



Full wwPDB EM Validation Report ⓘ

Nov 4, 2024 – 04:57 AM JST

PDB ID : 7EW6
EMDB ID : EMD-31348
Title : Barley photosystem I-LHCI-Lhca5 supercomplex
Authors : Wang, W.D.; Shen, L.; Tang, K.; Han, G.Y.; Zhang, X.; Shen, J.R.
Deposited on : 2021-05-24
Resolution : 3.40 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.dev113
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

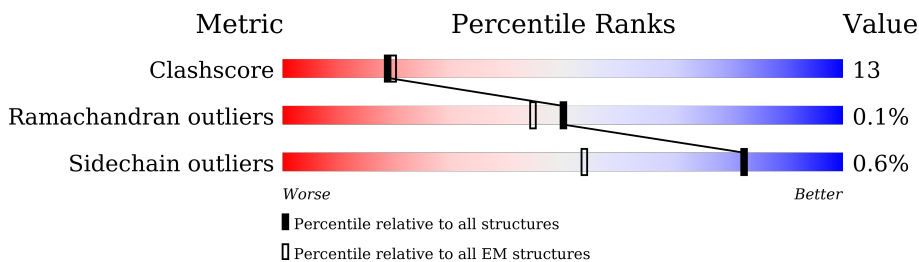
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.40 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.



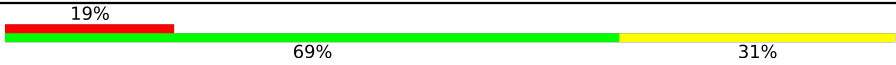

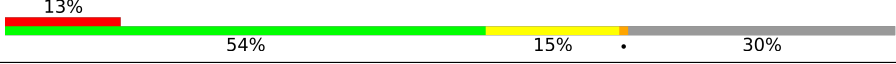
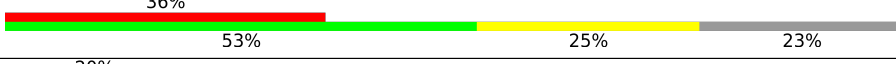

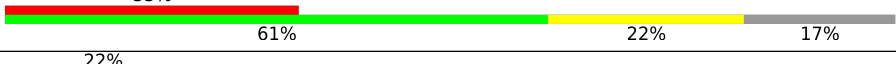

Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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

Mol	Chain	Length	Quality of chain
1	A	750	 77% 21%
2	B	734	 84% 15%
3	C	81	 73% 27%
4	D	205	 8% 53% 16% 31%
5	E	147	 38% 8% 54%
6	F	235	 49% 17% 33%
7	H	143	 20% 37% 6% 57%
8	I	36	 69% 14% 17%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
9	J	42	
10	K	131	
11	L	209	
12	1	247	
13	2	255	
14	3	269	
15	5	257	

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
16	CL0	A	801	X	-	-	-
17	CLA	1	504	X	-	-	-
17	CLA	1	505	X	-	-	-
17	CLA	1	506	X	-	-	-
17	CLA	1	507	X	-	-	-
17	CLA	1	508	X	-	-	-
17	CLA	1	510	X	-	-	-
17	CLA	1	511	X	-	-	-
17	CLA	1	515	X	-	-	-
17	CLA	2	504	X	-	-	-
17	CLA	2	506	X	-	-	-
17	CLA	2	507	X	-	-	-
17	CLA	2	508	X	-	-	-
17	CLA	2	509	X	-	-	-
17	CLA	2	510	X	-	-	-
17	CLA	2	511	X	-	-	-
17	CLA	2	514	X	-	-	-
17	CLA	3	301	X	-	-	-
17	CLA	3	306	X	-	-	-
17	CLA	3	307	X	-	-	-
17	CLA	3	308	X	-	-	-
17	CLA	3	310	X	-	-	-
17	CLA	3	311	X	-	-	-
17	CLA	3	312	X	-	-	-
17	CLA	3	313	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
17	CLA	3	314	X	-	-	-
17	CLA	3	316	X	-	-	-
17	CLA	3	317	X	-	-	-
17	CLA	3	318	X	-	-	-
17	CLA	5	305	X	-	-	-
17	CLA	5	306	X	-	-	-
17	CLA	5	307	X	-	-	-
17	CLA	5	308	X	-	-	-
17	CLA	5	309	X	-	-	-
17	CLA	5	310	X	-	-	-
17	CLA	5	311	X	-	-	-
17	CLA	5	312	X	-	-	-
17	CLA	5	313	X	-	-	-
17	CLA	5	316	X	-	-	-
17	CLA	A	802	X	-	-	-
17	CLA	A	803	X	-	-	-
17	CLA	A	804	X	-	-	-
17	CLA	A	805	X	-	-	-
17	CLA	A	806	X	-	-	-
17	CLA	A	807	X	-	-	-
17	CLA	A	808	X	-	-	-
17	CLA	A	809	X	-	-	-
17	CLA	A	810	X	-	-	-
17	CLA	A	811	X	-	-	-
17	CLA	A	812	X	-	-	-
17	CLA	A	813	X	-	-	-
17	CLA	A	814	X	-	-	-
17	CLA	A	815	X	-	-	-
17	CLA	A	816	X	-	-	-
17	CLA	A	817	X	-	-	-
17	CLA	A	818	X	-	-	-
17	CLA	A	819	X	-	-	-
17	CLA	A	820	X	-	-	-
17	CLA	A	821	X	-	-	-
17	CLA	A	822	X	-	-	-
17	CLA	A	823	X	-	-	-
17	CLA	A	824	X	-	-	-
17	CLA	A	825	X	-	-	-
17	CLA	A	826	X	-	-	-
17	CLA	A	827	X	-	-	-
17	CLA	A	828	X	-	-	-
17	CLA	A	829	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
17	CLA	A	830	X	-	-	-
17	CLA	A	831	X	-	-	-
17	CLA	A	832	X	-	-	-
17	CLA	A	833	X	-	-	-
17	CLA	A	834	X	-	-	-
17	CLA	A	835	X	-	-	-
17	CLA	A	836	X	-	-	-
17	CLA	A	837	X	-	-	-
17	CLA	A	838	X	-	-	-
17	CLA	A	839	X	-	-	-
17	CLA	A	840	X	-	-	-
17	CLA	A	842	X	-	-	-
17	CLA	A	852	X	-	-	-
17	CLA	B	801	X	-	-	-
17	CLA	B	802	X	-	-	-
17	CLA	B	803	X	-	-	-
17	CLA	B	804	X	-	-	-
17	CLA	B	805	X	-	-	-
17	CLA	B	806	X	-	-	-
17	CLA	B	807	X	-	-	-
17	CLA	B	808	X	-	-	-
17	CLA	B	809	X	-	-	-
17	CLA	B	810	X	-	-	-
17	CLA	B	811	X	-	-	-
17	CLA	B	812	X	-	-	-
17	CLA	B	813	X	-	-	-
17	CLA	B	814	X	-	-	-
17	CLA	B	815	X	-	-	-
17	CLA	B	816	X	-	-	-
17	CLA	B	817	X	-	-	-
17	CLA	B	818	X	-	-	-
17	CLA	B	819	X	-	-	-
17	CLA	B	820	X	-	-	-
17	CLA	B	821	X	-	-	-
17	CLA	B	822	X	-	-	-
17	CLA	B	823	X	-	-	-
17	CLA	B	824	X	-	-	-
17	CLA	B	825	X	-	-	-
17	CLA	B	826	X	-	-	-
17	CLA	B	827	X	-	-	-
17	CLA	B	828	X	-	-	-
17	CLA	B	829	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
17	CLA	B	830	X	-	-	-
17	CLA	B	831	X	-	-	-
17	CLA	B	832	X	-	-	-
17	CLA	B	833	X	-	-	-
17	CLA	B	834	X	-	-	-
17	CLA	B	835	X	-	-	-
17	CLA	B	837	X	-	-	-
17	CLA	B	838	X	-	-	-
17	CLA	B	839	X	-	-	-
17	CLA	B	840	X	-	-	-
17	CLA	B	841	X	-	-	-
17	CLA	B	842	X	-	-	-
17	CLA	F	802	X	-	-	-
17	CLA	F	803	X	-	-	-
17	CLA	J	101	X	-	-	-
17	CLA	K	201	X	-	-	-
17	CLA	K	202	X	-	-	-
17	CLA	K	203	X	-	-	-
17	CLA	K	205	X	-	-	-
17	CLA	L	301	X	-	-	-
17	CLA	L	302	X	-	-	-
17	CLA	L	303	X	-	-	-
17	CLA	L	304	X	-	-	-
25	CHL	1	512	X	-	-	-
25	CHL	1	514	X	-	-	-
25	CHL	1	517	X	-	-	-
25	CHL	2	512	X	-	-	-
25	CHL	2	513	X	-	-	-
25	CHL	2	515	X	-	-	-
25	CHL	2	516	X	-	-	-
25	CHL	3	302	X	-	-	-
25	CHL	3	315	X	-	-	-
25	CHL	5	314	X	-	-	-
25	CHL	5	315	X	-	-	-
25	CHL	5	317	X	-	-	-

2 Entry composition

There are 26 unique types of molecules in this entry. The entry contains 32973 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Photosystem I P700 chlorophyll a apoprotein A1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	742	Total	C	N	O	S	0	0
			5813	3812	983	1000	18		

- Molecule 2 is a protein called Photosystem I P700 chlorophyll a apoprotein A2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	733	Total	C	N	O	S	0	0
			5849	3834	995	1006	14		

- Molecule 3 is a protein called Photosystem I iron-sulfur center.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	81	Total	C	N	O	S	0	0
			610	376	105	117	12		

- Molecule 4 is a protein called Photosystem I reaction center subunit II, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	142	Total	C	N	O	S	0	0
			1113	716	193	201	3		

- Molecule 5 is a protein called Photosystem I reaction center subunit IV, chloroplastic.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	E	68	Total	C	N	O	0	0
			538	341	98	99		

- Molecule 6 is a protein called Photosystem I reaction center subunit III, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	158	Total	C	N	O	S	0	0
			1203	774	208	218	3		

- Molecule 7 is a protein called Photosystem I reaction center subunit VI, chloroplastic.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	H	61	Total	C	N	O	0	0
			454	303	76	75		

- Molecule 8 is a protein called Photosystem I reaction center subunit VIII.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	I	30	Total	C	N	O	0	0
			232	161	35	36		

- Molecule 9 is a protein called Photosystem I reaction center subunit IX.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	42	Total	C	N	O	S	0	0
			333	228	51	53	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	K	84	Total	C	N	O	S	0	0
			565	359	94	108	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	L	146	Total	C	N	O	S	0	0
			1088	716	174	197	1		

- Molecule 12 is a protein called Chlorophyll a-b binding protein Lhca1.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	1	191	Total	C	N	O	S	0	0
			1422	921	239	258	4		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	73	PHE	UNK	conflict	UNP A0A287WC32
1	74	GLU	UNK	conflict	UNP A0A287WC32
1	75	ARG	UNK	conflict	UNP A0A287WC32

- Molecule 13 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	2	203	Total	C	N	O	S	0	0
			1561	1018	257	283	3		

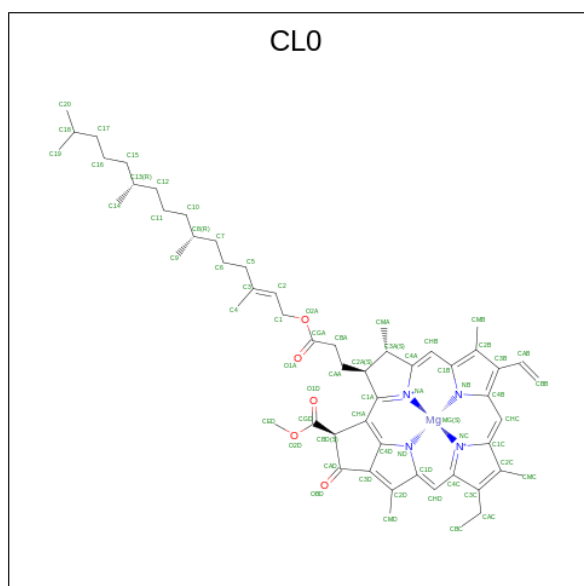
- Molecule 14 is a protein called Chlorophyll a-b binding protein, chloroplastic.

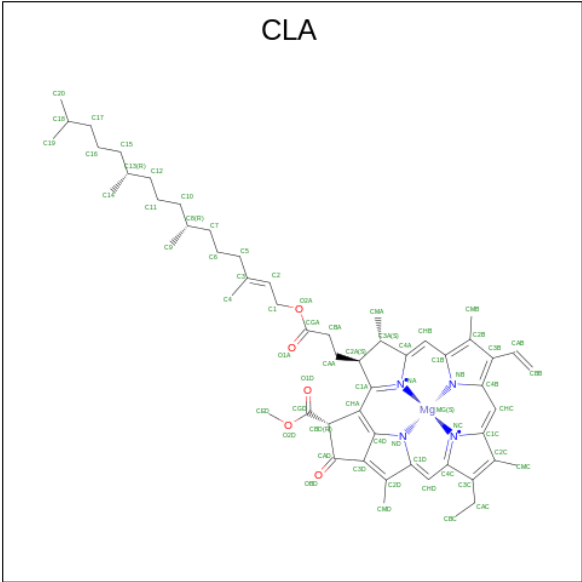
Mol	Chain	Residues	Atoms					AltConf	Trace
14	3	222	Total	C	N	O	S	0	0
			1629	1063	271	292	3		

- Molecule 15 is a protein called Chlorophyll a-b binding protein Lhca5.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	5	205	Total	C	N	O	S	0	0
			1486	962	247	270	7		

- Molecule 16 is CHLOROPHYLL A ISOMER (three-letter code: CL0) (formula: $C_{55}H_{72}MgN_4O_5$).





Mol	Chain	Residues	Atoms					AltConf
17	A	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
17	A	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
17	A	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
17	A	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
17	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	A	1	Total	C	Mg	N	O	0
			39	32	1	4	2	
17	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	A	1	Total	C	Mg	N	O	0
			39	32	1	4	2	
17	A	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
17	A	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
17	A	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
17	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
17	A	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
17	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
17	A	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
17	A	1	Total	C	Mg	N	O	0
			39	32	1	4	2	
17	A	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
17	A	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
17	A	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
17	A	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
17	A	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
17	A	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
17	A	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
17	A	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
17	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
17	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	A	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
17	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
17	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
17	A	1	Total	C	Mg	N	O	0
			63	53	1	4	5	
17	A	1	Total	C	Mg	N	O	0
			45	37	1	4	3	
17	A	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
17	A	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
17	A	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
17	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
17	A	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
17	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	A	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
17	A	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
17	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
17	A	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
17	B	1	Total	C	Mg	N	O	0
			39	31	1	4	3	
17	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
17	B	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
17	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
17	B	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
17	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
17	B	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
17	B	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
17	B	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
17	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
17	B	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
17	B	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
17	B	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
17	B	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
17	B	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
17	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			42	34	1	4	3	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
17	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
17	B	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
17	F	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
17	F	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
17	J	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
17	K	1	Total	C	Mg	N	O	0
			37	31	1	4	1	
17	K	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
17	K	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
17	K	1	Total	C	Mg	N	O	0
			39	31	1	4	3	
17	L	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
17	L	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
17	L	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
17	L	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
17	1	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
17	1	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
17	1	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
17	1	1	Total	C	Mg	N	O	0
			42	34	1	4	3	

Continued on next page...

Continued from previous page...

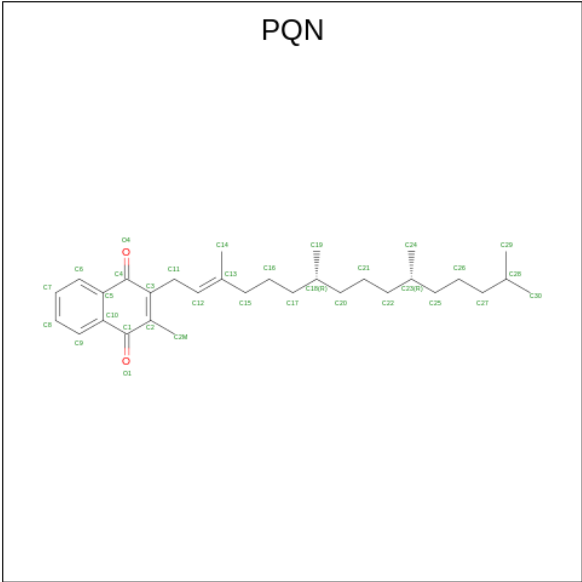
Mol	Chain	Residues	Atoms					AltConf
17	1	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
17	1	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
17	1	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
17	1	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
17	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	1	1	Total	C	Mg	N	O	0
			44	35	1	4	4	
17	2	1	Total	C	Mg	N	O	0
			36	30	1	4	1	
17	2	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
17	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	2	1	Total	C	Mg	N	O	0
			49	41	1	4	3	
17	2	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
17	2	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
17	2	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
17	2	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
17	2	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
17	3	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
17	3	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
17	3	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
17	3	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
17	3	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
17	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

Continued on next page...

Continued from previous page...

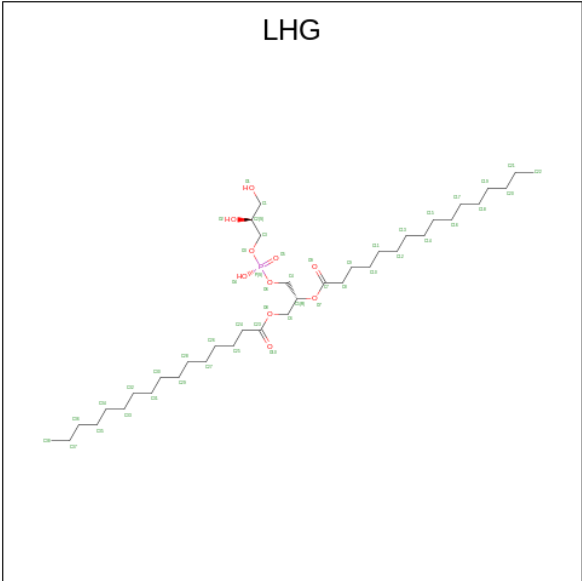
Mol	Chain	Residues	Atoms					AltConf
17	3	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
17	3	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
17	3	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
17	3	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
17	3	1	Total	C	Mg	N	O	0
			37	31	1	4	1	
17	3	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
17	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
17	5	1	Total	C	Mg	N	O	0
			38	30	1	4	3	
17	5	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
17	5	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	5	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
17	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
17	5	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
17	5	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
17	5	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
17	5	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
17	5	1	Total	C	Mg	N	O	0
			41	33	1	4	3	

- Molecule 18 is PHYLLOQUINONE (three-letter code: PQN) (formula: C₃₁H₄₆O₂).



Mol	Chain	Residues	Atoms			AltConf
18	A	1	Total	C	O	0
			33	31	2	
18	B	1	Total	C	O	0
			30	28	2	

- Molecule 19 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: C₃₈H₇₅O₁₀P).



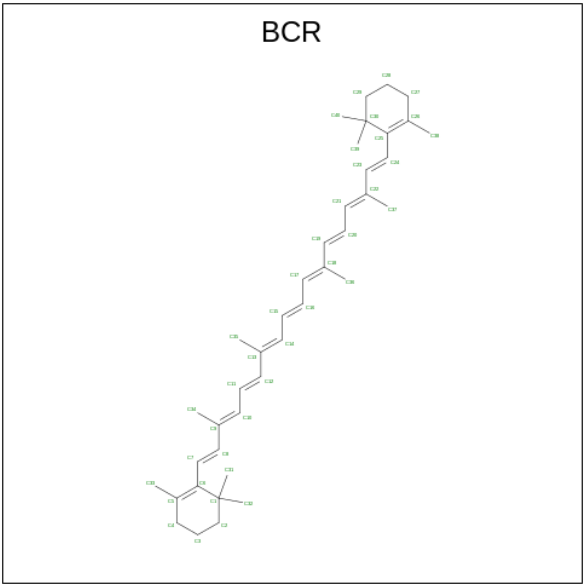
Mol	Chain	Residues	Atoms				AltConf
19	A	1	Total	C	O	P	0
			49	38	10	1	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf
19	A	1	Total	C	O	P	0
			30	19	10	1	
19	B	1	Total	C	O	P	0
			38	27	10	1	
19	1	1	Total	C	O	P	0
			49	38	10	1	
19	2	1	Total	C	O	P	0
			35	24	10	1	

- Molecule 20 is BETA-CAROTENE (three-letter code: BCR) (formula: C₄₀H₅₆).



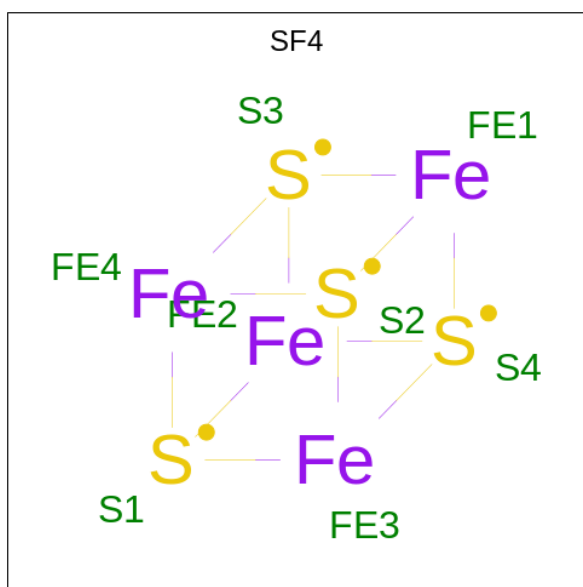
Mol	Chain	Residues	Atoms		AltConf
20	A	1	Total	C	0
			40	40	
20	A	1	Total	C	0
			40	40	
20	A	1	Total	C	0
			40	40	
20	A	1	Total	C	0
			40	40	
20	A	1	Total	C	0
			39	39	
20	A	1	Total	C	0
			40	40	
20	A	1	Total	C	0
			40	40	

Continued on next page...

Continued from previous page...

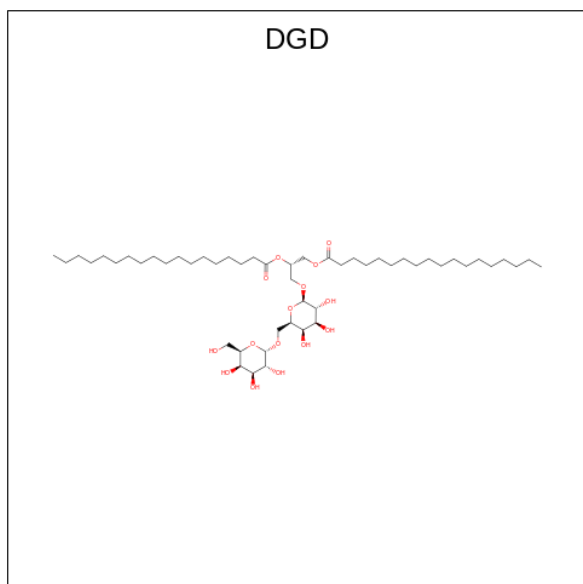
Mol	Chain	Residues	Atoms	AltConf
20	B	1	Total C 40 40	0
20	B	1	Total C 40 40	0
20	B	1	Total C 40 40	0
20	B	1	Total C 40 40	0
20	B	1	Total C 40 40	0
20	B	1	Total C 40 40	0
20	B	1	Total C 40 40	0
20	F	1	Total C 40 40	0
20	F	1	Total C 40 40	0
20	I	1	Total C 40 40	0
20	J	1	Total C 40 40	0
20	K	1	Total C 40 40	0
20	L	1	Total C 40 40	0
20	L	1	Total C 40 40	0
20	1	1	Total C 19 19	0
20	2	1	Total C 40 40	0
20	3	1	Total C 40 40	0
20	5	1	Total C 40 40	0

- Molecule 21 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



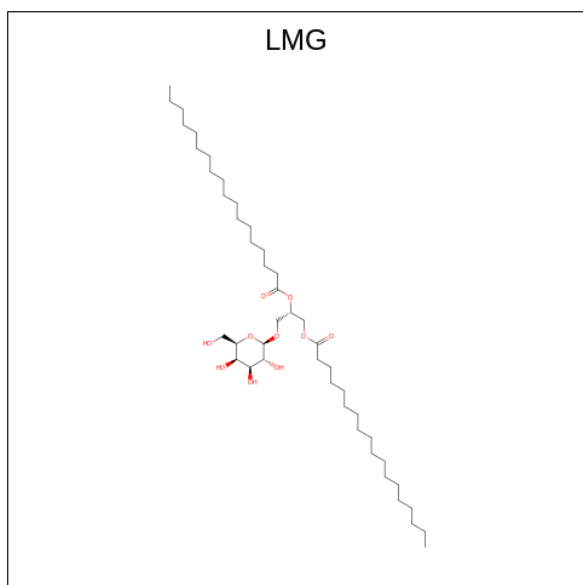
Mol	Chain	Residues	Atoms			AltConf
21	A	1	Total	Fe	S	0
			8	4	4	
21	C	1	Total	Fe	S	0
			8	4	4	
21	C	1	Total	Fe	S	0
			8	4	4	

- Molecule 22 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: $C_{51}H_{96}O_{15}$).



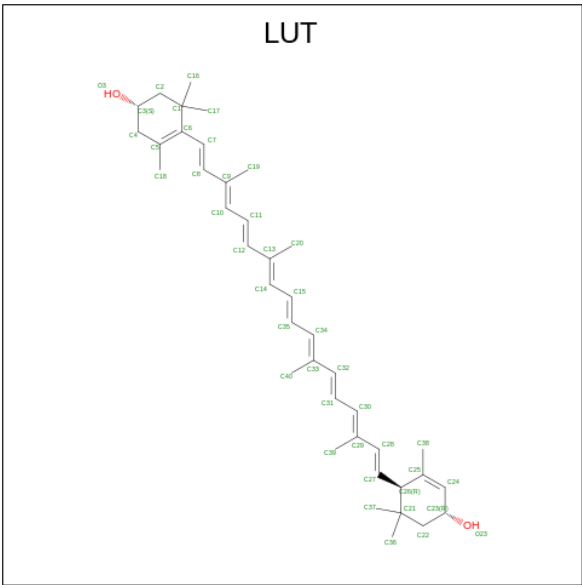
Mol	Chain	Residues	Atoms			AltConf
22	B	1	Total	C	O	0
			59	44	15	
22	J	1	Total	C	O	0
			66	51	15	

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



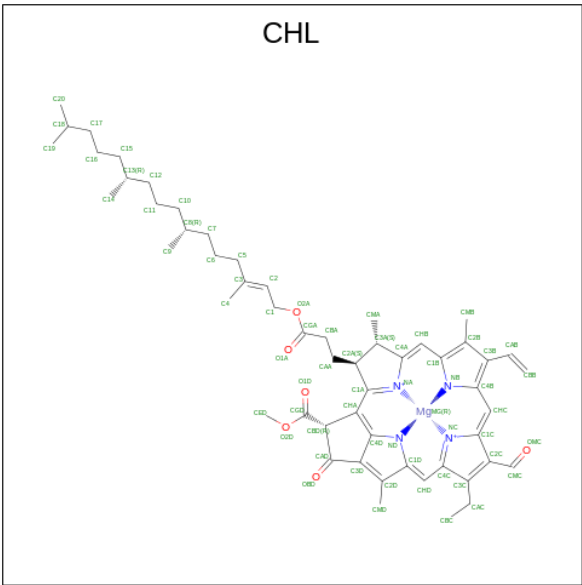
Mol	Chain	Residues	Atoms			AltConf
23	F	1	Total	C	O	0
			30	20	10	
23	F	1	Total	C	O	0
			45	35	10	
23	2	1	Total	C	O	0
			16	9	7	
23	2	1	Total	C	O	0
			36	26	10	
23	5	1	Total	C	O	0
			32	22	10	

- Molecule 24 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (three-letter code: LUT) (formula: $C_{40}H_{56}O_2$).



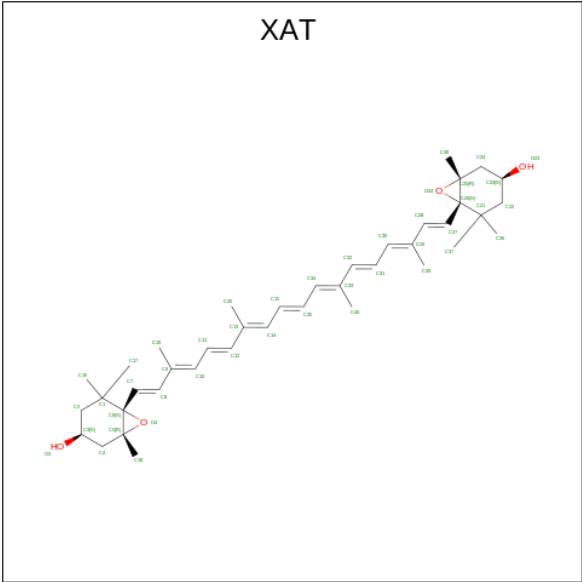
Mol	Chain	Residues	Atoms			AltConf
24	1	1	Total	C	O	0
			42	40	2	
24	1	1	Total	C	O	0
			42	40	2	
24	2	1	Total	C	O	0
			42	40	2	
24	3	1	Total	C	O	0
			42	40	2	
24	3	1	Total	C	O	0
			42	40	2	
24	5	1	Total	C	O	0
			42	40	2	

- Molecule 25 is CHLOROPHYLL B (three-letter code: CHL) (formula: C₅₅H₇₀MgN₄O₆).



Mol	Chain	Residues	Atoms					AltConf
25	1	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
25	1	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
25	1	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
25	2	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
25	2	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
25	2	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
25	2	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
25	3	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
25	3	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
25	5	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
25	5	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
25	5	1	Total	C	Mg	N	O	0
			40	31	1	4	4	

- Molecule 26 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).

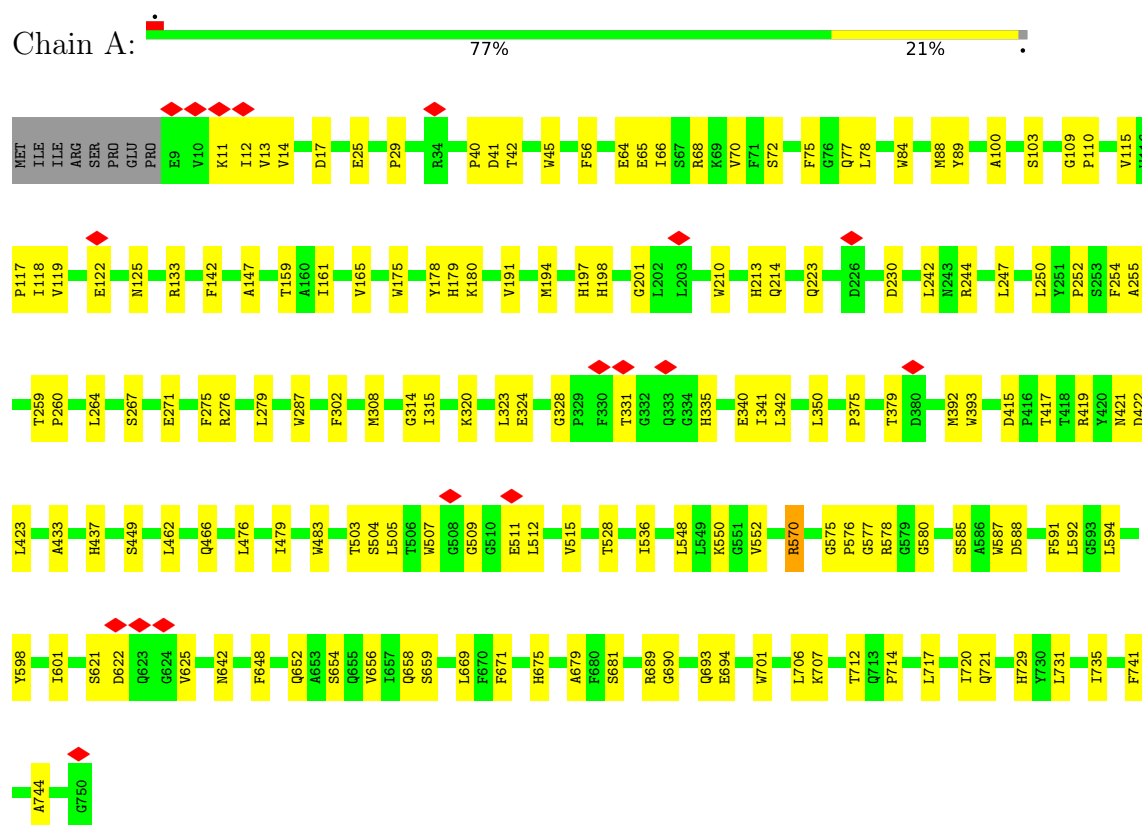


Mol	Chain	Residues	Atoms			AltConf
26	2	1	Total	C	O	0
			44	40	4	
26	5	1	Total	C	O	0
			44	40	4	

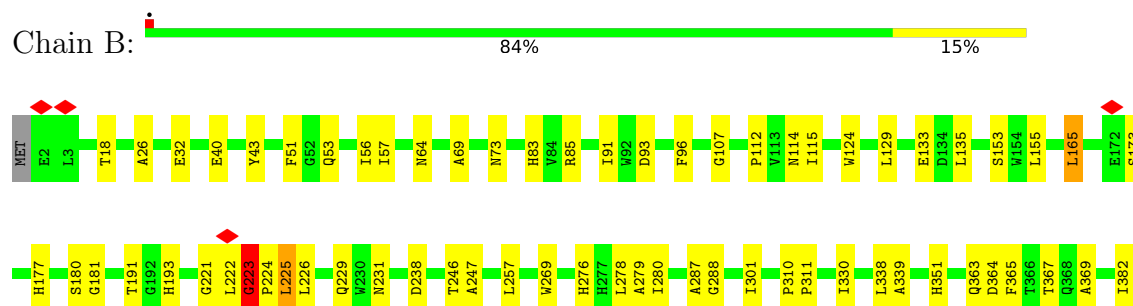
3 Residue-property plots

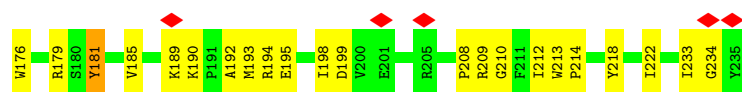
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

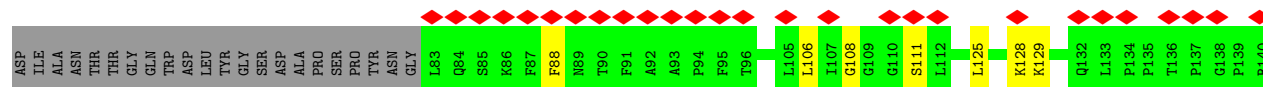
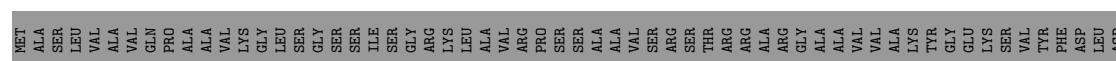
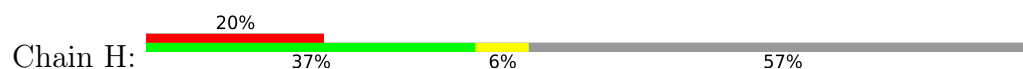


- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

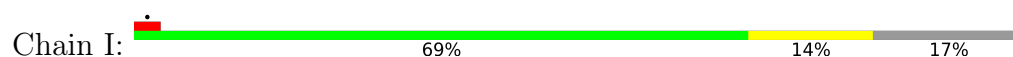




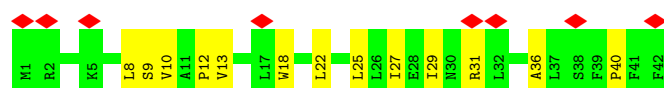
- Molecule 7: Photosystem I reaction center subunit VI, chloroplastic



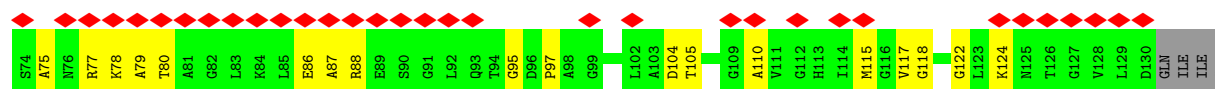
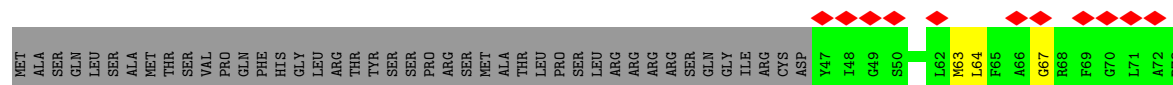
- Molecule 8: Photosystem I reaction center subunit VIII



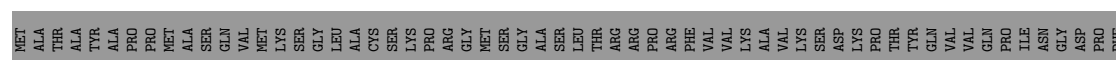
- Molecule 9: Photosystem I reaction center subunit IX

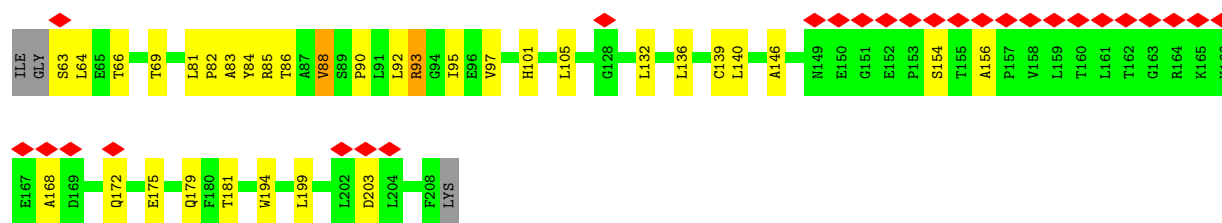


- Molecule 10: Photosystem I reaction center subunit psaK, chloroplastic

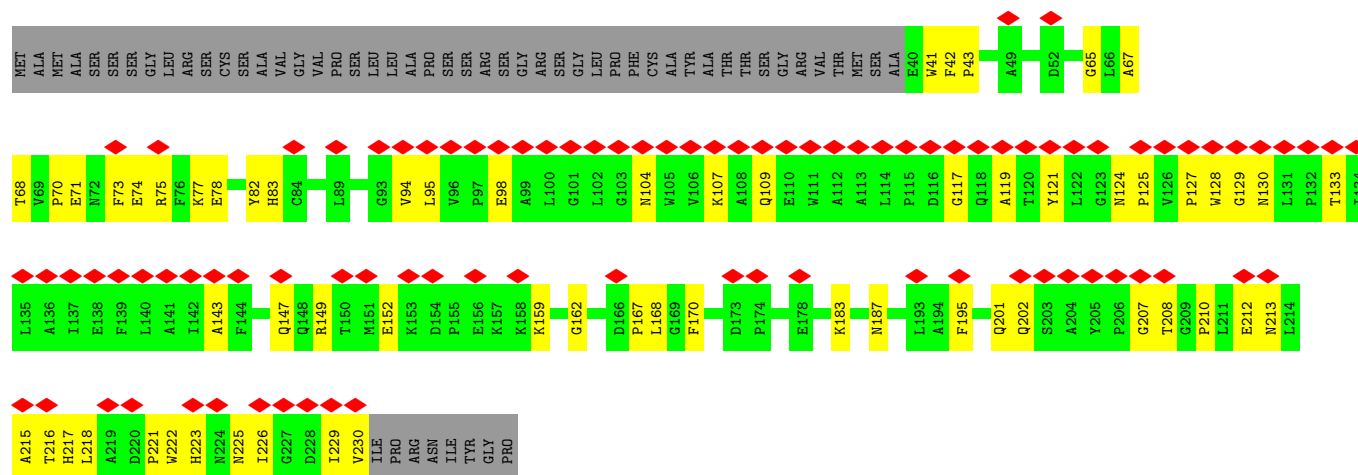


- Molecule 11: Photosystem I reaction center subunit XI, chloroplastic

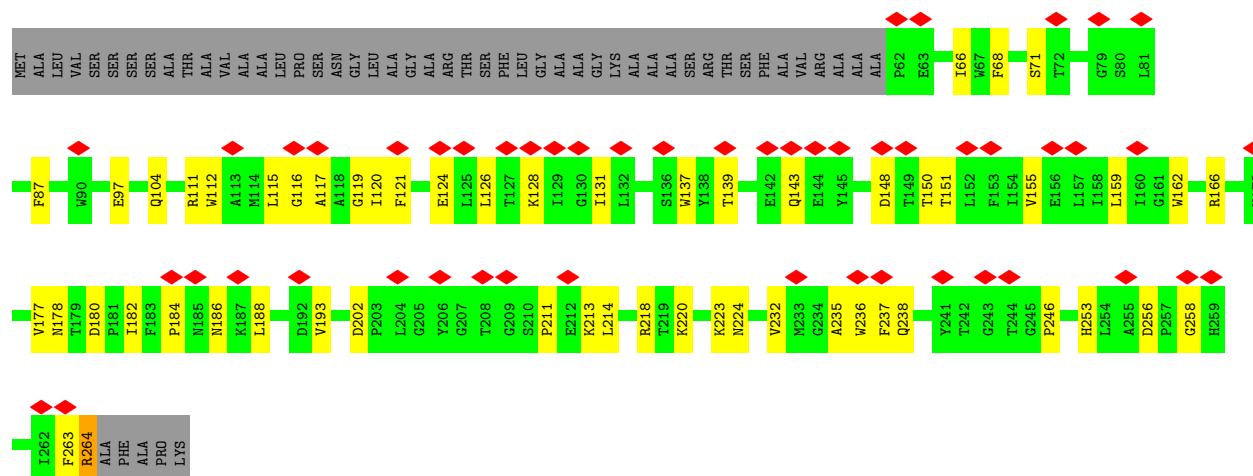




• Molecule 12: Chlorophyll a-b binding protein Lhca1

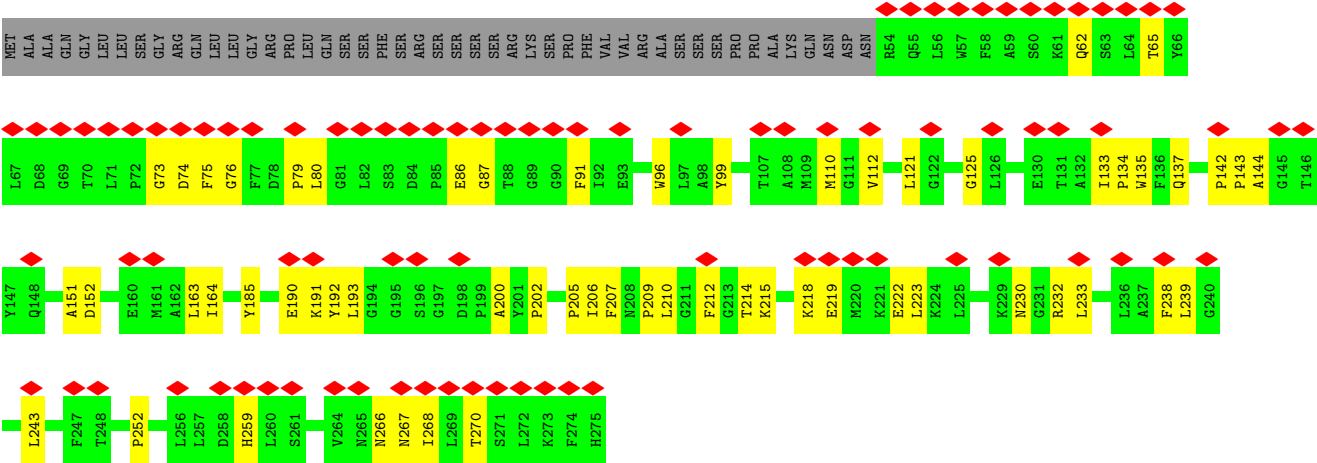


• Molecule 13: Chlorophyll a-b binding protein, chloroplastic

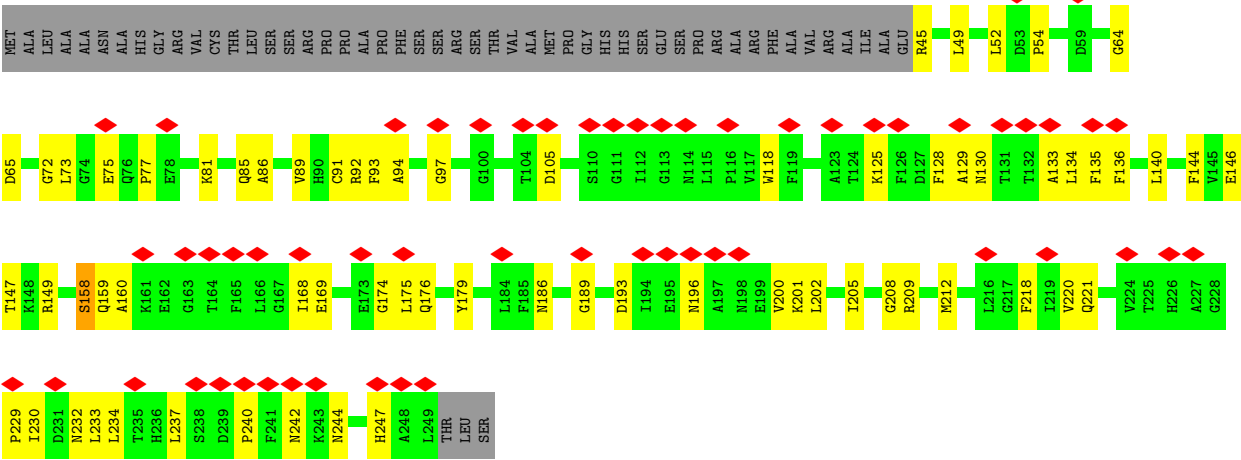


• Molecule 14: Chlorophyll a-b binding protein, chloroplastic





● Molecule 15: Chlorophyll a-b binding protein Lhca5



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	103844	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	5.056	Depositor
Minimum map value	-2.079	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.082	Depositor
Recommended contour level	0.72	Depositor
Map size (Å)	575.08, 575.08, 575.08	wwPDB
Map dimensions	440, 440, 440	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.307, 1.307, 1.307	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.66	0/6010	0.49	0/8202
2	B	0.69	0/6058	0.51	1/8273 (0.0%)
3	C	0.73	0/621	0.53	0/840
4	D	0.61	0/1142	0.53	0/1542
5	E	0.65	0/551	0.49	0/751
6	F	0.63	2/1229 (0.2%)	0.48	0/1664
7	H	0.37	0/467	0.46	0/631
8	I	0.55	0/238	0.48	0/324
9	J	0.54	0/343	0.58	0/467
10	K	0.38	0/571	0.55	0/775
11	L	0.57	0/1120	0.52	0/1534
12	1	0.36	0/1467	0.43	0/2008
13	2	0.42	0/1616	0.46	0/2215
14	3	0.41	0/1682	0.50	0/2295
15	5	0.45	0/1527	0.50	0/2085
All	All	0.59	2/24642 (0.0%)	0.50	1/33606 (0.0%)

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

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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	F	181	TYR	CE1-CZ	-8.91	1.26	1.38
6	F	181	TYR	CG-CD1	-5.10	1.32	1.39

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	223	GLY	N-CA-C	-5.13	100.26	113.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	222	LEU	Mainchain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5813	0	5633	132	0
2	B	5849	0	5600	95	0
3	C	610	0	597	22	0
4	D	1113	0	1113	27	0
5	E	538	0	537	8	0
6	F	1203	0	1199	42	0
7	H	454	0	487	6	0
8	I	232	0	254	4	0
9	J	333	0	347	12	0
10	K	565	0	557	18	0
11	L	1088	0	1079	30	0
12	1	1422	0	1324	50	0
13	2	1561	0	1485	57	0
14	3	1629	0	1496	47	0
15	5	1486	0	1389	58	0
16	A	61	0	62	4	0
17	1	471	0	375	27	0
17	2	454	0	383	23	0
17	3	590	0	442	33	0
17	5	468	0	375	21	0
17	A	2024	0	1724	73	0
17	B	2118	0	1848	86	0
17	F	83	0	60	5	0
17	J	42	0	31	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	K	157	0	107	7	0
17	L	193	0	152	8	0
18	A	33	0	46	2	0
18	B	30	0	37	1	0
19	1	49	0	74	5	0
19	2	35	0	40	2	0
19	A	79	0	104	8	0
19	B	38	0	46	0	0
20	1	19	0	26	3	0
20	2	40	0	56	4	0
20	3	40	0	56	4	0
20	5	40	0	56	6	0
20	A	279	0	389	18	0
20	B	280	0	392	20	0
20	F	80	0	112	5	0
20	I	40	0	56	4	0
20	J	40	0	56	1	0
20	K	40	0	56	2	0
20	L	80	0	112	10	0
21	A	8	0	0	0	0
21	C	16	0	0	1	0
22	B	59	0	79	4	0
22	J	66	0	96	3	0
23	2	52	0	55	3	0
23	5	32	0	34	1	0
23	F	75	0	90	3	0
24	1	84	0	112	11	0
24	2	42	0	56	9	0
24	3	84	0	112	14	0
24	5	42	0	56	8	0
25	1	129	0	83	7	0
25	2	174	0	110	13	0
25	3	90	0	60	2	0
25	5	133	0	80	8	0
26	2	44	0	56	7	0
26	5	44	0	56	5	0
All	All	32973	0	31505	816	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 13.

All (816) 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)
6:F:181:TYR:CE1	6:F:185:VAL:CG1	2.51	0.92
6:F:181:TYR:HE1	6:F:185:VAL:CG1	1.82	0.92
6:F:181:TYR:CE1	6:F:185:VAL:HG11	2.07	0.88
16:A:801:CL0:H13	17:B:802:CLA:OBD	1.77	0.84
6:F:181:TYR:CE1	6:F:185:VAL:HG13	2.18	0.78
2:B:124:TRP:CZ2	2:B:124:TRP:CD2	2.75	0.74
15:5:129:ALA:HB1	15:5:134:LEU:HD11	1.71	0.73
2:B:26:ALA:HB2	22:B:850:DGD:HA42	1.72	0.71
17:A:821:CLA:HAA2	10:K:79:ALA:HB3	1.73	0.71
9:J:10:VAL:HG13	9:J:12:PRO:HD2	1.72	0.71
1:A:175:TRP:HB2	17:A:810:CLA:HMC3	1.73	0.70
5:E:92:LYS:NZ	5:E:102:ASN:OD1	2.23	0.70
14:3:219:GLU:O	14:3:223:LEU:N	2.24	0.70
1:A:714:PRO:HB3	17:A:852:CLA:HMC3	1.73	0.69
12:1:128:TRP:HE1	17:1:515:CLA:CAD	2.06	0.69
12:1:83:HIS:HD2	24:1:502:LUT:H35	1.58	0.69
10:K:95:GLY:C	17:K:201:CLA:H3A	2.13	0.69
13:2:186:ASN:HB3	25:2:516:CHL:C1D	2.23	0.68
11:L:156:ALA:HB2	11:L:172:GLN:HG3	1.76	0.68
4:D:104:GLU:N	4:D:104:GLU:OE1	2.27	0.68
15:5:135:PHE:HB2	25:5:314:CHL:HBC1	1.75	0.67
14:3:112:VAL:HG11	24:3:303:LUT:H12	1.77	0.66
17:B:807:CLA:H51	22:B:850:DGD:HB71	1.76	0.66
12:1:67:ALA:HB1	12:1:73:PHE:HD1	1.60	0.66
1:A:570:ARG:NH2	19:A:843:LHG:O10	2.29	0.66
1:A:40:PRO:HG2	6:F:192:ALA:HB1	1.77	0.66
6:F:181:TYR:HE1	6:F:185:VAL:HG11	1.48	0.66
17:B:826:CLA:HMA1	20:B:848:BCR:H14C	1.78	0.65
14:3:209:PRO:HD2	24:3:303:LUT:H23	1.79	0.65
1:A:264:LEU:HD21	10:K:117:VAL:HG22	1.78	0.65
11:L:88:VAL:HG23	11:L:93:ARG:HD3	1.78	0.65
12:1:98:GLU:HG2	12:1:104:ASN:HA	1.79	0.65
2:B:476:ILE:HG22	2:B:477:LEU:H	1.62	0.64
15:5:118:TRP:HE1	15:5:229:PRO:HD3	1.63	0.64
17:B:823:CLA:HAB	17:B:842:CLA:HED1	1.80	0.64
17:L:301:CLA:HBB1	17:L:301:CLA:HMB1	1.78	0.64
12:1:149:ARG:HA	17:1:513:CLA:HBC3	1.80	0.64
1:A:275:PHE:HE2	17:A:817:CLA:HBB1	1.63	0.64
17:A:806:CLA:H41	19:A:843:LHG:H271	1.80	0.64
25:1:517:CHL:HED1	15:5:147:THR:HB	1.79	0.64
17:A:820:CLA:HMB1	17:A:820:CLA:HBB1	1.78	0.64
10:K:63:MET:HE1	10:K:115:MET:HB2	1.80	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:238:ASP:HB2	2:B:269:TRP:HZ3	1.62	0.63
12:1:229:ILE:HG13	12:1:230:VAL:H	1.63	0.63
4:D:167:VAL:HG21	4:D:173:ASN:HD21	1.64	0.63
12:1:119:ALA:H	12:1:129:GLY:HA3	1.63	0.63
13:2:186:ASN:HB3	25:2:516:CHL:C2D	2.29	0.63
1:A:314:GLY:HA2	10:K:88:ARG:HH22	1.63	0.63
22:J:103:DGD:O5E	22:J:103:DGD:O4E	2.09	0.63
12:1:183:LYS:O	12:1:187:ASN:ND2	2.24	0.63
1:A:341:ILE:HG22	1:A:419:ARG:HB3	1.79	0.63
2:B:339:ALA:HB2	20:B:848:BCR:H372	1.79	0.63
2:B:246:THR:OG1	2:B:247:ALA:N	2.32	0.62
13:2:258:GLY:HA3	14:3:151:ALA:HA	1.81	0.62
17:5:309:CLA:HMB1	17:5:309:CLA:HBB1	1.80	0.62
17:B:802:CLA:HMB1	17:B:802:CLA:HBB1	1.82	0.62
14:3:268:ILE:HD11	17:3:308:CLA:H11	1.81	0.62
24:3:303:LUT:O23	17:3:306:CLA:O1A	2.16	0.62
1:A:117:PRO:HB3	1:A:122:GLU:HB3	1.79	0.62
1:A:694:GLU:OE1	2:B:536:LYS:NZ	2.29	0.62
17:B:805:CLA:HBC3	17:B:830:CLA:H41	1.82	0.62
15:5:209:ARG:NH1	17:5:308:CLA:O2D	2.33	0.62
2:B:223:GLY:O	2:B:226:LEU:N	2.33	0.61
2:B:124:TRP:HB3	2:B:129:LEU:HD12	1.81	0.61
2:B:53:GLN:HB2	17:B:806:CLA:HMB2	1.81	0.61
1:A:65:GLU:N	1:A:65:GLU:OE1	2.33	0.61
2:B:330:ILE:HG21	17:B:806:CLA:HAC1	1.83	0.61
15:5:85:GLN:OE1	15:5:85:GLN:N	2.34	0.61
17:A:816:CLA:HBB1	17:A:816:CLA:HMB1	1.83	0.60
15:5:176:GLN:NE2	15:5:193:ASP:O	2.35	0.60
6:F:213:TRP:CD1	6:F:214:PRO:HD3	2.37	0.60
13:2:104:GLN:HE21	13:2:193:VAL:HG12	1.65	0.60
1:A:331:THR:HG21	19:A:844:LHG:HC11	1.82	0.60
13:2:166:ARG:NH2	13:2:177:VAL:O	2.34	0.60
17:A:802:CLA:HBB1	17:A:802:CLA:HMB1	1.83	0.60
2:B:279:ALA:HA	17:B:817:CLA:HMC3	1.84	0.60
2:B:133:GLU:N	2:B:133:GLU:OE1	2.34	0.59
14:3:112:VAL:HG11	24:3:303:LUT:H10	1.84	0.59
17:A:802:CLA:CGA	17:A:802:CLA:H3A	2.32	0.59
2:B:721:TYR:HB2	17:B:803:CLA:HED3	1.83	0.59
13:2:220:LYS:O	13:2:224:ASN:ND2	2.31	0.59
1:A:244:ARG:NH2	1:A:255:ALA:O	2.36	0.59
17:A:837:CLA:HBB1	17:A:837:CLA:HMB1	1.86	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:191:THR:HG21	2:B:278:LEU:HB2	1.85	0.58
2:B:85:ARG:HB3	2:B:115:ILE:HD12	1.85	0.58
1:A:656:VAL:HG21	1:A:741:PHE:HA	1.85	0.58
1:A:656:VAL:HG22	1:A:744:ALA:HB3	1.85	0.58
12:1:229:ILE:HG13	12:1:230:VAL:N	2.18	0.58
1:A:279:LEU:HG	1:A:505:LEU:HD23	1.85	0.58
17:A:815:CLA:HED2	17:A:815:CLA:H2A	1.85	0.58
2:B:257:LEU:HD21	2:B:493:TRP:HE3	1.67	0.58
5:E:108:VAL:HG23	5:E:109:THR:HG22	1.86	0.58
3:C:62:PHE:O	3:C:63:LEU:HG	2.03	0.58
17:5:308:CLA:HBB1	17:5:308:CLA:HMB1	1.86	0.58
1:A:267:SER:O	1:A:267:SER:OG	2.17	0.57
17:B:806:CLA:HMB1	17:B:806:CLA:HBB1	1.85	0.57
17:A:838:CLA:H91	17:F:802:CLA:HBC3	1.85	0.57
3:C:1:MET:N	3:C:45:THR:OG1	2.37	0.57
17:F:803:CLA:HMB2	20:F:804:BCR:H24C	1.85	0.57
6:F:190:LYS:HE2	6:F:193:MET:HG2	1.85	0.57
17:A:810:CLA:HMB1	17:A:810:CLA:HBB1	1.85	0.57
13:2:139:THR:O	13:2:143:GLN:NE2	2.32	0.57
17:B:818:CLA:H8	17:B:835:CLA:H11	1.85	0.57
15:5:75:GLU:N	15:5:75:GLU:OE1	2.37	0.57
20:A:845:BCR:H383	20:A:853:BCR:H10C	1.86	0.57
15:5:240:PRO:O	15:5:244:ASN:ND2	2.38	0.57
1:A:75:PHE:CZ	17:3:301:CLA:HBB1	2.40	0.57
1:A:476:LEU:HB2	1:A:528:THR:HG23	1.87	0.57
1:A:466:GLN:OE1	1:A:466:GLN:N	2.36	0.57
6:F:106:LEU:HB2	6:F:119:ILE:HG21	1.87	0.57
4:D:155:ASN:OD1	4:D:156:GLY:N	2.38	0.56
4:D:162:HIS:HB3	4:D:163:PRO:HD3	1.87	0.56
17:3:308:CLA:CGA	17:3:308:CLA:HBD	2.35	0.56
12:1:147:GLN:HG3	25:1:514:CHL:HMB3	1.85	0.56
13:2:166:ARG:CZ	25:2:516:CHL:HMC	2.35	0.56
17:A:840:CLA:HBB2	20:L:305:BCR:H372	1.87	0.56
2:B:83:HIS:HA	7:H:143:ILE:HB	1.86	0.56
8:I:3:ASN:O	8:I:6:SER:OG	2.21	0.56
17:L:302:CLA:C1B	17:L:303:CLA:HED1	2.35	0.56
13:2:112:TRP:HD1	17:2:514:CLA:HMD3	1.70	0.56
19:2:517:LHG:HC91	19:2:517:LHG:H281	1.87	0.56
15:5:196:ASN:O	15:5:200:VAL:N	2.30	0.56
4:D:68:GLN:HB3	4:D:150:TYR:OH	2.06	0.56
11:L:82:PRO:O	11:L:93:ARG:NH1	2.38	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:1:501:LUT:H32	17:1:504:CLA:CAB	2.36	0.56
14:3:79:PRO:HD2	24:3:304:LUT:H23	1.87	0.56
1:A:64:GLU:OE2	1:A:68:ARG:NH2	2.38	0.56
15:5:234:LEU:HD23	15:5:237:LEU:HD21	1.87	0.56
17:A:827:CLA:HBB1	17:A:827:CLA:HMB1	1.87	0.56
17:2:509:CLA:H12	25:2:515:CHL:CAD	2.35	0.56
23:5:301:LMG:O5	23:5:301:LMG:O4	2.23	0.56
13:2:115:LEU:O	13:2:119:GLY:N	2.38	0.56
1:A:507:TRP:O	1:A:509:GLY:N	2.38	0.56
17:A:815:CLA:HBB1	17:A:815:CLA:HMB1	1.88	0.56
15:5:91:CYS:HB2	15:5:208:GLY:HA3	1.88	0.56
15:5:233:LEU:HD23	15:5:237:LEU:HD23	1.88	0.56
1:A:247:LEU:HB3	1:A:254:PHE:HD2	1.70	0.55
1:A:717:LEU:HD23	1:A:721:GLN:HG2	1.88	0.55
6:F:173:TRP:CD1	6:F:210:GLY:HA3	2.41	0.55
19:1:516:LHG:H241	25:1:517:CHL:C1C	2.37	0.55
17:B:812:CLA:O1D	17:B:812:CLA:H2A	2.06	0.55
1:A:585:SER:OG	1:A:588:ASP:OD2	2.25	0.55
15:5:218:PHE:HE1	24:5:303:LUT:H41	1.70	0.55
6:F:198:ILE:O	9:J:9:SER:OG	2.25	0.55
4:D:137:ASN:OD1	4:D:140:ARG:NH2	2.25	0.55
12:1:217:HIS:HB2	17:1:506:CLA:HAA2	1.90	0.55
15:5:125:LYS:HE3	15:5:129:ALA:H	1.72	0.55
11:L:136:LEU:HD13	20:L:305:BCR:H401	1.88	0.54
1:A:315:ILE:HB	17:A:821:CLA:HMD1	1.89	0.54
15:5:169:GLU:OE1	15:5:169:GLU:N	2.39	0.54
15:5:221:GLN:HB3	15:5:232:ASN:ND2	2.21	0.54
13:2:121:PHE:CE2	24:2:501:LUT:H28	2.43	0.54
1:A:276:ARG:HD2	1:A:287:TRP:CD1	2.42	0.54
17:3:313:CLA:C1B	17:3:313:CLA:H2	2.38	0.54
19:1:516:LHG:H162	19:1:516:LHG:H282	1.89	0.54
13:2:214:LEU:O	13:2:218:ARG:N	2.27	0.54
2:B:18:THR:HG23	2:B:696:LYS:O	2.08	0.54
17:3:307:CLA:HMD2	17:3:312:CLA:C1D	2.37	0.54
14:3:267:ASN:OD1	14:3:270:THR:OG1	2.26	0.54
1:A:11:LYS:HG3	1:A:13:VAL:HG23	1.90	0.54
17:A:831:CLA:O1D	17:A:831:CLA:H2A	2.08	0.53
17:B:801:CLA:HBB1	17:B:801:CLA:HMB1	1.89	0.53
4:D:108:GLU:OE2	4:D:138:ARG:NH1	2.41	0.53
13:2:180:ASP:HB2	13:2:186:ASN:HB2	1.89	0.53
14:3:73:GLY:O	14:3:232:ARG:NH2	2.38	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:L:304:CLA:HBC3	17:L:304:CLA:HHD	1.89	0.53
2:B:450:GLU:OE2	6:F:129:ARG:NH2	2.30	0.53
1:A:133:ARG:NH1	6:F:109:TYR:OH	2.41	0.53
2:B:73:ASN:ND2	2:B:107:GLY:O	2.27	0.53
14:3:135:TRP:CD1	14:3:252:PRO:HG3	2.44	0.53
1:A:392:MET:HG3	1:A:601:ILE:HD12	1.91	0.53
11:L:83:ALA:HB2	17:L:303:CLA:HMD1	1.90	0.53
11:L:199:LEU:HD13	17:L:304:CLA:HED2	1.89	0.53
1:A:588:ASP:HA	1:A:591:PHE:HB3	1.89	0.53
17:B:816:CLA:HBC3	20:B:844:BCR:H391	1.90	0.53
12:1:167:PRO:HD2	24:1:501:LUT:H23	1.91	0.53
17:B:827:CLA:HBB1	17:B:827:CLA:HMB1	1.90	0.53
1:A:275:PHE:CE2	17:A:817:CLA:HBB1	2.44	0.53
1:A:504:SER:OG	1:A:505:LEU:N	2.40	0.53
17:B:811:CLA:HHC	17:B:811:CLA:HBB1	1.90	0.53
17:B:828:CLA:HBB1	17:B:828:CLA:HMB1	1.90	0.53
11:L:85:ARG:HH22	17:L:302:CLA:HMD3	1.74	0.53
12:1:43:PRO:HD2	25:1:517:CHL:O1D	2.09	0.53
3:C:61:ASP:HA	5:E:135:ASN:HD22	1.73	0.53
15:5:92:ARG:NH1	25:5:315:CHL:OBD	2.40	0.53
1:A:89:TYR:HD2	1:A:159:THR:HG1	1.58	0.52
14:3:62:GLN:O	14:3:65:THR:OG1	2.27	0.52
2:B:363:GLN:OE1	2:B:363:GLN:N	2.42	0.52
17:1:508:CLA:HMB1	17:1:508:CLA:HBB1	1.91	0.52
1:A:210:TRP:NE1	1:A:214:GLN:OE1	2.42	0.52
2:B:338:LEU:HD22	2:B:382:ILE:HG23	1.90	0.52
15:5:174:GLY:HA3	15:5:179:TYR:O	2.10	0.52
17:A:803:CLA:C4D	9:J:12:PRO:HG3	2.40	0.52
12:1:202:GLN:OE1	12:1:207:GLY:N	2.41	0.52
17:3:309:CLA:HMB1	17:3:310:CLA:HAA1	1.90	0.52
17:5:310:CLA:H12	25:5:317:CHL:C3D	2.40	0.52
13:2:258:GLY:O	14:3:152:ASP:N	2.30	0.52
15:5:158:SER:O	15:5:158:SER:OG	2.22	0.52
17:B:822:CLA:H11	20:B:844:BCR:HC22	1.92	0.52
17:2:506:CLA:HMB2	17:2:511:CLA:HAC1	1.90	0.52
14:3:164:ILE:HD13	17:3:316:CLA:HMC3	1.92	0.52
2:B:582:TRP:CH2	17:B:802:CLA:HAB	2.45	0.52
13:2:111:ARG:HH11	25:2:513:CHL:CAD	2.23	0.52
6:F:86:LYS:HB3	6:F:134:GLY:O	2.10	0.51
1:A:25:GLU:HB2	17:A:810:CLA:HAA2	1.91	0.51
25:5:315:CHL:HHC	25:5:315:CHL:HBB1	1.90	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:503:THR:HG21	17:A:833:CLA:HMA2	1.90	0.51
17:B:837:CLA:HBB1	17:B:837:CLA:HMB1	1.92	0.51
12:1:143:ALA:O	12:1:147:GLN:N	2.41	0.51
24:3:303:LUT:H26	17:3:306:CLA:H12	1.92	0.51
2:B:449:PRO:HG2	6:F:94:ARG:HH11	1.75	0.51
2:B:658:ALA:HB3	17:B:804:CLA:HBB2	1.93	0.51
17:B:808:CLA:HAA2	17:B:810:CLA:HED1	1.92	0.51
20:I:101:BCR:H382	20:I:101:BCR:H23C	1.93	0.51
11:L:203:ASP:OD1	11:L:203:ASP:N	2.43	0.51
13:2:162:TRP:CH2	20:2:503:BCR:H321	2.46	0.51
17:3:314:CLA:O1D	17:3:314:CLA:H2A	2.11	0.51
1:A:340:GLU:OE1	1:A:340:GLU:N	2.42	0.51
17:B:822:CLA:HMD2	20:B:844:BCR:HC8	1.93	0.51
17:3:311:CLA:H2A	17:3:311:CLA:HED2	1.93	0.51
4:D:184:ARG:NH1	4:D:189:ASN:OD1	2.40	0.51
13:2:104:GLN:NE2	13:2:193:VAL:HG12	2.25	0.51
17:3:314:CLA:C1B	17:3:314:CLA:H52	2.41	0.51
2:B:394:PHE:O	2:B:542:ARG:NH1	2.44	0.51
2:B:461:GLN:HG2	2:B:472:TYR:CZ	2.46	0.51
12:1:195:PHE:CE2	24:1:502:LUT:H34	2.46	0.51
14:3:214:THR:HG23	14:3:215:LYS:H	1.75	0.51
2:B:369:ALA:HB1	2:B:725:LEU:HD11	1.92	0.51
2:B:658:ALA:O	17:B:804:CLA:HAB	2.11	0.51
17:B:810:CLA:HMB1	17:B:810:CLA:HBB1	1.93	0.51
6:F:101:LYS:O	6:F:104:SER:OG	2.20	0.51
25:2:513:CHL:HHC	25:2:513:CHL:HBB1	1.92	0.51
2:B:155:LEU:HD21	17:B:812:CLA:HMD3	1.92	0.50
12:1:221:PRO:O	12:1:225:ASN:ND2	2.44	0.50
15:5:105:ASP:HB3	15:5:230:ILE:HD12	1.93	0.50
1:A:415:ASP:OD1	1:A:417:THR:OG1	2.28	0.50
17:1:509:CLA:HMB1	17:1:509:CLA:HBB1	1.92	0.50
25:2:515:CHL:HBA2	25:2:515:CHL:HBD	1.92	0.50
15:5:233:LEU:HD12	24:5:303:LUT:H163	1.92	0.50
17:A:827:CLA:C4A	17:A:827:CLA:HBA2	2.41	0.50
4:D:97:ILE:HG13	4:D:148:GLN:O	2.12	0.50
17:A:813:CLA:HMB1	17:A:813:CLA:HBB1	1.93	0.50
20:A:851:BCR:H331	17:J:101:CLA:HBC3	1.93	0.50
17:F:802:CLA:C4B	9:J:22:LEU:HD21	2.41	0.50
17:1:507:CLA:H2A	17:1:507:CLA:HED2	1.94	0.50
19:1:516:LHG:H241	25:1:517:CHL:NC	2.26	0.50
2:B:32:GLU:OE1	2:B:32:GLU:N	2.44	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:5:179:TYR:HB3	17:5:305:CLA:O1D	2.11	0.50
13:2:116:GLY:HA2	26:2:502:XAT:H161	1.94	0.50
15:5:144:PHE:CE2	20:5:302:BCR:H12C	2.47	0.50
1:A:331:THR:HB	1:A:423:LEU:HD21	1.94	0.50
17:A:804:CLA:H43	17:A:810:CLA:HMC2	1.94	0.50
3:C:52:LYS:HE3	3:C:67:VAL:HB	1.94	0.50
6:F:218:TYR:CZ	6:F:222:ILE:HD11	2.47	0.50
14:3:193:LEU:HD12	25:3:315:CHL:CMC	2.41	0.50
17:A:816:CLA:CHD	17:A:817:CLA:HBB2	2.42	0.50
17:B:801:CLA:OBD	17:B:803:CLA:HMB3	2.12	0.50
17:A:838:CLA:HAB	17:A:838:CLA:H122	1.93	0.49
13:2:246:PRO:O	24:2:501:LUT:O23	2.26	0.49
14:3:210:LEU:HD23	14:3:212:PHE:HE1	1.77	0.49
1:A:230:ASP:N	1:A:230:ASP:OD1	2.45	0.49
1:A:421:ASN:OD1	1:A:422:ASP:N	2.45	0.49
6:F:172:GLY:O	6:F:176:TRP:N	2.31	0.49
13:2:182:ILE:O	13:2:184:PRO:HD3	2.12	0.49
24:3:303:LUT:C15	17:3:307:CLA:HBB1	2.41	0.49
2:B:560:ASP:OD1	3:C:52:LYS:NZ	2.45	0.49
4:D:95:TYR:HD2	4:D:150:TYR:O	1.94	0.49
1:A:694:GLU:OE2	2:B:544:SER:OG	2.28	0.49
2:B:301:ILE:HG23	17:B:820:CLA:HED2	1.95	0.49
6:F:194:ARG:HH21	6:F:199:ASP:HB2	1.77	0.49
1:A:320:LYS:NZ	1:A:324:GLU:OE2	2.33	0.49
13:2:112:TRP:CD1	17:2:514:CLA:HMD3	2.48	0.49
2:B:177:HIS:O	2:B:181:GLY:N	2.43	0.49
7:H:88:PHE:CG	11:L:95:ILE:HD13	2.48	0.49
12:1:78:GLU:HG2	12:1:82:TYR:CE2	2.47	0.49
12:1:109:GLN:HG2	17:1:515:CLA:HMC1	1.95	0.49
17:B:824:CLA:HAB	17:B:831:CLA:HMD2	1.94	0.49
13:2:236:TRP:CZ3	25:2:512:CHL:HHB	2.47	0.49
14:3:137:GLN:HG2	14:3:144:ALA:O	2.12	0.49
24:3:303:LUT:H162	17:3:308:CLA:HMB3	1.94	0.49
1:A:147:ALA:HB2	1:A:375:PRO:HD2	1.94	0.49
2:B:91:ILE:HB	2:B:112:PRO:HB2	1.95	0.49
2:B:276:HIS:CE1	2:B:280:ILE:HD13	2.46	0.49
22:B:850:DGD:O1B	22:B:850:DGD:HB42	2.13	0.49
13:2:202:ASP:OD1	17:2:504:CLA:HBD	2.12	0.49
14:3:230:ASN:OD1	17:3:312:CLA:HMD1	2.13	0.49
1:A:735:ILE:HG21	17:A:827:CLA:HMC2	1.95	0.49
2:B:43:TYR:CZ	2:B:330:ILE:HD11	2.47	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:687:LEU:HD23	11:L:84:TYR:HE1	1.77	0.49
20:1:503:BCR:H333	17:1:509:CLA:C1B	2.43	0.49
17:2:506:CLA:HMC2	17:2:506:CLA:H92	1.94	0.49
15:5:97:GLY:HA2	26:5:304:XAT:H181	1.95	0.49
1:A:72:SER:OG	1:A:178:TYR:HB2	2.13	0.48
10:K:77:ARG:HA	10:K:87:ALA:HA	1.94	0.48
14:3:266:ASN:HD21	17:3:313:CLA:HED3	1.78	0.48
1:A:328:GLY:HA3	19:A:844:LHG:HC32	1.94	0.48
2:B:694:ARG:NH1	11:L:146:ALA:O	2.46	0.48
25:1:517:CHL:HMD2	20:5:302:BCR:HC22	1.94	0.48
1:A:110:PRO:HB3	1:A:142:PHE:CD2	2.48	0.48
2:B:180:SER:HB3	2:B:288:GLY:HA3	1.95	0.48
17:B:826:CLA:HBB1	17:B:826:CLA:HMB1	1.95	0.48
3:C:28:MET:HB3	4:D:172:VAL:HG12	1.95	0.48
4:D:80:GLY:C	11:L:64:LEU:HD21	2.34	0.48
13:2:66:ILE:HG22	13:2:68:PHE:H	1.77	0.48
13:2:87:PHE:HE2	26:2:502:XAT:H383	1.77	0.48
17:A:802:CLA:H102	17:A:839:CLA:HMC2	1.95	0.48
2:B:351:HIS:ND1	17:B:818:CLA:OBD	2.47	0.48
20:A:846:BCR:H341	20:A:846:BCR:H11C	1.73	0.48
2:B:687:LEU:HD21	11:L:81:LEU:HD11	1.95	0.48
13:2:120:ILE:O	13:2:124:GLU:HG2	2.13	0.48
17:3:316:CLA:HBB1	17:3:316:CLA:HMB1	1.94	0.48
17:A:818:CLA:HBB1	17:A:818:CLA:HMB1	1.96	0.48
17:A:836:CLA:HHC	17:A:836:CLA:HBB1	1.96	0.48
3:C:32:ASP:OD1	3:C:32:ASP:N	2.45	0.48
13:2:117:ALA:HB1	24:2:501:LUT:H32	1.96	0.48
1:A:259:THR:HG23	1:A:260:PRO:HD3	1.94	0.48
1:A:577:GLY:O	1:A:580:GLY:N	2.39	0.48
22:J:103:DGD:HO4E	22:J:103:DGD:HO5E	1.60	0.48
13:2:166:ARG:NH2	13:2:177:VAL:HG12	2.29	0.48
2:B:93:ASP:HB3	2:B:96:PHE:CD1	2.49	0.48
12:1:71:GLU:OE1	12:1:71:GLU:N	2.38	0.48
1:A:575:GLY:HA2	2:B:562:PRO:HD3	1.95	0.48
14:3:218:LYS:O	14:3:222:GLU:N	2.30	0.48
20:A:848:BCR:H15C	20:A:848:BCR:H351	1.74	0.47
2:B:457:PRO:HB3	2:B:517:PHE:HB2	1.95	0.47
3:C:43:PRO:HB2	4:D:177:GLN:HE21	1.78	0.47
20:F:801:BCR:C10	17:F:802:CLA:HAB	2.44	0.47
17:3:306:CLA:H92	17:3:306:CLA:H61	1.74	0.47
1:A:118:ILE:HG13	20:A:851:BCR:H322	1.95	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:684:ARG:HE	11:L:63:SER:HB3	1.78	0.47
17:1:510:CLA:H2A	17:1:510:CLA:O2D	2.14	0.47
15:5:220:VAL:HG12	17:5:307:CLA:HMD3	1.96	0.47
24:1:502:LUT:H383	17:1:509:CLA:C3B	2.45	0.47
17:A:852:CLA:H101	9:J:18:TRP:CZ3	2.49	0.47
15:5:45:ARG:HH21	15:5:54:PRO:HG3	1.79	0.47
20:A:853:BCR:C12	20:K:204:BCR:H333	2.45	0.47
2:B:365:PHE:CD2	2:B:734:GLY:HA2	2.50	0.47
17:B:838:CLA:HMB2	17:B:839:CLA:C2D	2.45	0.47
20:B:844:BCR:H351	20:B:844:BCR:H15C	1.60	0.47
12:1:215:ALA:HA	12:1:218:LEU:HB2	1.97	0.47
17:2:506:CLA:HMA1	17:2:511:CLA:HBC3	1.97	0.47
1:A:118:ILE:HG22	1:A:119:VAL:HG13	1.97	0.47
17:A:803:CLA:H2A	17:A:803:CLA:O2D	2.15	0.47
17:B:835:CLA:HMD2	17:B:836:CLA:CHC	2.45	0.47
13:2:236:TRP:HZ3	25:2:512:CHL:HHB	1.80	0.47
20:2:503:BCR:H361	20:2:503:BCR:H21C	1.95	0.47
14:3:185:TYR:HA	14:3:190:GLU:OE2	2.15	0.47
20:5:302:BCR:HC8	20:5:302:BCR:H311	1.96	0.47
1:A:741:PHE:CD2	16:A:801:CL0:H25	2.49	0.47
2:B:364:ASP:OD2	2:B:367:THR:OG1	2.24	0.47
4:D:104:GLU:OE2	4:D:119:GLU:HB2	2.15	0.47
11:L:105:LEU:HD12	11:L:132:LEU:HD23	1.96	0.47
13:2:97:GLU:OE2	23:2:518:LMG:O2	2.28	0.47
15:5:64:GLY:H	15:5:202:LEU:HD13	1.79	0.47
1:A:223:GLN:HE22	1:A:250:LEU:HD22	1.79	0.47
1:A:340:GLU:HG2	1:A:419:ARG:HH11	1.79	0.47
18:A:841:PQN:H193	18:A:841:PQN:H211	1.70	0.47
2:B:310:PRO:HG3	17:B:842:CLA:HBD	1.97	0.47
2:B:658:ALA:CB	17:B:804:CLA:HBB2	2.44	0.47
4:D:149:PHE:CZ	4:D:162:HIS:HB2	2.50	0.47
6:F:194:ARG:NH2	23:F:805:LMG:O3	2.37	0.47
14:3:202:PRO:HD3	25:3:315:CHL:HMD2	1.97	0.47
6:F:181:TYR:O	6:F:181:TYR:CD1	2.67	0.47
17:5:310:CLA:HBB1	17:5:310:CLA:HMB1	1.97	0.47
1:A:689:ARG:NH2	2:B:565:GLY:O	2.48	0.46
17:B:818:CLA:H91	17:B:818:CLA:H111	1.71	0.46
11:L:139:CYS:CB	20:L:305:BCR:H19C	2.45	0.46
13:2:159:LEU:HB3	20:2:503:BCR:C15	2.44	0.46
1:A:77:GLN:HB2	17:A:805:CLA:HMB2	1.96	0.46
1:A:721:GLN:HB2	19:A:843:LHG:HC42	1.96	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:676:GLU:HG2	3:C:81:TYR:HE1	1.80	0.46
10:K:118:GLY:HA3	17:K:202:CLA:C2C	2.46	0.46
12:1:167:PRO:HG2	17:1:513:CLA:H122	1.97	0.46
13:2:121:PHE:HE1	13:2:235:ALA:HB2	1.79	0.46
17:B:817:CLA:H2A	17:B:817:CLA:HED3	1.96	0.46
7:H:106:LEU:HD13	8:I:19:ILE:HG12	1.97	0.46
12:1:78:GLU:HB2	12:1:159:LYS:HE2	1.98	0.46
12:1:117:GLY:O	12:1:130:ASN:HA	2.16	0.46
17:2:506:CLA:H192	17:2:506:CLA:H161	1.74	0.46
19:2:517:LHG:H301	19:2:517:LHG:H112	1.97	0.46
20:3:305:BCR:H11C	20:3:305:BCR:H341	1.79	0.46
15:5:86:ALA:N	17:5:316:CLA:HED2	2.30	0.46
13:2:112:TRP:CE2	25:2:513:CHL:HED2	2.51	0.46
14:3:74:ASP:OD1	14:3:76:GLY:N	2.41	0.46
20:3:305:BCR:H272	17:3:311:CLA:C1C	2.46	0.46
12:1:223:HIS:HA	15:5:130:ASN:ND2	2.30	0.46
17:2:508:CLA:OBD	17:2:514:CLA:H2	2.15	0.46
1:A:197:HIS:O	1:A:201:GLY:N	2.44	0.46
1:A:247:LEU:HB3	1:A:254:PHE:CD2	2.50	0.46
1:A:335:HIS:CE1	19:A:844:LHG:HC12	2.50	0.46
2:B:64:ASN:ND2	17:B:828:CLA:HED1	2.30	0.46
17:1:506:CLA:HHC	17:1:506:CLA:HBB1	1.96	0.46
24:2:501:LUT:H11	24:2:501:LUT:H191	1.73	0.46
17:A:805:CLA:H2	17:A:805:CLA:H62	1.77	0.46
3:C:27:GLU:OE2	4:D:176:ARG:HD3	2.16	0.46
12:1:41:TRP:CD2	12:1:42:PHE:HB2	2.50	0.46
17:3:308:CLA:H12	17:3:313:CLA:CAD	2.46	0.46
1:A:29:PRO:HA	17:A:803:CLA:HBC1	1.97	0.46
16:A:801:CL0:CMB	17:B:802:CLA:OBD	2.57	0.46
12:1:104:ASN:OD1	12:1:107:LYS:HG2	2.16	0.46
15:5:49:LEU:HD23	15:5:52:LEU:HB2	1.97	0.46
17:A:827:CLA:H141	17:A:827:CLA:H161	1.73	0.46
10:K:63:MET:O	10:K:67:GLY:N	2.42	0.46
17:L:303:CLA:CHA	17:L:303:CLA:HBA1	2.45	0.46
14:3:223:LEU:HB3	17:3:306:CLA:HMA1	1.97	0.46
10:K:80:THR:HG23	10:K:86:GLU:HG3	1.98	0.46
1:A:707:LYS:HB2	6:F:179:ARG:HH12	1.81	0.45
3:C:8:TYR:HE1	4:D:182:ASN:HD22	1.64	0.45
12:1:95:LEU:HD11	12:1:210:PRO:HB2	1.97	0.45
17:5:308:CLA:H102	17:5:309:CLA:HMB3	1.98	0.45
2:B:718:ILE:HG23	17:B:828:CLA:HAB	1.97	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:K:64:LEU:HB3	17:K:201:CLA:HMC1	1.97	0.45
12:1:222:TRP:HB3	15:5:128:PHE:O	2.16	0.45
14:3:238:PHE:CD2	24:3:304:LUT:H12	2.52	0.45
15:5:72:GLY:HA2	15:5:75:GLU:OE2	2.16	0.45
25:2:512:CHL:C4C	23:2:519:LMG:H312	2.45	0.45
14:3:110:MET:O	17:3:311:CLA:HAB	2.15	0.45
20:3:305:BCR:H15C	20:3:305:BCR:H351	1.64	0.45
1:A:393:TRP:HB3	17:A:827:CLA:HMC3	1.98	0.45
2:B:287:ALA:HB2	17:B:820:CLA:HBC2	1.98	0.45
20:B:846:BCR:H371	20:B:846:BCR:H24C	1.62	0.45
24:2:501:LUT:H35	24:2:501:LUT:H401	1.74	0.45
15:5:221:GLN:HB3	15:5:232:ASN:HD22	1.80	0.45
1:A:125:ASN:O	1:A:133:ARG:NH2	2.50	0.45
1:A:594:LEU:HD13	1:A:594:LEU:HA	1.83	0.45
17:A:823:CLA:HMB3	19:A:844:LHG:HC2	1.99	0.45
17:B:838:CLA:H112	17:B:838:CLA:H142	1.71	0.45
6:F:213:TRP:CG	6:F:214:PRO:HD3	2.52	0.45
17:2:508:CLA:H2	17:2:508:CLA:HED3	1.98	0.45
15:5:242:ASN:HA	15:5:247:HIS:CE1	2.51	0.45
1:A:621:SER:OG	1:A:625:VAL:N	2.50	0.45
17:A:821:CLA:HMB1	17:A:821:CLA:HBB1	1.98	0.45
20:A:851:BCR:H15C	20:A:851:BCR:H351	1.72	0.45
20:1:503:BCR:C10	17:1:515:CLA:H3A	2.47	0.45
13:2:166:ARG:NE	25:2:513:CHL:OMC	2.48	0.45
14:3:74:ASP:HA	17:3:309:CLA:O1D	2.16	0.45
2:B:676:GLU:HG2	3:C:81:TYR:CE1	2.52	0.45
10:K:78:LYS:O	10:K:86:GLU:HB2	2.16	0.45
1:A:507:TRP:CH2	17:A:835:CLA:HED1	2.51	0.45
17:A:825:CLA:H141	17:A:835:CLA:H52	1.98	0.45
13:2:180:ASP:CB	13:2:186:ASN:HB2	2.46	0.45
24:2:501:LUT:H362	17:2:506:CLA:HMB3	1.99	0.45
17:2:507:CLA:H93	17:2:507:CLA:H62	1.83	0.45
1:A:12:ILE:O	1:A:14:VAL:HG13	2.16	0.45
2:B:615:TYR:OH	2:B:621:ARG:NH2	2.50	0.45
17:B:833:CLA:HBC1	17:B:838:CLA:H192	1.98	0.45
22:B:850:DGD:O5E	22:B:850:DGD:O4E	2.31	0.45
12:1:162:GLY:N	17:1:504:CLA:OBD	2.33	0.45
13:2:178:ASN:HB2	13:2:188:LEU:HB2	1.99	0.45
1:A:706:LEU:O	6:F:179:ARG:NH1	2.50	0.45
2:B:91:ILE:HD11	2:B:114:ASN:OD1	2.16	0.45
17:1:511:CLA:HED1	15:5:133:ALA:HB1	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:1:516:LHG:H242	19:1:516:LHG:H131	1.99	0.45
1:A:576:PRO:HD3	2:B:561:GLY:HA2	1.98	0.44
1:A:642:ASN:HB2	2:B:651:LEU:HD11	1.99	0.44
1:A:701:TRP:CE3	2:B:416:GLU:HB3	2.52	0.44
17:A:805:CLA:H162	17:A:805:CLA:H122	1.74	0.44
17:A:829:CLA:H62	17:A:829:CLA:H41	1.72	0.44
20:A:853:BCR:H15C	20:A:853:BCR:H351	1.74	0.44
17:B:824:CLA:HBA2	20:B:847:BCR:H16C	1.97	0.44
11:L:140:LEU:HD23	20:L:305:BCR:H23C	1.98	0.44
12:1:74:GLU:OE2	12:1:75:ARG:HG3	2.17	0.44
12:1:152:GLU:HB3	17:1:513:CLA:HBC1	1.99	0.44
17:1:511:CLA:O2D	17:1:511:CLA:H2A	2.17	0.44
13:2:223:LYS:HD3	17:2:510:CLA:O1D	2.18	0.44
17:2:508:CLA:HBA1	17:2:508:CLA:H3A	1.71	0.44
4:D:167:VAL:HB	4:D:173:ASN:OD1	2.17	0.44
6:F:212:ILE:HD12	15:5:73:LEU:HD22	2.00	0.44
13:2:162:TRP:HH2	20:2:503:BCR:H321	1.81	0.44
24:5:303:LUT:H15	24:5:303:LUT:H201	1.82	0.44
17:A:836:CLA:H3A	17:A:836:CLA:HBA2	1.76	0.44
20:A:849:BCR:H24C	20:A:849:BCR:H371	1.75	0.44
19:1:516:LHG:H151	19:1:516:LHG:H262	1.99	0.44
13:2:256:ASP:OD1	13:2:256:ASP:N	2.50	0.44
14:3:267:ASN:HB3	17:3:308:CLA:OBD	2.18	0.44
17:3:308:CLA:H43	17:3:313:CLA:OBD	2.18	0.44
2:B:173:SER:O	2:B:177:HIS:ND1	2.38	0.44
2:B:655:LEU:HD13	17:B:801:CLA:HAA1	2.00	0.44
17:B:825:CLA:HMB1	17:B:825:CLA:HBB1	2.00	0.44
18:B:843:PQN:H171	20:B:849:BCR:H382	2.00	0.44
13:2:263:PHE:C	13:2:264:ARG:HD3	2.38	0.44
17:2:505:CLA:HED2	17:2:510:CLA:H61	1.99	0.44
17:2:510:CLA:HMB1	17:2:510:CLA:HBB1	1.99	0.44
14:3:99:TYR:HE1	14:3:200:ALA:HA	1.82	0.44
15:5:175:LEU:HD13	15:5:175:LEU:HA	1.89	0.44
20:5:302:BCR:H352	20:5:302:BCR:H10C	2.00	0.44
17:A:809:CLA:HMA1	9:J:27:ILE:HD13	2.00	0.44
17:B:833:CLA:H61	20:F:804:BCR:HC32	1.99	0.44
8:I:11:LEU:HD23	8:I:11:LEU:HA	1.83	0.44
1:A:449:SER:HB3	1:A:536:ILE:HD13	1.98	0.44
1:A:570:ARG:HB3	1:A:587:TRP:HB2	1.98	0.44
2:B:193:HIS:HB2	17:B:815:CLA:CHC	2.48	0.44
2:B:225:LEU:HD22	20:B:844:BCR:H292	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:656:VAL:HG22	17:B:841:CLA:HMB3	1.99	0.44
17:B:811:CLA:HHC	17:B:811:CLA:CBB	2.48	0.44
20:B:844:BCR:H24C	20:B:844:BCR:H371	1.72	0.44
3:C:32:ASP:O	3:C:37:LYS:NZ	2.47	0.44
4:D:97:ILE:HB	4:D:149:PHE:HB3	2.00	0.44
20:F:804:BCR:H11C	20:F:804:BCR:H341	1.67	0.44
1:A:11:LYS:NZ	14:3:86:GLU:OE1	2.39	0.44
20:A:845:BCR:H20C	20:A:845:BCR:H361	1.77	0.44
17:B:824:CLA:HMA1	17:B:842:CLA:HED3	1.99	0.44
6:F:233:ILE:HG13	6:F:234:GLY:N	2.32	0.44
14:3:191:LYS:HE2	14:3:192:TYR:CZ	2.53	0.44
1:A:41:ASP:OD1	1:A:42:THR:N	2.44	0.44
1:A:194:MET:HB3	17:A:824:CLA:HMD1	1.99	0.44
1:A:379:THR:HG21	1:A:515:VAL:HB	1.99	0.44
1:A:693:GLN:HG2	2:B:546:LEU:HD22	1.98	0.44
2:B:40:GLU:HG2	2:B:165:LEU:HD23	2.00	0.44
20:B:845:BCR:H15C	20:B:845:BCR:H351	1.69	0.44
11:L:97:VAL:HG13	11:L:101:HIS:CE1	2.53	0.44
14:3:91:PHE:HA	14:3:96:TRP:CD1	2.53	0.44
14:3:192:TYR:HD1	14:3:205:PRO:HD2	1.83	0.44
24:5:303:LUT:C11	17:5:306:CLA:HMC2	2.48	0.44
17:5:307:CLA:NA	17:5:307:CLA:H12	2.33	0.44
17:B:828:CLA:H2A	17:B:828:CLA:O1D	2.18	0.43
20:1:503:BCR:H341	20:1:503:BCR:H11C	1.67	0.43
13:2:232:VAL:HG21	26:2:502:XAT:H12	2.00	0.43
26:5:304:XAT:H183	17:5:310:CLA:C3B	2.48	0.43
2:B:124:TRP:CZ2	2:B:124:TRP:NE1	2.86	0.43
17:B:802:CLA:H91	17:B:802:CLA:H111	1.74	0.43
17:B:820:CLA:CMB	17:B:825:CLA:HMA3	2.48	0.43
17:B:826:CLA:O1A	17:B:837:CLA:HMA1	2.18	0.43
11:L:66:THR:H	11:L:69:THR:HG22	1.83	0.43
24:2:501:LUT:H12	17:2:504:CLA:CAB	2.47	0.43
24:3:304:LUT:H35	24:3:304:LUT:H401	1.67	0.43
15:5:234:LEU:O	15:5:237:LEU:HG	2.19	0.43
1:A:84:TRP:O	1:A:88:MET:HG2	2.18	0.43
1:A:259:THR:CG2	1:A:260:PRO:HD3	2.48	0.43
2:B:443:MET:HG3	2:B:451:LYS:O	2.18	0.43
5:E:79:LYS:N	5:E:80:PRO:HD2	2.33	0.43
5:E:90:LYS:HE3	5:E:104:THR:HG21	2.00	0.43
11:L:194:TRP:CE3	20:L:306:BCR:H333	2.54	0.43
13:2:211:PRO:C	13:2:213:LYS:H	2.20	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:5:304:XAT:H15	26:5:304:XAT:H201	1.85	0.43
1:A:213:HIS:HB2	17:A:813:CLA:C1C	2.48	0.43
17:A:812:CLA:HMB1	17:A:812:CLA:HBB1	1.99	0.43
20:B:848:BCR:H11C	20:B:848:BCR:H341	1.86	0.43
7:H:108:GLY:O	7:H:111:SER:OG	2.27	0.43
10:K:105:THR:CB	17:K:201:CLA:HAB	2.48	0.43
20:L:305:BCR:H15C	20:L:305:BCR:H351	1.82	0.43
12:1:128:TRP:HB2	12:1:133:THR:HG21	2.00	0.43
24:1:501:LUT:H15	24:1:501:LUT:H201	1.90	0.43
24:1:501:LUT:H161	24:1:501:LUT:H8	1.99	0.43
2:B:276:HIS:HB2	17:B:818:CLA:C1B	2.47	0.43
17:B:819:CLA:HBB1	17:B:819:CLA:HMB1	2.01	0.43
7:H:125:LEU:HD23	7:H:128:LYS:HB2	2.01	0.43
13:2:120:ILE:HG13	26:2:502:XAT:C16	2.48	0.43
17:5:307:CLA:H12	17:5:307:CLA:HBA2	1.80	0.43
17:A:805:CLA:H112	17:A:805:CLA:H91	1.70	0.43
17:A:808:CLA:H202	17:A:808:CLA:H161	1.87	0.43
2:B:43:TYR:CE2	2:B:330:ILE:HD11	2.54	0.43
2:B:459:PHE:CD1	17:F:803:CLA:HMC2	2.53	0.43
20:B:852:BCR:H15C	20:B:852:BCR:H351	1.65	0.43
6:F:158:GLY:HA2	6:F:162:THR:HB	2.01	0.43
20:I:101:BCR:H15C	20:I:101:BCR:H351	1.79	0.43
12:1:127:PRO:HG2	12:1:128:TRP:CE3	2.54	0.43
1:A:17:ASP:HA	1:A:179:HIS:O	2.18	0.43
1:A:40:PRO:HA	1:A:45:TRP:CG	2.54	0.43
1:A:669:LEU:HB3	17:B:802:CLA:H62	2.01	0.43
1:A:712:THR:OG1	6:F:195:GLU:OE1	2.33	0.43
17:A:820:CLA:HMB2	17:A:824:CLA:HMA3	2.00	0.43
20:A:853:BCR:H20C	20:A:853:BCR:H361	1.80	0.43
3:C:28:MET:O	4:D:176:ARG:HD2	2.19	0.43
11:L:64:LEU:HD23	11:L:64:LEU:HA	1.71	0.43
1:A:159:THR:HG22	17:A:813:CLA:CGA	2.49	0.43
1:A:654:SER:O	1:A:658:GLN:HG2	2.18	0.43
2:B:53:GLN:O	2:B:53:GLN:NE2	2.50	0.43
2:B:56:ILE:HG21	17:B:807:CLA:HMD2	2.01	0.43
2:B:582:TRP:HH2	17:B:802:CLA:HAB	1.81	0.43
6:F:113:SER:OG	6:F:115:PRO:HD2	2.19	0.43
17:L:301:CLA:H62	17:L:301:CLA:H41	1.75	0.43
12:1:94:VAL:HG12	12:1:95:LEU:HD22	1.99	0.43
15:5:149:ARG:HA	25:5:315:CHL:HAC2	2.00	0.43
15:5:218:PHE:CE1	24:5:303:LUT:H41	2.53	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:100:ALA:O	1:A:103:SER:OG	2.31	0.43
1:A:252:PRO:HG2	1:A:271:GLU:OE1	2.18	0.43
17:A:816:CLA:C4A	17:A:816:CLA:HBA2	2.48	0.43
20:A:845:BCR:H11C	20:A:845:BCR:H341	1.87	0.43
17:B:837:CLA:HBC2	17:B:837:CLA:HHD	2.00	0.43
7:H:129:LYS:HE3	7:H:129:LYS:HB2	1.86	0.43
11:L:64:LEU:O	11:L:69:THR:HG21	2.19	0.43
11:L:175:GLU:O	11:L:179:GLN:HG2	2.18	0.43
12:1:42:PHE:CE1	25:1:517:CHL:HED3	2.54	0.43
12:1:82:TYR:CE2	12:1:149:ARG:HD2	2.54	0.43
12:1:201:GLN:HB3	12:1:213:ASN:ND2	2.33	0.43
15:5:159:GLN:HG2	25:5:315:CHL:HMC	2.01	0.43
1:A:308:MET:HE1	17:A:820:CLA:HMD3	2.01	0.43
17:A:804:CLA:HMB1	17:A:804:CLA:HBB1	1.99	0.43
2:B:229:GLN:C	2:B:231:ASN:H	2.22	0.43
6:F:181:TYR:OH	6:F:194:ARG:O	2.35	0.43
12:1:124:ASN:HA	12:1:125:PRO:HD3	1.94	0.43
12:1:168:LEU:O	12:1:168:LEU:HD23	2.19	0.43
13:2:253:HIS:ND1	17:2:506:CLA:HAA2	2.34	0.43
1:A:77:GLN:O	1:A:77:GLN:NE2	2.52	0.42
1:A:109:GLY:HA2	1:A:110:PRO:HD3	1.92	0.42
1:A:598:TYR:HB2	1:A:731:LEU:HD11	2.01	0.42
4:D:86:LEU:HA	4:D:86:LEU:HD23	1.75	0.42
6:F:94:ARG:NH2	6:F:143:ASP:O	2.51	0.42
12:1:149:ARG:HA	17:1:513:CLA:CBC	2.49	0.42
17:2:505:CLA:O1D	17:2:505:CLA:H12	2.19	0.42
15:5:65:ASP:HA	17:5:308:CLA:O1D	2.19	0.42
1:A:17:ASP:OD1	1:A:180:LYS:HD3	2.19	0.42
1:A:78:LEU:HD12	1:A:78:LEU:HA	1.84	0.42
1:A:576:PRO:HD2	3:C:52:LYS:HG2	2.00	0.42
17:A:806:CLA:H91	17:A:806:CLA:H112	1.75	0.42
17:B:831:CLA:HMB2	17:B:832:CLA:C2D	2.49	0.42
4:D:163:PRO:C	4:D:165:ASP:H	2.23	0.42
6:F:208:PRO:HG3	23:F:806:LMG:H111	2.00	0.42
9:J:31:ARG:NH2	17:J:101:CLA:O1D	2.53	0.42
12:1:109:GLN:NE2	24:1:502:LUT:H372	2.34	0.42
13:2:236:TRP:HD1	13:2:237:PHE:CD1	2.38	0.42
13:2:237:PHE:HB2	17:2:506:CLA:HAC2	2.01	0.42
17:2:510:CLA:H12	17:2:510:CLA:HBA1	1.81	0.42
14:3:259:HIS:CG	17:3:308:CLA:HAA2	2.54	0.42
15:5:146:GLU:HG3	17:5:316:CLA:C4B	2.50	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:5:212:MET:HE1	17:5:308:CLA:HAB	2.01	0.42
1:A:191:VAL:HA	1:A:194:MET:HB2	2.00	0.42
17:A:822:CLA:HMB3	17:A:842:CLA:HBC3	2.00	0.42
20:A:848:BCR:H20C	20:A:848:BCR:H361	1.83	0.42
20:L:306:BCR:H15C	20:L:306:BCR:H351	1.70	0.42
12:1:77:LYS:HB2	12:1:159:LYS:NZ	2.34	0.42
13:2:126:LEU:O	13:2:131:ILE:HG22	2.19	0.42
2:B:458:ILE:HG21	6:F:151:SER:HB3	2.00	0.42
20:B:849:BCR:H20C	20:B:849:BCR:H361	1.84	0.42
3:C:25:VAL:HG13	3:C:44:ARG:O	2.18	0.42
6:F:136:PHE:CD2	9:J:40:PRO:HG3	2.53	0.42
9:J:8:LEU:HD23	9:J:13:VAL:HG11	2.01	0.42
12:1:70:PRO:HA	12:1:73:PHE:HB3	2.02	0.42
12:1:212:GLU:O	12:1:216:THR:OG1	2.32	0.42
17:3:316:CLA:HMB2	17:3:318:CLA:C4B	2.50	0.42
15:5:77:PRO:O	15:5:81:LYS:HG2	2.19	0.42
15:5:89:VAL:HG21	15:5:149:ARG:NH1	2.35	0.42
15:5:93:PHE:CE2	17:5:316:CLA:HAC2	2.54	0.42
1:A:314:GLY:HA2	10:K:88:ARG:NH2	2.34	0.42
17:A:806:CLA:H161	17:A:828:CLA:HBB2	2.00	0.42
2:B:69:ALA:HB2	2:B:135:LEU:HD12	2.01	0.42
17:B:841:CLA:O1D	17:B:841:CLA:H2A	2.19	0.42
11:L:81:LEU:HB2	11:L:82:PRO:HD2	2.01	0.42
25:2:512:CHL:C1A	23:2:519:LMG:H152	2.49	0.42
14:3:233:LEU:CD2	24:3:303:LUT:H11	2.49	0.42
17:3:311:CLA:HMA2	17:3:317:CLA:HBC2	2.00	0.42
15:5:212:MET:HE2	17:5:308:CLA:HHC	2.01	0.42
20:A:846:BCR:H20C	20:A:846:BCR:H361	1.89	0.42
17:B:822:CLA:HBB1	17:B:822:CLA:HMB1	2.01	0.42
3:C:27:GLU:OE1	3:C:44:ARG:NH2	2.52	0.42
3:C:58:CYS:HA	21:C:102:SF4:S4	2.59	0.42
13:2:148:ASP:OD2	13:2:150:THR:OG1	2.36	0.42
1:A:13:VAL:HA	14:3:87:GLY:HA2	2.02	0.42
1:A:161:ILE:O	1:A:165:VAL:HG23	2.20	0.42
1:A:511:GLU:OE1	1:A:512:LEU:HG	2.19	0.42
1:A:690:GLY:N	2:B:568:CYS:O	2.52	0.42
20:A:851:BCR:H321	20:A:851:BCR:HC8	2.00	0.42
17:B:824:CLA:HED3	17:B:824:CLA:H2A	2.01	0.42
20:B:847:BCR:H341	20:B:847:BCR:H11C	1.73	0.42
17:J:101:CLA:HMC1	17:J:101:CLA:HBC2	2.00	0.42
17:1:506:CLA:HHC	17:1:506:CLA:CBB	2.49	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:5:94:ALA:HB2	26:5:304:XAT:C13	2.50	0.42
15:5:136:PHE:O	15:5:140:LEU:HG	2.19	0.42
1:A:302:PHE:HE1	17:A:820:CLA:HAB	1.85	0.42
1:A:592:LEU:HA	1:A:592:LEU:HD23	1.86	0.42
1:A:671:PHE:CE2	1:A:675:HIS:HE1	2.36	0.42
6:F:181:TYR:CD1	6:F:185:VAL:HG13	2.53	0.42
11:L:140:LEU:HB3	11:L:181:THR:HG22	2.02	0.42
12:1:65:GLY:O	12:1:68:THR:HG23	2.19	0.42
14:3:210:LEU:HD23	14:3:212:PHE:CE1	2.55	0.42
1:A:75:PHE:HZ	17:3:301:CLA:HBB1	1.84	0.42
1:A:622:ASP:N	1:A:622:ASP:OD1	2.51	0.42
19:A:843:LHG:H242	19:A:843:LHG:H272	1.75	0.42
2:B:64:ASN:HD21	17:B:828:CLA:HED1	1.84	0.42
17:B:813:CLA:HBA1	17:B:813:CLA:H3A	1.72	0.42
10:K:110:ALA:HA	20:K:204:BCR:C11	2.50	0.42
17:1:506:CLA:HBA2	17:1:506:CLA:H3A	1.77	0.42
17:2:506:CLA:C4C	17:2:506:CLA:H51	2.50	0.42
26:5:304:XAT:H173	26:5:304:XAT:H3	1.71	0.42
1:A:323:LEU:O	1:A:335:HIS:HB2	2.20	0.42
1:A:648:PHE:O	1:A:652:GLN:HB2	2.20	0.42
18:A:841:PQN:H222	18:A:841:PQN:H262	1.77	0.42
6:F:136:PHE:CE2	9:J:40:PRO:HG3	2.54	0.42
6:F:181:TYR:CD1	6:F:181:TYR:C	2.85	0.42
14:3:163:LEU:O	20:3:305:BCR:H16C	2.20	0.42
20:A:846:BCR:H351	20:A:846:BCR:H15C	1.78	0.41
17:B:815:CLA:H91	17:B:815:CLA:H112	1.88	0.41
10:K:122:GLY:HA2	10:K:124:LYS:NZ	2.34	0.41
12:1:208:THR:HG21	12:1:213:ASN:HD21	1.85	0.41
15:5:160:ALA:HB1	15:5:168:ILE:O	2.19	0.41
1:A:242:LEU:HD23	1:A:242:LEU:HA	1.82	0.41
1:A:550:LYS:HD3	2:B:670:TYR:HE1	1.85	0.41
1:A:681:SER:HB3	1:A:729:HIS:HB2	2.03	0.41
2:B:221:GLY:HA3	17:B:816:CLA:HMD1	2.02	0.41
17:B:822:CLA:C1D	20:B:844:BCR:H323	2.49	0.41
6:F:150:VAL:HG12	6:F:160:PHE:HB2	2.02	0.41
10:K:97:PRO:HD3	17:K:201:CLA:CAA	2.50	0.41
11:L:92:LEU:HA	11:L:95:ILE:HG22	2.01	0.41
24:1:502:LUT:H11	24:1:502:LUT:H191	1.92	0.41
24:3:304:LUT:C32	17:3:310:CLA:HMB2	2.50	0.41
1:A:314:GLY:HA3	10:K:75:ALA:HB1	2.02	0.41
1:A:342:LEU:HA	1:A:342:LEU:HD23	1.73	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:B:822:CLA:CAD	20:B:844:BCR:HC41	2.50	0.41
5:E:94:LEU:HD13	5:E:94:LEU:HA	1.89	0.41
13:2:87:PHE:HB3	17:2:507:CLA:CAD	2.50	0.41
13:2:121:PHE:CD2	24:2:501:LUT:H28	2.55	0.41
14:3:142:PRO:HD2	17:3:314:CLA:HMB3	2.02	0.41
24:3:304:LUT:H15	24:3:304:LUT:H201	1.94	0.41
15:5:174:GLY:O	15:5:175:LEU:HB2	2.20	0.41
20:5:302:BCR:H351	20:5:302:BCR:H15C	1.73	0.41
1:A:223:GLN:NE2	1:A:250:LEU:HD22	2.35	0.41
1:A:741:PHE:CG	16:A:801:CL0:H25	2.54	0.41
2:B:429:LEU:HA	2:B:429:LEU:HD23	1.80	0.41
2:B:492:LEU:HD13	2:B:492:LEU:HA	1.76	0.41
17:B:808:CLA:H2	20:I:101:BCR:HC31	2.03	0.41
17:B:811:CLA:H2A	17:B:811:CLA:O1D	2.21	0.41
20:B:844:BCR:H11C	20:B:844:BCR:H341	1.71	0.41
14:3:142:PRO:N	14:3:143:PRO:HD2	2.35	0.41
20:5:302:BCR:C37	25:5:317:CHL:HHB	2.50	0.41
1:A:66:ILE:O	1:A:70:VAL:HG13	2.20	0.41
1:A:194:MET:SD	1:A:198:HIS:CE1	3.13	0.41
1:A:679:ALA:HB3	17:A:802:CLA:HBB2	2.01	0.41
17:A:820:CLA:H92	17:A:820:CLA:H62	1.89	0.41
17:A:827:CLA:H151	20:J:102:BCR:H351	2.02	0.41
2:B:310:PRO:HA	2:B:311:PRO:HD3	1.93	0.41
3:C:27:GLU:OE1	3:C:44:ARG:NH1	2.54	0.41
11:L:154:SER:HB2	11:L:168:ALA:HB1	2.02	0.41
12:1:226:ILE:HB	17:1:506:CLA:H11	2.01	0.41
14:3:239:LEU:HD12	14:3:239:LEU:HA	1.88	0.41
15:5:186:ASN:ND2	15:5:189:GLY:HA2	2.35	0.41
1:A:56:PHE:CD2	17:A:805:CLA:HMC2	2.55	0.41
1:A:350:LEU:HB2	17:A:805:CLA:HMD3	2.03	0.41
1:A:548:LEU:O	1:A:552:VAL:HG23	2.21	0.41
3:C:62:PHE:HD2	4:D:186:ILE:HG21	1.86	0.41
6:F:209:ARG:HH22	15:5:72:GLY:HA3	1.84	0.41
9:J:25:LEU:O	9:J:29:ILE:HG13	2.21	0.41
26:2:502:XAT:H35	26:2:502:XAT:H401	1.81	0.41
17:3:309:CLA:O2D	17:3:309:CLA:H2A	2.21	0.41
17:3:311:CLA:C4A	17:3:311:CLA:HBA2	2.51	0.41
24:5:303:LUT:H11	24:5:303:LUT:H191	1.93	0.41
17:A:827:CLA:H143	17:A:827:CLA:H111	1.84	0.41
2:B:53:GLN:HE21	2:B:57:ILE:HG13	1.86	0.41
5:E:95:ARG:HD2	5:E:98:SER:HB2	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:2:120:ILE:HG12	13:2:137:TRP:CG	2.55	0.41
13:2:128:LYS:HA	13:2:128:LYS:HD2	1.91	0.41
15:5:200:VAL:HG12	17:5:305:CLA:HMA1	2.02	0.41
1:A:41:ASP:OD1	1:A:45:TRP:HB2	2.21	0.41
17:B:826:CLA:H102	17:B:838:CLA:H2	2.01	0.41
17:B:838:CLA:H192	17:B:838:CLA:H162	1.76	0.41
17:B:838:CLA:H151	20:F:804:BCR:H402	2.02	0.41
6:F:212:ILE:HD12	15:5:73:LEU:HD13	2.02	0.41
17:1:510:CLA:HBA1	17:1:510:CLA:H3A	1.69	0.41
13:2:68:PHE:HD2	13:2:71:SER:HB3	1.85	0.41
14:3:80:LEU:N	24:3:304:LUT:O23	2.54	0.41
20:A:847:BCR:H371	20:A:847:BCR:H24C	1.82	0.41
2:B:193:HIS:HB2	17:B:815:CLA:C1C	2.51	0.41
2:B:395:ILE:HD11	2:B:541:ALA:HB1	2.03	0.41
17:B:806:CLA:HBC2	17:B:830:CLA:CMA	2.51	0.41
17:B:807:CLA:H61	17:B:807:CLA:H93	1.73	0.41
17:B:811:CLA:HBA2	17:B:811:CLA:HBD	2.03	0.41
17:B:815:CLA:H112	17:B:815:CLA:H142	1.85	0.41
17:B:833:CLA:HBB1	17:B:833:CLA:HMB1	2.03	0.41
20:B:844:BCR:H20C	20:B:844:BCR:H361	1.80	0.41
4:D:101:SER:OG	4:D:117:MET:SD	2.66	0.41
4:D:133:LEU:HA	4:D:133:LEU:HD12	1.84	0.41
5:E:135:ASN:N	5:E:135:ASN:OD1	2.52	0.41
20:L:305:BCR:C8	20:L:305:BCR:H331	2.50	0.41
24:1:502:LUT:H201	24:1:502:LUT:H15	1.74	0.41
26:2:502:XAT:H15	26:2:502:XAT:H201	1.83	0.41
14:3:121:LEU:O	14:3:125:GLY:N	2.54	0.41
14:3:243:LEU:HD13	14:3:243:LEU:HA	1.95	0.41
25:5:314:CHL:CMC	25:5:317:CHL:HHC	2.50	0.41
1:A:479:ILE:O	1:A:483:TRP:N	2.48	0.41
3:C:3:HIS:ND1	3:C:69:LEU:HA	2.36	0.41
12:1:121:TYR:CE1	17:1:509:CLA:H2	2.56	0.41
17:A:836:CLA:C1A	17:A:836:CLA:CGA	2.99	0.40
2:B:51:PHE:HB2	2:B:153:SER:HB3	2.03	0.40
17:B:811:CLA:HAC2	20:I:101:BCR:H373	2.03	0.40
10:K:124:LYS:HE3	17:K:202:CLA:HMA3	2.03	0.40
24:1:502:LUT:H12	17:1:507:CLA:CBB	2.50	0.40
13:2:238:GLN:OE1	24:2:501:LUT:H24	2.22	0.40
17:5:309:CLA:HMD2	17:5:316:CLA:CHD	2.51	0.40
1:A:433:ALA:O	1:A:437:HIS:ND1	2.40	0.40
17:A:806:CLA:H193	17:A:806:CLA:HED2	2.02	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:A:806:CLA:H203	17:A:806:CLA:H162	1.71	0.40
17:A:816:CLA:HMD2	17:K:202:CLA:OBD	2.22	0.40
17:A:831:CLA:H12	17:A:831:CLA:H52	1.97	0.40
4:D:139:LEU:HB3	4:D:145:ILE:CG2	2.52	0.40
6:F:189:LYS:HG3	6:F:190:LYS:N	2.36	0.40
8:I:19:ILE:HA	8:I:22:THR:HG22	2.03	0.40
9:J:8:LEU:HD23	9:J:8:LEU:HA	1.93	0.40
22:J:103:DGD:HAG2	22:J:103:DGD:HAN1	1.76	0.40
24:5:303:LUT:H401	24:5:303:LUT:H35	1.61	0.40
1:A:462:LEU:HD22	2:B:96:PHE:HA	2.03	0.40
1:A:656:VAL:O	1:A:659:SER:OG	2.26	0.40
17:A:804:CLA:H62	17:A:804:CLA:H2	1.80	0.40
17:A:831:CLA:H192	20:L:305:BCR:H10C	2.02	0.40
20:A:845:BCR:H351	20:A:845:BCR:H15C	1.72	0.40
2:B:408:LEU:HD12	2:B:408:LEU:HA	1.81	0.40
3:C:10:THR:HB	3:C:64:SER:OG	2.21	0.40
6:F:209:ARG:NH1	23:F:806:LMG:O5	2.55	0.40
13:2:151:THR:O	13:2:155:VAL:HG23	2.21	0.40
24:5:303:LUT:H183	17:5:307:CLA:C3B	2.51	0.40
1:A:115:VAL:HG22	1:A:125:ASN:OD1	2.21	0.40
2:B:472:TYR:OH	2:B:512:ILE:O	2.39	0.40
17:B:804:CLA:CGA	17:B:804:CLA:H3A	2.44	0.40
4:D:139:LEU:O	4:D:145:ILE:HG22	2.20	0.40
11:L:84:TYR:O	11:L:86:THR:HG23	2.22	0.40
11:L:90:PRO:HA	11:L:93:ARG:HG3	2.03	0.40
11:L:136:LEU:HA	11:L:136:LEU:HD23	1.88	0.40
20:L:305:BCR:H11C	20:L:305:BCR:H341	1.74	0.40
12:1:226:ILE:HG21	17:1:506:CLA:H42	2.04	0.40
14:3:74:ASP:OD1	14:3:75:PHE:N	2.53	0.40
14:3:206:ILE:HG23	14:3:207:PHE:CD1	2.57	0.40
15:5:201:LYS:O	15:5:205:ILE:HG12	2.21	0.40
17:B:807:CLA:H152	17:B:807:CLA:H111	1.90	0.40
17:1:506:CLA:H41	17:1:506:CLA:H62	1.83	0.40
13:2:87:PHE:CE2	26:2:502:XAT:H383	2.56	0.40
13:2:120:ILE:HG23	13:2:137:TRP:CD1	2.56	0.40
14:3:133:ILE:HG22	14:3:134:PRO:O	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	740/750 (99%)	690 (93%)	50 (7%)	0	100	100
2	B	731/734 (100%)	688 (94%)	42 (6%)	1 (0%)	48	78
3	C	79/81 (98%)	70 (89%)	9 (11%)	0	100	100
4	D	140/205 (68%)	118 (84%)	22 (16%)	0	100	100
5	E	66/147 (45%)	61 (92%)	5 (8%)	0	100	100
6	F	156/235 (66%)	150 (96%)	6 (4%)	0	100	100
7	H	59/143 (41%)	58 (98%)	1 (2%)	0	100	100
8	I	28/36 (78%)	28 (100%)	0	0	100	100
9	J	40/42 (95%)	37 (92%)	2 (5%)	1 (2%)	4	22
10	K	82/131 (63%)	73 (89%)	9 (11%)	0	100	100
11	L	144/209 (69%)	135 (94%)	9 (6%)	0	100	100
12	1	189/247 (76%)	179 (95%)	10 (5%)	0	100	100
13	2	201/255 (79%)	185 (92%)	16 (8%)	0	100	100
14	3	220/269 (82%)	195 (89%)	25 (11%)	0	100	100
15	5	203/257 (79%)	173 (85%)	30 (15%)	0	100	100
All	All	3078/3741 (82%)	2840 (92%)	236 (8%)	2 (0%)	50	78

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	223	GLY
9	J	36	ALA

5.3.2 Protein sidechains

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

entries.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	592/608 (97%)	589 (100%)	3 (0%)	86	91
2	B	594/601 (99%)	590 (99%)	4 (1%)	81	88
3	C	70/71 (99%)	69 (99%)	1 (1%)	62	77
4	D	119/160 (74%)	119 (100%)	0	100	100
5	E	58/112 (52%)	58 (100%)	0	100	100
6	F	120/183 (66%)	120 (100%)	0	100	100
7	H	48/110 (44%)	48 (100%)	0	100	100
8	I	26/33 (79%)	26 (100%)	0	100	100
9	J	35/36 (97%)	35 (100%)	0	100	100
10	K	52/102 (51%)	51 (98%)	1 (2%)	52	71
11	L	112/166 (68%)	110 (98%)	2 (2%)	54	73
12	1	134/196 (68%)	133 (99%)	1 (1%)	81	88
13	2	156/194 (80%)	155 (99%)	1 (1%)	84	90
14	3	147/216 (68%)	147 (100%)	0	100	100
15	5	139/202 (69%)	138 (99%)	1 (1%)	81	88
All	All	2402/2990 (80%)	2388 (99%)	14 (1%)	82	90

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	570	ARG
1	A	578	ARG
1	A	720	ILE
2	B	165	LEU
2	B	224	PRO
2	B	225	LEU
2	B	437	TYR
3	C	47	ASP
10	K	104	ASP
11	L	88	VAL
11	L	93	ARG
12	1	170	PHE
13	2	264	ARG
15	5	158	SER

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

Mol	Chain	Res	Type
4	D	68	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

199 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
17	CLA	B	804	-	65,73,73	1.42	11 (16%)	76,113,113	1.42	6 (7%)
20	BCR	B	852	-	41,41,41	1.22	3 (7%)	56,56,56	2.06	18 (32%)
17	CLA	2	509	-	50,58,73	1.60	7 (14%)	58,95,113	1.63	8 (13%)
19	LHG	B	851	-	37,37,48	1.08	2 (5%)	40,43,54	1.17	4 (10%)
17	CLA	A	814	-	42,50,73	1.82	10 (23%)	48,85,113	1.73	9 (18%)
24	LUT	3	304	-	42,43,43	0.91	2 (4%)	51,60,60	1.56	10 (19%)
24	LUT	5	303	-	42,43,43	0.95	2 (4%)	51,60,60	1.83	13 (25%)
17	CLA	B	812	-	54,62,73	1.59	8 (14%)	67,100,113	1.57	13 (19%)
17	CLA	B	816	-	43,51,73	1.67	9 (20%)	49,86,113	1.66	6 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	CLA	1	515	-	45,52,73	1.81	9 (20%)	47,87,113	1.61	6 (12%)
20	BCR	2	503	-	41,41,41	0.89	1 (2%)	56,56,56	3.62	27 (48%)
17	CLA	K	203	-	39,48,73	1.71	10 (25%)	45,82,113	1.68	8 (17%)
17	CLA	A	835	-	51,59,73	1.62	10 (19%)	59,96,113	1.75	9 (15%)
24	LUT	1	501	-	42,43,43	0.89	1 (2%)	51,60,60	1.65	11 (21%)
16	CL0	A	801	-	61,69,73	1.64	10 (16%)	70,107,113	2.21	16 (22%)
17	CLA	B	826	-	62,70,73	1.40	10 (16%)	72,109,113	1.52	10 (13%)
17	CLA	3	309	-	41,48,73	2.19	11 (26%)	50,82,113	1.57	6 (12%)
23	LMG	5	301	-	32,32,55	1.18	2 (6%)	40,40,63	1.15	3 (7%)
25	CHL	3	302	13	47,55,74	2.24	15 (31%)	50,91,114	2.81	18 (36%)
22	DGD	B	850	-	60,60,67	0.88	2 (3%)	74,74,81	1.39	11 (14%)
17	CLA	2	505	-	52,60,73	1.58	7 (13%)	60,97,113	1.53	6 (10%)
17	CLA	3	318	-	45,53,73	1.67	7 (15%)	56,89,113	1.59	8 (14%)
17	CLA	A	852	-	57,65,73	1.61	9 (15%)	66,103,113	1.43	9 (13%)
17	CLA	5	310	-	50,58,73	1.65	8 (16%)	58,95,113	1.59	8 (13%)
17	CLA	1	509	-	50,58,73	1.63	7 (14%)	58,95,113	1.60	7 (12%)
26	XAT	2	502	-	39,47,47	1.13	4 (10%)	54,74,74	2.84	20 (37%)
17	CLA	L	304	-	45,53,73	1.65	10 (22%)	52,89,113	1.88	11 (21%)
17	CLA	K	205	10	37,47,73	1.93	7 (18%)	42,81,113	1.73	8 (19%)
17	CLA	A	802	-	58,66,73	1.54	9 (15%)	67,104,113	1.51	7 (10%)
17	CLA	A	804	17	52,60,73	1.56	9 (17%)	60,97,113	1.60	7 (11%)
17	CLA	5	316	-	41,49,73	1.73	9 (21%)	47,84,113	1.80	9 (19%)
17	CLA	1	505	-	42,50,73	1.86	7 (16%)	48,85,113	1.58	8 (16%)
17	CLA	A	831	-	63,71,73	1.50	10 (15%)	77,110,113	1.53	12 (15%)
17	CLA	B	821	-	50,58,73	1.71	9 (18%)	58,95,113	1.62	8 (13%)
20	BCR	L	306	-	41,41,41	0.85	1 (2%)	56,56,56	1.96	19 (33%)
24	LUT	1	502	-	42,43,43	0.90	2 (4%)	51,60,60	1.68	11 (21%)
24	LUT	3	303	-	42,43,43	0.89	2 (4%)	51,60,60	1.51	10 (19%)
17	CLA	A	811	-	39,48,73	1.73	9 (23%)	45,82,113	1.74	10 (22%)
17	CLA	2	506	-	65,73,73	1.44	9 (13%)	76,113,113	1.51	7 (9%)
23	LMG	F	806	-	45,45,55	0.95	2 (4%)	53,53,63	1.07	4 (7%)
20	BCR	F	801	-	41,41,41	0.99	2 (4%)	56,56,56	2.09	17 (30%)
20	BCR	J	102	-	41,41,41	1.01	2 (4%)	56,56,56	2.18	24 (42%)
20	BCR	3	305	-	41,41,41	0.90	2 (4%)	56,56,56	1.98	13 (23%)
17	CLA	B	808	-	52,60,73	1.68	9 (17%)	60,97,113	1.57	9 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CHL	2	512	-	46,54,74	2.17	14 (30%)	53,90,114	2.91	20 (37%)
17	CLA	B	822	-	47,55,73	1.72	10 (21%)	54,91,113	1.75	7 (12%)
17	CLA	5	311	-	42,50,73	1.72	7 (16%)	48,85,113	1.74	8 (16%)
17	CLA	B	828	-	41,49,73	1.74	10 (24%)	47,84,113	1.81	12 (25%)
17	CLA	A	813	-	45,53,73	1.69	9 (20%)	52,89,113	1.63	7 (13%)
20	BCR	B	848	-	41,41,41	1.05	2 (4%)	56,56,56	1.98	18 (32%)
25	CHL	5	317	-	41,48,74	2.34	15 (36%)	42,82,114	3.07	22 (52%)
25	CHL	2	513	-	40,48,74	2.49	16 (40%)	37,81,114	3.16	19 (51%)
17	CLA	3	314	14	55,63,73	1.58	6 (10%)	64,101,113	1.55	10 (15%)
17	CLA	A	824	-	39,48,73	1.77	8 (20%)	45,82,113	1.68	8 (17%)
17	CLA	3	313	-	48,56,73	1.71	6 (12%)	55,92,113	1.66	9 (16%)
17	CLA	2	508	-	47,55,73	1.72	7 (14%)	54,91,113	1.49	6 (11%)
17	CLA	3	316	-	38,45,73	1.80	5 (13%)	43,78,113	1.82	8 (18%)
17	CLA	5	306	-	39,48,73	1.78	6 (15%)	44,83,113	1.70	7 (15%)
17	CLA	A	808	1	65,73,73	1.42	10 (15%)	76,113,113	1.44	7 (9%)
17	CLA	3	317	-	41,49,73	1.79	8 (19%)	47,84,113	1.74	10 (21%)
20	BCR	L	305	-	41,41,41	1.00	1 (2%)	56,56,56	2.16	18 (32%)
17	CLA	A	810	17	54,62,73	1.59	10 (18%)	62,99,113	1.66	7 (11%)
17	CLA	B	833	-	65,73,73	1.39	8 (12%)	76,113,113	1.57	10 (13%)
17	CLA	B	836	-	42,50,73	1.84	9 (21%)	48,85,113	1.56	7 (14%)
17	CLA	L	301	-	56,64,73	1.59	11 (19%)	65,102,113	1.50	8 (12%)
17	CLA	1	511	-	46,54,73	1.71	9 (19%)	53,90,113	1.61	7 (13%)
23	LMG	2	519	-	36,36,55	1.09	2 (5%)	44,44,63	1.37	8 (18%)
25	CHL	1	512	-	47,55,74	2.31	16 (34%)	50,91,114	2.77	20 (40%)
17	CLA	A	838	-	65,73,73	1.46	10 (15%)	76,113,113	1.45	10 (13%)
26	XAT	5	304	-	39,47,47	1.24	5 (12%)	54,74,74	2.53	18 (33%)
17	CLA	3	307	-	39,48,73	2.01	9 (23%)	45,82,113	1.58	7 (15%)
17	CLA	A	832	-	44,53,73	1.68	10 (22%)	52,88,113	1.78	8 (15%)
17	CLA	B	806	-	38,47,73	1.98	12 (31%)	46,80,113	1.77	10 (21%)
17	CLA	B	825	-	42,50,73	1.70	10 (23%)	48,85,113	1.69	7 (14%)
17	CLA	A	826	-	60,68,73	1.48	8 (13%)	70,107,113	1.54	9 (12%)
25	CHL	1	517	12	40,49,74	2.29	14 (35%)	42,83,114	3.16	20 (47%)
17	CLA	B	830	-	56,64,73	1.72	11 (19%)	65,102,113	1.45	7 (10%)
20	BCR	A	847	-	41,41,41	0.97	2 (4%)	56,56,56	2.00	20 (35%)
22	DGD	J	103	-	67,67,67	0.83	2 (2%)	81,81,81	1.11	4 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	LUT	2	501	-	42,43,43	0.94	1 (2%)	51,60,60	1.94	15 (29%)
25	CHL	1	514	-	40,49,74	2.55	15 (37%)	42,83,114	3.00	19 (45%)
17	CLA	B	838	-	65,73,73	1.47	10 (15%)	76,113,113	1.49	8 (10%)
17	CLA	5	305	-	38,46,73	2.22	10 (26%)	47,79,113	1.71	10 (21%)
17	CLA	B	835	-	60,68,73	1.49	9 (15%)	70,107,113	1.50	11 (15%)
17	CLA	B	823	-	42,50,73	1.76	9 (21%)	48,85,113	1.68	7 (14%)
17	CLA	A	828	-	41,49,73	1.76	10 (24%)	47,84,113	1.68	7 (14%)
17	CLA	1	510	19	46,54,73	1.73	8 (17%)	53,90,113	1.56	7 (13%)
17	CLA	1	508	-	39,48,73	1.83	6 (15%)	45,82,113	1.71	7 (15%)
17	CLA	B	837	-	50,58,73	1.62	10 (20%)	58,95,113	1.62	10 (17%)
17	CLA	B	827	-	41,49,73	1.78	10 (24%)	47,84,113	1.86	10 (21%)
23	LMG	F	805	-	30,30,55	1.22	2 (6%)	38,38,63	1.21	3 (7%)
17	CLA	A	812	-	42,50,73	1.75	10 (23%)	48,85,113	1.76	10 (20%)
25	CHL	2	515	-	45,53,74	2.23	14 (31%)	52,89,114	2.82	21 (40%)
21	SF4	C	102	3	0,12,12	-	-	-	-	-
20	BCR	B	847	-	41,41,41	1.03	2 (4%)	56,56,56	2.35	19 (33%)
17	CLA	B	817	-	49,57,73	1.68	11 (22%)	55,93,113	1.59	7 (12%)
19	LHG	A	843	-	48,48,48	0.90	3 (6%)	51,54,54	1.29	5 (9%)
17	CLA	A	842	19	50,58,73	1.66	10 (20%)	58,95,113	1.52	8 (13%)
17	CLA	B	805	-	41,49,73	1.79	9 (21%)	47,84,113	1.75	10 (21%)
17	CLA	B	811	-	55,63,73	1.58	11 (20%)	64,101,113	1.53	7 (10%)
17	CLA	J	101	9	42,50,73	1.79	6 (14%)	48,85,113	1.68	7 (14%)
17	CLA	A	834	1	41,49,73	1.82	9 (21%)	47,84,113	1.62	7 (14%)
17	CLA	A	818	-	39,48,73	1.75	10 (25%)	45,82,113	1.74	9 (20%)
17	CLA	B	801	-	65,73,73	1.47	11 (16%)	76,113,113	1.47	10 (13%)
17	CLA	K	202	-	41,49,73	1.75	8 (19%)	47,84,113	1.70	8 (17%)
25	CHL	5	315	-	46,54,74	2.23	15 (32%)	49,90,114	2.89	21 (42%)
20	BCR	B	845	-	41,41,41	1.04	1 (2%)	56,56,56	2.07	17 (30%)
20	BCR	A	853	-	41,41,41	0.97	2 (4%)	56,56,56	2.24	18 (32%)
19	LHG	2	517	17	34,34,48	1.07	2 (5%)	37,40,54	1.21	4 (10%)
17	CLA	K	201	-	38,45,73	1.92	9 (23%)	43,78,113	1.66	6 (13%)
17	CLA	5	312	-	46,54,73	1.73	8 (17%)	53,90,113	1.50	7 (13%)
17	CLA	B	832	-	43,51,73	1.67	9 (20%)	49,86,113	1.62	5 (10%)
17	CLA	A	830	-	50,58,73	1.59	9 (18%)	58,95,113	1.64	6 (10%)
20	BCR	B	849	-	41,41,41	1.07	2 (4%)	56,56,56	2.01	17 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	CLA	B	820	-	53,61,73	1.68	10 (18%)	61,98,113	1.48	8 (13%)
20	BCR	5	302	-	41,41,41	0.83	0	56,56,56	1.97	13 (23%)
17	CLA	A	809	1	38,47,73	1.83	9 (23%)	39,80,113	1.63	5 (12%)
17	CLA	A	815	-	45,53,73	1.71	9 (20%)	52,89,113	1.61	8 (15%)
17	CLA	A	822	-	41,49,73	1.80	9 (21%)	47,84,113	1.79	9 (19%)
17	CLA	B	831	-	43,51,73	1.80	9 (20%)	49,86,113	1.62	7 (14%)
19	LHG	1	516	17	48,48,48	0.91	2 (4%)	51,54,54	1.16	4 (7%)
17	CLA	L	303	-	52,60,73	1.62	9 (17%)	60,97,113	1.73	10 (16%)
17	CLA	F	802	-	42,50,73	1.78	9 (21%)	48,85,113	1.68	7 (14%)
17	CLA	B	818	-	59,67,73	1.50	10 (16%)	68,105,113	1.59	9 (13%)
23	LMG	2	518	-	16,16,55	0.47	0	22,22,63	0.99	2 (9%)
17	CLA	B	819	-	41,49,73	1.77	10 (24%)	47,84,113	1.83	12 (25%)
18	PQN	B	843	-	31,31,34	1.36	2 (6%)	38,41,45	1.49	5 (13%)
20	BCR	A	846	-	41,41,41	1.05	2 (4%)	56,56,56	2.07	17 (30%)
17	CLA	A	805	-	64,72,73	1.50	12 (18%)	74,111,113	1.57	10 (13%)
17	CLA	B	810	2	39,48,73	1.75	10 (25%)	45,82,113	1.81	9 (20%)
20	BCR	I	101	-	41,41,41	1.22	3 (7%)	56,56,56	2.08	19 (33%)
17	CLA	5	308	-	60,68,73	1.52	9 (15%)	70,107,113	1.57	8 (11%)
20	BCR	F	804	-	41,41,41	1.03	1 (2%)	56,56,56	1.97	18 (32%)
17	CLA	1	513	-	65,73,73	1.53	7 (10%)	76,113,113	1.36	7 (9%)
20	BCR	B	844	-	41,41,41	0.85	1 (2%)	56,56,56	2.59	19 (33%)
17	CLA	B	802	-	64,72,73	1.46	10 (15%)	74,111,113	1.49	10 (13%)
17	CLA	B	809	-	39,48,73	1.81	10 (25%)	45,82,113	1.69	6 (13%)
17	CLA	A	829	-	55,63,73	1.60	10 (18%)	64,101,113	1.59	9 (14%)
17	CLA	3	301	-	41,49,73	1.80	9 (21%)	47,84,113	1.74	10 (21%)
21	SF4	C	101	3	0,12,12	-	-	-	-	-
25	CHL	5	314	-	47,55,74	2.22	15 (31%)	50,91,114	2.82	21 (42%)
17	CLA	A	840	-	41,49,73	1.82	9 (21%)	47,84,113	1.64	8 (17%)
20	BCR	B	846	-	41,41,41	1.05	3 (7%)	56,56,56	2.31	18 (32%)
17	CLA	B	842	-	57,65,73	1.55	8 (14%)	66,103,113	1.46	7 (10%)
17	CLA	B	803	-	65,73,73	1.45	9 (13%)	76,113,113	1.40	10 (13%)
17	CLA	B	815	-	65,73,73	1.50	11 (16%)	76,113,113	1.44	10 (13%)
17	CLA	A	819	-	39,48,73	1.82	9 (23%)	45,82,113	1.67	7 (15%)
17	CLA	5	313	15	39,48,73	1.80	9 (23%)	45,82,113	1.64	8 (17%)
17	CLA	A	825	-	59,67,73	1.55	10 (16%)	68,105,113	1.47	8 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	CLA	B	824	-	45,53,73	1.74	9 (20%)	52,89,113	1.54	6 (11%)
17	CLA	A	816	-	59,67,73	1.47	8 (13%)	68,105,113	1.56	8 (11%)
25	CHL	3	315	-	43,51,74	2.17	14 (32%)	45,86,114	3.02	19 (42%)
20	BCR	A	848	-	41,41,41	1.06	2 (4%)	56,56,56	2.00	12 (21%)
17	CLA	F	803	-	41,49,73	1.77	9 (21%)	47,84,113	1.65	8 (17%)
17	CLA	3	308	-	55,63,73	1.49	9 (16%)	64,101,113	1.54	9 (14%)
17	CLA	2	504	13	34,44,73	2.06	10 (29%)	42,76,113	1.87	10 (23%)
17	CLA	3	306	-	52,60,73	1.60	7 (13%)	65,97,113	1.75	11 (16%)
17	CLA	2	511	-	39,48,73	1.82	10 (25%)	45,82,113	1.93	11 (24%)
17	CLA	2	507	13	47,56,73	1.97	9 (19%)	54,91,113	1.81	10 (18%)
20	BCR	A	849	-	40,40,41	1.04	2 (5%)	54,54,56	1.90	15 (27%)
25	CHL	2	516	13	43,51,74	2.19	13 (30%)	49,86,114	3.04	19 (38%)
19	LHG	A	844	17	29,29,48	1.20	3 (10%)	32,35,54	1.19	3 (9%)
17	CLA	5	307	15	65,73,73	1.47	8 (12%)	76,113,113	1.35	8 (10%)
17	CLA	5	309	-	45,53,73	1.72	8 (17%)	52,89,113	1.65	7 (13%)
17	CLA	A	837	-	41,49,73	1.84	11 (26%)	47,84,113	1.87	10 (21%)
17	CLA	A	820	-	57,65,73	1.53	8 (14%)	66,103,113	1.69	9 (13%)
17	CLA	A	806	1	65,73,73	1.44	9 (13%)	76,113,113	1.41	8 (10%)
17	CLA	B	829	-	39,48,73	1.77	11 (28%)	45,82,113	1.73	9 (20%)
20	BCR	K	204	-	41,41,41	0.99	2 (4%)	56,56,56	2.02	16 (28%)
17	CLA	A	807	-	37,47,73	1.78	10 (27%)	41,80,113	1.76	8 (19%)
17	CLA	B	840	-	41,49,73	1.75	9 (21%)	47,84,113	1.80	8 (17%)
17	CLA	B	841	-	54,62,73	1.56	10 (18%)	62,99,113	1.53	9 (14%)
18	PQN	A	841	-	34,34,34	1.38	2 (5%)	42,45,45	1.24	4 (9%)
17	CLA	A	817	-	39,47,73	2.03	13 (33%)	42,81,113	1.80	7 (16%)
17	CLA	B	839	-	47,55,73	1.66	9 (19%)	54,91,113	1.73	9 (16%)
17	CLA	A	821	-	42,50,73	1.78	9 (21%)	48,85,113	1.79	8 (16%)
17	CLA	A	836	-	55,63,73	1.65	10 (18%)	64,101,113	1.60	10 (15%)
17	CLA	1	507	12	42,50,73	1.71	9 (21%)	48,85,113	1.68	9 (18%)
17	CLA	B	834	-	45,53,73	1.73	9 (20%)	52,89,113	1.66	10 (19%)
17	CLA	B	814	-	41,49,73	1.78	11 (26%)	47,84,113	1.77	12 (25%)
21	SF4	A	850	1,2	0,12,12	-	-	-	-	-
17	CLA	A	803	-	41,49,73	1.80	10 (24%)	47,84,113	1.79	10 (21%)
17	CLA	A	823	-	55,62,73	1.74	11 (20%)	60,99,113	1.54	10 (16%)
17	CLA	3	310	-	45,53,73	1.77	7 (15%)	52,89,113	1.63	9 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	CLA	3	311	-	50,58,73	1.51	7 (14%)	58,95,113	1.74	11 (18%)
17	CLA	A	827	-	65,73,73	1.42	12 (18%)	76,113,113	1.51	9 (11%)
17	CLA	1	504	-	41,49,73	1.78	7 (17%)	47,84,113	1.60	6 (12%)
17	CLA	2	514	-	55,63,73	1.55	10 (18%)	64,101,113	1.47	8 (12%)
17	CLA	B	807	2	65,73,73	1.46	11 (16%)	76,113,113	1.42	6 (7%)
17	CLA	2	510	19	60,68,73	1.50	7 (11%)	70,107,113	1.51	9 (12%)
17	CLA	3	312	-	41,49,73	1.84	7 (17%)	47,84,113	1.63	8 (17%)
20	BCR	1	503	-	19,19,41	0.67	0	26,26,56	2.04	7 (26%)
20	BCR	A	845	-	41,41,41	1.17	4 (9%)	56,56,56	2.29	20 (35%)
17	CLA	L	302	-	41,48,73	1.92	9 (21%)	45,82,113	1.80	8 (17%)
17	CLA	B	813	-	43,51,73	1.72	9 (20%)	49,86,113	1.69	9 (18%)
17	CLA	A	833	-	39,48,73	1.74	10 (25%)	45,82,113	1.77	9 (20%)
17	CLA	1	506	-	55,63,73	1.62	8 (14%)	64,101,113	1.50	8 (12%)
20	BCR	A	851	-	41,41,41	0.91	1 (2%)	56,56,56	2.17	20 (35%)
17	CLA	A	839	-	42,50,73	1.81	10 (23%)	48,85,113	1.73	7 (14%)

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
17	CLA	B	804	-	1/1/15/20	14/37/115/115	-
20	BCR	B	852	-	-	6/29/63/63	0/2/2/2
17	CLA	2	509	-	1/1/12/20	10/19/97/115	-
19	LHG	B	851	-	-	18/42/42/53	-
17	CLA	A	814	-	1/1/10/20	1/10/88/115	-
24	LUT	3	304	-	-	2/29/67/67	0/2/2/2
24	LUT	5	303	-	-	2/29/67/67	0/2/2/2
17	CLA	B	812	-	1/1/13/20	6/25/101/115	-
17	CLA	B	816	-	1/1/10/20	4/11/89/115	-
17	CLA	1	515	-	1/1/10/20	6/13/87/115	-
20	BCR	2	503	-	-	8/29/63/63	0/2/2/2
17	CLA	K	203	-	1/1/9/20	5/8/82/115	-
17	CLA	A	835	-	1/1/12/20	12/21/99/115	-
24	LUT	1	501	-	-	2/29/67/67	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	CL0	A	801	-	3/3/18/25	5/33/125/135	-
17	CLA	B	826	-	1/1/14/20	8/34/112/115	-
17	CLA	3	309	-	-	4/10/86/115	-
23	LMG	5	301	-	-	8/27/47/70	0/1/1/1
25	CHL	3	302	13	3/3/16/26	3/17/115/137	-
22	DGD	B	850	-	-	19/48/88/95	0/2/2/2
17	CLA	3	318	-	1/1/11/20	6/15/91/115	-
17	CLA	2	505	-	-	11/22/100/115	-
17	CLA	A	852	-	1/1/13/20	9/28/106/115	-
17	CLA	5	310	-	1/1/12/20	10/19/97/115	-
17	CLA	1	509	-	-	6/19/97/115	-
26	XAT	2	502	-	-	6/31/93/93	0/4/4/4
17	CLA	L	304	-	1/1/11/20	6/13/91/115	-
17	CLA	K	205	10	1/1/9/20	0/6/80/115	-
17	CLA	A	802	-	1/1/13/20	12/29/107/115	-
17	CLA	A	804	17	1/1/12/20	5/22/100/115	-
17	CLA	5	316	-	1/1/10/20	2/8/86/115	-
17	CLA	1	505	-	1/1/10/20	3/10/88/115	-
17	CLA	A	831	-	1/1/14/20	17/35/111/115	-
17	CLA	B	821	-	1/1/12/20	5/19/97/115	-
20	BCR	L	306	-	-	6/29/63/63	0/2/2/2
24	LUT	1	502	-	-	4/29/67/67	0/2/2/2
24	LUT	3	303	-	-	2/29/67/67	0/2/2/2
17	CLA	A	811	-	1/1/9/20	2/8/82/115	-
17	CLA	2	506	-	1/1/15/20	16/37/115/115	-
23	LMG	F	806	-	-	18/40/60/70	0/1/1/1
20	BCR	F	801	-	-	6/29/63/63	0/2/2/2
20	BCR	J	102	-	-	3/29/63/63	0/2/2/2
20	BCR	3	305	-	-	8/29/63/63	0/2/2/2
17	CLA	B	808	-	1/1/12/20	7/22/100/115	-
25	CHL	2	512	-	3/3/16/26	3/17/113/137	-
17	CLA	B	822	-	1/1/11/20	4/16/94/115	-
17	CLA	5	311	-	1/1/10/20	4/10/88/115	-
17	CLA	B	828	-	1/1/10/20	3/8/86/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	A	813	-	1/1/11/20	9/13/91/115	-
25	CHL	5	317	-	3/3/14/26	4/8/102/137	-
20	BCR	B	848	-	-	2/29/63/63	0/2/2/2
25	CHL	2	513	-	3/3/13/26	5/10/100/137	-
17	CLA	3	314	14	1/1/13/20	13/25/103/115	-
17	CLA	A	824	-	1/1/9/20	5/8/82/115	-
17	CLA	3	313	-	1/1/11/20	10/17/95/115	-
17	CLA	2	508	-	1/1/11/20	2/15/93/115	-
17	CLA	3	316	-	1/1/8/20	0/2/76/115	-
17	CLA	5	306	-	1/1/10/20	2/6/84/115	-
17	CLA	A	808	1	1/1/15/20	8/37/115/115	-
17	CLA	3	317	-	1/1/10/20	4/8/86/115	-
20	BCR	L	305	-	-	9/29/63/63	0/2/2/2
17	CLA	A	810	17	1/1/12/20	5/24/102/115	-
17	CLA	B	833	-	1/1/15/20	4/37/115/115	-
17	CLA	B	836	-	-	4/10/88/115	-
17	CLA	L	301	-	1/1/13/20	5/27/105/115	-
17	CLA	1	511	-	1/1/11/20	5/15/93/115	-
25	CHL	1	512	-	3/3/16/26	8/17/115/137	-
23	LMG	2	519	-	-	14/31/51/70	0/1/1/1
17	CLA	A	838	-	1/1/15/20	15/37/115/115	-
26	XAT	5	304	-	-	2/31/93/93	0/4/4/4
17	CLA	3	307	-	1/1/9/20	3/8/82/115	-
17	CLA	A	832	-	1/1/10/20	5/11/89/115	-
17	CLA	B	806	-	1/1/8/20	4/8/79/115	-
17	CLA	B	825	-	1/1/10/20	3/10/88/115	-
17	CLA	A	826	-	1/1/14/20	13/31/109/115	-
25	CHL	1	517	12	3/3/14/26	5/10/104/137	-
17	CLA	B	830	-	1/1/13/20	11/27/105/115	-
20	BCR	A	847	-	-	2/29/63/63	0/2/2/2
22	DGD	J	103	-	-	26/55/95/95	0/2/2/2
24	LUT	2	501	-	-	0/29/67/67	0/2/2/2
25	CHL	1	514	-	3/3/14/26	4/10/104/137	-
17	CLA	B	838	-	1/1/15/20	4/37/115/115	-
17	CLA	5	305	-	1/1/9/20	1/8/80/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	B	835	-	1/1/14/20	6/31/109/115	-
17	CLA	B	823	-	1/1/10/20	4/10/88/115	-
17	CLA	A	828	-	1/1/10/20	2/8/86/115	-
17	CLA	1	510	19	1/1/11/20	7/15/93/115	-
17	CLA	1	508	-	1/1/9/20	3/8/82/115	-
17	CLA	B	837	-	1/1/12/20	5/19/97/115	-
17	CLA	B	827	-	1/1/10/20	3/8/86/115	-
23	LMG	F	805	-	-	4/25/45/70	0/1/1/1
17	CLA	A	812	-	1/1/10/20	3/10/88/115	-
25	CHL	2	515	-	3/3/16/26	6/15/111/137	-
21	SF4	C	102	3	-	-	0/6/5/5
20	BCR	B	847	-	-	5/29/63/63	0/2/2/2
17	CLA	B	817	-	1/1/11/20	7/18/96/115	-
19	LHG	A	843	-	-	13/53/53/53	-
17	CLA	A	842	19	1/1/12/20	9/19/97/115	-
17	CLA	B	805	-	1/1/10/20	2/8/86/115	-
17	CLA	B	811	-	1/1/13/20	12/25/103/115	-
17	CLA	J	101	9	1/1/10/20	7/10/88/115	-
17	CLA	A	834	1	1/1/10/20	4/8/86/115	-
17	CLA	A	818	-	1/1/9/20	4/8/82/115	-
17	CLA	B	801	-	1/1/15/20	9/37/115/115	-
17	CLA	K	202	-	1/1/10/20	2/8/86/115	-
25	CHL	5	315	-	3/3/16/26	4/15/113/137	-
20	BCR	B	845	-	-	6/29/63/63	0/2/2/2
20	BCR	A	853	-	-	2/29/63/63	0/2/2/2
19	LHG	2	517	17	-	5/39/39/53	-
17	CLA	K	201	-	1/1/8/20	0/2/76/115	-
17	CLA	5	312	-	1/1/11/20	7/15/93/115	-
17	CLA	B	832	-	1/1/10/20	3/11/89/115	-
17	CLA	A	830	-	1/1/12/20	3/19/97/115	-
20	BCR	B	849	-	-	3/29/63/63	0/2/2/2
17	CLA	B	820	-	1/1/12/20	5/23/101/115	-
20	BCR	5	302	-	-	9/29/63/63	0/2/2/2
17	CLA	A	809	1	1/1/9/20	1/4/84/115	-
17	CLA	A	815	-	1/1/11/20	4/13/91/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	A	822	-	1/1/10/20	2/8/86/115	-
17	CLA	B	831	-	1/1/10/20	1/11/89/115	-
19	LHG	1	516	17	-	23/53/53/53	-
17	CLA	L	303	-	1/1/12/20	12/22/100/115	-
17	CLA	F	802	-	1/1/10/20	2/10/88/115	-
17	CLA	B	818	-	1/1/13/20	16/30/108/115	-
23	LMG	2	518	-	-	3/7/27/70	0/1/1/1
17	CLA	B	819	-	1/1/10/20	0/8/86/115	-
18	PQN	B	843	-	-	7/20/40/43	0/2/2/2
20	BCR	A	846	-	-	7/29/63/63	0/2/2/2
17	CLA	A	805	-	1/1/14/20	18/36/114/115	-
17	CLA	B	810	2	1/1/9/20	2/8/82/115	-
20	BCR	I	101	-	-	4/29/63/63	0/2/2/2
17	CLA	5	308	-	1/1/14/20	14/31/109/115	-
20	BCR	F	804	-	-	2/29/63/63	0/2/2/2
17	CLA	1	513	-	-	19/37/115/115	-
20	BCR	B	844	-	-	4/29/63/63	0/2/2/2
17	CLA	B	802	-	1/1/14/20	6/35/113/115	-
17	CLA	B	809	-	1/1/9/20	2/8/82/115	-
17	CLA	A	829	-	1/1/13/20	6/25/103/115	-
17	CLA	3	301	-	1/1/10/20	2/8/86/115	-
25	CHL	5	314	-	3/3/16/26	7/17/115/137	-
21	SF4	C	101	3	-	-	0/6/5/5
17	CLA	A	840	-	1/1/10/20	2/8/86/115	-
20	BCR	B	846	-	-	6/29/63/63	0/2/2/2
17	CLA	B	842	-	1/1/13/20	15/28/106/115	-
17	CLA	B	803	-	1/1/15/20	16/37/115/115	-
17	CLA	B	815	-	1/1/15/20	7/37/115/115	-
17	CLA	A	819	-	1/1/9/20	3/8/82/115	-
17	CLA	5	313	15	1/1/9/20	2/8/82/115	-
17	CLA	A	825	-	1/1/13/20	8/30/108/115	-
17	CLA	B	824	-	1/1/11/20	6/13/91/115	-
17	CLA	A	816	-	1/1/13/20	12/29/107/115	-
25	CHL	3	315	-	3/3/15/26	3/12/110/137	-
20	BCR	A	848	-	-	6/29/63/63	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	F	803	-	1/1/10/20	3/8/86/115	-
17	CLA	3	308	-	1/1/13/20	14/25/103/115	-
17	CLA	2	504	13	1/1/7/20	0/2/73/115	-
17	CLA	3	306	-	1/1/13/20	14/23/99/115	-
17	CLA	2	511	-	1/1/9/20	1/8/82/115	-
17	CLA	2	507	13	2/2/11/20	5/14/88/115	-
20	BCR	A	849	-	-	2/27/61/63	0/2/2/2
25	CHL	2	516	13	3/3/15/26	8/13/109/137	-
19	LHG	A	844	17	-	11/34/34/53	-
17	CLA	5	307	15	1/1/15/20	17/37/115/115	-
17	CLA	5	309	-	1/1/11/20	5/13/91/115	-
17	CLA	A	837	-	1/1/10/20	4/8/86/115	-
17	CLA	A	820	-	1/1/13/20	10/28/106/115	-
17	CLA	A	806	1	1/1/15/20	20/37/115/115	-
17	CLA	B	829	-	1/1/9/20	2/8/82/115	-
20	BCR	K	204	-	-	8/29/63/63	0/2/2/2
17	CLA	A	807	-	1/1/8/20	1/5/79/115	-
17	CLA	B	840	-	1/1/10/20	1/8/86/115	-
17	CLA	B	841	-	1/1/12/20	8/24/102/115	-
18	PQN	A	841	-	-	13/23/43/43	0/2/2/2
17	CLA	A	817	-	1/1/9/20	0/2/82/115	-
17	CLA	B	839	-	1/1/11/20	5/16/94/115	-
17	CLA	A	821	-	1/1/10/20	2/10/88/115	-
17	CLA	A	836	-	1/1/13/20	11/25/103/115	-
17	CLA	1	507	12	1/1/10/20	4/10/88/115	-
17	CLA	B	834	-	1/1/11/20	6/13/91/115	-
17	CLA	B	814	-	1/1/10/20	5/8/86/115	-
21	SF4	A	850	1,2	-	-	0/6/5/5
17	CLA	A	803	-	1/1/10/20	0/8/86/115	-
17	CLA	A	823	-	1/1/12/20	13/25/99/115	-
17	CLA	3	310	-	1/1/11/20	4/13/91/115	-
17	CLA	3	311	-	1/1/12/20	8/19/97/115	-
17	CLA	A	827	-	1/1/15/20	17/37/115/115	-
17	CLA	1	504	-	1/1/10/20	5/8/86/115	-
17	CLA	2	514	-	1/1/13/20	8/25/103/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	B	807	2	1/1/15/20	11/37/115/115	-
17	CLA	2	510	19	1/1/14/20	16/31/109/115	-
17	CLA	3	312	-	1/1/10/20	5/8/86/115	-
20	BCR	1	503	-	-	4/11/28/63	0/1/1/2
20	BCR	A	845	-	-	6/29/63/63	0/2/2/2
17	CLA	L	302	-	1/1/9/20	1/8/82/115	-
17	CLA	B	813	-	1/1/10/20	3/11/89/115	-
17	CLA	A	833	-	1/1/9/20	1/8/82/115	-
17	CLA	1	506	-	1/1/13/20	9/25/103/115	-
20	BCR	A	851	-	-	6/29/63/63	0/2/2/2
17	CLA	A	839	-	1/1/10/20	3/10/88/115	-

All (1514) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	3	307	CLA	C4B-NB	8.26	1.42	1.35
17	3	309	CLA	C3B-C4B	7.94	1.48	1.39
17	1	513	CLA	C4B-NB	7.88	1.42	1.35
17	3	313	CLA	C4B-NB	7.60	1.42	1.35
17	1	505	CLA	C4B-NB	7.57	1.42	1.35
17	3	310	CLA	C4B-NB	7.57	1.42	1.35
17	K	205	CLA	C4B-NB	7.56	1.42	1.35
16	A	801	CL0	MG-NA	7.46	2.24	2.06
17	5	305	CLA	C3B-C4B	7.40	1.48	1.39
17	1	510	CLA	C4B-NB	7.38	1.41	1.35
17	3	314	CLA	C4B-NB	7.33	1.41	1.35
17	B	830	CLA	C4B-NB	7.29	1.41	1.35
17	1	506	CLA	C4B-NB	7.27	1.41	1.35
17	3	312	CLA	C4B-NB	7.20	1.41	1.35
17	2	510	CLA	C4B-NB	7.17	1.41	1.35
17	A	821	CLA	C4B-NB	7.14	1.41	1.35
17	1	508	CLA	C4B-NB	7.12	1.41	1.35
17	3	316	CLA	C4B-NB	7.06	1.41	1.35
17	2	507	CLA	C4B-NB	7.06	1.41	1.35
17	B	836	CLA	C4B-NB	7.05	1.41	1.35
17	5	310	CLA	C4B-NB	7.04	1.41	1.35
17	B	821	CLA	C4B-NB	7.03	1.41	1.35
17	J	101	CLA	C4B-NB	7.02	1.41	1.35
17	1	515	CLA	C4B-NB	7.01	1.41	1.35
17	3	317	CLA	C4B-NB	7.00	1.41	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	1	509	CLA	C4B-NB	6.99	1.41	1.35
17	B	820	CLA	C4B-NB	6.95	1.41	1.35
17	K	201	CLA	C4B-NB	6.92	1.41	1.35
17	B	822	CLA	C4B-NB	6.91	1.41	1.35
17	B	842	CLA	C4B-NB	6.87	1.41	1.35
17	5	312	CLA	C4B-NB	6.85	1.41	1.35
17	A	842	CLA	C4B-NB	6.84	1.41	1.35
17	A	839	CLA	C4B-NB	6.80	1.41	1.35
17	5	311	CLA	C4B-NB	6.78	1.41	1.35
17	A	822	CLA	C4B-NB	6.75	1.41	1.35
17	A	837	CLA	C4B-NB	6.75	1.41	1.35
18	A	841	PQN	C3-C2	6.73	1.47	1.35
17	5	307	CLA	C4B-NB	6.72	1.41	1.35
17	2	507	CLA	C2-C3	6.66	1.52	1.33
17	2	508	CLA	C4B-NB	6.64	1.41	1.35
25	2	513	CHL	C4D-C3D	-6.64	1.31	1.45
17	2	511	CLA	C4B-NB	6.64	1.41	1.35
17	B	831	CLA	C4B-NB	6.62	1.41	1.35
17	B	808	CLA	C4B-NB	6.62	1.41	1.35
17	5	305	CLA	C4B-NB	6.60	1.41	1.35
17	2	514	CLA	C4B-NB	6.60	1.41	1.35
17	5	306	CLA	C4B-NB	6.59	1.41	1.35
17	F	802	CLA	C4B-NB	6.59	1.41	1.35
17	3	306	CLA	C4B-NB	6.56	1.41	1.35
17	A	834	CLA	C4B-NB	6.56	1.41	1.35
17	1	504	CLA	C4B-NB	6.56	1.41	1.35
17	2	505	CLA	C4B-NB	6.56	1.41	1.35
17	F	803	CLA	C4B-NB	6.46	1.41	1.35
17	L	302	CLA	C4B-NB	6.45	1.41	1.35
17	K	202	CLA	C4B-NB	6.44	1.41	1.35
17	2	506	CLA	C4B-NB	6.43	1.40	1.35
17	1	511	CLA	C4B-NB	6.43	1.40	1.35
17	3	301	CLA	C4B-NB	6.43	1.40	1.35
17	A	852	CLA	C4B-NB	6.40	1.40	1.35
17	L	303	CLA	C4B-NB	6.39	1.40	1.35
17	B	824	CLA	C4B-NB	6.37	1.40	1.35
17	5	313	CLA	C4B-NB	6.35	1.40	1.35
17	A	803	CLA	C4B-NB	6.35	1.40	1.35
17	1	507	CLA	C4B-NB	6.34	1.40	1.35
17	A	814	CLA	C4B-NB	6.34	1.40	1.35
17	B	802	CLA	C4B-NB	6.33	1.40	1.35
17	B	834	CLA	C4B-NB	6.30	1.40	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	B	839	CLA	C4B-NB	6.30	1.40	1.35
17	B	823	CLA	C4B-NB	6.29	1.40	1.35
17	B	805	CLA	C4B-NB	6.26	1.40	1.35
17	B	810	CLA	C4B-NB	6.24	1.40	1.35
17	A	825	CLA	C4B-NB	6.24	1.40	1.35
17	B	838	CLA	C4B-NB	6.23	1.40	1.35
17	B	817	CLA	C4B-NB	6.22	1.40	1.35
18	B	843	PQN	C3-C2	6.20	1.46	1.35
17	2	504	CLA	C4B-NB	6.19	1.40	1.35
17	A	840	CLA	C4B-NB	6.19	1.40	1.35
17	5	309	CLA	C4B-NB	6.18	1.40	1.35
17	B	818	CLA	C4B-NB	6.18	1.40	1.35
17	5	308	CLA	C4B-NB	6.18	1.40	1.35
17	A	836	CLA	C4B-NB	6.17	1.40	1.35
17	A	810	CLA	C4B-NB	6.15	1.40	1.35
17	B	833	CLA	C4B-NB	6.15	1.40	1.35
17	A	809	CLA	C4B-NB	6.15	1.40	1.35
17	A	823	CLA	C4B-NB	6.14	1.40	1.35
17	A	815	CLA	C4B-NB	6.12	1.40	1.35
17	B	840	CLA	C4B-NB	6.12	1.40	1.35
17	5	316	CLA	C4B-NB	6.09	1.40	1.35
17	3	309	CLA	C4B-NB	6.09	1.40	1.35
17	B	835	CLA	C4B-NB	6.08	1.40	1.35
17	A	813	CLA	C4B-NB	6.05	1.40	1.35
17	A	808	CLA	C4B-NB	6.02	1.40	1.35
17	B	801	CLA	C4B-NB	6.01	1.40	1.35
17	A	816	CLA	C4B-NB	6.00	1.40	1.35
17	3	318	CLA	C4B-NB	6.00	1.40	1.35
17	A	829	CLA	C4B-NB	5.99	1.40	1.35
17	L	301	CLA	C4B-NB	5.95	1.40	1.35
17	A	807	CLA	C4B-NB	5.95	1.40	1.35
17	B	825	CLA	C4B-NB	5.95	1.40	1.35
17	B	806	CLA	C4B-NB	5.94	1.40	1.35
17	A	831	CLA	C4B-NB	5.94	1.40	1.35
17	A	805	CLA	C4B-NB	5.91	1.40	1.35
17	B	827	CLA	C4B-NB	5.91	1.40	1.35
17	2	509	CLA	C4B-NB	5.91	1.40	1.35
17	A	828	CLA	C4B-NB	5.90	1.40	1.35
17	3	308	CLA	C4B-NB	5.89	1.40	1.35
17	A	819	CLA	C4B-NB	5.89	1.40	1.35
17	A	802	CLA	C4B-NB	5.86	1.40	1.35
17	B	812	CLA	C4B-NB	5.84	1.40	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	B	807	CLA	C4B-NB	5.84	1.40	1.35
17	K	203	CLA	C4B-NB	5.83	1.40	1.35
17	B	809	CLA	C4B-NB	5.81	1.40	1.35
17	B	837	CLA	C4B-NB	5.80	1.40	1.35
17	A	806	CLA	C4B-NB	5.78	1.40	1.35
17	A	817	CLA	C4B-NB	5.78	1.40	1.35
17	B	811	CLA	C4B-NB	5.77	1.40	1.35
17	A	820	CLA	C4B-NB	5.76	1.40	1.35
17	A	826	CLA	C4B-NB	5.76	1.40	1.35
17	L	304	CLA	C4B-NB	5.74	1.40	1.35
17	A	812	CLA	C4B-NB	5.73	1.40	1.35
17	A	838	CLA	C4B-NB	5.71	1.40	1.35
17	B	828	CLA	C4B-NB	5.68	1.40	1.35
17	B	815	CLA	C4B-NB	5.68	1.40	1.35
17	B	819	CLA	C4B-NB	5.66	1.40	1.35
17	B	832	CLA	C4B-NB	5.65	1.40	1.35
17	A	804	CLA	C4B-NB	5.61	1.40	1.35
17	A	833	CLA	C4B-NB	5.60	1.40	1.35
17	A	835	CLA	C4B-NB	5.56	1.40	1.35
17	A	830	CLA	C4B-NB	5.54	1.40	1.35
25	5	315	CHL	C3D-C4D	-5.53	1.31	1.44
17	B	841	CLA	C4B-NB	5.52	1.40	1.35
17	A	818	CLA	C4B-NB	5.51	1.40	1.35
17	A	811	CLA	C4B-NB	5.47	1.40	1.35
17	B	803	CLA	C4B-NB	5.41	1.40	1.35
17	3	311	CLA	C4B-NB	5.36	1.40	1.35
17	A	824	CLA	C4B-NB	5.36	1.40	1.35
17	B	826	CLA	C4B-NB	5.35	1.40	1.35
17	A	827	CLA	C4B-NB	5.29	1.39	1.35
17	B	813	CLA	C4B-NB	5.26	1.39	1.35
17	A	832	CLA	C4B-NB	5.26	1.39	1.35
25	2	512	CHL	O2D-CGD	5.25	1.46	1.33
17	B	816	CLA	C4B-NB	5.25	1.39	1.35
25	1	514	CHL	CHC-C1C	5.23	1.48	1.35
25	1	512	CHL	O2D-CGD	5.18	1.45	1.33
17	B	829	CLA	C4B-NB	5.15	1.39	1.35
25	1	514	CHL	C3B-C2B	5.09	1.47	1.40
25	2	513	CHL	O2D-CGD	5.05	1.45	1.33
25	2	516	CHL	C3D-C4D	-5.04	1.32	1.44
25	1	514	CHL	C3D-C4D	-5.04	1.32	1.44
25	5	317	CHL	O2D-CGD	5.04	1.45	1.33
25	1	517	CHL	C3D-C4D	-5.04	1.32	1.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	2	515	CHL	O2D-CGD	5.03	1.45	1.33
25	1	517	CHL	O2D-CGD	5.02	1.45	1.33
25	3	315	CHL	O2D-CGD	5.02	1.45	1.33
25	2	515	CHL	C3D-C4D	-5.02	1.32	1.44
25	5	314	CHL	O2D-CGD	5.00	1.45	1.33
25	3	302	CHL	C3D-C4D	-4.98	1.32	1.44
25	3	315	CHL	CHC-C1C	4.97	1.47	1.35
25	1	517	CHL	CHC-C1C	4.95	1.47	1.35
25	1	514	CHL	CHD-C1D	4.94	1.48	1.38
25	1	512	CHL	CHC-C1C	4.93	1.47	1.35
25	3	315	CHL	C3D-C4D	-4.93	1.33	1.44
17	B	814	CLA	C4B-NB	4.92	1.39	1.35
25	3	302	CHL	CHC-C1C	4.92	1.47	1.35
25	2	516	CHL	O2D-CGD	4.92	1.45	1.33
25	5	317	CHL	C3D-C4D	-4.91	1.33	1.44
25	2	512	CHL	C3D-C4D	-4.89	1.33	1.44
25	1	514	CHL	C2C-C3C	4.87	1.47	1.36
25	2	512	CHL	CHC-C1C	4.85	1.47	1.35
25	1	514	CHL	O2D-CGD	4.84	1.45	1.33
17	L	302	CLA	CHB-C4A	4.84	1.38	1.34
25	5	314	CHL	C3D-C4D	-4.83	1.33	1.44
25	1	512	CHL	C3B-C2B	4.83	1.47	1.40
17	B	804	CLA	C4B-NB	4.81	1.39	1.35
25	1	512	CHL	C3D-C4D	-4.77	1.33	1.44
25	5	314	CHL	CHC-C1C	4.75	1.47	1.35
25	2	516	CHL	CHC-C1C	4.71	1.47	1.35
25	3	302	CHL	O2D-CGD	4.67	1.44	1.33
25	2	513	CHL	C3D-C2D	4.66	1.46	1.36
25	5	315	CHL	O2D-CGD	4.64	1.44	1.33
25	2	515	CHL	CHC-C1C	4.64	1.46	1.35
25	2	513	CHL	CHC-C1C	4.64	1.46	1.35
25	1	512	CHL	CHD-C1D	4.58	1.47	1.38
25	5	317	CHL	CHC-C1C	4.58	1.46	1.35
17	A	823	CLA	CHB-C4A	4.57	1.38	1.34
17	2	504	CLA	CHB-C4A	4.57	1.38	1.34
17	B	806	CLA	CHB-C4A	4.55	1.38	1.34
25	1	514	CHL	CHD-C4C	4.51	1.49	1.39
17	L	301	CLA	C4D-ND	-4.50	1.31	1.37
25	5	314	CHL	C3B-C2B	4.49	1.46	1.40
25	2	515	CHL	CHD-C1D	4.47	1.47	1.38
25	2	515	CHL	O2A-CGA	4.47	1.45	1.30
25	1	512	CHL	C2C-C3C	4.45	1.46	1.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	3	302	CHL	C3B-C2B	4.43	1.46	1.40
25	5	315	CHL	O2A-CGA	4.43	1.45	1.30
25	5	315	CHL	CHC-C1C	4.42	1.46	1.35
25	5	317	CHL	C2C-C3C	4.41	1.46	1.37
25	2	516	CHL	CHD-C1D	4.38	1.46	1.38
25	1	517	CHL	CHD-C1D	4.38	1.46	1.38
25	2	515	CHL	C2C-C3C	4.37	1.46	1.36
25	2	512	CHL	CHD-C1D	4.36	1.46	1.38
25	3	302	CHL	CHD-C1D	4.35	1.46	1.38
25	5	317	CHL	CHD-C1D	4.35	1.46	1.38
23	F	805	LMG	O8-C28	4.35	1.46	1.33
25	2	513	CHL	C2C-C3C	4.34	1.46	1.36
23	5	301	LMG	O8-C28	4.33	1.46	1.33
25	5	317	CHL	C3B-C2B	4.32	1.46	1.40
19	A	844	LHG	O8-C23	4.31	1.45	1.33
25	5	314	CHL	C2C-C3C	4.29	1.45	1.36
25	1	517	CHL	C3B-C2B	4.26	1.46	1.40
25	5	315	CHL	CHD-C1D	4.25	1.46	1.38
19	B	851	LHG	O7-C7	4.25	1.46	1.34
16	A	801	CL0	C2A-C1A	-4.24	1.50	1.53
19	B	851	LHG	O8-C23	4.24	1.45	1.33
25	2	513	CHL	CHD-C1D	4.23	1.46	1.38
25	3	302	CHL	C2C-C3C	4.21	1.45	1.36
25	2	512	CHL	O2A-CGA	4.20	1.46	1.33
25	5	314	CHL	CHD-C1D	4.20	1.46	1.38
23	2	519	LMG	O8-C28	4.15	1.45	1.33
19	1	516	LHG	O8-C23	4.15	1.45	1.33
22	B	850	DGD	O1G-C1A	4.14	1.45	1.33
25	5	314	CHL	O2A-CGA	4.13	1.46	1.33
17	B	812	CLA	CAB-C3B	-4.13	1.43	1.51
22	J	103	DGD	O1G-C1A	4.12	1.45	1.33
17	3	309	CLA	C4D-ND	-4.11	1.32	1.37
25	1	517	CHL	C2C-C3C	4.09	1.45	1.36
17	B	804	CLA	C4D-ND	-4.08	1.32	1.37
17	B	827	CLA	C4D-ND	-4.07	1.32	1.37
25	3	315	CHL	C2C-C3C	4.06	1.45	1.36
25	1	512	CHL	O2A-CGA	4.06	1.45	1.33
23	2	519	LMG	O7-C10	4.05	1.45	1.34
23	5	301	LMG	O7-C10	4.04	1.45	1.34
17	A	817	CLA	O1D-CGD	4.04	1.36	1.19
25	2	515	CHL	CHD-C4C	4.03	1.48	1.39
23	F	805	LMG	O7-C10	4.03	1.45	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	1	512	CHL	CHD-C4C	4.03	1.48	1.39
25	2	516	CHL	C2C-C3C	4.03	1.45	1.36
17	2	505	CLA	C4D-ND	-4.03	1.32	1.37
17	1	511	CLA	C1D-ND	4.01	1.42	1.37
17	A	820	CLA	C4D-ND	-4.01	1.32	1.37
17	A	805	CLA	C4D-ND	-4.01	1.32	1.37
17	3	309	CLA	C4B-CHC	-4.01	1.35	1.43
22	J	103	DGD	O2G-C1B	4.00	1.45	1.34
19	A	843	LHG	O8-C23	3.99	1.45	1.33
25	5	315	CHL	C3B-C2B	3.98	1.45	1.40
25	2	512	CHL	C2C-C3C	3.98	1.45	1.36
17	5	305	CLA	C4D-ND	-3.98	1.32	1.37
17	A	819	CLA	C4D-ND	-3.97	1.32	1.37
17	A	825	CLA	C4D-ND	-3.95	1.32	1.37
25	5	317	CHL	CHD-C4C	3.94	1.48	1.39
17	A	812	CLA	C4D-ND	-3.93	1.32	1.37
17	1	510	CLA	C4D-ND	-3.93	1.32	1.37
19	2	517	LHG	O8-C23	3.92	1.44	1.33
17	A	829	CLA	CMB-C2B	-3.91	1.43	1.51
23	F	806	LMG	O8-C28	3.91	1.44	1.33
25	3	302	CHL	O2A-CGA	3.91	1.45	1.33
23	F	806	LMG	O7-C10	3.90	1.45	1.34
25	5	315	CHL	C2C-C3C	3.90	1.45	1.36
17	A	811	CLA	C4D-ND	-3.89	1.32	1.37
19	2	517	LHG	O7-C7	3.89	1.45	1.34
25	2	516	CHL	CHD-C4C	3.88	1.48	1.39
17	A	822	CLA	C4D-ND	-3.87	1.32	1.37
25	5	314	CHL	CHD-C4C	3.87	1.48	1.39
17	B	815	CLA	C3B-C2B	-3.87	1.35	1.40
17	A	817	CLA	C4D-ND	-3.87	1.32	1.37
17	B	814	CLA	C4D-ND	-3.87	1.32	1.37
17	A	831	CLA	C4D-ND	-3.86	1.32	1.37
25	1	514	CHL	OBD-CAD	3.85	1.29	1.22
17	B	832	CLA	C4D-ND	-3.85	1.32	1.37
25	2	512	CHL	CHD-C4C	3.84	1.48	1.39
17	B	807	CLA	C4D-ND	-3.84	1.32	1.37
17	B	841	CLA	C4D-ND	-3.84	1.32	1.37
17	3	308	CLA	C4D-ND	-3.83	1.32	1.37
25	2	513	CHL	C3B-C2B	3.83	1.45	1.40
19	1	516	LHG	O7-C7	3.83	1.45	1.34
17	B	811	CLA	C4D-ND	-3.83	1.32	1.37
17	A	831	CLA	CAB-C3B	-3.78	1.43	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	3	302	CHL	CHD-C4C	3.77	1.47	1.39
17	5	308	CLA	C4D-ND	-3.77	1.32	1.37
17	A	813	CLA	C4D-ND	-3.76	1.32	1.37
17	A	810	CLA	C4D-ND	-3.75	1.32	1.37
17	B	842	CLA	C4D-ND	-3.75	1.32	1.37
17	1	513	CLA	C1D-ND	3.75	1.42	1.37
17	A	836	CLA	C3B-C2B	-3.75	1.35	1.40
17	5	305	CLA	C4B-CHC	-3.74	1.36	1.43
17	1	504	CLA	C4D-ND	-3.74	1.32	1.37
19	A	844	LHG	O7-C7	3.74	1.44	1.34
17	A	824	CLA	C4D-ND	-3.74	1.32	1.37
17	2	508	CLA	C1D-ND	3.74	1.42	1.37
17	2	507	CLA	C4D-ND	-3.72	1.32	1.37
17	3	307	CLA	C1D-ND	3.72	1.42	1.37
25	1	512	CHL	OBD-CAD	3.71	1.28	1.22
20	I	101	BCR	C30-C25	-3.71	1.48	1.53
25	3	315	CHL	CHD-C1D	3.71	1.45	1.38
25	3	315	CHL	C3B-C2B	3.71	1.45	1.40
17	A	814	CLA	C4D-ND	-3.71	1.32	1.37
25	5	315	CHL	CHD-C4C	3.69	1.47	1.39
17	B	808	CLA	C4D-ND	-3.68	1.32	1.37
17	B	828	CLA	C4D-ND	-3.68	1.32	1.37
25	1	517	CHL	CHD-C4C	3.68	1.47	1.39
19	A	843	LHG	O7-C7	3.68	1.44	1.34
17	A	808	CLA	C4D-ND	-3.68	1.32	1.37
17	3	312	CLA	C1D-ND	3.67	1.42	1.37
17	B	837	CLA	C4D-ND	-3.67	1.32	1.37
17	L	304	CLA	C4D-ND	-3.66	1.32	1.37
17	A	828	CLA	C4D-ND	-3.66	1.32	1.37
17	A	852	CLA	C3B-C2B	-3.65	1.35	1.40
25	2	513	CHL	CHD-C4C	3.65	1.47	1.39
22	B	850	DGD	O2G-C1B	3.65	1.44	1.34
17	1	504	CLA	C1D-ND	3.65	1.42	1.37
17	A	852	CLA	C4D-ND	-3.65	1.32	1.37
18	A	841	PQN	C10-C5	3.64	1.46	1.40
17	B	830	CLA	C4D-ND	-3.63	1.32	1.37
17	B	829	CLA	C4D-ND	-3.63	1.32	1.37
17	L	303	CLA	C4D-ND	-3.63	1.32	1.37
17	3	311	CLA	C4D-ND	-3.62	1.32	1.37
17	B	836	CLA	C4D-ND	-3.62	1.32	1.37
17	A	816	CLA	C4D-ND	-3.61	1.32	1.37
17	B	813	CLA	C1D-ND	3.59	1.42	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	3	315	CHL	OBD-CAD	3.59	1.28	1.22
17	2	504	CLA	C1D-ND	3.59	1.42	1.37
17	5	309	CLA	C4D-ND	-3.59	1.32	1.37
17	A	836	CLA	C4D-ND	-3.59	1.32	1.37
17	A	829	CLA	C4D-ND	-3.59	1.32	1.37
17	3	313	CLA	C1D-ND	3.59	1.42	1.37
17	A	818	CLA	C4D-ND	-3.58	1.32	1.37
17	1	509	CLA	C1D-ND	3.58	1.42	1.37
17	B	820	CLA	C4D-ND	-3.58	1.32	1.37
17	B	823	CLA	C4D-ND	-3.58	1.32	1.37
17	F	803	CLA	C4D-ND	-3.57	1.32	1.37
17	B	830	CLA	CMB-C2B	-3.57	1.44	1.51
17	A	824	CLA	C3B-C2B	-3.57	1.35	1.40
17	B	840	CLA	C4D-ND	-3.57	1.32	1.37
20	I	101	BCR	C1-C6	-3.56	1.48	1.53
17	A	837	CLA	C4D-ND	-3.56	1.32	1.37
17	B	810	CLA	C4D-ND	-3.56	1.32	1.37
17	5	307	CLA	C4D-ND	-3.56	1.32	1.37
17	A	806	CLA	C4D-ND	-3.56	1.32	1.37
17	B	803	CLA	C4D-ND	-3.56	1.32	1.37
17	B	829	CLA	CMB-C2B	-3.56	1.44	1.51
17	K	202	CLA	C1D-ND	3.56	1.42	1.37
17	B	802	CLA	C4D-ND	-3.55	1.32	1.37
17	A	827	CLA	C4D-ND	-3.54	1.32	1.37
17	B	838	CLA	C4D-ND	-3.54	1.32	1.37
17	B	830	CLA	C3B-C2B	-3.53	1.35	1.40
17	A	836	CLA	CMB-C2B	-3.53	1.44	1.51
17	K	201	CLA	C4D-ND	-3.53	1.32	1.37
20	B	852	BCR	C30-C25	-3.53	1.48	1.53
17	A	809	CLA	C4D-ND	-3.53	1.32	1.37
17	A	838	CLA	C1D-ND	3.53	1.42	1.37
17	A	839	CLA	C4D-ND	-3.52	1.32	1.37
17	A	838	CLA	C4D-ND	-3.52	1.32	1.37
17	L	302	CLA	C1D-ND	3.52	1.42	1.37
17	3	318	CLA	CAB-C3B	-3.51	1.44	1.51
17	3	306	CLA	C1D-ND	3.51	1.42	1.37
17	2	514	CLA	C4D-ND	-3.51	1.32	1.37
17	5	311	CLA	C4D-ND	-3.50	1.32	1.37
17	1	515	CLA	C1D-ND	3.50	1.42	1.37
17	5	312	CLA	C4D-ND	-3.50	1.32	1.37
17	B	801	CLA	C4D-ND	-3.50	1.32	1.37
25	3	302	CHL	OBD-CAD	3.50	1.28	1.22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	A	835	CLA	C4D-ND	-3.49	1.32	1.37
17	B	817	CLA	C4D-ND	-3.49	1.32	1.37
17	B	821	CLA	C1D-ND	3.48	1.42	1.37
17	F	802	CLA	C1D-ND	3.48	1.42	1.37
17	B	809	CLA	C4D-ND	-3.48	1.32	1.37
17	2	510	CLA	C4D-ND	-3.47	1.32	1.37
17	A	840	CLA	C3B-C2B	-3.47	1.35	1.40
16	A	801	CL0	C1D-ND	-3.47	1.33	1.37
20	B	845	BCR	C30-C25	-3.46	1.49	1.53
17	K	203	CLA	C4D-ND	-3.46	1.32	1.37
17	A	815	CLA	C1D-ND	3.46	1.42	1.37
17	2	509	CLA	C4D-ND	-3.46	1.32	1.37
17	A	804	CLA	C4D-ND	-3.45	1.32	1.37
17	A	833	CLA	C4D-ND	-3.45	1.32	1.37
17	J	101	CLA	C1D-ND	3.45	1.42	1.37
17	2	509	CLA	C1D-ND	3.45	1.42	1.37
17	B	818	CLA	C4D-ND	-3.44	1.33	1.37
17	A	803	CLA	C4D-ND	-3.43	1.33	1.37
17	B	834	CLA	C4D-ND	-3.43	1.33	1.37
17	5	316	CLA	C4D-ND	-3.43	1.33	1.37
17	B	812	CLA	C4D-ND	-3.42	1.33	1.37
17	F	802	CLA	C4D-ND	-3.42	1.33	1.37
25	5	314	CHL	OBD-CAD	3.41	1.28	1.22
17	2	507	CLA	C1D-ND	3.41	1.42	1.37
17	3	301	CLA	C3B-C2B	-3.41	1.35	1.40
25	2	516	CHL	OBD-CAD	3.40	1.28	1.22
17	A	830	CLA	C4D-ND	-3.40	1.33	1.37
17	2	511	CLA	C4D-ND	-3.40	1.33	1.37
17	B	806	CLA	C4D-ND	-3.40	1.33	1.37
17	A	834	CLA	C4D-ND	-3.40	1.33	1.37
17	B	813	CLA	C4D-ND	-3.40	1.33	1.37
17	1	508	CLA	C4D-ND	-3.39	1.33	1.37
17	5	312	CLA	C1D-ND	3.39	1.42	1.37
17	A	817	CLA	C3B-C2B	-3.39	1.35	1.40
17	5	313	CLA	C4D-ND	-3.38	1.33	1.37
17	A	829	CLA	C3B-C2B	-3.38	1.35	1.40
17	A	818	CLA	CMB-C2B	-3.38	1.44	1.51
25	3	315	CHL	CHD-C4C	3.37	1.46	1.39
17	B	815	CLA	CMB-C2B	-3.37	1.44	1.51
17	3	318	CLA	C4D-ND	-3.37	1.33	1.37
17	A	802	CLA	C4D-ND	-3.37	1.33	1.37
17	B	822	CLA	C4D-ND	-3.36	1.33	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	A	832	CLA	C4D-ND	-3.36	1.33	1.37
17	5	310	CLA	C4D-ND	-3.35	1.33	1.37
20	F	804	BCR	C1-C6	-3.35	1.49	1.53
17	3	314	CLA	C4D-ND	-3.35	1.33	1.37
17	B	820	CLA	CMB-C2B	-3.35	1.44	1.51
17	A	823	CLA	C2A-C1A	-3.35	1.50	1.53
17	A	807	CLA	C4D-ND	-3.34	1.33	1.37
17	5	306	CLA	C4D-ND	-3.34	1.33	1.37
25	1	514	CHL	C3D-C2D	3.34	1.48	1.39
17	B	835	CLA	C4D-ND	-3.34	1.33	1.37
17	3	307	CLA	C4D-ND	-3.34	1.33	1.37
17	B	819	CLA	C4D-ND	-3.33	1.33	1.37
17	A	819	CLA	C3B-C2B	-3.33	1.35	1.40
17	2	511	CLA	C1D-ND	3.33	1.41	1.37
17	A	823	CLA	C1D-ND	3.33	1.41	1.37
17	B	839	CLA	C4D-ND	-3.33	1.33	1.37
17	J	101	CLA	C4D-ND	-3.33	1.33	1.37
17	1	507	CLA	C4D-ND	-3.32	1.33	1.37
17	5	310	CLA	C1D-ND	3.32	1.41	1.37
25	2	512	CHL	OBD-CAD	3.32	1.28	1.22
17	B	833	CLA	C4D-ND	-3.32	1.33	1.37
17	2	504	CLA	C4D-ND	-3.31	1.33	1.37
17	5	307	CLA	C1D-ND	3.31	1.41	1.37
20	A	845	BCR	C1-C6	-3.30	1.49	1.53
17	B	803	CLA	C3B-C2B	-3.30	1.35	1.40
17	1	511	CLA	C4D-ND	-3.30	1.33	1.37
17	A	821	CLA	C4D-ND	-3.30	1.33	1.37
17	2	506	CLA	C4D-ND	-3.30	1.33	1.37
17	1	506	CLA	C1D-ND	3.30	1.41	1.37
18	B	843	PQN	C10-C5	3.30	1.46	1.40
17	1	505	CLA	C1D-ND	3.29	1.41	1.37
17	B	814	CLA	C3B-C2B	-3.28	1.35	1.40
17	B	815	CLA	C4D-ND	-3.28	1.33	1.37
17	1	515	CLA	CAD-C3D	-3.28	1.45	1.50
17	3	316	CLA	C4D-ND	-3.27	1.33	1.37
25	5	317	CHL	OBD-CAD	3.27	1.28	1.22
17	A	842	CLA	CHC-C1C	3.27	1.43	1.35
17	F	803	CLA	C1D-ND	3.27	1.41	1.37
17	B	829	CLA	C3B-C2B	-3.26	1.35	1.40
17	B	826	CLA	C4D-ND	-3.26	1.33	1.37
17	1	508	CLA	C1D-ND	3.26	1.41	1.37
17	3	310	CLA	C1D-ND	3.26	1.41	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	B	805	CLA	C4D-ND	-3.26	1.33	1.37
25	5	315	CHL	OBD-CAD	3.26	1.28	1.22
25	1	517	CHL	OBD-CAD	3.26	1.28	1.22
17	3	308	CLA	C1D-ND	3.26	1.41	1.37
17	A	840	CLA	C4D-ND	-3.26	1.33	1.37
25	2	513	CHL	C1D-ND	-3.25	1.33	1.37
17	A	817	CLA	CHC-C1C	3.25	1.43	1.35
17	3	312	CLA	C4D-ND	-3.24	1.33	1.37
17	A	815	CLA	C4D-ND	-3.24	1.33	1.37
17	K	205	CLA	C1D-ND	3.24	1.41	1.37
20	A	845	BCR	C30-C25	-3.24	1.49	1.53
17	A	803	CLA	C1D-ND	3.24	1.41	1.37
17	B	824	CLA	C4D-ND	-3.24	1.33	1.37
17	K	202	CLA	CHC-C1C	3.24	1.43	1.35
17	3	307	CLA	CHC-C1C	3.23	1.43	1.35
17	2	506	CLA	C1D-ND	3.23	1.41	1.37
17	A	824	CLA	CMB-C2B	-3.23	1.44	1.51
17	3	306	CLA	CAB-C3B	-3.23	1.44	1.51
17	3	301	CLA	CMB-C2B	-3.22	1.44	1.51
17	K	205	CLA	CHC-C1C	3.22	1.43	1.35
25	1	514	CHL	MG-NA	-3.22	1.98	2.06
17	A	826	CLA	C4D-ND	-3.21	1.33	1.37
17	3	317	CLA	C4D-ND	-3.21	1.33	1.37
17	B	821	CLA	C4D-ND	-3.21	1.33	1.37
17	A	833	CLA	CMB-C2B	-3.21	1.45	1.51
17	A	817	CLA	CMB-C2B	-3.20	1.45	1.51
17	A	825	CLA	C1D-ND	3.20	1.41	1.37
17	A	814	CLA	C3B-C2B	-3.20	1.35	1.40
25	2	515	CHL	OBD-CAD	3.19	1.28	1.22
17	2	508	CLA	CHC-C1C	3.19	1.43	1.35
17	B	838	CLA	C1D-ND	3.18	1.41	1.37
17	3	310	CLA	C4D-ND	-3.18	1.33	1.37
17	B	801	CLA	C3B-C2B	-3.18	1.36	1.40
17	1	506	CLA	C4D-ND	-3.18	1.33	1.37
17	3	301	CLA	C4D-ND	-3.18	1.33	1.37
17	B	831	CLA	C4D-ND	-3.18	1.33	1.37
17	L	303	CLA	CMB-C2B	-3.18	1.45	1.51
17	A	802	CLA	C3B-C2B	-3.18	1.36	1.40
17	J	101	CLA	CHC-C1C	3.17	1.43	1.35
17	A	842	CLA	C1D-ND	3.17	1.41	1.37
20	B	847	BCR	C30-C25	-3.16	1.49	1.53
17	B	809	CLA	C3B-C2B	-3.16	1.36	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	A	819	CLA	CMB-C2B	-3.16	1.45	1.51
17	B	838	CLA	CMB-C2B	-3.15	1.45	1.51
17	1	505	CLA	C4D-ND	-3.15	1.33	1.37
17	A	820	CLA	CMB-C2B	-3.15	1.45	1.51
17	B	808	CLA	C3B-C2B	-3.15	1.36	1.40
17	B	805	CLA	CHC-C1C	3.14	1.43	1.35
17	A	842	CLA	C4D-ND	-3.14	1.33	1.37
17	A	810	CLA	CMB-C2B	-3.14	1.45	1.51
17	B	837	CLA	CHC-C1C	3.13	1.43	1.35
26	5	304	XAT	C22-C21	-3.13	1.49	1.54
17	K	201	CLA	CHC-C1C	3.13	1.43	1.35
17	5	309	CLA	C1D-ND	3.13	1.41	1.37
17	B	812	CLA	CMB-C2B	-3.13	1.45	1.51
17	B	822	CLA	CHC-C1C	3.13	1.43	1.35
17	B	815	CLA	CHC-C1C	3.13	1.43	1.35
17	1	505	CLA	CHC-C1C	3.13	1.43	1.35
17	2	508	CLA	C4D-ND	-3.13	1.33	1.37
17	2	507	CLA	CHC-C1C	3.13	1.43	1.35
17	3	306	CLA	C2C-C1C	3.12	1.45	1.40
17	B	806	CLA	C1D-ND	3.12	1.41	1.37
17	A	832	CLA	CMB-C2B	-3.12	1.45	1.51
17	A	826	CLA	CHC-C1C	3.12	1.43	1.35
17	B	831	CLA	C1D-ND	3.12	1.41	1.37
17	B	816	CLA	C4D-ND	-3.12	1.33	1.37
17	A	833	CLA	C3B-C2B	-3.11	1.36	1.40
17	K	201	CLA	C3B-C2B	-3.11	1.36	1.40
17	3	317	CLA	C1D-ND	3.11	1.41	1.37
17	A	836	CLA	CHC-C1C	3.11	1.42	1.35
17	B	825	CLA	C4D-ND	-3.11	1.33	1.37
17	B	836	CLA	CHC-C1C	3.10	1.42	1.35
17	B	834	CLA	CMB-C2B	-3.10	1.45	1.51
17	B	808	CLA	C3B-CAB	-3.09	1.41	1.47
17	3	306	CLA	C4D-ND	-3.09	1.33	1.37
17	1	508	CLA	CHC-C1C	3.09	1.42	1.35
17	A	834	CLA	C1D-ND	3.09	1.41	1.37
17	B	824	CLA	CMB-C2B	-3.09	1.45	1.51
17	1	509	CLA	C4D-ND	-3.09	1.33	1.37
17	B	820	CLA	CHC-C1C	3.08	1.42	1.35
17	B	811	CLA	CMB-C2B	-3.08	1.45	1.51
17	B	827	CLA	CHC-C1C	3.08	1.42	1.35
17	B	819	CLA	C3B-C2B	-3.08	1.36	1.40
17	B	809	CLA	CMB-C2B	-3.08	1.45	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	A	823	CLA	C4D-ND	-3.08	1.33	1.37
17	3	318	CLA	C1D-ND	3.07	1.41	1.37
20	B	852	BCR	C1-C6	-3.07	1.49	1.53
17	B	809	CLA	C1D-ND	3.07	1.41	1.37
17	A	852	CLA	CMB-C2B	-3.07	1.45	1.51
17	B	836	CLA	C1D-ND	3.07	1.41	1.37
17	3	314	CLA	CHC-C1C	3.07	1.42	1.35
17	B	833	CLA	C1D-ND	3.07	1.41	1.37
17	A	835	CLA	CMB-C2B	-3.07	1.45	1.51
17	2	510	CLA	CHC-C1C	3.06	1.42	1.35
17	3	317	CLA	CHC-C1C	3.06	1.42	1.35
17	B	819	CLA	CMB-C2B	-3.06	1.45	1.51
17	A	805	CLA	C3B-C2B	-3.06	1.36	1.40
17	B	828	CLA	CHC-C1C	3.06	1.42	1.35
17	B	831	CLA	CMB-C2B	-3.06	1.45	1.51
17	A	835	CLA	C3B-C2B	-3.06	1.36	1.40
17	2	505	CLA	CHC-C1C	3.06	1.42	1.35
17	A	819	CLA	CHC-C1C	3.05	1.42	1.35
17	A	802	CLA	CHC-C1C	3.05	1.42	1.35
17	A	840	CLA	CHC-C1C	3.05	1.42	1.35
17	B	823	CLA	CHC-C1C	3.05	1.42	1.35
17	L	302	CLA	C4D-ND	-3.05	1.33	1.37
17	B	814	CLA	CHC-C1C	3.05	1.42	1.35
17	B	841	CLA	CHC-C1C	3.05	1.42	1.35
17	A	817	CLA	C3B-CAB	-3.05	1.41	1.47
17	1	504	CLA	CHC-C1C	3.05	1.42	1.35
17	A	830	CLA	CMB-C2B	-3.05	1.45	1.51
17	5	310	CLA	CHC-C1C	3.04	1.42	1.35
17	5	308	CLA	C1D-ND	3.04	1.41	1.37
17	5	313	CLA	C1D-ND	3.04	1.41	1.37
17	3	313	CLA	CHC-C1C	3.04	1.42	1.35
17	2	506	CLA	CMB-C2B	-3.04	1.45	1.51
17	B	813	CLA	CMB-C2B	-3.04	1.45	1.51
17	A	838	CLA	CMB-C2B	-3.04	1.45	1.51
17	A	837	CLA	CHC-C1C	3.04	1.42	1.35
17	A	802	CLA	C1D-ND	3.04	1.41	1.37
17	A	834	CLA	CMB-C2B	-3.03	1.45	1.51
25	2	516	CHL	C1D-C2D	3.03	1.51	1.45
17	L	301	CLA	CHC-C1C	3.03	1.42	1.35
17	B	835	CLA	CHC-C1C	3.03	1.42	1.35
17	B	805	CLA	CMB-C2B	-3.03	1.45	1.51
17	5	305	CLA	CHC-C1C	3.03	1.42	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	A	832	CLA	C3B-C2B	-3.03	1.36	1.40
17	A	806	CLA	CMB-C2B	-3.03	1.45	1.51
17	5	309	CLA	CHC-C1C	3.02	1.42	1.35
17	A	810	CLA	CHC-C1C	3.02	1.42	1.35
17	1	515	CLA	C4D-ND	-3.02	1.33	1.37
17	1	506	CLA	CHC-C1C	3.02	1.42	1.35
17	B	816	CLA	C1D-ND	3.02	1.41	1.37
17	5	308	CLA	CHC-C1C	3.02	1.42	1.35
17	A	816	CLA	C1D-ND	3.02	1.41	1.37
17	1	515	CLA	CHC-C1C	3.02	1.42	1.35
20	A	846	BCR	C1-C6	-3.02	1.49	1.53
17	A	807	CLA	CMB-C2B	-3.01	1.45	1.51
17	A	818	CLA	C3B-C2B	-3.01	1.36	1.40
17	B	827	CLA	CMB-C2B	-3.01	1.45	1.51
17	1	513	CLA	C4D-ND	-3.01	1.33	1.37
17	1	513	CLA	CHC-C1C	3.01	1.42	1.35
17	A	823	CLA	CMB-C2B	-3.01	1.45	1.51
17	2	511	CLA	CHC-C1C	3.01	1.42	1.35
17	B	807	CLA	CMB-C2B	-3.01	1.45	1.51
17	A	821	CLA	CHC-C1C	3.01	1.42	1.35
17	5	306	CLA	C1D-ND	3.00	1.41	1.37
17	A	830	CLA	C3B-C2B	-3.00	1.36	1.40
17	1	510	CLA	CHC-C1C	3.00	1.42	1.35
17	1	511	CLA	CHC-C1C	3.00	1.42	1.35
17	A	838	CLA	CHC-C1C	3.00	1.42	1.35
17	3	316	CLA	CHC-C1C	3.00	1.42	1.35
17	B	830	CLA	C3B-CAB	-2.99	1.41	1.47
17	A	803	CLA	CMB-C2B	-2.99	1.45	1.51
17	K	202	CLA	C4D-ND	-2.99	1.33	1.37
17	B	842	CLA	C1D-ND	2.99	1.41	1.37
17	5	307	CLA	CHC-C1C	2.99	1.42	1.35
17	B	803	CLA	CMB-C2B	-2.99	1.45	1.51
17	2	509	CLA	CHC-C1C	2.99	1.42	1.35
17	B	802	CLA	C1D-ND	2.99	1.41	1.37
17	B	835	CLA	C1D-ND	2.99	1.41	1.37
17	A	802	CLA	CMB-C2B	-2.99	1.45	1.51
17	A	812	CLA	CHC-C1C	2.99	1.42	1.35
17	L	301	CLA	C3B-C2B	-2.98	1.36	1.40
17	B	809	CLA	CHC-C1C	2.98	1.42	1.35
17	B	816	CLA	CMB-C2B	-2.98	1.45	1.51
25	1	512	CHL	C1D-C2D	2.98	1.51	1.45
17	A	834	CLA	C3B-C2B	-2.97	1.36	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	1	512	CHL	C3D-C2D	2.97	1.47	1.39
26	5	304	XAT	O24-C25	-2.97	1.42	1.46
17	A	840	CLA	CMB-C2B	-2.97	1.45	1.51
17	A	813	CLA	CHC-C1C	2.97	1.42	1.35
17	A	823	CLA	CHC-C1C	2.96	1.42	1.35
17	B	805	CLA	C3B-C2B	-2.96	1.36	1.40
17	B	802	CLA	CHC-C1C	2.96	1.42	1.35
17	B	831	CLA	C3B-C2B	-2.96	1.36	1.40
17	A	852	CLA	C1D-ND	2.96	1.41	1.37
17	B	840	CLA	CMB-C2B	-2.96	1.45	1.51
17	A	804	CLA	CHC-C1C	2.95	1.42	1.35
17	B	817	CLA	C1D-ND	2.95	1.41	1.37
17	B	801	CLA	CHC-C1C	2.95	1.42	1.35
25	5	317	CHL	C3D-C2D	2.95	1.47	1.39
17	3	309	CLA	C1D-ND	2.95	1.41	1.37
17	F	802	CLA	CHC-C1C	2.95	1.42	1.35
17	L	301	CLA	CMB-C2B	-2.95	1.45	1.51
17	B	839	CLA	C1D-ND	2.95	1.41	1.37
17	5	316	CLA	C1D-ND	2.95	1.41	1.37
17	B	823	CLA	C1D-ND	2.94	1.41	1.37
17	5	316	CLA	CHC-C1C	2.94	1.42	1.35
17	3	308	CLA	CHC-C1C	2.94	1.42	1.35
17	L	303	CLA	CHC-C1C	2.94	1.42	1.35
17	A	834	CLA	CHC-C1C	2.94	1.42	1.35
17	A	835	CLA	CHC-C1C	2.94	1.42	1.35
17	B	817	CLA	C3B-CAB	-2.94	1.41	1.47
17	L	304	CLA	CHC-C1C	2.94	1.42	1.35
17	3	309	CLA	CHC-C1C	2.94	1.42	1.35
17	A	830	CLA	CHC-C1C	2.94	1.42	1.35
17	B	834	CLA	C1D-ND	2.93	1.41	1.37
17	A	839	CLA	CHC-C1C	2.93	1.42	1.35
17	B	802	CLA	CMB-C2B	-2.93	1.45	1.51
17	2	510	CLA	C1D-ND	2.93	1.41	1.37
17	5	312	CLA	CHC-C1C	2.93	1.42	1.35
17	2	504	CLA	CMB-C2B	-2.93	1.45	1.51
25	1	517	CHL	C1D-C2D	2.93	1.51	1.45
17	B	813	CLA	CHC-C1C	2.92	1.42	1.35
17	B	835	CLA	CMB-C2B	-2.92	1.45	1.51
17	A	825	CLA	CHC-C1C	2.92	1.42	1.35
17	A	828	CLA	CMB-C2B	-2.92	1.45	1.51
17	1	509	CLA	CHC-C1C	2.92	1.42	1.35
17	B	816	CLA	CHC-C1C	2.92	1.42	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	B	824	CLA	CHC-C1C	2.92	1.42	1.35
25	1	514	CHL	C1D-C2D	2.92	1.51	1.45
17	B	839	CLA	CHC-C1C	2.91	1.42	1.35
17	A	827	CLA	CHC-C1C	2.91	1.42	1.35
17	3	310	CLA	CHC-C1C	2.91	1.42	1.35
17	B	808	CLA	CHC-C1C	2.91	1.42	1.35
17	L	303	CLA	C3B-C2B	-2.91	1.36	1.40
17	B	801	CLA	CMB-C2B	-2.91	1.45	1.51
17	A	809	CLA	CHC-C1C	2.91	1.42	1.35
17	A	820	CLA	CHC-C1C	2.91	1.42	1.35
17	B	818	CLA	CHC-C1C	2.91	1.42	1.35
17	B	813	CLA	C3B-C2B	-2.90	1.36	1.40
17	A	814	CLA	C3B-CAB	-2.90	1.42	1.47
17	B	810	CLA	CMB-C2B	-2.90	1.45	1.51
17	B	832	CLA	CMB-C2B	-2.90	1.45	1.51
17	B	831	CLA	CHC-C1C	2.90	1.42	1.35
17	A	822	CLA	C1D-ND	2.90	1.41	1.37
17	A	821	CLA	CMB-C2B	-2.90	1.45	1.51
17	B	828	CLA	C3B-C2B	-2.89	1.36	1.40
17	B	804	CLA	C3B-C2B	-2.89	1.36	1.40
17	B	836	CLA	CMB-C2B	-2.89	1.45	1.51
17	A	814	CLA	CHC-C1C	2.89	1.42	1.35
17	B	817	CLA	C3B-C2B	-2.89	1.36	1.40
17	1	507	CLA	CHC-C1C	2.89	1.42	1.35
17	K	205	CLA	C4D-ND	-2.89	1.33	1.37
17	1	510	CLA	C1D-ND	2.89	1.41	1.37
17	3	312	CLA	CHC-C1C	2.89	1.42	1.35
17	A	831	CLA	CHC-C1C	2.89	1.42	1.35
17	B	829	CLA	CHC-C1C	2.89	1.42	1.35
17	B	815	CLA	CMC-C2C	-2.89	1.44	1.50
17	3	314	CLA	C1D-ND	2.89	1.41	1.37
17	B	811	CLA	CHC-C1C	2.89	1.42	1.35
17	B	822	CLA	CMB-C2B	-2.89	1.45	1.51
17	A	809	CLA	C3B-C2B	-2.88	1.36	1.40
17	A	805	CLA	C1D-ND	2.88	1.41	1.37
17	B	806	CLA	C3B-CAB	-2.88	1.42	1.47
17	B	833	CLA	CHC-C1C	2.88	1.42	1.35
17	B	842	CLA	CHC-C1C	2.88	1.42	1.35
17	A	835	CLA	CMC-C2C	-2.88	1.44	1.50
17	B	837	CLA	CMB-C2B	-2.88	1.45	1.51
20	B	844	BCR	C30-C25	-2.88	1.49	1.53
17	A	808	CLA	CMB-C2B	-2.88	1.45	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	5	313	CLA	CHC-C1C	2.88	1.42	1.35
25	5	314	CHL	C1D-C2D	2.88	1.51	1.45
17	A	815	CLA	CMB-C2B	-2.88	1.45	1.51
17	3	311	CLA	CMB-C2B	-2.88	1.45	1.51
17	A	803	CLA	CHC-C1C	2.87	1.42	1.35
25	2	513	CHL	CAD-CBD	-2.87	1.49	1.54
17	B	804	CLA	CMB-C2B	-2.87	1.45	1.51
17	A	828	CLA	CHC-C1C	2.87	1.42	1.35
17	A	828	CLA	C3B-C2B	-2.87	1.36	1.40
17	A	828	CLA	C1D-ND	2.87	1.41	1.37
17	K	203	CLA	CHC-C1C	2.87	1.42	1.35
25	3	302	CHL	C3D-C2D	2.87	1.46	1.39
17	B	807	CLA	CHC-C1C	2.87	1.42	1.35
17	3	311	CLA	CHC-C1C	2.87	1.42	1.35
17	A	822	CLA	CHC-C1C	2.87	1.42	1.35
17	A	824	CLA	CHC-C1C	2.87	1.42	1.35
25	2	512	CHL	C1D-C2D	2.87	1.51	1.45
20	B	848	BCR	C30-C25	-2.86	1.49	1.53
17	A	805	CLA	CMB-C2B	-2.86	1.45	1.51
17	A	832	CLA	CHC-C1C	2.86	1.42	1.35
25	5	315	CHL	C1D-ND	-2.86	1.34	1.37
17	B	806	CLA	CMB-C2B	-2.86	1.45	1.51
17	A	812	CLA	C3B-C2B	-2.86	1.36	1.40
17	A	811	CLA	CHC-C1C	2.86	1.42	1.35
17	B	816	CLA	C3B-C2B	-2.86	1.36	1.40
20	K	204	BCR	C30-C25	-2.85	1.49	1.53
17	B	821	CLA	CHC-C1C	2.85	1.42	1.35
17	A	819	CLA	C1D-ND	2.85	1.41	1.37
17	A	833	CLA	CHC-C1C	2.85	1.42	1.35
17	B	838	CLA	CHC-C1C	2.85	1.42	1.35
25	5	317	CHL	C1D-C2D	2.85	1.50	1.45
25	5	314	CHL	C3D-C2D	2.85	1.46	1.39
17	3	313	CLA	C4D-ND	-2.85	1.33	1.37
17	B	817	CLA	CMB-C2B	-2.85	1.45	1.51
17	3	301	CLA	CHC-C1C	2.85	1.42	1.35
17	3	318	CLA	CHC-C1C	2.85	1.42	1.35
17	B	808	CLA	CMB-C2B	-2.84	1.45	1.51
17	B	818	CLA	CMB-C2B	-2.84	1.45	1.51
17	B	841	CLA	CMB-C2B	-2.84	1.45	1.51
17	B	811	CLA	C3B-C2B	-2.84	1.36	1.40
17	B	813	CLA	CMD-C2D	-2.84	1.44	1.50
17	2	514	CLA	CHC-C1C	2.84	1.42	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	A	809	CLA	CMB-C2B	-2.84	1.45	1.51
17	1	507	CLA	C1D-ND	2.84	1.41	1.37
17	2	507	CLA	CMB-C2B	-2.84	1.45	1.51
17	2	514	CLA	C1D-ND	2.83	1.41	1.37
17	5	306	CLA	CHC-C1C	2.83	1.42	1.35
17	B	841	CLA	C3B-C2B	-2.83	1.36	1.40
17	B	812	CLA	CHC-C1C	2.83	1.42	1.35
17	A	807	CLA	C1D-ND	2.83	1.41	1.37
17	A	831	CLA	CMB-C2B	-2.83	1.45	1.51
17	B	834	CLA	CHC-C1C	2.83	1.42	1.35
17	B	817	CLA	CHC-C1C	2.83	1.42	1.35
17	A	826	CLA	C3B-C2B	-2.83	1.36	1.40
17	3	311	CLA	C1D-ND	2.82	1.41	1.37
17	A	808	CLA	CHC-C1C	2.82	1.42	1.35
17	A	816	CLA	CHC-C1C	2.82	1.42	1.35
17	5	305	CLA	CMB-C2B	-2.82	1.45	1.51
17	B	821	CLA	CMB-C2B	-2.82	1.45	1.51
17	2	508	CLA	CMB-C2B	-2.82	1.45	1.51
17	A	820	CLA	C1D-ND	2.82	1.41	1.37
17	B	837	CLA	C3B-C2B	-2.82	1.36	1.40
20	A	849	BCR	C30-C25	-2.82	1.49	1.53
17	1	506	CLA	CMB-C2B	-2.81	1.45	1.51
17	B	815	CLA	C3B-CAB	-2.81	1.42	1.47
17	B	824	CLA	C1D-ND	2.81	1.41	1.37
17	A	806	CLA	CHC-C1C	2.80	1.42	1.35
17	L	302	CLA	CHC-C1C	2.80	1.42	1.35
17	B	814	CLA	C1D-ND	2.80	1.41	1.37
17	A	814	CLA	CMB-C2B	-2.80	1.45	1.51
17	3	301	CLA	C1D-ND	2.80	1.41	1.37
17	L	304	CLA	C1D-ND	2.80	1.41	1.37
17	A	826	CLA	CMB-C2B	-2.80	1.45	1.51
17	B	823	CLA	CMB-C2B	-2.80	1.45	1.51
17	A	818	CLA	CHC-C1C	2.80	1.42	1.35
17	B	803	CLA	CHC-C1C	2.80	1.42	1.35
17	A	810	CLA	C1D-ND	2.79	1.41	1.37
17	5	313	CLA	CMB-C2B	-2.79	1.45	1.51
17	B	832	CLA	CHC-C1C	2.79	1.42	1.35
17	2	504	CLA	CHC-C1C	2.79	1.42	1.35
17	2	509	CLA	CMB-C2B	-2.79	1.45	1.51
17	2	505	CLA	C1D-ND	2.79	1.41	1.37
17	A	809	CLA	C2D-C1D	2.79	1.47	1.42
17	B	832	CLA	C3B-C2B	-2.79	1.36	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	A	812	CLA	CMB-C2B	-2.79	1.45	1.51
17	A	827	CLA	CMB-C2B	-2.79	1.45	1.51
17	B	819	CLA	C1D-ND	2.79	1.41	1.37
17	5	311	CLA	CMB-C2B	-2.78	1.45	1.51
25	3	315	CHL	C3D-C2D	2.78	1.46	1.39
20	L	306	BCR	C1-C6	-2.78	1.49	1.53
17	A	811	CLA	CMB-C2B	-2.77	1.45	1.51
17	A	840	CLA	C3B-CAB	-2.77	1.42	1.47
17	L	302	CLA	CMB-C2B	-2.77	1.45	1.51
17	B	826	CLA	CHC-C1C	2.76	1.42	1.35
17	A	804	CLA	CMB-C2B	-2.76	1.45	1.51
17	B	825	CLA	CHC-C1C	2.76	1.42	1.35
17	5	309	CLA	CMB-C2B	-2.76	1.45	1.51
17	B	806	CLA	C3B-C2B	-2.76	1.36	1.40
17	B	824	CLA	C3B-C2B	-2.76	1.36	1.40
17	B	834	CLA	C3B-C2B	-2.75	1.36	1.40
17	A	807	CLA	CHC-C1C	2.75	1.42	1.35
24	1	501	LUT	C22-C21	-2.75	1.51	1.54
17	1	505	CLA	CMB-C2B	-2.75	1.45	1.51
17	A	826	CLA	CMC-C2C	-2.75	1.45	1.50
17	A	806	CLA	C3B-C2B	-2.75	1.36	1.40
17	B	814	CLA	CMB-C2B	-2.75	1.45	1.51
17	B	830	CLA	C1D-ND	2.75	1.41	1.37
17	5	316	CLA	CMB-C2B	-2.74	1.45	1.51
17	B	820	CLA	CMC-C2C	-2.74	1.45	1.50
17	A	817	CLA	C3A-C2A	-2.74	1.52	1.54
17	A	808	CLA	C1D-ND	2.74	1.41	1.37
25	2	515	CHL	C1D-C2D	2.74	1.50	1.45
17	5	308	CLA	CMB-C2B	-2.74	1.45	1.51
17	A	807	CLA	C3B-C2B	-2.74	1.36	1.40
17	A	825	CLA	CMB-C2B	-2.74	1.45	1.51
17	B	810	CLA	CMC-C2C	-2.73	1.45	1.50
17	B	805	CLA	C3B-CAB	-2.73	1.42	1.47
16	A	801	CL0	MG-NC	2.73	2.12	2.06
17	A	805	CLA	CHC-C1C	2.73	1.42	1.35
17	B	840	CLA	CHC-C1C	2.73	1.42	1.35
17	B	830	CLA	CMC-C2C	-2.72	1.45	1.50
17	2	514	CLA	CMB-C2B	-2.72	1.46	1.51
17	F	802	CLA	CMB-C2B	-2.72	1.46	1.51
17	3	316	CLA	CMB-C2B	-2.72	1.46	1.51
17	L	301	CLA	C1D-ND	2.72	1.41	1.37
17	K	205	CLA	CMB-C2B	-2.71	1.46	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	A	823	CLA	C3B-C2B	-2.71	1.36	1.40
17	B	819	CLA	CHC-C1C	2.71	1.41	1.35
17	B	809	CLA	CMD-C2D	-2.71	1.45	1.50
17	A	852	CLA	CHC-C1C	2.71	1.41	1.35
17	A	832	CLA	C1D-ND	2.71	1.41	1.37
17	A	813	CLA	CMB-C2B	-2.71	1.46	1.51
17	A	839	CLA	CMB-C2B	-2.71	1.46	1.51
17	5	311	CLA	CHC-C1C	2.71	1.41	1.35
20	3	305	BCR	C30-C25	-2.71	1.50	1.53
17	B	804	CLA	C1D-ND	2.71	1.41	1.37
17	K	201	CLA	C3B-CAB	-2.71	1.42	1.47
17	A	818	CLA	C1D-ND	2.71	1.41	1.37
17	A	839	CLA	C1D-ND	2.71	1.41	1.37
17	A	842	CLA	CMB-C2B	-2.70	1.46	1.51
17	B	829	CLA	C1D-ND	2.70	1.41	1.37
17	A	815	CLA	CHC-C1C	2.70	1.41	1.35
17	B	816	CLA	CMD-C2D	-2.70	1.45	1.50
25	2	515	CHL	C3D-C2D	2.70	1.46	1.39
17	A	811	CLA	C3B-C2B	-2.70	1.36	1.40
17	B	804	CLA	CHC-C1C	2.70	1.41	1.35
17	2	511	CLA	CMB-C2B	-2.70	1.46	1.51
17	F	803	CLA	CHC-C1C	2.70	1.41	1.35
17	B	822	CLA	C1D-ND	2.70	1.41	1.37
17	B	821	CLA	CMD-C2D	-2.70	1.45	1.50
17	B	808	CLA	C1D-ND	2.70	1.41	1.37
17	B	835	CLA	C3B-C2B	-2.69	1.36	1.40
17	B	803	CLA	CMC-C2C	-2.69	1.45	1.50
17	B	801	CLA	CMC-C2C	-2.69	1.45	1.50
17	A	837	CLA	CMB-C2B	-2.69	1.46	1.51
17	B	810	CLA	CHC-C1C	2.68	1.41	1.35
17	B	827	CLA	C1D-ND	2.68	1.41	1.37
17	A	811	CLA	CMD-C2D	-2.68	1.45	1.50
17	B	827	CLA	CMD-C2D	-2.68	1.45	1.50
17	A	822	CLA	CMB-C2B	-2.68	1.46	1.51
17	B	833	CLA	CMB-C2B	-2.68	1.46	1.51
17	A	804	CLA	C3B-C2B	-2.68	1.36	1.40
20	B	846	BCR	C30-C25	-2.68	1.50	1.53
25	1	514	CHL	C4B-CHC	2.68	1.48	1.41
17	5	312	CLA	CMB-C2B	-2.68	1.46	1.51
25	2	515	CHL	MG-NA	-2.68	1.99	2.06
16	A	801	CL0	CHC-C1C	2.67	1.41	1.35
17	1	510	CLA	CMB-C2B	-2.67	1.46	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	A	840	CLA	C1D-ND	2.67	1.41	1.37
17	1	507	CLA	CMB-C2B	-2.67	1.46	1.51
17	A	812	CLA	CMC-C2C	-2.67	1.45	1.50
17	K	201	CLA	C1D-ND	2.67	1.41	1.37
17	5	311	CLA	C1D-ND	2.67	1.41	1.37
17	B	820	CLA	C3B-C2B	-2.67	1.36	1.40
25	2	513	CHL	C1D-C2D	2.67	1.50	1.45
20	L	305	BCR	C30-C25	-2.66	1.50	1.53
17	B	815	CLA	C1D-ND	2.66	1.41	1.37
17	A	805	CLA	C3B-CAB	-2.66	1.42	1.47
17	A	837	CLA	C1D-ND	2.66	1.41	1.37
17	B	838	CLA	C3B-C2B	-2.66	1.36	1.40
20	A	848	BCR	C1-C6	-2.66	1.50	1.53
17	B	836	CLA	C3B-C2B	-2.66	1.36	1.40
17	A	838	CLA	CMD-C2D	-2.66	1.45	1.50
16	A	801	CL0	C1C-NC	-2.66	1.33	1.37
17	A	806	CLA	C1D-ND	2.65	1.41	1.37
17	5	307	CLA	CMB-C2B	-2.65	1.46	1.51
17	B	806	CLA	CHC-C1C	2.65	1.41	1.35
17	2	506	CLA	CHC-C1C	2.65	1.41	1.35
20	A	849	BCR	C1-C6	-2.65	1.50	1.53
25	2	516	CHL	C3D-C2D	2.65	1.46	1.39
17	B	811	CLA	C1D-ND	2.64	1.41	1.37
17	B	826	CLA	C3B-C2B	-2.64	1.36	1.40
17	A	831	CLA	C1D-ND	2.64	1.41	1.37
17	5	313	CLA	C3B-C2B	-2.64	1.36	1.40
17	B	814	CLA	CMD-C2D	-2.64	1.45	1.50
17	A	829	CLA	CHC-C1C	2.64	1.41	1.35
17	3	310	CLA	CMB-C2B	-2.64	1.46	1.51
17	A	816	CLA	CMD-C2D	-2.64	1.45	1.50
17	B	824	CLA	CMD-C2D	-2.64	1.45	1.50
16	A	801	CL0	C4C-C3C	2.64	1.49	1.45
17	A	839	CLA	C3B-C2B	-2.63	1.36	1.40
20	J	102	BCR	C1-C6	-2.63	1.50	1.53
17	B	812	CLA	C1D-ND	2.63	1.41	1.37
17	B	837	CLA	C1D-ND	2.63	1.41	1.37
17	K	202	CLA	CMB-C2B	-2.62	1.46	1.51
17	B	819	CLA	CMD-C2D	-2.62	1.45	1.50
17	B	828	CLA	CMB-C2B	-2.62	1.46	1.51
17	2	505	CLA	CMB-C2B	-2.62	1.46	1.51
17	A	814	CLA	CMD-C2D	-2.62	1.45	1.50
17	B	806	CLA	CMD-C2D	-2.62	1.45	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	B	826	CLA	CMB-C2B	-2.62	1.46	1.51
17	B	825	CLA	CMB-C2B	-2.62	1.46	1.51
17	F	803	CLA	CMB-C2B	-2.62	1.46	1.51
17	B	840	CLA	C3B-C2B	-2.61	1.36	1.40
17	B	839	CLA	CMB-C2B	-2.61	1.46	1.51
17	K	201	CLA	CMB-C2B	-2.61	1.46	1.51
17	L	304	CLA	CMD-C2D	-2.61	1.45	1.50
17	3	317	CLA	CMB-C2B	-2.61	1.46	1.51
17	A	809	CLA	CMC-C2C	-2.61	1.45	1.50
17	L	301	CLA	C3B-CAB	-2.60	1.42	1.47
17	A	836	CLA	C1D-ND	2.60	1.41	1.37
17	A	810	CLA	C3B-C2B	-2.60	1.36	1.40
17	B	803	CLA	C3B-CAB	-2.60	1.42	1.47
25	5	315	CHL	C1D-C2D	2.60	1.50	1.45
17	B	803	CLA	C1D-ND	2.60	1.41	1.37
17	B	820	CLA	C1D-ND	2.60	1.41	1.37
17	B	823	CLA	C3B-C2B	-2.60	1.36	1.40
25	5	317	CHL	MG-NA	-2.60	2.00	2.06
17	A	831	CLA	CMC-C2C	-2.60	1.45	1.50
17	5	306	CLA	CMB-C2B	-2.60	1.46	1.51
17	A	803	CLA	C3B-C2B	-2.60	1.36	1.40
17	A	852	CLA	C3B-CAB	-2.59	1.42	1.47
25	3	302	CHL	MG-NA	-2.59	2.00	2.06
17	A	812	CLA	C1D-ND	2.59	1.41	1.37
17	B	831	CLA	CMD-C2D	-2.59	1.45	1.50
20	K	204	BCR	C1-C6	-2.59	1.50	1.53
17	A	828	CLA	CMD-C2D	-2.59	1.45	1.50
17	B	816	CLA	CMC-C2C	-2.59	1.45	1.50
17	A	814	CLA	C1D-ND	2.59	1.41	1.37
17	A	836	CLA	CMD-C2D	-2.58	1.45	1.50
24	5	303	LUT	C1-C6	-2.58	1.50	1.53
17	B	821	CLA	C3B-C2B	-2.58	1.36	1.40
17	A	833	CLA	C1D-ND	2.58	1.41	1.37
17	A	806	CLA	CMC-C2C	-2.58	1.45	1.50
20	A	853	BCR	C1-C6	-2.58	1.50	1.53
17	B	838	CLA	CMD-C2D	-2.57	1.45	1.50
17	B	826	CLA	CMD-C2D	-2.57	1.45	1.50
17	B	813	CLA	CMC-C2C	-2.57	1.45	1.50
17	B	807	CLA	CMC-C2C	-2.57	1.45	1.50
17	B	826	CLA	C1D-ND	2.57	1.40	1.37
17	3	309	CLA	CMB-C2B	-2.57	1.45	1.51
17	A	824	CLA	C1D-ND	2.57	1.40	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	A	848	BCR	C30-C25	-2.57	1.50	1.53
17	B	808	CLA	CMD-C2D	-2.57	1.45	1.50
17	1	515	CLA	CMD-C2D	-2.57	1.45	1.50
17	B	814	CLA	CMC-C2C	-2.56	1.45	1.50
17	A	804	CLA	CMD-C2D	-2.56	1.45	1.50
17	5	305	CLA	CMC-C2C	-2.56	1.45	1.50
17	2	504	CLA	C3B-C2B	-2.56	1.36	1.40
25	1	517	CHL	C3D-C2D	2.56	1.46	1.39
17	A	832	CLA	CMD-C2D	-2.56	1.45	1.50
17	J	101	CLA	CMB-C2B	-2.56	1.46	1.51
17	B	803	CLA	CMD-C2D	-2.56	1.45	1.50
17	B	806	CLA	CMC-C2C	-2.56	1.45	1.50
17	B	830	CLA	CHC-C1C	2.56	1.41	1.35
17	B	841	CLA	C1D-ND	2.56	1.40	1.37
17	B	842	CLA	CMB-C2B	-2.56	1.46	1.51
17	A	837	CLA	CMD-C2D	-2.56	1.45	1.50
17	A	825	CLA	CMD-C2D	-2.55	1.45	1.50
17	B	801	CLA	C1D-ND	2.55	1.40	1.37
17	A	830	CLA	C1D-ND	2.55	1.40	1.37
17	A	830	CLA	CMD-C2D	-2.55	1.45	1.50
25	2	512	CHL	C3D-C2D	2.55	1.46	1.39
25	3	315	CHL	C1D-ND	-2.55	1.34	1.37
17	2	511	CLA	C3B-C2B	-2.55	1.36	1.40
17	B	811	CLA	CMC-C2C	-2.54	1.45	1.50
17	A	824	CLA	CMD-C2D	-2.54	1.45	1.50
17	K	203	CLA	CMD-C2D	-2.54	1.45	1.50
17	L	304	CLA	CMB-C2B	-2.54	1.46	1.51
17	3	307	CLA	C3B-C2B	-2.54	1.36	1.40
17	B	804	CLA	CMD-C2D	-2.54	1.45	1.50
17	A	833	CLA	CMD-C2D	-2.54	1.45	1.50
17	5	312	CLA	C3B-C2B	-2.54	1.36	1.40
17	A	823	CLA	CMC-C2C	-2.53	1.45	1.50
17	K	203	CLA	CMB-C2B	-2.53	1.46	1.51
17	3	312	CLA	CMB-C2B	-2.53	1.46	1.51
17	A	826	CLA	CMD-C2D	-2.52	1.45	1.50
17	B	840	CLA	CMD-C2D	-2.52	1.45	1.50
17	A	836	CLA	C3B-CAB	-2.52	1.42	1.47
17	A	823	CLA	CMD-C2D	-2.52	1.45	1.50
17	5	313	CLA	C3B-CAB	-2.51	1.42	1.47
17	A	811	CLA	CMC-C2C	-2.51	1.45	1.50
17	B	807	CLA	CMD-C2D	-2.51	1.45	1.50
17	A	825	CLA	C3B-C2B	-2.51	1.36	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	3	314	CLA	CMB-C2B	-2.51	1.46	1.51
17	A	833	CLA	CMC-C2C	-2.51	1.45	1.50
17	B	825	CLA	CMD-C2D	-2.51	1.45	1.50
17	B	830	CLA	CMD-C2D	-2.51	1.45	1.50
25	1	512	CHL	MG-NA	-2.51	2.00	2.06
17	A	832	CLA	C3B-CAB	-2.51	1.42	1.47
17	A	803	CLA	CMD-C2D	-2.51	1.45	1.50
17	A	827	CLA	CMD-C2D	-2.51	1.45	1.50
17	1	504	CLA	CMB-C2B	-2.51	1.46	1.51
17	3	313	CLA	CMB-C2B	-2.51	1.46	1.51
17	B	802	CLA	C3B-C2B	-2.50	1.36	1.40
17	A	821	CLA	CMD-C2D	-2.50	1.45	1.50
25	3	315	CHL	C1D-C2D	2.50	1.50	1.45
17	5	308	CLA	CMC-C2C	-2.50	1.45	1.50
17	A	829	CLA	CMC-C2C	-2.50	1.45	1.50
17	A	839	CLA	C3B-CAB	-2.50	1.42	1.47
17	1	513	CLA	CMB-C2B	-2.50	1.46	1.51
17	A	820	CLA	C3B-C2B	-2.50	1.36	1.40
17	L	303	CLA	C1D-ND	2.50	1.40	1.37
17	2	510	CLA	CMB-C2B	-2.50	1.46	1.51
25	5	314	CHL	MG-NA	-2.50	2.00	2.06
17	B	834	CLA	CMC-C2C	-2.50	1.45	1.50
17	B	837	CLA	C3B-CAB	-2.49	1.42	1.47
17	1	511	CLA	CMB-C2B	-2.49	1.46	1.51
17	A	831	CLA	CMD-C2D	-2.49	1.45	1.50
17	B	807	CLA	C3B-C2B	-2.49	1.36	1.40
17	A	839	CLA	CMD-C2D	-2.49	1.45	1.50
17	2	508	CLA	CMD-C2D	-2.49	1.45	1.50
17	5	305	CLA	CMD-C2D	-2.49	1.45	1.50
17	A	852	CLA	CMC-C2C	-2.49	1.45	1.50
17	B	817	CLA	CMC-C2C	-2.49	1.45	1.50
17	1	508	CLA	CMB-C2B	-2.48	1.46	1.51
17	B	822	CLA	CMD-C2D	-2.48	1.45	1.50
17	B	822	CLA	C3B-C2B	-2.48	1.36	1.40
20	A	847	BCR	C30-C25	-2.48	1.50	1.53
17	A	852	CLA	CMD-C2D	-2.47	1.45	1.50
17	B	826	CLA	CMC-C2C	-2.47	1.45	1.50
17	A	804	CLA	C1D-ND	2.47	1.40	1.37
17	B	815	CLA	CMD-C2D	-2.47	1.45	1.50
17	B	829	CLA	C3B-CAB	-2.47	1.42	1.47
17	B	827	CLA	C3B-C2B	-2.47	1.36	1.40
17	5	305	CLA	C1D-ND	2.47	1.40	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	5	304	XAT	O4-C5	-2.47	1.42	1.46
17	B	840	CLA	C1D-ND	2.47	1.40	1.37
17	K	203	CLA	C1D-ND	2.47	1.40	1.37
25	1	514	CHL	C1D-ND	-2.46	1.34	1.37
17	A	816	CLA	CMC-C2C	-2.46	1.45	1.50
17	A	826	CLA	C1D-ND	2.46	1.40	1.37
17	A	821	CLA	MG-ND	-2.46	2.00	2.05
25	1	512	CHL	C4C-C3C	2.46	1.49	1.45
17	B	825	CLA	C1D-ND	2.46	1.40	1.37
17	B	825	CLA	CMC-C2C	-2.46	1.45	1.50
17	5	307	CLA	C3B-C2B	-2.45	1.37	1.40
25	5	315	CHL	C1C-NC	-2.45	1.34	1.37
17	3	301	CLA	C3B-CAB	-2.45	1.43	1.47
17	A	813	CLA	C1D-ND	2.45	1.40	1.37
26	2	502	XAT	O4-C5	-2.45	1.42	1.46
17	A	813	CLA	CMD-C2D	-2.44	1.45	1.50
17	A	839	CLA	CMC-C2C	-2.44	1.45	1.50
17	B	823	CLA	CMD-C2D	-2.44	1.45	1.50
17	A	840	CLA	CMD-C2D	-2.44	1.45	1.50
17	L	303	CLA	C3B-CAB	-2.44	1.43	1.47
17	3	301	CLA	CMC-C2C	-2.44	1.45	1.50
17	B	802	CLA	CMC-C2C	-2.44	1.45	1.50
17	A	803	CLA	C3B-CAB	-2.44	1.43	1.47
17	A	835	CLA	CMD-C2D	-2.44	1.45	1.50
17	B	837	CLA	CMC-C2C	-2.43	1.45	1.50
17	B	810	CLA	C3B-C2B	-2.43	1.37	1.40
17	2	509	CLA	C3B-C2B	-2.43	1.37	1.40
25	1	514	CHL	C4C-C3C	2.43	1.49	1.45
17	A	827	CLA	CMC-C2C	-2.43	1.45	1.50
17	3	318	CLA	CMB-C2B	-2.43	1.46	1.51
17	B	839	CLA	C3B-C2B	-2.43	1.37	1.40
17	1	504	CLA	CMC-C2C	-2.43	1.45	1.50
17	B	837	CLA	CMD-C2D	-2.42	1.45	1.50
17	B	839	CLA	C3B-CAB	-2.42	1.43	1.47
17	B	827	CLA	CMC-C2C	-2.42	1.45	1.50
17	A	808	CLA	CMC-C2C	-2.42	1.45	1.50
17	B	804	CLA	CMC-C2C	-2.42	1.45	1.50
20	A	853	BCR	C30-C25	-2.42	1.50	1.53
17	A	821	CLA	CMC-C2C	-2.42	1.45	1.50
17	1	515	CLA	CMB-C2B	-2.42	1.46	1.51
17	F	802	CLA	CMD-C2D	-2.42	1.45	1.50
17	B	825	CLA	C3B-CAB	-2.41	1.43	1.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	F	801	BCR	C30-C25	-2.41	1.50	1.53
16	A	801	CL0	C1D-C2D	2.41	1.50	1.45
17	A	810	CLA	CMD-C2D	-2.41	1.45	1.50
17	A	827	CLA	C3B-C2B	-2.41	1.37	1.40
17	B	818	CLA	C3B-CAB	-2.41	1.43	1.47
17	A	813	CLA	C3B-C2B	-2.41	1.37	1.40
17	3	306	CLA	CMD-C2D	-2.41	1.45	1.50
17	B	825	CLA	C3B-C2B	-2.41	1.37	1.40
17	B	835	CLA	CMC-C2C	-2.41	1.45	1.50
17	B	838	CLA	CMC-C2C	-2.41	1.45	1.50
17	B	811	CLA	CMD-C2D	-2.40	1.45	1.50
17	B	841	CLA	CMD-C2D	-2.40	1.45	1.50
17	3	307	CLA	CMB-C2B	-2.40	1.46	1.51
17	5	308	CLA	CMD-C2D	-2.40	1.45	1.50
17	A	829	CLA	CMD-C2D	-2.40	1.45	1.50
17	B	801	CLA	CMD-C2D	-2.40	1.45	1.50
17	A	809	CLA	C3B-CAB	-2.40	1.43	1.47
17	1	506	CLA	C3B-C2B	-2.39	1.37	1.40
17	A	804	CLA	C3B-CAB	-2.39	1.43	1.47
17	A	823	CLA	C3B-CAB	-2.39	1.43	1.47
17	A	822	CLA	CMD-C2D	-2.39	1.45	1.50
17	B	816	CLA	C3B-CAB	-2.39	1.43	1.47
25	5	317	CHL	CHB-C4A	-2.38	1.33	1.34
17	A	813	CLA	CMC-C2C	-2.38	1.45	1.50
17	B	812	CLA	CMD-C2D	-2.38	1.45	1.50
20	A	851	BCR	C1-C6	-2.38	1.50	1.53
25	1	514	CHL	C1B-CHB	2.38	1.47	1.41
26	2	502	XAT	C2-C1	-2.38	1.50	1.54
17	A	802	CLA	CMC-C2C	-2.38	1.45	1.50
17	A	837	CLA	CMC-C2C	-2.38	1.45	1.50
17	B	818	CLA	C3B-C2B	-2.38	1.37	1.40
17	F	802	CLA	C3B-C2B	-2.38	1.37	1.40
17	L	301	CLA	CMD-C2D	-2.38	1.45	1.50
17	3	313	CLA	CMD-C2D	-2.38	1.45	1.50
25	5	315	CHL	MG-NA	-2.38	2.00	2.06
17	A	812	CLA	CMD-C2D	-2.38	1.45	1.50
17	A	820	CLA	CMD-C2D	-2.38	1.45	1.50
17	B	814	CLA	C3B-CAB	-2.38	1.43	1.47
20	B	849	BCR	C30-C25	-2.37	1.50	1.53
17	B	802	CLA	CMD-C2D	-2.37	1.45	1.50
17	B	841	CLA	C3B-CAB	-2.37	1.43	1.47
17	5	310	CLA	CMC-C2C	-2.37	1.45	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	5	308	CLA	C3B-CAB	-2.37	1.43	1.47
20	A	847	BCR	C1-C6	-2.37	1.50	1.53
17	A	805	CLA	CMC-C2C	-2.37	1.45	1.50
17	B	812	CLA	CMC-C2C	-2.37	1.45	1.50
17	B	817	CLA	CMD-C2D	-2.37	1.45	1.50
25	3	315	CHL	C4B-CHC	2.36	1.47	1.41
17	B	801	CLA	C3B-CAB	-2.36	1.43	1.47
17	A	819	CLA	CMC-C2C	-2.36	1.45	1.50
17	L	301	CLA	CMC-C2C	-2.36	1.45	1.50
17	A	816	CLA	CMB-C2B	-2.36	1.46	1.51
25	3	315	CHL	MG-NA	-2.36	2.00	2.06
17	F	802	CLA	CMC-C2C	-2.36	1.45	1.50
17	B	824	CLA	C3B-CAB	-2.36	1.43	1.47
17	A	814	CLA	CMC-C2C	-2.36	1.45	1.50
17	A	805	CLA	CMD-C2D	-2.36	1.45	1.50
17	B	839	CLA	CMC-C2C	-2.36	1.45	1.50
17	A	811	CLA	C3B-CAB	-2.36	1.43	1.47
17	A	829	CLA	C3B-CAB	-2.36	1.43	1.47
17	A	819	CLA	C3B-CAB	-2.35	1.43	1.47
17	A	825	CLA	CMC-C2C	-2.35	1.45	1.50
17	1	504	CLA	MG-ND	-2.35	2.01	2.05
17	A	820	CLA	CMC-C2C	-2.35	1.45	1.50
17	A	810	CLA	CMC-C2C	-2.35	1.45	1.50
17	B	808	CLA	CMC-C2C	-2.35	1.45	1.50
17	B	819	CLA	CMC-C2C	-2.35	1.45	1.50
17	A	840	CLA	CMC-C2C	-2.35	1.45	1.50
17	K	203	CLA	CMC-C2C	-2.34	1.45	1.50
17	B	829	CLA	CMD-C2D	-2.34	1.45	1.50
26	5	304	XAT	C2-C1	-2.34	1.50	1.54
17	2	507	CLA	CMD-C2D	-2.34	1.45	1.50
17	B	807	CLA	C1D-ND	2.34	1.40	1.37
17	5	309	CLA	CMD-C2D	-2.34	1.45	1.50
17	A	817	CLA	C1D-ND	2.34	1.40	1.37
17	B	831	CLA	CMC-C2C	-2.34	1.45	1.50
17	A	822	CLA	C3B-C2B	-2.34	1.37	1.40
25	3	302	CHL	C1D-C2D	2.34	1.49	1.45
25	1	517	CHL	C4B-CHC	2.34	1.47	1.41
16	A	801	CL0	O2A-CGA	-2.34	1.31	1.42
20	B	847	BCR	C1-C6	-2.34	1.50	1.53
17	5	316	CLA	CMD-C2D	-2.33	1.45	1.50
17	A	806	CLA	CMD-C2D	-2.33	1.45	1.50
17	B	820	CLA	CMD-C2D	-2.33	1.45	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	B	842	CLA	CMC-C2C	-2.33	1.45	1.50
17	B	828	CLA	CMC-C2C	-2.33	1.45	1.50
25	5	317	CHL	C4B-CHC	2.33	1.47	1.41
17	A	811	CLA	C1D-ND	2.33	1.40	1.37
17	A	802	CLA	CMD-C2D	-2.33	1.45	1.50
17	B	839	CLA	CMD-C2D	-2.33	1.45	1.50
17	A	807	CLA	CMC-C2C	-2.33	1.45	1.50
17	B	840	CLA	CMC-C2C	-2.33	1.45	1.50
17	B	817	CLA	MG-ND	-2.33	2.01	2.05
25	5	315	CHL	C3D-C2D	2.33	1.45	1.39
17	A	803	CLA	CMC-C2C	-2.32	1.45	1.50
17	B	805	CLA	CMC-C2C	-2.32	1.45	1.50
17	B	834	CLA	C3B-CAB	-2.32	1.43	1.47
17	B	818	CLA	C1D-ND	2.32	1.40	1.37
17	B	818	CLA	CMD-C2D	-2.32	1.45	1.50
17	1	509	CLA	CMD-C2D	-2.32	1.45	1.50
17	A	808	CLA	C3B-C2B	-2.32	1.37	1.40
17	B	818	CLA	CMC-C2C	-2.32	1.45	1.50
17	3	311	CLA	CMD-C2D	-2.31	1.45	1.50
24	3	304	LUT	C22-C21	-2.31	1.51	1.54
17	F	803	CLA	C3B-C2B	-2.31	1.37	1.40
17	A	819	CLA	CMD-C2D	-2.31	1.45	1.50
17	L	304	CLA	CMC-C2C	-2.31	1.45	1.50
25	1	512	CHL	C4B-CHC	2.31	1.47	1.41
17	A	827	CLA	C1D-ND	2.31	1.40	1.37
17	B	822	CLA	C3B-CAB	-2.31	1.43	1.47
17	B	824	CLA	CMC-C2C	-2.31	1.45	1.50
17	B	823	CLA	CMC-C2C	-2.30	1.45	1.50
17	A	818	CLA	CMC-C2C	-2.30	1.45	1.50
24	3	303	LUT	C22-C21	-2.30	1.51	1.54
17	5	316	CLA	C3B-C2B	-2.30	1.37	1.40
17	K	202	CLA	C3B-C2B	-2.30	1.37	1.40
17	B	802	CLA	C3B-CAB	-2.30	1.43	1.47
25	2	516	CHL	C1D-ND	-2.30	1.35	1.37
25	2	512	CHL	C1D-ND	-2.30	1.35	1.37
17	2	505	CLA	CMC-C2C	-2.30	1.45	1.50
17	A	815	CLA	MG-ND	-2.30	2.01	2.05
17	K	201	CLA	CMC-C2C	-2.30	1.45	1.50
17	A	838	CLA	CMC-C2C	-2.29	1.45	1.50
17	3	308	CLA	CMB-C2B	-2.29	1.46	1.51
17	A	842	CLA	CMC-C2C	-2.29	1.45	1.50
26	2	502	XAT	O24-C25	-2.29	1.42	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	B	836	CLA	CMC-C2C	-2.29	1.45	1.50
17	B	831	CLA	C3B-CAB	-2.29	1.43	1.47
17	5	307	CLA	C3B-CAB	-2.29	1.43	1.47
17	A	817	CLA	MG-ND	-2.28	2.01	2.05
17	B	809	CLA	C3B-CAB	-2.28	1.43	1.47
17	B	822	CLA	CMC-C2C	-2.28	1.46	1.50
17	A	815	CLA	C3B-C2B	-2.28	1.37	1.40
24	5	303	LUT	C22-C21	-2.28	1.51	1.54
17	B	829	CLA	CMC-C2C	-2.28	1.46	1.50
17	2	511	CLA	C3B-CAB	-2.28	1.43	1.47
17	3	307	CLA	CMD-C2D	-2.28	1.46	1.50
17	A	809	CLA	CBD-CGD	-2.28	1.49	1.51
17	B	842	CLA	CMD-C2D	-2.27	1.46	1.50
17	1	505	CLA	C3B-C2B	-2.27	1.37	1.40
17	1	511	CLA	C3B-CAB	-2.27	1.43	1.47
17	B	833	CLA	CMD-C2D	-2.27	1.46	1.50
17	A	837	CLA	C3B-CAB	-2.27	1.43	1.47
17	F	803	CLA	CMC-C2C	-2.27	1.46	1.50
17	3	306	CLA	CMB-C2B	-2.27	1.46	1.51
25	1	512	CHL	C1B-CHB	2.27	1.47	1.41
17	B	836	CLA	CMD-C2D	-2.27	1.46	1.50
17	A	808	CLA	CMD-C2D	-2.27	1.46	1.50
17	A	812	CLA	C3B-CAB	-2.27	1.43	1.47
17	A	832	CLA	CMC-C2C	-2.26	1.46	1.50
20	B	849	BCR	C1-C6	-2.26	1.50	1.53
17	A	815	CLA	CMD-C2D	-2.26	1.46	1.50
17	B	832	CLA	CMC-C2C	-2.26	1.46	1.50
17	A	825	CLA	MG-ND	-2.26	2.01	2.05
17	2	514	CLA	CMD-C2D	-2.26	1.46	1.50
17	5	313	CLA	CMD-C2D	-2.26	1.46	1.50
25	3	302	CHL	C1D-ND	-2.25	1.35	1.37
17	2	506	CLA	CMD-C2D	-2.25	1.46	1.50
17	K	201	CLA	MG-ND	-2.25	2.01	2.05
17	1	506	CLA	CMC-C2C	-2.25	1.46	1.50
17	B	836	CLA	C3B-CAB	-2.25	1.43	1.47
17	3	301	CLA	CMD-C2D	-2.25	1.46	1.50
17	B	805	CLA	C1D-ND	2.25	1.40	1.37
17	A	822	CLA	C3B-CAB	-2.25	1.43	1.47
25	2	516	CHL	MG-NA	-2.25	2.00	2.06
24	1	502	LUT	C1-C6	-2.25	1.50	1.53
25	2	515	CHL	C4B-CHC	2.25	1.47	1.41
17	B	828	CLA	C3B-CAB	-2.25	1.43	1.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	1	517	CHL	MG-NA	-2.25	2.00	2.06
17	A	830	CLA	CMC-C2C	-2.24	1.46	1.50
17	2	508	CLA	C3B-C2B	-2.24	1.37	1.40
17	1	513	CLA	CMD-C2D	-2.24	1.46	1.50
17	B	841	CLA	CMC-C2C	-2.24	1.46	1.50
17	A	818	CLA	CMD-C2D	-2.24	1.46	1.50
17	5	310	CLA	CMB-C2B	-2.24	1.47	1.51
17	A	834	CLA	C3B-CAB	-2.24	1.43	1.47
17	3	316	CLA	C1D-ND	2.24	1.40	1.37
17	B	832	CLA	CMD-C2D	-2.24	1.46	1.50
17	A	817	CLA	CMC-C2C	-2.24	1.46	1.50
17	B	835	CLA	CMD-C2D	-2.23	1.46	1.50
17	1	511	CLA	C3B-C2B	-2.23	1.37	1.40
25	5	317	CHL	C4C-C3C	2.23	1.48	1.44
17	2	511	CLA	CMD-C2D	-2.23	1.46	1.50
17	A	838	CLA	C3B-C2B	-2.23	1.37	1.40
17	F	803	CLA	CMD-C2D	-2.23	1.46	1.50
17	K	202	CLA	CMD-C2D	-2.23	1.46	1.50
17	5	308	CLA	C3B-C2B	-2.23	1.37	1.40
17	B	832	CLA	MG-ND	-2.23	2.01	2.05
17	B	819	CLA	C3B-CAB	-2.23	1.43	1.47
17	2	504	CLA	CMC-C2C	-2.23	1.46	1.50
17	2	510	CLA	MG-ND	-2.22	2.01	2.05
17	3	317	CLA	CMC-C2C	-2.22	1.46	1.50
17	A	836	CLA	CMC-C2C	-2.22	1.46	1.50
17	B	810	CLA	C1D-ND	2.22	1.40	1.37
25	2	512	CHL	MG-NA	-2.22	2.01	2.06
25	5	314	CHL	C4B-CHC	2.22	1.47	1.41
17	2	506	CLA	C3B-C2B	-2.22	1.37	1.40
20	3	305	BCR	C1-C6	-2.22	1.50	1.53
17	5	309	CLA	C3B-C2B	-2.22	1.37	1.40
17	1	508	CLA	CMD-C2D	-2.21	1.46	1.50
17	A	828	CLA	CMC-C2C	-2.21	1.46	1.50
17	B	820	CLA	C3B-CAB	-2.21	1.43	1.47
17	B	840	CLA	C3B-CAB	-2.21	1.43	1.47
17	3	307	CLA	CMC-C2C	-2.21	1.46	1.50
17	5	316	CLA	CMC-C2C	-2.21	1.46	1.50
17	B	828	CLA	C3A-C2A	-2.21	1.52	1.54
20	F	801	BCR	C1-C6	-2.21	1.50	1.53
17	A	815	CLA	CMC-C2C	-2.21	1.46	1.50
17	A	824	CLA	CMC-C2C	-2.21	1.46	1.50
24	2	501	LUT	C1-C6	-2.21	1.50	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	A	802	CLA	C3B-CAB	-2.21	1.43	1.47
17	B	821	CLA	CMC-C2C	-2.20	1.46	1.50
17	A	816	CLA	C3B-CAB	-2.20	1.43	1.47
17	B	810	CLA	CMD-C2D	-2.20	1.46	1.50
17	A	814	CLA	CAC-C3C	-2.20	1.45	1.51
20	A	845	BCR	C14-C13	-2.20	1.32	1.35
25	5	317	CHL	C1D-ND	-2.20	1.35	1.37
17	A	834	CLA	CMD-C2D	-2.20	1.46	1.50
17	A	827	CLA	MG-ND	-2.20	2.01	2.05
17	B	832	CLA	C1D-ND	2.20	1.40	1.37
17	2	514	CLA	MG-ND	-2.20	2.01	2.05
17	B	834	CLA	CMD-C2D	-2.20	1.46	1.50
17	B	823	CLA	C3B-CAB	-2.19	1.43	1.47
17	A	807	CLA	CMD-C2D	-2.19	1.46	1.50
17	A	829	CLA	MG-ND	-2.19	2.01	2.05
17	A	833	CLA	C3B-CAB	-2.19	1.43	1.47
17	B	829	CLA	MG-ND	-2.19	2.01	2.05
17	3	314	CLA	CMD-C2D	-2.19	1.46	1.50
16	A	801	CL0	CHB-C4A	2.19	1.36	1.34
17	A	817	CLA	CMD-C2D	-2.19	1.46	1.50
17	A	835	CLA	C3B-CAB	-2.19	1.43	1.47
17	B	807	CLA	MG-ND	-2.19	2.01	2.05
17	1	507	CLA	CMC-C2C	-2.18	1.46	1.50
17	2	507	CLA	C3B-CAB	-2.18	1.43	1.47
25	2	516	CHL	C1B-NB	-2.18	1.33	1.35
17	A	807	CLA	C3B-CAB	-2.18	1.43	1.47
17	3	311	CLA	CMC-C2C	-2.18	1.46	1.50
17	2	510	CLA	CMD-C2D	-2.18	1.46	1.50
17	B	825	CLA	MG-ND	-2.18	2.01	2.05
17	A	839	CLA	MG-ND	-2.18	2.01	2.05
17	1	510	CLA	CMC-C2C	-2.18	1.46	1.50
17	A	837	CLA	MG-ND	-2.18	2.01	2.05
17	A	842	CLA	C3B-CAB	-2.18	1.43	1.47
17	3	308	CLA	C3B-C2B	-2.18	1.37	1.40
17	K	203	CLA	C3B-C2B	-2.17	1.37	1.40
17	2	504	CLA	CMD-C2D	-2.17	1.46	1.50
17	5	312	CLA	CMD-C2D	-2.17	1.46	1.50
17	L	301	CLA	CAC-C3C	-2.17	1.45	1.51
17	B	809	CLA	CMC-C2C	-2.17	1.46	1.50
17	B	801	CLA	CAC-C3C	-2.17	1.45	1.51
17	A	821	CLA	C3B-CAB	-2.17	1.43	1.47
17	1	506	CLA	C3B-CAB	-2.17	1.43	1.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	B	830	CLA	CAC-C3C	-2.16	1.45	1.51
17	A	837	CLA	C3A-C2A	-2.16	1.52	1.54
17	L	303	CLA	CMC-C2C	-2.16	1.46	1.50
25	3	302	CHL	C1C-NC	-2.16	1.34	1.37
17	5	309	CLA	CMC-C2C	-2.16	1.46	1.50
17	A	829	CLA	C1D-ND	2.16	1.40	1.37
17	B	806	CLA	C4B-CHC	-2.16	1.35	1.41
17	B	804	CLA	C3B-CAB	-2.16	1.43	1.47
17	B	838	CLA	MG-ND	-2.16	2.01	2.05
17	1	507	CLA	C3B-CAB	-2.16	1.43	1.47
17	3	309	CLA	CMC-C2C	-2.16	1.46	1.50
17	K	203	CLA	C3B-CAB	-2.16	1.43	1.47
17	A	836	CLA	CAA-C2A	-2.15	1.50	1.54
17	2	506	CLA	C3B-CAB	-2.15	1.43	1.47
17	A	818	CLA	C3B-CAB	-2.15	1.43	1.47
17	L	303	CLA	CMD-C2D	-2.15	1.46	1.50
25	2	513	CHL	C3A-C4A	-2.15	1.47	1.51
17	B	828	CLA	MG-ND	-2.15	2.01	2.05
17	A	822	CLA	CMC-C2C	-2.15	1.46	1.50
17	A	828	CLA	C3B-CAB	-2.15	1.43	1.47
17	1	507	CLA	CMD-C2D	-2.15	1.46	1.50
24	3	304	LUT	C1-C6	-2.15	1.50	1.53
17	2	514	CLA	CMC-C2C	-2.14	1.46	1.50
17	K	203	CLA	MG-ND	-2.14	2.01	2.05
25	5	315	CHL	C1B-CHB	2.14	1.46	1.41
17	B	815	CLA	MG-ND	-2.14	2.01	2.05
20	J	102	BCR	C30-C25	-2.14	1.50	1.53
17	A	821	CLA	C1D-ND	2.14	1.40	1.37
17	3	317	CLA	CMD-C2D	-2.14	1.46	1.50
17	A	833	CLA	MG-ND	-2.14	2.01	2.05
17	B	835	CLA	C3B-CAB	-2.14	1.43	1.47
17	L	302	CLA	C3B-C2B	-2.14	1.37	1.40
17	A	832	CLA	C4B-CHC	-2.14	1.35	1.41
17	L	301	CLA	MG-ND	-2.14	2.01	2.05
17	K	205	CLA	C3B-CAB	-2.13	1.43	1.47
17	2	511	CLA	CMC-C2C	-2.13	1.46	1.50
20	B	848	BCR	C1-C6	-2.13	1.50	1.53
25	2	512	CHL	C4B-CHC	2.13	1.46	1.41
17	B	811	CLA	CAA-C2A	-2.13	1.50	1.54
17	A	835	CLA	C1D-ND	2.13	1.40	1.37
17	1	511	CLA	CMD-C2D	-2.13	1.46	1.50
17	B	807	CLA	CAC-C3C	-2.13	1.45	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	B	814	CLA	MG-ND	-2.13	2.01	2.05
17	B	821	CLA	C3B-CAB	-2.12	1.43	1.47
17	B	801	CLA	MG-ND	-2.12	2.01	2.05
24	3	303	LUT	C34-C33	-2.12	1.33	1.35
17	J	101	CLA	CMD-C2D	-2.12	1.46	1.50
25	1	512	CHL	C1D-ND	-2.12	1.35	1.37
17	A	828	CLA	MG-ND	-2.12	2.01	2.05
17	2	514	CLA	C3B-C2B	-2.12	1.37	1.40
17	1	509	CLA	CMB-C2B	-2.12	1.47	1.51
17	A	813	CLA	C3B-CAB	-2.12	1.43	1.47
17	1	507	CLA	C3B-C2B	-2.12	1.37	1.40
17	A	830	CLA	C3B-CAB	-2.11	1.43	1.47
17	5	312	CLA	CMC-C2C	-2.11	1.46	1.50
17	B	811	CLA	CMA-C3A	-2.11	1.48	1.53
17	A	818	CLA	MG-ND	-2.11	2.01	2.05
17	B	837	CLA	MG-ND	-2.11	2.01	2.05
17	5	310	CLA	CMD-C2D	-2.11	1.46	1.50
20	B	846	BCR	C1-C6	-2.11	1.50	1.53
25	2	513	CHL	C4B-CHC	2.11	1.46	1.41
17	A	838	CLA	C3B-CAB	-2.11	1.43	1.47
17	2	504	CLA	C3B-CAB	-2.11	1.43	1.47
20	A	845	BCR	C17-C18	-2.11	1.33	1.35
17	A	827	CLA	C4B-CHC	-2.11	1.35	1.41
17	L	302	CLA	C3B-CAB	-2.11	1.43	1.47
24	1	502	LUT	C22-C21	-2.10	1.52	1.54
20	B	846	BCR	C14-C13	-2.10	1.33	1.35
17	5	311	CLA	CMD-C2D	-2.10	1.46	1.50
17	2	507	CLA	CMC-C2C	-2.10	1.46	1.50
17	B	804	CLA	CAC-C3C	-2.10	1.45	1.51
17	5	313	CLA	CMC-C2C	-2.10	1.46	1.50
17	B	806	CLA	CAC-C3C	-2.10	1.45	1.51
17	B	805	CLA	CMD-C2D	-2.10	1.46	1.50
17	2	505	CLA	MG-ND	-2.10	2.01	2.05
25	2	513	CHL	C1C-NC	-2.10	1.34	1.37
20	A	846	BCR	C10-C9	-2.10	1.33	1.35
17	3	318	CLA	CMD-C2D	-2.09	1.46	1.50
20	B	852	BCR	C14-C13	-2.09	1.33	1.35
17	1	515	CLA	CMC-C2C	-2.09	1.46	1.50
26	5	304	XAT	C22-C23	-2.09	1.49	1.52
17	A	812	CLA	MG-ND	-2.09	2.01	2.05
17	B	809	CLA	CAC-C3C	-2.09	1.45	1.51
17	A	804	CLA	CMC-C2C	-2.09	1.46	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	2	516	CHL	C1C-NC	-2.09	1.34	1.37
17	B	807	CLA	C3B-CAB	-2.09	1.43	1.47
17	B	838	CLA	C3B-CAB	-2.08	1.43	1.47
17	A	806	CLA	MG-ND	-2.08	2.01	2.05
17	B	827	CLA	C3B-CAB	-2.08	1.43	1.47
17	B	833	CLA	C3B-C2B	-2.08	1.37	1.40
17	2	509	CLA	CMD-C2D	-2.08	1.46	1.50
17	B	833	CLA	CMC-C2C	-2.08	1.46	1.50
17	5	307	CLA	CMD-C2D	-2.08	1.46	1.50
25	2	515	CHL	C1D-ND	-2.08	1.35	1.37
17	A	842	CLA	C3B-C2B	-2.08	1.37	1.40
17	2	511	CLA	CAC-C3C	-2.08	1.45	1.51
17	3	309	CLA	CMD-C2D	-2.08	1.46	1.50
17	3	312	CLA	CMC-C2C	-2.08	1.46	1.50
17	A	827	CLA	C3B-CAB	-2.08	1.43	1.47
17	A	810	CLA	CAC-C3C	-2.08	1.45	1.51
17	B	822	CLA	CAC-C3C	-2.07	1.45	1.51
17	B	810	CLA	C3B-CAB	-2.07	1.43	1.47
17	1	510	CLA	CMD-C2D	-2.07	1.46	1.50
17	B	827	CLA	MG-ND	-2.07	2.01	2.05
17	5	316	CLA	C3B-CAB	-2.07	1.43	1.47
17	B	804	CLA	MG-ND	-2.07	2.01	2.05
17	L	304	CLA	C3B-C2B	-2.07	1.37	1.40
17	B	817	CLA	C4B-CHC	-2.07	1.35	1.41
17	B	813	CLA	CAC-C3C	-2.07	1.45	1.51
17	A	838	CLA	MG-ND	-2.07	2.01	2.05
17	2	514	CLA	C3B-CAB	-2.07	1.43	1.47
17	K	205	CLA	CMD-C2D	-2.06	1.46	1.50
17	1	505	CLA	CMC-C2C	-2.06	1.46	1.50
17	F	802	CLA	C3B-CAB	-2.06	1.43	1.47
17	B	819	CLA	C3A-C2A	-2.06	1.52	1.54
17	A	835	CLA	MG-ND	-2.06	2.01	2.05
26	2	502	XAT	C22-C21	-2.06	1.51	1.54
25	5	314	CHL	C1D-ND	-2.06	1.35	1.37
17	3	309	CLA	CAA-C2A	-2.06	1.49	1.54
19	A	844	LHG	O7-C5	-2.06	1.41	1.46
17	K	202	CLA	C3B-CAB	-2.06	1.43	1.47
17	3	308	CLA	MG-ND	-2.06	2.01	2.05
25	3	315	CHL	C1B-CHB	2.06	1.46	1.41
25	2	513	CHL	C1B-CHB	2.06	1.46	1.41
25	3	302	CHL	C4B-CHC	2.05	1.46	1.41
17	3	308	CLA	CMC-C2C	-2.05	1.46	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	B	830	CLA	MG-ND	-2.05	2.01	2.05
25	1	517	CHL	C1D-ND	-2.05	1.35	1.37
17	B	814	CLA	CAC-C3C	-2.05	1.45	1.51
17	B	842	CLA	MG-ND	-2.05	2.01	2.05
17	B	828	CLA	C1D-ND	2.05	1.40	1.37
17	B	802	CLA	MG-ND	-2.05	2.01	2.05
17	5	305	CLA	MG-ND	-2.05	2.01	2.05
17	B	811	CLA	C3B-CAB	-2.05	1.43	1.47
17	A	810	CLA	C3B-CAB	-2.05	1.43	1.47
17	L	302	CLA	CMC-C2C	-2.05	1.46	1.50
17	B	818	CLA	C4B-CHC	-2.05	1.35	1.41
17	A	834	CLA	CMC-C2C	-2.05	1.46	1.50
17	3	308	CLA	CMD-C2D	-2.04	1.46	1.50
25	2	513	CHL	MG-NA	-2.04	2.01	2.06
17	A	803	CLA	MG-ND	-2.04	2.01	2.05
17	1	515	CLA	MG-ND	-2.04	2.01	2.05
17	B	820	CLA	MG-ND	-2.04	2.01	2.05
17	1	510	CLA	MG-ND	-2.04	2.01	2.05
25	2	512	CHL	C1B-CHB	2.04	1.46	1.41
17	A	817	CLA	CBD-CGD	-2.04	1.49	1.51
17	L	304	CLA	MG-ND	-2.04	2.01	2.05
20	I	101	BCR	C21-C22	-2.04	1.33	1.35
25	2	515	CHL	C4C-C3C	2.04	1.48	1.45
17	B	841	CLA	CAA-C2A	-2.04	1.50	1.54
17	3	307	CLA	C3B-CAB	-2.04	1.43	1.47
17	A	805	CLA	CAA-C2A	-2.04	1.50	1.54
17	A	842	CLA	CMD-C2D	-2.04	1.46	1.50
17	5	306	CLA	CMD-C2D	-2.04	1.46	1.50
17	1	511	CLA	CMC-C2C	-2.03	1.46	1.50
17	A	837	CLA	C3B-C2B	-2.03	1.37	1.40
17	A	827	CLA	CAA-C2A	-2.03	1.50	1.54
17	A	808	CLA	CAC-C3C	-2.03	1.45	1.51
17	A	842	CLA	MG-ND	-2.03	2.01	2.05
17	3	310	CLA	CMC-C2C	-2.03	1.46	1.50
17	A	807	CLA	MG-ND	-2.02	2.01	2.05
17	1	513	CLA	CMC-C2C	-2.02	1.46	1.50
17	A	805	CLA	CMA-C3A	-2.02	1.48	1.53
17	B	815	CLA	CAC-C3C	-2.02	1.45	1.51
17	3	310	CLA	CMD-C2D	-2.02	1.46	1.50
17	B	826	CLA	C3B-CAB	-2.02	1.43	1.47
19	A	843	LHG	O7-C5	-2.02	1.41	1.46
17	A	825	CLA	C3B-CAB	-2.02	1.43	1.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	L	304	CLA	C4B-CHC	-2.02	1.35	1.41
17	A	831	CLA	CAA-C2A	-2.02	1.50	1.54
17	B	810	CLA	CAC-C3C	-2.02	1.45	1.51
17	3	317	CLA	MG-ND	-2.01	2.01	2.05
17	3	312	CLA	MG-ND	-2.01	2.01	2.05
17	A	805	CLA	CAC-C3C	-2.01	1.45	1.51
17	2	506	CLA	CMC-C2C	-2.01	1.46	1.50
17	5	311	CLA	CMC-C2C	-2.01	1.46	1.50
25	5	314	CHL	C4C-C3C	2.01	1.48	1.45
17	5	310	CLA	C3B-CAB	-2.01	1.43	1.47
17	A	831	CLA	CAC-C3C	-2.01	1.46	1.51
17	B	826	CLA	CAC-C3C	-2.01	1.46	1.51
17	B	829	CLA	C4B-CHC	-2.01	1.35	1.41
25	1	517	CHL	C1B-CHB	2.00	1.46	1.41
17	A	808	CLA	C3B-CAB	-2.00	1.43	1.47
17	F	803	CLA	MG-ND	-2.00	2.01	2.05
17	3	309	CLA	MG-ND	-2.00	2.01	2.05
20	2	503	BCR	C1-C6	-2.00	1.51	1.53
17	1	509	CLA	CMC-C2C	-2.00	1.46	1.50

All (2004) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	2	503	BCR	C40-C30-C25	-12.70	89.71	110.30
16	A	801	CL0	C4A-NA-C1A	10.86	111.59	106.71
25	5	315	CHL	CMD-C2D-C1D	9.11	140.76	124.71
20	2	503	BCR	C20-C21-C22	-8.87	114.64	127.31
25	2	516	CHL	CMD-C2D-C1D	8.70	140.05	124.71
25	2	512	CHL	CMD-C2D-C1D	8.61	139.90	124.71
20	2	503	BCR	C40-C30-C39	-8.44	82.63	108.53
25	2	513	CHL	C2C-C3C-C4C	-8.33	100.55	106.49
25	1	512	CHL	CMD-C2D-C1D	8.31	139.35	124.71
25	2	515	CHL	CMD-C2D-C1D	8.28	139.30	124.71
25	1	517	CHL	CMD-C2D-C1D	8.24	139.23	124.71
17	3	308	CLA	C4A-NA-C1A	8.23	110.41	106.71
25	5	314	CHL	CMD-C2D-C1D	8.22	139.20	124.71
25	3	302	CHL	C2C-C3C-C4C	-8.20	100.64	106.49
17	A	810	CLA	C4A-NA-C1A	8.14	110.37	106.71
25	2	513	CHL	CMD-C2D-C1D	8.14	139.06	124.71
25	3	315	CHL	CMD-C2D-C1D	8.11	139.00	124.71
25	5	317	CHL	CMD-C2D-C1D	8.04	138.88	124.71
17	A	835	CLA	C4A-NA-C1A	8.00	110.30	106.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	847	BCR	C15-C14-C13	-7.99	115.90	127.31
25	2	516	CHL	C2C-C3C-C4C	-7.97	100.81	106.49
25	1	514	CHL	CMD-C2D-C1D	7.95	138.72	124.71
17	2	511	CLA	C4A-NA-C1A	7.89	110.25	106.71
25	1	514	CHL	CHD-C1D-ND	-7.86	117.23	124.45
17	A	832	CLA	C4A-NA-C1A	7.86	110.24	106.71
17	B	804	CLA	C4A-NA-C1A	7.75	110.19	106.71
17	L	303	CLA	C4A-NA-C1A	7.71	110.17	106.71
17	A	820	CLA	C4A-NA-C1A	7.69	110.16	106.71
17	3	306	CLA	C4A-NA-C1A	7.68	110.16	106.71
17	B	839	CLA	C4A-NA-C1A	7.60	110.12	106.71
17	2	506	CLA	C4A-NA-C1A	7.57	110.11	106.71
25	2	512	CHL	C2C-C3C-C4C	-7.56	101.10	106.49
17	2	509	CLA	C4A-NA-C1A	7.55	110.10	106.71
17	A	821	CLA	C4A-NA-C1A	7.53	110.09	106.71
17	A	830	CLA	C4A-NA-C1A	7.51	110.08	106.71
17	3	313	CLA	C4A-NA-C1A	7.51	110.08	106.71
17	B	822	CLA	C4A-NA-C1A	7.47	110.06	106.71
17	A	839	CLA	C4A-NA-C1A	7.47	110.06	106.71
17	5	311	CLA	C4A-NA-C1A	7.45	110.06	106.71
17	L	302	CLA	C4A-NA-C1A	7.45	110.06	106.71
26	5	304	XAT	O4-C5-C4	7.42	118.95	113.38
17	2	504	CLA	C4A-NA-C1A	7.41	110.04	106.71
25	5	315	CHL	C2C-C3C-C4C	-7.37	101.24	106.49
17	3	311	CLA	C4A-NA-C1A	7.37	110.02	106.71
25	3	302	CHL	CMD-C2D-C1D	7.36	137.68	124.71
25	1	512	CHL	C2C-C3C-C4C	-7.34	101.25	106.49
25	5	314	CHL	C2C-C3C-C4C	-7.32	101.27	106.49
20	B	844	BCR	C7-C8-C9	-7.31	115.18	126.23
17	A	836	CLA	C4A-NA-C1A	7.30	109.99	106.71
17	B	816	CLA	C4A-NA-C1A	7.27	109.97	106.71
17	B	821	CLA	C4A-NA-C1A	7.25	109.96	106.71
17	B	840	CLA	C4A-NA-C1A	7.24	109.96	106.71
17	3	301	CLA	C4A-NA-C1A	7.24	109.96	106.71
17	A	816	CLA	C4A-NA-C1A	7.22	109.95	106.71
25	1	517	CHL	C2C-C3C-C4C	-7.21	101.35	106.49
17	B	838	CLA	C4A-NA-C1A	7.19	109.94	106.71
17	A	822	CLA	C4A-NA-C1A	7.18	109.93	106.71
17	A	808	CLA	C4A-NA-C1A	7.18	109.93	106.71
17	B	818	CLA	C4A-NA-C1A	7.16	109.93	106.71
25	2	516	CHL	CHD-C1D-ND	-7.10	117.93	124.45
17	A	802	CLA	C4A-NA-C1A	7.09	109.89	106.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	3	310	CLA	C4A-NA-C1A	7.07	109.89	106.71
20	A	853	BCR	C24-C23-C22	-7.03	115.61	126.23
17	3	316	CLA	C4A-NA-C1A	7.02	109.86	106.71
17	5	306	CLA	C4A-NA-C1A	7.00	109.85	106.71
26	2	502	XAT	C38-C25-C26	-6.99	110.54	122.26
17	A	828	CLA	C4A-NA-C1A	6.98	109.85	106.71
20	B	844	BCR	C20-C21-C22	-6.97	117.36	127.31
25	5	317	CHL	C2C-C3C-C4C	-6.96	101.32	106.49
17	B	832	CLA	C4A-NA-C1A	6.96	109.83	106.71
25	5	315	CHL	CHD-C1D-ND	-6.95	118.06	124.45
17	B	817	CLA	C4A-NA-C1A	6.95	109.83	106.71
17	5	316	CLA	C4A-NA-C1A	6.94	109.83	106.71
25	2	512	CHL	C1B-C2B-C3B	-6.94	100.46	106.92
20	B	846	BCR	C7-C8-C9	-6.91	115.80	126.23
17	1	507	CLA	C4A-NA-C1A	6.90	109.81	106.71
17	2	510	CLA	C4A-NA-C1A	6.88	109.80	106.71
17	2	505	CLA	C4A-NA-C1A	6.87	109.80	106.71
20	F	801	BCR	C24-C23-C22	-6.86	115.86	126.23
17	3	318	CLA	C4A-NA-C1A	6.85	109.79	106.71
25	2	515	CHL	C2C-C3C-C4C	-6.84	101.61	106.49
26	2	502	XAT	C18-C5-C6	-6.84	110.80	122.26
17	B	833	CLA	C4A-NA-C1A	6.83	109.78	106.71
26	5	304	XAT	O24-C25-C24	6.82	118.50	113.38
17	1	506	CLA	C4A-NA-C1A	6.80	109.76	106.71
17	B	812	CLA	C4A-NA-C1A	6.80	109.76	106.71
17	B	835	CLA	C4A-NA-C1A	6.77	109.75	106.71
25	2	515	CHL	C1B-C2B-C3B	-6.76	100.63	106.92
17	A	805	CLA	C4A-NA-C1A	6.76	109.74	106.71
17	B	814	CLA	C4A-NA-C1A	6.75	109.74	106.71
17	3	314	CLA	C4A-NA-C1A	6.74	109.74	106.71
20	B	844	BCR	C15-C14-C13	-6.74	117.69	127.31
17	A	803	CLA	C4A-NA-C1A	6.73	109.73	106.71
17	B	829	CLA	C4A-NA-C1A	6.71	109.72	106.71
17	A	807	CLA	C4A-NA-C1A	6.70	109.72	106.71
17	A	809	CLA	C4A-NA-C1A	6.69	109.71	106.71
25	1	512	CHL	CHD-C1D-ND	-6.68	118.32	124.45
25	1	514	CHL	C2C-C3C-C4C	-6.65	101.75	106.49
26	2	502	XAT	C11-C10-C9	-6.65	117.82	127.31
17	A	814	CLA	C4A-NA-C1A	6.65	109.69	106.71
17	3	317	CLA	C4A-NA-C1A	6.64	109.69	106.71
17	B	808	CLA	C4A-NA-C1A	6.64	109.69	106.71
17	1	511	CLA	C4A-NA-C1A	6.63	109.69	106.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	B	841	CLA	C4A-NA-C1A	6.63	109.69	106.71
17	5	310	CLA	C4A-NA-C1A	6.62	109.68	106.71
17	A	840	CLA	C4A-NA-C1A	6.62	109.68	106.71
17	F	803	CLA	C4A-NA-C1A	6.61	109.68	106.71
17	1	505	CLA	C4A-NA-C1A	6.58	109.66	106.71
17	A	827	CLA	C4A-NA-C1A	6.57	109.66	106.71
17	2	514	CLA	C4A-NA-C1A	6.56	109.66	106.71
26	2	502	XAT	O4-C5-C4	6.56	118.31	113.38
17	F	802	CLA	C4A-NA-C1A	6.56	109.65	106.71
17	A	804	CLA	C4A-NA-C1A	6.55	109.65	106.71
17	B	823	CLA	C4A-NA-C1A	6.54	109.65	106.71
17	A	842	CLA	C4A-NA-C1A	6.54	109.64	106.71
25	1	517	CHL	CHD-C1D-ND	-6.54	118.45	124.45
17	B	807	CLA	C4A-NA-C1A	6.53	109.64	106.71
17	B	831	CLA	C4A-NA-C1A	6.53	109.64	106.71
26	5	304	XAT	C38-C25-C26	-6.52	111.34	122.26
17	B	809	CLA	C4A-NA-C1A	6.51	109.63	106.71
25	3	315	CHL	C2C-C3C-C4C	-6.51	101.85	106.49
17	A	806	CLA	C4A-NA-C1A	6.51	109.63	106.71
17	5	308	CLA	C4A-NA-C1A	6.50	109.63	106.71
25	2	516	CHL	C1B-C2B-C3B	-6.48	100.89	106.92
17	L	304	CLA	C4A-NA-C1A	6.47	109.61	106.71
20	B	845	BCR	C7-C8-C9	-6.47	116.46	126.23
25	5	317	CHL	CHD-C1D-ND	-6.46	118.51	124.45
17	3	309	CLA	C4A-NA-C1A	6.45	109.61	106.71
17	1	510	CLA	C4A-NA-C1A	6.44	109.60	106.71
17	5	307	CLA	C4A-NA-C1A	6.44	109.60	106.71
17	A	811	CLA	C4A-NA-C1A	6.43	109.60	106.71
17	1	509	CLA	C4A-NA-C1A	6.42	109.59	106.71
17	B	819	CLA	C4A-NA-C1A	6.41	109.59	106.71
25	2	512	CHL	CHD-C1D-ND	-6.41	118.56	124.45
25	2	513	CHL	CHD-C1D-ND	-6.40	118.57	124.45
24	5	303	LUT	C35-C34-C33	-6.40	118.17	127.31
17	B	803	CLA	C4A-NA-C1A	6.40	109.58	106.71
17	A	826	CLA	C4A-NA-C1A	6.39	109.58	106.71
17	B	813	CLA	C4A-NA-C1A	6.39	109.58	106.71
17	A	813	CLA	C4A-NA-C1A	6.38	109.57	106.71
20	2	503	BCR	C24-C23-C22	-6.38	116.60	126.23
17	A	837	CLA	C4A-NA-C1A	6.36	109.57	106.71
17	A	817	CLA	C4A-NA-C1A	6.35	109.56	106.71
25	5	314	CHL	CHD-C1D-ND	-6.35	118.62	124.45
17	A	831	CLA	C4A-NA-C1A	6.35	109.56	106.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	A	852	CLA	C4A-NA-C1A	6.35	109.56	106.71
25	3	315	CHL	CHD-C1D-ND	-6.33	118.64	124.45
17	B	810	CLA	C4A-NA-C1A	6.32	109.55	106.71
17	B	827	CLA	C4A-NA-C1A	6.32	109.55	106.71
17	K	201	CLA	C4A-NA-C1A	6.31	109.54	106.71
17	B	802	CLA	C4A-NA-C1A	6.29	109.53	106.71
17	B	825	CLA	C4A-NA-C1A	6.26	109.52	106.71
17	A	833	CLA	C4A-NA-C1A	6.25	109.52	106.71
17	1	513	CLA	C4A-NA-C1A	6.25	109.52	106.71
17	A	834	CLA	C4A-NA-C1A	6.24	109.51	106.71
17	B	842	CLA	C4A-NA-C1A	6.24	109.51	106.71
17	B	834	CLA	C4A-NA-C1A	6.20	109.50	106.71
17	2	507	CLA	C4A-NA-C1A	6.19	109.49	106.71
17	1	508	CLA	C4A-NA-C1A	6.18	109.48	106.71
17	A	825	CLA	C4A-NA-C1A	6.17	109.48	106.71
17	5	312	CLA	C4A-NA-C1A	6.14	109.47	106.71
17	B	811	CLA	C4A-NA-C1A	6.14	109.47	106.71
20	2	503	BCR	C15-C14-C13	6.12	136.05	127.31
20	A	848	BCR	C28-C27-C26	-6.12	103.14	114.08
17	A	838	CLA	C4A-NA-C1A	6.12	109.46	106.71
17	B	837	CLA	C4A-NA-C1A	6.12	109.46	106.71
17	K	202	CLA	C4A-NA-C1A	6.11	109.45	106.71
17	L	301	CLA	C4A-NA-C1A	6.11	109.45	106.71
17	5	313	CLA	C4A-NA-C1A	6.09	109.44	106.71
25	2	515	CHL	CHD-C1D-ND	-6.09	118.86	124.45
17	A	812	CLA	C4A-NA-C1A	6.08	109.44	106.71
17	B	806	CLA	C4A-NA-C1A	6.08	109.44	106.71
17	B	828	CLA	C4A-NA-C1A	6.08	109.44	106.71
16	A	801	CL0	CMD-C2D-C1D	6.06	135.40	124.71
17	A	829	CLA	C4A-NA-C1A	6.06	109.43	106.71
17	J	101	CLA	C4A-NA-C1A	6.06	109.43	106.71
17	A	815	CLA	C4A-NA-C1A	6.05	109.43	106.71
17	K	205	CLA	C4A-NA-C1A	6.05	109.42	106.71
17	B	805	CLA	C4A-NA-C1A	6.04	109.42	106.71
20	J	102	BCR	C28-C27-C26	-6.03	103.30	114.08
17	B	815	CLA	C4A-NA-C1A	6.02	109.41	106.71
17	3	307	CLA	C4A-NA-C1A	6.02	109.41	106.71
25	3	302	CHL	CHD-C1D-ND	-6.01	118.93	124.45
25	5	317	CHL	C2A-C3A-C4A	-5.98	99.67	106.26
20	L	305	BCR	C28-C27-C26	-5.98	103.39	114.08
26	5	304	XAT	C18-C5-C6	-5.98	112.24	122.26
17	3	312	CLA	C4A-NA-C1A	5.98	109.39	106.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	3	302	CHL	O2D-CGD-CBD	5.97	121.88	111.27
20	B	846	BCR	C24-C23-C22	-5.96	117.23	126.23
17	1	504	CLA	C4A-NA-C1A	5.96	109.39	106.71
17	A	824	CLA	C4A-NA-C1A	5.95	109.38	106.71
17	B	830	CLA	C4A-NA-C1A	5.95	109.38	106.71
17	B	836	CLA	C4A-NA-C1A	5.93	109.37	106.71
17	K	203	CLA	C4A-NA-C1A	5.89	109.35	106.71
17	5	309	CLA	C4A-NA-C1A	5.89	109.35	106.71
20	2	503	BCR	C40-C30-C29	-5.87	85.44	108.91
17	A	818	CLA	C4A-NA-C1A	5.85	109.33	106.71
20	3	305	BCR	C15-C14-C13	-5.83	118.99	127.31
20	B	846	BCR	C15-C14-C13	-5.83	118.99	127.31
17	A	819	CLA	C4A-NA-C1A	5.81	109.32	106.71
17	B	826	CLA	C4A-NA-C1A	5.81	109.32	106.71
17	B	820	CLA	C4A-NA-C1A	5.80	109.31	106.71
17	2	508	CLA	C4A-NA-C1A	5.80	109.31	106.71
20	1	503	BCR	C11-C10-C9	-5.78	119.06	127.31
20	B	844	BCR	C11-C10-C9	-5.75	119.10	127.31
16	A	801	CL0	C1B-C2B-C3B	-5.72	101.59	106.92
17	5	305	CLA	C4A-NA-C1A	5.71	109.27	106.71
20	A	845	BCR	C15-C14-C13	-5.69	119.19	127.31
17	A	823	CLA	C4A-NA-C1A	5.68	109.26	106.71
24	1	502	LUT	C15-C14-C13	-5.68	119.21	127.31
20	A	848	BCR	C24-C23-C22	-5.67	117.67	126.23
20	B	852	BCR	C7-C8-C9	-5.64	117.71	126.23
17	B	824	CLA	C4A-NA-C1A	5.64	109.24	106.71
20	2	503	BCR	C15-C16-C17	-5.61	111.98	123.47
20	B	844	BCR	C16-C17-C18	-5.59	119.33	127.31
20	B	844	BCR	C24-C23-C22	-5.56	117.83	126.23
25	2	515	CHL	O2D-CGD-CBD	5.55	121.13	111.27
25	1	517	CHL	O2D-CGD-CBD	5.55	121.13	111.27
20	2	503	BCR	C39-C30-C25	5.54	119.29	110.30
20	A	849	BCR	C7-C8-C9	-5.54	117.87	126.23
20	A	845	BCR	C16-C17-C18	-5.53	119.41	127.31
20	A	851	BCR	C15-C14-C13	-5.51	119.45	127.31
20	F	801	BCR	C28-C27-C26	-5.48	104.30	114.08
17	B	801	CLA	C4A-NA-C1A	5.46	109.16	106.71
25	1	514	CHL	C1B-CHB-C4A	-5.45	119.33	130.12
20	B	852	BCR	C15-C14-C13	-5.43	119.56	127.31
20	L	305	BCR	C16-C17-C18	-5.41	119.59	127.31
25	3	302	CHL	C3C-C4C-NC	5.41	116.64	110.57
20	I	101	BCR	C24-C23-C22	-5.40	118.08	126.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	2	502	XAT	O24-C25-C38	5.39	121.51	115.06
20	F	804	BCR	C11-C10-C9	-5.38	119.63	127.31
17	2	507	CLA	C4-C3-C2	-5.37	110.14	121.98
17	1	515	CLA	C4A-NA-C1A	5.37	109.12	106.71
20	K	204	BCR	C16-C17-C18	-5.33	119.70	127.31
25	3	315	CHL	O2D-CGD-CBD	5.32	120.72	111.27
20	B	849	BCR	C20-C21-C22	-5.30	119.75	127.31
25	2	516	CHL	C3C-C4C-NC	5.29	116.51	110.57
25	3	315	CHL	C3C-C4C-NC	5.23	116.43	110.57
20	A	853	BCR	C28-C27-C26	-5.22	104.76	114.08
26	2	502	XAT	O4-C5-C18	5.20	121.28	115.06
25	2	512	CHL	C3C-C4C-NC	5.19	116.39	110.57
20	F	801	BCR	C20-C21-C22	-5.17	119.93	127.31
20	2	503	BCR	C16-C15-C14	5.17	134.06	123.47
20	A	847	BCR	C15-C14-C13	-5.17	119.94	127.31
25	3	315	CHL	CHD-C4C-C3C	-5.16	117.26	124.84
25	1	514	CHL	O2D-CGD-CBD	5.14	120.41	111.27
20	5	302	BCR	C33-C5-C6	-5.14	118.76	124.53
25	1	517	CHL	C3C-C4C-NC	5.11	116.30	110.57
25	1	514	CHL	C4A-NA-C1A	5.06	108.98	106.71
25	2	513	CHL	O2D-CGD-CBD	5.06	119.93	111.49
20	A	845	BCR	C33-C5-C6	-5.05	118.85	124.53
20	A	845	BCR	C20-C21-C22	-5.02	120.14	127.31
20	A	846	BCR	C16-C17-C18	-5.00	120.17	127.31
25	2	513	CHL	C3C-C4C-NC	5.00	116.18	110.57
18	B	843	PQN	C11-C12-C13	-4.96	118.53	126.79
20	I	101	BCR	C20-C21-C22	-4.92	120.29	127.31
25	5	314	CHL	O2D-CGD-CBD	4.91	120.00	111.27
20	B	847	BCR	C7-C8-C9	-4.91	118.82	126.23
24	3	304	LUT	C35-C34-C33	-4.90	120.32	127.31
25	3	315	CHL	C3D-C2D-C1D	-4.90	99.15	105.83
25	5	317	CHL	C3C-C4C-NC	4.88	115.90	110.57
19	A	843	LHG	O7-C7-C8	4.85	121.96	111.50
23	2	519	LMG	O7-C10-C11	4.85	121.95	111.50
20	L	306	BCR	C15-C14-C13	-4.82	120.43	127.31
25	1	517	CHL	C3D-C2D-C1D	-4.82	99.26	105.83
17	5	308	CLA	CMB-C2B-C1B	-4.80	121.08	128.46
24	2	501	LUT	C7-C8-C9	-4.78	119.01	126.23
20	A	846	BCR	C11-C10-C9	-4.77	120.50	127.31
20	B	847	BCR	C15-C16-C17	-4.76	113.72	123.47
26	2	502	XAT	O24-C25-C24	4.76	116.96	113.38
24	1	501	LUT	C18-C5-C6	-4.76	119.19	124.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	2	512	CHL	O2D-CGD-CBD	4.75	119.70	111.27
20	B	849	BCR	C24-C23-C22	-4.74	119.07	126.23
25	5	314	CHL	C3D-C2D-C1D	-4.74	99.37	105.83
20	5	302	BCR	C7-C8-C9	-4.74	119.08	126.23
25	5	317	CHL	O2D-CGD-CBD	4.73	119.67	111.27
17	A	837	CLA	CMB-C2B-C1B	-4.71	121.23	128.46
25	1	512	CHL	O2D-CGD-CBD	4.69	119.61	111.27
20	A	846	BCR	C24-C23-C22	-4.67	119.17	126.23
25	5	314	CHL	C3C-C4C-NC	4.66	115.80	110.57
20	J	102	BCR	C16-C17-C18	-4.66	120.66	127.31
20	A	851	BCR	C28-C27-C26	-4.66	105.76	114.08
24	2	501	LUT	C15-C14-C13	-4.65	120.68	127.31
25	2	512	CHL	C3D-C2D-C1D	-4.63	99.51	105.83
20	K	204	BCR	C28-C27-C26	-4.61	105.84	114.08
17	A	829	CLA	CMB-C2B-C1B	-4.60	121.40	128.46
25	5	315	CHL	O2D-CGD-CBD	4.60	119.44	111.27
25	2	516	CHL	C3D-C2D-C1D	-4.59	99.57	105.83
20	3	305	BCR	C24-C23-C22	-4.58	119.31	126.23
20	B	845	BCR	C15-C14-C13	-4.58	120.77	127.31
25	1	512	CHL	C3C-C4C-NC	4.58	115.71	110.57
17	1	508	CLA	CMB-C2B-C1B	-4.58	121.43	128.46
25	3	315	CHL	C2D-C1D-ND	4.58	113.48	110.10
17	5	309	CLA	CMB-C2B-C1B	-4.56	121.46	128.46
20	A	848	BCR	C20-C21-C22	-4.55	120.81	127.31
17	B	827	CLA	CMB-C2B-C1B	-4.55	121.47	128.46
17	A	821	CLA	CMB-C2B-C1B	-4.55	121.47	128.46
25	5	315	CHL	C3D-C2D-C1D	-4.54	99.64	105.83
17	A	820	CLA	CMB-C2B-C1B	-4.53	121.50	128.46
26	5	304	XAT	C26-C27-C28	-4.53	116.41	125.99
17	B	825	CLA	CMB-C2B-C1B	-4.53	121.50	128.46
20	B	846	BCR	C16-C17-C18	-4.52	120.85	127.31
20	A	851	BCR	C38-C26-C25	-4.51	119.46	124.53
17	A	812	CLA	CMB-C2B-C1B	-4.50	121.55	128.46
25	3	302	CHL	C3D-C2D-C1D	-4.50	99.69	105.83
20	B	848	BCR	C15-C14-C13	-4.49	120.90	127.31
20	L	305	BCR	C11-C10-C9	-4.49	120.91	127.31
20	F	804	BCR	C15-C14-C13	-4.48	120.92	127.31
25	5	317	CHL	C3D-C2D-C1D	-4.47	99.73	105.83
20	B	849	BCR	C16-C17-C18	-4.47	120.93	127.31
17	A	805	CLA	CAA-C2A-C3A	-4.46	100.58	112.78
17	A	810	CLA	CMB-C2B-C1B	-4.45	121.62	128.46
20	A	849	BCR	C20-C21-C22	-4.45	120.96	127.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	1	512	CHL	C3D-C2D-C1D	-4.44	99.77	105.83
20	B	848	BCR	C24-C23-C22	-4.44	119.53	126.23
17	A	827	CLA	CMB-C2B-C1B	-4.43	121.65	128.46
17	2	510	CLA	CMB-C2B-C1B	-4.43	121.66	128.46
20	J	102	BCR	C3-C4-C5	-4.42	106.18	114.08
20	A	851	BCR	C3-C4-C5	-4.42	106.18	114.08
20	K	204	BCR	C20-C21-C22	-4.42	121.00	127.31
20	B	847	BCR	C11-C10-C9	-4.41	121.01	127.31
25	5	315	CHL	C3C-C4C-NC	4.40	115.51	110.57
25	1	517	CHL	C1D-ND-C4D	-4.39	103.22	106.33
20	A	845	BCR	C38-C26-C25	-4.39	119.60	124.53
25	2	516	CHL	O2D-CGD-CBD	4.38	119.05	111.27
20	B	848	BCR	C38-C26-C25	-4.38	119.61	124.53
25	1	517	CHL	CHD-C4C-C3C	-4.37	118.42	124.84
17	L	304	CLA	CAC-C3C-C4C	4.37	130.48	124.81
20	A	848	BCR	C15-C14-C13	-4.36	121.08	127.31
17	A	838	CLA	CMB-C2B-C1B	-4.36	121.76	128.46
17	L	301	CLA	CMB-C2B-C1B	-4.36	121.76	128.46
25	2	516	CHL	CHD-C4C-C3C	-4.36	118.43	124.84
23	5	301	LMG	O7-C10-C11	4.36	120.89	111.50
17	3	316	CLA	CMB-C2B-C1B	-4.36	121.77	128.46
19	B	851	LHG	O7-C7-C8	4.35	120.88	111.50
25	2	513	CHL	C1D-C2D-C3D	-4.35	100.59	106.94
20	2	503	BCR	C33-C5-C6	-4.34	119.65	124.53
17	B	833	CLA	CMB-C2B-C1B	-4.34	121.80	128.46
24	1	501	LUT	C35-C34-C33	-4.33	121.14	127.31
20	K	204	BCR	C38-C26-C25	-4.32	119.67	124.53
17	A	802	CLA	CMB-C2B-C1B	-4.32	121.82	128.46
20	B	845	BCR	C30-C25-C26	-4.32	116.53	122.61
20	A	846	BCR	C15-C14-C13	-4.30	121.17	127.31
17	A	818	CLA	CMB-C2B-C1B	-4.30	121.86	128.46
20	I	101	BCR	C7-C8-C9	-4.30	119.74	126.23
16	A	801	CL0	CHD-C1D-ND	-4.29	120.51	124.45
20	J	102	BCR	C15-C14-C13	-4.29	121.19	127.31
17	A	817	CLA	CAA-C2A-C3A	-4.28	106.11	116.10
17	B	826	CLA	CMB-C2B-C1B	-4.28	121.89	128.46
17	B	801	CLA	CMB-C2B-C1B	-4.28	121.89	128.46
17	B	820	CLA	CMB-C2B-C1B	-4.27	121.90	128.46
17	1	509	CLA	CMB-C2B-C1B	-4.27	121.91	128.46
25	1	514	CHL	C3D-C2D-C1D	-4.25	100.03	105.83
25	2	515	CHL	C3C-C4C-NC	4.24	115.32	110.57
24	2	501	LUT	C11-C10-C9	-4.24	121.27	127.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	3	305	BCR	C38-C26-C25	-4.23	119.78	124.53
17	L	304	CLA	CMB-C2B-C1B	-4.21	121.99	128.46
17	5	310	CLA	CMB-C2B-C1B	-4.21	121.99	128.46
20	B	845	BCR	C33-C5-C6	-4.21	119.80	124.53
22	B	850	DGD	O2G-C1B-C2B	4.21	120.57	111.50
24	5	303	LUT	C18-C5-C6	-4.20	119.81	124.53
20	1	503	BCR	C33-C5-C6	-4.20	119.81	124.53
20	L	306	BCR	C24-C23-C22	-4.19	119.90	126.23
17	B	818	CLA	CMB-C2B-C1B	-4.17	122.06	128.46
17	A	829	CLA	O2D-CGD-O1D	-4.16	115.70	123.84
17	5	316	CLA	CMB-C2B-C1B	-4.16	122.08	128.46
20	A	853	BCR	C16-C17-C18	-4.15	121.39	127.31
17	L	303	CLA	CMB-C2B-C1B	-4.15	122.08	128.46
25	2	515	CHL	C3D-C2D-C1D	-4.15	100.17	105.83
17	2	507	CLA	C5-C3-C2	-4.14	110.69	122.80
25	1	517	CHL	C2D-C1D-ND	4.14	113.15	110.10
17	B	822	CLA	CMB-C2B-C1B	-4.13	122.12	128.46
25	1	512	CHL	CAC-C3C-C4C	4.13	130.16	124.81
17	1	504	CLA	CMB-C2B-C1B	-4.12	122.13	128.46
17	B	811	CLA	CMB-C2B-C1B	-4.12	122.14	128.46
17	5	308	CLA	CMB-C2B-C3B	4.11	132.36	124.68
26	2	502	XAT	C26-C27-C28	-4.10	117.31	125.99
20	B	852	BCR	C33-C5-C6	-4.10	119.92	124.53
17	B	806	CLA	CMB-C2B-C1B	-4.09	122.17	128.46
25	5	315	CHL	CAC-C3C-C4C	4.09	130.11	124.81
19	1	516	LHG	O7-C7-C8	4.08	120.30	111.50
26	2	502	XAT	C31-C30-C29	-4.08	121.49	127.31
17	1	515	CLA	CMB-C2B-C1B	-4.07	122.21	128.46
20	A	851	BCR	C16-C17-C18	-4.07	121.50	127.31
17	A	808	CLA	CMB-C2B-C1B	-4.07	122.21	128.46
20	L	305	BCR	C7-C8-C9	-4.07	120.08	126.23
17	A	816	CLA	CMB-C2B-C1B	-4.07	122.21	128.46
25	3	302	CHL	CAC-C3C-C4C	4.07	130.09	124.81
24	2	501	LUT	C35-C34-C33	-4.07	121.50	127.31
20	A	845	BCR	C24-C23-C22	-4.07	120.09	126.23
17	B	807	CLA	CMB-C2B-C1B	-4.06	122.23	128.46
17	B	837	CLA	CMB-C2B-C1B	-4.05	122.24	128.46
17	B	839	CLA	CMB-C2B-C1B	-4.05	122.25	128.46
23	F	805	LMG	O7-C10-C11	4.04	120.22	111.50
24	5	303	LUT	C15-C14-C13	-4.04	121.54	127.31
17	L	302	CLA	CMB-C2B-C1B	-4.03	122.27	128.46
17	A	823	CLA	CMB-C2B-C1B	-4.03	122.27	128.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	B	802	CLA	CMB-C2B-C1B	-4.02	122.28	128.46
20	3	305	BCR	C11-C10-C9	-4.02	121.57	127.31
25	5	314	CHL	CHD-C4C-C3C	-4.02	118.93	124.84
17	A	836	CLA	O2D-CGD-O1D	-4.02	115.98	123.84
20	A	853	BCR	C20-C21-C22	-4.02	121.58	127.31
20	2	503	BCR	C30-C25-C26	-4.01	116.97	122.61
17	B	838	CLA	CMB-C2B-C1B	-4.01	122.31	128.46
25	3	302	CHL	CHD-C4C-C3C	-4.00	118.96	124.84
25	2	512	CHL	CHD-C4C-C3C	-4.00	118.96	124.84
25	3	315	CHL	C1D-ND-C4D	-4.00	103.49	106.33
25	1	517	CHL	C3B-C4B-NB	4.00	114.38	109.21
20	B	852	BCR	C38-C26-C25	-4.00	120.04	124.53
20	B	844	BCR	C3-C4-C5	-3.99	106.95	114.08
19	A	844	LHG	O7-C7-C8	3.99	120.10	111.50
17	5	311	CLA	CMB-C2B-C1B	-3.99	122.33	128.46
20	F	801	BCR	C16-C17-C18	-3.99	121.62	127.31
19	2	517	LHG	O7-C7-C8	3.97	120.06	111.50
17	B	840	CLA	CMB-C2B-C1B	-3.97	122.36	128.46
17	A	815	CLA	CMB-C2B-C1B	-3.97	122.37	128.46
17	A	806	CLA	CMB-C2B-C1B	-3.95	122.39	128.46
17	A	825	CLA	CMB-C2B-C1B	-3.95	122.40	128.46
17	2	508	CLA	CMB-C2B-C1B	-3.94	122.40	128.46
17	K	205	CLA	CMB-C2B-C1B	-3.94	122.41	128.46
17	A	811	CLA	CMB-C2B-C1B	-3.93	122.43	128.46
17	K	203	CLA	CMB-C2B-C1B	-3.92	122.44	128.46
20	A	846	BCR	C20-C21-C22	-3.92	121.72	127.31
20	2	503	BCR	C23-C22-C21	3.91	124.94	118.94
17	A	837	CLA	CMB-C2B-C3B	3.91	131.99	124.68
17	B	831	CLA	CMB-C2B-C1B	-3.90	122.47	128.46
17	A	827	CLA	CMB-C2B-C3B	3.90	131.98	124.68
17	B	842	CLA	CMB-C2B-C1B	-3.90	122.47	128.46
20	I	101	BCR	C15-C14-C13	-3.90	121.75	127.31
20	5	302	BCR	C15-C14-C13	-3.88	121.77	127.31
20	5	302	BCR	C34-C9-C10	-3.88	117.49	122.92
20	A	849	BCR	C24-C23-C22	-3.88	120.37	126.23
17	A	833	CLA	O2D-CGD-O1D	-3.88	116.25	123.84
20	L	306	BCR	C1-C6-C5	-3.87	117.16	122.61
25	5	315	CHL	C3B-C4B-NB	3.87	114.21	109.21
17	2	506	CLA	CMB-C2B-C1B	-3.87	122.52	128.46
24	3	304	LUT	C21-C26-C27	-3.87	107.81	112.70
17	A	813	CLA	CMB-C2B-C1B	-3.86	122.53	128.46
17	3	306	CLA	CAB-C3B-C4B	-3.85	122.54	128.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	849	BCR	C3-C4-C5	-3.85	107.20	114.08
17	A	826	CLA	CMB-C2B-C1B	-3.85	122.55	128.46
17	B	805	CLA	CMB-C2B-C1B	-3.85	122.55	128.46
25	5	314	CHL	C2D-C1D-ND	3.84	112.93	110.10
20	B	852	BCR	C28-C27-C26	-3.83	107.23	114.08
17	B	830	CLA	CMB-C2B-C1B	-3.83	122.58	128.46
20	K	204	BCR	C33-C5-C6	-3.83	120.23	124.53
17	A	832	CLA	CMB-C2B-C1B	-3.82	122.59	128.46
25	2	513	CHL	CBD-CHA-C1A	3.82	132.10	128.06
17	B	813	CLA	CMB-C2B-C1B	-3.82	122.60	128.46
17	B	829	CLA	CMB-C2B-C1B	-3.81	122.61	128.46
25	2	512	CHL	CAC-C3C-C4C	3.81	129.75	124.81
25	2	516	CHL	C1D-ND-C4D	-3.81	103.63	106.33
20	F	804	BCR	C7-C8-C9	-3.80	120.50	126.23
20	A	853	BCR	C27-C26-C25	-3.79	117.22	122.73
17	1	510	CLA	CMB-C2B-C1B	-3.79	122.64	128.46
20	B	848	BCR	C15-C16-C17	-3.79	115.71	123.47
17	B	816	CLA	CMB-C2B-C1B	-3.79	122.64	128.46
20	L	305	BCR	C38-C26-C25	-3.79	120.27	124.53
17	A	804	CLA	CMB-C2B-C1B	-3.78	122.65	128.46
17	B	828	CLA	O2D-CGD-O1D	-3.78	116.45	123.84
20	A	853	BCR	C15-C14-C13	-3.78	121.92	127.31
17	3	311	CLA	CMB-C2B-C1B	-3.77	122.66	128.46
17	A	819	CLA	CMB-C2B-C1B	-3.76	122.68	128.46
17	2	504	CLA	CBD-CHA-C1A	3.76	132.04	128.06
17	3	318	CLA	CAB-C3B-C4B	-3.76	122.69	128.46
24	3	303	LUT	C31-C30-C29	-3.75	121.95	127.31
25	2	513	CHL	CAC-C3C-C4C	3.75	129.68	124.81
20	B	847	BCR	C33-C5-C6	-3.75	120.32	124.53
20	A	851	BCR	C33-C5-C6	-3.75	120.32	124.53
17	2	505	CLA	CMB-C2B-C1B	-3.75	122.71	128.46
17	A	819	CLA	O2D-CGD-O1D	-3.75	116.51	123.84
25	2	512	CHL	C2D-C1D-ND	3.74	112.86	110.10
22	J	103	DGD	O2G-C1B-C2B	3.74	119.57	111.50
17	1	508	CLA	CMB-C2B-C3B	3.74	131.68	124.68
20	I	101	BCR	C16-C17-C18	-3.74	121.97	127.31
20	A	845	BCR	C28-C27-C26	-3.74	107.40	114.08
17	A	836	CLA	CMB-C2B-C1B	-3.74	122.72	128.46
20	L	305	BCR	C3-C4-C5	-3.73	107.42	114.08
22	B	850	DGD	C4D-C3D-C2D	-3.73	104.31	110.82
25	2	513	CHL	CHD-C4C-C3C	-3.73	119.36	124.84
20	F	804	BCR	C28-C27-C26	-3.71	107.44	114.08

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	1	509	CLA	CMB-C2B-C3B	3.71	131.62	124.68
20	B	848	BCR	C7-C8-C9	-3.71	120.62	126.23
18	A	841	PQN	C11-C12-C13	-3.71	120.62	126.79
20	A	847	BCR	C16-C17-C18	-3.71	122.02	127.31
17	B	825	CLA	CMB-C2B-C3B	3.71	131.61	124.68
17	B	810	CLA	CMB-C2B-C1B	-3.70	122.77	128.46
25	1	517	CHL	C3D-C4D-ND	3.70	116.23	110.24
17	A	835	CLA	CMB-C2B-C1B	-3.70	122.77	128.46
20	J	102	BCR	C20-C21-C22	-3.70	122.03	127.31
17	B	827	CLA	CMB-C2B-C3B	3.70	131.60	124.68
17	B	823	CLA	CMB-C2B-C1B	-3.69	122.79	128.46
17	B	826	CLA	CMB-C2B-C3B	3.69	131.58	124.68
26	2	502	XAT	C35-C34-C33	-3.69	122.05	127.31
17	5	305	CLA	CBD-CHA-C1A	3.69	132.85	128.50
17	A	805	CLA	CMB-C2B-C1B	-3.68	122.80	128.46
25	5	314	CHL	C3B-C4B-NB	3.68	113.97	109.21
17	A	822	CLA	CMB-C2B-C1B	-3.68	122.81	128.46
25	2	512	CHL	C1D-ND-C4D	-3.68	103.72	106.33
20	B	849	BCR	C33-C5-C6	-3.67	120.41	124.53
17	J	101	CLA	CMB-C2B-C1B	-3.67	122.83	128.46
18	B	843	PQN	C2M-C2-C3	-3.67	118.42	124.40
17	1	513	CLA	CMB-C2B-C1B	-3.67	122.83	128.46
17	B	819	CLA	CMB-C2B-C1B	-3.66	122.83	128.46
26	2	502	XAT	C8-C9-C10	3.66	124.56	118.94
17	K	202	CLA	O2D-CGD-O1D	-3.66	116.68	123.84
17	1	506	CLA	CMB-C2B-C1B	-3.66	122.84	128.46
25	3	302	CHL	C1B-CHB-C4A	-3.66	122.87	130.12
16	A	801	CL0	C1-C2-C3	-3.65	119.73	126.04
25	2	516	CHL	C3D-C4D-ND	3.65	116.14	110.24
26	2	502	XAT	C24-C23-C22	-3.64	103.73	110.77
17	F	802	CLA	CMB-C2B-C1B	-3.64	122.86	128.46
20	A	848	BCR	C38-C26-C25	-3.64	120.44	124.53
17	3	314	CLA	O2D-CGD-O1D	-3.63	116.73	123.84
17	A	824	CLA	CMB-C2B-C1B	-3.63	122.88	128.46
20	2	503	BCR	C29-C30-C25	3.63	116.07	110.48
17	A	820	CLA	CMB-C2B-C3B	3.63	131.47	124.68
17	3	312	CLA	CMB-C2B-C1B	-3.63	122.89	128.46
17	A	812	CLA	CMB-C2B-C3B	3.63	131.47	124.68
17	B	832	CLA	CMB-C2B-C1B	-3.62	122.89	128.46
20	A	853	BCR	C2-C1-C6	3.62	116.06	110.48
17	A	838	CLA	CMB-C2B-C3B	3.62	131.46	124.68
20	3	305	BCR	C33-C5-C6	-3.62	120.46	124.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	A	838	CLA	O2D-CGD-O1D	-3.62	116.76	123.84
20	2	503	BCR	C37-C22-C21	-3.62	117.86	122.92
25	1	512	CHL	C1B-CHB-C4A	-3.61	122.96	130.12
17	A	837	CLA	CAA-C2A-C3A	-3.61	107.68	116.10
17	A	830	CLA	CMB-C2B-C1B	-3.61	122.92	128.46
17	A	834	CLA	CMB-C2B-C1B	-3.61	122.92	128.46
20	1	503	BCR	C7-C8-C9	-3.60	120.79	126.23
20	A	847	BCR	C8-C7-C6	-3.60	117.09	127.20
17	A	833	CLA	CMB-C2B-C1B	-3.60	122.93	128.46
25	5	317	CHL	CHD-C4C-C3C	-3.60	119.36	124.98
17	K	202	CLA	CAA-C2A-C3A	-3.59	107.72	116.10
17	2	507	CLA	CMB-C2B-C1B	-3.59	122.95	128.46
17	3	314	CLA	CMB-C2B-C1B	-3.59	122.95	128.46
17	B	806	CLA	CMB-C2B-C3B	3.59	131.39	124.68
17	B	828	CLA	CMB-C2B-C1B	-3.58	122.95	128.46
25	2	516	CHL	C2D-C1D-ND	3.58	112.75	110.10
20	B	848	BCR	C33-C5-C6	-3.58	120.50	124.53
20	5	302	BCR	C38-C26-C25	-3.58	120.51	124.53
17	B	822	CLA	O2D-CGD-O1D	-3.57	116.85	123.84
20	I	101	BCR	C11-C10-C9	-3.57	122.21	127.31
17	A	831	CLA	CMB-C2B-C1B	-3.57	122.97	128.46
17	2	509	CLA	CMB-C2B-C1B	-3.57	122.98	128.46
20	A	845	BCR	C30-C25-C26	-3.57	117.59	122.61
17	B	801	CLA	CMB-C2B-C3B	3.57	131.35	124.68
17	L	304	CLA	O2D-CGD-O1D	-3.56	116.87	123.84
20	B	847	BCR	C38-C26-C25	-3.56	120.53	124.53
17	A	803	CLA	CMB-C2B-C1B	-3.56	122.99	128.46
17	3	317	CLA	CMB-C2B-C1B	-3.56	122.99	128.46
17	B	818	CLA	CMB-C2B-C3B	3.56	131.34	124.68
20	B	845	BCR	C28-C27-C26	-3.56	107.73	114.08
26	5	304	XAT	C10-C11-C12	-3.56	112.12	123.22
16	A	801	CL0	CAB-C3B-C4B	-3.55	123.00	128.46
17	A	839	CLA	O2D-CGD-O1D	-3.55	116.89	123.84
17	5	309	CLA	CMB-C2B-C3B	3.55	131.31	124.68
17	A	814	CLA	O2D-CGD-O1D	-3.55	116.90	123.84
17	1	507	CLA	CMB-C2B-C1B	-3.54	123.02	128.46
23	F	806	LMG	O7-C10-C11	3.54	119.14	111.50
20	2	503	BCR	C39-C30-C29	3.54	123.08	108.91
17	3	306	CLA	C1-C2-C3	-3.54	119.92	126.04
17	3	301	CLA	CMB-C2B-C1B	-3.54	123.03	128.46
20	A	847	BCR	C33-C5-C4	3.54	120.41	113.62
17	5	306	CLA	CMB-C2B-C1B	-3.53	123.03	128.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	L	303	CLA	O2D-CGD-O1D	-3.53	116.93	123.84
20	L	305	BCR	C15-C14-C13	-3.53	122.27	127.31
25	3	315	CHL	C3D-C4D-ND	3.53	115.94	110.24
17	A	816	CLA	CMB-C2B-C3B	3.52	131.27	124.68
20	A	848	BCR	C33-C5-C6	-3.52	120.57	124.53
17	B	819	CLA	CAA-C2A-C3A	-3.52	107.89	116.10
25	2	515	CHL	CHD-C4C-C3C	-3.52	119.67	124.84
20	B	847	BCR	C3-C4-C5	-3.52	107.80	114.08
17	B	814	CLA	CMB-C2B-C1B	-3.51	123.07	128.46
25	5	317	CHL	C1B-CHB-C4A	-3.51	123.17	130.12
17	A	830	CLA	O2D-CGD-O1D	-3.51	116.98	123.84
17	B	815	CLA	O2D-CGD-O1D	-3.51	116.98	123.84
25	5	314	CHL	C1D-ND-C4D	-3.51	103.84	106.33
20	B	846	BCR	C8-C9-C10	3.50	124.32	118.94
20	2	503	BCR	C12-C13-C14	-3.50	113.57	118.94
17	B	817	CLA	CMB-C2B-C1B	-3.50	123.08	128.46
24	1	502	LUT	C3-C4-C5	-3.50	104.88	111.85
17	B	833	CLA	CMB-C2B-C3B	3.49	131.22	124.68
17	A	803	CLA	O2D-CGD-O1D	-3.49	117.01	123.84
25	5	315	CHL	CMD-C2D-C3D	-3.49	119.58	127.61
17	B	826	CLA	O2D-CGD-O1D	-3.49	117.01	123.84
17	B	802	CLA	CMB-C2B-C3B	3.49	131.21	124.68
20	5	302	BCR	C16-C17-C18	-3.49	122.33	127.31
17	L	301	CLA	CMB-C2B-C3B	3.49	131.21	124.68
20	L	306	BCR	C28-C27-C26	-3.49	107.85	114.08
17	B	836	CLA	CMB-C2B-C1B	-3.49	123.10	128.46
17	A	835	CLA	O2D-CGD-O1D	-3.49	117.02	123.84
22	J	103	DGD	C1E-O6E-C5E	3.48	120.53	113.69
17	2	510	CLA	CMB-C2B-C3B	3.48	131.19	124.68
17	A	802	CLA	CMB-C2B-C3B	3.48	131.18	124.68
20	A	845	BCR	C38-C26-C27	3.47	120.29	113.62
17	A	839	CLA	CMB-C2B-C1B	-3.47	123.12	128.46
17	F	803	CLA	CMB-C2B-C1B	-3.47	123.13	128.46
17	1	515	CLA	CMB-C2B-C3B	3.47	131.16	124.68
20	B	844	BCR	C28-C27-C26	-3.47	107.89	114.08
20	J	102	BCR	C24-C23-C22	-3.47	121.00	126.23
20	A	853	BCR	C3-C4-C5	-3.46	107.89	114.08
17	A	818	CLA	O2D-CGD-O1D	-3.46	117.07	123.84
17	L	304	CLA	CMB-C2B-C3B	3.46	131.15	124.68
25	5	314	CHL	C3D-C4D-ND	3.46	115.83	110.24
17	A	807	CLA	CMB-C2B-C1B	-3.46	123.15	128.46
25	2	512	CHL	C3D-C4D-ND	3.45	115.83	110.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	847	BCR	C12-C13-C14	3.45	124.24	118.94
25	5	314	CHL	CAC-C3C-C4C	3.45	129.29	124.81
17	A	817	CLA	CMB-C2B-C1B	-3.45	123.16	128.46
17	1	504	CLA	CMB-C2B-C3B	3.45	131.13	124.68
17	K	201	CLA	C1B-CHB-C4A	-3.45	123.29	130.12
26	2	502	XAT	C4-C3-C2	-3.45	104.12	110.77
17	5	305	CLA	O2D-CGD-O1D	-3.44	117.11	123.84
22	B	850	DGD	C2G-O2G-C1B	-3.44	109.33	117.79
17	5	310	CLA	CMB-C2B-C3B	3.43	131.10	124.68
25	2	515	CHL	C3D-C4D-ND	3.43	115.79	110.24
20	A	847	BCR	C33-C5-C6	-3.43	120.67	124.53
26	5	304	XAT	C38-C25-C24	3.43	118.14	114.28
26	5	304	XAT	O24-C25-C38	3.43	119.17	115.06
25	3	315	CHL	C3B-C4B-NB	3.43	113.64	109.21
20	K	204	BCR	C3-C4-C5	-3.43	107.96	114.08
19	1	516	LHG	O8-C23-C24	3.42	122.66	111.91
25	1	514	CHL	C3C-C4C-NC	3.42	114.41	110.57
17	A	812	CLA	O2D-CGD-O1D	-3.42	117.15	123.84
17	B	839	CLA	CMB-C2B-C3B	3.42	131.07	124.68
20	2	503	BCR	C38-C26-C25	-3.41	120.70	124.53
25	3	302	CHL	C2D-C1D-ND	3.41	112.61	110.10
17	5	316	CLA	CMB-C2B-C3B	3.41	131.05	124.68
25	5	315	CHL	CHD-C4C-C3C	-3.41	119.83	124.84
20	F	804	BCR	C11-C12-C13	-3.41	116.85	126.42
17	A	823	CLA	CMB-C2B-C3B	3.41	131.05	124.68
20	A	853	BCR	C29-C30-C25	3.41	115.72	110.48
20	2	503	BCR	C7-C8-C9	-3.40	121.09	126.23
17	3	316	CLA	CMB-C2B-C3B	3.40	131.05	124.68
20	B	848	BCR	C3-C4-C5	-3.40	108.00	114.08
17	A	821	CLA	CMB-C2B-C3B	3.40	131.04	124.68
17	A	826	CLA	O2D-CGD-O1D	-3.40	117.19	123.84
17	B	802	CLA	O2D-CGD-O1D	-3.40	117.20	123.84
24	5	303	LUT	C7-C8-C9	-3.40	121.11	126.23
17	A	836	CLA	O2D-CGD-CBD	3.39	117.29	111.27
17	B	816	CLA	CMB-C2B-C3B	3.39	131.02	124.68
20	A	848	BCR	C16-C17-C18	-3.39	122.47	127.31
17	A	804	CLA	CMB-C2B-C3B	3.39	131.02	124.68
17	B	801	CLA	O2D-CGD-O1D	-3.39	117.22	123.84
24	2	501	LUT	C3-C4-C5	-3.39	105.11	111.85
17	B	828	CLA	CMB-C2B-C3B	3.38	131.01	124.68
20	J	102	BCR	C38-C26-C25	-3.38	120.73	124.53
20	B	844	BCR	C11-C12-C13	-3.38	116.92	126.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	B	822	CLA	CMB-C2B-C3B	3.37	130.99	124.68
20	A	847	BCR	C20-C21-C22	-3.37	122.50	127.31
26	5	304	XAT	O4-C5-C18	3.37	119.10	115.06
20	A	849	BCR	C3-C4-C5	-3.37	108.06	114.08
17	A	831	CLA	O2D-CGD-O1D	-3.37	117.25	123.84
17	B	804	CLA	CMB-C2B-C1B	-3.37	123.28	128.46
20	5	302	BCR	C11-C10-C9	-3.37	122.50	127.31
17	A	804	CLA	O2D-CGD-O1D	-3.36	117.26	123.84
17	B	808	CLA	O2D-CGD-O1D	-3.36	117.28	123.84
17	3	310	CLA	CMB-C2B-C1B	-3.35	123.31	128.46
17	1	506	CLA	O2D-CGD-O1D	-3.35	117.28	123.84
17	K	202	CLA	CMB-C2B-C1B	-3.35	123.32	128.46
20	F	801	BCR	C33-C5-C6	-3.35	120.77	124.53
17	5	307	CLA	CMB-C2B-C1B	-3.35	123.32	128.46
17	A	825	CLA	O2D-CGD-O1D	-3.35	117.30	123.84
17	A	842	CLA	CMB-C2B-C1B	-3.34	123.33	128.46
25	2	515	CHL	CAC-C3C-C4C	3.34	129.15	124.81
17	A	813	CLA	CMB-C2B-C3B	3.34	130.93	124.68
25	3	302	CHL	C3B-C4B-NB	3.34	113.53	109.21
17	3	311	CLA	CMB-C2B-C3B	3.34	130.92	124.68
17	A	810	CLA	CMB-C2B-C3B	3.34	130.92	124.68
20	A	851	BCR	C38-C26-C27	3.33	120.02	113.62
20	3	305	BCR	C16-C17-C18	-3.33	122.56	127.31
20	L	306	BCR	C33-C5-C6	-3.33	120.79	124.53
17	A	831	CLA	CAB-C3B-C4B	-3.33	123.35	128.46
17	A	823	CLA	O2D-CGD-O1D	-3.33	117.34	123.84
17	B	815	CLA	CMB-C2B-C1B	-3.33	123.35	128.46
20	A	846	BCR	C33-C5-C6	-3.32	120.80	124.53
17	2	511	CLA	CMB-C2B-C1B	-3.32	123.36	128.46
17	3	313	CLA	CMB-C2B-C1B	-3.32	123.37	128.46
17	B	842	CLA	CMB-C2B-C3B	3.32	130.88	124.68
17	A	828	CLA	CMB-C2B-C1B	-3.32	123.37	128.46
20	J	102	BCR	C38-C26-C27	3.32	119.98	113.62
26	5	304	XAT	C15-C14-C13	-3.31	122.58	127.31
20	B	847	BCR	C23-C24-C25	-3.31	117.90	127.20
25	1	517	CHL	CAC-C3C-C4C	3.31	129.10	124.81
20	A	847	BCR	C3-C4-C5	-3.31	108.17	114.08
17	3	307	CLA	CBD-CHA-C1A	3.31	132.40	128.50
17	A	827	CLA	O2D-CGD-O1D	-3.31	117.38	123.84
20	5	302	BCR	C8-C9-C10	3.30	124.01	118.94
17	B	837	CLA	CMB-C2B-C3B	3.30	130.85	124.68
17	A	829	CLA	CMB-C2B-C3B	3.30	130.85	124.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	5	313	CLA	CMB-C2B-C1B	-3.30	123.39	128.46
20	L	305	BCR	C20-C21-C22	-3.30	122.60	127.31
17	2	504	CLA	CMB-C2B-C1B	-3.30	123.40	128.46
25	1	512	CHL	C3D-C4D-ND	3.30	115.57	110.24
20	B	846	BCR	C34-C9-C10	-3.29	118.31	122.92
17	B	835	CLA	CMB-C2B-C1B	-3.29	123.40	128.46
20	I	101	BCR	C30-C25-C26	-3.29	117.98	122.61
20	L	306	BCR	C33-C5-C4	3.29	119.93	113.62
25	3	315	CHL	C1C-C2C-C3C	-3.29	104.50	107.11
17	A	814	CLA	CMB-C2B-C1B	-3.29	123.41	128.46
17	B	810	CLA	O2D-CGD-O1D	-3.29	117.41	123.84
25	1	512	CHL	CHD-C4C-C3C	-3.29	120.01	124.84
17	L	303	CLA	CMB-C2B-C3B	3.28	130.82	124.68
17	B	827	CLA	O2D-CGD-O1D	-3.28	117.42	123.84
17	A	852	CLA	CMB-C2B-C1B	-3.28	123.42	128.46
17	B	841	CLA	O2D-CGD-O1D	-3.28	117.42	123.84
25	1	514	CHL	CAC-C3C-C4C	3.28	129.07	124.81
17	3	306	CLA	CMB-C2B-C1B	-3.28	123.43	128.46
17	B	807	CLA	CMB-C2B-C3B	3.28	130.81	124.68
17	1	510	CLA	O2D-CGD-O1D	-3.27	117.44	123.84
25	2	516	CHL	CAC-C3C-C4C	3.27	129.06	124.81
17	B	834	CLA	CMB-C2B-C1B	-3.27	123.44	128.46
17	5	312	CLA	CMB-C2B-C1B	-3.27	123.44	128.46
25	1	512	CHL	C3B-C4B-NB	3.27	113.43	109.21
17	B	838	CLA	O2D-CGD-O1D	-3.27	117.45	123.84
20	B	849	BCR	C28-C27-C26	-3.26	108.25	114.08
17	A	811	CLA	O2D-CGD-O1D	-3.26	117.47	123.84
17	B	841	CLA	CMB-C2B-C1B	-3.24	123.48	128.46
19	1	516	LHG	C5-O7-C7	-3.24	109.81	117.79
20	B	845	BCR	C16-C17-C18	-3.24	122.69	127.31
17	K	203	CLA	CMB-C2B-C3B	3.24	130.73	124.68
20	B	846	BCR	C35-C13-C14	-3.23	118.39	122.92
17	2	511	CLA	O2D-CGD-O1D	-3.23	117.52	123.84
20	B	847	BCR	C35-C13-C14	-3.23	118.40	122.92
17	J	101	CLA	O2D-CGD-O1D	-3.23	117.52	123.84
17	A	808	CLA	CMB-C2B-C3B	3.23	130.72	124.68
24	3	304	LUT	C7-C8-C9	-3.22	121.36	126.23
17	B	812	CLA	CMB-C2B-C1B	-3.22	123.51	128.46
17	B	824	CLA	CMB-C2B-C1B	-3.22	123.52	128.46
17	A	837	CLA	O2D-CGD-O1D	-3.22	117.54	123.84
25	5	315	CHL	C3D-C4D-ND	3.22	115.45	110.24
20	B	849	BCR	C37-C22-C21	-3.21	118.42	122.92

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	B	809	CLA	CMB-C2B-C1B	-3.21	123.53	128.46
17	B	803	CLA	O2D-CGD-O1D	-3.21	117.57	123.84
17	B	812	CLA	O2D-CGD-O1D	-3.21	117.57	123.84
17	A	818	CLA	CMB-C2B-C3B	3.20	130.67	124.68
17	B	817	CLA	O2D-CGD-O1D	-3.20	117.58	123.84
17	2	505	CLA	O2D-CGD-O1D	-3.20	117.59	123.84
20	B	852	BCR	C34-C9-C10	-3.19	118.45	122.92
20	F	801	BCR	C20-C19-C18	-3.19	117.45	126.42
17	B	821	CLA	CMB-C2B-C1B	-3.19	123.56	128.46
17	2	509	CLA	CMB-C2B-C3B	3.19	130.65	124.68
25	3	315	CHL	CHB-C4A-NA	3.19	128.92	124.51
25	5	317	CHL	C3D-C4D-ND	3.19	115.40	110.24
25	5	317	CHL	C2D-C1D-ND	3.19	112.45	110.10
17	K	205	CLA	CMB-C2B-C3B	3.18	130.63	124.68
22	B	850	DGD	O1G-C1A-C2A	3.17	121.87	111.91
17	1	511	CLA	CMB-C2B-C1B	-3.17	123.59	128.46
17	B	813	CLA	CMB-C2B-C3B	3.17	130.60	124.68
20	B	849	BCR	C10-C11-C12	-3.16	113.35	123.22
24	3	303	LUT	C22-C23-C24	3.16	115.34	111.74
17	B	811	CLA	CMB-C2B-C3B	3.15	130.58	124.68
17	2	514	CLA	CMB-C2B-C1B	-3.15	123.62	128.46
26	2	502	XAT	C19-C9-C10	-3.15	118.51	122.92
24	1	502	LUT	C18-C5-C6	-3.15	120.99	124.53
20	B	852	BCR	C38-C26-C27	3.15	119.66	113.62
25	2	516	CHL	CMD-C2D-C3D	-3.14	120.38	127.61
17	A	842	CLA	O2D-CGD-O1D	-3.14	117.69	123.84
17	B	808	CLA	CMB-C2B-C1B	-3.14	123.64	128.46
17	B	809	CLA	CBD-CHA-C1A	3.14	132.20	128.50
17	K	201	CLA	CMB-C2B-C1B	-3.14	123.64	128.46
20	B	844	BCR	C38-C26-C25	-3.14	121.00	124.53
17	2	508	CLA	CMB-C2B-C3B	3.14	130.55	124.68
17	3	306	CLA	C1C-NC-C4C	3.14	108.12	106.71
20	A	851	BCR	C20-C21-C22	-3.13	122.84	127.31
17	A	806	CLA	CMB-C2B-C3B	3.13	130.54	124.68
17	B	819	CLA	O2D-CGD-O1D	-3.13	117.72	123.84
25	5	317	CHL	C3B-C4B-NB	3.13	113.25	109.21
17	A	832	CLA	CMB-C2B-C3B	3.12	130.52	124.68
20	K	204	BCR	C15-C14-C13	-3.12	122.86	127.31
23	F	805	LMG	O8-C28-C29	3.12	119.56	111.38
17	A	827	CLA	C1-C2-C3	-3.12	120.65	126.04
17	A	817	CLA	CMA-C3A-C2A	-3.11	108.83	116.10
20	L	305	BCR	C38-C26-C27	3.11	119.59	113.62

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	B	832	CLA	O2D-CGD-O1D	-3.11	117.75	123.84
17	A	825	CLA	CMB-C2B-C3B	3.11	130.50	124.68
17	B	810	CLA	C2D-C1D-ND	-3.11	107.81	110.10
20	B	844	BCR	C36-C18-C17	-3.11	118.57	122.92
17	A	807	CLA	CBD-CHA-C1A	3.10	131.34	128.06
20	I	101	BCR	C33-C5-C6	-3.10	121.05	124.53
17	A	813	CLA	O2D-CGD-O1D	-3.10	117.78	123.84
17	A	832	CLA	CBD-CHA-C1A	3.10	132.39	127.43
17	B	818	CLA	O2D-CGD-O1D	-3.10	117.78	123.84
24	2	501	LUT	C18-C5-C6	-3.09	121.05	124.53
20	B	846	BCR	C1-C6-C5	-3.09	118.26	122.61
17	A	822	CLA	O2D-CGD-O1D	-3.09	117.79	123.84
17	2	506	CLA	CMB-C2B-C3B	3.09	130.46	124.68
20	B	846	BCR	C33-C5-C6	-3.09	121.06	124.53
18	A	841	PQN	C2M-C2-C3	-3.09	119.36	124.40
25	5	315	CHL	C1B-CHB-C4A	-3.09	124.00	130.12
20	A	848	BCR	C38-C26-C27	3.09	119.54	113.62
17	B	837	CLA	CAC-C3C-C4C	3.08	128.81	124.81
25	2	515	CHL	CMD-C2D-C3D	-3.08	120.53	127.61
17	B	805	CLA	CMB-C2B-C3B	3.08	130.44	124.68
17	5	311	CLA	CMB-C2B-C3B	3.08	130.44	124.68
20	2	503	BCR	C10-C11-C12	-3.08	113.61	123.22
17	3	317	CLA	CMB-C2B-C3B	3.08	130.44	124.68
17	A	811	CLA	CMB-C2B-C3B	3.07	130.43	124.68
17	J	101	CLA	CMB-C2B-C3B	3.07	130.43	124.68
17	B	814	CLA	O2D-CGD-O1D	-3.07	117.83	123.84
17	B	840	CLA	CAA-C2A-C3A	-3.07	108.94	116.10
17	B	820	CLA	CMB-C2B-C3B	3.07	130.42	124.68
17	B	810	CLA	CMB-C2B-C3B	3.07	130.42	124.68
20	B	847	BCR	C33-C5-C4	3.07	119.51	113.62
17	1	513	CLA	CMB-C2B-C3B	3.07	130.41	124.68
25	1	517	CHL	C2A-C1A-CHA	-3.07	117.96	122.71
25	5	317	CHL	CAC-C3C-C4C	3.06	129.70	125.04
17	B	829	CLA	CMB-C2B-C3B	3.05	130.39	124.68
17	A	803	CLA	CAA-C2A-C3A	-3.05	108.98	116.10
25	2	512	CHL	CMD-C2D-C3D	-3.05	120.60	127.61
25	1	512	CHL	C2D-C1D-ND	3.05	112.35	110.10
20	L	306	BCR	C16-C17-C18	-3.05	122.96	127.31
17	A	806	CLA	C1-C2-C3	-3.05	120.77	126.04
17	1	513	CLA	O2D-CGD-O1D	-3.05	117.88	123.84
17	3	301	CLA	CAA-C2A-C3A	-3.04	108.99	116.10
17	B	805	CLA	CAA-C2A-C3A	-3.04	109.00	116.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	B	842	CLA	O2D-CGD-O1D	-3.04	117.89	123.84
20	B	846	BCR	C3-C4-C5	-3.04	108.65	114.08
20	L	305	BCR	C36-C18-C17	-3.04	118.67	122.92
17	A	805	CLA	CMB-C2B-C3B	3.04	130.36	124.68
17	L	303	CLA	CHB-C4A-NA	3.04	128.71	124.51
17	A	826	CLA	CMB-C2B-C3B	3.04	130.36	124.68
20	2	503	BCR	C21-C20-C19	3.04	132.69	123.22
17	2	504	CLA	C3A-C4A-CHB	-3.04	120.19	123.91
17	B	840	CLA	CMB-C2B-C3B	3.04	130.36	124.68
17	B	832	CLA	CMB-C2B-C3B	3.03	130.35	124.68
17	3	316	CLA	CAA-C2A-C3A	-3.03	109.02	116.10
20	B	846	BCR	C33-C5-C4	3.03	119.44	113.62
17	B	823	CLA	CMB-C2B-C3B	3.03	130.35	124.68
20	B	852	BCR	C3-C4-C5	-3.03	108.66	114.08
17	A	826	CLA	C1-C2-C3	-3.03	120.80	126.04
17	3	306	CLA	CMB-C2B-C3B	3.03	130.62	124.69
18	B	843	PQN	C2M-C2-C1	3.03	121.28	116.27
17	A	832	CLA	CHB-C4A-NA	3.02	128.69	124.51
20	A	846	BCR	C7-C8-C9	-3.02	121.67	126.23
25	3	302	CHL	C3D-C4D-ND	3.02	115.13	110.24
19	A	843	LHG	O8-C23-C24	3.02	121.39	111.91
17	B	838	CLA	CMB-C2B-C3B	3.02	130.33	124.68
17	1	507	CLA	CMB-C2B-C3B	3.02	130.32	124.68
24	3	303	LUT	C10-C11-C12	-3.01	113.81	123.22
17	B	830	CLA	O2D-CGD-O1D	-3.01	117.94	123.84
17	3	311	CLA	C1-C2-C3	-3.01	121.88	126.75
20	A	845	BCR	C11-C10-C9	-3.01	123.01	127.31
17	B	839	CLA	O2D-CGD-O1D	-3.01	117.95	123.84
20	A	851	BCR	C2-C1-C6	3.01	115.11	110.48
17	1	508	CLA	CBD-CHA-C1A	2.99	132.03	128.50
20	3	305	BCR	C3-C4-C5	-2.99	108.73	114.08
17	L	301	CLA	O2D-CGD-O1D	-2.99	117.99	123.84
17	B	804	CLA	CMB-C2B-C3B	2.99	130.27	124.68
25	3	302	CHL	O2D-CGD-O1D	-2.99	117.99	123.84
17	3	308	CLA	CMB-C2B-C1B	-2.99	123.87	128.46
20	B	849	BCR	C15-C14-C13	-2.98	123.05	127.31
17	A	822	CLA	CAA-C2A-C3A	-2.98	109.13	116.10
17	B	812	CLA	CAB-C3B-C4B	-2.98	123.88	128.46
17	3	317	CLA	O2D-CGD-O1D	-2.98	118.01	123.84
17	A	835	CLA	CMB-C2B-C3B	2.98	130.25	124.68
19	2	517	LHG	O8-C23-C24	2.98	121.25	111.91
20	A	853	BCR	C38-C26-C27	2.98	119.33	113.62

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	B	827	CLA	CAA-C2A-C3A	-2.97	109.16	116.10
20	5	302	BCR	C35-C13-C12	2.97	122.76	118.08
17	B	804	CLA	O2D-CGD-O1D	-2.97	118.03	123.84
17	B	833	CLA	O2D-CGD-O1D	-2.97	118.03	123.84
26	5	304	XAT	C18-C5-C4	2.97	117.62	114.28
17	1	511	CLA	C1B-CHB-C4A	-2.96	124.25	130.12
17	K	201	CLA	CHB-C4A-NA	2.96	128.61	124.51
17	B	809	CLA	O2D-CGD-O1D	-2.96	118.05	123.84
20	J	102	BCR	C33-C5-C6	-2.96	121.20	124.53
17	A	815	CLA	CMB-C2B-C3B	2.96	130.21	124.68
23	2	519	LMG	C7-O1-C1	-2.96	107.96	113.74
20	K	204	BCR	C38-C26-C27	2.96	119.29	113.62
17	B	807	CLA	O2D-CGD-O1D	-2.95	118.06	123.84
25	2	516	CHL	C2A-C1A-CHA	-2.95	118.70	123.86
17	3	312	CLA	CMB-C2B-C3B	2.95	130.20	124.68
20	A	849	BCR	C34-C9-C10	-2.95	118.79	122.92
20	B	852	BCR	C16-C17-C18	-2.95	123.11	127.31
17	B	819	CLA	CMB-C2B-C3B	2.95	130.19	124.68
20	B	848	BCR	C20-C21-C22	-2.94	123.11	127.31
17	B	813	CLA	O2D-CGD-O1D	-2.94	118.08	123.84
17	K	201	CLA	CMB-C2B-C3B	2.94	130.18	124.68
20	B	844	BCR	C33-C5-C6	-2.94	121.23	124.53
20	A	847	BCR	C38-C26-C25	-2.93	121.24	124.53
25	1	512	CHL	CMD-C2D-C3D	-2.93	120.87	127.61
25	2	516	CHL	CMB-C2B-C3B	2.93	130.43	124.69
20	5	302	BCR	C35-C13-C14	-2.93	118.82	122.92
17	B	833	CLA	C1-C2-C3	-2.93	120.98	126.04
26	5	304	XAT	C6-C7-C8	-2.93	119.80	125.99
20	B	848	BCR	C33-C5-C4	2.93	119.24	113.62
17	2	511	CLA	CHB-C4A-NA	2.93	128.56	124.51
24	3	303	LUT	C18-C5-C6	-2.93	121.24	124.53
17	A	803	CLA	CMB-C2B-C3B	2.93	130.15	124.68
17	5	313	CLA	O2D-CGD-O1D	-2.92	118.12	123.84
17	A	833	CLA	CMB-C2B-C3B	2.92	130.14	124.68
20	B	848	BCR	C11-C10-C9	-2.92	123.14	127.31
17	A	820	CLA	O2D-CGD-O1D	-2.92	118.13	123.84
17	B	836	CLA	O2D-CGD-O1D	-2.92	118.13	123.84
17	B	802	CLA	O2D-CGD-CBD	2.92	116.45	111.27
20	A	853	BCR	C35-C13-C14	-2.92	118.84	122.92
26	5	304	XAT	C24-C23-C22	-2.91	105.15	110.77
20	B	845	BCR	C8-C9-C10	2.91	123.41	118.94
17	A	820	CLA	CHD-C1D-ND	-2.91	121.78	124.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	B	811	CLA	CAA-C2A-C3A	-2.91	104.80	112.78
17	3	318	CLA	O2D-CGD-O1D	-2.91	118.14	123.84
19	A	843	LHG	C5-O7-C7	-2.91	110.63	117.79
25	5	315	CHL	C1D-ND-C4D	-2.91	104.27	106.33
17	K	202	CLA	CMB-C2B-C3B	2.91	130.12	124.68
17	B	831	CLA	CMB-C2B-C3B	2.91	130.12	124.68
25	5	315	CHL	C2D-C1D-ND	2.91	112.25	110.10
17	B	815	CLA	CMB-C2B-C3B	2.90	130.11	124.68
17	F	802	CLA	CMB-C2B-C3B	2.90	130.11	124.68
17	A	824	CLA	CMB-C2B-C3B	2.90	130.11	124.68
17	L	302	CLA	CMB-C2B-C3B	2.90	130.10	124.68
17	5	310	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
17	3	314	CLA	CMB-C2B-C3B	2.90	130.10	124.68
17	B	835	CLA	O2D-CGD-O1D	-2.90	118.18	123.84
17	B	814	CLA	CMB-C2B-C3B	2.90	130.10	124.68
20	A	846	BCR	C33-C5-C4	2.89	119.18	113.62
25	5	317	CHL	C1C-C2C-C3C	-2.89	104.82	107.11
17	F	802	CLA	O2D-CGD-O1D	-2.89	118.19	123.84
24	5	303	LUT	C16-C1-C6	-2.89	105.61	110.30
17	A	840	CLA	O2D-CGD-O1D	-2.89	118.19	123.84
17	B	821	CLA	O2D-CGD-O1D	-2.89	118.19	123.84
20	3	305	BCR	C7-C8-C9	-2.88	121.88	126.23
17	A	816	CLA	O2D-CGD-O1D	-2.88	118.20	123.84
17	1	505	CLA	CMB-C2B-C1B	-2.88	124.03	128.46
25	2	513	CHL	C1D-ND-C4D	-2.88	104.29	106.33
17	A	820	CLA	CHB-C4A-NA	2.88	128.50	124.51
17	2	507	CLA	CMB-C2B-C3B	2.88	130.07	124.68
22	B	850	DGD	O6D-C1D-O3G	-2.88	103.16	109.97
20	A	849	BCR	C15-C14-C13	-2.88	123.20	127.31
17	1	510	CLA	CMB-C2B-C3B	2.88	130.06	124.68
17	3	317	CLA	CAA-C2A-C3A	-2.87	109.39	116.10
25	1	514	CHL	C3D-C4D-ND	2.87	114.88	110.24
20	3	305	BCR	C20-C21-C22	-2.87	123.21	127.31
17	3	313	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
25	2	515	CHL	C1D-ND-C4D	-2.87	104.30	106.33
20	B	852	BCR	C24-C23-C22	-2.87	121.90	126.23
24	5	303	LUT	C35-C15-C14	-2.87	117.60	123.47
22	B	850	DGD	C1D-O6D-C5D	2.87	119.31	113.69
20	B	846	BCR	C38-C26-C25	-2.86	121.31	124.53
20	2	503	BCR	C36-C18-C19	2.86	122.58	118.08
17	B	835	CLA	CMB-C2B-C3B	2.86	130.03	124.68
17	3	318	CLA	CMB-C2B-C1B	-2.86	124.07	128.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	A	839	CLA	CHB-C4A-NA	2.85	128.46	124.51
17	A	821	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
17	1	511	CLA	CMB-C2B-C3B	2.85	130.00	124.68
17	3	309	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
17	3	308	CLA	CMB-C2B-C3B	2.84	130.00	124.68
17	2	505	CLA	CMB-C2B-C3B	2.84	130.00	124.68
17	A	835	CLA	CHB-C4A-NA	2.84	128.44	124.51
17	B	822	CLA	CHB-C4A-NA	2.84	128.44	124.51
17	A	835	CLA	C1-C2-C3	-2.84	121.13	126.04
26	2	502	XAT	C38-C25-C24	2.84	117.48	114.28
24	3	303	LUT	C15-C35-C34	-2.84	117.66	123.47
17	B	824	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
20	B	847	BCR	C28-C27-C26	-2.83	109.02	114.08
25	2	516	CHL	C4B-C3B-C2B	-2.83	104.28	106.92
25	3	315	CHL	C2A-C1A-CHA	-2.83	118.91	123.86
17	1	509	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
17	2	508	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
25	5	317	CHL	CMB-C2B-C3B	2.82	129.96	124.68
17	B	802	CLA	C1B-CHB-C4A	-2.82	124.53	130.12
17	3	306	CLA	CHB-C4A-NA	2.82	128.41	124.51
20	K	204	BCR	C7-C8-C9	-2.82	121.97	126.23
17	3	306	CLA	CAB-C3B-C2B	2.82	130.21	124.69
17	F	803	CLA	CAA-C2A-C3A	-2.82	109.52	116.10
24	1	502	LUT	C8-C7-C6	-2.82	119.28	127.20
17	A	834	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
20	A	846	BCR	C38-C26-C25	-2.82	121.36	124.53
17	A	826	CLA	C2D-C1D-ND	-2.82	108.03	110.10
17	1	511	CLA	CHB-C4A-NA	2.82	128.41	124.51
20	F	804	BCR	C16-C17-C18	-2.82	123.29	127.31
17	A	820	CLA	C1B-CHB-C4A	-2.82	124.54	130.12
22	B	850	DGD	O3G-C3G-C2G	-2.81	104.11	110.90
23	F	806	LMG	O8-C28-C29	2.81	120.73	111.91
26	5	304	XAT	C4-C3-C2	-2.81	105.34	110.77
17	B	801	CLA	C1B-CHB-C4A	-2.81	124.55	130.12
17	A	822	CLA	CMB-C2B-C3B	2.81	129.94	124.68
26	2	502	XAT	C15-C14-C13	-2.81	123.30	127.31
20	L	306	BCR	C38-C26-C27	2.81	119.02	113.62
17	5	312	CLA	O2D-CGD-O1D	-2.81	118.35	123.84
17	B	834	CLA	O2D-CGD-O1D	-2.81	118.35	123.84
19	A	844	LHG	C5-O7-C7	-2.81	110.88	117.79
20	B	846	BCR	C37-C22-C21	-2.81	118.99	122.92
24	1	501	LUT	C7-C8-C9	-2.81	122.00	126.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	3	304	LUT	C40-C33-C34	-2.81	118.99	122.92
17	3	308	CLA	CHB-C4A-NA	2.81	128.39	124.51
17	F	803	CLA	CMB-C2B-C3B	2.80	129.93	124.68
17	3	306	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
25	2	513	CHL	C3B-C4B-NB	2.80	112.83	109.21
20	J	102	BCR	C11-C10-C9	-2.80	123.32	127.31
17	1	511	CLA	O2D-CGD-O1D	-2.80	118.37	123.84
17	A	830	CLA	CMB-C2B-C3B	2.79	129.90	124.68
25	5	314	CHL	C1B-CHB-C4A	-2.79	124.60	130.12
17	A	807	CLA	CMB-C2B-C3B	2.79	129.89	124.68
25	1	514	CHL	CHD-C1D-C2D	2.79	131.33	125.48
17	A	817	CLA	CMB-C2B-C3B	2.79	129.89	124.68
17	5	305	CLA	CMB-C2B-C3B	2.78	130.02	124.93
17	2	509	CLA	CHB-C4A-NA	2.78	128.36	124.51
17	A	842	CLA	CMB-C2B-C3B	2.78	129.88	124.68
20	B	847	BCR	C34-C9-C10	-2.78	119.03	122.92
17	B	831	CLA	O2D-CGD-O1D	-2.78	118.40	123.84
17	3	311	CLA	O2D-CGD-O1D	-2.78	118.41	123.84
17	3	313	CLA	CHB-C4A-NA	2.78	128.35	124.51
20	F	804	BCR	C38-C26-C25	-2.77	121.42	124.53
25	1	517	CHL	O2D-CGD-O1D	-2.77	118.42	123.84
17	2	511	CLA	O2D-CGD-CBD	2.77	116.19	111.27
17	B	837	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
25	1	514	CHL	CMD-C2D-C3D	-2.77	121.24	127.61
17	B	833	CLA	CHB-C4A-NA	2.77	128.34	124.51
20	B	846	BCR	C23-C22-C21	2.77	123.19	118.94
24	2	501	LUT	C18-C5-C4	2.76	119.47	114.36
20	A	851	BCR	C7-C8-C9	-2.76	122.06	126.23
17	B	823	CLA	O2D-CGD-O1D	-2.76	118.44	123.84
17	3	301	CLA	O2D-CGD-O1D	-2.76	118.44	123.84
17	B	829	CLA	O2D-CGD-O1D	-2.76	118.44	123.84
17	1	515	CLA	O2D-CGD-O1D	-2.76	118.44	123.84
22	B	850	DGD	O2G-C1B-O1B	-2.76	117.04	123.70
17	L	304	CLA	CHB-C4A-NA	2.75	128.32	124.51
20	L	306	BCR	C38-C26-C25	-2.75	121.44	124.53
17	5	312	CLA	CMB-C2B-C3B	2.75	129.82	124.68
25	5	314	CHL	OMC-CMC-C2C	-2.75	119.47	125.69
17	B	828	CLA	CAA-C2A-C3A	-2.75	109.68	116.10
17	3	310	CLA	CMB-C2B-C3B	2.75	129.82	124.68
17	B	825	CLA	CHB-C4A-NA	2.75	128.31	124.51
17	B	836	CLA	CMB-C2B-C3B	2.75	129.82	124.68
17	A	829	CLA	O2D-CGD-CBD	2.75	116.15	111.27

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	I	101	BCR	C28-C27-C26	-2.75	109.17	114.08
17	B	834	CLA	CMB-C2B-C3B	2.74	129.81	124.68
17	3	318	CLA	CAB-C3B-C2B	2.74	130.05	124.69
17	L	302	CLA	C2A-C3A-C4A	-2.74	103.24	106.26
20	A	853	BCR	C37-C22-C21	-2.74	119.09	122.92
17	1	504	CLA	O2D-CGD-O1D	-2.74	118.48	123.84
17	3	317	CLA	CHD-C1D-ND	-2.74	121.94	124.45
17	5	308	CLA	C1B-CHB-C4A	-2.74	124.69	130.12
17	A	803	CLA	O2D-CGD-CBD	2.74	116.13	111.27
25	1	517	CHL	CMB-C2B-C3B	2.74	129.80	124.68
20	1	503	BCR	C34-C9-C10	-2.73	119.09	122.92
17	A	809	CLA	CMB-C2B-C1B	-2.73	124.26	128.46
17	B	805	CLA	CHB-C4A-NA	2.73	128.29	124.51
17	B	806	CLA	O2D-CGD-O1D	-2.73	118.50	123.84
25	5	317	CHL	C1D-ND-C4D	-2.73	104.40	106.33
17	B	838	CLA	O2D-CGD-CBD	2.73	116.12	111.27
17	5	308	CLA	O2D-CGD-O1D	-2.73	118.50	123.84
17	A	814	CLA	CMB-C2B-C3B	2.73	129.78	124.68
17	A	842	CLA	C1-C2-C3	-2.73	122.34	126.75
20	A	847	BCR	C7-C8-C9	-2.73	122.12	126.23
24	2	501	LUT	C30-C31-C32	-2.73	114.71	123.22
17	B	821	CLA	CHB-C4A-NA	2.72	128.28	124.51
17	A	828	CLA	CMB-C2B-C3B	2.72	129.77	124.68
17	1	507	CLA	O2D-CGD-O1D	-2.72	118.52	123.84
17	A	831	CLA	CAB-C3B-C2B	2.72	130.02	124.69
20	L	306	BCR	C3-C4-C5	-2.72	109.22	114.08
17	B	835	CLA	CHB-C4A-NA	2.72	128.27	124.51
17	B	808	CLA	CHD-C1D-ND	-2.72	121.96	124.45
20	B	845	BCR	C34-C9-C10	-2.71	119.12	122.92
17	1	504	CLA	C1B-CHB-C4A	-2.71	124.75	130.12
19	2	517	LHG	C5-O7-C7	-2.71	111.12	117.79
17	A	803	CLA	CHB-C4A-NA	2.71	128.26	124.51
25	5	317	CHL	CMD-C2D-C3D	-2.71	121.38	127.61
17	1	505	CLA	O2D-CGD-O1D	-2.71	118.54	123.84
20	A	847	BCR	C11-C10-C9	-2.71	123.45	127.31
17	3	306	CLA	C1B-CHB-C4A	-2.71	124.76	130.12
17	1	510	CLA	CHB-C4A-NA	2.71	128.25	124.51
20	I	101	BCR	C15-C16-C17	-2.70	117.93	123.47
20	A	846	BCR	C28-C27-C26	-2.70	109.26	114.08
25	3	315	CHL	CMB-C2B-C3B	2.70	129.73	124.68
20	A	847	BCR	C24-C23-C22	-2.70	122.16	126.23
17	B	841	CLA	CMB-C2B-C3B	2.70	129.72	124.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	B	825	CLA	O2D-CGD-O1D	-2.70	118.57	123.84
20	2	503	BCR	C34-C9-C10	-2.70	119.15	122.92
25	3	302	CHL	C1D-ND-C4D	-2.70	104.42	106.33
24	1	502	LUT	C15-C35-C34	-2.70	117.95	123.47
17	A	815	CLA	O2D-CGD-O1D	-2.69	118.57	123.84
20	A	849	BCR	C28-C27-C26	-2.69	109.27	114.08
17	B	817	CLA	CMB-C2B-C3B	2.69	129.72	124.68
17	A	805	CLA	C1B-CHB-C4A	-2.69	124.78	130.12
17	3	316	CLA	CHB-C4A-NA	2.69	128.24	124.51
17	3	317	CLA	CHB-C4A-NA	2.69	128.24	124.51
17	A	819	CLA	CMB-C2B-C3B	2.69	129.71	124.68
17	A	840	CLA	CAA-C2A-C3A	-2.69	109.82	116.10
17	B	830	CLA	CMB-C2B-C3B	2.69	129.71	124.68
17	A	831	CLA	CMB-C2B-C3B	2.69	129.95	124.69
20	B	845	BCR	C27-C26-C25	-2.69	118.83	122.73
20	3	305	BCR	C35-C13-C14	-2.69	119.16	122.92
25	5	314	CHL	CMD-C2D-C3D	-2.69	121.44	127.61
17	B	813	CLA	C2D-C1D-ND	-2.69	108.12	110.10
17	B	811	CLA	O2D-CGD-O1D	-2.69	118.59	123.84
19	A	843	LHG	C6-C5-C4	-2.68	105.44	111.79
17	A	810	CLA	O2D-CGD-O1D	-2.68	118.59	123.84
17	5	316	CLA	CAA-C2A-C3A	-2.68	109.84	116.10
20	B	844	BCR	C15-C16-C17	-2.68	117.98	123.47
17	A	805	CLA	CHB-C4A-NA	2.68	128.22	124.51
17	1	506	CLA	C1-C2-C3	-2.68	121.41	126.04
17	5	310	CLA	C1-C2-C3	-2.68	122.42	126.75
20	F	804	BCR	C3-C4-C5	-2.68	109.29	114.08
17	A	839	CLA	CMB-C2B-C3B	2.68	129.69	124.68
20	L	305	BCR	C29-C30-C25	2.68	114.60	110.48
17	B	814	CLA	CAA-C2A-C3A	-2.68	109.86	116.10
17	5	312	CLA	C1B-CHB-C4A	-2.67	124.82	130.12
20	B	845	BCR	C3-C4-C5	-2.67	109.30	114.08
17	3	311	CLA	CHB-C4A-NA	2.67	128.21	124.51
17	A	834	CLA	CAA-C2A-C3A	-2.67	109.87	116.10
16	A	801	CL0	C2D-C1D-ND	2.67	112.07	110.10
17	B	820	CLA	C1B-CHB-C4A	-2.67	124.83	130.12
17	B	818	CLA	CHB-C4A-NA	2.67	128.20	124.51
20	A	853	BCR	C32-C1-C6	-2.67	105.97	110.30
17	K	203	CLA	O2D-CGD-O1D	-2.67	118.62	123.84
16	A	801	CL0	O2D-CGD-O1D	-2.67	118.03	124.09
20	B	847	BCR	C36-C18-C19	2.67	122.28	118.08
25	3	302	CHL	CMB-C2B-C3B	2.66	129.66	124.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	B	810	CLA	CBD-CHA-C1A	2.66	131.64	128.50
17	3	310	CLA	CHB-C4A-NA	2.66	128.19	124.51
17	A	811	CLA	O2D-CGD-CBD	2.66	115.99	111.27
17	5	313	CLA	CMB-C2B-C3B	2.66	129.65	124.68
25	1	517	CHL	CMD-C2D-C3D	-2.66	121.50	127.61
17	5	306	CLA	CMB-C2B-C3B	2.65	129.64	124.68
20	A	846	BCR	C38-C26-C27	2.65	118.71	113.62
20	F	801	BCR	C10-C11-C12	-2.65	114.95	123.22
17	B	808	CLA	CMB-C2B-C3B	2.65	129.63	124.68
20	B	846	BCR	C36-C18-C17	-2.65	119.21	122.92
25	2	515	CHL	C2D-C1D-ND	2.65	112.05	110.10
25	2	512	CHL	C2A-C1A-CHA	-2.65	119.23	123.86
25	2	512	CHL	CMB-C2B-C3B	2.64	129.87	124.69
20	B	845	BCR	C35-C13-C14	-2.64	119.22	122.92
20	F	801	BCR	C15-C14-C13	-2.64	123.54	127.31
17	B	840	CLA	O2D-CGD-O1D	-2.64	118.67	123.84
17	2	510	CLA	O2D-CGD-O1D	-2.64	118.67	123.84
17	A	828	CLA	O2D-CGD-O1D	-2.64	118.68	123.84
20	B	847	BCR	C1-C6-C5	-2.64	118.90	122.61
20	A	851	BCR	C23-C24-C25	-2.64	119.79	127.20
17	2	507	CLA	O2D-CGD-O1D	-2.64	118.68	123.84
17	A	840	CLA	CMB-C2B-C1B	-2.64	124.41	128.46
20	K	204	BCR	C10-C11-C12	-2.64	114.99	123.22
16	A	801	CL0	CMB-C2B-C3B	2.63	129.85	124.69
17	A	805	CLA	O2D-CGD-O1D	-2.63	118.69	123.84
24	3	303	LUT	C20-C13-C12	2.63	122.23	118.08
20	A	849	BCR	C38-C26-C25	-2.63	121.57	124.53
17	B	835	CLA	C1-C2-C3	-2.63	121.49	126.04
20	A	847	BCR	C4-C5-C6	-2.63	118.91	122.73
17	2	504	CLA	C1B-CHB-C4A	-2.63	124.91	130.12
17	3	309	CLA	CMB-C2B-C3B	2.63	129.74	124.93
17	3	314	CLA	CHB-C4A-NA	2.63	128.14	124.51
25	1	512	CHL	C1D-ND-C4D	-2.63	104.47	106.33
18	B	843	PQN	C14-C13-C15	2.63	119.69	115.27
17	1	508	CLA	C1B-CHB-C4A	-2.62	124.92	130.12
25	1	512	CHL	OMC-CMC-C2C	-2.62	119.76	125.69
17	B	807	CLA	CHB-C4A-NA	2.62	128.14	124.51
20	K	204	BCR	C36-C18-C17	-2.62	119.25	122.92
24	3	304	LUT	C18-C5-C6	-2.62	121.59	124.53
17	3	311	CLA	CAC-C3C-C4C	2.62	128.21	124.81
17	5	310	CLA	CHB-C4A-NA	2.62	128.13	124.51
17	5	309	CLA	CAA-CBA-CGA	-2.62	105.56	112.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	J	101	CLA	CHB-C4A-NA	2.62	128.13	124.51
20	L	306	BCR	C21-C20-C19	-2.62	115.06	123.22
25	2	516	CHL	CHB-C4A-NA	2.61	128.13	124.51
17	B	837	CLA	O2A-CGA-O1A	-2.61	116.99	123.59
17	1	504	CLA	CHB-C4A-NA	2.61	128.12	124.51
17	B	820	CLA	O2D-CGD-O1D	-2.61	118.74	123.84
17	B	839	CLA	O2A-CGA-O1A	-2.60	117.02	123.59
20	A	846	BCR	C30-C25-C26	-2.60	118.95	122.61
17	B	803	CLA	CMB-C2B-C1B	-2.60	124.46	128.46
17	B	819	CLA	CMA-C3A-C2A	-2.60	110.02	116.10
16	A	801	CL0	CMD-C2D-C3D	-2.60	121.63	127.61
25	5	314	CHL	CMB-C2B-C3B	2.60	129.54	124.68
17	1	515	CLA	C2D-C1D-ND	-2.60	108.19	110.10
17	B	830	CLA	C1B-CHB-C4A	-2.60	124.97	130.12
17	5	316	CLA	CHB-C4A-NA	2.60	128.10	124.51
17	A	836	CLA	O2A-CGA-O1A	-2.59	117.04	123.59
20	F	804	BCR	C21-C20-C19	-2.59	115.12	123.22
20	B	844	BCR	C35-C13-C14	-2.59	119.29	122.92
19	B	851	LHG	O8-C23-C24	2.59	120.04	111.91
20	A	846	BCR	C8-C7-C6	-2.59	119.92	127.20
17	B	827	CLA	CHB-C4A-NA	2.59	128.09	124.51
17	5	307	CLA	CMB-C2B-C3B	2.59	129.52	124.68
17	A	824	CLA	O2D-CGD-O1D	-2.59	118.78	123.84
17	2	506	CLA	O2D-CGD-O1D	-2.59	118.78	123.84
17	A	834	CLA	CMB-C2B-C3B	2.59	129.52	124.68
20	L	306	BCR	C31-C1-C6	-2.59	106.10	110.30
17	B	827	CLA	C2D-C1D-ND	-2.59	108.20	110.10
17	3	312	CLA	CAA-C2A-C3A	-2.59	110.06	116.10
25	1	514	CHL	CBD-CHA-C1A	2.59	131.55	128.50
17	B	816	CLA	CHB-C4A-NA	2.59	128.09	124.51
17	L	303	CLA	C1B-CHB-C4A	-2.59	124.99	130.12
17	B	826	CLA	C2D-C1D-ND	-2.59	108.20	110.10
17	A	833	CLA	O2D-CGD-CBD	2.59	115.86	111.27
17	A	852	CLA	O2D-CGD-O1D	-2.58	118.79	123.84
24	1	502	LUT	C38-C25-C24	-2.58	118.03	123.56
17	2	511	CLA	C1B-CHB-C4A	-2.58	125.00	130.12
17	1	506	CLA	CMB-C2B-C3B	2.58	129.50	124.68
16	A	801	CL0	C6-C5-C3	-2.58	106.69	113.45
20	J	102	BCR	C29-C30-C25	2.58	114.45	110.48
17	A	802	CLA	O2D-CGD-O1D	-2.58	118.80	123.84
17	B	809	CLA	C2A-C1A-CHA	2.57	126.70	122.71
17	B	833	CLA	O2A-CGA-O1A	-2.57	117.10	123.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	851	BCR	C29-C30-C25	2.57	114.44	110.48
25	1	512	CHL	CMB-C2B-C3B	2.57	129.49	124.68
20	A	851	BCR	C33-C5-C4	2.57	118.56	113.62
17	B	834	CLA	CHD-C1D-ND	-2.57	122.09	124.45
17	B	805	CLA	CMA-C3A-C2A	-2.57	110.10	116.10
17	2	509	CLA	O2D-CGD-O1D	-2.57	118.81	123.84
24	1	502	LUT	C18-C5-C4	2.57	119.11	114.36
17	A	818	CLA	C2D-C1D-ND	-2.57	108.21	110.10
20	A	847	BCR	C28-C27-C26	-2.57	109.49	114.08
20	I	101	BCR	C36-C18-C19	2.57	122.12	118.08
17	1	505	CLA	CHB-C4A-NA	2.57	128.06	124.51
20	B	847	BCR	C1-C6-C7	2.57	123.04	115.78
17	B	815	CLA	C2D-C1D-ND	-2.56	108.21	110.10
17	A	828	CLA	C1B-CHB-C4A	-2.56	125.04	130.12
17	B	803	CLA	C1B-CHB-C4A	-2.56	125.04	130.12
17	5	305	CLA	C4B-CHC-C1C	-2.56	125.69	129.64
17	2	514	CLA	CHB-C4A-NA	2.56	128.06	124.51
17	A	811	CLA	CBD-CHA-C1A	2.56	131.52	128.50
18	A	841	PQN	C2M-C2-C1	2.56	120.52	116.27
17	3	311	CLA	C1B-CHB-C4A	-2.56	125.04	130.12
20	F	804	BCR	C24-C23-C22	-2.56	122.36	126.23
17	3	307	CLA	O2D-CGD-O1D	-2.56	118.83	123.84
17	B	834	CLA	CHB-C4A-NA	2.56	128.05	124.51
20	L	305	BCR	C34-C9-C10	-2.56	119.34	122.92
20	L	306	BCR	C7-C8-C9	-2.56	122.37	126.23
20	F	804	BCR	C33-C5-C6	-2.55	121.66	124.53
17	5	313	CLA	CBD-CHA-C1A	2.55	131.51	128.50
17	A	816	CLA	C1B-CHB-C4A	-2.55	125.06	130.12
17	2	505	CLA	C1B-CHB-C4A	-2.55	125.06	130.12
25	5	314	CHL	O2D-CGD-O1D	-2.55	118.86	123.84
17	B	806	CLA	C3A-C4A-CHB	-2.55	120.79	123.91
20	A	846	BCR	C3-C4-C5	-2.55	109.53	114.08
17	B	834	CLA	C1B-CHB-C4A	-2.55	125.08	130.12
17	5	316	CLA	C1B-CHB-C4A	-2.54	125.08	130.12
20	3	305	BCR	C8-C7-C6	-2.54	120.06	127.20
17	B	808	CLA	O2A-CGA-O1A	-2.54	117.18	123.59
17	L	303	CLA	O2D-CGD-CBD	2.54	115.78	111.27
20	F	804	BCR	C29-C30-C25	2.54	114.39	110.48
24	3	303	LUT	C8-C7-C6	-2.54	120.08	127.20
17	B	834	CLA	O2A-CGA-O1A	-2.54	116.98	123.30
17	A	852	CLA	CMB-C2B-C3B	2.54	129.42	124.68
24	2	501	LUT	C39-C29-C28	2.53	122.07	118.08

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	B	838	CLA	CHB-C4A-NA	2.53	128.02	124.51
25	5	315	CHL	OMC-CMC-C2C	-2.53	119.96	125.69
25	2	515	CHL	C2A-C1A-CHA	-2.53	119.43	123.86
25	2	515	CHL	O2D-CGD-O1D	-2.53	118.89	123.84
17	3	313	CLA	CMB-C2B-C3B	2.53	129.41	124.68
17	2	514	CLA	CMB-C2B-C3B	2.53	129.41	124.68
17	B	805	CLA	O2D-CGD-O1D	-2.53	118.89	123.84
20	B	847	BCR	C21-C20-C19	-2.53	115.33	123.22
25	3	315	CHL	OMC-CMC-C2C	-2.53	119.97	125.69
17	5	306	CLA	CAA-C2A-C3A	-2.53	110.20	116.10
17	B	823	CLA	CHB-C4A-NA	2.52	128.00	124.51
17	2	514	CLA	O2D-CGD-O1D	-2.52	118.90	123.84
17	5	305	CLA	C2A-C1A-CHA	2.52	126.62	122.71
17	B	821	CLA	C1-C2-C3	-2.52	122.67	126.75
17	A	833	CLA	CHB-C4A-NA	2.52	128.00	124.51
17	A	831	CLA	C1-C2-C3	-2.52	121.69	126.04
17	2	511	CLA	CMB-C2B-C3B	2.52	129.39	124.68
17	A	814	CLA	CHB-C4A-NA	2.52	127.99	124.51
17	A	822	CLA	CHB-C4A-NA	2.52	127.99	124.51
17	3	301	CLA	CHB-C4A-NA	2.52	127.99	124.51
17	B	824	CLA	CMB-C2B-C3B	2.52	129.39	124.68
17	1	508	CLA	O2D-CGD-O1D	-2.52	118.92	123.84
17	3	311	CLA	O2A-CGA-O1A	-2.51	117.25	123.59
17	A	817	CLA	C1B-CHB-C4A	-2.51	125.14	130.12
20	B	845	BCR	C24-C23-C22	-2.51	122.44	126.23
25	2	513	CHL	CMB-C2B-C3B	2.51	129.38	124.68
17	B	802	CLA	O2A-CGA-O1A	-2.51	117.25	123.59
23	F	806	LMG	C8-O7-C10	-2.51	111.61	117.79
17	K	205	CLA	O2D-CGD-O1D	-2.51	118.39	124.09
26	2	502	XAT	C40-C33-C34	-2.51	119.41	122.92
20	B	846	BCR	C28-C27-C26	-2.51	109.60	114.08
25	3	315	CHL	CMD-C2D-C3D	-2.51	121.84	127.61
17	5	308	CLA	CHB-C4A-NA	2.51	127.98	124.51
23	2	519	LMG	O7-C10-O9	-2.51	117.65	123.70
20	1	503	BCR	C33-C5-C4	2.50	118.43	113.62
17	A	816	CLA	CHB-C4A-NA	2.50	127.97	124.51
19	B	851	LHG	C5-O7-C7	-2.50	111.63	117.79
17	3	317	CLA	CMA-C3A-C2A	-2.50	110.26	116.10
17	B	826	CLA	CHD-C1D-ND	-2.50	122.15	124.45
17	A	825	CLA	C1B-CHB-C4A	-2.50	125.16	130.12
17	B	836	CLA	C1B-CHB-C4A	-2.50	125.16	130.12
25	2	512	CHL	CHB-C4A-NA	2.50	127.97	124.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	848	BCR	C21-C20-C19	-2.50	115.41	123.22
17	1	507	CLA	CHB-C4A-NA	2.50	127.97	124.51
17	2	510	CLA	CHB-C4A-NA	2.50	127.97	124.51
17	3	310	CLA	O2D-CGD-O1D	-2.50	118.95	123.84
20	A	849	BCR	C16-C15-C14	-2.50	118.36	123.47
17	L	304	CLA	C1B-CHB-C4A	-2.49	125.18	130.12
17	5	307	CLA	O2D-CGD-O1D	-2.49	118.96	123.84
17	B	817	CLA	CHB-C4A-NA	2.49	127.96	124.51
20	A	845	BCR	C37-C22-C21	-2.49	119.43	122.92
20	J	102	BCR	C31-C1-C6	-2.49	106.26	110.30
25	1	514	CHL	CMB-C2B-C3B	2.49	129.34	124.68
17	B	823	CLA	C2D-C1D-ND	-2.49	108.27	110.10
24	2	501	LUT	C40-C33-C32	2.49	122.00	118.08
17	A	818	CLA	O2D-CGD-CBD	2.49	115.69	111.27
20	B	849	BCR	C29-C30-C25	2.49	114.31	110.48
20	I	101	BCR	C10-C11-C12	-2.49	115.45	123.22
17	A	836	CLA	CMB-C2B-C3B	2.49	129.33	124.68
20	2	503	BCR	C35-C13-C12	2.49	121.99	118.08
20	5	302	BCR	C21-C20-C19	-2.48	115.46	123.22
17	B	819	CLA	C2D-C1D-ND	-2.48	108.28	110.10
17	5	316	CLA	O2D-CGD-O1D	-2.48	118.99	123.84
17	5	309	CLA	O2D-CGD-O1D	-2.48	119.00	123.84
17	F	802	CLA	C1B-CHB-C4A	-2.48	125.21	130.12
20	B	852	BCR	C8-C9-C10	2.48	122.74	118.94
20	F	801	BCR	C29-C30-C25	2.48	114.29	110.48
17	B	839	CLA	CHD-C1D-ND	-2.48	122.18	124.45
17	B	814	CLA	CAC-C3C-C4C	2.47	128.02	124.81
17	5	311	CLA	O2D-CGD-O1D	-2.47	119.00	123.84
17	2	514	CLA	O2A-CGA-O1A	-2.47	117.35	123.59
17	B	841	CLA	CHB-C4A-NA	2.47	127.93	124.51
17	A	828	CLA	CHB-C4A-NA	2.47	127.93	124.51
17	B	822	CLA	O2D-CGD-CBD	2.47	115.66	111.27
17	F	802	CLA	CHD-C1D-ND	-2.47	122.19	124.45
17	B	821	CLA	C2D-C1D-ND	-2.47	108.29	110.10
17	2	504	CLA	CAC-C3C-C4C	2.47	128.01	124.81
17	1	510	CLA	O2D-CGD-CBD	2.46	115.64	111.27
17	B	812	CLA	C2D-C1D-ND	-2.46	108.29	110.10
17	B	837	CLA	CHB-C4A-NA	2.46	127.91	124.51
20	B	844	BCR	C20-C19-C18	-2.46	119.51	126.42
17	B	838	CLA	C1B-CHB-C4A	-2.46	125.25	130.12
20	J	102	BCR	C34-C9-C8	2.46	121.95	118.08
24	3	304	LUT	C10-C11-C12	-2.46	115.55	123.22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	A	801	CL0	CAB-C3B-C2B	2.46	129.50	124.69
17	A	810	CLA	CHB-C4A-NA	2.46	127.91	124.51
20	B	852	BCR	C23-C24-C25	-2.46	120.30	127.20
17	A	824	CLA	C2A-C1A-CHA	2.46	126.52	122.71
17	K	205	CLA	C1B-CHB-C4A	-2.46	125.25	130.12
25	2	515	CHL	OMC-CMC-C2C	-2.46	120.14	125.69
17	1	506	CLA	CHB-C4A-NA	2.45	127.91	124.51
24	5	303	LUT	C39-C29-C28	2.45	121.94	118.08
17	A	822	CLA	C1B-CHB-C4A	-2.45	125.26	130.12
17	B	829	CLA	O2D-CGD-CBD	2.45	115.63	111.27
17	B	806	CLA	CHD-C1D-ND	-2.45	122.20	124.45
17	A	831	CLA	C2D-C1D-ND	-2.45	108.30	110.10
17	A	832	CLA	C1B-CHB-C4A	-2.45	125.26	130.12
17	B	826	CLA	CHB-C4A-NA	2.45	127.90	124.51
17	A	806	CLA	CHB-C4A-NA	2.45	127.90	124.51
22	J	103	DGD	O1G-C1A-C2A	2.45	119.59	111.91
17	2	510	CLA	O2A-CGA-O1A	-2.45	117.41	123.59
23	2	518	LMG	O6-C1-C2	-2.45	105.17	110.35
20	L	306	BCR	C4-C5-C6	-2.45	119.18	122.73
17	B	835	CLA	O2A-CGA-O1A	-2.45	117.42	123.59
17	3	310	CLA	O2A-CGA-O1A	-2.44	117.21	123.30
17	2	504	CLA	CMB-C2B-C3B	2.44	129.25	124.68
17	B	809	CLA	CMB-C2B-C3B	2.44	129.25	124.68
17	A	807	CLA	CHB-C4A-NA	2.44	127.89	124.51
25	3	315	CHL	O1D-CGD-CBD	-2.44	119.49	124.48
17	F	803	CLA	CHB-C4A-NA	2.44	127.89	124.51
20	B	852	BCR	C30-C25-C26	-2.44	119.18	122.61
17	A	808	CLA	O2D-CGD-O1D	-2.44	119.07	123.84
17	L	303	CLA	CAA-C2A-C3A	-2.44	106.10	112.78
25	2	513	CHL	O2D-CGD-O1D	-2.44	119.07	123.84
17	2	505	CLA	CHB-C4A-NA	2.44	127.88	124.51
17	5	310	CLA	C1B-CHB-C4A	-2.44	125.29	130.12
20	A	845	BCR	C36-C18-C17	-2.44	119.51	122.92
24	2	501	LUT	C19-C9-C10	-2.43	119.51	122.92
20	1	503	BCR	C8-C7-C6	-2.43	120.37	127.20
23	2	519	LMG	O8-C28-C29	2.43	119.54	111.91
17	B	812	CLA	CHB-C4A-NA	2.43	127.88	124.51
17	B	839	CLA	CHB-C4A-NA	2.43	127.88	124.51
17	A	831	CLA	O2A-CGA-O1A	-2.43	117.46	123.59
17	F	802	CLA	CHB-C4A-NA	2.43	127.87	124.51
17	1	510	CLA	C1B-CHB-C4A	-2.43	125.31	130.12
17	A	806	CLA	O2D-CGD-O1D	-2.43	119.09	123.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	3	307	CLA	CMB-C2B-C1B	-2.43	124.73	128.46
17	5	307	CLA	O2A-CGA-O1A	-2.43	117.47	123.59
17	3	318	CLA	CMB-C2B-C3B	2.43	129.44	124.69
17	A	824	CLA	C2D-C1D-ND	-2.42	108.32	110.10
17	B	840	CLA	CHB-C4A-NA	2.42	127.86	124.51
17	1	513	CLA	C1B-CHB-C4A	-2.42	125.31	130.12
17	B	839	CLA	C1B-CHB-C4A	-2.42	125.32	130.12
20	J	102	BCR	C2-C1-C6	2.42	114.21	110.48
20	A	849	BCR	C8-C9-C10	2.42	122.66	118.94
17	5	307	CLA	CHD-C1D-ND	-2.42	122.23	124.45
17	1	509	CLA	C1B-CHB-C4A	-2.42	125.33	130.12
17	A	814	CLA	CAA-C2A-C3A	-2.42	108.22	114.26
17	3	309	CLA	CAA-C2A-C3A	-2.41	108.23	114.26
17	A	803	CLA	C1B-CHB-C4A	-2.41	125.34	130.12
17	3	301	CLA	CMB-C2B-C3B	2.41	129.19	124.68
20	L	305	BCR	C37-C22-C21	-2.41	119.54	122.92
17	B	812	CLA	C1-C2-C3	-2.41	121.87	126.04
17	3	316	CLA	C1B-CHB-C4A	-2.41	125.34	130.12
17	A	815	CLA	C2D-C1D-ND	-2.41	108.33	110.10
17	B	820	CLA	O2A-CGA-O1A	-2.41	117.51	123.59
16	A	801	CL0	CHA-C4D-ND	2.41	137.54	132.50
20	3	305	BCR	C15-C16-C17	-2.41	118.54	123.47
17	B	803	CLA	C1-C2-C3	-2.41	121.88	126.04
17	A	838	CLA	C1B-CHB-C4A	-2.41	125.35	130.12
17	3	312	CLA	O2D-CGD-O1D	-2.41	119.14	123.84
17	A	807	CLA	C1B-CHB-C4A	-2.41	125.35	130.12
17	5	311	CLA	CHB-C4A-NA	2.41	127.84	124.51
20	2	503	BCR	C20-C19-C18	2.40	133.17	126.42
24	3	304	LUT	C38-C25-C24	-2.40	118.41	123.56
22	J	103	DGD	C6D-O5D-C1E	-2.40	109.04	113.74
20	A	846	BCR	C37-C22-C21	-2.40	119.56	122.92
17	A	837	CLA	CMA-C3A-C2A	-2.40	110.49	116.10
17	A	825	CLA	O2A-CGA-O1A	-2.40	117.53	123.59
18	B	843	PQN	C11-C3-C4	2.40	121.07	118.50
17	B	812	CLA	CAB-C3B-C2B	2.40	129.39	124.69
17	3	308	CLA	O2D-CGD-O1D	-2.40	119.15	123.84
20	J	102	BCR	C27-C26-C25	-2.40	119.25	122.73
17	3	318	CLA	CHB-C4A-NA	2.40	127.83	124.51
24	3	304	LUT	C16-C1-C6	-2.40	106.41	110.30
23	2	519	LMG	O1-C1-C2	2.40	112.05	108.30
17	A	802	CLA	CHB-C4A-NA	2.40	127.83	124.51
20	A	851	BCR	C31-C1-C6	-2.39	106.42	110.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	2	515	CHL	C1C-C2C-C3C	-2.39	105.21	107.11
17	B	818	CLA	CHD-C1D-ND	-2.39	122.25	124.45
20	F	801	BCR	C37-C22-C21	-2.39	119.57	122.92
17	L	301	CLA	CHB-C4A-NA	2.39	127.82	124.51
17	2	511	CLA	CHD-C1D-ND	-2.39	122.26	124.45
20	A	845	BCR	C8-C7-C6	-2.39	120.49	127.20
20	B	852	BCR	C35-C13-C14	-2.39	119.58	122.92
20	F	804	BCR	C33-C5-C4	2.39	118.20	113.62
20	A	847	BCR	C1-C6-C5	-2.39	119.25	122.61
25	1	514	CHL	OMC-CMC-C2C	-2.39	120.29	125.69
17	1	509	CLA	CHB-C4A-NA	2.39	127.81	124.51
19	1	516	LHG	O8-C23-O10	-2.39	117.57	123.59
17	5	307	CLA	C1B-CHB-C4A	-2.39	125.39	130.12
17	3	314	CLA	C1B-CHB-C4A	-2.39	125.39	130.12
17	A	836	CLA	CHD-C1D-ND	-2.39	122.26	124.45
17	3	311	CLA	O1D-CGD-CBD	2.38	129.36	124.48
17	A	817	CLA	CHB-C4A-NA	2.38	127.81	124.51
17	B	842	CLA	CHB-C4A-NA	2.38	127.81	124.51
20	I	101	BCR	C27-C26-C25	-2.38	119.27	122.73
20	J	102	BCR	C36-C18-C19	2.38	121.83	118.08
17	B	821	CLA	CMB-C2B-C3B	2.38	129.14	124.68
17	B	812	CLA	CMB-C2B-C3B	2.38	129.35	124.69
25	1	517	CHL	CHB-C4A-NA	2.38	127.81	124.51
17	J	101	CLA	C1B-CHB-C4A	-2.38	125.40	130.12
17	A	827	CLA	C1B-CHB-C4A	-2.38	125.40	130.12
17	B	829	CLA	C1B-CHB-C4A	-2.38	125.40	130.12
20	L	306	BCR	C30-C25-C26	-2.38	119.26	122.61
17	B	815	CLA	C1B-CHB-C4A	-2.38	125.40	130.12
17	5	306	CLA	CMA-C3A-C2A	-2.38	110.54	116.10
23	F	805	LMG	C8-O7-C10	-2.38	111.93	117.79
17	L	302	CLA	C1B-CHB-C4A	-2.38	125.41	130.12
20	L	305	BCR	C39-C30-C25	-2.38	106.44	110.30
17	A	832	CLA	O2A-CGA-O1A	-2.37	117.60	123.59
20	B	848	BCR	C36-C18-C19	2.37	121.82	118.08
25	1	517	CHL	C1C-C2C-C3C	-2.37	105.23	107.11
25	2	513	CHL	C2D-C1D-ND	2.37	111.85	110.10
17	B	813	CLA	CHB-C4A-NA	2.37	127.79	124.51
20	K	204	BCR	C33-C5-C4	2.37	118.17	113.62
17	B	828	CLA	C2D-C1D-ND	-2.37	108.36	110.10
20	A	853	BCR	C39-C30-C25	-2.37	106.45	110.30
17	A	823	CLA	C1B-CHB-C4A	-2.37	125.42	130.12
17	2	511	CLA	CBD-CHA-C1A	2.37	131.29	128.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	849	BCR	C38-C26-C25	-2.37	121.87	124.53
20	J	102	BCR	C10-C11-C12	-2.37	115.83	123.22
17	B	804	CLA	CHB-C4A-NA	2.37	127.79	124.51
20	A	847	BCR	C15-C16-C17	-2.37	118.62	123.47
17	A	837	CLA	CHB-C4A-NA	2.37	127.78	124.51
17	K	205	CLA	CHD-C1D-ND	-2.37	122.28	124.45
17	A	830	CLA	O1D-CGD-CBD	2.37	129.32	124.48
17	B	810	CLA	O2D-CGD-CBD	2.37	115.47	111.27
25	5	315	CHL	C4A-NA-C1A	2.36	107.77	106.71
17	B	817	CLA	C1B-CHB-C4A	-2.36	125.43	130.12
20	B	845	BCR	C29-C28-C27	-2.36	106.09	111.38
17	B	805	CLA	C1B-CHB-C4A	-2.36	125.44	130.12
17	A	804	CLA	CHB-C4A-NA	2.36	127.77	124.51
17	B	818	CLA	C1B-CHB-C4A	-2.36	125.44	130.12
17	B	805	CLA	C2D-C1D-ND	-2.36	108.37	110.10
23	2	519	LMG	O6-C5-C4	2.36	113.98	109.69
25	5	314	CHL	C2A-C1A-CHA	-2.36	119.74	123.86
17	B	833	CLA	C1B-CHB-C4A	-2.36	125.45	130.12
17	1	509	CLA	O2A-CGA-O1A	-2.36	117.64	123.59
17	A	810	CLA	C1B-CHB-C4A	-2.36	125.45	130.12
17	B	833	CLA	C2D-C1D-ND	-2.36	108.37	110.10
23	2	519	LMG	C3-C4-C5	2.36	114.44	110.24
17	A	809	CLA	CHB-C4A-NA	2.36	127.77	124.51
17	B	814	CLA	CHB-C4A-NA	2.35	127.77	124.51
17	2	508	CLA	C1B-CHB-C4A	-2.35	125.46	130.12
20	5	302	BCR	C36-C18-C17	-2.35	119.63	122.92
17	3	312	CLA	CHB-C4A-NA	2.35	127.76	124.51
20	A	848	BCR	C8-C7-C6	-2.35	120.60	127.20
17	A	820	CLA	O2A-CGA-O1A	-2.35	117.66	123.59
17	L	302	CLA	CHB-C4A-NA	2.35	127.93	124.34
17	A	838	CLA	C1-C2-C3	-2.35	121.98	126.04
20	A	845	BCR	C20-C19-C18	-2.35	119.82	126.42
20	A	846	BCR	C34-C9-C10	-2.35	119.64	122.92
17	3	310	CLA	CHD-C1D-ND	-2.35	122.30	124.45
24	1	501	LUT	C20-C13-C12	2.35	121.77	118.08
17	L	303	CLA	CHD-C1D-ND	-2.34	122.30	124.45
17	A	821	CLA	O1D-CGD-CBD	2.34	129.28	124.48
20	A	847	BCR	C34-C9-C8	2.34	121.77	118.08
24	2	501	LUT	C40-C33-C34	-2.34	119.64	122.92
17	3	307	CLA	C2D-C1D-ND	-2.34	108.38	110.10
25	1	514	CHL	O2D-CGD-O1D	-2.34	119.26	123.84
17	B	836	CLA	CHB-C4A-NA	2.34	127.75	124.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	B	837	CLA	C1B-CHB-C4A	-2.34	125.48	130.12
24	1	501	LUT	C15-C14-C13	-2.34	123.97	127.31
17	B	824	CLA	O2A-CGA-O1A	-2.34	117.47	123.30
17	2	506	CLA	CHB-C4A-NA	2.34	127.74	124.51
17	A	852	CLA	CHD-C1D-ND	-2.33	122.31	124.45
17	A	828	CLA	CAA-C2A-C3A	-2.33	110.65	116.10
17	F	803	CLA	C1B-CHB-C4A	-2.33	125.50	130.12
17	A	820	CLA	O2D-CGD-CBD	2.33	115.41	111.27
17	B	830	CLA	O1D-CGD-CBD	2.33	129.25	124.48
17	3	316	CLA	CHD-C1D-ND	-2.33	122.31	124.45
20	A	849	BCR	C10-C11-C12	-2.33	115.95	123.22
20	B	849	BCR	C40-C30-C25	-2.32	106.53	110.30
17	A	839	CLA	C1B-CHB-C4A	-2.32	125.51	130.12
17	B	827	CLA	C1B-CHB-C4A	-2.32	125.51	130.12
17	B	803	CLA	CMB-C2B-C3B	2.32	129.03	124.68
17	A	829	CLA	C1B-CHB-C4A	-2.32	125.52	130.12
17	5	305	CLA	C1B-CHB-C4A	-2.32	125.52	130.12
20	F	801	BCR	C2-C1-C6	2.32	114.06	110.48
17	A	808	CLA	CHB-C4A-NA	2.32	127.72	124.51
17	B	802	CLA	C2D-C1D-ND	-2.32	108.39	110.10
17	K	205	CLA	CHB-C4A-NA	2.32	127.72	124.51
17	B	828	CLA	CMA-C3A-C2A	-2.32	110.68	116.10
17	3	310	CLA	C1B-CHB-C4A	-2.32	125.52	130.12
20	A	851	BCR	C21-C20-C19	-2.32	115.98	123.22
17	A	812	CLA	CHB-C4A-NA	2.32	127.71	124.51
17	A	829	CLA	O2A-CGA-O1A	-2.31	117.75	123.59
17	A	823	CLA	CHD-C1D-ND	-2.31	122.33	124.45
17	B	826	CLA	C1B-CHB-C4A	-2.31	125.53	130.12
17	2	509	CLA	C1B-CHB-C4A	-2.31	125.53	130.12
17	3	308	CLA	C1-C2-C3	-2.31	122.04	126.04
20	I	101	BCR	C35-C13-C12	2.31	121.72	118.08
17	3	312	CLA	C1B-CHB-C4A	-2.31	125.54	130.12
20	B	849	BCR	C16-C15-C14	-2.31	118.74	123.47
25	2	515	CHL	C1B-CHB-C4A	-2.31	125.54	130.12
20	F	801	BCR	C27-C26-C25	-2.31	119.38	122.73
17	A	842	CLA	CHB-C4A-NA	2.31	127.70	124.51
17	3	308	CLA	C1B-CHB-C4A	-2.31	125.54	130.12
17	A	819	CLA	O1D-CGD-CBD	2.31	129.21	124.48
17	A	823	CLA	O1D-CGD-CBD	2.31	129.21	124.48
17	3	301	CLA	O1D-CGD-CBD	2.30	129.20	124.48
17	A	833	CLA	CBD-CHA-C1A	2.30	131.21	128.50
17	B	815	CLA	O2D-CGD-CBD	2.30	115.36	111.27

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	2	504	CLA	CHB-C4A-NA	2.30	127.86	124.34
17	3	309	CLA	C4B-CHC-C1C	-2.30	126.09	129.64
17	A	825	CLA	CHB-C4A-NA	2.30	127.69	124.51
24	1	501	LUT	C38-C25-C24	-2.30	118.64	123.56
17	B	806	CLA	CBD-CHA-C1A	2.30	131.21	128.50
17	A	837	CLA	C1B-CHB-C4A	-2.30	125.57	130.12
20	B	849	BCR	C8-C7-C6	-2.30	120.75	127.20
17	1	506	CLA	C1B-CHB-C4A	-2.30	125.57	130.12
17	2	514	CLA	C2D-C1D-ND	-2.29	108.41	110.10
17	A	840	CLA	CHB-C4A-NA	2.29	127.69	124.51
20	F	801	BCR	C8-C7-C6	-2.29	120.76	127.20
20	J	102	BCR	C8-C7-C6	-2.29	120.76	127.20
17	3	308	CLA	O2D-CGD-CBD	2.29	115.34	111.27
17	A	805	CLA	CHD-C1D-ND	-2.29	122.35	124.45
25	5	315	CHL	O2A-CGA-CBA	2.29	121.40	114.03
17	A	852	CLA	CHB-C4A-NA	2.29	127.68	124.51
17	B	842	CLA	CHD-C1D-ND	-2.29	122.35	124.45
20	2	503	BCR	C38-C26-C27	2.29	118.02	113.62
17	A	831	CLA	C1B-CHB-C4A	-2.29	125.58	130.12
17	B	841	CLA	O2A-CGA-O1A	-2.29	117.82	123.59
17	3	311	CLA	CHD-C1D-ND	-2.29	122.35	124.45
26	2	502	XAT	C39-C29-C30	-2.29	119.72	122.92
17	B	812	CLA	CAA-CBA-CGA	-2.29	106.57	113.25
17	B	808	CLA	O2D-CGD-CBD	2.28	115.33	111.27
17	B	835	CLA	C2D-C1D-ND	-2.28	108.42	110.10
17	A	824	CLA	CBD-CHA-C1A	2.28	131.19	128.50
17	B	823	CLA	C1B-CHB-C4A	-2.28	125.60	130.12
17	A	814	CLA	O2D-CGD-CBD	2.28	115.32	111.27
17	B	827	CLA	CMA-C3A-C2A	-2.28	110.78	116.10
17	B	805	CLA	CHD-C1D-ND	-2.28	122.36	124.45
17	L	304	CLA	CAC-C3C-C2C	-2.28	123.63	127.53
17	5	305	CLA	C1B-NB-C4B	2.28	108.41	106.32
20	A	846	BCR	C16-C15-C14	-2.28	118.81	123.47
20	A	853	BCR	C33-C5-C6	-2.28	121.97	124.53
20	B	845	BCR	C33-C5-C4	2.28	117.99	113.62
24	1	501	LUT	C30-C31-C32	-2.28	116.11	123.22
17	B	801	CLA	C1-C2-C3	-2.28	122.11	126.04
17	A	821	CLA	CHB-C4A-NA	2.28	127.66	124.51
24	3	304	LUT	C15-C14-C13	-2.27	124.06	127.31
17	B	819	CLA	CHB-C4A-NA	2.27	127.66	124.51
17	A	822	CLA	CMA-C3A-C2A	-2.27	110.79	116.10
17	3	318	CLA	C1B-CHB-C4A	-2.27	125.61	130.12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	B	825	CLA	C1B-CHB-C4A	-2.27	125.61	130.12
17	A	814	CLA	C2D-C1D-ND	-2.27	108.43	110.10
17	L	301	CLA	C1B-CHB-C4A	-2.27	125.62	130.12
20	A	851	BCR	C35-C13-C14	-2.27	119.74	122.92
17	B	822	CLA	C1B-CHB-C4A	-2.27	125.62	130.12
25	1	514	CHL	C3B-C4B-NB	2.27	112.15	109.21
17	B	837	CLA	CHD-C1D-ND	-2.27	122.37	124.45
17	A	835	CLA	O2D-CGD-CBD	2.27	115.30	111.27
17	B	828	CLA	CAC-C3C-C4C	2.27	127.75	124.81
20	A	845	BCR	C16-C15-C14	-2.27	118.83	123.47
17	2	514	CLA	C1B-CHB-C4A	-2.27	125.63	130.12
25	5	317	CHL	OMC-CMC-C2C	-2.27	120.56	125.69
17	B	818	CLA	O2D-CGD-CBD	2.27	115.29	111.27
17	A	822	CLA	C2D-C1D-ND	-2.26	108.44	110.10
17	5	310	CLA	O2A-CGA-O1A	-2.26	117.88	123.59
25	5	315	CHL	CMB-C2B-C3B	2.26	128.91	124.68
25	5	315	CHL	C1C-C2C-C3C	-2.26	105.32	107.11
24	1	501	LUT	C18-C5-C4	2.26	118.55	114.36
17	2	507	CLA	C1B-CHB-C4A	-2.26	125.64	130.12
17	B	820	CLA	CHB-C4A-NA	2.26	127.64	124.51
17	1	513	CLA	CHB-C4A-NA	2.26	127.63	124.51
17	B	811	CLA	C1B-CHB-C4A	-2.26	125.65	130.12
17	A	812	CLA	C2D-C1D-ND	-2.26	108.44	110.10
17	B	801	CLA	C2D-C1D-ND	-2.26	108.44	110.10
20	L	305	BCR	C33-C5-C6	-2.26	121.99	124.53
17	B	821	CLA	C1B-CHB-C4A	-2.26	125.65	130.12
17	B	842	CLA	C1B-CHB-C4A	-2.26	125.65	130.12
17	A	818	CLA	CBD-CHA-C1A	2.25	131.16	128.50
17	B	816	CLA	C1B-CHB-C4A	-2.25	125.65	130.12
17	3	314	CLA	O2D-CGD-CBD	2.25	115.27	111.27
17	A	808	CLA	C1B-CHB-C4A	-2.25	125.65	130.12
25	5	317	CHL	O2D-CGD-O1D	-2.25	119.43	123.84
18	A	841	PQN	C14-C13-C15	2.25	119.06	115.27
20	A	847	BCR	C21-C20-C19	-2.25	116.19	123.22
17	5	307	CLA	CHB-C4A-NA	2.25	127.63	124.51
17	B	829	CLA	CHB-C4A-NA	2.25	127.63	124.51
17	1	505	CLA	CMB-C2B-C3B	2.25	128.89	124.68
17	A	826	CLA	CHB-C4A-NA	2.25	127.62	124.51
17	B	802	CLA	CHB-C4A-NA	2.25	127.62	124.51
17	B	811	CLA	CHB-C4A-NA	2.25	127.62	124.51
17	2	510	CLA	C1B-CHB-C4A	-2.25	125.66	130.12
20	A	845	BCR	C10-C11-C12	-2.25	116.20	123.22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	B	802	CLA	C7-C6-C5	-2.25	109.61	114.49
17	B	835	CLA	C1B-CHB-C4A	-2.25	125.67	130.12
25	2	513	CHL	CED-O2D-CGD	2.25	121.02	115.94
17	3	307	CLA	C1B-CHB-C4A	-2.25	125.67	130.12
17	L	302	CLA	C3A-C4A-CHB	-2.25	120.20	124.24
19	A	843	LHG	O7-C7-O9	-2.24	118.28	123.70
25	5	314	CHL	C1C-C2C-C3C	-2.24	105.33	107.11
17	B	826	CLA	C3C-C4C-NC	-2.24	108.06	110.57
20	J	102	BCR	C23-C24-C25	-2.24	120.90	127.20
17	A	815	CLA	C1B-CHB-C4A	-2.24	125.68	130.12
25	1	512	CHL	C1C-C2C-C3C	-2.24	105.34	107.11
17	A	842	CLA	C1B-CHB-C4A	-2.24	125.69	130.12
17	F	803	CLA	O2D-CGD-O1D	-2.24	119.47	123.84
17	A	852	CLA	O2A-CGA-O1A	-2.24	117.95	123.59
20	B	846	BCR	C4-C5-C6	-2.24	119.49	122.73
17	3	301	CLA	C2D-C1D-ND	-2.23	108.46	110.10
25	2	513	CHL	C3A-C4A-CHB	-2.23	118.12	124.01
20	L	305	BCR	C23-C24-C25	-2.23	120.94	127.20
17	B	838	CLA	O2A-CGA-O1A	-2.23	117.96	123.59
20	F	804	BCR	C15-C16-C17	-2.23	118.91	123.47
20	A	851	BCR	C37-C22-C21	-2.23	119.80	122.92
17	B	812	CLA	CHD-C1D-ND	-2.23	122.41	124.45
17	A	806	CLA	CHD-C1D-ND	-2.23	122.41	124.45
24	3	303	LUT	C1-C6-C5	-2.23	119.48	122.61
17	2	506	CLA	O2A-CGA-O1A	-2.23	117.97	123.59
17	2	511	CLA	C3C-C4C-NC	-2.23	108.07	110.57
17	B	831	CLA	CHD-C1D-ND	-2.23	122.41	124.45
17	1	505	CLA	CAA-C2A-C3A	-2.23	108.70	114.26
17	A	818	CLA	C1B-CHB-C4A	-2.23	125.71	130.12
17	5	312	CLA	CHB-C4A-NA	2.23	127.59	124.51
17	B	819	CLA	O2D-CGD-CBD	2.22	115.22	111.27
25	1	517	CHL	C3A-C4A-CHB	-2.22	118.16	124.01
17	L	302	CLA	O2D-CGD-O1D	-2.22	119.50	123.84
20	I	101	BCR	C3-C4-C5	-2.22	110.11	114.08
17	A	835	CLA	C1B-CHB-C4A	-2.22	125.72	130.12
25	1	517	CHL	OMC-CMC-C2C	-2.22	120.67	125.69
17	A	813	CLA	CHB-C4A-NA	2.22	127.58	124.51
17	5	311	CLA	C1B-CHB-C4A	-2.22	125.72	130.12
17	K	203	CLA	C1B-CHB-C4A	-2.22	125.72	130.12
17	A	804	CLA	C1B-CHB-C4A	-2.22	125.72	130.12
17	3	312	CLA	CAC-C3C-C4C	2.22	127.69	124.81
17	A	838	CLA	CHB-C4A-NA	2.21	127.57	124.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	A	804	CLA	C2D-C1D-ND	-2.21	108.47	110.10
25	2	512	CHL	O2D-CGD-O1D	-2.21	119.51	123.84
25	2	516	CHL	C1C-C2C-C3C	-2.21	105.36	107.11
17	L	304	CLA	O2A-CGA-O1A	-2.21	117.79	123.30
17	1	507	CLA	C1B-CHB-C4A	-2.21	125.74	130.12
17	A	840	CLA	C2D-C1D-ND	-2.21	108.47	110.10
22	B	850	DGD	C3G-C2G-C1G	-2.21	106.56	111.79
22	B	850	DGD	C6D-O5D-C1E	-2.21	109.42	113.74
20	A	853	BCR	C31-C1-C6	-2.21	106.71	110.30
17	A	812	CLA	CAA-C2A-C3A	-2.21	108.74	114.26
17	B	819	CLA	C1B-CHB-C4A	-2.21	125.74	130.12
17	A	830	CLA	CHB-C4A-NA	2.21	127.56	124.51
17	B	816	CLA	O2D-CGD-O1D	-2.20	119.53	123.84
20	F	804	BCR	C34-C9-C10	-2.20	119.84	122.92
25	2	515	CHL	O1D-CGD-CBD	-2.20	119.98	124.48
17	B	830	CLA	O2A-CGA-O1A	-2.20	118.04	123.59
17	A	838	CLA	C2D-C1D-ND	-2.20	108.48	110.10
17	L	303	CLA	O2A-CGA-O1A	-2.20	118.04	123.59
20	I	101	BCR	C16-C15-C14	-2.20	118.97	123.47
20	B	848	BCR	C39-C30-C25	-2.20	106.73	110.30
17	1	508	CLA	CHB-C4A-NA	2.20	127.55	124.51
24	1	502	LUT	C30-C31-C32	-2.20	116.36	123.22
17	A	834	CLA	C1B-CHB-C4A	-2.20	125.77	130.12
17	3	313	CLA	CHD-C1D-ND	-2.20	122.44	124.45
17	B	834	CLA	CAA-C2A-C3A	-2.20	106.76	112.78
24	1	501	LUT	C10-C11-C12	-2.20	116.36	123.22
17	A	852	CLA	C1B-CHB-C4A	-2.20	125.77	130.12
17	B	806	CLA	C1B-CHB-C4A	-2.20	125.77	130.12
17	2	506	CLA	C1B-CHB-C4A	-2.20	125.77	130.12
17	5	311	CLA	C2D-C1D-ND	-2.20	108.49	110.10
20	A	847	BCR	C11-C12-C13	-2.20	120.25	126.42
17	A	829	CLA	CHD-C1D-ND	-2.19	122.44	124.45
17	5	309	CLA	C1B-CHB-C4A	-2.19	125.77	130.12
20	L	306	BCR	C27-C26-C25	-2.19	119.55	122.73
17	5	309	CLA	CHB-C4A-NA	2.19	127.55	124.51
17	A	819	CLA	CHD-C1D-ND	-2.19	122.44	124.45
17	A	825	CLA	CHD-C1D-ND	-2.19	122.44	124.45
17	A	812	CLA	C1B-CHB-C4A	-2.19	125.78	130.12
17	B	841	CLA	C1B-CHB-C4A	-2.19	125.78	130.12
20	B	847	BCR	C19-C18-C17	-2.19	115.58	118.94
17	L	304	CLA	CHD-C1D-ND	-2.19	122.44	124.45
20	B	844	BCR	C40-C30-C25	-2.19	106.75	110.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	A	809	CLA	CMB-C2B-C3B	2.19	128.77	124.68
17	5	308	CLA	C2D-C1D-ND	-2.19	108.49	110.10
17	1	507	CLA	CAA-C2A-C3A	-2.19	108.80	114.26
20	B	844	BCR	C33-C5-C4	2.19	117.82	113.62
17	2	509	CLA	C1-C2-C3	-2.19	123.22	126.75
17	B	803	CLA	C2D-C1D-ND	-2.18	108.49	110.10
17	2	507	CLA	O1D-CGD-CBD	2.18	128.95	124.48
26	5	304	XAT	C31-C30-C29	-2.18	124.19	127.31
17	B	831	CLA	CHB-C4A-NA	2.18	127.53	124.51
17	A	818	CLA	C2A-C1A-CHA	2.18	126.10	122.71
17	B	818	CLA	O2A-CGA-O1A	-2.18	118.08	123.59
24	2	501	LUT	C35-C15-C14	-2.18	119.00	123.47
17	A	811	CLA	C1B-CHB-C4A	-2.18	125.79	130.12
17	5	316	CLA	C2D-C1D-ND	-2.18	108.50	110.10
17	A	827	CLA	CHB-C4A-NA	2.18	127.53	124.51
19	2	517	LHG	O8-C23-O10	-2.18	118.08	123.59
20	B	848	BCR	C35-C13-C14	-2.18	119.87	122.92
20	A	845	BCR	C7-C8-C9	-2.18	122.94	126.23
17	K	203	CLA	CBD-CHA-C1A	2.18	131.07	128.50
17	A	806	CLA	C1B-CHB-C4A	-2.18	125.80	130.12
17	2	507	CLA	C2D-C1D-ND	-2.18	108.50	110.10
25	2	515	CHL	CMB-C2B-C3B	2.18	128.95	124.69
17	B	814	CLA	CMA-C3A-C2A	-2.18	111.02	116.10
17	A	840	CLA	C1B-CHB-C4A	-2.18	125.81	130.12
17	5	305	CLA	C3B-C4B-NB	-2.18	107.77	110.36
20	B	847	BCR	C38-C26-C27	2.18	117.80	113.62
17	A	816	CLA	CHD-C1D-ND	-2.17	122.46	124.45
20	A	845	BCR	C23-C24-C25	-2.17	121.10	127.20
17	3	309	CLA	C1B-CHB-C4A	-2.17	125.81	130.12
25	2	516	CHL	O2D-CGD-O1D	-2.17	119.59	123.84
20	B	848	BCR	C38-C26-C27	2.17	117.79	113.62
17	3	313	CLA	C1B-CHB-C4A	-2.17	125.82	130.12
17	A	824	CLA	C1B-CHB-C4A	-2.17	125.82	130.12
20	A	845	BCR	C33-C5-C4	2.17	117.78	113.62
17	A	813	CLA	O2A-CGA-O1A	-2.17	117.89	123.30
16	A	801	CL0	C1-O2A-CGA	2.17	121.57	112.41
24	5	303	LUT	C40-C33-C34	-2.17	119.89	122.92
17	2	510	CLA	C2D-C1D-ND	-2.17	108.51	110.10
25	3	302	CHL	CMD-C2D-C3D	-2.17	122.63	127.61
25	2	513	CHL	C1B-CHB-C4A	-2.17	125.83	130.12
20	F	804	BCR	C31-C1-C6	-2.17	106.78	110.30
25	2	512	CHL	OMC-CMC-C2C	-2.17	120.79	125.69

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	1	507	CLA	O1D-CGD-CBD	2.17	128.91	124.48
20	B	848	BCR	C23-C24-C25	-2.16	121.12	127.20
17	A	815	CLA	O2A-CGA-O1A	-2.16	117.90	123.30
25	5	317	CHL	C3A-C4A-CHB	-2.16	120.34	124.24
17	A	835	CLA	O2A-CGA-O1A	-2.16	118.13	123.59
17	L	301	CLA	C1-C2-C3	-2.16	122.30	126.04
17	B	813	CLA	C1B-CHB-C4A	-2.16	125.83	130.12
20	2	503	BCR	C3-C2-C1	-2.16	106.87	114.60
17	5	313	CLA	CHB-C4A-NA	2.16	127.50	124.51
17	B	824	CLA	CHB-C4A-NA	2.16	127.50	124.51
17	B	808	CLA	C1B-CHB-C4A	-2.16	125.84	130.12
17	5	306	CLA	CHB-C4A-NA	2.16	127.50	124.51
17	5	313	CLA	C2D-C1D-ND	-2.16	108.51	110.10
17	A	836	CLA	C3A-C2A-C1A	2.16	104.57	101.34
17	2	504	CLA	C2D-C1D-ND	-2.15	108.52	110.10
23	5	301	LMG	O7-C10-O9	-2.15	118.50	123.70
20	B	849	BCR	C33-C5-C4	2.15	117.75	113.62
17	A	807	CLA	CHD-C1D-ND	-2.15	122.47	124.45
20	L	306	BCR	C35-C13-C14	-2.15	119.91	122.92
24	1	501	LUT	C21-C26-C27	-2.15	109.98	112.70
22	B	850	DGD	O3G-C1D-C2D	-2.15	104.94	108.30
17	A	823	CLA	O2A-CGA-O1A	-2.15	118.16	123.59
17	1	506	CLA	O2A-CGA-O1A	-2.15	118.16	123.59
17	A	837	CLA	C2D-C1D-ND	-2.15	108.52	110.10
17	F	803	CLA	CHD-C1D-ND	-2.15	122.48	124.45
17	B	826	CLA	O2A-CGA-O1A	-2.15	118.17	123.59
24	3	303	LUT	C19-C9-C8	2.15	121.46	118.08
17	A	831	CLA	CHB-C4A-NA	2.15	127.48	124.51
20	K	204	BCR	C2-C1-C6	2.15	113.79	110.48
20	K	204	BCR	C24-C23-C22	-2.15	122.99	126.23
17	1	515	CLA	C1B-CHB-C4A	-2.15	125.86	130.12
17	B	833	CLA	CHD-C1D-ND	-2.14	122.48	124.45
17	B	815	CLA	CHB-C4A-NA	2.14	127.48	124.51
20	A	851	BCR	C11-C10-C9	-2.14	124.25	127.31
17	B	819	CLA	CHD-C1D-ND	-2.14	122.49	124.45
20	B	849	BCR	C23-C22-C21	2.14	122.23	118.94
20	L	306	BCR	C20-C21-C22	-2.14	124.25	127.31
17	A	807	CLA	C2D-C1D-ND	-2.14	108.53	110.10
25	3	302	CHL	O1D-CGD-CBD	-2.14	120.10	124.48
17	B	810	CLA	C2A-C1A-CHA	2.14	126.03	122.71
17	A	803	CLA	CMA-C3A-C2A	-2.14	111.10	116.10
17	K	202	CLA	C1B-CHB-C4A	-2.14	125.88	130.12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	848	BCR	C37-C22-C21	-2.14	119.93	122.92
17	B	828	CLA	CHB-C4A-NA	2.14	127.47	124.51
17	K	203	CLA	CHB-C4A-NA	2.14	127.47	124.51
25	1	512	CHL	O2D-CGD-O1D	-2.14	119.66	123.84
20	L	305	BCR	C33-C5-C4	2.14	117.72	113.62
17	A	838	CLA	O2A-CGA-O1A	-2.14	118.20	123.59
17	B	834	CLA	CAA-C2A-C1A	-2.14	104.97	111.97
17	A	833	CLA	C2D-C1D-ND	-2.14	108.53	110.10
17	B	813	CLA	C3C-C4C-NC	-2.14	108.18	110.57
20	F	801	BCR	C35-C13-C12	2.14	121.44	118.08
17	A	814	CLA	C3C-C4C-NC	-2.13	108.18	110.57
17	2	510	CLA	O2D-CGD-CBD	2.13	115.06	111.27
17	5	312	CLA	C2D-C1D-ND	-2.13	108.53	110.10
17	3	317	CLA	O2D-CGD-CBD	2.13	115.06	111.27
17	B	820	CLA	CHD-C1D-ND	-2.13	122.50	124.45
17	A	802	CLA	C1B-CHB-C4A	-2.13	125.90	130.12
20	B	845	BCR	C21-C20-C19	-2.13	116.58	123.22
26	5	304	XAT	C30-C31-C32	-2.13	116.58	123.22
17	2	508	CLA	CHB-C4A-NA	2.13	127.45	124.51
20	1	503	BCR	C11-C12-C13	-2.13	120.44	126.42
25	2	512	CHL	C1C-C2C-C3C	-2.13	105.43	107.11
17	A	823	CLA	CHB-C4A-NA	2.12	127.59	124.34
17	A	809	CLA	C1B-CHB-C4A	-2.12	125.91	130.12
20	A	848	BCR	C3-C4-C5	-2.12	110.28	114.08
17	A	815	CLA	CHB-C4A-NA	2.12	127.45	124.51
25	2	513	CHL	CMD-C2D-C3D	-2.12	120.36	126.12
17	B	803	CLA	CHB-C4A-NA	2.12	127.45	124.51
24	1	502	LUT	C16-C1-C6	-2.12	106.86	110.30
17	B	807	CLA	C1B-CHB-C4A	-2.12	125.91	130.12
20	I	101	BCR	C38-C26-C27	2.12	117.69	113.62
17	5	313	CLA	C1B-CHB-C4A	-2.12	125.92	130.12
17	A	832	CLA	CHD-C1D-ND	-2.12	122.50	124.45
17	5	306	CLA	C1B-CHB-C4A	-2.12	125.92	130.12
20	J	102	BCR	C36-C18-C17	-2.12	119.95	122.92
23	5	301	LMG	O8-C28-C29	2.12	118.56	111.91
20	B	845	BCR	C10-C11-C12	-2.12	116.61	123.22
17	K	201	CLA	C2A-C1A-CHA	2.12	127.55	123.85
17	B	840	CLA	C2D-C1D-ND	-2.12	108.54	110.10
20	3	305	BCR	C23-C24-C25	-2.12	121.25	127.20
26	5	304	XAT	C35-C34-C33	-2.12	124.29	127.31
17	A	834	CLA	CHB-C4A-NA	2.12	127.44	124.51
17	B	803	CLA	O2A-CGA-O1A	-2.11	118.25	123.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	B	819	CLA	C3C-C4C-NC	-2.11	108.20	110.57
20	A	849	BCR	C35-C13-C12	2.11	121.41	118.08
20	F	801	BCR	C34-C9-C8	2.11	121.41	118.08
17	A	813	CLA	C1B-CHB-C4A	-2.11	125.93	130.12
17	K	202	CLA	CHB-C4A-NA	2.11	127.43	124.51
23	2	518	LMG	O6-C5-C4	2.11	113.31	109.52
17	A	827	CLA	CHD-C1D-ND	-2.11	122.51	124.45
17	3	301	CLA	C1B-CHB-C4A	-2.11	125.94	130.12
17	B	828	CLA	C1B-CHB-C4A	-2.11	125.94	130.12
25	3	302	CHL	O2A-CGA-CBA	2.11	120.56	112.23
20	K	204	BCR	C23-C24-C25	-2.11	121.28	127.20
17	B	801	CLA	O2D-CGD-CBD	2.10	115.01	111.27
17	A	802	CLA	C2D-C1D-ND	-2.10	108.55	110.10
17	3	313	CLA	O2A-CGA-O1A	-2.10	118.28	123.59
17	B	841	CLA	C2D-C1D-ND	-2.10	108.55	110.10
17	B	827	CLA	O2D-CGD-CBD	2.10	115.00	111.27
17	B	803	CLA	O1D-CGD-CBD	2.10	128.78	124.48
17	A	811	CLA	CHB-C4A-NA	2.10	127.42	124.51
17	2	511	CLA	C2D-C1D-ND	-2.10	108.56	110.10
20	L	305	BCR	C16-C15-C14	-2.10	119.18	123.47
17	3	313	CLA	C3C-C4C-NC	-2.10	108.22	110.57
26	5	304	XAT	C19-C9-C8	2.10	121.38	118.08
25	2	513	CHL	CHB-C4A-NA	2.10	127.41	124.51
17	2	507	CLA	CBD-CHA-C1A	2.10	130.97	128.50
17	B	815	CLA	O2A-CGA-O1A	-2.09	118.31	123.59
17	L	301	CLA	O2A-CGA-O1A	-2.09	118.31	123.59
20	F	801	BCR	C16-C15-C14	-2.09	119.19	123.47
16	A	801	CL0	C3D-C2D-C1D	-2.09	102.97	105.83
17	B	806	CLA	C2A-C1A-CHA	2.09	125.96	122.71
20	L	306	BCR	C34-C9-C8	2.09	121.37	118.08
17	B	814	CLA	CHD-C1D-ND	-2.09	122.53	124.45
20	A	845	BCR	C39-C30-C25	-2.09	106.91	110.30
24	3	303	LUT	C12-C13-C14	-2.09	115.73	118.94
17	J	101	CLA	C2D-C1D-ND	-2.09	108.56	110.10
17	A	837	CLA	O2D-CGD-CBD	2.09	114.98	111.27
20	B	848	BCR	C35-C13-C12	2.09	121.37	118.08
20	A	851	BCR	C10-C11-C12	-2.09	116.70	123.22
20	A	849	BCR	C18-C19-C20	-2.09	120.17	124.81
17	1	505	CLA	CHD-C1D-ND	-2.09	122.54	124.45
20	A	853	BCR	C30-C25-C26	-2.09	119.67	122.61
17	A	833	CLA	C1B-CHB-C4A	-2.09	125.98	130.12
24	1	501	LUT	C35-C15-C14	-2.09	119.20	123.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	B	840	CLA	C1B-CHB-C4A	-2.09	125.99	130.12
16	A	801	CL0	C4-C3-C5	2.08	118.78	115.27
20	I	101	BCR	C37-C22-C21	-2.08	120.00	122.92
24	3	304	LUT	C2-C3-C4	-2.08	107.45	110.30
20	A	847	BCR	C36-C18-C19	2.08	121.36	118.08
17	1	513	CLA	O2D-CGD-CBD	2.08	114.96	111.27
17	B	831	CLA	C1B-CHB-C4A	-2.08	126.00	130.12
20	J	102	BCR	C33-C5-C4	2.08	117.61	113.62
17	B	832	CLA	CHB-C4A-NA	2.08	127.38	124.51
20	A	851	BCR	C36-C18-C17	-2.08	120.02	122.92
20	I	101	BCR	C33-C5-C4	2.08	117.60	113.62
17	5	305	CLA	O1D-CGD-CBD	2.07	128.73	124.48
17	B	825	CLA	C2A-C1A-CHA	2.07	127.49	123.86
17	A	808	CLA	C1-C2-C3	-2.07	122.46	126.04
17	A	826	CLA	C1B-CHB-C4A	-2.07	126.01	130.12
25	3	315	CHL	O2D-CGD-O1D	-2.07	119.79	123.84
17	A	823	CLA	C2D-C1D-ND	-2.07	108.58	110.10
17	A	821	CLA	CAA-C2A-C1A	-2.07	107.56	112.14
17	A	852	CLA	C1-C2-C3	-2.07	122.46	126.04
20	B	852	BCR	C21-C20-C19	-2.07	116.76	123.22
17	A	839	CLA	O2D-CGD-CBD	2.07	114.94	111.27
20	F	801	BCR	C3-C4-C5	-2.07	110.39	114.08
17	A	819	CLA	CBD-CHA-C1A	2.07	130.94	128.50
17	A	827	CLA	O1D-CGD-CBD	2.07	128.71	124.48
17	B	836	CLA	CHD-C1D-ND	-2.07	122.56	124.45
17	A	840	CLA	CMB-C2B-C3B	2.06	128.54	124.68
20	K	204	BCR	C31-C1-C6	-2.06	106.95	110.30
20	J	102	BCR	C15-C16-C17	-2.06	119.25	123.47
17	A	836	CLA	CHB-C4A-NA	2.06	127.37	124.51
17	A	821	CLA	C1B-CHB-C4A	-2.06	126.03	130.12
17	A	811	CLA	CHD-C1D-ND	-2.06	122.56	124.45
17	B	839	CLA	O1D-CGD-CBD	2.06	128.71	124.48
17	1	511	CLA	CAA-C2A-C3A	-2.06	107.13	112.78
17	B	835	CLA	C3C-C4C-NC	-2.06	108.26	110.57
17	B	828	CLA	O2D-CGD-CBD	2.06	114.93	111.27
17	A	810	CLA	O2A-CGA-O1A	-2.06	118.39	123.59
24	5	303	LUT	C11-C10-C9	-2.06	124.37	127.31
17	5	316	CLA	CMA-C3A-C2A	-2.06	111.29	116.10
17	B	813	CLA	CHD-C1D-ND	-2.06	122.56	124.45
17	A	826	CLA	O1D-CGD-CBD	2.06	128.69	124.48
17	3	317	CLA	C1B-CHB-C4A	-2.06	126.04	130.12
24	5	303	LUT	C30-C31-C32	-2.06	116.80	123.22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	2	501	LUT	C38-C25-C24	-2.05	119.17	123.56
17	B	837	CLA	CHA-C1A-NA	-2.05	121.70	126.40
25	5	317	CHL	C4D-CHA-C1A	-2.05	118.75	121.25
25	5	315	CHL	O1D-CGD-CBD	-2.05	120.29	124.48
17	A	811	CLA	C2A-C1A-CHA	2.05	125.89	122.71
24	1	502	LUT	C39-C29-C28	2.05	121.31	118.08
17	A	831	CLA	C3C-C4C-NC	-2.05	108.27	110.57
17	B	812	CLA	C1B-CHB-C4A	-2.05	126.06	130.12
17	3	307	CLA	C2A-C1A-CHA	2.05	125.89	122.71
17	K	205	CLA	C2D-C1D-ND	-2.05	108.59	110.10
17	B	817	CLA	O2A-CGA-O1A	-2.05	118.42	123.59
25	5	317	CHL	C2A-C1A-CHA	-2.05	120.36	123.81
17	A	816	CLA	O2A-CGA-O1A	-2.05	118.42	123.59
17	B	810	CLA	C1B-CHB-C4A	-2.05	126.06	130.12
17	1	505	CLA	C1B-CHB-C4A	-2.05	126.06	130.12
17	3	306	CLA	C3C-C4C-NC	-2.05	108.34	110.57
17	A	838	CLA	O1D-CGD-CBD	2.05	128.67	124.48
26	2	502	XAT	O4-C5-C6	-2.04	57.27	58.96
20	J	102	BCR	C21-C20-C19	-2.04	116.84	123.22
25	5	314	CHL	O2A-CGA-CBA	2.04	120.30	112.23
20	B	848	BCR	C8-C7-C6	-2.04	121.47	127.20
17	A	805	CLA	C2D-C1D-ND	-2.04	108.60	110.10
25	2	512	CHL	C4B-C3B-C2B	-2.04	105.02	106.92
20	2	503	BCR	C28-C29-C30	-2.04	107.31	114.60
19	A	844	LHG	O8-C23-C24	2.04	118.31	111.91
24	5	303	LUT	C28-C29-C30	-2.04	115.81	118.94
17	3	301	CLA	CMA-C3A-C2A	-2.04	111.34	116.10
17	3	316	CLA	CMA-C3A-C2A	-2.04	111.34	116.10
24	5	303	LUT	C8-C7-C6	-2.04	121.48	127.20
17	3	314	CLA	O2A-CGA-O1A	-2.04	118.45	123.59
17	A	836	CLA	C1B-CHB-C4A	-2.04	126.08	130.12
17	L	304	CLA	C2D-C1D-ND	-2.04	108.60	110.10
20	A	849	BCR	C33-C5-C6	-2.04	122.24	124.53
17	B	829	CLA	CBD-CHA-C1A	2.04	130.90	128.50
17	B	814	CLA	CHA-C1A-NA	-2.04	121.74	126.40
17	1	507	CLA	C2D-C1D-ND	-2.04	108.60	110.10
20	A	849	BCR	C37-C22-C21	-2.04	120.07	122.92
20	B	849	BCR	C2-C1-C6	2.04	113.61	110.48
24	2	501	LUT	C21-C26-C27	-2.03	110.13	112.70
17	B	801	CLA	CHD-C1D-ND	-2.03	122.58	124.45
17	K	203	CLA	CHD-C1D-ND	-2.03	122.58	124.45
25	1	514	CHL	O1D-CGD-CBD	-2.03	120.32	124.48

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	1	512	CHL	O2A-CGA-CBA	2.03	120.27	112.23
17	B	835	CLA	CHD-C1D-ND	-2.03	122.59	124.45
17	B	808	CLA	CHB-C4A-NA	2.03	127.32	124.51
20	B	844	BCR	C38-C26-C27	2.03	117.52	113.62
20	B	852	BCR	C20-C21-C22	-2.03	124.41	127.31
17	3	308	CLA	C3A-C2A-C1A	2.03	104.38	101.34
20	B	852	BCR	C33-C5-C4	2.03	117.52	113.62
17	A	829	CLA	CHB-C4A-NA	2.03	127.32	124.51
17	A	812	CLA	CHD-C1D-ND	-2.03	122.59	124.45
17	2	504	CLA	C2A-C1A-CHA	2.03	125.86	122.71
17	B	814	CLA	C1B-CHB-C4A	-2.03	126.10	130.12
17	B	806	CLA	C3C-C4C-NC	-2.03	108.30	110.57
20	J	102	BCR	C37-C22-C21	-2.03	120.08	122.92
17	A	803	CLA	CHD-C1D-ND	-2.03	122.59	124.45
20	B	844	BCR	C23-C24-C25	-2.03	121.51	127.20
17	A	812	CLA	O2D-CGD-CBD	2.03	114.87	111.27
17	A	805	CLA	CAA-C2A-C1A	-2.03	105.34	111.97
20	B	845	BCR	C38-C26-C27	2.02	117.50	113.62
17	B	814	CLA	C2A-C1A-CHA	2.02	127.39	123.85
17	K	202	CLA	O2D-CGD-CBD	2.02	114.86	111.27
20	F	804	BCR	C12-C13-C14	2.02	122.05	118.94
25	1	514	CHL	C1C-C2C-C3C	-2.02	105.51	107.11
20	A	853	BCR	C36-C18-C17	-2.02	120.09	122.92
23	2	519	LMG	C8-O7-C10	-2.02	112.81	117.79
17	B	804	CLA	C1B-CHB-C4A	-2.02	126.11	130.12
17	2	509	CLA	O2A-CGA-O1A	-2.02	118.49	123.59
20	5	302	BCR	C24-C23-C22	-2.02	123.18	126.23
20	A	847	BCR	C23-C24-C25	-2.02	121.53	127.20
17	B	815	CLA	C3C-C4C-NC	-2.02	108.31	110.57
20	B	846	BCR	C36-C18-C19	2.02	121.26	118.08
26	2	502	XAT	C20-C13-C14	-2.02	120.10	122.92
24	1	502	LUT	C35-C34-C33	-2.02	124.43	127.31
20	A	848	BCR	C35-C13-C14	-2.02	120.10	122.92
17	3	314	CLA	C1-C2-C3	-2.02	122.56	126.04
25	5	314	CHL	CHB-C4A-NA	2.01	127.30	124.51
25	2	515	CHL	C4B-C3B-C2B	-2.01	105.05	106.92
17	A	842	CLA	CHD-C1D-ND	-2.01	122.60	124.45
17	B	829	CLA	C2A-C1A-CHA	2.01	125.83	122.71
17	B	828	CLA	O1D-CGD-CBD	2.01	128.60	124.48
20	F	804	BCR	C1-C6-C5	-2.01	119.78	122.61
25	1	512	CHL	CED-O2D-CGD	2.01	120.48	115.94
17	B	801	CLA	C3C-C4C-NC	-2.01	108.32	110.57

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	B	841	CLA	O1D-CGD-CBD	2.01	128.59	124.48
23	F	806	LMG	C9-C8-C7	-2.01	107.04	111.79
17	3	310	CLA	O1A-CGA-CBA	2.01	129.53	123.08
17	5	308	CLA	CAC-C3C-C4C	2.00	127.41	124.81
24	5	303	LUT	C10-C11-C12	-2.00	116.97	123.22
17	B	812	CLA	O2A-CGA-O1A	-2.00	118.54	123.59
25	5	315	CHL	CHD-C1D-C2D	2.00	129.68	125.48
20	B	852	BCR	C2-C3-C4	-2.00	106.90	111.38
17	5	311	CLA	CAA-C2A-C3A	-2.00	109.26	114.26
19	B	851	LHG	O7-C7-O9	-2.00	118.87	123.70
17	3	314	CLA	C2D-C1D-ND	-2.00	108.63	110.10

All (171) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
16	A	801	CL0	ND
16	A	801	CL0	NA
16	A	801	CL0	NC
17	A	802	CLA	ND
17	A	803	CLA	ND
17	A	804	CLA	ND
17	A	805	CLA	ND
17	A	806	CLA	ND
17	A	807	CLA	ND
17	A	808	CLA	ND
17	A	809	CLA	ND
17	A	810	CLA	ND
17	A	811	CLA	ND
17	A	812	CLA	ND
17	A	813	CLA	ND
17	A	814	CLA	ND
17	A	815	CLA	ND
17	A	816	CLA	ND
17	A	817	CLA	ND
17	A	818	CLA	ND
17	A	819	CLA	ND
17	A	820	CLA	ND
17	A	821	CLA	ND
17	A	822	CLA	ND
17	A	823	CLA	ND
17	A	824	CLA	ND
17	A	825	CLA	ND

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
17	A	826	CLA	ND
17	A	827	CLA	ND
17	A	828	CLA	ND
17	A	829	CLA	ND
17	A	830	CLA	ND
17	A	831	CLA	ND
17	A	832	CLA	ND
17	A	833	CLA	ND
17	A	834	CLA	ND
17	A	835	CLA	ND
17	A	836	CLA	ND
17	A	837	CLA	ND
17	A	838	CLA	ND
17	A	839	CLA	ND
17	A	840	CLA	ND
17	A	842	CLA	ND
17	A	852	CLA	ND
17	B	801	CLA	ND
17	B	802	CLA	ND
17	B	803	CLA	ND
17	B	804	CLA	ND
17	B	805	CLA	ND
17	B	806	CLA	ND
17	B	807	CLA	ND
17	B	808	CLA	ND
17	B	809	CLA	ND
17	B	810	CLA	ND
17	B	811	CLA	ND
17	B	812	CLA	ND
17	B	813	CLA	ND
17	B	814	CLA	ND
17	B	815	CLA	ND
17	B	816	CLA	ND
17	B	817	CLA	ND
17	B	818	CLA	ND
17	B	819	CLA	ND
17	B	820	CLA	ND
17	B	821	CLA	ND
17	B	822	CLA	ND
17	B	823	CLA	ND
17	B	824	CLA	ND
17	B	825	CLA	ND

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
17	B	826	CLA	ND
17	B	827	CLA	ND
17	B	828	CLA	ND
17	B	829	CLA	ND
17	B	830	CLA	ND
17	B	831	CLA	ND
17	B	832	CLA	ND
17	B	833	CLA	ND
17	B	834	CLA	ND
17	B	835	CLA	ND
17	B	837	CLA	ND
17	B	838	CLA	ND
17	B	839	CLA	ND
17	B	840	CLA	ND
17	B	841	CLA	ND
17	B	842	CLA	ND
17	F	802	CLA	ND
17	F	803	CLA	ND
17	J	101	CLA	ND
17	K	201	CLA	ND
17	K	202	CLA	ND
17	K	203	CLA	ND
17	K	205	CLA	ND
17	L	301	CLA	ND
17	L	302	CLA	ND
17	L	303	CLA	ND
17	L	304	CLA	ND
17	1	504	CLA	ND
17	1	505	CLA	ND
17	1	506	CLA	ND
17	1	507	CLA	ND
17	1	508	CLA	ND
17	1	510	CLA	ND
17	1	511	CLA	ND
17	1	515	CLA	ND
17	2	504	CLA	ND
17	2	506	CLA	ND
17	2	507	CLA	ND
17	2	507	CLA	C8
17	2	508	CLA	ND
17	2	509	CLA	ND
17	2	510	CLA	ND

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
17	2	511	CLA	ND
17	2	514	CLA	ND
17	3	301	CLA	ND
17	3	306	CLA	ND
17	3	307	CLA	ND
17	3	308	CLA	ND
17	3	310	CLA	ND
17	3	311	CLA	ND
17	3	312	CLA	ND
17	3	313	CLA	ND
17	3	314	CLA	ND
17	3	316	CLA	ND
17	3	317	CLA	ND
17	3	318	CLA	ND
17	5	305	CLA	ND
17	5	306	CLA	ND
17	5	307	CLA	ND
17	5	308	CLA	ND
17	5	309	CLA	ND
17	5	310	CLA	ND
17	5	311	CLA	ND
17	5	312	CLA	ND
17	5	313	CLA	ND
17	5	316	CLA	ND
25	1	512	CHL	ND
25	1	512	CHL	NA
25	1	512	CHL	NC
25	1	514	CHL	ND
25	1	514	CHL	NA
25	1	514	CHL	NC
25	1	517	CHL	ND
25	1	517	CHL	NA
25	1	517	CHL	NC
25	2	512	CHL	ND
25	2	512	CHL	NA
25	2	512	CHL	NC
25	2	513	CHL	ND
25	2	513	CHL	NA
25	2	513	CHL	NC
25	2	515	CHL	ND
25	2	515	CHL	NA
25	2	515	CHL	NC

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
25	2	516	CHL	ND
25	2	516	CHL	NA
25	2	516	CHL	NC
25	3	302	CHL	ND
25	3	302	CHL	NA
25	3	302	CHL	NC
25	3	315	CHL	ND
25	3	315	CHL	NA
25	3	315	CHL	NC
25	5	314	CHL	ND
25	5	314	CHL	NA
25	5	314	CHL	NC
25	5	315	CHL	ND
25	5	315	CHL	NA
25	5	315	CHL	NC
25	5	317	CHL	ND
25	5	317	CHL	NA
25	5	317	CHL	NC

All (1257) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
16	A	801	CL0	C1A-C2A-CAA-CBA
16	A	801	CL0	CHA-CBD-CGD-O2D
17	A	802	CLA	CHA-CBD-CGD-O1D
17	A	802	CLA	CHA-CBD-CGD-O2D
17	A	802	CLA	C6-C7-C8-C9
17	A	804	CLA	C1A-C2A-CAA-CBA
17	A	804	CLA	C3A-C2A-CAA-CBA
17	A	805	CLA	C1A-C2A-CAA-CBA
17	A	805	CLA	CHA-CBD-CGD-O1D
17	A	805	CLA	CHA-CBD-CGD-O2D
17	A	806	CLA	CHA-CBD-CGD-O1D
17	A	806	CLA	CHA-CBD-CGD-O2D
17	A	807	CLA	CAD-CBD-CGD-O2D
17	A	809	CLA	C1A-C2A-CAA-CBA
17	A	816	CLA	CBD-CGD-O2D-CED
17	A	818	CLA	CHA-CBD-CGD-O1D
17	A	818	CLA	CHA-CBD-CGD-O2D
17	A	821	CLA	C1A-C2A-CAA-CBA
17	A	821	CLA	C3A-C2A-CAA-CBA
17	A	822	CLA	CBD-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
17	A	823	CLA	C1A-C2A-CAA-CBA
17	A	823	CLA	CHA-CBD-CGD-O1D
17	A	823	CLA	CHA-CBD-CGD-O2D
17	A	827	CLA	CBD-CGD-O2D-CED
17	A	831	CLA	C2A-CAA-CBA-CGA
17	A	831	CLA	CAD-CBD-CGD-O1D
17	A	831	CLA	CAD-CBD-CGD-O2D
17	A	831	CLA	CBD-CGD-O2D-CED
17	A	835	CLA	CAD-CBD-CGD-O1D
17	A	835	CLA	CAD-CBD-CGD-O2D
17	A	835	CLA	C2-C3-C5-C6
17	A	838	CLA	CHA-CBD-CGD-O1D
17	A	838	CLA	CHA-CBD-CGD-O2D
17	A	842	CLA	C1A-C2A-CAA-CBA
17	A	842	CLA	C3A-C2A-CAA-CBA
17	A	842	CLA	CHA-CBD-CGD-O2D
17	A	842	CLA	CBD-CGD-O2D-CED
17	A	852	CLA	CBD-CGD-O2D-CED
17	B	803	CLA	CHA-CBD-CGD-O1D
17	B	803	CLA	CHA-CBD-CGD-O2D
17	B	804	CLA	C3A-C2A-CAA-CBA
17	B	804	CLA	CBD-CGD-O2D-CED
17	B	805	CLA	CBD-CGD-O2D-CED
17	B	806	CLA	CHA-CBD-CGD-O1D
17	B	806	CLA	CHA-CBD-CGD-O2D
17	B	806	CLA	CAD-CBD-CGD-O1D
17	B	810	CLA	CHA-CBD-CGD-O1D
17	B	810	CLA	CHA-CBD-CGD-O2D
17	B	811	CLA	C1A-C2A-CAA-CBA
17	B	811	CLA	CHA-CBD-CGD-O1D
17	B	811	CLA	CHA-CBD-CGD-O2D
17	B	811	CLA	CAD-CBD-CGD-O1D
17	B	811	CLA	CAD-CBD-CGD-O2D
17	B	812	CLA	CBD-CGD-O2D-CED
17	B	815	CLA	CBD-CGD-O2D-CED
17	B	817	CLA	CBD-CGD-O2D-CED
17	B	818	CLA	C1A-C2A-CAA-CBA
17	B	818	CLA	C3A-C2A-CAA-CBA
17	B	818	CLA	C2-C3-C5-C6
17	B	818	CLA	C4-C3-C5-C6
17	B	822	CLA	CHA-CBD-CGD-O1D
17	B	822	CLA	CHA-CBD-CGD-O2D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
17	B	823	CLA	C1A-C2A-CAA-CBA
17	B	823	CLA	C3A-C2A-CAA-CBA
17	B	824	CLA	C1A-C2A-CAA-CBA
17	B	824	CLA	C3A-C2A-CAA-CBA
17	B	824	CLA	CHA-CBD-CGD-O1D
17	B	824	CLA	CHA-CBD-CGD-O2D
17	B	826	CLA	C11-C12-C13-C14
17	B	832	CLA	CBD-CGD-O2D-CED
17	B	834	CLA	C1A-C2A-CAA-CBA
17	B	835	CLA	CBD-CGD-O2D-CED
17	B	836	CLA	C3A-C2A-CAA-CBA
17	B	838	CLA	CHA-CBD-CGD-O1D
17	B	838	CLA	CHA-CBD-CGD-O2D
17	B	842	CLA	C1A-C2A-CAA-CBA
17	B	842	CLA	C3A-C2A-CAA-CBA
17	J	101	CLA	CHA-CBD-CGD-O1D
17	J	101	CLA	CHA-CBD-CGD-O2D
17	K	203	CLA	CBD-CGD-O2D-CED
17	L	303	CLA	C1A-C2A-CAA-CBA
17	L	303	CLA	C3-C5-C6-C7
17	L	304	CLA	CHA-CBD-CGD-O1D
17	L	304	CLA	CHA-CBD-CGD-O2D
17	1	505	CLA	C1A-C2A-CAA-CBA
17	1	505	CLA	C3A-C2A-CAA-CBA
17	1	506	CLA	C1A-C2A-CAA-CBA
17	1	506	CLA	C3A-C2A-CAA-CBA
17	1	507	CLA	CBD-CGD-O2D-CED
17	1	508	CLA	CBD-CGD-O2D-CED
17	1	509	CLA	CHA-CBD-CGD-O1D
17	1	509	CLA	CHA-CBD-CGD-O2D
17	1	510	CLA	C1A-C2A-CAA-CBA
17	1	510	CLA	C3A-C2A-CAA-CBA
17	1	510	CLA	CBD-CGD-O2D-CED
17	1	511	CLA	CBA-CGA-O2A-C1
17	1	511	CLA	CBD-CGD-O2D-CED
17	2	505	CLA	CBD-CGD-O2D-CED
17	2	505	CLA	C3-C5-C6-C7
17	2	506	CLA	CHA-CBD-CGD-O1D
17	2	506	CLA	CHA-CBD-CGD-O2D
17	2	509	CLA	C1A-C2A-CAA-CBA
17	2	510	CLA	CBA-CGA-O2A-C1
17	3	306	CLA	C1A-C2A-CAA-CBA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
17	3	306	CLA	C3A-C2A-CAA-CBA
17	3	306	CLA	C2-C1-O2A-CGA
17	3	306	CLA	CBD-CGD-O2D-CED
17	3	308	CLA	CHA-CBD-CGD-O1D
17	3	308	CLA	CHA-CBD-CGD-O2D
17	3	308	CLA	CBD-CGD-O2D-CED
17	3	309	CLA	CHA-CBD-CGD-O1D
17	3	309	CLA	CHA-CBD-CGD-O2D
17	3	309	CLA	CBD-CGD-O2D-CED
17	3	311	CLA	CBD-CGD-O2D-CED
17	3	312	CLA	CBD-CGD-O2D-CED
17	3	313	CLA	CHA-CBD-CGD-O1D
17	3	313	CLA	CBD-CGD-O2D-CED
17	3	317	CLA	CHA-CBD-CGD-O1D
17	3	317	CLA	CHA-CBD-CGD-O2D
17	5	307	CLA	CBA-CGA-O2A-C1
17	5	307	CLA	O1A-CGA-O2A-C1
17	5	307	CLA	CHA-CBD-CGD-O1D
17	5	307	CLA	CHA-CBD-CGD-O2D
17	5	307	CLA	C2-C3-C5-C6
17	5	307	CLA	C4-C3-C5-C6
17	5	310	CLA	CHA-CBD-CGD-O1D
17	5	310	CLA	CHA-CBD-CGD-O2D
17	5	312	CLA	CHA-CBD-CGD-O1D
17	5	312	CLA	CHA-CBD-CGD-O2D
17	5	312	CLA	CBD-CGD-O2D-CED
17	5	313	CLA	CAD-CBD-CGD-O1D
17	5	313	CLA	CAD-CBD-CGD-O2D
19	A	843	LHG	C3-O3-P-O4
19	A	844	LHG	C4-O6-P-O4
19	A	844	LHG	C4-O6-P-O5
19	B	851	LHG	C4-O6-P-O4
19	1	516	LHG	C4-O6-P-O3
19	1	516	LHG	C4-O6-P-O5
19	2	517	LHG	C4-O6-P-O5
20	A	845	BCR	C21-C22-C23-C24
20	A	845	BCR	C37-C22-C23-C24
20	A	848	BCR	C23-C24-C25-C26
20	A	851	BCR	C5-C6-C7-C8
20	B	844	BCR	C1-C6-C7-C8
20	B	845	BCR	C21-C22-C23-C24
20	B	845	BCR	C37-C22-C23-C24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
20	B	847	BCR	C1-C6-C7-C8
20	B	847	BCR	C5-C6-C7-C8
20	B	849	BCR	C21-C22-C23-C24
20	B	849	BCR	C37-C22-C23-C24
20	F	801	BCR	C17-C18-C19-C20
20	F	801	BCR	C36-C18-C19-C20
20	F	801	BCR	C37-C22-C23-C24
20	I	101	BCR	C21-C22-C23-C24
20	I	101	BCR	C37-C22-C23-C24
20	I	101	BCR	C23-C24-C25-C26
20	I	101	BCR	C23-C24-C25-C30
20	K	204	BCR	C1-C6-C7-C8
20	K	204	BCR	C23-C24-C25-C26
20	L	305	BCR	C17-C18-C19-C20
20	L	305	BCR	C36-C18-C19-C20
20	L	305	BCR	C21-C22-C23-C24
20	L	305	BCR	C37-C22-C23-C24
20	2	503	BCR	C21-C22-C23-C24
20	2	503	BCR	C37-C22-C23-C24
20	3	305	BCR	C7-C8-C9-C34
20	5	302	BCR	C1-C6-C7-C8
20	5	302	BCR	C5-C6-C7-C8
20	5	302	BCR	C11-C12-C13-C14
20	5	302	BCR	C11-C12-C13-C35
22	B	850	DGD	C2B-C1B-O2G-C2G
22	B	850	DGD	O1B-C1B-O2G-C2G
22	J	103	DGD	C2E-C1E-O5D-C6D
22	J	103	DGD	O6E-C1E-O5D-C6D
23	F	806	LMG	C2-C1-O1-C7
23	F	806	LMG	O6-C1-O1-C7
23	2	519	LMG	O9-C10-O7-C8
24	1	501	LUT	C1-C6-C7-C8
24	1	501	LUT	C5-C6-C7-C8
24	3	303	LUT	C1-C6-C7-C8
25	1	512	CHL	C3C-C2C-CMC-OMC
25	1	517	CHL	C3C-C2C-CMC-OMC
25	2	515	CHL	C1A-C2A-CAA-CBA
25	2	515	CHL	C3C-C2C-CMC-OMC
25	2	516	CHL	CHA-CBD-CGD-O1D
25	2	516	CHL	CHA-CBD-CGD-O2D
25	2	516	CHL	CAD-CBD-CGD-O1D
25	3	315	CHL	C1A-C2A-CAA-CBA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
25	5	314	CHL	C3C-C2C-CMC-OMC
25	5	315	CHL	C3C-C2C-CMC-OMC
25	5	317	CHL	C3C-C2C-CMC-OMC
26	2	502	XAT	C5-C6-C7-C8
26	2	502	XAT	O4-C6-C7-C8
26	2	502	XAT	C7-C8-C9-C10
26	2	502	XAT	C7-C8-C9-C19
26	2	502	XAT	C27-C28-C29-C30
26	2	502	XAT	C27-C28-C29-C39
17	B	836	CLA	O1D-CGD-O2D-CED
17	2	509	CLA	O1D-CGD-O2D-CED
17	A	806	CLA	O1D-CGD-O2D-CED
17	A	852	CLA	O1D-CGD-O2D-CED
17	B	803	CLA	O1D-CGD-O2D-CED
17	B	804	CLA	O1D-CGD-O2D-CED
17	B	812	CLA	O1D-CGD-O2D-CED
17	B	832	CLA	O1D-CGD-O2D-CED
17	3	301	CLA	O1D-CGD-O2D-CED
17	3	306	CLA	O1D-CGD-O2D-CED
17	3	308	CLA	O1D-CGD-O2D-CED
17	3	312	CLA	O1D-CGD-O2D-CED
17	3	317	CLA	O1D-CGD-O2D-CED
17	5	307	CLA	O1D-CGD-O2D-CED
17	A	806	CLA	CBD-CGD-O2D-CED
17	A	810	CLA	CBD-CGD-O2D-CED
17	A	813	CLA	CBD-CGD-O2D-CED
17	A	815	CLA	CBD-CGD-O2D-CED
17	A	820	CLA	CBD-CGD-O2D-CED
17	A	828	CLA	CBD-CGD-O2D-CED
17	B	803	CLA	CBD-CGD-O2D-CED
17	B	811	CLA	CBD-CGD-O2D-CED
17	B	814	CLA	CBD-CGD-O2D-CED
17	B	816	CLA	CBD-CGD-O2D-CED
17	B	820	CLA	CBD-CGD-O2D-CED
17	B	823	CLA	CBD-CGD-O2D-CED
17	B	836	CLA	CBD-CGD-O2D-CED
17	F	802	CLA	CBD-CGD-O2D-CED
17	1	506	CLA	CBD-CGD-O2D-CED
17	1	509	CLA	CBD-CGD-O2D-CED
17	1	513	CLA	CBD-CGD-O2D-CED
17	1	515	CLA	CBD-CGD-O2D-CED
17	2	509	CLA	CBD-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
17	2	514	CLA	CBD-CGD-O2D-CED
17	3	301	CLA	CBD-CGD-O2D-CED
17	3	307	CLA	CBD-CGD-O2D-CED
17	3	317	CLA	CBD-CGD-O2D-CED
17	5	307	CLA	CBD-CGD-O2D-CED
17	5	309	CLA	CBD-CGD-O2D-CED
25	2	513	CHL	CBD-CGD-O2D-CED
25	5	315	CHL	CBD-CGD-O2D-CED
17	L	303	CLA	O1A-CGA-O2A-C1
17	1	509	CLA	O1A-CGA-O2A-C1
17	2	510	CLA	O1A-CGA-O2A-C1
17	A	816	CLA	O1D-CGD-O2D-CED
17	A	820	CLA	O1D-CGD-O2D-CED
17	B	815	CLA	O1D-CGD-O2D-CED
17	1	513	CLA	O1D-CGD-O2D-CED
17	3	307	CLA	O1D-CGD-O2D-CED
17	5	309	CLA	O1D-CGD-O2D-CED
17	A	831	CLA	O1D-CGD-O2D-CED
17	B	835	CLA	O1D-CGD-O2D-CED
17	1	507	CLA	O1D-CGD-O2D-CED
17	1	508	CLA	O1D-CGD-O2D-CED
17	1	510	CLA	O1D-CGD-O2D-CED
17	1	511	CLA	O1D-CGD-O2D-CED
17	1	509	CLA	CBA-CGA-O2A-C1
17	L	304	CLA	CBD-CGD-O2D-CED
17	2	507	CLA	CBD-CGD-O2D-CED
17	5	308	CLA	CBD-CGD-O2D-CED
17	5	316	CLA	CBD-CGD-O2D-CED
25	2	516	CHL	CBD-CGD-O2D-CED
25	3	315	CHL	CBD-CGD-O2D-CED
17	A	831	CLA	O1A-CGA-O2A-C1
17	3	308	CLA	O1A-CGA-O2A-C1
17	5	310	CLA	O1A-CGA-O2A-C1
23	F	806	LMG	O10-C28-O8-C9
17	1	511	CLA	O1A-CGA-O2A-C1
17	A	827	CLA	O1D-CGD-O2D-CED
17	B	817	CLA	O1D-CGD-O2D-CED
17	2	505	CLA	O1D-CGD-O2D-CED
17	A	822	CLA	O1D-CGD-O2D-CED
17	A	842	CLA	O1D-CGD-O2D-CED
17	K	203	CLA	O1D-CGD-O2D-CED
17	3	309	CLA	O1D-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
17	3	311	CLA	O1D-CGD-O2D-CED
17	5	312	CLA	O1D-CGD-O2D-CED
25	1	512	CHL	CBD-CGD-O2D-CED
17	B	805	CLA	O1D-CGD-O2D-CED
17	B	823	CLA	O1D-CGD-O2D-CED
17	1	515	CLA	O1D-CGD-O2D-CED
17	3	313	CLA	O1D-CGD-O2D-CED
17	3	318	CLA	CBA-CGA-O2A-C1
17	3	318	CLA	O1A-CGA-O2A-C1
17	B	807	CLA	C3-C5-C6-C7
17	B	811	CLA	C3-C5-C6-C7
17	B	841	CLA	C3-C5-C6-C7
17	3	306	CLA	C3-C5-C6-C7
18	A	841	PQN	C13-C15-C16-C17
17	A	831	CLA	CBA-CGA-O2A-C1
17	A	835	CLA	CBA-CGA-O2A-C1
17	L	303	CLA	CBA-CGA-O2A-C1
17	3	308	CLA	CBA-CGA-O2A-C1
22	J	103	DGD	C2A-C1A-O1G-C1G
23	F	806	LMG	C29-C28-O8-C9
17	L	304	CLA	C2C-C3C-CAC-CBC
23	2	519	LMG	C11-C10-O7-C8
17	B	816	CLA	O1D-CGD-O2D-CED
17	3	318	CLA	CBD-CGD-O2D-CED
17	2	514	CLA	O1A-CGA-O2A-C1
17	A	836	CLA	C4-C3-C5-C6
17	B	841	CLA	C4-C3-C5-C6
17	L	303	CLA	C4-C3-C5-C6
17	3	308	CLA	C4-C3-C5-C6
17	2	506	CLA	CBD-CGD-O2D-CED
17	2	510	CLA	CBD-CGD-O2D-CED
17	5	310	CLA	CBD-CGD-O2D-CED
17	B	801	CLA	C2A-CAA-CBA-CGA
17	3	308	CLA	C2A-CAA-CBA-CGA
17	3	314	CLA	C2A-CAA-CBA-CGA
25	2	512	CHL	C2A-CAA-CBA-CGA
25	5	314	CHL	C2A-CAA-CBA-CGA
17	B	820	CLA	O1D-CGD-O2D-CED
17	A	836	CLA	C3-C5-C6-C7
17	B	835	CLA	C3-C5-C6-C7
17	3	314	CLA	C3-C5-C6-C7
17	A	816	CLA	CBA-CGA-O2A-C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
17	B	822	CLA	CBA-CGA-O2A-C1
17	B	830	CLA	CBA-CGA-O2A-C1
17	5	310	CLA	CBA-CGA-O2A-C1
22	B	850	DGD	C5B-C6B-C7B-C8B
17	1	509	CLA	O1D-CGD-O2D-CED
25	5	315	CHL	O1D-CGD-O2D-CED
17	B	824	CLA	CBD-CGD-O2D-CED
17	F	803	CLA	CBD-CGD-O2D-CED
17	A	813	CLA	O1D-CGD-O2D-CED
17	B	811	CLA	O1D-CGD-O2D-CED
17	F	802	CLA	O1D-CGD-O2D-CED
17	1	506	CLA	O1D-CGD-O2D-CED
25	2	513	CHL	O1D-CGD-O2D-CED
17	B	818	CLA	O1A-CGA-O2A-C1
17	2	506	CLA	O1A-CGA-O2A-C1
22	J	103	DGD	O1A-C1A-O1G-C1G
20	2	503	BCR	C13-C14-C15-C16
17	J	101	CLA	C2C-C3C-CAC-CBC
17	A	802	CLA	CBD-CGD-O2D-CED
17	A	824	CLA	CBD-CGD-O2D-CED
17	A	826	CLA	CBD-CGD-O2D-CED
17	B	834	CLA	CBD-CGD-O2D-CED
17	1	504	CLA	CBD-CGD-O2D-CED
17	A	815	CLA	O1D-CGD-O2D-CED
19	1	516	LHG	O2-C2-C3-O3
17	B	818	CLA	CBA-CGA-O2A-C1
17	2	506	CLA	CBA-CGA-O2A-C1
17	2	514	CLA	CBA-CGA-O2A-C1
17	A	816	CLA	O1A-CGA-O2A-C1
17	A	835	CLA	O1A-CGA-O2A-C1
17	A	811	CLA	CBD-CGD-O2D-CED
17	A	825	CLA	CBD-CGD-O2D-CED
17	3	310	CLA	CBD-CGD-O2D-CED
17	A	828	CLA	O1D-CGD-O2D-CED
17	L	304	CLA	C4C-C3C-CAC-CBC
17	B	830	CLA	CBD-CGD-O2D-CED
17	A	820	CLA	CBA-CGA-O2A-C1
17	B	814	CLA	O1D-CGD-O2D-CED
23	2	519	LMG	O6-C5-C6-O5
17	B	830	CLA	O1A-CGA-O2A-C1
17	B	841	CLA	C2-C3-C5-C6
17	J	101	CLA	CBD-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
17	A	827	CLA	C2A-CAA-CBA-CGA
17	2	514	CLA	O1D-CGD-O2D-CED
17	B	822	CLA	O1A-CGA-O2A-C1
22	J	103	DGD	O6D-C1D-O3G-C3G
23	2	518	LMG	O6-C1-O1-C7
17	J	101	CLA	C4C-C3C-CAC-CBC
17	3	314	CLA	CBA-CGA-O2A-C1
19	B	851	LHG	C24-C23-O8-C6
17	A	810	CLA	O1D-CGD-O2D-CED
17	L	304	CLA	O1D-CGD-O2D-CED
25	3	315	CHL	O1D-CGD-O2D-CED
17	A	820	CLA	O1A-CGA-O2A-C1
19	B	851	LHG	O10-C23-O8-C6
17	A	852	CLA	C3-C5-C6-C7
17	A	810	CLA	CBA-CGA-O2A-C1
17	A	836	CLA	CBA-CGA-O2A-C1
17	B	812	CLA	CBA-CGA-O2A-C1
17	B	842	CLA	CBA-CGA-O2A-C1
17	L	301	CLA	CBA-CGA-O2A-C1
17	5	308	CLA	CBA-CGA-O2A-C1
16	A	801	CL0	CAA-CBA-CGA-O2A
17	A	805	CLA	C10-C11-C12-C13
17	2	506	CLA	C15-C16-C17-C18
17	2	510	CLA	C5-C6-C7-C8
23	2	518	LMG	C2-C1-O1-C7
17	L	301	CLA	O1A-CGA-O2A-C1
22	J	103	DGD	O6E-C5E-C6E-O5E
17	A	836	CLA	C2-C3-C5-C6
17	L	303	CLA	C2-C3-C5-C6
17	3	308	CLA	C2-C3-C5-C6
17	A	826	CLA	C6-C7-C8-C9
17	A	827	CLA	C14-C13-C15-C16
17	A	838	CLA	C11-C12-C13-C14
17	B	818	CLA	C11-C10-C8-C9
17	2	506	CLA	C11-C12-C13-C14
18	A	841	PQN	C19-C18-C20-C21
18	B	843	PQN	C19-C18-C20-C21
17	2	507	CLA	O1D-CGD-O2D-CED
17	A	808	CLA	C2A-CAA-CBA-CGA
20	A	847	BCR	C7-C8-C9-C34
20	A	851	BCR	C37-C22-C23-C24
20	A	853	BCR	C37-C22-C23-C24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
20	B	844	BCR	C7-C8-C9-C34
20	L	305	BCR	C7-C8-C9-C34
20	L	306	BCR	C11-C12-C13-C35
26	5	304	XAT	C27-C28-C29-C39
20	A	847	BCR	C7-C8-C9-C10
20	A	853	BCR	C21-C22-C23-C24
20	B	844	BCR	C7-C8-C9-C10
20	F	801	BCR	C21-C22-C23-C24
20	L	305	BCR	C7-C8-C9-C10
23	2	519	LMG	C4-C5-C6-O5
23	2	519	LMG	C28-C29-C30-C31
17	A	805	CLA	C8-C10-C11-C12
18	B	843	PQN	C15-C16-C17-C18
17	1	510	CLA	CBA-CGA-O2A-C1
17	3	306	CLA	CBA-CGA-O2A-C1
17	B	802	CLA	C10-C11-C12-C13
17	B	802	CLA	C15-C16-C17-C18
17	2	514	CLA	C5-C6-C7-C8
18	A	841	PQN	C18-C20-C21-C22
17	A	838	CLA	C5-C6-C7-C8
17	B	838	CLA	C5-C6-C7-C8
17	2	507	CLA	C5-C6-C7-C8
17	3	308	CLA	C5-C6-C7-C8
17	5	308	CLA	C10-C11-C12-C13
17	K	202	CLA	CBD-CGD-O2D-CED
25	2	516	CHL	O1D-CGD-O2D-CED
17	5	308	CLA	C5-C6-C7-C8
23	F	806	LMG	C14-C15-C16-C17
17	2	514	CLA	C2-C1-O2A-CGA
17	B	835	CLA	C5-C6-C7-C8
17	A	838	CLA	CBD-CGD-O2D-CED
25	2	516	CHL	C2A-CAA-CBA-CGA
17	B	818	CLA	C5-C6-C7-C8
17	5	307	CLA	C10-C11-C12-C13
17	A	806	CLA	C6-C7-C8-C10
17	5	308	CLA	C11-C10-C8-C7
17	3	308	CLA	C3-C5-C6-C7
17	A	810	CLA	O1A-CGA-O2A-C1
17	3	306	CLA	O1A-CGA-O2A-C1
17	5	308	CLA	O1A-CGA-O2A-C1
17	A	823	CLA	C2A-CAA-CBA-CGA
17	5	308	CLA	O1D-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
17	5	316	CLA	O1D-CGD-O2D-CED
25	1	512	CHL	O1D-CGD-O2D-CED
17	A	823	CLA	C5-C6-C7-C8
17	A	827	CLA	C10-C11-C12-C13
17	B	826	CLA	C8-C10-C11-C12
17	3	306	CLA	C5-C6-C7-C8
17	A	836	CLA	O1A-CGA-O2A-C1
17	B	842	CLA	O1A-CGA-O2A-C1
17	A	827	CLA	C8-C10-C11-C12
17	B	837	CLA	C2C-C3C-CAC-CBC
17	3	318	CLA	O1D-CGD-O2D-CED
19	B	851	LHG	O2-C2-C3-O3
17	B	842	CLA	C3-C5-C6-C7
17	A	805	CLA	C5-C6-C7-C8
17	B	812	CLA	O1A-CGA-O2A-C1
17	3	314	CLA	O1A-CGA-O2A-C1
17	A	802	CLA	C5-C6-C7-C8
17	A	806	CLA	C13-C15-C16-C17
17	B	803	CLA	C10-C11-C12-C13
22	B	850	DGD	O6D-C5D-C6D-O5D
19	A	844	LHG	C3-O3-P-O6
19	A	844	LHG	C4-O6-P-O3
19	B	851	LHG	C3-O3-P-O6
19	B	851	LHG	C4-O6-P-O3
19	1	516	LHG	C3-O3-P-O6
19	1	516	LHG	C23-C24-C25-C26
17	2	510	CLA	C3-C5-C6-C7
17	A	804	CLA	CBA-CGA-O2A-C1
17	A	825	CLA	CBA-CGA-O2A-C1
23	F	805	LMG	O9-C10-O7-C8
17	A	829	CLA	C4-C3-C5-C6
17	A	829	CLA	C5-C6-C7-C8
17	A	816	CLA	C2A-CAA-CBA-CGA
17	B	802	CLA	C2A-CAA-CBA-CGA
17	5	307	CLA	C2A-CAA-CBA-CGA
17	5	308	CLA	C2A-CAA-CBA-CGA
17	1	506	CLA	C6-C7-C8-C9
17	5	307	CLA	C16-C17-C18-C20
22	B	850	DGD	C4D-C5D-C6D-O5D
23	5	301	LMG	C11-C12-C13-C14
17	B	824	CLA	O1D-CGD-O2D-CED
17	5	310	CLA	O1D-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
17	B	842	CLA	CBD-CGD-O2D-CED
23	F	805	LMG	C11-C10-O7-C8
23	F	806	LMG	C11-C10-O7-C8
17	B	834	CLA	O1D-CGD-O2D-CED
17	F	803	CLA	O1D-CGD-O2D-CED
17	2	510	CLA	O1D-CGD-O2D-CED
17	A	823	CLA	C6-C7-C8-C9
17	2	510	CLA	C11-C12-C13-C14
17	3	308	CLA	C6-C7-C8-C9
17	3	314	CLA	C6-C7-C8-C9
17	5	308	CLA	C11-C12-C13-C14
23	F	806	LMG	O9-C10-O7-C8
22	J	103	DGD	C7B-C8B-C9B-CAB
17	2	506	CLA	O1D-CGD-O2D-CED
25	3	302	CHL	CBA-CGA-O2A-C1
19	A	844	LHG	C7-C8-C9-C10
22	J	103	DGD	C1A-C2A-C3A-C4A
17	1	504	CLA	O1D-CGD-O2D-CED
19	A	843	LHG	C27-C28-C29-C30
19	1	516	LHG	C34-C35-C36-C37
17	A	831	CLA	C15-C16-C17-C18
23	2	519	LMG	C11-C12-C13-C14
17	B	807	CLA	C6-C7-C8-C9
17	1	513	CLA	C6-C7-C8-C9
17	1	513	CLA	C11-C12-C13-C14
17	A	824	CLA	O1D-CGD-O2D-CED
17	B	842	CLA	C8-C10-C11-C12
23	F	806	LMG	C28-C29-C30-C31
17	B	821	CLA	C2A-CAA-CBA-CGA
17	2	509	CLA	C2A-CAA-CBA-CGA
17	5	312	CLA	C2A-CAA-CBA-CGA
20	A	848	BCR	C37-C22-C23-C24
20	K	204	BCR	C37-C22-C23-C24
20	1	503	BCR	C7-C8-C9-C34
20	3	305	BCR	C37-C22-C23-C24
19	A	844	LHG	O1-C1-C2-C3
20	A	848	BCR	C21-C22-C23-C24
20	K	204	BCR	C21-C22-C23-C24
20	1	503	BCR	C7-C8-C9-C10
20	3	305	BCR	C7-C8-C9-C10
20	3	305	BCR	C21-C22-C23-C24
22	J	103	DGD	O1B-C1B-O2G-C2G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
22	J	103	DGD	C2B-C1B-O2G-C2G
17	B	841	CLA	C5-C6-C7-C8
19	A	843	LHG	C14-C15-C16-C17
17	A	831	CLA	C13-C15-C16-C17
23	F	806	LMG	C12-C13-C14-C15
17	2	510	CLA	C11-C12-C13-C15
17	3	314	CLA	C6-C7-C8-C10
17	5	308	CLA	C11-C12-C13-C15
17	A	802	CLA	O1D-CGD-O2D-CED
25	1	512	CHL	CBA-CGA-O2A-C1
25	2	512	CHL	CBA-CGA-O2A-C1
25	5	314	CHL	CBA-CGA-O2A-C1
17	B	821	CLA	CBD-CGD-O2D-CED
19	1	516	LHG	C14-C15-C16-C17
17	2	505	CLA	CBA-CGA-O2A-C1
19	B	851	LHG	C29-C30-C31-C32
22	B	850	DGD	CDB-CEB-CFB-CGB
17	A	805	CLA	C3A-C2A-CAA-CBA
17	A	852	CLA	C3A-C2A-CAA-CBA
17	B	834	CLA	C3A-C2A-CAA-CBA
17	L	303	CLA	C3A-C2A-CAA-CBA
17	3	310	CLA	C3A-C2A-CAA-CBA
17	3	318	CLA	C3A-C2A-CAA-CBA
17	5	309	CLA	C3A-C2A-CAA-CBA
25	2	516	CHL	C3A-C2A-CAA-CBA
25	5	314	CHL	C3A-C2A-CAA-CBA
17	A	806	CLA	C5-C6-C7-C8
17	A	806	CLA	C15-C16-C17-C18
22	J	103	DGD	CEA-CFA-CGA-CHA
17	A	804	CLA	O1A-CGA-O2A-C1
17	A	825	CLA	O1A-CGA-O2A-C1
17	3	308	CLA	C6-C7-C8-C10
22	J	103	DGD	C6B-C7B-C8B-C9B
17	A	826	CLA	O1D-CGD-O2D-CED
25	1	514	CHL	CBD-CGD-O2D-CED
19	A	843	LHG	C29-C30-C31-C32
17	A	823	CLA	C6-C7-C8-C10
17	A	826	CLA	C3-C5-C6-C7
19	A	843	LHG	C31-C32-C33-C34
19	1	516	LHG	C1-C2-C3-O3
17	3	314	CLA	C2-C1-O2A-CGA
17	5	310	CLA	C2-C1-O2A-CGA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
19	1	516	LHG	C9-C10-C11-C12
17	A	805	CLA	C13-C15-C16-C17
17	A	831	CLA	C5-C6-C7-C8
19	1	516	LHG	C7-C8-C9-C10
17	A	818	CLA	CBD-CGD-O2D-CED
20	A	845	BCR	C1-C6-C7-C8
20	A	845	BCR	C5-C6-C7-C8
20	A	848	BCR	C23-C24-C25-C30
20	A	851	BCR	C1-C6-C7-C8
20	A	851	BCR	C23-C24-C25-C26
20	A	851	BCR	C23-C24-C25-C30
20	B	844	BCR	C5-C6-C7-C8
20	K	204	BCR	C5-C6-C7-C8
20	K	204	BCR	C23-C24-C25-C30
20	L	306	BCR	C23-C24-C25-C26
20	L	306	BCR	C23-C24-C25-C30
20	1	503	BCR	C1-C6-C7-C8
20	1	503	BCR	C5-C6-C7-C8
20	2	503	BCR	C1-C6-C7-C8
20	2	503	BCR	C5-C6-C7-C8
20	3	305	BCR	C1-C6-C7-C8
20	3	305	BCR	C5-C6-C7-C8
24	3	303	LUT	C5-C6-C7-C8
17	A	842	CLA	CBA-CGA-O2A-C1
17	3	311	CLA	CBA-CGA-O2A-C1
17	A	806	CLA	C10-C11-C12-C13
18	A	841	PQN	C25-C26-C27-C28
17	2	507	CLA	C4-C3-C5-C6
17	3	313	CLA	O2A-C1-C2-C3
17	2	505	CLA	O1A-CGA-O2A-C1
17	5	308	CLA	C8-C10-C11-C12
17	A	805	CLA	C2-C3-C5-C6
17	A	825	CLA	C11-C10-C8-C7
17	1	513	CLA	C6-C7-C8-C10
17	1	513	CLA	C11-C12-C13-C15
19	B	851	LHG	C9-C10-C11-C12
17	L	303	CLA	CBD-CGD-O2D-CED
25	5	317	CHL	CBD-CGD-O2D-CED
17	1	510	CLA	O1A-CGA-O2A-C1
23	5	301	LMG	C29-C28-O8-C9
17	B	817	CLA	C2A-CAA-CBA-CGA
17	5	310	CLA	C2A-CAA-CBA-CGA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
17	3	311	CLA	O1A-CGA-O2A-C1
17	A	811	CLA	O1D-CGD-O2D-CED
17	A	825	CLA	O1D-CGD-O2D-CED
22	B	850	DGD	C2B-C3B-C4B-C5B
17	3	310	CLA	O1D-CGD-O2D-CED
17	B	807	CLA	C15-C16-C17-C18
17	B	830	CLA	O1D-CGD-O2D-CED
17	A	842	CLA	O1A-CGA-O2A-C1
18	A	841	PQN	C26-C27-C28-C30
17	A	827	CLA	C5-C6-C7-C8
19	A	844	LHG	C8-C7-O7-C5
19	1	516	LHG	C8-C7-O7-C5
17	B	833	CLA	C5-C6-C7-C8
17	B	829	CLA	CBD-CGD-O2D-CED
19	A	844	LHG	O9-C7-O7-C5
19	A	843	LHG	C10-C11-C12-C13
17	A	836	CLA	C6-C7-C8-C9
17	A	805	CLA	C4-C3-C5-C6
17	A	829	CLA	C2-C3-C5-C6
17	B	830	CLA	C6-C7-C8-C9
17	5	308	CLA	C11-C10-C8-C9
17	A	820	CLA	C2A-CAA-CBA-CGA
17	B	808	CLA	C2A-CAA-CBA-CGA
17	2	506	CLA	C2A-CAA-CBA-CGA
17	3	306	CLA	C2A-CAA-CBA-CGA
24	1	502	LUT	C7-C8-C9-C19
17	A	835	CLA	CBD-CGD-O2D-CED
23	F	806	LMG	C38-C39-C40-C41
17	J	101	CLA	O1D-CGD-O2D-CED
17	A	852	CLA	C1A-C2A-CAA-CBA
17	B	804	CLA	C1A-C2A-CAA-CBA
17	B	820	CLA	C1A-C2A-CAA-CBA
17	B	821	CLA	C1A-C2A-CAA-CBA
17	3	308	CLA	C1A-C2A-CAA-CBA
17	3	310	CLA	C1A-C2A-CAA-CBA
17	3	313	CLA	C1A-C2A-CAA-CBA
17	3	314	CLA	C1A-C2A-CAA-CBA
17	5	309	CLA	C1A-C2A-CAA-CBA
25	2	516	CHL	C1A-C2A-CAA-CBA
17	1	506	CLA	C6-C7-C8-C10
17	5	307	CLA	C16-C17-C18-C19
19	1	516	LHG	O9-C7-O7-C5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
17	A	839	CLA	CBD-CGD-O2D-CED
17	A	825	CLA	C5-C6-C7-C8
22	B	850	DGD	C4A-C5A-C6A-C7A
23	F	805	LMG	C13-C14-C15-C16
23	F	806	LMG	C11-C12-C13-C14
22	J	103	DGD	C6A-C7A-C8A-C9A
17	L	301	CLA	C4-C3-C5-C6
23	5	301	LMG	O10-C28-O8-C9
22	B	850	DGD	CCB-CDB-CEB-CFB
22	J	103	DGD	O1G-C1G-C2G-C3G
22	J	103	DGD	C1G-C2G-C3G-O3G
22	J	103	DGD	C5D-C6D-O5D-C1E
17	A	838	CLA	O1D-CGD-O2D-CED
17	A	805	CLA	C16-C17-C18-C19
17	A	825	CLA	C11-C12-C13-C14
17	A	836	CLA	C6-C7-C8-C10
17	A	823	CLA	CBD-CGD-O2D-CED
23	5	301	LMG	O6-C5-C6-O5
17	A	816	CLA	C3-C5-C6-C7
17	A	806	CLA	C4-C3-C5-C6
19	2	517	LHG	C7-C8-C9-C10
17	B	841	CLA	C6-C7-C8-C9
17	A	837	CLA	CBD-CGD-O2D-CED
17	B	818	CLA	C8-C10-C11-C12
17	1	513	CLA	C2-C1-O2A-CGA
22	B	850	DGD	C4B-C5B-C6B-C7B
17	5	307	CLA	C8-C10-C11-C12
22	B	850	DGD	C3B-C4B-C5B-C6B
17	A	806	CLA	CBA-CGA-O2A-C1
23	2	519	LMG	C29-C28-O8-C9
18	A	841	PQN	C26-C27-C28-C29
25	1	514	CHL	O1D-CGD-O2D-CED
17	A	827	CLA	C13-C15-C16-C17
17	B	830	CLA	C4-C3-C5-C6
17	2	506	CLA	C4-C3-C5-C6
17	A	805	CLA	C6-C7-C8-C10
17	A	806	CLA	C2-C3-C5-C6
17	B	803	CLA	C12-C13-C15-C16
17	B	807	CLA	C12-C13-C15-C16
17	B	826	CLA	C11-C12-C13-C15
17	B	830	CLA	C2-C3-C5-C6
17	B	830	CLA	C6-C7-C8-C10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
17	2	506	CLA	C2-C3-C5-C6
17	5	307	CLA	C12-C13-C15-C16
18	A	841	PQN	C17-C18-C20-C21
18	B	843	PQN	C17-C18-C20-C21
16	A	801	CL0	C3-C5-C6-C7
17	A	831	CLA	C10-C11-C12-C13
17	A	805	CLA	C6-C7-C8-C9
17	A	806	CLA	C6-C7-C8-C9
17	A	808	CLA	C11-C12-C13-C14
17	A	816	CLA	C6-C7-C8-C9
17	A	825	CLA	C11-C10-C8-C9
17	B	807	CLA	C14-C13-C15-C16
17	5	307	CLA	C14-C13-C15-C16
17	A	832	CLA	CBA-CGA-O2A-C1
17	B	804	CLA	CBA-CGA-O2A-C1
17	K	202	CLA	O1D-CGD-O2D-CED
25	3	302	CHL	O1A-CGA-O2A-C1
20	B	847	BCR	C11-C12-C13-C35
20	B	852	BCR	C37-C22-C23-C24
20	K	204	BCR	C11-C12-C13-C35
20	2	503	BCR	C7-C8-C9-C34
20	B	847	BCR	C11-C12-C13-C14
17	1	513	CLA	C5-C6-C7-C8
17	B	803	CLA	C15-C16-C17-C18
19	A	843	LHG	C23-C24-C25-C26
23	F	806	LMG	C10-C11-C12-C13
17	A	829	CLA	CBA-CGA-O2A-C1
17	A	852	CLA	C4-C3-C5-C6
18	A	841	PQN	C15-C16-C17-C18
17	B	808	CLA	CBA-CGA-O2A-C1
17	1	506	CLA	CBA-CGA-O2A-C1
25	5	317	CHL	O1D-CGD-O2D-CED
17	A	813	CLA	C3A-C2A-CAA-CBA
17	A	826	CLA	C3A-C2A-CAA-CBA
17	B	813	CLA	C3A-C2A-CAA-CBA
25	2	515	CHL	C3A-C2A-CAA-CBA
22	J	103	DGD	CFA-CGA-CHA-CIA
17	2	508	CLA	O2A-C1-C2-C3
17	2	506	CLA	C13-C15-C16-C17
19	1	516	LHG	C4-C5-C6-O8
19	1	516	LHG	C11-C10-C9-C8
17	A	806	CLA	O1A-CGA-O2A-C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
22	J	103	DGD	C4B-C5B-C6B-C7B
25	1	512	CHL	O1A-CGA-O2A-C1
17	B	804	CLA	O2A-C1-C2-C3
17	A	802	CLA	C8-C10-C11-C12
17	B	833	CLA	C3-C5-C6-C7
22	B	850	DGD	C6A-C7A-C8A-C9A
17	A	827	CLA	C4-C3-C5-C6
17	B	842	CLA	O1D-CGD-O2D-CED
17	5	311	CLA	CBD-CGD-O2D-CED
25	2	513	CHL	C2C-C3C-CAC-CBC
17	B	829	CLA	O1D-CGD-O2D-CED
19	A	843	LHG	C3-O3-P-O6
25	1	514	CHL	C3C-C2C-CMC-OMC
19	B	851	LHG	O6-C4-C5-O7
17	A	838	CLA	CBA-CGA-O2A-C1
17	1	506	CLA	O1A-CGA-O2A-C1
17	B	818	CLA	CBD-CGD-O2D-CED
25	1	517	CHL	CBD-CGD-O2D-CED
22	B	850	DGD	CEB-CFB-CGB-CHB
17	A	832	CLA	O1A-CGA-O2A-C1
17	B	804	CLA	O1A-CGA-O2A-C1
17	B	830	CLA	C3-C5-C6-C7
23	2	519	LMG	O1-C7-C8-O7
23	5	301	LMG	O1-C7-C8-O7
17	A	806	CLA	C16-C17-C18-C19
17	A	827	CLA	C16-C17-C18-C19
17	3	306	CLA	C6-C7-C8-C9
17	B	803	CLA	C4-C3-C5-C6
17	A	826	CLA	C2-C1-O2A-CGA
17	B	817	CLA	C2-C1-O2A-CGA
17	A	852	CLA	C2-C3-C5-C6
17	A	831	CLA	C11-C10-C8-C9
17	A	838	CLA	C11-C10-C8-C9
17	B	802	CLA	C6-C7-C8-C9
17	2	510	CLA	C11-C10-C8-C9
25	2	512	CHL	O1A-CGA-O2A-C1
17	2	510	CLA	C10-C11-C12-C13
18	A	841	PQN	C20-C21-C22-C23
17	A	835	CLA	C4-C3-C5-C6
19	B	851	LHG	C2-C3-O3-P
19	1	516	LHG	C2-C3-O3-P
20	A	846	BCR	C23-C24-C25-C26

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
20	A	848	BCR	C5-C6-C7-C8
20	B	845	BCR	C5-C6-C7-C8
20	J	102	BCR	C23-C24-C25-C26
20	J	102	BCR	C23-C24-C25-C30
20	L	305	BCR	C23-C24-C25-C26
20	L	305	BCR	C23-C24-C25-C30
24	5	303	LUT	C5-C6-C7-C8
20	A	846	BCR	C7-C8-C9-C34
20	F	801	BCR	C7-C8-C9-C34
24	3	304	LUT	C7-C8-C9-C19
17	J	101	CLA	C1A-C2A-CAA-CBA
17	1	504	CLA	C1A-C2A-CAA-CBA
17	1	507	CLA	C1A-C2A-CAA-CBA
20	L	306	BCR	C11-C12-C13-C14
26	5	304	XAT	C27-C28-C29-C30
19	1	516	LHG	C28-C29-C30-C31
17	A	827	CLA	C16-C17-C18-C20
17	B	828	CLA	CBD-CGD-O2D-CED
17	B	837	CLA	C4C-C3C-CAC-CBC
17	B	803	CLA	CAA-CBA-CGA-O2A
19	A	843	LHG	C35-C36-C37-C38
17	A	802	CLA	C6-C7-C8-C10
17	A	806	CLA	C12-C13-C15-C16
17	A	808	CLA	C11-C12-C13-C15
17	A	816	CLA	C6-C7-C8-C10
17	B	803	CLA	C2-C3-C5-C6
17	B	803	CLA	C6-C7-C8-C10
17	B	818	CLA	C11-C10-C8-C7
17	1	513	CLA	C12-C13-C15-C16
17	2	510	CLA	C11-C10-C8-C7
17	A	806	CLA	C16-C17-C18-C20
17	B	815	CLA	CBA-CGA-O2A-C1
23	2	519	LMG	O10-C28-O8-C9
17	B	815	CLA	C2A-CAA-CBA-CGA
17	B	839	CLA	CBA-CGA-O2A-C1
25	5	314	CHL	O1A-CGA-O2A-C1
17	A	804	CLA	CAD-CBD-CGD-O2D
17	A	814	CLA	CAD-CBD-CGD-O2D
17	A	833	CLA	CAD-CBD-CGD-O2D
17	A	837	CLA	CAD-CBD-CGD-O2D
17	A	852	CLA	CAD-CBD-CGD-O2D
17	B	804	CLA	CAD-CBD-CGD-O2D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
17	B	806	CLA	CAD-CBD-CGD-O2D
17	B	836	CLA	CAD-CBD-CGD-O2D
17	B	840	CLA	CAD-CBD-CGD-O2D
17	F	803	CLA	CAD-CBD-CGD-O2D
17	1	505	CLA	CAD-CBD-CGD-O2D
17	1	508	CLA	CAD-CBD-CGD-O2D
17	1	511	CLA	CAD-CBD-CGD-O2D
17	3	307	CLA	CAD-CBD-CGD-O2D
17	5	305	CLA	CAD-CBD-CGD-O2D
22	J	103	DGD	C1G-C2G-O2G-C1B
17	A	835	CLA	O1D-CGD-O2D-CED
23	2	519	LMG	C7-C8-C9-O8
17	5	312	CLA	CAA-CBA-CGA-O2A
17	A	839	CLA	O1D-CGD-O2D-CED
17	A	808	CLA	CHA-CBD-CGD-O1D
17	A	812	CLA	CHA-CBD-CGD-O1D
17	A	812	CLA	CHA-CBD-CGD-O2D
17	A	813	CLA	CHA-CBD-CGD-O1D
17	A	813	CLA	CHA-CBD-CGD-O2D
17	A	815	CLA	CHA-CBD-CGD-O1D
17	A	815	CLA	CHA-CBD-CGD-O2D
17	A	819	CLA	CHA-CBD-CGD-O1D
17	A	819	CLA	CHA-CBD-CGD-O2D
17	A	824	CLA	CHA-CBD-CGD-O1D
17	A	824	CLA	CHA-CBD-CGD-O2D
17	A	830	CLA	CHA-CBD-CGD-O1D
17	A	834	CLA	CHA-CBD-CGD-O1D
17	A	834	CLA	CHA-CBD-CGD-O2D
17	A	842	CLA	CHA-CBD-CGD-O1D
17	B	809	CLA	CHA-CBD-CGD-O1D
17	B	809	CLA	CHA-CBD-CGD-O2D
17	B	814	CLA	CHA-CBD-CGD-O1D
17	B	825	CLA	CHA-CBD-CGD-O1D
17	B	825	CLA	CHA-CBD-CGD-O2D
17	B	827	CLA	CHA-CBD-CGD-O1D
17	B	827	CLA	CHA-CBD-CGD-O2D
17	B	834	CLA	CHA-CBD-CGD-O1D
17	B	834	CLA	CHA-CBD-CGD-O2D
17	B	837	CLA	CHA-CBD-CGD-O1D
17	B	839	CLA	CHA-CBD-CGD-O1D
17	B	839	CLA	CHA-CBD-CGD-O2D
17	L	303	CLA	CHA-CBD-CGD-O1D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
17	L	303	CLA	CHA-CBD-CGD-O2D
17	2	510	CLA	CHA-CBD-CGD-O1D
17	2	510	CLA	CHA-CBD-CGD-O2D
17	3	312	CLA	CHA-CBD-CGD-O1D
17	3	312	CLA	CHA-CBD-CGD-O2D
17	3	313	CLA	CHA-CBD-CGD-O2D
17	5	308	CLA	CHA-CBD-CGD-O1D
17	5	308	CLA	CHA-CBD-CGD-O2D
17	A	840	CLA	CBD-CGD-O2D-CED
17	A	832	CLA	O2A-C1-C2-C3
22	J	103	DGD	O1G-C1G-C2G-O2G
22	J	103	DGD	C3A-C4A-C5A-C6A
22	J	103	DGD	C4E-C5E-C6E-O5E
17	A	829	CLA	O1A-CGA-O2A-C1
17	B	821	CLA	O1D-CGD-O2D-CED
19	A	843	LHG	C30-C31-C32-C33
17	B	808	CLA	O1A-CGA-O2A-C1
17	1	513	CLA	C13-C15-C16-C17
17	1	513	CLA	C14-C13-C15-C16
22	J	103	DGD	C9B-CAB-CBB-CCB
25	1	512	CHL	C2A-CAA-CBA-CGA
17	A	838	CLA	O1A-CGA-O2A-C1
17	B	815	CLA	O1A-CGA-O2A-C1
17	3	313	CLA	CBA-CGA-O2A-C1
20	A	846	BCR	C37-C22-C23-C24
20	B	846	BCR	C7-C8-C9-C34
24	3	304	LUT	C7-C8-C9-C10
17	L	303	CLA	O1D-CGD-O2D-CED
17	A	826	CLA	C1A-C2A-CAA-CBA
17	A	835	CLA	C1A-C2A-CAA-CBA
17	2	505	CLA	C1A-C2A-CAA-CBA
17	3	318	CLA	C1A-C2A-CAA-CBA
17	5	306	CLA	CHA-CBD-CGD-O2D
17	1	513	CLA	C16-C17-C18-C20
17	A	808	CLA	C15-C16-C17-C18
17	A	837	CLA	O1D-CGD-O2D-CED
17	B	818	CLA	O1D-CGD-O2D-CED
19	A	843	LHG	C4-O6-P-O3
25	2	513	CHL	CAD-CBD-CGD-O2D
18	B	843	PQN	C14-C13-C15-C16
17	5	311	CLA	O1D-CGD-O2D-CED
17	B	839	CLA	O1A-CGA-O2A-C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
19	A	843	LHG	C3-O3-P-O5
19	A	844	LHG	C3-O3-P-O5
19	B	851	LHG	C3-O3-P-O4
19	B	851	LHG	C3-O3-P-O5
19	1	516	LHG	C3-O3-P-O5
19	B	851	LHG	O6-C4-C5-C6
17	A	823	CLA	O1D-CGD-O2D-CED
17	A	838	CLA	C2A-CAA-CBA-CGA
17	A	805	CLA	CAD-CBD-CGD-O1D
17	A	806	CLA	CAD-CBD-CGD-O1D
17	A	812	CLA	CAD-CBD-CGD-O1D
17	A	813	CLA	CAD-CBD-CGD-O1D
17	A	819	CLA	CAD-CBD-CGD-O1D
17	A	823	CLA	CAD-CBD-CGD-O1D
17	A	824	CLA	CAD-CBD-CGD-O1D
17	B	812	CLA	CAD-CBD-CGD-O1D
17	B	814	CLA	CAD-CBD-CGD-O1D
17	B	827	CLA	CAD-CBD-CGD-O1D
17	B	837	CLA	CAD-CBD-CGD-O1D
17	B	841	CLA	CAD-CBD-CGD-O1D
17	2	505	CLA	CAD-CBD-CGD-O1D
17	3	312	CLA	CAD-CBD-CGD-O1D
19	2	517	LHG	C23-C24-C25-C26
17	B	820	CLA	C2C-C3C-CAC-CBC
16	A	801	CL0	C2-C1-O2A-CGA
17	3	306	CLA	C6-C7-C8-C10
17	A	835	CLA	C3A-C2A-CAA-CBA
17	A	838	CLA	C11-C10-C8-C7
17	B	811	CLA	C3A-C2A-CAA-CBA
17	B	826	CLA	C6-C7-C8-C10
17	2	505	CLA	C3A-C2A-CAA-CBA
22	B	850	DGD	C1A-C2A-C3A-C4A
17	3	313	CLA	O1A-CGA-O2A-C1
17	1	513	CLA	C15-C16-C17-C18
17	A	823	CLA	C3A-C2A-CAA-CBA
22	B	850	DGD	C3A-C4A-C5A-C6A
23	2	519	LMG	O1-C7-C8-C9
23	5	301	LMG	O1-C7-C8-C9
25	1	512	CHL	C1C-C2C-CMC-OMC
25	1	514	CHL	C1C-C2C-CMC-OMC
25	1	517	CHL	C1C-C2C-CMC-OMC
25	2	515	CHL	C1C-C2C-CMC-OMC

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
25	5	314	CHL	C1C-C2C-CMC-OMC
25	5	315	CHL	C1C-C2C-CMC-OMC
25	5	317	CHL	C1C-C2C-CMC-OMC
22	J	103	DGD	O2G-C2G-C3G-O3G
19	1	516	LHG	C24-C23-O8-C6
17	A	805	CLA	C11-C10-C8-C9
17	A	806	CLA	C14-C13-C15-C16
17	B	803	CLA	C6-C7-C8-C9
17	B	807	CLA	C11-C10-C8-C9
25	1	517	CHL	O1D-CGD-O2D-CED
20	2	503	BCR	C18-C19-C20-C21
20	5	302	BCR	C10-C11-C12-C13
20	B	848	BCR	C36-C18-C19-C20
23	2	519	LMG	C14-C15-C16-C17
19	1	516	LHG	O10-C23-O8-C6
18	B	843	PQN	C12-C13-C15-C16
17	B	803	CLA	C8-C10-C11-C12
17	B	820	CLA	C5-C6-C7-C8
17	B	817	CLA	C1-C2-C3-C4
17	A	840	CLA	O1D-CGD-O2D-CED
23	F	806	LMG	C9-C8-O7-C10
17	A	816	CLA	C2-C1-O2A-CGA
17	B	812	CLA	C2-C1-O2A-CGA
17	A	808	CLA	C3-C5-C6-C7
17	1	515	CLA	CHA-CBD-CGD-O1D
17	1	515	CLA	CHA-CBD-CGD-O2D
19	B	851	LHG	C7-C8-C9-C10
17	B	835	CLA	C4-C3-C5-C6
18	A	841	PQN	C14-C13-C15-C16
20	A	848	BCR	C1-C6-C7-C8
20	B	845	BCR	C1-C6-C7-C8
20	B	852	BCR	C5-C6-C7-C8
20	3	305	BCR	C23-C24-C25-C26
20	3	305	BCR	C23-C24-C25-C30
24	1	502	LUT	C1-C6-C7-C8
24	5	303	LUT	C1-C6-C7-C8
17	B	804	CLA	C13-C15-C16-C17
17	1	513	CLA	C16-C17-C18-C19
19	1	516	LHG	C11-C12-C13-C14
19	2	517	LHG	C3-O3-P-O6
19	2	517	LHG	C4-O6-P-O3
25	2	513	CHL	C4C-C3C-CAC-CBC

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
17	3	314	CLA	C4-C3-C5-C6
17	A	838	CLA	C12-C13-C15-C16
17	B	807	CLA	C6-C7-C8-C10
17	B	801	CLA	C8-C10-C11-C12
20	B	848	BCR	C17-C18-C19-C20
24	1	502	LUT	C7-C8-C9-C10
17	B	835	CLA	C2-C3-C5-C6
17	B	802	CLA	C8-C10-C11-C12
17	3	311	CLA	C2A-CAA-CBA-CGA
20	B	847	BCR	C19-C20-C21-C22
18	B	843	PQN	C13-C15-C16-C17
17	A	818	CLA	O1D-CGD-O2D-CED
22	J	103	DGD	C1B-C2B-C3B-C4B
17	A	820	CLA	C4-C3-C5-C6
22	J	103	DGD	CDA-CEA-CFA-CGA
17	A	820	CLA	C2-C3-C5-C6
19	A	843	LHG	C11-C12-C13-C14
22	B	850	DGD	C2G-C1G-O1G-C1A
23	2	518	LMG	O1-C7-C8-O7
17	A	831	CLA	C11-C12-C13-C15
17	B	801	CLA	C16-C17-C18-C19
17	A	836	CLA	CBD-CGD-O2D-CED
17	A	820	CLA	C6-C7-C8-C9
17	A	827	CLA	C11-C10-C8-C9
17	B	804	CLA	C14-C13-C15-C16
17	B	826	CLA	C11-C10-C8-C9
20	A	849	BCR	C11-C10-C9-C34
20	B	845	BCR	C11-C10-C9-C34
20	B	846	BCR	C11-C10-C9-C34
20	B	846	BCR	C20-C21-C22-C37
20	B	852	BCR	C11-C10-C9-C34
20	F	804	BCR	C35-C13-C14-C15
20	5	302	BCR	C11-C10-C9-C34
25	1	512	CHL	CAA-CBA-CGA-O2A
23	2	519	LMG	C7-C8-O7-C10
23	2	519	LMG	C9-C8-O7-C10
17	A	808	CLA	C1A-C2A-CAA-CBA
17	A	813	CLA	C1A-C2A-CAA-CBA
17	B	801	CLA	C1A-C2A-CAA-CBA
17	B	813	CLA	C1A-C2A-CAA-CBA
17	B	832	CLA	C1A-C2A-CAA-CBA
17	B	839	CLA	C1A-C2A-CAA-CBA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
17	2	510	CLA	C1A-C2A-CAA-CBA
25	5	314	CHL	C1A-C2A-CAA-CBA
17	A	805	CLA	C12-C13-C15-C16
17	A	826	CLA	C6-C7-C8-C10
17	A	838	CLA	C11-C12-C13-C15
17	B	804	CLA	C6-C7-C8-C10
17	B	804	CLA	C11-C10-C8-C7
17	B	842	CLA	C11-C10-C8-C7
17	5	307	CLA	C11-C10-C8-C7
23	F	806	LMG	C29-C30-C31-C32
17	5	307	CLA	C5-C6-C7-C8
17	B	811	CLA	C4-C3-C5-C6
17	1	513	CLA	C4-C3-C5-C6
17	B	801	CLA	C13-C15-C16-C17
20	A	849	BCR	C11-C10-C9-C8
20	B	845	BCR	C11-C10-C9-C8
20	B	846	BCR	C11-C10-C9-C8
20	B	846	BCR	C20-C21-C22-C23
20	B	852	BCR	C11-C10-C9-C8
20	F	804	BCR	C12-C13-C14-C15
20	5	302	BCR	C11-C10-C9-C8
19	1	516	LHG	O7-C5-C6-O8
17	B	826	CLA	CBA-CGA-O2A-C1
19	A	844	LHG	C24-C23-O8-C6
17	2	505	CLA	C2A-CAA-CBA-CGA
20	L	306	BCR	C19-C20-C21-C22
17	1	515	CLA	CAA-CBA-CGA-O1A
17	1	515	CLA	CAA-CBA-CGA-O2A
19	B	851	LHG	C1-C2-C3-O3
17	A	823	CLA	C2-C1-O2A-CGA
17	B	815	CLA	C2-C1-O2A-CGA
17	A	813	CLA	CAA-CBA-CGA-O2A
17	B	826	CLA	O1A-CGA-O2A-C1
17	A	838	CLA	C3-C5-C6-C7
17	A	805	CLA	CAA-CBA-CGA-O2A
17	1	510	CLA	CAA-CBA-CGA-O2A
20	A	845	BCR	C23-C24-C25-C30
20	A	846	BCR	C23-C24-C25-C30
20	B	849	BCR	C1-C6-C7-C8
20	B	852	BCR	C1-C6-C7-C8
20	J	102	BCR	C1-C6-C7-C8
20	L	305	BCR	C1-C6-C7-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
20	5	302	BCR	C23-C24-C25-C30
23	F	806	LMG	C31-C32-C33-C34
17	B	842	CLA	C4-C3-C5-C6
17	5	311	CLA	C1A-C2A-CAA-CBA
20	A	846	BCR	C21-C22-C23-C24
20	B	852	BCR	C21-C22-C23-C24
20	F	801	BCR	C7-C8-C9-C10
17	A	827	CLA	C2-C3-C5-C6
17	L	301	CLA	C2-C3-C5-C6
17	3	314	CLA	C2-C3-C5-C6
18	A	841	PQN	C12-C13-C15-C16
17	A	823	CLA	C3-C5-C6-C7
22	B	850	DGD	C5D-C6D-O5D-C1E
23	F	806	LMG	C8-C7-O1-C1
17	B	830	CLA	C11-C10-C8-C9
17	B	828	CLA	O1D-CGD-O2D-CED
17	A	831	CLA	C3-C5-C6-C7
17	B	841	CLA	O1A-CGA-O2A-C1
17	B	815	CLA	C4-C3-C5-C6
17	B	841	CLA	CBA-CGA-O2A-C1
20	A	846	BCR	C19-C20-C21-C22
17	3	311	CLA	CAA-CBA-CGA-O2A
23	F	806	LMG	O1-C7-C8-O7
25	2	515	CHL	CAA-CBA-CGA-O2A
17	A	826	CLA	C4-C3-C5-C6
17	1	506	CLA	C4-C3-C5-C6
18	B	843	PQN	C20-C21-C22-C23
17	1	513	CLA	C2-C3-C5-C6
17	B	842	CLA	CAA-CBA-CGA-O2A
17	A	838	CLA	C14-C13-C15-C16
17	B	804	CLA	C6-C7-C8-C9
17	B	818	CLA	C6-C7-C8-C9
17	B	826	CLA	C6-C7-C8-C9
17	A	836	CLA	C3A-C2A-CAA-CBA
17	2	514	CLA	C3A-C2A-CAA-CBA
17	A	802	CLA	O1A-CGA-O2A-C1
17	A	816	CLA	C2-C3-C5-C6
17	A	813	CLA	CAA-CBA-CGA-O1A
17	A	810	CLA	CAD-CBD-CGD-O2D
17	A	829	CLA	CAD-CBD-CGD-O2D
17	A	836	CLA	CAD-CBD-CGD-O2D
17	B	813	CLA	CAD-CBD-CGD-O2D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
17	B	818	CLA	CAD-CBD-CGD-O2D
17	B	821	CLA	CAD-CBD-CGD-O2D
17	B	828	CLA	CAD-CBD-CGD-O2D
17	B	830	CLA	CAD-CBD-CGD-O2D
17	B	833	CLA	CAD-CBD-CGD-O2D
17	B	842	CLA	CAD-CBD-CGD-O2D
17	L	301	CLA	CAD-CBD-CGD-O2D
17	L	302	CLA	CAD-CBD-CGD-O2D
17	1	507	CLA	CAD-CBD-CGD-O2D
17	2	507	CLA	CAD-CBD-CGD-O2D
17	2	511	CLA	CAD-CBD-CGD-O2D
25	3	302	CHL	CAD-CBD-CGD-O2D
17	B	801	CLA	C16-C17-C18-C20
17	2	506	CLA	C3-C5-C6-C7
17	A	831	CLA	C2-C1-O2A-CGA
17	B	817	CLA	CAA-CBA-CGA-O2A
17	B	811	CLA	C2-C3-C5-C6
20	A	846	BCR	C7-C8-C9-C10
20	A	851	BCR	C21-C22-C23-C24
20	K	204	BCR	C11-C12-C13-C14
20	L	306	BCR	C21-C22-C23-C24
20	2	503	BCR	C7-C8-C9-C10
17	B	807	CLA	C5-C6-C7-C8
23	F	806	LMG	C7-C8-C9-O8
17	K	203	CLA	C4C-C3C-CAC-CBC
17	B	811	CLA	O2A-C1-C2-C3
17	2	509	CLA	CBA-CGA-O2A-C1
19	1	516	LHG	O8-C23-C24-C25
19	A	844	LHG	O10-C23-O8-C6
17	A	808	CLA	CHA-CBD-CGD-O2D
17	A	830	CLA	CHA-CBD-CGD-O2D
17	A	835	CLA	CHA-CBD-CGD-O1D
17	A	835	CLA	CHA-CBD-CGD-O2D
17	A	837	CLA	CHA-CBD-CGD-O1D
17	B	801	CLA	CHA-CBD-CGD-O2D
17	B	808	CLA	CHA-CBD-CGD-O1D
17	B	808	CLA	CHA-CBD-CGD-O2D
17	B	814	CLA	CHA-CBD-CGD-O2D
17	B	816	CLA	CHA-CBD-CGD-O1D
17	B	816	CLA	CHA-CBD-CGD-O2D
17	B	831	CLA	CHA-CBD-CGD-O1D
17	B	837	CLA	CHA-CBD-CGD-O2D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
17	K	203	CLA	CHA-CBD-CGD-O1D
17	K	203	CLA	CHA-CBD-CGD-O2D
17	1	504	CLA	CHA-CBD-CGD-O1D
17	1	504	CLA	CHA-CBD-CGD-O2D
17	2	508	CLA	CHA-CBD-CGD-O2D
17	2	509	CLA	CHA-CBD-CGD-O1D
17	2	509	CLA	CHA-CBD-CGD-O2D
17	3	306	CLA	CHA-CBD-CGD-O1D
17	3	306	CLA	CHA-CBD-CGD-O2D
17	3	311	CLA	CHA-CBD-CGD-O2D
25	1	517	CHL	CHA-CBD-CGD-O2D
17	B	804	CLA	C15-C16-C17-C18
17	B	801	CLA	C4-C3-C5-C6
17	A	834	CLA	CBD-CGD-O2D-CED
17	A	816	CLA	CAA-CBA-CGA-O2A
17	A	805	CLA	O1D-CGD-O2D-CED
17	B	818	CLA	CAA-CBA-CGA-O2A
17	A	832	CLA	CAA-CBA-CGA-O2A
17	B	833	CLA	CAA-CBA-CGA-O2A
22	B	850	DGD	C8A-C9A-CAA-CBA
17	A	826	CLA	C2-C3-C5-C6
17	A	827	CLA	C12-C13-C15-C16
17	1	513	CLA	C11-C10-C8-C7
18	A	841	PQN	C16-C17-C18-C20
17	A	852	CLA	C6-C7-C8-C9
17	B	803	CLA	C14-C13-C15-C16
17	B	842	CLA	C11-C10-C8-C9
17	1	513	CLA	C11-C10-C8-C9
18	A	841	PQN	C16-C17-C18-C19
17	A	826	CLA	C11-C12-C13-C15
25	2	515	CHL	CAA-CBA-CGA-O1A
17	L	303	CLA	C2A-CAA-CBA-CGA
17	5	310	CLA	CAA-CBA-CGA-O2A
17	B	802	CLA	C2-C3-C5-C6
17	B	842	CLA	CAA-CBA-CGA-O1A
17	2	510	CLA	C4-C3-C5-C6
17	B	817	CLA	CAA-CBA-CGA-O1A
17	1	513	CLA	C1A-C2A-CAA-CBA
17	2	514	CLA	C1A-C2A-CAA-CBA
22	B	850	DGD	C7B-C8B-C9B-CAB
17	A	802	CLA	CBA-CGA-O2A-C1
17	A	827	CLA	CBA-CGA-O2A-C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
17	A	802	CLA	C2A-CAA-CBA-CGA
17	A	836	CLA	C2A-CAA-CBA-CGA
17	3	311	CLA	CAA-CBA-CGA-O1A
17	3	314	CLA	CBD-CGD-O2D-CED
17	A	832	CLA	CAA-CBA-CGA-O1A
19	1	516	LHG	O10-C23-C24-C25
17	2	509	CLA	O1A-CGA-O2A-C1
19	B	851	LHG	C26-C27-C28-C29
17	2	506	CLA	C16-C17-C18-C19
17	B	803	CLA	CAA-CBA-CGA-O1A
17	A	802	CLA	CAA-CBA-CGA-O2A
23	5	301	LMG	O6-C1-O1-C7
20	A	845	BCR	C23-C24-C25-C26
20	5	302	BCR	C23-C24-C25-C26
24	1	502	LUT	C5-C6-C7-C8
17	A	816	CLA	CAA-CBA-CGA-O1A
17	A	827	CLA	O1A-CGA-O2A-C1
17	A	820	CLA	CAA-CBA-CGA-O2A
17	A	806	CLA	C2A-CAA-CBA-CGA
17	2	510	CLA	C8-C10-C11-C12
17	3	314	CLA	O1D-CGD-O2D-CED
17	B	842	CLA	C2-C3-C5-C6
17	A	830	CLA	CAD-CBD-CGD-O1D
17	A	839	CLA	CAD-CBD-CGD-O1D
17	B	825	CLA	CAD-CBD-CGD-O1D
17	2	509	CLA	CAD-CBD-CGD-O1D
17	3	314	CLA	CAD-CBD-CGD-O1D
17	5	309	CLA	CAD-CBD-CGD-O1D
17	5	311	CLA	CAD-CBD-CGD-O1D
23	5	301	LMG	C28-C29-C30-C31
17	A	826	CLA	C11-C10-C8-C9
23	F	805	LMG	O7-C10-C11-C12
17	B	838	CLA	C10-C11-C12-C13
17	A	826	CLA	O1A-CGA-O2A-C1
17	A	834	CLA	O1D-CGD-O2D-CED
17	B	807	CLA	CAA-CBA-CGA-O2A
17	3	313	CLA	CAA-CBA-CGA-O2A
17	B	803	CLA	O1A-CGA-O2A-C1
17	A	820	CLA	CAA-CBA-CGA-O1A
17	A	831	CLA	C11-C10-C8-C7
17	B	801	CLA	C3A-C2A-CAA-CBA
17	B	807	CLA	C11-C10-C8-C7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
17	2	506	CLA	C11-C12-C13-C15
17	2	509	CLA	C3A-C2A-CAA-CBA
17	3	313	CLA	C3A-C2A-CAA-CBA
17	5	306	CLA	CHA-CBD-CGD-O1D
17	5	310	CLA	CAA-CBA-CGA-O1A
17	A	827	CLA	CAA-CBA-CGA-O2A
17	B	808	CLA	CAA-CBA-CGA-O2A
17	2	505	CLA	CAA-CBA-CGA-O2A
17	2	506	CLA	CAA-CBA-CGA-O2A
19	B	851	LHG	O7-C7-C8-C9
20	B	846	BCR	C7-C8-C9-C10
17	A	831	CLA	CAA-CBA-CGA-O2A
17	B	808	CLA	CAA-CBA-CGA-O1A
17	B	818	CLA	CAA-CBA-CGA-O1A
17	2	505	CLA	CAA-CBA-CGA-O1A
17	B	807	CLA	CAA-CBA-CGA-O1A
17	A	842	CLA	C2A-CAA-CBA-CGA
17	5	312	CLA	CAA-CBA-CGA-O1A
19	B	851	LHG	C10-C11-C12-C13

There are no ring outliers.

174 monomers are involved in 434 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	B	804	CLA	4	0
20	B	852	BCR	1	0
17	2	509	CLA	1	0
24	3	304	LUT	6	0
24	5	303	LUT	8	0
17	B	812	CLA	2	0
17	B	816	CLA	2	0
17	1	515	CLA	3	0
20	2	503	BCR	4	0
17	A	835	CLA	2	0
24	1	501	LUT	4	0
16	A	801	CL0	4	0
17	B	826	CLA	4	0
17	3	309	CLA	3	0
23	5	301	LMG	1	0
22	B	850	DGD	4	0
17	2	505	CLA	2	0
17	3	318	CLA	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	A	852	CLA	2	0
17	5	310	CLA	3	0
17	1	509	CLA	4	0
26	2	502	XAT	7	0
17	L	304	CLA	2	0
17	A	802	CLA	4	0
17	A	804	CLA	3	0
17	5	316	CLA	4	0
17	A	831	CLA	3	0
20	L	306	BCR	2	0
24	1	502	LUT	7	0
24	3	303	LUT	8	0
17	2	506	CLA	8	0
23	F	806	LMG	2	0
20	F	801	BCR	1	0
20	J	102	BCR	1	0
20	3	305	BCR	4	0
17	B	808	CLA	2	0
25	2	512	CHL	4	0
17	B	822	CLA	5	0
17	B	828	CLA	5	0
17	A	813	CLA	3	0
20	B	848	BCR	3	0
25	5	317	CHL	3	0
25	2	513	CHL	4	0
17	3	314	CLA	3	0
17	A	824	CLA	2	0
17	3	313	CLA	4	0
17	2	508	CLA	3	0
17	3	316	CLA	3	0
17	5	306	CLA	1	0
17	A	808	CLA	1	0
17	3	317	CLA	1	0
20	L	305	BCR	8	0
17	A	810	CLA	4	0
17	B	833	CLA	3	0
17	B	836	CLA	1	0
17	L	301	CLA	2	0
17	1	511	CLA	2	0
23	2	519	LMG	2	0
17	A	838	CLA	2	0
26	5	304	XAT	5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	3	307	CLA	2	0
17	B	806	CLA	4	0
17	B	825	CLA	2	0
25	1	517	CHL	6	0
17	B	830	CLA	2	0
20	A	847	BCR	1	0
22	J	103	DGD	3	0
24	2	501	LUT	9	0
25	1	514	CHL	1	0
17	B	838	CLA	6	0
17	5	305	CLA	2	0
17	B	835	CLA	2	0
17	B	823	CLA	1	0
17	A	828	CLA	1	0
17	1	510	CLA	2	0
17	1	508	CLA	1	0
17	B	837	CLA	3	0
17	B	827	CLA	1	0
23	F	805	LMG	1	0
17	A	812	CLA	1	0
25	2	515	CHL	2	0
21	C	102	SF4	1	0
20	B	847	BCR	2	0
17	B	817	CLA	2	0
19	A	843	LHG	4	0
17	A	842	CLA	1	0
17	B	805	CLA	1	0
17	B	811	CLA	5	0
17	J	101	CLA	3	0
17	A	818	CLA	1	0
17	B	801	CLA	3	0
17	K	202	CLA	3	0
25	5	315	CHL	4	0
20	B	845	BCR	1	0
20	A	853	BCR	4	0
19	2	517	LHG	2	0
17	K	201	CLA	4	0
17	B	832	CLA	1	0
20	B	849	BCR	2	0
17	B	820	CLA	3	0
20	5	302	BCR	6	0
17	A	809	CLA	1	0

Continued on next page...

Continued from previous page...

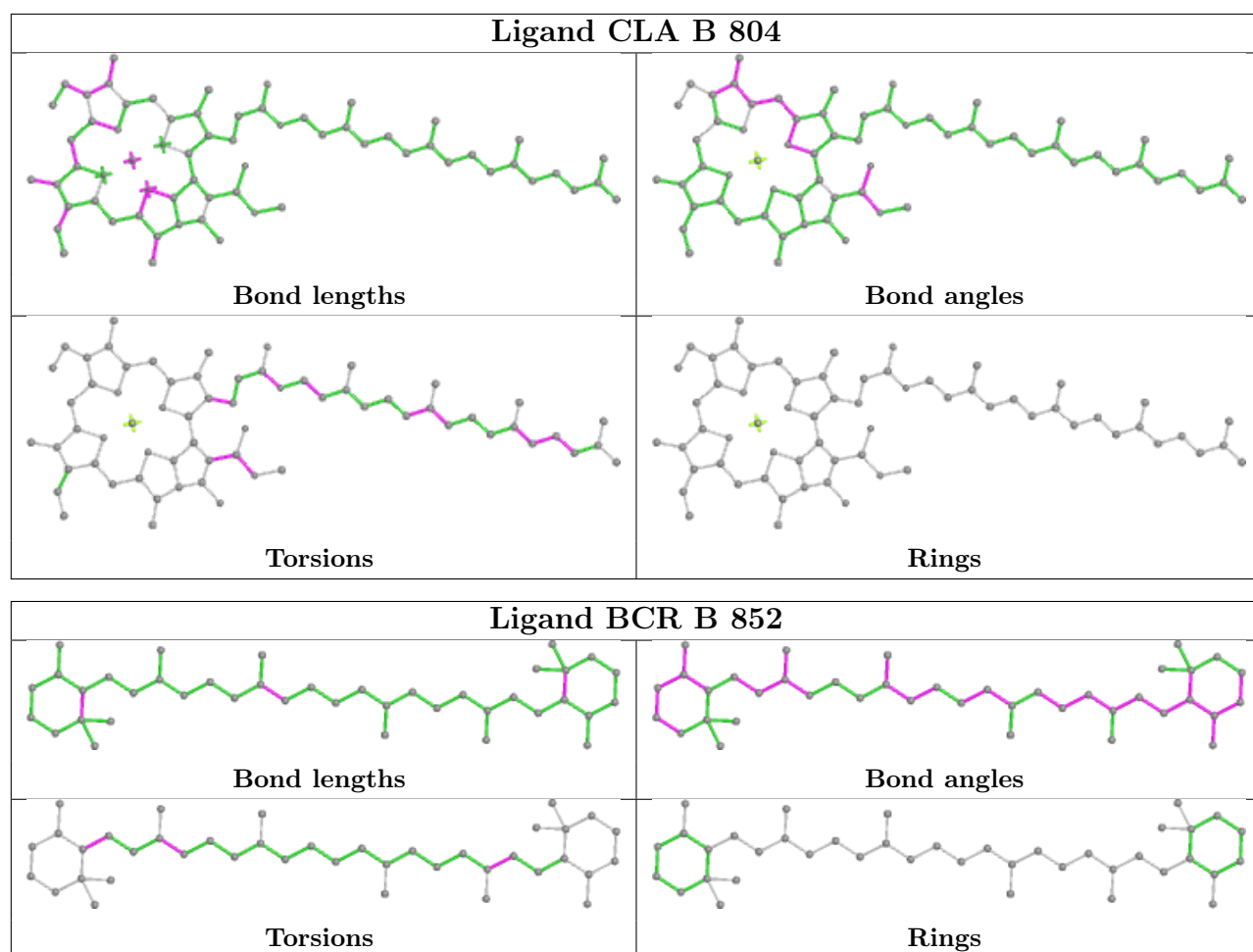
Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	A	815	CLA	2	0
17	A	822	CLA	1	0
17	B	831	CLA	2	0
19	1	516	LHG	5	0
17	L	303	CLA	3	0
17	F	802	CLA	3	0
17	B	818	CLA	4	0
23	2	518	LMG	1	0
17	B	819	CLA	1	0
18	B	843	PQN	1	0
20	A	846	BCR	3	0
17	A	805	CLA	6	0
17	B	810	CLA	2	0
20	I	101	BCR	4	0
17	5	308	CLA	6	0
20	F	804	BCR	4	0
17	1	513	CLA	4	0
20	B	844	BCR	10	0
17	B	802	CLA	7	0
17	A	829	CLA	1	0
17	3	301	CLA	2	0
25	5	314	CHL	2	0
17	A	840	CLA	1	0
20	B	846	BCR	1	0
17	B	842	CLA	3	0
17	B	803	CLA	2	0
17	B	815	CLA	4	0
17	A	825	CLA	1	0
17	B	824	CLA	4	0
17	A	816	CLA	4	0
25	3	315	CHL	2	0
20	A	848	BCR	2	0
17	F	803	CLA	2	0
17	3	308	CLA	7	0
17	2	504	CLA	2	0
17	3	306	CLA	4	0
17	2	511	CLA	2	0
17	2	507	CLA	2	0
20	A	849	BCR	1	0
25	2	516	CHL	3	0
19	A	844	LHG	4	0
17	5	307	CLA	4	0

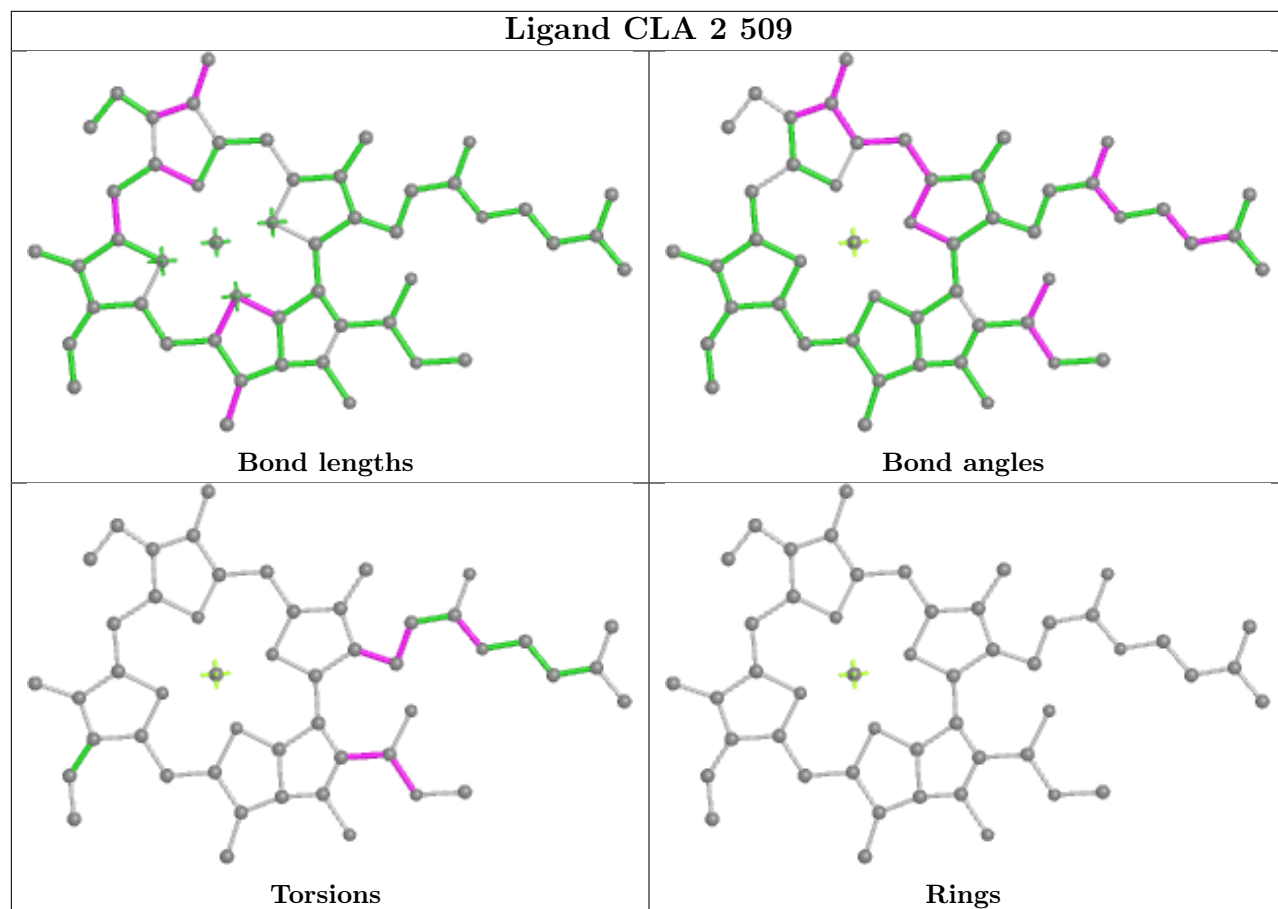
Continued on next page...

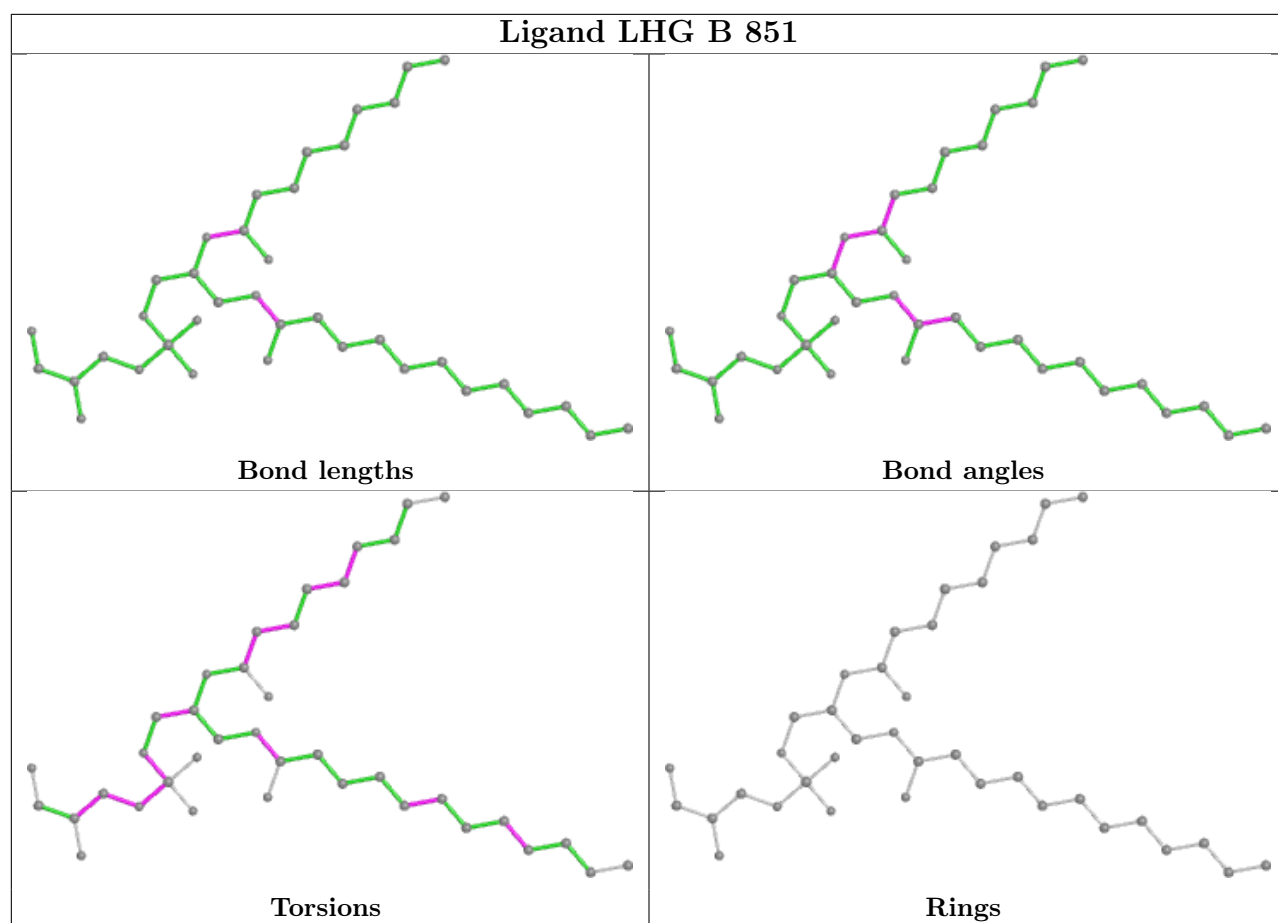
Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	5	309	CLA	3	0
17	A	837	CLA	1	0
17	A	820	CLA	5	0
17	A	806	CLA	5	0
20	K	204	BCR	2	0
17	B	841	CLA	2	0
18	A	841	PQN	2	0
17	A	817	CLA	3	0
17	B	839	CLA	1	0
17	A	821	CLA	3	0
17	A	836	CLA	3	0
17	1	507	CLA	2	0
17	A	803	CLA	3	0
17	A	823	CLA	1	0
17	3	310	CLA	2	0
17	3	311	CLA	5	0
17	A	827	CLA	7	0
17	1	504	CLA	2	0
17	2	514	CLA	3	0
17	B	807	CLA	4	0
17	2	510	CLA	4	0
17	3	312	CLA	2	0
20	1	503	BCR	3	0
20	A	845	BCR	4	0
17	L	302	CLA	2	0
17	B	813	CLA	1	0
17	A	833	CLA	1	0
17	1	506	CLA	7	0
20	A	851	BCR	4	0
17	A	839	CLA	1	0

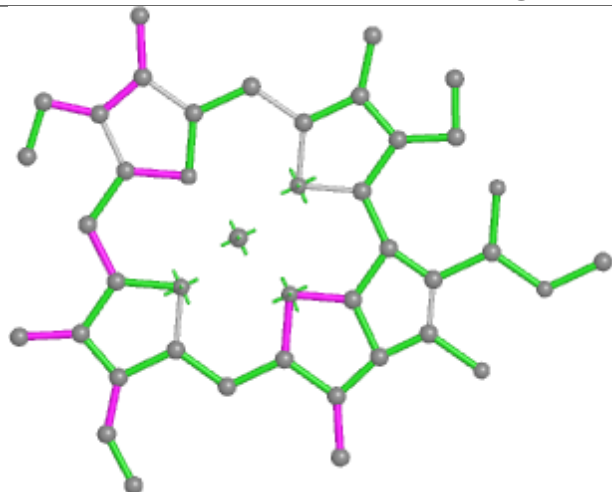
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



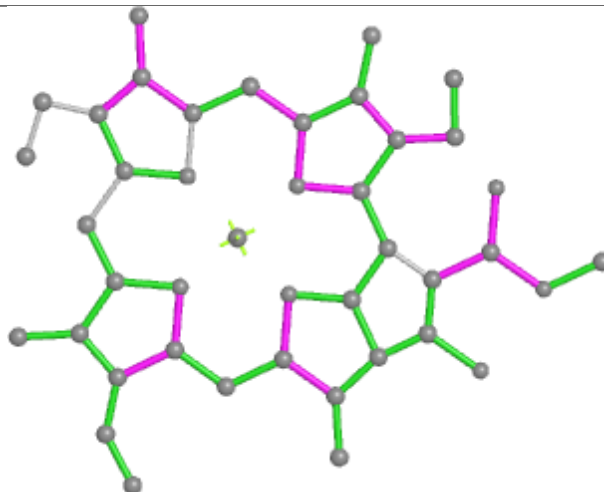




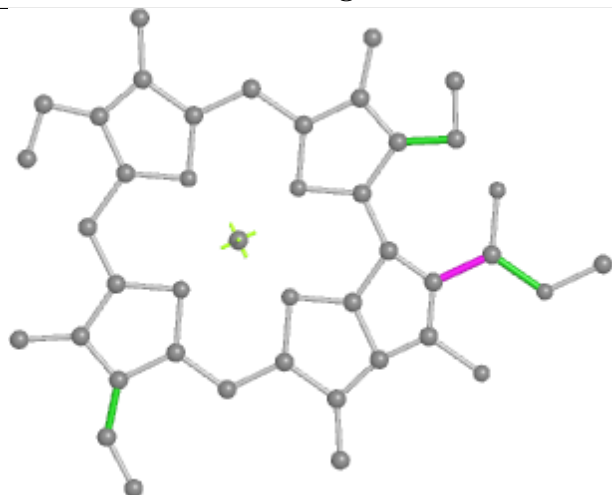
Ligand CLA A 814



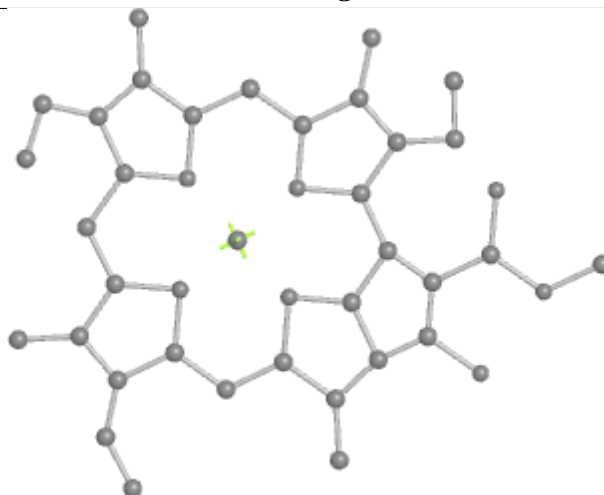
Bond lengths



Bond angles

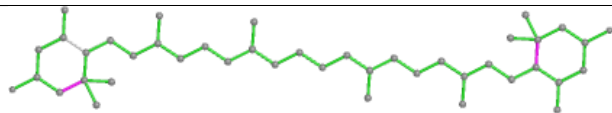


Torsions

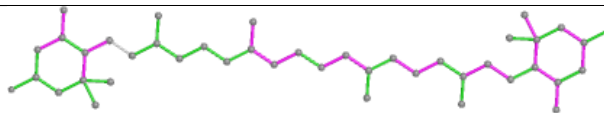


Rings

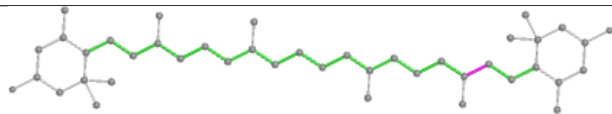
Ligand LUT 3 304



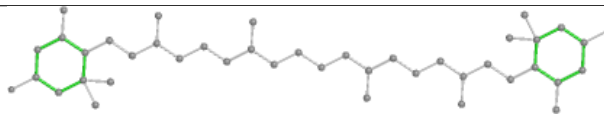
Bond lengths



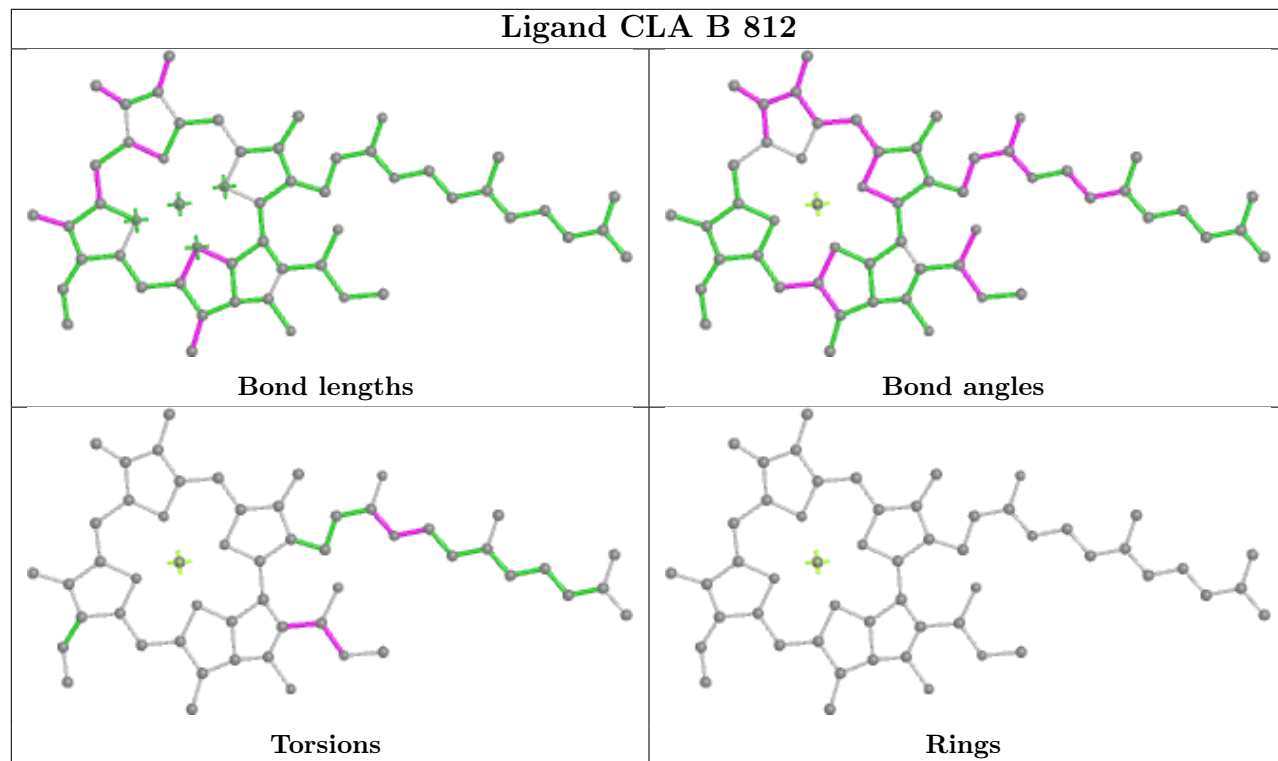
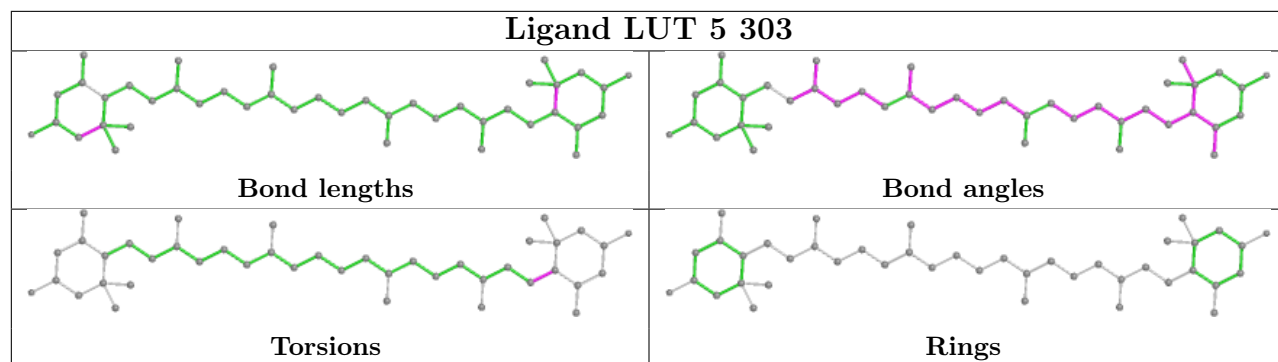
Bond angles



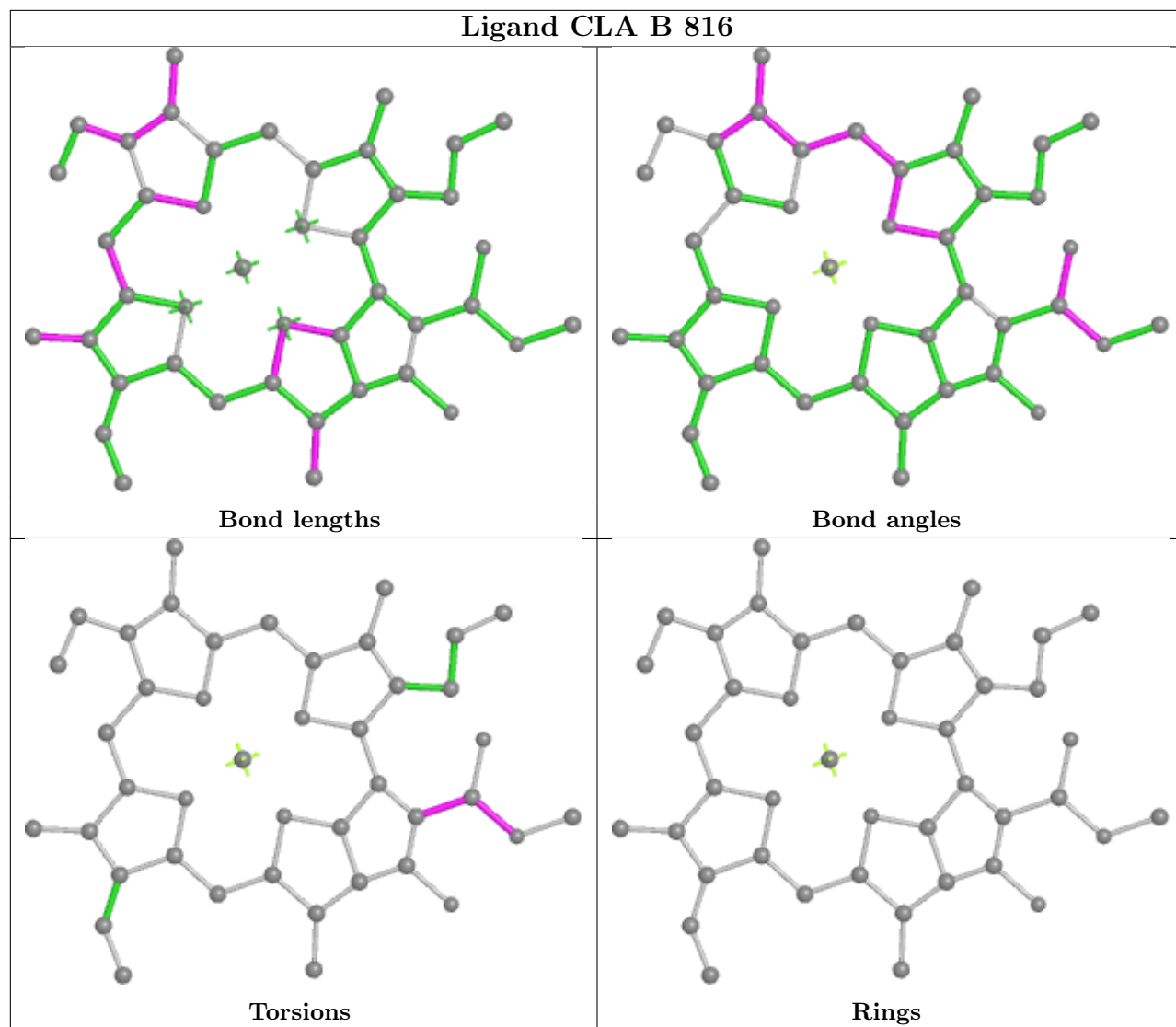
Torsions



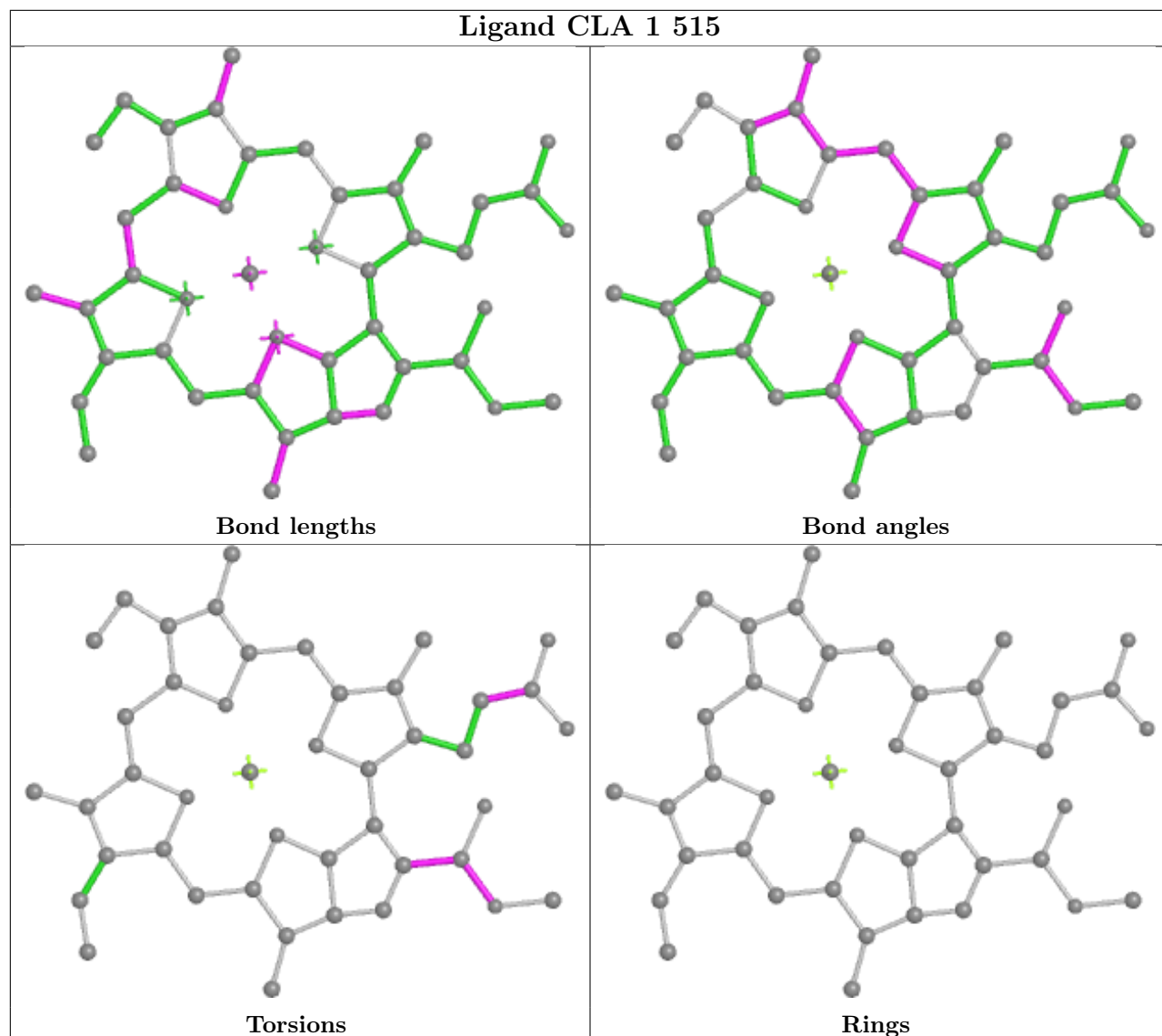
Rings



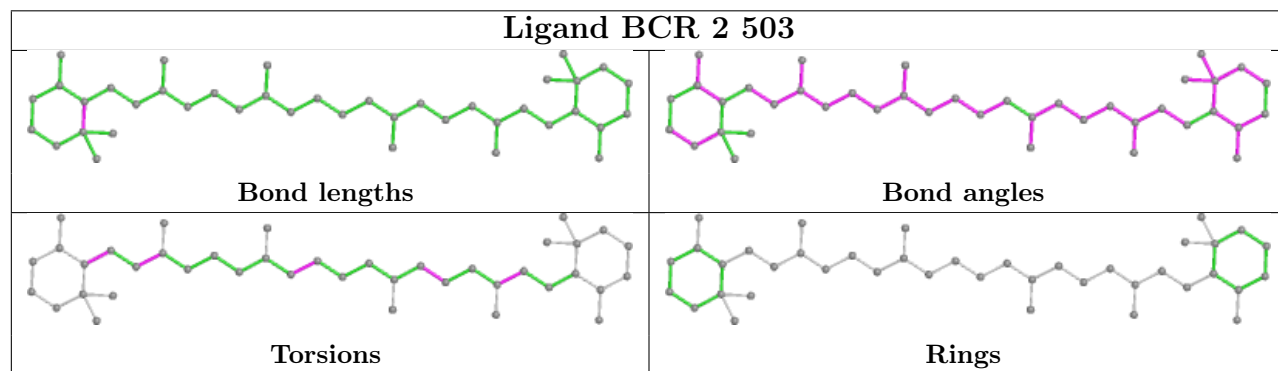
Ligand CLA B 816



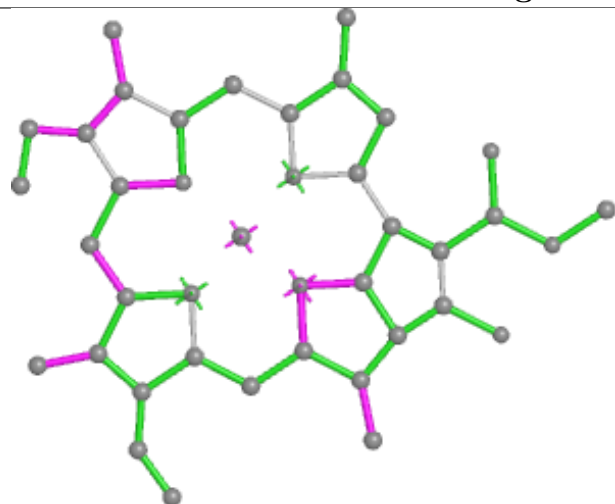
Ligand CLA 1 515



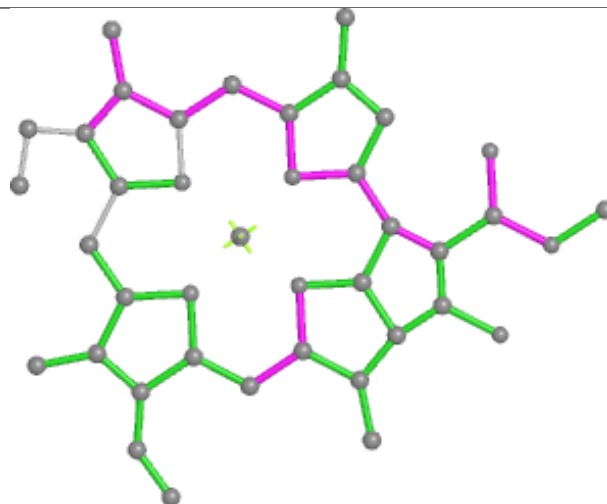
Ligand BCR 2 503



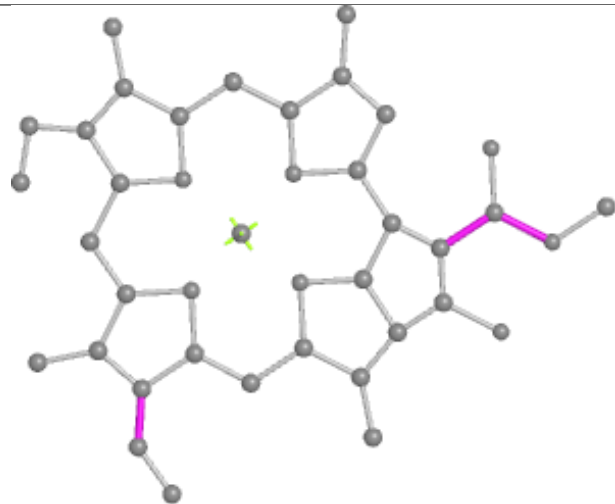
Ligand CLA K 203



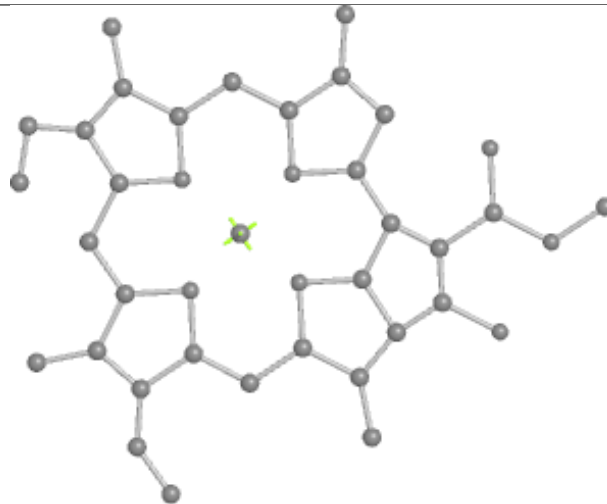
Bond lengths



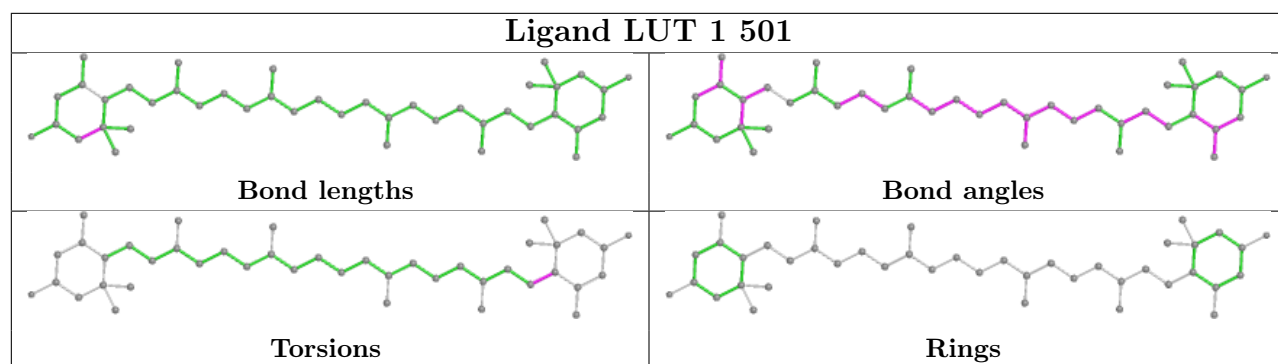
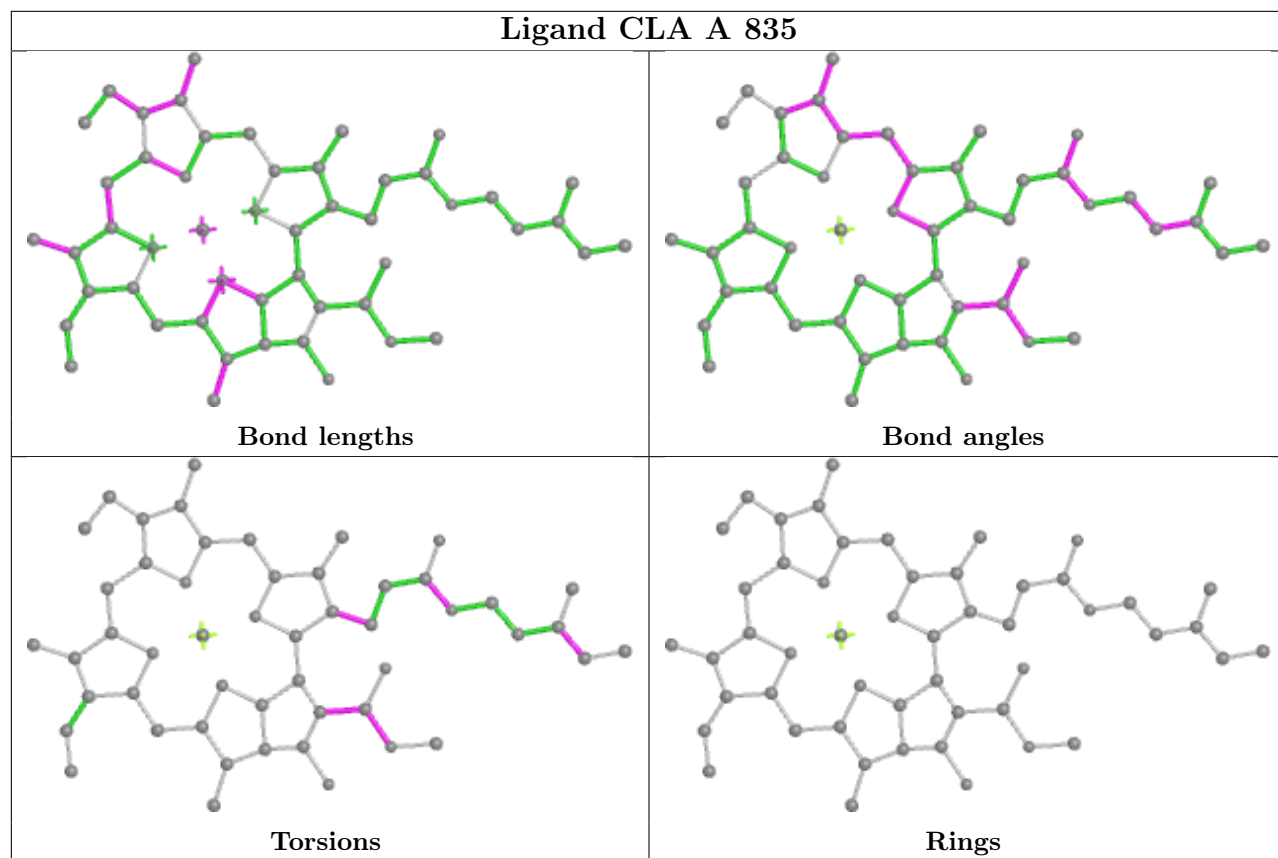
Bond angles



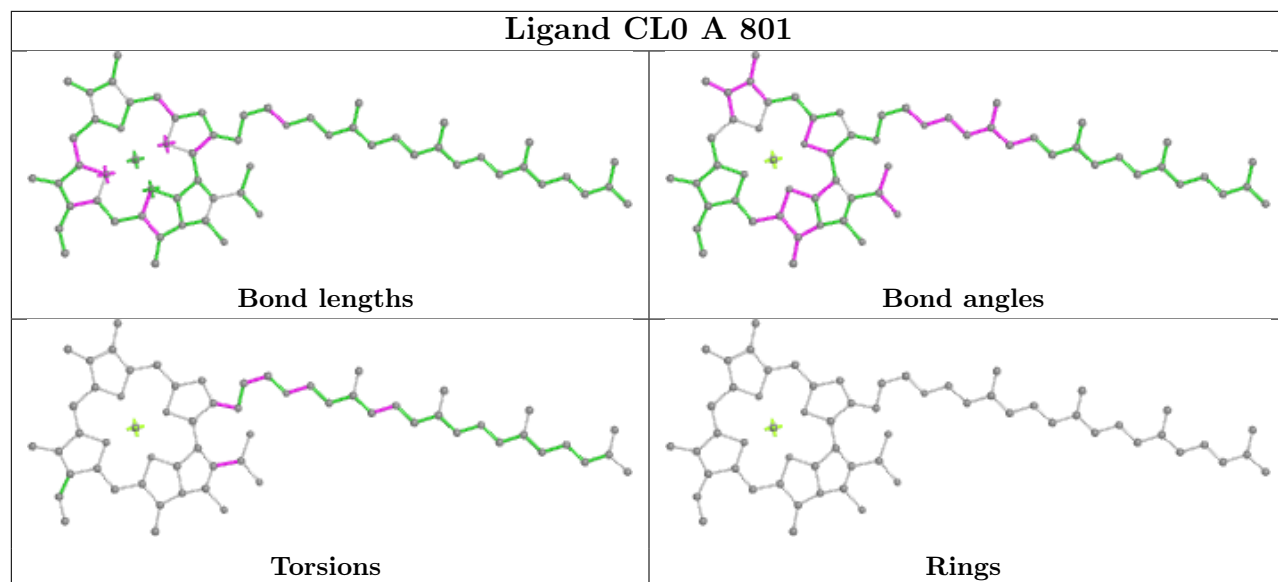
Torsions



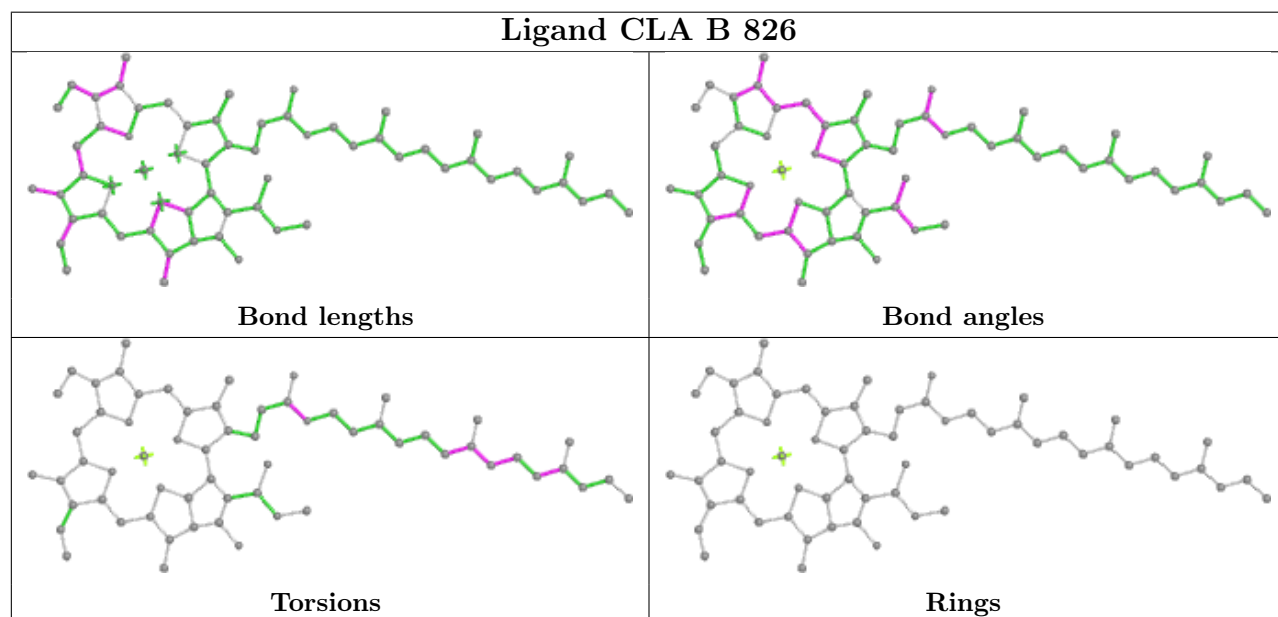
Rings



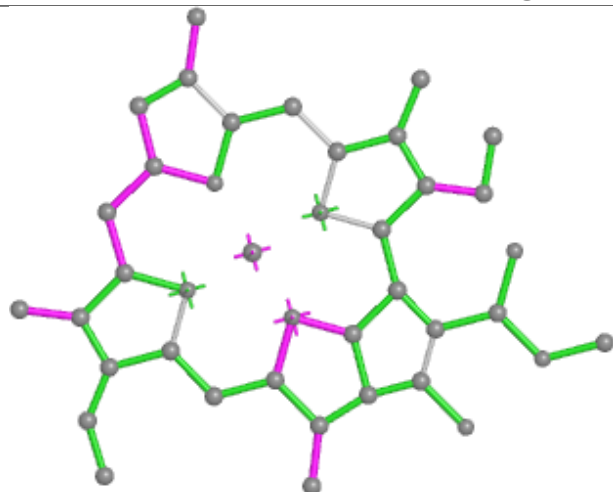
Ligand CL0 A 801



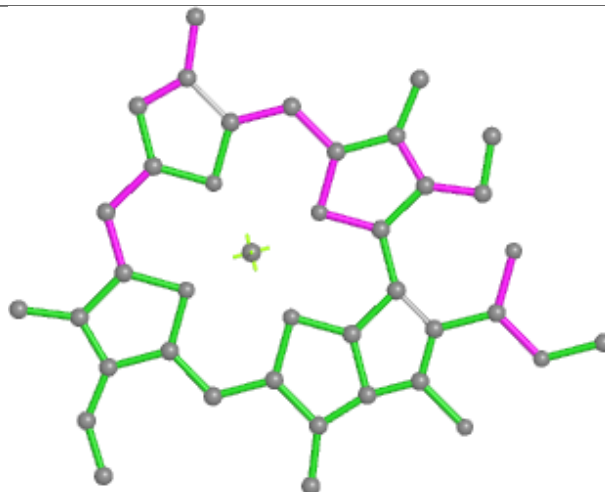
Ligand CLA B 826



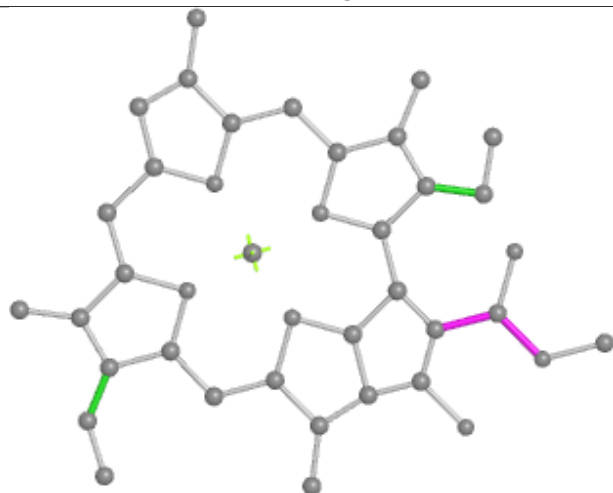
Ligand CLA 3 309



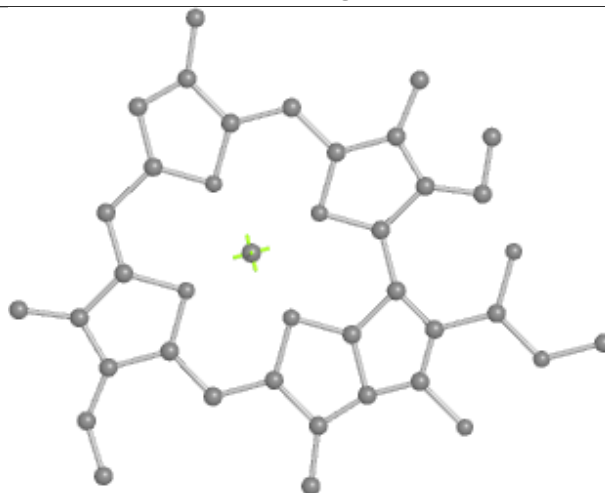
Bond lengths



Bond angles

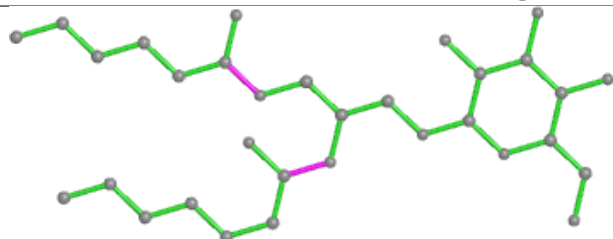


Torsions

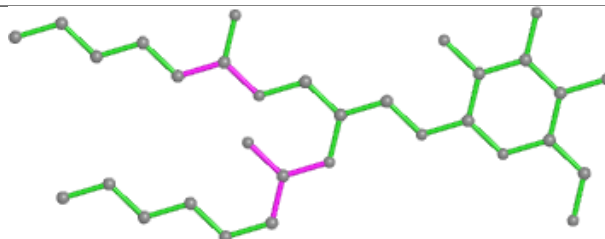


Rings

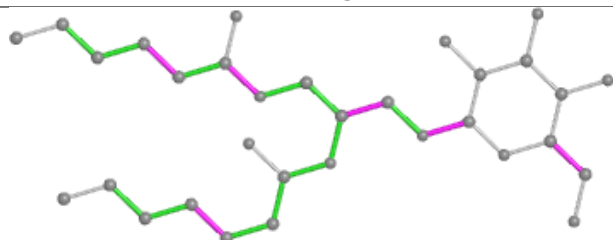
Ligand LMG 5 301



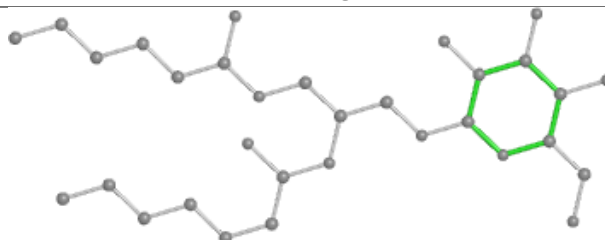
Bond lengths



Bond angles

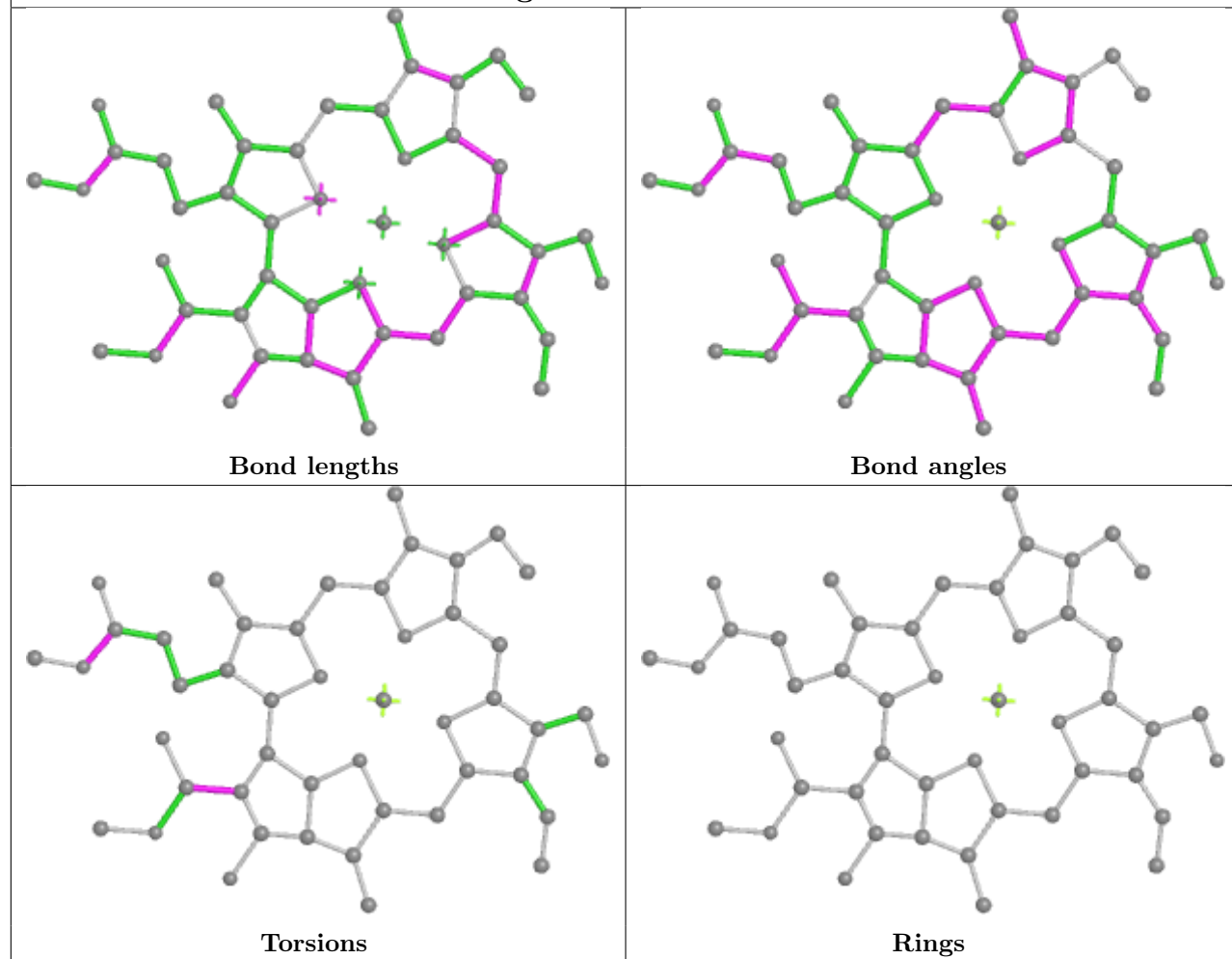


Torsions

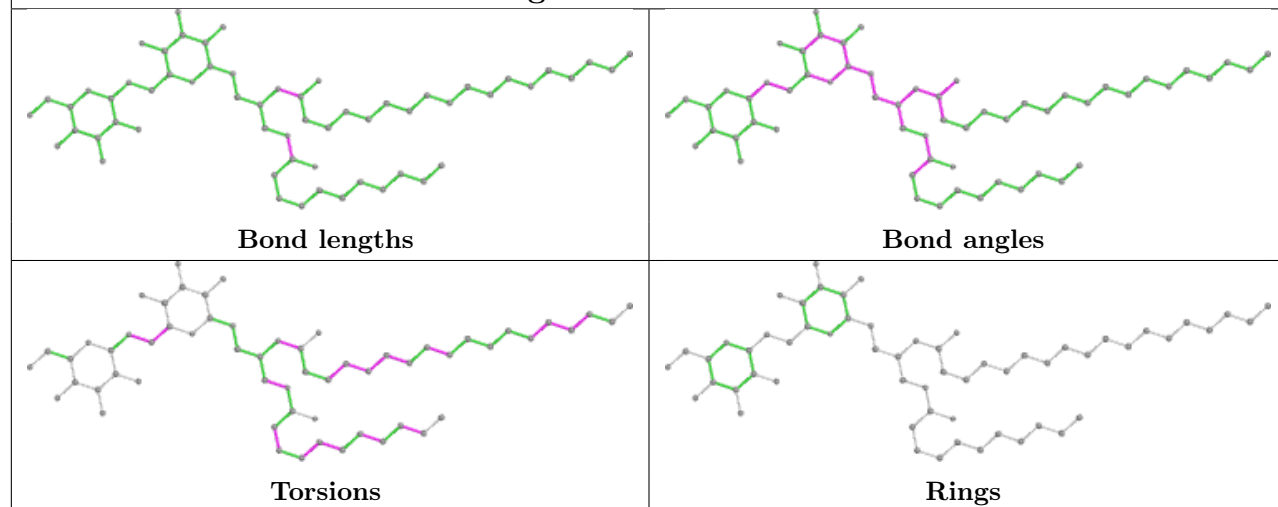


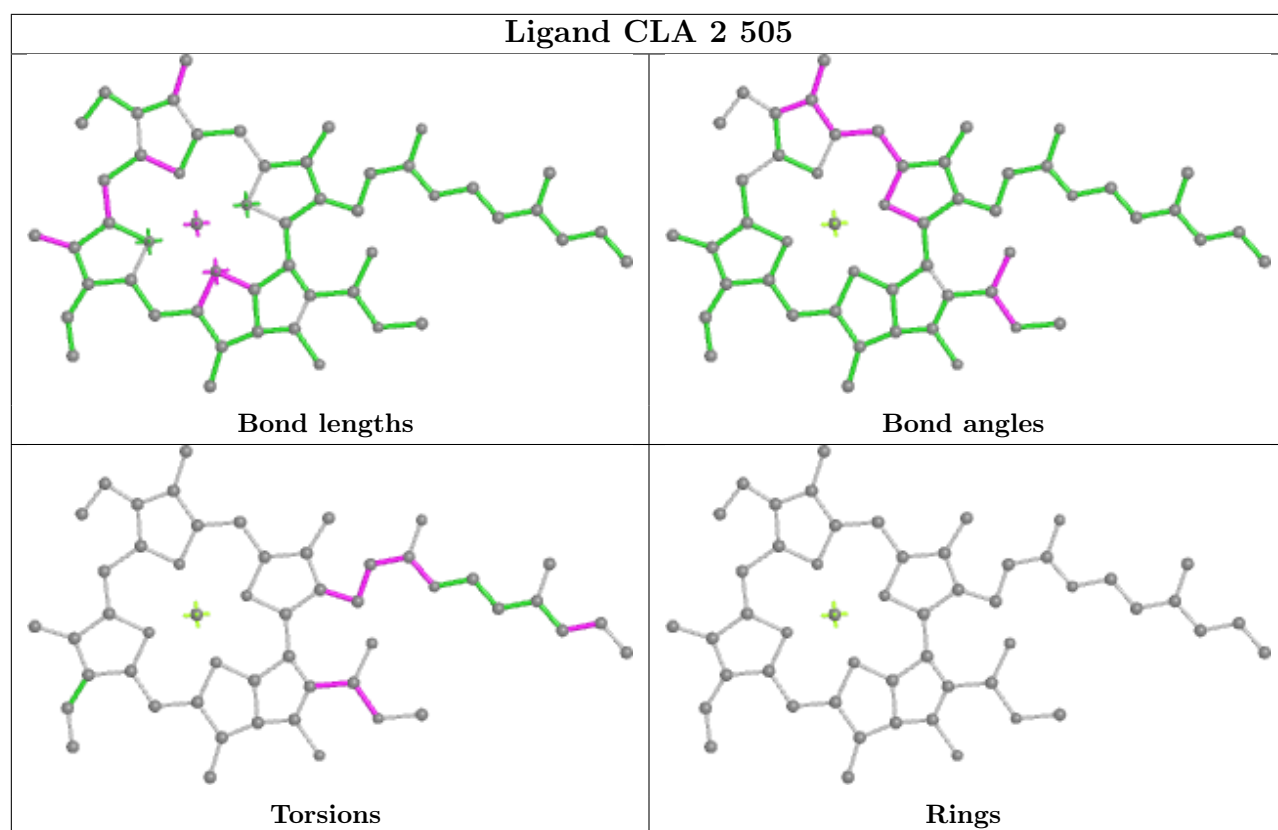
Rings

Ligand CHL 3 302

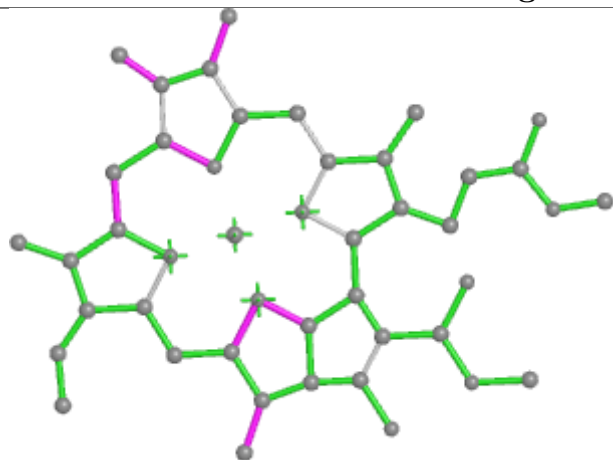


Ligand DGD B 850

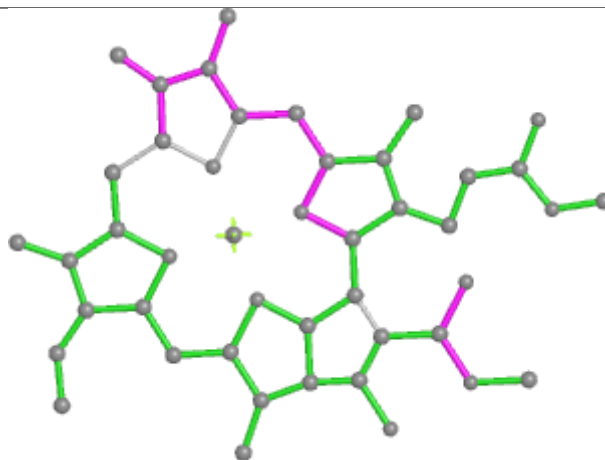




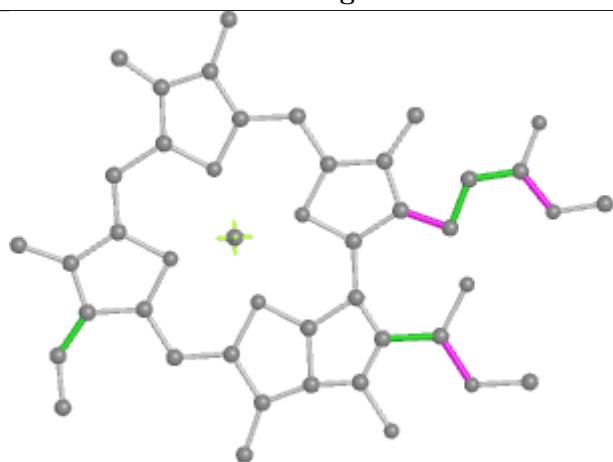
Ligand CLA 3 318



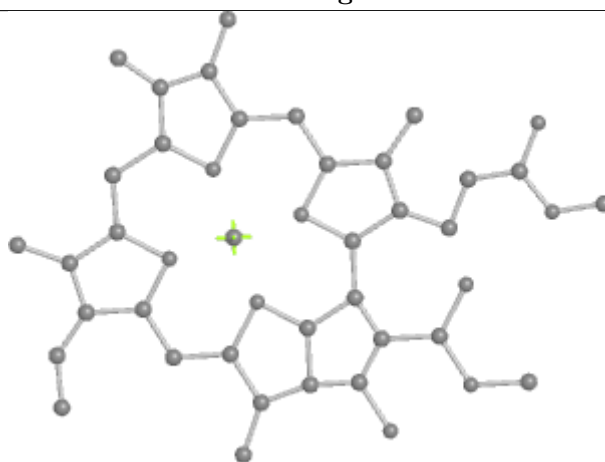
Bond lengths



Bond angles

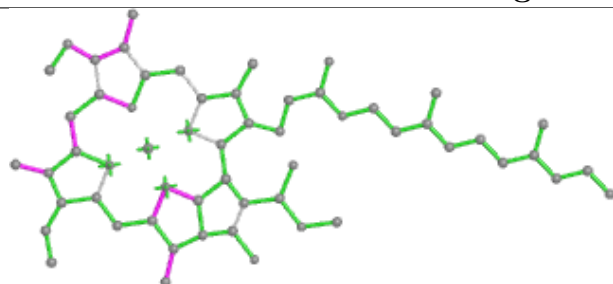


Torsions

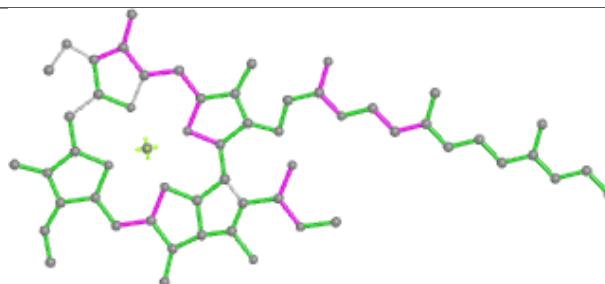


Rings

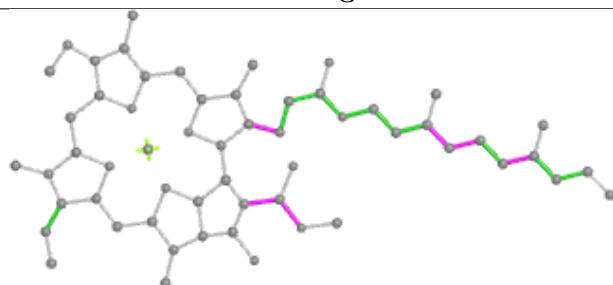
Ligand CLA A 852



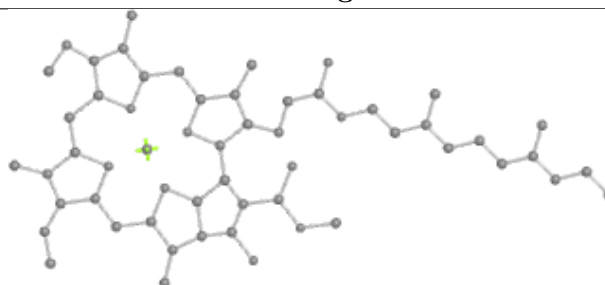
Bond lengths



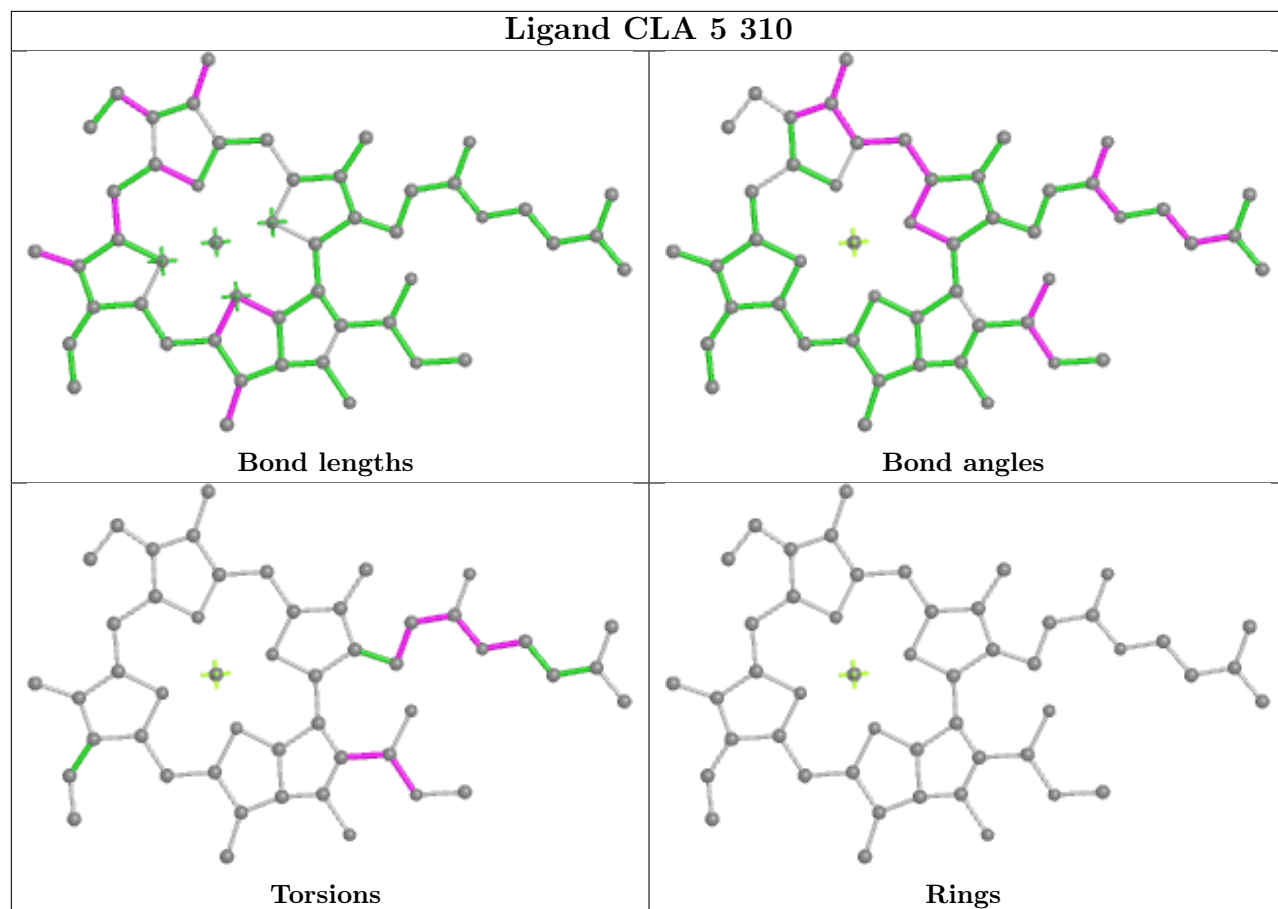
Bond angles



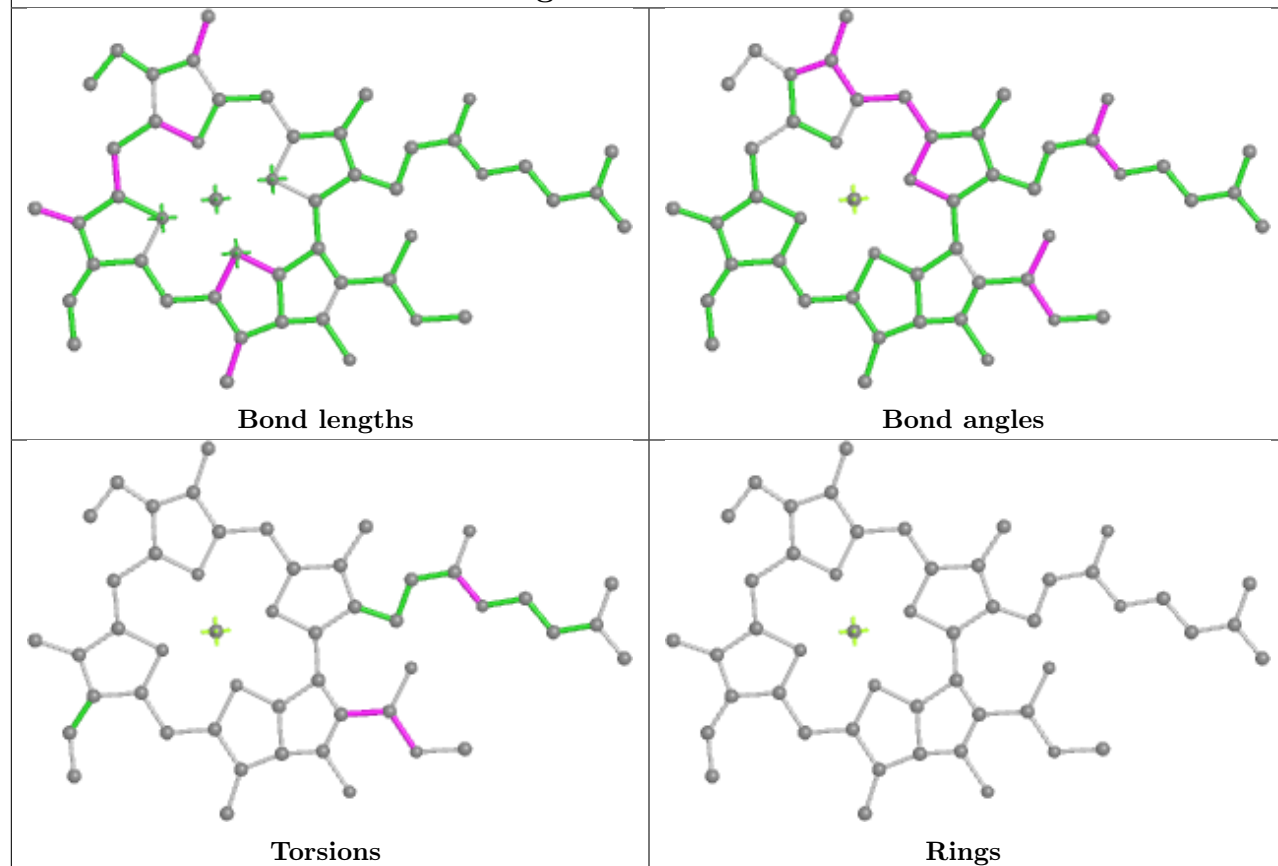
Torsions



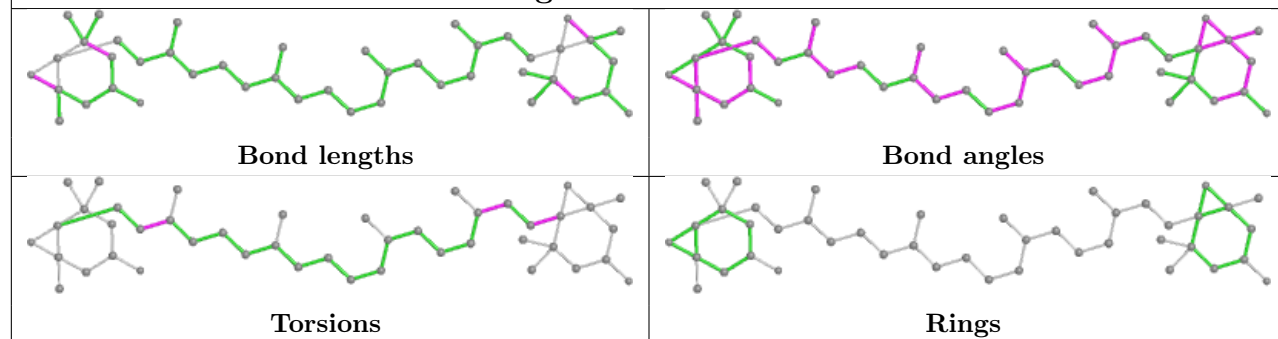
Rings



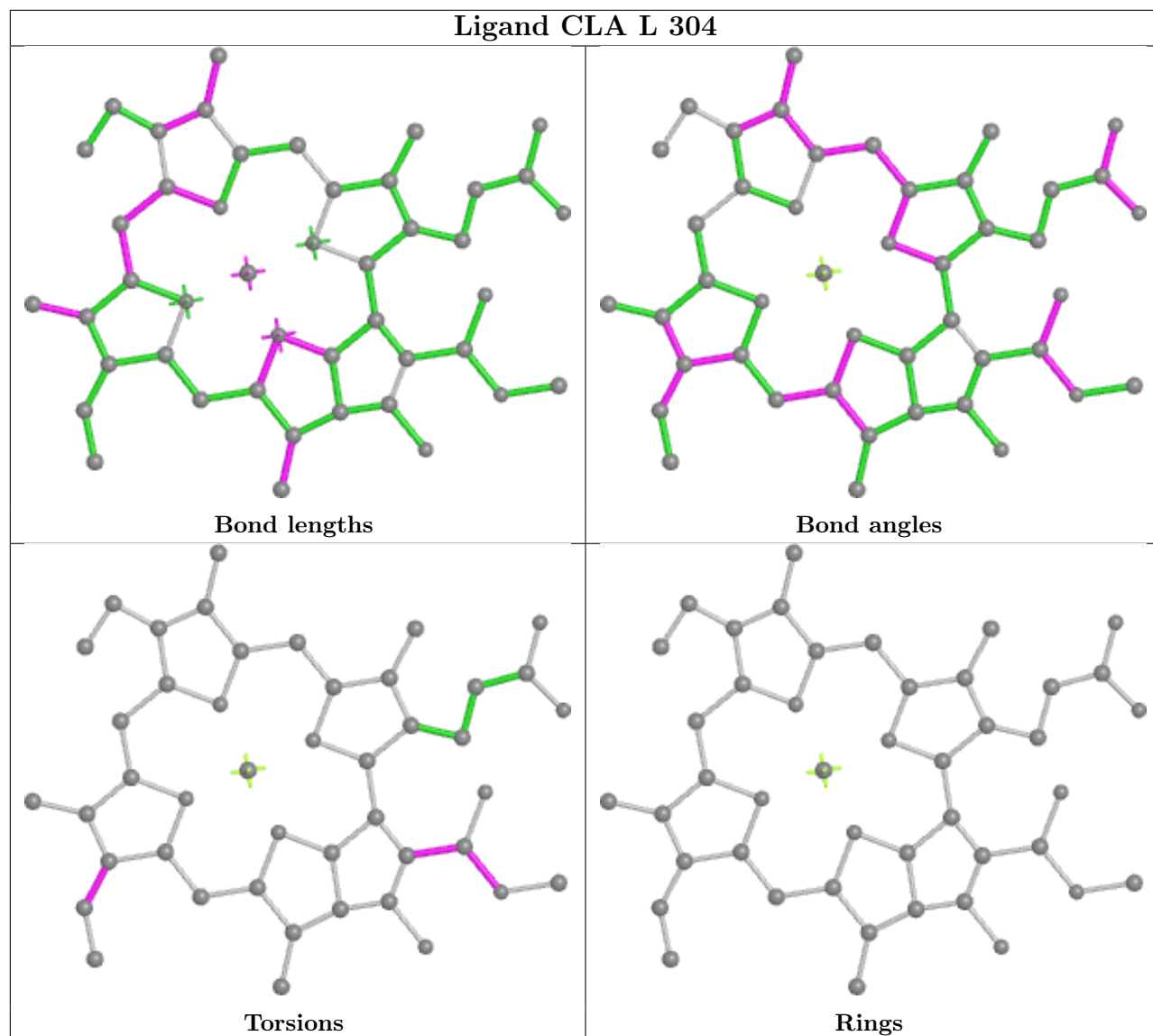
Ligand CLA 1 509



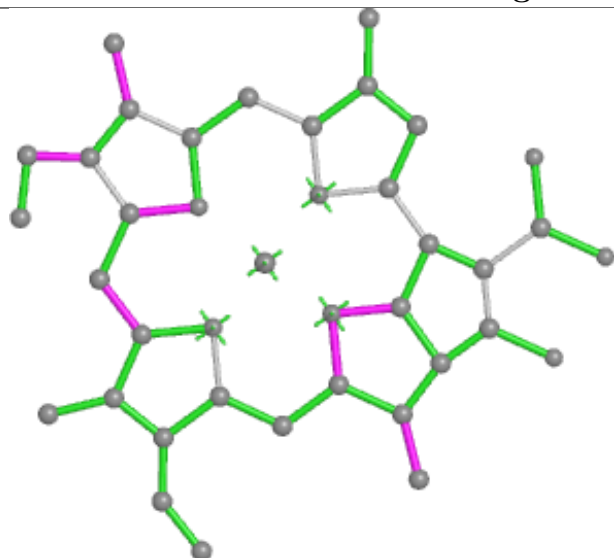
Ligand XAT 2 502



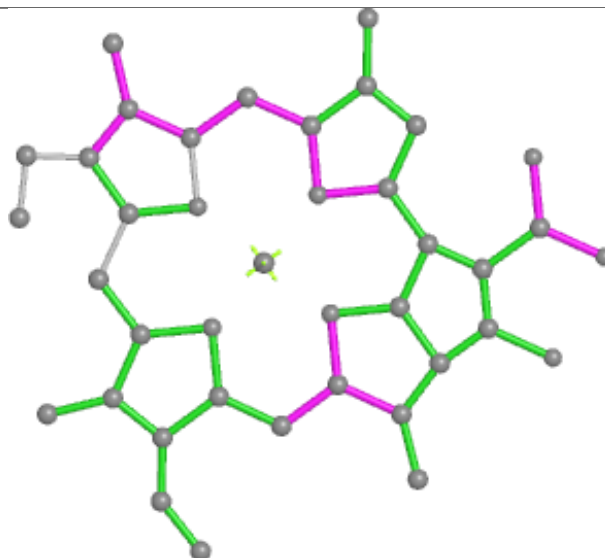
Ligand CLA L 304



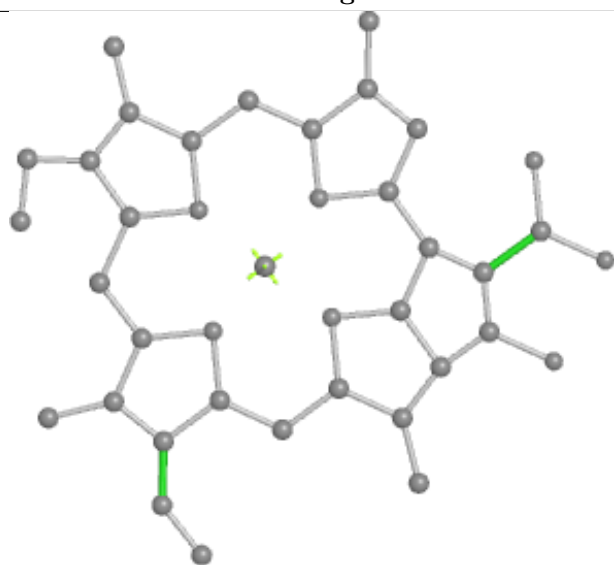
Ligand CLA K 205



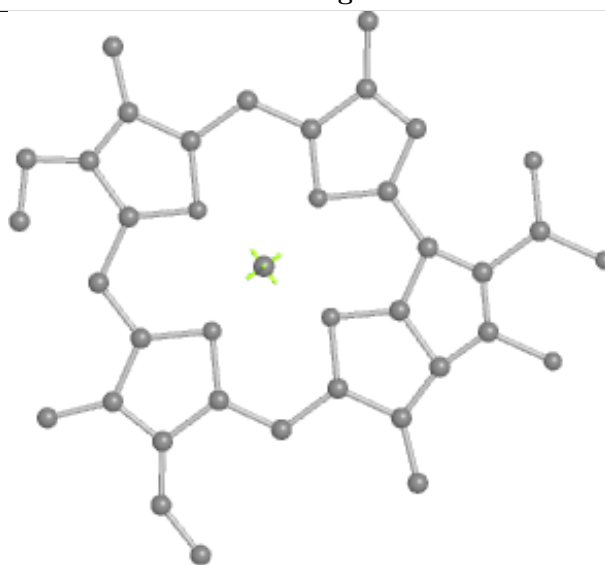
Bond lengths



Bond angles

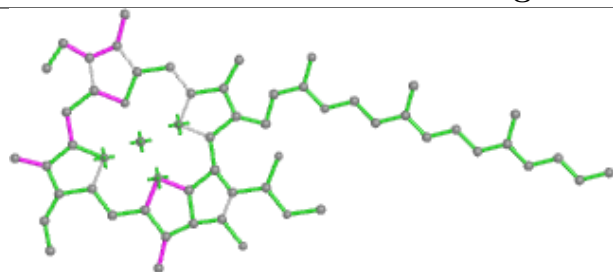


Torsions

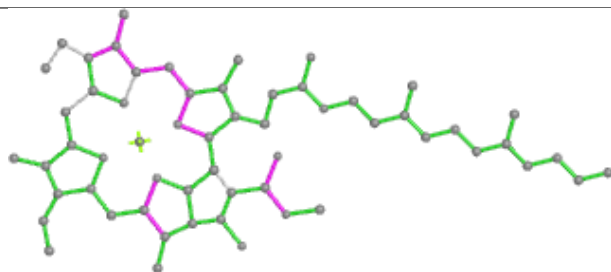


Rings

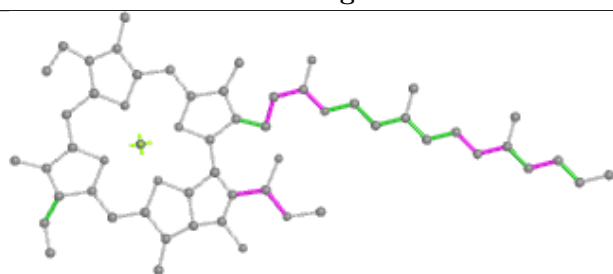
Ligand CLA A 802



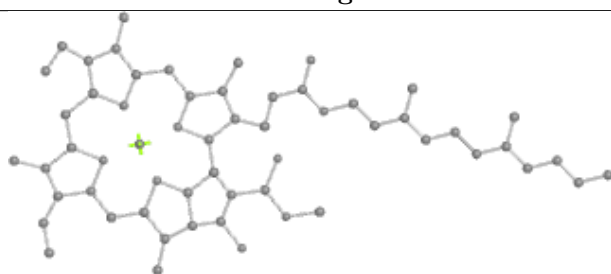
Bond lengths



Bond angles

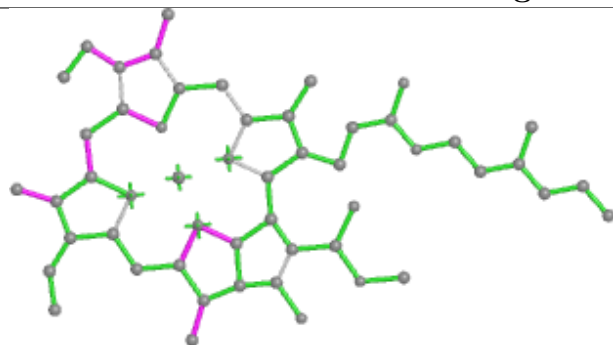


Torsions

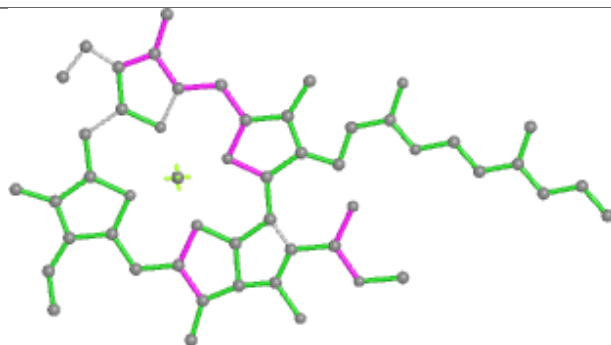


Rings

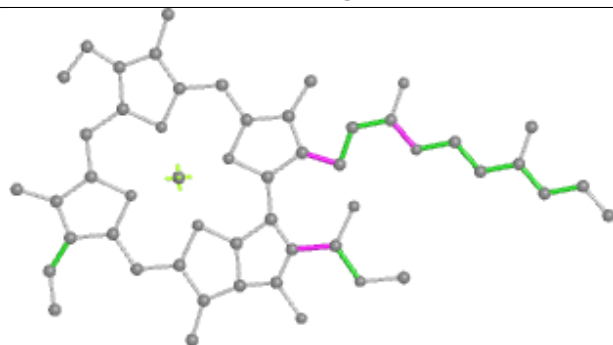
Ligand CLA A 804



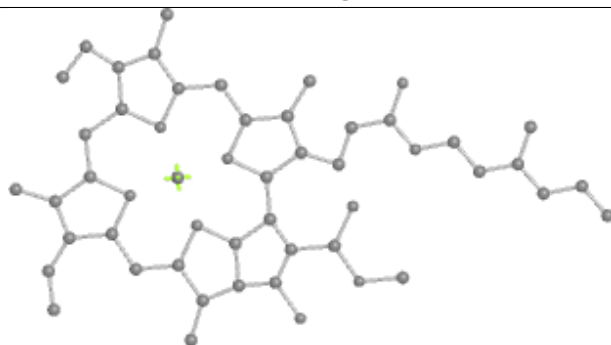
Bond lengths



Bond angles

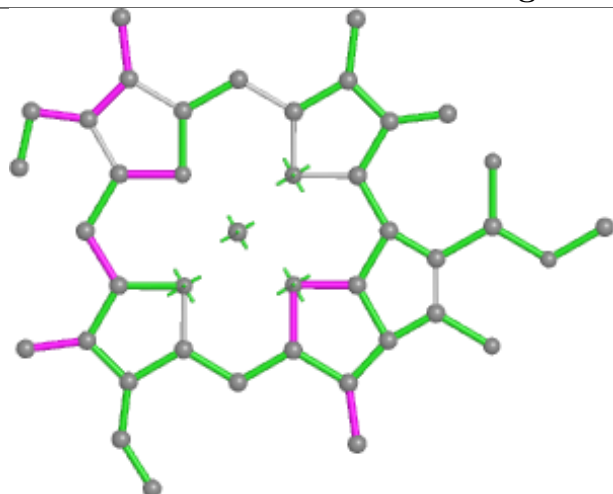


Torsions

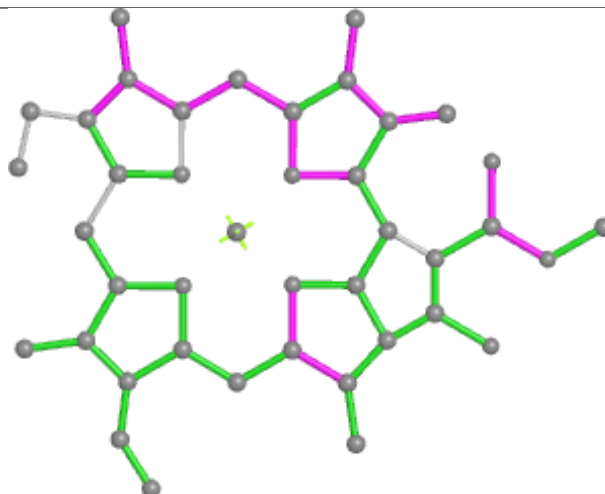


Rings

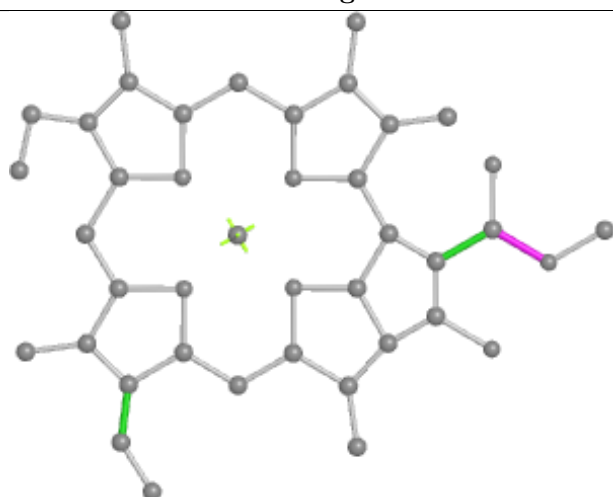
Ligand CLA 5 316



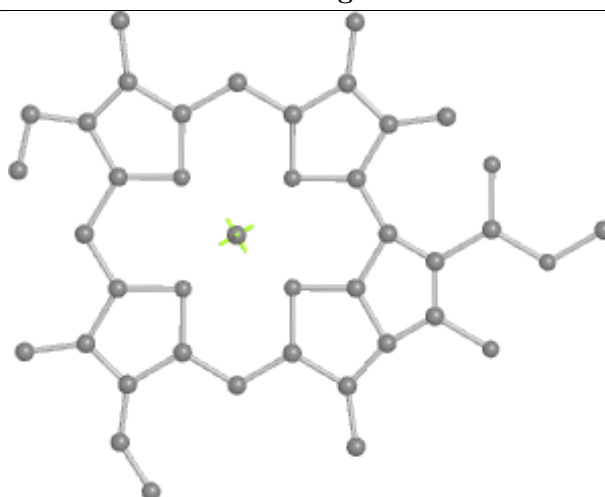
Bond lengths



Bond angles

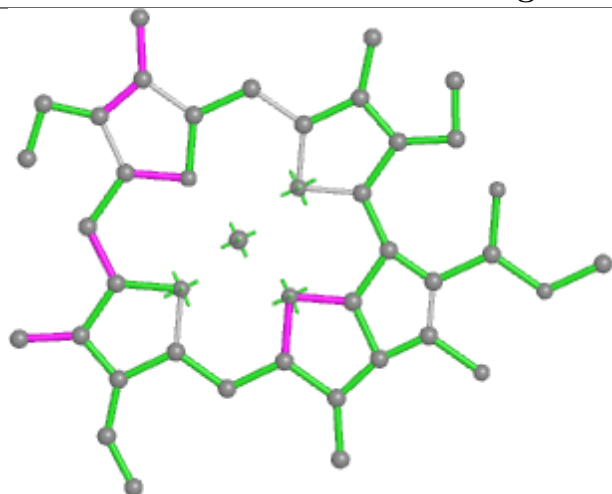


Torsions

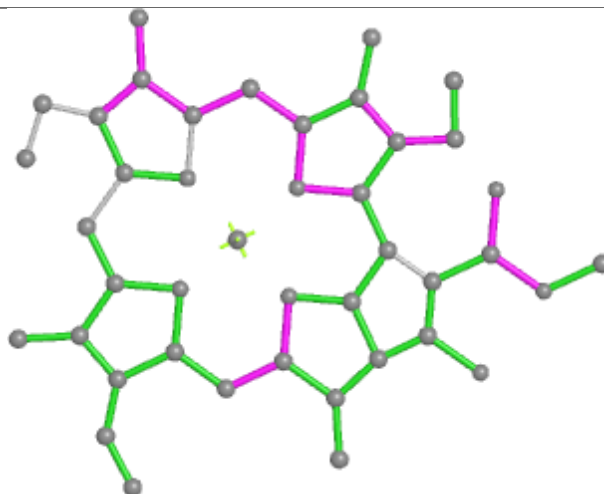


Rings

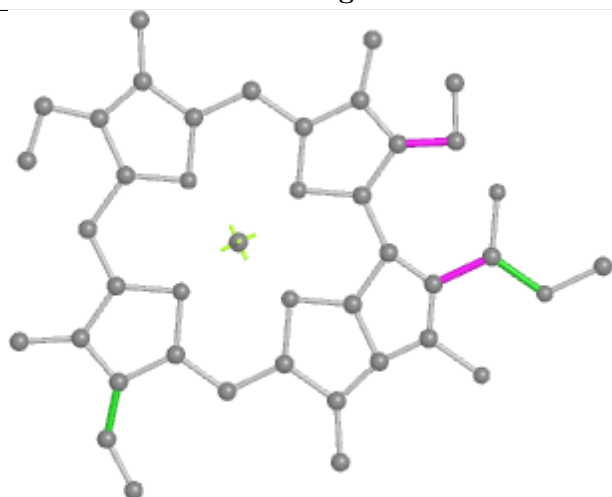
Ligand CLA 1 505



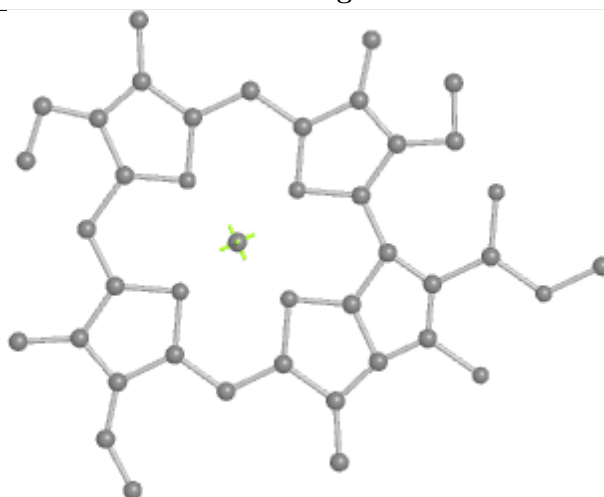
Bond lengths



Bond angles

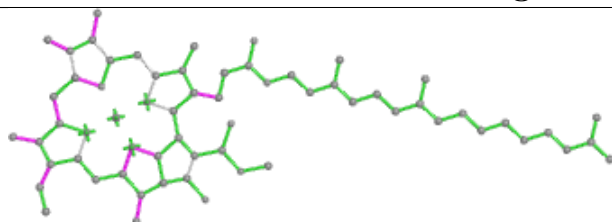


Torsions

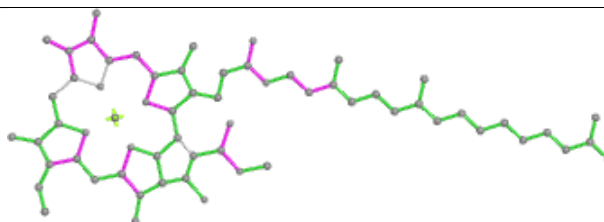


Rings

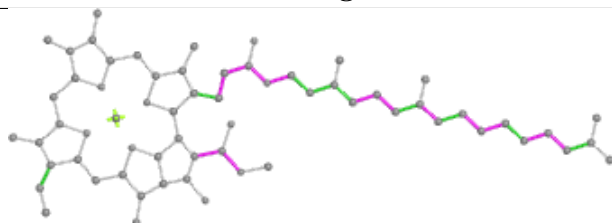
Ligand CLA A 831



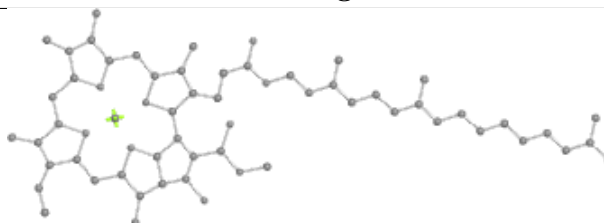
Bond lengths



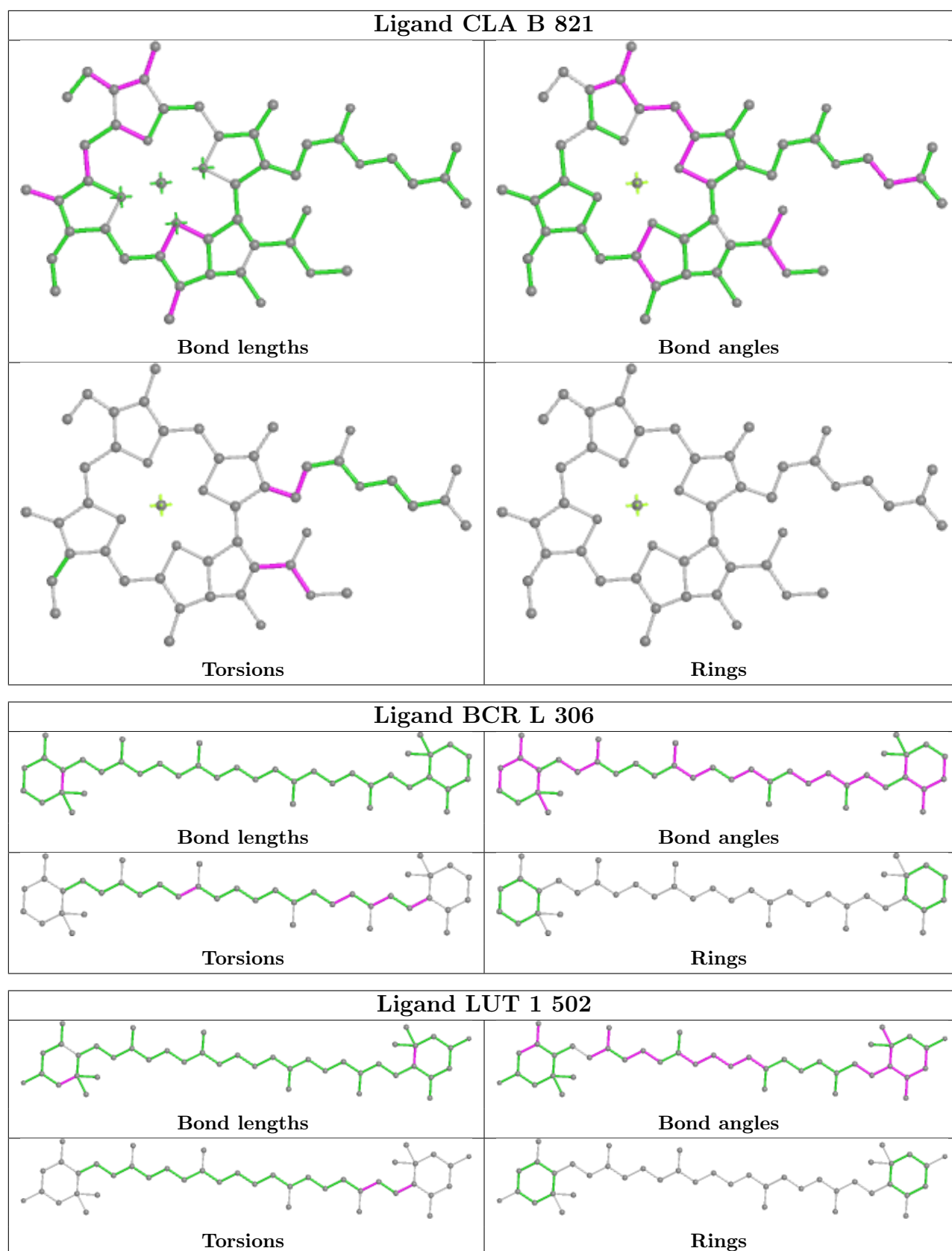
Bond angles



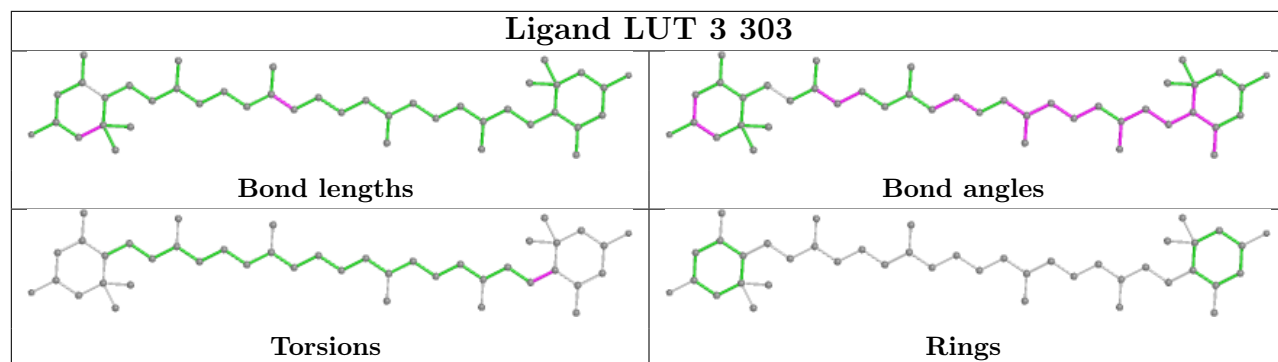
Torsions



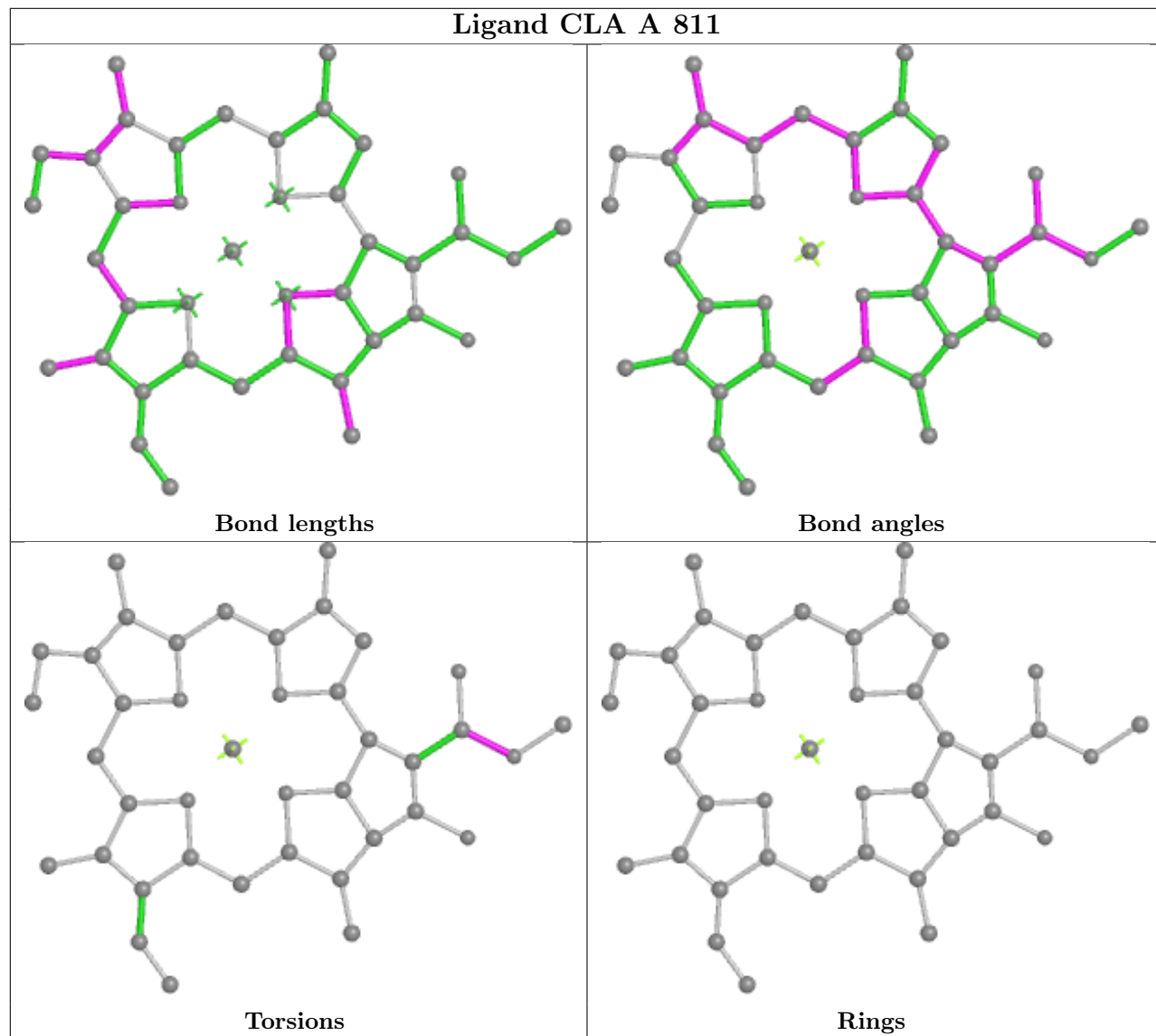
Rings



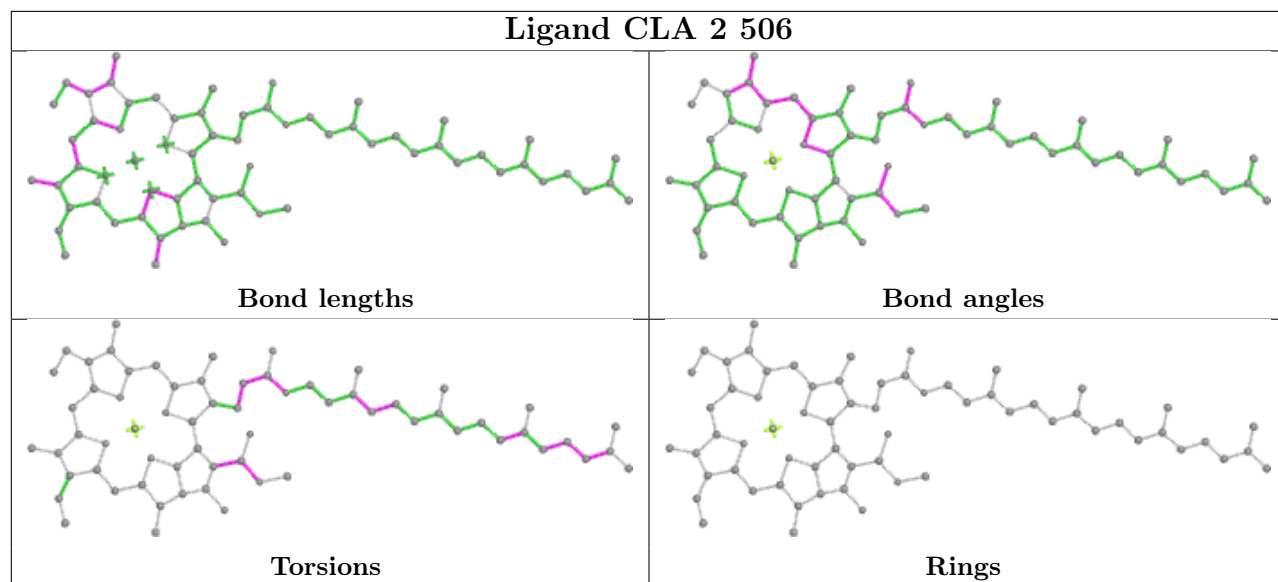
Ligand LUT 3 303



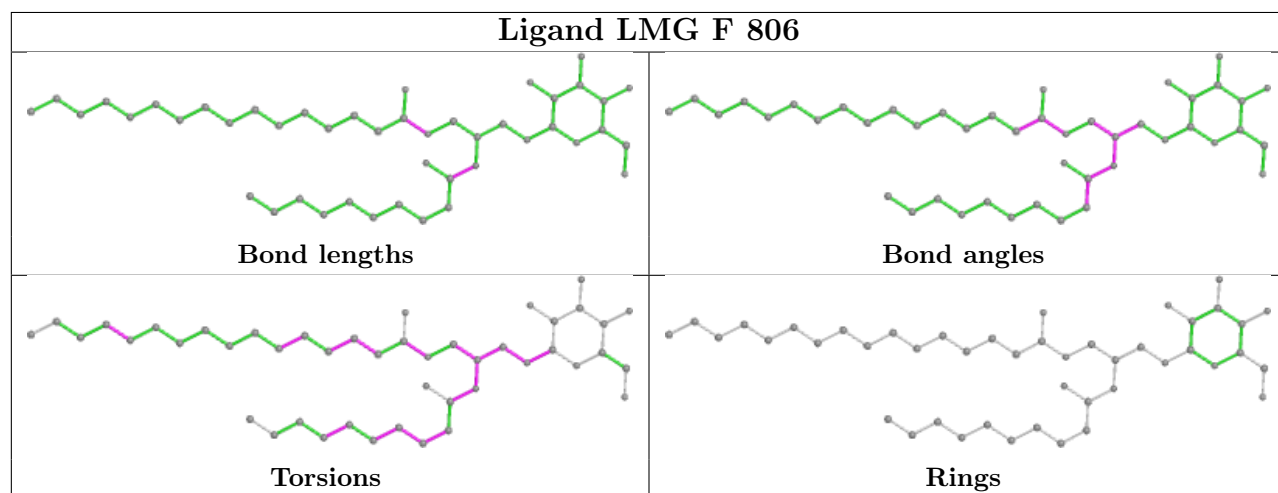
Ligand CLA A 811



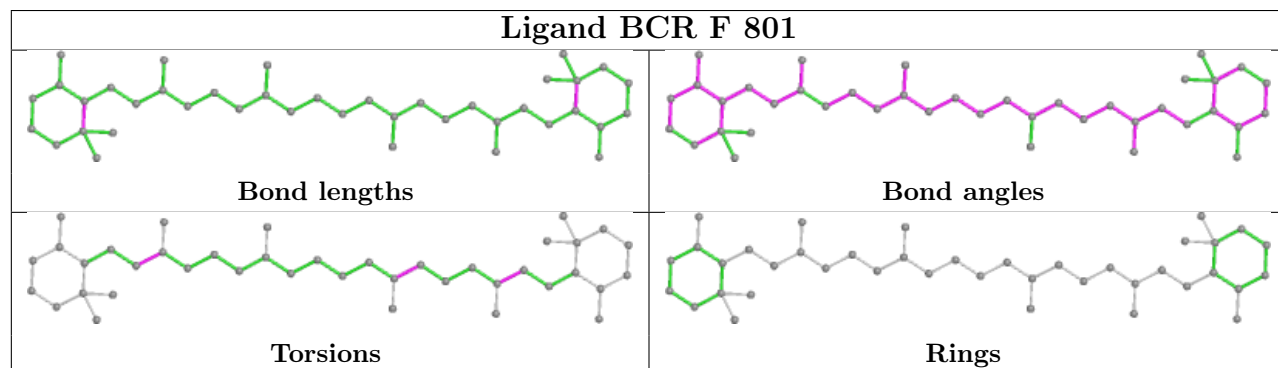
Ligand CLA 2 506

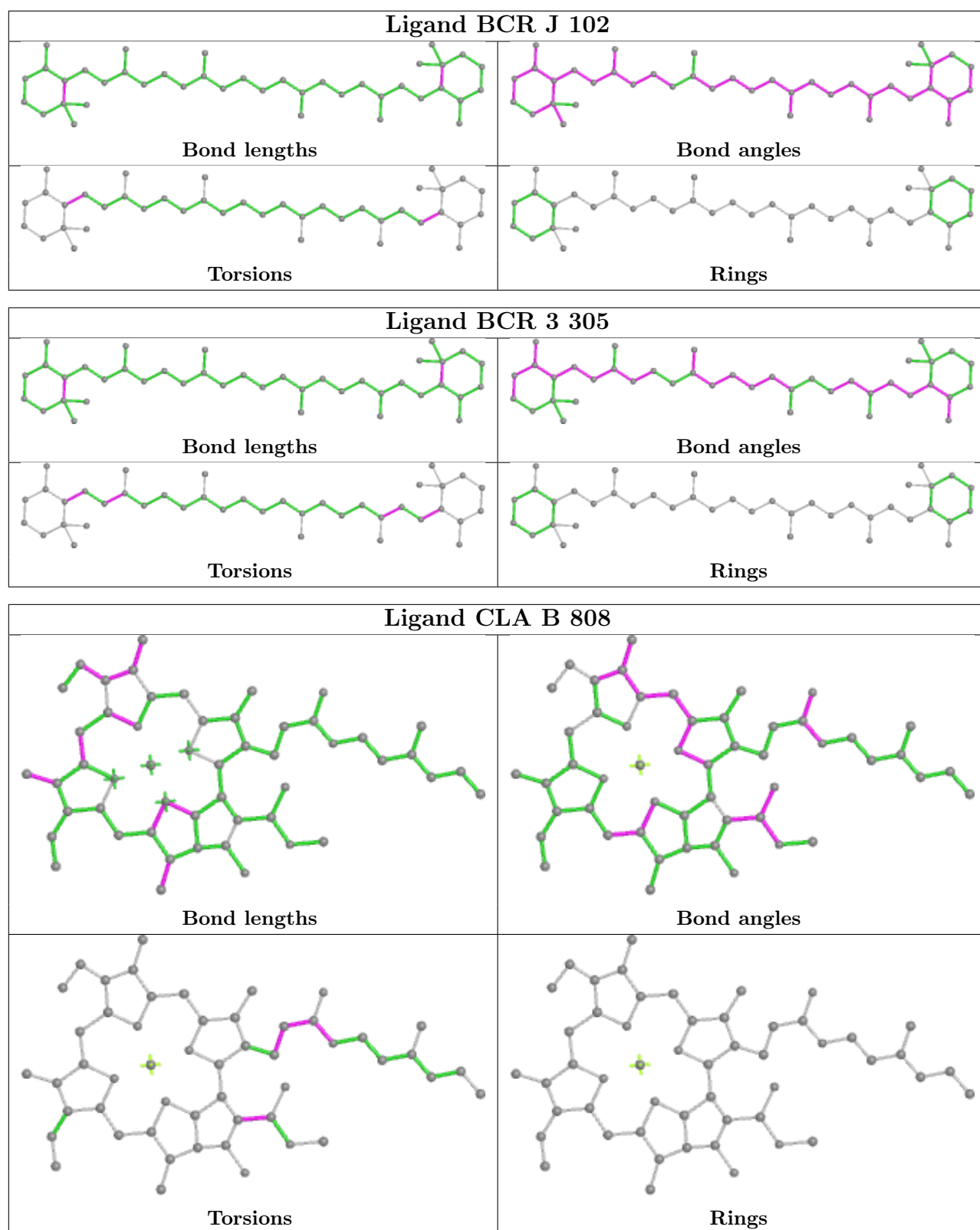


Ligand LMG F 806

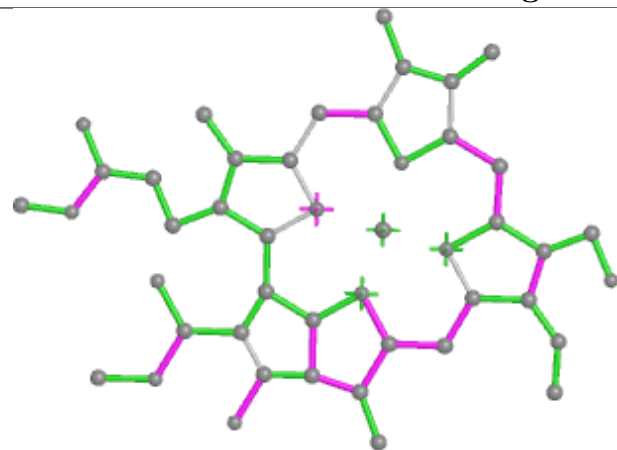


Ligand BCR F 801

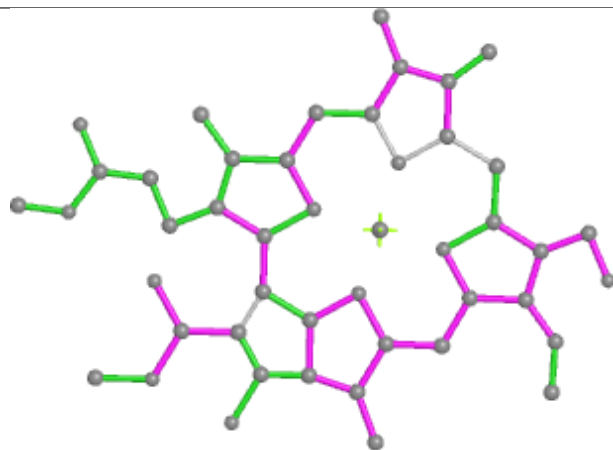




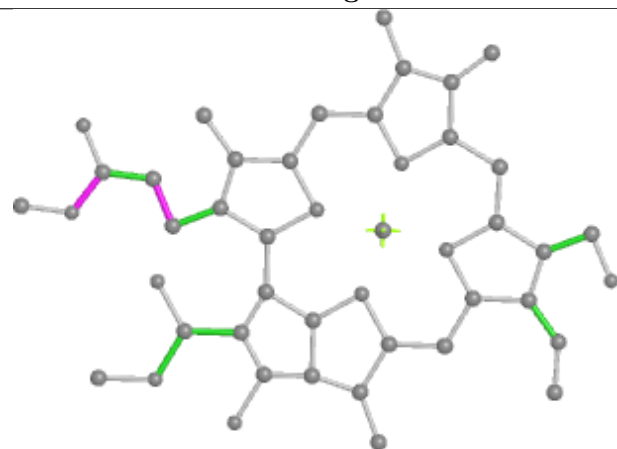
Ligand CHL 2 512



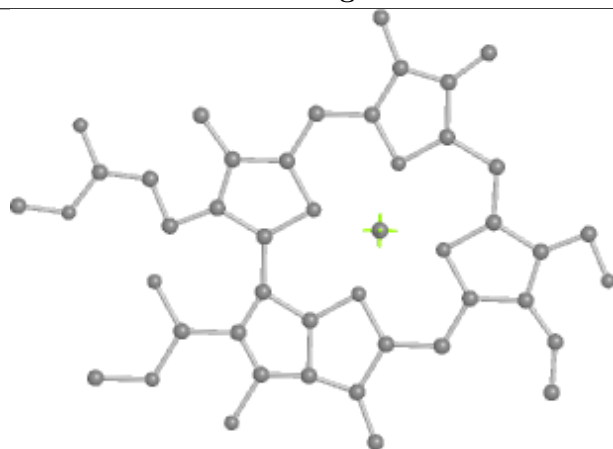
Bond lengths



Bond angles

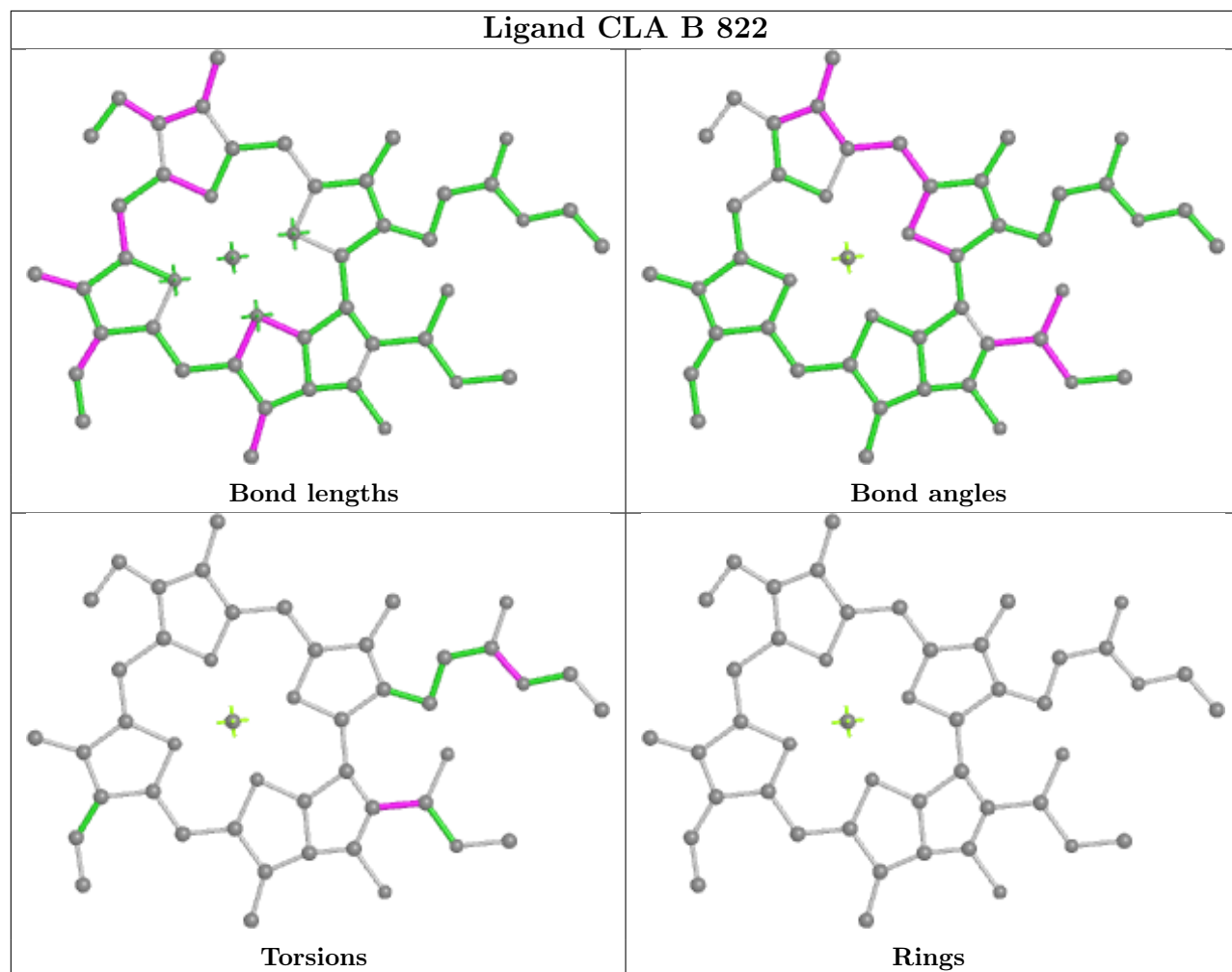


Torsions

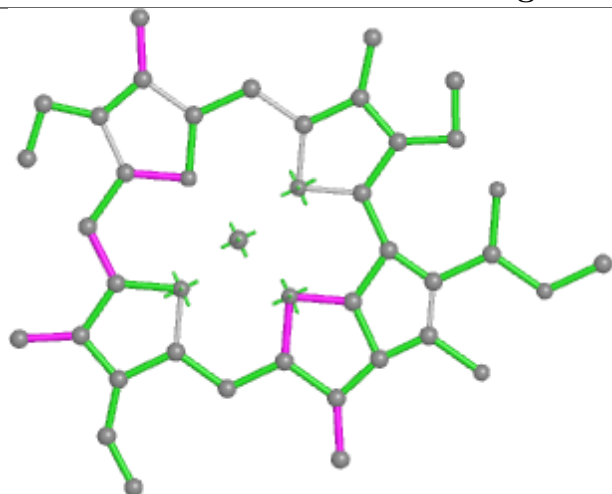


Rings

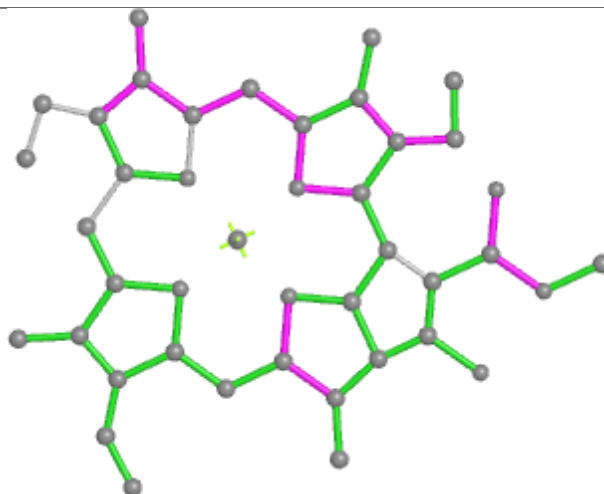
Ligand CLA B 822



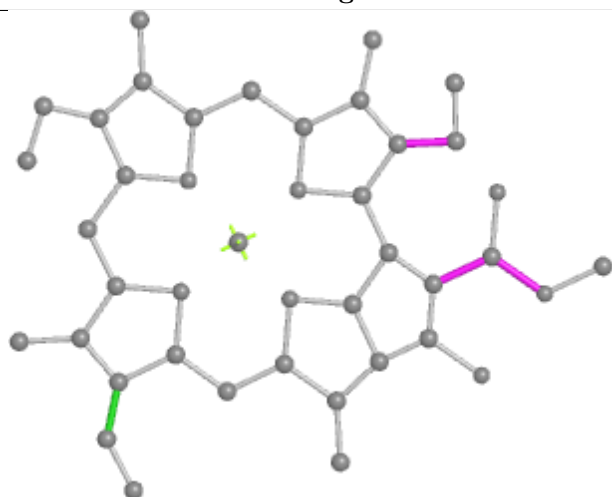
Ligand CLA 5 311



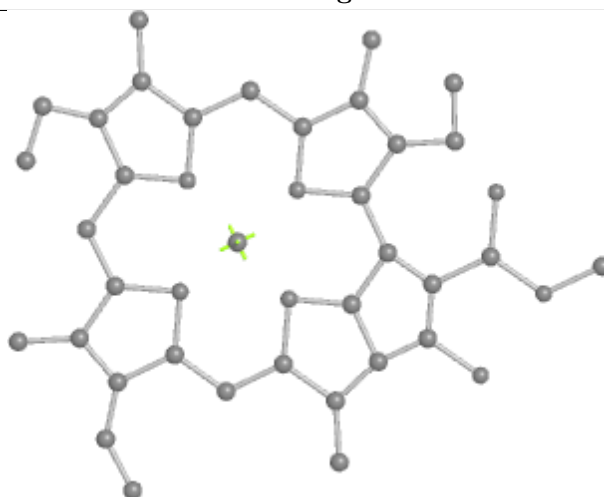
Bond lengths



Bond angles

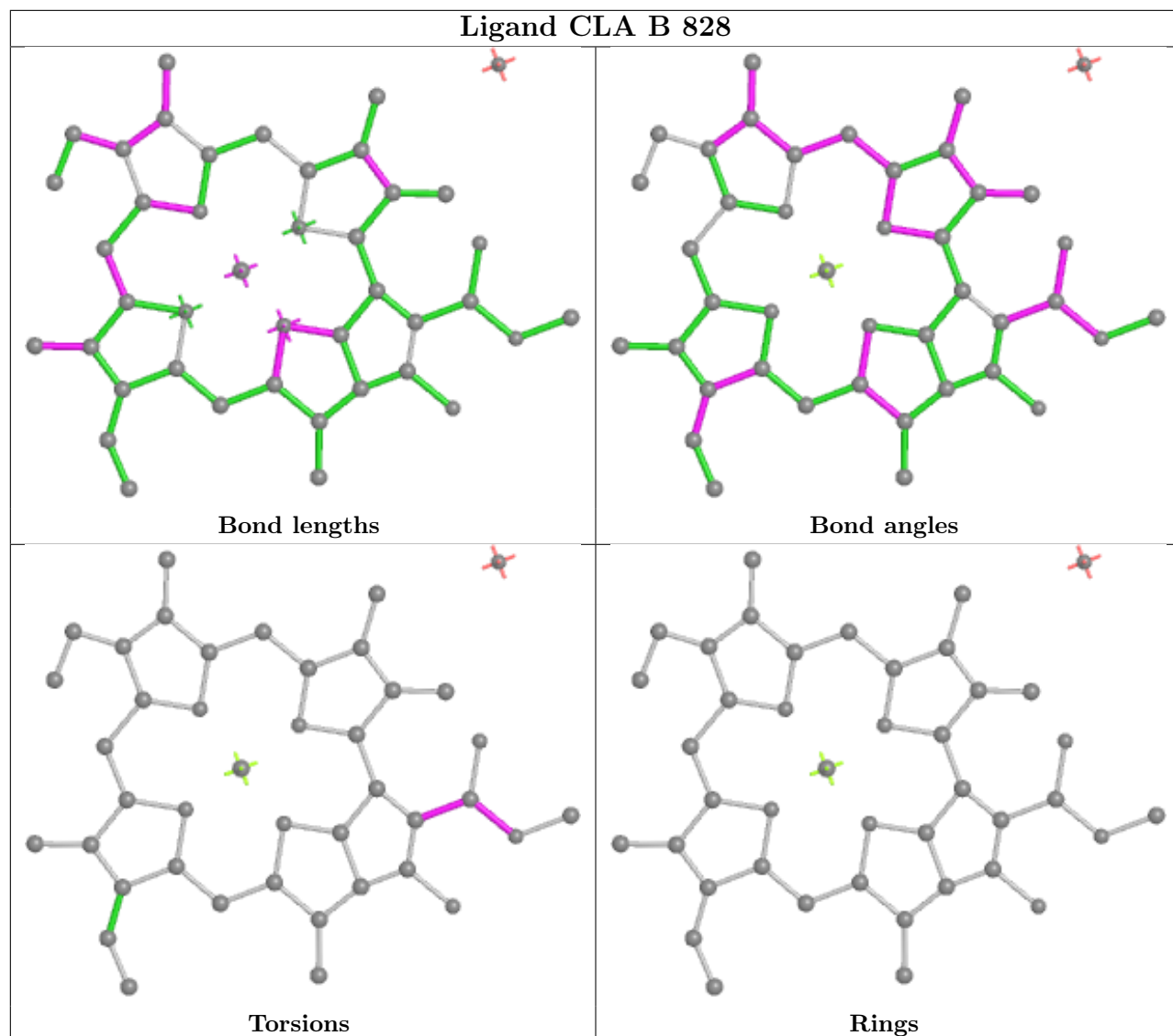


Torsions

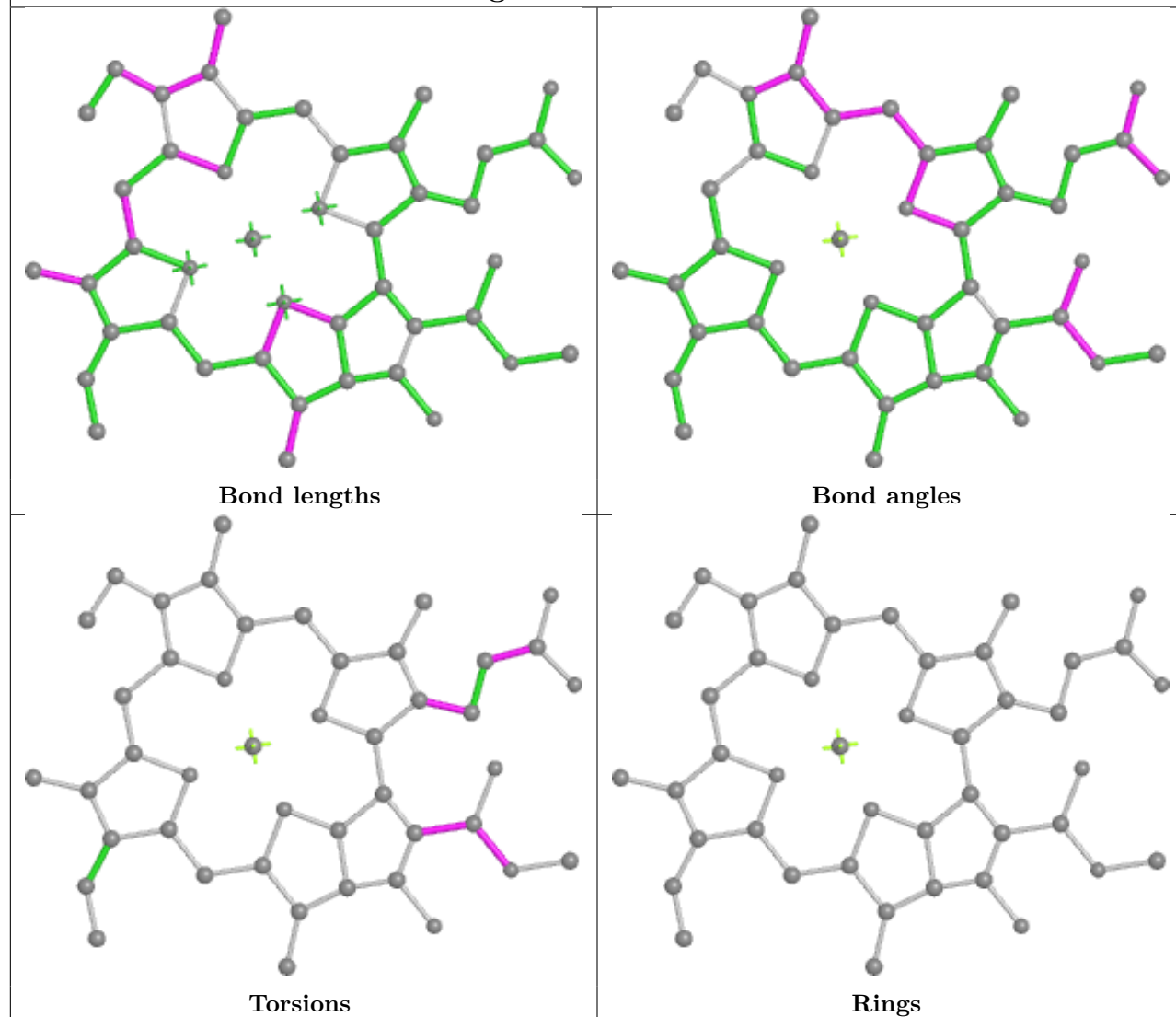


Rings

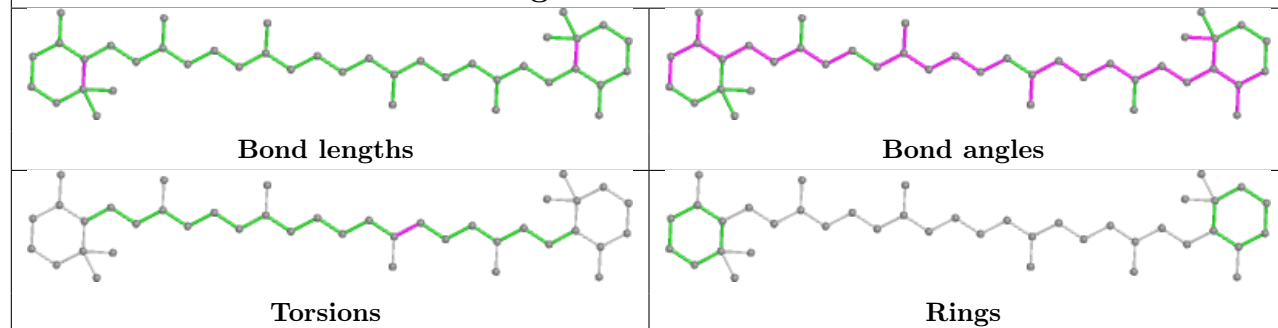
Ligand CLA B 828



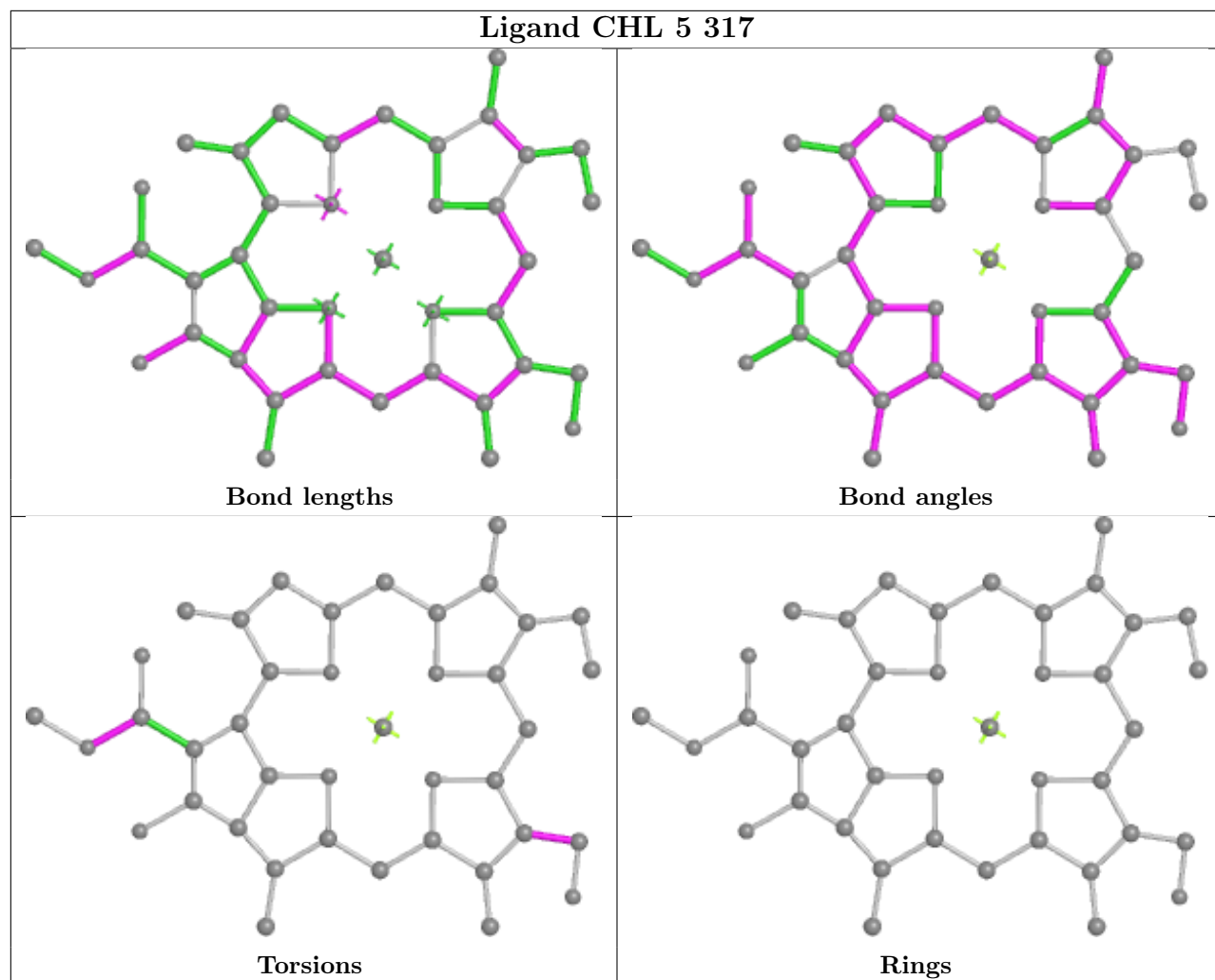
Ligand CLA A 813



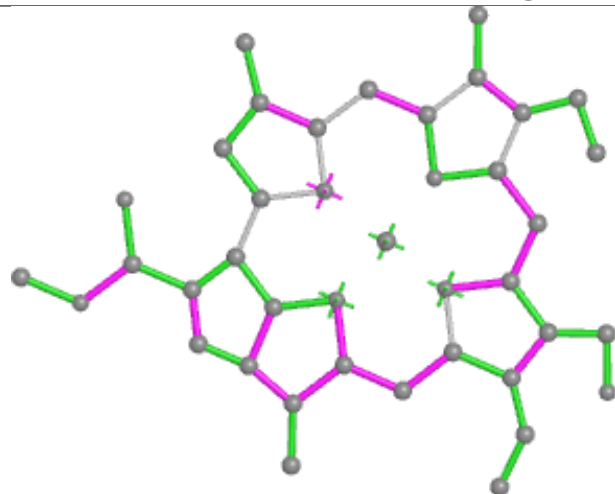
Ligand BCR B 848



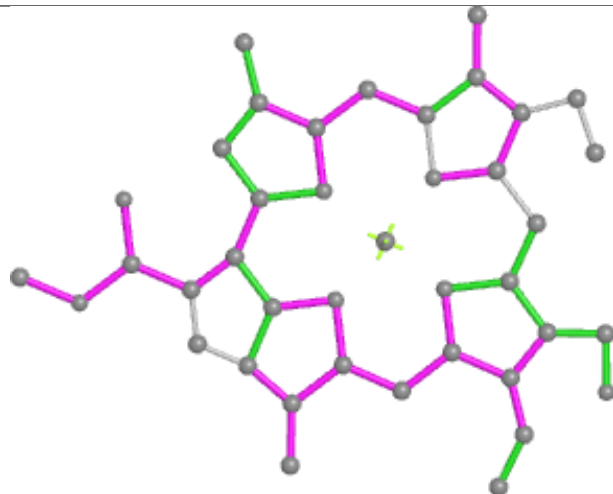
Ligand CHL 5 317



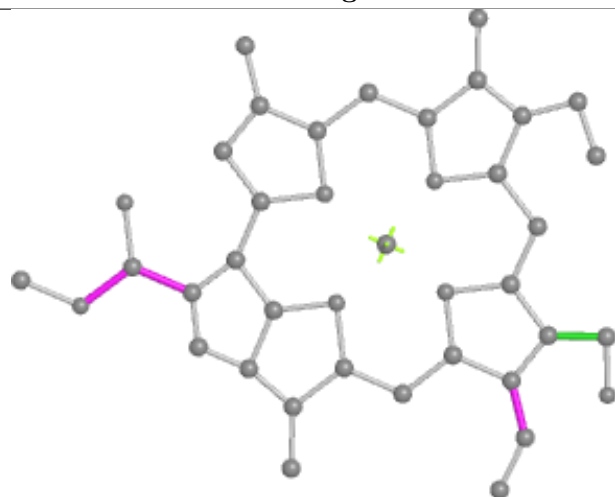
Ligand CHL 2 513



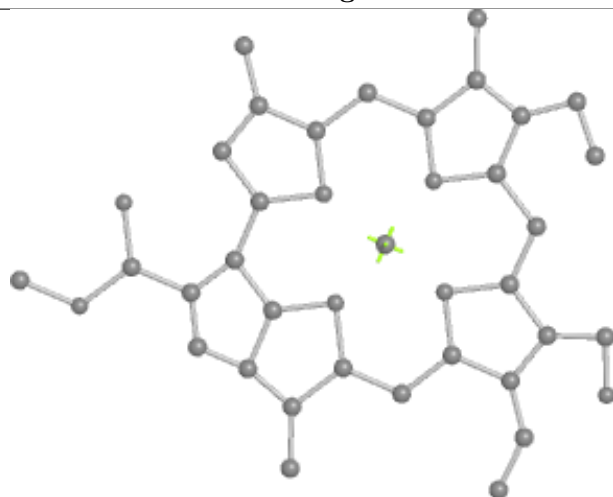
Bond lengths



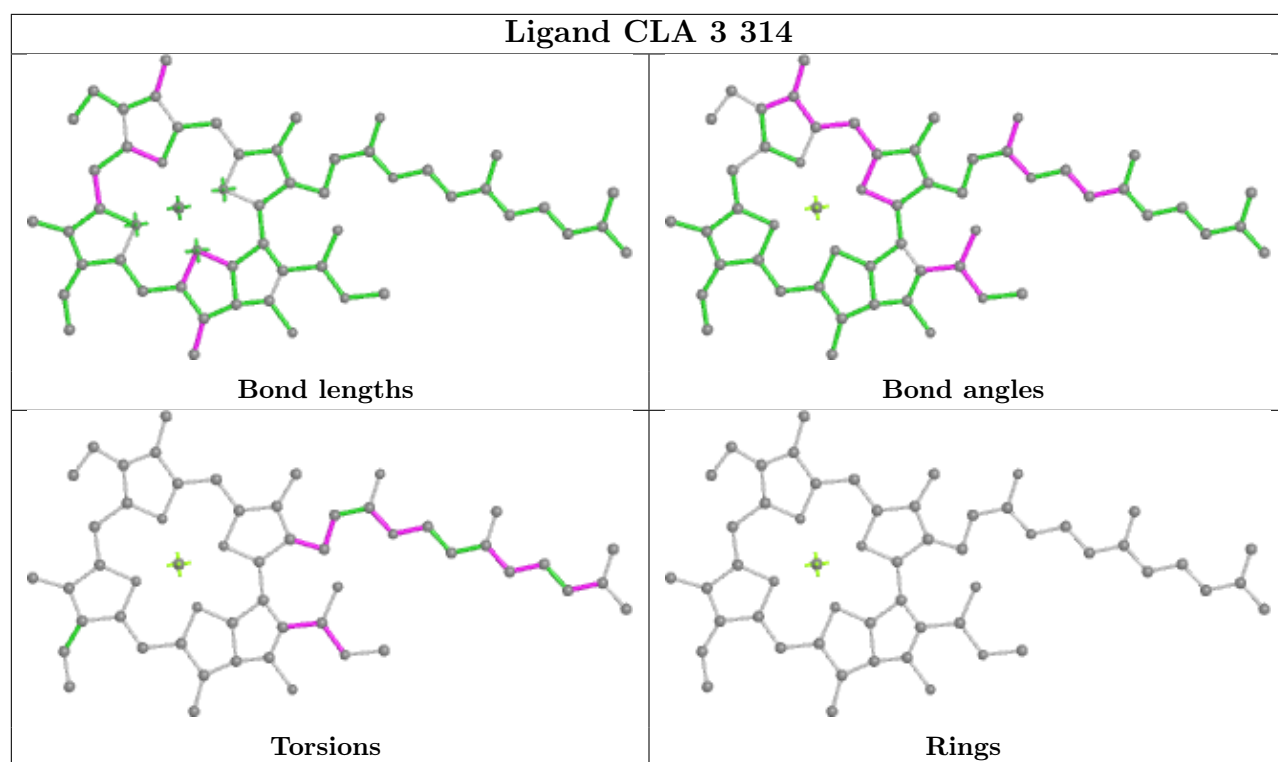
Bond angles



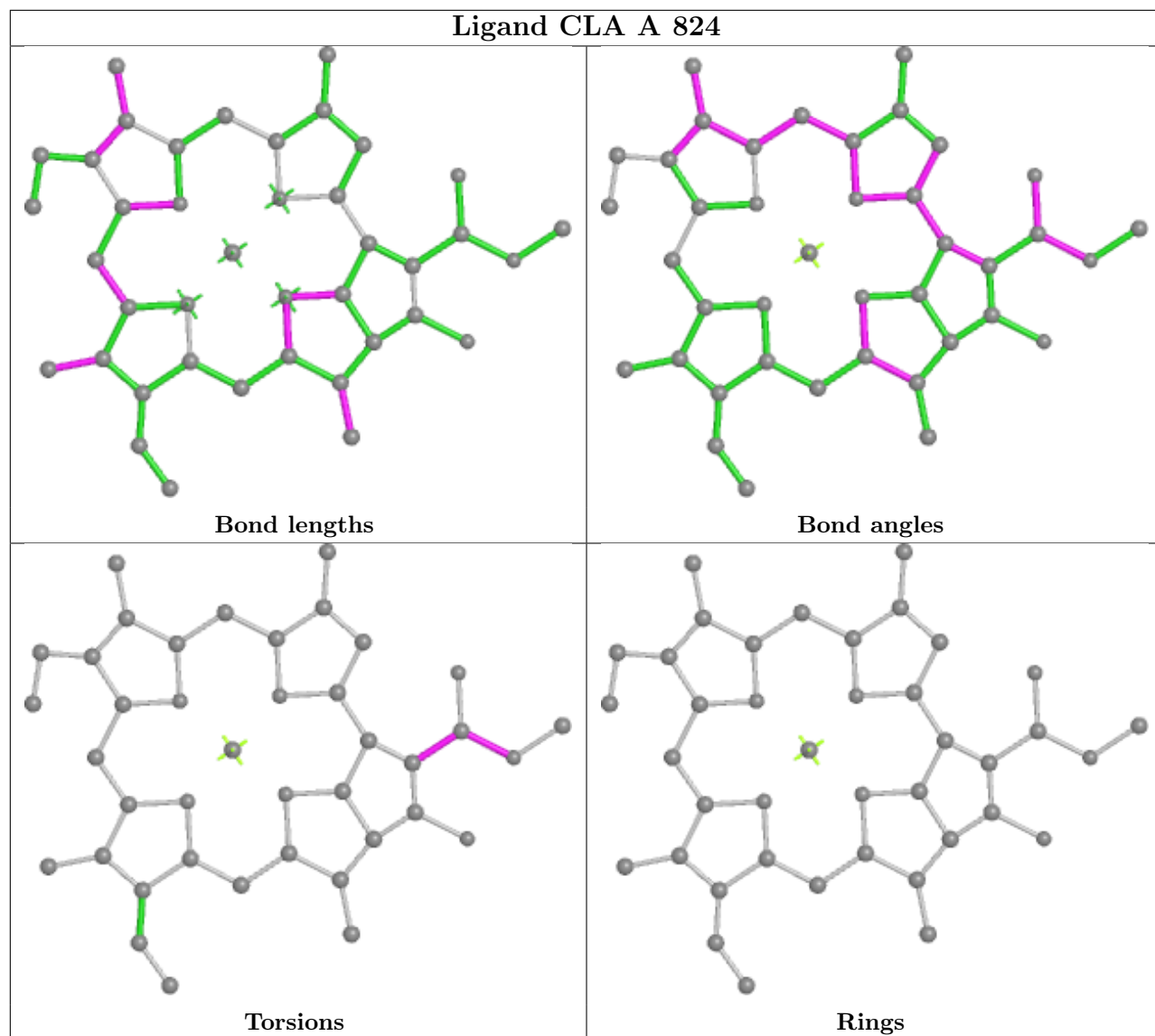
Torsions

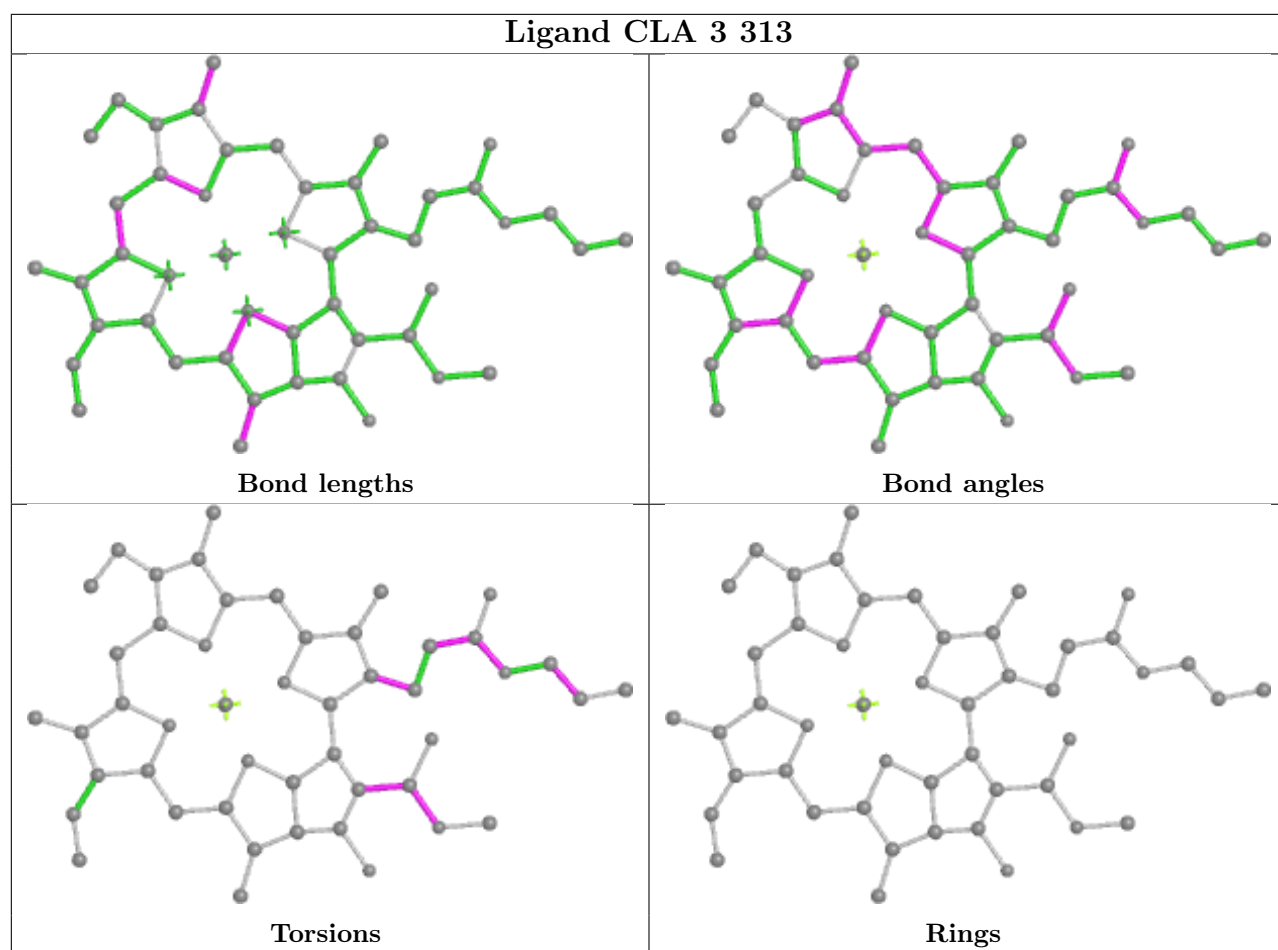


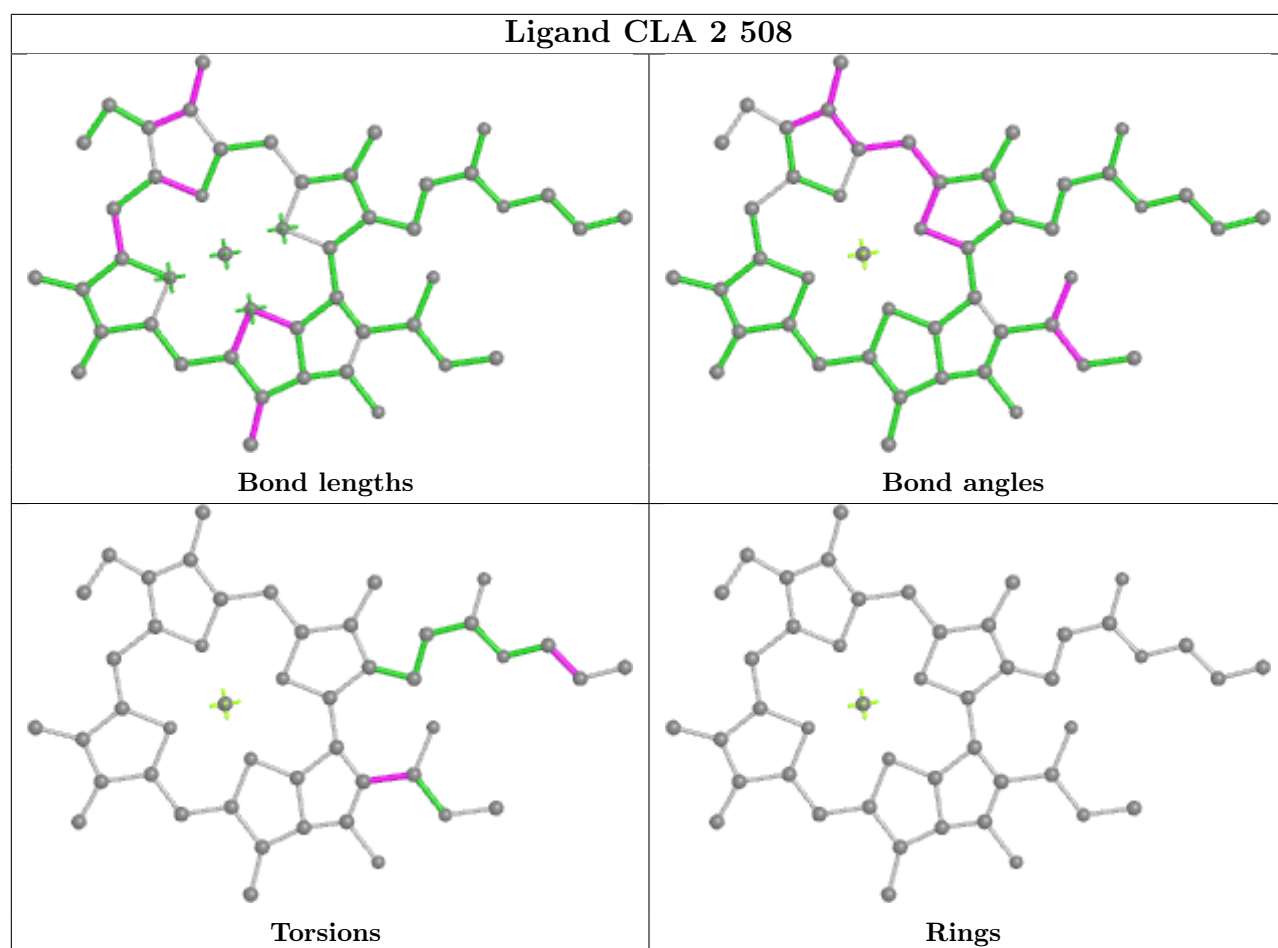
Rings



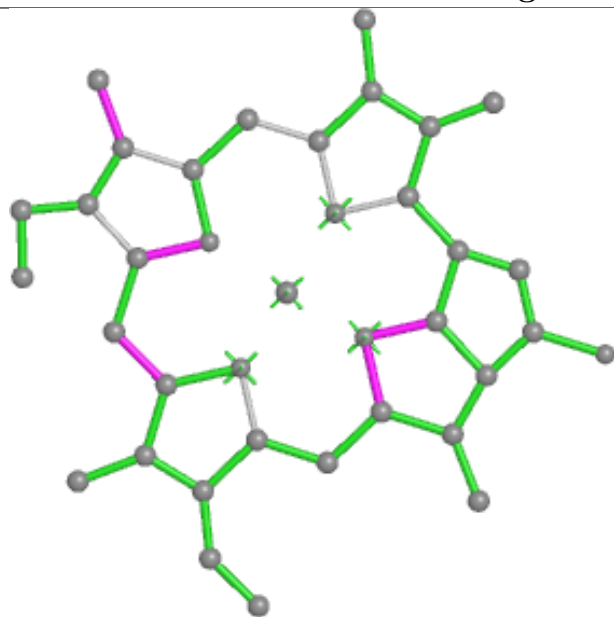
Ligand CLA A 824



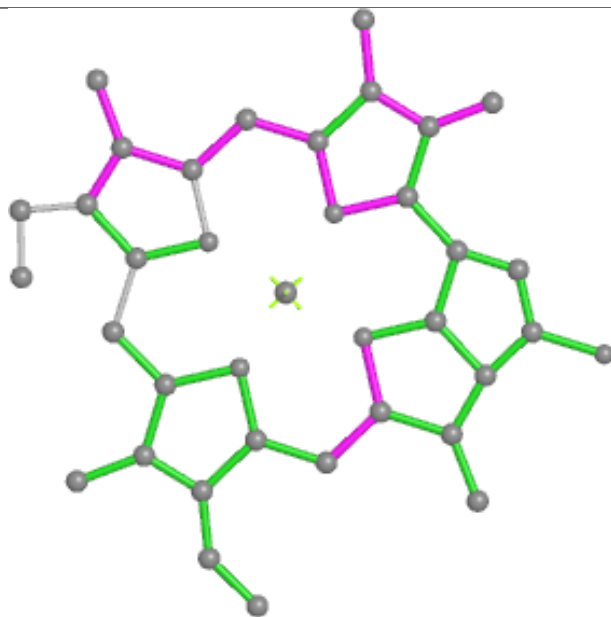




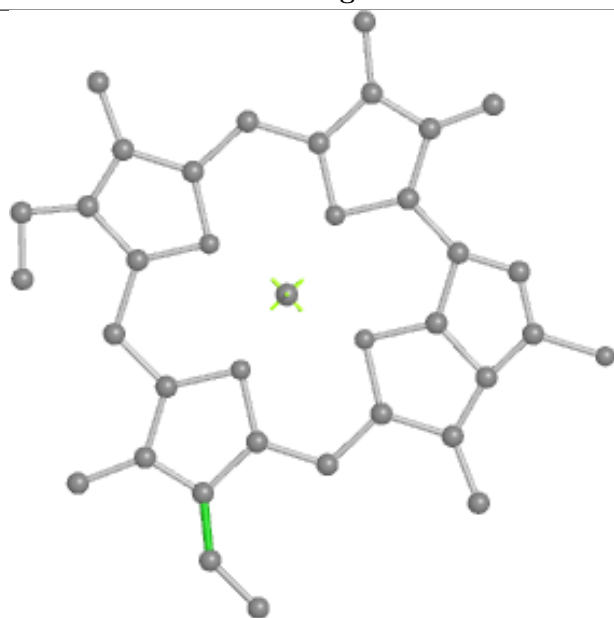
Ligand CLA 3 316



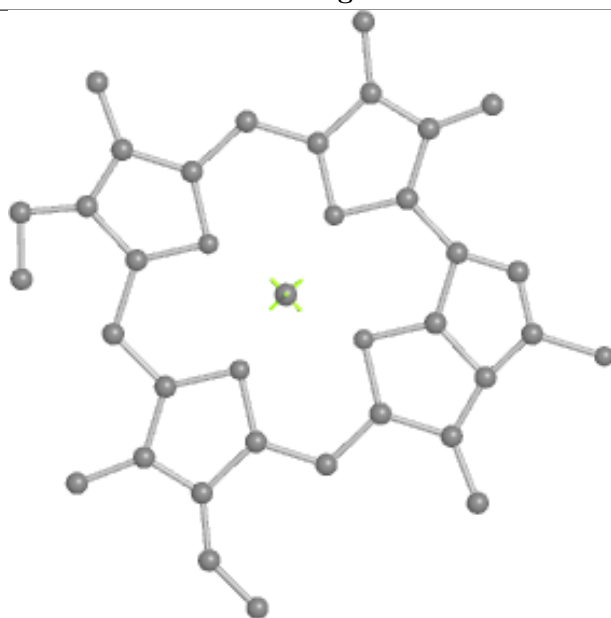
Bond lengths



Bond angles

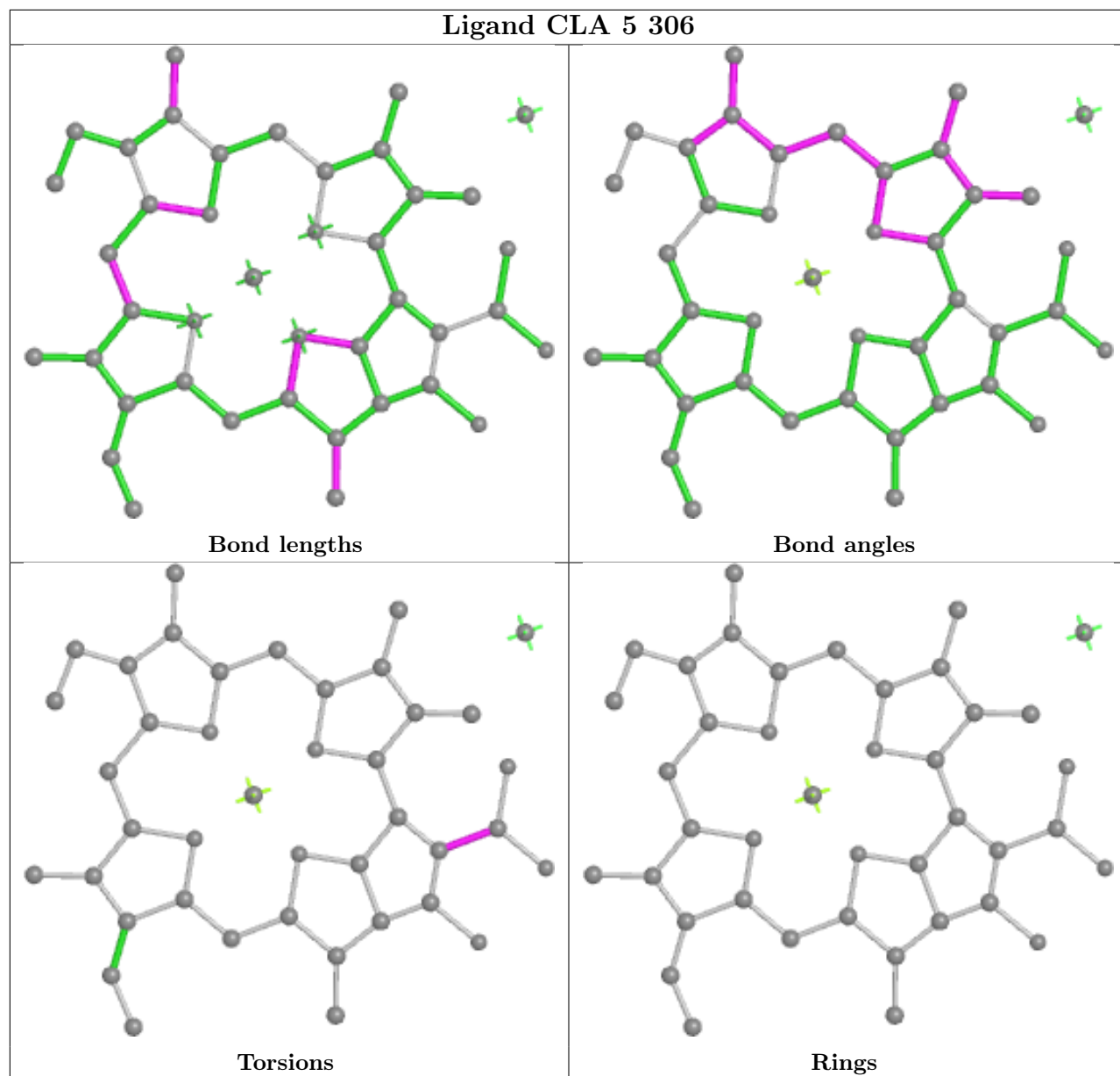


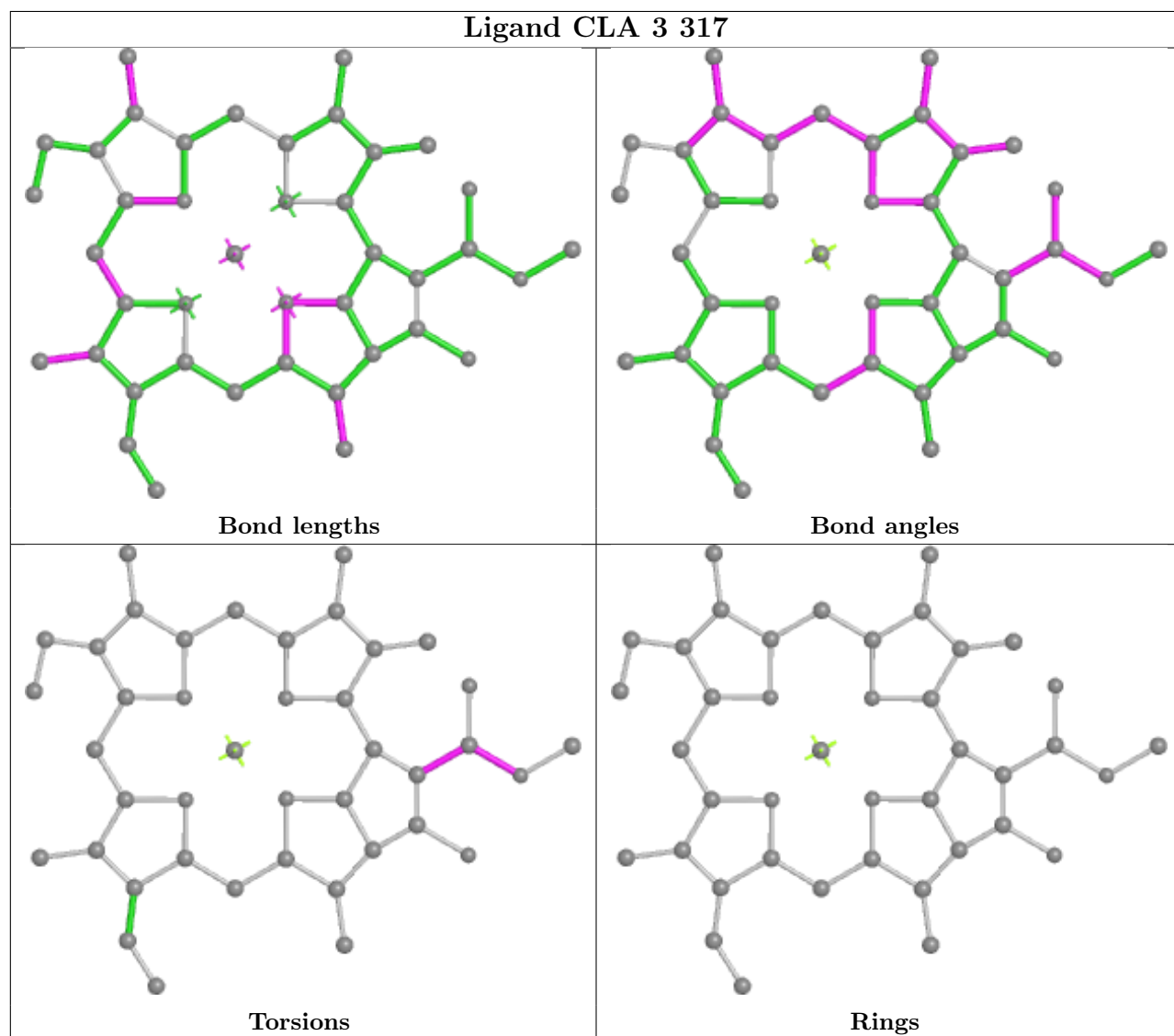
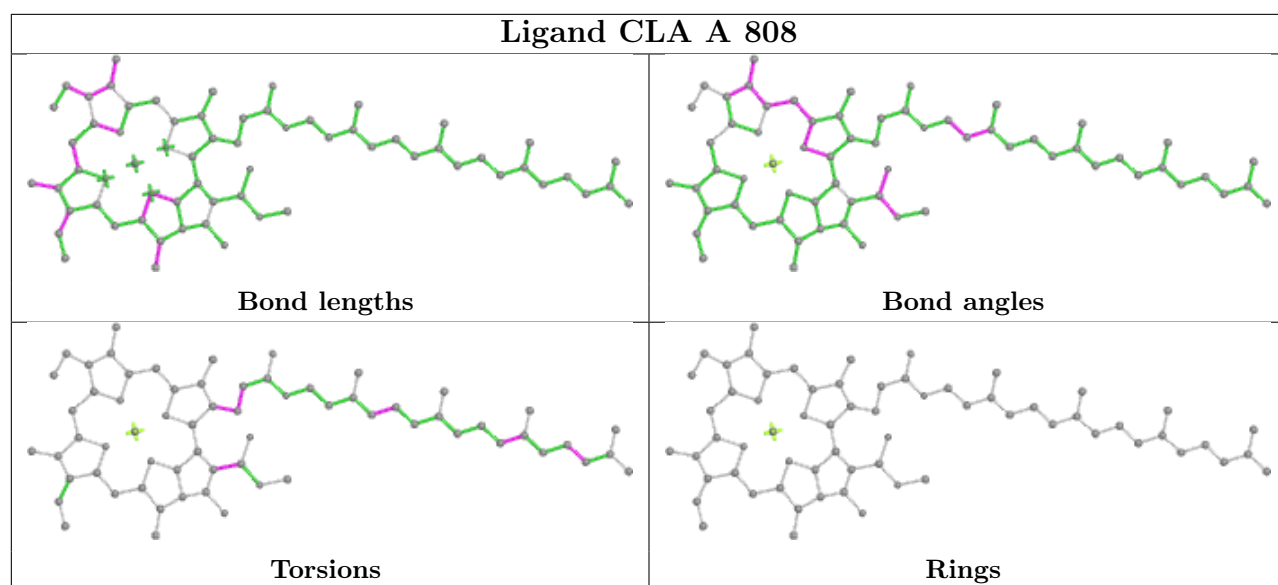
Torsions

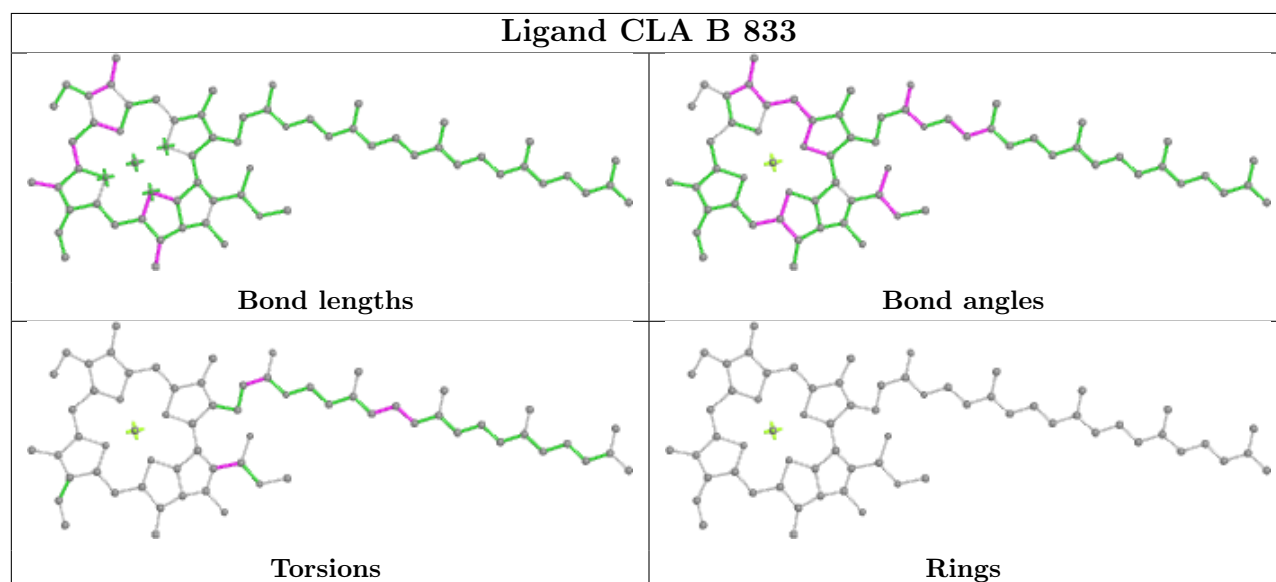
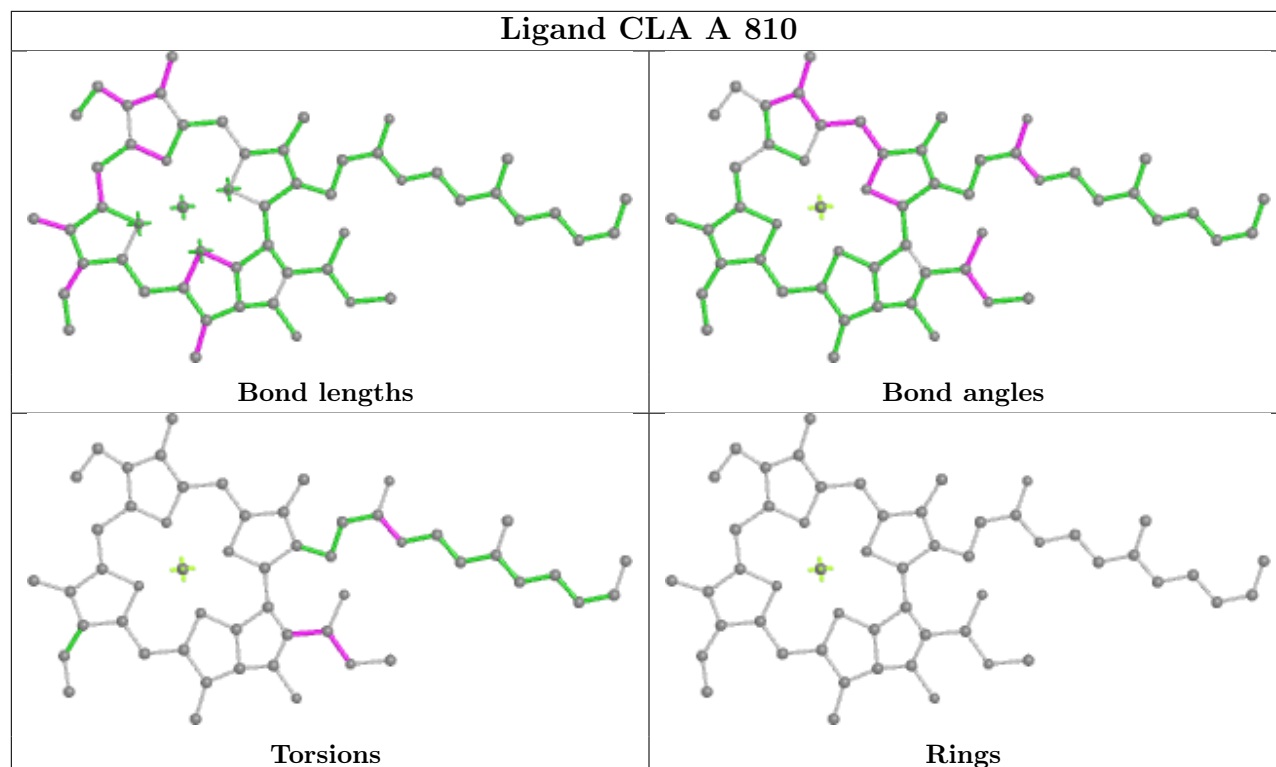
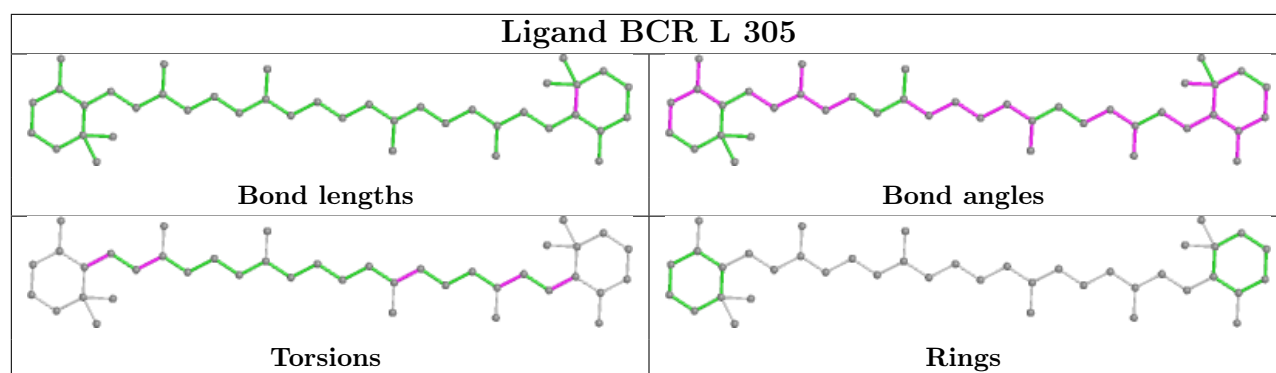


Rings

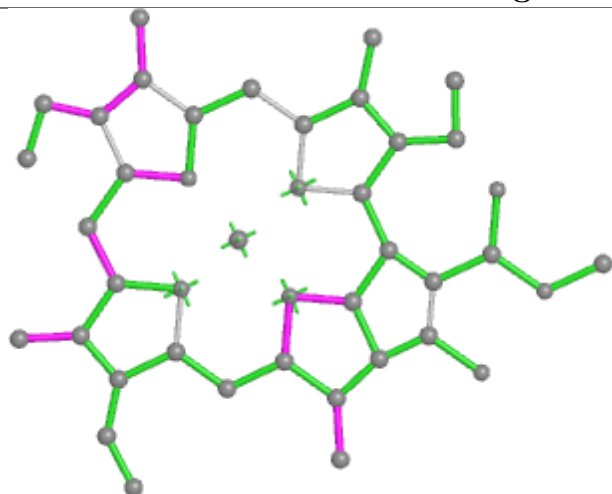
Ligand CLA 5 306



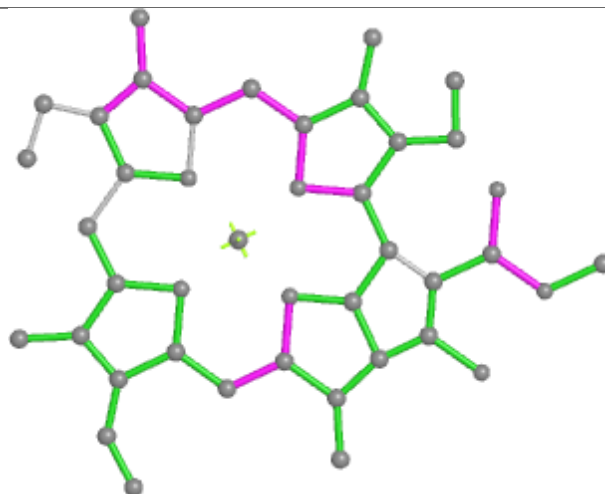




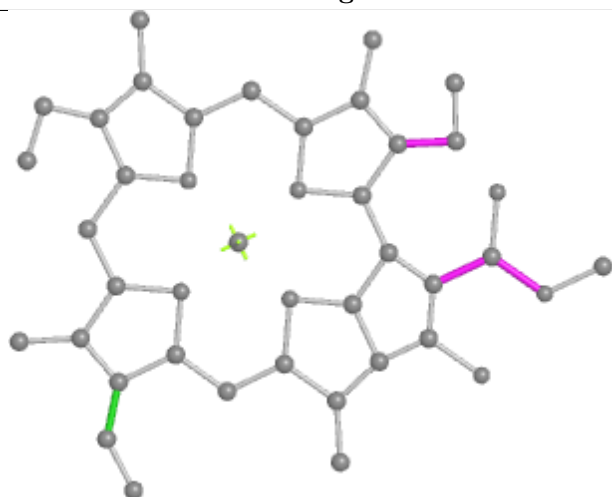
Ligand CLA B 836



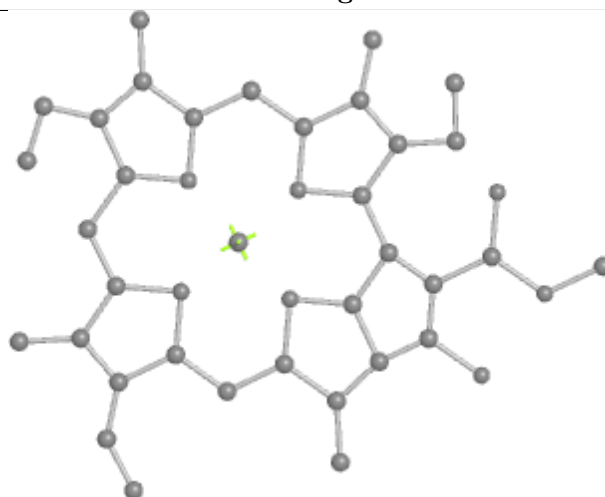
Bond lengths



Bond angles

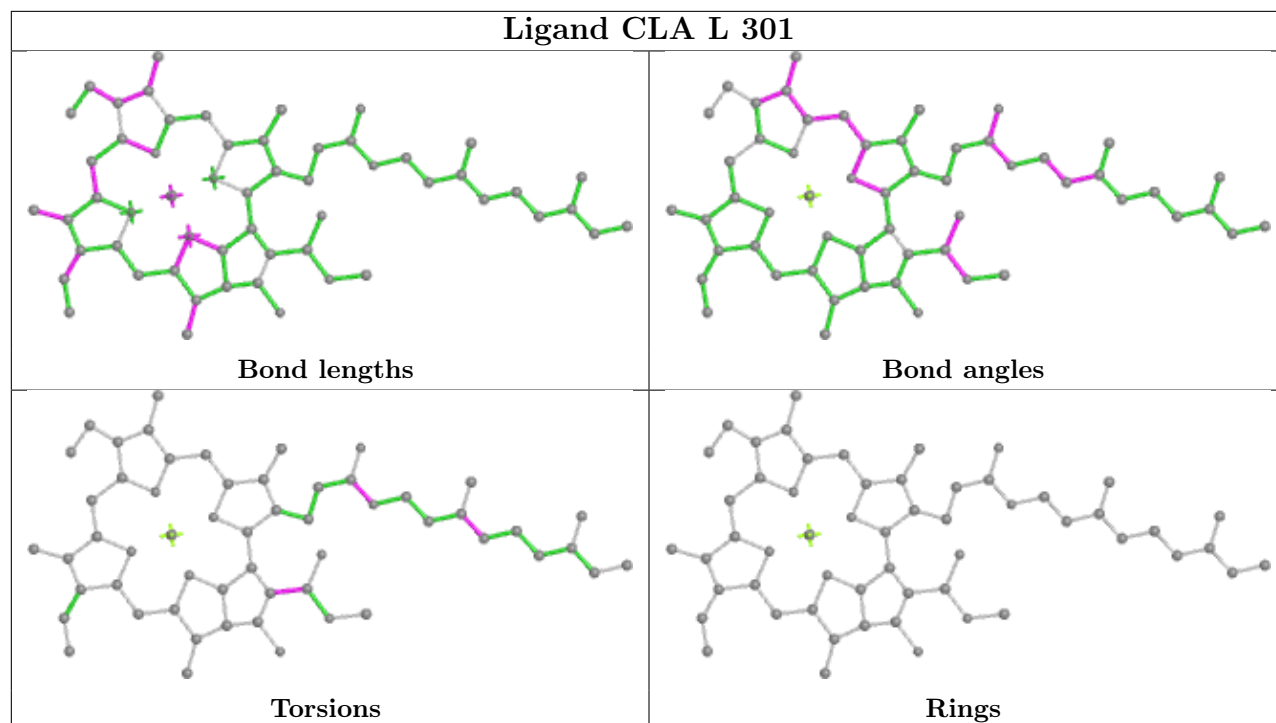


Torsions

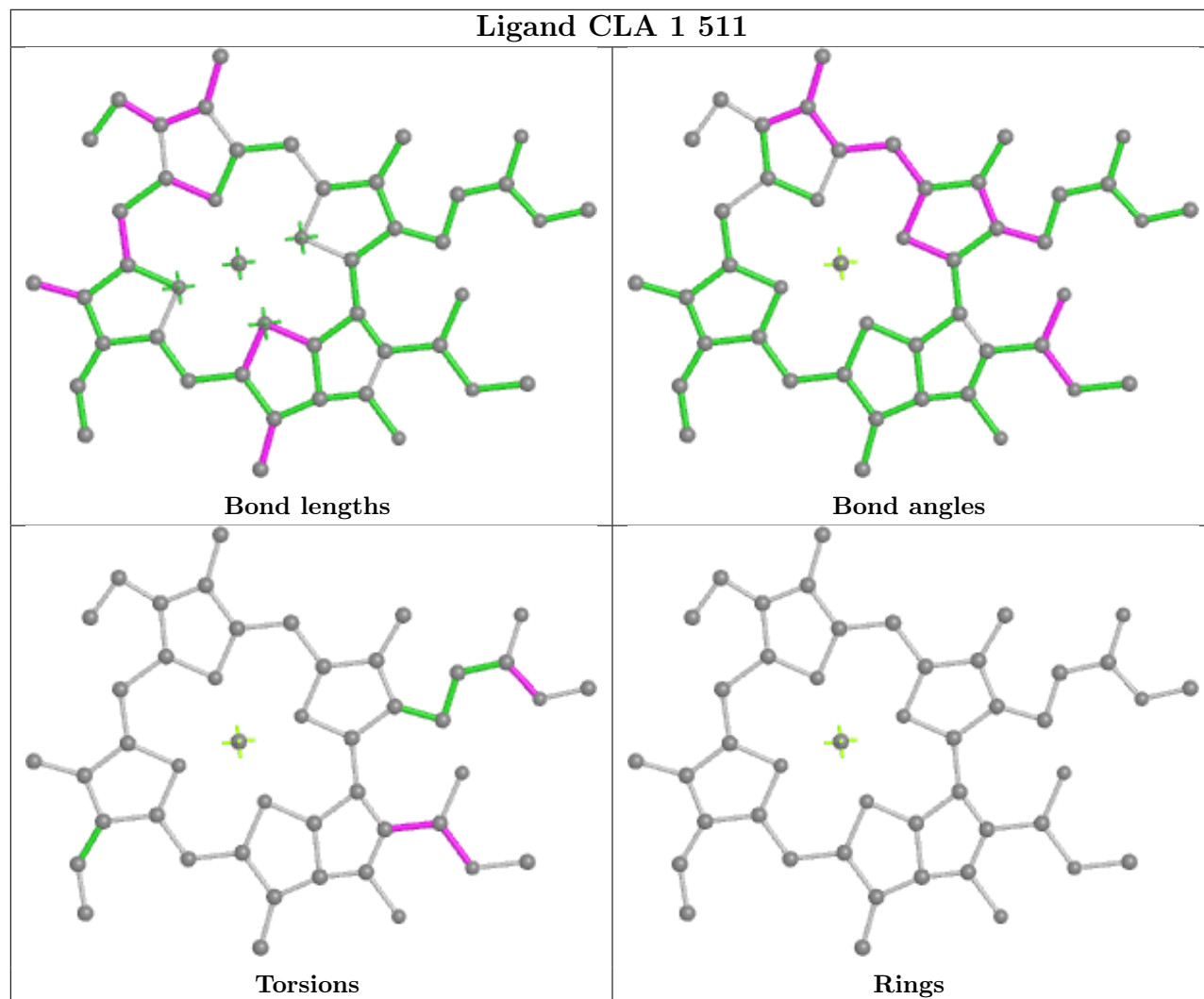


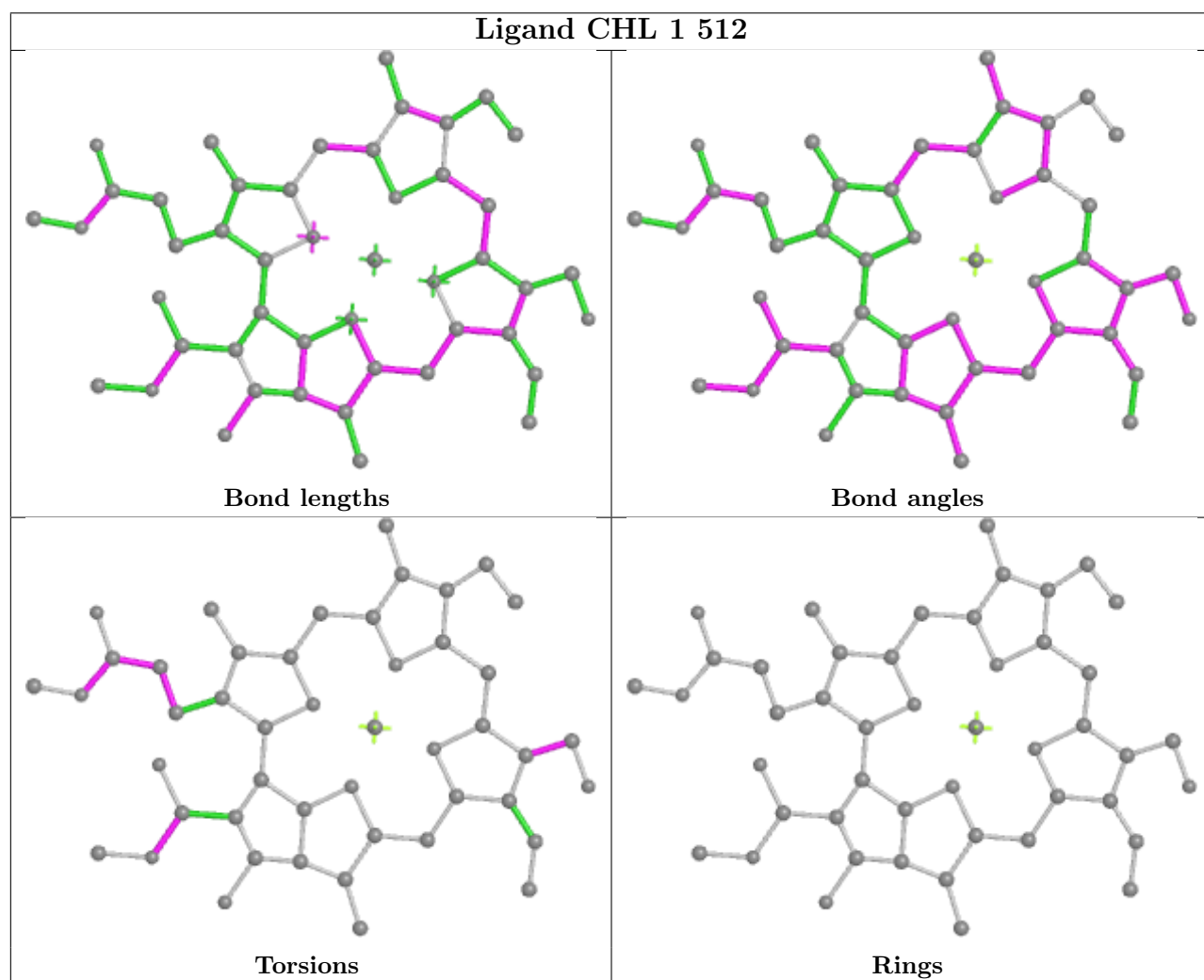
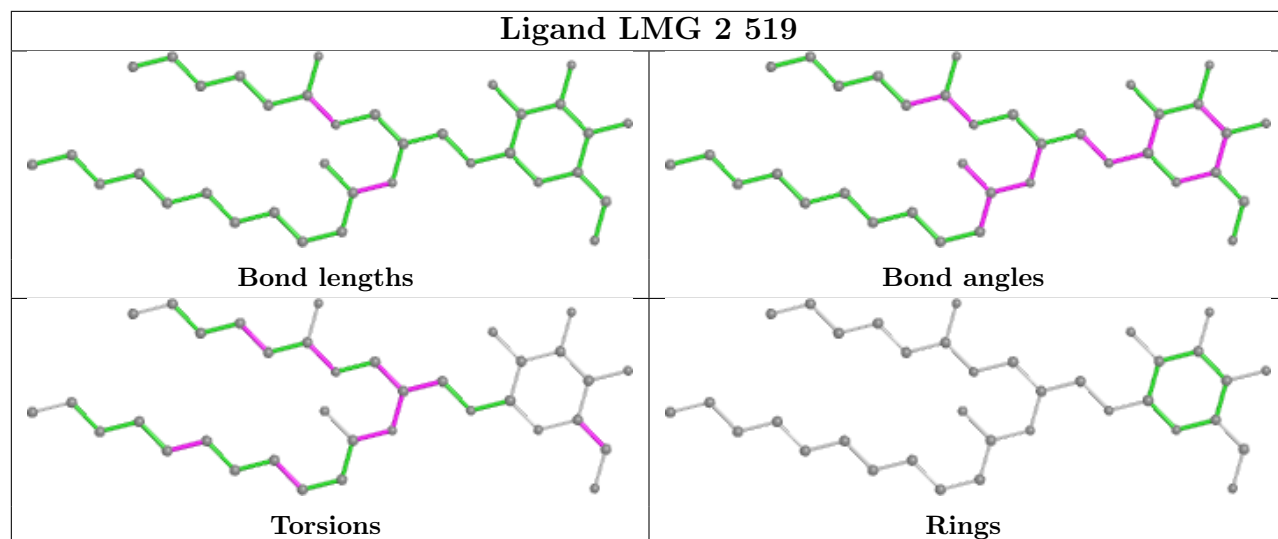
Rings

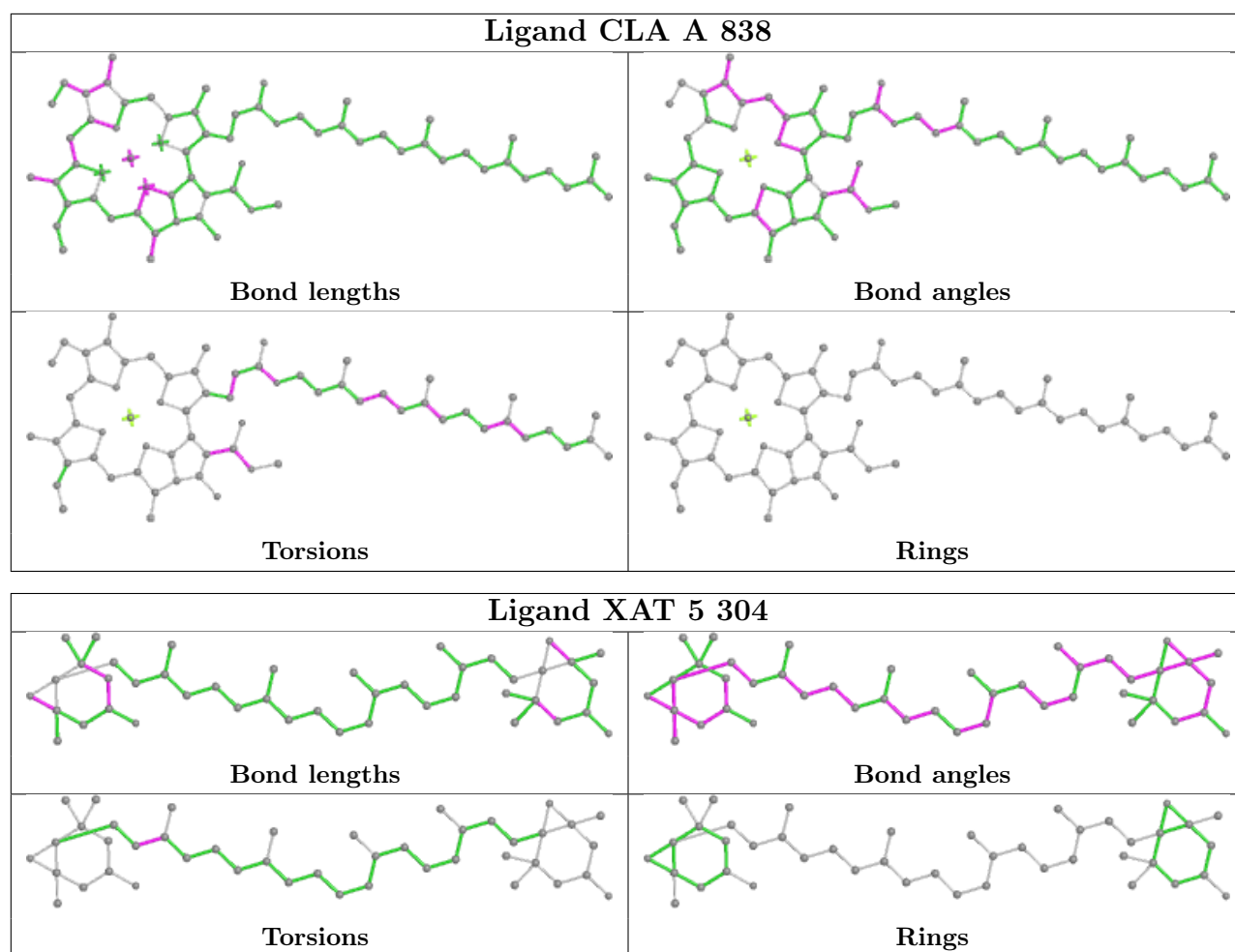
Ligand CLA L 301



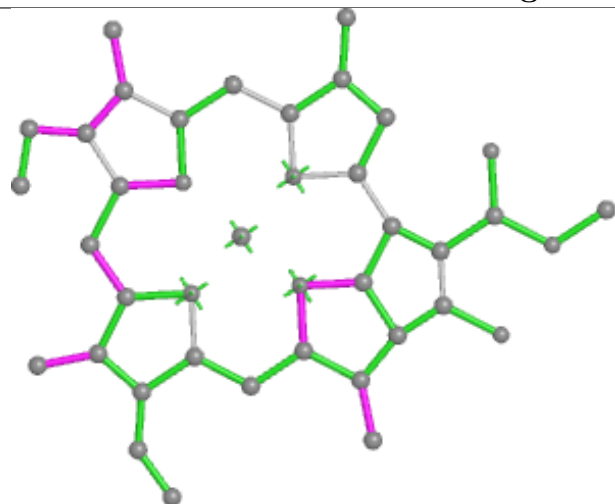
Ligand CLA 1 511



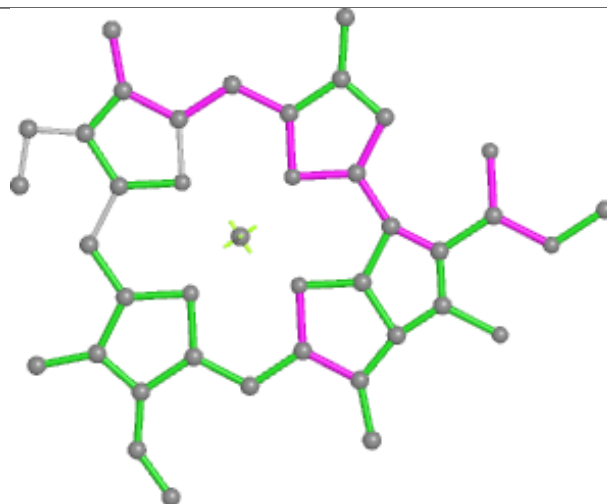




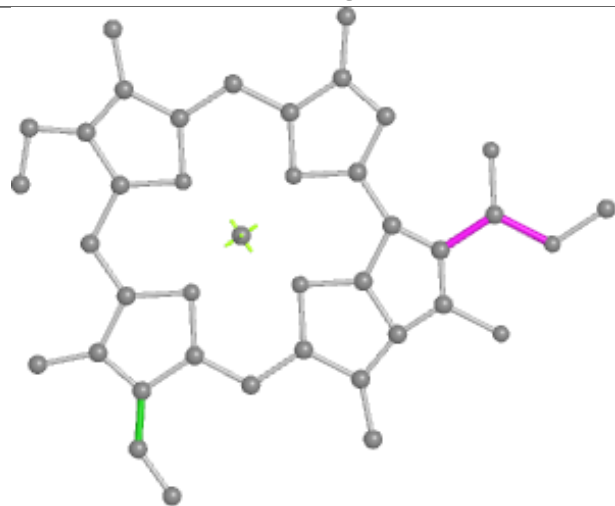
Ligand CLA 3 307



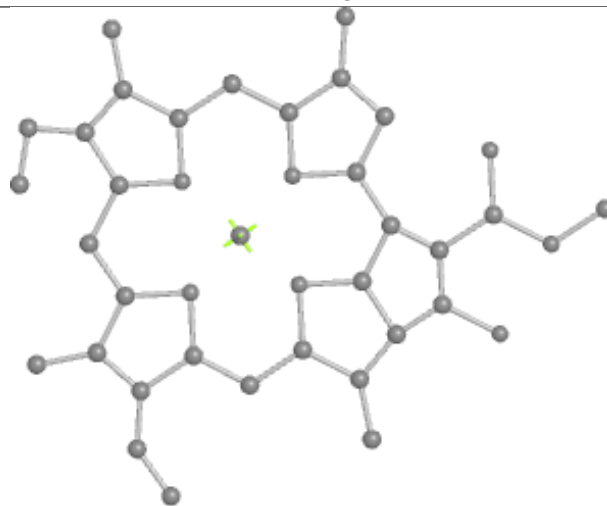
Bond lengths



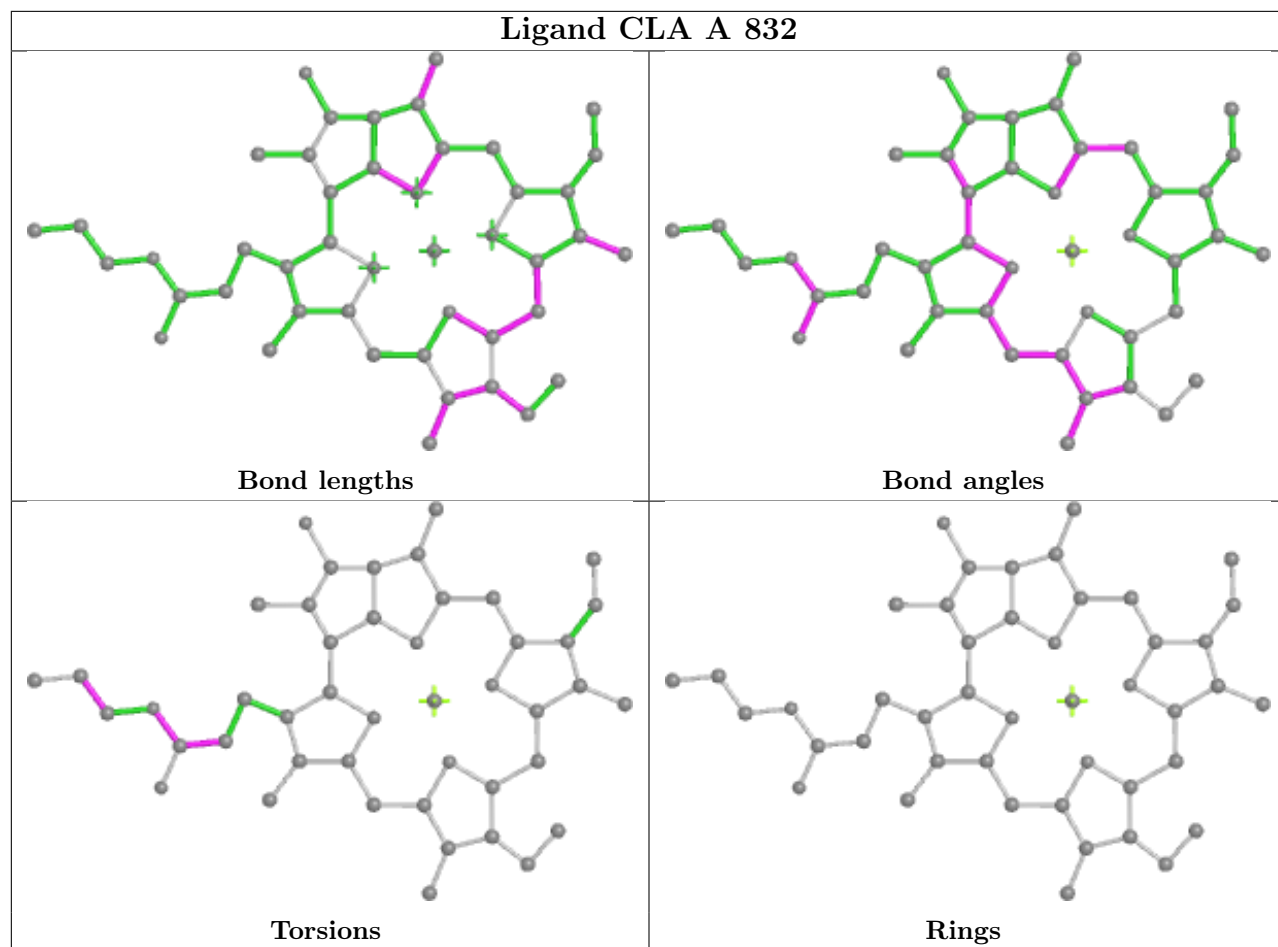
Bond angles



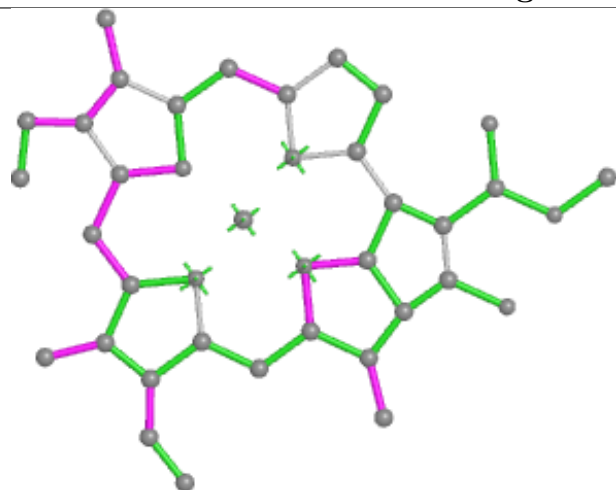
Torsions



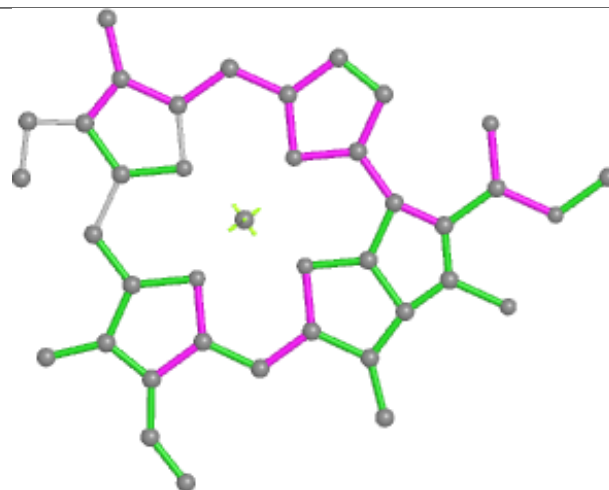
Rings



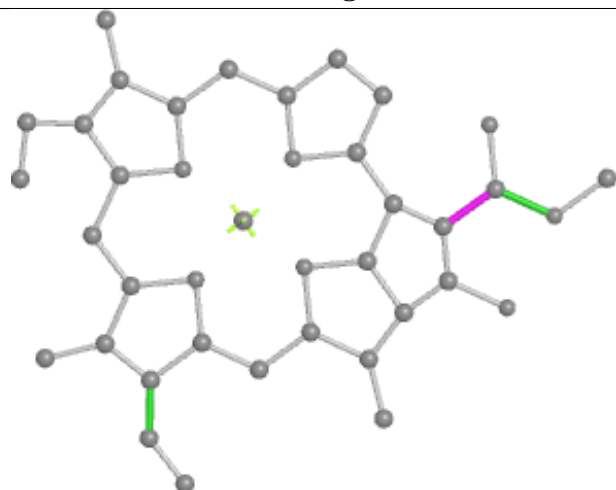
Ligand CLA B 806



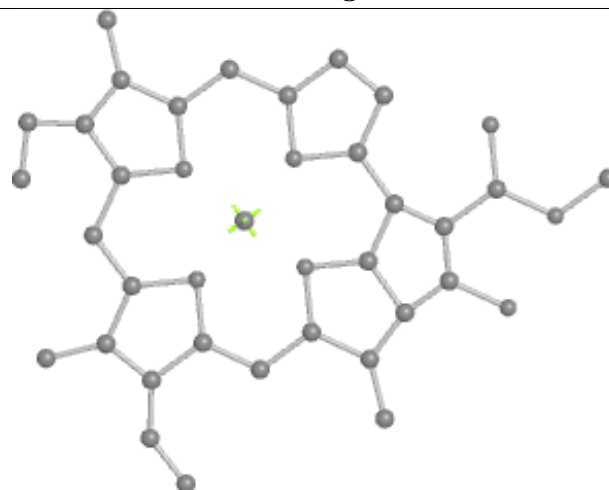
Bond lengths



Bond angles

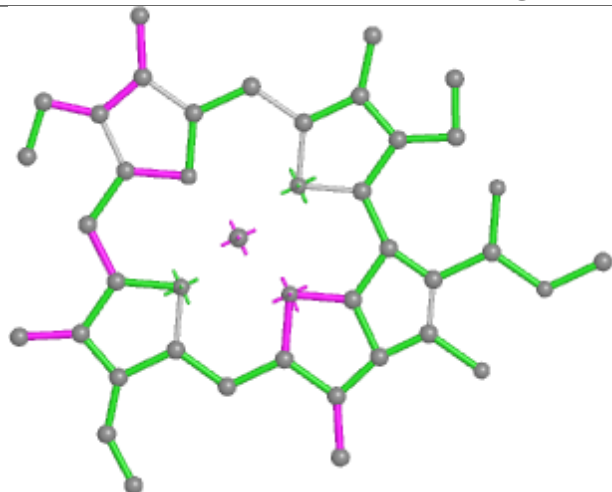


Torsions

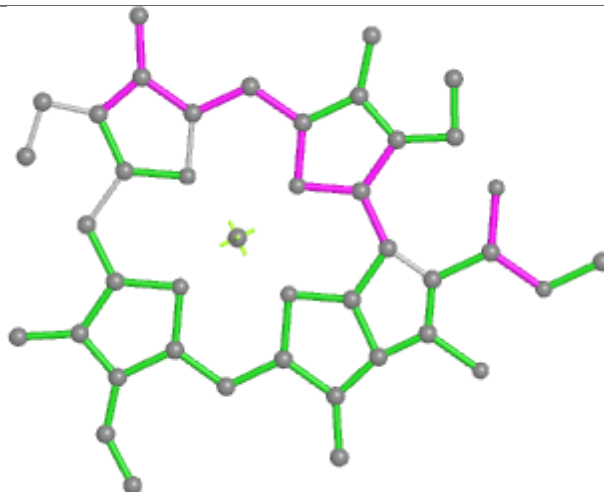


Rings

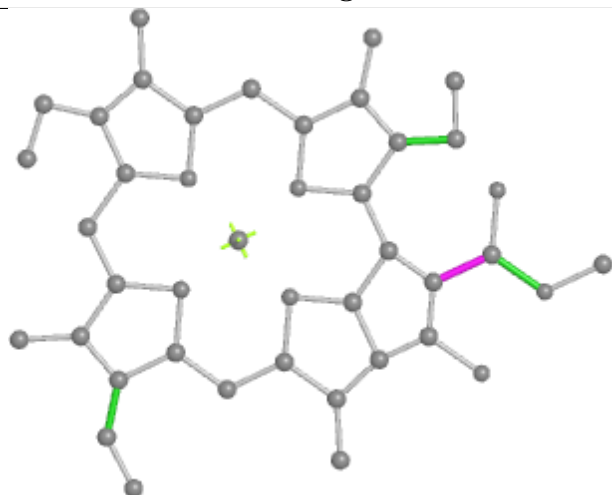
Ligand CLA B 825



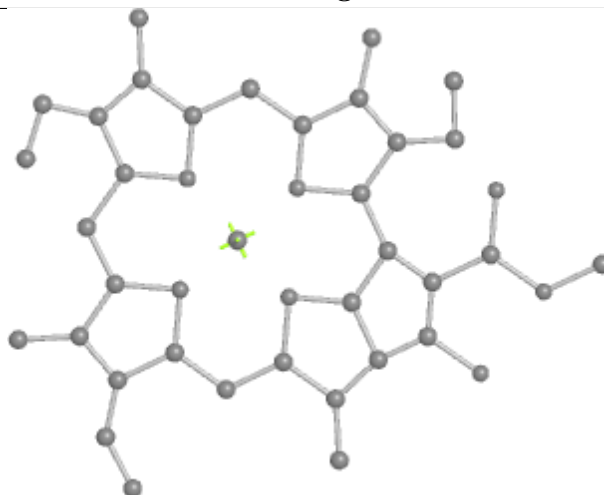
Bond lengths



Bond angles

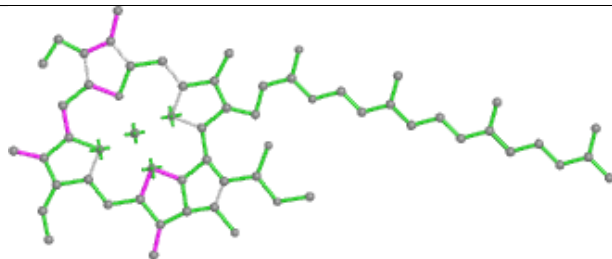


Torsions

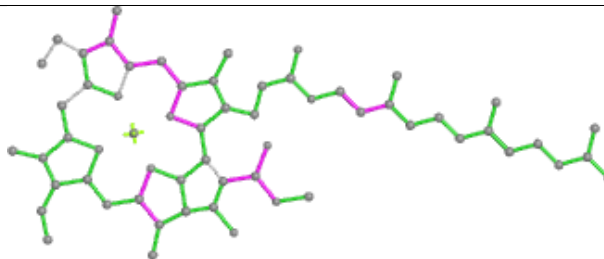


Rings

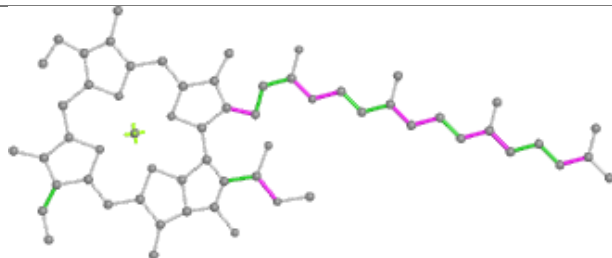
Ligand CLA A 826



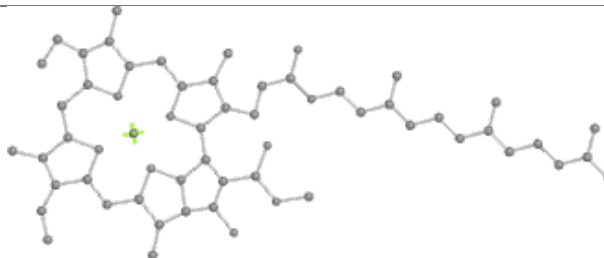
Bond lengths



Bond angles

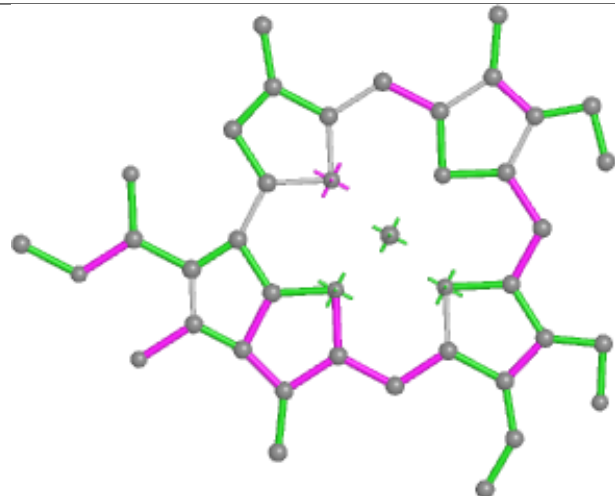


Torsions

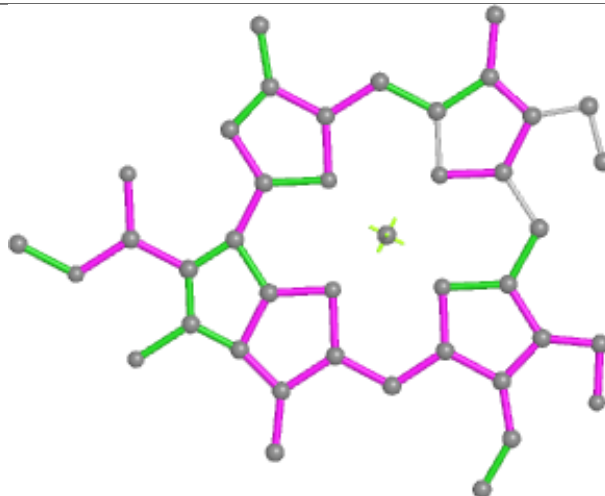


Rings

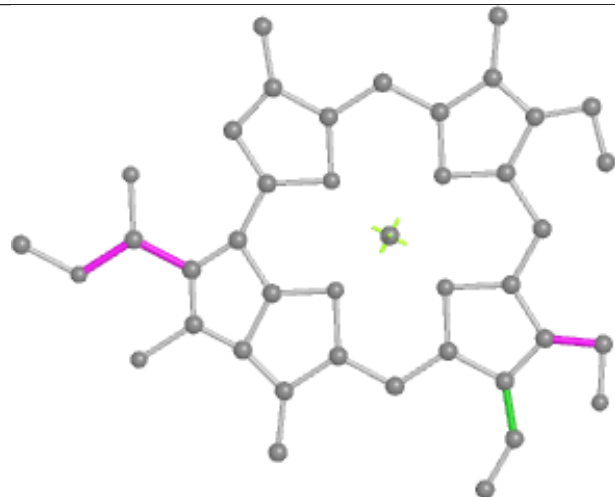
Ligand CHL 1 517



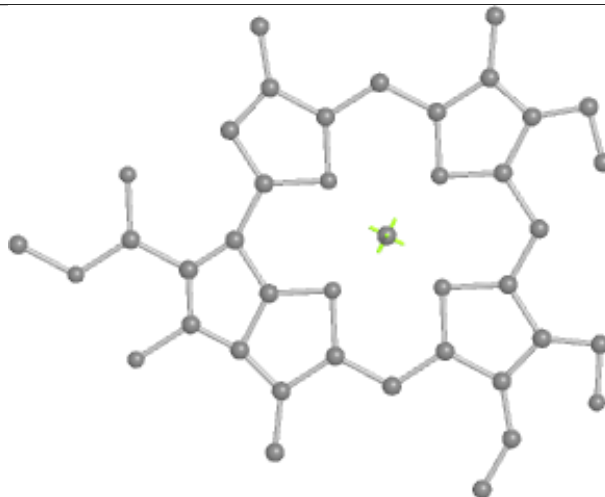
Bond lengths



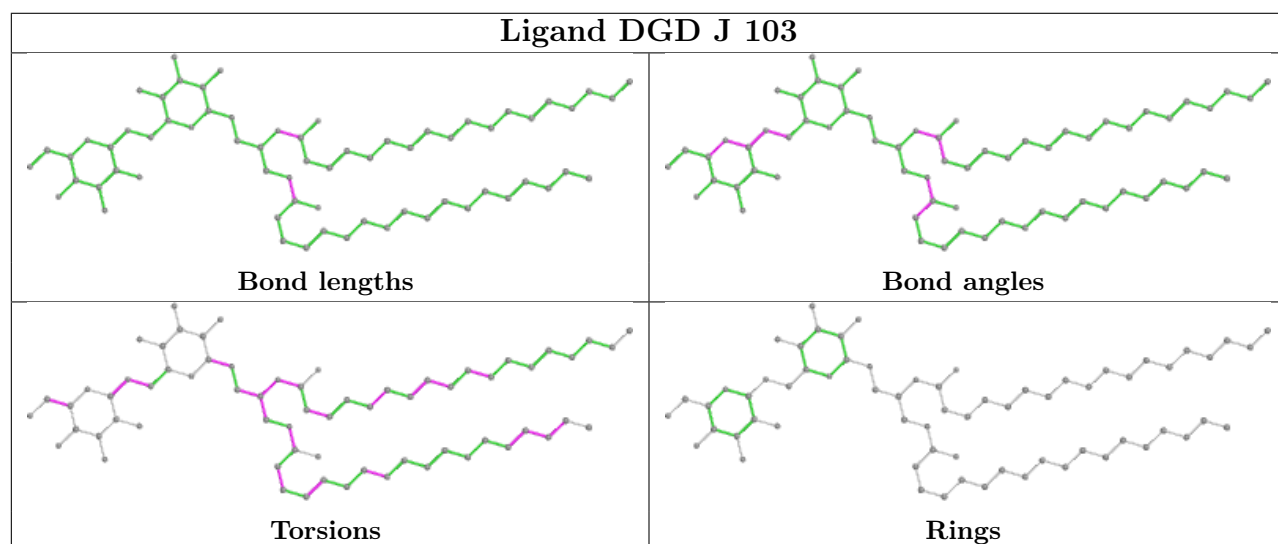
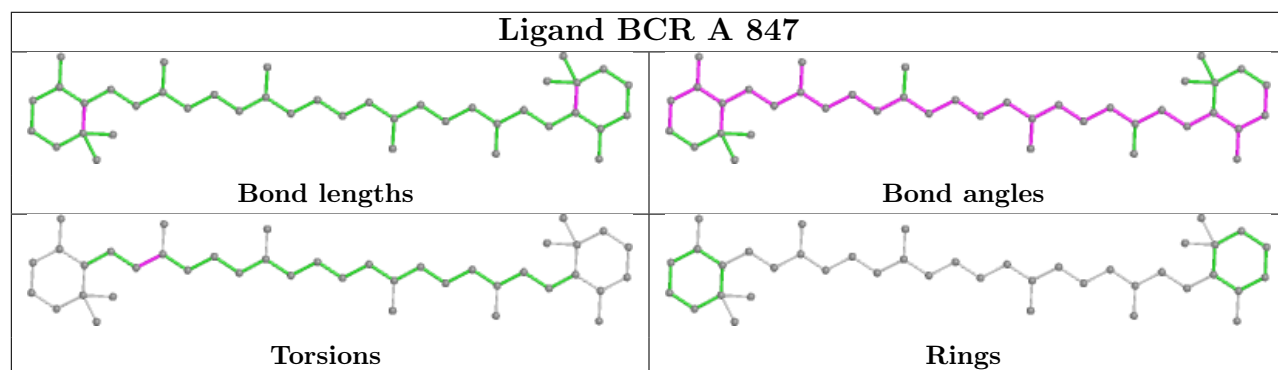
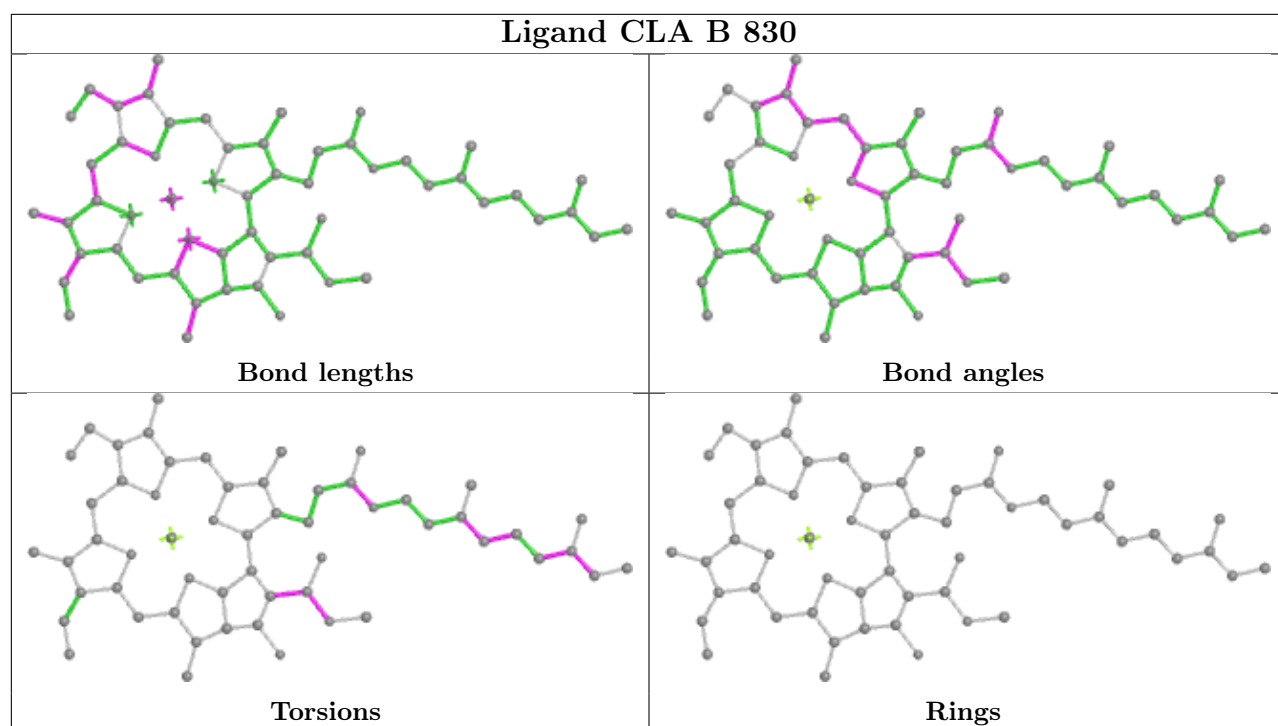
Bond angles

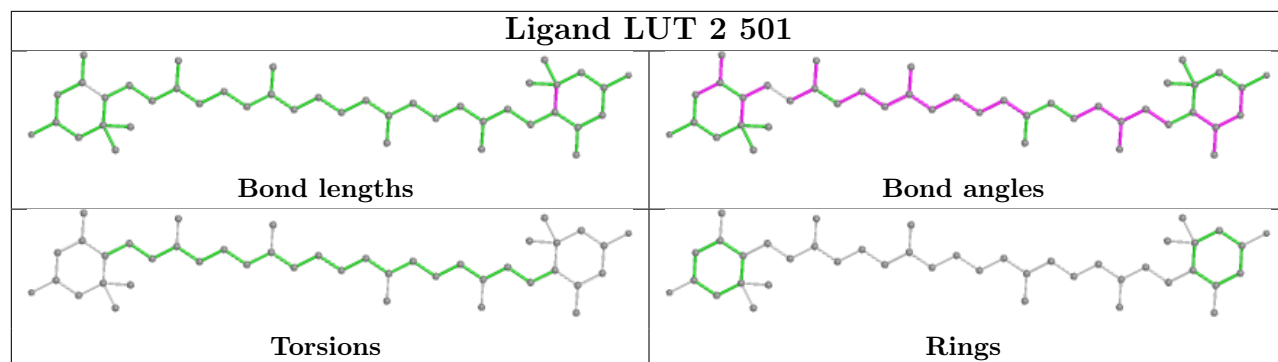
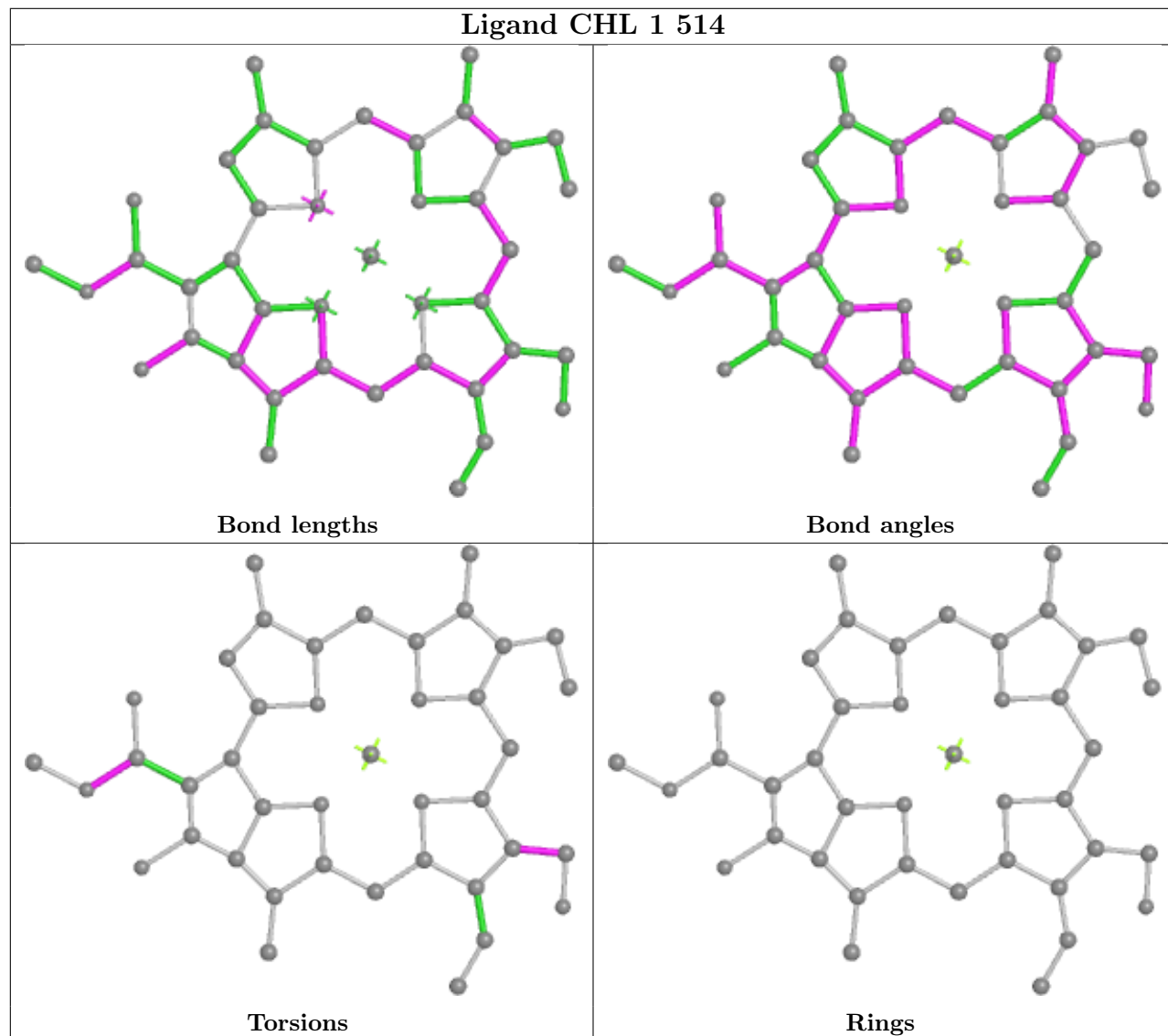


Torsions

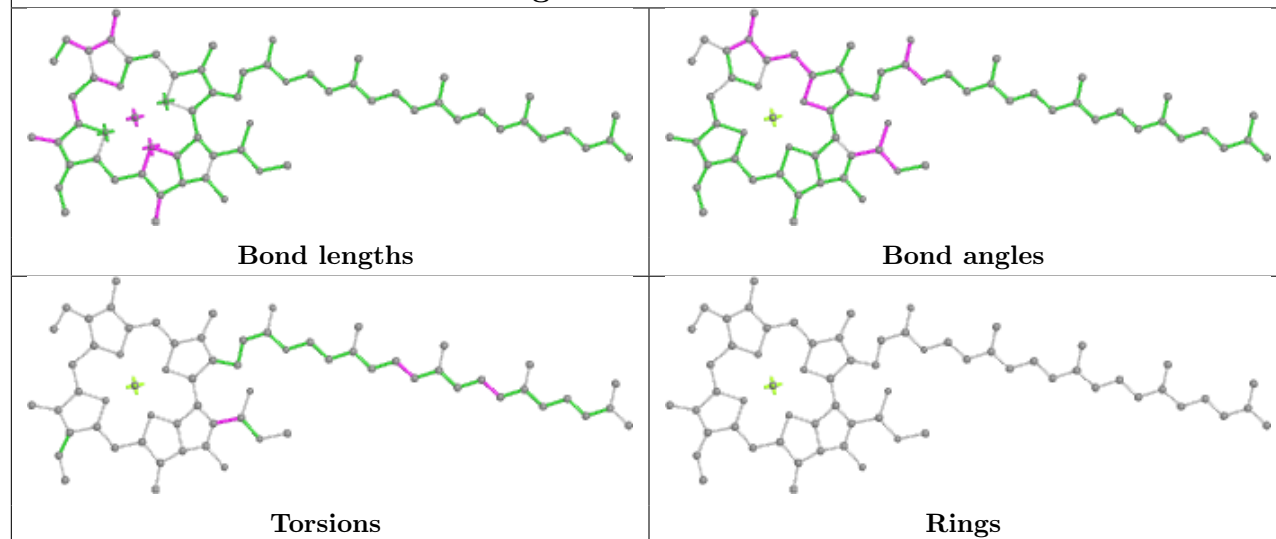


Rings

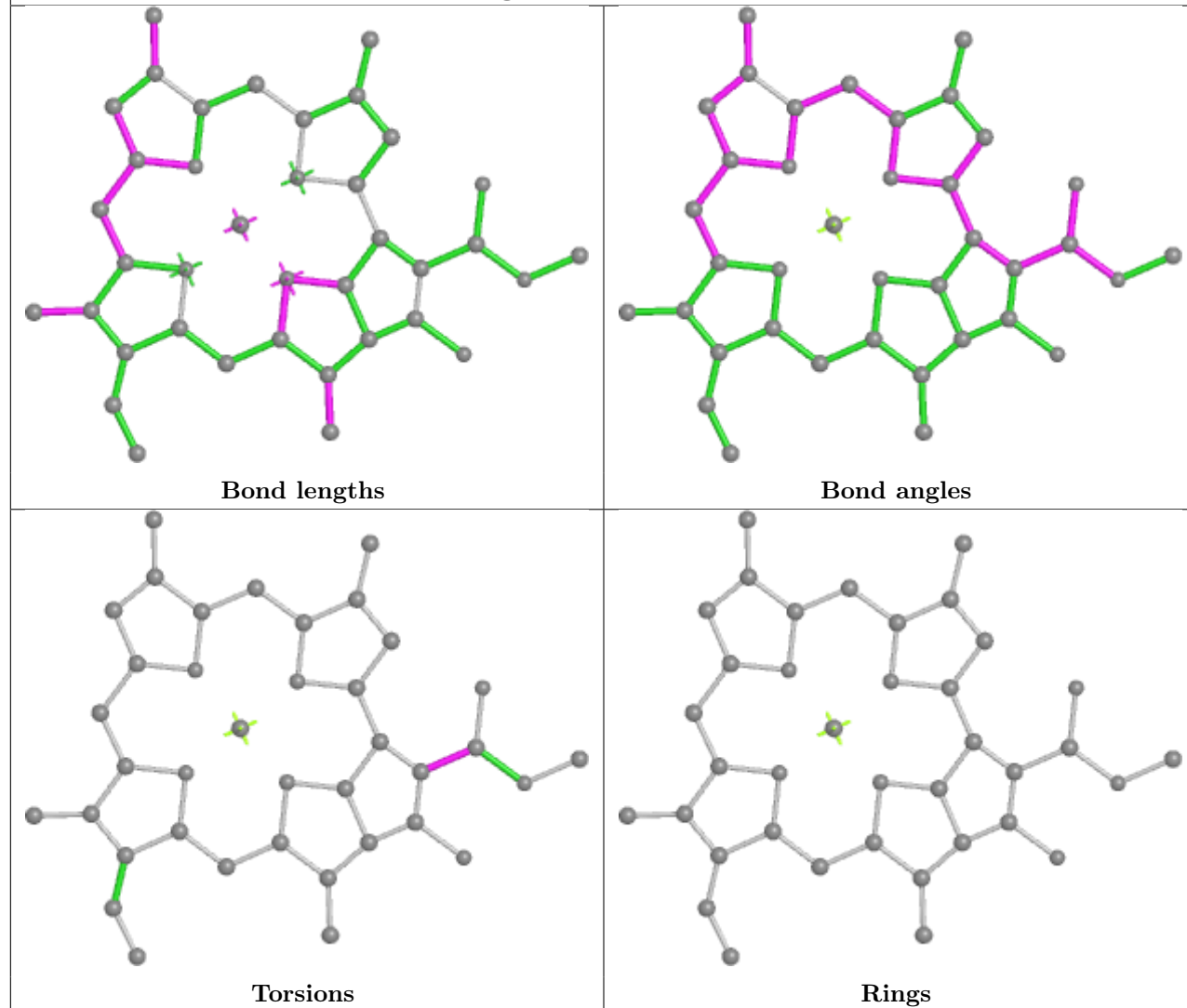


Ligand LUT 2 501**Ligand CHL 1 514**

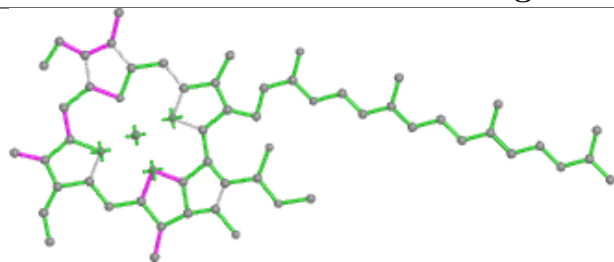
Ligand CLA B 838



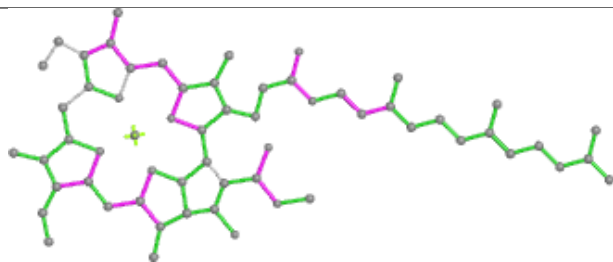
Ligand CLA 5 305



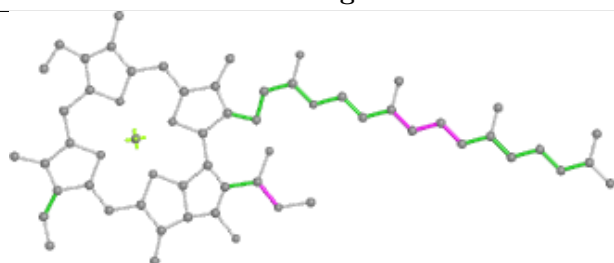
Ligand CLA B 835



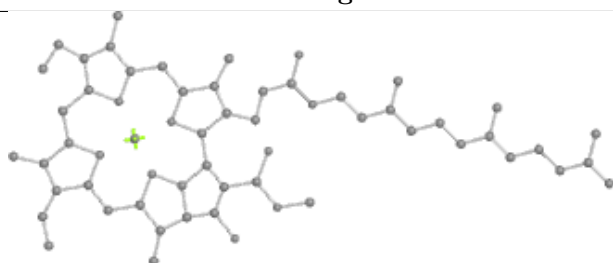
Bond lengths



Bond angles

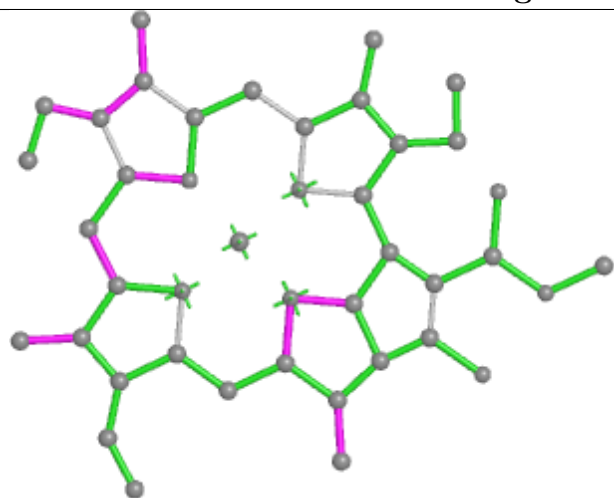


Torsions

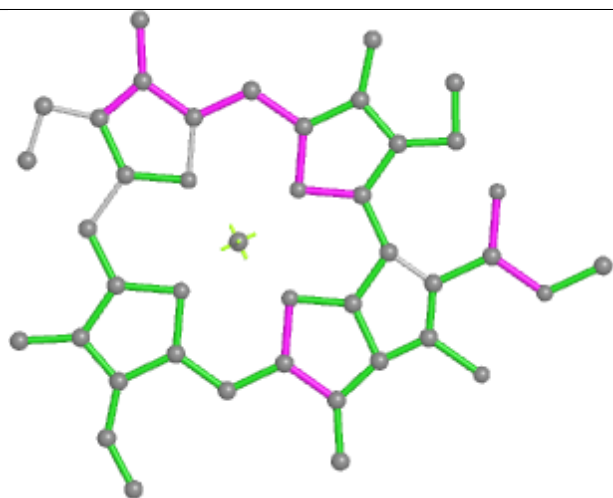


Rings

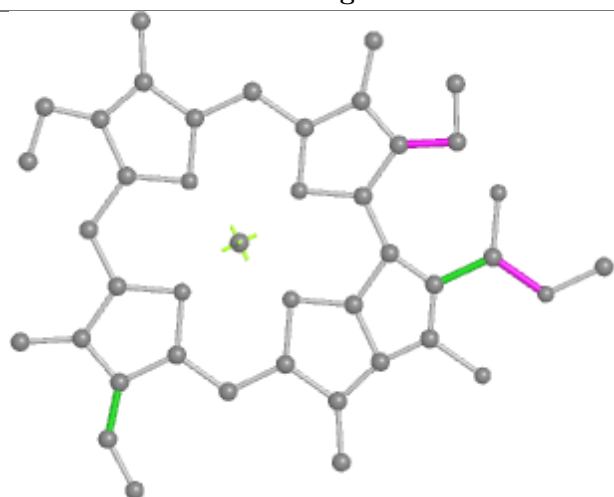
Ligand CLA B 823



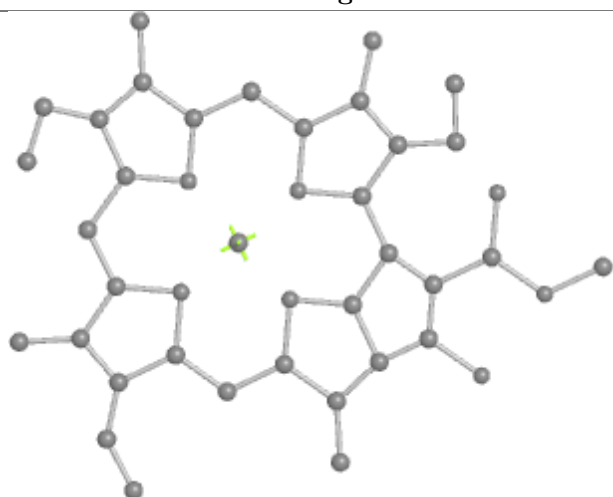
Bond lengths



Bond angles

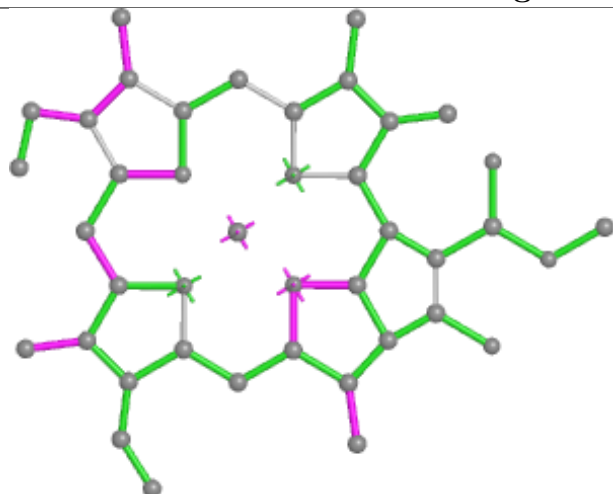


Torsions

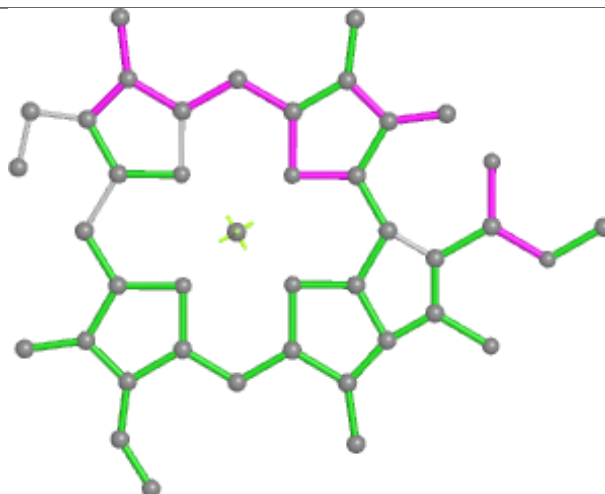


Rings

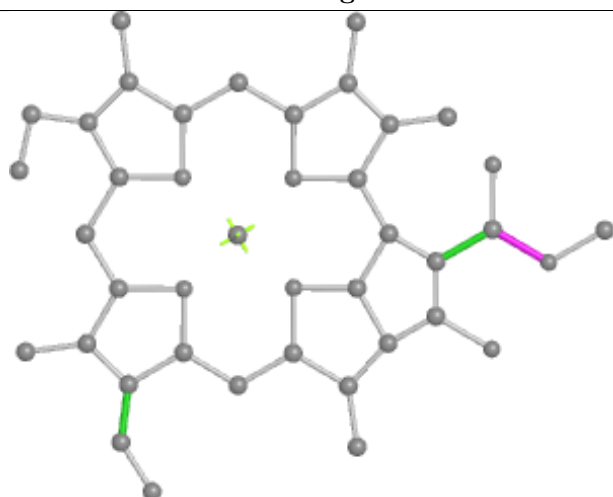
Ligand CLA A 828



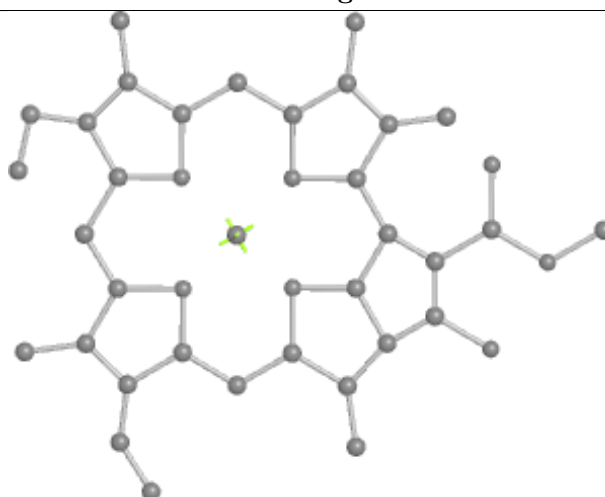
Bond lengths



Bond angles

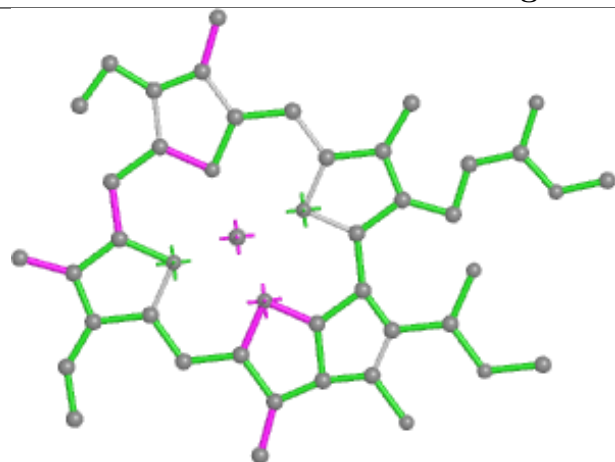


Torsions

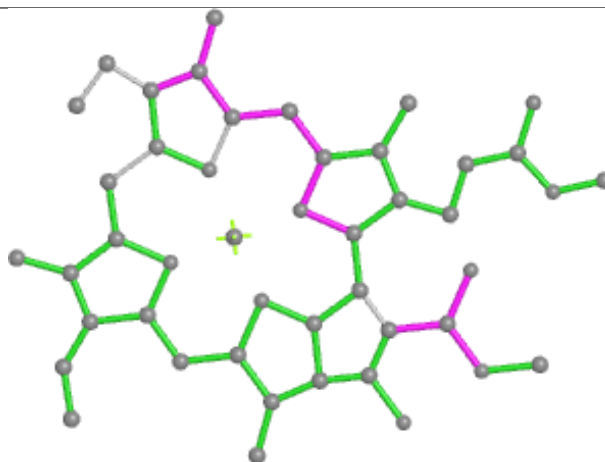


Rings

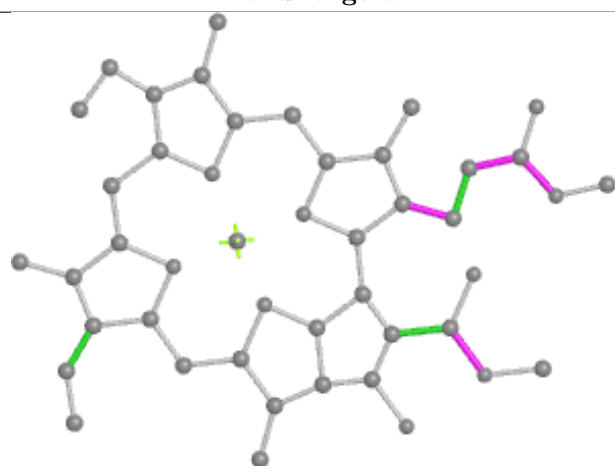
Ligand CLA 1 510



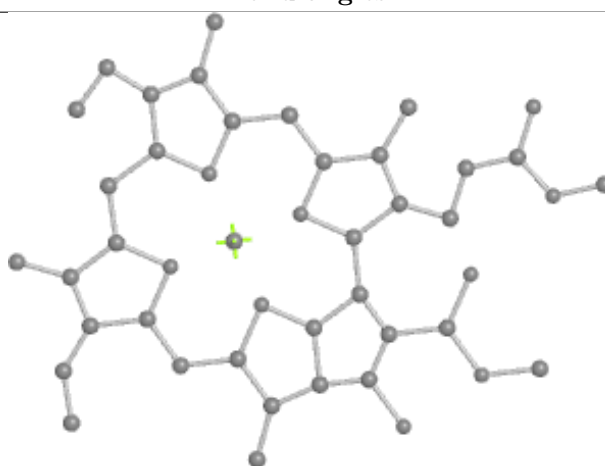
Bond lengths



Bond angles

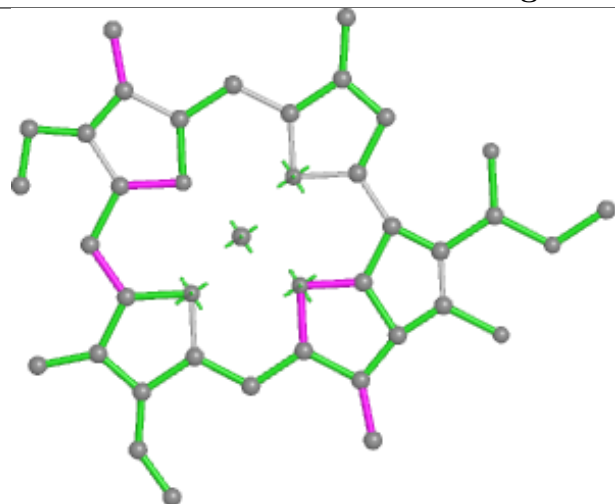


Torsions

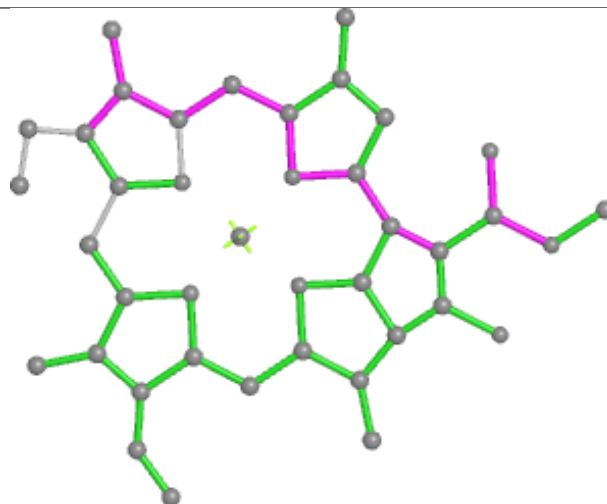


Rings

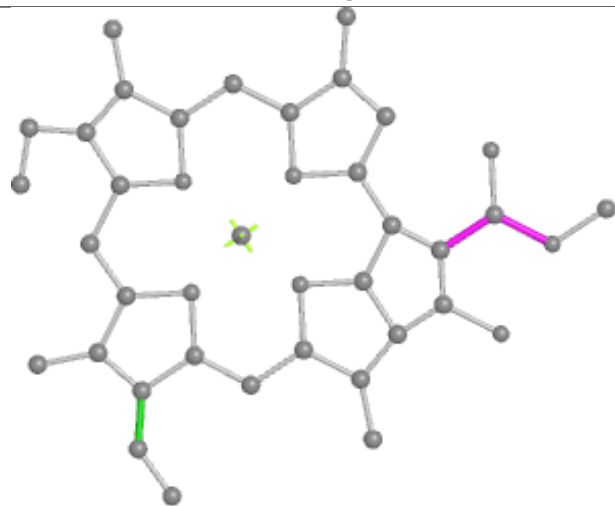
Ligand CLA 1 508



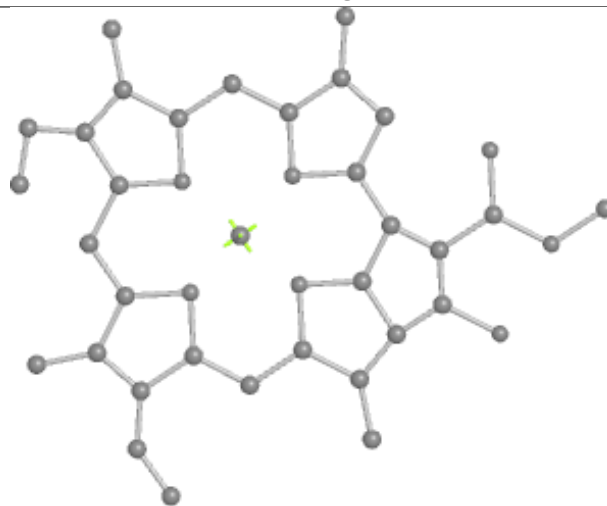
Bond lengths



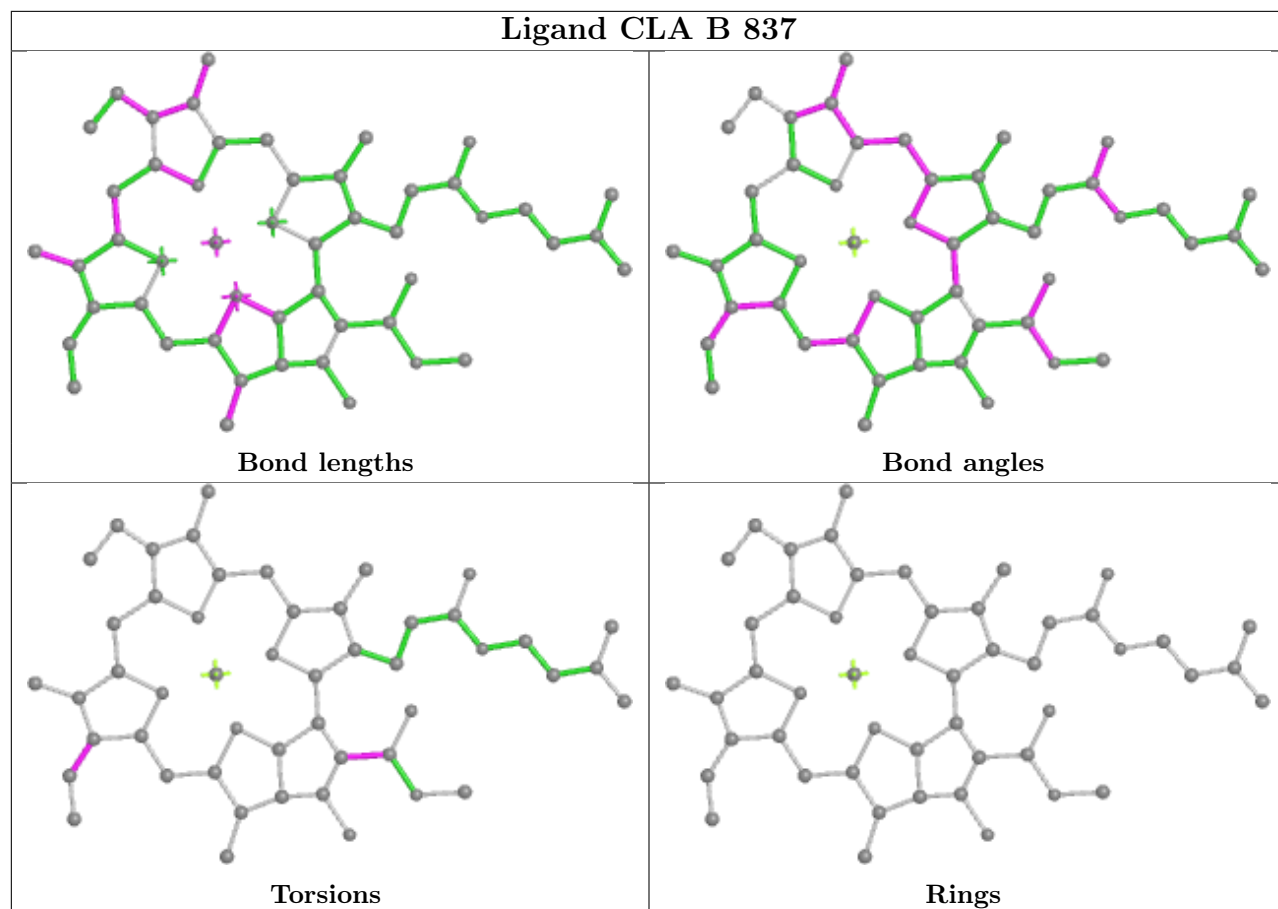
Bond angles



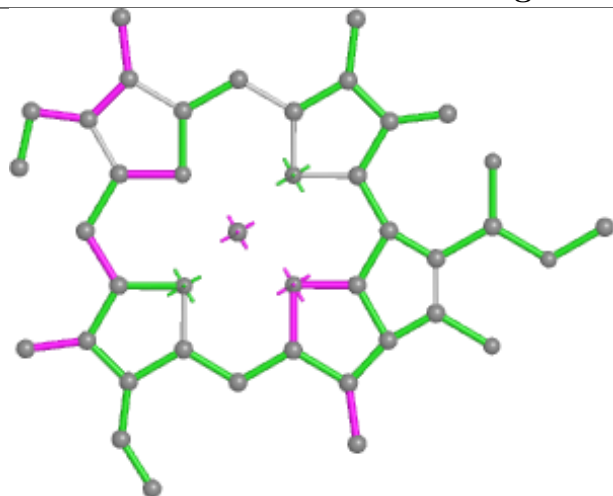
Torsions



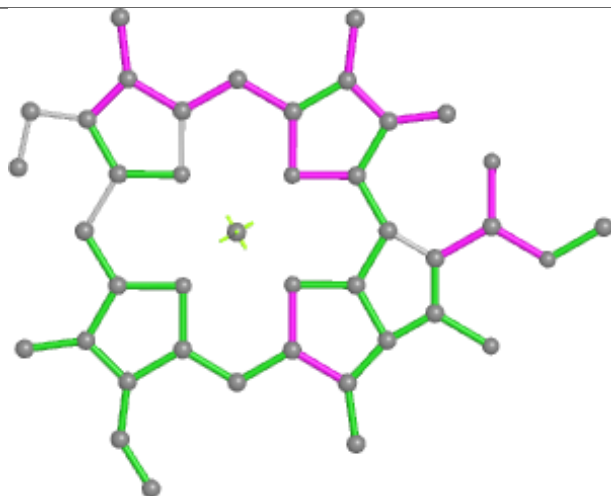
Rings



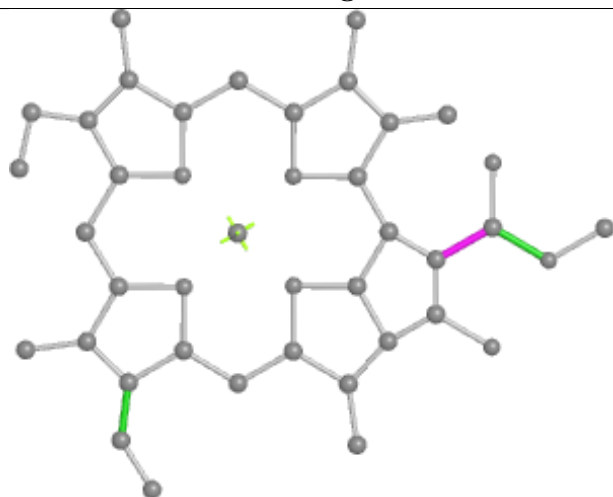
Ligand CLA B 827



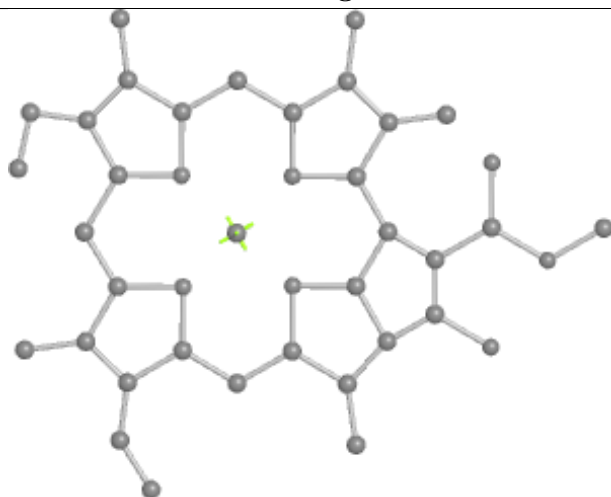
Bond lengths



Bond angles

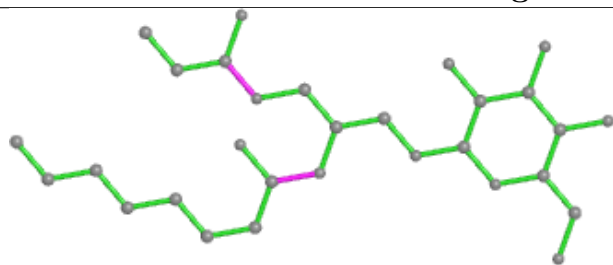


Torsions

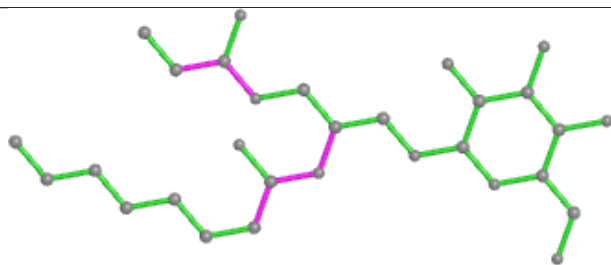


Rings

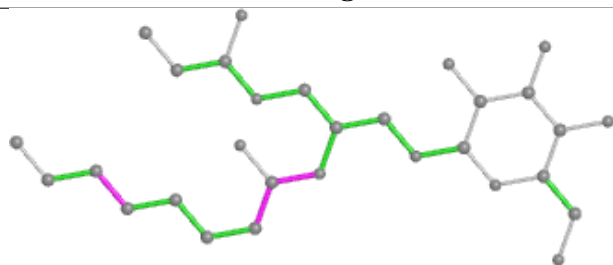
Ligand LMG F 805



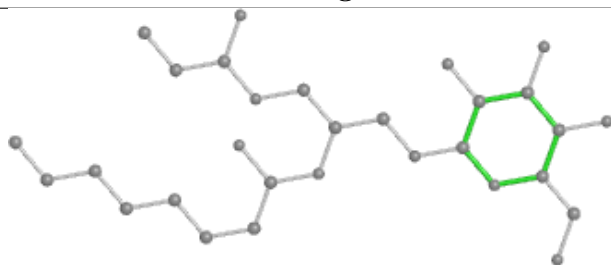
Bond lengths



Bond angles

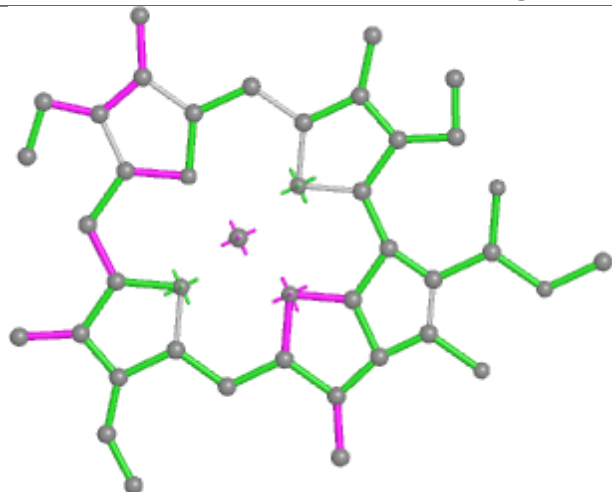


Torsions

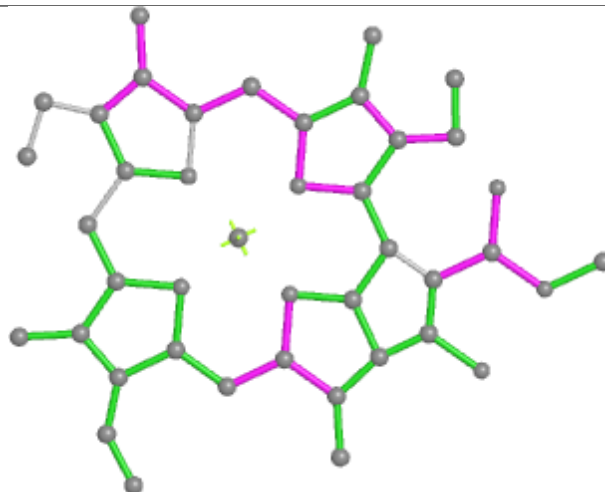


Rings

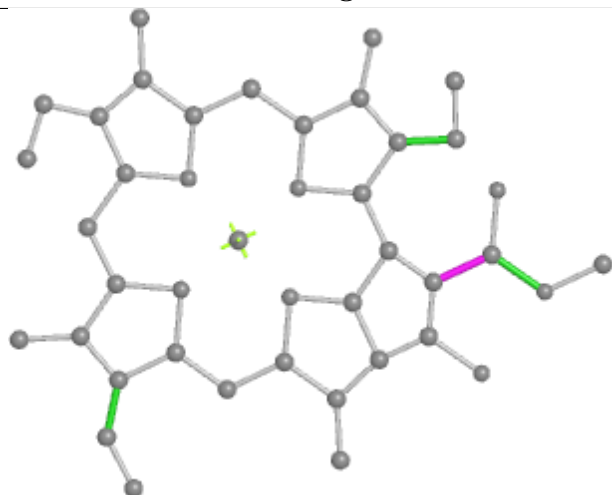
Ligand CLA A 812



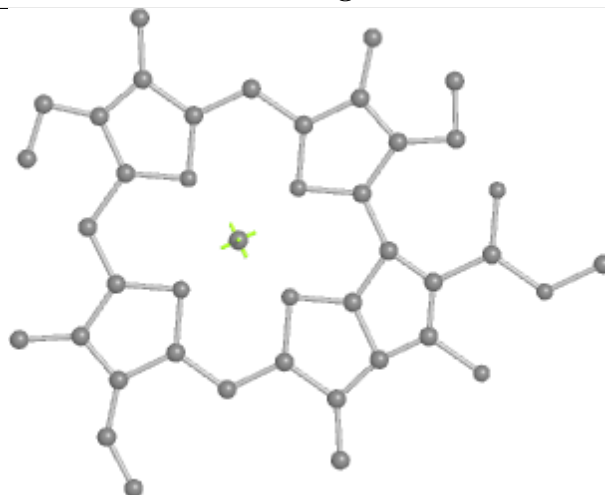
Bond lengths



Bond angles

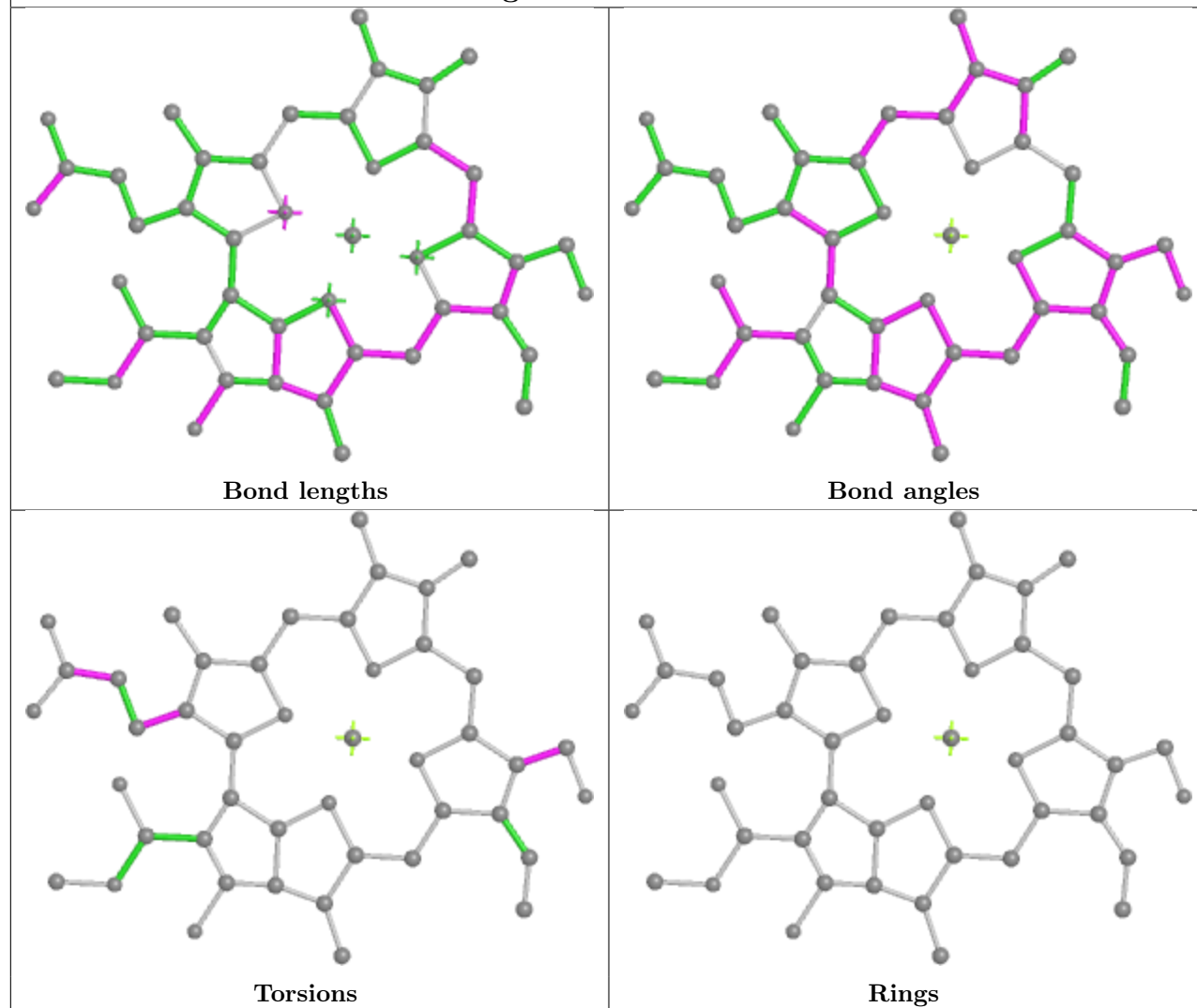


Torsions

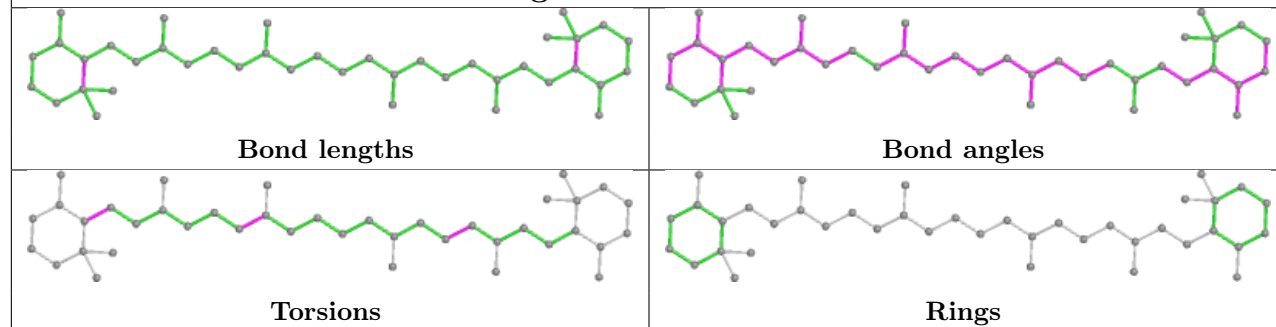


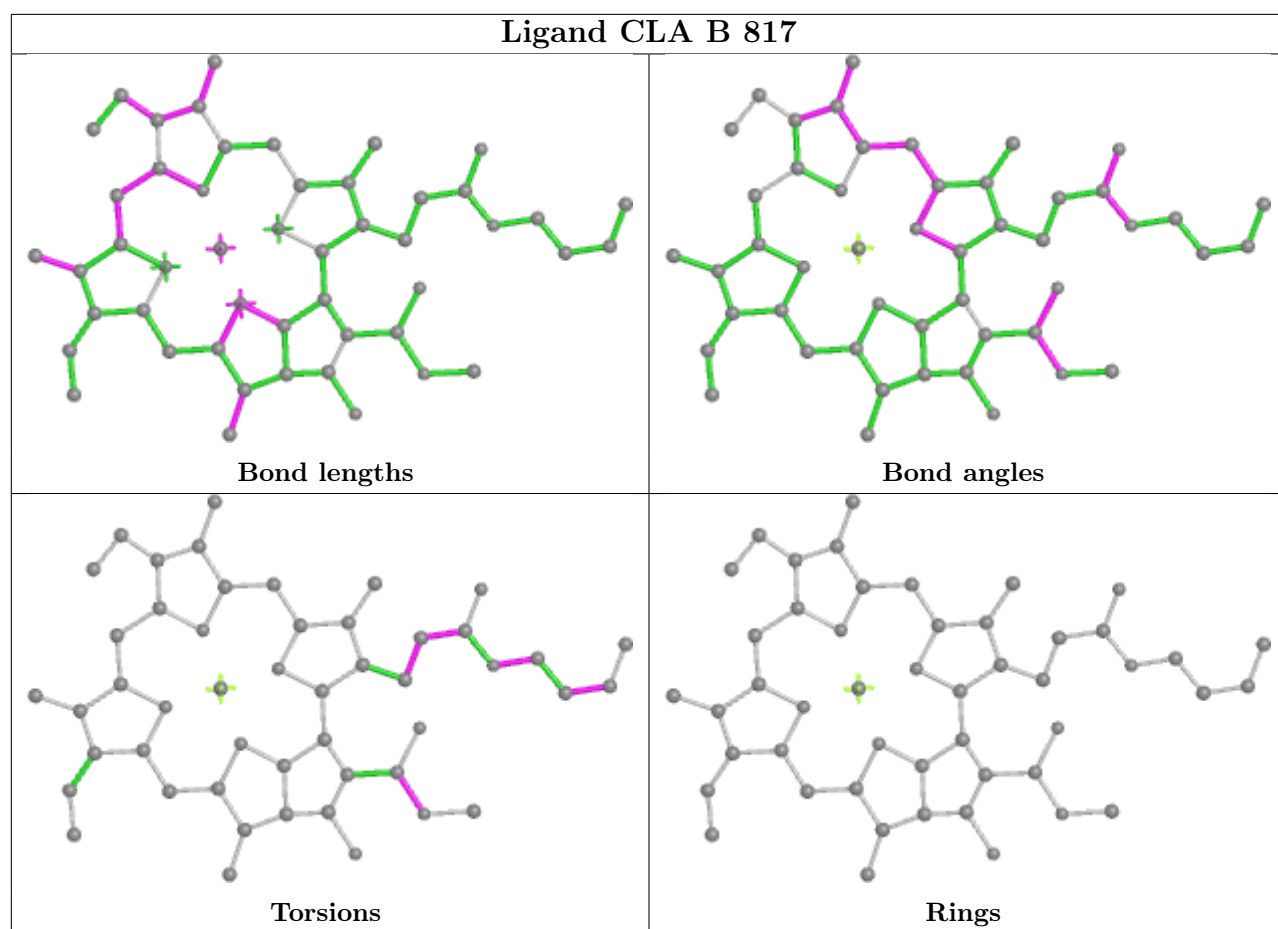
Rings

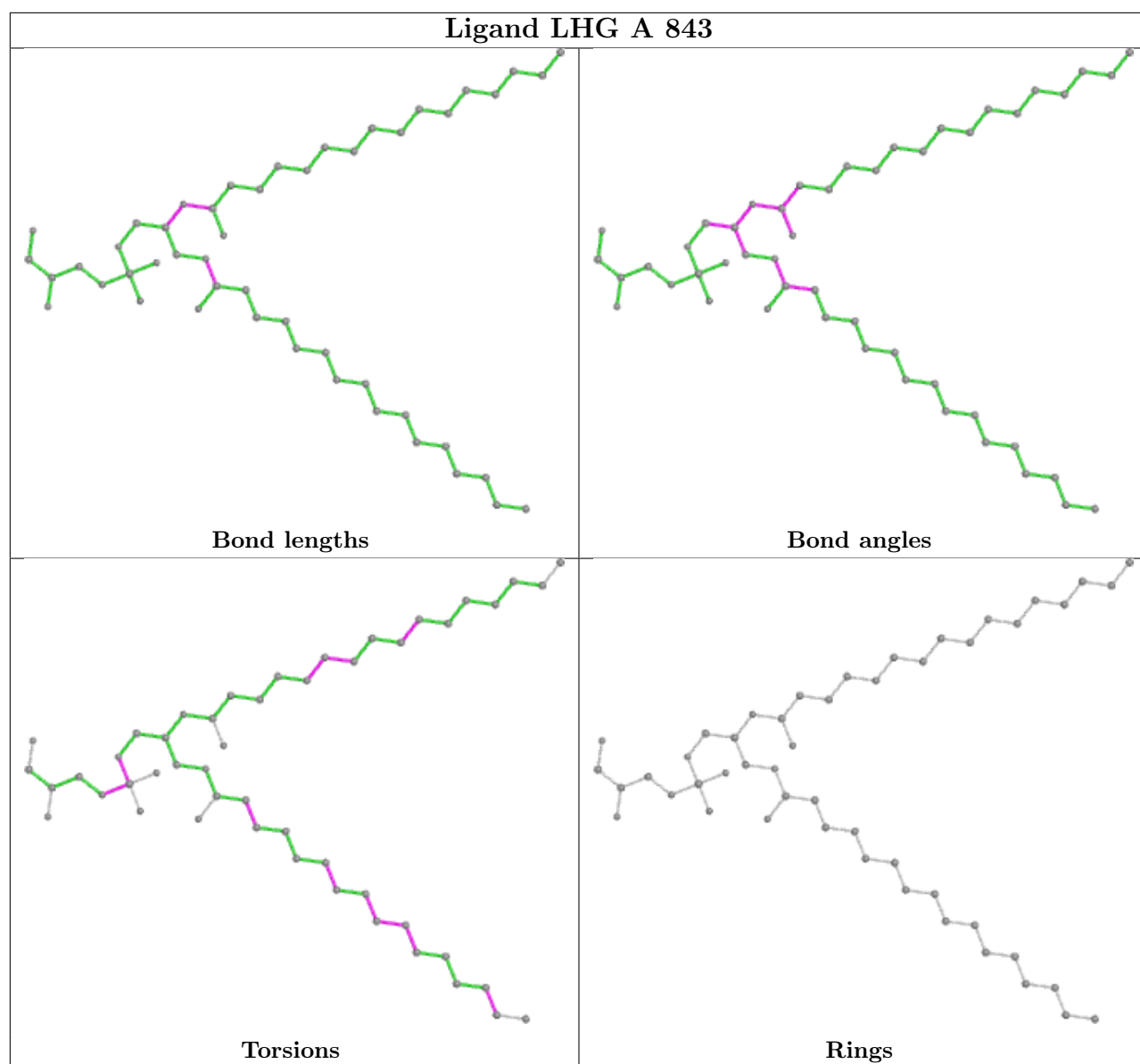
Ligand CHL 2 515

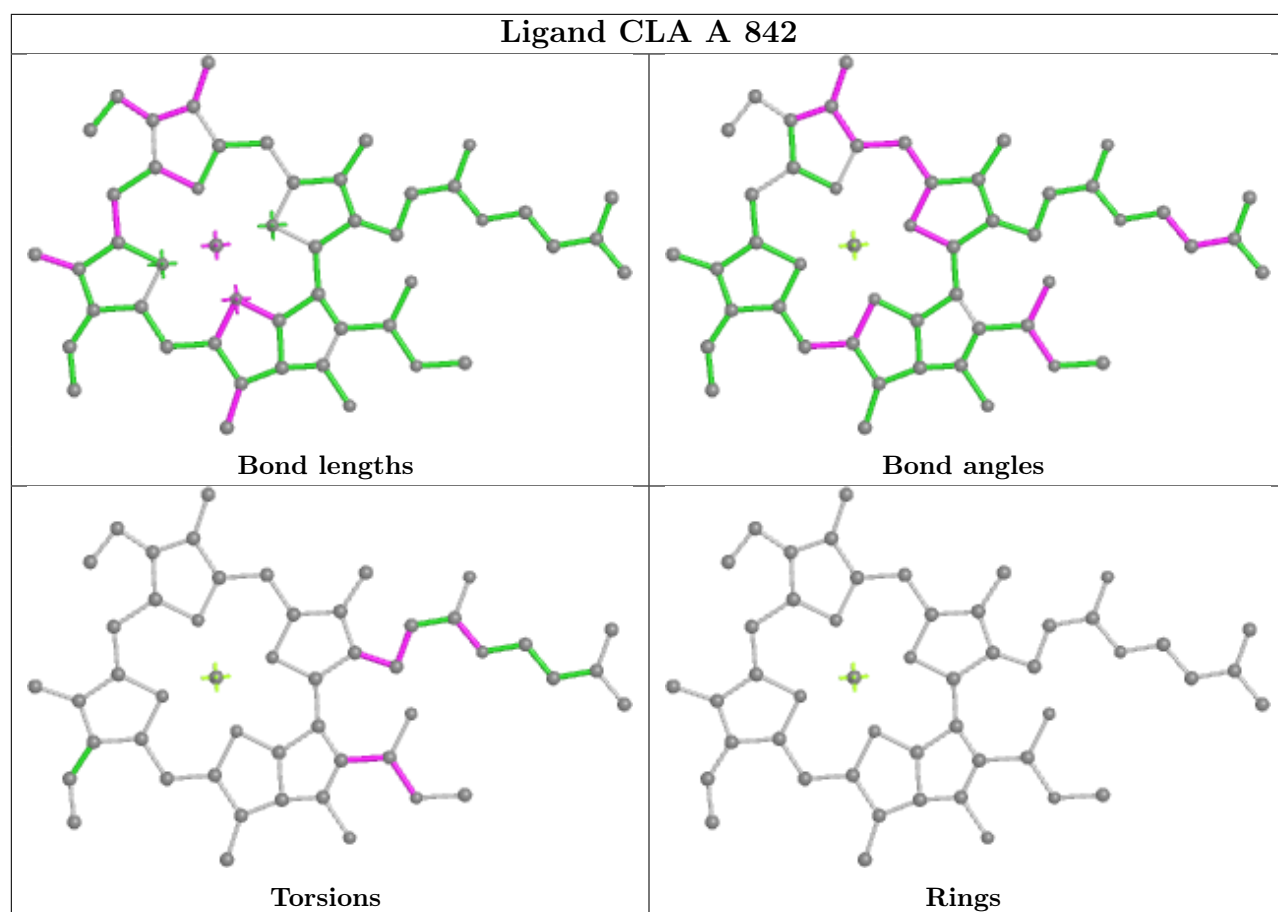


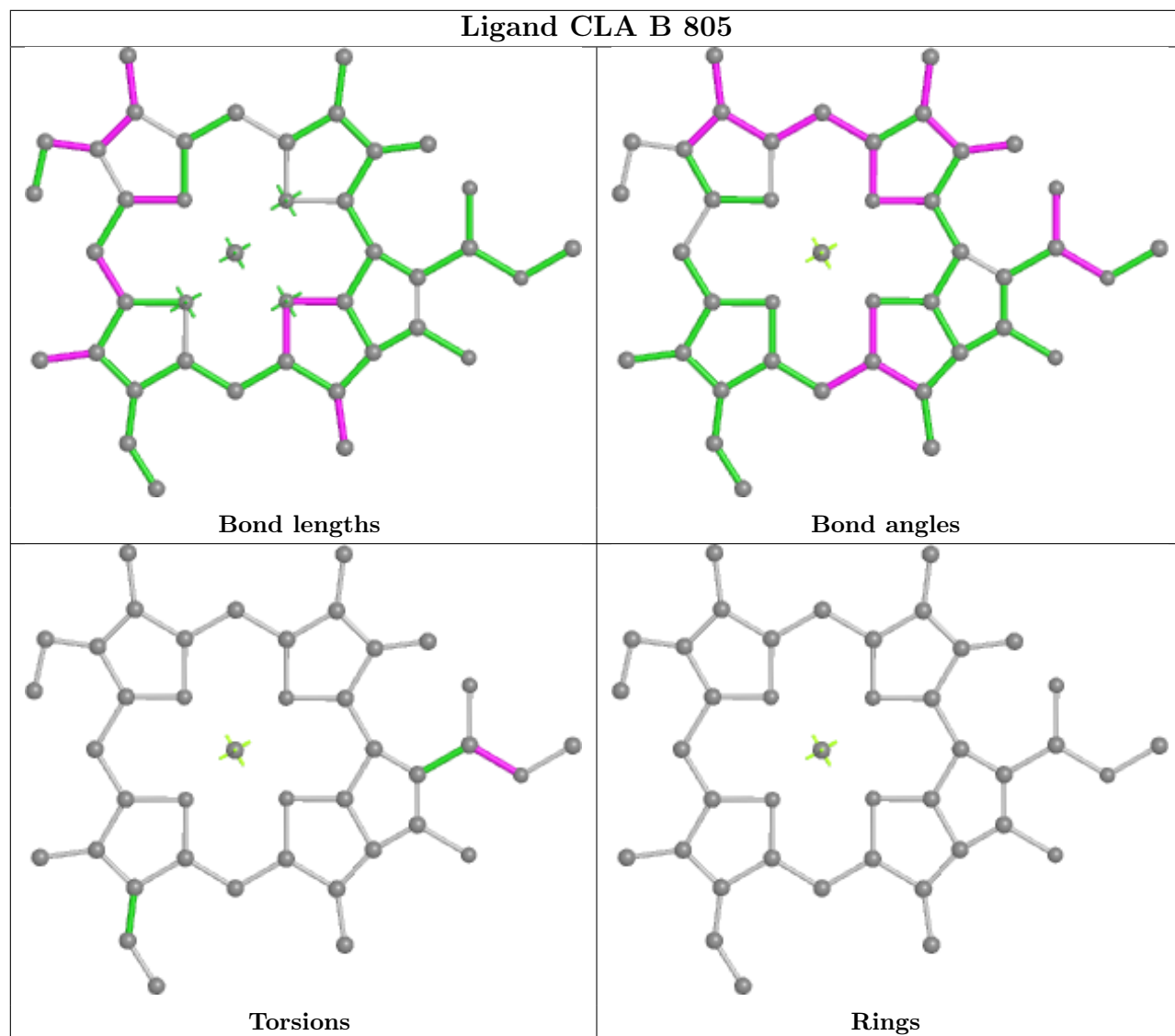
Ligand BCR B 847

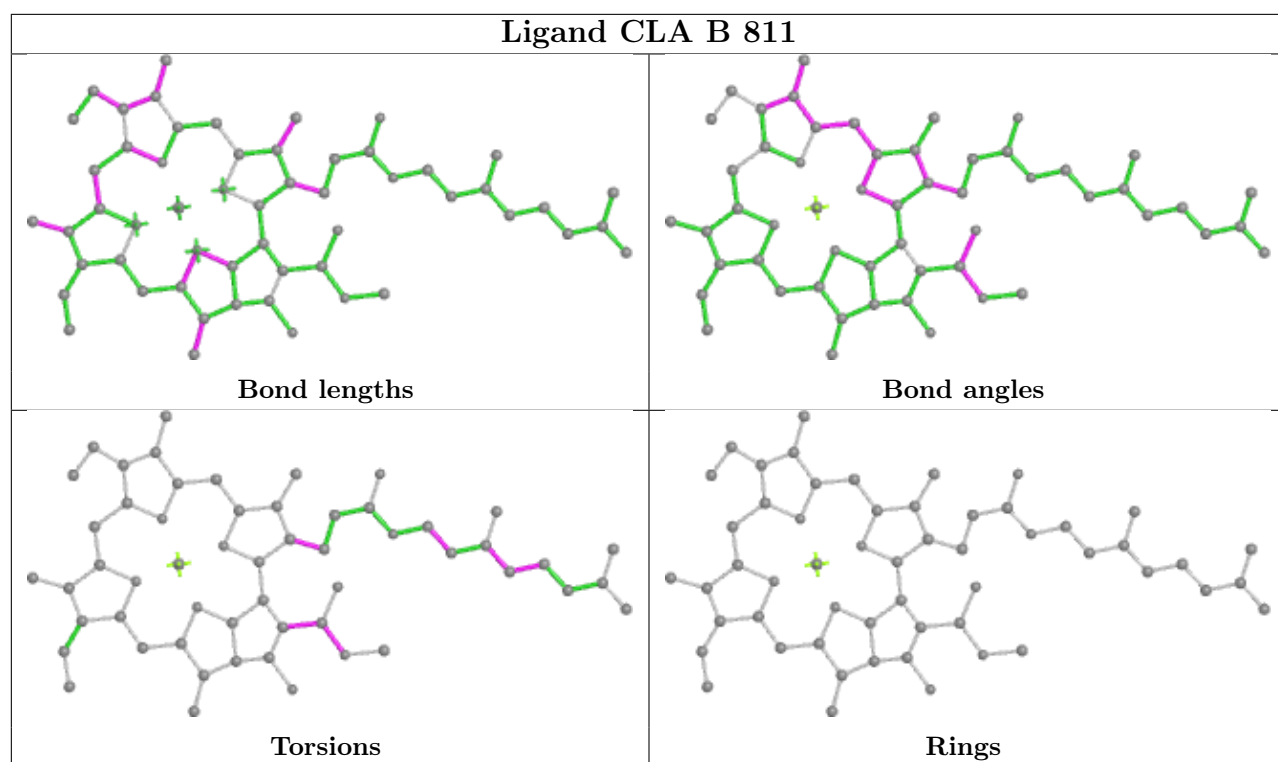




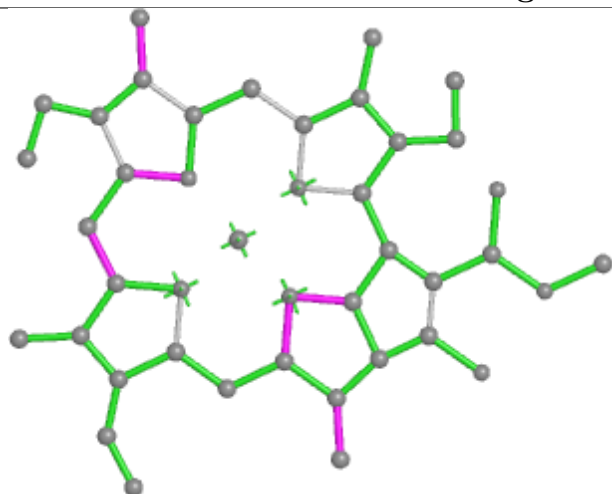




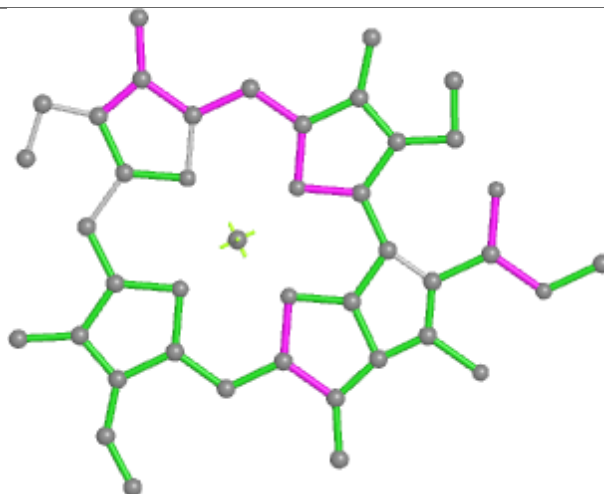




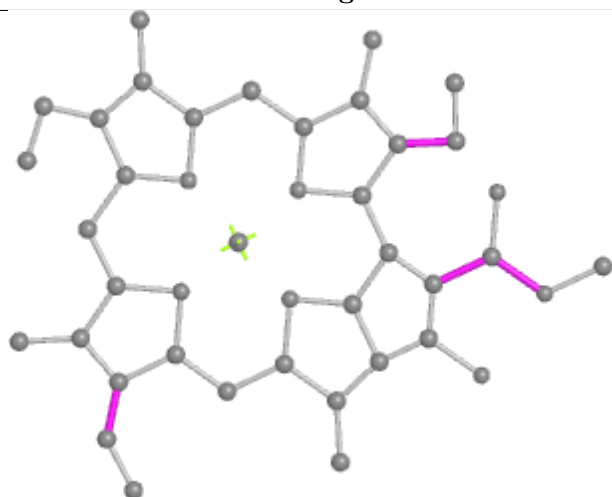
Ligand CLA J 101



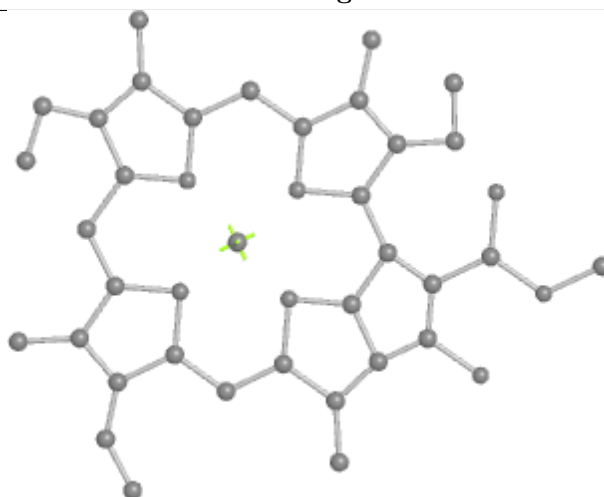
Bond lengths



Bond angles

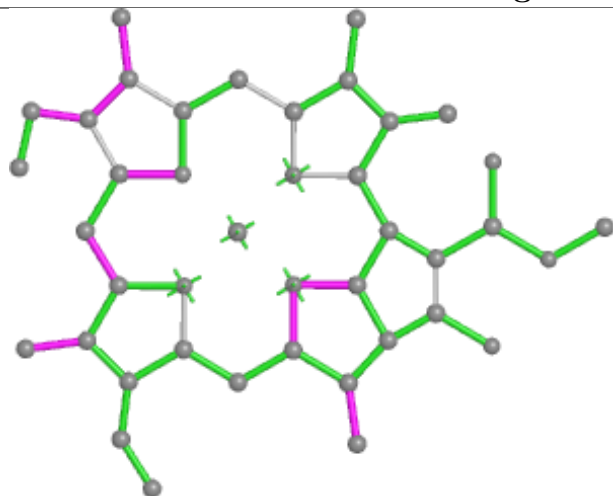


Torsions

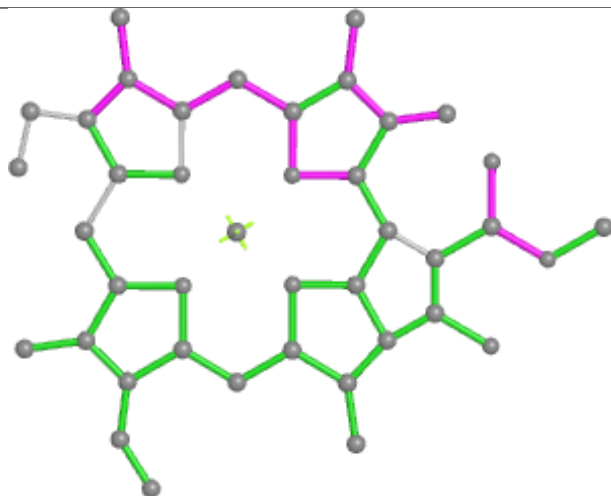


Rings

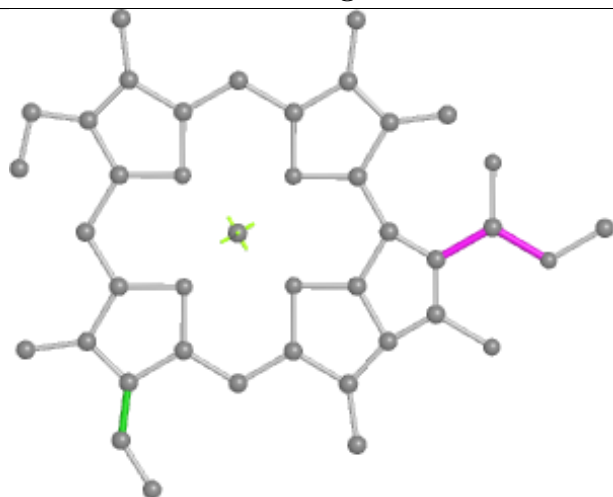
Ligand CLA A 834



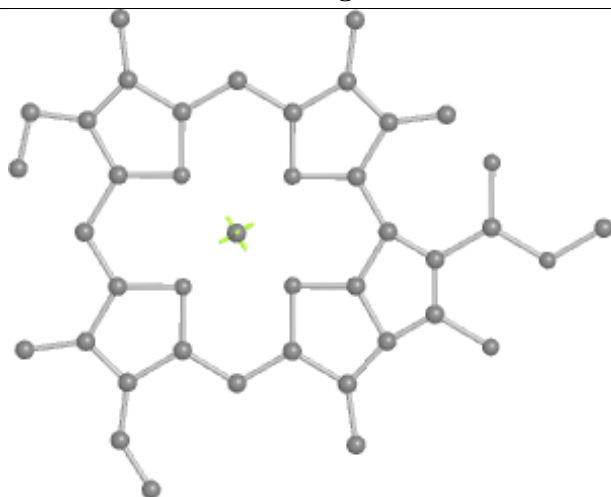
Bond lengths



Bond angles

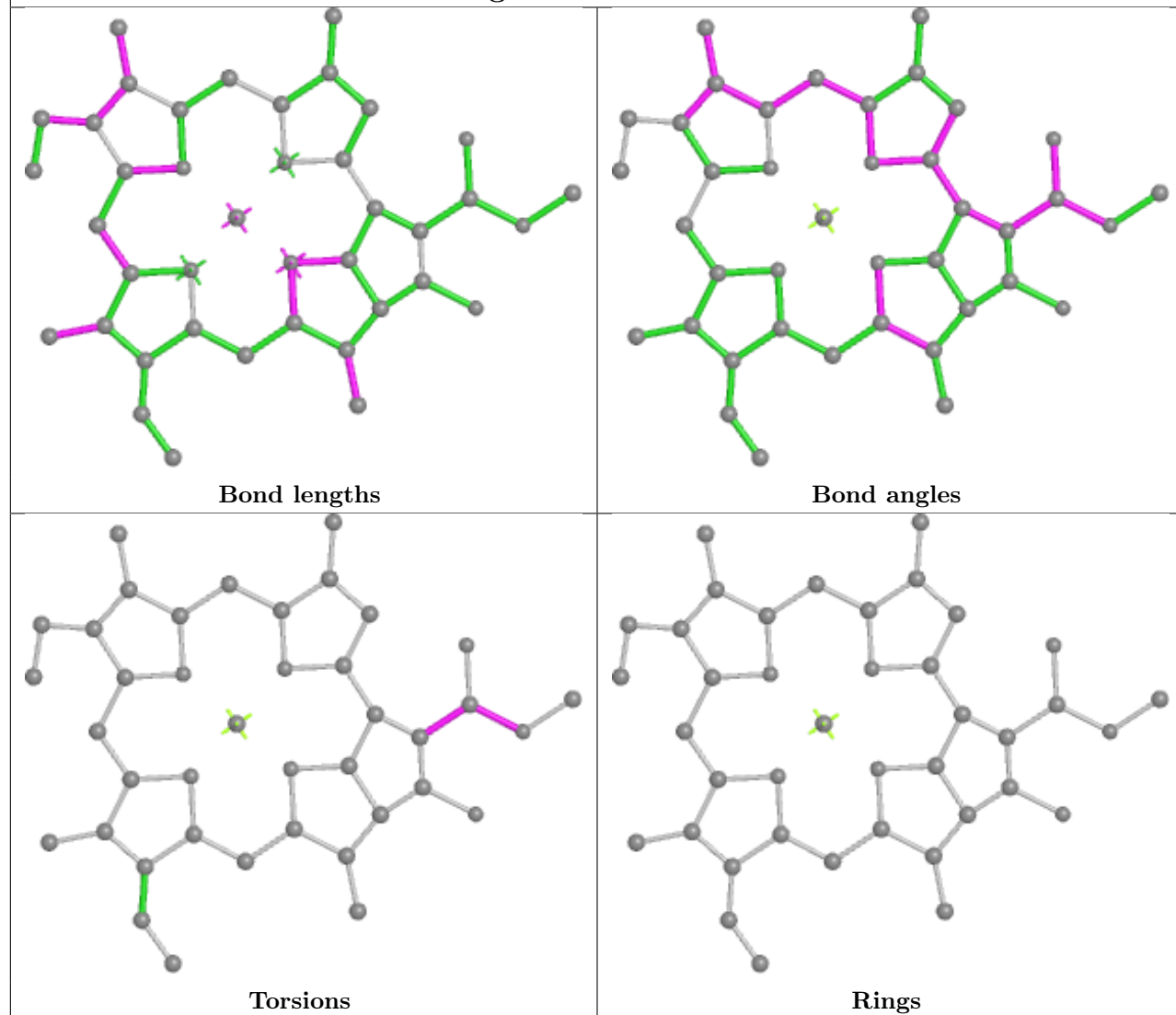


Torsions

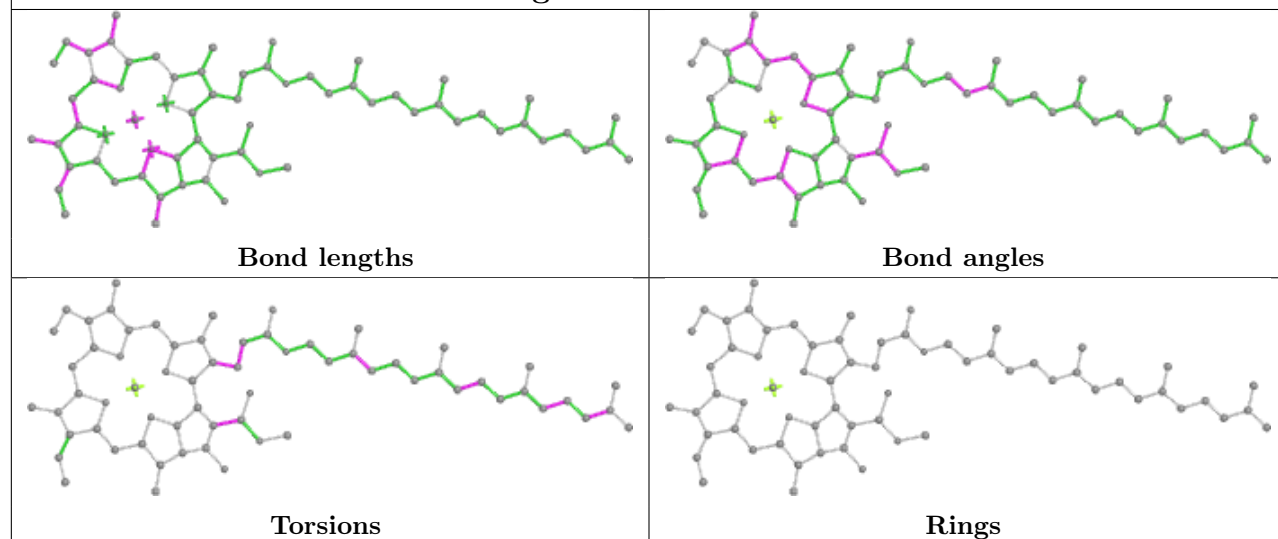


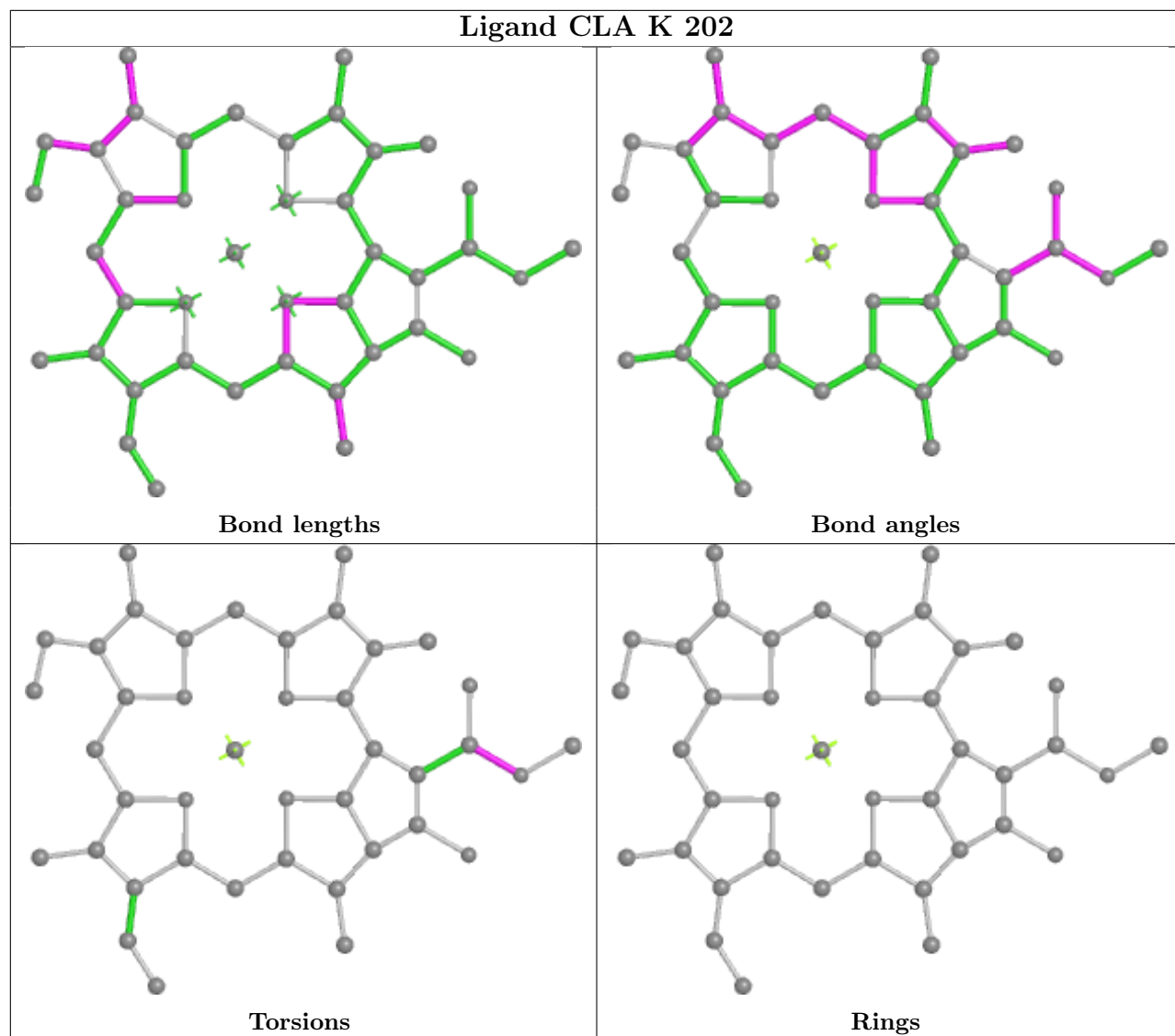
Rings

Ligand CLA A 818

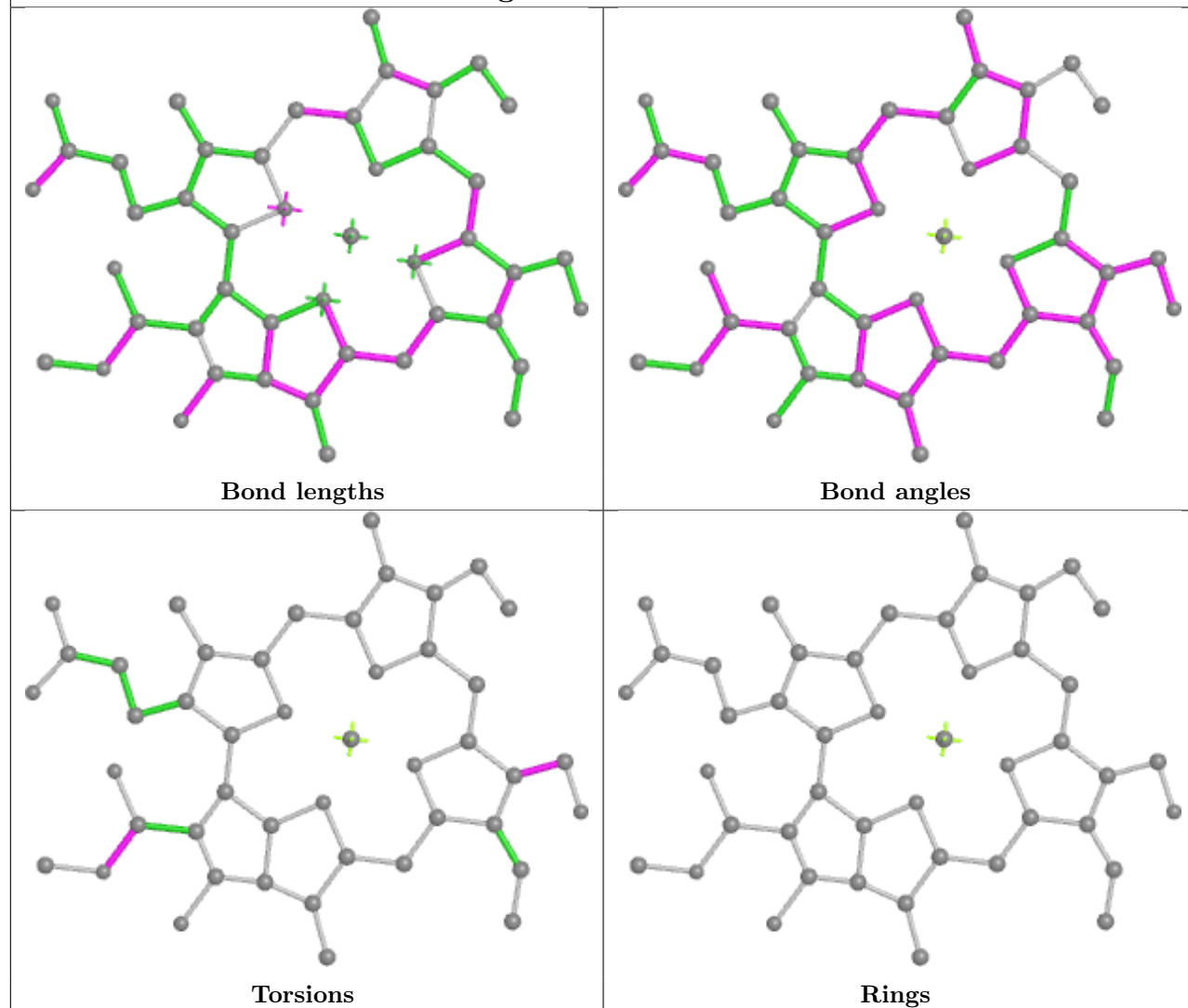


Ligand CLA B 801

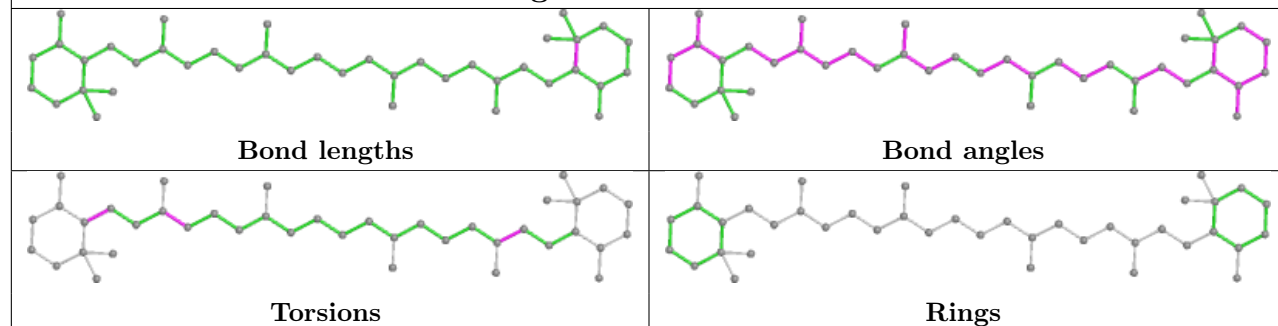


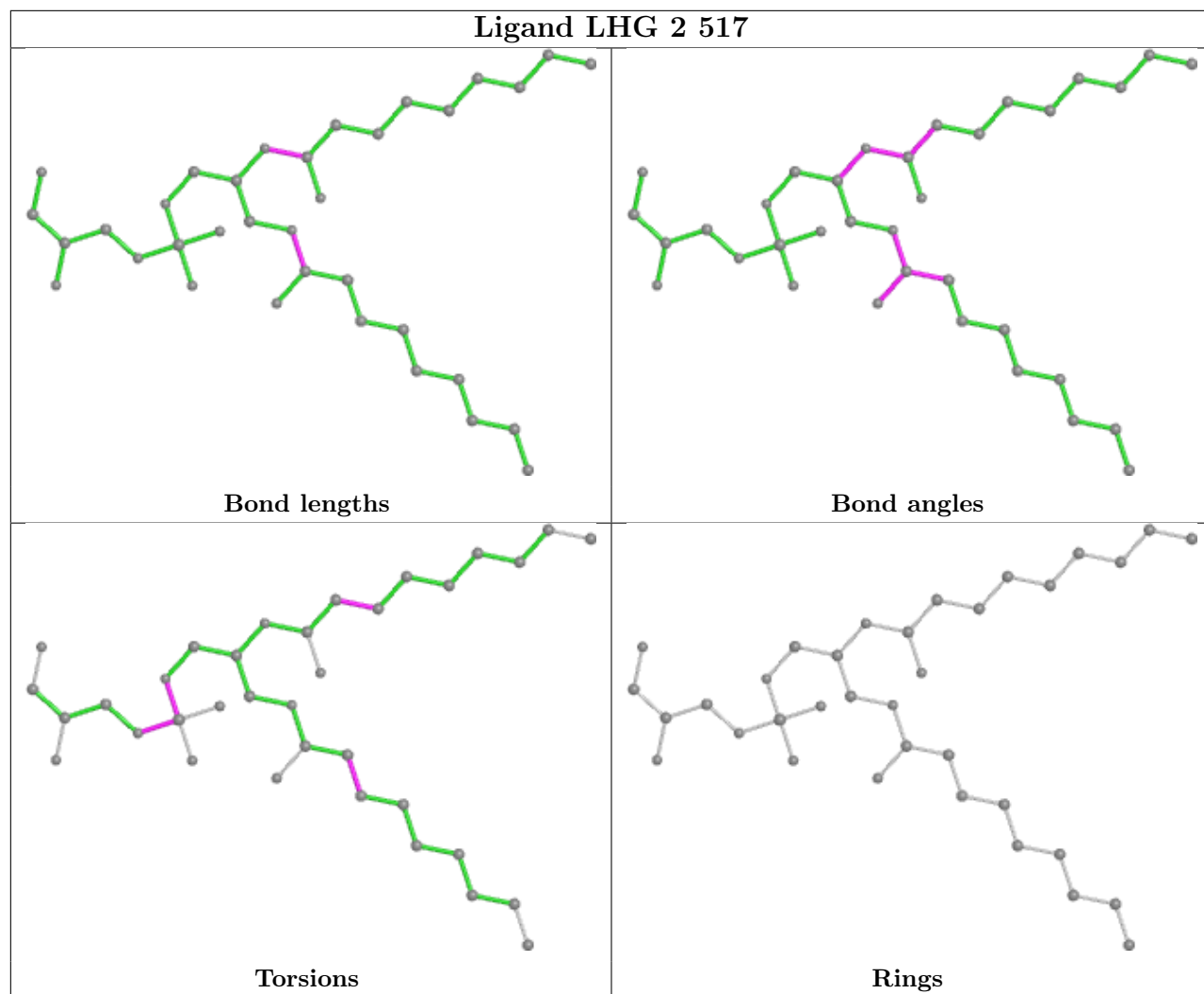
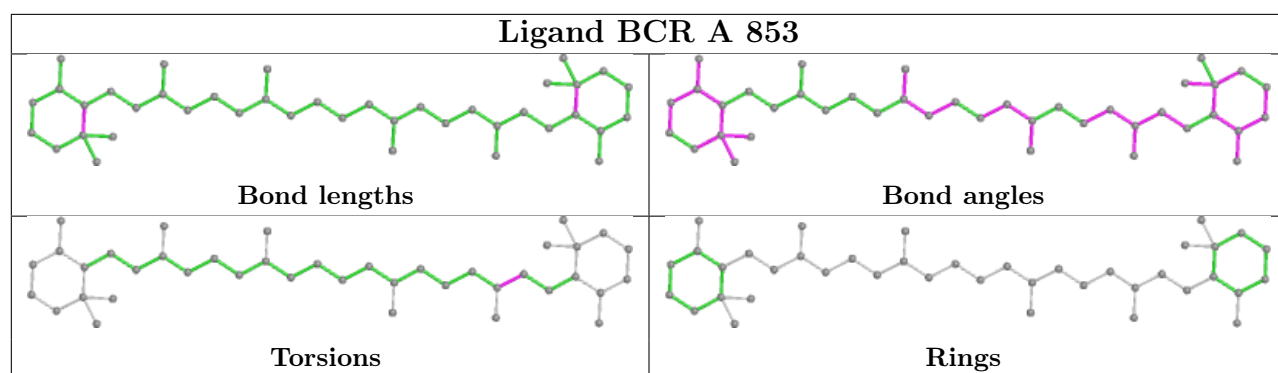


Ligand CHL 5 315

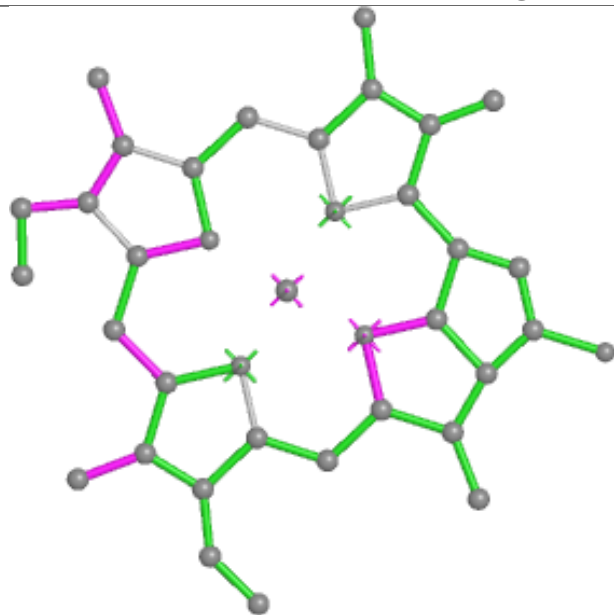


Ligand BCR B 845

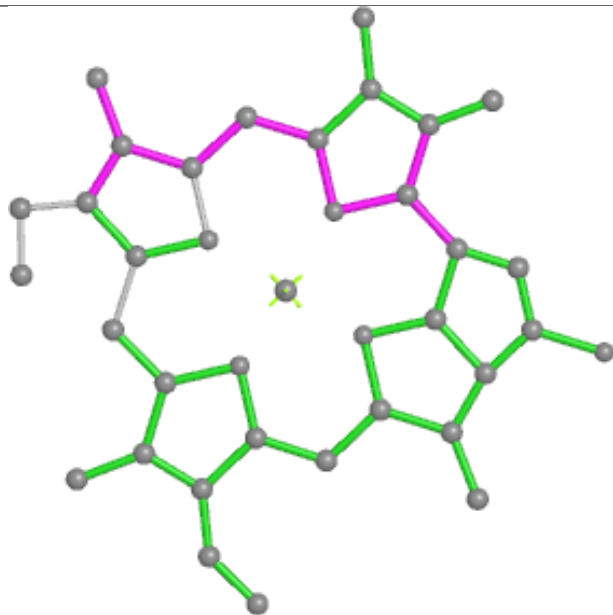




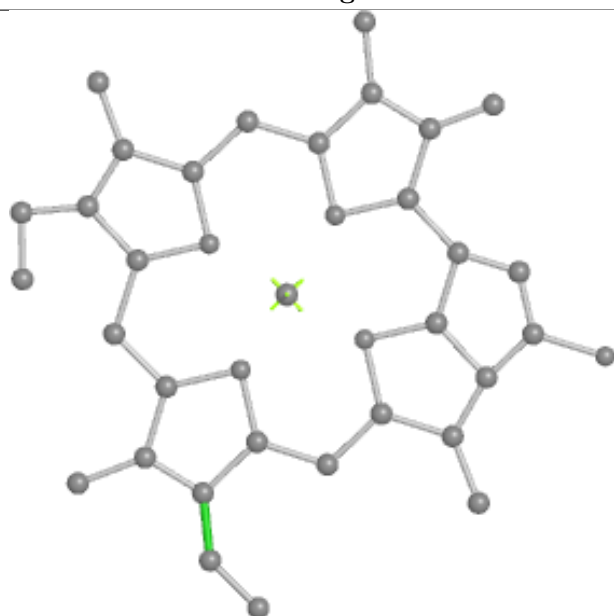
Ligand CLA K 201



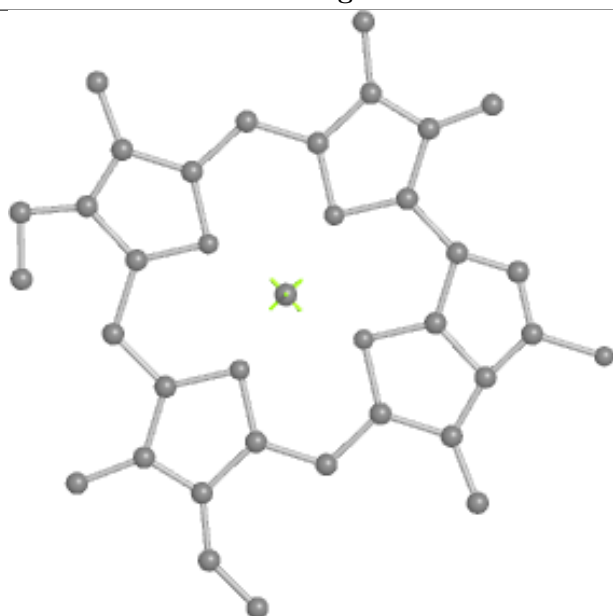
Bond lengths



Bond angles

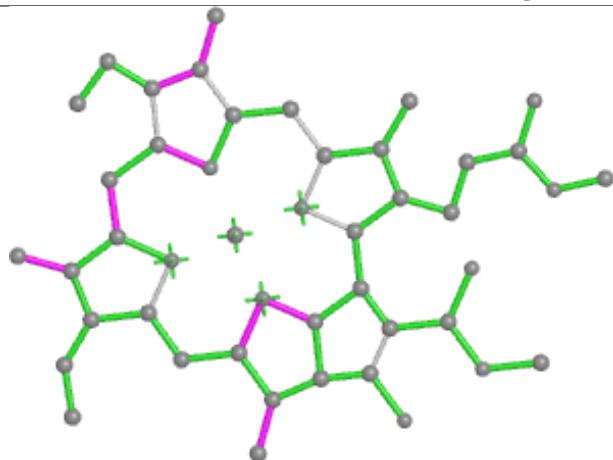


Torsions

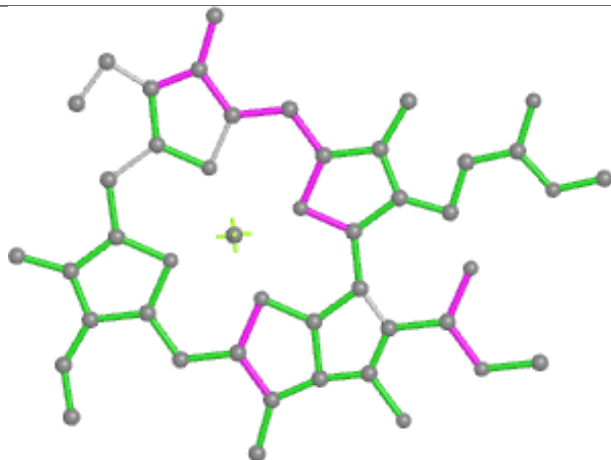


Rings

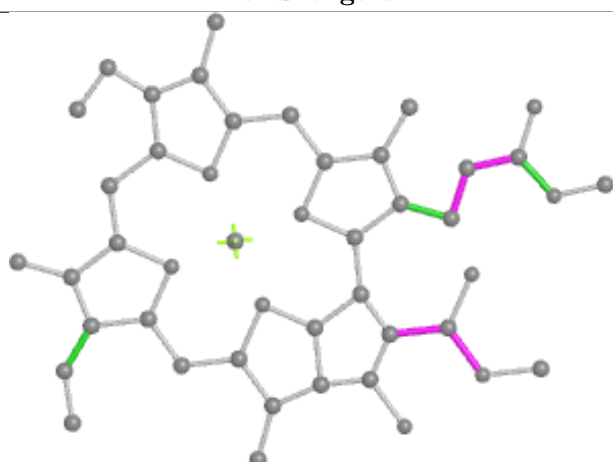
Ligand CLA 5 312



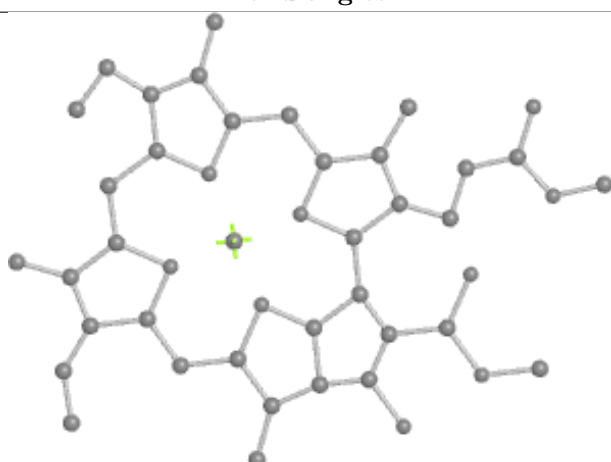
Bond lengths



Bond angles

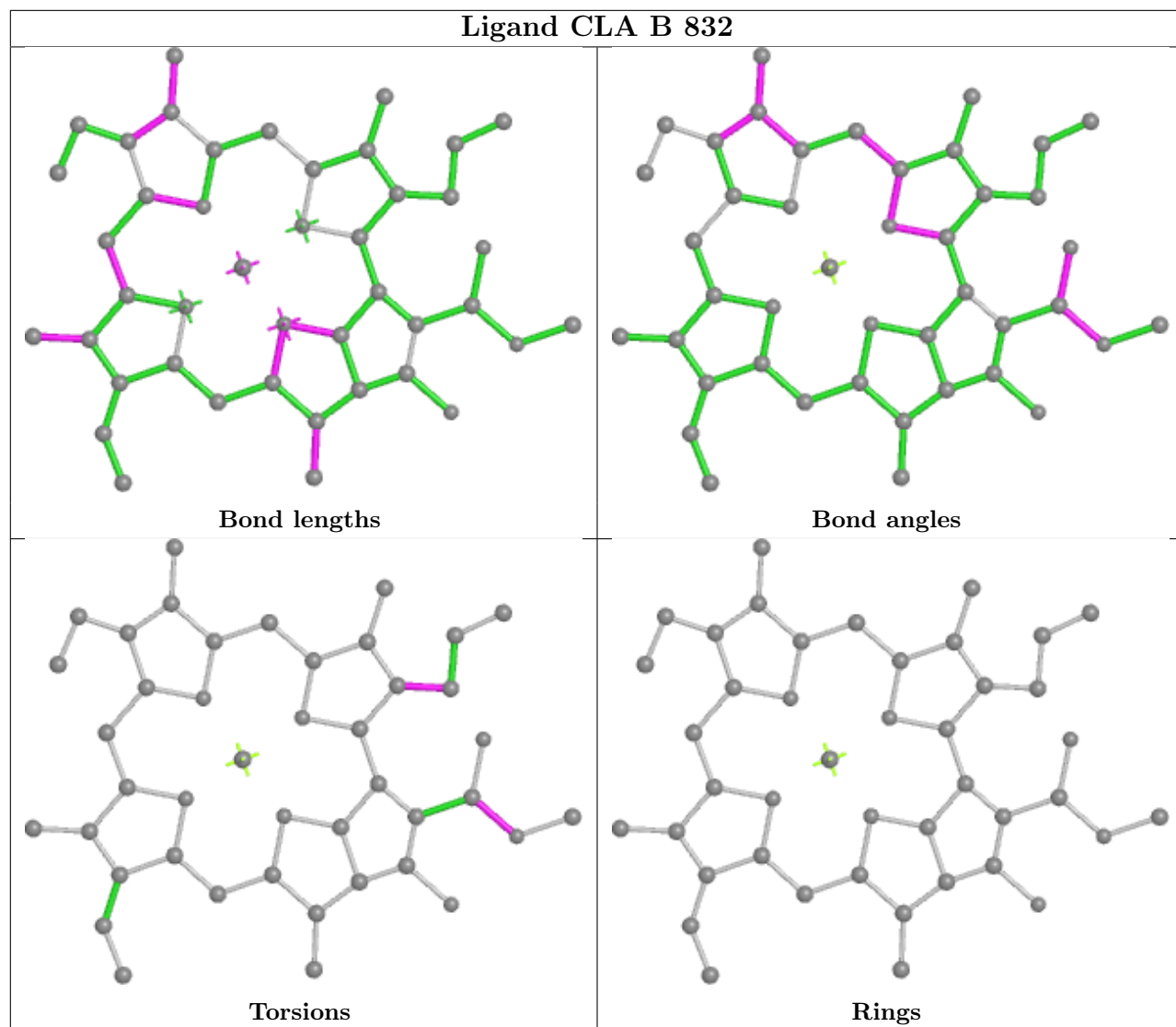


Torsions

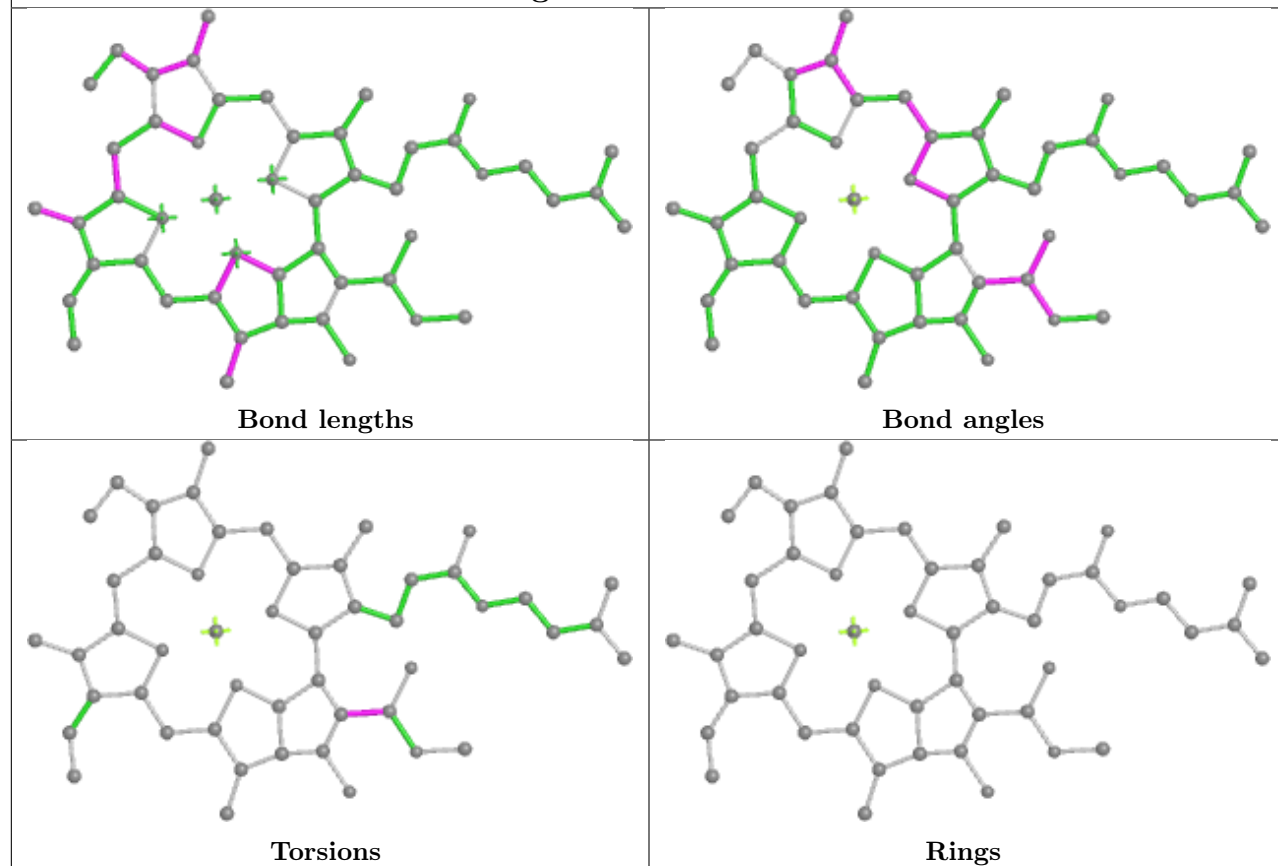


Rings

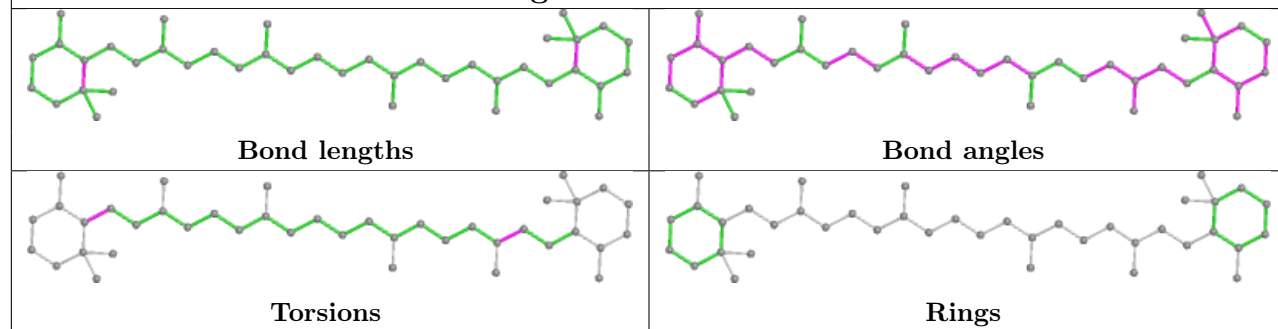
Ligand CLA B 832



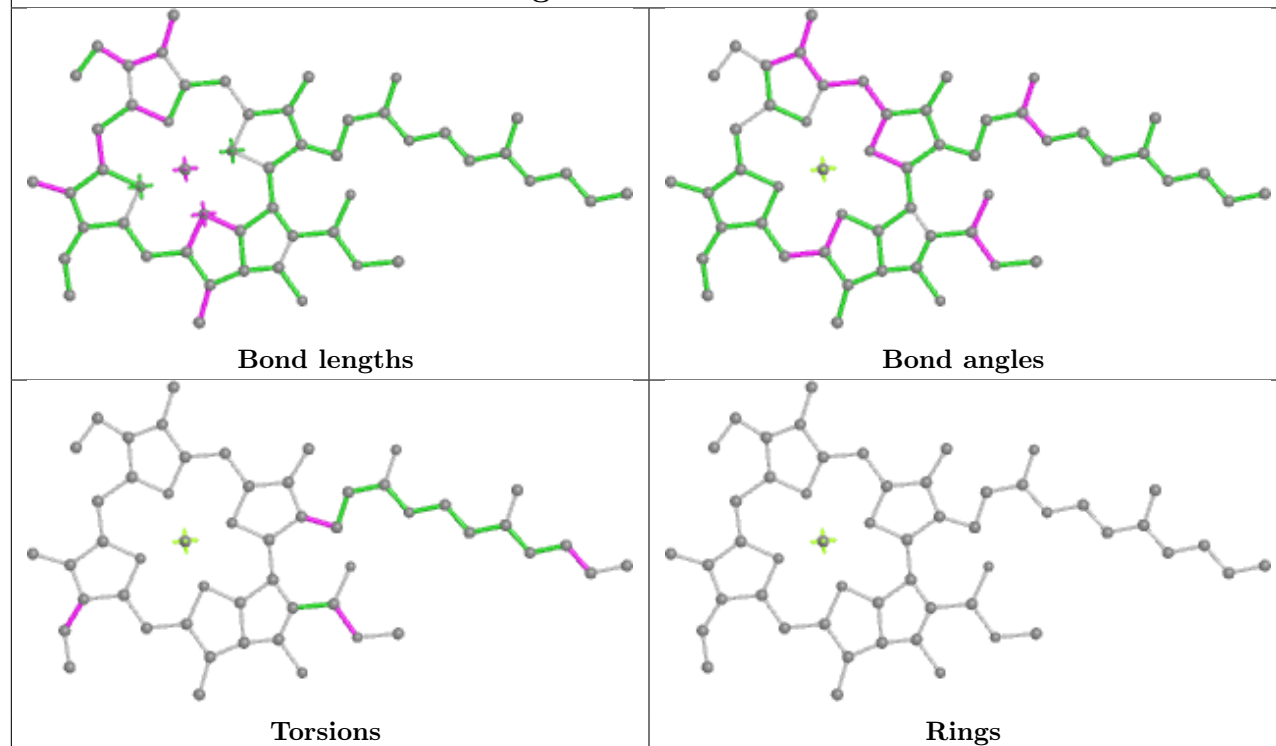
Ligand CLA A 830



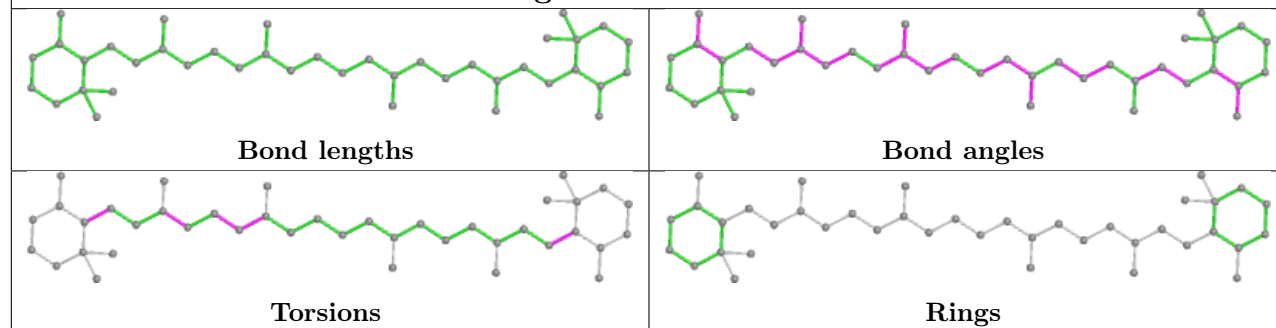
Ligand BCR B 849



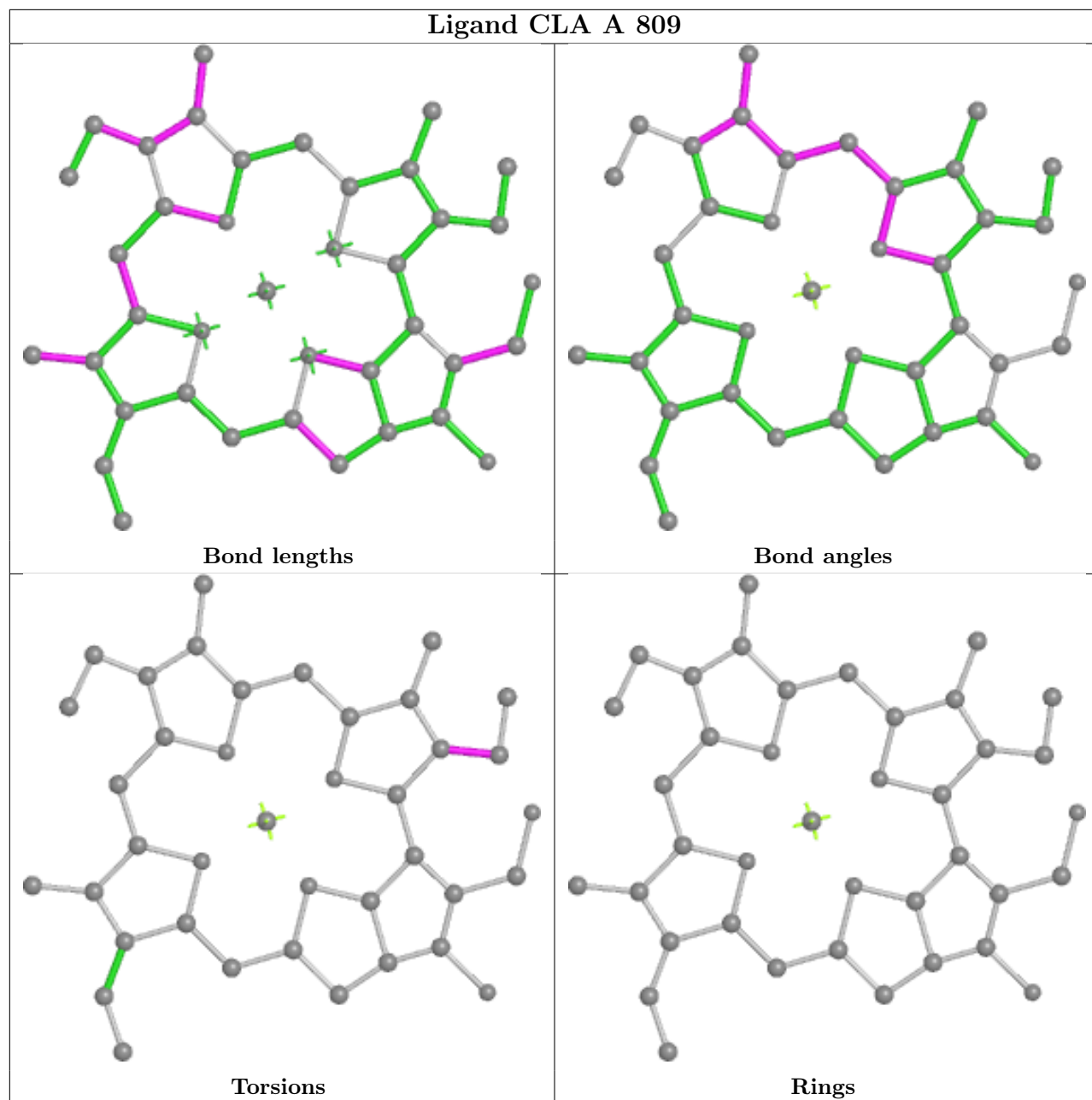
Ligand CLA B 820



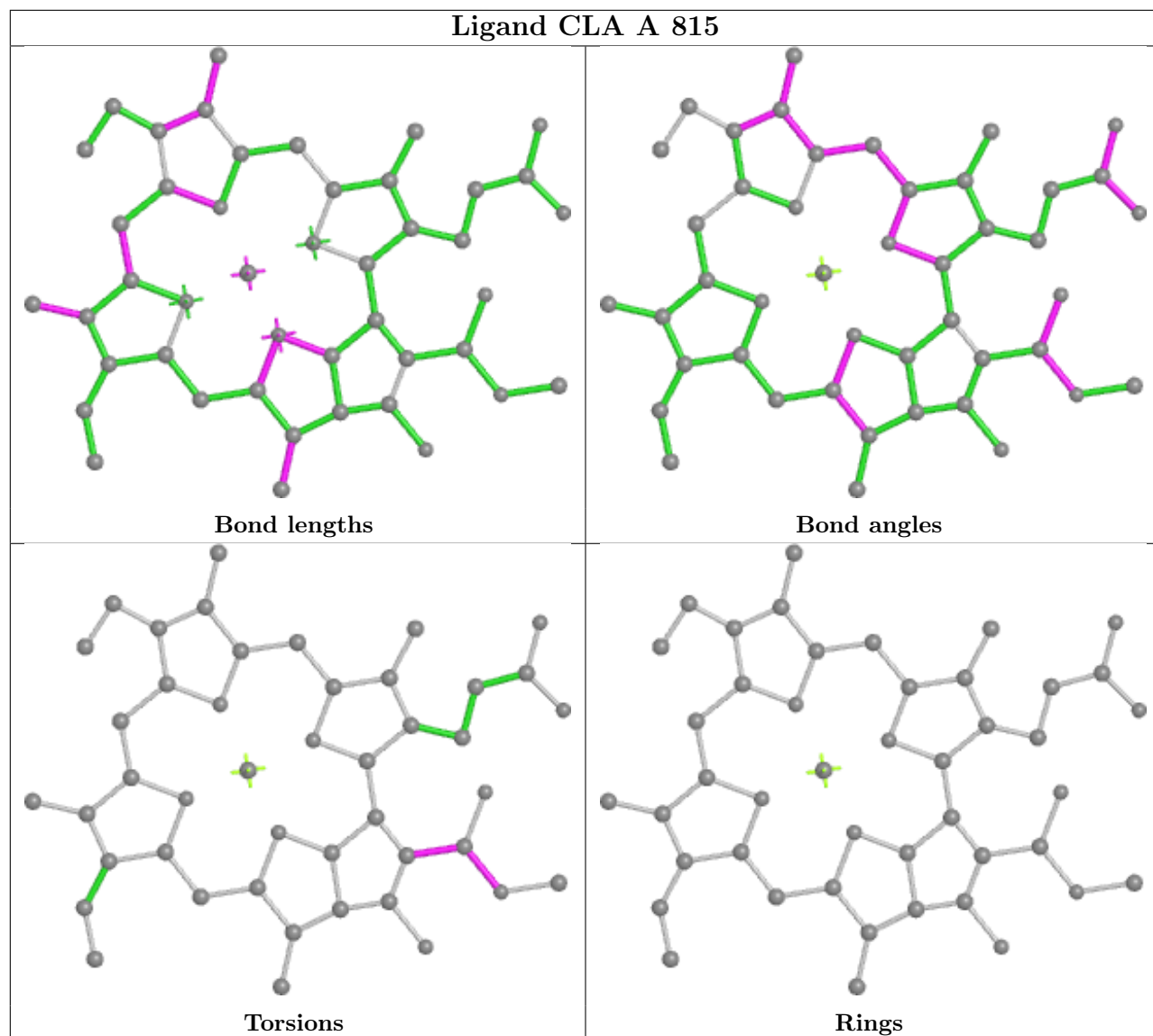
Ligand BCR 5 302



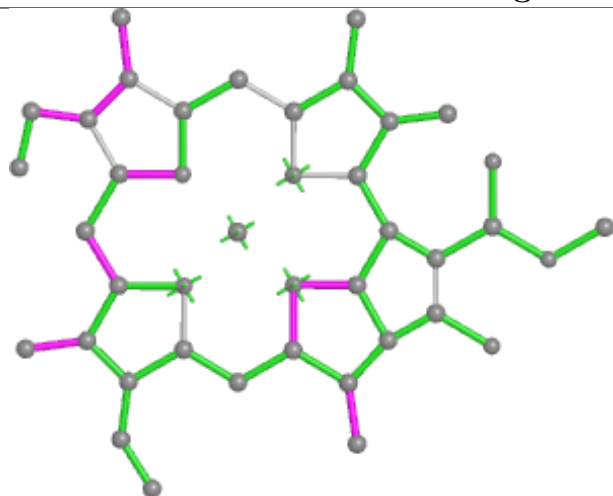
Ligand CLA A 809



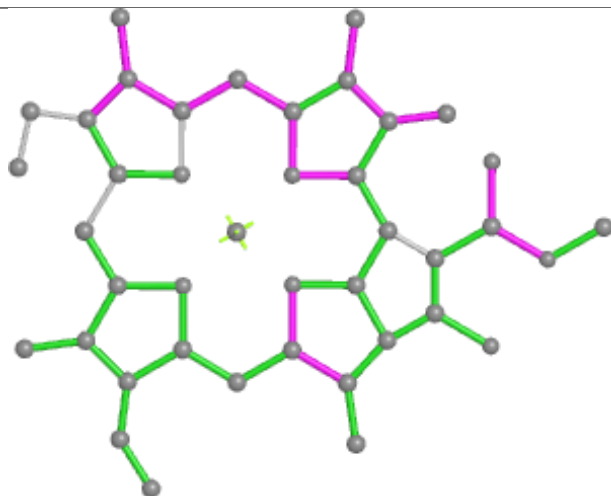
Ligand CLA A 815



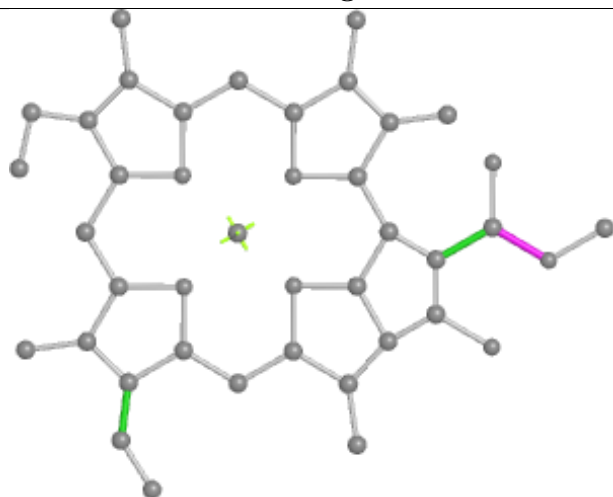
Ligand CLA A 822



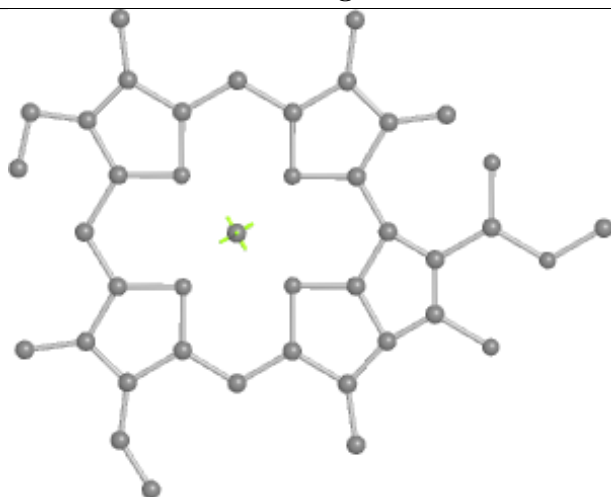
Bond lengths



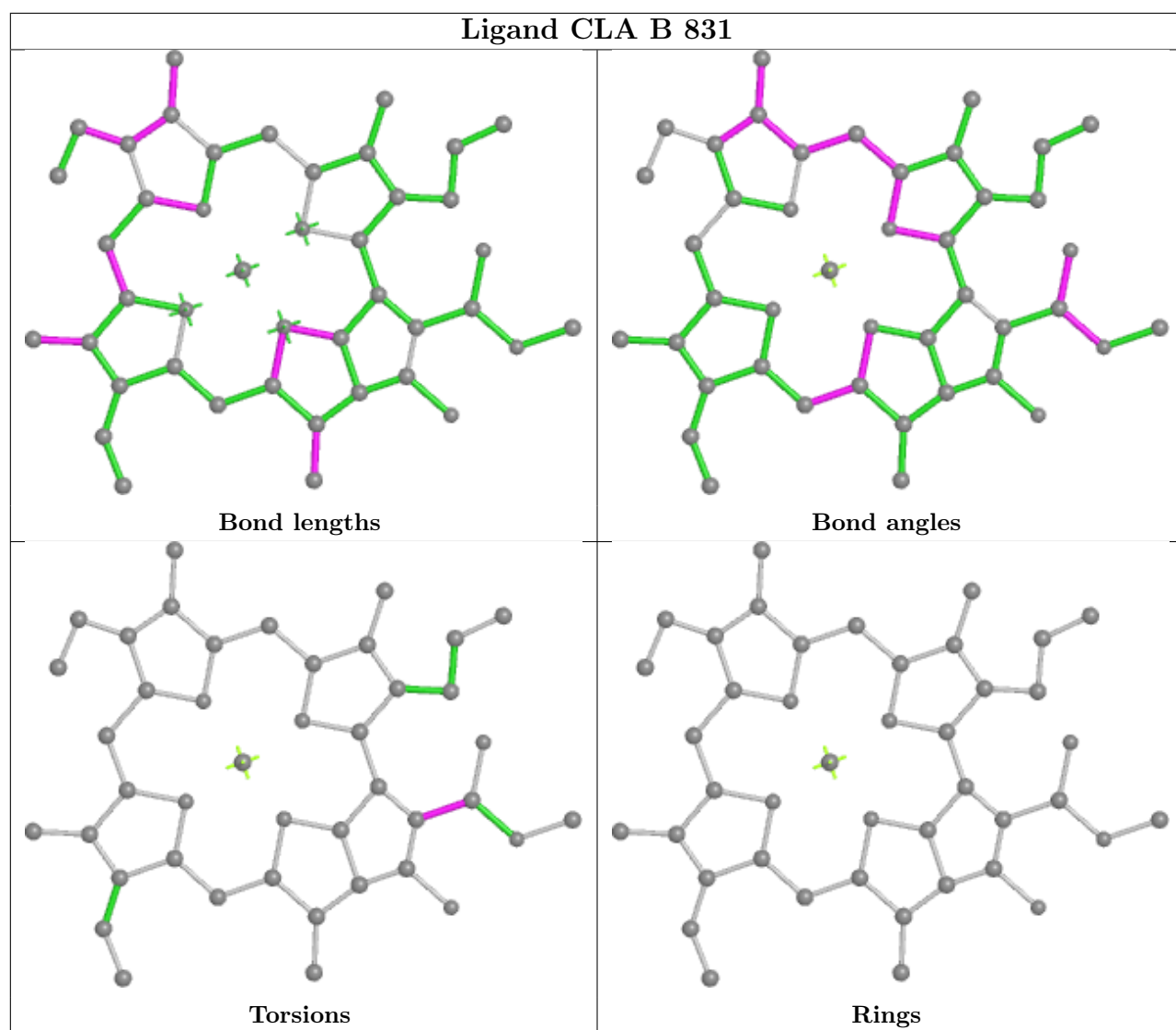
Bond angles

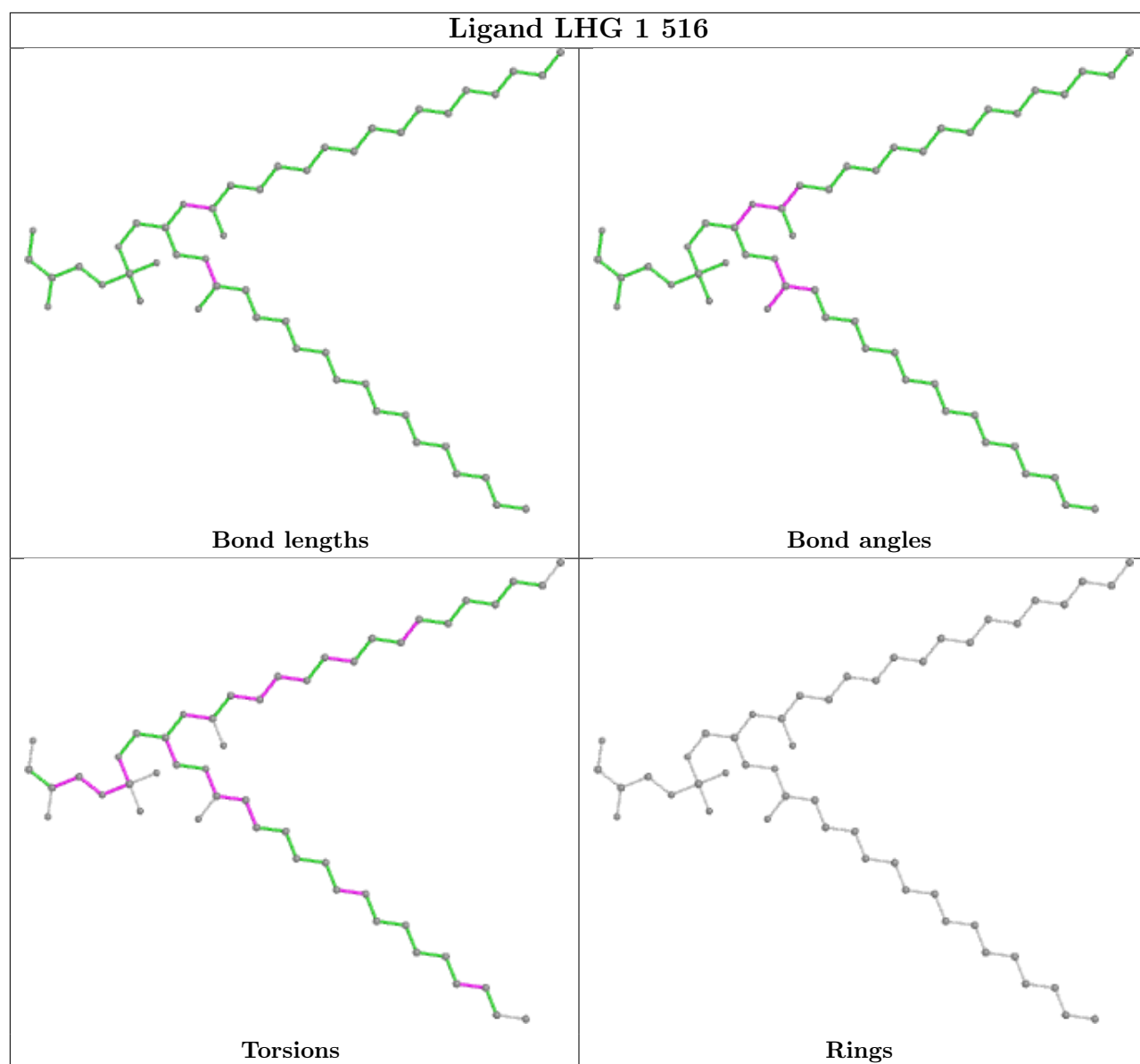


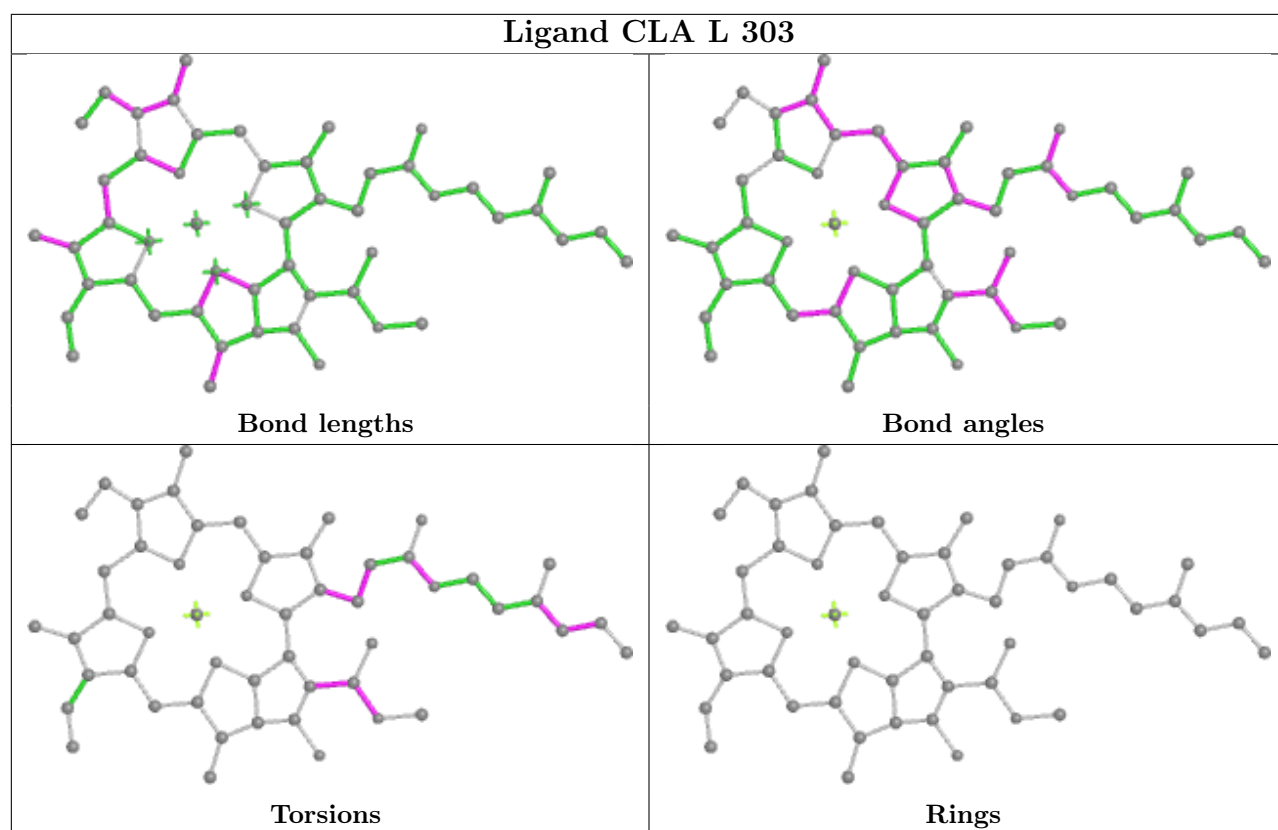
Torsions



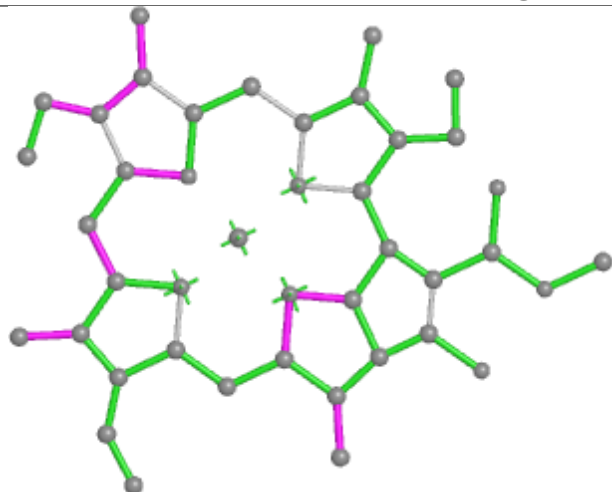
Rings



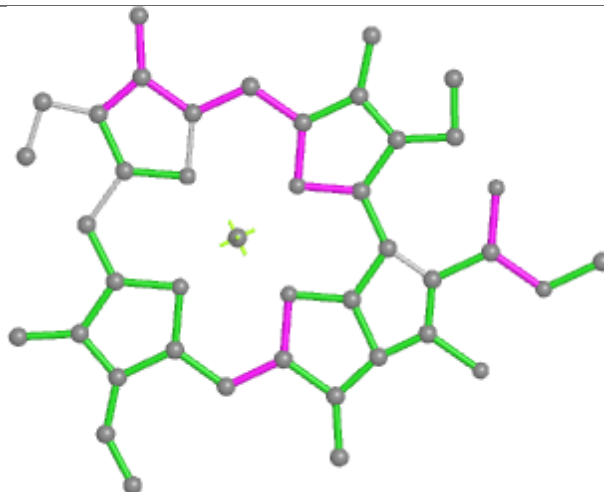




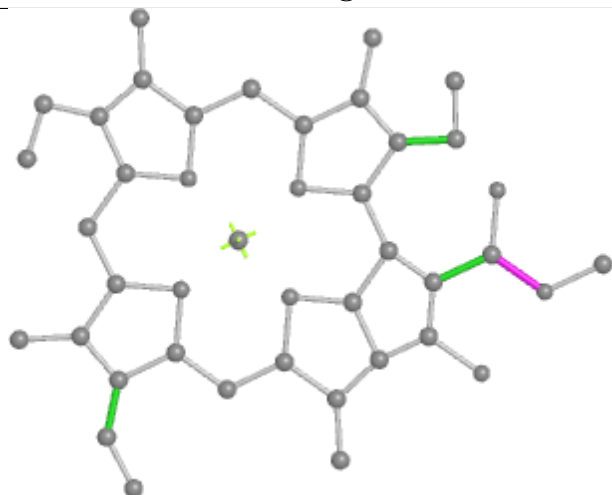
Ligand CLA F 802



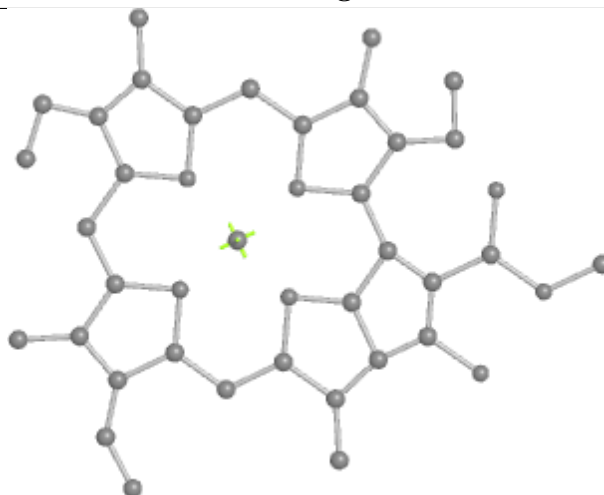
Bond lengths



Bond angles

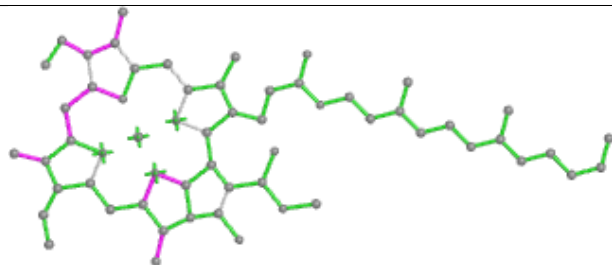


Torsions

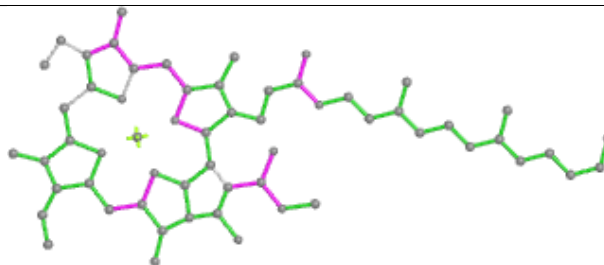


Rings

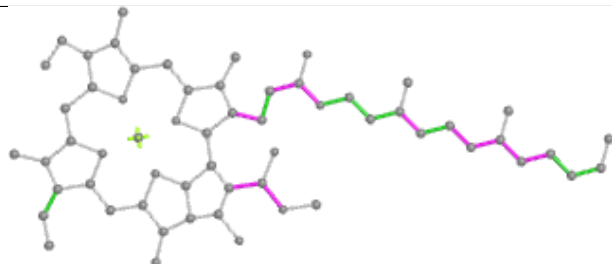
Ligand CLA B 818



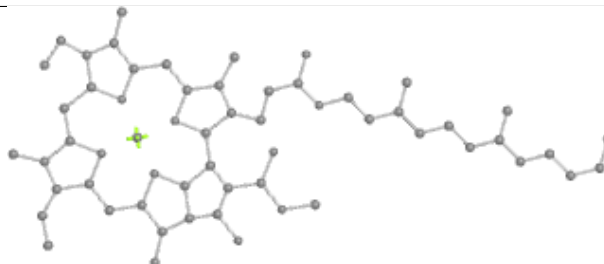
Bond lengths



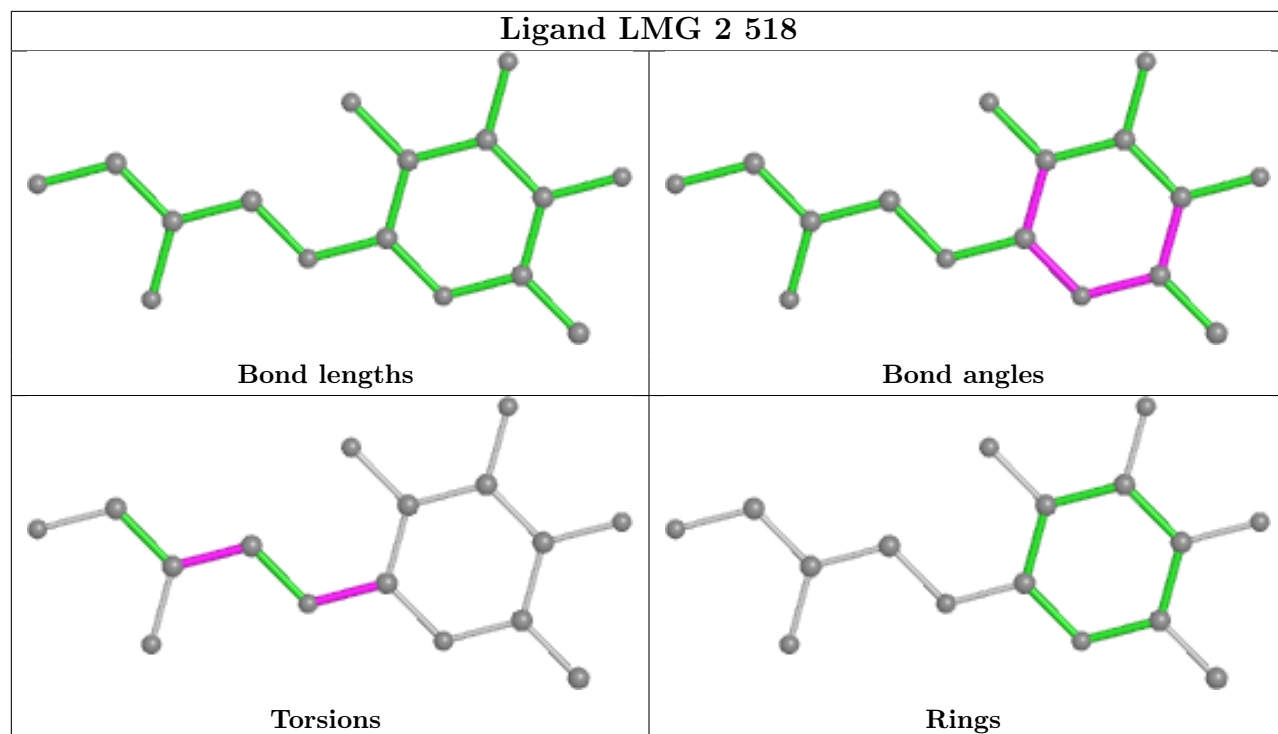
Bond angles



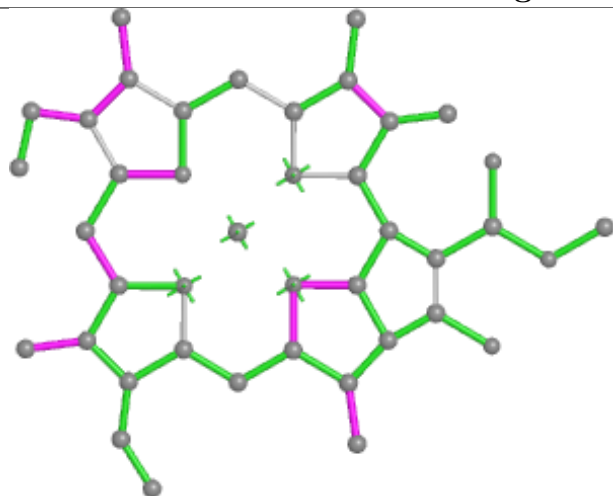
Torsions



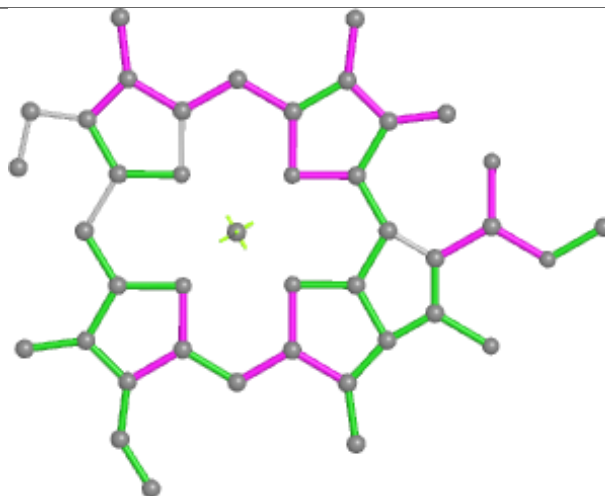
Rings



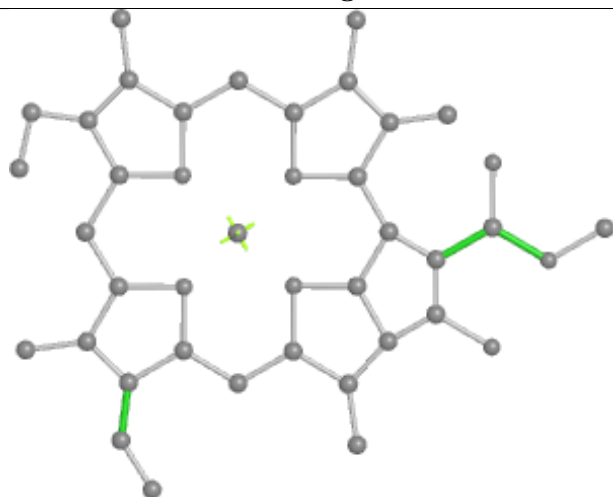
Ligand CLA B 819



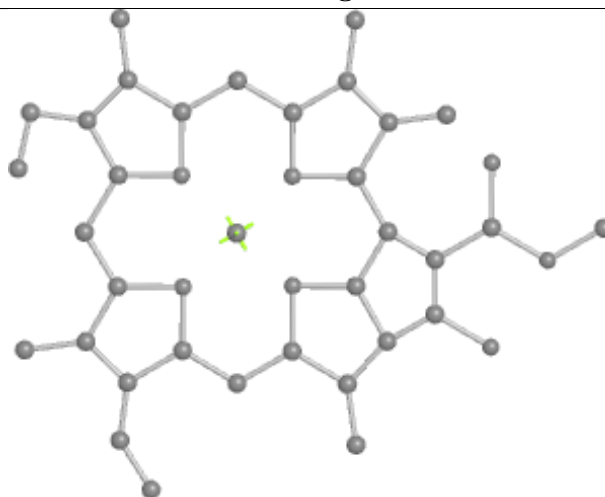
Bond lengths



Bond angles

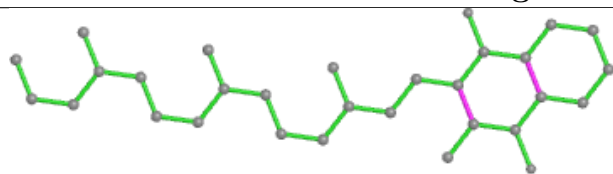


Torsions

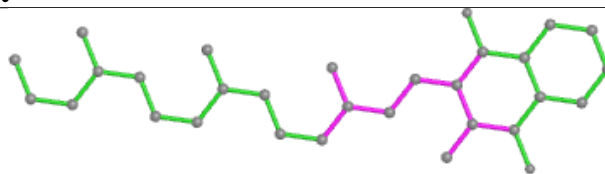


Rings

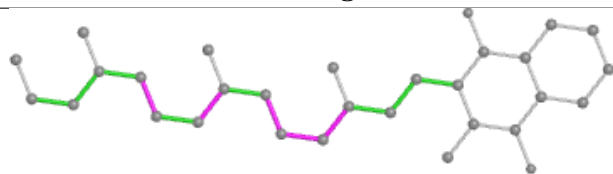
Ligand PQN B 843



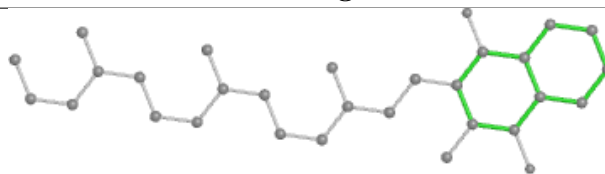
Bond lengths



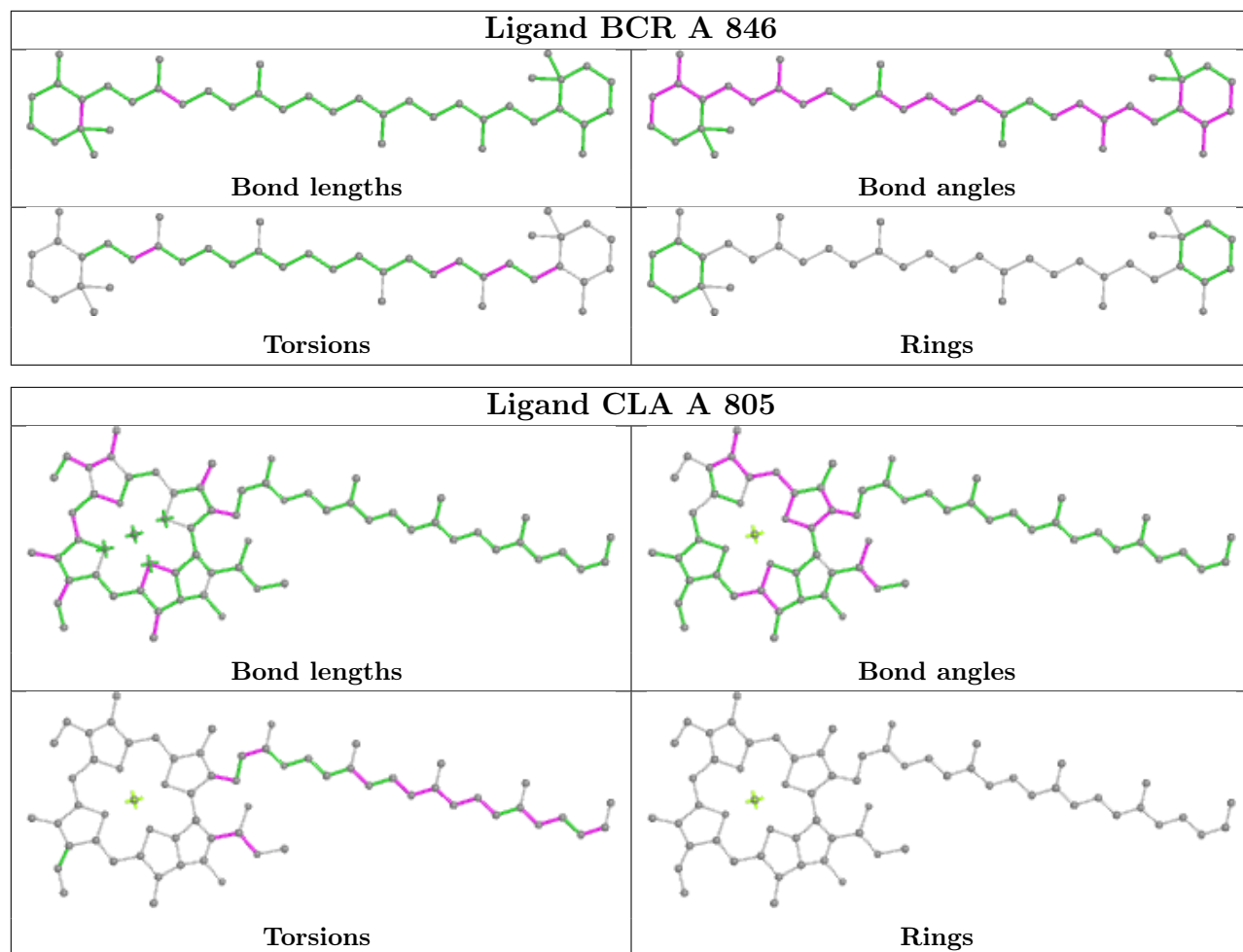
Bond angles



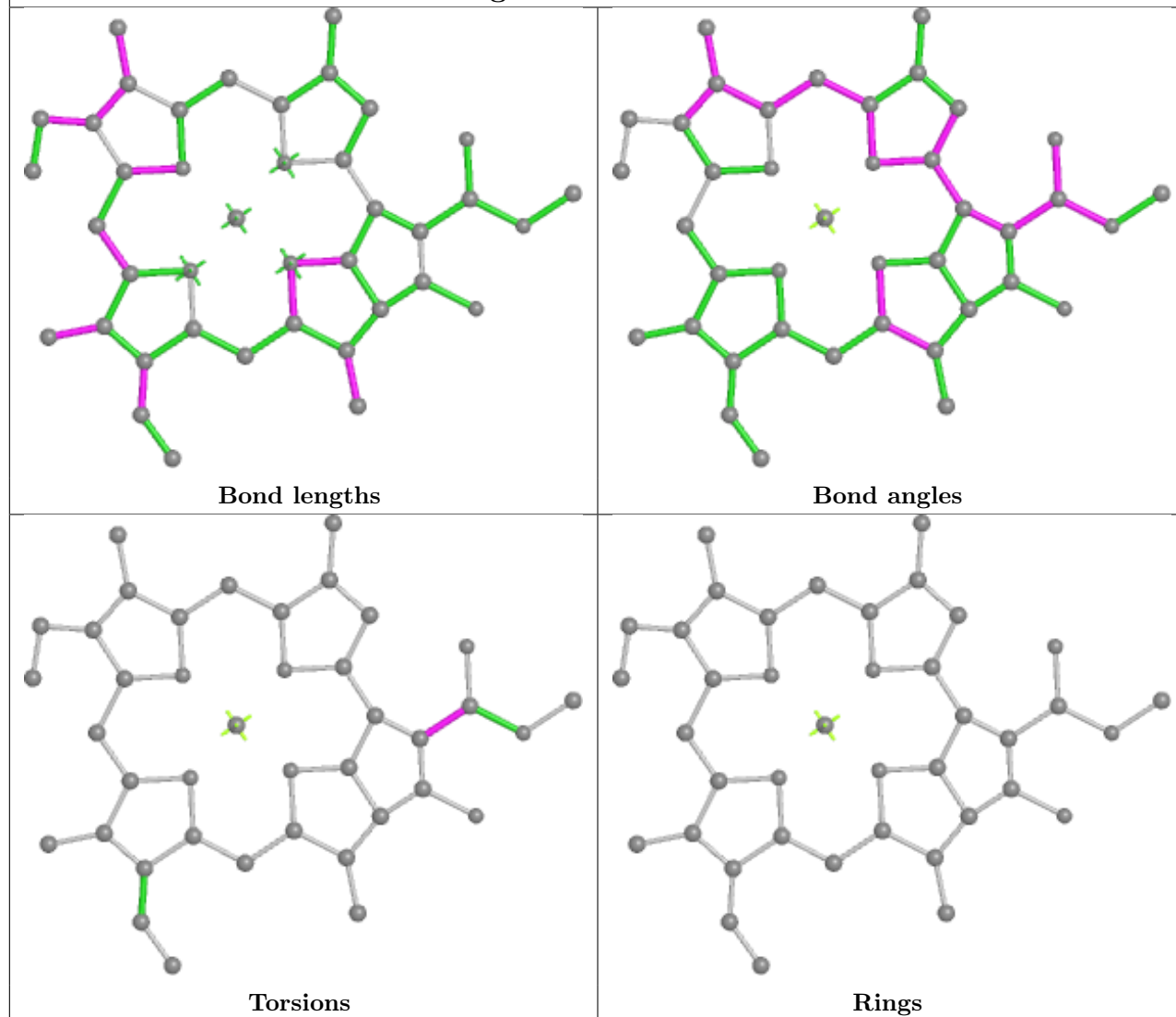
Torsions



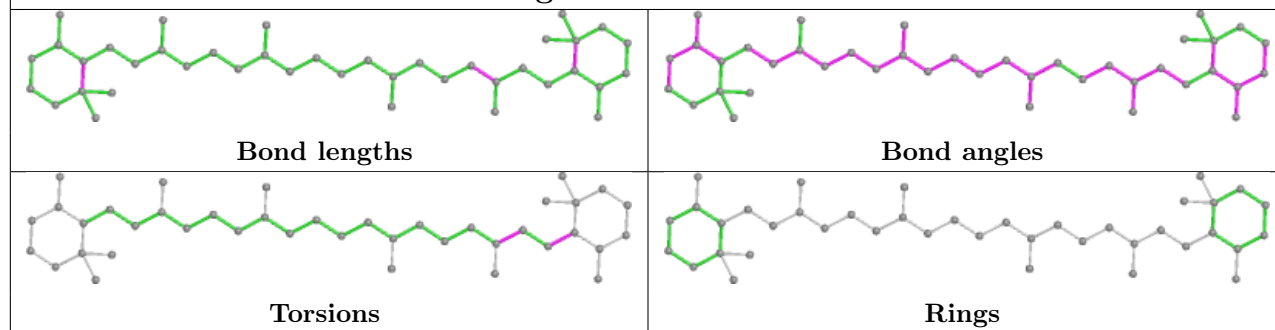
Rings

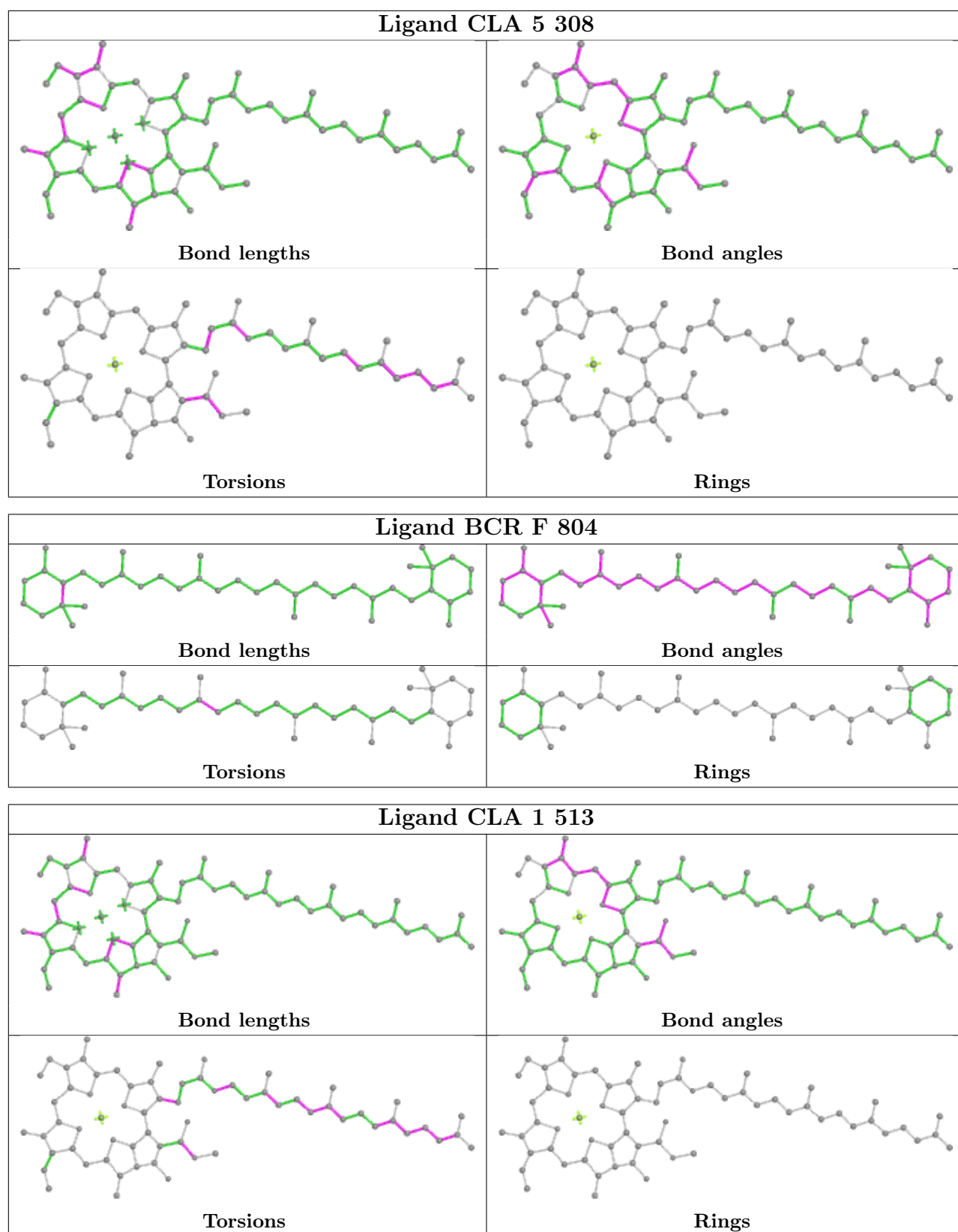


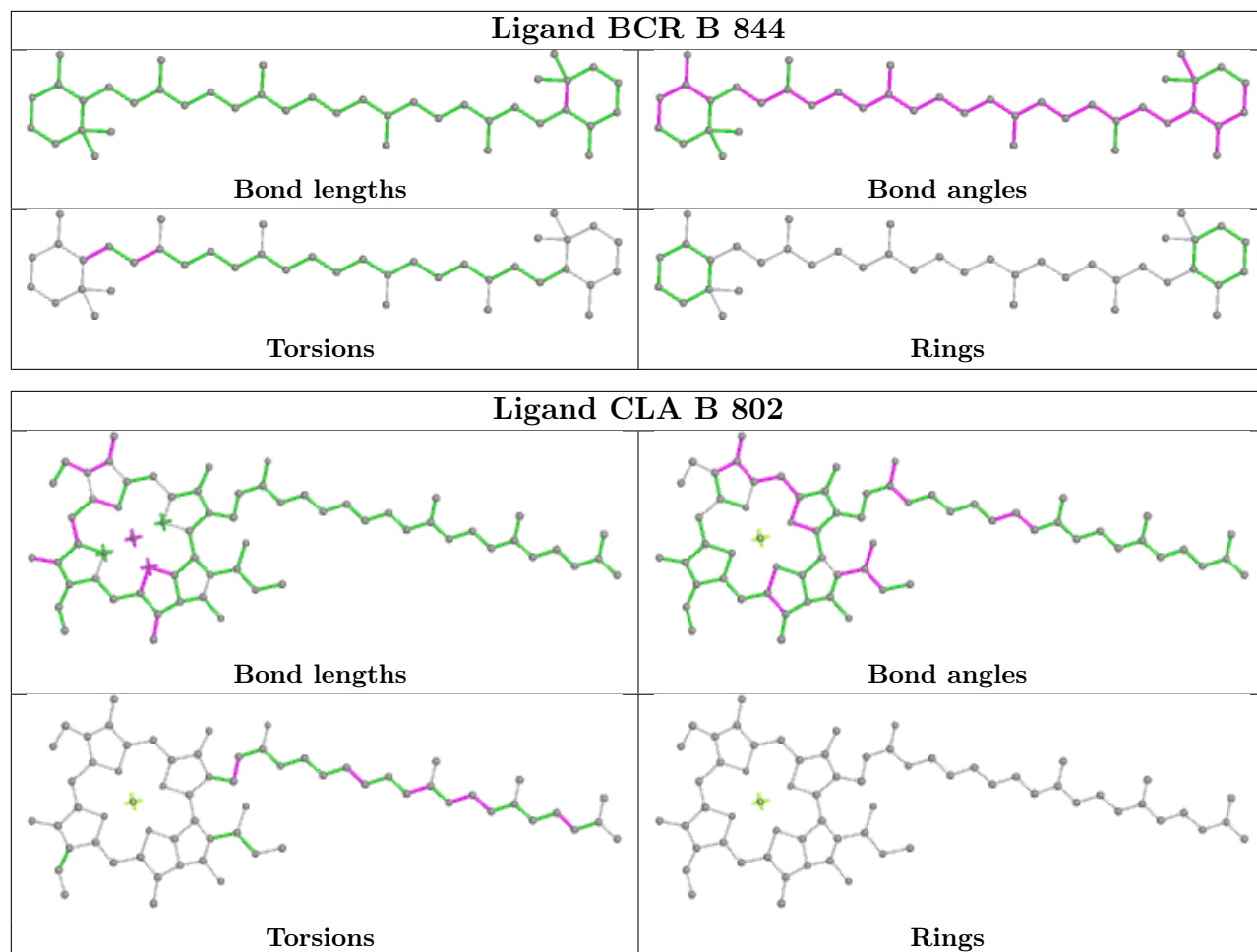
Ligand CLA B 810



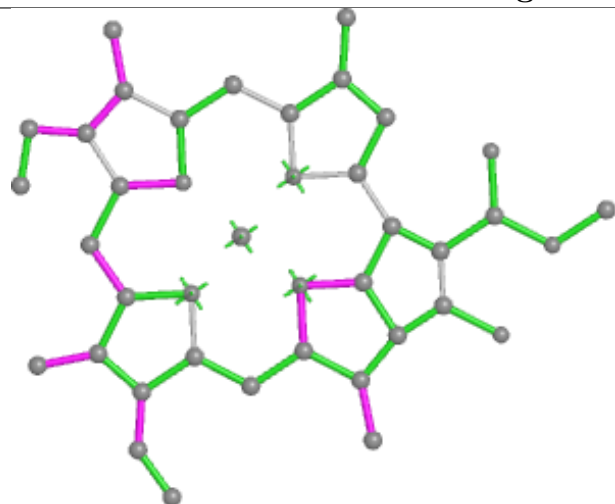
Ligand BCR I 101



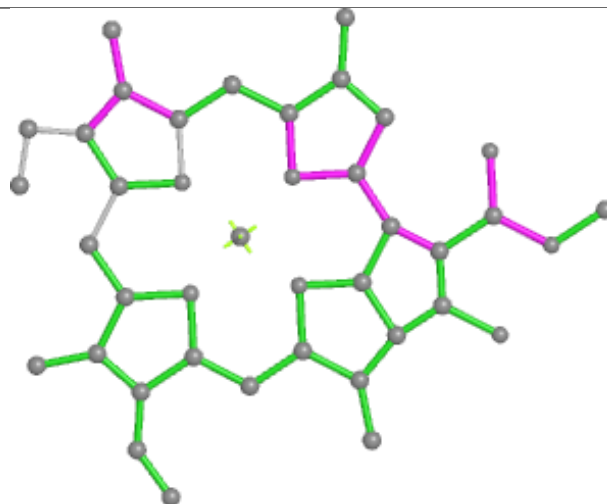




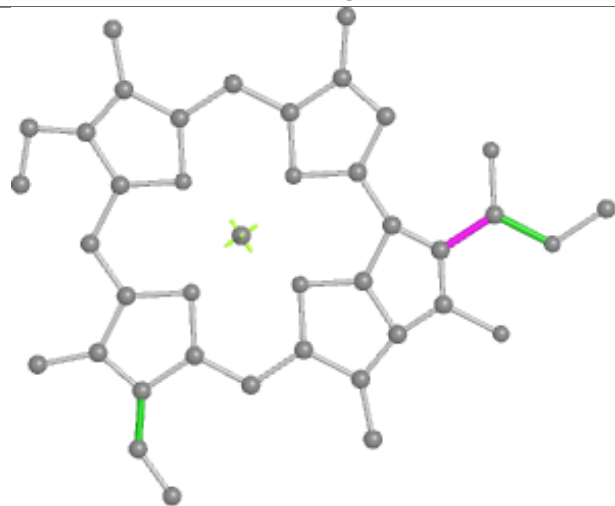
Ligand CLA B 809



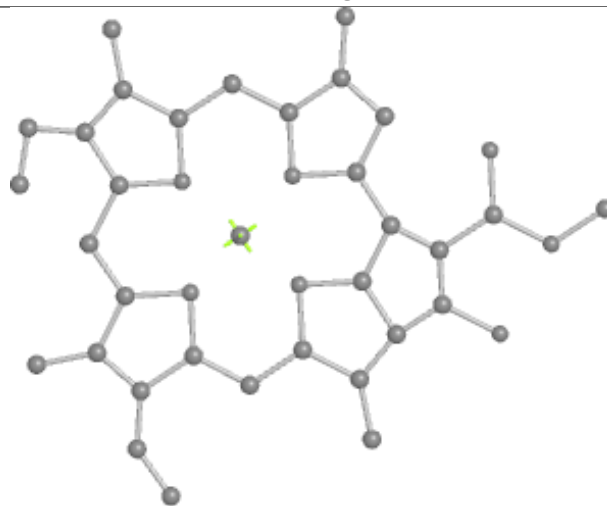
Bond lengths



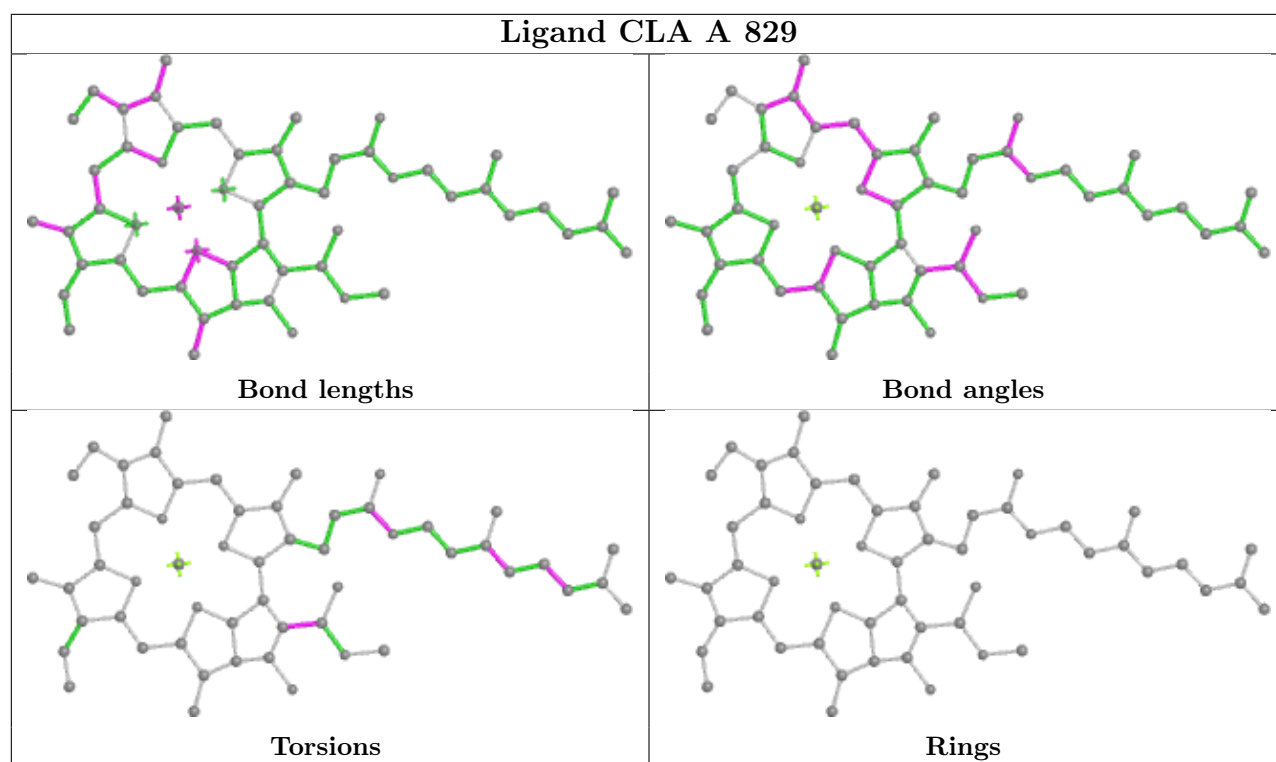
Bond angles



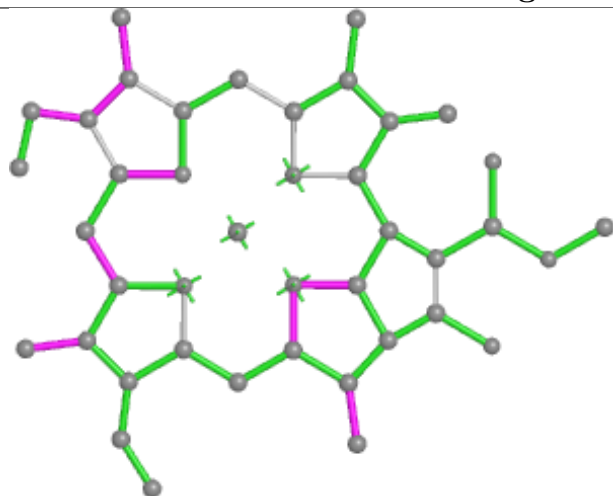
Torsions



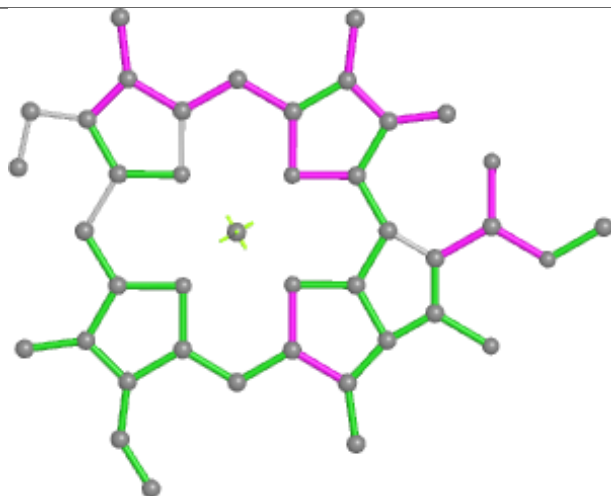
Rings



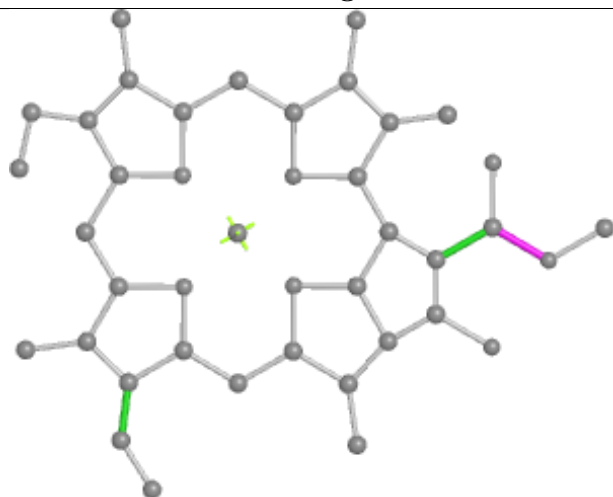
Ligand CLA 3 301



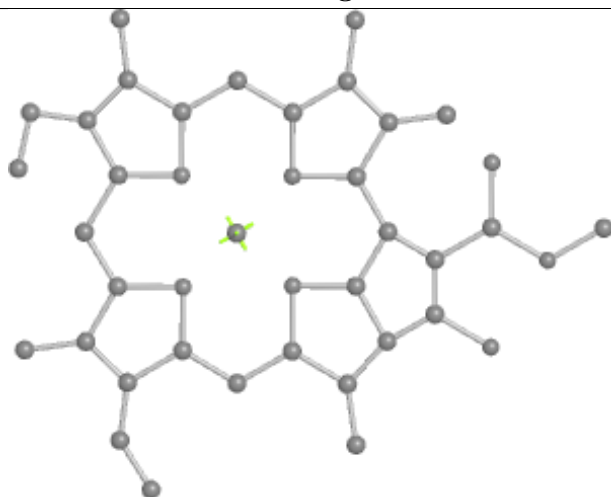
Bond lengths



Bond angles

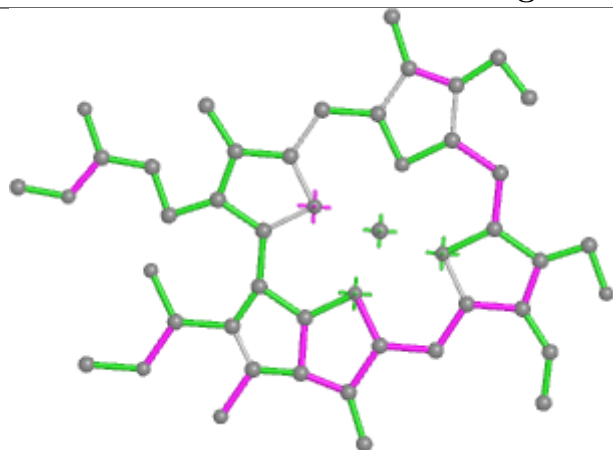


Torsions

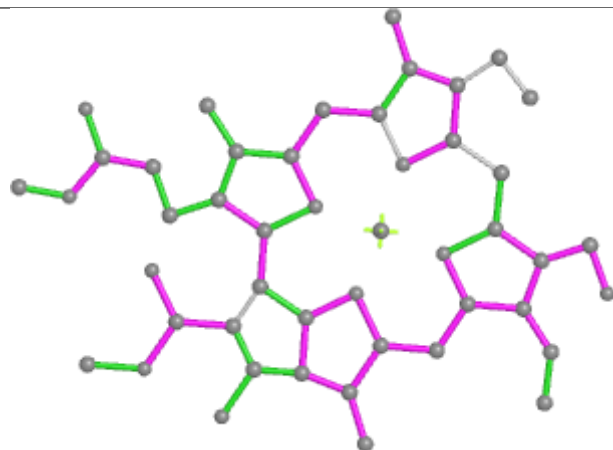


Rings

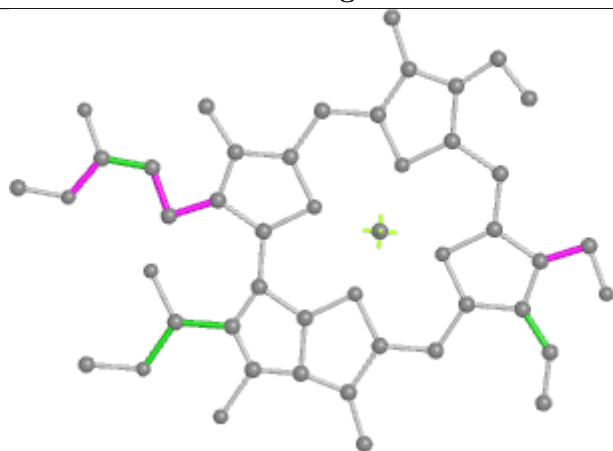
Ligand CHL 5 314



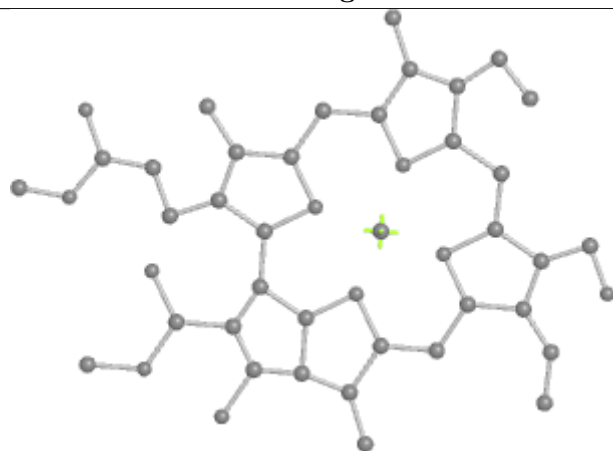
Bond lengths



Bond angles

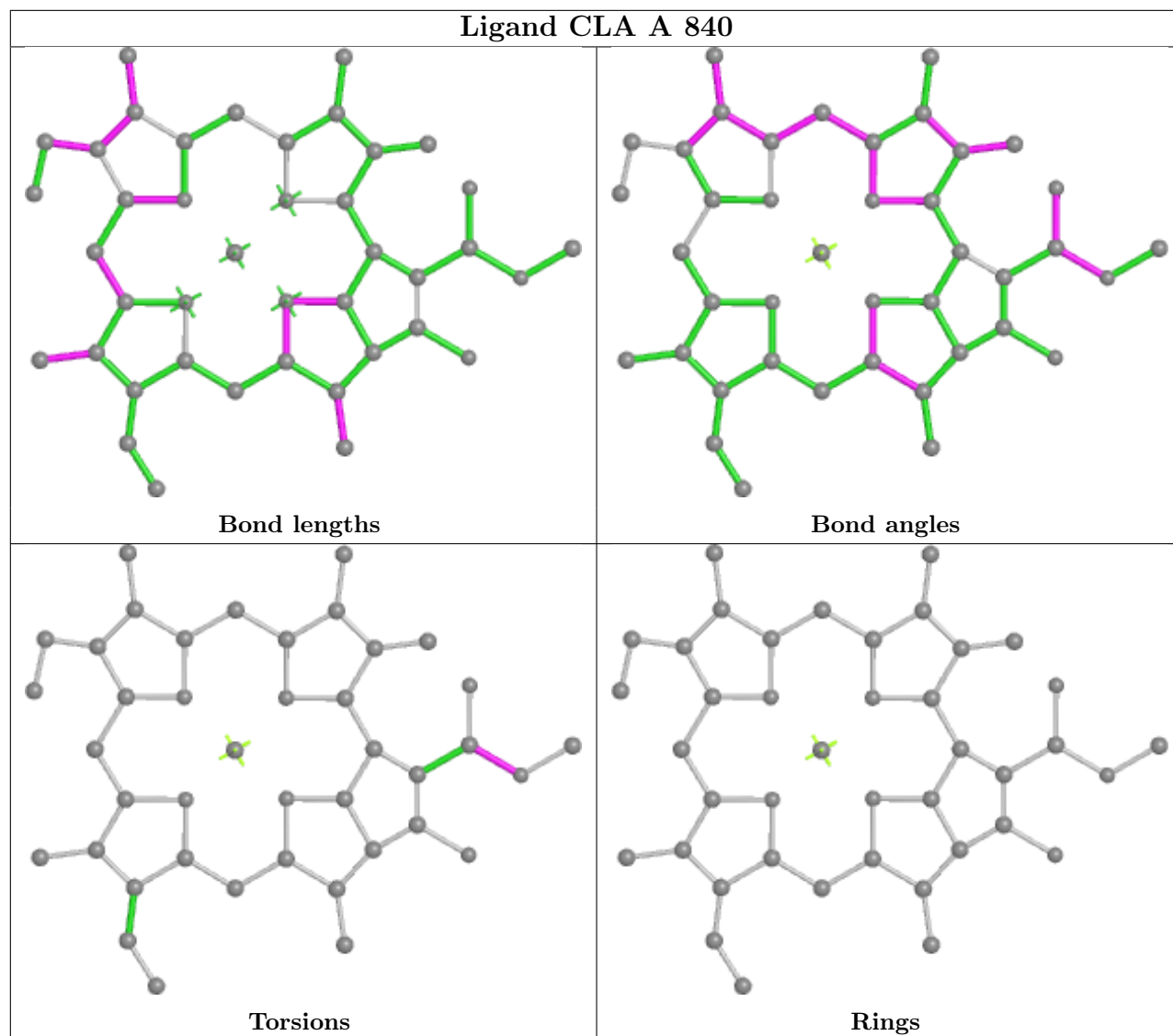


Torsions

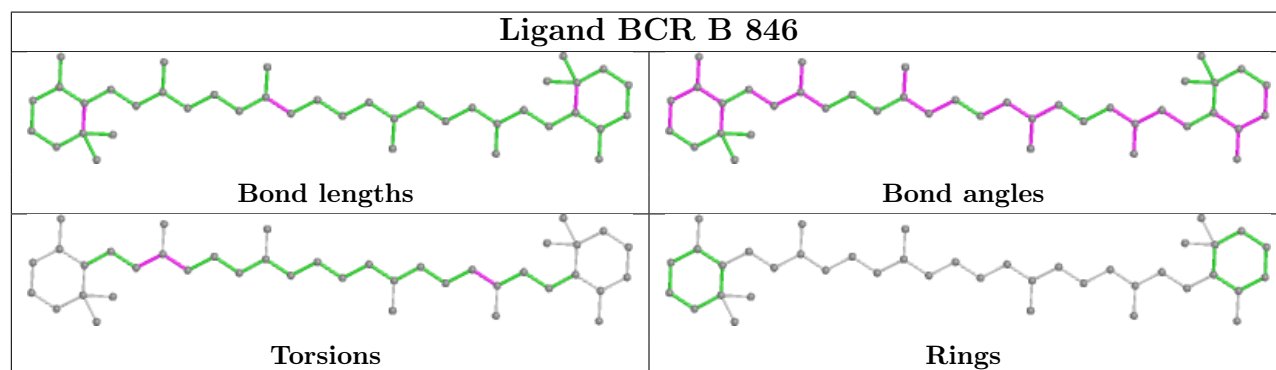


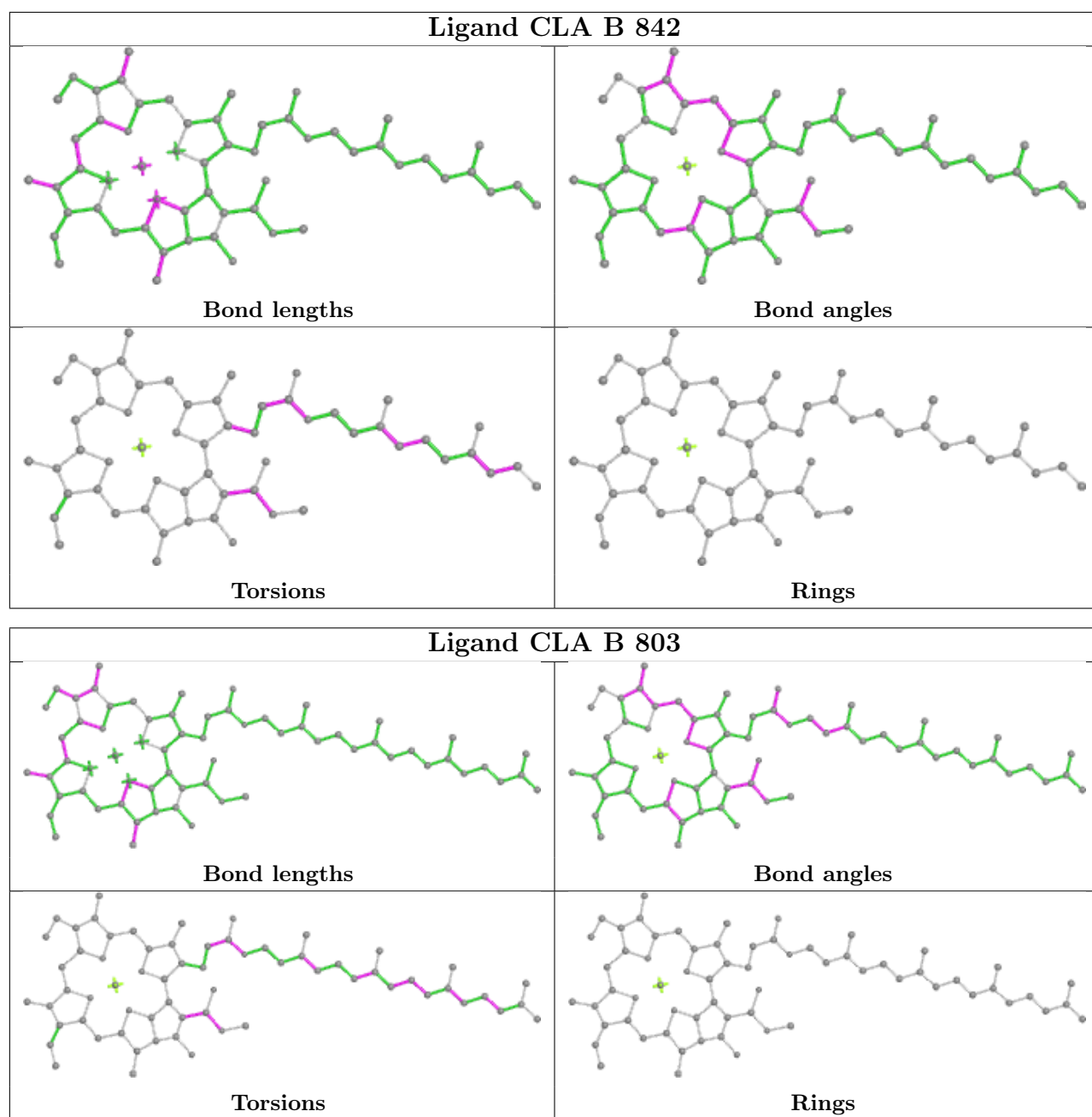
Rings

Ligand CLA A 840

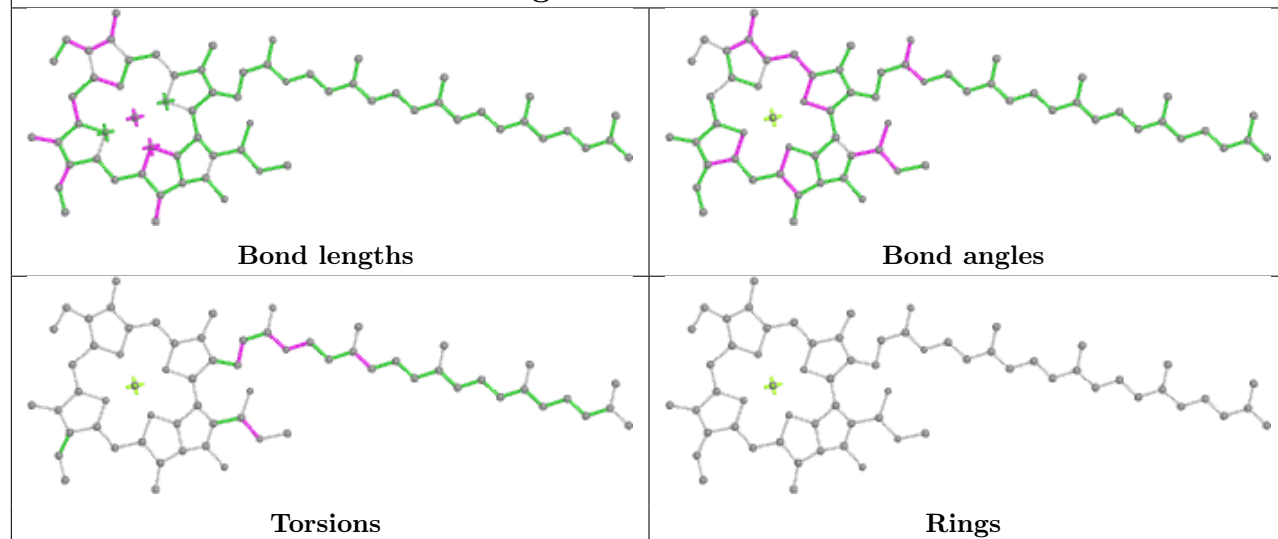


Ligand BCR B 846

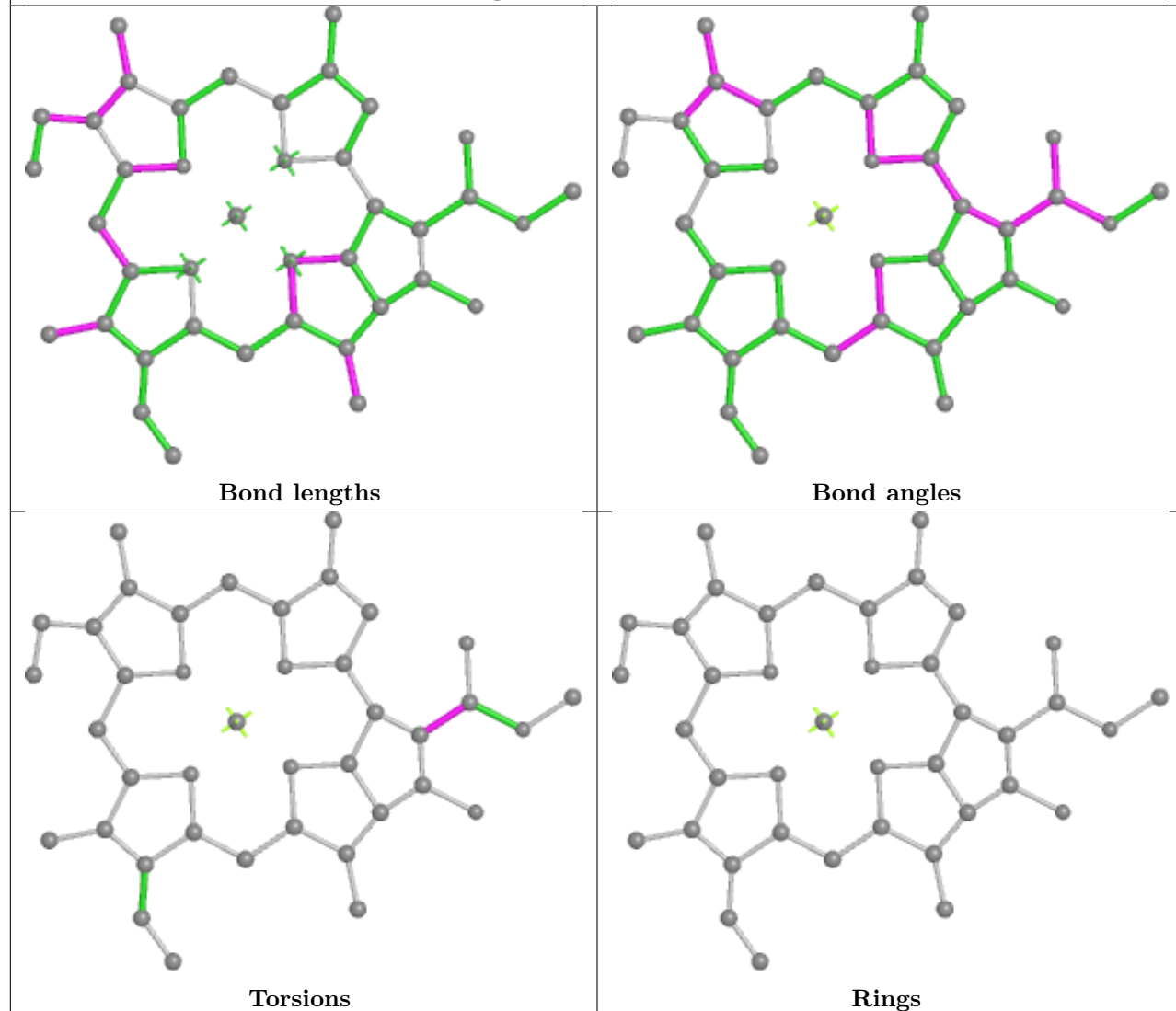




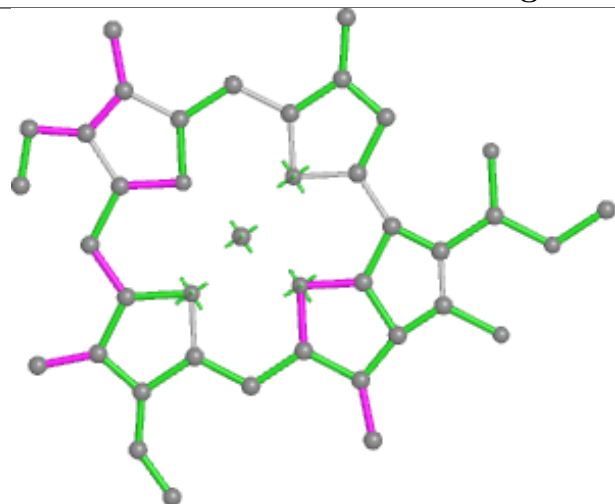
Ligand CLA B 815



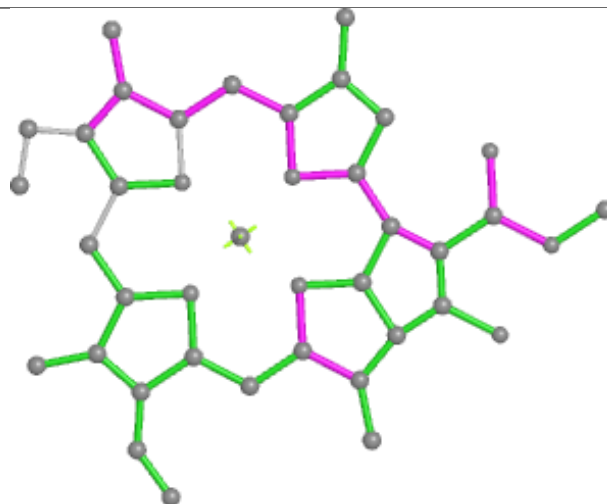
Ligand CLA A 819



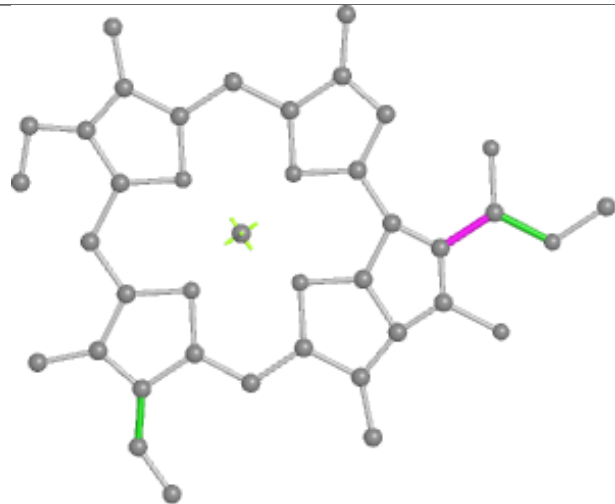
Ligand CLA 5 313



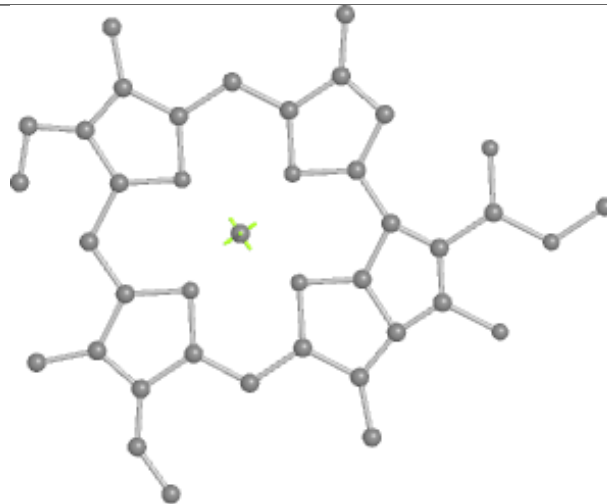
Bond lengths



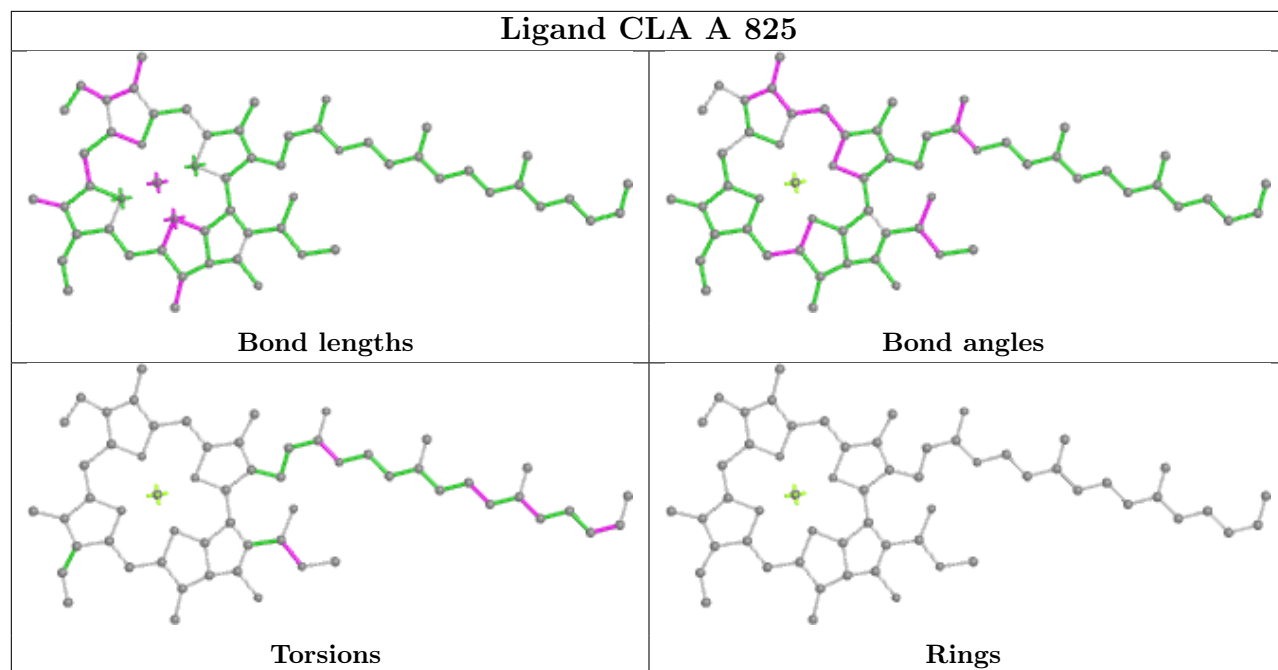
Bond angles



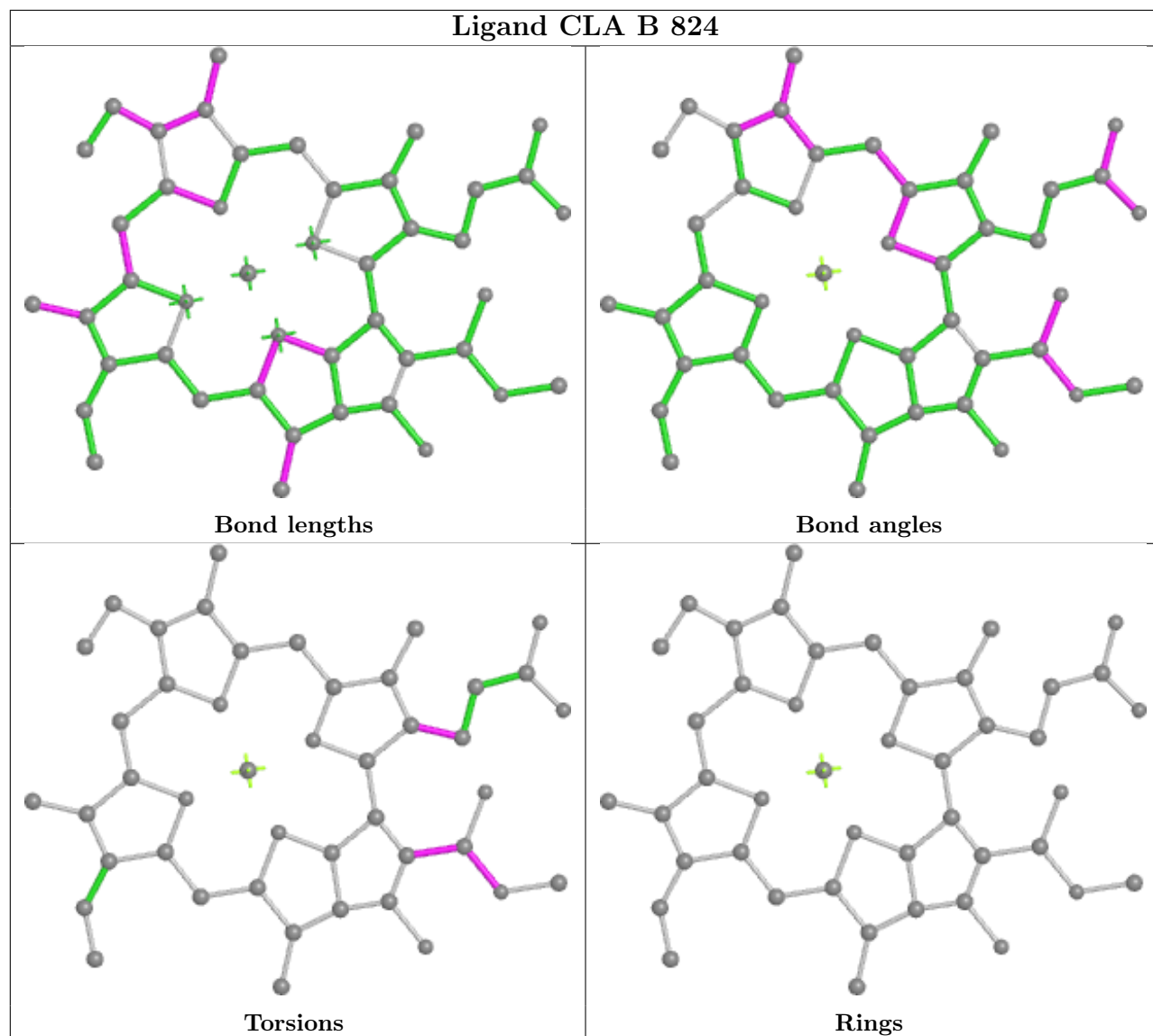
Torsions



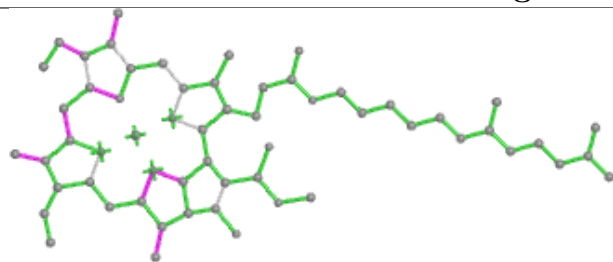
Rings



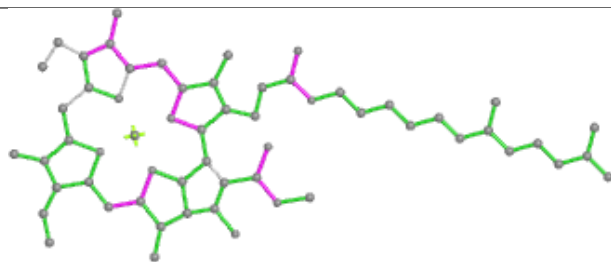
Ligand CLA B 824



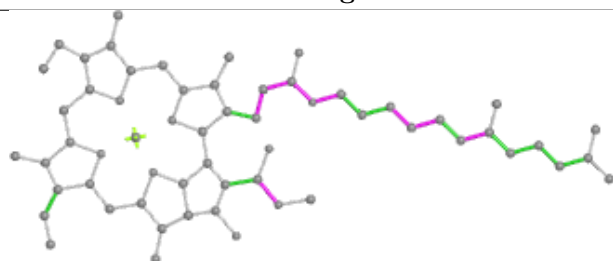
Ligand CLA A 816



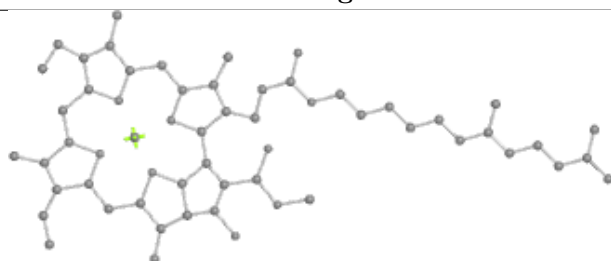
Bond lengths



Bond angles

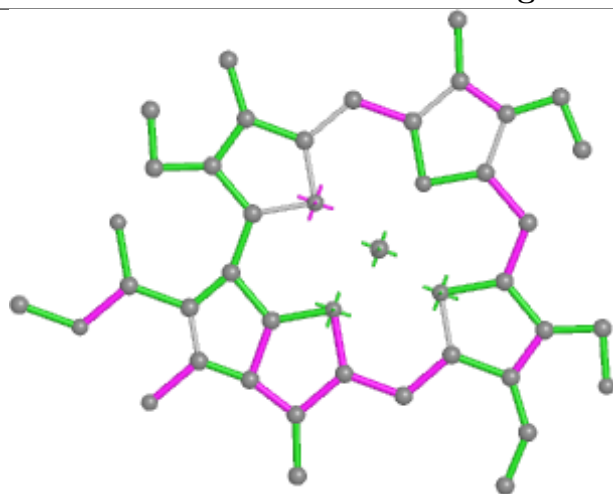


Torsions

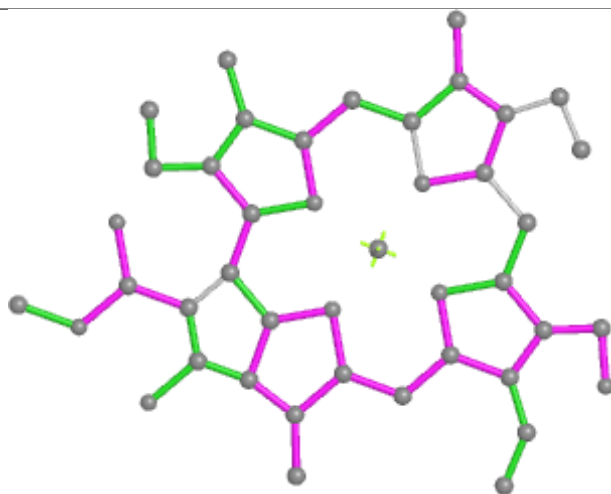


Rings

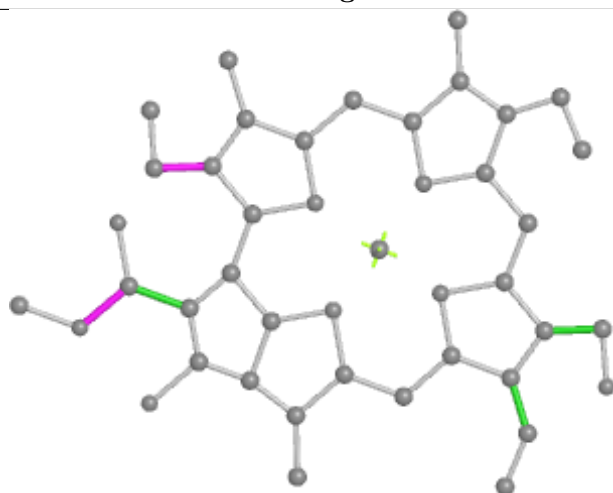
Ligand CHL 3 315



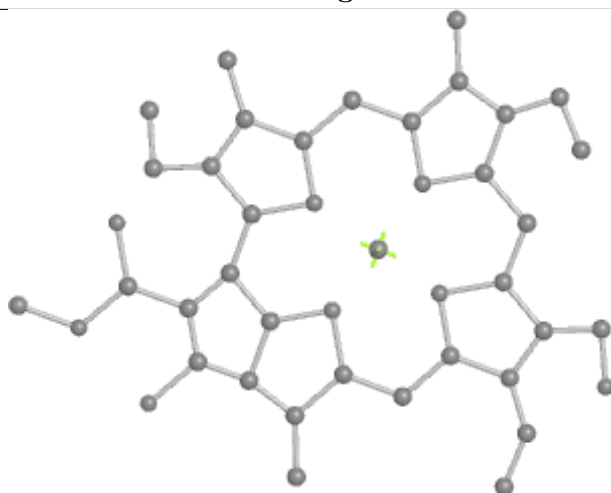
Bond lengths



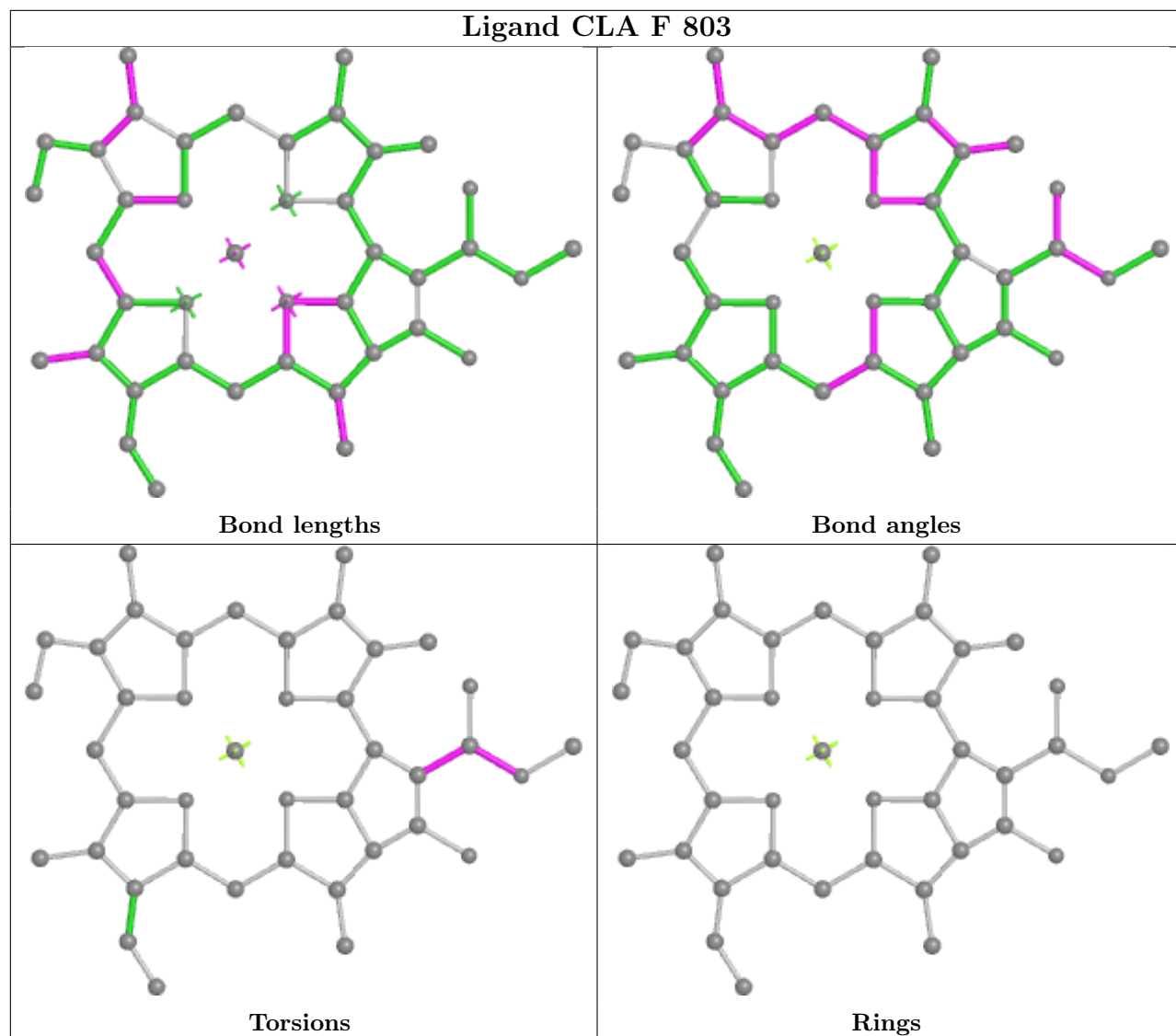
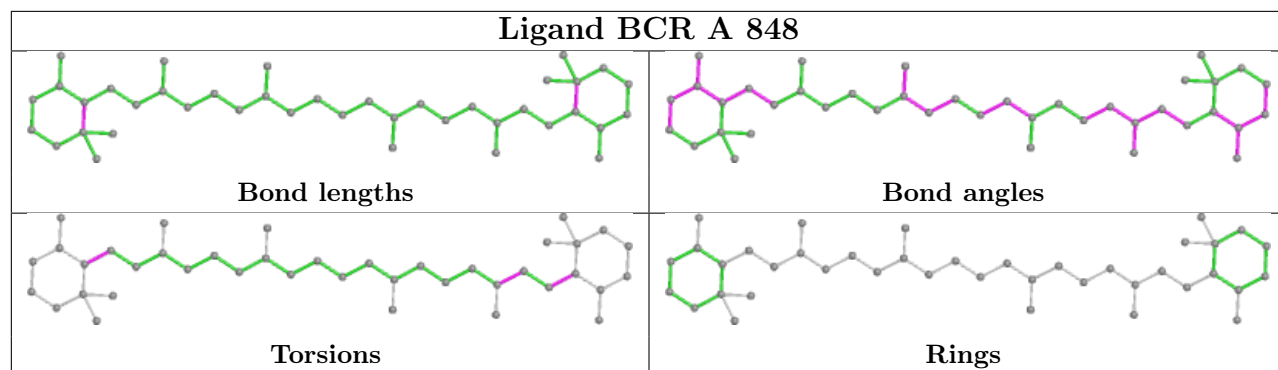
Bond angles

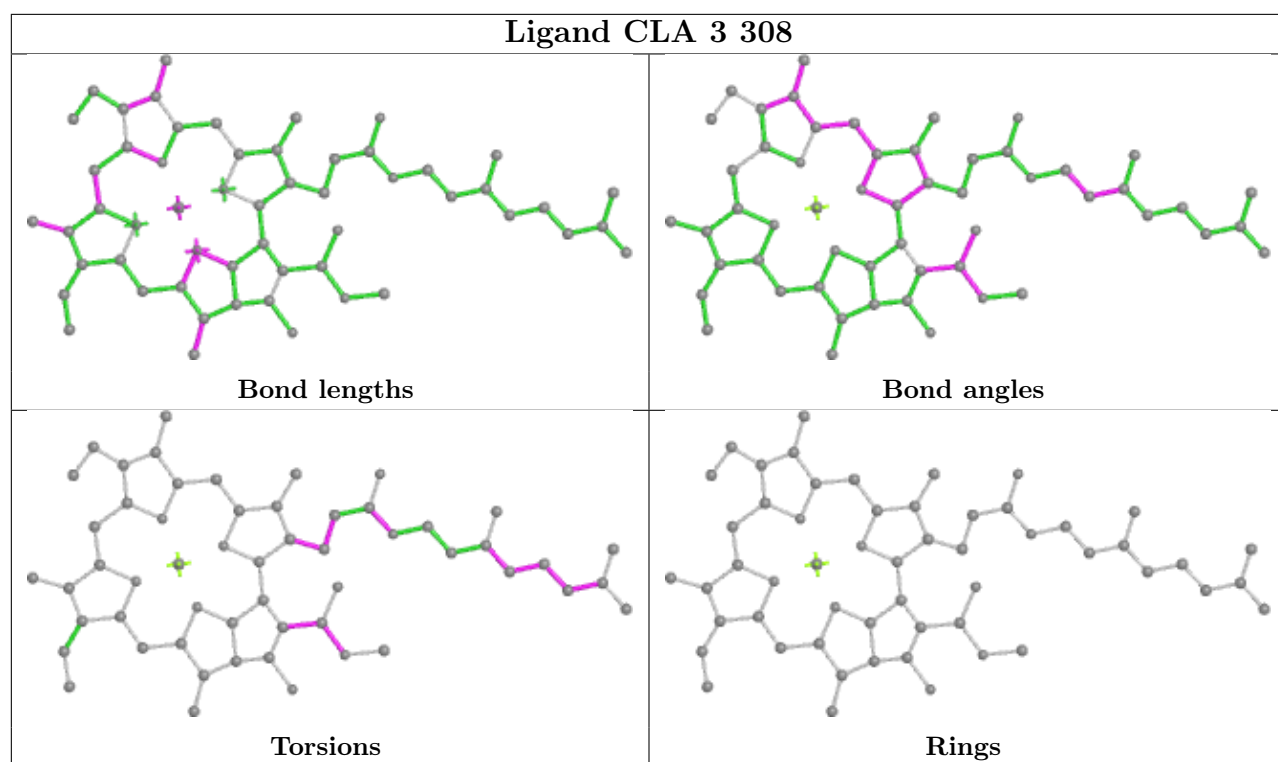


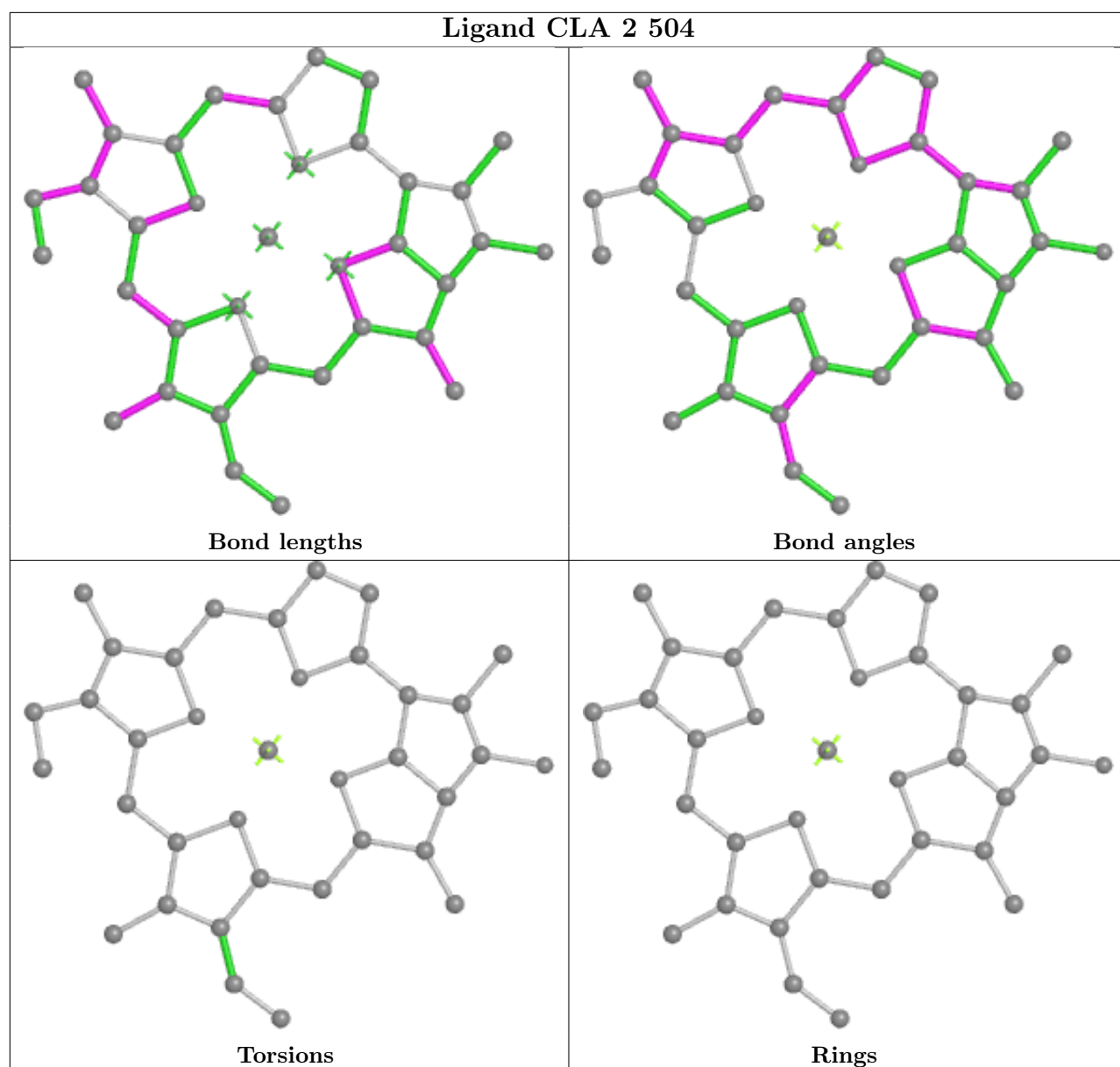
Torsions

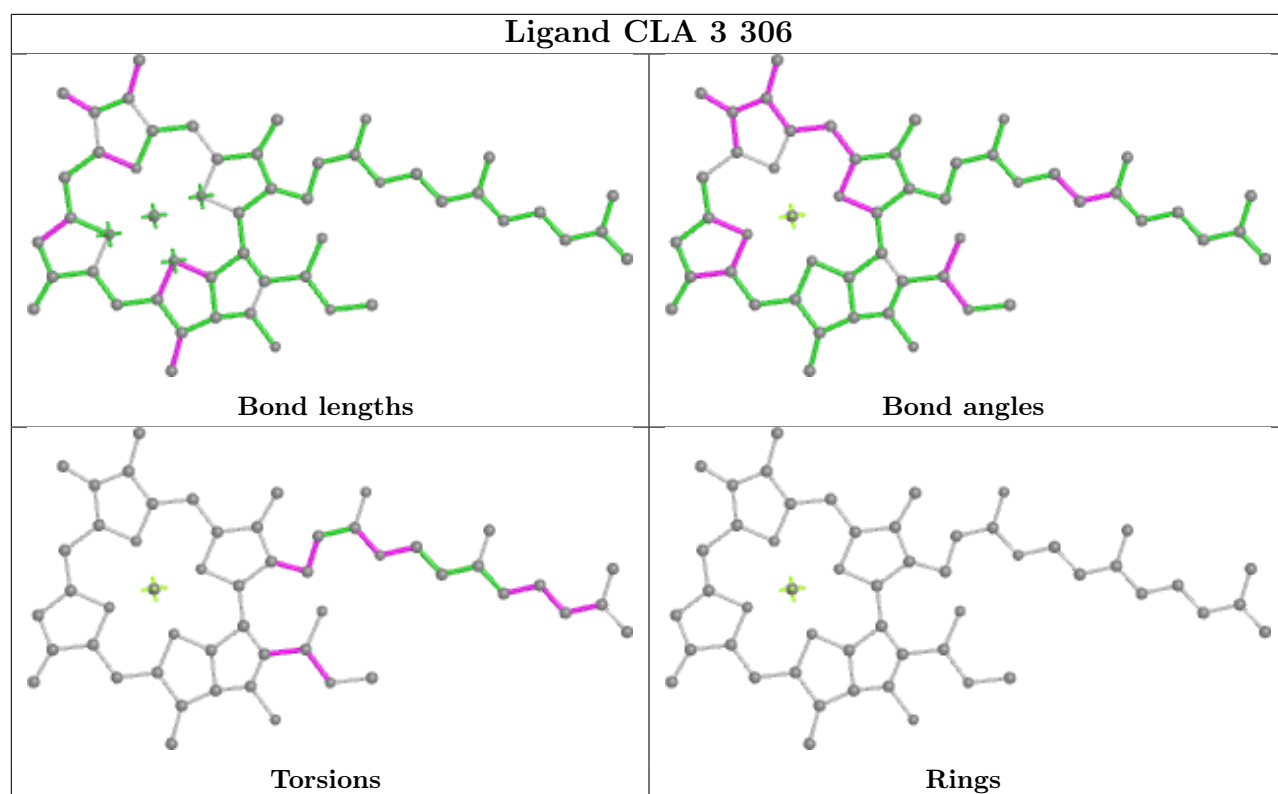


Rings

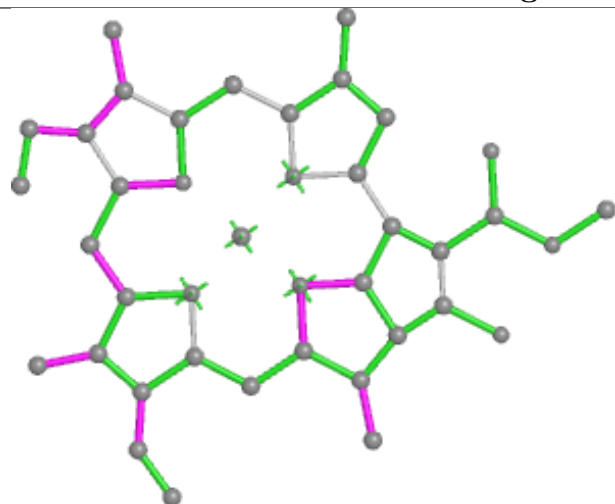




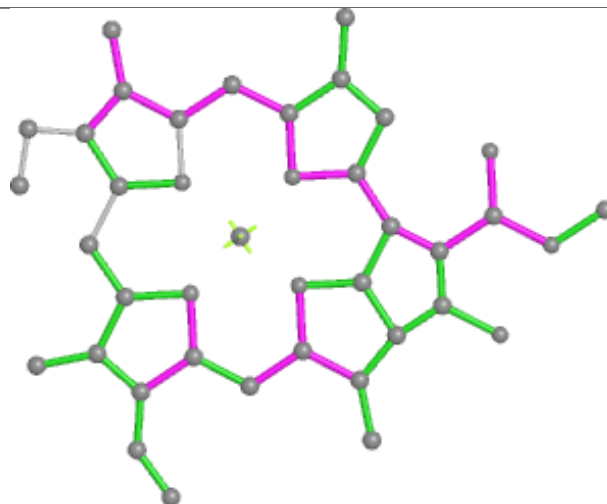




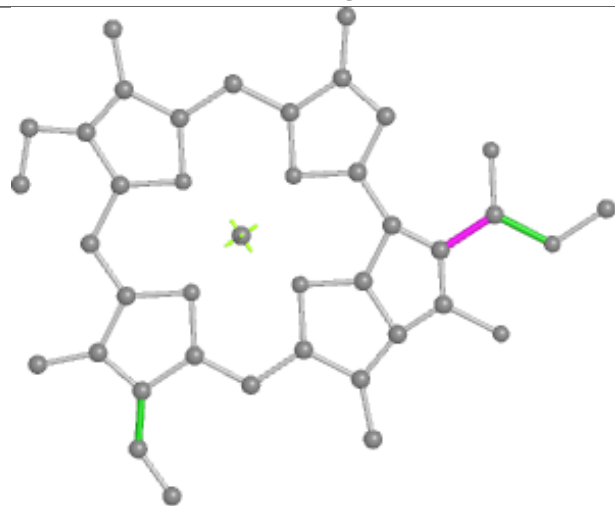
Ligand CLA 2 511



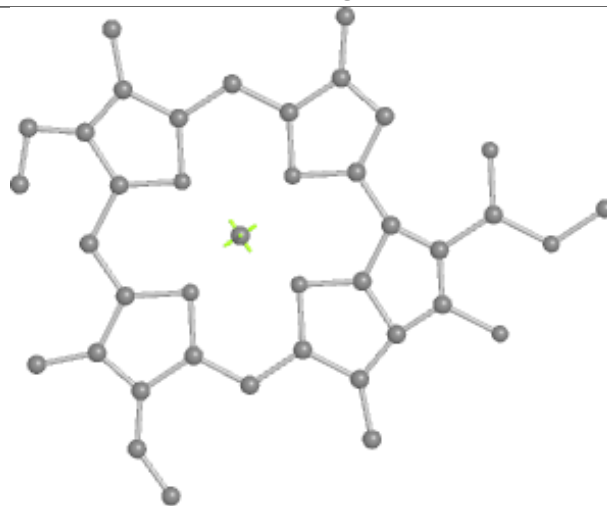
Bond lengths



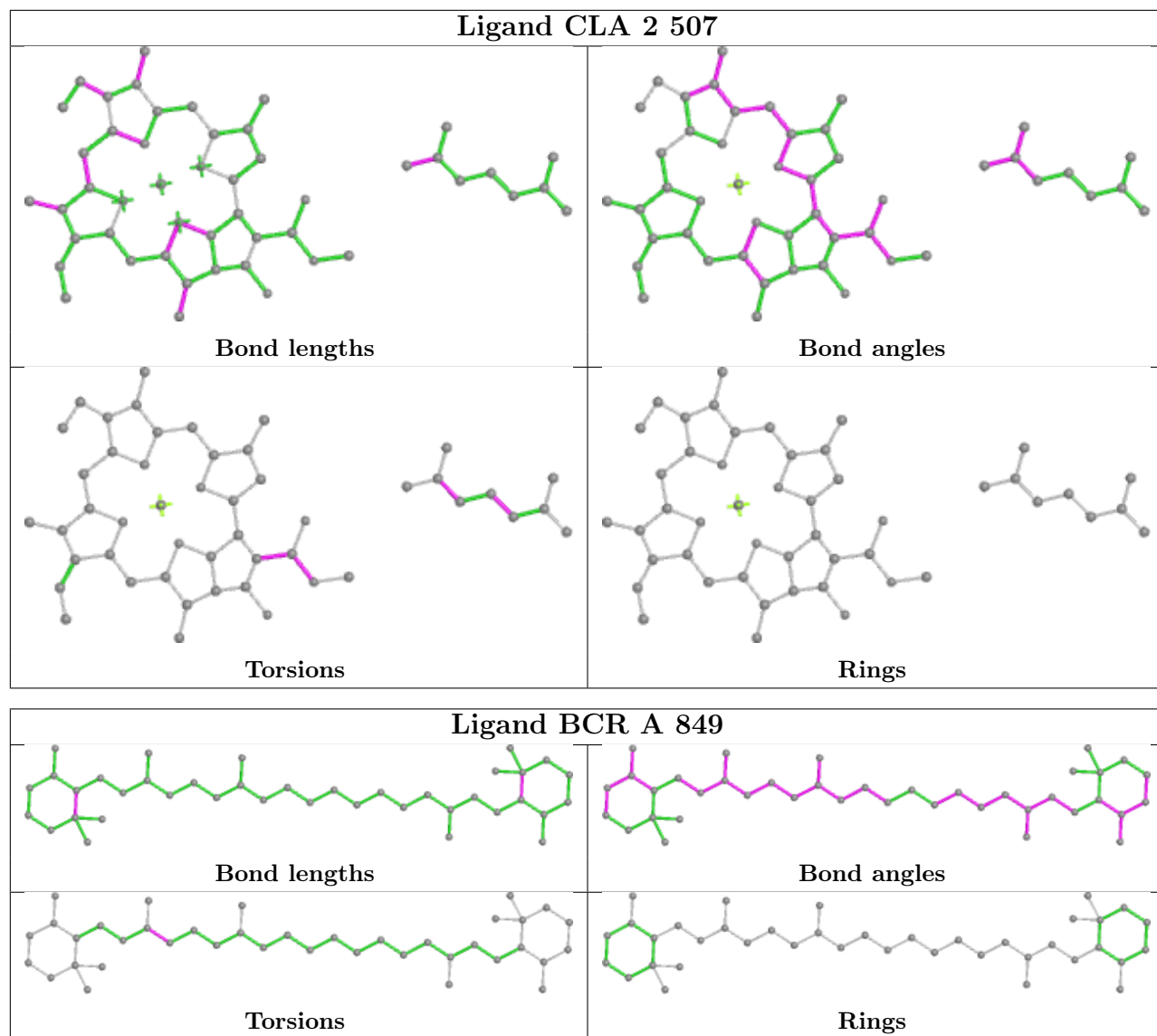
Bond angles



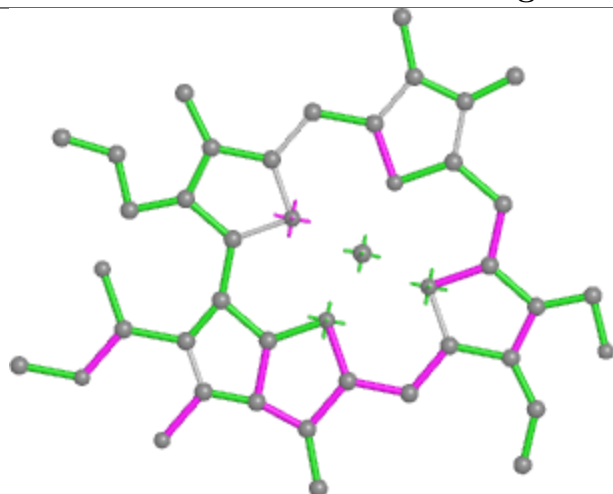
Torsions



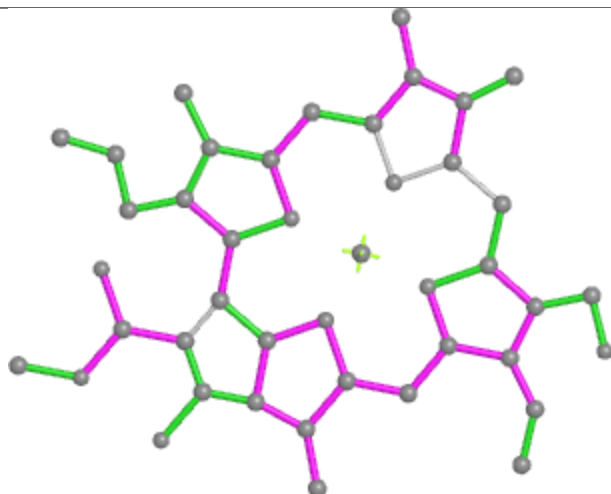
Rings



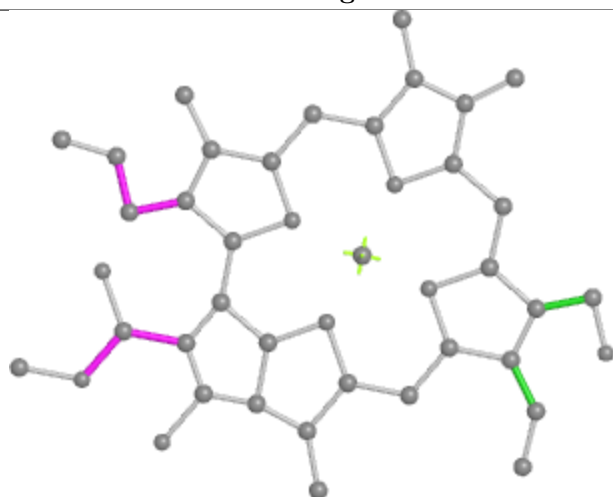
Ligand CHL 2 516



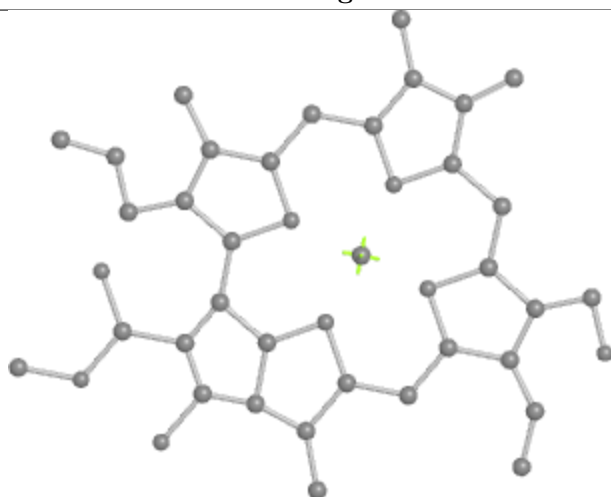
Bond lengths



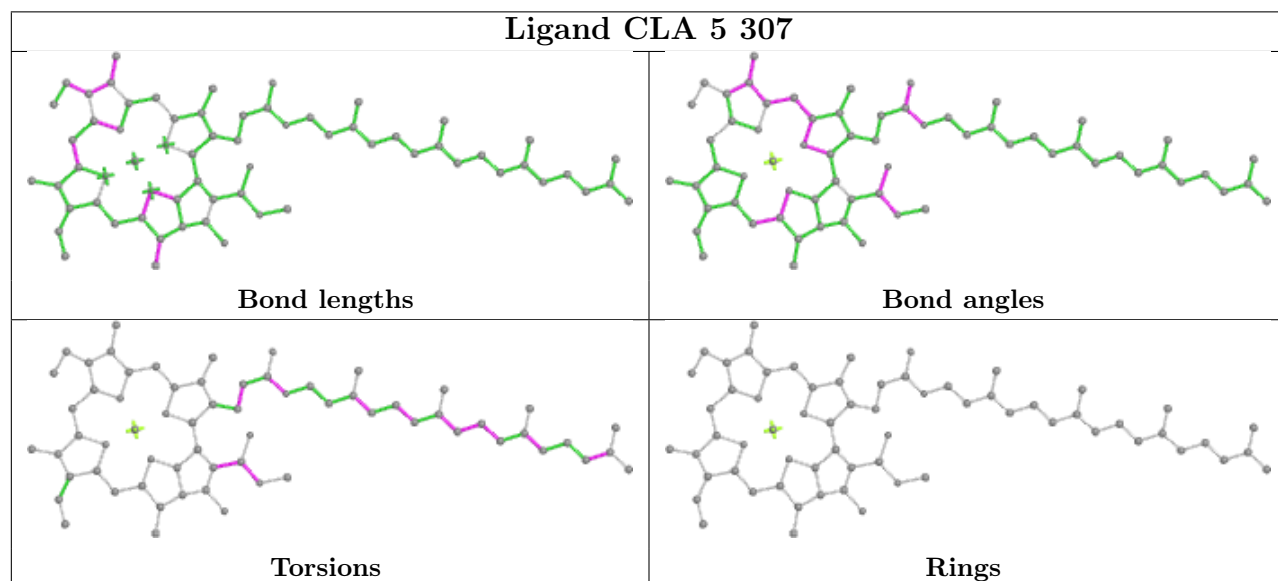
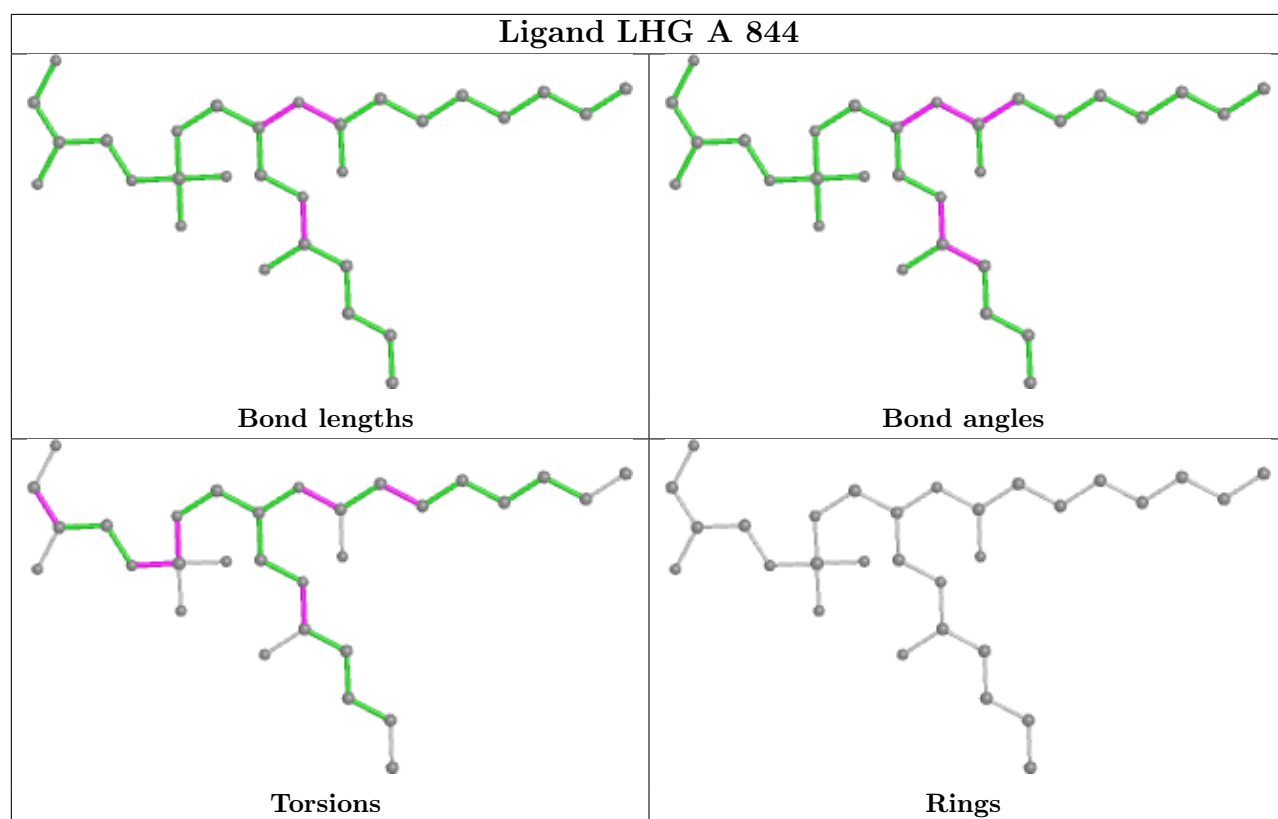
Bond angles



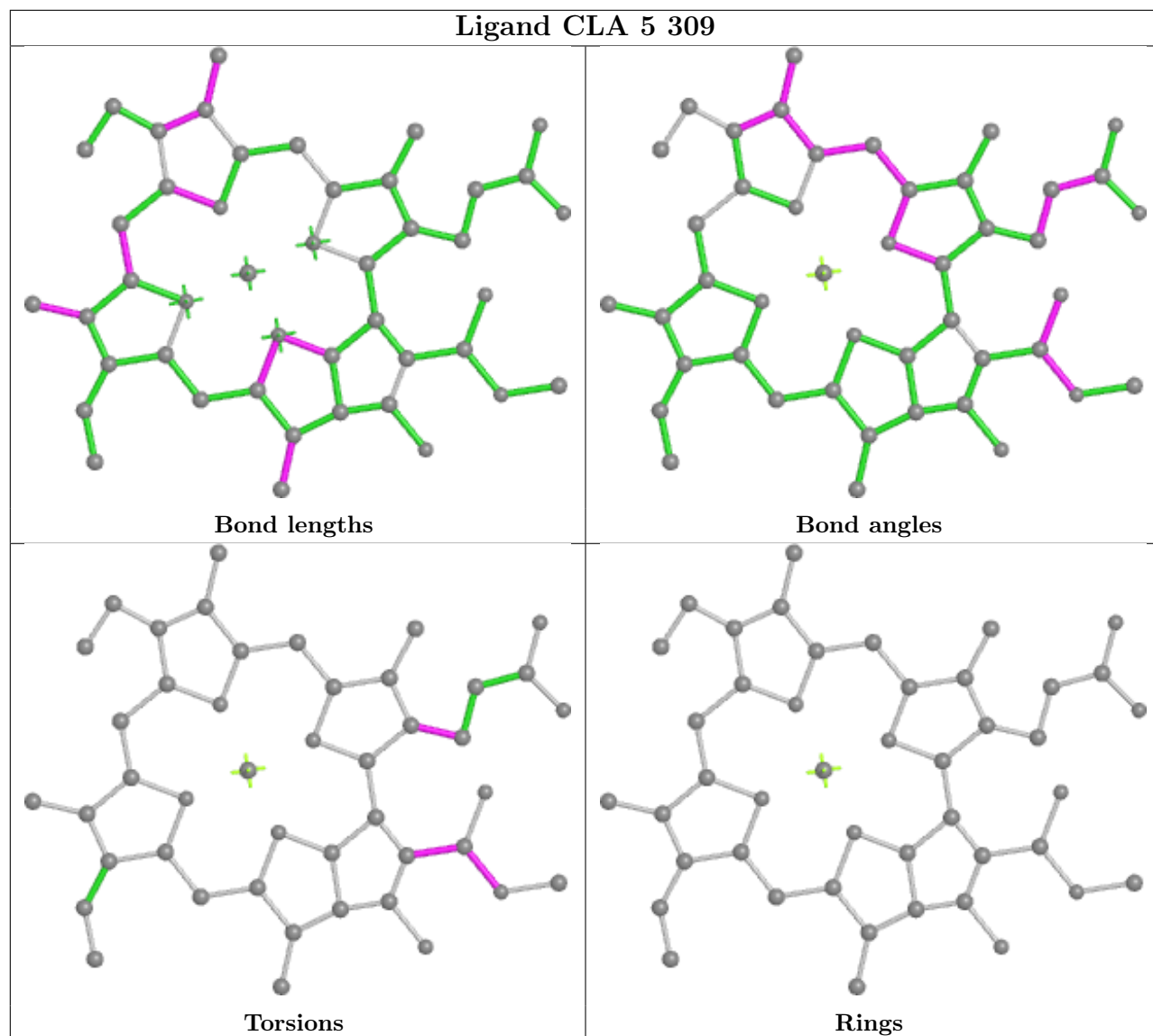
Torsions



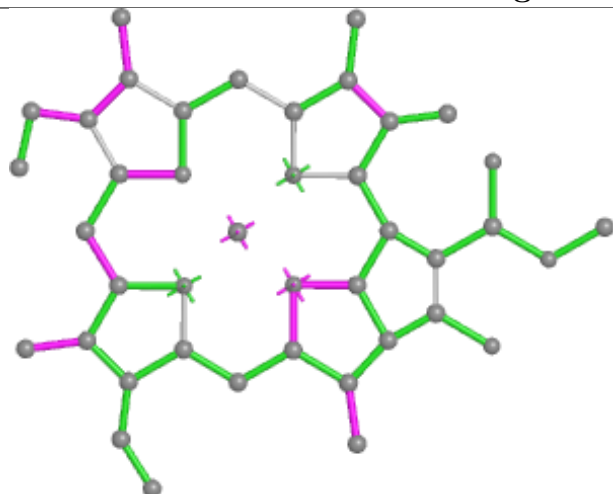
Rings



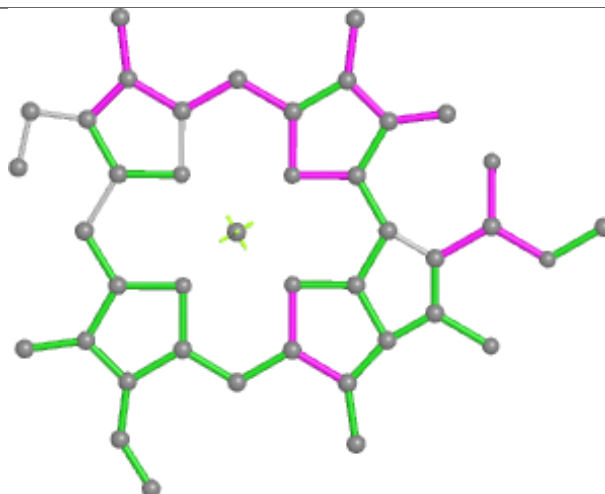
Ligand CLA 5 309



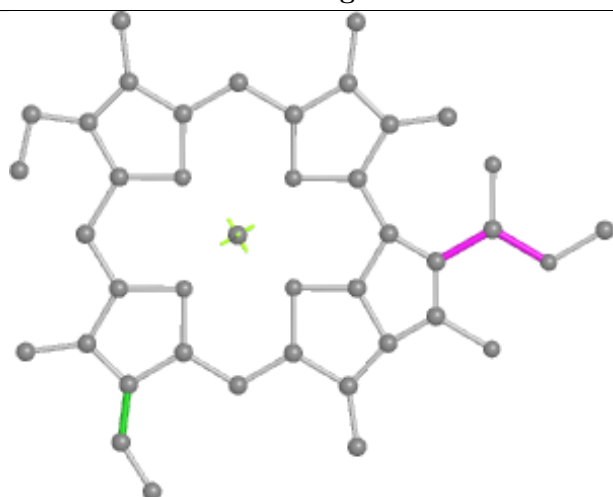
Ligand CLA A 837



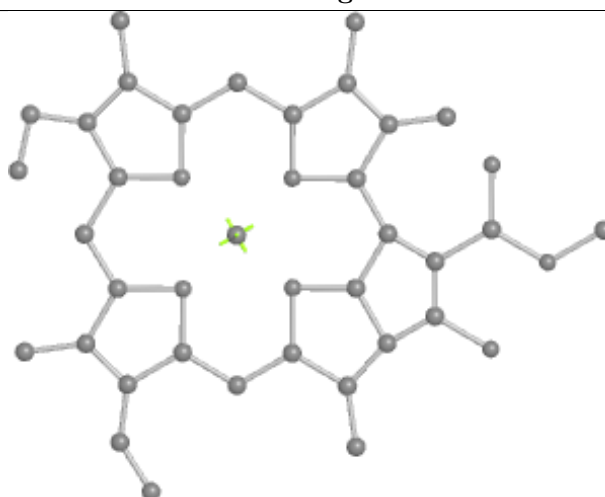
Bond lengths



Bond angles

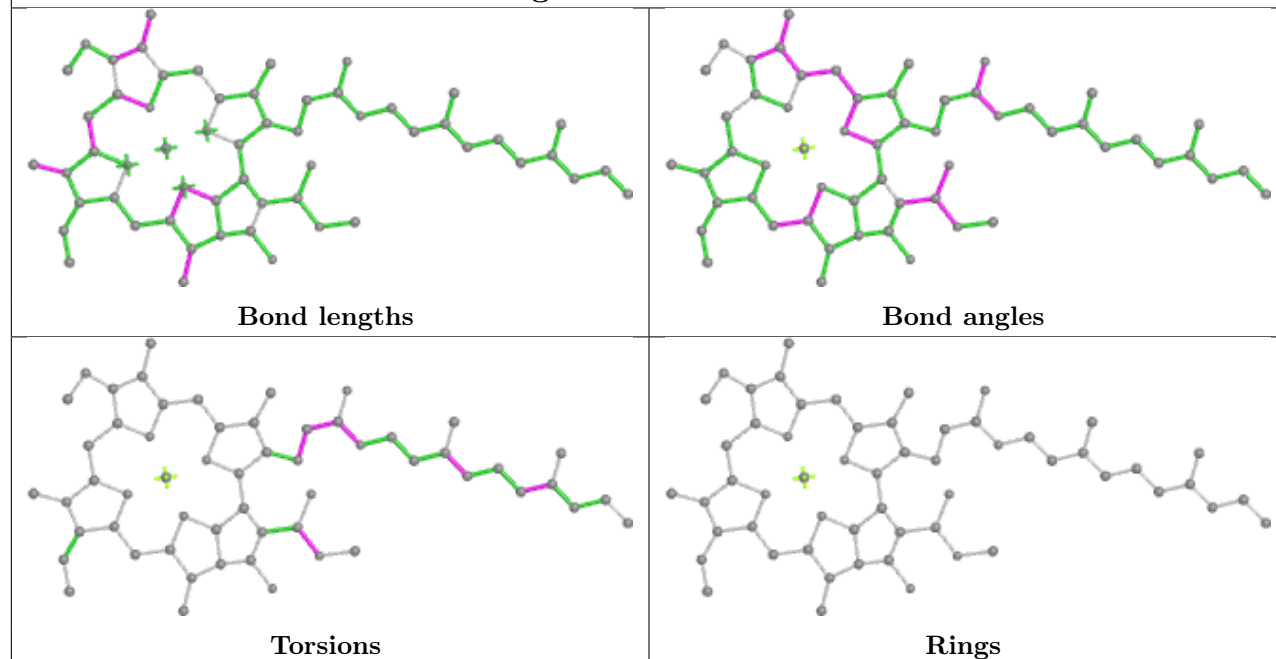


Torsions

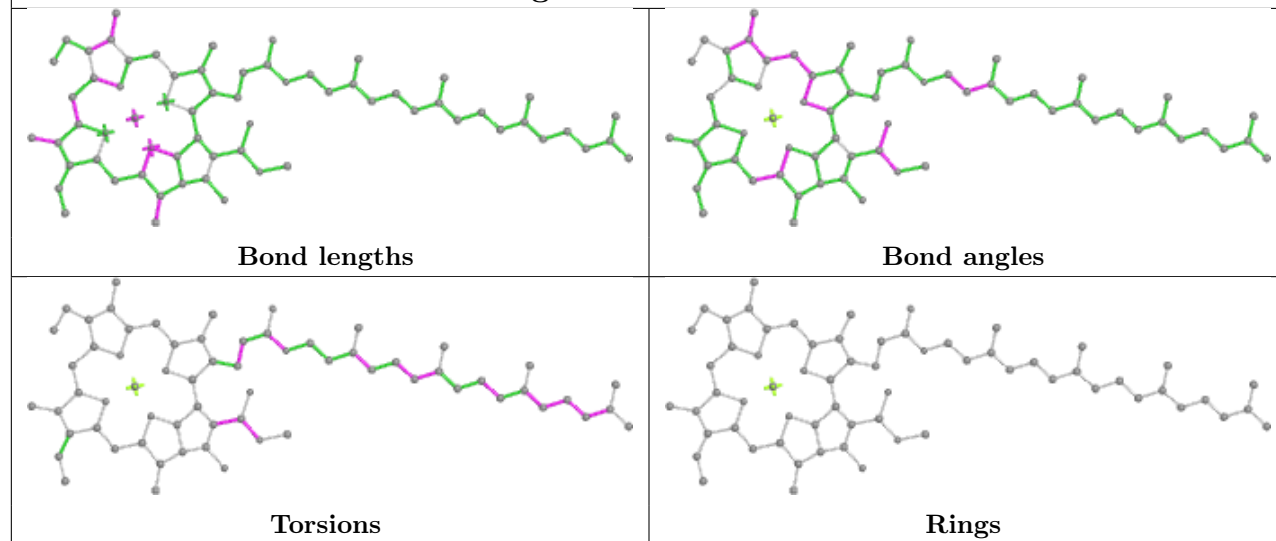


Rings

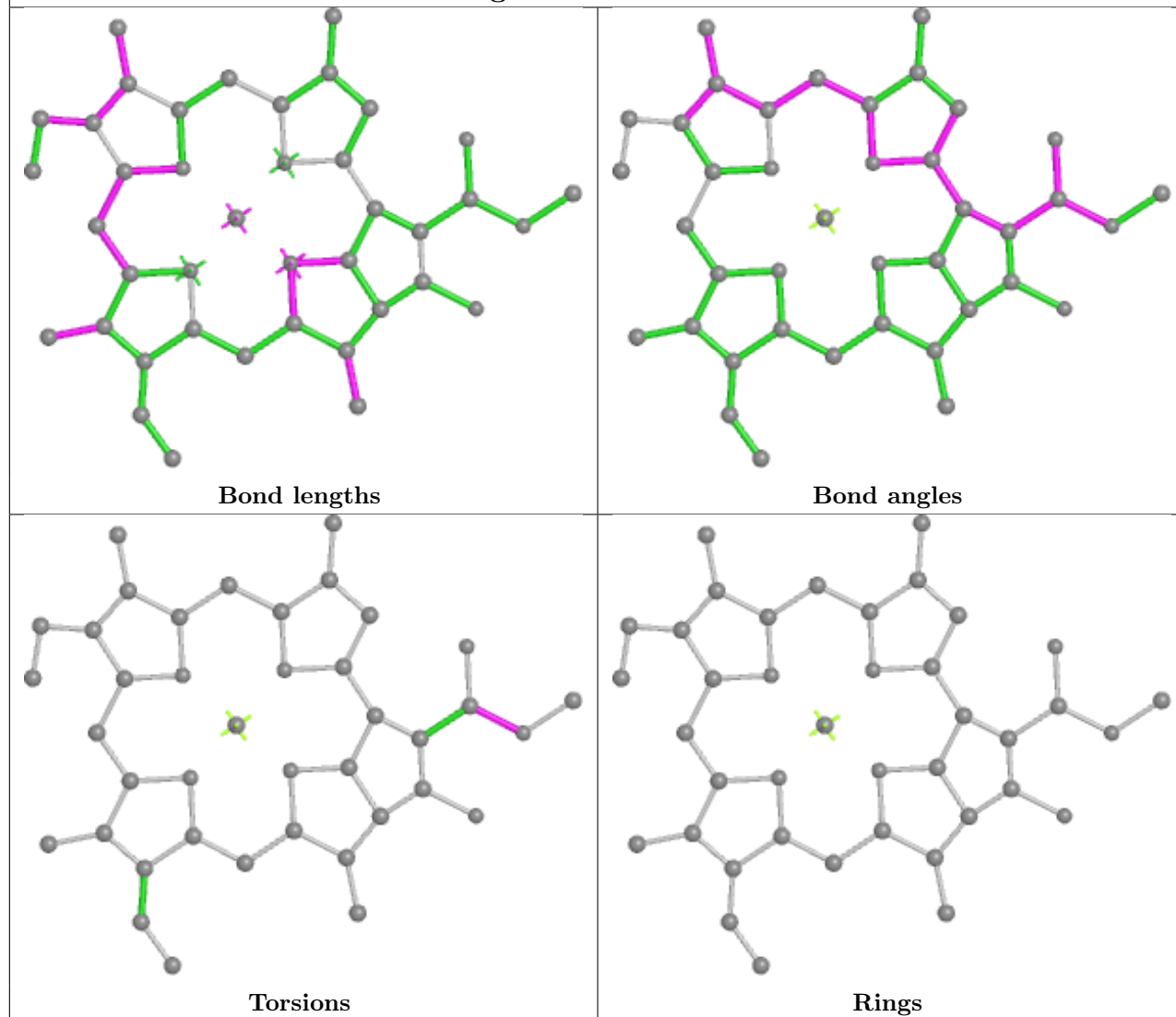
Ligand CLA A 820



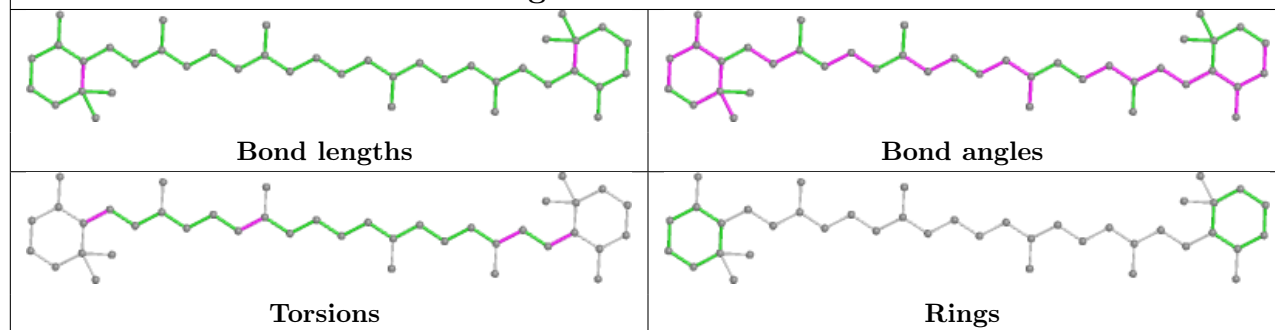
Ligand CLA A 806



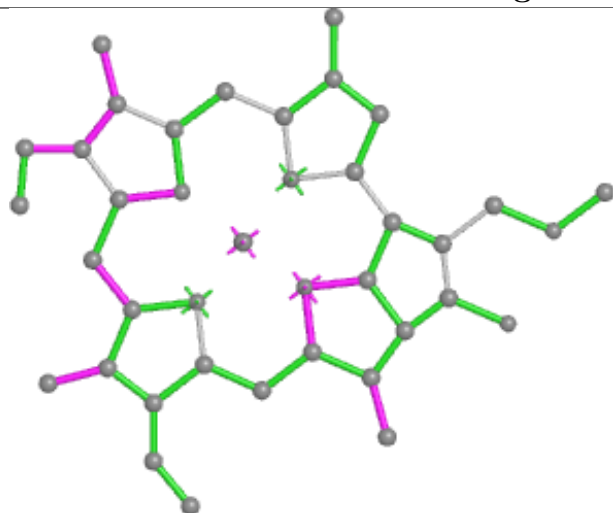
Ligand CLA B 829



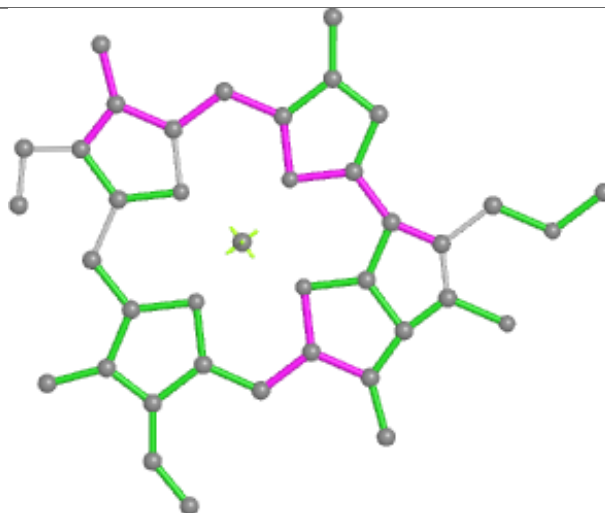
Ligand BCR K 204



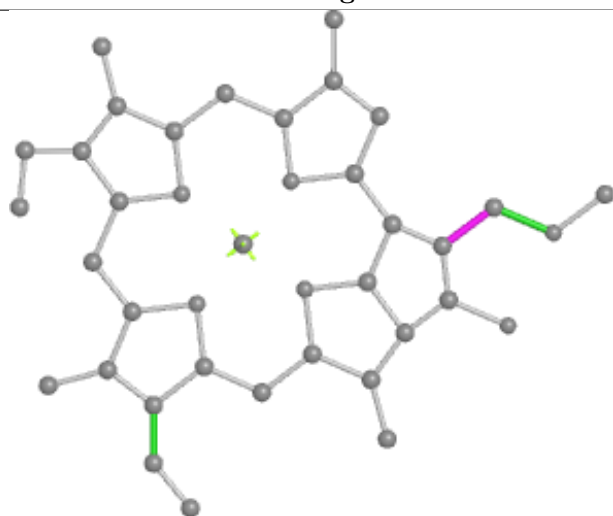
Ligand CLA A 807



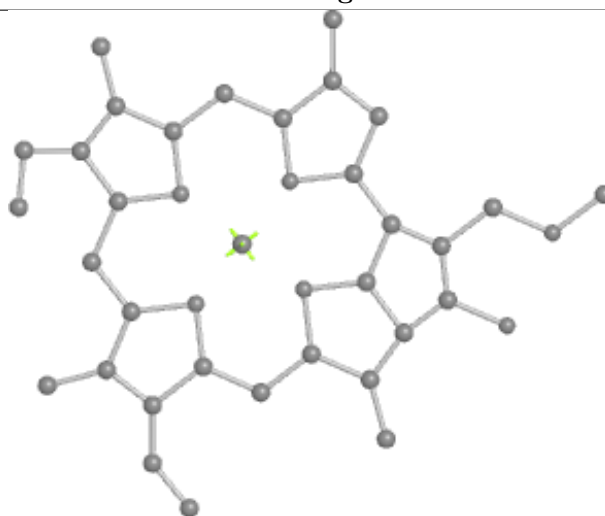
Bond lengths



Bond angles

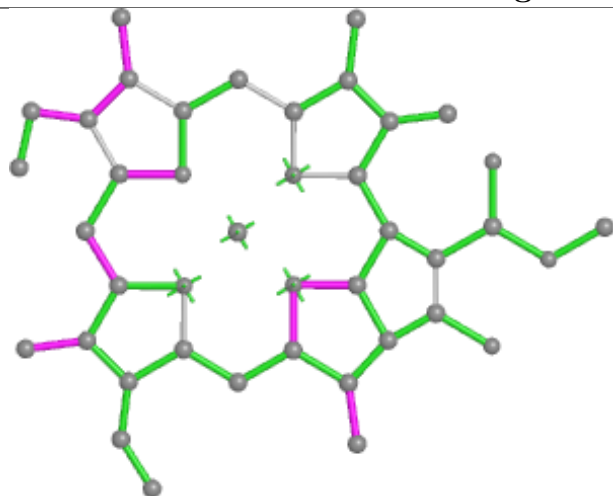


Torsions

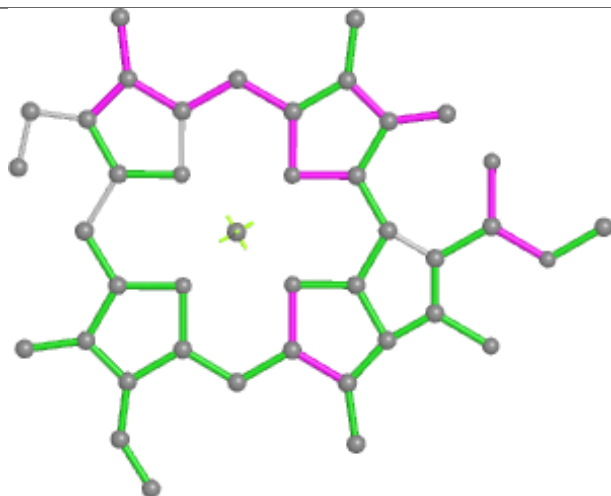


Rings

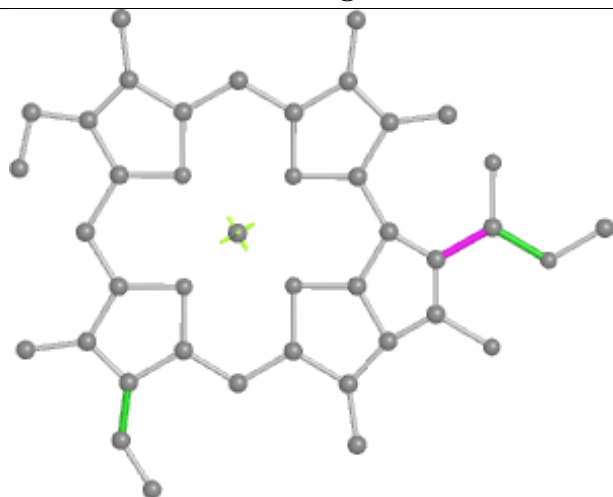
Ligand CLA B 840



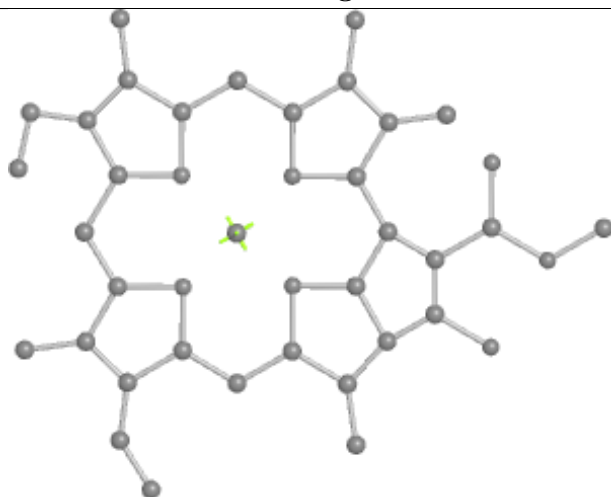
Bond lengths



Bond angles

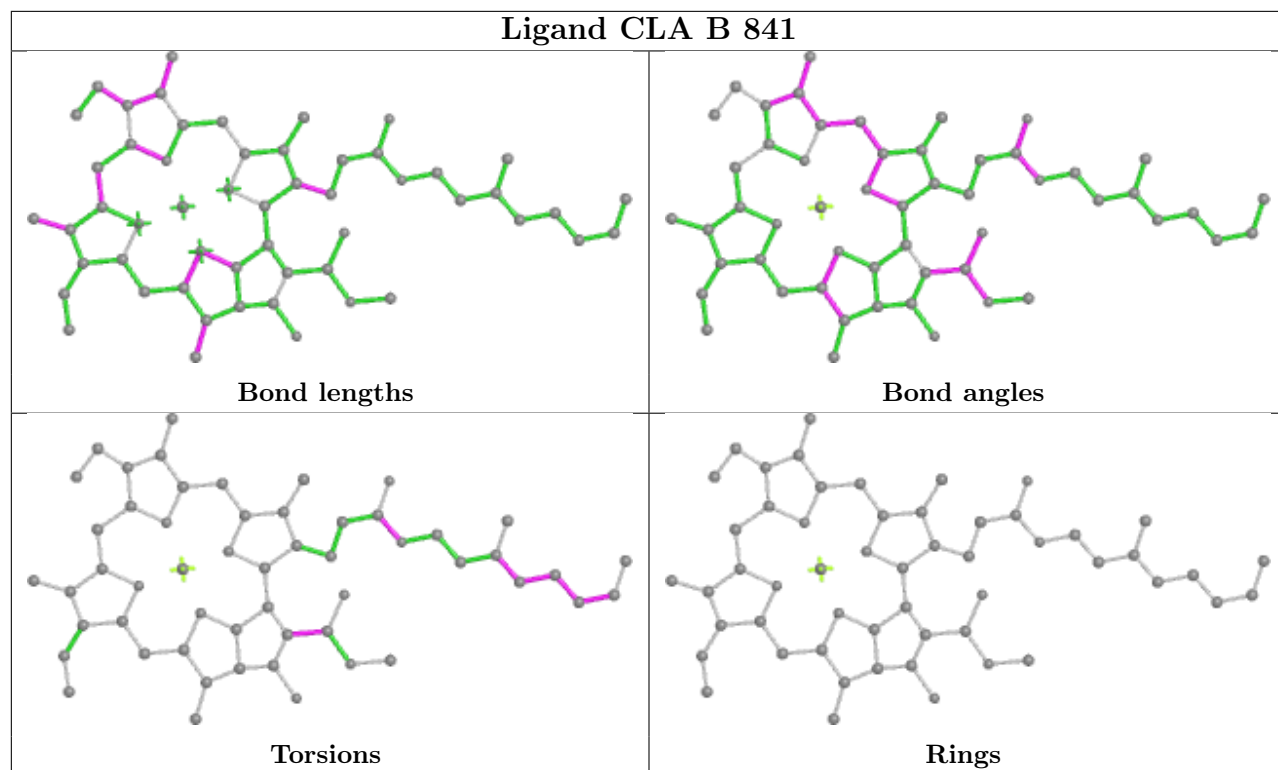


Torsions

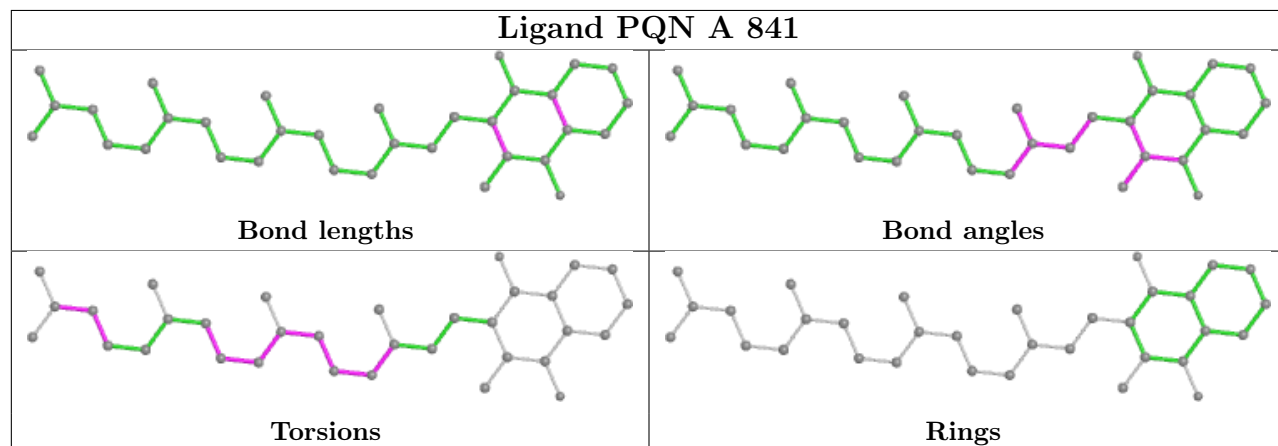


Rings

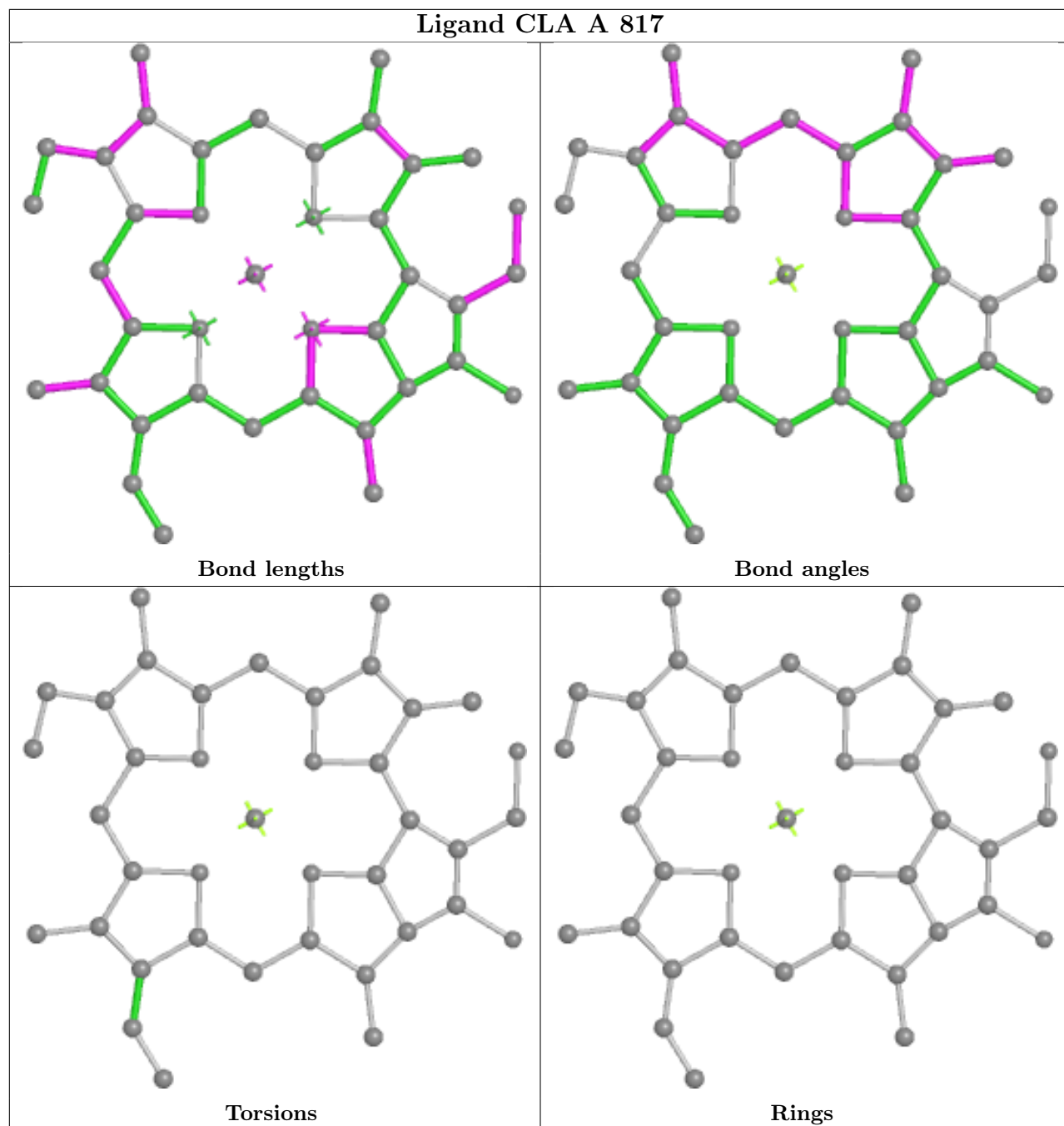
Ligand CLA B 841



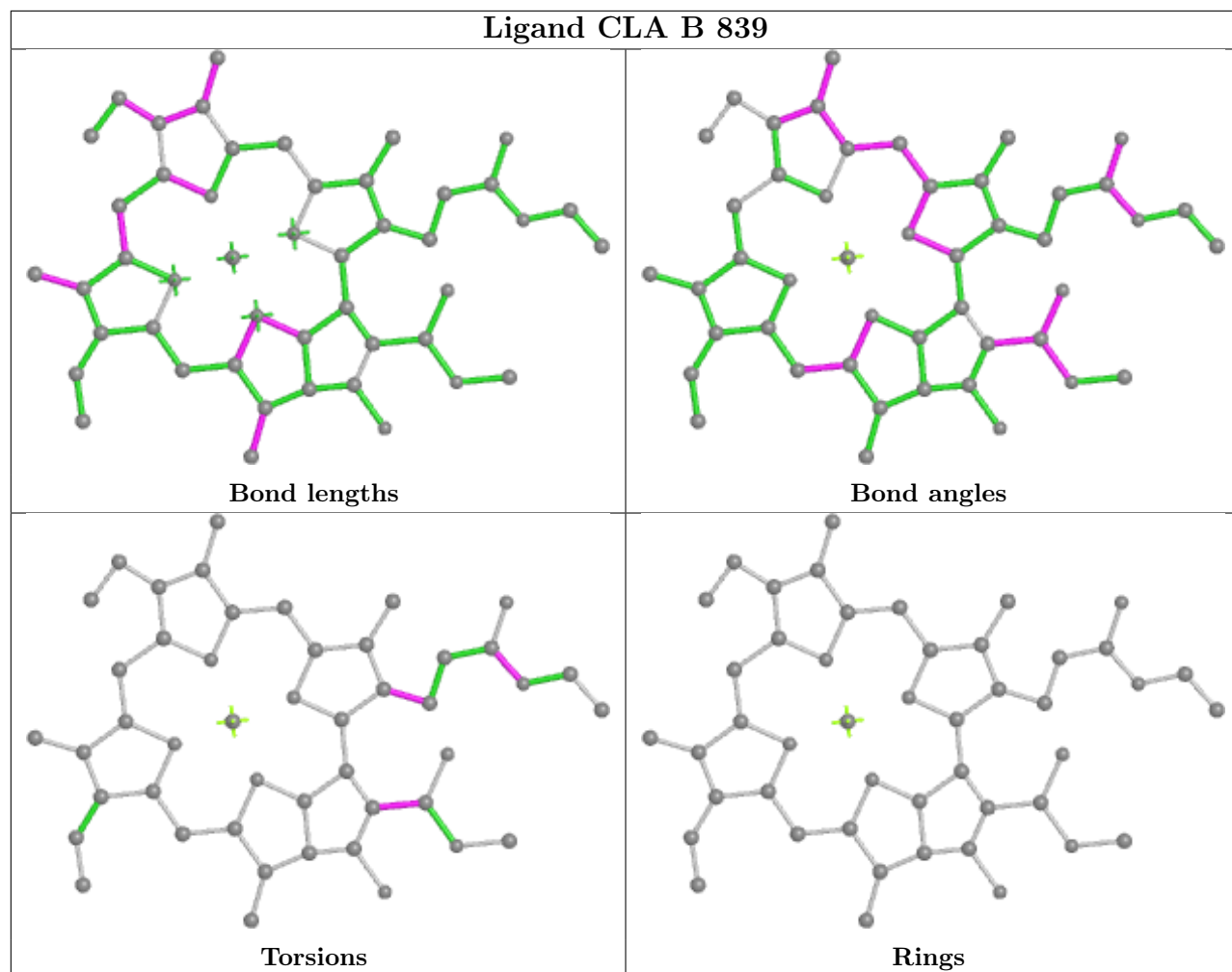
Ligand PQN A 841



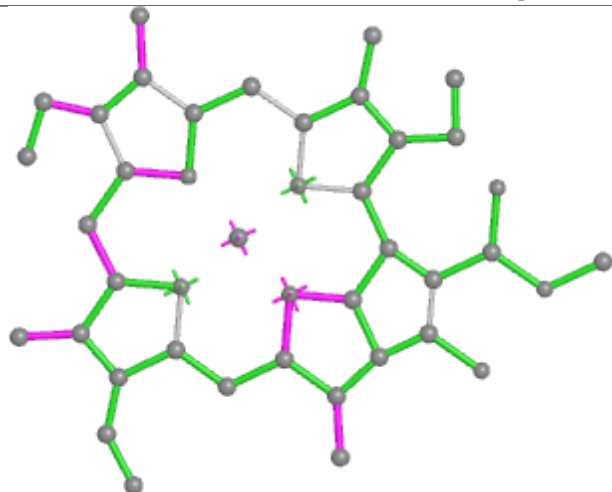
Ligand CLA A 817



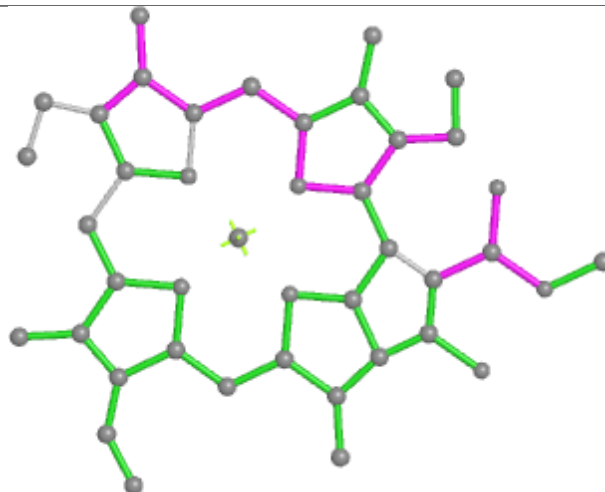
Ligand CLA B 839



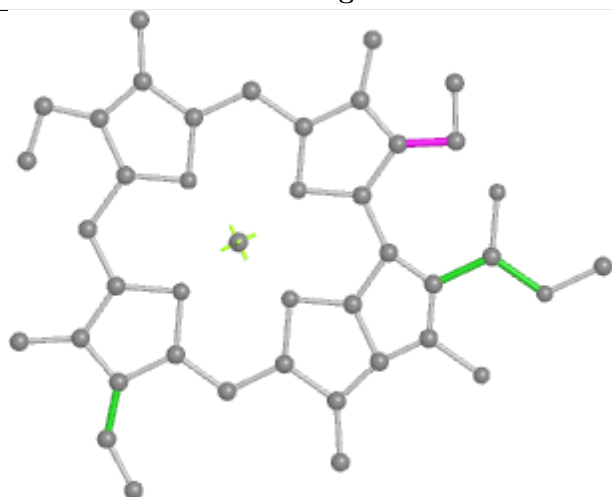
Ligand CLA A 821



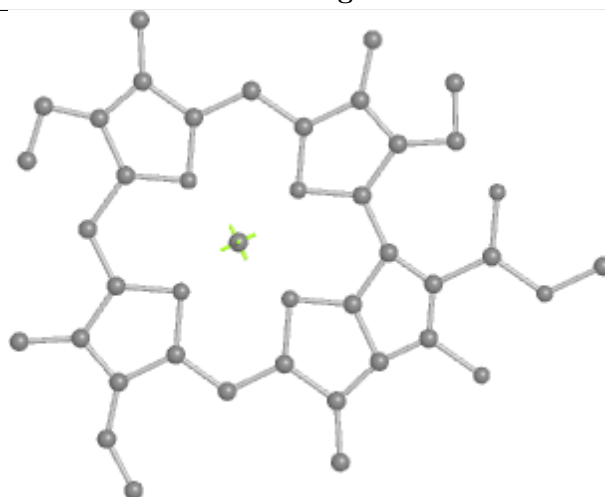
Bond lengths



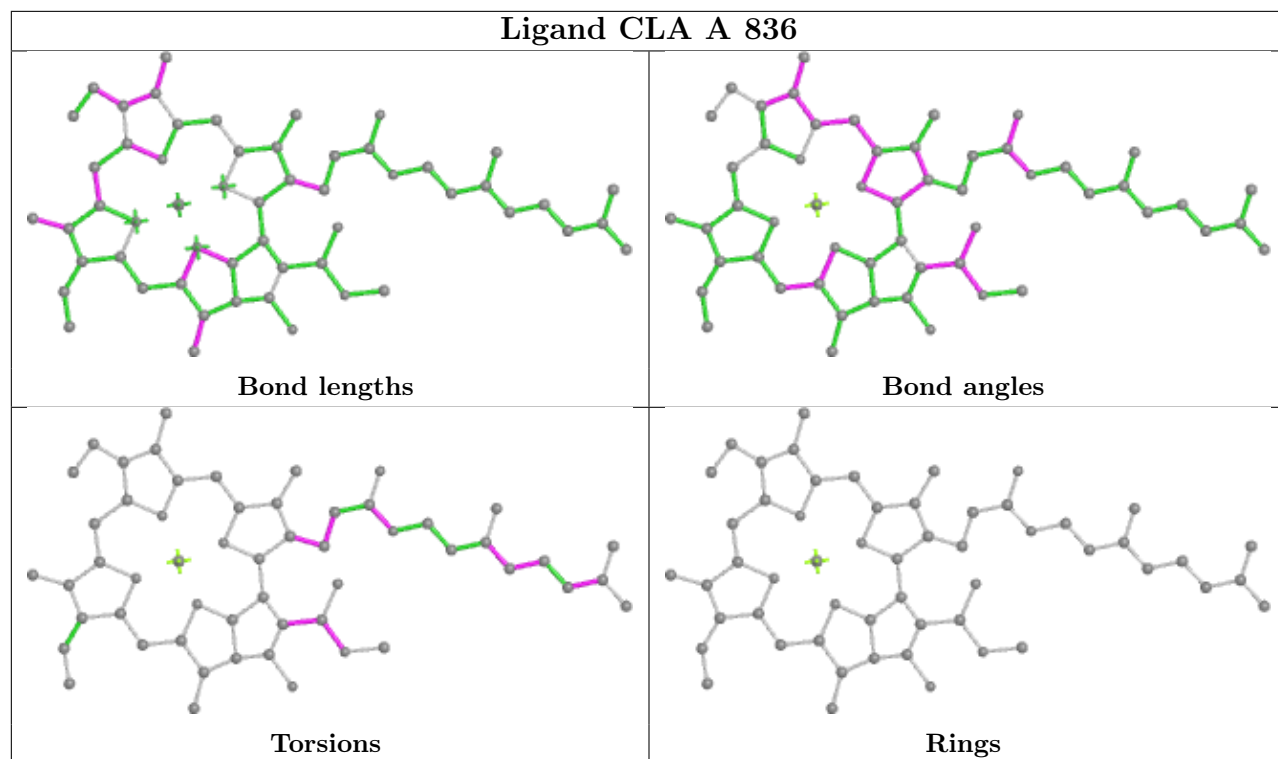
Bond angles



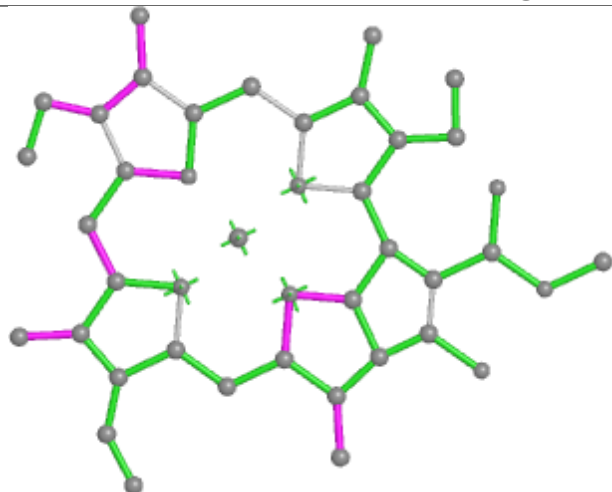
Torsions



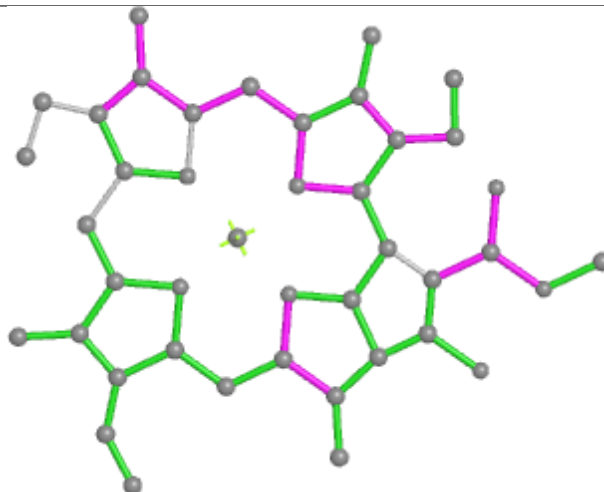
Rings



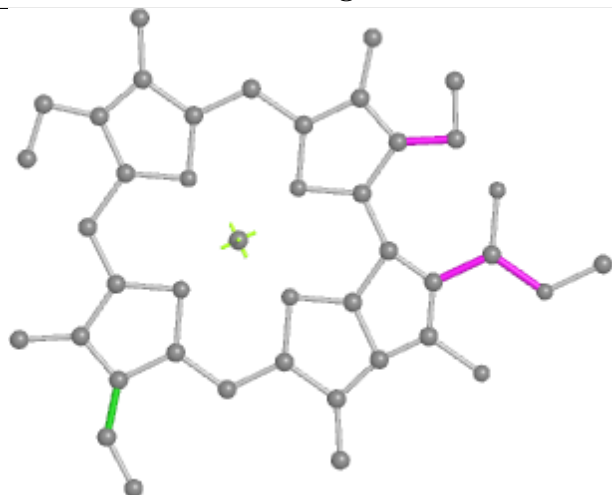
Ligand CLA 1 507



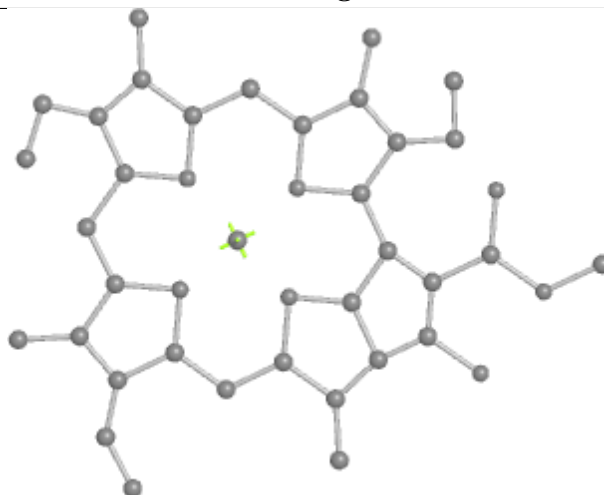
Bond lengths



Bond angles

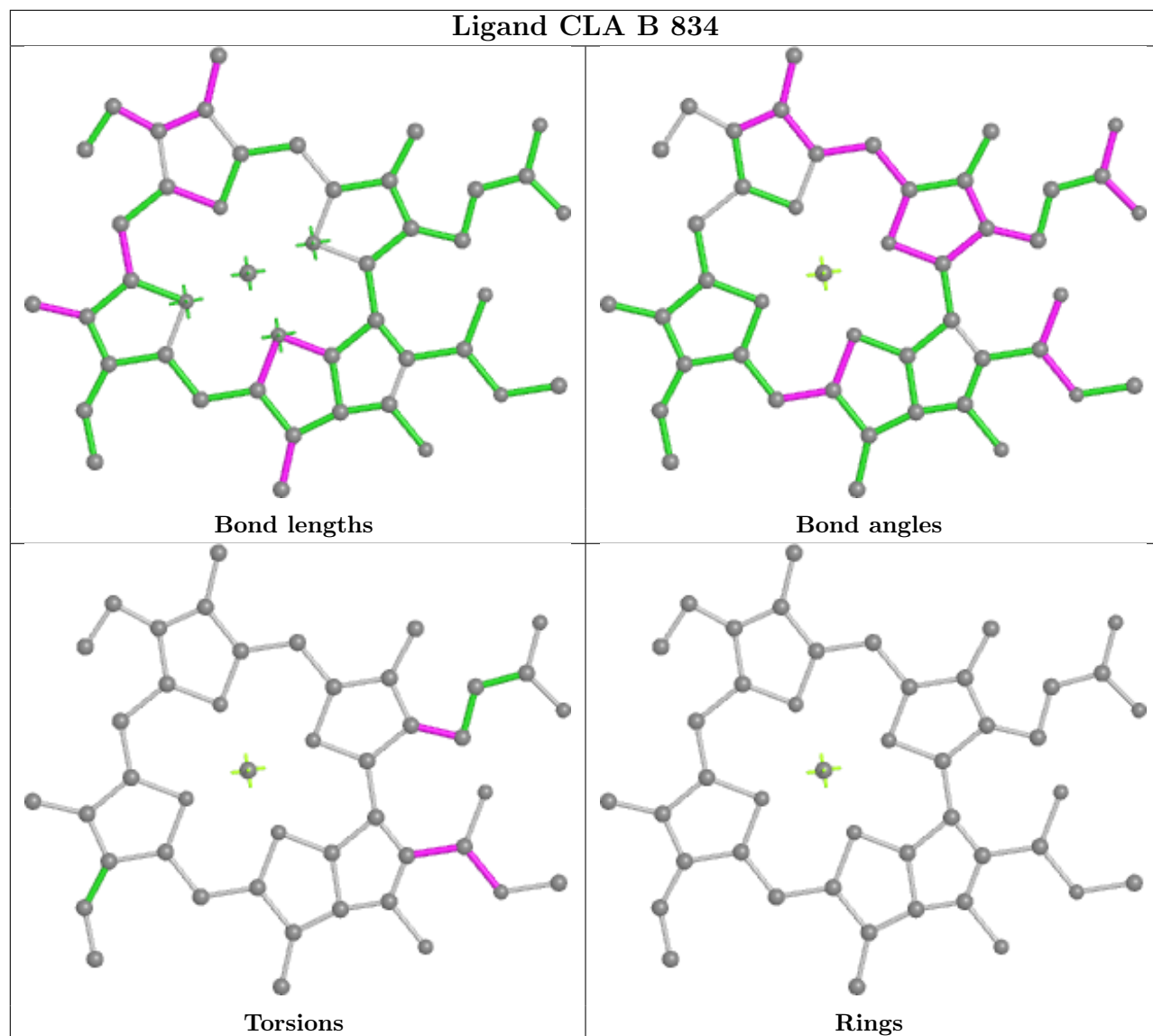


Torsions

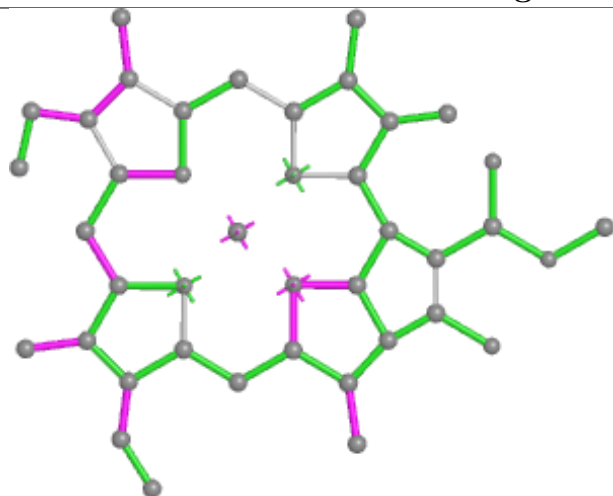


Rings

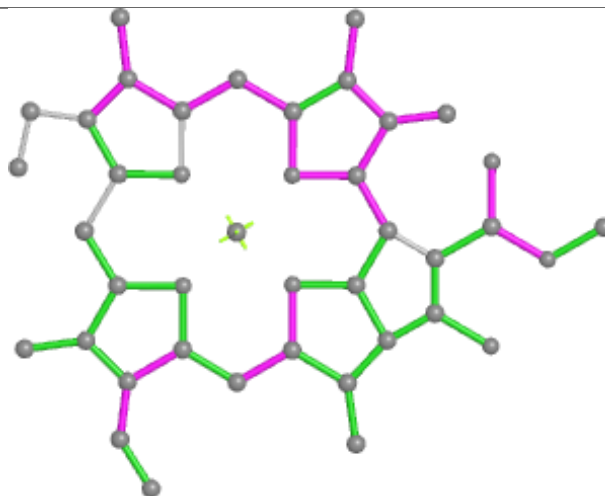
Ligand CLA B 834



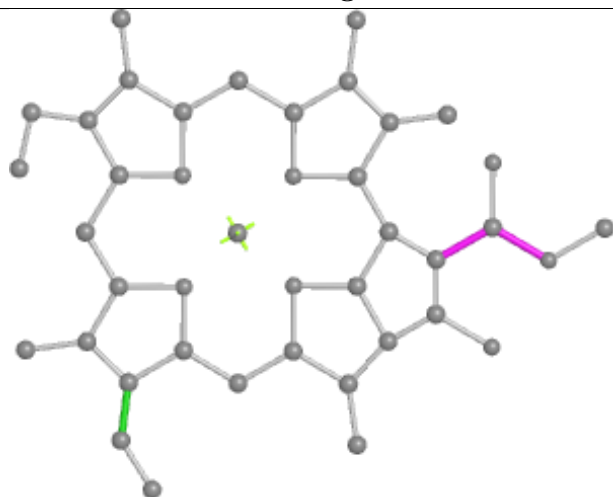
Ligand CLA B 814



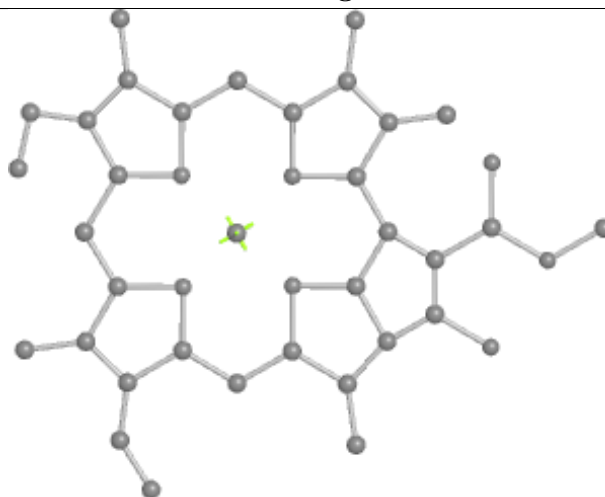
Bond lengths



Bond angles

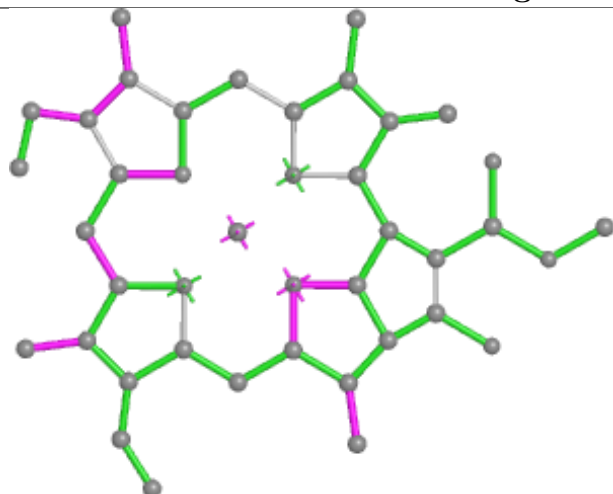


Torsions

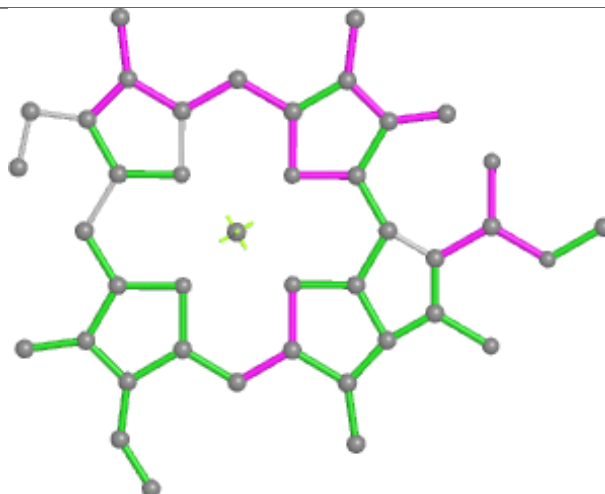


Rings

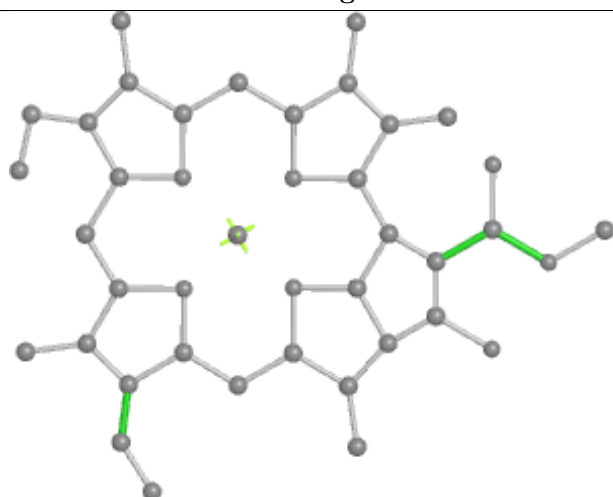
Ligand CLA A 803



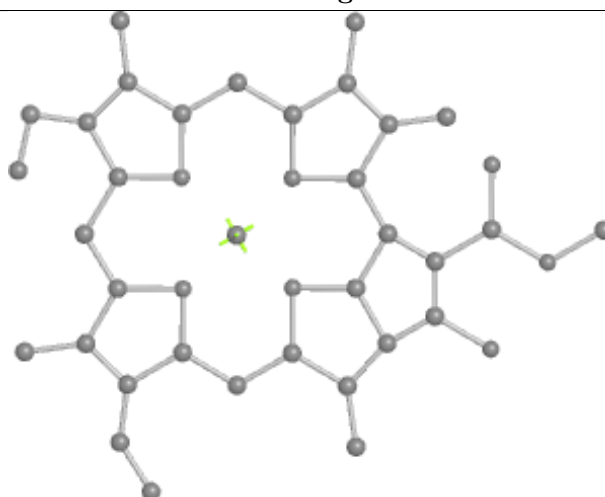
Bond lengths



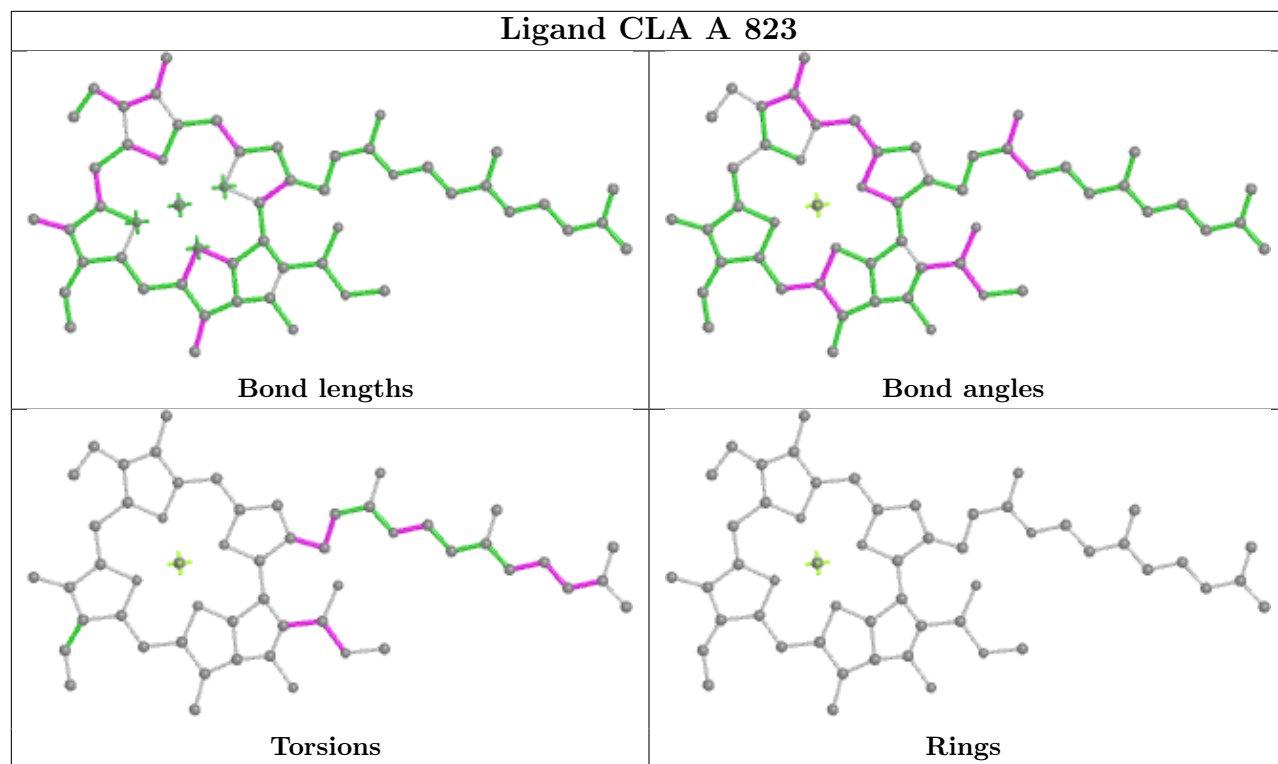
Bond angles



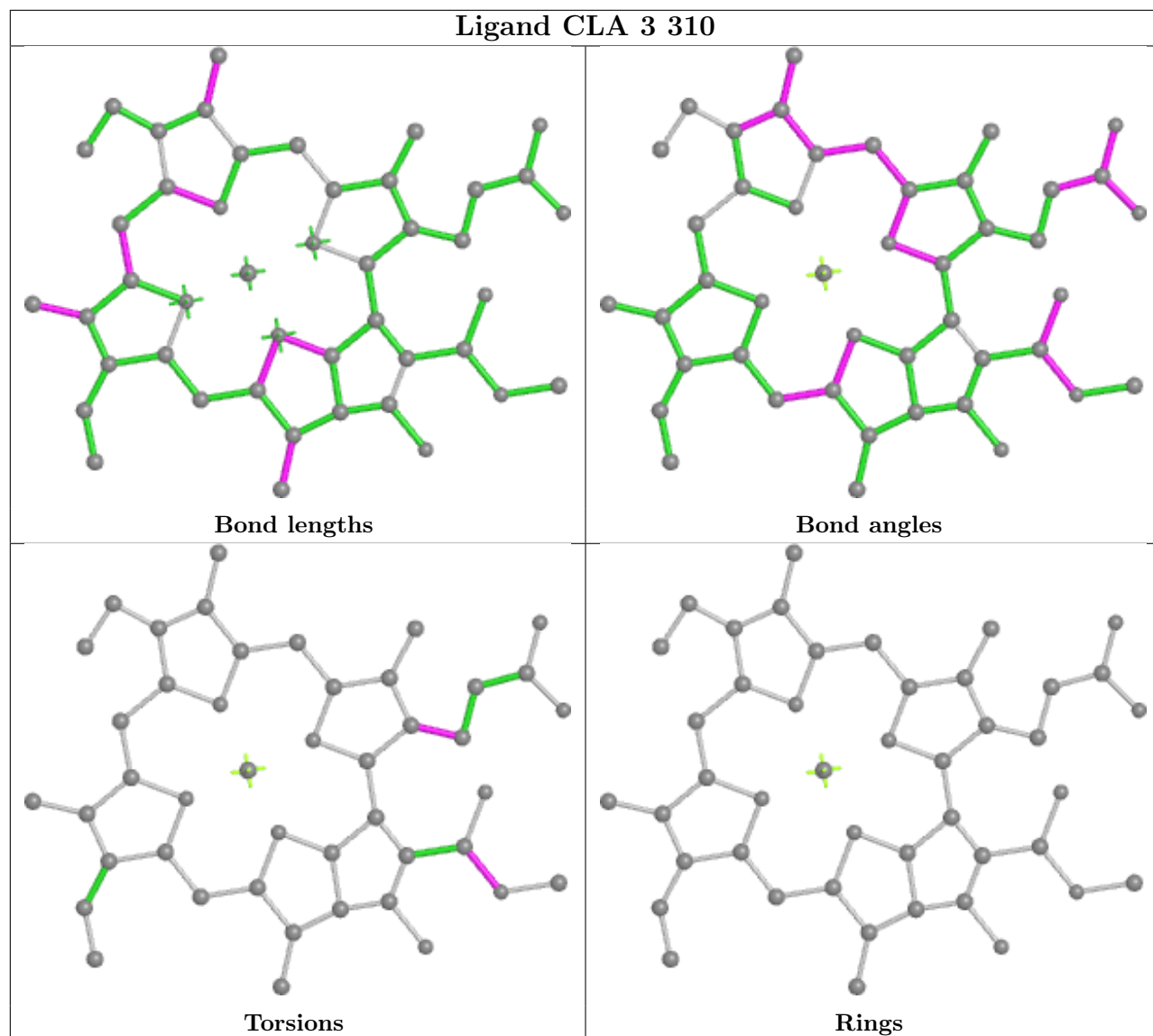
Torsions



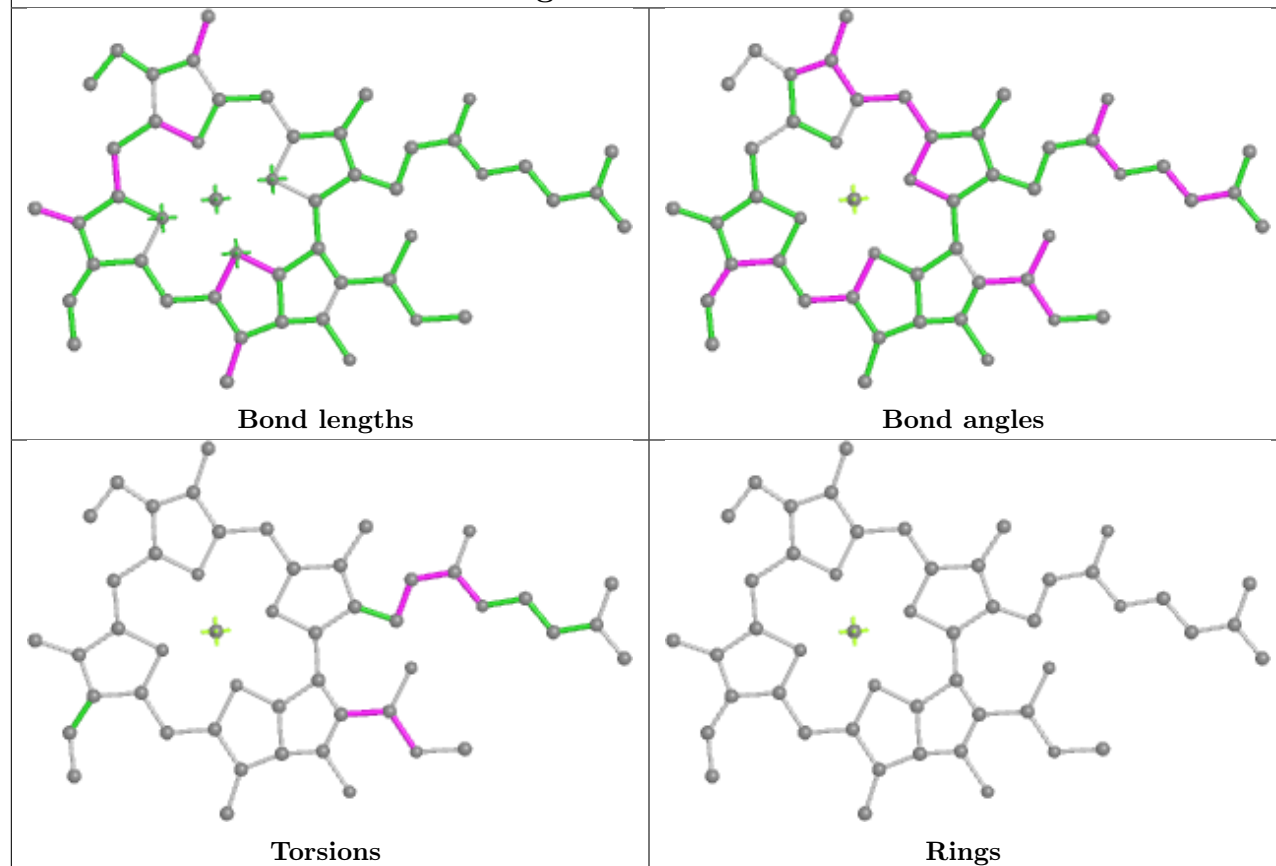
Rings



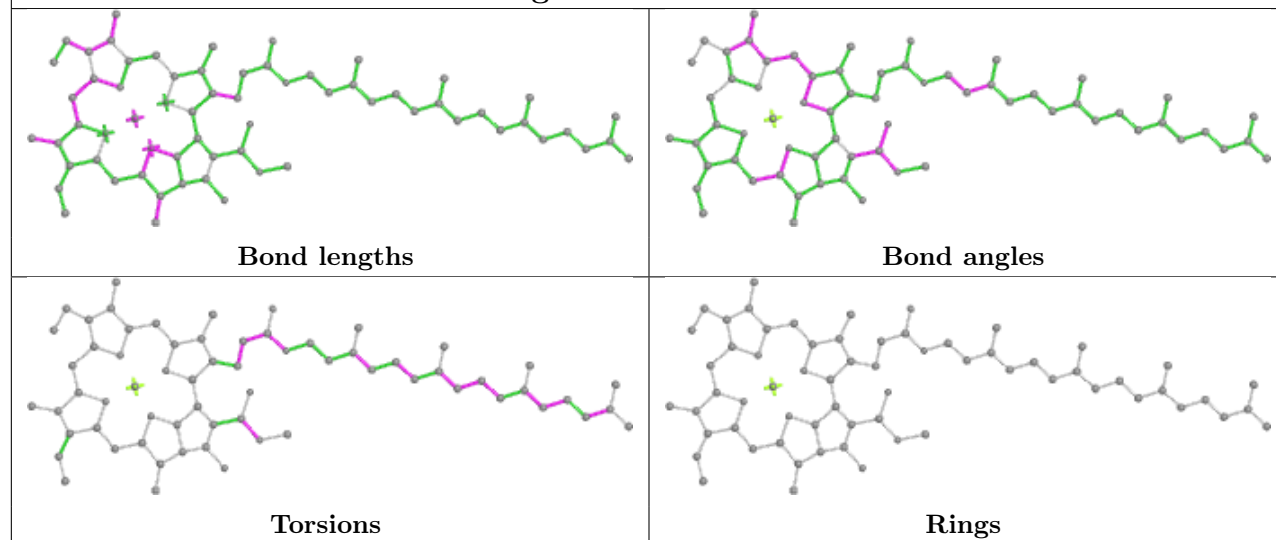
Ligand CLA 3 310



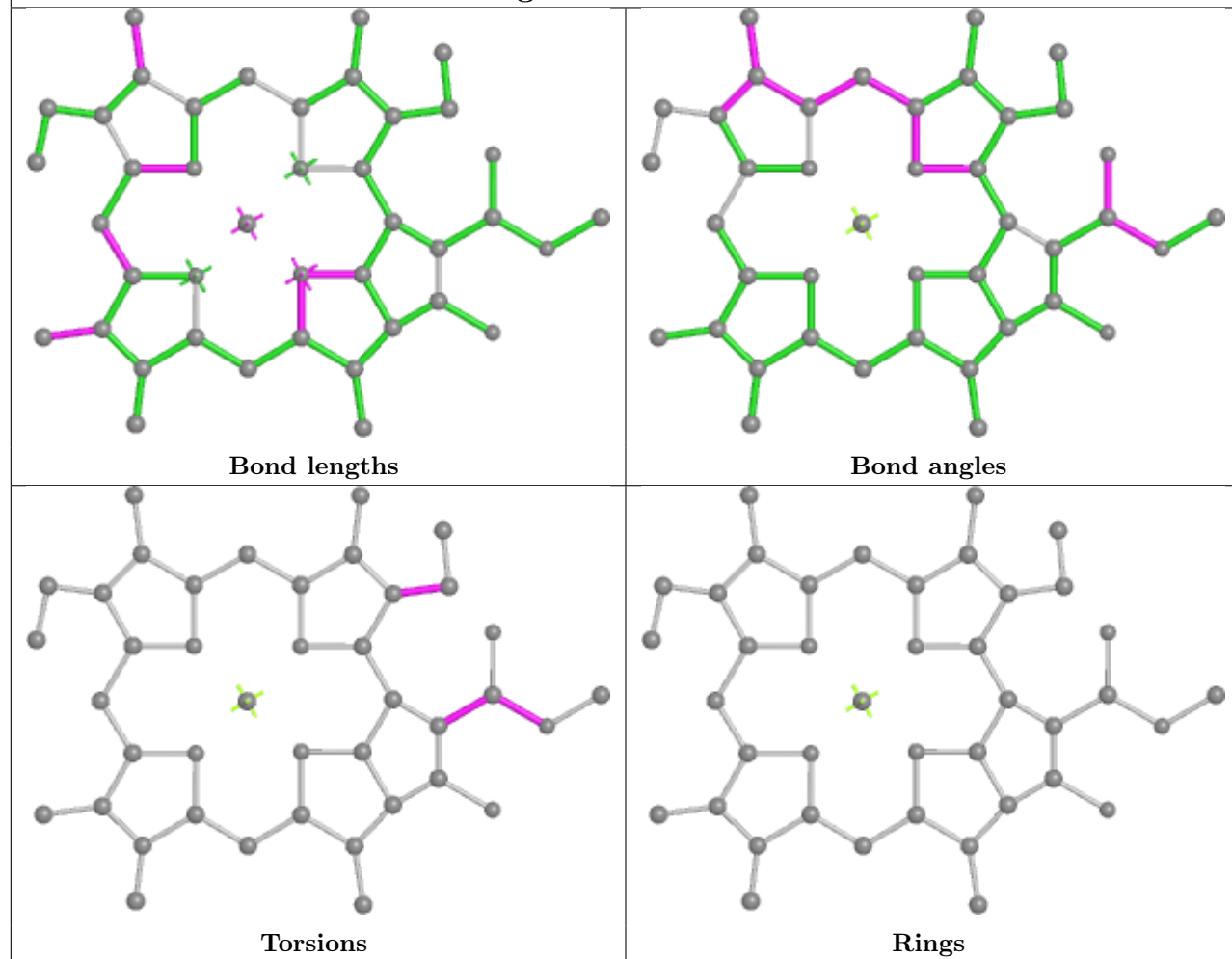
Ligand CLA 3 311



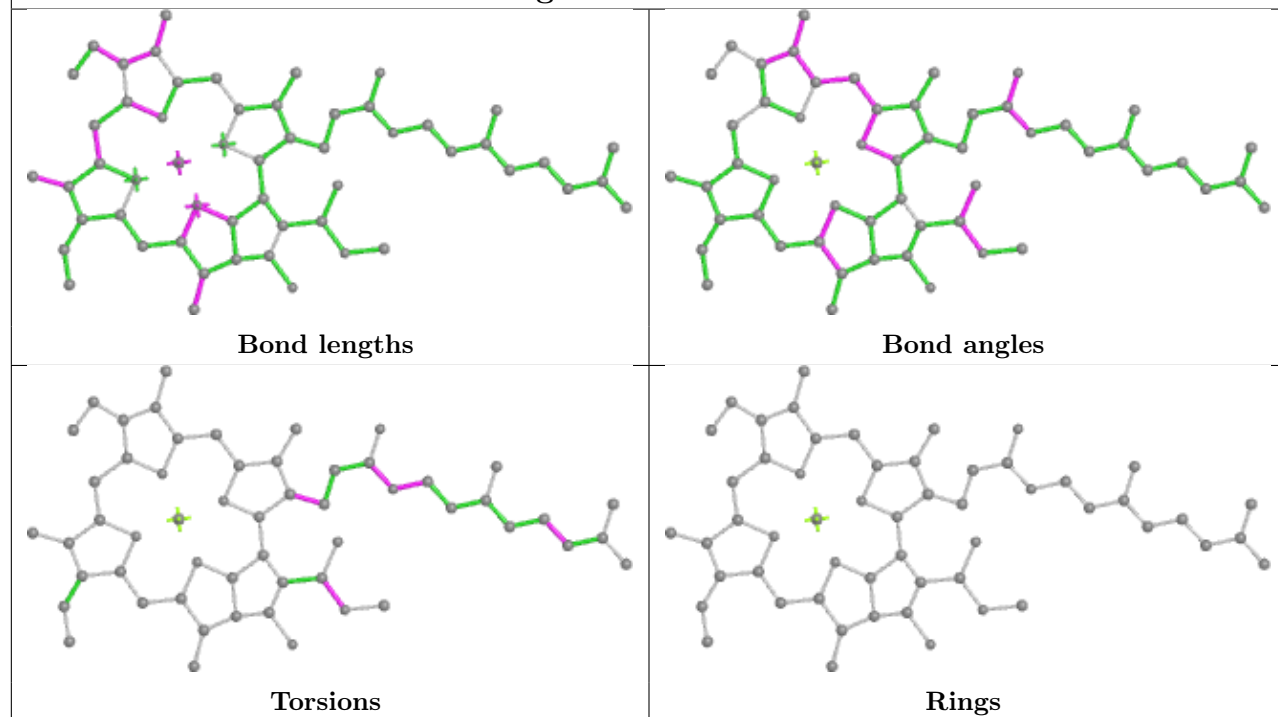
Ligand CLA A 827



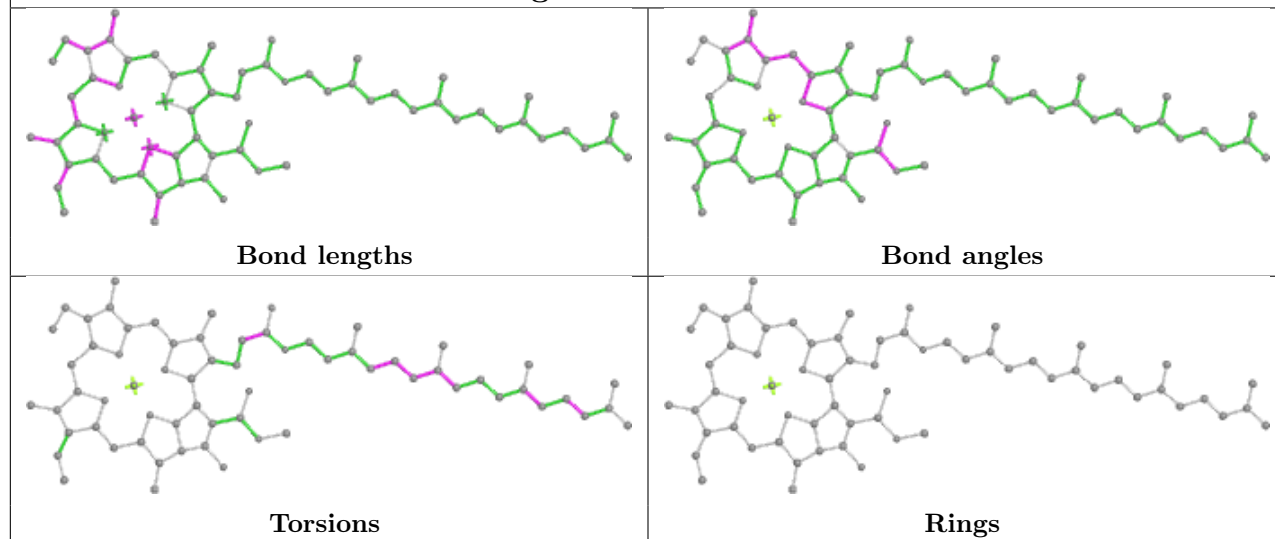
Ligand CLA 1 504



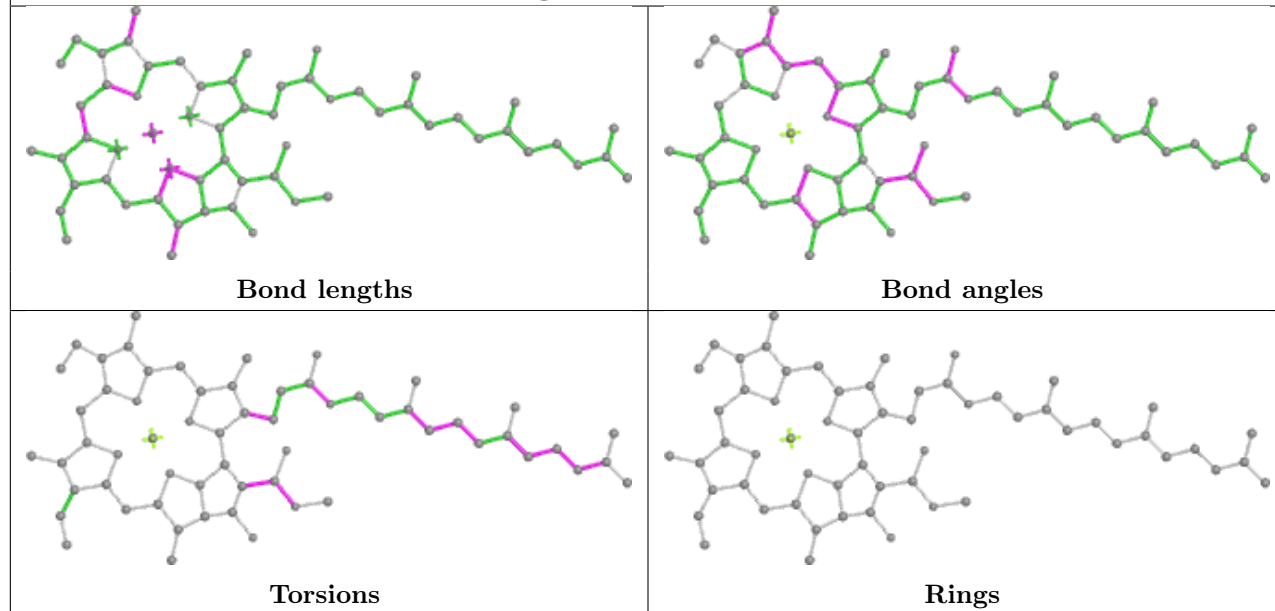
Ligand CLA 2 514



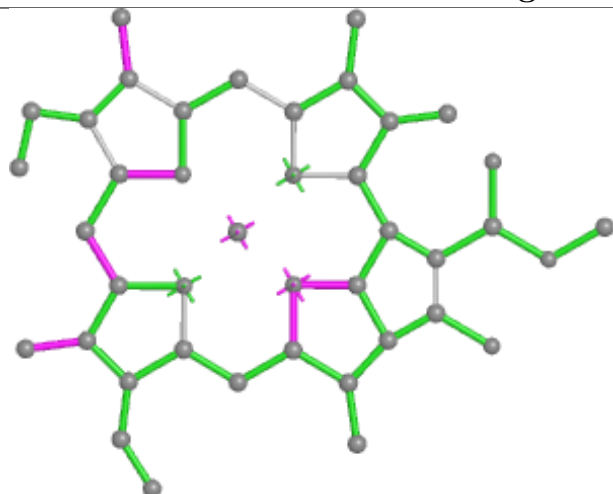
Ligand CLA B 807



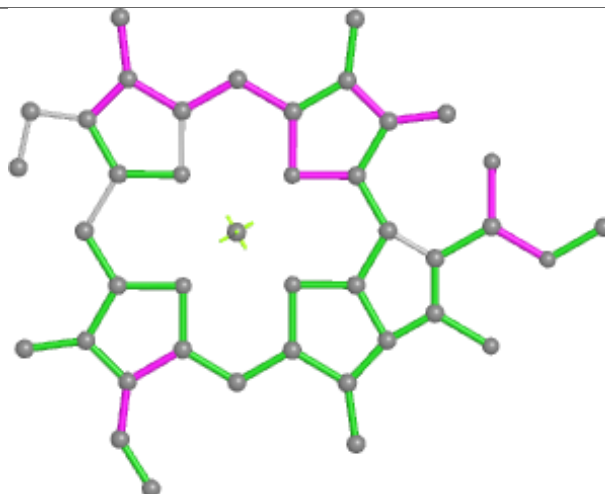
Ligand CLA 2 510



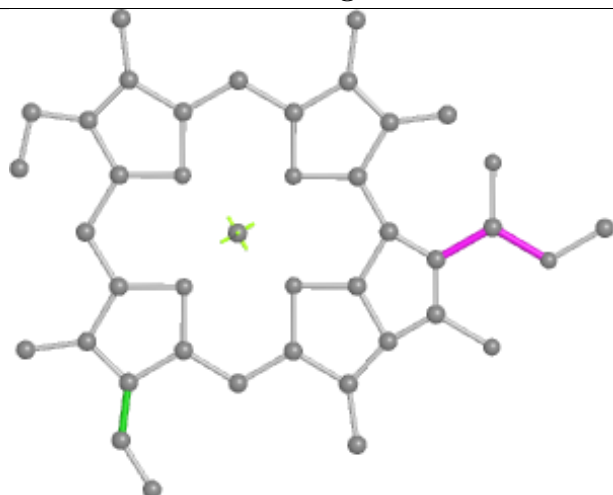
Ligand CLA 3 312



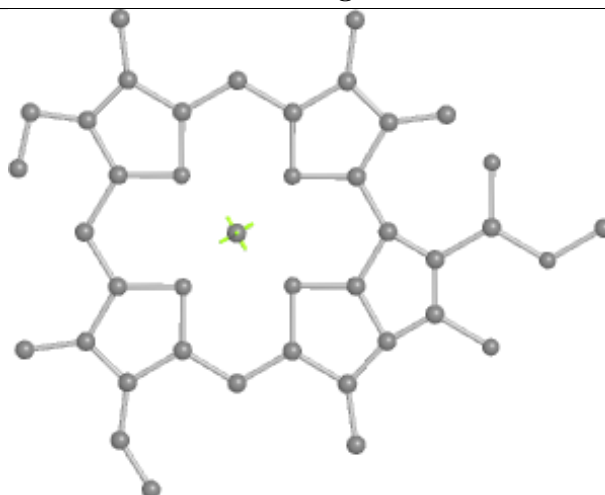
Bond lengths



Bond angles

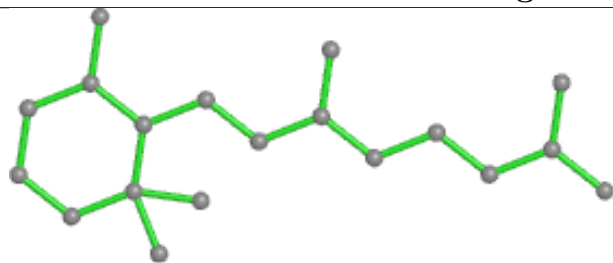


Torsions

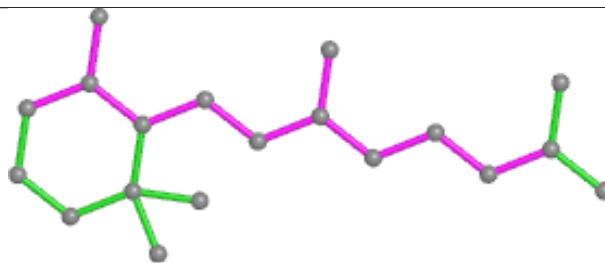


Rings

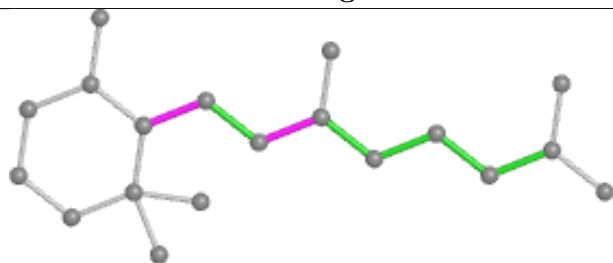
Ligand BCR 1 503



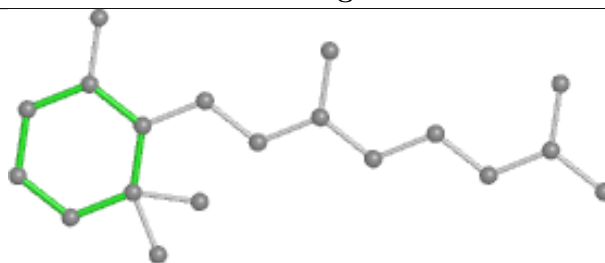
Bond lengths



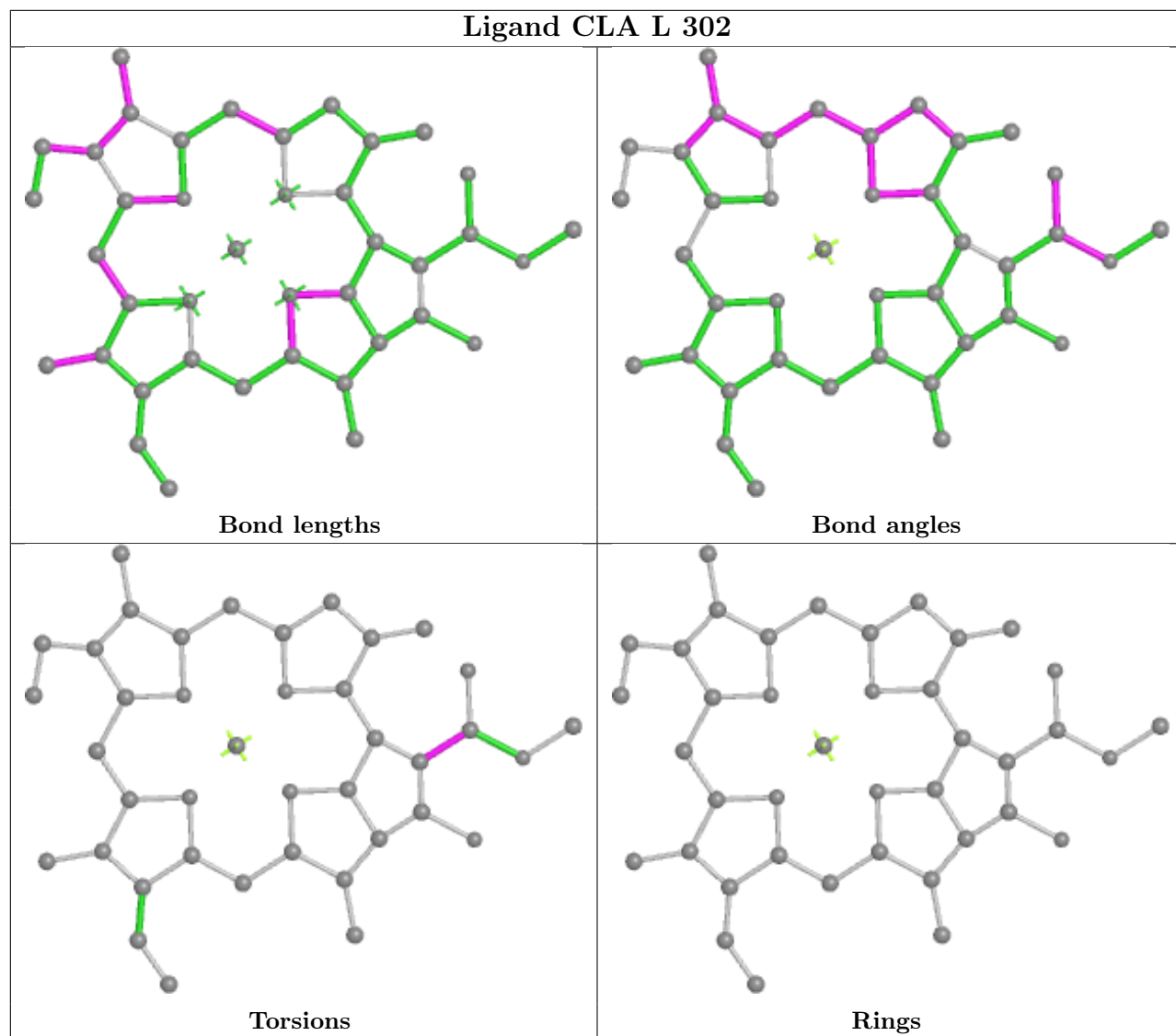
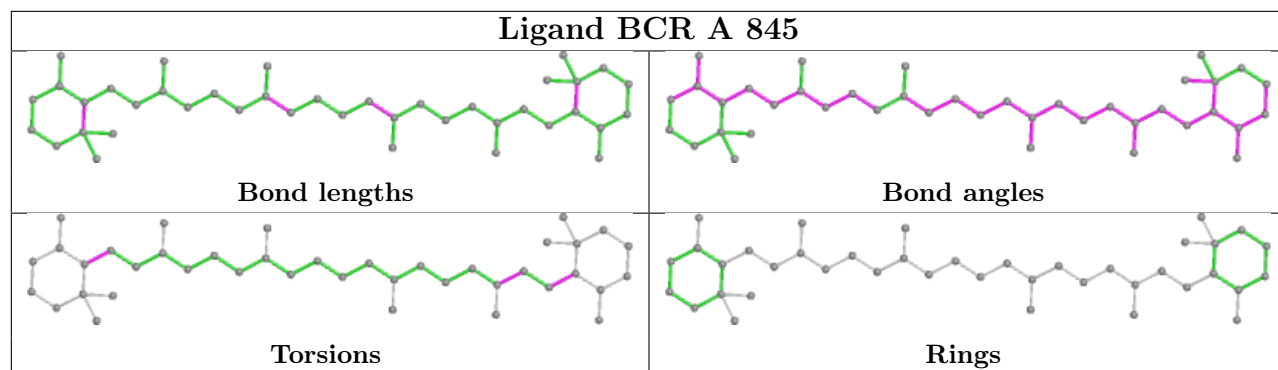
Bond angles



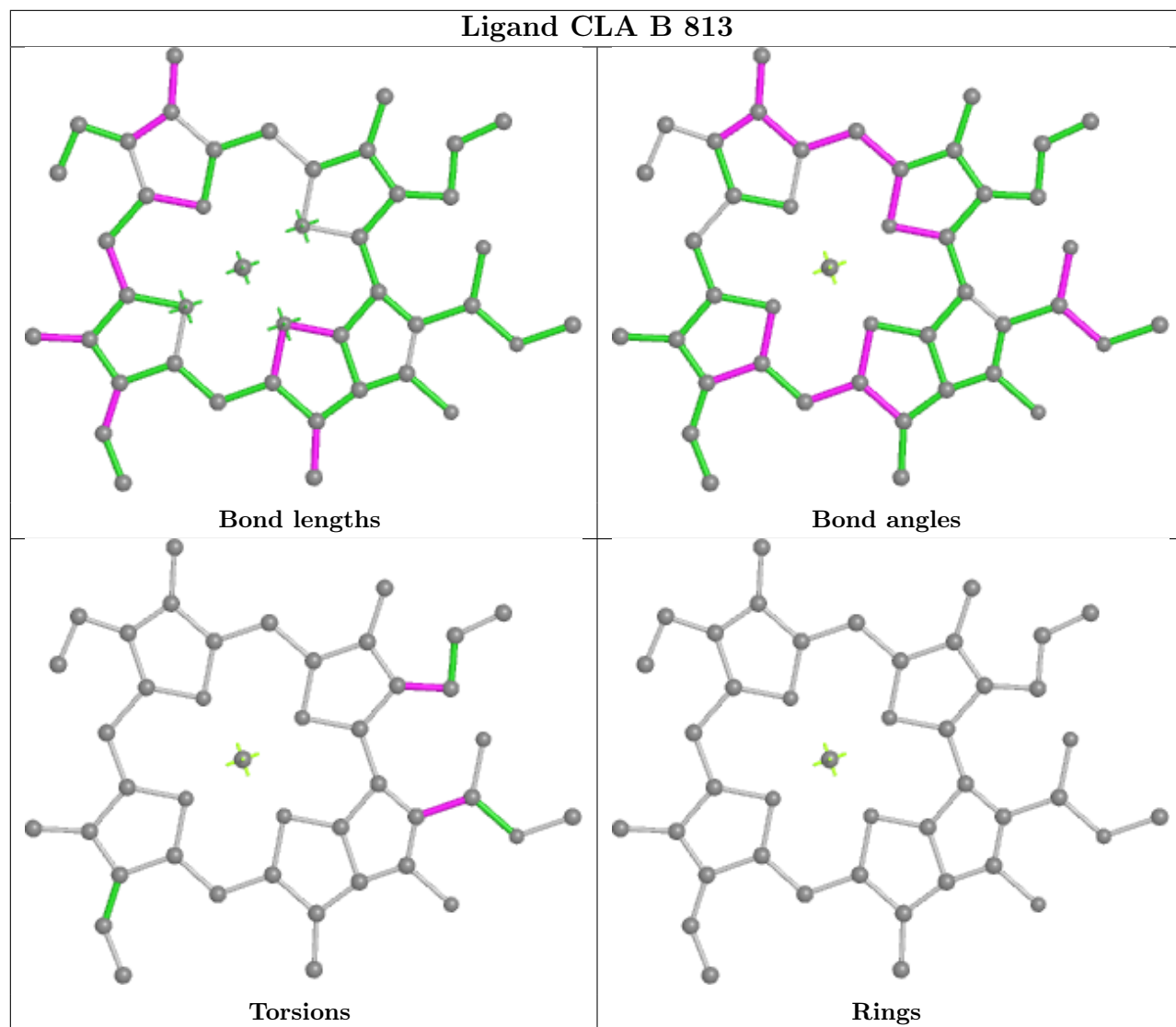
Torsions



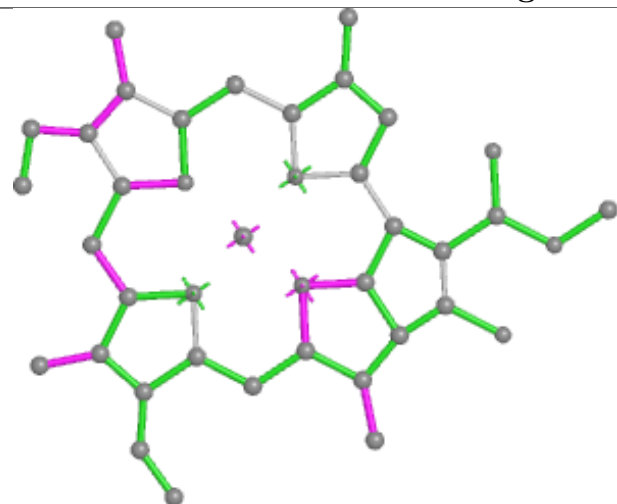
Rings



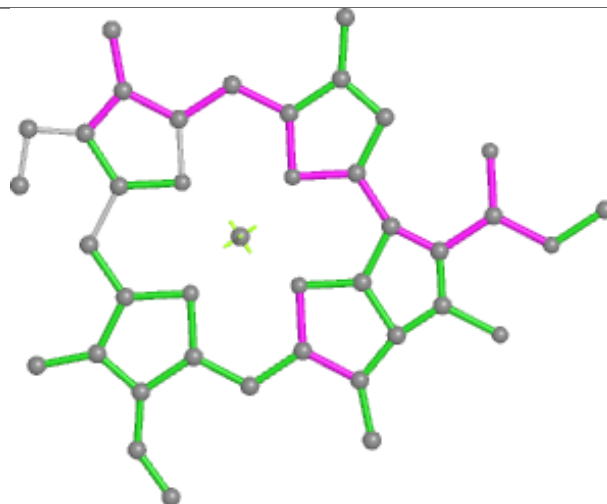
Ligand CLA B 813



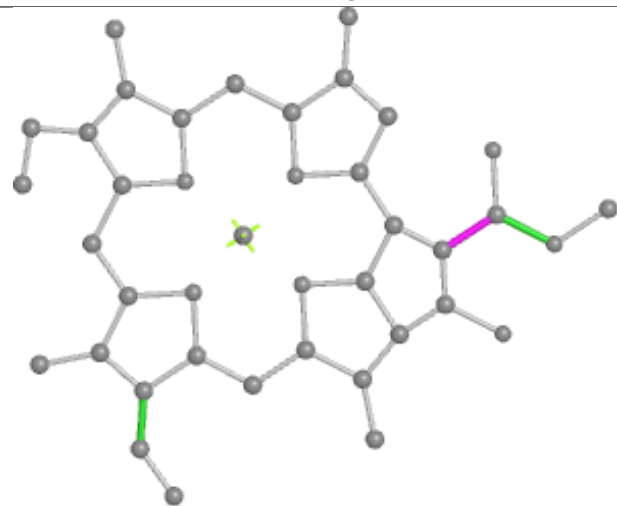
Ligand CLA A 833



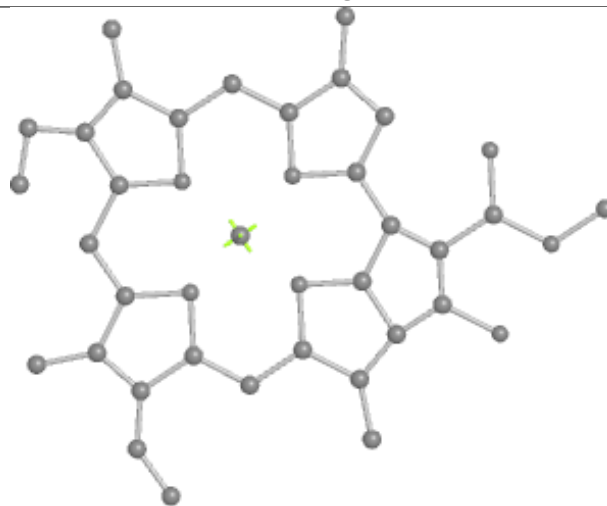
Bond lengths



Bond angles

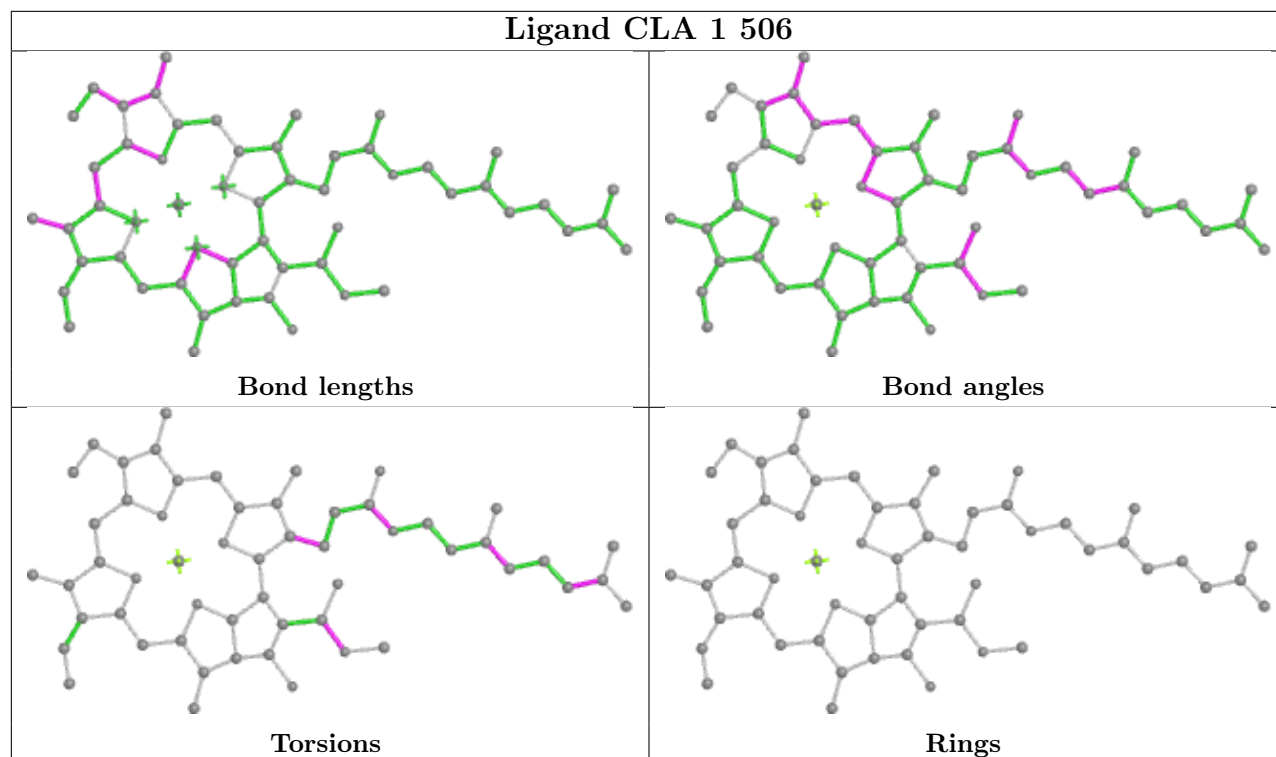


Torsions

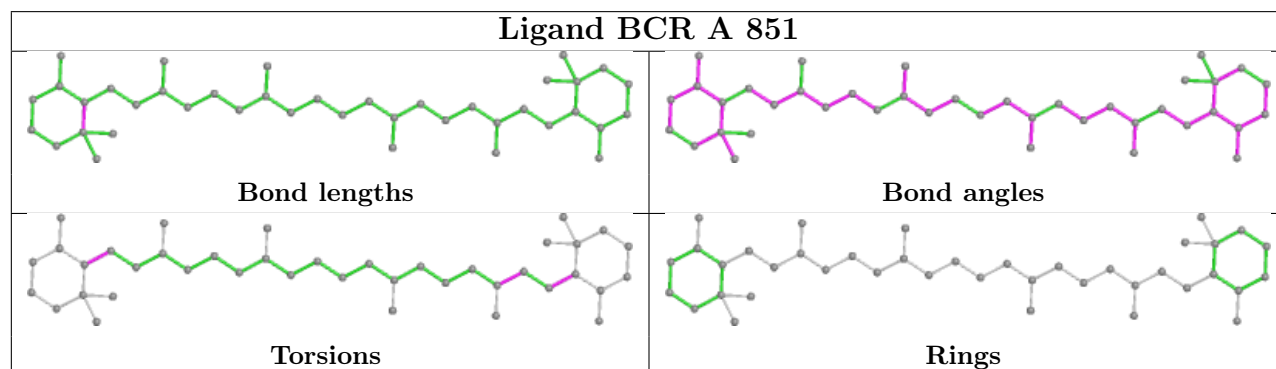


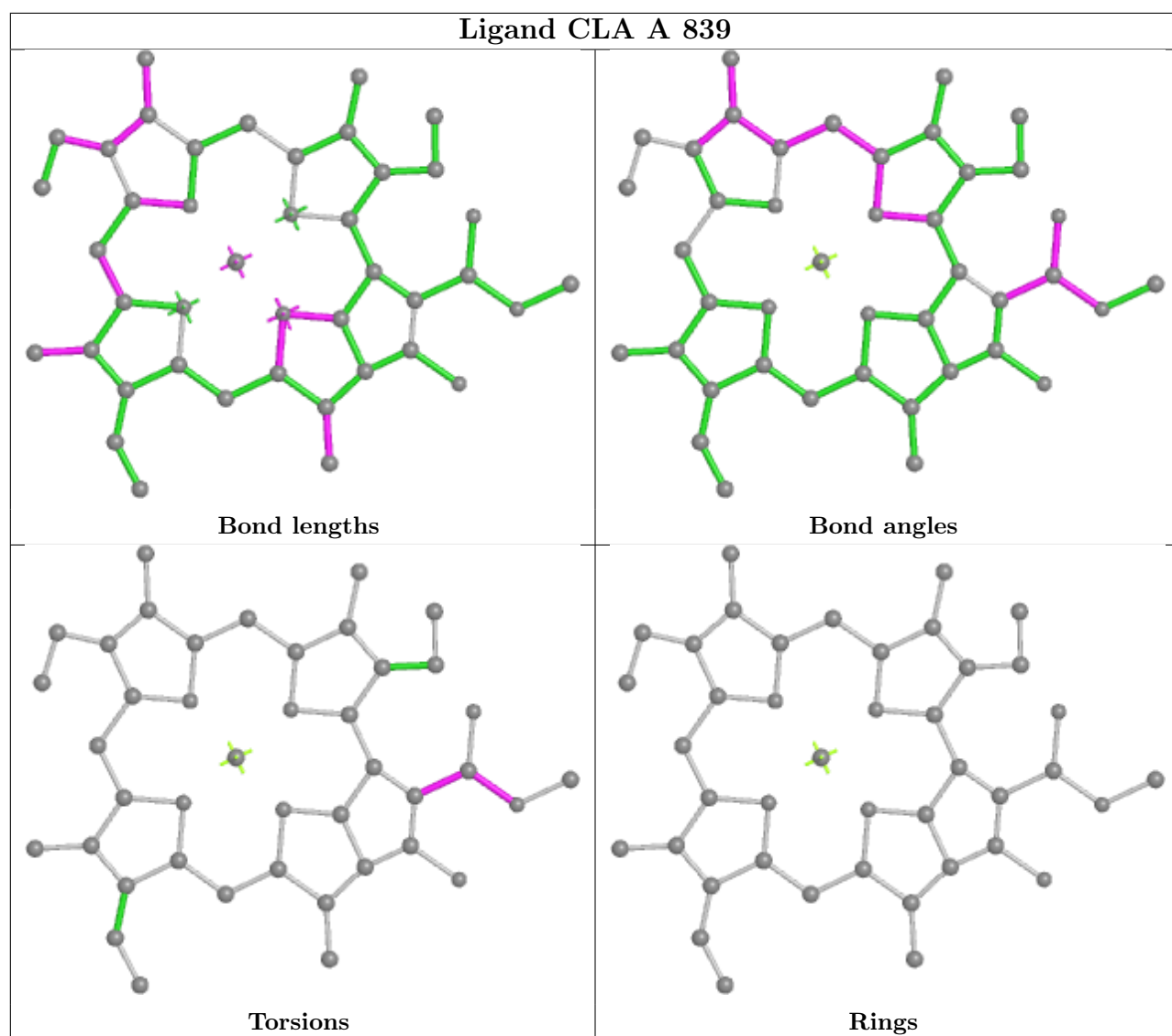
Rings

Ligand CLA 1 506



Ligand BCR A 851





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.

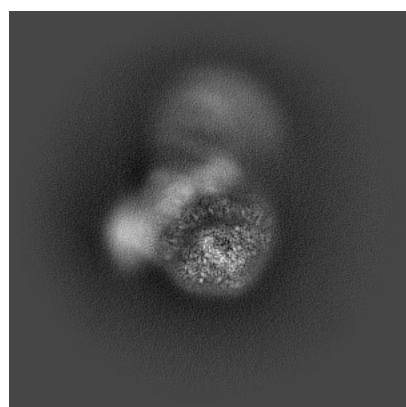
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-31348. These allow visual inspection of the internal detail of the map and identification of artifacts.

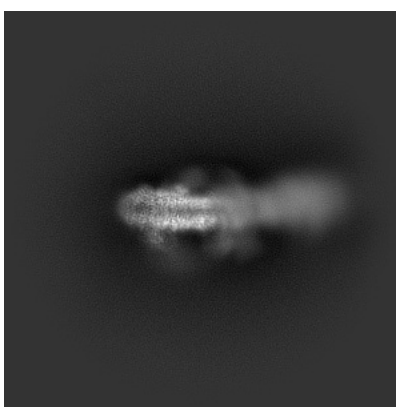
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

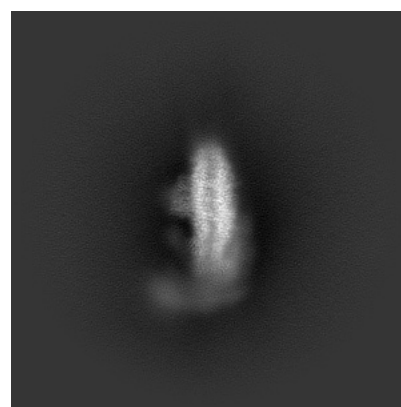
6.1.1 Primary map



X



Y

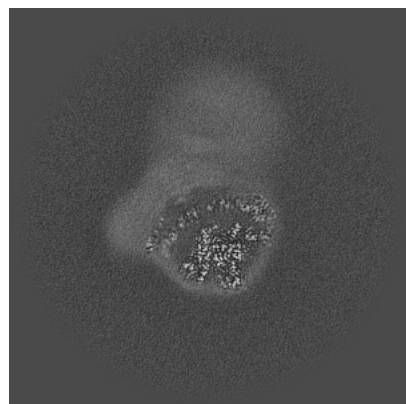


Z

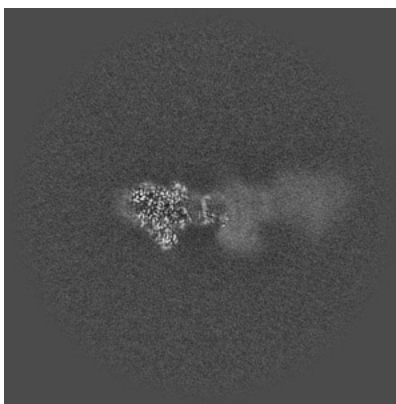
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

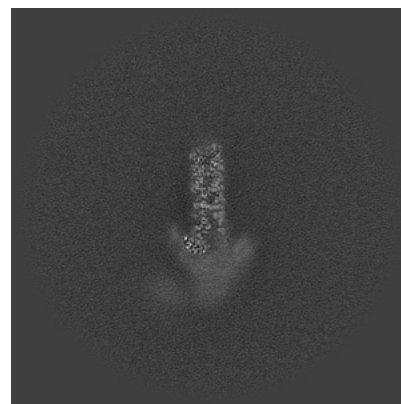
6.2.1 Primary map



X Index: 220



Y Index: 220

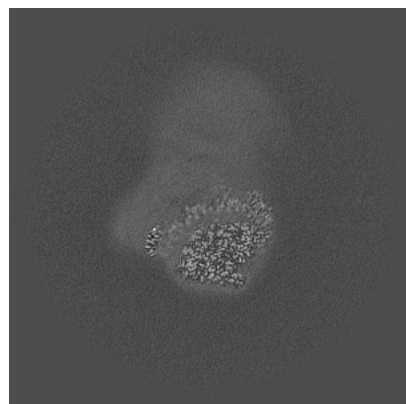


Z Index: 220

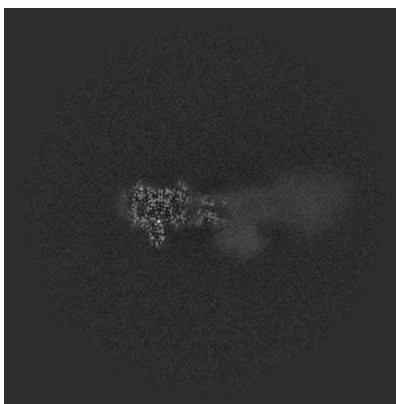
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

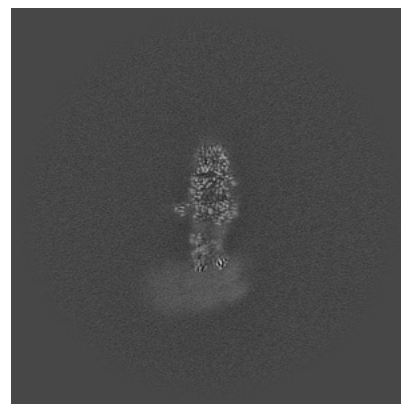
6.3.1 Primary map



X Index: 229



Y Index: 231

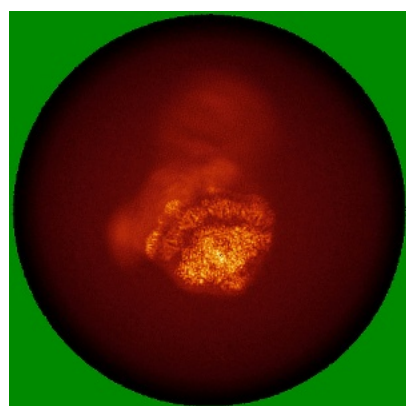


Z Index: 188

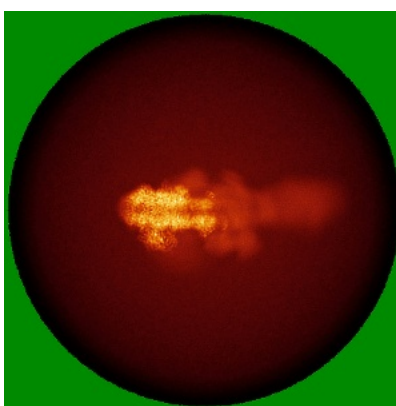
The images above show the largest variance slices of the map in three orthogonal directions.

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

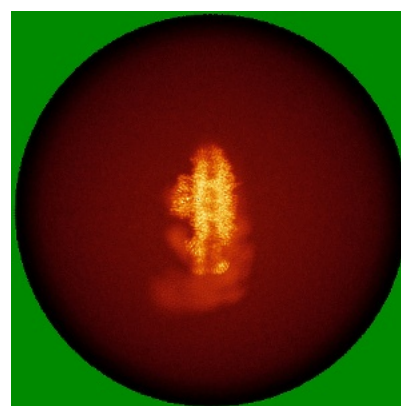
6.4.1 Primary map



X



Y

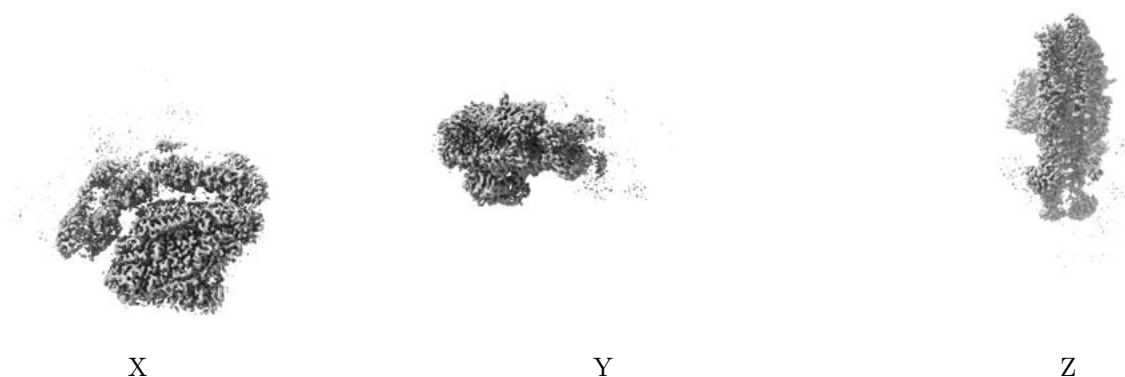


Z

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 0.72. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

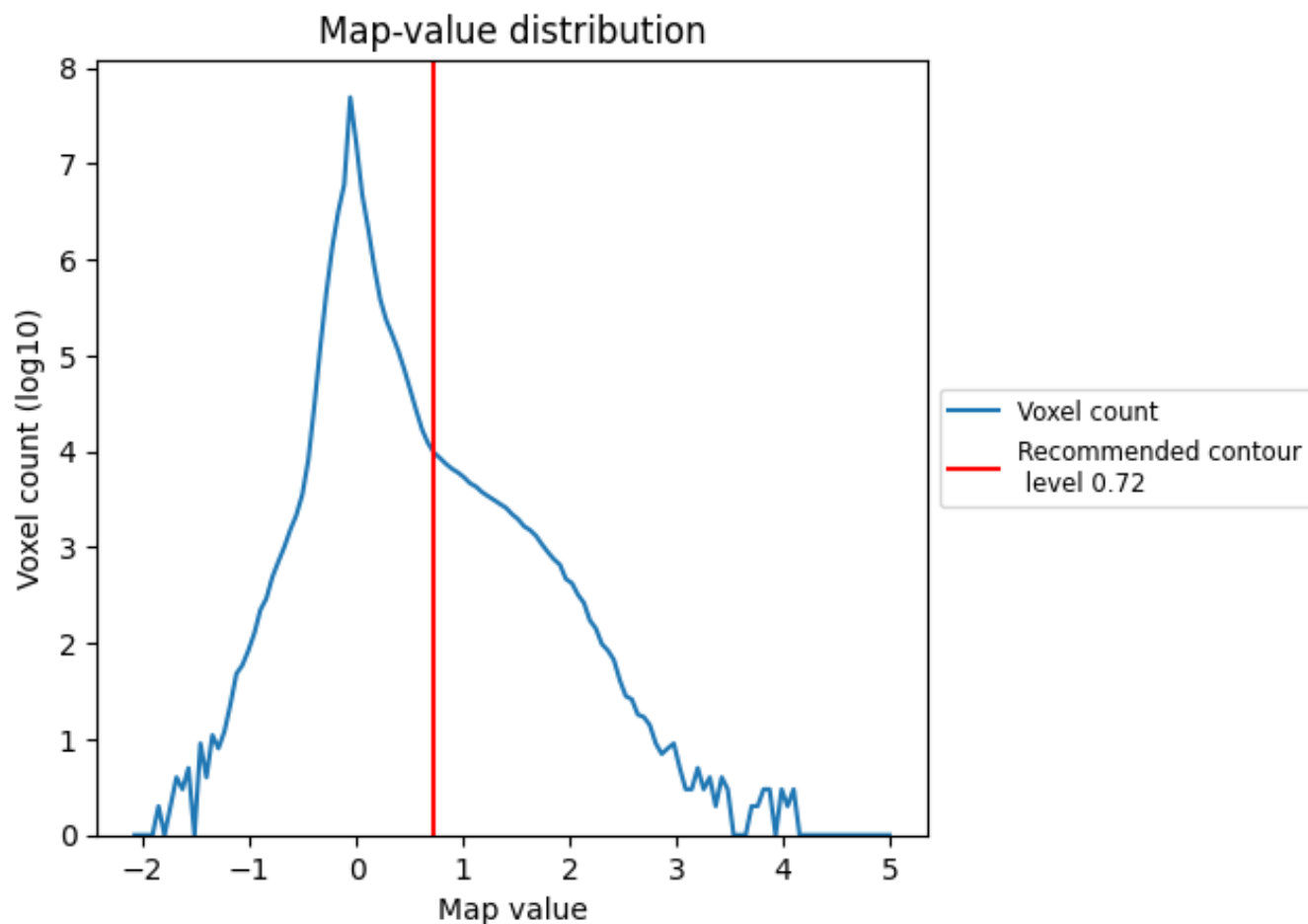
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

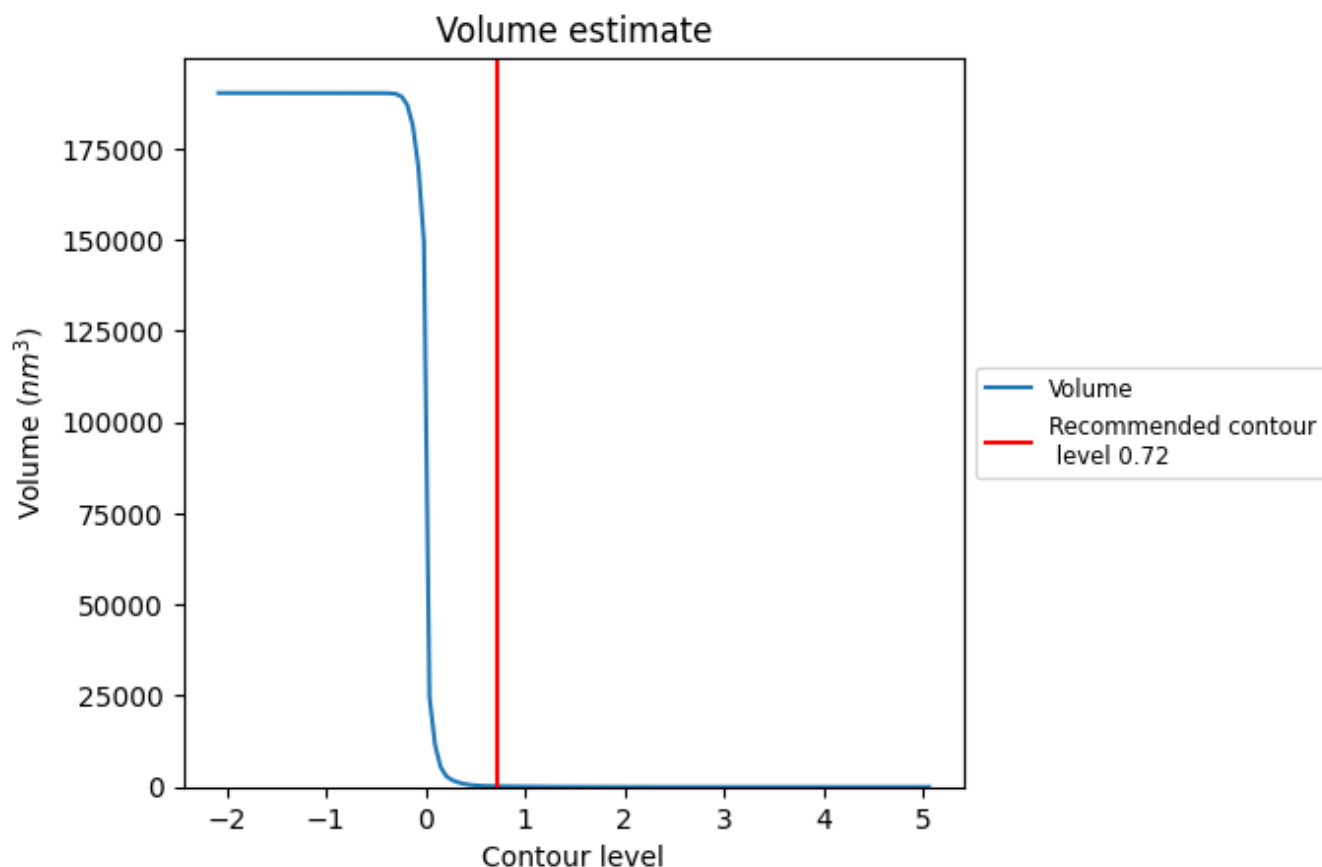
This section contains the results of statistical analysis of the map.

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.

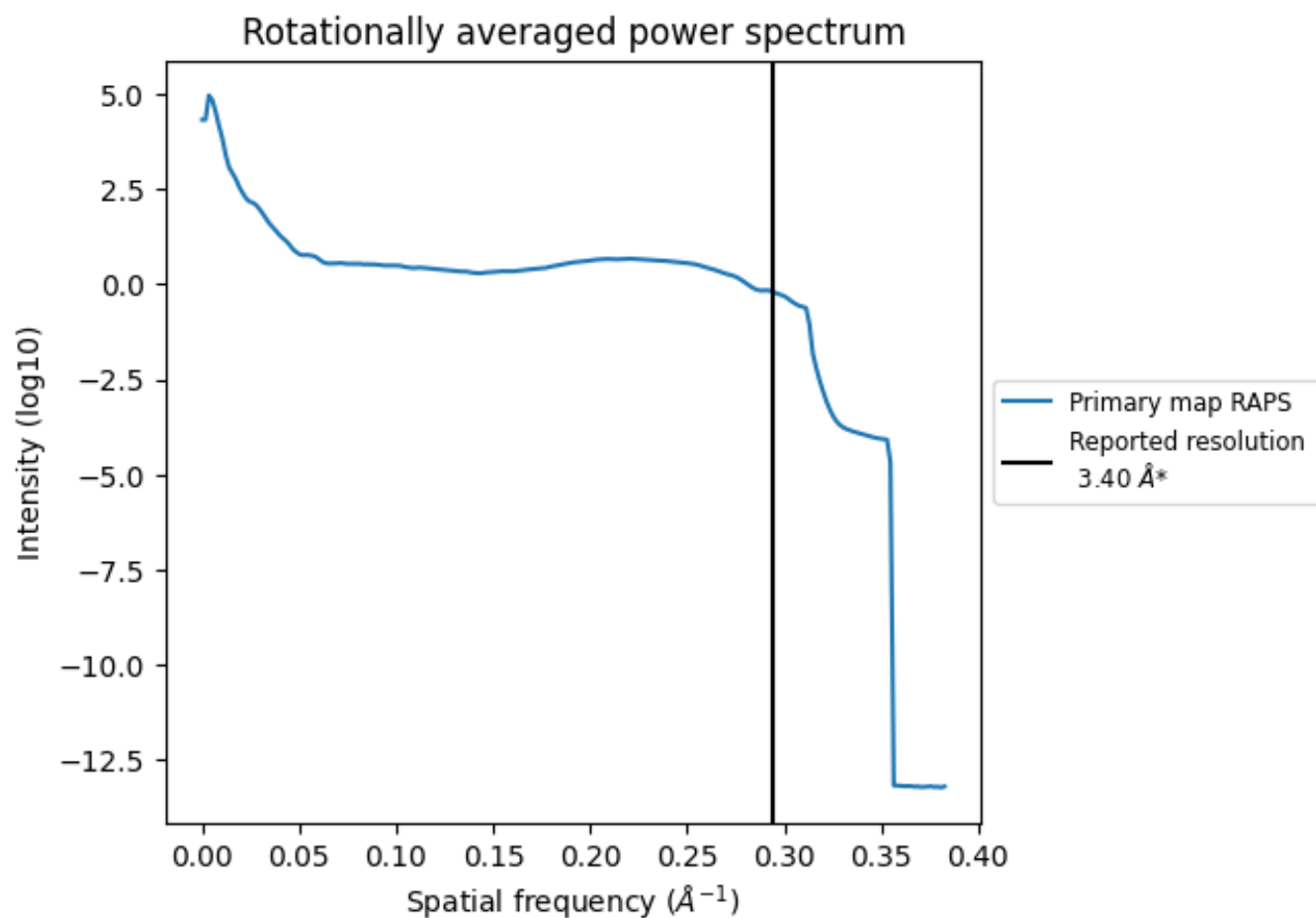
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 189 nm^3 ; this corresponds to an approximate mass of 170 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 0.294 Å⁻¹

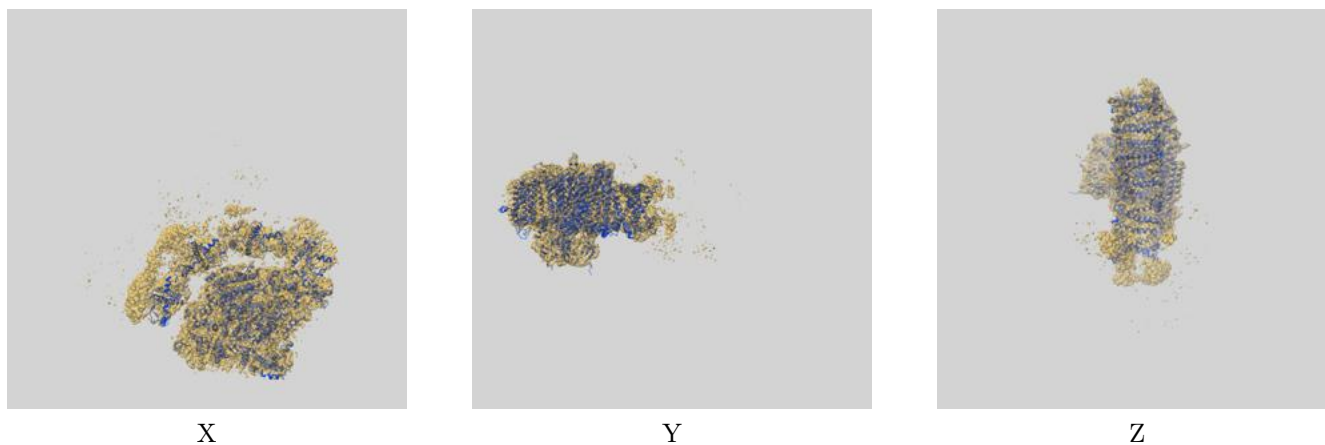
8 Fourier-Shell correlation ⓘ

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

9 Map-model fit [i](#)

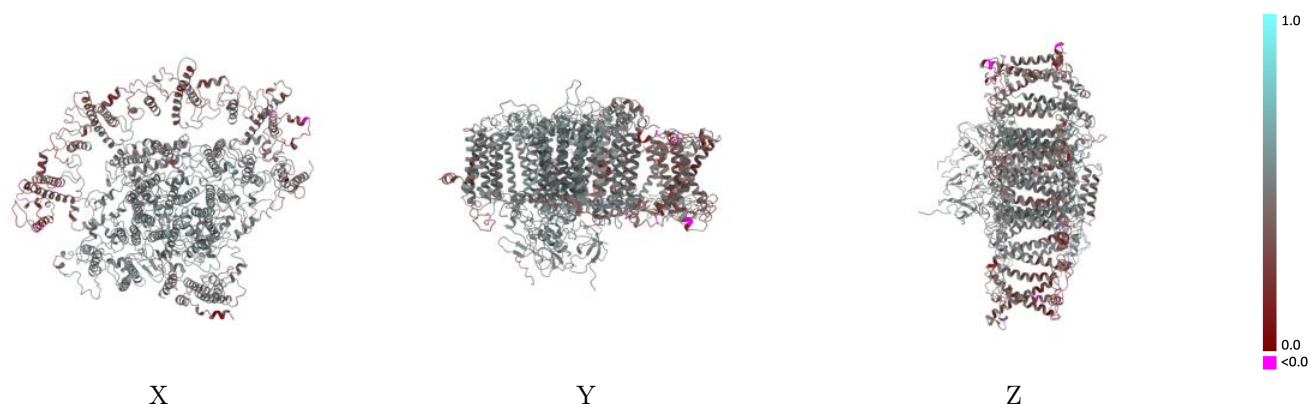
This section contains information regarding the fit between EMDB map EMD-31348 and PDB model 7EW6. Per-residue inclusion information can be found in section [3](#) on page [25](#).

9.1 Map-model overlay [i](#)



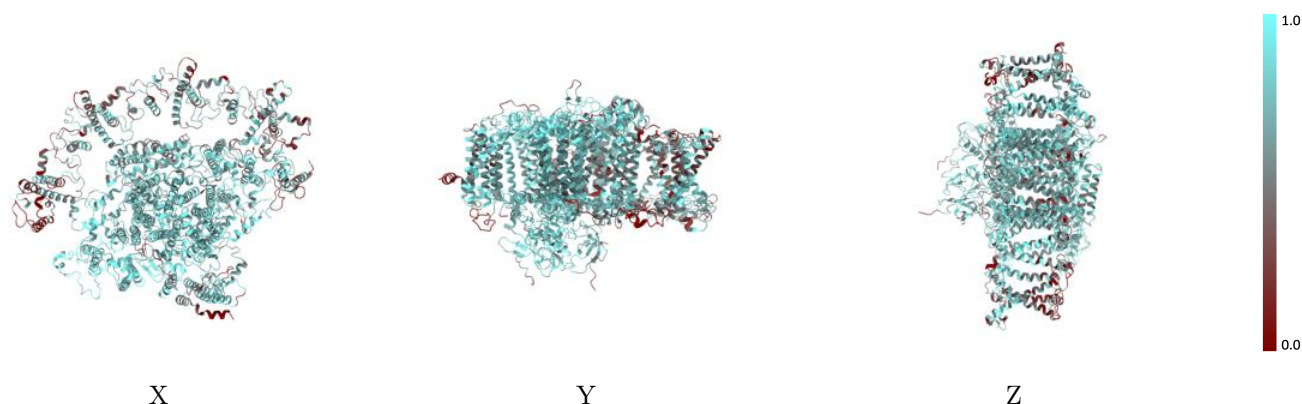
The images above show the 3D surface view of the map at the recommended contour level 0.72 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



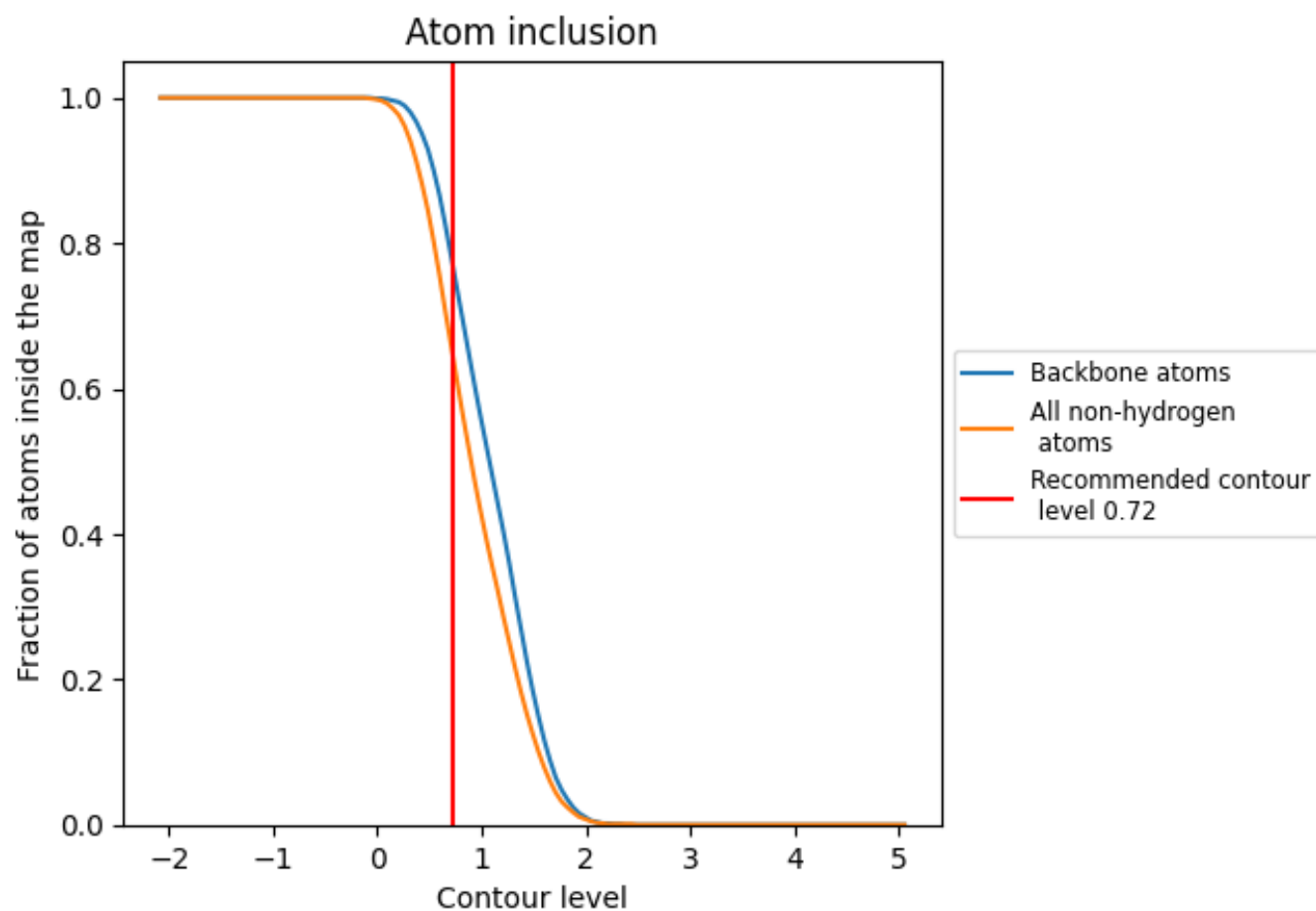
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.72).

9.4 Atom inclusion [i](#)



At the recommended contour level, 77% of all backbone atoms, 65% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.72) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.6480	<div></div> 0.4660
1	<div></div> 0.3980	<div></div> 0.3020
2	<div></div> 0.5250	<div></div> 0.3870
3	<div></div> 0.4570	<div></div> 0.3520
5	<div></div> 0.5640	<div></div> 0.3970
A	<div></div> 0.7350	<div></div> 0.5220
B	<div></div> 0.7690	<div></div> 0.5240
C	<div></div> 0.8610	<div></div> 0.5200
D	<div></div> 0.6940	<div></div> 0.4910
E	<div></div> 0.6980	<div></div> 0.4810
F	<div></div> 0.6450	<div></div> 0.4880
H	<div></div> 0.3740	<div></div> 0.3900
I	<div></div> 0.6750	<div></div> 0.5100
J	<div></div> 0.4840	<div></div> 0.4810
K	<div></div> 0.3900	<div></div> 0.3820
L	<div></div> 0.6170	<div></div> 0.4580

1.0

0.0

<0.0