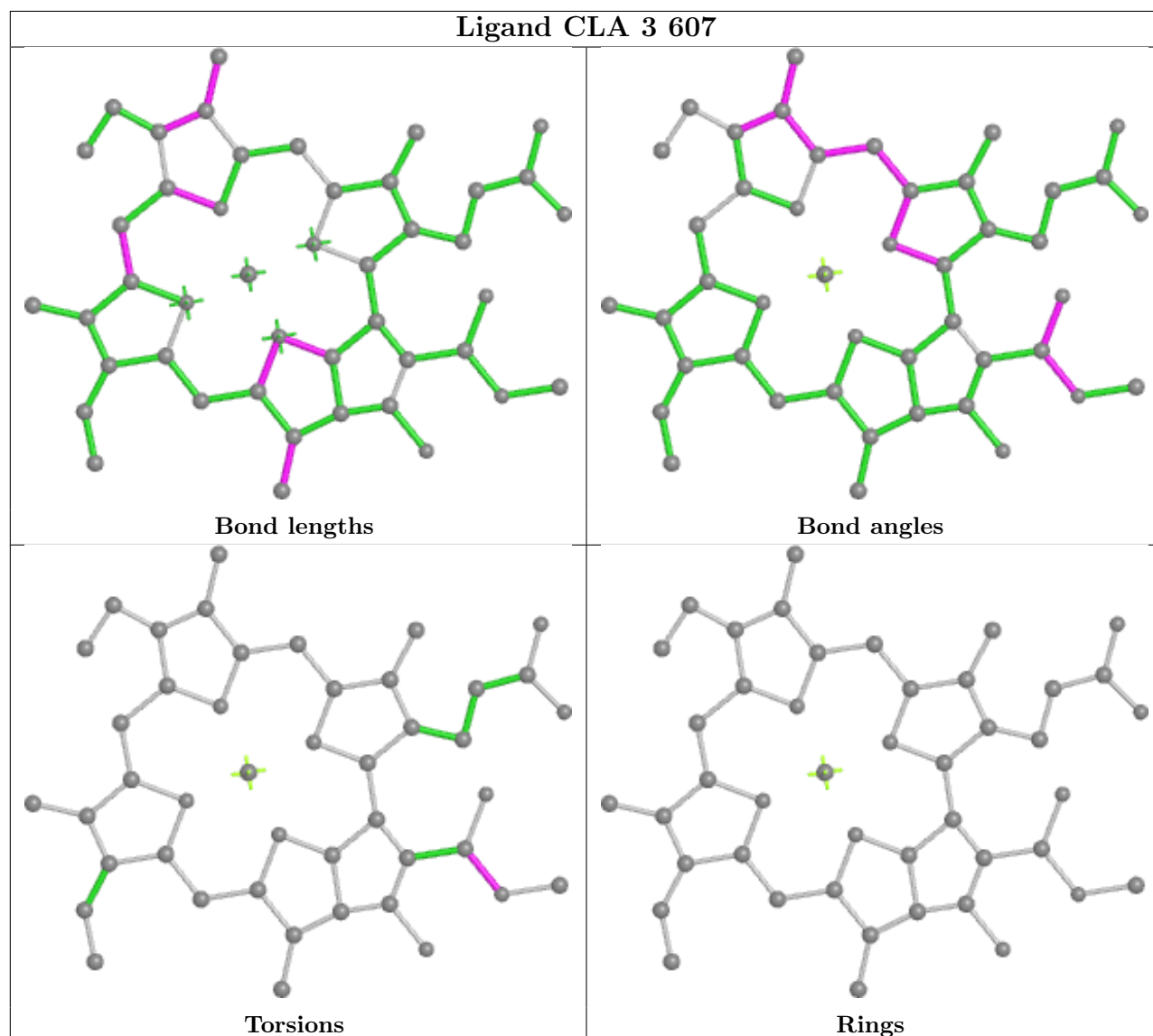




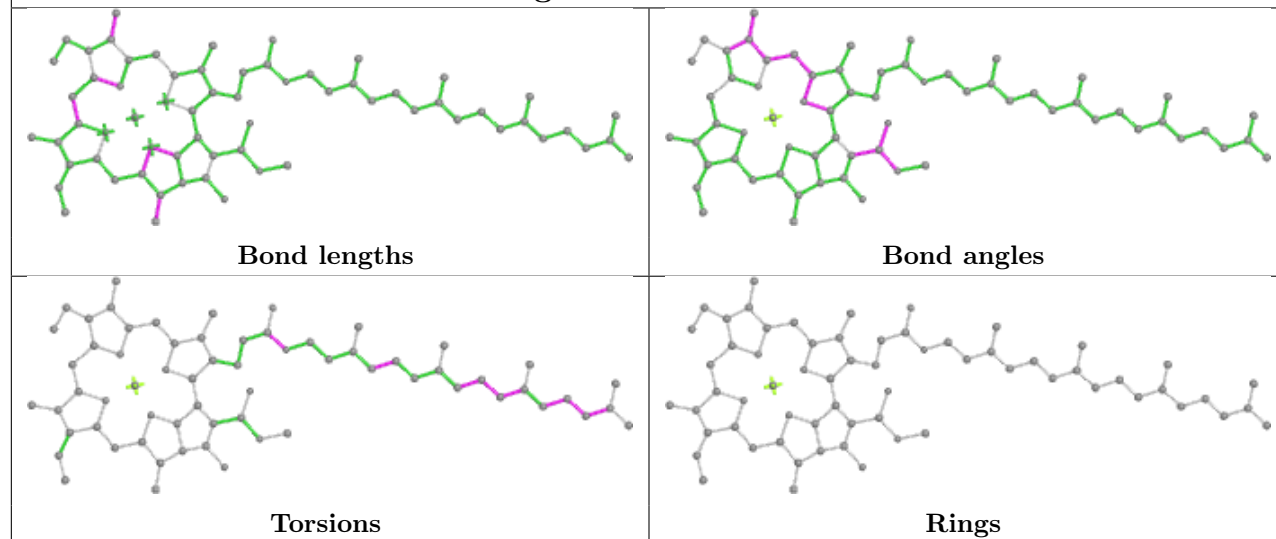
Ligand CLA A 807



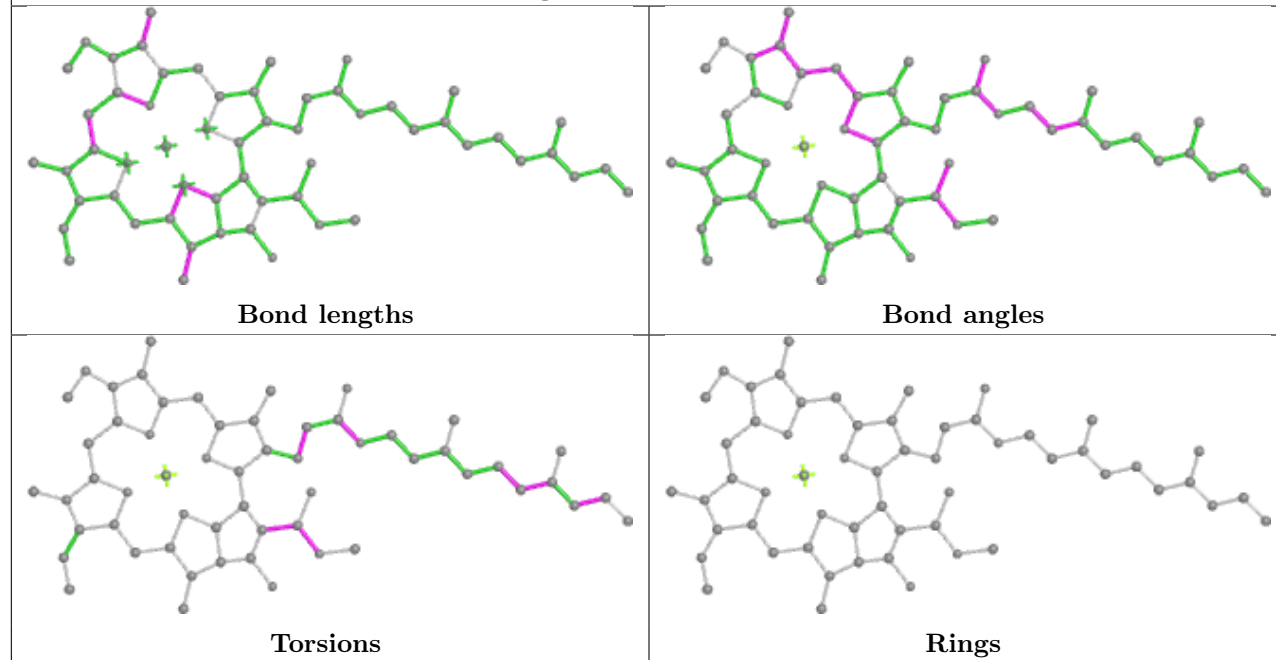
Ligand CLA 3 607



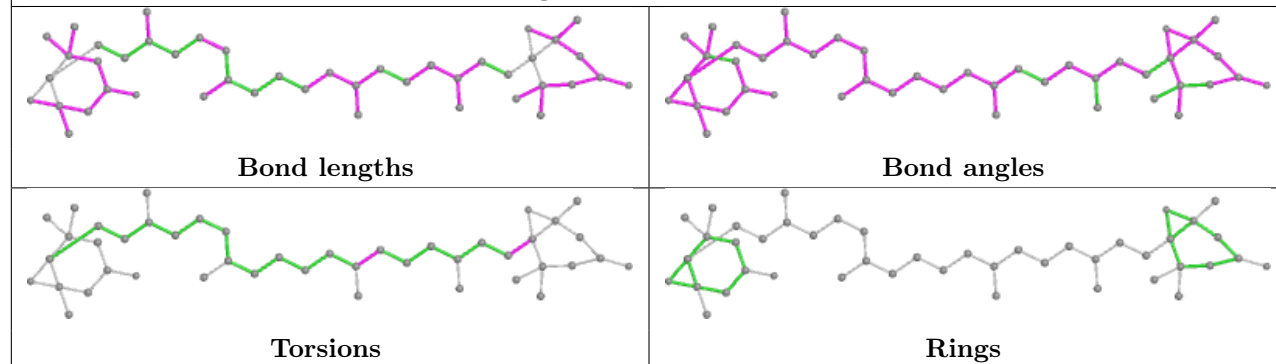
Ligand CLA L 303

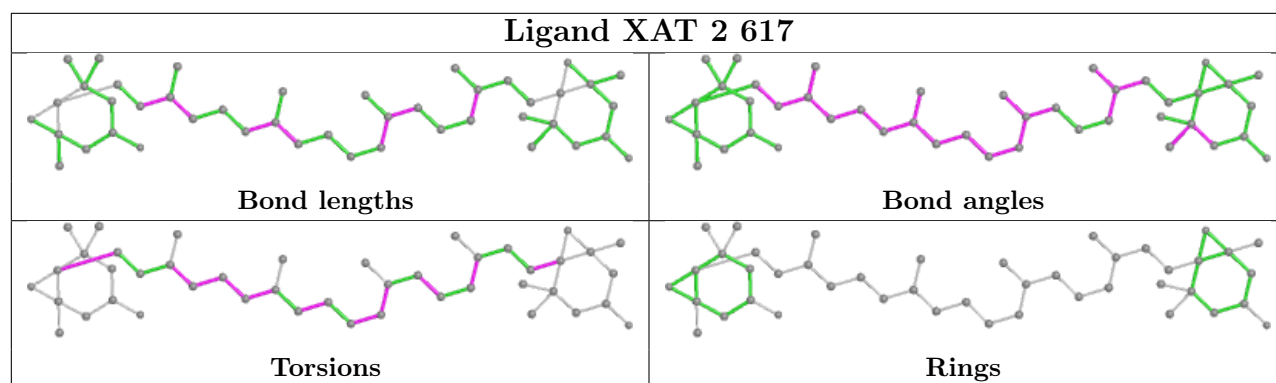
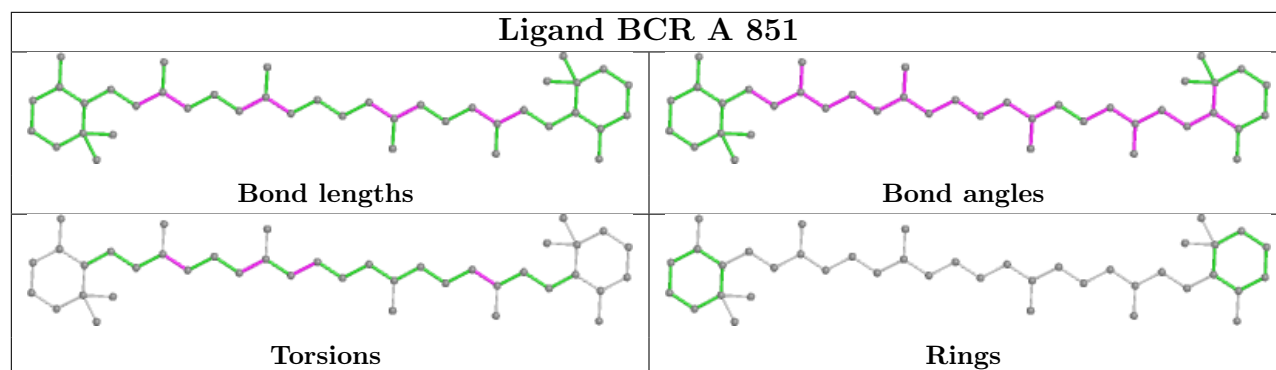
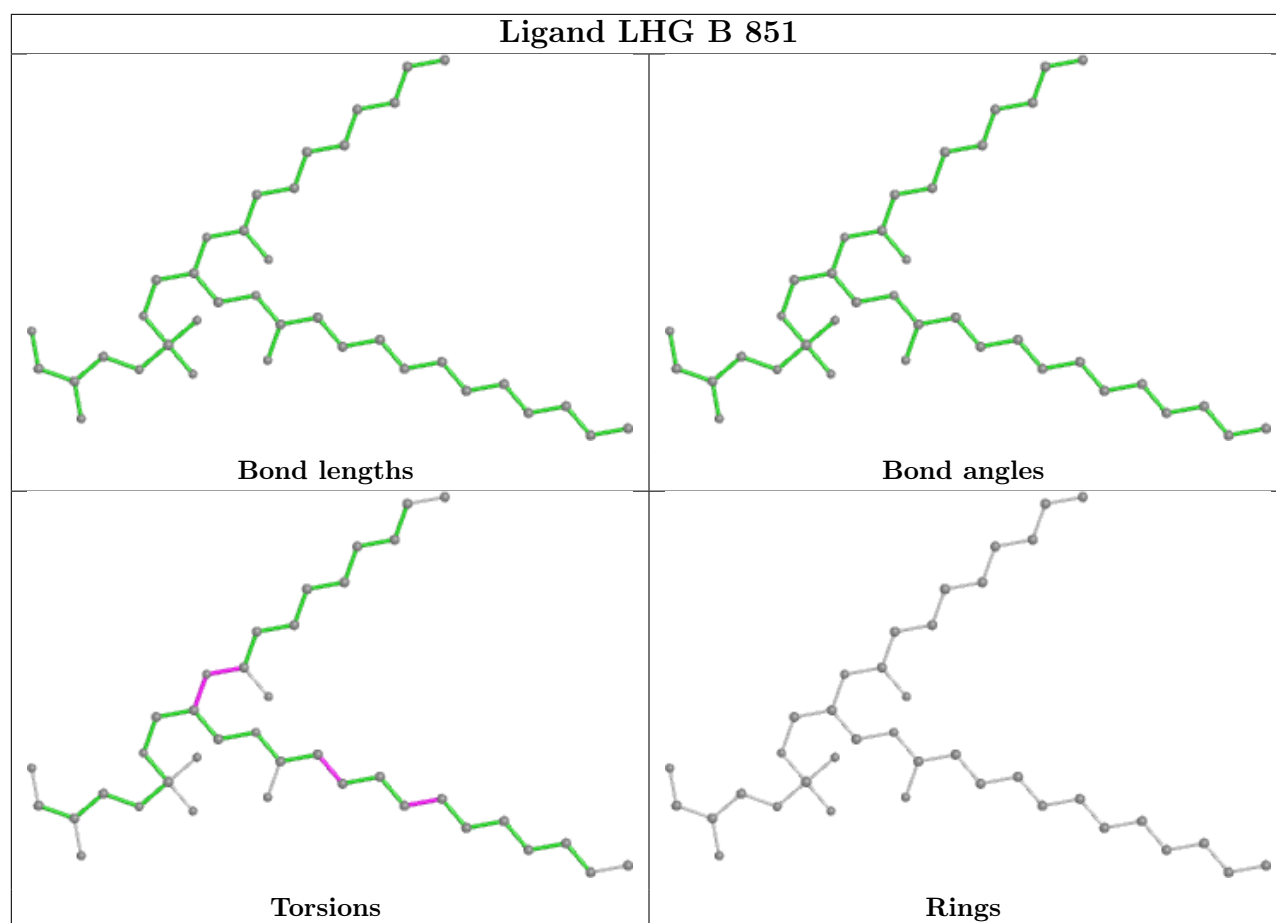


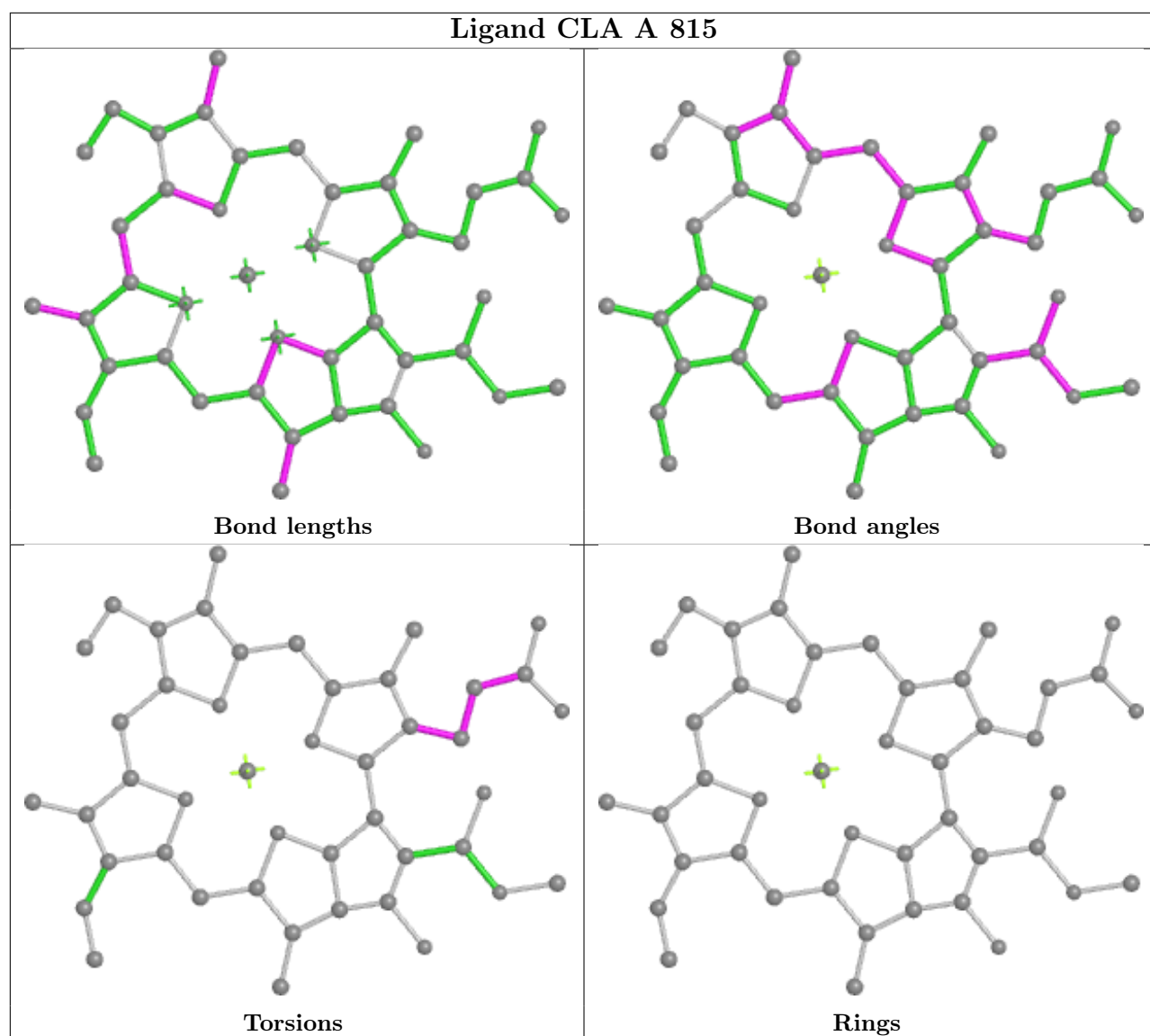
Ligand CLA 4 612



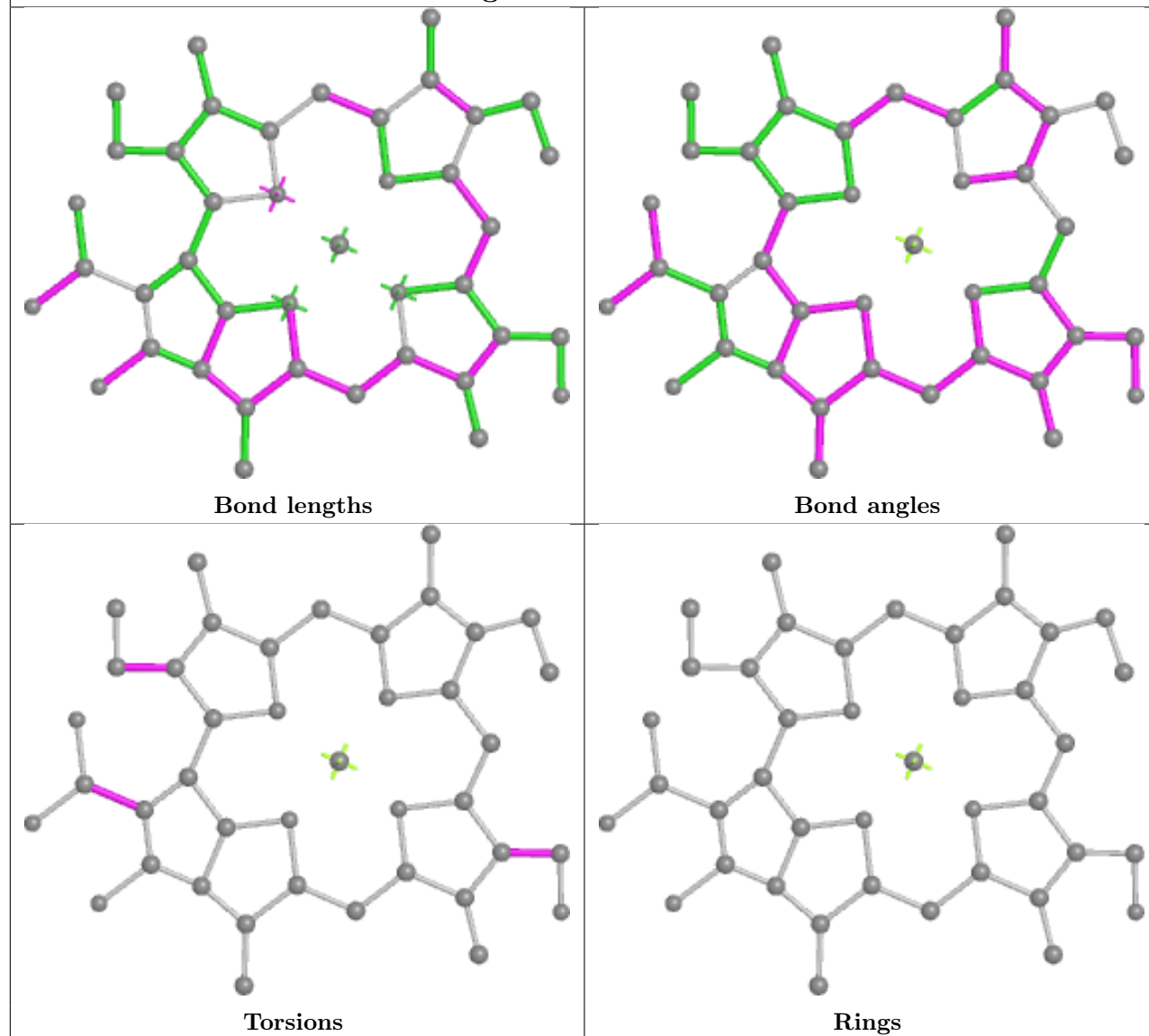
Ligand XAT 4 617



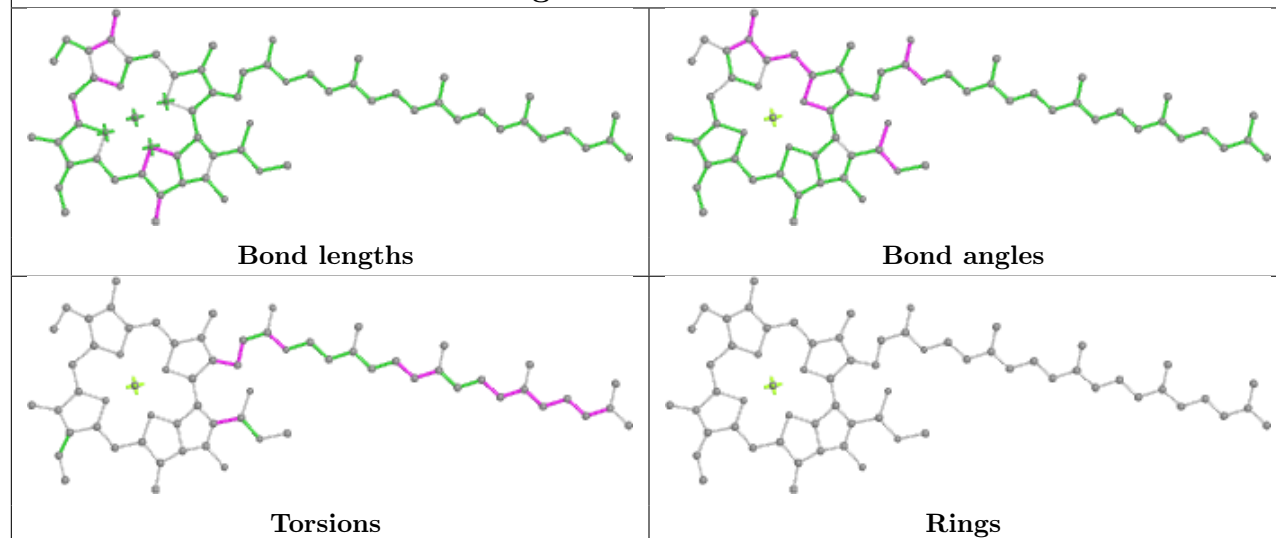


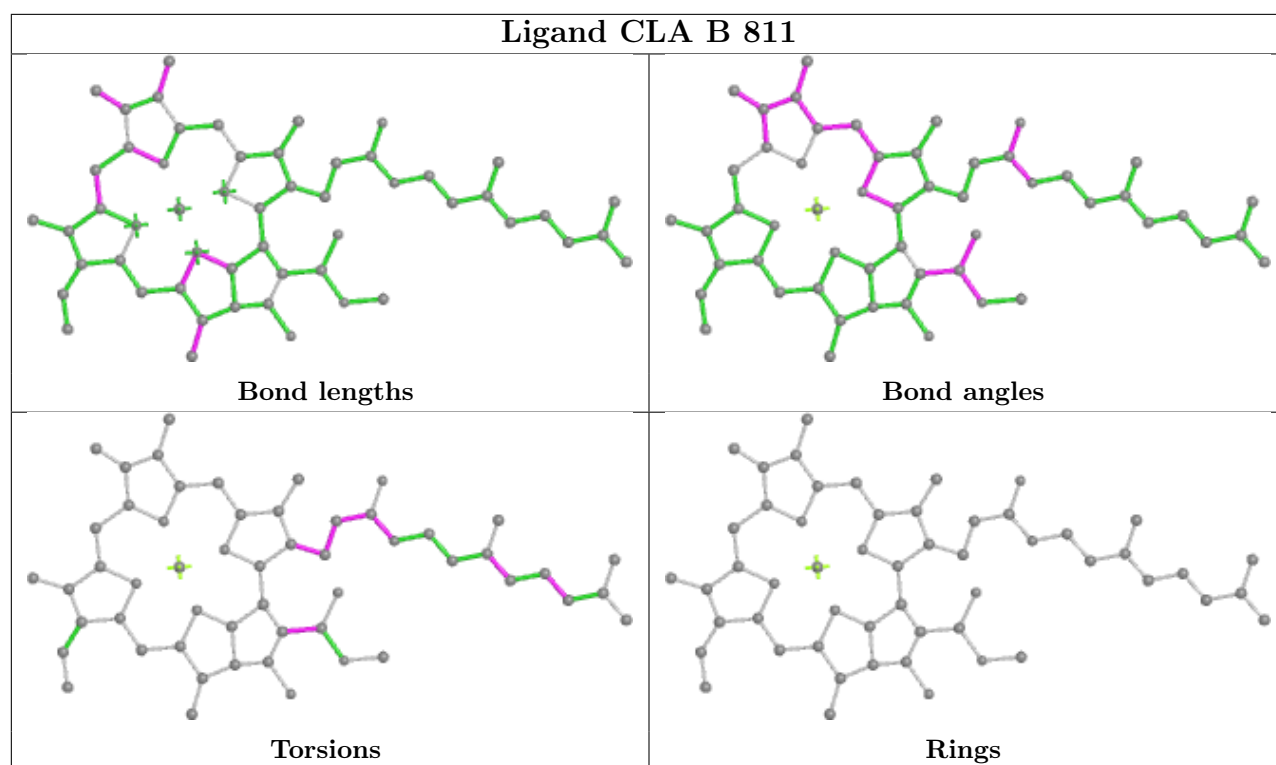


Ligand CHL 4 605

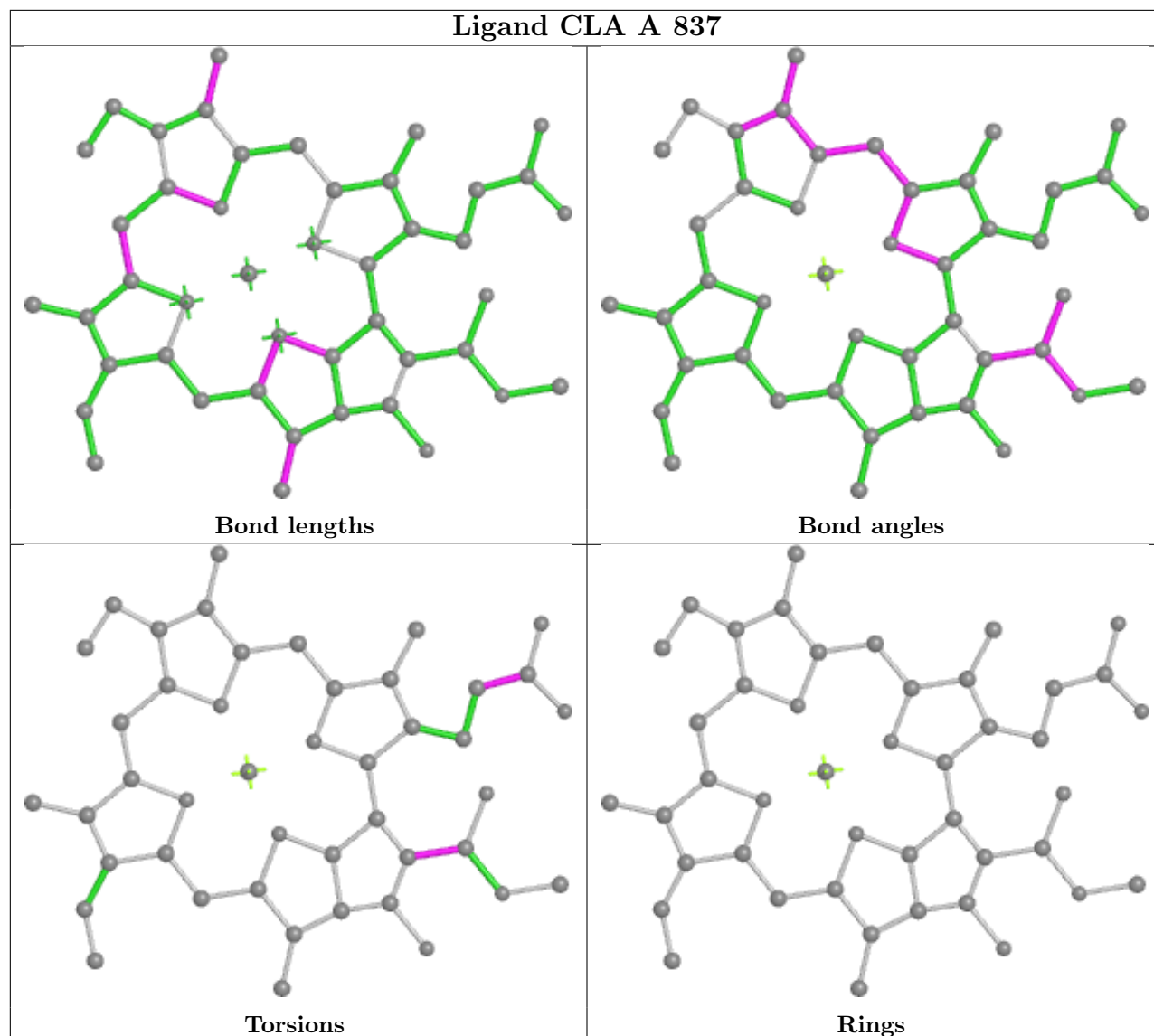


Ligand CLA B 828

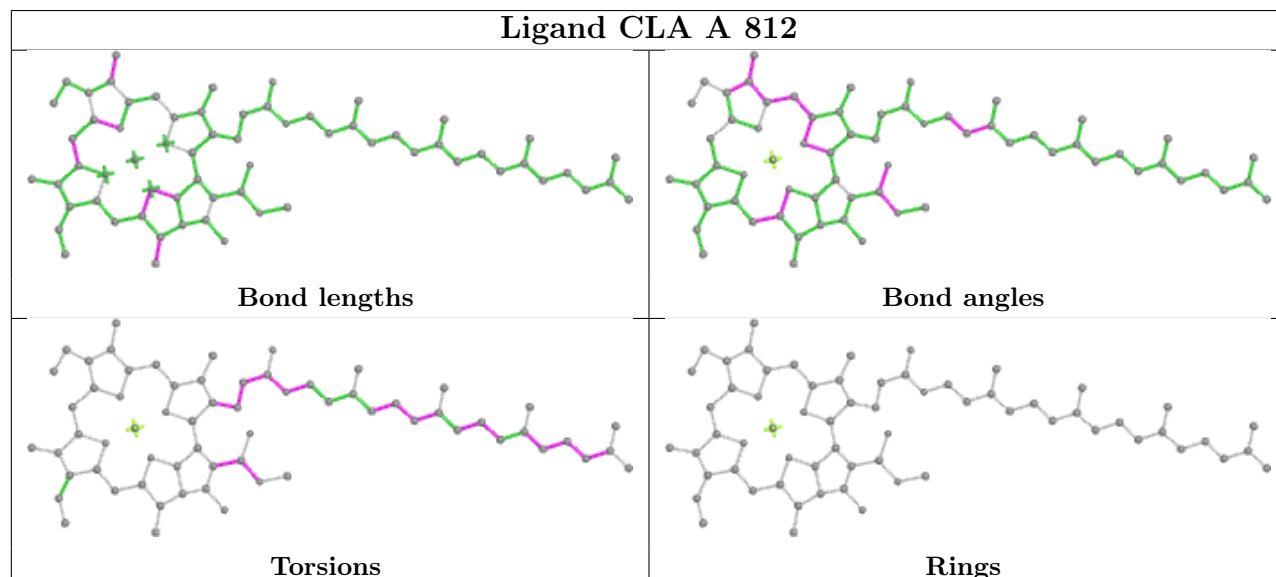




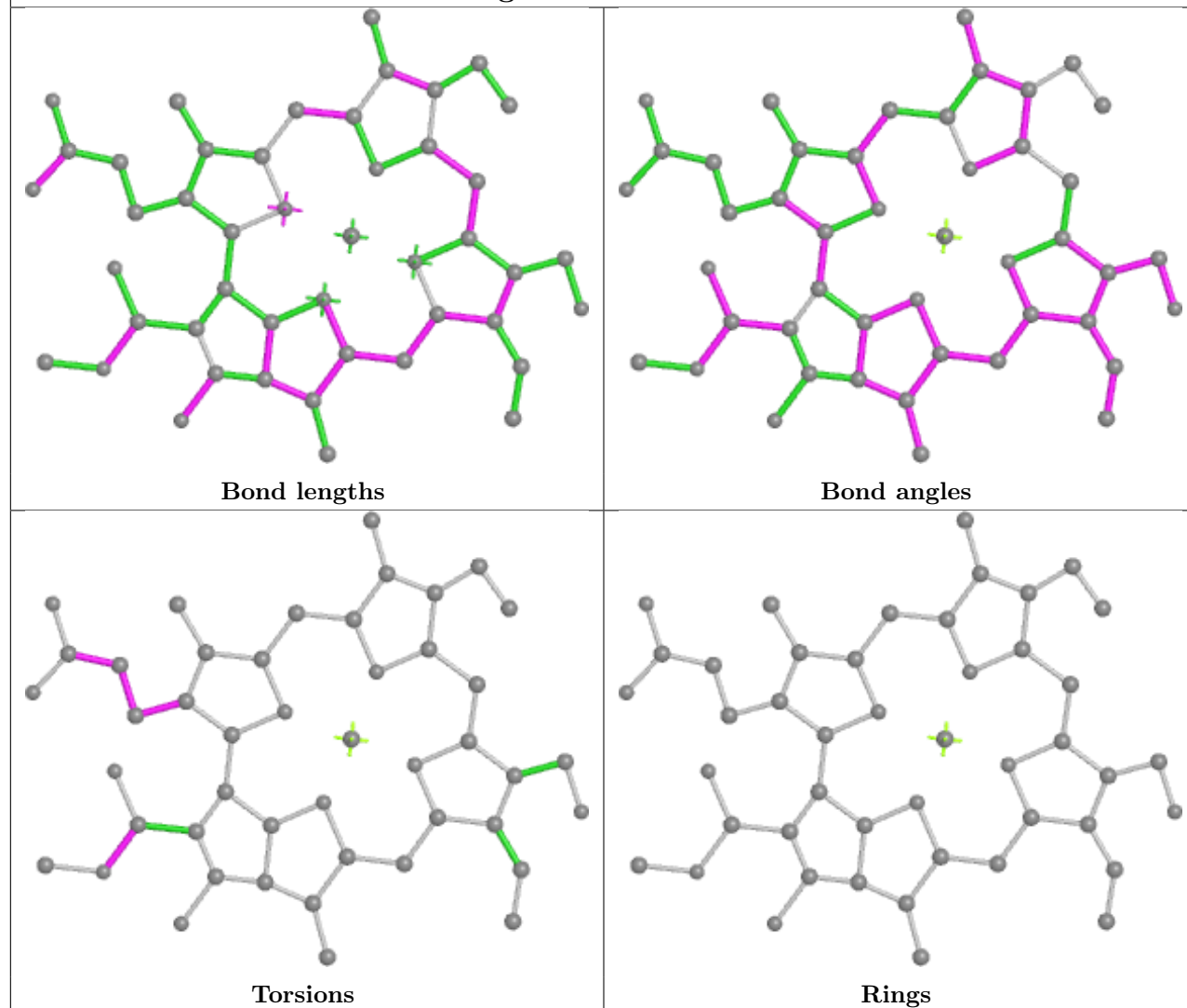
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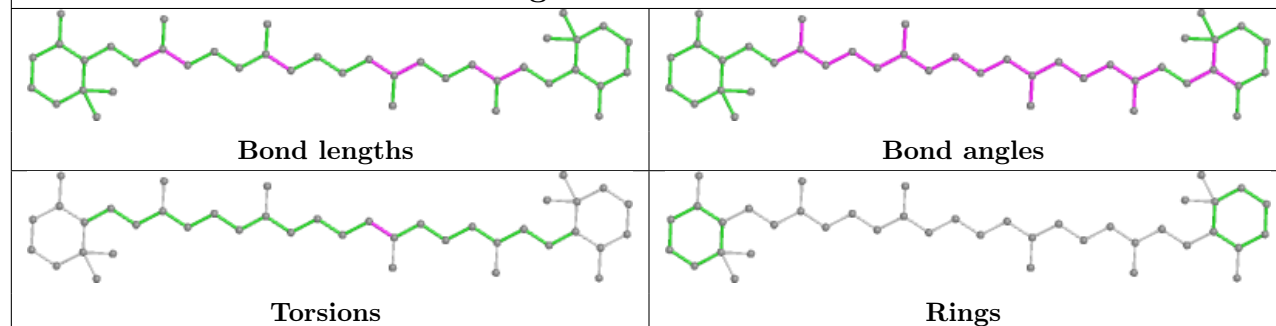
Ligand CLA A 812



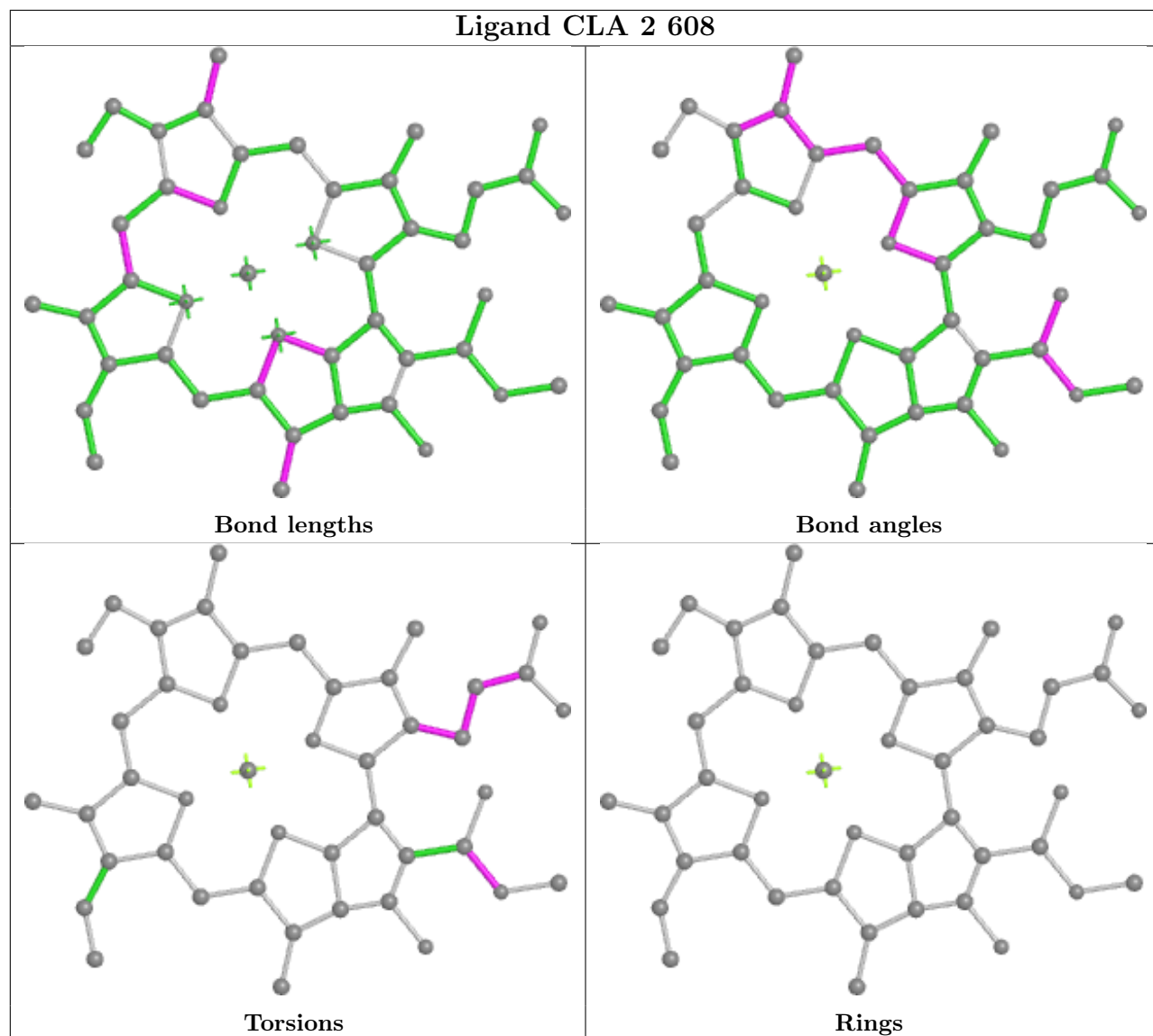
Ligand CHL 4 607



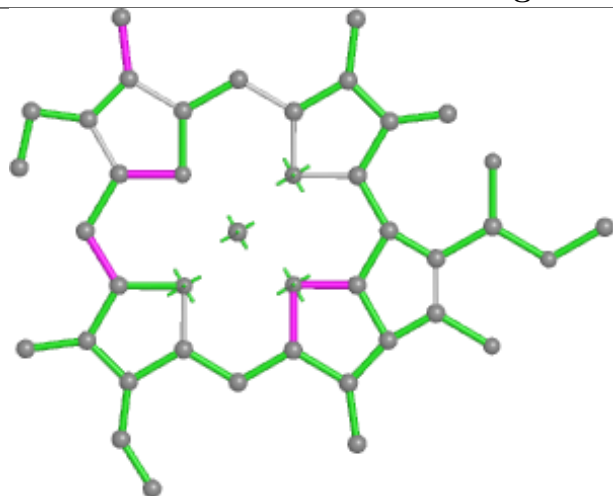
Ligand BCR K 202



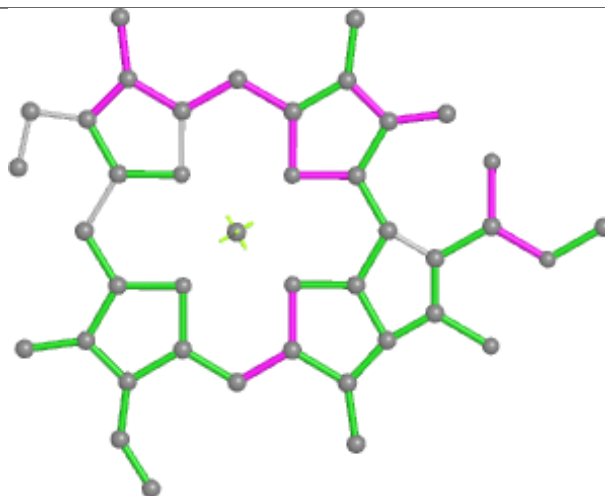
Ligand CLA 2 608



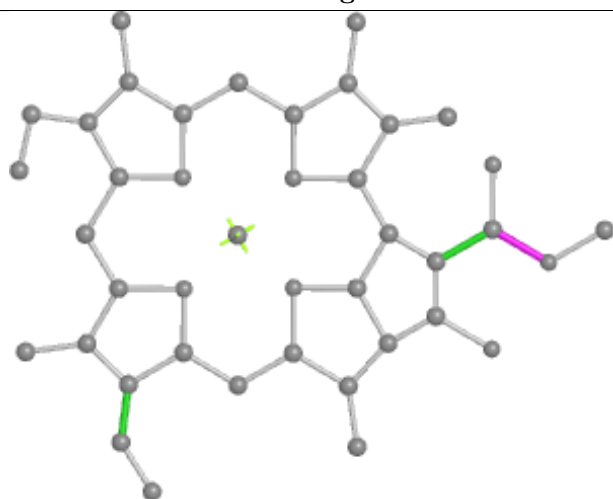
Ligand CLA A 824



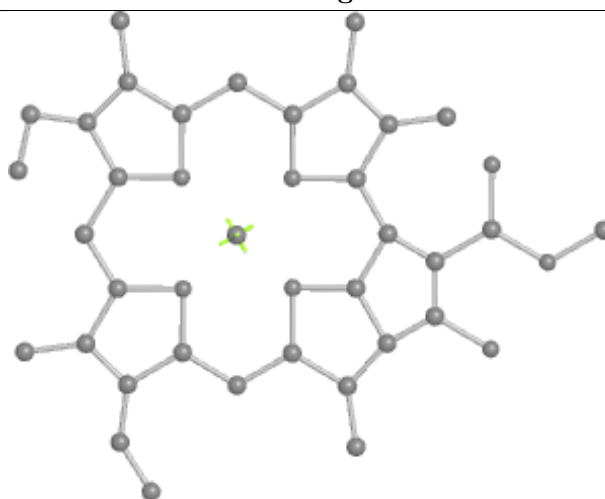
Bond lengths



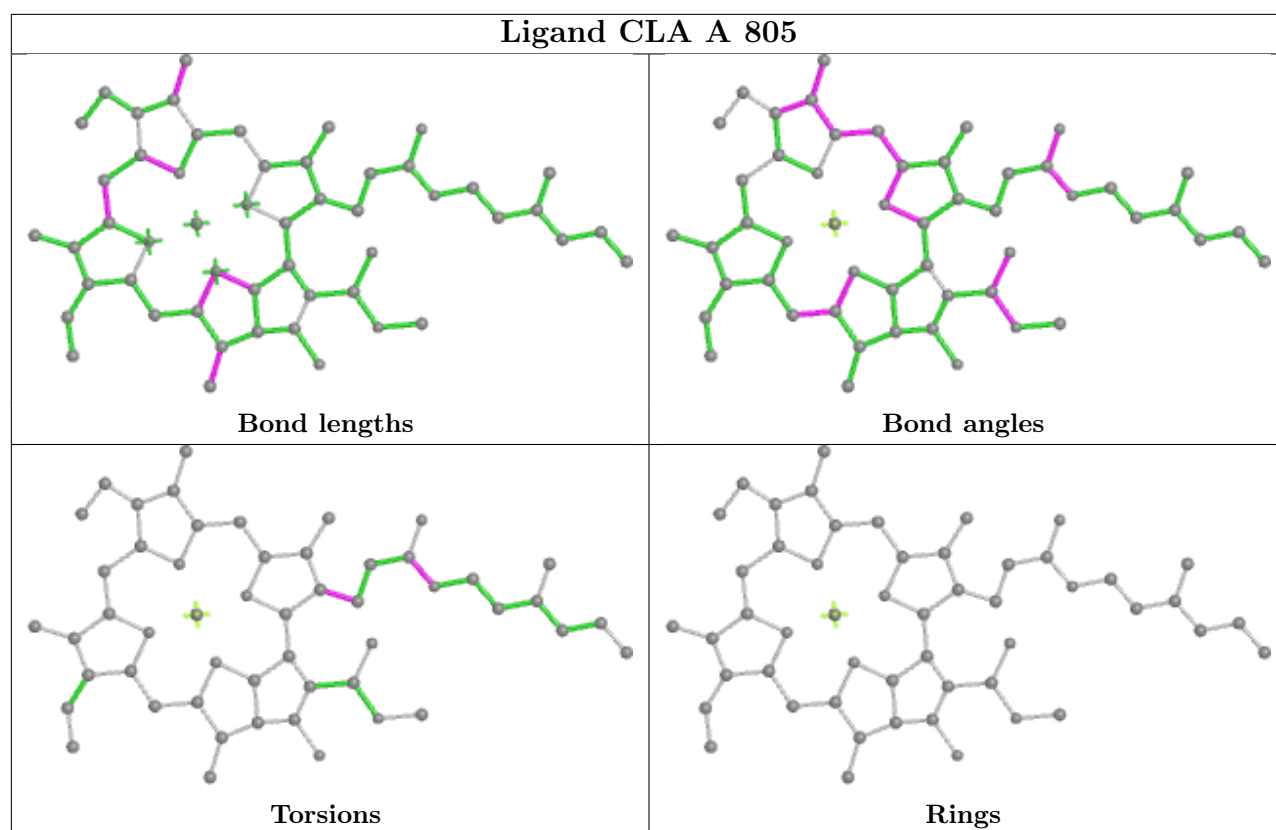
Bond angles



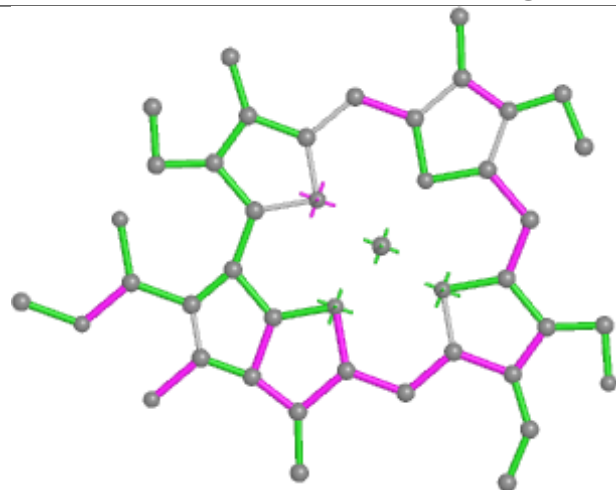
Torsions



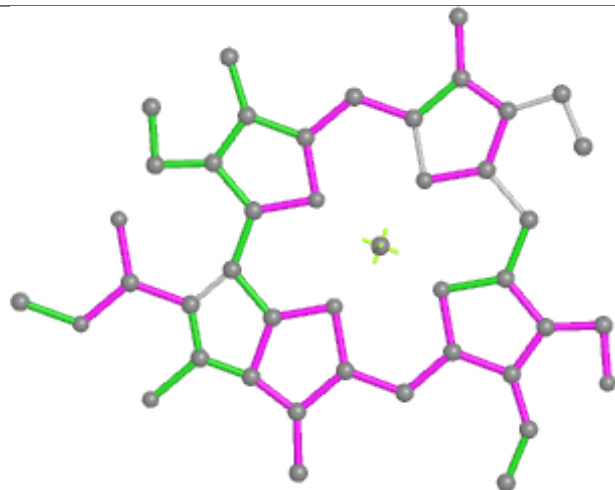
Rings



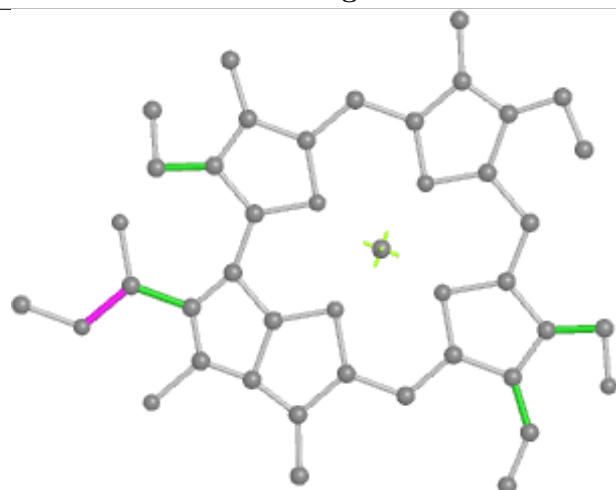
Ligand CHL 2 606



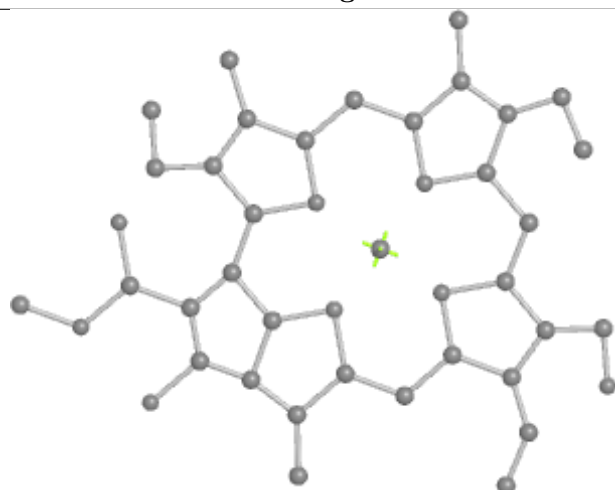
Bond lengths



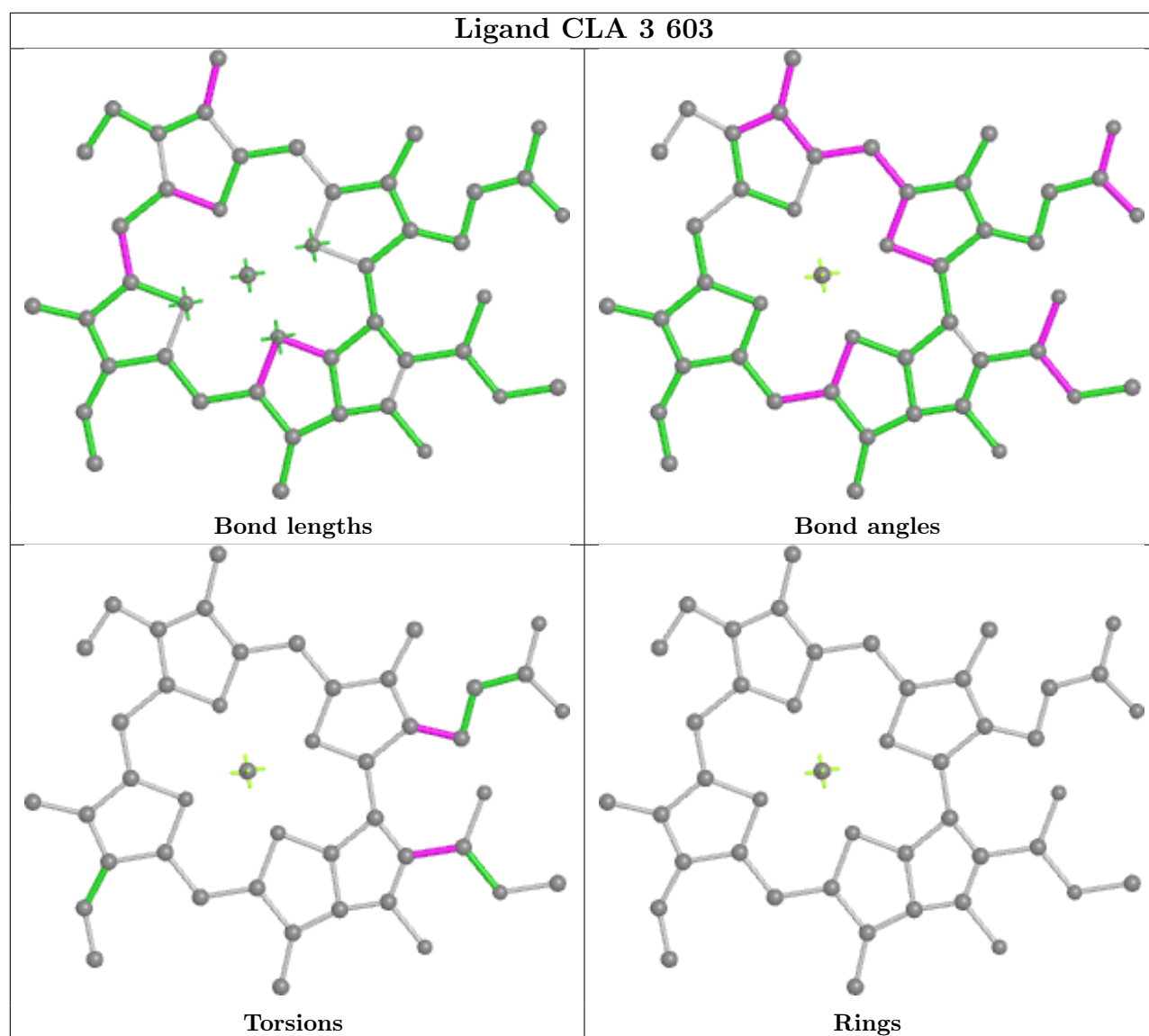
Bond angles



Torsions



Rings



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

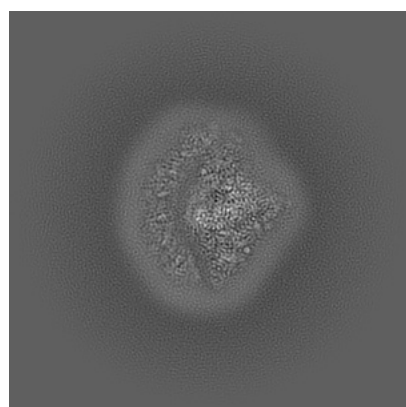
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-36036. These allow visual inspection of the internal detail of the map and identification of artifacts.

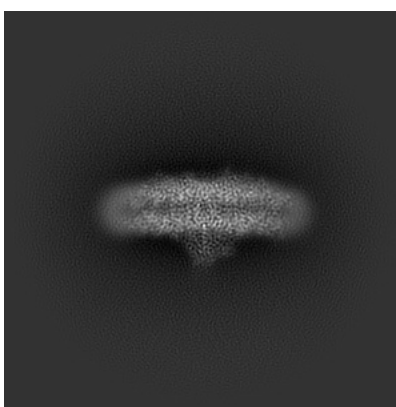
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

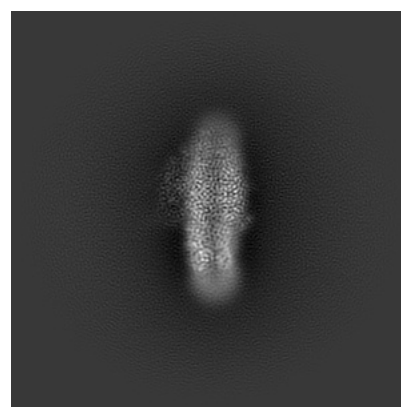
6.1.1 Primary map



X



Y

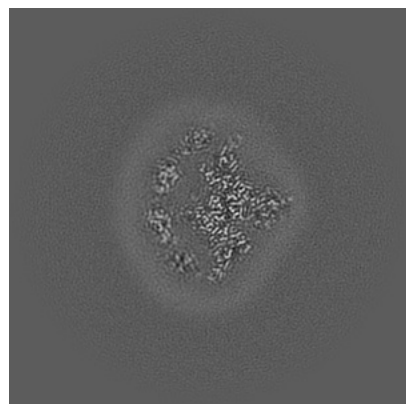


Z

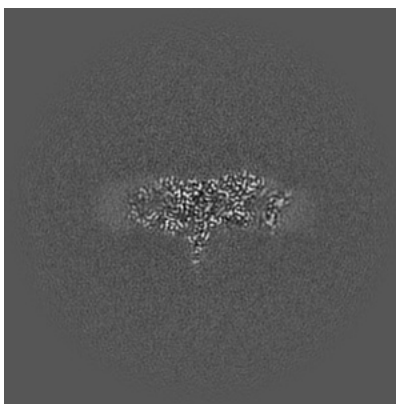
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

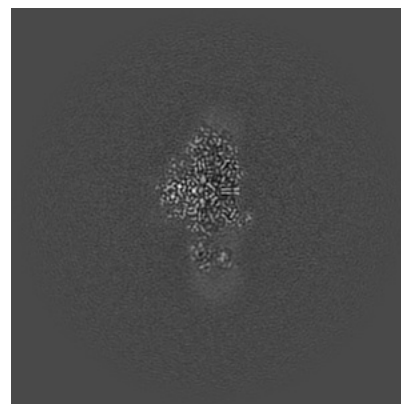
6.2.1 Primary map



X Index: 192



Y Index: 192

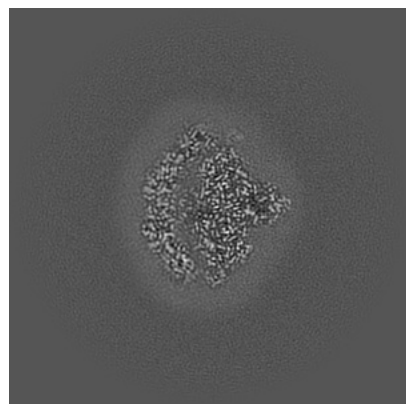


Z Index: 192

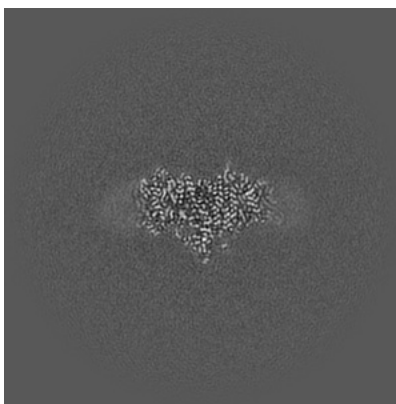
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

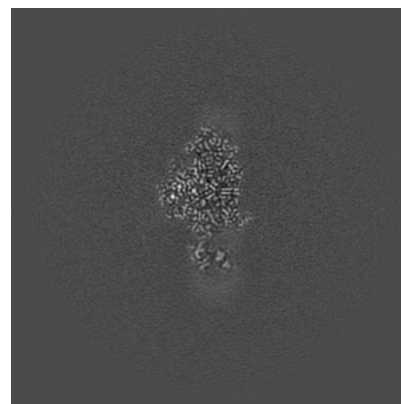
6.3.1 Primary map



X Index: 182



Y Index: 211

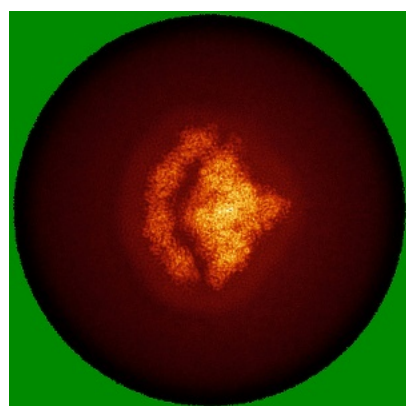


Z Index: 191

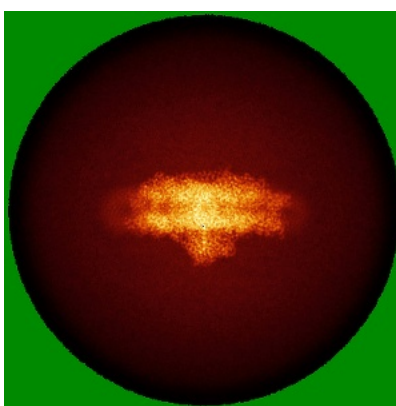
The images above show the largest variance slices of the map in three orthogonal directions.

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

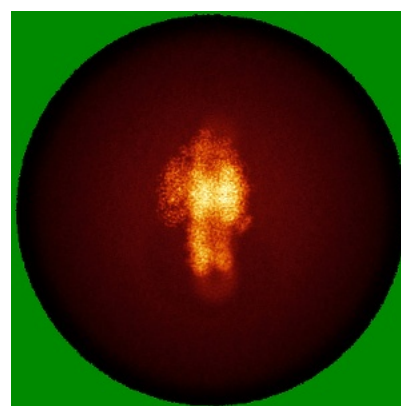
6.4.1 Primary map



X



Y

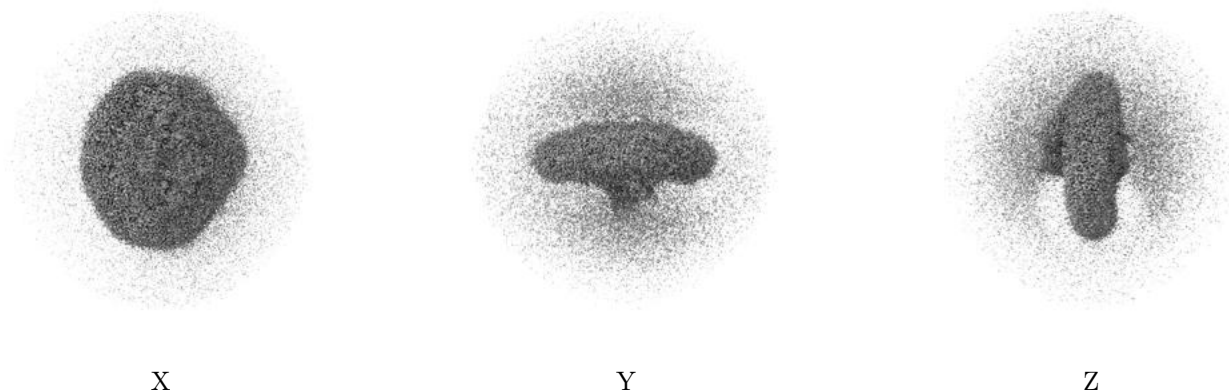


Z

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 [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 2.57. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

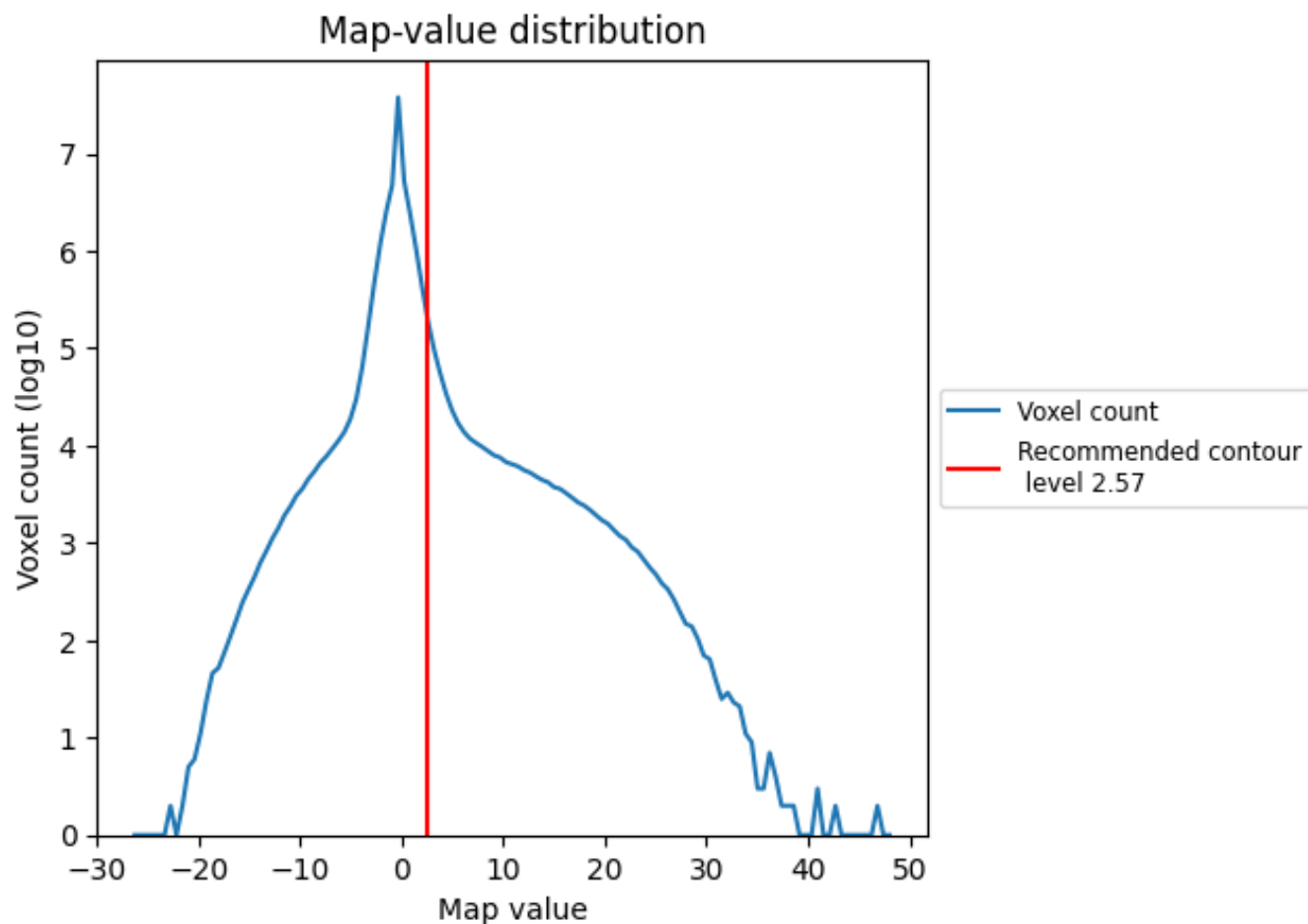
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

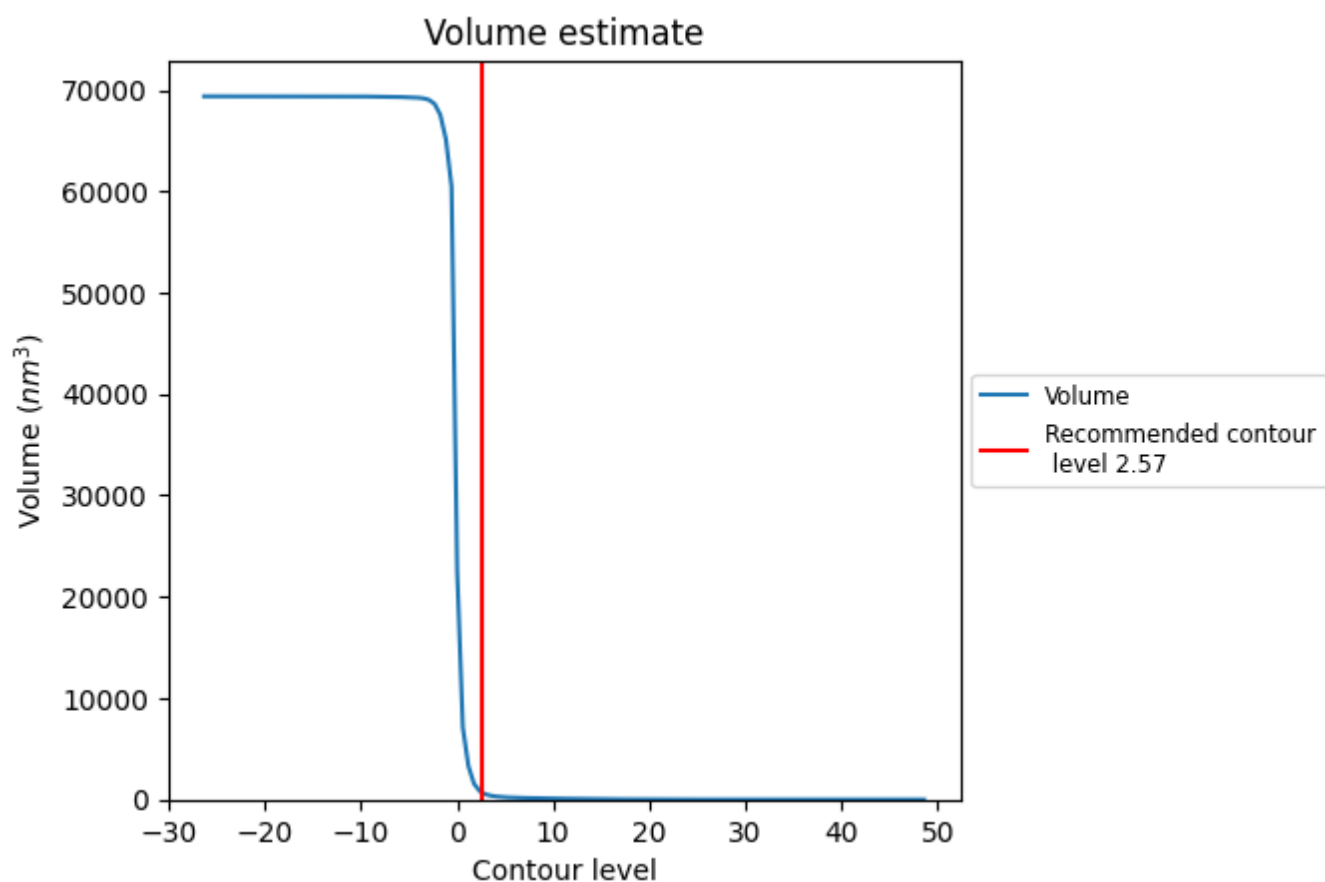
This section contains the results of statistical analysis of the map.

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.

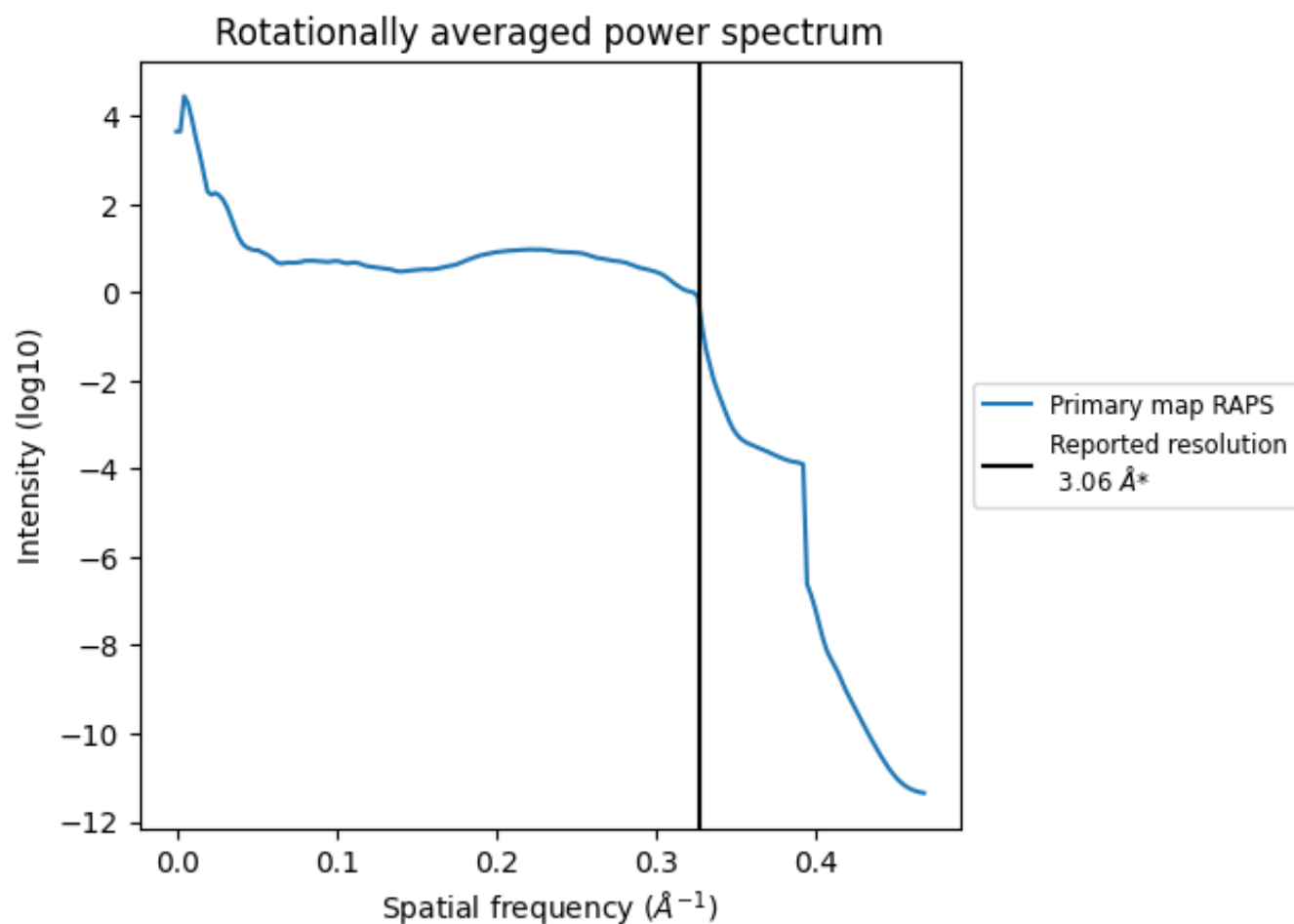
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 724 nm^3 ; this corresponds to an approximate mass of 654 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 0.327 Å⁻¹

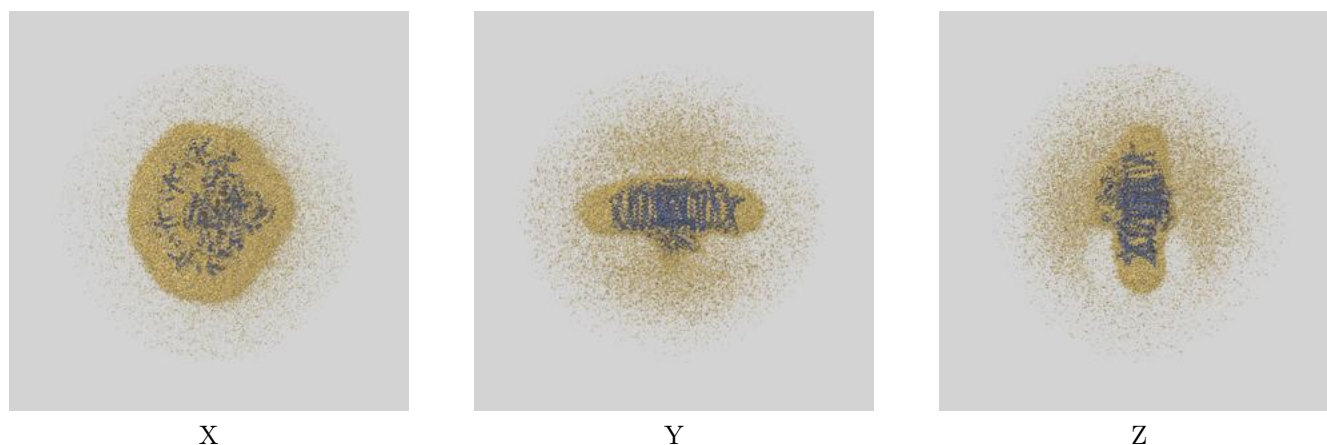
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

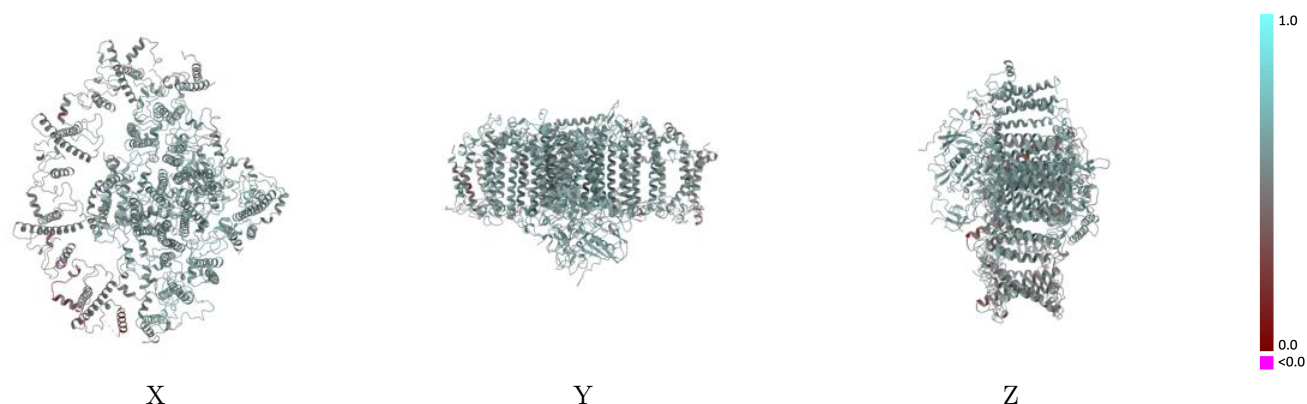
This section contains information regarding the fit between EMDB map EMD-36036 and PDB model 8J7A. Per-residue inclusion information can be found in [section 3](#) on [page 26](#).

9.1 Map-model overlay [i](#)



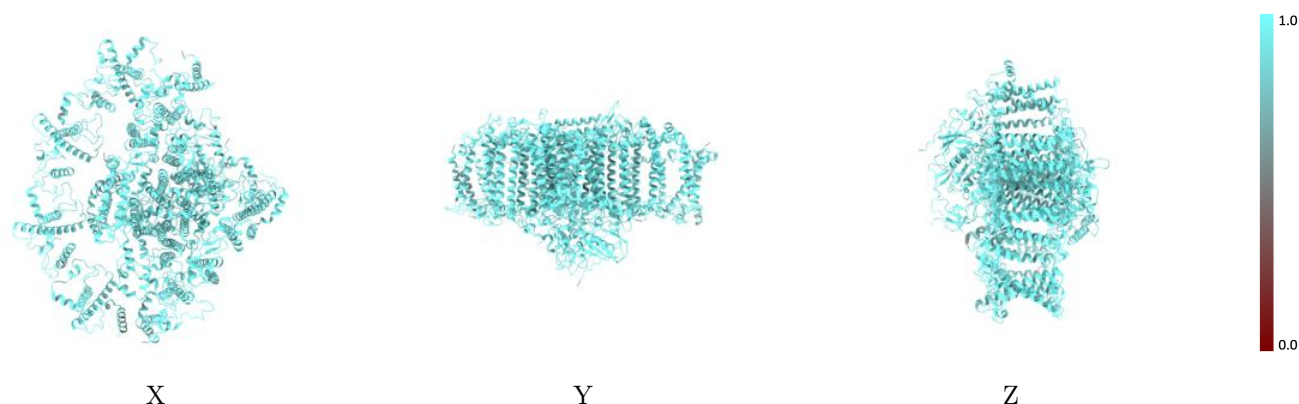
The images above show the 3D surface view of the map at the recommended contour level 2.57 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



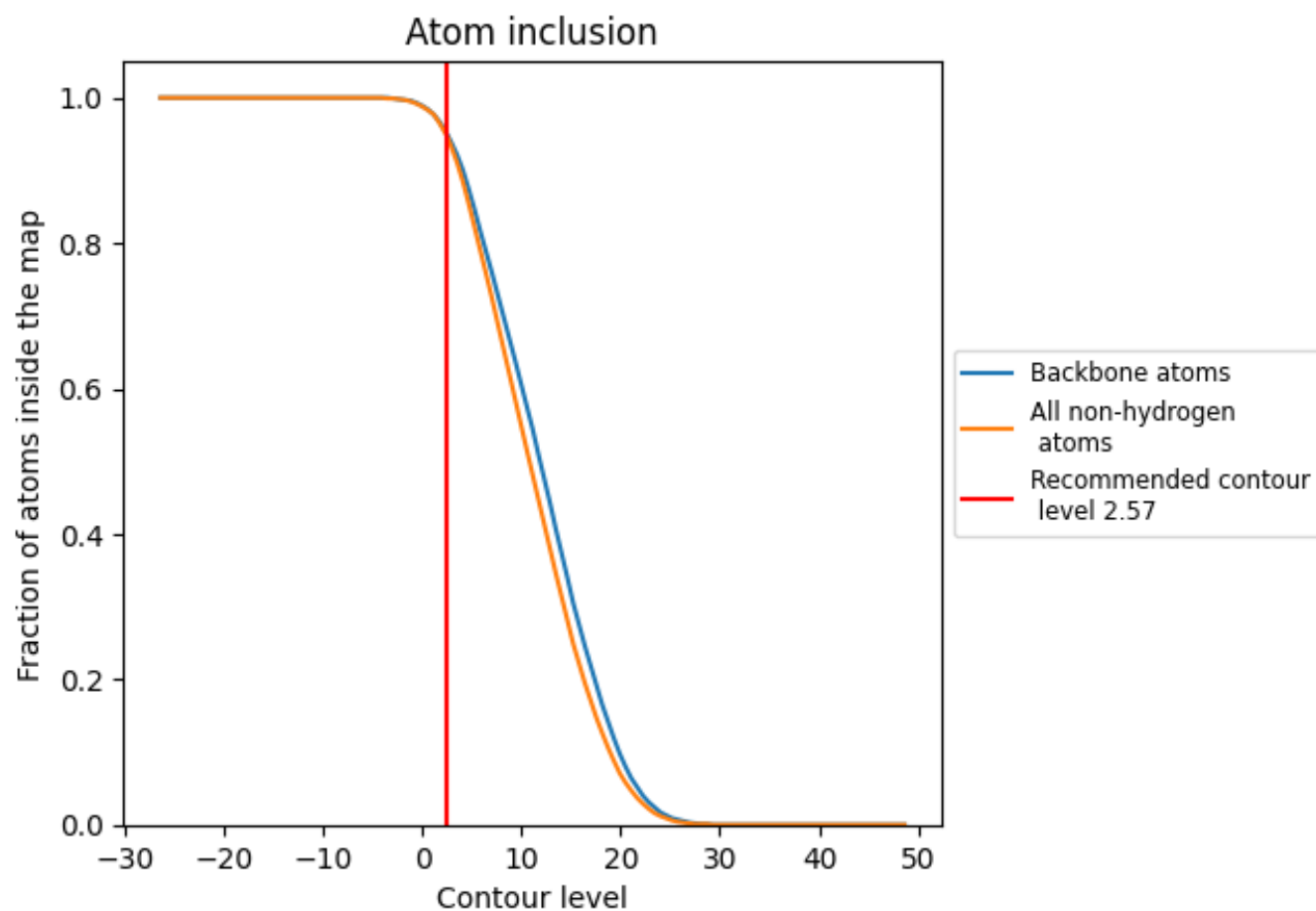
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (2.57).

9.4 Atom inclusion [i](#)



At the recommended contour level, 95% 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 (2.57) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.9460	<div><div></div></div> 0.5490
1	<div><div></div></div> 0.8790	<div><div></div></div> 0.3980
2	<div><div></div></div> 0.9350	<div><div></div></div> 0.5010
3	<div><div></div></div> 0.9320	<div><div></div></div> 0.5130
4	<div><div></div></div> 0.9280	<div><div></div></div> 0.4910
A	<div><div></div></div> 0.9570	<div><div></div></div> 0.5800
B	<div><div></div></div> 0.9640	<div><div></div></div> 0.5900
C	<div><div></div></div> 0.9870	<div><div></div></div> 0.5880
D	<div><div></div></div> 0.9750	<div><div></div></div> 0.5830
E	<div><div></div></div> 0.9880	<div><div></div></div> 0.5750
F	<div><div></div></div> 0.9370	<div><div></div></div> 0.5560
G	<div><div></div></div> 0.9340	<div><div></div></div> 0.5440
H	<div><div></div></div> 0.9420	<div><div></div></div> 0.5440
I	<div><div></div></div> 0.9610	<div><div></div></div> 0.5630
J	<div><div></div></div> 0.8390	<div><div></div></div> 0.4940
K	<div><div></div></div> 0.8610	<div><div></div></div> 0.4450
L	<div><div></div></div> 0.9580	<div><div></div></div> 0.5700

1.0

0.0

<0.0