



Full wwPDB EM Validation Report ⓘ

Oct 14, 2024 – 11:27 PM JST

PDB ID : 7YCA
EMDB ID : EMD-33737
Title : Cryo-EM structure of the PSI-LHCI-Lhcp supercomplex from *Ostreococcus tauri*
Authors : Shan, J.; Sheng, X.; Ishii, A.; Watanabe, A.; Song, C.; Murata, K.; Minagawa, J.; Liu, Z.
Deposited on : 2022-07-01
Resolution : 2.94 Å (reported)
Based on initial models : 7D0J, 5ZJI

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

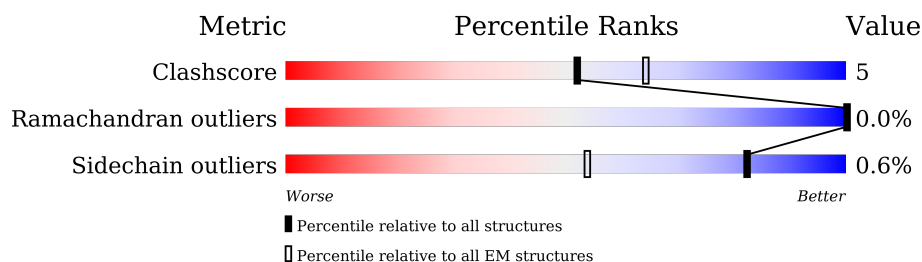
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.94 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	1	225	
2	2	242	
3	3	272	
4	4	236	
5	5	217	
6	6	249	
7	A	751	
8	B	733	

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Mol	Chain	Length	Quality of chain
9	C	81	
10	D	188	
11	E	101	
12	F	231	
13	G	132	
14	H	166	
15	I	35	
16	J	42	
17	K	131	
18	L	204	
19	M	31	
20	N	139	
21	O	136	
22	P	233	
22	R	233	
22	S	233	
22	T	233	
22	U	233	
22	V	233	
22	W	233	
22	X	233	
23	Q	226	

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
24	CHL	1	601	X	-	-	-
24	CHL	1	604	X	-	-	-
24	CHL	2	601	X	-	-	-
24	CHL	2	605	X	-	-	-
24	CHL	2	607	X	-	-	-
24	CHL	2	615	X	-	-	-
24	CHL	3	306	X	-	-	-
24	CHL	4	302	X	-	-	-
24	CHL	4	306	X	-	-	-
24	CHL	4	307	X	-	-	-
24	CHL	4	308	X	-	-	-
24	CHL	5	605	X	-	-	-
24	CHL	6	601	X	-	-	-
24	CHL	6	605	X	-	-	-
24	CHL	6	606	X	-	-	-
24	CHL	P	304	X	-	-	-
24	CHL	P	305	X	-	-	-
24	CHL	P	306	X	-	-	-
24	CHL	P	307	X	-	-	-
24	CHL	P	314	X	-	-	-
24	CHL	Q	307	X	-	-	-
24	CHL	Q	308	X	-	-	-
24	CHL	Q	309	X	-	-	-
24	CHL	Q	316	X	-	-	-
24	CHL	R	302	X	-	-	-
24	CHL	R	308	X	-	-	-
24	CHL	R	309	X	-	-	-
24	CHL	R	310	X	-	-	-
24	CHL	R	311	X	-	-	-
24	CHL	R	318	X	-	-	-
24	CHL	S	304	X	-	-	-
24	CHL	S	305	X	-	-	-
24	CHL	S	306	X	-	-	-
24	CHL	S	307	X	-	-	-
24	CHL	S	314	X	-	-	-
24	CHL	T	304	X	-	-	-
24	CHL	T	305	X	-	-	-
24	CHL	T	306	X	-	-	-
24	CHL	T	307	X	-	-	-
24	CHL	T	314	X	-	-	-
24	CHL	T	320	X	-	-	-
24	CHL	U	304	X	-	-	-
24	CHL	U	305	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	CHL	U	306	X	-	-	-
24	CHL	U	313	X	-	-	-
24	CHL	V	304	X	-	-	-
24	CHL	V	305	X	-	-	-
24	CHL	V	306	X	-	-	-
24	CHL	V	307	X	-	-	-
24	CHL	V	314	X	-	-	-
24	CHL	W	304	X	-	-	-
24	CHL	W	305	X	-	-	-
24	CHL	W	306	X	-	-	-
24	CHL	W	307	X	-	-	-
24	CHL	W	314	X	-	-	-
24	CHL	X	305	X	-	-	-
24	CHL	X	306	X	-	-	-
24	CHL	X	307	X	-	-	-
24	CHL	X	308	X	-	-	-
24	CHL	X	315	X	-	-	-
25	CLA	1	602	X	-	-	-
25	CLA	1	603	X	-	-	-
25	CLA	1	605	X	-	-	-
25	CLA	1	606	X	-	-	-
25	CLA	1	607	X	-	-	-
25	CLA	1	608	X	-	-	-
25	CLA	1	609	X	-	-	-
25	CLA	1	613	X	-	-	-
25	CLA	2	602	X	-	-	-
25	CLA	2	603	X	-	-	-
25	CLA	2	604	X	-	-	-
25	CLA	2	606	X	-	-	-
25	CLA	2	608	X	-	-	-
25	CLA	2	609	X	-	-	-
25	CLA	2	610	X	-	-	-
25	CLA	2	611	X	-	-	-
25	CLA	2	612	X	-	-	-
25	CLA	2	613	X	-	-	-
25	CLA	2	614	X	-	-	-
25	CLA	3	301	X	-	-	-
25	CLA	3	302	X	-	-	-
25	CLA	3	303	X	-	-	-
25	CLA	3	304	X	-	-	-
25	CLA	3	305	X	-	-	-
25	CLA	3	307	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CLA	3	308	X	-	-	-
25	CLA	3	309	X	-	-	-
25	CLA	3	310	X	-	-	-
25	CLA	3	311	X	-	-	-
25	CLA	3	312	X	-	-	-
25	CLA	3	313	X	-	-	-
25	CLA	4	303	X	-	-	-
25	CLA	4	304	X	-	-	-
25	CLA	4	305	X	-	-	-
25	CLA	4	309	X	-	-	-
25	CLA	4	310	X	-	-	-
25	CLA	4	311	X	-	-	-
25	CLA	4	312	X	-	-	-
25	CLA	4	314	X	-	-	-
25	CLA	4	315	X	-	-	-
25	CLA	4	316	X	-	-	-
25	CLA	5	601	X	-	-	-
25	CLA	5	602	X	-	-	-
25	CLA	5	603	X	-	-	-
25	CLA	5	604	X	-	-	-
25	CLA	5	606	X	-	-	-
25	CLA	5	607	X	-	-	-
25	CLA	5	608	X	-	-	-
25	CLA	5	609	X	-	-	-
25	CLA	5	610	X	-	-	-
25	CLA	6	602	X	-	-	-
25	CLA	6	603	X	-	-	-
25	CLA	6	604	X	-	-	-
25	CLA	6	607	X	-	-	-
25	CLA	6	608	X	-	-	-
25	CLA	6	609	X	-	-	-
25	CLA	6	610	X	-	-	-
25	CLA	6	611	X	-	-	-
25	CLA	6	612	X	-	-	-
25	CLA	A	803	X	-	-	-
25	CLA	A	804	X	-	-	-
25	CLA	A	805	X	-	-	-
25	CLA	A	806	X	-	-	-
25	CLA	A	807	X	-	-	-
25	CLA	A	808	X	-	-	-
25	CLA	A	809	X	-	-	-
25	CLA	A	810	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CLA	A	811	X	-	-	-
25	CLA	A	812	X	-	-	-
25	CLA	A	813	X	-	-	-
25	CLA	A	814	X	-	-	-
25	CLA	A	815	X	-	-	-
25	CLA	A	816	X	-	-	-
25	CLA	A	818	X	-	-	-
25	CLA	A	819	X	-	-	-
25	CLA	A	820	X	-	-	-
25	CLA	A	821	X	-	-	-
25	CLA	A	822	X	-	-	-
25	CLA	A	823	X	-	-	-
25	CLA	A	824	X	-	-	-
25	CLA	A	825	X	-	-	-
25	CLA	A	826	X	-	-	-
25	CLA	A	827	X	-	-	-
25	CLA	A	829	X	-	-	-
25	CLA	A	830	X	-	-	-
25	CLA	A	831	X	-	-	-
25	CLA	A	832	X	-	-	-
25	CLA	A	834	X	-	-	-
25	CLA	A	835	X	-	-	-
25	CLA	A	836	X	-	-	-
25	CLA	A	837	X	-	-	-
25	CLA	A	839	X	-	-	-
25	CLA	A	841	X	-	-	-
25	CLA	A	842	X	-	-	-
25	CLA	A	843	X	-	-	-
25	CLA	A	845	X	-	-	-
25	CLA	A	856	X	-	-	-
25	CLA	B	802	X	-	-	-
25	CLA	B	803	X	-	-	-
25	CLA	B	804	X	-	-	-
25	CLA	B	805	X	-	-	-
25	CLA	B	806	X	-	-	-
25	CLA	B	807	X	-	-	-
25	CLA	B	808	X	-	-	-
25	CLA	B	809	X	-	-	-
25	CLA	B	810	X	-	-	-
25	CLA	B	811	X	-	-	-
25	CLA	B	812	X	-	-	-
25	CLA	B	813	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CLA	B	814	X	-	-	-
25	CLA	B	815	X	-	-	-
25	CLA	B	816	X	-	-	-
25	CLA	B	817	X	-	-	-
25	CLA	B	818	X	-	-	-
25	CLA	B	819	X	-	-	-
25	CLA	B	820	X	-	-	-
25	CLA	B	821	X	-	-	-
25	CLA	B	822	X	-	-	-
25	CLA	B	823	X	-	-	-
25	CLA	B	824	X	-	-	-
25	CLA	B	825	X	-	-	-
25	CLA	B	826	X	-	-	-
25	CLA	B	827	X	-	-	-
25	CLA	B	828	X	-	-	-
25	CLA	B	829	X	-	-	-
25	CLA	B	830	X	-	-	-
25	CLA	B	831	X	-	-	-
25	CLA	B	832	X	-	-	-
25	CLA	B	833	X	-	-	-
25	CLA	B	834	X	-	-	-
25	CLA	B	835	X	-	-	-
25	CLA	B	837	X	-	-	-
25	CLA	B	838	X	-	-	-
25	CLA	B	839	X	-	-	-
25	CLA	B	841	X	-	-	-
25	CLA	B	842	X	-	-	-
25	CLA	B	843	X	-	-	-
25	CLA	F	802	X	-	-	-
25	CLA	F	803	X	-	-	-
25	CLA	G	202	X	-	-	-
25	CLA	G	203	X	-	-	-
25	CLA	G	204	X	-	-	-
25	CLA	H	301	X	-	-	-
25	CLA	H	302	X	-	-	-
25	CLA	H	304	X	-	-	-
25	CLA	J	102	X	-	-	-
25	CLA	K	201	X	-	-	-
25	CLA	K	203	X	-	-	-
25	CLA	K	204	X	-	-	-
25	CLA	K	206	X	-	-	-
25	CLA	L	301	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CLA	L	303	X	-	-	-
25	CLA	L	304	X	-	-	-
25	CLA	N	202	X	-	-	-
25	CLA	N	203	X	-	-	-
25	CLA	O	2001	X	-	-	-
25	CLA	O	2002	X	-	-	-
25	CLA	O	2003	X	-	-	-
25	CLA	O	2004	X	-	-	-
25	CLA	O	2005	X	-	-	-
25	CLA	P	301	X	-	-	-
25	CLA	P	302	X	-	-	-
25	CLA	P	303	X	-	-	-
25	CLA	P	309	X	-	-	-
25	CLA	P	310	X	-	-	-
25	CLA	P	311	X	-	-	-
25	CLA	P	312	X	-	-	-
25	CLA	Q	301	X	-	-	-
25	CLA	Q	304	X	-	-	-
25	CLA	Q	305	X	-	-	-
25	CLA	Q	306	X	-	-	-
25	CLA	Q	311	X	-	-	-
25	CLA	Q	312	X	-	-	-
25	CLA	Q	313	X	-	-	-
25	CLA	Q	314	X	-	-	-
25	CLA	Q	315	X	-	-	-
25	CLA	R	305	X	-	-	-
25	CLA	R	306	X	-	-	-
25	CLA	R	307	X	-	-	-
25	CLA	R	313	X	-	-	-
25	CLA	R	314	X	-	-	-
25	CLA	R	315	X	-	-	-
25	CLA	R	316	X	-	-	-
25	CLA	S	301	X	-	-	-
25	CLA	S	302	X	-	-	-
25	CLA	S	303	X	-	-	-
25	CLA	S	309	X	-	-	-
25	CLA	S	310	X	-	-	-
25	CLA	S	311	X	-	-	-
25	CLA	S	312	X	-	-	-
25	CLA	S	313	X	-	-	-
25	CLA	T	301	X	-	-	-
25	CLA	T	302	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CLA	T	303	X	-	-	-
25	CLA	T	309	X	-	-	-
25	CLA	T	310	X	-	-	-
25	CLA	T	311	X	-	-	-
25	CLA	T	312	X	-	-	-
25	CLA	T	313	X	-	-	-
25	CLA	U	301	X	-	-	-
25	CLA	U	302	X	-	-	-
25	CLA	U	303	X	-	-	-
25	CLA	U	308	X	-	-	-
25	CLA	U	309	X	-	-	-
25	CLA	U	310	X	-	-	-
25	CLA	U	311	X	-	-	-
25	CLA	U	312	X	-	-	-
25	CLA	V	301	X	-	-	-
25	CLA	V	302	X	-	-	-
25	CLA	V	303	X	-	-	-
25	CLA	V	309	X	-	-	-
25	CLA	V	310	X	-	-	-
25	CLA	V	311	X	-	-	-
25	CLA	V	313	X	-	-	-
25	CLA	W	301	X	-	-	-
25	CLA	W	302	X	-	-	-
25	CLA	W	303	X	-	-	-
25	CLA	W	309	X	-	-	-
25	CLA	W	310	X	-	-	-
25	CLA	W	311	X	-	-	-
25	CLA	W	312	X	-	-	-
25	CLA	W	313	X	-	-	-
25	CLA	X	302	X	-	-	-
25	CLA	X	303	X	-	-	-
25	CLA	X	304	X	-	-	-
25	CLA	X	310	X	-	-	-
25	CLA	X	311	X	-	-	-
25	CLA	X	312	X	-	-	-
25	CLA	X	313	X	-	-	-
25	CLA	X	314	X	-	-	-
33	CL0	A	802	X	-	-	-

2 Entry composition

There are 39 unique types of molecules in this entry. The entry contains 64832 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 Lhca1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	159	Total	C	N	O	S	0	0
			1209	768	219	213	9		

- Molecule 2 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	205	Total	C	N	O	S	0	0
			1583	1023	265	286	9		

- Molecule 3 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	3	227	Total	C	N	O	S	0	0
			1717	1111	279	311	16		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	4	203	Total	C	N	O	S	0	0
			1579	1021	267	280	11		

- Molecule 5 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	5	166	Total	C	N	O	S	0	0
			1278	826	215	226	11		

- Molecule 6 is a protein called Lhca6.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	6	194	Total	C	N	O	S	0	0
			1484	963	243	269	9		

- Molecule 7 is a protein called Photosystem I P700 chlorophyll a apoprotein A1.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	A	742	Total	C	N	O	S	0	0
			5819	3802	990	1000	27		

- Molecule 8 is a protein called Photosystem I P700 chlorophyll a apoprotein A2.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	B	732	Total	C	N	O	S	0	0
			5773	3793	966	996	18		

- Molecule 9 is a protein called Photosystem I iron-sulfur center.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	C	80	Total	C	N	O	S	0	0
			593	364	103	115	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	D	143	Total	C	N	O	S	0	0
			1116	717	197	196	6		

- Molecule 11 is a protein called Photosystem I reaction centre subunit IV.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	E	62	Total	C	N	O	S	0	0
			503	324	84	94	1		

- Molecule 12 is a protein called Photosystem I reaction center subunit III.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	F	165	Total	C	N	O	S	0	0
			1259	808	212	235	4		

- Molecule 13 is a protein called PsaG.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	G	95	Total	C	N	O	S	0	0
			717	453	124	137	3		

- Molecule 14 is a protein called Photosystem I PsuH, reaction centre subunit VI.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	H	96	Total	C	N	O	0	0
			721	456	122	143		

- Molecule 15 is a protein called Photosystem I reaction center subunit VIII.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	I	35	Total	C	N	O	S	0	0
			264	181	37	44	2		

- Molecule 16 is a protein called Photosystem I reaction center subunit IX.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	J	41	Total	C	N	O	S	0	0
			328	225	49	53	1		

- Molecule 17 is a protein called Photosystem I PsaG/PsaK protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	K	87	Total	C	N	O	S	0	0
			625	393	106	121	5		

- Molecule 18 is a protein called PSI subunit V.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	L	158	Total	C	N	O	S	0	0
			1169	759	190	217	3		

- Molecule 19 is a protein called Photosystem I reaction center subunit XII.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	M	31	Total	C	N	O	S	0	0
			239	159	37	42	1		

- Molecule 20 is a protein called Photosystem I PsaN, reaction centre subunit N.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	N	91	Total	C	N	O	S	0	0
			676	415	118	138	5		

- Molecule 21 is a protein called PsaO.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	O	96	Total	C	N	O	S	0	0
			759	498	123	132	6		

- Molecule 22 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	P	201	Total	C	N	O	S	0	0
			1507	968	246	287	6		
22	R	201	Total	C	N	O	S	0	0
			1507	968	246	287	6		
22	S	202	Total	C	N	O	S	0	0
			1512	971	247	288	6		
22	T	201	Total	C	N	O	S	0	0
			1507	968	246	287	6		
22	U	201	Total	C	N	O	S	0	0
			1507	968	246	287	6		
22	V	197	Total	C	N	O	S	0	0
			1484	956	242	280	6		
22	W	200	Total	C	N	O	S	0	0
			1499	964	245	284	6		
22	X	196	Total	C	N	O	S	0	0
			1474	949	241	278	6		

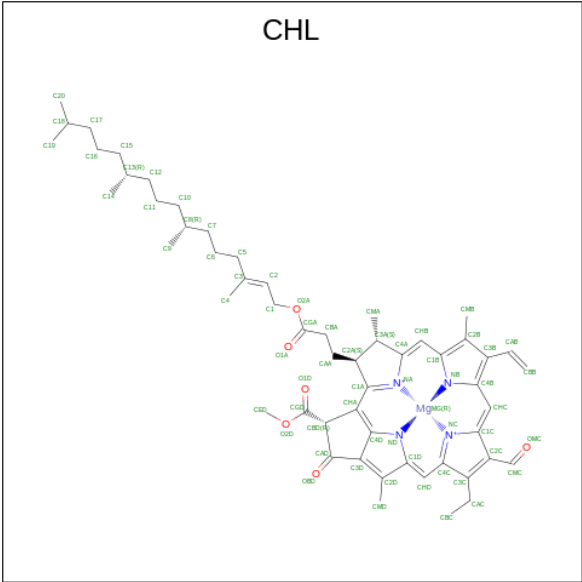
- Molecule 23 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms						AltConf	Trace
23	Q	226	Total	C	N	O	P	S	0	0
			1706	1100	285	313	1	7		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q	28	ACE	-	acetylation	UNP A0A090LYE8

- Molecule 24 is CHLOROPHYLL B (three-letter code: CHL) (formula: $C_{55}H_{70}MgN_4O_6$).



Mol	Chain	Residues	Atoms					AltConf
24	1	1	Total	C	Mg	N	O	0
			55	44	1	4	6	
24	1	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
24	2	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
24	2	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
24	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
24	2	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
24	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
24	4	1	Total	C	Mg	N	O	0
			52	41	1	4	6	
24	4	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
24	4	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
24	4	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
24	5	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
24	6	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
24	6	1	Total	C	Mg	N	O	0
			42	33	1	4	4	

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Mol	Chain	Residues	Atoms					AltConf
24	6	1	Total 43	C 34	Mg 1	N 4	O 4	0
24	P	1	Total 46	C 35	Mg 1	N 4	O 6	0
24	P	1	Total 46	C 35	Mg 1	N 4	O 6	0
24	P	1	Total 52	C 41	Mg 1	N 4	O 6	0
24	P	1	Total 44	C 35	Mg 1	N 4	O 4	0
24	P	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	Q	1	Total 46	C 35	Mg 1	N 4	O 6	0
24	Q	1	Total 50	C 39	Mg 1	N 4	O 6	0
24	Q	1	Total 44	C 35	Mg 1	N 4	O 4	0
24	Q	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	R	1	Total 47	C 36	Mg 1	N 4	O 6	0
24	R	1	Total 46	C 35	Mg 1	N 4	O 6	0
24	R	1	Total 50	C 39	Mg 1	N 4	O 6	0
24	R	1	Total 52	C 41	Mg 1	N 4	O 6	0
24	R	1	Total 44	C 35	Mg 1	N 4	O 4	0
24	R	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	S	1	Total 42	C 33	Mg 1	N 4	O 4	0
24	S	1	Total 42	C 33	Mg 1	N 4	O 4	0
24	S	1	Total 52	C 41	Mg 1	N 4	O 6	0
24	S	1	Total 42	C 33	Mg 1	N 4	O 4	0
24	S	1	Total 45	C 35	Mg 1	N 4	O 5	0

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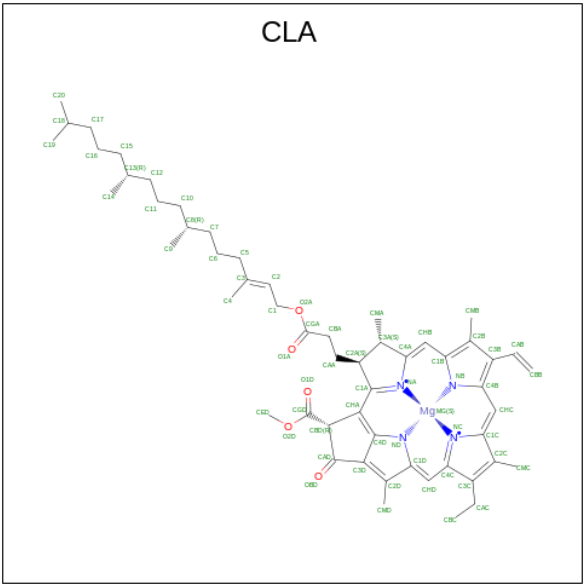
Mol	Chain	Residues	Atoms					AltConf
24	T	1	Total 43	C 34	Mg 1	N 4	O 4	0
24	T	1	Total 49	C 38	Mg 1	N 4	O 6	0
24	T	1	Total 52	C 41	Mg 1	N 4	O 6	0
24	T	1	Total 44	C 35	Mg 1	N 4	O 4	0
24	T	1	Total 42	C 33	Mg 1	N 4	O 4	0
24	T	1	Total 52	C 41	Mg 1	N 4	O 6	0
24	U	1	Total 42	C 33	Mg 1	N 4	O 4	0
24	U	1	Total 46	C 35	Mg 1	N 4	O 6	0
24	U	1	Total 44	C 35	Mg 1	N 4	O 4	0
24	U	1	Total 43	C 34	Mg 1	N 4	O 4	0
24	V	1	Total 46	C 35	Mg 1	N 4	O 6	0
24	V	1	Total 43	C 34	Mg 1	N 4	O 4	0
24	V	1	Total 44	C 35	Mg 1	N 4	O 4	0
24	V	1	Total 44	C 35	Mg 1	N 4	O 4	0
24	V	1	Total 44	C 35	Mg 1	N 4	O 4	0
24	W	1	Total 42	C 33	Mg 1	N 4	O 4	0
24	W	1	Total 42	C 33	Mg 1	N 4	O 4	0
24	W	1	Total 52	C 41	Mg 1	N 4	O 6	0
24	W	1	Total 66	C 55	Mg 1	N 4	O 6	0
24	W	1	Total 41	C 32	Mg 1	N 4	O 4	0
24	X	1	Total 42	C 33	Mg 1	N 4	O 4	0

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Mol	Chain	Residues	Atoms					AltConf
24	X	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
24	X	1	Total	C	Mg	N	O	0
			52	41	1	4	6	
24	X	1	Total	C	Mg	N	O	0
			44	35	1	4	4	
24	X	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

- Molecule 25 is CHLOROPHYLL A (three-letter code: CLA) (formula: C₅₅H₇₂MgN₄O₅).



Mol	Chain	Residues	Atoms					AltConf
25	1	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
25	1	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
25	1	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
25	1	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
25	1	1	Total	C	Mg	N	O	0
			37	30	1	4	2	
25	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	1	1	Total	C	Mg	N	O	0
			38	30	1	4	3	

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Mol	Chain	Residues	Atoms					AltConf
25	1	1	Total 40	C 32	Mg 1	N 4	O 3	0
25	1	1	Total 52	C 42	Mg 1	N 4	O 5	0
25	2	1	Total 61	C 51	Mg 1	N 4	O 5	0
25	2	1	Total 44	C 34	Mg 1	N 4	O 5	0
25	2	1	Total 43	C 34	Mg 1	N 4	O 4	0
25	2	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	2	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	2	1	Total 55	C 45	Mg 1	N 4	O 5	0
25	2	1	Total 42	C 34	Mg 1	N 4	O 3	0
25	2	1	Total 44	C 34	Mg 1	N 4	O 5	0
25	2	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	2	1	Total 42	C 34	Mg 1	N 4	O 3	0
25	2	1	Total 44	C 35	Mg 1	N 4	O 4	0
25	3	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	3	1	Total 55	C 45	Mg 1	N 4	O 5	0
25	3	1	Total 43	C 33	Mg 1	N 4	O 5	0
25	3	1	Total 41	C 33	Mg 1	N 4	O 3	0
25	3	1	Total 41	C 33	Mg 1	N 4	O 3	0
25	3	1	Total 61	C 51	Mg 1	N 4	O 5	0
25	3	1	Total 41	C 33	Mg 1	N 4	O 3	0
25	3	1	Total 42	C 34	Mg 1	N 4	O 3	0

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Mol	Chain	Residues	Atoms					AltConf
25	3	1	Total 43	C 35	Mg 1	N 4	O 3	0
25	3	1	Total 54	C 44	Mg 1	N 4	O 5	0
25	3	1	Total 40	C 32	Mg 1	N 4	O 3	0
25	3	1	Total 41	C 33	Mg 1	N 4	O 3	0
25	3	1	Total 40	C 32	Mg 1	N 4	O 3	0
25	4	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	4	1	Total 44	C 34	Mg 1	N 4	O 5	0
25	4	1	Total 43	C 33	Mg 1	N 4	O 5	0
25	4	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	4	1	Total 54	C 44	Mg 1	N 4	O 5	0
25	4	1	Total 42	C 34	Mg 1	N 4	O 3	0
25	4	1	Total 41	C 33	Mg 1	N 4	O 3	0
25	4	1	Total 57	C 47	Mg 1	N 4	O 5	0
25	4	1	Total 41	C 33	Mg 1	N 4	O 3	0
25	4	1	Total 41	C 33	Mg 1	N 4	O 3	0
25	4	1	Total 42	C 34	Mg 1	N 4	O 3	0
25	5	1	Total 46	C 36	Mg 1	N 4	O 5	0
25	5	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	5	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	5	1	Total 38	C 30	Mg 1	N 4	O 3	0
25	5	1	Total 40	C 32	Mg 1	N 4	O 3	0

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Mol	Chain	Residues	Atoms					AltConf
25	5	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	5	1	Total 41	C 33	Mg 1	N 4	O 3	0
25	5	1	Total 54	C 44	Mg 1	N 4	O 5	0
25	5	1	Total 41	C 33	Mg 1	N 4	O 3	0
25	6	1	Total 62	C 52	Mg 1	N 4	O 5	0
25	6	1	Total 44	C 34	Mg 1	N 4	O 5	0
25	6	1	Total 43	C 34	Mg 1	N 4	O 4	0
25	6	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	6	1	Total 42	C 34	Mg 1	N 4	O 3	0
25	6	1	Total 44	C 34	Mg 1	N 4	O 5	0
25	6	1	Total 61	C 51	Mg 1	N 4	O 5	0
25	6	1	Total 43	C 35	Mg 1	N 4	O 3	0
25	6	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	6	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	A	1	Total 52	C 42	Mg 1	N 4	O 5	0
25	A	1	Total 64	C 54	Mg 1	N 4	O 5	0
25	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	A	1	Total 50	C 40	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
25	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
25	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
25	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	A	1	Total 50	C 40	Mg 1	N 4	O 5	0
25	A	1	Total 56	C 46	Mg 1	N 4	O 5	0
25	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
25	A	1	Total 50	C 40	Mg 1	N 4	O 5	0
25	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	A	1	Total 50	C 40	Mg 1	N 4	O 5	0
25	A	1	Total 57	C 47	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
25	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
25	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 43	C 35	Mg 1	N 4	O 3	0
25	B	1	Total 43	C 35	Mg 1	N 4	O 3	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	B	1	Total 42	C 34	Mg 1	N 4	O 3	0
25	B	1	Total 50	C 40	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 47	C 37	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	F	1	Total 42	C 34	Mg 1	N 4	O 3	0
25	F	1	Total 41	C 33	Mg 1	N 4	O 3	0
25	G	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	G	1	Total 42	C 34	Mg 1	N 4	O 3	0
25	G	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	H	1	Total 44	C 35	Mg 1	N 4	O 4	0

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Mol	Chain	Residues	Atoms					AltConf
25	H	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	H	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	J	1	Total 42	C 34	Mg 1	N 4	O 3	0
25	K	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	K	1	Total 62	C 52	Mg 1	N 4	O 5	0
25	K	1	Total 46	C 36	Mg 1	N 4	O 5	0
25	K	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	L	1	Total 41	C 33	Mg 1	N 4	O 3	0
25	L	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	L	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	L	1	Total 42	C 34	Mg 1	N 4	O 3	0
25	N	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	N	1	Total 42	C 34	Mg 1	N 4	O 3	0
25	O	1	Total 59	C 49	Mg 1	N 4	O 5	0
25	O	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	O	1	Total 41	C 33	Mg 1	N 4	O 3	0
25	O	1	Total 41	C 33	Mg 1	N 4	O 3	0
25	O	1	Total 41	C 33	Mg 1	N 4	O 3	0
25	P	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	P	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	P	1	Total 50	C 40	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
25	P	1	Total 64	C 54	Mg 1	N 4	O 5	0
25	P	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	P	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	P	1	Total 55	C 45	Mg 1	N 4	O 5	0
25	P	1	Total 48	C 38	Mg 1	N 4	O 5	0
25	Q	1	Total 55	C 45	Mg 1	N 4	O 5	0
25	Q	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	Q	1	Total 44	C 35	Mg 1	N 4	O 4	0
25	Q	1	Total 50	C 40	Mg 1	N 4	O 5	0
25	Q	1	Total 55	C 45	Mg 1	N 4	O 5	0
25	Q	1	Total 42	C 34	Mg 1	N 4	O 3	0
25	Q	1	Total 46	C 36	Mg 1	N 4	O 5	0
25	Q	1	Total 53	C 43	Mg 1	N 4	O 5	0
25	Q	1	Total 48	C 38	Mg 1	N 4	O 5	0
25	R	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	R	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	R	1	Total 50	C 40	Mg 1	N 4	O 5	0
25	R	1	Total 64	C 54	Mg 1	N 4	O 5	0
25	R	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	R	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	R	1	Total 55	C 45	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
25	R	1	Total 48	C 38	Mg 1	N 4	O 5	0
25	S	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	S	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	S	1	Total 50	C 40	Mg 1	N 4	O 5	0
25	S	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	S	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	S	1	Total 47	C 37	Mg 1	N 4	O 5	0
25	S	1	Total 55	C 45	Mg 1	N 4	O 5	0
25	S	1	Total 41	C 33	Mg 1	N 4	O 3	0
25	T	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	T	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	T	1	Total 50	C 40	Mg 1	N 4	O 5	0
25	T	1	Total 59	C 49	Mg 1	N 4	O 5	0
25	T	1	Total 42	C 34	Mg 1	N 4	O 3	0
25	T	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	T	1	Total 55	C 45	Mg 1	N 4	O 5	0
25	T	1	Total 42	C 34	Mg 1	N 4	O 3	0
25	U	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	U	1	Total 56	C 46	Mg 1	N 4	O 5	0
25	U	1	Total 50	C 40	Mg 1	N 4	O 5	0
25	U	1	Total 41	C 33	Mg 1	N 4	O 3	0

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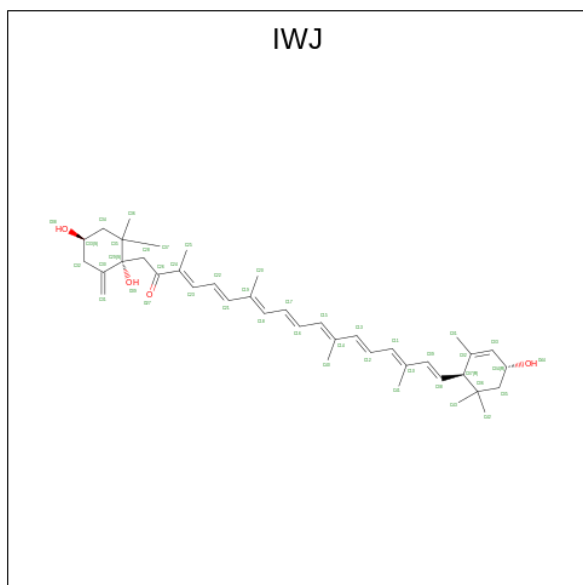
Mol	Chain	Residues	Atoms					AltConf
25	U	1	Total 46	C 36	Mg 1	N 4	O 5	0
25	U	1	Total 44	C 35	Mg 1	N 4	O 4	0
25	U	1	Total 55	C 45	Mg 1	N 4	O 5	0
25	U	1	Total 41	C 33	Mg 1	N 4	O 3	0
25	V	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	V	1	Total 50	C 40	Mg 1	N 4	O 5	0
25	V	1	Total 50	C 40	Mg 1	N 4	O 5	0
25	V	1	Total 42	C 34	Mg 1	N 4	O 3	0
25	V	1	Total 47	C 37	Mg 1	N 4	O 5	0
25	V	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	V	1	Total 55	C 45	Mg 1	N 4	O 5	0
25	V	1	Total 48	C 38	Mg 1	N 4	O 5	0
25	W	1	Total 55	C 45	Mg 1	N 4	O 5	0
25	W	1	Total 55	C 45	Mg 1	N 4	O 5	0
25	W	1	Total 50	C 40	Mg 1	N 4	O 5	0
25	W	1	Total 64	C 54	Mg 1	N 4	O 5	0
25	W	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	W	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	W	1	Total 55	C 45	Mg 1	N 4	O 5	0
25	W	1	Total 43	C 35	Mg 1	N 4	O 3	0
25	X	1	Total 55	C 45	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
25	X	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
25	X	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
25	X	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
25	X	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
25	X	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
25	X	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
25	X	1	Total	C	Mg	N	O	0
			41	33	1	4	3	

- Molecule 26 is (3 {E},5 {E},7 {E},9 {E},11 {E},13 {E},15 {E},17 {E})-1-[(1 {S},4 {S})-2,2-dimethyl-6-methylidene-1,4-bis(oxidanyl)cyclohexyl]-3,7,12,16-tetramethyl-18-[(1 {R},4 {R})-2,6,6-trimethyl-4-oxidanyl-cyclohex-2-en-1-yl]octadeca-3,5,7,9,11,13,15,17-octaen-2-one (three-letter code: IWJ) (formula: C₄₀H₅₆O₄) (labeled as "Ligand of Interest" by depositor).



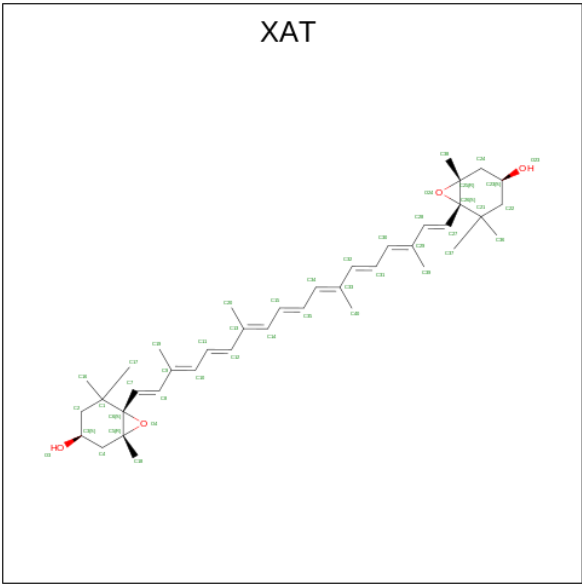
Mol	Chain	Residues	Atoms			AltConf
26	1	1	Total	C	O	0
			44	40	4	
26	3	1	Total	C	O	0
			44	40	4	

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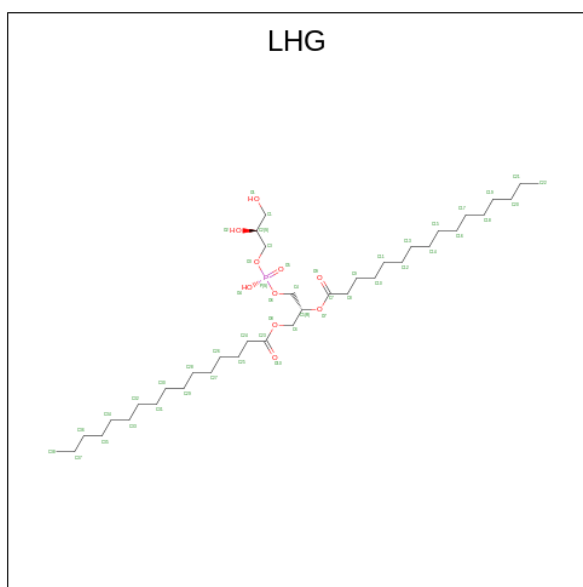
Mol	Chain	Residues	Atoms			AltConf
26	4	1	Total	C	O	0
			44	40	4	
26	4	1	Total	C	O	0
			44	40	4	
26	5	1	Total	C	O	0
			44	40	4	
26	6	1	Total	C	O	0
			44	40	4	
26	P	1	Total	C	O	0
			44	40	4	
26	P	1	Total	C	O	0
			44	40	4	
26	Q	1	Total	C	O	0
			44	40	4	
26	Q	1	Total	C	O	0
			44	40	4	
26	R	1	Total	C	O	0
			44	40	4	
26	R	1	Total	C	O	0
			44	40	4	
26	S	1	Total	C	O	0
			44	40	4	
26	S	1	Total	C	O	0
			44	40	4	
26	S	1	Total	C	O	0
			44	40	4	
26	T	1	Total	C	O	0
			44	40	4	
26	T	1	Total	C	O	0
			44	40	4	
26	U	1	Total	C	O	0
			44	40	4	
26	V	1	Total	C	O	0
			44	40	4	
26	V	1	Total	C	O	0
			44	40	4	
26	V	1	Total	C	O	0
			44	40	4	
26	W	1	Total	C	O	0
			44	40	4	
26	X	1	Total	C	O	0
			44	40	4	

- Molecule 27 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).



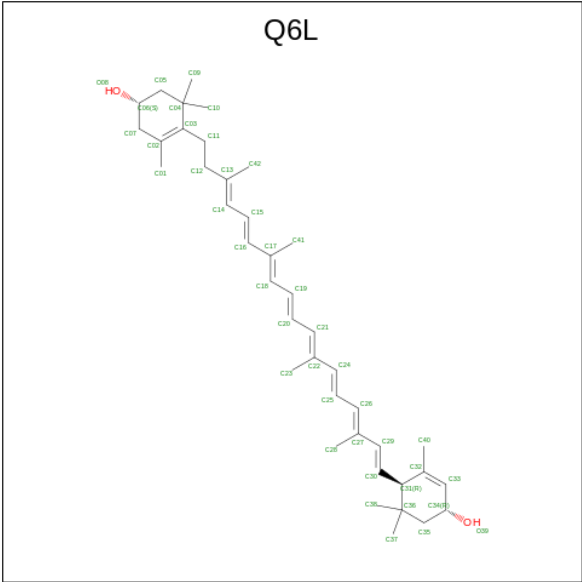
Mol	Chain	Residues	Atoms			AltConf
27	1	1	Total	C	O	0
			44	40	4	
27	2	1	Total	C	O	0
			44	40	4	
27	3	1	Total	C	O	0
			44	40	4	
27	4	1	Total	C	O	0
			44	40	4	
27	5	1	Total	C	O	0
			44	40	4	
27	6	1	Total	C	O	0
			44	40	4	

- Molecule 28 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: C₃₈H₇₅O₁₀P).



Mol	Chain	Residues	Atoms				AltConf
28	1	1	Total	C	O	P	0
			35	24	10	1	
28	2	1	Total	C	O	P	0
			33	22	10	1	
28	3	1	Total	C	O	P	0
			23	13	9	1	
28	3	1	Total	C	O	P	0
			43	32	10	1	
28	3	1	Total	C	O	P	0
			36	25	10	1	
28	3	1	Total	C	O	P	0
			43	32	10	1	
28	6	1	Total	C	O	P	0
			46	35	10	1	
28	A	1	Total	C	O	P	0
			49	38	10	1	
28	A	1	Total	C	O	P	0
			30	19	10	1	
28	Q	1	Total	C	O	P	0
			35	24	10	1	

- Molecule 29 is (1 {S})-3,5,5-trimethyl-4-[(3 {E},5 {E},7 {E},9 {E},11 {E},13 {E},15 {E},17 {E})-3,7,12,16-tetramethyl-18-[(1 {R},4 {R})-2,6,6-trimethyl-4-oxidanyl-cyclohex-2-en-1-yl] octadeca-3,5,7,9,11,13,15,17-octaenyl]cyclohex-3-en-1-ol (three-letter code: Q6L) (formula: C₄₀H₅₈O₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
29	2	1	Total	C	O	0
			42	40	2	
29	O	1	Total	C	O	0
			42	40	2	
29	O	1	Total	C	O	0
			42	40	2	
29	P	1	Total	C	O	0
			42	40	2	
29	P	1	Total	C	O	0
			42	40	2	
29	P	1	Total	C	O	0
			42	40	2	
29	P	1	Total	C	O	0
			42	40	2	
29	Q	1	Total	C	O	0
			42	40	2	
29	Q	1	Total	C	O	0
			42	40	2	
29	Q	1	Total	C	O	0
			42	40	2	
29	R	1	Total	C	O	0
			42	40	2	
29	R	1	Total	C	O	0
			42	40	2	
29	R	1	Total	C	O	0
			42	40	2	
29	R	1	Total	C	O	0
			42	40	2	

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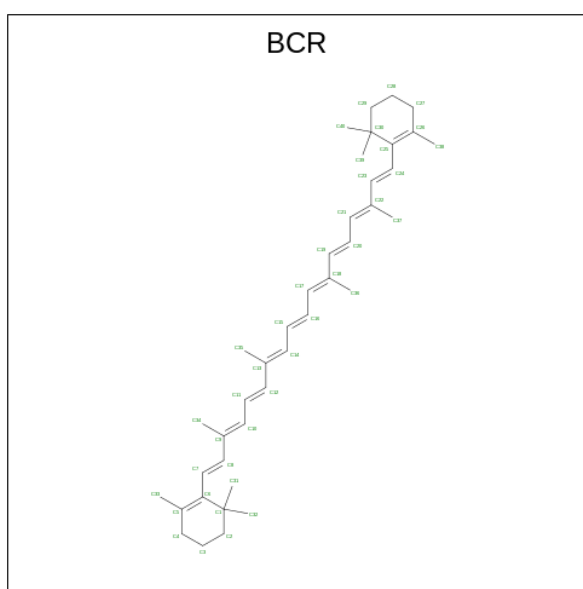
Mol	Chain	Residues	Atoms			AltConf
29	R	1	Total 42	C 40	O 2	0
29	S	1	Total 42	C 40	O 2	0
29	S	1	Total 42	C 40	O 2	0
29	S	1	Total 42	C 40	O 2	0
29	S	1	Total 42	C 40	O 2	0
29	S	1	Total 42	C 40	O 2	0
29	T	1	Total 42	C 40	O 2	0
29	T	1	Total 42	C 40	O 2	0
29	T	1	Total 42	C 40	O 2	0
29	T	1	Total 42	C 40	O 2	0
29	U	1	Total 42	C 40	O 2	0
29	U	1	Total 42	C 40	O 2	0
29	U	1	Total 42	C 40	O 2	0
29	V	1	Total 42	C 40	O 2	0
29	V	1	Total 42	C 40	O 2	0
29	V	1	Total 42	C 40	O 2	0
29	V	1	Total 42	C 40	O 2	0
29	W	1	Total 42	C 40	O 2	0
29	W	1	Total 42	C 40	O 2	0
29	W	1	Total 42	C 40	O 2	0
29	W	1	Total 42	C 40	O 2	0

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Mol	Chain	Residues	Atoms			AltConf
29	X	1	Total	C	O	0
			42	40	2	
29	X	1	Total	C		0
			40	40		
29	X	1	Total	C	O	0
			42	40	2	
29	X	1	Total	C	O	0
			42	40	2	

- Molecule 30 is BETA-CAROTENE (three-letter code: BCR) (formula: C₄₀H₅₆).



Mol	Chain	Residues	Atoms		AltConf
30	2	1	Total	C	0
			40	40	
30	3	1	Total	C	0
			40	40	
30	3	1	Total	C	0
			40	40	
30	3	1	Total	C	0
			40	40	
30	4	1	Total	C	0
			40	40	
30	A	1	Total	C	0
			40	40	
30	A	1	Total	C	0
			40	40	

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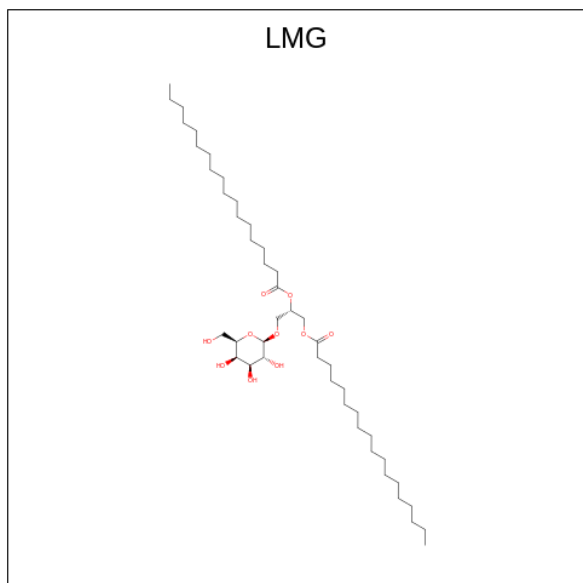
Mol	Chain	Residues	Atoms	AltConf
30	A	1	Total C 40 40	0
30	A	1	Total C 40 40	0
30	A	1	Total C 40 40	0
30	B	1	Total C 40 40	0
30	B	1	Total C 40 40	0
30	B	1	Total C 40 40	0
30	B	1	Total C 40 40	0
30	B	1	Total C 40 40	0
30	B	1	Total C 40 40	0
30	F	1	Total C 40 40	0
30	F	1	Total C 40 40	0
30	G	1	Total C 40 40	0
30	G	1	Total C 40 40	0
30	H	1	Total C 40 40	0
30	I	1	Total C 40 40	0
30	J	1	Total C 40 40	0
30	J	1	Total C 40 40	0
30	K	1	Total C 40 40	0
30	K	1	Total C 40 40	0
30	K	1	Total C 40 40	0
30	L	1	Total C 40 40	0
30	L	1	Total C 40 40	0

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Mol	Chain	Residues	Atoms	AltConf
30	L	1	Total C 40 40	0
30	M	1	Total C 40 40	0

- Molecule 31 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: $C_{45}H_{86}O_{10}$).



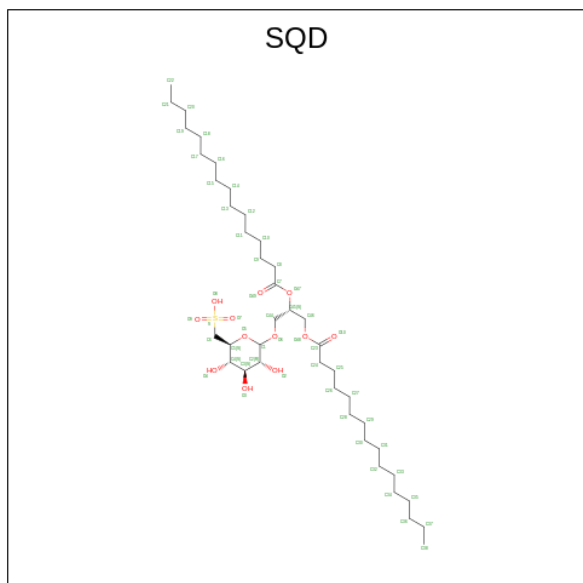
Mol	Chain	Residues	Atoms	AltConf
31	2	1	Total C O 31 21 10	0
31	5	1	Total C O 54 44 10	0
31	A	1	Total C O 31 21 10	0
31	A	1	Total C O 27 17 10	0
31	A	1	Total C O 46 36 10	0
31	B	1	Total C O 38 28 10	0
31	F	1	Total C O 31 21 10	0
31	J	1	Total C O 46 36 10	0
31	L	1	Total C O 31 21 10	0

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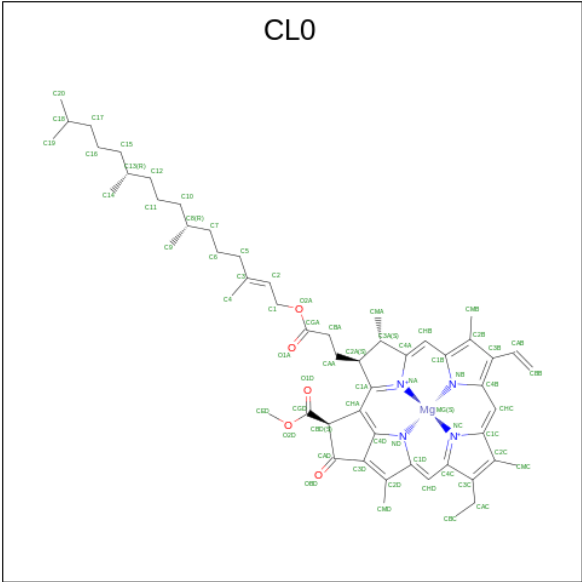
Mol	Chain	Residues	Atoms			AltConf
31	N	1	Total	C	O	0
			55	45	10	
31	O	1	Total	C	O	0
			39	29	10	

- Molecule 32 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula: C₄₁H₇₈O₁₂S).



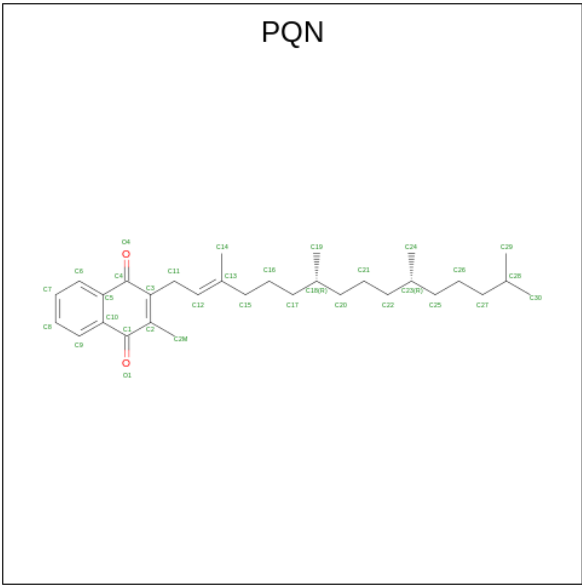
Mol	Chain	Residues	Atoms				AltConf
32	6	1	Total	C	O	S	0
			54	41	12	1	
32	H	1	Total	C	O	S	0
			48	35	12	1	

- Molecule 33 is CHLOROPHYLL A ISOMER (three-letter code: CL0) (formula: C₅₅H₇₂MgN₄O₅) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 34 is PHYLLOQUINONE (three-letter code: PQN) (formula: C₃₁H₄₆O₂).



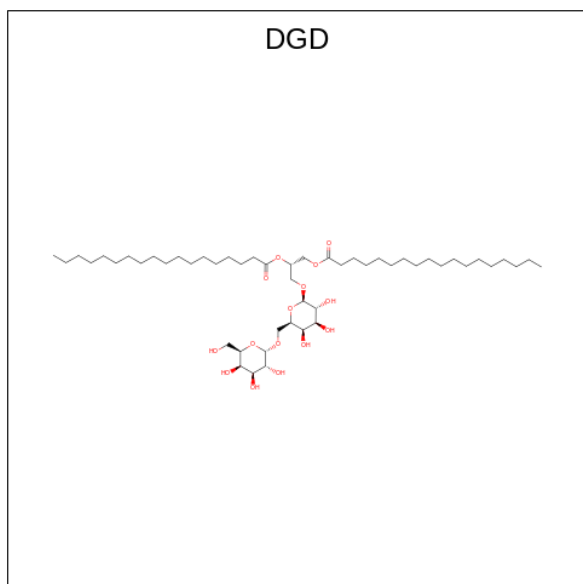
Mol	Chain	Residues	Atoms			AltConf
34	A	1	Total	C	O	0
			33	31	2	
34	B	1	Total	C	O	0
			33	31	2	

- Molecule 35 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



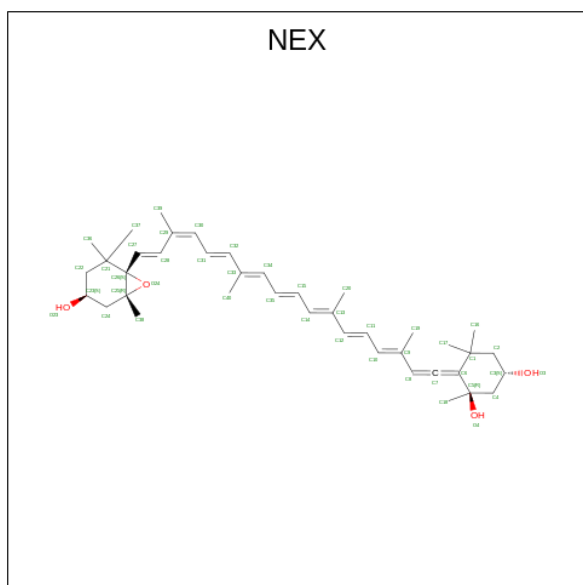
Mol	Chain	Residues	Atoms			AltConf
35	A	1	Total	Fe	S	0
			8	4	4	
35	C	1	Total	Fe	S	0
			8	4	4	
35	C	1	Total	Fe	S	0
			8	4	4	

- Molecule 36 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: $C_{51}H_{96}O_{15}$).



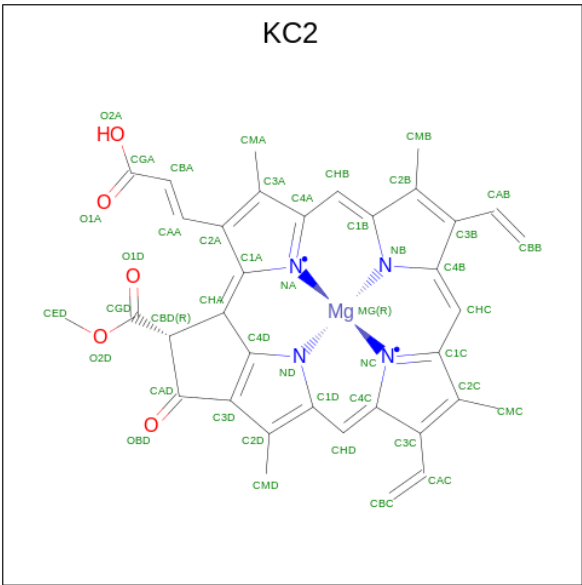
Mol	Chain	Residues	Atoms			AltConf
36	A	1	Total	C	O	0
			51	36	15	
36	B	1	Total	C	O	0
			59	44	15	

- Molecule 37 is (1R,3R)-6-[(3E,5E,7E,9E,11E,13E,15E,17E)-18-[(1S,4R,6R)-4-HYDROXY-2,2,6-TRIMETHYL-7-OXABICYCLO[4.1.0]HEPT-1-YL]-3,7,12,16-TETRAMETHYLOCTA DECA-1,3,5,7,9,11,13,15,17-NONAENYLIDENE}-1,5,5-TRIMETHYLCYCLOHEXANE-1,3-DIOL (three-letter code: NEX) (formula: $C_{40}H_{56}O_4$).



Mol	Chain	Residues	Atoms			AltConf
37	H	1	Total	C	O	0
			44	40	4	
37	P	1	Total	C	O	0
			44	40	4	
37	R	1	Total	C	O	0
			44	40	4	
37	S	1	Total	C	O	0
			44	40	4	
37	T	1	Total	C	O	0
			44	40	4	
37	W	1	Total	C	O	0
			44	40	4	

- Molecule 38 is Chlorophyll c2 (three-letter code: KC2) (formula: $C_{35}H_{28}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
38	P	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
38	Q	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
38	R	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
38	S	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
38	T	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
38	U	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
38	V	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
38	W	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
38	X	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

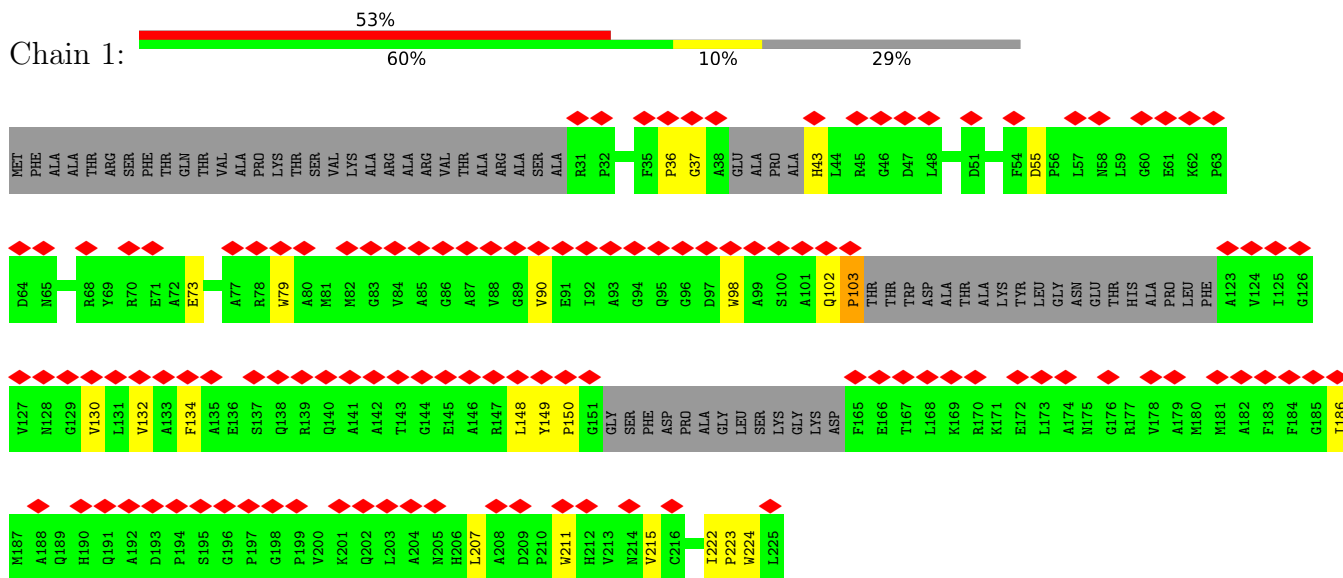
- Molecule 39 is water.

Mol	Chain	Residues	Atoms		AltConf
39	A	3	Total	O	0
			3	3	
39	Q	1	Total	O	0
			1	1	

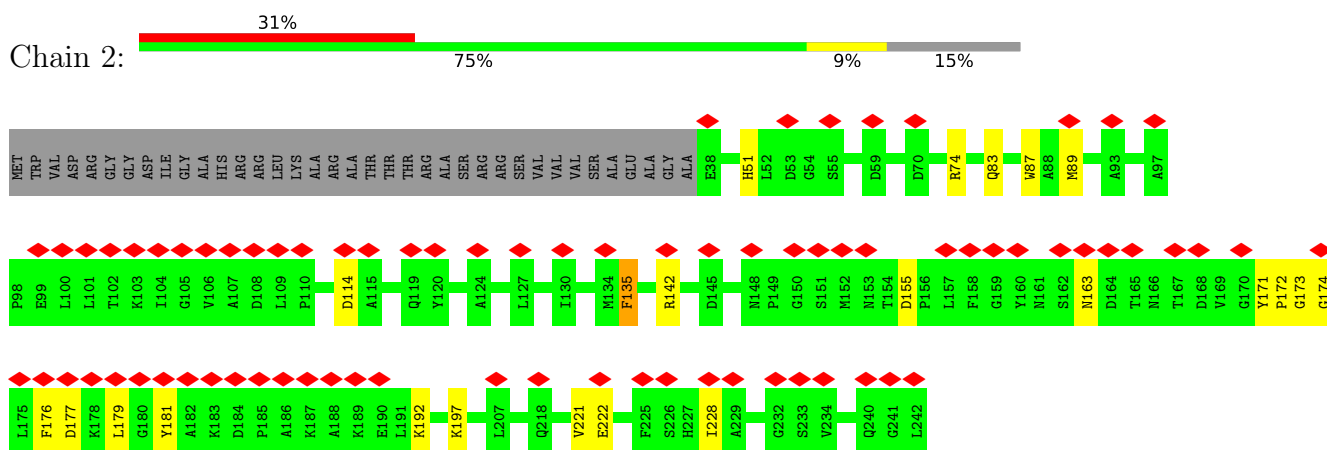
3 Residue-property plots

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: Lhca1

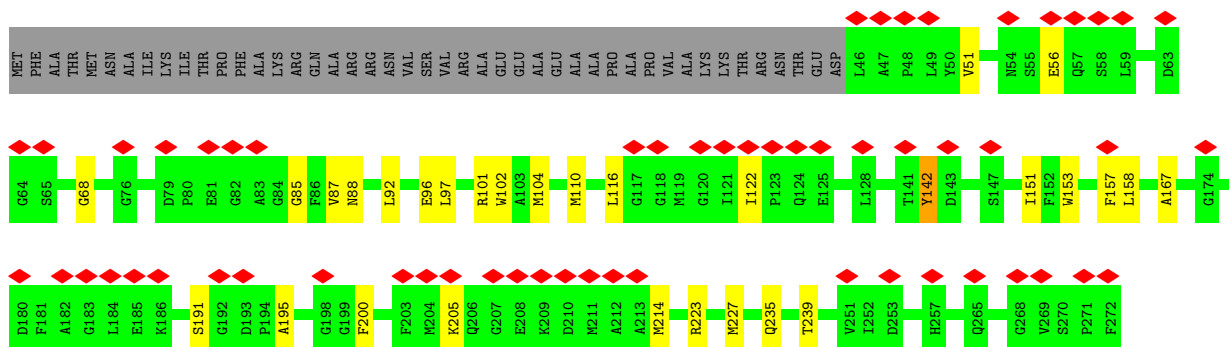


- Molecule 2: Chlorophyll a-b binding protein, chloroplastic

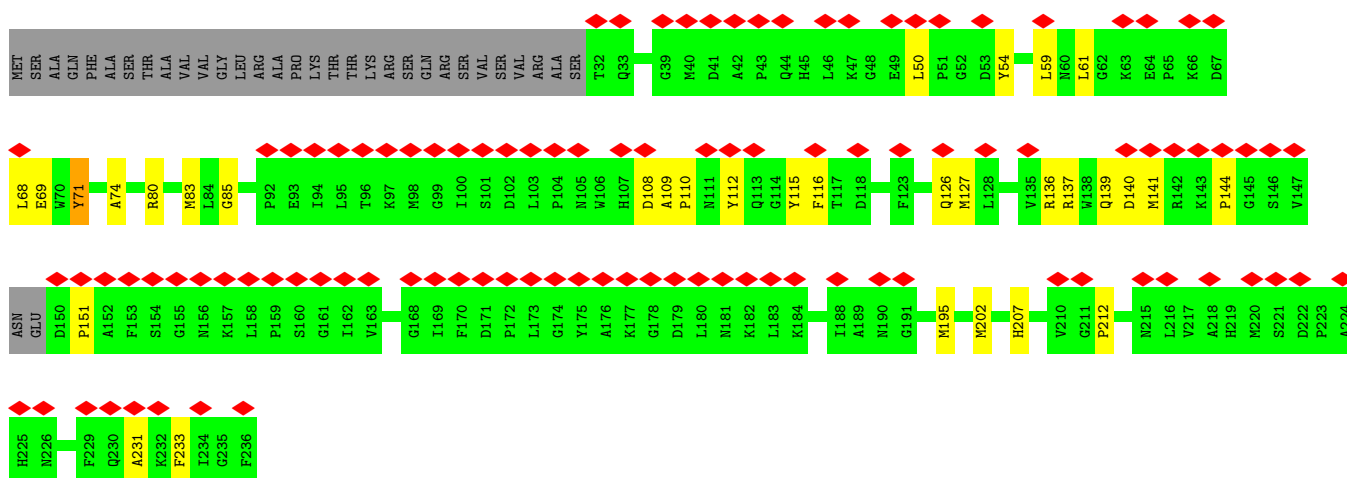
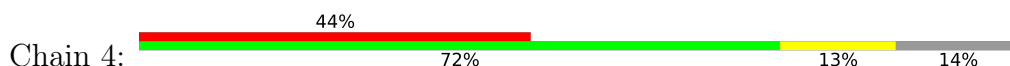


- Molecule 3: Chlorophyll a-b binding protein, chloroplastic

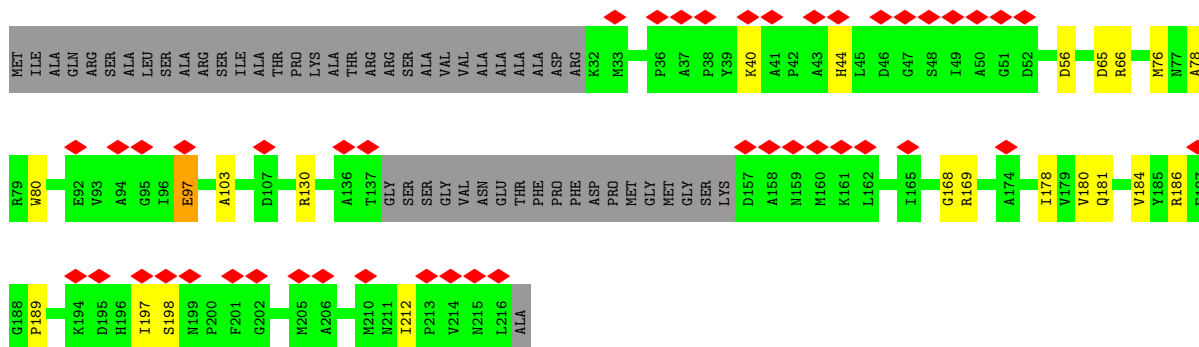




• Molecule 4: Chlorophyll a-b binding protein, chloroplastic

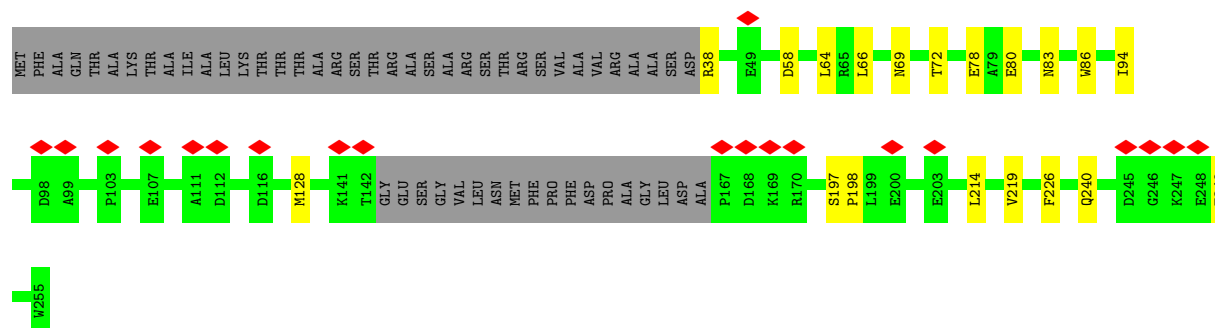


• Molecule 5: Chlorophyll a-b binding protein, chloroplastic

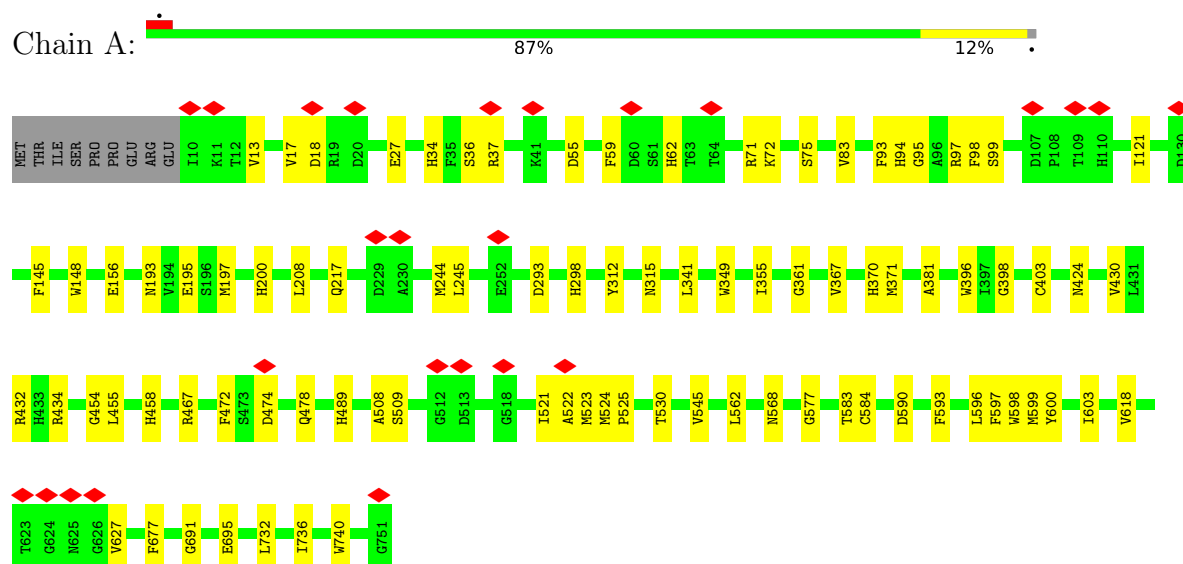


• Molecule 6: Lhca6

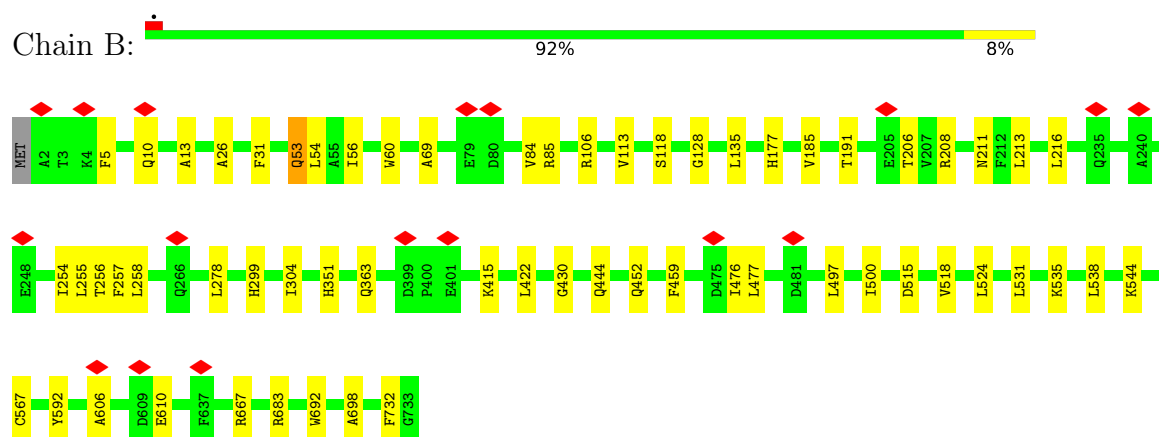




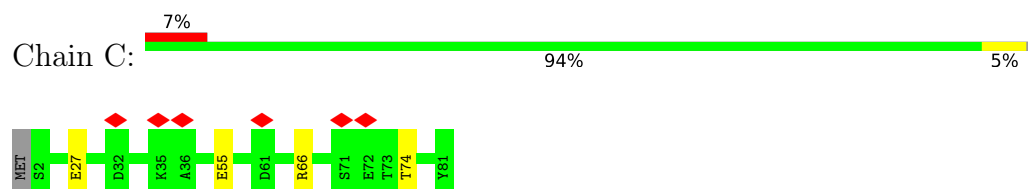
- Molecule 7: Photosystem I P700 chlorophyll a apoprotein A1



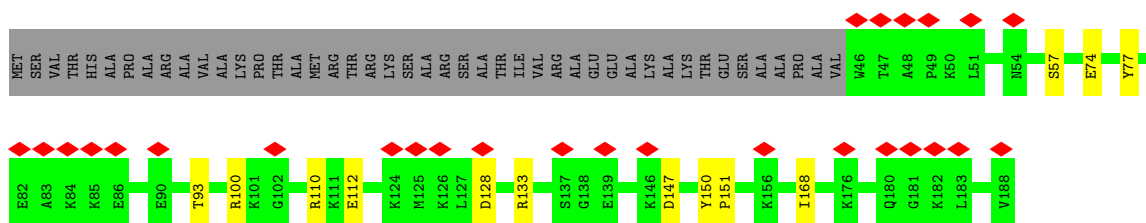
- Molecule 8: Photosystem I P700 chlorophyll a apoprotein A2



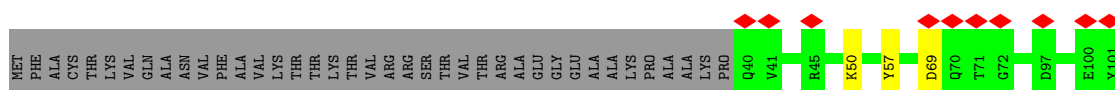
- Molecule 9: Photosystem I iron-sulfur center



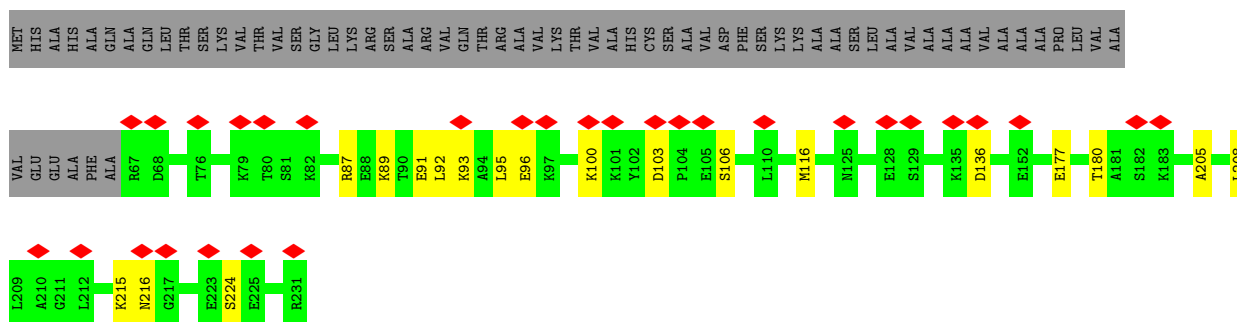
- Chain D: 



- Chain E: 



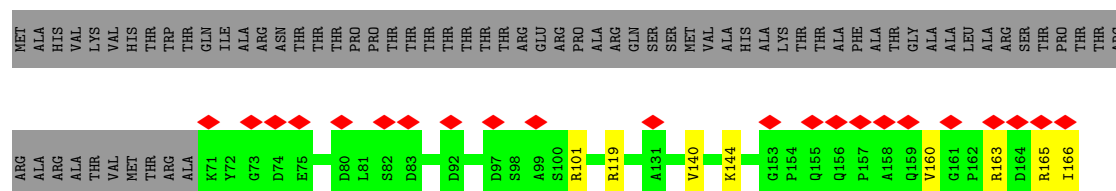
- Chain F:  13% 63% 8% 18%



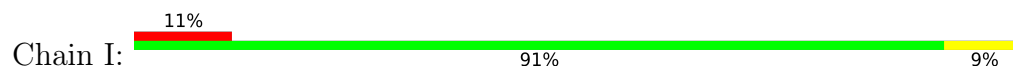
- Chain G: 



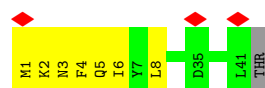
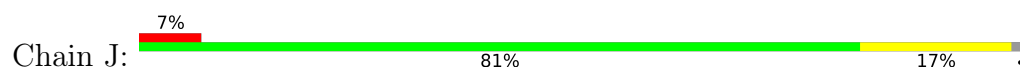
- Chain H: 



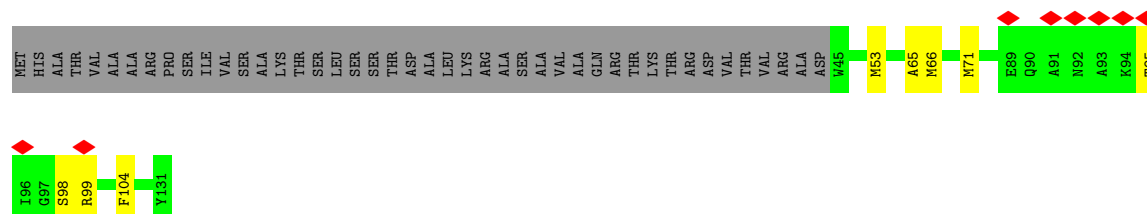
• Molecule 15: Photosystem I reaction center subunit VIII



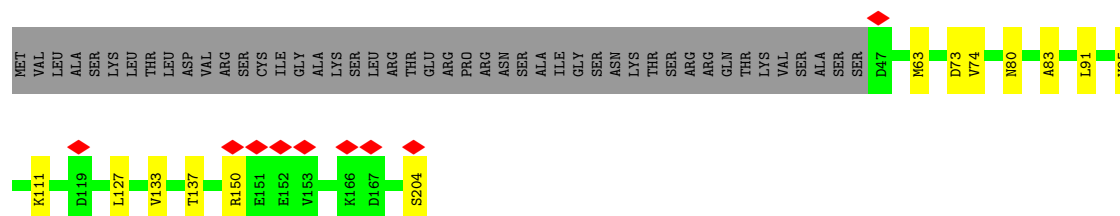
• Molecule 16: Photosystem I reaction center subunit IX



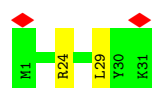
• Molecule 17: Photosystem I PsaG/PsaK protein



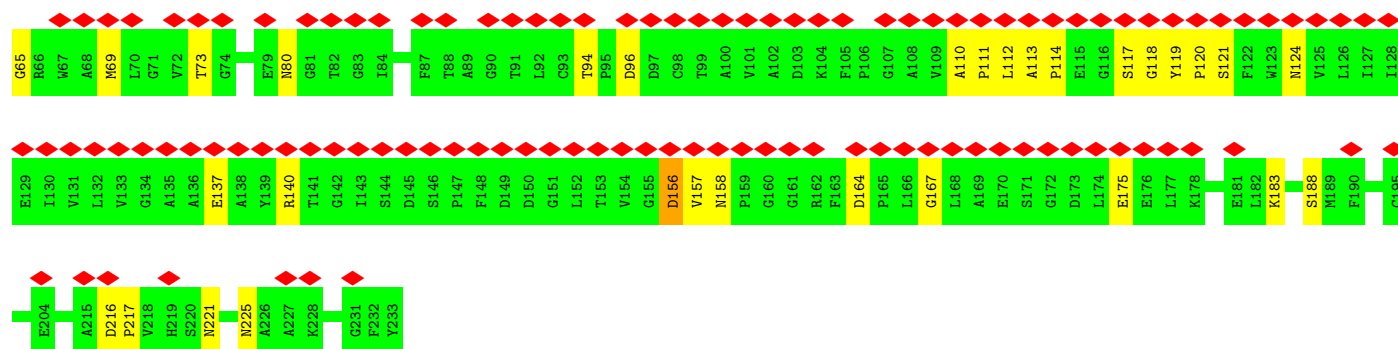
• Molecule 18: PSI subunit V



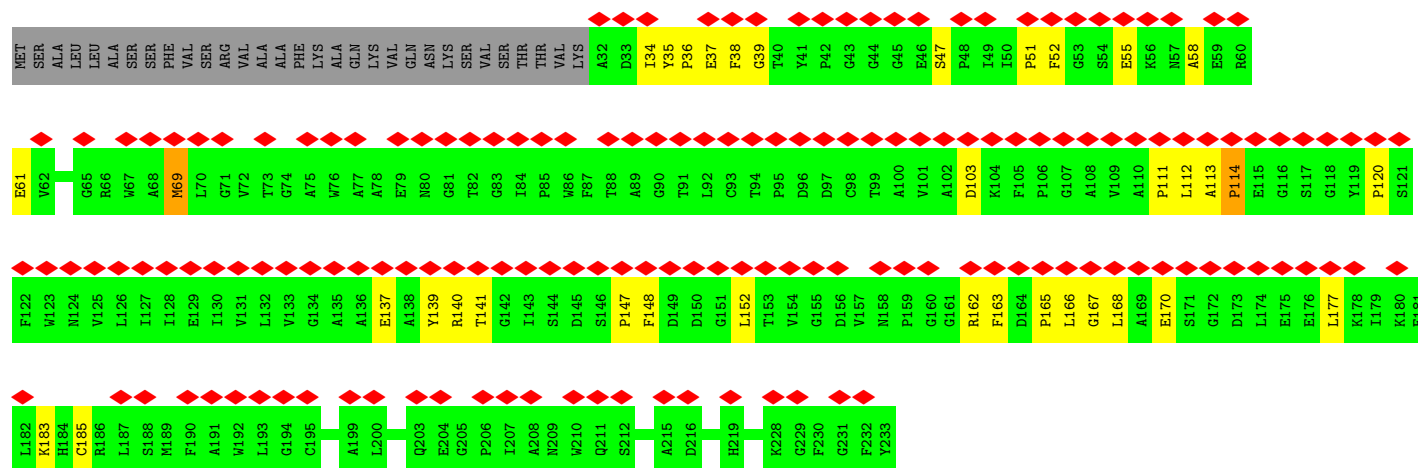
• Molecule 19: Photosystem I reaction center subunit XII



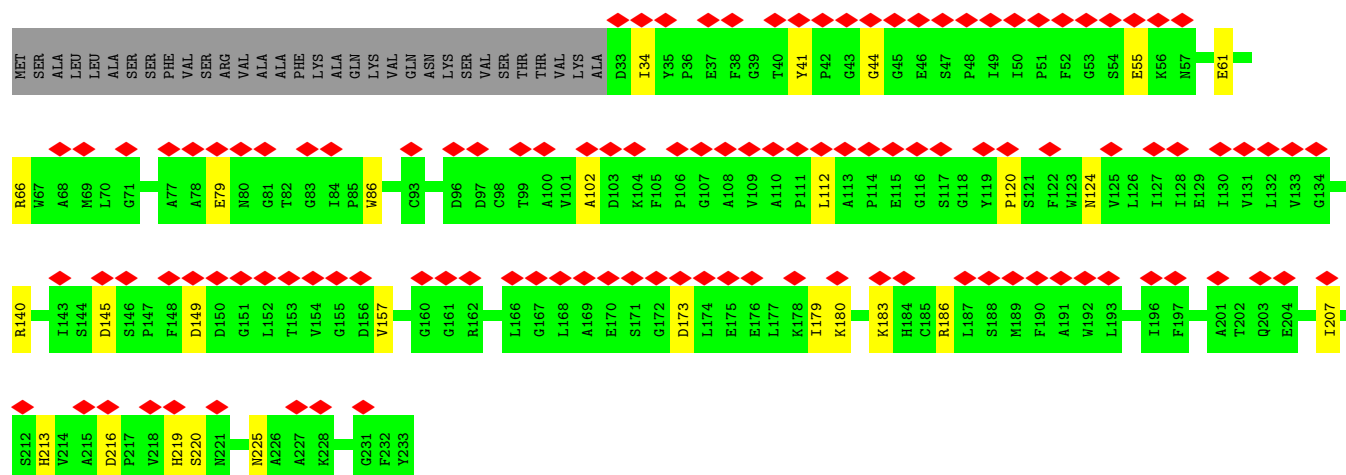
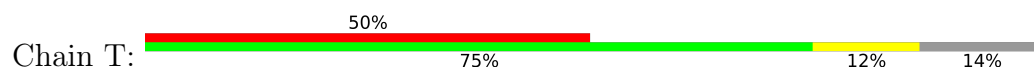
- Chain R:
-
- | Amino Acid | Percentage |
|------------|------------|
| MET | 0.55% |
| SER | 0.55% |
| ALA | 0.55% |
| LEU | 0.55% |
| SER | 0.55% |
| PHE | 0.55% |
| VAL | 0.55% |
| ARG | 0.55% |
| SER | 0.55% |
| VAL | 0.55% |
| ALA | 0.55% |
| PHE | 0.55% |
| LYS | 0.55% |
| ALA | 0.55% |
| GLN | 0.55% |
| LYS | 0.55% |
| VAL | 0.55% |
| GLN | 0.55% |
| ASN | 0.55% |
| LYS | 0.55% |
| SER | 0.55% |
| VAL | 0.55% |
| SER | 0.55% |
| THR | 0.55% |
| THR | 0.55% |
| VAL | 0.55% |
| LYS | 0.55% |
| ALA | 0.55% |
| D33 | 0.55% |
| I34 | 0.55% |
| E37 | 0.55% |
| F38 | 0.55% |
| G39 | 0.55% |
| T40 | 0.55% |
| Y41 | 0.55% |
| P42 | 0.55% |
| G43 | 0.55% |
| G44 | 0.55% |
| G45 | 0.55% |
| E46 | 0.55% |
| S47 | 0.55% |
| P48 | 0.55% |
| F52 | 0.55% |
| G53 | 0.55% |
| S54 | 0.55% |
| E55 | 0.55% |
| K56 | 0.55% |
| N57 | 0.55% |
| A58 | 0.55% |
| E59 | 0.55% |
| R60 | 0.55% |
| E61 | 0.55% |
| V62 | 0.55% |



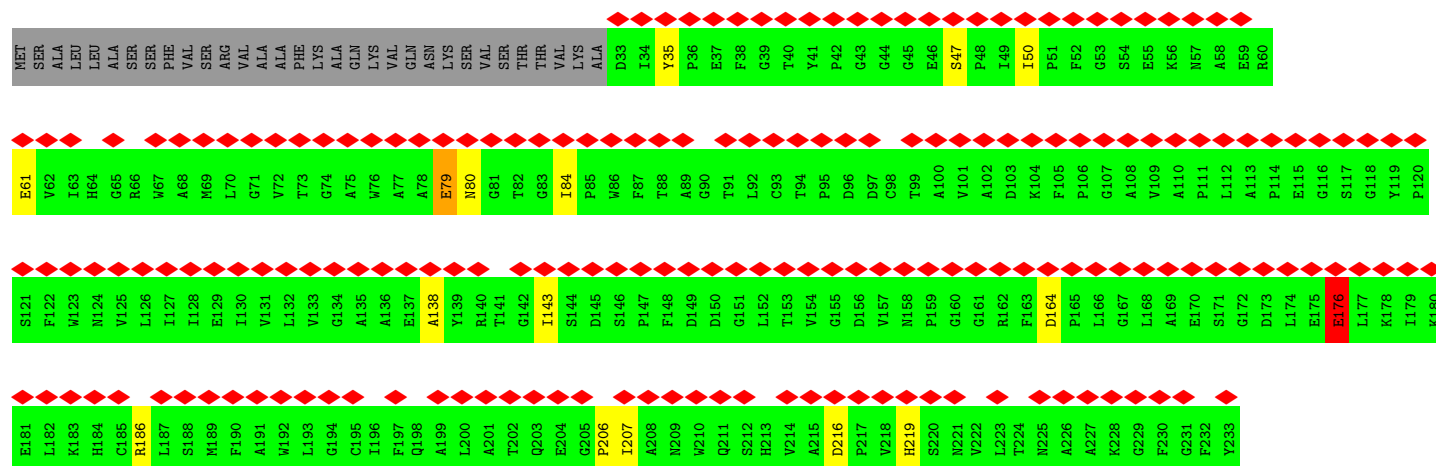
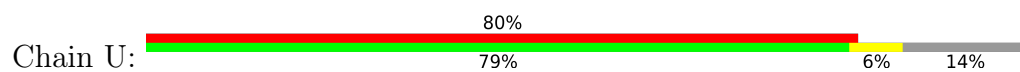
- Molecule 22: Chlorophyll a-b binding protein, chloroplastic



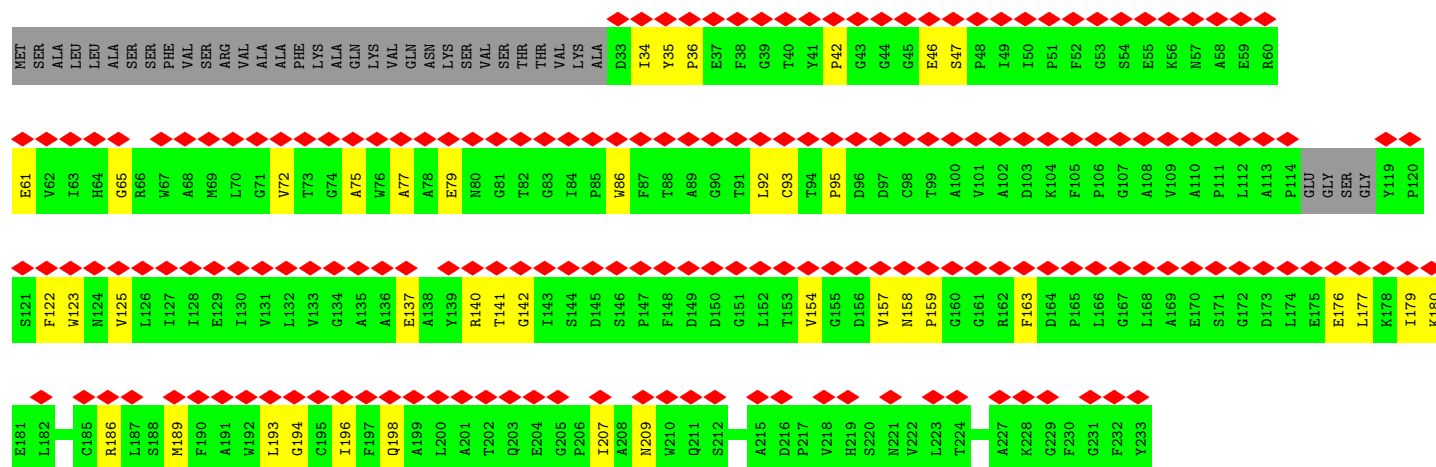
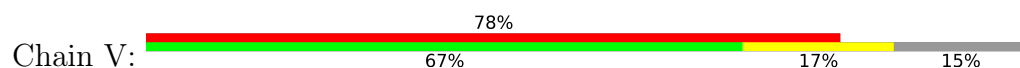
- Molecule 22: Chlorophyll a-b binding protein, chloroplastic



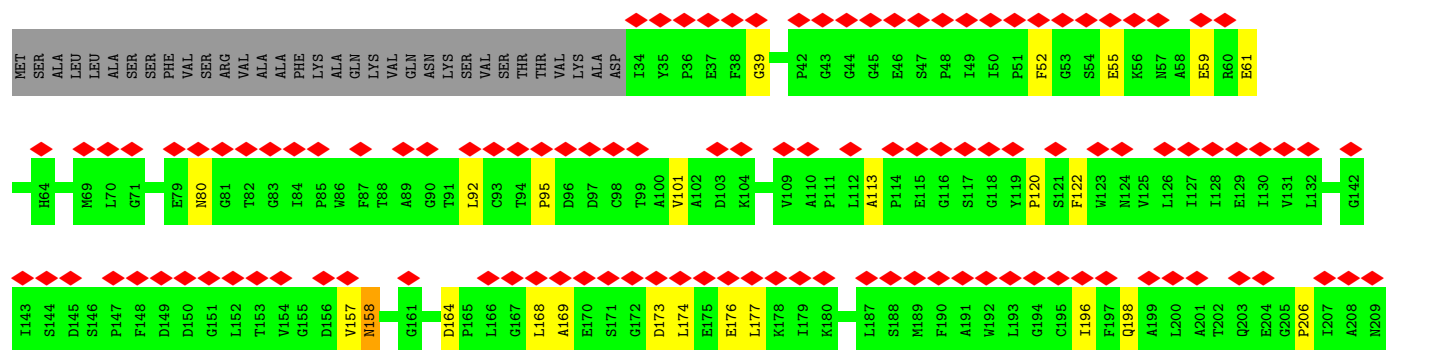
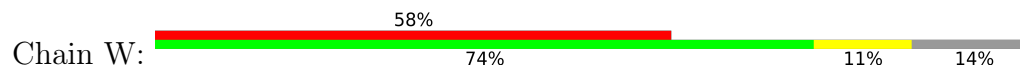
- Molecule 22: Chlorophyll a-b binding protein, chloroplastic

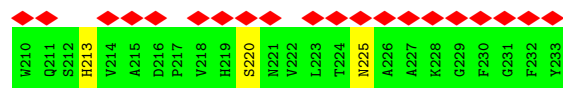


• Molecule 22: Chlorophyll a-b binding protein, chloroplastic



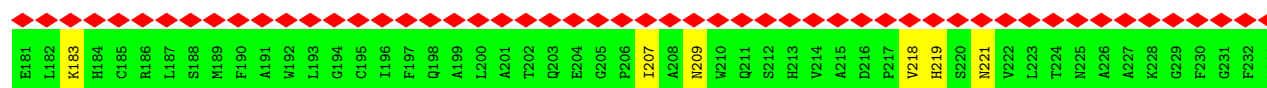
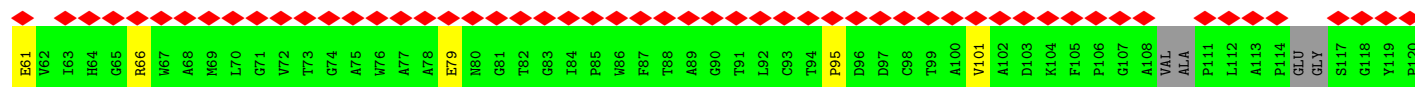
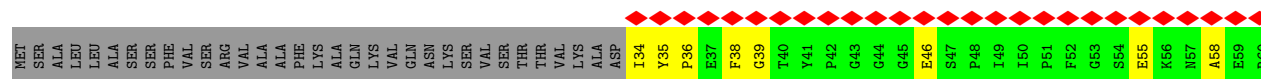
• Molecule 22: Chlorophyll a-b binding protein, chloroplastic





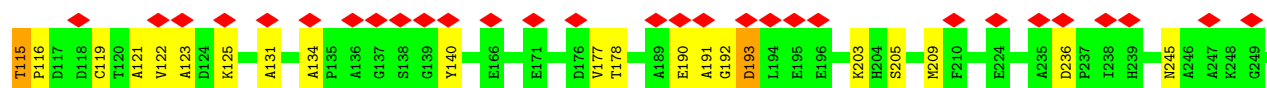
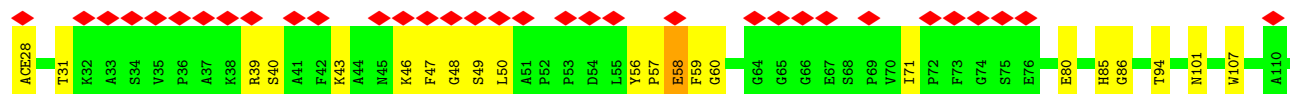
- Molecule 22: Chlorophyll a-b binding protein, chloroplastic

Chain X:



- Molecule 23: Chlorophyll a-b binding protein, chloroplastic

Chain Q:



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	80366	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60.0	Depositor
Minimum defocus (nm)	1800	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K2 BASE (4k x 4k)	Depositor
Maximum map value	0.135	Depositor
Minimum map value	-0.074	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.025	Depositor
Map size (\AA)	399.36, 399.36, 399.36	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.04, 1.04, 1.04	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: LHG, CHL, CL0, BCR, CLA, SQD, PQN, ACE, Q6L, XAT, LMG, SF4, TPO, NEX, DGD, IWJ, KC2

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	1	0.61	2/1242 (0.2%)	0.79	3/1686 (0.2%)
2	2	0.57	3/1634 (0.2%)	0.70	1/2224 (0.0%)
3	3	0.56	1/1768 (0.1%)	0.78	1/2394 (0.0%)
4	4	0.54	2/1630 (0.1%)	0.71	1/2215 (0.0%)
5	5	0.54	1/1312 (0.1%)	0.73	1/1783 (0.1%)
6	6	0.46	0/1522	0.65	1/2068 (0.0%)
7	A	0.46	1/6017 (0.0%)	0.64	2/8202 (0.0%)
8	B	0.47	0/5981	0.64	0/8166
9	C	0.48	0/603	0.74	0/818
10	D	0.53	0/1142	0.82	2/1537 (0.1%)
11	E	0.46	0/516	0.77	1/703 (0.1%)
12	F	0.46	0/1286	0.67	0/1739
13	G	0.51	0/732	0.73	0/995
14	H	0.43	0/736	0.68	0/1001
15	I	0.59	0/270	0.72	0/368
16	J	0.46	0/338	0.61	0/462
17	K	0.45	0/635	0.66	0/860
18	L	0.46	0/1197	0.62	0/1635
19	M	0.46	0/242	0.62	0/328
20	N	0.49	0/685	0.75	1/921 (0.1%)
21	O	0.42	0/787	0.63	0/1070
22	P	0.50	1/1553 (0.1%)	0.73	1/2122 (0.0%)
22	R	0.49	0/1553	0.78	6/2122 (0.3%)
22	S	0.52	0/1558	0.72	3/2129 (0.1%)
22	T	0.48	0/1553	0.68	1/2122 (0.0%)
22	U	0.57	2/1553 (0.1%)	0.69	1/2122 (0.0%)
22	V	0.55	1/1529 (0.1%)	0.70	2/2089 (0.1%)
22	W	0.56	1/1545 (0.1%)	0.67	1/2111 (0.0%)
22	X	0.50	0/1518	0.68	1/2070 (0.0%)
23	Q	0.58	2/1746 (0.1%)	0.76	3/2379 (0.1%)
All	All	0.51	17/44383 (0.0%)	0.69	33/60441 (0.1%)

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
22	U	0	1

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	U	79	GLU	CG-CD	-9.89	1.37	1.51
1	1	103	PRO	CB-CG	9.36	1.96	1.50
23	Q	80	GLU	CD-OE1	-9.19	1.15	1.25
4	4	69	GLU	CD-OE1	-7.71	1.17	1.25
4	4	71	TYR	CD1-CE1	-6.08	1.30	1.39
2	2	221	VAL	CB-CG1	-5.92	1.40	1.52
2	2	135	PHE	CD2-CE2	-5.59	1.28	1.39
22	W	55	GLU	CB-CG	5.45	1.62	1.52
7	A	367	VAL	CB-CG1	-5.37	1.41	1.52
23	Q	115	THR	C-N	5.34	1.44	1.34
22	P	76	TRP	CB-CG	5.28	1.59	1.50
3	3	142	TYR	CD1-CE1	-5.21	1.31	1.39
5	5	40	LYS	CE-NZ	-5.16	1.36	1.49
2	2	222	GLU	CB-CG	5.15	1.61	1.52
1	1	224	TRP	CB-CG	5.12	1.59	1.50
22	U	176	GLU	CD-OE1	5.11	1.31	1.25
22	V	93	CYS	CB-SG	-5.04	1.73	1.81

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	4	69	GLU	OE1-CD-OE2	-11.52	109.47	123.30
10	D	147	ASP	CB-CG-OD1	10.91	128.12	118.30
1	1	102	GLN	C-N-CD	8.90	147.10	128.40
22	R	216	ASP	CB-CG-OD1	8.57	126.02	118.30
11	E	69	ASP	CB-CG-OD2	-8.19	110.93	118.30
22	R	111	PRO	CA-N-CD	-8.16	100.07	111.50
23	Q	236	ASP	CB-CG-OD1	7.88	125.39	118.30
20	N	125	CYS	CA-CB-SG	7.69	127.85	114.00
23	Q	28	ACE	O-C-N	-7.25	111.10	122.70
22	U	176	GLU	CG-CD-OE1	6.91	132.12	118.30
22	S	114	PRO	CA-N-CD	-6.88	101.88	111.50
22	S	103	ASP	CB-CG-OD1	-6.82	112.17	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	W	55	GLU	OE1-CD-OE2	-6.73	115.22	123.30
6	6	78	GLU	OE1-CD-OE2	-6.68	115.28	123.30
10	D	147	ASP	OD1-CG-OD2	-6.55	110.86	123.30
22	R	175	GLU	CG-CD-OE2	6.45	131.19	118.30
3	3	200	PHE	CB-CG-CD1	6.42	125.29	120.80
1	1	103	PRO	CB-CG-CD	-6.41	81.50	106.50
23	Q	193	ASP	CB-CG-OD1	6.24	123.92	118.30
22	P	97	ASP	CB-CG-OD1	6.18	123.86	118.30
5	5	97	GLU	OE1-CD-OE2	-6.10	115.98	123.30
22	T	55	GLU	OE1-CD-OE2	-5.95	116.16	123.30
22	R	110	ALA	C-N-CD	5.84	140.68	128.40
2	2	155	ASP	CB-CG-OD1	5.76	123.49	118.30
1	1	73	GLU	OE1-CD-OE2	-5.75	116.39	123.30
22	R	175	GLU	OE1-CD-OE2	-5.71	116.45	123.30
22	S	69	MET	CG-SD-CE	-5.58	91.27	100.20
22	R	156	ASP	CB-CG-OD1	5.43	123.19	118.30
22	X	174	LEU	CA-CB-CG	5.33	127.56	115.30
22	V	36	PRO	CA-N-CD	-5.28	104.11	111.50
22	V	92	LEU	CB-CG-CD1	-5.25	102.07	111.00
7	A	371	MET	CG-SD-CE	-5.13	91.99	100.20
7	A	455	LEU	CA-CB-CG	5.08	126.97	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
22	U	176	GLU	Mainchain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	1209	0	1167	18	0
2	2	1583	0	1529	19	0
3	3	1717	0	1657	23	0
4	4	1579	0	1521	27	0
5	5	1278	0	1267	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	6	1484	0	1465	13	0
7	A	5819	0	5655	69	0
8	B	5773	0	5540	48	0
9	C	593	0	573	4	0
10	D	1116	0	1151	9	0
11	E	503	0	489	2	0
12	F	1259	0	1285	15	0
13	G	717	0	685	34	0
14	H	721	0	698	8	0
15	I	264	0	286	10	0
16	J	328	0	341	6	0
17	K	625	0	625	10	0
18	L	1169	0	1186	8	0
19	M	239	0	262	2	0
20	N	676	0	650	13	0
21	O	759	0	722	7	0
22	P	1507	0	1429	19	0
22	R	1507	0	1429	40	0
22	S	1512	0	1434	33	0
22	T	1507	0	1429	19	0
22	U	1507	0	1429	11	0
22	V	1484	0	1411	35	0
22	W	1499	0	1425	23	0
22	X	1474	0	1401	26	0
23	Q	1706	0	1649	36	0
24	1	96	0	68	1	0
24	2	177	0	115	2	0
24	3	45	0	30	1	0
24	4	181	0	117	3	0
24	5	41	0	24	0	0
24	6	127	0	77	0	0
24	P	233	0	163	1	0
24	Q	185	0	130	1	0
24	R	284	0	200	9	0
24	S	223	0	151	7	0
24	T	282	0	199	1	0
24	U	175	0	118	1	0
24	V	221	0	153	3	0
24	W	243	0	189	1	0
24	X	225	0	155	2	0
25	1	424	0	334	9	0
25	2	530	0	430	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	3	602	0	470	13	0
25	4	510	0	396	6	0
25	5	430	0	345	8	0
25	6	494	0	412	9	0
25	A	2557	0	2585	28	0
25	B	2465	0	2485	38	0
25	F	83	0	60	2	0
25	G	132	0	97	3	0
25	H	154	0	138	1	0
25	J	42	0	31	1	0
25	K	218	0	201	3	0
25	L	188	0	152	2	0
25	N	87	0	61	1	0
25	O	247	0	217	2	0
25	P	467	0	454	5	0
25	Q	458	0	387	10	0
25	R	467	0	454	8	0
25	S	443	0	414	13	0
25	T	438	0	411	3	0
25	U	378	0	296	1	0
25	V	412	0	347	15	0
25	W	427	0	379	11	0
25	X	373	0	290	9	0
26	1	44	0	0	0	0
26	3	44	0	0	2	0
26	4	88	0	0	3	0
26	5	44	0	0	0	0
26	6	44	0	0	2	0
26	P	88	0	0	2	0
26	Q	88	0	0	1	0
26	R	88	0	0	1	0
26	S	132	0	0	2	0
26	T	88	0	0	2	0
26	U	44	0	0	0	0
26	V	132	0	0	2	0
26	W	44	0	0	2	0
26	X	44	0	0	0	0
27	1	44	0	56	0	0
27	2	44	0	56	1	0
27	3	44	0	56	2	0
27	4	44	0	56	1	0
27	5	44	0	56	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
27	6	44	0	56	2	0
28	1	35	0	40	1	0
28	2	33	0	36	1	0
28	3	145	0	180	0	0
28	6	46	0	65	1	0
28	A	79	0	104	0	0
28	Q	35	0	40	0	0
29	2	42	0	0	2	0
29	O	84	0	0	1	0
29	P	168	0	0	1	0
29	Q	126	0	0	1	0
29	R	210	0	0	2	0
29	S	210	0	0	1	0
29	T	168	0	0	1	0
29	U	126	0	0	2	0
29	V	168	0	0	1	0
29	W	168	0	0	2	0
29	X	166	0	0	1	0
30	2	40	0	56	0	0
30	3	120	0	168	1	0
30	4	40	0	56	2	0
30	A	200	0	280	5	0
30	B	200	0	280	2	0
30	F	80	0	112	1	0
30	G	80	0	112	5	0
30	H	40	0	56	0	0
30	I	40	0	56	0	0
30	J	80	0	112	4	0
30	K	120	0	168	2	0
30	L	120	0	168	3	0
30	M	40	0	56	1	0
31	2	31	0	32	0	0
31	5	54	0	81	0	0
31	A	104	0	121	1	0
31	B	38	0	46	0	0
31	F	31	0	32	1	0
31	J	46	0	65	0	0
31	L	31	0	32	0	0
31	N	55	0	86	0	0
31	O	39	0	48	0	0
32	6	54	0	78	0	0
32	H	48	0	60	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
33	A	65	0	72	0	0
34	A	33	0	46	1	0
34	B	33	0	46	0	0
35	A	8	0	0	0	0
35	C	16	0	0	0	0
36	A	51	0	60	1	0
36	B	59	0	79	1	0
37	H	44	0	56	0	0
37	P	44	0	56	1	0
37	R	44	0	56	0	0
37	S	44	0	56	0	0
37	T	44	0	56	0	0
37	W	44	0	56	0	0
38	P	45	0	0	1	0
38	Q	45	0	0	0	0
38	R	45	0	0	2	0
38	S	45	0	0	1	0
38	T	45	0	0	1	0
38	U	45	0	0	0	0
38	V	45	0	0	1	0
38	W	45	0	0	0	0
38	X	45	0	0	0	0
39	A	3	0	0	0	0
39	Q	1	0	0	0	0
All	All	64832	0	59326	634	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 5.

All (634) 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)
1:1:103:PRO:CG	1:1:103:PRO:CB	1.96	1.39
7:A:489:HIS:NE2	21:O:101:ASP:OD1	1.65	1.30
5:5:97:GLU:OE2	5:5:103:ALA:HB2	1.12	1.28
5:5:97:GLU:OE2	5:5:103:ALA:CB	1.84	1.25
13:G:53:TYR:CE1	13:G:57:PHE:CE2	2.38	1.12
13:G:53:TYR:CD1	13:G:57:PHE:CE2	2.38	1.11
23:Q:209:MET:CE	25:Q:304:CLA:HAB	1.81	1.10
13:G:53:TYR:CD1	13:G:57:PHE:HE2	1.70	1.08
25:B:842:CLA:H72	15:I:23:MET:CE	1.83	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:S:39:GLY:HA3	25:S:301:CLA:HMD1	1.34	1.07
23:Q:209:MET:HE1	25:Q:304:CLA:HAB	1.35	1.03
25:B:842:CLA:H72	15:I:23:MET:HE3	1.06	1.02
22:P:66:ARG:HH22	22:P:158:ASN:HB3	1.23	1.01
25:B:842:CLA:C7	15:I:23:MET:HE3	1.98	0.91
13:G:66:GLN:O	13:G:70:VAL:HG12	1.72	0.88
15:I:23:MET:CE	30:L:305:BCR:H352	2.03	0.88
22:R:114:PRO:HB2	22:R:117:SER:HB3	1.56	0.87
13:G:53:TYR:CE1	13:G:57:PHE:CD2	2.62	0.86
7:A:197:MET:HG2	25:A:815:CLA:HBC2	1.59	0.83
23:Q:209:MET:HE2	25:Q:304:CLA:HAB	1.62	0.80
22:V:177:LEU:HG	25:V:309:CLA:H3A	1.62	0.80
7:A:508:ALA:HB3	7:A:523:MET:HG3	1.62	0.80
22:R:114:PRO:HG3	24:R:308:CHL:C3B	2.12	0.80
22:W:174:LEU:HD12	25:W:309:CLA:HMA2	1.65	0.78
23:Q:121:ALA:O	23:Q:125:LYS:NZ	2.11	0.78
22:R:114:PRO:HG2	22:R:119:TYR:HD1	1.51	0.76
25:B:824:CLA:HED3	13:G:69:ARG:HH12	1.50	0.76
22:U:47:SER:OG	22:U:50:ILE:O	1.99	0.76
17:K:65:ALA:HB1	17:K:71:MET:HG3	1.68	0.76
22:R:94:THR:OG1	22:R:96:ASP:OD1	2.03	0.76
15:I:23:MET:HE2	30:L:305:BCR:H352	1.68	0.76
22:S:52:PHE:HZ	22:S:55:GLU:HA	1.48	0.76
13:G:53:TYR:HD1	13:G:57:PHE:HE2	1.32	0.75
12:F:215:LYS:NZ	12:F:216:ASN:OD1	2.19	0.75
15:I:23:MET:HE1	30:L:305:BCR:H352	1.69	0.75
13:G:63:GLN:HE22	30:G:201:BCR:H313	1.51	0.75
8:B:257:PHE:CD1	25:B:819:CLA:HMB2	2.22	0.74
8:B:363:GLN:O	14:H:163:ARG:NH1	2.20	0.74
22:P:66:ARG:NH2	22:P:158:ASN:HB3	2.01	0.74
22:V:137:GLU:OE1	38:V:308:KC2:C4C	2.34	0.73
22:W:169:ALA:HB1	22:W:174:LEU:HD13	1.70	0.72
22:S:52:PHE:CD1	25:S:301:CLA:HMA2	2.24	0.72
22:R:65:GLY:O	22:R:69:MET:HG3	1.89	0.72
13:G:63:GLN:NE2	30:G:201:BCR:H313	2.05	0.71
13:G:97:THR:HG22	13:G:99:ASP:H	1.55	0.70
10:D:128:ASP:OD1	10:D:150:TYR:OH	2.08	0.70
13:G:53:TYR:CD1	13:G:57:PHE:CD2	2.79	0.70
5:5:130:ARG:NH2	25:5:607:CLA:O1D	2.25	0.70
8:B:256:THR:HA	25:B:818:CLA:HED1	1.74	0.70
1:1:36:PRO:O	4:4:139:GLN:NE2	2.24	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:K:71:MET:HG2	25:K:206:CLA:CHC	2.22	0.69
1:1:215:VAL:HG21	25:1:610:CLA:HMD3	1.72	0.69
8:B:732:PHE:O	14:H:163:ARG:NE	2.26	0.69
7:A:489:HIS:NE2	21:O:101:ASP:CG	2.46	0.68
17:K:65:ALA:HB3	17:K:71:MET:SD	2.34	0.68
22:R:80:ASN:ND2	26:R:322:IWJ:O44	2.26	0.68
5:5:97:GLU:OE2	5:5:103:ALA:CA	2.40	0.68
22:U:84:ILE:O	22:U:84:ILE:HD12	1.94	0.68
13:G:63:GLN:NE2	30:G:201:BCR:C31	2.57	0.68
7:A:509:SER:HA	7:A:525:PRO:HA	1.76	0.68
24:V:307:CHL:HMB1	24:V:307:CHL:HBB1	1.75	0.68
22:X:36:PRO:HD2	22:X:183:LYS:NZ	2.09	0.68
22:W:169:ALA:CB	22:W:174:LEU:HD13	2.24	0.67
3:3:227:MET:SD	25:3:301:CLA:HMC1	2.35	0.67
7:A:94:HIS:HA	7:A:98:PHE:HD2	1.58	0.67
7:A:18:ASP:OD2	7:A:71:ARG:NH2	2.28	0.67
25:B:824:CLA:CED	13:G:69:ARG:HH12	2.08	0.66
12:F:95:LEU:HD13	12:F:116:MET:HA	1.77	0.66
14:H:140:VAL:O	14:H:144:LYS:NZ	2.28	0.66
22:V:180:LYS:HZ1	25:V:311:CLA:HBD	1.59	0.66
3:3:96:GLU:OE1	25:3:301:CLA:C4A	2.43	0.65
22:X:39:GLY:HA3	25:X:302:CLA:HMD1	1.78	0.65
22:W:92:LEU:CD2	25:W:303:CLA:H2A	2.26	0.65
22:X:36:PRO:HD2	22:X:183:LYS:HZ1	1.60	0.65
22:S:52:PHE:HD1	25:S:301:CLA:HMA2	1.60	0.65
13:G:56:ARG:HH22	13:G:100:PRO:HD2	1.62	0.65
7:A:695:GLU:OE1	8:B:535:LYS:NZ	2.29	0.65
22:V:198:GLN:HE21	22:V:209:ASN:HD22	1.44	0.64
13:G:66:GLN:OE1	13:G:69:ARG:NH2	2.30	0.64
22:P:66:ARG:HH22	22:P:158:ASN:CB	2.07	0.64
22:R:137:GLU:OE1	38:R:312:KC2:NB	2.30	0.64
22:S:34:ILE:O	22:S:36:PRO:HD3	1.98	0.64
22:R:62:VAL:HG11	22:R:157:VAL:HG11	1.81	0.63
2:2:177:ASP:OD1	25:2:609:CLA:HBD	1.98	0.63
23:Q:177:VAL:HG23	23:Q:178:THR:HG23	1.79	0.63
6:6:38:ARG:NH1	6:6:58:ASP:O	2.32	0.63
25:B:842:CLA:C7	15:I:23:MET:CE	2.68	0.63
22:W:61:GLU:OE1	25:W:301:CLA:C4A	2.46	0.63
7:A:467:ARG:NH2	25:A:836:CLA:O1D	2.32	0.63
20:N:106:LYS:HD2	20:N:107:PHE:CE2	2.33	0.63
22:X:35:TYR:CD2	22:X:183:LYS:HE2	2.34	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:O:101:ASP:OD1	21:O:101:ASP:O	2.17	0.62
22:X:35:TYR:HD2	22:X:183:LYS:HE2	1.64	0.62
25:V:301:CLA:H72	25:V:302:CLA:HMD1	1.82	0.62
7:A:489:HIS:CD2	21:O:101:ASP:OD1	2.51	0.62
22:R:113:ALA:HB1	22:R:118:GLY:HA2	1.81	0.62
22:V:163:PHE:CD2	25:V:309:CLA:HMD1	2.34	0.62
26:P:320:IWJ:O27	26:P:320:IWJ:O39	2.17	0.62
13:G:63:GLN:HE22	30:G:201:BCR:C31	2.13	0.62
8:B:53:GLN:OE1	25:B:808:CLA:NC	2.33	0.62
17:K:71:MET:HG2	25:K:206:CLA:C4B	2.30	0.61
22:S:168:LEU:HD13	25:S:309:CLA:H42	1.81	0.61
22:U:35:TYR:OH	22:U:186:ARG:NH1	2.34	0.61
1:1:148:LEU:HA	25:1:605:CLA:HMD2	1.83	0.61
22:R:69:MET:HG2	22:R:188:SER:OG	2.01	0.61
22:R:56:LYS:HB3	22:R:60:ARG:NH1	2.16	0.60
25:B:842:CLA:H101	15:I:23:MET:HE1	1.82	0.60
13:G:56:ARG:HE	13:G:101:ALA:HB3	1.65	0.60
26:T:318:IWJ:O27	26:T:318:IWJ:O39	2.16	0.60
21:O:123:GLN:OE1	29:O:2006:Q6L:O39	2.19	0.60
23:Q:209:MET:HE1	25:Q:304:CLA:CAB	2.23	0.60
6:6:226:PHE:HB2	25:6:612:CLA:HMC1	1.83	0.60
22:S:52:PHE:CZ	22:S:55:GLU:HA	2.34	0.60
4:4:212:PRO:O	26:4:317:IWJ:O38	2.20	0.60
26:W:318:IWJ:O27	26:W:318:IWJ:O39	2.15	0.60
1:1:79:TRP:CD1	25:1:606:CLA:HMD3	2.37	0.59
22:S:167:GLY:O	22:S:170:GLU:HG2	2.02	0.59
7:A:600:TYR:HB2	7:A:732:LEU:HD11	1.84	0.59
22:R:39:GLY:HA3	25:R:305:CLA:HMD1	1.83	0.59
22:W:92:LEU:HG	22:W:101:VAL:HG22	1.84	0.59
25:A:856:CLA:HMC2	30:F:801:BCR:H381	1.84	0.59
22:T:41:TYR:CE1	22:T:44:GLY:N	2.71	0.59
1:1:148:LEU:O	25:1:607:CLA:HBB2	2.03	0.59
7:A:197:MET:CG	25:A:815:CLA:HBC2	2.32	0.59
22:X:174:LEU:HG	22:X:178:LYS:HZ2	1.68	0.59
22:V:194:GLY:O	22:V:198:GLN:HG3	2.03	0.58
22:R:114:PRO:HD2	22:R:119:TYR:H	1.69	0.58
5:5:197:ILE:HD11	25:5:610:CLA:HMC3	1.85	0.58
7:A:381:ALA:HB1	7:A:522:ALA:O	2.03	0.58
22:R:164:ASP:OD1	22:R:167:GLY:N	2.36	0.58
8:B:254:ILE:HG13	8:B:255:LEU:HG	1.84	0.58
22:W:39:GLY:HA3	25:W:301:CLA:HMD1	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:85:GLY:O	3:3:88:ASN:ND2	2.37	0.58
30:B:847:BCR:H313	30:B:848:BCR:H272	1.85	0.57
22:W:173:ASP:HB2	22:W:176:GLU:HB2	1.85	0.57
8:B:256:THR:HA	25:B:818:CLA:CED	2.34	0.57
7:A:75:SER:HB2	25:A:813:CLA:HMD3	1.86	0.57
1:1:132:VAL:HG11	25:1:606:CLA:HMC3	1.87	0.57
4:4:109:ALA:O	4:4:112:TYR:HB3	2.04	0.57
13:G:98:ASN:HB2	25:G:204:CLA:CAD	2.34	0.57
22:W:206:PRO:O	29:W:315:Q6L:O08	2.23	0.57
22:X:34:ILE:HG12	22:X:36:PRO:HD3	1.87	0.57
7:A:736:ILE:HG21	25:A:830:CLA:HMC2	1.87	0.57
4:4:195:MET:HE2	25:4:303:CLA:HMC3	1.87	0.56
7:A:521:ILE:HD11	7:A:627:VAL:HG13	1.86	0.56
22:X:209:ASN:N	22:X:209:ASN:OD1	2.36	0.56
1:1:43:HIS:NE2	1:1:55:ASP:OD2	2.38	0.56
3:3:56:GLU:OE2	17:K:95:THR:OG1	2.24	0.56
13:G:129:GLN:HE21	25:G:202:CLA:CAD	2.17	0.56
20:N:65:ASP:OD1	20:N:68:ARG:NH2	2.38	0.56
22:P:39:GLY:HA3	25:P:301:CLA:HMD1	1.87	0.56
25:V:301:CLA:H3A	25:V:301:CLA:O1A	2.06	0.56
22:X:61:GLU:OE1	25:X:302:CLA:C4A	2.53	0.56
22:R:112:LEU:HD21	24:R:308:CHL:CHD	2.36	0.56
8:B:683:ARG:HE	18:L:63:MET:HB2	1.71	0.56
2:2:135:PHE:CD2	25:2:608:CLA:HMC3	2.41	0.56
22:P:158:ASN:HB2	25:P:309:CLA:CGD	2.36	0.56
22:U:206:PRO:O	29:U:314:Q6L:O08	2.24	0.56
8:B:106:ARG:NH2	8:B:113:VAL:O	2.38	0.56
25:B:823:CLA:HMD2	30:G:201:BCR:HC7	1.87	0.56
22:V:86:TRP:CH2	22:V:196:ILE:HG22	2.41	0.56
23:Q:58:GLU:OE1	23:Q:203:LYS:NZ	2.34	0.56
25:X:304:CLA:H2A	25:X:304:CLA:HED3	1.87	0.56
4:4:137:ARG:O	4:4:141:MET:HG3	2.06	0.55
7:A:156:GLU:OE2	20:N:75:ASN:ND2	2.38	0.55
22:X:101:VAL:HG11	24:X:306:CHL:HBC1	1.88	0.55
22:W:80:ASN:ND2	26:W:318:IWJ:O44	2.39	0.55
22:X:218:VAL:O	22:X:221:ASN:ND2	2.39	0.55
23:Q:60:GLY:HA3	25:Q:304:CLA:HMD1	1.87	0.55
22:T:61:GLU:OE2	22:T:186:ARG:NH2	2.39	0.55
4:4:71:TYR:HH	12:F:208:LEU:HD11	1.71	0.55
16:J:1:MET:O	16:J:5:GLN:HG3	2.06	0.55
23:Q:85:HIS:HB3	23:Q:209:MET:CE	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:74:ALA:HB2	25:4:309:CLA:HED3	1.89	0.55
14:H:101:ARG:NH2	18:L:80:ASN:O	2.40	0.55
26:6:614:IWJ:O27	26:6:614:IWJ:O39	2.21	0.55
23:Q:40:SER:HB3	23:Q:43:LYS:HB2	1.88	0.55
23:Q:57:PRO:HG2	23:Q:58:GLU:OE2	2.06	0.55
22:V:86:TRP:HH2	22:V:196:ILE:HG22	1.70	0.54
3:3:151:ILE:HD13	25:3:304:CLA:HMD3	1.87	0.54
6:6:128:MET:HG3	25:6:607:CLA:HMC3	1.90	0.54
4:4:50:LEU:HD21	4:4:68:LEU:HD11	1.88	0.54
31:F:805:LMG:HC61	16:J:2:LYS:HD2	1.89	0.54
7:A:600:TYR:HB2	7:A:732:LEU:CD1	2.37	0.54
13:G:55:GLY:O	13:G:60:LEU:HB2	2.07	0.54
20:N:95:GLY:HA2	25:N:202:CLA:HMD2	1.90	0.54
7:A:83:VAL:HG11	25:A:808:CLA:HMD2	1.89	0.54
23:Q:49:SER:HB3	23:Q:193:ASP:HB3	1.90	0.54
22:V:61:GLU:OE2	22:V:186:ARG:NE	2.40	0.54
25:A:810:CLA:HMC3	25:A:811:CLA:HMD2	1.88	0.54
18:L:83:ALA:HB2	25:L:302:CLA:HMD1	1.90	0.53
26:S:322:IWJ:O27	26:S:322:IWJ:O39	2.26	0.53
11:E:50:LYS:NZ	12:F:224:SER:O	2.41	0.53
23:Q:57:PRO:HD2	23:Q:203:LYS:HZ1	1.73	0.53
22:R:37:GLU:OE1	22:R:183:LYS:NZ	2.42	0.53
17:K:65:ALA:CB	17:K:71:MET:SD	2.96	0.53
22:R:42:PRO:HA	25:R:305:CLA:HED3	1.90	0.53
22:V:35:TYR:OH	22:V:186:ARG:NH1	2.41	0.53
10:D:110:ARG:NH2	10:D:112:GLU:OE1	2.40	0.53
22:R:114:PRO:CD	22:R:119:TYR:H	2.22	0.53
22:S:139:TYR:CD2	22:S:147:PRO:HD3	2.43	0.53
7:A:34:HIS:NE2	25:A:813:CLA:O1A	2.39	0.53
7:A:562:LEU:O	10:D:110:ARG:NH1	2.42	0.53
22:S:112:LEU:O	24:S:304:CHL:C4D	2.56	0.53
22:U:216:ASP:OD2	22:U:219:HIS:CD2	2.61	0.53
12:F:87:ARG:NH2	12:F:136:ASP:OD1	2.42	0.53
22:V:177:LEU:CG	25:V:309:CLA:H3A	2.35	0.53
22:W:52:PHE:HA	25:W:301:CLA:HBA1	1.90	0.53
25:5:609:CLA:H92	25:5:609:CLA:HMC2	1.91	0.53
23:Q:101:ASN:ND2	26:Q:320:IWJ:O44	2.41	0.53
8:B:54:LEU:HD11	25:B:815:CLA:HBA2	1.91	0.52
8:B:444:GLN:NE2	8:B:452:GLN:OE1	2.41	0.52
2:2:83:GLN:OE1	2:2:142:ARG:NH1	2.41	0.52
22:U:79:GLU:HB2	22:U:207:ILE:HD13	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:176:PHE:CD2	25:2:609:CLA:HMD1	2.43	0.52
7:A:193:ASN:O	7:A:197:MET:HG3	2.10	0.52
8:B:128:GLY:O	8:B:208:ARG:NH2	2.42	0.52
13:G:56:ARG:NE	13:G:101:ALA:HB3	2.25	0.52
22:P:61:GLU:OE1	25:P:301:CLA:C4A	2.56	0.52
22:P:137:GLU:OE1	38:P:308:KC2:C4A	2.55	0.52
23:Q:123:ALA:HB1	23:Q:134:ALA:H	1.75	0.52
22:R:62:VAL:CG1	22:R:157:VAL:HG11	2.40	0.52
22:R:120:PRO:HG3	24:R:308:CHL:C4C	2.39	0.52
22:R:69:MET:CG	22:R:188:SER:OG	2.58	0.52
2:2:87:TRP:CD1	25:2:608:CLA:HMD3	2.45	0.52
8:B:5:PHE:HB2	15:I:30:ILE:HA	1.91	0.52
22:V:79:GLU:OE1	22:V:207:ILE:HB	2.10	0.52
4:4:112:TYR:HD1	4:4:115:TYR:CE2	2.28	0.52
6:6:240:GLN:OE1	19:M:24:ARG:NH2	2.43	0.52
17:K:53:MET:HG2	24:W:314:CHL:H3A	1.92	0.52
5:5:184:VAL:HG21	25:5:609:CLA:HMD1	1.91	0.51
22:T:140:ARG:NH1	38:T:308:KC2:O1D	2.39	0.51
3:3:87:VAL:HA	3:3:92:LEU:HD11	1.93	0.51
7:A:36:SER:OG	7:A:37:ARG:N	2.44	0.51
7:A:349:TRP:HE3	25:A:807:CLA:HMD2	1.74	0.51
23:Q:85:HIS:HB3	23:Q:209:MET:HE3	1.92	0.51
5:5:78:ALA:HB1	5:5:168:GLY:HA3	1.92	0.51
8:B:56:ILE:HG21	25:B:808:CLA:HMD2	1.92	0.51
23:Q:245:ASN:ND2	25:Q:314:CLA:OBD	2.42	0.51
5:5:80:TRP:CD1	25:5:607:CLA:HMD3	2.45	0.51
13:G:96:SER:O	13:G:96:SER:OG	2.27	0.51
23:Q:46:LYS:HD2	23:Q:191:ALA:O	2.11	0.51
2:2:51:HIS:O	2:2:74:ARG:NH1	2.44	0.51
5:5:180:VAL:HG12	25:5:609:CLA:HMD3	1.92	0.51
7:A:244:MET:HE2	7:A:245:LEU:CD2	2.41	0.51
22:P:66:ARG:NH1	22:P:157:VAL:HG12	2.25	0.51
7:A:97:ARG:HG2	36:A:854:DGD:O5E	2.11	0.51
13:G:48:ASN:OD1	13:G:112:GLY:HA2	2.11	0.51
22:V:176:GLU:O	22:V:180:LYS:HG3	2.11	0.51
34:A:844:PQN:H291	25:F:802:CLA:HMC1	1.91	0.51
25:B:825:CLA:HAB	25:B:832:CLA:HMD2	1.91	0.51
25:P:301:CLA:HMC2	29:P:316:Q6L:C15	2.40	0.50
4:4:109:ALA:N	4:4:110:PRO:HD2	2.26	0.50
7:A:27:GLU:HA	16:J:3:ASN:HD22	1.76	0.50
16:J:4:PHE:O	16:J:8:LEU:HG	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:Q:39:ARG:NE	22:T:149:ASP:OD1	2.43	0.50
30:A:852:BCR:H24C	25:B:835:CLA:HMC2	1.93	0.50
22:R:156:ASP:OD1	22:R:158:ASN:N	2.41	0.50
22:R:114:PRO:HG2	22:R:119:TYR:CD1	2.40	0.50
2:2:228:ILE:HD11	25:2:613:CLA:HMC3	1.94	0.50
4:4:126:GLN:OE1	4:4:127:MET:SD	2.69	0.50
7:A:244:MET:HE2	7:A:245:LEU:HD21	1.94	0.50
7:A:434:ARG:NH2	10:D:93:THR:O	2.43	0.50
8:B:54:LEU:HD12	25:B:815:CLA:HED1	1.93	0.50
12:F:95:LEU:HB3	12:F:116:MET:HG2	1.94	0.50
22:V:198:GLN:HG2	25:V:312:CLA:ND	2.26	0.50
26:P:318:IWJ:O27	26:P:318:IWJ:O39	2.29	0.50
22:R:114:PRO:HG3	24:R:308:CHL:C2B	2.41	0.50
1:1:130:VAL:HG11	13:G:50:LEU:HD21	1.93	0.50
2:2:172:PRO:HG2	2:2:176:PHE:CE2	2.47	0.50
22:V:34:ILE:HD11	22:V:179:ILE:HG21	1.94	0.50
3:3:235:GLN:NE2	26:3:315:IWJ:O38	2.45	0.50
21:O:129:ARG:NH1	25:O:2002:CLA:OBD	2.44	0.50
22:P:153:THR:O	22:P:156:ASP:HB3	2.11	0.50
22:T:216:ASP:OD1	22:T:219:HIS:ND1	2.45	0.50
25:X:311:CLA:H2A	25:X:311:CLA:HED3	1.93	0.50
9:C:55:GLU:OE2	9:C:66:ARG:NH1	2.45	0.49
12:F:92:LEU:O	12:F:96:GLU:HG2	2.12	0.49
23:Q:71:ILE:HG22	25:Q:304:CLA:HBA2	1.93	0.49
25:R:305:CLA:HMC2	29:R:320:Q6L:C15	2.42	0.49
22:S:137:GLU:OE1	38:S:308:KC2:NB	2.45	0.49
22:X:36:PRO:HG3	25:X:311:CLA:HMA3	1.93	0.49
25:6:602:CLA:HMC2	27:6:615:XAT:C31	2.42	0.49
22:V:42:PRO:HD3	22:V:186:ARG:NH2	2.27	0.49
22:V:46:GLU:OE2	22:V:47:SER:OG	2.30	0.49
10:D:77:TYR:OH	10:D:133:ARG:NH1	2.45	0.49
4:4:71:TYR:OH	12:F:208:LEU:HD11	2.12	0.49
8:B:667:ARG:NH1	8:B:698:ALA:O	2.45	0.49
25:3:301:CLA:HMC2	27:3:316:XAT:C31	2.42	0.49
25:A:824:CLA:HMA1	30:K:207:BCR:H343	1.95	0.49
8:B:84:VAL:HA	14:H:166:ILE:HG12	1.94	0.49
22:U:61:GLU:OE1	25:U:301:CLA:C4A	2.56	0.49
26:V:317:IWJ:O27	26:V:317:IWJ:O39	2.30	0.49
1:1:37:GLY:O	4:4:139:GLN:NE2	2.43	0.49
22:T:66:ARG:NH2	22:T:157:VAL:O	2.45	0.49
25:W:309:CLA:O1D	25:W:309:CLA:H2A	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:521:ILE:HD13	7:A:524:MET:HE1	1.95	0.49
7:A:195:GLU:OE1	7:A:312:TYR:HB3	2.12	0.49
22:P:210:TRP:CZ3	22:P:214:VAL:HG21	2.48	0.49
22:T:225:ASN:ND2	25:T:312:CLA:OBD	2.45	0.49
1:1:207:LEU:HD21	25:1:609:CLA:HMC3	1.95	0.49
3:3:101:ARG:NH1	24:3:306:CHL:OBD	2.44	0.49
12:F:92:LEU:HA	12:F:95:LEU:HD12	1.94	0.49
18:L:133:VAL:O	18:L:137:THR:OG1	2.30	0.49
25:A:811:CLA:HAB	25:B:835:CLA:HMD2	1.94	0.49
22:R:140:ARG:HG3	24:R:311:CHL:C1D	2.43	0.49
2:2:179:LEU:HB3	2:2:181:TYR:CE1	2.48	0.48
8:B:206:THR:O	8:B:211:ASN:ND2	2.38	0.48
22:V:189:MET:HB3	25:V:301:CLA:HMC3	1.94	0.48
13:G:54:LEU:HD12	13:G:58:VAL:HG21	1.95	0.48
30:J:101:BCR:H313	25:J:102:CLA:HMD3	1.95	0.48
8:B:606:ALA:O	8:B:610:GLU:HG3	2.14	0.48
22:R:69:MET:HG2	22:R:188:SER:CB	2.43	0.48
22:T:79:GLU:HG2	22:T:207:ILE:HB	1.95	0.48
4:4:54:TYR:N	25:4:303:CLA:OBD	2.45	0.48
22:T:102:ALA:HA	22:T:112:LEU:HD23	1.95	0.48
7:A:584:CYS:N	8:B:667:ARG:O	2.46	0.48
25:3:303:CLA:HMD2	25:3:313:CLA:HAB	1.95	0.48
17:K:98:SER:OG	17:K:104:PHE:O	2.31	0.48
22:U:138:ALA:HA	22:U:143:ILE:HD12	1.95	0.48
13:G:55:GLY:HA3	13:G:111:TRP:CE2	2.48	0.48
22:W:158:ASN:HB2	25:W:309:CLA:CGD	2.44	0.48
2:2:173:GLY:O	2:2:177:ASP:HB2	2.12	0.48
7:A:370:HIS:ND1	25:A:820:CLA:OBD	2.46	0.48
23:Q:48:GLY:N	23:Q:192:GLY:HA2	2.28	0.48
22:R:140:ARG:HG3	24:R:311:CHL:CHD	2.44	0.48
22:S:147:PRO:CD	22:S:148:PHE:H	2.27	0.48
7:A:508:ALA:HB3	7:A:523:MET:CG	2.37	0.48
8:B:351:HIS:ND1	25:B:819:CLA:OBD	2.44	0.48
20:N:77:GLU:HG2	20:N:107:PHE:HD2	1.78	0.48
22:X:66:ARG:NH1	24:X:308:CHL:OBD	2.45	0.48
26:4:301:IWJ:O27	26:4:301:IWJ:O39	2.29	0.47
25:B:808:CLA:HBC3	25:B:808:CLA:HHD	1.95	0.47
22:R:58:ALA:HA	25:R:305:CLA:HMA1	1.95	0.47
22:T:66:ARG:NH1	24:T:307:CHL:OBD	2.44	0.47
22:S:47:SER:OG	22:S:51:PRO:HA	2.13	0.47
2:2:197:LYS:NZ	28:2:619:LHG:O5	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:J:2:LYS:O	16:J:6:ILE:HG13	2.14	0.47
22:S:114:PRO:HD2	24:S:304:CHL:C1B	2.45	0.47
22:T:86:TRP:O	29:T:316:Q6L:O39	2.32	0.47
7:A:577:GLY:O	7:A:583:THR:OG1	2.27	0.47
22:S:137:GLU:O	22:S:141:THR:HG22	2.15	0.47
22:V:125:VAL:HG21	24:V:305:CHL:C3D	2.44	0.47
22:V:142:GLY:HA2	22:V:154:VAL:HG11	1.95	0.47
22:X:36:PRO:HG3	25:X:311:CLA:CMA	2.45	0.47
5:5:76:MET:SD	5:5:130:ARG:NE	2.88	0.47
8:B:60:TRP:NE1	25:B:829:CLA:OBD	2.48	0.47
22:R:121:SER:H	22:R:124:ASN:HB2	1.80	0.47
1:1:222:ILE:HD12	1:1:223:PRO:O	2.14	0.47
22:U:164:ASP:OD1	29:U:314:Q6L:O39	2.33	0.47
3:3:191:SER:O	3:3:191:SER:OG	2.32	0.47
25:B:815:CLA:O1A	25:B:815:CLA:H3A	2.15	0.47
20:N:112:MET:O	20:N:115:GLU:HG2	2.15	0.47
22:S:163:PHE:HZ	24:S:307:CHL:NB	2.13	0.47
22:T:180:LYS:HD3	25:T:311:CLA:HBD	1.96	0.47
22:V:61:GLU:OE1	25:V:301:CLA:C4A	2.57	0.47
22:V:142:GLY:CA	22:V:154:VAL:HG11	2.45	0.47
25:B:834:CLA:HMB1	25:B:834:CLA:HBB1	1.96	0.46
22:P:148:PHE:HB3	22:P:162:ARG:NH1	2.30	0.46
4:4:80:ARG:NH1	24:4:308:CHL:OBD	2.44	0.46
5:5:44:HIS:NE2	5:5:56:ASP:OD2	2.49	0.46
7:A:599:MET:O	7:A:603:ILE:HG12	2.15	0.46
22:V:72:VAL:O	22:V:75:ALA:HB3	2.15	0.46
22:W:198:GLN:HG2	25:W:312:CLA:ND	2.30	0.46
25:2:602:CLA:HMC2	27:2:617:XAT:C31	2.46	0.46
14:H:160:VAL:HG12	14:H:166:ILE:HG22	1.97	0.46
18:L:111:LYS:NZ	18:L:204:SER:O	2.41	0.46
22:W:113:ALA:HB3	22:W:120:PRO:HG3	1.96	0.46
22:W:164:ASP:OD1	29:W:315:Q6L:O39	2.33	0.46
5:5:186:ARG:HH22	8:B:213:LEU:HB3	1.81	0.46
22:S:52:PHE:CE1	25:S:301:CLA:HMA2	2.51	0.46
1:1:90:VAL:HG23	1:1:98:TRP:HA	1.97	0.46
22:R:73:THR:HG23	25:R:307:CLA:HMC3	1.97	0.46
24:2:607:CHL:HMB1	24:2:607:CHL:HBB1	1.97	0.46
25:6:610:CLA:H143	25:6:611:CLA:HMD2	1.98	0.46
37:P:317:NEX:H162	37:P:317:NEX:H193	1.96	0.46
22:R:56:LYS:NZ	38:R:312:KC2:O2A	2.47	0.46
22:S:61:GLU:OE1	25:S:301:CLA:C4A	2.63	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:V:320:IWJ:O27	26:V:320:IWJ:O39	2.34	0.46
7:A:454:GLY:O	7:A:458:HIS:HB3	2.16	0.46
13:G:53:TYR:HE1	13:G:57:PHE:CE2	2.21	0.46
13:G:104:ASN:O	13:G:108:VAL:HG23	2.15	0.46
22:W:213:HIS:HA	22:W:220:SER:HB2	1.98	0.46
3:3:214:MET:HE3	25:3:308:CLA:HBB	1.97	0.46
8:B:26:ALA:HB2	36:B:850:DGD:HA31	1.97	0.46
25:H:301:CLA:HMC2	18:L:127:LEU:HD13	1.98	0.46
22:S:177:LEU:HG	25:S:309:CLA:H3A	1.98	0.46
2:2:89:MET:HE3	25:2:609:CLA:HMC3	1.98	0.46
9:C:27:GLU:HA	10:D:151:PRO:HB2	1.98	0.46
23:Q:56:TYR:HE1	23:Q:59:PHE:O	1.98	0.46
6:6:80:GLU:OE1	25:6:602:CLA:C4A	2.63	0.46
22:W:95:PRO:HA	22:W:122:PHE:HB3	1.97	0.46
16:J:4:PHE:CZ	16:J:8:LEU:HD21	2.51	0.45
22:S:168:LEU:CD1	25:S:309:CLA:H42	2.46	0.45
25:A:825:CLA:HAA1	30:K:207:BCR:H342	1.97	0.45
8:B:422:LEU:HD13	8:B:531:LEU:HA	1.97	0.45
17:K:66:MET:HG3	17:K:104:PHE:HE1	1.82	0.45
23:Q:47:PHE:CE2	23:Q:191:ALA:HB3	2.52	0.45
31:A:857:LMG:H352	25:L:303:CLA:HMC2	1.98	0.45
20:N:106:LYS:O	20:N:106:LYS:HD3	2.16	0.45
22:X:34:ILE:N	22:X:179:ILE:HG21	2.31	0.45
22:X:79:GLU:OE2	22:X:207:ILE:N	2.46	0.45
7:A:341:LEU:HD13	25:A:826:CLA:HMD3	1.97	0.45
7:A:596:LEU:HD21	25:A:832:CLA:HBC1	1.98	0.45
8:B:518:VAL:HG21	8:B:592:TYR:HB2	1.97	0.45
22:V:123:TRP:HZ2	22:X:218:VAL:HG21	1.82	0.45
22:V:137:GLU:HA	22:V:140:ARG:HG2	1.98	0.45
2:2:171:TYR:CZ	2:2:192:LYS:HG2	2.52	0.45
3:3:102:TRP:CD1	25:3:307:CLA:HMD3	2.52	0.45
7:A:396:TRP:HB3	25:A:830:CLA:HMC3	1.98	0.45
13:G:72:MET:HG2	13:G:79:THR:CG2	2.47	0.45
23:Q:43:LYS:HD2	22:T:145:ASP:HB2	1.99	0.45
22:X:174:LEU:HD11	25:X:310:CLA:HED2	1.98	0.45
2:2:163:ASN:ND2	2:2:174:GLY:HA3	2.30	0.45
25:B:808:CLA:HBB2	25:B:830:CLA:HMC2	1.98	0.45
18:L:91:LEU:O	18:L:95:VAL:HG23	2.17	0.45
22:P:66:ARG:HH12	22:P:157:VAL:HG12	1.81	0.45
22:S:168:LEU:HD22	25:S:309:CLA:H11	1.99	0.45
26:T:321:IWJ:O27	26:T:321:IWJ:O39	2.35	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:Q:49:SER:HB3	23:Q:193:ASP:CB	2.47	0.45
25:B:808:CLA:CBB	25:B:830:CLA:HMC2	2.47	0.45
22:T:213:HIS:HA	22:T:220:SER:HB2	1.99	0.45
13:G:56:ARG:HH22	13:G:100:PRO:CD	2.29	0.45
13:G:56:ARG:NH1	13:G:99:ASP:OD1	2.50	0.45
20:N:105:VAL:HB	20:N:109:SER:H	1.82	0.45
22:R:57:ASN:OD1	25:R:306:CLA:HED3	2.17	0.45
8:B:185:VAL:HG11	30:B:845:BCR:H341	1.98	0.44
22:P:62:VAL:CG1	22:P:157:VAL:HG11	2.47	0.44
22:P:153:THR:HG23	22:P:156:ASP:CB	2.47	0.44
23:Q:119:CYS:O	23:Q:122:VAL:HG12	2.17	0.44
25:Q:312:CLA:C4B	25:S:310:CLA:H43	2.47	0.44
4:4:108:ASP:O	4:4:112:TYR:N	2.49	0.44
7:A:59:PHE:CD2	25:A:807:CLA:HMC2	2.52	0.44
7:A:93:PHE:CE2	25:A:809:CLA:HMD3	2.52	0.44
7:A:472:PHE:O	7:A:530:THR:HG21	2.17	0.44
22:R:120:PRO:HG3	24:R:308:CHL:C3C	2.47	0.44
7:A:424:ASN:OD1	7:A:432:ARG:NH1	2.46	0.44
5:5:97:GLU:CD	5:5:103:ALA:HB2	2.14	0.44
25:5:602:CLA:HMC2	27:5:612:XAT:C31	2.46	0.44
7:A:355:ILE:HD11	30:A:850:BCR:H24C	1.97	0.44
22:X:46:GLU:HA	25:X:302:CLA:HED1	1.99	0.44
22:X:175:GLU:HA	22:X:178:LYS:HZ3	1.83	0.44
4:4:115:TYR:CD1	24:4:306:CHL:HMD2	2.53	0.44
6:6:64:LEU:HB2	6:6:66:LEU:CD2	2.47	0.44
12:F:91:GLU:O	12:F:95:LEU:HG	2.18	0.44
22:S:162:ARG:O	22:S:165:PRO:HD3	2.17	0.44
3:3:68:GLY:O	3:3:223:ARG:NH2	2.48	0.44
28:6:616:LHG:H151	15:I:21:VAL:HG12	1.99	0.44
7:A:430:VAL:HG23	25:A:833:CLA:HMD3	1.99	0.44
25:A:808:CLA:HMD3	30:J:103:BCR:H322	1.99	0.44
22:V:65:GLY:HA2	22:V:189:MET:HG3	1.99	0.44
22:W:59:GLU:OE2	22:W:157:VAL:HG13	2.18	0.44
3:3:157:PHE:CE1	3:3:158:LEU:HD22	2.52	0.44
5:5:169:ARG:HB3	25:5:602:CLA:HBC3	1.98	0.44
7:A:208:LEU:HD21	25:A:822:CLA:HMC1	1.99	0.44
12:F:89:LYS:O	12:F:93:LYS:HG3	2.18	0.44
23:Q:48:GLY:CA	23:Q:192:GLY:HA2	2.47	0.44
22:X:139:TYR:CE2	22:X:147:PRO:HB3	2.53	0.44
6:6:86:TRP:CD1	25:6:607:CLA:HMD3	2.52	0.44
7:A:474:ASP:O	7:A:478:GLN:NE2	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:S:37:GLU:OE2	22:S:183:LYS:HD3	2.17	0.44
22:X:175:GLU:HA	22:X:178:LYS:NZ	2.33	0.44
7:A:13:VAL:N	7:A:315:ASN:OD1	2.47	0.44
7:A:95:GLY:HA3	7:A:148:TRP:CH2	2.53	0.44
7:A:677:PHE:CG	30:A:852:BCR:H363	2.53	0.44
8:B:177:HIS:CG	25:B:815:CLA:HMC2	2.53	0.43
25:V:301:CLA:H3A	25:V:301:CLA:CGA	2.48	0.43
3:3:51:VAL:HG21	17:K:99:ARG:HB2	2.00	0.43
28:1:614:LHG:O4	25:B:843:CLA:NB	2.52	0.43
7:A:403:CYS:SG	7:A:596:LEU:HA	2.58	0.43
7:A:695:GLU:HB2	8:B:535:LYS:HZ1	1.84	0.43
25:A:814:CLA:HMC1	30:A:849:BCR:H371	2.00	0.43
12:F:96:GLU:O	12:F:100:LYS:HG3	2.18	0.43
7:A:593:PHE:CE1	7:A:597:PHE:HE2	2.36	0.43
23:Q:50:LEU:HB3	25:S:310:CLA:HMB3	2.00	0.43
22:S:163:PHE:CZ	24:S:307:CHL:NC	2.86	0.43
22:W:225:ASN:ND2	25:W:312:CLA:OBD	2.51	0.43
3:3:110:MET:HG3	27:3:316:XAT:H163	2.00	0.43
7:A:545:VAL:HG11	7:A:598:TRP:CE2	2.54	0.43
7:A:590:ASP:O	7:A:593:PHE:HB3	2.18	0.43
8:B:191:THR:HG21	8:B:278:LEU:HB2	2.01	0.43
13:G:99:ASP:OD2	13:G:103:PHE:HB3	2.17	0.43
22:V:158:ASN:ND2	25:V:309:CLA:O1D	2.51	0.43
22:V:193:LEU:O	22:V:196:ILE:HG12	2.18	0.43
3:3:151:ILE:CD1	25:3:304:CLA:HMD3	2.49	0.43
22:P:158:ASN:H	24:P:307:CHL:HMD1	1.82	0.43
22:T:34:ILE:HD11	22:T:179:ILE:HG13	2.01	0.43
25:4:310:CLA:HMC2	26:4:317:IWJ:C12	2.49	0.43
7:A:72:LYS:NZ	25:A:813:CLA:OBD	2.44	0.43
7:A:121:ILE:HD13	30:J:101:BCR:H332	2.01	0.43
20:N:77:GLU:HG2	20:N:107:PHE:CD2	2.54	0.43
22:S:166:LEU:HD22	29:S:315:Q6L:C35	2.48	0.43
3:3:104:MET:HE3	25:3:308:CLA:HMC3	2.01	0.43
8:B:430:GLY:HA2	8:B:524:LEU:HD22	2.00	0.43
25:B:806:CLA:H3A	19:M:29:LEU:HD13	2.01	0.43
22:P:99:THR:HG22	22:P:120:PRO:HG2	2.01	0.43
25:2:613:CLA:OBD	3:3:153:TRP:NE1	2.50	0.43
7:A:55:ASP:O	7:A:62:HIS:NE2	2.45	0.43
18:L:73:ASP:OD1	18:L:74:VAL:N	2.52	0.43
23:Q:86:GLY:HA3	23:Q:205:SER:HB3	2.00	0.43
29:V:321:Q6L:C28	22:W:196:ILE:HG23	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:172:PRO:HG2	2:2:176:PHE:HE2	1.84	0.42
25:3:304:CLA:HBB1	25:3:307:CLA:HMC1	2.01	0.42
6:6:198:PRO:O	26:6:614:IWJ:O44	2.37	0.42
22:U:176:GLU:C	22:U:176:GLU:OE1	2.57	0.42
22:V:95:PRO:HA	22:V:122:PHE:CD2	2.54	0.42
7:A:740:TRP:NE1	25:A:830:CLA:O1A	2.48	0.42
3:3:97:LEU:HD23	3:3:195:ALA:HB1	2.02	0.42
8:B:497:LEU:HA	8:B:500:ILE:HG22	2.01	0.42
20:N:114:ILE:HG12	20:N:114:ILE:O	2.20	0.42
22:P:210:TRP:CH2	22:P:214:VAL:HG11	2.54	0.42
6:6:219:VAL:HG21	25:6:612:CLA:HMD3	2.00	0.42
8:B:69:ALA:HB2	8:B:135:LEU:HB2	2.01	0.42
12:F:103:ASP:OD1	12:F:103:ASP:N	2.52	0.42
21:O:115:LEU:HD21	25:O:2001:CLA:C3B	2.49	0.42
22:S:52:PHE:CE1	22:S:58:ALA:HB2	2.54	0.42
22:S:69:MET:HE2	22:S:185:CYS:HA	2.00	0.42
2:2:171:TYR:CE2	2:2:192:LYS:HG2	2.54	0.42
4:4:207:HIS:HB3	4:4:231:ALA:HB1	2.01	0.42
23:Q:131:ALA:HB1	24:Q:307:CHL:HMA3	2.01	0.42
23:Q:134:ALA:HA	23:Q:140:TYR:HA	2.01	0.42
22:R:58:ALA:O	22:R:62:VAL:HG23	2.19	0.42
22:S:111:PRO:HB2	22:S:113:ALA:O	2.20	0.42
22:V:140:ARG:HG3	22:V:141:THR:HG23	2.01	0.42
22:X:150:ASP:HB3	22:X:152:LEU:HD23	2.02	0.42
6:6:214:LEU:HD13	25:6:610:CLA:HMD2	2.01	0.42
7:A:93:PHE:CZ	7:A:97:ARG:HD2	2.54	0.42
7:A:524:MET:HE3	7:A:524:MET:HB2	1.86	0.42
8:B:118:SER:HA	25:B:829:CLA:HMA2	2.01	0.42
25:K:201:CLA:HMC2	22:W:168:LEU:HD11	2.01	0.42
20:N:74:ALA:HB1	20:N:108:LEU:HD23	2.02	0.42
22:P:169:ALA:HB2	25:P:309:CLA:HAA2	2.01	0.42
22:S:140:ARG:HA	24:S:307:CHL:C4C	2.50	0.42
22:X:95:PRO:HA	22:X:122:PHE:HB3	2.01	0.42
5:5:66:ARG:NH2	25:B:813:CLA:OBD	2.53	0.42
8:B:459:PHE:CD1	25:F:803:CLA:HMC2	2.55	0.42
25:B:827:CLA:HMB2	25:B:840:CLA:HBA1	2.02	0.42
30:M:101:BCR:H15C	30:M:101:BCR:H351	1.87	0.42
22:R:225:ASN:ND2	25:R:316:CLA:OBD	2.51	0.42
22:S:35:TYR:CE1	22:S:37:GLU:HB2	2.54	0.42
22:T:102:ALA:HB2	22:T:120:PRO:HG2	2.00	0.42
4:4:83:MET:HE3	25:4:310:CLA:HMC3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:99:SER:HB2	7:A:145:PHE:HZ	1.84	0.42
22:U:79:GLU:CB	22:U:207:ILE:HD13	2.49	0.42
22:V:198:GLN:HG2	25:V:312:CLA:C1D	2.50	0.42
14:H:119:ARG:NH2	32:H:303:SQD:O10	2.53	0.42
20:N:101:GLU:HA	20:N:112:MET:HG2	2.01	0.42
22:R:120:PRO:HG3	24:R:308:CHL:C1C	2.50	0.42
22:S:47:SER:HB3	25:S:301:CLA:OBD	2.19	0.42
22:S:152:LEU:HB3	24:S:307:CHL:HBC3	2.01	0.42
8:B:256:THR:CG2	8:B:258:LEU:HG	2.50	0.42
9:C:74:THR:HG21	10:D:74:GLU:OE2	2.20	0.42
10:D:57:SER:O	10:D:100:ARG:NH1	2.53	0.42
24:U:304:CHL:HBB1	24:V:314:CHL:HBB	2.02	0.42
22:V:180:LYS:NZ	25:V:311:CLA:HAA2	2.35	0.42
1:1:98:TRP:CZ2	1:1:186:ILE:HG22	2.55	0.41
24:1:601:CHL:OBD	4:4:136:ARG:NH1	2.52	0.41
5:5:212:ILE:HG22	8:B:216:LEU:HD21	2.02	0.41
7:A:524:MET:HB3	7:A:618:VAL:HG13	2.02	0.41
25:S:310:CLA:H2A	25:S:310:CLA:O2D	2.20	0.41
22:T:41:TYR:CD1	22:T:44:GLY:N	2.88	0.41
2:2:135:PHE:HD2	25:2:608:CLA:HMC3	1.84	0.41
4:4:140:ASP:CG	4:4:144:PRO:HA	2.40	0.41
25:A:803:CLA:H161	25:B:803:CLA:H151	2.02	0.41
23:Q:85:HIS:CB	23:Q:209:MET:HE1	2.50	0.41
25:X:313:CLA:O2D	25:X:313:CLA:H2A	2.20	0.41
4:4:115:TYR:HB3	24:4:306:CHL:HMD3	2.02	0.41
8:B:515:ASP:HA	8:B:518:VAL:HG12	2.03	0.41
26:S:319:IWJ:O27	26:S:319:IWJ:O39	2.38	0.41
1:1:148:LEU:O	25:1:605:CLA:HMD2	2.20	0.41
30:4:319:BCR:H15C	30:4:319:BCR:H351	1.96	0.41
7:A:691:GLY:N	8:B:567:CYS:O	2.48	0.41
30:J:101:BCR:H351	30:J:101:BCR:H15C	1.88	0.41
22:R:217:PRO:O	22:R:221:ASN:ND2	2.53	0.41
1:1:211:TRP:CE3	4:4:116:PHE:HE2	2.38	0.41
25:3:308:CLA:HMC2	26:3:315:IWJ:C12	2.50	0.41
4:4:151:PRO:HB2	30:4:319:BCR:H401	2.02	0.41
8:B:476:ILE:HG13	8:B:477:LEU:N	2.36	0.41
23:Q:107:TRP:O	29:Q:319:Q6L:O08	2.38	0.41
25:R:313:CLA:HMC2	29:R:319:Q6L:C25	2.51	0.41
22:W:177:LEU:HD13	25:W:309:CLA:O1A	2.21	0.41
25:2:609:CLA:HMC2	29:2:616:Q6L:C15	2.51	0.41
22:R:114:PRO:HG3	24:R:308:CHL:CAB	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:X:38:PHE:O	29:X:319:Q6L:O39	2.38	0.41
1:1:149:TYR:CD1	25:1:607:CLA:HHC	2.56	0.41
2:2:176:PHE:CG	25:2:609:CLA:HMD1	2.56	0.41
8:B:10:GLN:O	8:B:13:ALA:N	2.54	0.41
23:Q:115:THR:CG2	23:Q:116:PRO:HD2	2.51	0.41
22:R:65:GLY:O	22:R:69:MET:CG	2.65	0.41
22:S:163:PHE:HE1	24:S:307:CHL:NA	2.19	0.41
22:V:77:ALA:O	25:V:303:CLA:HMD3	2.20	0.41
6:6:94:ILE:HD11	27:6:615:XAT:O4	2.21	0.41
8:B:31:PHE:CD2	25:B:807:CLA:HMC2	2.56	0.41
8:B:692:TRP:HE3	25:B:841:CLA:HMD3	1.86	0.41
25:B:824:CLA:CED	13:G:69:ARG:NH1	2.81	0.41
22:R:96:ASP:OD1	22:R:96:ASP:N	2.54	0.41
3:3:116:LEU:HB3	3:3:122:ILE:HG12	2.02	0.41
4:4:85:GLY:HA2	27:4:318:XAT:H181	2.02	0.41
30:A:852:BCR:H402	25:B:834:CLA:HMB3	2.02	0.41
8:B:544:LYS:HD2	11:E:57:TYR:HA	2.03	0.41
9:C:66:ARG:HG3	10:D:168:ILE:CD1	2.51	0.41
22:W:177:LEU:HB3	25:W:309:CLA:H3A	2.03	0.41
22:X:55:GLU:O	22:X:58:ALA:N	2.54	0.41
7:A:17:VAL:HG21	25:A:812:CLA:HED2	2.01	0.41
7:A:200:HIS:ND1	25:A:815:CLA:HMC2	2.36	0.41
8:B:299:HIS:HB3	8:B:304:ILE:HD11	2.02	0.41
20:N:105:VAL:H	20:N:109:SER:CB	2.34	0.41
22:P:221:ASN:OD1	22:P:221:ASN:N	2.53	0.41
2:2:179:LEU:HB2	29:2:616:Q6L:O08	2.21	0.40
3:3:102:TRP:HD1	25:3:307:CLA:HMD3	1.86	0.40
3:3:167:ALA:HB2	25:3:307:CLA:CMA	2.51	0.40
4:4:59:LEU:O	4:4:61:LEU:N	2.54	0.40
8:B:85:ARG:HG3	14:H:165:ARG:HB3	2.03	0.40
25:B:825:CLA:HMD1	25:B:826:CLA:HMC2	2.03	0.40
22:V:157:VAL:C	22:V:159:PRO:HD3	2.42	0.40
1:1:149:TYR:HD1	25:1:607:CLA:HAB	1.85	0.40
5:5:178:ILE:HG23	5:5:189:PRO:HG3	2.04	0.40
13:G:45:SER:OG	25:G:203:CLA:HBD	2.21	0.40
23:Q:39:ARG:NH2	22:T:149:ASP:HA	2.37	0.40
3:3:235:GLN:O	3:3:239:THR:OG1	2.21	0.40
6:6:83:ASN:ND2	25:6:607:CLA:OBD	2.53	0.40
7:A:361:GLY:HA2	7:A:398:GLY:HA2	2.03	0.40
12:F:177:GLU:O	12:F:180:THR:OG1	2.39	0.40
24:2:601:CHL:HMD2	30:3:317:BCR:HC21	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:207:HIS:HA	4:4:233:PHE:HA	2.03	0.40
6:6:69:ASN:HB3	6:6:72:THR:HG22	2.03	0.40
25:B:809:CLA:H3A	25:B:810:CLA:HMB3	2.03	0.40
25:Q:314:CLA:H2	25:Q:315:CLA:HMD1	2.03	0.40
22:V:180:LYS:NZ	25:V:311:CLA:HBD	2.30	0.40
25:4:303:CLA:H93	12:F:205:ALA:HB2	2.03	0.40
7:A:217:GLN:OE1	7:A:298:HIS:ND1	2.52	0.40
8:B:415:LYS:HB2	8:B:538:LEU:HD13	2.03	0.40
23:Q:94:THR:OG1	25:Q:306:CLA:HMC3	2.21	0.40
22:T:183:LYS:HD2	25:T:310:CLA:C3D	2.52	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1	151/225 (67%)	144 (95%)	6 (4%)	1 (1%)	19	41
2	2	203/242 (84%)	197 (97%)	6 (3%)	0	100	100
3	3	225/272 (83%)	215 (96%)	10 (4%)	0	100	100
4	4	199/236 (84%)	190 (96%)	9 (4%)	0	100	100
5	5	162/217 (75%)	158 (98%)	4 (2%)	0	100	100
6	6	190/249 (76%)	187 (98%)	3 (2%)	0	100	100
7	A	740/751 (98%)	724 (98%)	16 (2%)	0	100	100
8	B	730/733 (100%)	706 (97%)	24 (3%)	0	100	100
9	C	78/81 (96%)	77 (99%)	1 (1%)	0	100	100
10	D	141/188 (75%)	135 (96%)	6 (4%)	0	100	100
11	E	60/101 (59%)	59 (98%)	1 (2%)	0	100	100
12	F	163/231 (71%)	159 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	G	93/132 (70%)	89 (96%)	4 (4%)	0	100	100
14	H	94/166 (57%)	93 (99%)	1 (1%)	0	100	100
15	I	33/35 (94%)	32 (97%)	1 (3%)	0	100	100
16	J	39/42 (93%)	37 (95%)	2 (5%)	0	100	100
17	K	85/131 (65%)	84 (99%)	1 (1%)	0	100	100
18	L	156/204 (76%)	153 (98%)	3 (2%)	0	100	100
19	M	29/31 (94%)	29 (100%)	0	0	100	100
20	N	89/139 (64%)	83 (93%)	6 (7%)	0	100	100
21	O	94/136 (69%)	93 (99%)	1 (1%)	0	100	100
22	P	199/233 (85%)	191 (96%)	8 (4%)	0	100	100
22	R	199/233 (85%)	185 (93%)	14 (7%)	0	100	100
22	S	200/233 (86%)	190 (95%)	9 (4%)	1 (0%)	25	50
22	T	199/233 (85%)	189 (95%)	10 (5%)	0	100	100
22	U	199/233 (85%)	191 (96%)	8 (4%)	0	100	100
22	V	193/233 (83%)	188 (97%)	5 (3%)	0	100	100
22	W	198/233 (85%)	188 (95%)	10 (5%)	0	100	100
22	X	190/233 (82%)	184 (97%)	6 (3%)	0	100	100
23	Q	223/226 (99%)	212 (95%)	11 (5%)	0	100	100
All	All	5554/6632 (84%)	5362 (96%)	190 (3%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
22	S	120	PRO
1	1	150	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1	118/166 (71%)	117 (99%)	1 (1%)	79	87
2	2	160/186 (86%)	159 (99%)	1 (1%)	84	90
3	3	173/208 (83%)	171 (99%)	2 (1%)	67	81
4	4	159/186 (86%)	158 (99%)	1 (1%)	84	90
5	5	127/163 (78%)	124 (98%)	3 (2%)	44	68
6	6	148/188 (79%)	146 (99%)	2 (1%)	62	79
7	A	600/609 (98%)	598 (100%)	2 (0%)	91	95
8	B	584/585 (100%)	583 (100%)	1 (0%)	92	96
9	C	66/67 (98%)	66 (100%)	0	100	100
10	D	118/150 (79%)	118 (100%)	0	100	100
11	E	55/85 (65%)	55 (100%)	0	100	100
12	F	130/176 (74%)	129 (99%)	1 (1%)	79	87
13	G	73/99 (74%)	72 (99%)	1 (1%)	62	79
14	H	72/128 (56%)	72 (100%)	0	100	100
15	I	29/29 (100%)	29 (100%)	0	100	100
16	J	35/36 (97%)	35 (100%)	0	100	100
17	K	66/101 (65%)	66 (100%)	0	100	100
18	L	125/165 (76%)	124 (99%)	1 (1%)	79	87
19	M	27/27 (100%)	27 (100%)	0	100	100
20	N	72/103 (70%)	72 (100%)	0	100	100
21	O	80/110 (73%)	80 (100%)	0	100	100
22	P	153/179 (86%)	152 (99%)	1 (1%)	81	89
22	R	153/179 (86%)	152 (99%)	1 (1%)	81	89
22	S	153/179 (86%)	152 (99%)	1 (1%)	81	89
22	T	153/179 (86%)	151 (99%)	2 (1%)	65	80
22	U	153/179 (86%)	152 (99%)	1 (1%)	81	89
22	V	151/179 (84%)	151 (100%)	0	100	100
22	W	152/179 (85%)	151 (99%)	1 (1%)	81	89
22	X	150/179 (84%)	148 (99%)	2 (1%)	65	80
23	Q	167/167 (100%)	165 (99%)	2 (1%)	67	81
All	All	4402/5166 (85%)	4375 (99%)	27 (1%)	82	90

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	134	PHE
2	2	114	ASP
3	3	142	TYR
3	3	205	LYS
4	4	202	MET
5	5	65	ASP
5	5	181	GLN
5	5	198	SER
6	6	197	SER
6	6	249	GLU
7	A	293	ASP
7	A	568	ASN
8	B	53	GLN
12	F	106	SER
13	G	125	SER
18	L	150	ARG
22	P	178	LYS
23	Q	58	GLU
23	Q	190	GLU
22	R	60	ARG
22	S	38	PHE
22	T	124	ASN
22	T	173	ASP
22	U	80	ASN
22	W	158	ASN
22	X	123	TRP
22	X	219	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
4	4	113	GLN
13	G	63	GLN
13	G	129	GLN
16	J	3	ASN
16	J	5	GLN
22	P	158	ASN
22	U	219	HIS
22	V	209	ASN
22	W	209	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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$
23	TPO	Q	31	23	8,10,11	1.69	1 (12%)	10,14,16	1.11	1 (10%)

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
23	TPO	Q	31	23	-	2/9/11/13	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	Q	31	TPO	P-O1P	3.45	1.61	1.50

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	Q	31	TPO	P-OG1-CB	-2.28	116.33	123.21

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	Q	31	TPO	O-C-CA-CB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	Q	31	TPO	CB-OG1-P-O1P

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

449 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	$\# Z > 2$
31	LMG	F	805	-	31,31,55	1.15	2 (6%)	39,39,63	1.12	3 (7%)
31	LMG	O	2008	-	39,39,55	1.06	2 (5%)	47,47,63	1.14	3 (6%)
25	CLA	V	301	22	60,68,73	1.48	5 (8%)	70,107,113	1.74	11 (15%)
24	CHL	5	605	-	40,49,74	1.81	6 (15%)	41,84,114	1.72	7 (17%)
29	Q6L	T	319	-	42,43,43	1.85	7 (16%)	47,60,60	1.46	5 (10%)
25	CLA	W	312	22	55,63,73	1.60	7 (12%)	64,101,113	1.79	13 (20%)
25	CLA	A	813	-	65,73,73	1.46	8 (12%)	76,113,113	1.28	7 (9%)
25	CLA	B	803	-	65,73,73	1.47	7 (10%)	76,113,113	1.69	15 (19%)
25	CLA	H	302	-	65,73,73	1.47	7 (10%)	76,113,113	1.59	12 (15%)
25	CLA	B	821	-	55,63,73	1.71	8 (14%)	64,101,113	1.49	11 (17%)
35	SF4	C	101	9	0,12,12	-	-	-	-	-
24	CHL	T	307	-	44,52,74	1.76	6 (13%)	46,87,114	1.75	6 (13%)
25	CLA	R	316	22	55,63,73	1.62	5 (9%)	64,101,113	1.74	11 (17%)
25	CLA	A	823	39	65,73,73	1.57	9 (13%)	76,113,113	1.55	13 (17%)
24	CHL	2	605	-	42,50,74	1.92	8 (19%)	45,85,114	1.47	5 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	R	313	22	64,72,73	1.54	7 (10%)	74,111,113	1.51	11 (14%)
24	CHL	R	318	22	45,53,74	1.80	6 (13%)	46,88,114	1.54	8 (17%)
25	CLA	B	836	8	60,68,73	1.58	8 (13%)	70,107,113	1.46	9 (12%)
25	CLA	Q	315	-	48,56,73	1.70	7 (14%)	55,92,113	1.62	10 (18%)
24	CHL	2	607	-	45,53,74	1.77	8 (17%)	46,88,114	1.58	8 (17%)
30	BCR	4	319	-	41,41,41	1.33	5 (12%)	56,56,56	2.31	23 (41%)
25	CLA	V	309	22	42,50,73	2.12	9 (21%)	48,85,113	2.06	14 (29%)
25	CLA	N	202	20	44,53,73	1.81	7 (15%)	50,89,113	1.45	5 (10%)
25	CLA	A	826	-	55,63,73	1.59	8 (14%)	64,101,113	1.47	7 (10%)
24	CHL	W	306	-	52,60,74	1.60	8 (15%)	56,97,114	2.11	14 (25%)
25	CLA	A	828	-	59,67,73	1.53	10 (16%)	68,105,113	1.42	11 (16%)
34	PQN	B	844	-	34,34,34	2.96	11 (32%)	42,45,45	2.05	7 (16%)
24	CHL	T	314	22	42,50,74	1.79	6 (14%)	44,85,114	1.69	8 (18%)
25	CLA	K	201	17	45,53,73	1.77	5 (11%)	52,89,113	1.96	12 (23%)
30	BCR	J	101	-	41,41,41	1.25	4 (9%)	56,56,56	2.59	24 (42%)
31	LMG	2	620	-	31,31,55	1.18	2 (6%)	39,39,63	1.28	4 (10%)
24	CHL	V	304	22	46,54,74	1.78	8 (17%)	49,90,114	1.49	8 (16%)
35	SF4	A	853	7,8	0,12,12	-	-	-	-	-
30	BCR	L	305	-	41,41,41	1.05	1 (2%)	56,56,56	2.31	20 (35%)
30	BCR	I	101	-	41,41,41	1.02	3 (7%)	56,56,56	2.42	22 (39%)
25	CLA	S	309	22	60,68,73	1.58	8 (13%)	70,107,113	1.36	10 (14%)
25	CLA	6	604	-	43,51,73	1.82	7 (16%)	48,86,113	1.53	7 (14%)
28	LHG	3	323	-	42,42,48	1.00	2 (4%)	45,48,54	0.92	3 (6%)
25	CLA	B	817	-	43,51,73	1.78	8 (18%)	49,86,113	1.57	7 (14%)
24	CHL	X	305	22	42,50,74	1.85	5 (11%)	44,85,114	1.43	8 (18%)
30	BCR	B	848	-	41,41,41	1.30	4 (9%)	56,56,56	2.23	18 (32%)
25	CLA	R	307	-	50,58,73	1.71	7 (14%)	58,95,113	1.50	7 (12%)
25	CLA	S	311	-	47,55,73	1.69	6 (12%)	54,91,113	1.71	9 (16%)
25	CLA	A	816	-	45,53,73	1.73	8 (17%)	52,89,113	1.64	8 (15%)
25	CLA	5	601	5	46,54,73	1.76	8 (17%)	53,90,113	1.76	13 (24%)
25	CLA	W	302	-	55,63,73	1.61	8 (14%)	64,101,113	1.34	8 (12%)
25	CLA	B	826	-	65,73,73	1.52	10 (15%)	76,113,113	1.67	15 (19%)
25	CLA	5	604	-	37,46,73	2.03	7 (18%)	46,81,113	1.50	8 (17%)
25	CLA	2	609	2	55,63,73	1.54	9 (16%)	64,101,113	1.44	10 (15%)
25	CLA	X	314	-	41,49,73	1.85	7 (17%)	47,84,113	1.55	8 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	Q	313	-	46,54,73	1.72	8 (17%)	53,90,113	1.66	9 (16%)
30	BCR	A	848	-	41,41,41	1.36	5 (12%)	56,56,56	2.12	19 (33%)
25	CLA	5	609	-	53,62,73	1.64	5 (9%)	61,100,113	1.43	8 (13%)
32	SQD	6	617	-	53,54,54	1.19	4 (7%)	62,65,65	1.13	5 (8%)
25	CLA	1	608	1	65,73,73	1.54	10 (15%)	76,113,113	1.36	10 (13%)
25	CLA	B	824	-	60,68,73	1.59	9 (15%)	70,107,113	1.46	7 (10%)
25	CLA	B	835	-	45,53,73	1.82	8 (17%)	52,89,113	1.36	8 (15%)
25	CLA	L	303	-	45,53,73	1.76	5 (11%)	52,89,113	1.86	13 (25%)
30	BCR	G	201	-	41,41,41	1.13	3 (7%)	56,56,56	2.21	19 (33%)
26	IWJ	V	320	-	43,45,45	1.16	5 (11%)	43,65,65	1.13	2 (4%)
25	CLA	B	839	-	65,73,73	1.55	9 (13%)	76,113,113	1.38	7 (9%)
25	CLA	B	811	8	65,73,73	1.48	11 (16%)	76,113,113	1.48	8 (10%)
29	Q6L	R	320	-	42,43,43	1.88	7 (16%)	47,60,60	1.40	5 (10%)
30	BCR	B	845	-	41,41,41	1.32	5 (12%)	56,56,56	2.71	25 (44%)
25	CLA	V	302	-	50,58,73	1.70	9 (18%)	58,95,113	1.47	11 (18%)
25	CLA	A	819	-	60,68,73	1.51	7 (11%)	70,107,113	1.59	10 (14%)
25	CLA	6	610	-	61,69,73	1.52	8 (13%)	71,108,113	1.32	10 (14%)
25	CLA	B	808	8	65,73,73	1.47	10 (15%)	76,113,113	1.44	14 (18%)
25	CLA	K	203	-	62,70,73	1.50	8 (12%)	72,109,113	1.56	11 (15%)
25	CLA	X	310	22	42,50,73	1.82	7 (16%)	48,85,113	1.58	9 (18%)
24	CHL	Q	307	23	46,54,74	1.63	4 (8%)	49,90,114	1.65	10 (20%)
36	DGD	A	854	-	52,52,67	1.05	3 (5%)	66,66,81	1.21	7 (10%)
25	CLA	5	606	-	40,48,73	1.89	6 (15%)	50,83,113	1.75	10 (20%)
25	CLA	W	303	-	50,58,73	1.65	8 (16%)	58,95,113	1.68	11 (18%)
25	CLA	R	305	22	65,73,73	1.52	7 (10%)	76,113,113	1.50	12 (15%)
24	CHL	4	302	4	52,60,74	1.63	9 (17%)	56,97,114	1.90	16 (28%)
25	CLA	A	824	-	42,50,73	1.86	7 (16%)	48,85,113	1.62	7 (14%)
25	CLA	S	312	22	55,63,73	1.63	8 (14%)	64,101,113	1.37	9 (14%)
25	CLA	4	315	-	41,49,73	1.85	5 (12%)	47,84,113	1.49	9 (19%)
24	CHL	V	314	22	44,52,74	1.79	7 (15%)	46,87,114	1.66	10 (21%)
37	NEX	T	317	-	38,46,46	1.26	4 (10%)	50,70,70	2.54	15 (30%)
30	BCR	K	202	-	41,41,41	1.26	7 (17%)	56,56,56	2.59	24 (42%)
32	SQD	H	303	-	47,48,54	1.30	4 (8%)	56,59,65	1.14	3 (5%)
26	IWJ	4	301	-	43,45,45	1.17	4 (9%)	43,65,65	1.09	2 (4%)
25	CLA	Q	305	-	44,52,73	1.76	8 (18%)	49,87,113	1.47	7 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	LHG	A	846	-	48,48,48	0.93	2 (4%)	51,54,54	0.98	2 (3%)
25	CLA	B	809	-	65,73,73	1.47	10 (15%)	76,113,113	1.46	14 (18%)
25	CLA	L	302	-	60,68,73	1.64	9 (15%)	70,107,113	1.58	9 (12%)
24	CHL	S	304	22	42,50,74	1.94	8 (19%)	44,85,114	1.77	9 (20%)
25	CLA	U	310	-	44,52,73	1.83	7 (15%)	49,87,113	1.46	10 (20%)
25	CLA	F	802	-	42,50,73	1.80	9 (21%)	48,85,113	1.59	11 (22%)
25	CLA	2	606	-	45,53,73	1.79	9 (20%)	52,89,113	1.66	8 (15%)
24	CHL	V	307	-	44,52,74	1.74	5 (11%)	46,87,114	1.53	9 (19%)
29	Q6L	R	319	-	42,43,43	1.90	7 (16%)	47,60,60	1.47	4 (8%)
30	BCR	3	318	-	41,41,41	1.30	6 (14%)	56,56,56	2.17	19 (33%)
25	CLA	P	309	22	64,72,73	1.45	5 (7%)	74,111,113	1.64	14 (18%)
25	CLA	3	310	-	43,51,73	1.76	6 (13%)	49,86,113	1.53	8 (16%)
25	CLA	B	829	-	65,73,73	1.44	8 (12%)	76,113,113	1.66	11 (14%)
29	Q6L	P	315	-	42,43,43	1.92	8 (19%)	47,60,60	1.38	5 (10%)
30	BCR	A	851	-	41,41,41	0.98	2 (4%)	56,56,56	2.42	22 (39%)
24	CHL	V	306	-	44,52,74	1.75	7 (15%)	46,87,114	1.96	12 (26%)
26	IWJ	Q	320	-	43,45,45	1.12	4 (9%)	43,65,65	1.29	7 (16%)
29	Q6L	T	322	-	42,43,43	1.91	8 (19%)	47,60,60	1.45	4 (8%)
24	CHL	W	314	22	40,49,74	1.84	6 (15%)	42,83,114	1.99	10 (23%)
25	CLA	2	611	2	43,52,73	1.75	6 (13%)	49,88,113	1.60	8 (16%)
29	Q6L	2	616	-	42,43,43	1.82	7 (16%)	47,60,60	1.54	8 (17%)
38	KC2	W	308	22	48,53,53	2.57	16 (33%)	54,89,89	2.32	20 (37%)
38	KC2	V	308	22	48,53,53	2.53	16 (33%)	54,89,89	2.21	19 (35%)
25	CLA	6	602	6	62,70,73	1.43	5 (8%)	72,109,113	1.63	11 (15%)
25	CLA	5	610	-	41,49,73	1.87	6 (14%)	47,84,113	1.46	8 (17%)
25	CLA	1	609	-	37,46,73	1.97	6 (16%)	46,81,113	1.74	11 (23%)
25	CLA	T	303	-	50,58,73	1.72	8 (16%)	58,95,113	1.51	6 (10%)
38	KC2	X	309	22	48,53,53	2.57	16 (33%)	54,89,89	2.54	21 (38%)
25	CLA	W	311	-	45,53,73	1.68	6 (13%)	52,89,113	1.62	8 (15%)
25	CLA	V	311	-	60,68,73	1.51	7 (11%)	70,107,113	1.40	11 (15%)
25	CLA	2	604	-	43,51,73	1.81	6 (13%)	48,86,113	1.53	8 (16%)
25	CLA	B	843	28	65,73,73	1.47	8 (12%)	76,113,113	1.59	10 (13%)
28	LHG	3	321	-	42,42,48	1.00	2 (4%)	45,48,54	0.89	1 (2%)
27	XAT	6	615	-	39,47,47	1.09	2 (5%)	54,74,74	2.99	25 (46%)
25	CLA	3	302	-	55,63,73	1.68	8 (14%)	64,101,113	1.93	17 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	Q6L	S	323	-	42,43,43	1.86	6 (14%)	47,60,60	1.81	11 (23%)
25	CLA	6	612	6	45,53,73	1.76	9 (20%)	52,89,113	1.43	6 (11%)
25	CLA	A	831	-	65,73,73	1.48	9 (13%)	76,113,113	1.49	12 (15%)
26	IWJ	R	322	-	43,45,45	1.16	4 (9%)	43,65,65	1.00	2 (4%)
24	CHL	R	308	22	46,54,74	1.72	5 (10%)	49,90,114	1.50	8 (16%)
25	CLA	Q	311	23	55,63,73	1.55	7 (12%)	64,101,113	1.41	10 (15%)
24	CHL	P	307	-	44,52,74	1.76	7 (15%)	46,87,114	1.88	10 (21%)
25	CLA	H	301	14	44,52,73	1.80	7 (15%)	49,87,113	1.50	9 (18%)
29	Q6L	O	2007	-	42,43,43	1.92	8 (19%)	47,60,60	1.34	4 (8%)
25	CLA	A	818	-	45,53,73	1.77	5 (11%)	52,89,113	1.70	7 (13%)
24	CHL	Q	309	-	44,52,74	1.73	6 (13%)	46,87,114	1.61	8 (17%)
29	Q6L	T	315	-	42,43,43	1.86	7 (16%)	47,60,60	1.39	6 (12%)
25	CLA	A	830	-	65,73,73	1.51	8 (12%)	76,113,113	1.77	15 (19%)
25	CLA	B	831	-	65,73,73	1.52	7 (10%)	76,113,113	1.68	13 (17%)
25	CLA	4	314	-	41,49,73	1.85	6 (14%)	47,84,113	1.63	9 (19%)
25	CLA	P	302	-	65,73,73	1.50	8 (12%)	76,113,113	1.45	12 (15%)
29	Q6L	W	319	-	42,43,43	1.88	7 (16%)	47,60,60	1.45	7 (14%)
29	Q6L	Q	317	-	42,43,43	1.82	6 (14%)	47,60,60	1.61	6 (12%)
37	NEX	W	317	-	38,46,46	1.13	4 (10%)	50,70,70	2.59	13 (26%)
25	CLA	3	314	3	39,48,73	1.90	4 (10%)	44,83,113	1.69	8 (18%)
29	Q6L	V	319	-	42,43,43	1.81	7 (16%)	47,60,60	1.79	12 (25%)
29	Q6L	Q	318	-	42,43,43	1.81	6 (14%)	47,60,60	1.58	6 (12%)
29	Q6L	S	316	-	42,43,43	1.87	7 (16%)	47,60,60	1.56	5 (10%)
30	BCR	B	847	-	41,41,41	1.33	6 (14%)	56,56,56	2.49	22 (39%)
25	CLA	A	820	-	59,67,73	1.64	10 (16%)	68,105,113	1.46	11 (16%)
28	LHG	2	619	25	32,32,48	1.12	2 (6%)	35,38,54	1.07	3 (8%)
24	CHL	R	309	-	50,58,74	1.73	6 (12%)	52,94,114	1.57	10 (19%)
25	CLA	B	810	-	65,73,73	1.51	10 (15%)	76,113,113	1.30	9 (11%)
38	KC2	R	312	22	48,53,53	2.61	14 (29%)	54,89,89	2.49	21 (38%)
29	Q6L	R	304	-	42,43,43	1.90	7 (16%)	47,60,60	1.45	3 (6%)
25	CLA	4	309	4	45,53,73	1.86	9 (20%)	52,89,113	1.90	12 (23%)
25	CLA	O	2001	-	59,67,73	1.52	8 (13%)	68,105,113	1.58	11 (16%)
25	CLA	G	203	-	42,50,73	1.83	7 (16%)	48,85,113	1.69	9 (18%)
25	CLA	S	310	22	60,68,73	1.59	9 (15%)	70,107,113	1.41	11 (15%)
30	BCR	B	849	-	41,41,41	1.08	3 (7%)	56,56,56	2.28	16 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	Q6L	Q	319	-	42,43,43	1.87	7 (16%)	47,60,60	1.71	10 (21%)
25	CLA	U	303	-	50,58,73	1.76	8 (16%)	58,95,113	1.49	9 (15%)
26	IWJ	6	614	-	43,45,45	1.16	4 (9%)	43,65,65	1.30	3 (6%)
26	IWJ	W	318	-	43,45,45	1.15	4 (9%)	43,65,65	1.36	6 (13%)
24	CHL	X	315	22	45,53,74	1.83	6 (13%)	46,88,114	1.36	5 (10%)
26	IWJ	V	318	-	43,45,45	1.14	4 (9%)	43,65,65	1.43	8 (18%)
25	CLA	B	841	-	65,73,73	1.56	9 (13%)	76,113,113	1.55	12 (15%)
25	CLA	B	830	-	65,73,73	1.47	9 (13%)	76,113,113	1.31	6 (7%)
30	BCR	B	846	-	41,41,41	1.11	4 (9%)	56,56,56	2.46	18 (32%)
24	CHL	4	306	-	40,49,74	1.78	6 (15%)	42,84,114	2.07	11 (26%)
25	CLA	L	304	-	42,50,73	1.79	8 (19%)	48,85,113	1.65	8 (16%)
25	CLA	N	203	-	42,50,73	1.89	9 (21%)	48,85,113	1.58	11 (22%)
25	CLA	A	835	-	65,73,73	1.54	9 (13%)	76,113,113	1.36	9 (11%)
28	LHG	3	320	25	22,22,48	1.10	1 (4%)	24,27,54	1.07	1 (4%)
25	CLA	3	309	28	42,50,73	1.86	6 (14%)	48,85,113	1.56	9 (18%)
25	CLA	R	306	-	65,73,73	1.45	8 (12%)	76,113,113	1.30	6 (7%)
25	CLA	X	302	22	55,63,73	1.64	10 (18%)	64,101,113	1.48	13 (20%)
25	CLA	F	803	12	41,49,73	1.83	9 (21%)	47,84,113	1.72	12 (25%)
25	CLA	S	301	22	65,73,73	1.55	9 (13%)	76,113,113	1.41	13 (17%)
24	CHL	6	601	6	42,50,74	1.75	6 (14%)	45,85,114	1.87	13 (28%)
24	CHL	P	306	-	52,60,74	1.61	8 (15%)	56,97,114	1.70	12 (21%)
25	CLA	1	610	1	40,48,73	1.93	6 (15%)	50,83,113	1.68	14 (28%)
25	CLA	6	611	-	43,51,73	1.76	6 (13%)	49,86,113	1.63	8 (16%)
25	CLA	A	822	-	45,53,73	1.72	7 (15%)	52,89,113	1.52	9 (17%)
25	CLA	1	605	-	40,49,73	1.87	6 (15%)	45,84,113	1.51	6 (13%)
29	Q6L	X	301	-	42,43,43	1.90	7 (16%)	47,60,60	1.52	5 (10%)
25	CLA	U	311	22	55,63,73	1.64	8 (14%)	64,101,113	1.67	10 (15%)
38	KC2	T	308	22	48,53,53	2.57	14 (29%)	54,89,89	2.41	19 (35%)
25	CLA	3	311	3	53,62,73	1.68	9 (16%)	61,100,113	1.89	14 (22%)
25	CLA	R	315	-	60,68,73	1.59	7 (11%)	70,107,113	1.49	12 (17%)
38	KC2	P	308	22	48,53,53	2.62	16 (33%)	54,89,89	2.65	21 (38%)
26	IWJ	T	321	-	43,45,45	1.20	5 (11%)	43,65,65	1.10	3 (6%)
25	CLA	B	832	-	43,51,73	1.97	11 (25%)	49,86,113	1.69	13 (26%)
25	CLA	A	840	-	55,63,73	1.60	7 (12%)	64,101,113	1.62	10 (15%)
31	LMG	A	801	-	31,31,55	1.14	2 (6%)	39,39,63	0.93	1 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	BCR	H	305	-	41,41,41	1.19	3 (7%)	56,56,56	1.80	17 (30%)
25	CLA	B	815	-	65,73,73	1.41	8 (12%)	76,113,113	1.87	10 (13%)
25	CLA	T	309	22	59,67,73	1.63	10 (16%)	68,105,113	1.46	12 (17%)
29	Q6L	V	321	-	42,43,43	1.86	7 (16%)	47,60,60	1.57	4 (8%)
24	CHL	W	305	-	42,50,74	1.81	6 (14%)	44,85,114	1.83	10 (22%)
24	CHL	Q	316	23	45,53,74	1.81	5 (11%)	46,88,114	1.57	11 (23%)
31	LMG	J	104	-	46,46,55	0.97	2 (4%)	54,54,63	0.88	2 (3%)
31	LMG	5	613	-	54,54,55	0.92	2 (3%)	62,62,63	0.84	1 (1%)
25	CLA	A	832	-	65,73,73	1.48	6 (9%)	76,113,113	1.35	7 (9%)
26	IWJ	U	316	-	43,45,45	1.15	4 (9%)	43,65,65	1.35	5 (11%)
24	CHL	X	307	-	52,60,74	1.58	10 (19%)	56,97,114	2.51	18 (32%)
26	IWJ	S	318	-	43,45,45	1.16	5 (11%)	43,65,65	1.38	6 (13%)
29	Q6L	V	316	-	42,43,43	1.94	7 (16%)	47,60,60	1.60	5 (10%)
24	CHL	T	304	22	43,51,74	1.76	5 (11%)	45,86,114	1.94	7 (15%)
30	BCR	J	103	-	41,41,41	1.12	4 (9%)	56,56,56	2.21	20 (35%)
30	BCR	L	306	-	41,41,41	1.18	4 (9%)	56,56,56	2.08	19 (33%)
24	CHL	P	304	22	46,54,74	1.78	6 (13%)	49,90,114	1.95	16 (32%)
26	IWJ	S	319	-	43,45,45	1.19	7 (16%)	43,65,65	1.26	6 (13%)
25	CLA	5	602	5	60,68,73	1.53	6 (10%)	70,107,113	1.51	12 (17%)
25	CLA	1	607	1	36,44,73	2.03	7 (19%)	39,74,113	2.98	11 (28%)
25	CLA	B	816	-	51,59,73	1.65	7 (13%)	59,96,113	1.52	7 (11%)
25	CLA	B	819	-	59,67,73	1.60	9 (15%)	68,105,113	1.42	11 (16%)
26	IWJ	R	303	-	43,45,45	1.18	5 (11%)	43,65,65	1.25	3 (6%)
29	Q6L	P	319	-	42,43,43	1.87	7 (16%)	47,60,60	1.60	7 (14%)
29	Q6L	W	320	-	42,43,43	1.88	7 (16%)	47,60,60	1.72	5 (10%)
26	IWJ	V	317	-	43,45,45	1.17	4 (9%)	43,65,65	1.20	2 (4%)
25	CLA	3	301	3	60,68,73	1.55	8 (13%)	70,107,113	1.57	9 (12%)
25	CLA	B	818	-	55,63,73	1.58	8 (14%)	64,101,113	1.61	13 (20%)
25	CLA	A	825	-	65,73,73	1.51	6 (9%)	76,113,113	1.80	17 (22%)
25	CLA	T	311	-	60,68,73	1.52	6 (10%)	70,107,113	1.55	9 (12%)
24	CHL	1	601	1	54,63,74	1.63	8 (14%)	58,101,114	1.43	11 (18%)
25	CLA	V	313	-	48,56,73	1.70	7 (14%)	55,92,113	1.37	8 (14%)
24	CHL	T	305	-	49,57,74	1.68	6 (12%)	52,93,114	1.88	11 (21%)
26	IWJ	T	318	-	43,45,45	1.17	5 (11%)	43,65,65	1.18	4 (9%)
25	CLA	5	603	5	45,53,73	1.78	5 (11%)	52,89,113	1.66	7 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	6	613	6	65,73,73	1.51	6 (9%)	76,113,113	1.45	11 (14%)
24	CHL	6	606	-	43,51,74	1.74	5 (11%)	45,86,114	1.76	10 (22%)
25	CLA	A	856	-	57,65,73	1.54	8 (14%)	66,103,113	1.81	14 (21%)
25	CLA	2	602	2	61,69,73	1.56	7 (11%)	71,108,113	1.83	17 (23%)
25	CLA	B	840	-	47,55,73	1.79	8 (17%)	54,91,113	1.56	9 (16%)
26	IWJ	P	318	-	43,45,45	1.16	4 (9%)	43,65,65	1.11	1 (2%)
25	CLA	B	842	-	65,73,73	1.49	8 (12%)	76,113,113	1.71	15 (19%)
37	NEX	H	306	-	38,46,46	1.33	7 (18%)	50,70,70	2.53	18 (36%)
25	CLA	6	603	6	43,52,73	1.87	8 (18%)	49,88,113	1.57	12 (24%)
24	CHL	2	601	2	47,55,74	1.73	9 (19%)	50,91,114	1.72	10 (20%)
25	CLA	A	805	-	65,73,73	1.44	7 (10%)	76,113,113	1.69	12 (15%)
24	CHL	S	306	-	52,60,74	1.67	11 (21%)	56,97,114	2.21	17 (30%)
31	LMG	N	201	-	55,55,55	0.90	2 (3%)	63,63,63	1.16	6 (9%)
24	CHL	X	306	-	42,50,74	1.79	6 (14%)	44,85,114	1.84	8 (18%)
25	CLA	R	314	22	60,68,73	1.59	6 (10%)	70,107,113	1.58	13 (18%)
25	CLA	G	204	13	45,53,73	1.78	6 (13%)	52,89,113	1.63	9 (17%)
25	CLA	P	312	22	55,63,73	1.65	5 (9%)	64,101,113	1.57	10 (15%)
28	LHG	6	616	-	45,45,48	0.95	2 (4%)	48,51,54	1.08	3 (6%)
25	CLA	W	313	-	43,51,73	1.77	6 (13%)	49,86,113	1.41	7 (14%)
29	Q6L	U	317	-	42,43,43	1.86	7 (16%)	47,60,60	1.57	5 (10%)
25	CLA	O	2003	-	41,49,73	1.84	5 (12%)	47,84,113	1.41	7 (14%)
30	BCR	A	850	-	41,41,41	1.25	7 (17%)	56,56,56	2.38	22 (39%)
25	CLA	A	814	-	54,62,73	1.67	7 (12%)	62,99,113	1.50	12 (19%)
25	CLA	2	610	28	42,50,73	1.82	5 (11%)	48,85,113	1.58	8 (16%)
25	CLA	W	310	22	60,68,73	1.55	6 (10%)	70,107,113	1.30	8 (11%)
25	CLA	X	311	22	50,58,73	1.65	7 (14%)	58,95,113	1.41	8 (13%)
25	CLA	V	310	22	47,55,73	1.74	8 (17%)	54,91,113	1.48	10 (18%)
25	CLA	A	842	-	65,73,73	1.50	9 (13%)	76,113,113	1.58	14 (18%)
30	BCR	A	849	-	41,41,41	1.15	4 (9%)	56,56,56	2.23	18 (32%)
24	CHL	W	304	22	42,50,74	1.88	5 (11%)	44,85,114	1.58	7 (15%)
26	IWJ	X	318	-	43,45,45	1.18	7 (16%)	43,65,65	1.39	7 (16%)
29	Q6L	P	321	-	42,43,43	1.89	8 (19%)	47,60,60	1.54	6 (12%)
30	BCR	L	307	-	41,41,41	1.16	3 (7%)	56,56,56	2.65	18 (32%)
24	CHL	S	307	-	42,50,74	1.85	6 (14%)	44,85,114	1.80	7 (15%)
25	CLA	U	309	22	46,54,73	1.75	7 (15%)	53,90,113	1.46	8 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	A	807	-	64,72,73	1.49	9 (14%)	74,111,113	1.50	10 (13%)
25	CLA	W	309	22	64,72,73	1.51	6 (9%)	74,111,113	1.59	14 (18%)
24	CHL	R	311	-	44,52,74	1.86	8 (18%)	46,87,114	1.59	10 (21%)
25	CLA	6	607	6	45,53,73	1.81	9 (20%)	52,89,113	1.65	7 (13%)
25	CLA	A	845	28	50,58,73	1.60	6 (12%)	58,95,113	1.50	10 (17%)
26	IWJ	4	317	-	43,45,45	1.20	6 (13%)	43,65,65	1.25	4 (9%)
25	CLA	A	803	-	65,73,73	1.44	5 (7%)	76,113,113	1.55	10 (13%)
26	IWJ	Q	303	-	43,45,45	1.21	4 (9%)	43,65,65	1.27	6 (13%)
25	CLA	X	312	-	51,59,73	1.66	8 (15%)	59,96,113	1.56	11 (18%)
24	CHL	U	306	-	44,52,74	1.76	7 (15%)	46,87,114	1.34	5 (10%)
24	CHL	6	605	-	42,50,74	1.82	7 (16%)	45,85,114	1.73	7 (15%)
25	CLA	B	814	-	65,73,73	1.49	6 (9%)	76,113,113	1.45	10 (13%)
24	CHL	T	320	-	52,60,74	1.66	7 (13%)	56,97,114	1.65	12 (21%)
25	CLA	B	805	-	65,73,73	1.51	9 (13%)	76,113,113	1.47	12 (15%)
25	CLA	4	313	4	57,65,73	1.56	8 (14%)	66,103,113	1.66	11 (16%)
29	Q6L	X	319	-	42,43,43	1.92	6 (14%)	47,60,60	1.77	7 (14%)
25	CLA	3	308	3	41,49,73	1.77	9 (21%)	47,84,113	1.53	10 (21%)
26	IWJ	5	611	-	43,45,45	1.17	3 (6%)	43,65,65	1.28	4 (9%)
25	CLA	3	303	-	43,51,73	1.88	9 (20%)	54,87,113	1.58	9 (16%)
25	CLA	T	313	-	42,50,73	1.87	8 (19%)	48,85,113	1.35	6 (12%)
29	Q6L	U	314	-	42,43,43	1.85	7 (16%)	47,60,60	1.65	6 (12%)
25	CLA	S	313	-	41,49,73	1.88	6 (14%)	47,84,113	1.43	8 (17%)
36	DGD	B	850	-	60,60,67	0.95	2 (3%)	74,74,81	0.96	4 (5%)
25	CLA	B	813	-	65,73,73	1.44	9 (13%)	76,113,113	1.69	21 (27%)
25	CLA	A	834	-	56,64,73	1.56	7 (12%)	65,102,113	1.45	9 (13%)
29	Q6L	X	317	-	42,43,43	1.86	7 (16%)	47,60,60	1.57	5 (10%)
30	BCR	A	852	-	41,41,41	1.14	4 (9%)	56,56,56	2.20	12 (21%)
25	CLA	B	806	-	65,73,73	1.52	9 (13%)	76,113,113	1.62	15 (19%)
34	PQN	A	844	-	34,34,34	2.98	12 (35%)	42,45,45	1.95	6 (14%)
25	CLA	Q	314	23	53,61,73	1.59	6 (11%)	61,98,113	1.50	9 (14%)
29	Q6L	T	316	-	42,43,43	1.86	7 (16%)	47,60,60	1.62	10 (21%)
30	BCR	2	618	-	41,41,41	1.17	3 (7%)	56,56,56	2.18	15 (26%)
24	CHL	3	306	-	45,53,74	1.94	8 (17%)	52,89,114	1.58	7 (13%)
29	Q6L	P	316	-	42,43,43	1.91	8 (19%)	47,60,60	1.44	6 (12%)
25	CLA	A	817	-	65,73,73	1.50	6 (9%)	76,113,113	1.45	10 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	K	206	17	65,73,73	1.48	4 (6%)	76,113,113	1.53	11 (14%)
25	CLA	Q	306	39	50,58,73	1.78	7 (14%)	58,95,113	1.78	11 (18%)
25	CLA	4	304	-	44,52,73	1.85	6 (13%)	55,88,113	1.84	11 (20%)
28	LHG	Q	302	-	34,34,48	1.09	2 (5%)	37,40,54	1.06	2 (5%)
26	IWJ	1	611	-	43,45,45	1.22	5 (11%)	43,65,65	1.12	3 (6%)
25	CLA	1	602	1	56,64,73	1.70	10 (17%)	65,102,113	1.45	10 (15%)
30	BCR	3	319	-	41,41,41	1.27	5 (12%)	56,56,56	2.04	15 (26%)
24	CHL	Q	308	23	50,58,74	1.71	7 (14%)	52,94,114	1.96	12 (23%)
25	CLA	3	312	-	39,48,73	1.88	6 (15%)	44,83,113	1.62	9 (20%)
25	CLA	B	802	-	65,73,73	1.47	6 (9%)	76,113,113	1.66	13 (17%)
25	CLA	5	607	5	65,73,73	1.52	8 (12%)	76,113,113	1.41	9 (11%)
25	CLA	2	603	-	43,52,73	1.82	8 (18%)	49,88,113	1.58	10 (20%)
24	CHL	S	305	22	42,50,74	1.77	8 (19%)	44,85,114	1.79	8 (18%)
25	CLA	P	313	-	48,56,73	1.74	6 (12%)	55,92,113	1.42	9 (16%)
25	CLA	T	301	22	65,73,73	1.54	8 (12%)	76,113,113	1.67	14 (18%)
25	CLA	A	806	-	52,60,73	1.68	6 (11%)	60,97,113	1.69	10 (16%)
25	CLA	A	833	-	50,58,73	1.80	10 (20%)	58,95,113	1.44	9 (15%)
27	XAT	2	617	-	39,47,47	1.12	3 (7%)	54,74,74	3.07	27 (50%)
30	BCR	G	205	-	41,41,41	1.25	5 (12%)	56,56,56	2.02	14 (25%)
28	LHG	1	614	25	34,34,48	1.11	2 (5%)	37,40,54	1.17	3 (8%)
25	CLA	P	310	22	60,68,73	1.58	6 (10%)	70,107,113	1.46	11 (15%)
24	CHL	U	305	-	46,54,74	1.75	6 (13%)	49,90,114	1.73	8 (16%)
25	CLA	K	204	-	46,54,73	1.68	8 (17%)	53,90,113	1.75	11 (20%)
25	CLA	O	2005	-	41,49,73	1.80	6 (14%)	47,84,113	1.66	8 (17%)
37	NEX	R	321	-	38,46,46	1.30	7 (18%)	50,70,70	2.71	17 (34%)
29	Q6L	X	316	-	40,41,43	1.86	5 (12%)	46,56,60	1.61	6 (13%)
30	BCR	K	207	-	41,41,41	1.26	5 (12%)	56,56,56	2.10	16 (28%)
26	IWJ	P	320	-	43,45,45	1.20	6 (13%)	43,65,65	1.36	5 (11%)
25	CLA	2	612	2	65,73,73	1.52	8 (12%)	76,113,113	1.48	15 (19%)
25	CLA	B	833	-	43,51,73	1.75	7 (16%)	49,86,113	1.74	8 (16%)
25	CLA	S	303	-	50,58,73	1.73	7 (14%)	58,95,113	1.66	10 (17%)
25	CLA	U	312	-	41,49,73	1.86	6 (14%)	47,84,113	1.41	6 (12%)
25	CLA	2	613	-	41,50,73	1.83	7 (17%)	46,85,113	1.54	10 (21%)
24	CHL	P	314	22	45,53,74	1.78	6 (13%)	46,88,114	1.50	8 (17%)
25	CLA	A	836	-	65,73,73	1.44	8 (12%)	76,113,113	1.50	8 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	J	102	16	42,50,73	1.77	9 (21%)	48,85,113	1.63	7 (14%)
30	BCR	F	804	-	41,41,41	1.18	3 (7%)	56,56,56	2.40	21 (37%)
25	CLA	B	837	-	42,50,73	1.84	6 (14%)	48,85,113	1.66	8 (16%)
29	Q6L	W	315	-	42,43,43	1.84	7 (16%)	47,60,60	1.54	7 (14%)
29	Q6L	V	315	-	42,43,43	1.91	7 (16%)	47,60,60	1.45	6 (12%)
25	CLA	H	304	18	45,53,73	1.71	9 (20%)	52,89,113	1.68	10 (19%)
25	CLA	X	313	22	41,49,73	1.86	8 (19%)	47,84,113	1.60	9 (19%)
24	CHL	W	307	-	66,74,74	1.46	6 (9%)	73,114,114	1.53	10 (13%)
25	CLA	1	606	1	40,48,73	1.91	7 (17%)	50,83,113	1.66	12 (24%)
25	CLA	B	820	-	60,68,73	1.50	9 (15%)	70,107,113	1.65	16 (22%)
25	CLA	X	304	-	42,50,73	1.86	8 (19%)	48,85,113	1.74	9 (18%)
25	CLA	B	804	-	65,73,73	1.51	7 (10%)	76,113,113	1.39	9 (11%)
25	CLA	U	301	22	45,53,73	1.76	10 (22%)	52,89,113	1.67	9 (17%)
25	CLA	B	827	-	50,58,73	1.60	4 (8%)	58,95,113	1.61	12 (20%)
30	BCR	M	101	-	41,41,41	1.40	8 (19%)	56,56,56	2.32	22 (39%)
24	CHL	2	615	2	43,51,74	1.67	7 (16%)	45,86,114	1.56	9 (20%)
25	CLA	B	823	-	47,55,73	1.83	8 (17%)	54,91,113	1.38	7 (12%)
25	CLA	A	839	-	65,73,73	1.41	6 (9%)	76,113,113	1.51	10 (13%)
35	SF4	C	102	9	0,12,12	-	-	-	-	-
29	Q6L	R	301	-	42,43,43	1.89	7 (16%)	47,60,60	1.73	6 (12%)
25	CLA	A	804	39	65,73,73	1.51	10 (15%)	76,113,113	1.65	16 (21%)
24	CHL	V	305	22	43,51,74	1.74	7 (16%)	45,86,114	1.76	7 (15%)
29	Q6L	W	316	-	42,43,43	1.91	9 (21%)	47,60,60	1.54	6 (12%)
25	CLA	P	303	-	50,58,73	1.70	5 (10%)	58,95,113	1.55	9 (15%)
38	KC2	S	308	22	48,53,53	2.58	15 (31%)	54,89,89	2.42	18 (33%)
25	CLA	B	822	-	50,58,73	1.68	7 (14%)	58,95,113	1.55	9 (15%)
29	Q6L	U	315	-	42,43,43	1.90	8 (19%)	47,60,60	1.73	9 (19%)
25	CLA	B	828	-	65,73,73	1.47	8 (12%)	76,113,113	1.43	10 (13%)
25	CLA	Q	301	14	55,63,73	1.59	8 (14%)	64,101,113	1.72	13 (20%)
26	IWJ	3	315	-	43,45,45	1.13	6 (13%)	43,65,65	1.24	2 (4%)
24	CHL	R	310	-	52,60,74	1.63	8 (15%)	56,97,114	1.73	11 (19%)
25	CLA	P	311	-	60,68,73	1.51	6 (10%)	70,107,113	1.56	14 (20%)
25	CLA	4	310	4	54,62,73	1.58	5 (9%)	62,99,113	1.59	14 (22%)
24	CHL	X	308	-	44,52,74	1.72	6 (13%)	46,87,114	1.77	10 (21%)
25	CLA	A	809	-	50,58,73	1.64	9 (18%)	58,95,113	1.64	10 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	B	812	-	65,73,73	1.41	10 (15%)	76,113,113	1.36	11 (14%)
25	CLA	3	307	3	61,69,73	1.56	11 (18%)	71,108,113	1.72	14 (19%)
25	CLA	4	312	4	40,49,73	1.85	6 (15%)	45,84,113	1.67	8 (17%)
25	CLA	R	317	-	48,56,73	1.68	7 (14%)	55,92,113	1.60	9 (16%)
31	LMG	B	801	-	38,38,55	1.14	3 (7%)	46,46,63	1.14	3 (6%)
25	CLA	3	305	3	41,49,73	1.93	8 (19%)	51,84,113	1.51	11 (21%)
37	NEX	S	317	-	38,46,46	1.32	4 (10%)	50,70,70	2.71	16 (32%)
24	CHL	1	604	1	40,49,74	1.81	8 (20%)	41,84,114	1.61	10 (24%)
37	NEX	P	317	-	38,46,46	1.26	6 (15%)	50,70,70	2.62	17 (34%)
38	KC2	U	307	22	48,53,53	2.57	14 (29%)	54,89,89	2.35	18 (33%)
25	CLA	T	312	22	55,63,73	1.63	7 (12%)	64,101,113	1.48	10 (15%)
25	CLA	A	829	-	65,73,73	1.40	10 (15%)	76,113,113	1.55	14 (18%)
25	CLA	U	302	-	56,64,73	1.63	11 (19%)	65,102,113	1.53	8 (12%)
25	CLA	A	815	-	65,73,73	1.47	7 (10%)	76,113,113	1.78	9 (11%)
25	CLA	4	305	-	43,51,73	1.92	8 (18%)	54,87,113	1.48	8 (14%)
31	LMG	A	857	-	46,46,55	0.97	2 (4%)	54,54,63	0.89	2 (3%)
25	CLA	6	608	6	42,50,73	1.76	6 (14%)	48,85,113	1.77	7 (14%)
26	IWJ	S	322	-	43,45,45	1.18	5 (11%)	43,65,65	1.18	3 (6%)
24	CHL	S	314	22	45,53,74	1.76	5 (11%)	46,88,114	1.62	6 (13%)
25	CLA	6	609	-	44,52,73	1.79	4 (9%)	51,88,113	1.90	10 (19%)
25	CLA	A	808	7	65,73,73	1.43	11 (16%)	76,113,113	1.56	9 (11%)
29	Q6L	S	320	-	42,43,43	1.92	7 (16%)	47,60,60	1.65	9 (19%)
25	CLA	B	825	-	45,53,73	1.67	8 (17%)	52,89,113	1.41	8 (15%)
29	Q6L	O	2006	-	42,43,43	1.90	7 (16%)	47,60,60	1.42	5 (10%)
25	CLA	X	303	-	51,59,73	1.72	8 (15%)	59,96,113	1.32	7 (11%)
25	CLA	W	301	22	55,63,73	1.59	9 (16%)	64,101,113	1.53	9 (14%)
28	LHG	3	322	-	35,35,48	1.04	2 (5%)	38,41,54	1.06	3 (7%)
30	BCR	3	317	-	41,41,41	1.08	3 (7%)	56,56,56	1.89	18 (32%)
25	CLA	5	608	5	41,49,73	1.87	8 (19%)	47,84,113	1.65	8 (17%)
25	CLA	O	2004	-	41,49,73	1.84	7 (17%)	47,84,113	1.68	8 (17%)
28	LHG	A	847	25	29,29,48	1.17	2 (6%)	32,35,54	1.05	2 (6%)
25	CLA	A	827	39	65,73,73	1.49	8 (12%)	76,113,113	1.69	15 (19%)
25	CLA	G	202	-	45,53,73	1.80	8 (17%)	52,89,113	1.39	7 (13%)
25	CLA	B	807	-	65,73,73	1.47	7 (10%)	76,113,113	1.65	10 (13%)
24	CHL	R	302	-	47,55,74	1.73	6 (12%)	50,91,114	1.71	13 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	B	838	-	50,58,73	1.57	5 (10%)	58,95,113	1.67	7 (12%)
25	CLA	U	308	22	41,49,73	1.90	10 (24%)	47,84,113	1.92	13 (27%)
27	XAT	1	612	-	39,47,47	1.34	6 (15%)	54,74,74	3.21	28 (51%)
25	CLA	L	301	18	41,49,73	1.82	8 (19%)	47,84,113	1.61	7 (14%)
25	CLA	P	301	22	65,73,73	1.43	7 (10%)	76,113,113	1.52	13 (17%)
33	CL0	A	802	-	65,73,73	1.54	10 (15%)	76,113,113	1.41	11 (14%)
31	LMG	A	855	-	27,27,55	1.27	2 (7%)	35,35,63	1.35	4 (11%)
38	KC2	Q	310	23	48,53,53	2.58	14 (29%)	54,89,89	2.51	18 (33%)
30	BCR	K	205	-	41,41,41	1.23	4 (9%)	56,56,56	2.07	16 (28%)
25	CLA	V	303	-	50,58,73	1.72	8 (16%)	58,95,113	1.73	8 (13%)
24	CHL	T	306	-	52,60,74	1.60	7 (13%)	56,97,114	1.63	11 (19%)
25	CLA	4	303	4	60,68,73	1.56	9 (15%)	70,107,113	1.39	12 (17%)
29	Q6L	S	315	-	42,43,43	1.76	5 (11%)	47,60,60	1.65	9 (19%)
25	CLA	A	843	-	65,73,73	1.47	7 (10%)	76,113,113	1.64	13 (17%)
25	CLA	2	614	2	44,52,73	1.73	8 (18%)	49,87,113	1.65	6 (12%)
25	CLA	T	310	22	42,50,73	1.89	7 (16%)	48,85,113	1.36	6 (12%)
30	BCR	F	801	-	41,41,41	1.14	4 (9%)	56,56,56	1.96	16 (28%)
25	CLA	A	841	-	50,58,73	1.72	7 (14%)	58,95,113	1.52	9 (15%)
25	CLA	1	603	-	55,63,73	1.62	8 (14%)	64,101,113	1.79	15 (23%)
25	CLA	1	613	-	52,60,73	1.68	5 (9%)	60,97,113	1.50	9 (15%)
25	CLA	A	810	7	65,73,73	1.46	9 (13%)	76,113,113	1.50	10 (13%)
25	CLA	3	304	3	40,49,73	1.87	7 (17%)	45,84,113	1.71	9 (20%)
25	CLA	4	316	4	42,50,73	1.83	6 (14%)	48,85,113	1.57	9 (18%)
24	CHL	U	313	22	43,51,74	1.81	6 (13%)	45,86,114	1.55	8 (17%)
25	CLA	A	838	7	65,73,73	1.52	7 (10%)	76,113,113	1.57	14 (18%)
29	Q6L	S	321	-	42,43,43	1.96	8 (19%)	47,60,60	1.41	6 (12%)
25	CLA	A	812	-	64,72,73	1.48	8 (12%)	74,111,113	1.43	9 (12%)
24	CHL	4	307	-	42,50,74	1.86	9 (21%)	48,85,114	2.11	13 (27%)
25	CLA	4	311	-	42,50,73	2.07	7 (16%)	48,85,113	1.75	12 (25%)
25	CLA	Q	304	23	65,73,73	1.45	10 (15%)	76,113,113	1.67	9 (11%)
24	CHL	P	305	-	46,54,74	1.77	6 (13%)	49,90,114	1.93	11 (22%)
27	XAT	5	612	-	39,47,47	1.03	2 (5%)	54,74,74	3.01	25 (46%)
31	LMG	L	308	-	31,31,55	1.20	2 (6%)	39,39,63	1.03	2 (5%)
25	CLA	V	312	22	55,63,73	1.60	9 (16%)	64,101,113	1.47	9 (14%)
29	Q6L	R	323	-	42,43,43	1.89	6 (14%)	47,60,60	1.73	7 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	XAT	3	316	-	39,47,47	1.23	5 (12%)	54,74,74	3.25	24 (44%)
25	CLA	Q	312	23	42,50,73	1.92	7 (16%)	48,85,113	1.41	7 (14%)
25	CLA	3	313	-	41,49,73	1.84	7 (17%)	47,84,113	1.55	8 (17%)
25	CLA	T	302	-	65,73,73	1.54	8 (12%)	76,113,113	1.34	9 (11%)
25	CLA	O	2002	-	65,73,73	1.46	9 (13%)	76,113,113	1.73	15 (19%)
25	CLA	A	821	-	65,73,73	1.50	7 (10%)	76,113,113	1.57	13 (17%)
25	CLA	S	302	-	65,73,73	1.53	10 (15%)	76,113,113	1.38	10 (13%)
25	CLA	A	811	7	50,58,73	1.60	4 (8%)	58,95,113	1.80	8 (13%)
24	CHL	4	308	-	46,54,74	1.75	6 (13%)	49,90,114	1.42	6 (12%)
25	CLA	B	834	-	65,73,73	1.44	8 (12%)	76,113,113	1.48	11 (14%)
25	CLA	2	608	2	45,53,73	1.79	6 (13%)	52,89,113	1.61	11 (21%)
27	XAT	4	318	-	39,47,47	1.10	5 (12%)	54,74,74	3.38	23 (42%)
25	CLA	A	837	-	65,73,73	1.57	7 (10%)	76,113,113	1.48	11 (14%)
24	CHL	U	304	22	42,50,74	1.82	9 (21%)	44,85,114	1.74	11 (25%)

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
31	LMG	F	805	-	-	2/26/46/70	0/1/1/1
31	LMG	O	2008	-	-	2/34/54/70	0/1/1/1
25	CLA	V	301	22	1/1/14/20	10/31/109/115	-
24	CHL	5	605	-	3/3/15/26	2/8/106/137	-
29	Q6L	T	319	-	-	8/29/67/67	0/2/2/2
25	CLA	W	312	22	1/1/13/20	9/25/103/115	-
25	CLA	A	813	-	1/1/15/20	13/37/115/115	-
25	CLA	B	803	-	1/1/15/20	10/37/115/115	-
25	CLA	H	302	-	1/1/15/20	12/37/115/115	-
25	CLA	B	821	-	1/1/13/20	7/25/103/115	-
35	SF4	C	101	9	-	-	0/6/5/5
24	CHL	T	307	-	3/3/15/26	3/13/111/137	-
25	CLA	R	316	22	1/1/13/20	9/25/103/115	-
25	CLA	A	823	39	1/1/15/20	10/37/115/115	-
24	CHL	2	605	-	3/3/15/26	7/10/108/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	R	313	22	1/1/14/20	17/36/114/115	-
24	CHL	R	318	22	3/3/15/26	4/13/112/137	-
25	CLA	B	836	8	-	6/31/109/115	-
25	CLA	Q	315	-	1/1/11/20	5/17/95/115	-
24	CHL	2	607	-	3/3/15/26	4/13/112/137	-
30	BCR	4	319	-	-	3/29/63/63	0/2/2/2
25	CLA	V	309	22	1/1/10/20	4/10/88/115	-
25	CLA	N	202	20	1/1/11/20	3/13/91/115	-
25	CLA	A	826	-	1/1/13/20	8/25/103/115	-
24	CHL	W	306	-	3/3/17/26	5/23/121/137	-
25	CLA	A	828	-	-	8/30/108/115	-
34	PQN	B	844	-	-	6/23/43/43	0/2/2/2
24	CHL	T	314	22	3/3/15/26	3/10/108/137	-
25	CLA	K	201	17	1/1/11/20	6/13/91/115	-
30	BCR	J	101	-	-	4/29/63/63	0/2/2/2
31	LMG	2	620	-	-	3/26/46/70	0/1/1/1
24	CHL	V	304	22	3/3/16/26	8/15/113/137	-
35	SF4	A	853	7,8	-	-	0/6/5/5
30	BCR	L	305	-	-	4/29/63/63	0/2/2/2
30	BCR	I	101	-	-	9/29/63/63	0/2/2/2
25	CLA	S	309	22	1/1/14/20	12/31/109/115	-
25	CLA	6	604	-	1/1/10/20	2/9/88/115	-
28	LHG	3	323	-	-	15/47/47/53	-
25	CLA	B	817	-	1/1/10/20	4/11/89/115	-
24	CHL	X	305	22	3/3/15/26	1/10/108/137	-
30	BCR	B	848	-	-	2/29/63/63	0/2/2/2
25	CLA	R	307	-	1/1/12/20	2/19/97/115	-
25	CLA	S	311	-	1/1/11/20	6/16/94/115	-
25	CLA	A	816	-	1/1/11/20	6/13/91/115	-
25	CLA	5	601	5	1/1/11/20	9/15/93/115	-
25	CLA	W	302	-	1/1/13/20	5/25/103/115	-
25	CLA	B	826	-	1/1/15/20	8/37/115/115	-
25	CLA	5	604	-	1/1/10/20	0/4/80/115	-
25	CLA	2	609	2	1/1/13/20	7/25/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	X	314	-	1/1/10/20	5/8/86/115	-
25	CLA	Q	313	-	1/1/11/20	7/15/93/115	-
30	BCR	A	848	-	-	3/29/63/63	0/2/2/2
25	CLA	5	609	-	1/1/13/20	7/23/101/115	-
32	SQD	6	617	-	-	13/49/69/69	0/1/1/1
25	CLA	1	608	1	1/1/15/20	10/37/115/115	-
25	CLA	B	824	-	1/1/14/20	6/31/109/115	-
25	CLA	B	835	-	1/1/11/20	3/13/91/115	-
25	CLA	L	303	-	1/1/11/20	5/13/91/115	-
30	BCR	G	201	-	-	2/29/63/63	0/2/2/2
26	IWJ	V	320	-	-	5/33/76/76	1/2/2/2
25	CLA	B	839	-	1/1/15/20	20/37/115/115	-
25	CLA	B	811	8	1/1/15/20	13/37/115/115	-
29	Q6L	R	320	-	-	0/29/67/67	0/2/2/2
30	BCR	B	845	-	-	3/29/63/63	0/2/2/2
25	CLA	V	302	-	1/1/12/20	9/19/97/115	-
25	CLA	A	819	-	1/1/14/20	13/31/109/115	-
25	CLA	6	610	-	1/1/14/20	13/33/111/115	-
25	CLA	B	808	8	1/1/15/20	23/37/115/115	-
25	CLA	K	203	-	1/1/14/20	4/34/112/115	-
25	CLA	X	310	22	1/1/10/20	3/10/88/115	-
24	CHL	Q	307	23	3/3/16/26	6/15/113/137	-
36	DGD	A	854	-	-	4/40/80/95	0/2/2/2
25	CLA	5	606	-	1/1/10/20	0/8/84/115	-
25	CLA	W	303	-	1/1/12/20	4/19/97/115	-
25	CLA	R	305	22	1/1/15/20	9/37/115/115	-
24	CHL	4	302	4	3/3/17/26	4/23/121/137	-
25	CLA	A	824	-	1/1/10/20	6/10/88/115	-
25	CLA	S	312	22	1/1/13/20	7/25/103/115	-
25	CLA	4	315	-	1/1/10/20	3/8/86/115	-
24	CHL	V	314	22	3/3/15/26	5/13/111/137	-
37	NEX	T	317	-	-	3/27/83/83	0/3/3/3
30	BCR	K	202	-	-	0/29/63/63	0/2/2/2
32	SQD	H	303	-	-	10/43/63/69	0/1/1/1
26	IWJ	4	301	-	-	7/33/76/76	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	Q	305	-	1/1/10/20	0/11/90/115	-
28	LHG	A	846	-	-	12/53/53/53	-
25	CLA	B	809	-	1/1/15/20	9/37/115/115	-
25	CLA	L	302	-	-	10/31/109/115	-
24	CHL	S	304	22	3/3/15/26	3/10/108/137	-
25	CLA	U	310	-	1/1/10/20	5/11/90/115	-
25	CLA	F	802	-	1/1/10/20	4/10/88/115	-
25	CLA	2	606	-	1/1/11/20	10/13/91/115	-
24	CHL	V	307	-	3/3/15/26	5/13/111/137	-
29	Q6L	R	319	-	-	10/29/67/67	0/2/2/2
30	BCR	3	318	-	-	2/29/63/63	0/2/2/2
25	CLA	P	309	22	1/1/14/20	15/36/114/115	-
25	CLA	3	310	-	1/1/10/20	6/11/89/115	-
25	CLA	B	829	-	1/1/15/20	16/37/115/115	-
29	Q6L	P	315	-	-	6/29/67/67	0/2/2/2
30	BCR	A	851	-	-	6/29/63/63	0/2/2/2
24	CHL	V	306	-	3/3/15/26	0/13/111/137	-
26	IWJ	Q	320	-	-	12/33/76/76	0/2/2/2
29	Q6L	T	322	-	-	8/29/67/67	0/2/2/2
24	CHL	W	314	22	3/3/14/26	5/10/104/137	-
25	CLA	2	611	2	1/1/11/20	5/11/89/115	-
29	Q6L	2	616	-	-	11/29/67/67	0/2/2/2
38	KC2	W	308	22	-	10/15/71/71	-
38	KC2	V	308	22	-	10/15/71/71	-
25	CLA	6	602	6	1/1/14/20	13/34/112/115	-
25	CLA	5	610	-	1/1/10/20	4/8/86/115	-
25	CLA	1	609	-	1/1/10/20	2/4/80/115	-
25	CLA	T	303	-	1/1/12/20	6/19/97/115	-
38	KC2	X	309	22	-	10/15/71/71	-
25	CLA	W	311	-	1/1/11/20	5/13/91/115	-
25	CLA	V	311	-	1/1/14/20	10/31/109/115	-
25	CLA	2	604	-	1/1/10/20	3/9/88/115	-
25	CLA	B	843	28	1/1/15/20	14/37/115/115	-
28	LHG	3	321	-	-	9/47/47/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	XAT	6	615	-	-	0/31/93/93	0/4/4/4
25	CLA	3	302	-	1/1/13/20	7/25/103/115	-
29	Q6L	S	323	-	-	9/29/67/67	0/2/2/2
25	CLA	6	612	6	1/1/11/20	5/13/91/115	-
25	CLA	A	831	-	1/1/15/20	15/37/115/115	-
26	IWJ	R	322	-	-	7/33/76/76	1/2/2/2
24	CHL	R	308	22	3/3/16/26	3/15/113/137	-
25	CLA	Q	311	23	1/1/13/20	8/25/103/115	-
24	CHL	P	307	-	3/3/15/26	3/13/111/137	-
25	CLA	H	301	14	1/1/10/20	6/11/90/115	-
29	Q6L	O	2007	-	-	6/29/67/67	0/2/2/2
25	CLA	A	818	-	1/1/11/20	5/13/91/115	-
24	CHL	Q	309	-	3/3/15/26	3/13/111/137	-
29	Q6L	T	315	-	-	6/29/67/67	0/2/2/2
25	CLA	A	830	-	1/1/15/20	21/37/115/115	-
25	CLA	B	831	-	1/1/15/20	12/37/115/115	-
25	CLA	4	314	-	1/1/10/20	5/8/86/115	-
25	CLA	P	302	-	1/1/15/20	15/37/115/115	-
29	Q6L	W	319	-	-	9/29/67/67	0/2/2/2
29	Q6L	Q	317	-	-	6/29/67/67	0/2/2/2
37	NEX	W	317	-	-	2/27/83/83	0/3/3/3
25	CLA	3	314	3	-	0/6/84/115	-
29	Q6L	V	319	-	-	9/29/67/67	0/2/2/2
29	Q6L	Q	318	-	-	6/29/67/67	0/2/2/2
29	Q6L	S	316	-	-	3/29/67/67	0/2/2/2
30	BCR	B	847	-	-	0/29/63/63	0/2/2/2
25	CLA	A	820	-	1/1/13/20	11/30/108/115	-
28	LHG	2	619	25	-	8/37/37/53	-
24	CHL	R	309	-	3/3/16/26	7/20/118/137	-
25	CLA	B	810	-	1/1/15/20	16/37/115/115	-
38	KC2	R	312	22	-	8/15/71/71	-
29	Q6L	R	304	-	-	5/29/67/67	0/2/2/2
25	CLA	4	309	4	1/1/11/20	8/13/91/115	-
25	CLA	O	2001	-	1/1/13/20	13/30/108/115	-
25	CLA	G	203	-	1/1/10/20	3/10/88/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	S	310	22	1/1/14/20	11/31/109/115	-
30	BCR	B	849	-	-	3/29/63/63	0/2/2/2
29	Q6L	Q	319	-	-	5/29/67/67	0/2/2/2
25	CLA	U	303	-	1/1/12/20	6/19/97/115	-
26	IWJ	6	614	-	-	3/33/76/76	0/2/2/2
26	IWJ	W	318	-	-	10/33/76/76	0/2/2/2
24	CHL	X	315	22	3/3/15/26	4/13/112/137	-
26	IWJ	V	318	-	-	4/33/76/76	0/2/2/2
25	CLA	B	841	-	1/1/15/20	6/37/115/115	-
25	CLA	B	830	-	1/1/15/20	13/37/115/115	-
30	BCR	B	846	-	-	4/29/63/63	0/2/2/2
24	CHL	4	306	-	3/3/15/26	3/8/106/137	-
25	CLA	L	304	-	1/1/10/20	4/10/88/115	-
25	CLA	N	203	-	1/1/10/20	4/10/88/115	-
25	CLA	A	835	-	1/1/15/20	12/37/115/115	-
28	LHG	3	320	25	-	4/26/26/53	-
25	CLA	3	309	28	1/1/10/20	3/10/88/115	-
25	CLA	R	306	-	1/1/15/20	11/37/115/115	-
25	CLA	X	302	22	1/1/13/20	8/25/103/115	-
25	CLA	F	803	12	1/1/10/20	4/8/86/115	-
25	CLA	S	301	22	1/1/15/20	9/37/115/115	-
24	CHL	6	601	6	3/3/15/26	3/10/108/137	-
24	CHL	P	306	-	3/3/17/26	7/23/121/137	-
25	CLA	6	611	-	1/1/10/20	6/11/89/115	-
25	CLA	A	822	-	1/1/11/20	3/13/91/115	-
25	CLA	1	610	1	-	5/8/84/115	-
25	CLA	1	605	-	1/1/10/20	3/8/86/115	-
29	Q6L	X	301	-	-	8/29/67/67	0/2/2/2
25	CLA	U	311	22	1/1/13/20	6/25/103/115	-
38	KC2	T	308	22	-	8/15/71/71	-
25	CLA	3	311	3	1/1/13/20	10/23/101/115	-
25	CLA	R	315	-	1/1/14/20	10/31/109/115	-
38	KC2	P	308	22	-	9/15/71/71	-
26	IWJ	T	321	-	-	4/33/76/76	1/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	B	832	-	1/1/10/20	3/11/89/115	-
25	CLA	A	840	-	-	7/25/103/115	-
31	LMG	A	801	-	-	1/26/46/70	0/1/1/1
30	BCR	H	305	-	-	6/29/63/63	0/2/2/2
25	CLA	B	815	-	1/1/15/20	14/37/115/115	-
25	CLA	T	309	22	1/1/13/20	10/30/108/115	-
29	Q6L	V	321	-	-	6/29/67/67	0/2/2/2
24	CHL	W	305	-	3/3/15/26	2/10/108/137	-
24	CHL	Q	316	23	3/3/15/26	3/13/112/137	-
31	LMG	J	104	-	-	6/41/61/70	0/1/1/1
31	LMG	5	613	-	-	5/49/69/70	0/1/1/1
25	CLA	A	832	-	1/1/15/20	12/37/115/115	-
26	IWJ	U	316	-	-	2/33/76/76	0/2/2/2
24	CHL	X	307	-	3/3/17/26	10/23/121/137	-
26	IWJ	S	318	-	-	4/33/76/76	0/2/2/2
29	Q6L	V	316	-	-	8/29/67/67	0/2/2/2
24	CHL	T	304	22	3/3/15/26	5/12/110/137	-
30	BCR	J	103	-	-	2/29/63/63	0/2/2/2
30	BCR	L	306	-	-	3/29/63/63	0/2/2/2
24	CHL	P	304	22	3/3/16/26	6/15/113/137	-
26	IWJ	S	319	-	-	7/33/76/76	1/2/2/2
25	CLA	5	602	5	1/1/14/20	12/31/109/115	-
25	CLA	1	607	1	1/1/7/20	2/6/68/115	-
25	CLA	B	816	-	1/1/12/20	5/21/99/115	-
25	CLA	B	819	-	1/1/13/20	10/30/108/115	-
26	IWJ	R	303	-	-	4/33/76/76	0/2/2/2
29	Q6L	P	319	-	-	6/29/67/67	0/2/2/2
29	Q6L	W	320	-	-	7/29/67/67	0/2/2/2
26	IWJ	V	317	-	-	6/33/76/76	0/2/2/2
25	CLA	3	301	3	1/1/14/20	7/31/109/115	-
25	CLA	B	818	-	1/1/13/20	9/25/103/115	-
25	CLA	A	825	-	1/1/15/20	18/37/115/115	-
25	CLA	T	311	-	1/1/14/20	15/31/109/115	-
24	CHL	1	601	1	3/3/18/26	8/25/123/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	V	313	-	1/1/11/20	4/17/95/115	-
24	CHL	T	305	-	3/3/16/26	5/19/117/137	-
26	IWJ	T	318	-	-	6/33/76/76	0/2/2/2
25	CLA	5	603	5	1/1/11/20	6/13/91/115	-
25	CLA	6	613	6	-	8/37/115/115	-
24	CHL	6	606	-	3/3/15/26	8/12/110/137	-
25	CLA	A	856	-	1/1/13/20	12/28/106/115	-
25	CLA	2	602	2	1/1/14/20	15/33/111/115	-
25	CLA	B	840	-	-	8/16/94/115	-
26	IWJ	P	318	-	-	2/33/76/76	0/2/2/2
25	CLA	B	842	-	1/1/15/20	18/37/115/115	-
37	NEX	H	306	-	-	3/27/83/83	0/3/3/3
25	CLA	6	603	6	1/1/11/20	2/11/89/115	-
24	CHL	2	601	2	3/3/16/26	2/17/115/137	-
25	CLA	A	805	-	1/1/15/20	13/37/115/115	-
24	CHL	S	306	-	3/3/17/26	7/23/121/137	-
31	LMG	N	201	-	-	3/50/70/70	0/1/1/1
24	CHL	X	306	-	3/3/15/26	2/10/108/137	-
25	CLA	R	314	22	1/1/14/20	13/31/109/115	-
25	CLA	G	204	13	1/1/11/20	10/13/91/115	-
25	CLA	P	312	22	1/1/13/20	12/25/103/115	-
28	LHG	6	616	-	-	10/50/50/53	-
25	CLA	W	313	-	1/1/10/20	2/11/89/115	-
29	Q6L	U	317	-	-	5/29/67/67	0/2/2/2
25	CLA	O	2003	-	1/1/10/20	0/8/86/115	-
30	BCR	A	850	-	-	1/29/63/63	0/2/2/2
25	CLA	A	814	-	1/1/12/20	7/24/102/115	-
25	CLA	2	610	28	1/1/10/20	3/10/88/115	-
25	CLA	W	310	22	1/1/14/20	9/31/109/115	-
25	CLA	X	311	22	1/1/12/20	8/19/97/115	-
25	CLA	V	310	22	1/1/11/20	8/16/94/115	-
25	CLA	A	842	-	1/1/15/20	14/37/115/115	-
30	BCR	A	849	-	-	5/29/63/63	0/2/2/2
24	CHL	W	304	22	3/3/15/26	0/10/108/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	IWJ	X	318	-	-	6/33/76/76	1/2/2/2
29	Q6L	P	321	-	-	7/29/67/67	0/2/2/2
30	BCR	L	307	-	-	4/29/63/63	0/2/2/2
24	CHL	S	307	-	3/3/15/26	5/10/108/137	-
25	CLA	U	309	22	1/1/11/20	9/15/93/115	-
25	CLA	A	807	-	1/1/14/20	18/36/114/115	-
25	CLA	W	309	22	1/1/14/20	7/36/114/115	-
24	CHL	R	311	-	3/3/15/26	3/13/111/137	-
25	CLA	6	607	6	1/1/11/20	2/13/91/115	-
25	CLA	A	845	28	1/1/12/20	7/19/97/115	-
26	IWJ	4	317	-	-	7/33/76/76	0/2/2/2
25	CLA	A	803	-	1/1/15/20	8/37/115/115	-
26	IWJ	Q	303	-	-	3/33/76/76	0/2/2/2
25	CLA	X	312	-	1/1/12/20	4/21/99/115	-
24	CHL	U	306	-	3/3/15/26	5/13/111/137	-
24	CHL	6	605	-	3/3/15/26	0/10/108/137	-
25	CLA	B	814	-	1/1/15/20	12/37/115/115	-
24	CHL	T	320	-	3/3/17/26	8/23/121/137	-
25	CLA	B	805	-	1/1/15/20	16/37/115/115	-
25	CLA	4	313	4	-	9/28/106/115	-
29	Q6L	X	319	-	-	10/29/67/67	0/2/2/2
25	CLA	3	308	3	1/1/10/20	2/8/86/115	-
26	IWJ	5	611	-	-	5/33/76/76	1/2/2/2
25	CLA	3	303	-	1/1/11/20	0/11/87/115	-
25	CLA	T	313	-	1/1/10/20	4/10/88/115	-
29	Q6L	U	314	-	-	7/29/67/67	0/2/2/2
25	CLA	S	313	-	1/1/10/20	1/8/86/115	-
36	DGD	B	850	-	-	12/48/88/95	0/2/2/2
25	CLA	B	813	-	1/1/15/20	14/37/115/115	-
25	CLA	A	834	-	1/1/13/20	4/27/105/115	-
29	Q6L	X	317	-	-	2/29/67/67	0/2/2/2
30	BCR	A	852	-	-	5/29/63/63	0/2/2/2
25	CLA	B	806	-	1/1/15/20	17/37/115/115	-
34	PQN	A	844	-	-	13/23/43/43	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	Q	314	23	1/1/12/20	12/23/101/115	-
29	Q6L	T	316	-	-	1/29/67/67	0/2/2/2
30	BCR	2	618	-	-	4/29/63/63	0/2/2/2
24	CHL	3	306	-	3/3/16/26	5/13/111/137	-
29	Q6L	P	316	-	-	2/29/67/67	0/2/2/2
25	CLA	A	817	-	-	12/37/115/115	-
25	CLA	K	206	17	1/1/15/20	13/37/115/115	-
25	CLA	Q	306	39	1/1/12/20	9/19/97/115	-
25	CLA	4	304	-	1/1/11/20	6/13/89/115	-
28	LHG	Q	302	-	-	6/39/39/53	-
26	IWJ	1	611	-	-	4/33/76/76	0/2/2/2
25	CLA	1	602	1	1/1/13/20	5/27/105/115	-
30	BCR	3	319	-	-	2/29/63/63	0/2/2/2
24	CHL	Q	308	23	3/3/16/26	4/20/118/137	-
25	CLA	3	312	-	1/1/10/20	0/6/84/115	-
25	CLA	B	802	-	1/1/15/20	13/37/115/115	-
25	CLA	5	607	5	1/1/15/20	13/37/115/115	-
25	CLA	2	603	-	1/1/11/20	3/11/89/115	-
24	CHL	S	305	22	3/3/15/26	4/10/108/137	-
25	CLA	T	301	22	1/1/15/20	13/37/115/115	-
25	CLA	P	313	-	-	4/17/95/115	-
25	CLA	A	806	-	1/1/12/20	7/22/100/115	-
25	CLA	A	833	-	-	5/19/97/115	-
27	XAT	2	617	-	-	0/31/93/93	0/4/4/4
30	BCR	G	205	-	-	2/29/63/63	0/2/2/2
28	LHG	1	614	25	-	12/39/39/53	-
25	CLA	P	310	22	1/1/14/20	10/31/109/115	-
24	CHL	U	305	-	3/3/16/26	6/15/113/137	-
25	CLA	K	204	-	1/1/11/20	7/15/93/115	-
25	CLA	O	2005	-	1/1/10/20	4/8/86/115	-
37	NEX	R	321	-	-	3/27/83/83	0/3/3/3
29	Q6L	X	316	-	-	7/29/63/67	0/2/2/2
30	BCR	K	207	-	-	3/29/63/63	0/2/2/2
26	IWJ	P	320	-	-	2/33/76/76	0/2/2/2
25	CLA	2	612	2	1/1/15/20	14/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	B	833	-	1/1/10/20	1/11/89/115	-
25	CLA	S	303	-	1/1/12/20	5/19/97/115	-
25	CLA	U	312	-	1/1/10/20	1/8/86/115	-
25	CLA	2	613	-	1/1/10/20	3/9/87/115	-
24	CHL	P	314	22	3/3/15/26	6/13/112/137	-
25	CLA	A	836	-	1/1/15/20	4/37/115/115	-
25	CLA	J	102	16	1/1/10/20	4/10/88/115	-
30	BCR	F	804	-	-	6/29/63/63	0/2/2/2
25	CLA	B	837	-	1/1/10/20	2/10/88/115	-
29	Q6L	W	315	-	-	4/29/67/67	0/2/2/2
29	Q6L	V	315	-	-	11/29/67/67	0/2/2/2
25	CLA	H	304	18	1/1/11/20	4/13/91/115	-
25	CLA	X	313	22	1/1/10/20	3/8/86/115	-
24	CHL	W	307	-	3/3/20/26	13/39/137/137	-
25	CLA	1	606	1	1/1/10/20	5/8/84/115	-
25	CLA	B	820	-	1/1/14/20	10/31/109/115	-
25	CLA	X	304	-	1/1/10/20	5/10/88/115	-
25	CLA	B	804	-	1/1/15/20	15/37/115/115	-
25	CLA	U	301	22	1/1/11/20	7/13/91/115	-
25	CLA	B	827	-	1/1/12/20	4/19/97/115	-
30	BCR	M	101	-	-	6/29/63/63	0/2/2/2
24	CHL	2	615	2	3/3/15/26	5/12/110/137	-
25	CLA	B	823	-	1/1/11/20	6/16/94/115	-
25	CLA	A	839	-	1/1/15/20	17/37/115/115	-
35	SF4	C	102	9	-	-	0/6/5/5
29	Q6L	R	301	-	-	11/29/67/67	0/2/2/2
25	CLA	A	804	39	1/1/15/20	14/37/115/115	-
24	CHL	V	305	22	3/3/15/26	2/12/110/137	-
29	Q6L	W	316	-	-	5/29/67/67	0/2/2/2
25	CLA	P	303	-	1/1/12/20	11/19/97/115	-
38	KC2	S	308	22	-	7/15/71/71	-
25	CLA	B	822	-	1/1/12/20	3/19/97/115	-
29	Q6L	U	315	-	-	2/29/67/67	0/2/2/2
25	CLA	B	828	-	1/1/15/20	5/37/115/115	-
25	CLA	Q	301	14	1/1/13/20	14/25/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	IWJ	3	315	-	-	3/33/76/76	1/2/2/2
24	CHL	R	310	-	3/3/17/26	6/23/121/137	-
25	CLA	P	311	-	1/1/14/20	10/31/109/115	-
25	CLA	4	310	4	1/1/12/20	6/24/102/115	-
24	CHL	X	308	-	3/3/15/26	8/13/111/137	-
25	CLA	A	809	-	1/1/12/20	6/19/97/115	-
25	CLA	B	812	-	1/1/15/20	12/37/115/115	-
25	CLA	3	307	3	1/1/14/20	10/33/111/115	-
25	CLA	4	312	4	1/1/10/20	3/8/86/115	-
25	CLA	R	317	-	-	6/17/95/115	-
31	LMG	B	801	-	-	4/33/53/70	0/1/1/1
25	CLA	3	305	3	1/1/10/20	2/10/86/115	-
37	NEX	S	317	-	-	3/27/83/83	0/3/3/3
24	CHL	1	604	1	3/3/15/26	0/8/106/137	-
37	NEX	P	317	-	-	2/27/83/83	0/3/3/3
38	KC2	U	307	22	-	11/15/71/71	-
25	CLA	T	312	22	1/1/13/20	12/25/103/115	-
25	CLA	A	829	-	1/1/15/20	16/37/115/115	-
25	CLA	U	302	-	1/1/13/20	11/27/105/115	-
25	CLA	A	815	-	1/1/15/20	12/37/115/115	-
25	CLA	4	305	-	1/1/11/20	2/11/87/115	-
31	LMG	A	857	-	-	9/41/61/70	0/1/1/1
25	CLA	6	608	6	1/1/10/20	5/10/88/115	-
26	IWJ	S	322	-	-	5/33/76/76	0/2/2/2
24	CHL	S	314	22	3/3/15/26	5/13/112/137	-
25	CLA	6	609	-	1/1/11/20	4/11/89/115	-
25	CLA	A	808	7	1/1/15/20	11/37/115/115	-
29	Q6L	S	320	-	-	7/29/67/67	0/2/2/2
25	CLA	B	825	-	1/1/11/20	6/13/91/115	-
29	Q6L	O	2006	-	-	9/29/67/67	0/2/2/2
25	CLA	X	303	-	1/1/12/20	9/21/99/115	-
25	CLA	W	301	22	1/1/13/20	10/25/103/115	-
28	LHG	3	322	-	-	10/40/40/53	-
30	BCR	3	317	-	-	2/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	5	608	5	1/1/10/20	4/8/86/115	-
25	CLA	O	2004	-	1/1/10/20	5/8/86/115	-
28	LHG	A	847	25	-	9/34/34/53	-
25	CLA	A	827	39	1/1/15/20	9/37/115/115	-
25	CLA	G	202	-	1/1/11/20	7/13/91/115	-
25	CLA	B	807	-	1/1/15/20	12/37/115/115	-
24	CHL	R	302	-	3/3/16/26	5/17/115/137	-
25	CLA	B	838	-	1/1/12/20	0/19/97/115	-
25	CLA	U	308	22	1/1/10/20	1/8/86/115	-
27	XAT	1	612	-	-	6/31/93/93	0/4/4/4
25	CLA	L	301	18	1/1/10/20	3/8/86/115	-
25	CLA	P	301	22	1/1/15/20	9/37/115/115	-
33	CL0	A	802	-	3/3/20/25	8/37/135/135	-
31	LMG	A	855	-	-	4/22/42/70	0/1/1/1
38	KC2	Q	310	23	-	6/15/71/71	-
30	BCR	K	205	-	-	3/29/63/63	0/2/2/2
25	CLA	V	303	-	1/1/12/20	5/19/97/115	-
24	CHL	T	306	-	3/3/17/26	6/23/121/137	-
25	CLA	4	303	4	1/1/14/20	15/31/109/115	-
29	Q6L	S	315	-	-	5/29/67/67	0/2/2/2
25	CLA	A	843	-	1/1/15/20	8/37/115/115	-
25	CLA	2	614	2	1/1/10/20	6/11/90/115	-
25	CLA	T	310	22	1/1/10/20	3/10/88/115	-
30	BCR	F	801	-	-	4/29/63/63	0/2/2/2
25	CLA	A	841	-	1/1/12/20	6/19/97/115	-
25	CLA	1	603	-	1/1/13/20	6/25/103/115	-
25	CLA	1	613	-	1/1/12/20	6/22/100/115	-
25	CLA	A	810	7	1/1/15/20	8/37/115/115	-
25	CLA	3	304	3	1/1/10/20	2/8/86/115	-
25	CLA	4	316	4	1/1/10/20	3/10/88/115	-
24	CHL	U	313	22	3/3/15/26	3/12/110/137	-
25	CLA	A	838	7	-	19/37/115/115	-
29	Q6L	S	321	-	-	11/29/67/67	0/2/2/2
25	CLA	A	812	-	1/1/14/20	10/36/114/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CHL	4	307	-	3/3/15/26	6/12/108/137	-
25	CLA	4	311	-	1/1/10/20	5/10/88/115	-
25	CLA	Q	304	23	1/1/15/20	9/37/115/115	-
24	CHL	P	305	-	3/3/16/26	4/15/113/137	-
27	XAT	5	612	-	-	0/31/93/93	0/4/4/4
31	LMG	L	308	-	-	6/26/46/70	0/1/1/1
25	CLA	V	312	22	-	7/25/103/115	-
29	Q6L	R	323	-	-	9/29/67/67	0/2/2/2
27	XAT	3	316	-	-	3/31/93/93	0/4/4/4
25	CLA	Q	312	23	1/1/10/20	3/10/88/115	-
25	CLA	3	313	-	1/1/10/20	4/8/86/115	-
25	CLA	T	302	-	1/1/15/20	14/37/115/115	-
25	CLA	O	2002	-	1/1/15/20	8/37/115/115	-
25	CLA	A	821	-	1/1/15/20	18/37/115/115	-
25	CLA	S	302	-	1/1/15/20	11/37/115/115	-
25	CLA	A	811	7	1/1/12/20	2/19/97/115	-
24	CHL	4	308	-	3/3/16/26	3/15/113/137	-
25	CLA	B	834	-	1/1/15/20	11/37/115/115	-
25	CLA	2	608	2	1/1/11/20	6/13/91/115	-
27	XAT	4	318	-	-	5/31/93/93	0/4/4/4
25	CLA	A	837	-	1/1/15/20	12/37/115/115	-
24	CHL	U	304	22	3/3/15/26	5/10/108/137	-

All (3027) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	V	309	CLA	C4B-NB	10.02	1.44	1.35
34	A	844	PQN	C12-C13	9.18	1.55	1.33
34	B	844	PQN	C12-C13	9.06	1.54	1.33
29	V	316	Q6L	C29-C30	8.77	1.53	1.32
38	V	308	KC2	C2A-C3A	8.64	1.54	1.37
29	P	321	Q6L	C29-C30	8.62	1.52	1.32
38	X	309	KC2	C2A-C3A	8.61	1.54	1.37
29	O	2007	Q6L	C29-C30	8.59	1.52	1.32
29	S	321	Q6L	C29-C30	8.59	1.52	1.32
38	S	308	KC2	C2A-C3A	8.56	1.54	1.37
24	S	304	CHL	C4B-NB	8.54	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	P	316	Q6L	C29-C30	8.51	1.52	1.32
29	X	319	Q6L	C29-C30	8.50	1.52	1.32
29	R	304	Q6L	C29-C30	8.49	1.52	1.32
29	O	2006	Q6L	C29-C30	8.47	1.52	1.32
29	R	301	Q6L	C29-C30	8.47	1.52	1.32
29	R	319	Q6L	C29-C30	8.45	1.52	1.32
29	U	315	Q6L	C29-C30	8.45	1.52	1.32
29	S	316	Q6L	C29-C30	8.45	1.52	1.32
29	P	319	Q6L	C29-C30	8.43	1.52	1.32
29	P	315	Q6L	C29-C30	8.43	1.52	1.32
29	T	322	Q6L	C29-C30	8.43	1.52	1.32
29	R	323	Q6L	C29-C30	8.43	1.52	1.32
29	X	301	Q6L	C29-C30	8.42	1.52	1.32
29	R	320	Q6L	C29-C30	8.41	1.52	1.32
29	W	319	Q6L	C29-C30	8.41	1.52	1.32
29	U	317	Q6L	C29-C30	8.41	1.52	1.32
29	T	319	Q6L	C29-C30	8.40	1.52	1.32
29	W	316	Q6L	C29-C30	8.39	1.52	1.32
29	X	316	Q6L	C29-C30	8.38	1.52	1.32
29	X	317	Q6L	C29-C30	8.37	1.52	1.32
29	T	316	Q6L	C29-C30	8.33	1.51	1.32
29	S	320	Q6L	C29-C30	8.32	1.51	1.32
29	W	320	Q6L	C29-C30	8.31	1.51	1.32
29	V	321	Q6L	C29-C30	8.29	1.51	1.32
38	Q	310	KC2	C2A-C3A	8.28	1.54	1.37
38	T	308	KC2	C2A-C3A	8.28	1.54	1.37
29	Q	317	Q6L	C29-C30	8.27	1.51	1.32
24	X	305	CHL	C4B-NB	8.25	1.42	1.35
29	T	315	Q6L	C29-C30	8.24	1.51	1.32
38	R	312	KC2	C2A-C3A	8.24	1.54	1.37
29	S	323	Q6L	C29-C30	8.24	1.51	1.32
25	Q	312	CLA	C4B-NB	8.23	1.42	1.35
34	A	844	PQN	O1-C1	8.23	1.40	1.23
29	Q	319	Q6L	C29-C30	8.23	1.51	1.32
29	V	315	Q6L	C29-C30	8.17	1.51	1.32
29	U	314	Q6L	C29-C30	8.17	1.51	1.32
24	3	306	CHL	C4B-NB	8.15	1.42	1.35
38	U	307	KC2	C2A-C3A	8.12	1.53	1.37
29	Q	318	Q6L	C29-C30	8.06	1.51	1.32
29	W	315	Q6L	C29-C30	8.06	1.51	1.32
24	W	304	CHL	C4B-NB	8.05	1.42	1.35
25	4	311	CLA	C4B-NB	8.03	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	2	616	Q6L	C29-C30	8.01	1.51	1.32
25	T	310	CLA	C4B-NB	7.99	1.42	1.35
24	P	314	CHL	C4B-NB	7.97	1.42	1.35
24	S	307	CHL	C4B-NB	7.93	1.42	1.35
29	S	315	Q6L	C29-C30	7.92	1.51	1.32
25	R	315	CLA	C4B-NB	7.92	1.42	1.35
38	W	308	KC2	C2A-C3A	7.90	1.53	1.37
34	B	844	PQN	O4-C4	7.90	1.39	1.23
25	R	313	CLA	C4B-NB	7.90	1.42	1.35
34	A	844	PQN	O4-C4	7.86	1.39	1.23
25	1	602	CLA	C4B-NB	7.84	1.42	1.35
38	P	308	KC2	C2A-C3A	7.83	1.53	1.37
24	X	315	CHL	C4B-NB	7.80	1.42	1.35
24	S	314	CHL	C4B-NB	7.78	1.42	1.35
25	6	609	CLA	C4B-NB	7.76	1.42	1.35
25	A	837	CLA	C4B-NB	7.75	1.42	1.35
25	A	824	CLA	C4B-NB	7.75	1.42	1.35
25	5	607	CLA	C4B-NB	7.75	1.42	1.35
25	3	314	CLA	C4B-NB	7.74	1.42	1.35
24	T	307	CHL	C4B-NB	7.74	1.42	1.35
24	X	308	CHL	C4B-NB	7.71	1.42	1.35
24	W	307	CHL	C4B-NB	7.70	1.42	1.35
24	R	311	CHL	C4B-NB	7.68	1.42	1.35
25	U	308	CLA	C4B-NB	7.67	1.42	1.35
34	B	844	PQN	O1-C1	7.67	1.39	1.23
24	W	314	CHL	C4B-NB	7.67	1.42	1.35
24	R	318	CHL	C4B-NB	7.67	1.42	1.35
24	U	313	CHL	C4B-NB	7.66	1.42	1.35
25	R	316	CLA	C4B-NB	7.65	1.42	1.35
25	S	309	CLA	C4B-NB	7.65	1.42	1.35
25	2	608	CLA	C4B-NB	7.65	1.42	1.35
25	1	609	CLA	C4B-NB	7.64	1.42	1.35
25	T	302	CLA	C4B-NB	7.64	1.42	1.35
24	T	304	CHL	C4B-NB	7.63	1.42	1.35
38	P	308	KC2	C1D-ND	7.62	1.42	1.35
24	R	309	CHL	C4B-NB	7.61	1.42	1.35
24	T	314	CHL	C4B-NB	7.61	1.42	1.35
24	4	308	CHL	C4B-NB	7.60	1.42	1.35
25	1	613	CLA	C4B-NB	7.60	1.42	1.35
24	P	305	CHL	C4B-NB	7.59	1.42	1.35
29	V	319	Q6L	C29-C30	7.59	1.50	1.32
24	T	305	CHL	C4B-NB	7.59	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	W	305	CHL	C4B-NB	7.59	1.42	1.35
25	S	313	CLA	C4B-NB	7.59	1.42	1.35
25	S	303	CLA	C4B-NB	7.58	1.42	1.35
24	6	605	CHL	C4B-NB	7.58	1.42	1.35
25	2	610	CLA	C4B-NB	7.58	1.42	1.35
25	2	602	CLA	C4B-NB	7.57	1.42	1.35
25	T	312	CLA	C4B-NB	7.57	1.42	1.35
25	4	310	CLA	C4B-NB	7.56	1.42	1.35
25	A	841	CLA	C4B-NB	7.55	1.41	1.35
25	A	818	CLA	C4B-NB	7.55	1.41	1.35
25	N	202	CLA	C4B-NB	7.55	1.41	1.35
25	A	825	CLA	C4B-NB	7.55	1.41	1.35
25	3	309	CLA	C4B-NB	7.53	1.41	1.35
25	A	806	CLA	C4B-NB	7.53	1.41	1.35
25	K	201	CLA	C4B-NB	7.52	1.41	1.35
24	V	314	CHL	C4B-NB	7.52	1.41	1.35
25	1	610	CLA	C4B-NB	7.52	1.41	1.35
25	A	843	CLA	C4B-NB	7.52	1.41	1.35
25	T	313	CLA	C4B-NB	7.51	1.41	1.35
38	R	312	KC2	C3D-C4D	7.51	1.47	1.40
25	X	313	CLA	C4B-NB	7.51	1.41	1.35
25	U	310	CLA	C4B-NB	7.50	1.41	1.35
24	2	605	CHL	C4B-NB	7.50	1.41	1.35
25	6	613	CLA	C4B-NB	7.50	1.41	1.35
25	T	303	CLA	C4B-NB	7.50	1.41	1.35
25	B	831	CLA	C4B-NB	7.50	1.41	1.35
25	4	316	CLA	C4B-NB	7.49	1.41	1.35
25	3	305	CLA	C4B-NB	7.48	1.41	1.35
25	U	312	CLA	C4B-NB	7.48	1.41	1.35
25	B	804	CLA	C4B-NB	7.48	1.41	1.35
38	S	308	KC2	C1D-ND	7.47	1.41	1.35
25	W	309	CLA	C4B-NB	7.47	1.41	1.35
25	B	823	CLA	C4B-NB	7.47	1.41	1.35
25	P	312	CLA	C4B-NB	7.46	1.41	1.35
25	W	312	CLA	C4B-NB	7.46	1.41	1.35
25	L	303	CLA	C4B-NB	7.46	1.41	1.35
25	R	307	CLA	C4B-NB	7.46	1.41	1.35
25	4	314	CLA	C4B-NB	7.45	1.41	1.35
24	Q	316	CHL	C4B-NB	7.44	1.41	1.35
25	1	607	CLA	C4B-NB	7.44	1.41	1.35
25	S	310	CLA	C4B-NB	7.42	1.41	1.35
25	B	814	CLA	C4B-NB	7.42	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	T	301	CLA	C4B-NB	7.41	1.41	1.35
25	B	840	CLA	C4B-NB	7.40	1.41	1.35
25	4	309	CLA	C4B-NB	7.39	1.41	1.35
25	4	312	CLA	C4B-NB	7.39	1.41	1.35
25	S	312	CLA	C4B-NB	7.38	1.41	1.35
25	B	824	CLA	C4B-NB	7.38	1.41	1.35
25	U	309	CLA	C4B-NB	7.38	1.41	1.35
24	5	605	CHL	C4B-NB	7.38	1.41	1.35
38	P	308	KC2	C3D-C4D	7.37	1.47	1.40
25	3	312	CLA	C4B-NB	7.37	1.41	1.35
25	A	815	CLA	C4B-NB	7.37	1.41	1.35
25	U	303	CLA	C4B-NB	7.36	1.41	1.35
24	V	307	CHL	C4B-NB	7.35	1.41	1.35
25	4	305	CLA	C4B-NB	7.35	1.41	1.35
38	U	307	KC2	C1D-ND	7.35	1.41	1.35
25	6	607	CLA	C4B-NB	7.34	1.41	1.35
25	B	837	CLA	C4B-NB	7.34	1.41	1.35
25	5	610	CLA	C4B-NB	7.34	1.41	1.35
25	P	313	CLA	C4B-NB	7.34	1.41	1.35
24	U	305	CHL	C4B-NB	7.34	1.41	1.35
24	6	606	CHL	C4B-NB	7.34	1.41	1.35
38	T	308	KC2	C1D-ND	7.33	1.41	1.35
25	T	311	CLA	C4B-NB	7.33	1.41	1.35
25	U	311	CLA	C4B-NB	7.33	1.41	1.35
25	X	310	CLA	C4B-NB	7.33	1.41	1.35
25	A	840	CLA	C4B-NB	7.33	1.41	1.35
38	Q	310	KC2	C3D-C4D	7.32	1.47	1.40
25	6	604	CLA	C4B-NB	7.32	1.41	1.35
25	S	311	CLA	C4B-NB	7.32	1.41	1.35
25	1	606	CLA	C4B-NB	7.32	1.41	1.35
24	P	304	CHL	C4B-NB	7.32	1.41	1.35
25	W	310	CLA	C4B-NB	7.32	1.41	1.35
25	Q	315	CLA	C4B-NB	7.31	1.41	1.35
25	T	309	CLA	C4B-NB	7.31	1.41	1.35
24	Q	309	CHL	C4B-NB	7.31	1.41	1.35
24	W	306	CHL	C4B-NB	7.31	1.41	1.35
24	V	306	CHL	C4B-NB	7.30	1.41	1.35
25	R	314	CLA	C4B-NB	7.30	1.41	1.35
25	5	603	CLA	C4B-NB	7.30	1.41	1.35
25	P	310	CLA	C4B-NB	7.29	1.41	1.35
25	3	304	CLA	C4B-NB	7.27	1.41	1.35
24	P	307	CHL	C4B-NB	7.26	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	3	311	CLA	C4B-NB	7.25	1.41	1.35
25	H	302	CLA	C4B-NB	7.24	1.41	1.35
25	O	2003	CLA	C4B-NB	7.24	1.41	1.35
24	R	302	CHL	C4B-NB	7.24	1.41	1.35
25	A	838	CLA	C4B-NB	7.24	1.41	1.35
25	P	303	CLA	C4B-NB	7.24	1.41	1.35
25	A	814	CLA	C4B-NB	7.24	1.41	1.35
25	4	304	CLA	C4B-NB	7.23	1.41	1.35
25	K	206	CLA	C4B-NB	7.22	1.41	1.35
25	B	835	CLA	C4B-NB	7.22	1.41	1.35
25	S	301	CLA	C4B-NB	7.21	1.41	1.35
24	U	304	CHL	C4B-NB	7.20	1.41	1.35
25	5	602	CLA	C4B-NB	7.19	1.41	1.35
25	2	604	CLA	C4B-NB	7.19	1.41	1.35
25	A	842	CLA	C4B-NB	7.18	1.41	1.35
25	2	612	CLA	C4B-NB	7.18	1.41	1.35
24	4	307	CHL	C4B-NB	7.18	1.41	1.35
25	X	314	CLA	C4B-NB	7.17	1.41	1.35
25	5	606	CLA	C4B-NB	7.16	1.41	1.35
25	G	202	CLA	C4B-NB	7.16	1.41	1.35
25	B	816	CLA	C4B-NB	7.15	1.41	1.35
25	3	310	CLA	C4B-NB	7.14	1.41	1.35
25	3	313	CLA	C4B-NB	7.14	1.41	1.35
25	B	841	CLA	C4B-NB	7.13	1.41	1.35
25	O	2005	CLA	C4B-NB	7.13	1.41	1.35
25	4	315	CLA	C4B-NB	7.13	1.41	1.35
24	U	306	CHL	C4B-NB	7.13	1.41	1.35
25	O	2004	CLA	C4B-NB	7.13	1.41	1.35
24	V	304	CHL	C4B-NB	7.12	1.41	1.35
25	V	302	CLA	C4B-NB	7.11	1.41	1.35
25	X	312	CLA	C4B-NB	7.11	1.41	1.35
25	P	311	CLA	C4B-NB	7.11	1.41	1.35
25	5	604	CLA	C4B-NB	7.11	1.41	1.35
25	P	309	CLA	C4B-NB	7.10	1.41	1.35
25	A	832	CLA	C4B-NB	7.10	1.41	1.35
25	2	606	CLA	C4B-NB	7.09	1.41	1.35
24	4	306	CHL	C4B-NB	7.08	1.41	1.35
25	B	821	CLA	C4B-NB	7.08	1.41	1.35
25	V	303	CLA	C4B-NB	7.06	1.41	1.35
25	P	302	CLA	C4B-NB	7.06	1.41	1.35
25	A	823	CLA	C4B-NB	7.05	1.41	1.35
25	6	611	CLA	C4B-NB	7.05	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	A	835	CLA	C4B-NB	7.05	1.41	1.35
25	A	803	CLA	C4B-NB	7.04	1.41	1.35
25	V	313	CLA	C4B-NB	7.04	1.41	1.35
25	X	303	CLA	C4B-NB	7.03	1.41	1.35
24	X	306	CHL	C4B-NB	7.03	1.41	1.35
25	A	817	CLA	C4B-NB	7.02	1.41	1.35
25	B	802	CLA	C4B-NB	7.01	1.41	1.35
25	B	827	CLA	C4B-NB	7.01	1.41	1.35
25	Q	313	CLA	C4B-NB	7.01	1.41	1.35
25	4	313	CLA	C4B-NB	7.00	1.41	1.35
25	B	822	CLA	C4B-NB	6.99	1.41	1.35
25	6	602	CLA	C4B-NB	6.98	1.41	1.35
25	A	827	CLA	C4B-NB	6.98	1.41	1.35
25	G	203	CLA	C4B-NB	6.98	1.41	1.35
25	R	317	CLA	C4B-NB	6.97	1.41	1.35
25	S	302	CLA	C4B-NB	6.96	1.41	1.35
24	6	601	CHL	C4B-NB	6.96	1.41	1.35
25	1	605	CLA	C4B-NB	6.95	1.41	1.35
25	3	303	CLA	C4B-NB	6.94	1.41	1.35
25	Q	305	CLA	C4B-NB	6.94	1.41	1.35
24	R	308	CHL	C4B-NB	6.93	1.41	1.35
25	U	302	CLA	C4B-NB	6.93	1.41	1.35
24	T	320	CHL	C4B-NB	6.91	1.41	1.35
25	A	819	CLA	C4B-NB	6.91	1.41	1.35
25	5	608	CLA	C4B-NB	6.90	1.41	1.35
25	1	603	CLA	C4B-NB	6.90	1.41	1.35
24	V	305	CHL	C4B-NB	6.90	1.41	1.35
24	1	601	CHL	C4B-NB	6.90	1.41	1.35
25	5	609	CLA	C4B-NB	6.90	1.41	1.35
25	K	203	CLA	C4B-NB	6.89	1.41	1.35
25	A	821	CLA	C4B-NB	6.89	1.41	1.35
25	B	842	CLA	C4B-NB	6.88	1.41	1.35
25	3	302	CLA	C4B-NB	6.87	1.41	1.35
25	B	839	CLA	C4B-NB	6.87	1.41	1.35
25	A	805	CLA	C4B-NB	6.87	1.41	1.35
25	2	613	CLA	C4B-NB	6.87	1.41	1.35
24	1	604	CHL	C4B-NB	6.85	1.41	1.35
25	X	304	CLA	C4B-NB	6.85	1.41	1.35
25	Q	306	CLA	C4B-NB	6.85	1.41	1.35
25	2	614	CLA	C4B-NB	6.84	1.41	1.35
25	B	834	CLA	C4B-NB	6.83	1.41	1.35
25	A	822	CLA	C4B-NB	6.83	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	Q	308	CHL	C4B-NB	6.83	1.41	1.35
25	2	611	CLA	C4B-NB	6.82	1.41	1.35
25	F	802	CLA	C4B-NB	6.82	1.41	1.35
25	R	305	CLA	C4B-NB	6.82	1.41	1.35
25	L	304	CLA	C4B-NB	6.82	1.41	1.35
24	P	306	CHL	C4B-NB	6.82	1.41	1.35
25	A	830	CLA	C4B-NB	6.81	1.41	1.35
38	X	309	KC2	C3D-C4D	6.80	1.46	1.40
25	L	301	CLA	C4B-NB	6.79	1.41	1.35
24	S	306	CHL	C4B-NB	6.79	1.41	1.35
25	V	311	CLA	C4B-NB	6.78	1.41	1.35
25	W	313	CLA	C4B-NB	6.78	1.41	1.35
25	W	302	CLA	C4B-NB	6.77	1.41	1.35
25	6	603	CLA	C4B-NB	6.77	1.41	1.35
25	B	807	CLA	C4B-NB	6.76	1.41	1.35
25	B	832	CLA	C4B-NB	6.76	1.41	1.35
25	H	301	CLA	C4B-NB	6.75	1.41	1.35
25	B	817	CLA	C4B-NB	6.74	1.41	1.35
25	4	303	CLA	C4B-NB	6.73	1.41	1.35
25	1	608	CLA	C4B-NB	6.73	1.41	1.35
24	T	306	CHL	C4B-NB	6.71	1.41	1.35
25	A	811	CLA	C4B-NB	6.71	1.41	1.35
24	S	305	CHL	C4B-NB	6.70	1.41	1.35
25	V	312	CLA	C4B-NB	6.70	1.41	1.35
24	R	310	CHL	C4B-NB	6.69	1.41	1.35
25	6	612	CLA	C4B-NB	6.69	1.41	1.35
38	W	308	KC2	C1D-ND	6.68	1.41	1.35
25	B	843	CLA	C4B-NB	6.68	1.41	1.35
25	6	608	CLA	C4B-NB	6.67	1.41	1.35
24	2	607	CHL	C4B-NB	6.67	1.41	1.35
25	6	610	CLA	C4B-NB	6.67	1.41	1.35
25	B	810	CLA	C4B-NB	6.66	1.41	1.35
38	Q	310	KC2	C1D-ND	6.66	1.41	1.35
25	V	310	CLA	C4B-NB	6.65	1.41	1.35
25	Q	314	CLA	C4B-NB	6.64	1.41	1.35
25	O	2001	CLA	C4B-NB	6.64	1.41	1.35
38	T	308	KC2	C3D-C4D	6.64	1.46	1.40
25	2	603	CLA	C4B-NB	6.63	1.41	1.35
25	A	856	CLA	C4B-NB	6.62	1.41	1.35
25	B	836	CLA	C4B-NB	6.61	1.41	1.35
25	B	815	CLA	C4B-NB	6.61	1.41	1.35
33	A	802	CL0	C4B-NB	6.60	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	A	831	CLA	C4B-NB	6.58	1.41	1.35
25	N	203	CLA	C4B-NB	6.58	1.41	1.35
25	B	818	CLA	C4B-NB	6.58	1.41	1.35
25	W	311	CLA	C4B-NB	6.56	1.41	1.35
38	W	308	KC2	C3D-C4D	6.56	1.46	1.40
25	B	833	CLA	C4B-NB	6.54	1.41	1.35
25	A	810	CLA	C4B-NB	6.54	1.41	1.35
38	R	312	KC2	C1D-ND	6.54	1.41	1.35
25	F	803	CLA	C4B-NB	6.53	1.41	1.35
25	A	833	CLA	C4B-NB	6.52	1.41	1.35
25	L	302	CLA	C4B-NB	6.51	1.41	1.35
25	5	601	CLA	C4B-NB	6.51	1.41	1.35
25	X	311	CLA	C4B-NB	6.51	1.41	1.35
25	B	803	CLA	C4B-NB	6.50	1.41	1.35
25	A	836	CLA	C4B-NB	6.49	1.41	1.35
25	B	819	CLA	C4B-NB	6.49	1.41	1.35
25	Q	311	CLA	C4B-NB	6.48	1.41	1.35
25	B	813	CLA	C4B-NB	6.47	1.41	1.35
25	H	304	CLA	C4B-NB	6.47	1.41	1.35
25	3	307	CLA	C4B-NB	6.45	1.41	1.35
25	B	806	CLA	C4B-NB	6.43	1.40	1.35
24	4	302	CHL	C4B-NB	6.43	1.40	1.35
25	3	301	CLA	C4B-NB	6.42	1.40	1.35
25	R	306	CLA	C4B-NB	6.42	1.40	1.35
38	U	307	KC2	C3D-C4D	6.41	1.46	1.40
25	B	838	CLA	C4B-NB	6.39	1.40	1.35
25	V	301	CLA	C4B-NB	6.39	1.40	1.35
25	A	809	CLA	C4B-NB	6.39	1.40	1.35
25	A	813	CLA	C4B-NB	6.39	1.40	1.35
25	W	303	CLA	C4B-NB	6.37	1.40	1.35
25	Q	301	CLA	C4B-NB	6.36	1.40	1.35
38	S	308	KC2	C3D-C4D	6.36	1.46	1.40
24	2	615	CHL	C4B-NB	6.34	1.40	1.35
25	B	805	CLA	C4B-NB	6.33	1.40	1.35
25	B	828	CLA	C4B-NB	6.33	1.40	1.35
38	Q	310	KC2	CBA-CAA	6.32	1.52	1.33
25	J	102	CLA	C4B-NB	6.31	1.40	1.35
25	A	807	CLA	C4B-NB	6.29	1.40	1.35
25	B	811	CLA	C4B-NB	6.29	1.40	1.35
25	B	809	CLA	C4B-NB	6.28	1.40	1.35
25	3	308	CLA	C4B-NB	6.28	1.40	1.35
38	V	308	KC2	CBA-CAA	6.28	1.52	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	Q	307	CHL	C4B-NB	6.27	1.40	1.35
25	A	816	CLA	C4B-NB	6.27	1.40	1.35
25	G	204	CLA	C4B-NB	6.27	1.40	1.35
25	A	826	CLA	C4B-NB	6.26	1.40	1.35
25	B	820	CLA	C4B-NB	6.25	1.40	1.35
25	O	2002	CLA	C4B-NB	6.24	1.40	1.35
38	X	309	KC2	C1D-ND	6.24	1.40	1.35
25	A	834	CLA	C4B-NB	6.23	1.40	1.35
24	2	601	CHL	C4B-NB	6.23	1.40	1.35
25	A	812	CLA	C4B-NB	6.23	1.40	1.35
25	P	301	CLA	C4B-NB	6.21	1.40	1.35
25	A	845	CLA	C4B-NB	6.21	1.40	1.35
25	K	204	CLA	C4B-NB	6.18	1.40	1.35
25	B	829	CLA	C4B-NB	6.17	1.40	1.35
25	W	301	CLA	C4B-NB	6.14	1.40	1.35
25	A	839	CLA	C4B-NB	6.10	1.40	1.35
38	U	307	KC2	CBA-CAA	6.08	1.51	1.33
25	B	826	CLA	C4B-NB	6.08	1.40	1.35
25	B	808	CLA	C4B-NB	6.06	1.40	1.35
38	W	308	KC2	CBA-CAA	6.05	1.51	1.33
24	X	307	CHL	C4B-NB	6.04	1.40	1.35
38	P	308	KC2	CBA-CAA	6.00	1.51	1.33
38	R	312	KC2	CBA-CAA	5.99	1.51	1.33
38	X	309	KC2	CBA-CAA	5.98	1.51	1.33
25	A	820	CLA	C4B-NB	5.98	1.40	1.35
38	T	308	KC2	CBA-CAA	5.97	1.51	1.33
25	B	825	CLA	C4B-NB	5.92	1.40	1.35
38	S	308	KC2	CBA-CAA	5.90	1.50	1.33
25	U	301	CLA	C4B-NB	5.88	1.40	1.35
25	B	830	CLA	C4B-NB	5.87	1.40	1.35
25	A	804	CLA	C4B-NB	5.86	1.40	1.35
25	X	302	CLA	C4B-NB	5.83	1.40	1.35
29	V	315	Q6L	C12-C11	-5.73	1.33	1.52
29	R	301	Q6L	C12-C11	-5.62	1.34	1.52
25	B	812	CLA	C4B-NB	5.61	1.40	1.35
25	Q	304	CLA	C4B-NB	5.58	1.40	1.35
29	R	323	Q6L	C12-C11	-5.55	1.34	1.52
25	A	828	CLA	C4B-NB	5.54	1.40	1.35
29	P	315	Q6L	C12-C11	-5.54	1.34	1.52
29	W	320	Q6L	C12-C11	-5.53	1.34	1.52
29	W	315	Q6L	C12-C11	-5.51	1.34	1.52
29	X	319	Q6L	C12-C11	-5.51	1.34	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	S	320	Q6L	C12-C11	-5.50	1.34	1.52
25	2	609	CLA	C4B-NB	5.50	1.40	1.35
29	S	321	Q6L	C12-C11	-5.47	1.34	1.52
29	T	315	Q6L	C12-C11	-5.47	1.34	1.52
29	U	314	Q6L	C12-C11	-5.47	1.34	1.52
29	V	316	Q6L	C12-C11	-5.47	1.34	1.52
29	W	316	Q6L	C12-C11	-5.46	1.34	1.52
29	Q	317	Q6L	C12-C11	-5.46	1.34	1.52
29	V	321	Q6L	C12-C11	-5.45	1.34	1.52
29	V	319	Q6L	C12-C11	-5.44	1.34	1.52
29	2	616	Q6L	C12-C11	-5.43	1.34	1.52
29	W	319	Q6L	C12-C11	-5.40	1.34	1.52
29	X	301	Q6L	C12-C11	-5.40	1.34	1.52
29	T	322	Q6L	C12-C11	-5.39	1.34	1.52
29	S	323	Q6L	C12-C11	-5.38	1.34	1.52
29	R	319	Q6L	C12-C11	-5.38	1.34	1.52
29	P	321	Q6L	C12-C11	-5.37	1.34	1.52
29	Q	319	Q6L	C12-C11	-5.37	1.34	1.52
29	O	2006	Q6L	C12-C11	-5.33	1.35	1.52
29	Q	318	Q6L	C12-C11	-5.33	1.35	1.52
29	S	315	Q6L	C12-C11	-5.32	1.35	1.52
29	R	304	Q6L	C12-C11	-5.30	1.35	1.52
25	A	808	CLA	C4B-NB	5.29	1.39	1.35
29	R	320	Q6L	C12-C11	-5.27	1.35	1.52
29	U	317	Q6L	C12-C11	-5.27	1.35	1.52
29	U	315	Q6L	C12-C11	-5.27	1.35	1.52
25	A	829	CLA	C4B-NB	5.26	1.39	1.35
38	V	308	KC2	C1D-ND	5.26	1.39	1.35
29	O	2007	Q6L	C12-C11	-5.24	1.35	1.52
29	X	316	Q6L	C12-C11	-5.24	1.35	1.52
29	T	319	Q6L	C12-C11	-5.23	1.35	1.52
29	P	316	Q6L	C12-C11	-5.23	1.35	1.52
29	P	319	Q6L	C12-C11	-5.21	1.35	1.52
29	S	316	Q6L	C12-C11	-5.17	1.35	1.52
29	X	317	Q6L	C12-C11	-5.16	1.35	1.52
25	4	311	CLA	CMB-C2B	-5.13	1.41	1.51
29	T	316	Q6L	C12-C11	-5.12	1.35	1.52
34	B	844	PQN	C2-C1	-5.00	1.37	1.48
38	V	308	KC2	C3D-C4D	4.97	1.44	1.40
25	Q	306	CLA	C4D-ND	-4.91	1.31	1.37
32	H	303	SQD	O8-S	4.62	1.64	1.47
36	A	854	DGD	O1G-C1A	4.58	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	6	617	SQD	O8-S	4.55	1.63	1.47
28	3	320	LHG	O7-C7	4.54	1.47	1.34
32	H	303	SQD	O47-C7	4.49	1.47	1.34
25	X	302	CLA	C4D-ND	-4.43	1.31	1.37
28	1	614	LHG	O8-C23	4.41	1.46	1.33
24	Q	308	CHL	CMD-C2D	-4.39	1.41	1.50
28	3	321	LHG	O7-C7	4.38	1.46	1.34
36	B	850	DGD	O2G-C1B	4.38	1.46	1.34
28	2	619	LHG	O7-C7	4.38	1.46	1.34
31	O	2008	LMG	O7-C10	4.37	1.46	1.34
32	H	303	SQD	O48-C23	4.36	1.46	1.33
36	B	850	DGD	O1G-C1A	4.34	1.46	1.33
32	6	617	SQD	O47-C7	4.34	1.46	1.34
31	N	201	LMG	O7-C10	4.33	1.46	1.34
31	A	855	LMG	O7-C10	4.30	1.46	1.34
38	R	312	KC2	C4A-C3A	4.30	1.52	1.44
28	Q	302	LHG	O7-C7	4.30	1.46	1.34
36	A	854	DGD	O2G-C1B	4.30	1.46	1.34
24	Q	316	CHL	C1D-ND	4.27	1.43	1.37
31	5	613	LMG	O8-C28	4.23	1.45	1.33
31	A	857	LMG	O8-C28	4.23	1.45	1.33
25	6	609	CLA	C1D-ND	4.22	1.43	1.37
28	A	846	LHG	O8-C23	4.22	1.45	1.33
31	L	308	LMG	O8-C28	4.21	1.45	1.33
28	A	847	LHG	O8-C23	4.21	1.45	1.33
32	6	617	SQD	O48-C23	4.20	1.45	1.33
25	G	203	CLA	C1D-ND	4.20	1.42	1.37
38	X	309	KC2	CMD-C2D	-4.19	1.42	1.51
31	L	308	LMG	O7-C10	4.18	1.46	1.34
25	B	832	CLA	C3B-C2B	-4.18	1.34	1.40
31	B	801	LMG	O7-C10	4.18	1.46	1.34
31	2	620	LMG	O8-C28	4.17	1.45	1.33
31	F	805	LMG	O7-C10	4.16	1.46	1.34
25	5	603	CLA	C1D-ND	4.14	1.42	1.37
25	G	204	CLA	CMB-C2B	-4.13	1.43	1.51
25	5	604	CLA	CAB-C3B	-4.13	1.43	1.51
34	B	844	PQN	C3-C2	4.13	1.42	1.35
38	S	308	KC2	C4A-C3A	4.12	1.52	1.44
38	W	308	KC2	C4A-C3A	4.11	1.52	1.44
31	A	855	LMG	O8-C28	4.11	1.45	1.33
25	B	833	CLA	C1D-ND	4.11	1.42	1.37
25	A	833	CLA	CMB-C2B	-4.10	1.43	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	A	823	CLA	CMB-C2B	-4.09	1.43	1.51
25	G	204	CLA	C1D-ND	4.09	1.42	1.37
28	3	322	LHG	O7-C7	4.09	1.45	1.34
25	N	203	CLA	CMD-C2D	-4.08	1.42	1.50
25	1	613	CLA	C1D-ND	4.08	1.42	1.37
38	P	308	KC2	C4A-C3A	4.08	1.52	1.44
28	3	323	LHG	O7-C7	4.08	1.45	1.34
38	V	308	KC2	CMD-C2D	-4.07	1.43	1.51
28	A	846	LHG	O7-C7	4.07	1.45	1.34
25	K	206	CLA	C1D-ND	4.07	1.42	1.37
25	A	833	CLA	C3B-C2B	-4.06	1.34	1.40
34	A	844	PQN	C3-C2	4.06	1.42	1.35
31	O	2008	LMG	O8-C28	4.06	1.45	1.33
25	L	302	CLA	C3B-C2B	-4.06	1.34	1.40
31	J	104	LMG	O8-C28	4.06	1.45	1.33
25	B	827	CLA	C1D-ND	4.05	1.42	1.37
25	2	610	CLA	C1D-ND	4.05	1.42	1.37
31	5	613	LMG	O7-C10	4.05	1.45	1.34
25	L	302	CLA	C4D-ND	-4.04	1.32	1.37
25	K	201	CLA	C1D-ND	4.04	1.42	1.37
25	V	309	CLA	CHC-C1C	4.03	1.45	1.35
25	5	608	CLA	C1D-ND	4.03	1.42	1.37
25	R	313	CLA	C1D-ND	4.03	1.42	1.37
25	V	301	CLA	C4D-ND	-4.03	1.32	1.37
25	P	310	CLA	C1D-ND	4.03	1.42	1.37
31	B	801	LMG	O8-C28	4.01	1.45	1.33
25	3	309	CLA	C1D-ND	4.01	1.42	1.37
31	A	857	LMG	O7-C10	4.00	1.45	1.34
25	3	301	CLA	C1D-ND	4.00	1.42	1.37
25	B	821	CLA	C3B-C2B	-3.99	1.34	1.40
25	U	308	CLA	C4D-ND	-3.99	1.32	1.37
25	B	823	CLA	C1D-ND	3.99	1.42	1.37
28	6	616	LHG	O7-C7	3.98	1.45	1.34
28	6	616	LHG	O8-C23	3.97	1.44	1.33
24	2	601	CHL	C4D-ND	-3.97	1.32	1.37
25	6	607	CLA	CMB-C2B	-3.97	1.43	1.51
25	U	301	CLA	C4D-ND	-3.97	1.32	1.37
25	B	821	CLA	CMB-C2B	-3.96	1.43	1.51
28	Q	302	LHG	O8-C23	3.96	1.44	1.33
25	1	606	CLA	C1D-ND	3.96	1.42	1.37
31	A	801	LMG	O7-C10	3.95	1.45	1.34
31	A	801	LMG	O8-C28	3.95	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	S	302	CLA	C1D-ND	3.94	1.42	1.37
25	X	303	CLA	C1D-ND	3.94	1.42	1.37
25	A	820	CLA	C1D-ND	3.94	1.42	1.37
25	2	602	CLA	C1D-ND	3.93	1.42	1.37
31	2	620	LMG	O7-C10	3.93	1.45	1.34
24	W	304	CHL	C1D-ND	3.93	1.42	1.37
25	A	825	CLA	C1D-ND	3.93	1.42	1.37
31	J	104	LMG	O7-C10	3.93	1.45	1.34
24	V	304	CHL	C1D-ND	3.92	1.42	1.37
25	6	603	CLA	CMB-C2B	-3.92	1.43	1.51
25	L	301	CLA	C1D-ND	3.92	1.42	1.37
38	T	308	KC2	C4A-C3A	3.92	1.52	1.44
38	U	307	KC2	C4A-C3A	3.92	1.52	1.44
25	W	303	CLA	C4D-ND	-3.91	1.32	1.37
28	3	321	LHG	O8-C23	3.91	1.44	1.33
25	5	610	CLA	C1D-ND	3.90	1.42	1.37
25	W	302	CLA	C1D-ND	3.90	1.42	1.37
24	6	606	CHL	C1D-ND	3.89	1.42	1.37
28	A	847	LHG	O7-C7	3.89	1.45	1.34
25	5	609	CLA	C1D-ND	3.89	1.42	1.37
25	O	2001	CLA	C1D-ND	3.89	1.42	1.37
25	T	301	CLA	C4D-ND	-3.88	1.32	1.37
30	K	207	BCR	C8-C9	3.88	1.54	1.45
25	B	822	CLA	C4D-ND	-3.87	1.32	1.37
25	5	601	CLA	C1D-ND	3.87	1.42	1.37
24	3	306	CHL	CMB-C2B	-3.87	1.43	1.51
25	B	802	CLA	C4D-ND	-3.86	1.32	1.37
25	A	813	CLA	C1D-ND	3.86	1.42	1.37
25	K	204	CLA	C1D-ND	3.86	1.42	1.37
25	R	314	CLA	C1D-ND	3.86	1.42	1.37
24	X	306	CHL	C1D-ND	3.86	1.42	1.37
25	4	312	CLA	C1D-ND	3.86	1.42	1.37
37	S	317	NEX	C7-C8	-3.85	1.25	1.32
25	3	314	CLA	C1D-ND	3.85	1.42	1.37
24	U	313	CHL	C1D-ND	3.85	1.42	1.37
25	4	311	CLA	C1D-ND	3.84	1.42	1.37
25	J	102	CLA	C4D-ND	-3.84	1.32	1.37
25	2	611	CLA	C1D-ND	3.84	1.42	1.37
31	N	201	LMG	O8-C28	3.84	1.44	1.33
25	W	312	CLA	C4D-ND	-3.84	1.32	1.37
25	W	310	CLA	C1D-ND	3.83	1.42	1.37
25	4	315	CLA	C1D-ND	3.83	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	A	834	CLA	C1D-ND	3.83	1.42	1.37
25	T	302	CLA	C1D-ND	3.83	1.42	1.37
28	1	614	LHG	O7-C7	3.83	1.45	1.34
25	B	842	CLA	C1D-ND	3.83	1.42	1.37
25	X	304	CLA	CMB-C2B	-3.83	1.43	1.51
25	V	311	CLA	C1D-ND	3.82	1.42	1.37
25	G	202	CLA	C1D-ND	3.82	1.42	1.37
25	B	828	CLA	C1D-ND	3.82	1.42	1.37
25	B	808	CLA	C4D-ND	-3.82	1.32	1.37
24	S	314	CHL	C1D-ND	3.81	1.42	1.37
25	S	301	CLA	C4D-ND	-3.81	1.32	1.37
38	V	308	KC2	C4A-C3A	3.81	1.51	1.44
25	W	313	CLA	C1D-ND	3.81	1.42	1.37
25	2	604	CLA	C1D-ND	3.80	1.42	1.37
25	A	839	CLA	C1D-ND	3.80	1.42	1.37
25	X	314	CLA	C1D-ND	3.80	1.42	1.37
25	6	604	CLA	C1D-ND	3.80	1.42	1.37
25	6	611	CLA	C1D-ND	3.80	1.42	1.37
28	3	323	LHG	O8-C23	3.79	1.44	1.33
25	A	832	CLA	C1D-ND	3.79	1.42	1.37
24	4	307	CHL	CAB-C3B	-3.79	1.43	1.51
25	W	301	CLA	C1D-ND	3.79	1.42	1.37
25	4	313	CLA	C1D-ND	3.79	1.42	1.37
25	4	316	CLA	C1D-ND	3.78	1.42	1.37
25	1	605	CLA	C1D-ND	3.78	1.42	1.37
25	B	823	CLA	C4D-ND	-3.78	1.32	1.37
25	5	606	CLA	C1D-ND	3.77	1.42	1.37
24	P	304	CHL	CHC-C1C	3.77	1.44	1.35
25	B	832	CLA	CMB-C2B	-3.77	1.43	1.51
24	4	306	CHL	C1D-ND	3.76	1.42	1.37
31	F	805	LMG	O8-C28	3.76	1.44	1.33
28	3	322	LHG	O8-C23	3.76	1.44	1.33
25	B	824	CLA	CMB-C2B	-3.76	1.43	1.51
25	R	305	CLA	C1D-ND	3.76	1.42	1.37
37	R	321	NEX	C7-C8	-3.76	1.25	1.32
38	X	309	KC2	C4A-C3A	3.76	1.51	1.44
25	O	2004	CLA	C1D-ND	3.76	1.42	1.37
25	B	819	CLA	C4D-ND	-3.75	1.32	1.37
25	B	817	CLA	C1D-ND	3.75	1.42	1.37
25	P	302	CLA	C1D-ND	3.75	1.42	1.37
25	P	303	CLA	C1D-ND	3.75	1.42	1.37
25	6	608	CLA	C1D-ND	3.74	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	P	313	CLA	C1D-ND	3.74	1.42	1.37
25	B	826	CLA	C4D-ND	-3.74	1.32	1.37
25	B	843	CLA	C4D-ND	-3.74	1.32	1.37
24	W	314	CHL	C1D-ND	3.74	1.42	1.37
25	Q	301	CLA	C1D-ND	3.73	1.42	1.37
25	U	311	CLA	C1D-ND	3.73	1.42	1.37
25	4	305	CLA	C1D-ND	3.73	1.42	1.37
25	2	613	CLA	C1D-ND	3.73	1.42	1.37
25	A	808	CLA	C4D-ND	-3.73	1.32	1.37
24	X	315	CHL	C1D-ND	3.73	1.42	1.37
34	A	844	PQN	C2-C1	-3.72	1.40	1.48
25	A	823	CLA	C3B-C2B	-3.72	1.35	1.40
25	4	309	CLA	C4D-ND	-3.71	1.32	1.37
25	B	818	CLA	C1D-ND	3.71	1.42	1.37
25	5	604	CLA	C1D-ND	3.71	1.42	1.37
25	A	822	CLA	C4D-ND	-3.70	1.32	1.37
25	V	310	CLA	C1D-ND	3.70	1.42	1.37
26	Q	303	IWJ	C09-C10	3.70	1.53	1.45
38	Q	310	KC2	C4A-C3A	3.70	1.51	1.44
25	B	840	CLA	C4D-ND	-3.70	1.32	1.37
25	4	309	CLA	C1D-ND	3.70	1.42	1.37
24	R	311	CHL	C1D-ND	3.69	1.42	1.37
25	L	302	CLA	CMB-C2B	-3.69	1.44	1.51
25	O	2005	CLA	C1D-ND	3.69	1.42	1.37
25	A	815	CLA	C1D-ND	3.68	1.42	1.37
25	U	302	CLA	C1D-ND	3.68	1.42	1.37
25	B	841	CLA	CMB-C2B	-3.68	1.44	1.51
25	U	310	CLA	C1D-ND	3.67	1.42	1.37
25	W	309	CLA	C1D-ND	3.67	1.42	1.37
24	P	307	CHL	C1D-ND	3.67	1.42	1.37
25	U	310	CLA	C4D-ND	-3.66	1.32	1.37
25	F	803	CLA	C1D-ND	3.66	1.42	1.37
25	A	845	CLA	C1D-ND	3.65	1.42	1.37
25	1	603	CLA	C1D-ND	3.65	1.42	1.37
25	U	303	CLA	C1D-ND	3.65	1.42	1.37
25	3	304	CLA	C1D-ND	3.65	1.42	1.37
25	R	316	CLA	C1D-ND	3.64	1.42	1.37
25	X	303	CLA	C4D-ND	-3.64	1.32	1.37
24	S	304	CHL	C4D-ND	-3.64	1.32	1.37
25	A	820	CLA	C3B-CAB	-3.63	1.40	1.47
24	R	309	CHL	C1D-ND	3.63	1.42	1.37
25	A	845	CLA	C4D-ND	-3.63	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	R	302	CHL	C1D-ND	3.63	1.42	1.37
25	O	2003	CLA	C1D-ND	3.63	1.42	1.37
25	3	312	CLA	C1D-ND	3.63	1.42	1.37
25	A	821	CLA	C1D-ND	3.62	1.42	1.37
38	W	308	KC2	CMD-C2D	-3.62	1.44	1.51
25	2	609	CLA	C1D-ND	3.62	1.42	1.37
25	R	317	CLA	C1D-ND	3.62	1.42	1.37
25	3	310	CLA	C1D-ND	3.62	1.42	1.37
24	T	320	CHL	C1D-ND	3.61	1.42	1.37
24	X	307	CHL	C1D-ND	3.61	1.42	1.37
25	5	606	CLA	CAB-C3B	-3.61	1.44	1.51
25	B	811	CLA	C4D-ND	-3.61	1.32	1.37
24	X	306	CHL	C4D-ND	-3.61	1.32	1.37
25	Q	311	CLA	C1D-ND	3.61	1.42	1.37
24	4	308	CHL	C1D-ND	3.60	1.42	1.37
25	X	311	CLA	C1D-ND	3.60	1.42	1.37
24	V	307	CHL	C1D-ND	3.60	1.42	1.37
25	A	810	CLA	C1D-ND	3.60	1.42	1.37
25	K	203	CLA	C1D-ND	3.60	1.42	1.37
25	1	607	CLA	C4D-CHA	3.60	1.44	1.39
25	3	311	CLA	C1D-ND	3.59	1.42	1.37
25	T	309	CLA	C1D-ND	3.59	1.42	1.37
24	R	318	CHL	C1D-ND	3.59	1.42	1.37
25	2	603	CLA	C1D-ND	3.59	1.42	1.37
25	P	311	CLA	C1D-ND	3.59	1.42	1.37
25	1	607	CLA	C1D-ND	3.59	1.42	1.37
25	B	837	CLA	CMB-C2B	-3.59	1.44	1.51
25	A	826	CLA	C1D-ND	3.58	1.42	1.37
25	V	301	CLA	C1D-ND	3.58	1.42	1.37
25	A	840	CLA	C1D-ND	3.58	1.42	1.37
25	3	305	CLA	CAB-C3B	-3.58	1.44	1.51
25	B	837	CLA	C1D-ND	3.58	1.42	1.37
24	R	311	CHL	CMD-C2D	-3.58	1.43	1.50
24	2	607	CHL	C4D-ND	-3.58	1.32	1.37
24	Q	307	CHL	C1D-ND	3.57	1.42	1.37
25	2	612	CLA	C1D-ND	3.57	1.42	1.37
24	T	304	CHL	C1D-ND	3.57	1.42	1.37
25	V	313	CLA	C1D-ND	3.57	1.42	1.37
25	T	313	CLA	C4D-ND	-3.57	1.32	1.37
25	3	313	CLA	C1D-ND	3.57	1.42	1.37
25	B	839	CLA	C4D-ND	-3.57	1.32	1.37
25	Q	305	CLA	C1D-ND	3.57	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	P	301	CLA	C1D-ND	3.57	1.42	1.37
25	T	310	CLA	C1D-ND	3.57	1.42	1.37
28	2	619	LHG	O8-C23	3.57	1.43	1.33
25	A	814	CLA	CMB-C2B	-3.57	1.44	1.51
25	X	312	CLA	C1D-ND	3.56	1.42	1.37
25	Q	306	CLA	C1D-ND	3.56	1.42	1.37
25	Q	315	CLA	C1D-ND	3.56	1.42	1.37
25	R	315	CLA	C1D-ND	3.56	1.42	1.37
25	A	806	CLA	C1D-ND	3.56	1.42	1.37
25	A	838	CLA	C1D-ND	3.56	1.42	1.37
24	2	605	CHL	C3B-C2B	-3.55	1.35	1.40
25	P	312	CLA	C4D-ND	-3.55	1.32	1.37
24	R	309	CHL	C4D-ND	-3.55	1.32	1.37
25	P	312	CLA	C1D-ND	3.55	1.42	1.37
25	Q	312	CLA	C1D-ND	3.55	1.42	1.37
25	N	202	CLA	C4D-ND	-3.55	1.32	1.37
25	W	301	CLA	C4D-ND	-3.55	1.32	1.37
25	N	202	CLA	C1D-ND	3.55	1.42	1.37
25	1	606	CLA	CAB-C3B	-3.54	1.44	1.51
25	U	309	CLA	C1D-ND	3.54	1.42	1.37
25	Q	304	CLA	C1D-ND	3.54	1.42	1.37
25	4	304	CLA	CAB-C3B	-3.54	1.44	1.51
25	3	303	CLA	CAB-C3B	-3.54	1.44	1.51
24	W	304	CHL	CHC-C1C	3.54	1.44	1.35
24	U	305	CHL	C1D-ND	3.54	1.42	1.37
25	A	825	CLA	C4D-ND	-3.54	1.32	1.37
30	M	101	BCR	C10-C9	3.53	1.40	1.35
25	L	303	CLA	C1D-ND	3.53	1.42	1.37
24	T	314	CHL	C1D-ND	3.53	1.42	1.37
25	A	835	CLA	C1D-ND	3.53	1.42	1.37
25	A	805	CLA	C1D-ND	3.53	1.42	1.37
25	A	829	CLA	C1D-ND	3.53	1.42	1.37
25	B	830	CLA	C4D-ND	-3.53	1.32	1.37
25	F	803	CLA	C4D-ND	-3.52	1.32	1.37
25	U	312	CLA	C1D-ND	3.51	1.42	1.37
25	4	310	CLA	C1D-ND	3.51	1.42	1.37
25	A	818	CLA	C1D-ND	3.51	1.42	1.37
25	2	608	CLA	C1D-ND	3.51	1.42	1.37
24	U	304	CHL	C1D-ND	3.51	1.42	1.37
24	U	306	CHL	C1D-ND	3.51	1.42	1.37
24	2	605	CHL	CMB-C2B	-3.51	1.44	1.51
25	A	817	CLA	C1D-ND	3.51	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	A	820	CLA	C3B-C2B	-3.50	1.35	1.40
25	A	806	CLA	CHC-C1C	3.50	1.43	1.35
24	T	304	CHL	CHC-C1C	3.50	1.43	1.35
25	S	313	CLA	C1D-ND	3.50	1.42	1.37
25	B	838	CLA	C1D-ND	3.49	1.42	1.37
25	1	610	CLA	CAB-C3B	-3.49	1.44	1.51
25	R	306	CLA	C4D-ND	-3.49	1.32	1.37
25	B	803	CLA	C4D-ND	-3.49	1.32	1.37
37	T	317	NEX	C7-C8	-3.49	1.26	1.32
25	A	812	CLA	C1D-ND	3.49	1.42	1.37
25	A	838	CLA	C4D-ND	-3.49	1.32	1.37
25	L	304	CLA	C1D-ND	3.49	1.42	1.37
25	A	827	CLA	C1D-ND	3.48	1.42	1.37
25	6	603	CLA	C1D-ND	3.48	1.42	1.37
25	H	302	CLA	C1D-ND	3.48	1.42	1.37
25	H	301	CLA	C1D-ND	3.48	1.42	1.37
24	5	605	CHL	C1D-ND	3.48	1.42	1.37
25	1	609	CLA	CAB-C3B	-3.48	1.44	1.51
25	T	311	CLA	C1D-ND	3.48	1.42	1.37
25	4	304	CLA	C4D-ND	-3.48	1.32	1.37
25	A	830	CLA	C1D-ND	3.47	1.42	1.37
25	A	819	CLA	C1D-ND	3.47	1.42	1.37
30	A	850	BCR	C30-C25	-3.47	1.49	1.53
24	4	302	CHL	C1D-ND	3.46	1.42	1.37
26	5	611	IWJ	C09-C10	3.46	1.53	1.45
25	3	305	CLA	C4D-ND	-3.46	1.32	1.37
25	Q	313	CLA	C1D-ND	3.46	1.42	1.37
25	A	809	CLA	C4D-ND	-3.46	1.32	1.37
24	6	601	CHL	C1D-ND	3.46	1.42	1.37
25	1	608	CLA	CMB-C2B	-3.46	1.44	1.51
25	A	833	CLA	C1D-ND	3.45	1.42	1.37
25	3	307	CLA	C1D-ND	3.45	1.42	1.37
25	A	837	CLA	CMB-C2B	-3.45	1.44	1.51
25	S	312	CLA	C1D-ND	3.45	1.42	1.37
24	Q	309	CHL	C1D-ND	3.45	1.42	1.37
24	V	305	CHL	C1D-ND	3.45	1.42	1.37
24	V	314	CHL	C4D-ND	-3.45	1.33	1.37
25	4	305	CLA	CAB-C3B	-3.45	1.44	1.51
25	X	313	CLA	C1D-ND	3.44	1.42	1.37
26	4	301	IWJ	C09-C10	3.44	1.53	1.45
25	B	820	CLA	C1D-ND	3.44	1.42	1.37
25	A	811	CLA	C4D-ND	-3.44	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	W	311	CLA	C1D-ND	3.44	1.42	1.37
26	T	321	IWJ	C09-C10	3.44	1.53	1.45
25	A	807	CLA	C1D-ND	3.44	1.42	1.37
25	A	808	CLA	C1D-ND	3.44	1.42	1.37
24	2	607	CHL	C1D-ND	3.43	1.42	1.37
24	P	304	CHL	C1D-ND	3.43	1.42	1.37
24	V	314	CHL	C1D-ND	3.43	1.42	1.37
25	3	302	CLA	C4D-ND	-3.43	1.33	1.37
25	V	302	CLA	C1D-ND	3.43	1.42	1.37
25	A	811	CLA	C1D-ND	3.43	1.42	1.37
30	M	101	BCR	C12-C13	3.43	1.53	1.45
24	P	305	CHL	C4D-ND	-3.43	1.33	1.37
26	1	611	IWJ	C09-C10	3.43	1.53	1.45
26	6	614	IWJ	C09-C10	3.43	1.53	1.45
25	A	841	CLA	C1D-ND	3.42	1.42	1.37
30	B	845	BCR	C12-C13	3.42	1.53	1.45
25	4	314	CLA	C1D-ND	3.42	1.42	1.37
25	5	602	CLA	C1D-ND	3.42	1.42	1.37
25	B	807	CLA	C1D-ND	3.41	1.42	1.37
25	4	304	CLA	C1D-ND	3.41	1.42	1.37
25	A	810	CLA	C4D-ND	-3.41	1.33	1.37
24	1	604	CHL	C1D-ND	3.41	1.42	1.37
24	1	601	CHL	C1D-ND	3.41	1.42	1.37
25	X	304	CLA	C3B-C2B	-3.40	1.35	1.40
25	B	837	CLA	C4D-ND	-3.40	1.33	1.37
25	S	301	CLA	CMC-C2C	-3.40	1.43	1.50
25	R	307	CLA	C1D-ND	3.40	1.42	1.37
25	O	2002	CLA	CMB-C2B	-3.40	1.44	1.51
24	P	304	CHL	C4D-ND	-3.40	1.33	1.37
25	W	313	CLA	C4D-ND	-3.40	1.33	1.37
25	B	819	CLA	CMB-C2B	-3.40	1.44	1.51
25	6	610	CLA	C1D-ND	3.40	1.42	1.37
25	B	806	CLA	C3B-CAB	-3.39	1.41	1.47
25	A	829	CLA	C4D-ND	-3.39	1.33	1.37
25	6	607	CLA	C4D-ND	-3.39	1.33	1.37
26	R	303	IWJ	C09-C10	3.39	1.53	1.45
25	A	815	CLA	C4D-ND	-3.39	1.33	1.37
25	B	826	CLA	CMB-C2B	-3.39	1.44	1.51
24	W	307	CHL	C1D-ND	3.39	1.41	1.37
25	N	203	CLA	CMB-C2B	-3.38	1.44	1.51
25	1	608	CLA	C1D-ND	3.38	1.41	1.37
25	2	614	CLA	C4D-ND	-3.38	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	A	824	CLA	C1D-ND	3.38	1.41	1.37
25	T	312	CLA	C1D-ND	3.38	1.41	1.37
25	B	838	CLA	C4D-ND	-3.38	1.33	1.37
24	2	601	CHL	C1D-ND	3.38	1.41	1.37
25	B	842	CLA	CMB-C2B	-3.38	1.44	1.51
26	T	318	IWJ	C09-C10	3.38	1.53	1.45
26	V	317	IWJ	C09-C10	3.38	1.53	1.45
25	B	810	CLA	C1D-ND	3.38	1.41	1.37
25	A	821	CLA	CMB-C2B	-3.38	1.44	1.51
25	Q	304	CLA	C4D-ND	-3.38	1.33	1.37
24	V	306	CHL	CHC-C1C	3.38	1.43	1.35
26	R	322	IWJ	C09-C10	3.38	1.53	1.45
25	A	823	CLA	C4D-ND	-3.38	1.33	1.37
25	H	304	CLA	C4D-ND	-3.38	1.33	1.37
25	2	603	CLA	CMB-C2B	-3.37	1.44	1.51
25	S	310	CLA	C1D-ND	3.37	1.41	1.37
25	A	824	CLA	C4D-ND	-3.37	1.33	1.37
25	X	304	CLA	C1D-ND	3.37	1.41	1.37
25	B	840	CLA	C1D-ND	3.37	1.41	1.37
24	S	307	CHL	CHC-C1C	3.37	1.43	1.35
25	S	303	CLA	C1D-ND	3.37	1.41	1.37
24	T	307	CHL	C4D-ND	-3.37	1.33	1.37
25	S	311	CLA	C1D-ND	3.37	1.41	1.37
24	W	306	CHL	C4D-ND	-3.37	1.33	1.37
26	S	322	IWJ	C09-C10	3.37	1.53	1.45
25	4	303	CLA	C4D-ND	-3.36	1.33	1.37
24	S	305	CHL	C1D-ND	3.36	1.41	1.37
25	A	804	CLA	C1D-ND	3.36	1.41	1.37
25	B	829	CLA	CMD-C2D	-3.36	1.43	1.50
26	S	319	IWJ	C09-C10	3.36	1.53	1.45
25	P	309	CLA	C1D-ND	3.36	1.41	1.37
25	3	303	CLA	C4D-ND	-3.36	1.33	1.37
26	V	320	IWJ	C09-C10	3.35	1.53	1.45
29	V	315	Q6L	C12-C13	-3.35	1.44	1.51
25	B	825	CLA	C4D-ND	-3.35	1.33	1.37
25	6	613	CLA	C1D-ND	3.35	1.41	1.37
25	A	824	CLA	CMB-C2B	-3.35	1.44	1.51
25	2	609	CLA	C4D-ND	-3.35	1.33	1.37
25	R	317	CLA	CHC-C1C	3.35	1.43	1.35
25	R	305	CLA	C4D-ND	-3.35	1.33	1.37
24	V	306	CHL	C1D-ND	3.35	1.41	1.37
25	A	820	CLA	C4D-ND	-3.35	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	1	602	CLA	C1D-ND	3.35	1.41	1.37
25	3	314	CLA	CHC-C1C	3.34	1.43	1.35
24	2	615	CHL	C1D-ND	3.34	1.41	1.37
25	A	809	CLA	C1D-ND	3.34	1.41	1.37
25	A	839	CLA	C4D-ND	-3.34	1.33	1.37
24	S	306	CHL	C4C-C3C	3.34	1.50	1.45
25	P	301	CLA	C4D-ND	-3.34	1.33	1.37
29	S	320	Q6L	C34-C33	3.34	1.54	1.50
25	4	311	CLA	C4D-ND	-3.34	1.33	1.37
25	1	605	CLA	C4D-ND	-3.34	1.33	1.37
25	A	828	CLA	C1D-ND	3.34	1.41	1.37
25	B	819	CLA	C1D-ND	3.34	1.41	1.37
24	R	310	CHL	C1D-ND	3.34	1.41	1.37
25	3	307	CLA	CMB-C2B	-3.34	1.44	1.51
24	X	308	CHL	C1D-ND	3.34	1.41	1.37
24	4	307	CHL	C1D-ND	3.34	1.41	1.37
37	H	306	NEX	C7-C8	-3.33	1.26	1.32
26	V	318	IWJ	C09-C10	3.33	1.53	1.45
25	V	303	CLA	CHC-C1C	3.33	1.43	1.35
25	B	814	CLA	C1D-ND	3.33	1.41	1.37
25	A	826	CLA	C4D-ND	-3.33	1.33	1.37
25	3	303	CLA	C1D-ND	3.33	1.41	1.37
25	A	835	CLA	C4D-ND	-3.33	1.33	1.37
25	3	301	CLA	C4D-ND	-3.33	1.33	1.37
25	R	306	CLA	C1D-ND	3.33	1.41	1.37
25	3	304	CLA	CMB-C2B	-3.32	1.44	1.51
26	U	316	IWJ	C09-C10	3.32	1.53	1.45
25	A	830	CLA	C4D-ND	-3.32	1.33	1.37
25	L	304	CLA	C4D-ND	-3.32	1.33	1.37
24	U	304	CHL	C4D-ND	-3.31	1.33	1.37
25	4	305	CLA	C4D-ND	-3.31	1.33	1.37
25	1	610	CLA	C1D-ND	3.31	1.41	1.37
25	A	820	CLA	CHC-C1C	3.31	1.43	1.35
25	A	822	CLA	C1D-ND	3.31	1.41	1.37
30	L	307	BCR	C8-C9	3.31	1.53	1.45
25	A	838	CLA	CMB-C2B	-3.31	1.44	1.51
25	6	612	CLA	C1D-ND	3.31	1.41	1.37
24	V	307	CHL	C4D-ND	-3.30	1.33	1.37
25	B	839	CLA	CHC-C1C	3.30	1.43	1.35
25	V	309	CLA	C1D-ND	3.30	1.41	1.37
25	B	832	CLA	C3B-CAB	-3.30	1.41	1.47
26	S	318	IWJ	C09-C10	3.30	1.53	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	1	608	CLA	C3B-C2B	-3.30	1.35	1.40
25	2	614	CLA	C1D-ND	3.30	1.41	1.37
24	T	306	CHL	C4D-ND	-3.30	1.33	1.37
26	W	318	IWJ	C09-C10	3.30	1.53	1.45
25	A	817	CLA	C4D-ND	-3.30	1.33	1.37
25	B	831	CLA	C1D-ND	3.30	1.41	1.37
25	X	310	CLA	C1D-ND	3.30	1.41	1.37
25	5	609	CLA	CHC-C1C	3.29	1.43	1.35
25	L	301	CLA	C4D-ND	-3.29	1.33	1.37
25	V	302	CLA	C4D-ND	-3.29	1.33	1.37
33	A	802	CL0	CMD-C2D	-3.29	1.43	1.50
25	3	313	CLA	CMB-C2B	-3.29	1.44	1.51
25	A	814	CLA	C1D-ND	3.29	1.41	1.37
25	S	310	CLA	C4D-ND	-3.29	1.33	1.37
24	R	302	CHL	C4D-ND	-3.29	1.33	1.37
25	A	818	CLA	C4D-ND	-3.29	1.33	1.37
25	K	204	CLA	C4D-ND	-3.29	1.33	1.37
25	A	833	CLA	C3B-CAB	-3.28	1.41	1.47
25	O	2002	CLA	C1D-ND	3.28	1.41	1.37
25	B	830	CLA	C3B-CAB	-3.28	1.41	1.47
25	3	308	CLA	C1D-ND	3.28	1.41	1.37
25	B	832	CLA	C1D-ND	3.28	1.41	1.37
24	T	307	CHL	C1D-ND	3.28	1.41	1.37
25	B	806	CLA	C4D-ND	-3.28	1.33	1.37
25	B	828	CLA	C4D-ND	-3.28	1.33	1.37
24	3	306	CHL	C4D-ND	-3.28	1.33	1.37
25	A	807	CLA	C4D-ND	-3.27	1.33	1.37
25	A	812	CLA	C4D-ND	-3.27	1.33	1.37
25	U	301	CLA	CHC-C1C	3.27	1.43	1.35
24	T	305	CHL	CHC-C1C	3.27	1.43	1.35
25	B	816	CLA	CHC-C1C	3.27	1.43	1.35
25	A	836	CLA	C1D-ND	3.27	1.41	1.37
24	R	311	CHL	CHC-C1C	3.27	1.43	1.35
25	A	828	CLA	C4D-ND	-3.27	1.33	1.37
25	B	811	CLA	CMB-C2B	-3.26	1.44	1.51
25	T	301	CLA	C1D-ND	3.26	1.41	1.37
25	3	302	CLA	CMD-C2D	-3.26	1.43	1.50
25	B	818	CLA	CHC-C1C	3.26	1.43	1.35
24	R	308	CHL	C4D-ND	-3.25	1.33	1.37
25	T	313	CLA	C1D-ND	3.25	1.41	1.37
25	B	824	CLA	C4D-ND	-3.25	1.33	1.37
24	T	306	CHL	C1D-ND	3.25	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	A	804	CLA	C4D-ND	-3.25	1.33	1.37
25	A	816	CLA	C4D-ND	-3.25	1.33	1.37
24	X	305	CHL	CHC-C1C	3.25	1.43	1.35
25	6	612	CLA	C4D-ND	-3.25	1.33	1.37
25	B	805	CLA	C1D-ND	3.24	1.41	1.37
24	P	306	CHL	C1D-ND	3.24	1.41	1.37
24	Q	316	CHL	C4D-ND	-3.24	1.33	1.37
25	4	314	CLA	C4D-ND	-3.24	1.33	1.37
25	A	833	CLA	C4D-ND	-3.24	1.33	1.37
25	2	606	CLA	C1D-ND	3.24	1.41	1.37
26	P	320	IWJ	C09-C10	3.23	1.52	1.45
24	4	307	CHL	CHC-C1C	3.23	1.43	1.35
25	U	309	CLA	C4D-ND	-3.23	1.33	1.37
26	3	315	IWJ	C09-C10	3.23	1.52	1.45
33	A	802	CL0	C4D-ND	-3.23	1.33	1.37
25	B	816	CLA	C1D-ND	3.23	1.41	1.37
24	U	304	CHL	CHC-C1C	3.22	1.43	1.35
24	S	305	CHL	CHC-C1C	3.22	1.43	1.35
25	6	603	CLA	C4D-ND	-3.22	1.33	1.37
25	A	831	CLA	C4D-ND	-3.22	1.33	1.37
25	B	841	CLA	C1D-ND	3.22	1.41	1.37
25	A	834	CLA	C4D-ND	-3.22	1.33	1.37
25	A	831	CLA	CMB-C2B	-3.22	1.44	1.51
33	A	802	CL0	CMB-C2B	-3.22	1.44	1.51
25	A	813	CLA	C4D-ND	-3.22	1.33	1.37
25	V	312	CLA	C4D-ND	-3.22	1.33	1.37
25	A	830	CLA	CMB-C2B	-3.21	1.45	1.51
26	Q	320	IWJ	C09-C10	3.21	1.52	1.45
25	Q	314	CLA	C1D-ND	3.21	1.41	1.37
25	B	817	CLA	CMB-C2B	-3.21	1.45	1.51
25	A	837	CLA	C1D-ND	3.21	1.41	1.37
24	V	304	CHL	CHC-C1C	3.21	1.43	1.35
25	B	812	CLA	C1D-ND	3.21	1.41	1.37
25	A	856	CLA	C1D-ND	3.20	1.41	1.37
25	P	311	CLA	C4D-ND	-3.20	1.33	1.37
26	4	317	IWJ	C09-C10	3.20	1.52	1.45
25	B	836	CLA	C4D-ND	-3.20	1.33	1.37
25	Q	314	CLA	C4D-ND	-3.20	1.33	1.37
25	1	603	CLA	C4D-ND	-3.20	1.33	1.37
25	B	812	CLA	C4D-ND	-3.19	1.33	1.37
24	X	315	CHL	C4D-ND	-3.19	1.33	1.37
38	V	308	KC2	MG-NA	3.19	2.13	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	P	318	IWJ	C09-C10	3.19	1.52	1.45
25	F	802	CLA	CMB-C2B	-3.19	1.45	1.51
25	4	311	CLA	C3B-C2B	-3.19	1.35	1.40
25	P	301	CLA	CHC-C1C	3.19	1.43	1.35
24	S	305	CHL	C4D-ND	-3.19	1.33	1.37
25	P	303	CLA	CHC-C1C	3.19	1.43	1.35
25	B	804	CLA	C4D-ND	-3.19	1.33	1.37
25	G	203	CLA	C4D-ND	-3.19	1.33	1.37
25	S	313	CLA	CHC-C1C	3.19	1.43	1.35
25	B	806	CLA	C1D-ND	3.19	1.41	1.37
25	R	315	CLA	CHC-C1C	3.19	1.43	1.35
24	6	605	CHL	C1D-ND	3.19	1.41	1.37
25	B	843	CLA	CHC-C1C	3.19	1.43	1.35
25	B	826	CLA	C1D-ND	3.18	1.41	1.37
25	U	303	CLA	C3B-C2B	-3.18	1.36	1.40
24	2	601	CHL	CHC-C1C	3.18	1.43	1.35
25	T	301	CLA	CHC-C1C	3.18	1.43	1.35
25	B	821	CLA	C1D-ND	3.18	1.41	1.37
24	X	308	CHL	CHC-C1C	3.18	1.43	1.35
24	X	305	CHL	C4D-ND	-3.18	1.33	1.37
25	B	836	CLA	C3B-C2B	-3.18	1.36	1.40
25	3	305	CLA	C1D-ND	3.18	1.41	1.37
25	4	303	CLA	C1D-ND	3.18	1.41	1.37
25	B	841	CLA	C4D-ND	-3.17	1.33	1.37
24	R	308	CHL	C1D-ND	3.17	1.41	1.37
24	2	605	CHL	C1D-ND	3.17	1.41	1.37
25	1	610	CLA	C4D-ND	-3.17	1.33	1.37
24	6	605	CHL	CMD-C2D	-3.17	1.44	1.50
25	2	612	CLA	C4D-ND	-3.17	1.33	1.37
25	K	201	CLA	C4D-ND	-3.16	1.33	1.37
25	B	833	CLA	C4D-ND	-3.16	1.33	1.37
25	A	817	CLA	CHC-C1C	3.16	1.43	1.35
24	W	304	CHL	C4D-ND	-3.16	1.33	1.37
24	W	307	CHL	CHC-C1C	3.16	1.43	1.35
25	B	809	CLA	C1D-ND	3.16	1.41	1.37
25	U	302	CLA	C4D-ND	-3.16	1.33	1.37
25	5	602	CLA	C4D-ND	-3.16	1.33	1.37
25	5	608	CLA	CHC-C1C	3.16	1.43	1.35
24	U	306	CHL	C4D-ND	-3.16	1.33	1.37
25	2	604	CLA	C4D-ND	-3.16	1.33	1.37
25	T	303	CLA	C4D-ND	-3.16	1.33	1.37
25	5	607	CLA	CMB-C2B	-3.15	1.45	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B	839	CLA	C3B-C2B	-3.15	1.36	1.40
25	1	606	CLA	C4D-ND	-3.15	1.33	1.37
25	5	607	CLA	C1D-ND	3.15	1.41	1.37
25	5	607	CLA	C4D-ND	-3.15	1.33	1.37
25	O	2002	CLA	C4D-ND	-3.15	1.33	1.37
25	F	802	CLA	C1D-ND	3.14	1.41	1.37
25	O	2003	CLA	C4D-ND	-3.14	1.33	1.37
25	3	307	CLA	C4D-ND	-3.14	1.33	1.37
25	S	301	CLA	CHC-C1C	3.14	1.43	1.35
25	T	311	CLA	C4D-ND	-3.14	1.33	1.37
25	5	610	CLA	CHC-C1C	3.14	1.43	1.35
25	B	830	CLA	CMD-C2D	-3.14	1.44	1.50
25	P	312	CLA	CHC-C1C	3.14	1.43	1.35
24	W	305	CHL	C4D-ND	-3.14	1.33	1.37
25	P	313	CLA	C4D-ND	-3.14	1.33	1.37
25	B	820	CLA	CMB-C2B	-3.14	1.45	1.51
25	U	301	CLA	C1D-ND	3.14	1.41	1.37
33	A	802	CL0	C1D-ND	3.14	1.41	1.37
25	6	602	CLA	C4D-ND	-3.13	1.33	1.37
25	3	302	CLA	C1D-ND	3.13	1.41	1.37
25	B	815	CLA	C4D-ND	-3.13	1.33	1.37
25	B	813	CLA	C1D-ND	3.13	1.41	1.37
25	4	305	CLA	CMB-C2B	-3.13	1.45	1.51
25	B	817	CLA	C4D-ND	-3.13	1.33	1.37
25	X	314	CLA	C4D-ND	-3.13	1.33	1.37
25	6	612	CLA	CMB-C2B	-3.13	1.45	1.51
25	U	303	CLA	CMB-C2B	-3.13	1.45	1.51
25	1	609	CLA	C4D-ND	-3.13	1.33	1.37
25	V	303	CLA	C4D-ND	-3.13	1.33	1.37
25	B	805	CLA	C3B-C2B	-3.13	1.36	1.40
25	2	603	CLA	C4D-ND	-3.13	1.33	1.37
25	2	613	CLA	CHC-C1C	3.12	1.43	1.35
25	B	829	CLA	C1D-ND	3.12	1.41	1.37
38	V	308	KC2	C4D-ND	-3.12	1.32	1.35
25	A	843	CLA	CMD-C2D	-3.12	1.44	1.50
25	A	842	CLA	C3B-C2B	-3.12	1.36	1.40
25	X	310	CLA	CHC-C1C	3.12	1.43	1.35
25	B	836	CLA	C1D-ND	3.12	1.41	1.37
25	X	311	CLA	C4D-ND	-3.12	1.33	1.37
24	T	305	CHL	C1D-ND	3.12	1.41	1.37
25	R	317	CLA	C4D-ND	-3.11	1.33	1.37
38	U	307	KC2	C4D-ND	-3.11	1.32	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	6	601	CHL	C4D-ND	-3.11	1.33	1.37
25	4	304	CLA	CHC-C1C	3.11	1.42	1.35
25	R	307	CLA	CHC-C1C	3.11	1.42	1.35
25	N	203	CLA	C1D-ND	3.11	1.41	1.37
38	P	308	KC2	C4B-NB	3.11	1.41	1.37
25	2	606	CLA	C4D-ND	-3.11	1.33	1.37
25	A	827	CLA	CMB-C2B	-3.11	1.45	1.51
24	5	605	CHL	C4D-ND	-3.11	1.33	1.37
24	V	306	CHL	C4D-ND	-3.11	1.33	1.37
25	B	834	CLA	C4D-ND	-3.10	1.33	1.37
25	S	311	CLA	C4D-ND	-3.10	1.33	1.37
24	1	601	CHL	CHC-C1C	3.10	1.42	1.35
25	S	309	CLA	CHC-C1C	3.10	1.42	1.35
24	R	318	CHL	CHC-C1C	3.10	1.42	1.35
24	W	305	CHL	C1D-ND	3.10	1.41	1.37
24	W	314	CHL	C4D-ND	-3.10	1.33	1.37
25	4	316	CLA	C4D-ND	-3.10	1.33	1.37
30	A	848	BCR	C12-C13	3.10	1.52	1.45
25	1	607	CLA	C4D-ND	-3.10	1.34	1.37
25	W	309	CLA	CHC-C1C	3.10	1.42	1.35
25	4	313	CLA	C4D-ND	-3.09	1.33	1.37
25	P	310	CLA	CHC-C1C	3.09	1.42	1.35
25	B	816	CLA	C4D-ND	-3.09	1.33	1.37
25	K	206	CLA	C4D-ND	-3.09	1.33	1.37
25	A	831	CLA	C1D-ND	3.09	1.41	1.37
25	A	828	CLA	C3B-C2B	-3.09	1.36	1.40
25	B	829	CLA	CMB-C2B	-3.09	1.45	1.51
25	B	839	CLA	C1D-ND	3.09	1.41	1.37
25	T	309	CLA	CHC-C1C	3.09	1.42	1.35
25	X	302	CLA	C3B-CAB	-3.08	1.41	1.47
25	3	305	CLA	CMB-C2B	-3.08	1.45	1.51
25	S	302	CLA	C4D-ND	-3.08	1.33	1.37
25	W	302	CLA	C4D-ND	-3.08	1.33	1.37
25	3	313	CLA	C4D-ND	-3.08	1.33	1.37
25	5	608	CLA	CMC-C2C	-3.08	1.44	1.50
25	B	821	CLA	C4D-ND	-3.08	1.33	1.37
25	U	301	CLA	CMD-C2D	-3.08	1.44	1.50
25	2	613	CLA	C4D-ND	-3.08	1.33	1.37
24	T	307	CHL	CHC-C1C	3.08	1.42	1.35
25	P	302	CLA	CHC-C1C	3.08	1.42	1.35
24	Q	309	CHL	C4D-ND	-3.08	1.33	1.37
25	5	604	CLA	CHC-C1C	3.08	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	T	302	CLA	C4D-ND	-3.08	1.33	1.37
25	B	803	CLA	CMB-C2B	-3.08	1.45	1.51
25	3	308	CLA	C3B-C2B	-3.08	1.36	1.40
25	3	309	CLA	C4D-ND	-3.07	1.33	1.37
24	P	307	CHL	C4D-ND	-3.07	1.33	1.37
24	P	305	CHL	C1D-ND	3.07	1.41	1.37
25	S	309	CLA	CMD-C2D	-3.07	1.44	1.50
25	V	310	CLA	C4D-ND	-3.07	1.33	1.37
25	O	2004	CLA	C4D-ND	-3.07	1.33	1.37
24	Q	308	CHL	CHC-C1C	3.07	1.42	1.35
25	U	311	CLA	CHC-C1C	3.07	1.42	1.35
25	X	312	CLA	C4D-ND	-3.07	1.33	1.37
25	B	824	CLA	C1D-ND	3.07	1.41	1.37
24	X	315	CHL	CHC-C1C	3.07	1.42	1.35
25	O	2003	CLA	CHC-C1C	3.07	1.42	1.35
25	L	301	CLA	CHC-C1C	3.07	1.42	1.35
25	B	810	CLA	C4D-ND	-3.07	1.33	1.37
25	W	311	CLA	C4D-ND	-3.07	1.33	1.37
24	2	607	CHL	CHC-C1C	3.06	1.42	1.35
25	F	802	CLA	C4D-ND	-3.06	1.33	1.37
24	3	306	CHL	C1D-ND	3.06	1.41	1.37
30	H	305	BCR	C8-C9	3.06	1.52	1.45
24	2	605	CHL	CHC-C1C	3.06	1.42	1.35
24	U	306	CHL	CHC-C1C	3.06	1.42	1.35
25	A	840	CLA	C4D-ND	-3.06	1.33	1.37
25	Q	313	CLA	C4D-ND	-3.06	1.33	1.37
25	Q	312	CLA	CHC-C1C	3.06	1.42	1.35
25	X	303	CLA	C3B-C2B	-3.06	1.36	1.40
26	1	611	IWJ	C04-C03	3.06	1.54	1.50
26	S	322	IWJ	C04-C03	3.05	1.54	1.50
25	X	302	CLA	C1D-ND	3.05	1.41	1.37
25	Q	315	CLA	C4D-ND	-3.05	1.33	1.37
25	O	2001	CLA	C4D-ND	-3.05	1.33	1.37
25	N	203	CLA	C3B-C2B	-3.05	1.36	1.40
25	A	814	CLA	C4D-ND	-3.05	1.33	1.37
25	K	203	CLA	C4D-ND	-3.05	1.33	1.37
25	5	601	CLA	C3B-C2B	-3.05	1.36	1.40
26	X	318	IWJ	C09-C10	3.05	1.52	1.45
25	3	312	CLA	CHC-C1C	3.05	1.42	1.35
25	A	816	CLA	CHC-C1C	3.05	1.42	1.35
25	5	604	CLA	C4D-ND	-3.05	1.33	1.37
25	W	301	CLA	CHC-C1C	3.05	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	S	312	CLA	C4D-ND	-3.04	1.33	1.37
25	T	312	CLA	C4D-ND	-3.04	1.33	1.37
25	6	602	CLA	C1D-ND	3.04	1.41	1.37
25	1	602	CLA	C4D-ND	-3.04	1.33	1.37
25	V	312	CLA	C1D-ND	3.04	1.41	1.37
25	4	303	CLA	CMB-C2B	-3.04	1.45	1.51
38	R	312	KC2	C4D-ND	-3.04	1.32	1.35
25	H	301	CLA	C3B-CAB	-3.04	1.41	1.47
25	T	313	CLA	CHC-C1C	3.04	1.42	1.35
25	S	312	CLA	CHC-C1C	3.04	1.42	1.35
25	P	309	CLA	CHC-C1C	3.04	1.42	1.35
25	A	828	CLA	CMB-C2B	-3.04	1.45	1.51
25	B	811	CLA	C1D-ND	3.04	1.41	1.37
25	B	807	CLA	C4D-ND	-3.04	1.33	1.37
25	V	303	CLA	C3B-C2B	-3.04	1.36	1.40
25	3	302	CLA	CHC-C1C	3.04	1.42	1.35
25	A	827	CLA	CMD-C2D	-3.04	1.44	1.50
24	U	305	CHL	CHC-C1C	3.04	1.42	1.35
25	3	303	CLA	CMC-C2C	-3.04	1.44	1.50
25	3	314	CLA	C4D-ND	-3.04	1.33	1.37
25	A	841	CLA	C4D-ND	-3.04	1.33	1.37
25	R	314	CLA	C4D-ND	-3.03	1.33	1.37
25	6	604	CLA	CHC-C1C	3.03	1.42	1.35
25	V	313	CLA	CHC-C1C	3.03	1.42	1.35
24	6	605	CHL	C4D-ND	-3.03	1.33	1.37
25	B	828	CLA	CHC-C1C	3.03	1.42	1.35
25	A	836	CLA	C3B-C2B	-3.03	1.36	1.40
25	6	613	CLA	C4D-ND	-3.03	1.33	1.37
24	P	307	CHL	CHC-C1C	3.03	1.42	1.35
25	H	301	CLA	C4D-ND	-3.03	1.33	1.37
24	T	305	CHL	CMD-C2D	-3.03	1.44	1.50
25	1	613	CLA	CHC-C1C	3.03	1.42	1.35
24	4	308	CHL	CHC-C1C	3.03	1.42	1.35
25	S	303	CLA	CHC-C1C	3.03	1.42	1.35
25	4	315	CLA	C4D-ND	-3.03	1.33	1.37
25	K	206	CLA	CHC-C1C	3.03	1.42	1.35
24	6	606	CHL	CHC-C1C	3.02	1.42	1.35
38	W	308	KC2	C4B-NB	3.02	1.41	1.37
30	B	847	BCR	C19-C18	3.02	1.52	1.45
30	G	205	BCR	C12-C13	3.02	1.52	1.45
26	5	611	IWJ	C04-C03	3.02	1.54	1.50
25	A	842	CLA	C1D-ND	3.02	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	A	837	CLA	C4D-ND	-3.02	1.33	1.37
25	U	310	CLA	CHC-C1C	3.02	1.42	1.35
24	U	305	CHL	C4D-ND	-3.02	1.33	1.37
25	T	303	CLA	C1D-ND	3.02	1.41	1.37
38	Q	310	KC2	C2A-C1A	3.02	1.53	1.44
25	4	309	CLA	CHC-C1C	3.02	1.42	1.35
24	S	304	CHL	CHC-C1C	3.02	1.42	1.35
25	V	303	CLA	CMB-C2B	-3.02	1.45	1.51
29	V	319	Q6L	C34-C33	3.02	1.54	1.50
25	A	807	CLA	CMB-C2B	-3.02	1.45	1.51
25	L	303	CLA	C4D-ND	-3.01	1.33	1.37
25	W	303	CLA	C1D-ND	3.01	1.41	1.37
25	W	310	CLA	CHC-C1C	3.01	1.42	1.35
34	A	844	PQN	C2M-C2	3.01	1.57	1.50
25	W	303	CLA	CMB-C2B	-3.01	1.45	1.51
25	1	605	CLA	CHC-C1C	3.01	1.42	1.35
25	P	313	CLA	CHC-C1C	3.01	1.42	1.35
25	A	810	CLA	CHC-C1C	3.01	1.42	1.35
25	G	204	CLA	CHC-C1C	3.01	1.42	1.35
25	3	312	CLA	C4D-ND	-3.01	1.33	1.37
25	3	311	CLA	CMB-C2B	-3.01	1.45	1.51
25	B	805	CLA	CMB-C2B	-3.01	1.45	1.51
25	S	313	CLA	C4D-ND	-3.01	1.33	1.37
25	B	835	CLA	CHC-C1C	3.01	1.42	1.35
25	B	841	CLA	CHC-C1C	3.01	1.42	1.35
25	U	312	CLA	CHC-C1C	3.01	1.42	1.35
25	B	805	CLA	C4D-ND	-3.01	1.33	1.37
29	X	319	Q6L	C34-C33	3.01	1.54	1.50
25	3	304	CLA	C4D-ND	-3.01	1.33	1.37
24	2	615	CHL	C4D-ND	-3.00	1.33	1.37
25	R	314	CLA	CHC-C1C	3.00	1.42	1.35
24	4	308	CHL	C4D-ND	-3.00	1.33	1.37
25	5	603	CLA	C4D-ND	-3.00	1.33	1.37
25	P	302	CLA	C4D-ND	-3.00	1.33	1.37
25	2	606	CLA	CHC-C1C	3.00	1.42	1.35
25	5	609	CLA	C4D-ND	-3.00	1.33	1.37
25	X	311	CLA	CHC-C1C	3.00	1.42	1.35
25	Q	306	CLA	CMB-C2B	-3.00	1.45	1.51
25	X	313	CLA	CHC-C1C	3.00	1.42	1.35
25	B	812	CLA	C3B-CAB	-2.99	1.41	1.47
25	6	610	CLA	C4D-ND	-2.99	1.33	1.37
25	A	806	CLA	C4D-ND	-2.99	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	U	312	CLA	C4D-ND	-2.99	1.33	1.37
25	X	313	CLA	C4D-ND	-2.99	1.33	1.37
29	P	315	Q6L	C34-C33	2.99	1.54	1.50
24	P	314	CHL	CHC-C1C	2.99	1.42	1.35
25	X	302	CLA	CHC-C1C	2.99	1.42	1.35
25	R	305	CLA	CMA-C3A	-2.99	1.46	1.53
25	B	814	CLA	C4D-ND	-2.99	1.33	1.37
25	T	310	CLA	CHC-C1C	2.99	1.42	1.35
24	V	304	CHL	C4D-ND	-2.99	1.33	1.37
25	V	313	CLA	C4D-ND	-2.99	1.33	1.37
25	5	606	CLA	CHC-C1C	2.99	1.42	1.35
25	6	613	CLA	CMB-C2B	-2.99	1.45	1.51
25	Q	304	CLA	CHC-C1C	2.98	1.42	1.35
26	R	322	IWJ	C04-C03	2.98	1.54	1.50
25	Q	305	CLA	CMD-C2D	-2.98	1.44	1.50
25	A	856	CLA	C4D-ND	-2.98	1.33	1.37
24	P	314	CHL	C4D-ND	-2.98	1.33	1.37
25	5	608	CLA	C4D-ND	-2.98	1.33	1.37
25	2	603	CLA	C3B-C2B	-2.98	1.36	1.40
25	B	835	CLA	C1D-ND	2.98	1.41	1.37
25	H	304	CLA	C1D-ND	2.98	1.41	1.37
25	U	303	CLA	C4D-ND	-2.98	1.33	1.37
25	X	304	CLA	C4D-ND	-2.98	1.33	1.37
29	R	323	Q6L	C34-C33	2.98	1.54	1.50
25	A	842	CLA	CMB-C2B	-2.98	1.45	1.51
25	3	305	CLA	CHC-C1C	2.98	1.42	1.35
25	A	808	CLA	C3B-CAB	-2.98	1.41	1.47
25	5	601	CLA	C3B-CAB	-2.98	1.41	1.47
29	Q	319	Q6L	C34-C33	2.98	1.54	1.50
25	R	313	CLA	CHC-C1C	2.98	1.42	1.35
24	6	605	CHL	CHC-C1C	2.98	1.42	1.35
25	B	804	CLA	C1D-ND	2.98	1.41	1.37
25	Q	311	CLA	C4D-ND	-2.97	1.33	1.37
25	A	837	CLA	CHC-C1C	2.97	1.42	1.35
26	V	317	IWJ	C29-C35	-2.97	1.51	1.56
25	Q	301	CLA	CMB-C2B	-2.97	1.45	1.51
25	W	313	CLA	CHC-C1C	2.97	1.42	1.35
25	P	310	CLA	C4D-ND	-2.97	1.33	1.37
25	4	305	CLA	CHC-C1C	2.97	1.42	1.35
25	6	603	CLA	CMD-C2D	-2.97	1.44	1.50
25	T	312	CLA	CHC-C1C	2.97	1.42	1.35
25	B	804	CLA	CHC-C1C	2.97	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	P	305	CHL	CHC-C1C	2.97	1.42	1.35
25	A	819	CLA	C4D-ND	-2.97	1.33	1.37
25	B	807	CLA	CHC-C1C	2.97	1.42	1.35
26	T	321	IWJ	C04-C03	2.97	1.54	1.50
25	P	303	CLA	C4D-ND	-2.97	1.33	1.37
25	L	303	CLA	CMB-C2B	-2.97	1.45	1.51
25	G	202	CLA	CHC-C1C	2.97	1.42	1.35
25	A	812	CLA	CHC-C1C	2.97	1.42	1.35
25	B	832	CLA	CHC-C1C	2.96	1.42	1.35
26	Q	320	IWJ	C04-C03	2.96	1.54	1.50
25	B	819	CLA	C3B-C2B	-2.96	1.36	1.40
26	P	318	IWJ	C29-C35	-2.96	1.51	1.56
25	6	613	CLA	CMD-C2D	-2.96	1.44	1.50
25	O	2004	CLA	CHC-C1C	2.96	1.42	1.35
25	B	809	CLA	C3B-C2B	-2.96	1.36	1.40
25	A	821	CLA	CHC-C1C	2.96	1.42	1.35
25	A	805	CLA	CMD-C2D	-2.96	1.44	1.50
24	Q	309	CHL	CHC-C1C	2.96	1.42	1.35
38	S	308	KC2	CMD-C2D	-2.96	1.45	1.51
25	3	302	CLA	CMB-C2B	-2.96	1.45	1.51
25	S	309	CLA	C1D-ND	2.96	1.41	1.37
38	X	309	KC2	C2A-C1A	2.96	1.53	1.44
24	T	320	CHL	C4D-ND	-2.96	1.33	1.37
25	Q	306	CLA	CHC-C1C	2.96	1.42	1.35
25	L	304	CLA	CHC-C1C	2.95	1.42	1.35
25	5	601	CLA	CHC-C1C	2.95	1.42	1.35
25	4	303	CLA	C3B-C2B	-2.95	1.36	1.40
25	B	836	CLA	C3B-CAB	-2.95	1.41	1.47
25	5	606	CLA	C4D-ND	-2.95	1.33	1.37
30	F	804	BCR	C12-C13	2.95	1.52	1.45
25	Q	311	CLA	CHC-C1C	2.95	1.42	1.35
24	X	308	CHL	C4D-ND	-2.95	1.33	1.37
26	X	318	IWJ	C04-C03	2.95	1.54	1.50
25	3	311	CLA	C4D-ND	-2.95	1.33	1.37
25	4	310	CLA	C4D-ND	-2.95	1.33	1.37
25	3	309	CLA	CHC-C1C	2.95	1.42	1.35
25	4	312	CLA	CHC-C1C	2.95	1.42	1.35
24	V	314	CHL	CHC-C1C	2.95	1.42	1.35
25	A	826	CLA	C3B-C2B	-2.95	1.36	1.40
25	R	316	CLA	CHC-C1C	2.94	1.42	1.35
26	U	316	IWJ	C04-C03	2.94	1.54	1.50
25	A	809	CLA	CHC-C1C	2.94	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	K	207	BCR	C12-C13	2.94	1.52	1.45
25	H	301	CLA	C3B-C2B	-2.94	1.36	1.40
25	2	610	CLA	CHC-C1C	2.94	1.42	1.35
25	B	835	CLA	C3B-C2B	-2.94	1.36	1.40
30	4	319	BCR	C8-C9	2.94	1.52	1.45
25	V	311	CLA	CHC-C1C	2.94	1.42	1.35
24	S	307	CHL	C4D-ND	-2.94	1.33	1.37
25	Q	315	CLA	CHC-C1C	2.94	1.42	1.35
25	B	829	CLA	C4D-ND	-2.94	1.33	1.37
25	4	310	CLA	CHC-C1C	2.94	1.42	1.35
38	P	308	KC2	C4D-ND	-2.94	1.32	1.35
29	T	322	Q6L	C34-C33	2.93	1.54	1.50
24	V	305	CHL	CHC-C1C	2.93	1.42	1.35
26	T	318	IWJ	C04-C03	2.93	1.54	1.50
25	6	608	CLA	C4D-ND	-2.93	1.33	1.37
25	A	803	CLA	C4D-ND	-2.93	1.33	1.37
25	U	311	CLA	C4D-ND	-2.93	1.33	1.37
25	A	816	CLA	C1D-ND	2.93	1.41	1.37
26	P	320	IWJ	C04-C03	2.93	1.54	1.50
24	4	307	CHL	C4D-ND	-2.93	1.33	1.37
25	2	611	CLA	CHC-C1C	2.93	1.42	1.35
25	Q	314	CLA	CHC-C1C	2.92	1.42	1.35
25	O	2005	CLA	C4D-ND	-2.92	1.33	1.37
25	1	608	CLA	CMD-C2D	-2.92	1.44	1.50
25	1	602	CLA	MG-NC	2.92	2.13	2.06
25	B	807	CLA	CMB-C2B	-2.92	1.45	1.51
25	J	102	CLA	C1D-ND	2.92	1.41	1.37
25	U	303	CLA	CHC-C1C	2.92	1.42	1.35
24	W	314	CHL	CHC-C1C	2.92	1.42	1.35
38	T	308	KC2	C4D-ND	-2.92	1.32	1.35
25	B	815	CLA	C1D-ND	2.92	1.41	1.37
27	1	612	XAT	C14-C13	-2.92	1.31	1.35
25	3	301	CLA	C4B-CHC	-2.92	1.32	1.41
25	T	303	CLA	CHC-C1C	2.91	1.42	1.35
24	X	306	CHL	CHC-C1C	2.91	1.42	1.35
25	B	827	CLA	C4D-ND	-2.91	1.33	1.37
26	S	319	IWJ	C04-C03	2.91	1.54	1.50
25	B	810	CLA	C3B-C2B	-2.91	1.36	1.40
25	3	310	CLA	CHC-C1C	2.91	1.42	1.35
25	A	835	CLA	CMB-C2B	-2.91	1.45	1.51
25	5	610	CLA	C4D-ND	-2.91	1.33	1.37
25	B	832	CLA	C4D-ND	-2.91	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	R	312	KC2	C4B-NB	2.90	1.41	1.37
25	2	612	CLA	CHC-C1C	2.90	1.42	1.35
25	S	311	CLA	CHC-C1C	2.90	1.42	1.35
26	R	303	IWJ	C04-C03	2.90	1.54	1.50
25	H	301	CLA	CHC-C1C	2.90	1.42	1.35
24	R	310	CHL	CMD-C2D	-2.90	1.44	1.50
25	B	839	CLA	CMB-C2B	-2.90	1.45	1.51
26	Q	303	IWJ	C04-C03	2.90	1.54	1.50
25	B	831	CLA	C4D-ND	-2.90	1.33	1.37
30	2	618	BCR	C23-C22	2.90	1.52	1.45
37	W	317	NEX	C7-C8	-2.90	1.27	1.32
29	R	301	Q6L	C12-C13	-2.90	1.45	1.51
26	S	318	IWJ	C04-C03	2.90	1.54	1.50
32	H	303	SQD	C6-S	-2.90	1.66	1.77
25	2	606	CLA	CMB-C2B	-2.89	1.45	1.51
24	R	318	CHL	C4D-ND	-2.89	1.33	1.37
25	1	606	CLA	CHC-C1C	2.89	1.42	1.35
25	A	803	CLA	CMB-C2B	-2.89	1.45	1.51
25	Q	313	CLA	CHC-C1C	2.89	1.42	1.35
29	O	2006	Q6L	C34-C33	2.89	1.54	1.50
25	3	312	CLA	CMB-C2B	-2.89	1.45	1.51
24	V	305	CHL	C4D-ND	-2.89	1.33	1.37
25	B	809	CLA	C4D-ND	-2.89	1.33	1.37
25	A	832	CLA	C4D-ND	-2.89	1.33	1.37
29	O	2006	Q6L	C02-C03	2.89	1.38	1.34
25	1	613	CLA	C4D-ND	-2.89	1.33	1.37
26	V	320	IWJ	C04-C03	2.89	1.54	1.50
25	6	604	CLA	C4D-ND	-2.89	1.33	1.37
30	3	318	BCR	C8-C9	2.89	1.52	1.45
38	V	308	KC2	C4B-NB	2.89	1.41	1.37
24	R	309	CHL	CHC-C1C	2.89	1.42	1.35
24	V	307	CHL	CHC-C1C	2.89	1.42	1.35
24	P	306	CHL	C4D-ND	-2.88	1.33	1.37
25	O	2005	CLA	CHC-C1C	2.88	1.42	1.35
24	1	604	CHL	C4D-ND	-2.88	1.33	1.37
29	U	317	Q6L	C02-C03	2.88	1.38	1.34
25	B	819	CLA	CHC-C1C	2.88	1.42	1.35
25	1	603	CLA	C3B-C2B	-2.88	1.36	1.40
25	1	608	CLA	C4D-ND	-2.88	1.33	1.37
25	B	835	CLA	C4D-ND	-2.88	1.33	1.37
29	P	315	Q6L	C12-C13	-2.88	1.45	1.51
25	H	304	CLA	CMB-C2B	-2.88	1.45	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	Q	312	CLA	C4D-ND	-2.88	1.33	1.37
25	R	307	CLA	C4D-ND	-2.88	1.33	1.37
38	V	308	KC2	C2A-C1A	2.88	1.53	1.44
25	6	608	CLA	CHC-C1C	2.87	1.42	1.35
25	V	312	CLA	CMB-C2B	-2.87	1.45	1.51
25	A	831	CLA	C3B-C2B	-2.87	1.36	1.40
25	B	834	CLA	CMB-C2B	-2.87	1.45	1.51
29	O	2007	Q6L	C34-C33	2.87	1.54	1.50
25	2	602	CLA	CMB-C2B	-2.87	1.45	1.51
25	V	312	CLA	CHC-C1C	2.87	1.42	1.35
25	1	602	CLA	CHC-C1C	2.87	1.42	1.35
25	B	825	CLA	C1D-ND	2.87	1.41	1.37
25	A	838	CLA	CHC-C1C	2.87	1.42	1.35
25	4	314	CLA	CHC-C1C	2.87	1.42	1.35
25	T	311	CLA	CHC-C1C	2.87	1.42	1.35
25	V	310	CLA	C3B-C2B	-2.87	1.36	1.40
29	X	319	Q6L	C12-C13	-2.87	1.45	1.51
25	V	301	CLA	CMB-C2B	-2.87	1.45	1.51
25	A	826	CLA	CHC-C1C	2.87	1.42	1.35
25	A	827	CLA	C4D-ND	-2.86	1.33	1.37
25	W	302	CLA	CHC-C1C	2.86	1.42	1.35
25	X	314	CLA	CHC-C1C	2.86	1.42	1.35
29	S	320	Q6L	C33-C32	2.86	1.36	1.33
24	T	320	CHL	CHC-C1C	2.86	1.42	1.35
25	A	837	CLA	C3B-C2B	-2.86	1.36	1.40
25	B	836	CLA	CMB-C2B	-2.86	1.45	1.51
25	6	611	CLA	CHC-C1C	2.86	1.42	1.35
25	V	311	CLA	C4D-ND	-2.86	1.33	1.37
25	4	315	CLA	CHC-C1C	2.86	1.42	1.35
32	6	617	SQD	C6-S	-2.86	1.66	1.77
25	U	309	CLA	CHC-C1C	2.86	1.42	1.35
25	T	310	CLA	C4D-ND	-2.86	1.33	1.37
25	B	842	CLA	C3B-C2B	-2.86	1.36	1.40
25	A	815	CLA	CHC-C1C	2.86	1.42	1.35
25	A	818	CLA	CMB-C2B	-2.86	1.45	1.51
25	3	310	CLA	C4D-ND	-2.85	1.33	1.37
25	B	814	CLA	CHC-C1C	2.85	1.42	1.35
29	P	316	Q6L	C02-C03	2.85	1.38	1.34
25	Q	301	CLA	C4D-ND	-2.85	1.33	1.37
25	B	828	CLA	CMB-C2B	-2.85	1.45	1.51
24	4	306	CHL	CHC-C1C	2.85	1.42	1.35
24	S	314	CHL	C4D-ND	-2.85	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	5	604	CLA	CMB-C2B	-2.85	1.45	1.51
26	4	317	IWJ	C04-C03	2.85	1.54	1.50
25	B	809	CLA	CMB-C2B	-2.85	1.45	1.51
25	P	311	CLA	CHC-C1C	2.85	1.42	1.35
25	4	303	CLA	CHC-C1C	2.85	1.42	1.35
25	V	310	CLA	CMB-C2B	-2.85	1.45	1.51
29	R	320	Q6L	C34-C33	2.85	1.54	1.50
25	5	608	CLA	C3B-C2B	-2.85	1.36	1.40
25	S	302	CLA	CHC-C1C	2.85	1.42	1.35
25	1	609	CLA	CHC-C1C	2.85	1.42	1.35
25	F	803	CLA	CMB-C2B	-2.84	1.45	1.51
25	A	822	CLA	CHC-C1C	2.84	1.42	1.35
25	1	607	CLA	CHC-C1C	2.84	1.42	1.35
25	3	307	CLA	C4B-CHC	-2.84	1.33	1.41
25	N	203	CLA	C4D-ND	-2.84	1.33	1.37
25	S	309	CLA	C4D-ND	-2.84	1.33	1.37
25	Q	305	CLA	C4D-ND	-2.84	1.33	1.37
25	6	607	CLA	CMD-C2D	-2.84	1.44	1.50
38	S	308	KC2	C4B-NB	2.84	1.41	1.37
25	A	807	CLA	CHC-C1C	2.84	1.42	1.35
25	P	309	CLA	C4D-ND	-2.84	1.33	1.37
29	S	321	Q6L	C34-C33	2.84	1.54	1.50
25	S	303	CLA	CMB-C2B	-2.84	1.45	1.51
25	5	602	CLA	CHC-C1C	2.83	1.42	1.35
29	S	323	Q6L	C12-C13	-2.83	1.45	1.51
25	H	302	CLA	C4D-ND	-2.83	1.33	1.37
38	U	307	KC2	C2A-C1A	2.83	1.53	1.44
29	W	316	Q6L	C12-C13	-2.83	1.45	1.51
24	T	314	CHL	CHC-C1C	2.83	1.42	1.35
38	W	308	KC2	C2A-C1A	2.83	1.53	1.44
24	6	601	CHL	CHC-C1C	2.83	1.42	1.35
25	A	813	CLA	CHC-C1C	2.82	1.42	1.35
38	Q	310	KC2	C4B-NB	2.82	1.41	1.37
30	A	848	BCR	C8-C9	2.82	1.52	1.45
24	T	314	CHL	C4D-ND	-2.82	1.33	1.37
25	U	308	CLA	MG-NC	2.82	2.13	2.06
38	T	308	KC2	CMD-C2D	-2.82	1.45	1.51
25	A	836	CLA	CHC-C1C	2.82	1.42	1.35
25	Q	301	CLA	C3B-C2B	-2.82	1.36	1.40
25	A	816	CLA	C3B-CAB	-2.82	1.42	1.47
25	F	802	CLA	C3B-C2B	-2.82	1.36	1.40
25	B	821	CLA	CHC-C1C	2.82	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	O	2001	CLA	CHC-C1C	2.81	1.42	1.35
25	R	316	CLA	C4D-ND	-2.81	1.33	1.37
25	A	819	CLA	CHC-C1C	2.81	1.42	1.35
25	W	310	CLA	C4D-ND	-2.81	1.33	1.37
25	B	810	CLA	CHC-C1C	2.81	1.42	1.35
25	Q	314	CLA	CMD-C2D	-2.81	1.44	1.50
37	P	317	NEX	C7-C8	-2.81	1.27	1.32
24	Q	316	CHL	CHC-C1C	2.81	1.42	1.35
24	S	307	CHL	CMB-C2B	-2.81	1.45	1.51
25	6	611	CLA	C4D-ND	-2.81	1.33	1.37
25	L	302	CLA	C3B-CAB	-2.81	1.42	1.47
25	2	608	CLA	CHC-C1C	2.81	1.42	1.35
25	T	303	CLA	CMB-C2B	-2.81	1.45	1.51
25	B	820	CLA	C4D-ND	-2.81	1.33	1.37
25	B	805	CLA	CHC-C1C	2.81	1.42	1.35
25	B	817	CLA	CHC-C1C	2.81	1.42	1.35
25	H	304	CLA	CHC-C1C	2.81	1.42	1.35
38	W	308	KC2	CMC-C2C	-2.81	1.44	1.50
25	2	602	CLA	C4D-ND	-2.80	1.33	1.37
25	2	608	CLA	C4D-ND	-2.80	1.33	1.37
25	B	840	CLA	C3B-C2B	-2.80	1.36	1.40
25	B	830	CLA	CMB-C2B	-2.80	1.45	1.51
26	P	318	IWJ	C04-C03	2.80	1.54	1.50
25	X	313	CLA	CMB-C2B	-2.80	1.45	1.51
24	T	306	CHL	CHC-C1C	2.80	1.42	1.35
30	A	848	BCR	C19-C18	2.80	1.52	1.45
25	B	840	CLA	CMB-C2B	-2.80	1.45	1.51
29	U	315	Q6L	C34-C33	2.80	1.54	1.50
25	1	603	CLA	CMB-C2B	-2.80	1.45	1.51
24	T	304	CHL	C4D-ND	-2.80	1.33	1.37
29	T	316	Q6L	C02-C03	2.80	1.38	1.34
38	U	307	KC2	CMD-C2D	-2.80	1.45	1.51
24	U	313	CHL	C4D-ND	-2.80	1.33	1.37
37	T	317	NEX	C22-C21	-2.80	1.50	1.54
24	Q	308	CHL	C4D-ND	-2.80	1.33	1.37
38	T	308	KC2	C2A-C1A	2.80	1.53	1.44
37	P	317	NEX	C12-C13	2.80	1.52	1.45
29	T	319	Q6L	C34-C33	2.80	1.54	1.50
25	6	609	CLA	C4D-ND	-2.80	1.33	1.37
30	J	101	BCR	C19-C18	2.80	1.51	1.45
25	B	836	CLA	CHC-C1C	2.79	1.42	1.35
24	3	306	CHL	CHC-C1C	2.79	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	U	313	CHL	CHC-C1C	2.79	1.42	1.35
30	K	202	BCR	C16-C15	-2.79	1.28	1.36
25	3	303	CLA	CMD-C2D	-2.79	1.44	1.50
29	S	321	Q6L	C12-C13	-2.79	1.45	1.51
25	A	833	CLA	CHC-C1C	2.79	1.42	1.35
30	K	202	BCR	C19-C18	2.79	1.51	1.45
26	6	614	IWJ	C04-C03	2.79	1.54	1.50
25	2	609	CLA	C3B-C2B	-2.79	1.36	1.40
25	G	204	CLA	C3B-C2B	-2.79	1.36	1.40
25	3	303	CLA	CHC-C1C	2.79	1.42	1.35
25	1	610	CLA	CHC-C1C	2.79	1.42	1.35
29	S	320	Q6L	C12-C13	-2.79	1.45	1.51
29	R	323	Q6L	C12-C13	-2.78	1.45	1.51
25	R	305	CLA	CHC-C1C	2.78	1.42	1.35
26	4	301	IWJ	C04-C03	2.78	1.54	1.50
25	B	823	CLA	CHC-C1C	2.78	1.42	1.35
25	6	609	CLA	CHC-C1C	2.78	1.42	1.35
25	L	303	CLA	CHC-C1C	2.78	1.42	1.35
25	S	310	CLA	CHC-C1C	2.78	1.42	1.35
25	S	301	CLA	C1D-ND	2.78	1.41	1.37
25	2	611	CLA	C4D-ND	-2.78	1.33	1.37
30	A	850	BCR	C12-C13	2.78	1.51	1.45
25	A	823	CLA	CHC-C1C	2.78	1.42	1.35
29	T	315	Q6L	C34-C33	2.78	1.54	1.50
25	X	310	CLA	C4D-ND	-2.77	1.33	1.37
25	B	835	CLA	CMD-C2D	-2.77	1.44	1.50
24	S	314	CHL	CHC-C1C	2.77	1.42	1.35
25	2	604	CLA	CMB-C2B	-2.77	1.45	1.51
25	A	843	CLA	C1D-ND	2.77	1.41	1.37
25	K	204	CLA	CHC-C1C	2.77	1.42	1.35
25	B	802	CLA	CMB-C2B	-2.77	1.45	1.51
24	1	601	CHL	C4D-ND	-2.77	1.33	1.37
25	A	842	CLA	C4D-ND	-2.77	1.33	1.37
25	2	604	CLA	CHC-C1C	2.77	1.42	1.35
25	X	312	CLA	CHC-C1C	2.77	1.42	1.35
26	V	318	IWJ	C04-C03	2.77	1.54	1.50
25	A	832	CLA	CHC-C1C	2.77	1.42	1.35
25	G	202	CLA	C4D-ND	-2.77	1.33	1.37
25	B	831	CLA	CMB-C2B	-2.77	1.45	1.51
25	B	804	CLA	CMC-C2C	-2.77	1.44	1.50
25	K	201	CLA	CHC-C1C	2.76	1.42	1.35
38	R	312	KC2	CMD-C2D	-2.76	1.45	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	Q	307	CHL	CHC-C1C	2.76	1.42	1.35
24	R	311	CHL	CMB-C2B	-2.76	1.45	1.51
25	1	609	CLA	C1D-ND	2.76	1.41	1.37
24	W	305	CHL	CHC-C1C	2.76	1.42	1.35
25	W	312	CLA	C1D-ND	2.76	1.41	1.37
25	U	302	CLA	CHC-C1C	2.76	1.42	1.35
25	V	302	CLA	CMB-C2B	-2.76	1.45	1.51
25	4	316	CLA	CHC-C1C	2.76	1.42	1.35
25	4	312	CLA	C4D-ND	-2.76	1.33	1.37
25	A	841	CLA	CMB-C2B	-2.76	1.45	1.51
30	4	319	BCR	C12-C13	2.76	1.51	1.45
24	X	305	CHL	C1D-ND	2.76	1.41	1.37
25	Q	305	CLA	CHC-C1C	2.76	1.42	1.35
38	R	312	KC2	C2A-C1A	2.76	1.53	1.44
25	A	804	CLA	C3B-C2B	-2.76	1.36	1.40
30	B	847	BCR	C1-C6	-2.76	1.50	1.53
25	3	303	CLA	CMB-C2B	-2.76	1.45	1.51
26	1	611	IWJ	C29-C35	-2.76	1.52	1.56
30	K	205	BCR	C8-C9	2.76	1.51	1.45
24	Q	308	CHL	C1D-ND	2.75	1.41	1.37
25	S	313	CLA	CMD-C2D	-2.75	1.45	1.50
29	R	304	Q6L	C34-C33	2.75	1.54	1.50
24	T	307	CHL	CMB-C2B	-2.75	1.45	1.51
38	Q	310	KC2	CMD-C2D	-2.75	1.45	1.51
30	B	847	BCR	C31-C1	-2.75	1.48	1.53
25	A	845	CLA	CHC-C1C	2.75	1.42	1.35
25	1	610	CLA	CMB-C2B	-2.74	1.45	1.51
25	A	803	CLA	CHC-C1C	2.74	1.42	1.35
25	B	812	CLA	C3B-C2B	-2.74	1.36	1.40
24	W	307	CHL	C4D-ND	-2.74	1.33	1.37
25	3	308	CLA	C4D-ND	-2.74	1.33	1.37
25	6	610	CLA	C3B-C2B	-2.74	1.36	1.40
29	V	321	Q6L	C12-C13	-2.74	1.45	1.51
25	L	301	CLA	CMC-C2C	-2.74	1.45	1.50
26	3	315	IWJ	C04-C03	2.74	1.54	1.50
25	B	826	CLA	C3B-C2B	-2.74	1.36	1.40
25	A	810	CLA	CMB-C2B	-2.74	1.45	1.51
29	R	319	Q6L	C02-C03	2.74	1.38	1.34
25	Q	301	CLA	C4B-CHC	-2.74	1.33	1.41
24	X	307	CHL	C4D-ND	-2.74	1.33	1.37
34	B	844	PQN	C3-C4	-2.74	1.40	1.47
24	4	306	CHL	CMB-C2B	-2.74	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	W	315	Q6L	C12-C13	-2.73	1.45	1.51
27	1	612	XAT	C35-C15	-2.73	1.28	1.36
29	T	316	Q6L	C34-C33	2.73	1.54	1.50
29	W	320	Q6L	C34-C33	2.73	1.54	1.50
29	W	320	Q6L	C12-C13	-2.73	1.45	1.51
25	O	2002	CLA	CHC-C1C	2.73	1.42	1.35
25	S	303	CLA	C4D-ND	-2.73	1.33	1.37
25	6	610	CLA	CHC-C1C	2.73	1.42	1.35
25	B	811	CLA	CMC-C2C	-2.73	1.45	1.50
25	R	306	CLA	CHC-C1C	2.73	1.42	1.35
34	A	844	PQN	C3-C4	-2.73	1.40	1.47
25	T	313	CLA	CMB-C2B	-2.73	1.46	1.51
25	B	830	CLA	MG-ND	-2.73	2.00	2.05
25	B	826	CLA	CHC-C1C	2.73	1.42	1.35
25	B	841	CLA	C3B-C2B	-2.73	1.36	1.40
25	A	817	CLA	CMB-C2B	-2.73	1.46	1.51
25	A	823	CLA	C1D-ND	2.73	1.41	1.37
25	5	607	CLA	CHC-C1C	2.72	1.41	1.35
25	L	302	CLA	CHC-C1C	2.72	1.41	1.35
25	J	102	CLA	C3B-CAB	-2.72	1.42	1.47
30	A	852	BCR	C37-C22	2.72	1.56	1.50
26	V	317	IWJ	C04-C03	2.72	1.54	1.50
25	B	808	CLA	C3B-C2B	-2.72	1.36	1.40
25	3	301	CLA	CMC-C2C	-2.72	1.45	1.50
25	6	607	CLA	C1D-ND	2.72	1.41	1.37
24	R	310	CHL	CHC-C1C	2.72	1.41	1.35
25	A	834	CLA	CHC-C1C	2.72	1.41	1.35
29	T	322	Q6L	C12-C13	-2.72	1.45	1.51
24	S	307	CHL	C1D-ND	2.72	1.41	1.37
25	P	302	CLA	C3B-C2B	-2.71	1.36	1.40
29	T	315	Q6L	C12-C13	-2.71	1.45	1.51
26	T	321	IWJ	C03-C02	2.71	1.36	1.33
24	1	604	CHL	CMD-C2D	-2.71	1.45	1.50
29	V	316	Q6L	C34-C33	2.71	1.54	1.50
25	B	831	CLA	CMD-C2D	-2.71	1.45	1.50
24	5	605	CHL	CHC-C1C	2.71	1.41	1.35
25	B	803	CLA	CHC-C1C	2.71	1.41	1.35
25	S	310	CLA	C3B-C2B	-2.71	1.36	1.40
29	X	301	Q6L	C33-C32	2.71	1.36	1.33
25	2	610	CLA	C4D-ND	-2.71	1.34	1.37
25	A	856	CLA	CMB-C2B	-2.71	1.46	1.51
26	5	611	IWJ	C03-C02	2.71	1.36	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	X	314	CLA	CMB-C2B	-2.71	1.46	1.51
34	B	844	PQN	C10-C5	-2.71	1.36	1.40
25	R	306	CLA	CMD-C2D	-2.71	1.45	1.50
26	Q	303	IWJ	C03-C02	2.71	1.36	1.33
25	4	314	CLA	CMB-C2B	-2.71	1.46	1.51
29	W	319	Q6L	C12-C13	-2.70	1.45	1.51
24	2	605	CHL	C4D-ND	-2.70	1.34	1.37
25	A	829	CLA	C3B-CAB	-2.70	1.42	1.47
25	H	302	CLA	CHC-C1C	2.70	1.41	1.35
24	Q	307	CHL	C4D-ND	-2.70	1.34	1.37
29	P	316	Q6L	C34-C33	2.70	1.54	1.50
30	B	845	BCR	C34-C9	2.70	1.56	1.50
29	Q	317	Q6L	C12-C13	-2.70	1.45	1.51
25	A	814	CLA	CMD-C2D	-2.70	1.45	1.50
25	X	311	CLA	CMB-C2B	-2.70	1.46	1.51
25	B	843	CLA	C1D-ND	2.70	1.41	1.37
25	1	608	CLA	CHC-C1C	2.70	1.41	1.35
25	3	307	CLA	C3B-C2B	-2.70	1.36	1.40
25	A	828	CLA	C3B-CAB	-2.69	1.42	1.47
25	B	818	CLA	C4D-ND	-2.69	1.34	1.37
25	B	833	CLA	CMB-C2B	-2.69	1.46	1.51
25	A	825	CLA	CHC-C1C	2.69	1.41	1.35
38	Q	310	KC2	C4D-ND	-2.69	1.32	1.35
24	T	305	CHL	C4D-ND	-2.69	1.34	1.37
27	4	318	XAT	C32-C33	2.69	1.51	1.45
25	W	303	CLA	CHC-C1C	2.69	1.41	1.35
25	5	603	CLA	CHC-C1C	2.69	1.41	1.35
25	4	304	CLA	CMB-C2B	-2.69	1.46	1.51
25	B	822	CLA	CHC-C1C	2.69	1.41	1.35
29	Q	319	Q6L	C33-C32	2.69	1.36	1.33
24	4	306	CHL	C4D-ND	-2.69	1.34	1.37
25	A	821	CLA	C4D-ND	-2.69	1.34	1.37
25	2	609	CLA	C3B-CAB	-2.69	1.42	1.47
26	S	319	IWJ	C03-C02	2.69	1.36	1.33
25	W	302	CLA	C3B-C2B	-2.69	1.36	1.40
25	B	822	CLA	CMB-C2B	-2.69	1.46	1.51
25	S	302	CLA	CMB-C2B	-2.68	1.46	1.51
25	6	603	CLA	C3B-C2B	-2.68	1.36	1.40
25	A	819	CLA	C3B-C2B	-2.68	1.36	1.40
24	4	302	CHL	CHC-C1C	2.68	1.41	1.35
25	2	609	CLA	CHC-C1C	2.68	1.41	1.35
30	F	801	BCR	C19-C18	2.68	1.51	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	W	316	Q6L	C34-C33	2.68	1.54	1.50
25	A	804	CLA	CMB-C2B	-2.68	1.46	1.51
29	S	321	Q6L	C33-C32	2.68	1.36	1.33
25	H	302	CLA	CMB-C2B	-2.68	1.46	1.51
25	A	804	CLA	CMA-C3A	-2.68	1.47	1.53
25	U	312	CLA	CMD-C2D	-2.68	1.45	1.50
38	P	308	KC2	CMD-C2D	-2.68	1.46	1.51
37	S	317	NEX	C22-C21	-2.68	1.50	1.54
25	A	804	CLA	CHC-C1C	2.68	1.41	1.35
25	3	302	CLA	CMC-C2C	-2.68	1.45	1.50
29	U	314	Q6L	C34-C33	2.68	1.54	1.50
26	W	318	IWJ	C04-C03	2.68	1.54	1.50
29	O	2007	Q6L	C33-C32	2.68	1.36	1.33
30	J	101	BCR	C16-C15	-2.67	1.29	1.36
25	5	602	CLA	CMB-C2B	-2.67	1.46	1.51
25	1	602	CLA	CMD-C2D	-2.67	1.45	1.50
24	W	305	CHL	CMD-C2D	-2.67	1.45	1.50
29	X	301	Q6L	C34-C33	2.67	1.54	1.50
25	X	310	CLA	CMB-C2B	-2.67	1.46	1.51
29	O	2007	Q6L	C02-C03	2.67	1.37	1.34
25	A	812	CLA	C3B-C2B	-2.67	1.36	1.40
24	V	305	CHL	CMD-C2D	-2.67	1.45	1.50
25	B	815	CLA	CHC-C1C	2.67	1.41	1.35
24	S	306	CHL	C1D-ND	2.67	1.41	1.37
29	U	314	Q6L	C12-C13	-2.67	1.45	1.51
29	R	320	Q6L	C12-C13	-2.67	1.45	1.51
25	W	312	CLA	CMB-C2B	-2.67	1.46	1.51
25	A	830	CLA	CMC-C2C	-2.67	1.45	1.50
25	B	830	CLA	C1D-ND	2.66	1.41	1.37
26	4	317	IWJ	C29-C35	-2.66	1.52	1.56
25	B	813	CLA	C4D-ND	-2.66	1.34	1.37
25	3	304	CLA	CHC-C1C	2.66	1.41	1.35
29	V	319	Q6L	C12-C13	-2.66	1.45	1.51
34	B	844	PQN	C2M-C2	2.66	1.56	1.50
24	S	304	CHL	CMB-C2B	-2.66	1.46	1.51
25	V	312	CLA	CMD-C2D	-2.66	1.45	1.50
25	A	830	CLA	CMD-C2D	-2.66	1.45	1.50
25	K	203	CLA	CHC-C1C	2.66	1.41	1.35
25	R	316	CLA	CMB-C2B	-2.66	1.46	1.51
24	2	615	CHL	CHC-C1C	2.66	1.41	1.35
25	A	809	CLA	CMB-C2B	-2.66	1.46	1.51
25	B	836	CLA	CMD-C2D	-2.66	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B	806	CLA	C3B-C2B	-2.66	1.36	1.40
29	X	316	Q6L	C02-C03	2.66	1.37	1.34
30	M	101	BCR	C34-C9	2.66	1.56	1.50
25	A	811	CLA	CHC-C1C	2.65	1.41	1.35
29	X	317	Q6L	C02-C03	2.65	1.37	1.34
25	B	810	CLA	CMC-C2C	-2.65	1.45	1.50
25	N	203	CLA	MG-ND	-2.65	2.00	2.05
29	S	316	Q6L	C34-C33	2.65	1.53	1.50
25	V	310	CLA	C4B-CHC	-2.65	1.33	1.41
30	3	318	BCR	C12-C13	2.65	1.51	1.45
30	A	849	BCR	C19-C18	2.65	1.51	1.45
25	B	820	CLA	CHC-C1C	2.65	1.41	1.35
25	Q	305	CLA	CMB-C2B	-2.65	1.46	1.51
25	R	307	CLA	CMB-C2B	-2.65	1.46	1.51
25	A	834	CLA	CMB-C2B	-2.65	1.46	1.51
38	X	309	KC2	CMC-C2C	-2.65	1.45	1.50
25	N	202	CLA	CHC-C1C	2.65	1.41	1.35
25	A	816	CLA	CMD-C2D	-2.65	1.45	1.50
24	5	605	CHL	CMB-C2B	-2.65	1.46	1.51
25	4	311	CLA	C4B-CHC	-2.64	1.33	1.41
24	X	307	CHL	CMB-C2B	-2.64	1.46	1.51
26	P	320	IWJ	O39-C29	-2.64	1.39	1.43
25	B	808	CLA	CMB-C2B	-2.64	1.46	1.51
25	B	819	CLA	C3B-CAB	-2.64	1.42	1.47
25	A	818	CLA	CHC-C1C	2.64	1.41	1.35
30	2	618	BCR	C19-C18	2.64	1.51	1.45
25	W	311	CLA	CHC-C1C	2.64	1.41	1.35
25	B	829	CLA	CHC-C1C	2.64	1.41	1.35
25	B	834	CLA	C1D-ND	2.64	1.41	1.37
25	A	813	CLA	CMB-C2B	-2.64	1.46	1.51
26	U	316	IWJ	C03-C02	2.64	1.36	1.33
25	A	814	CLA	CHC-C1C	2.64	1.41	1.35
25	S	310	CLA	CMB-C2B	-2.64	1.46	1.51
38	X	309	KC2	C4B-NB	2.64	1.41	1.37
25	A	805	CLA	C4D-ND	-2.64	1.34	1.37
29	2	616	Q6L	C34-C33	2.63	1.53	1.50
25	B	802	CLA	C1D-ND	2.63	1.41	1.37
38	T	308	KC2	C4B-NB	2.63	1.41	1.37
26	1	611	IWJ	C03-C02	2.63	1.36	1.33
38	U	307	KC2	C4B-NB	2.63	1.41	1.37
25	A	823	CLA	C3B-CAB	-2.63	1.42	1.47
25	4	315	CLA	CMB-C2B	-2.63	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	S	322	IWJ	C03-C02	2.63	1.36	1.33
25	3	307	CLA	CMA-C3A	-2.63	1.47	1.53
26	W	318	IWJ	C03-C02	2.63	1.36	1.33
25	6	613	CLA	CHC-C1C	2.63	1.41	1.35
25	A	805	CLA	CHC-C1C	2.63	1.41	1.35
25	B	814	CLA	CMB-C2B	-2.63	1.46	1.51
29	S	323	Q6L	C02-C03	2.63	1.37	1.34
24	3	306	CHL	CMD-C2D	-2.63	1.45	1.50
25	J	102	CLA	CMB-C2B	-2.63	1.46	1.51
38	S	308	KC2	C2A-C1A	2.63	1.52	1.44
26	4	301	IWJ	C03-C02	2.63	1.36	1.33
25	A	816	CLA	C3B-C2B	-2.62	1.36	1.40
25	T	309	CLA	C3B-C2B	-2.62	1.36	1.40
25	W	309	CLA	C4D-ND	-2.62	1.34	1.37
25	B	826	CLA	CMC-C2C	-2.62	1.45	1.50
25	X	312	CLA	CMB-C2B	-2.62	1.46	1.51
25	B	825	CLA	CHC-C1C	2.62	1.41	1.35
25	S	301	CLA	CMD-C2D	-2.62	1.45	1.50
30	G	201	BCR	C17-C18	-2.62	1.32	1.35
38	V	308	KC2	CMC-C2C	-2.62	1.45	1.50
29	X	317	Q6L	C34-C33	2.62	1.53	1.50
30	K	205	BCR	C12-C13	2.62	1.51	1.45
29	R	319	Q6L	C12-C13	-2.62	1.45	1.51
29	P	319	Q6L	C02-C03	2.62	1.37	1.34
24	S	306	CHL	CMB-C2B	-2.62	1.46	1.51
25	K	203	CLA	CMB-C2B	-2.62	1.46	1.51
25	B	812	CLA	CMD-C2D	-2.62	1.45	1.50
24	4	302	CHL	C4D-ND	-2.62	1.34	1.37
25	3	301	CLA	CHC-C1C	2.62	1.41	1.35
25	B	838	CLA	CMB-C2B	-2.62	1.46	1.51
29	P	319	Q6L	C33-C32	2.61	1.36	1.33
25	N	203	CLA	C3B-CAB	-2.61	1.42	1.47
29	U	314	Q6L	C02-C03	2.61	1.37	1.34
25	A	820	CLA	CMB-C2B	-2.61	1.46	1.51
24	S	306	CHL	C4D-ND	-2.61	1.34	1.37
37	H	306	NEX	C12-C13	2.61	1.51	1.45
30	A	850	BCR	C1-C6	-2.61	1.50	1.53
25	4	309	CLA	CMB-C2B	-2.61	1.46	1.51
24	1	601	CHL	C3B-C2B	-2.61	1.36	1.40
24	V	314	CHL	CMD-C2D	-2.61	1.45	1.50
24	R	302	CHL	CHC-C1C	2.61	1.41	1.35
25	A	839	CLA	CHC-C1C	2.61	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B	823	CLA	CMB-C2B	-2.61	1.46	1.51
25	A	840	CLA	CHC-C1C	2.61	1.41	1.35
25	S	303	CLA	CMD-C2D	-2.60	1.45	1.50
25	6	603	CLA	MG-ND	-2.60	2.00	2.05
25	V	302	CLA	C3B-C2B	-2.60	1.36	1.40
30	4	319	BCR	C16-C15	-2.60	1.29	1.36
25	2	612	CLA	CMB-C2B	-2.60	1.46	1.51
25	A	839	CLA	C3B-CAB	-2.60	1.42	1.47
26	R	322	IWJ	C03-C02	2.60	1.36	1.33
30	L	306	BCR	C12-C13	2.60	1.51	1.45
24	R	308	CHL	CHC-C1C	2.60	1.41	1.35
25	4	316	CLA	CMB-C2B	-2.60	1.46	1.51
25	3	308	CLA	C4B-CHC	-2.60	1.33	1.41
25	4	313	CLA	CHC-C1C	2.60	1.41	1.35
25	A	835	CLA	C3B-C2B	-2.60	1.36	1.40
29	P	316	Q6L	C12-C13	-2.60	1.45	1.51
25	3	311	CLA	CHC-C1C	2.60	1.41	1.35
25	L	302	CLA	C1D-ND	2.59	1.41	1.37
25	B	826	CLA	C4B-CHC	-2.59	1.33	1.41
24	2	607	CHL	C3B-C2B	-2.59	1.36	1.40
29	X	301	Q6L	C12-C13	-2.59	1.45	1.51
34	A	844	PQN	C10-C5	-2.59	1.36	1.40
25	G	203	CLA	CHC-C1C	2.59	1.41	1.35
25	4	313	CLA	CMB-C2B	-2.59	1.46	1.51
25	B	803	CLA	C1D-ND	2.59	1.41	1.37
24	Q	309	CHL	CMB-C2B	-2.59	1.46	1.51
25	5	601	CLA	C4D-ND	-2.59	1.34	1.37
25	A	832	CLA	CMB-C2B	-2.59	1.46	1.51
25	A	813	CLA	CMD-C2D	-2.59	1.45	1.50
24	T	320	CHL	C3B-C2B	-2.59	1.36	1.40
24	W	306	CHL	C1D-ND	2.58	1.41	1.37
25	B	809	CLA	C4B-CHC	-2.58	1.33	1.41
25	A	842	CLA	CMD-C2D	-2.58	1.45	1.50
25	R	313	CLA	C4D-ND	-2.58	1.34	1.37
25	1	606	CLA	CMB-C2B	-2.58	1.46	1.51
29	W	319	Q6L	C34-C33	2.58	1.53	1.50
24	R	310	CHL	C4D-ND	-2.58	1.34	1.37
25	F	803	CLA	C3B-C2B	-2.58	1.36	1.40
25	B	825	CLA	C3B-CAB	-2.58	1.42	1.47
25	B	806	CLA	CHC-C1C	2.58	1.41	1.35
24	V	304	CHL	C3B-C2B	-2.58	1.36	1.40
25	3	313	CLA	CHC-C1C	2.58	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B	822	CLA	C1D-ND	2.58	1.41	1.37
25	V	311	CLA	CMB-C2B	-2.58	1.46	1.51
29	V	316	Q6L	C12-C13	-2.58	1.45	1.51
25	X	303	CLA	CHC-C1C	2.58	1.41	1.35
25	W	302	CLA	CMB-C2B	-2.58	1.46	1.51
37	H	306	NEX	C22-C21	-2.58	1.50	1.54
25	T	309	CLA	C4D-ND	-2.58	1.34	1.37
25	A	830	CLA	C3B-C2B	-2.58	1.36	1.40
25	A	843	CLA	CMB-C2B	-2.58	1.46	1.51
24	S	306	CHL	C1D-C2D	2.57	1.50	1.45
29	U	315	Q6L	C02-C03	2.57	1.37	1.34
25	R	305	CLA	C3B-C2B	-2.57	1.36	1.40
25	V	303	CLA	C1D-ND	2.57	1.40	1.37
25	A	843	CLA	C4D-ND	-2.57	1.34	1.37
25	T	303	CLA	CMD-C2D	-2.57	1.45	1.50
25	A	813	CLA	C4B-CHC	-2.57	1.33	1.41
29	R	301	Q6L	C34-C33	2.57	1.53	1.50
29	V	315	Q6L	C34-C33	2.57	1.53	1.50
26	T	318	IWJ	C03-C02	2.57	1.36	1.33
25	A	836	CLA	C4B-CHC	-2.57	1.33	1.41
25	3	301	CLA	CMB-C2B	-2.57	1.46	1.51
25	5	607	CLA	C3B-C2B	-2.57	1.36	1.40
24	2	607	CHL	CMB-C2B	-2.57	1.46	1.51
24	Q	308	CHL	CMB-C2B	-2.57	1.46	1.51
25	U	311	CLA	CMB-C2B	-2.57	1.46	1.51
29	W	316	Q6L	C02-C03	2.56	1.37	1.34
30	B	845	BCR	C10-C9	2.56	1.39	1.35
38	R	312	KC2	CMC-C2C	-2.56	1.45	1.50
24	6	606	CHL	C4D-ND	-2.56	1.34	1.37
25	R	315	CLA	CMB-C2B	-2.56	1.46	1.51
25	A	842	CLA	CHC-C1C	2.56	1.41	1.35
25	P	313	CLA	CMB-C2B	-2.56	1.46	1.51
25	B	810	CLA	CMD-C2D	-2.56	1.45	1.50
25	B	802	CLA	CMD-C2D	-2.56	1.45	1.50
25	T	302	CLA	CHC-C1C	2.56	1.41	1.35
25	T	309	CLA	CMB-C2B	-2.56	1.46	1.51
25	A	826	CLA	C3B-CAB	-2.56	1.42	1.47
25	U	302	CLA	C3B-CAB	-2.56	1.42	1.47
25	X	304	CLA	CHC-C1C	2.56	1.41	1.35
25	T	301	CLA	CMB-C2B	-2.56	1.46	1.51
29	V	319	Q6L	C02-C03	2.55	1.37	1.34
26	P	320	IWJ	C03-C02	2.55	1.36	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	R	306	CLA	CMB-C2B	-2.55	1.46	1.51
30	J	103	BCR	C23-C22	2.55	1.51	1.45
25	R	317	CLA	CMC-C2C	-2.55	1.45	1.50
25	W	309	CLA	CMB-C2B	-2.55	1.46	1.51
24	2	601	CHL	C3B-CAB	-2.55	1.42	1.47
27	3	316	XAT	C12-C13	2.55	1.51	1.45
25	S	302	CLA	CMD-C2D	-2.55	1.45	1.50
25	W	310	CLA	CMB-C2B	-2.55	1.46	1.51
25	Q	312	CLA	CMB-C2B	-2.55	1.46	1.51
25	3	302	CLA	MG-ND	-2.55	2.00	2.05
25	A	835	CLA	CHC-C1C	2.55	1.41	1.35
24	3	306	CHL	C3B-C2B	-2.55	1.36	1.40
27	4	318	XAT	O24-C25	-2.55	1.42	1.46
29	R	304	Q6L	C12-C13	-2.54	1.46	1.51
25	6	610	CLA	CMD-C2D	-2.54	1.45	1.50
26	W	318	IWJ	C29-C35	-2.54	1.52	1.56
30	3	319	BCR	C19-C18	2.54	1.51	1.45
25	G	203	CLA	CMB-C2B	-2.54	1.46	1.51
30	3	319	BCR	C12-C13	2.54	1.51	1.45
38	P	308	KC2	C2A-C1A	2.54	1.52	1.44
26	R	303	IWJ	C03-C02	2.54	1.36	1.33
29	S	320	Q6L	C02-C03	2.54	1.37	1.34
25	B	806	CLA	CMD-C2D	-2.54	1.45	1.50
26	4	317	IWJ	C03-C02	2.54	1.36	1.33
25	W	313	CLA	CMB-C2B	-2.54	1.46	1.51
33	A	802	CL0	C3B-CAB	-2.53	1.42	1.47
24	W	306	CHL	CHC-C1C	2.53	1.41	1.35
25	5	603	CLA	CMB-C2B	-2.53	1.46	1.51
29	Q	318	Q6L	C02-C03	2.53	1.37	1.34
25	A	841	CLA	CHC-C1C	2.53	1.41	1.35
25	F	803	CLA	CHC-C1C	2.53	1.41	1.35
29	W	315	Q6L	C34-C33	2.53	1.53	1.50
24	V	304	CHL	C3B-CAB	-2.53	1.42	1.47
25	5	606	CLA	CMB-C2B	-2.53	1.46	1.51
25	B	803	CLA	CMC-C2C	-2.53	1.45	1.50
25	B	842	CLA	C4B-CHC	-2.53	1.34	1.41
24	S	306	CHL	CMC-C2C	2.53	1.50	1.45
25	6	612	CLA	C3B-C2B	-2.53	1.36	1.40
29	2	616	Q6L	C12-C13	-2.53	1.46	1.51
25	A	830	CLA	CHC-C1C	2.53	1.41	1.35
25	A	836	CLA	C4D-ND	-2.53	1.34	1.37
25	T	310	CLA	CMD-C2D	-2.53	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	G	202	CLA	C3B-C2B	-2.53	1.36	1.40
30	3	319	BCR	C8-C9	2.53	1.51	1.45
25	1	605	CLA	CMB-C2B	-2.52	1.46	1.51
25	U	302	CLA	CMD-C2D	-2.52	1.45	1.50
25	6	610	CLA	CMB-C2B	-2.52	1.46	1.51
25	B	806	CLA	CMB-C2B	-2.52	1.46	1.51
29	S	316	Q6L	C02-C03	2.52	1.37	1.34
25	W	311	CLA	CMB-C2B	-2.52	1.46	1.51
25	B	821	CLA	C3B-CAB	-2.52	1.42	1.47
25	5	608	CLA	CMB-C2B	-2.52	1.46	1.51
29	Q	318	Q6L	C12-C13	-2.52	1.46	1.51
25	X	310	CLA	CMD-C2D	-2.52	1.45	1.50
29	R	319	Q6L	C34-C33	2.52	1.53	1.50
25	2	606	CLA	C3B-C2B	-2.52	1.36	1.40
25	Q	304	CLA	C3B-C2B	-2.52	1.36	1.40
26	V	320	IWJ	C03-C02	2.52	1.36	1.33
25	J	102	CLA	CMC-C2C	-2.52	1.45	1.50
24	X	315	CHL	CMB-C2B	-2.52	1.46	1.51
25	A	831	CLA	MG-ND	-2.52	2.00	2.05
26	X	318	IWJ	C29-C35	-2.52	1.52	1.56
29	2	616	Q6L	C02-C03	2.52	1.37	1.34
24	4	307	CHL	CMB-C2B	-2.51	1.46	1.51
25	A	840	CLA	CMB-C2B	-2.51	1.46	1.51
25	A	826	CLA	CMB-C2B	-2.51	1.46	1.51
29	P	321	Q6L	C12-C13	-2.51	1.46	1.51
25	O	2003	CLA	CMB-C2B	-2.51	1.46	1.51
25	B	831	CLA	CHC-C1C	2.51	1.41	1.35
25	A	856	CLA	C3B-CAB	-2.51	1.42	1.47
25	3	311	CLA	C4-C3	-2.51	1.44	1.50
30	B	846	BCR	C8-C9	2.51	1.51	1.45
25	O	2004	CLA	CMB-C2B	-2.51	1.46	1.51
24	1	601	CHL	C3B-CAB	-2.51	1.42	1.47
30	L	307	BCR	C19-C18	2.51	1.51	1.45
25	B	834	CLA	C3B-C2B	-2.51	1.36	1.40
25	Q	304	CLA	CAA-C2A	-2.51	1.49	1.54
26	V	318	IWJ	C03-C02	2.51	1.36	1.33
29	S	315	Q6L	C12-C13	-2.51	1.46	1.51
25	B	830	CLA	C3B-C2B	-2.51	1.36	1.40
29	U	317	Q6L	C34-C33	2.51	1.53	1.50
24	R	311	CHL	C4D-ND	-2.51	1.34	1.37
24	W	306	CHL	CMB-C2B	-2.51	1.46	1.51
24	W	304	CHL	CMB-C2B	-2.51	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	P	307	CHL	CMB-C2B	-2.50	1.46	1.51
25	Q	301	CLA	CHC-C1C	2.50	1.41	1.35
26	6	614	IWJ	C03-C02	2.50	1.36	1.33
27	2	617	XAT	C22-C21	-2.50	1.50	1.54
24	2	605	CHL	CMD-C2D	-2.50	1.45	1.50
33	A	802	CL0	MG-ND	-2.50	2.00	2.05
25	2	609	CLA	CMB-C2B	-2.50	1.46	1.51
25	3	307	CLA	CMC-C2C	-2.50	1.45	1.50
25	G	202	CLA	CMB-C2B	-2.50	1.46	1.51
25	6	604	CLA	CMB-C2B	-2.50	1.46	1.51
38	V	308	KC2	O2A-CGA	2.50	1.36	1.30
25	B	813	CLA	CHC-C1C	2.50	1.41	1.35
25	T	302	CLA	CMB-C2B	-2.50	1.46	1.51
38	V	308	KC2	CHD-C4C	2.50	1.41	1.35
25	A	820	CLA	CMC-C2C	-2.49	1.45	1.50
25	5	610	CLA	CMB-C2B	-2.49	1.46	1.51
24	P	314	CHL	C1D-ND	2.49	1.40	1.37
25	U	309	CLA	CMB-C2B	-2.49	1.46	1.51
24	2	615	CHL	CMD-C2D	-2.49	1.45	1.50
25	A	837	CLA	CMD-C2D	-2.49	1.45	1.50
25	1	607	CLA	CMB-C2B	-2.49	1.46	1.51
30	A	851	BCR	C16-C15	-2.49	1.29	1.36
38	Q	310	KC2	CHD-C4C	2.49	1.41	1.35
25	B	811	CLA	C3B-C2B	-2.49	1.36	1.40
38	X	309	KC2	CMB-C2B	-2.49	1.45	1.50
38	Q	310	KC2	C1B-C2B	2.49	1.50	1.45
25	O	2002	CLA	C3B-C2B	-2.49	1.36	1.40
25	B	804	CLA	CMB-C2B	-2.49	1.46	1.51
25	L	301	CLA	CMB-C2B	-2.49	1.46	1.51
29	R	304	Q6L	C02-C03	2.49	1.37	1.34
29	R	301	Q6L	C33-C32	2.49	1.36	1.33
25	2	610	CLA	CMB-C2B	-2.49	1.46	1.51
25	2	603	CLA	CHC-C1C	2.49	1.41	1.35
25	T	312	CLA	CMB-C2B	-2.49	1.46	1.51
25	A	841	CLA	CMD-C2D	-2.49	1.45	1.50
29	X	319	Q6L	C02-C03	2.49	1.37	1.34
30	4	319	BCR	C30-C25	-2.48	1.50	1.53
29	V	321	Q6L	C34-C33	2.48	1.53	1.50
25	B	813	CLA	CMD-C2D	-2.48	1.45	1.50
25	3	308	CLA	C3B-CAB	-2.48	1.42	1.47
25	P	302	CLA	C3B-CAB	-2.48	1.42	1.47
29	W	320	Q6L	C02-C03	2.48	1.37	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	R	314	CLA	CMB-C2B	-2.48	1.46	1.51
25	A	827	CLA	CHC-C1C	2.48	1.41	1.35
25	3	309	CLA	CMB-C2B	-2.48	1.46	1.51
24	W	306	CHL	CAC-C3C	-2.48	1.44	1.51
25	B	824	CLA	CHC-C1C	2.48	1.41	1.35
38	U	307	KC2	CMC-C2C	-2.48	1.45	1.50
25	A	822	CLA	CMB-C2B	-2.48	1.46	1.51
24	X	307	CHL	CHC-C1C	2.48	1.41	1.35
29	T	322	Q6L	C02-C03	2.48	1.37	1.34
30	J	103	BCR	C19-C18	2.48	1.51	1.45
24	X	307	CHL	C4B-CHC	-2.48	1.34	1.41
29	V	315	Q6L	C11-C03	-2.48	1.47	1.51
24	T	306	CHL	CMB-C2B	-2.48	1.46	1.51
25	Q	313	CLA	CMB-C2B	-2.47	1.46	1.51
26	S	318	IWJ	C03-C02	2.47	1.36	1.33
25	2	614	CLA	CMB-C2B	-2.47	1.46	1.51
25	U	303	CLA	C3B-CAB	-2.47	1.42	1.47
25	T	301	CLA	CMC-C2C	-2.47	1.45	1.50
25	1	607	CLA	C3D-C4D	2.47	1.48	1.42
24	T	320	CHL	CMB-C2B	-2.47	1.46	1.51
29	Q	317	Q6L	C34-C33	2.47	1.53	1.50
29	V	315	Q6L	C02-C03	2.47	1.37	1.34
26	Q	320	IWJ	C03-C02	2.47	1.36	1.33
29	W	315	Q6L	C02-C03	2.47	1.37	1.34
26	4	317	IWJ	C26-C24	-2.47	1.45	1.49
25	O	2005	CLA	CMB-C2B	-2.47	1.46	1.51
25	X	302	CLA	C3B-C2B	-2.47	1.36	1.40
25	A	836	CLA	CMB-C2B	-2.46	1.46	1.51
25	U	302	CLA	CMB-C2B	-2.46	1.46	1.51
29	V	316	Q6L	C02-C03	2.46	1.37	1.34
38	S	308	KC2	CMB-C2B	-2.46	1.45	1.50
24	P	306	CHL	CMB-C2B	-2.46	1.46	1.51
25	6	612	CLA	CHC-C1C	2.46	1.41	1.35
29	Q	319	Q6L	C12-C13	-2.46	1.46	1.51
25	P	302	CLA	CMB-C2B	-2.46	1.46	1.51
38	Q	310	KC2	O2A-CGA	2.46	1.36	1.30
24	X	305	CHL	CMB-C2B	-2.46	1.46	1.51
25	X	302	CLA	CMB-C2B	-2.46	1.46	1.51
24	W	314	CHL	CMD-C2D	-2.46	1.45	1.50
25	L	302	CLA	CMC-C2C	-2.46	1.45	1.50
25	B	833	CLA	C3B-C2B	-2.46	1.37	1.40
29	T	322	Q6L	C33-C32	2.46	1.36	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	O	2006	Q6L	C12-C13	-2.46	1.46	1.51
25	A	845	CLA	CMC-C2C	-2.46	1.45	1.50
24	S	304	CHL	C3B-C2B	-2.46	1.37	1.40
30	A	851	BCR	C8-C9	2.46	1.51	1.45
25	A	804	CLA	MG-ND	-2.46	2.00	2.05
25	V	313	CLA	CMB-C2B	-2.45	1.46	1.51
25	B	839	CLA	C3B-CAB	-2.45	1.42	1.47
25	B	824	CLA	C4B-CHC	-2.45	1.34	1.41
38	U	307	KC2	CMB-C2B	-2.45	1.45	1.50
25	5	601	CLA	CMB-C2B	-2.45	1.46	1.51
38	Q	310	KC2	CMC-C2C	-2.45	1.45	1.50
25	B	805	CLA	C3B-CAB	-2.45	1.42	1.47
25	V	309	CLA	C1A-CHA	-2.45	1.32	1.43
30	4	319	BCR	C19-C18	2.45	1.51	1.45
27	3	316	XAT	C35-C15	-2.45	1.29	1.36
30	K	207	BCR	C19-C18	2.45	1.51	1.45
29	X	316	Q6L	C12-C13	-2.44	1.46	1.51
25	T	310	CLA	CMB-C2B	-2.44	1.46	1.51
25	B	825	CLA	C3B-C2B	-2.44	1.37	1.40
25	A	828	CLA	CHC-C1C	2.44	1.41	1.35
25	H	301	CLA	CMB-C2B	-2.44	1.46	1.51
34	B	844	PQN	C10-C1	-2.44	1.43	1.48
29	Q	319	Q6L	C02-C03	2.44	1.37	1.34
25	A	812	CLA	C3B-CAB	-2.44	1.43	1.47
25	T	309	CLA	CMD-C2D	-2.44	1.45	1.50
25	S	312	CLA	CMB-C2B	-2.44	1.46	1.51
25	A	813	CLA	C3B-C2B	-2.43	1.37	1.40
25	P	301	CLA	CMB-C2B	-2.43	1.46	1.51
25	G	203	CLA	C4B-CHC	-2.43	1.34	1.41
29	X	319	Q6L	C33-C32	2.43	1.36	1.33
25	F	802	CLA	CMD-C2D	-2.43	1.45	1.50
25	6	611	CLA	CMB-C2B	-2.43	1.46	1.51
25	L	304	CLA	CMB-C2B	-2.43	1.46	1.51
25	R	315	CLA	C4D-ND	-2.43	1.34	1.37
25	6	610	CLA	C3B-CAB	-2.43	1.43	1.47
25	A	809	CLA	C3B-C2B	-2.43	1.37	1.40
26	X	318	IWJ	C03-C02	2.43	1.36	1.33
26	4	317	IWJ	C28-C29	-2.43	1.51	1.54
25	P	309	CLA	CMB-C2B	-2.43	1.46	1.51
25	V	312	CLA	C3B-C2B	-2.43	1.37	1.40
30	J	103	BCR	C12-C13	2.43	1.51	1.45
25	B	827	CLA	CHC-C1C	2.43	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	W	301	CLA	C3B-C2B	-2.43	1.37	1.40
25	B	808	CLA	CHC-C1C	2.43	1.41	1.35
34	B	844	PQN	C11-C12	2.43	1.54	1.50
26	3	315	IWJ	C03-C02	2.43	1.36	1.33
25	B	809	CLA	CHC-C1C	2.43	1.41	1.35
38	T	308	KC2	CMC-C2C	-2.42	1.45	1.50
29	P	319	Q6L	C34-C33	2.42	1.53	1.50
38	U	307	KC2	O2A-CGA	2.42	1.36	1.30
25	B	833	CLA	CHC-C1C	2.42	1.41	1.35
30	G	205	BCR	C8-C9	2.42	1.51	1.45
30	A	852	BCR	C8-C9	2.42	1.51	1.45
38	P	308	KC2	CMC-C2C	-2.42	1.45	1.50
24	S	304	CHL	MG-ND	-2.42	2.01	2.05
25	U	301	CLA	CMC-C2C	-2.42	1.45	1.50
30	F	801	BCR	C37-C22	2.42	1.55	1.50
25	W	309	CLA	C3B-C2B	-2.42	1.37	1.40
29	V	316	Q6L	C33-C32	2.42	1.36	1.33
29	S	315	Q6L	C02-C03	2.42	1.37	1.34
27	1	612	XAT	O24-C25	-2.41	1.42	1.46
25	T	309	CLA	C1B-NB	2.41	1.37	1.35
29	R	304	Q6L	C33-C32	2.41	1.36	1.33
25	S	302	CLA	C3B-C2B	-2.41	1.37	1.40
25	X	303	CLA	CMB-C2B	-2.41	1.46	1.51
25	B	837	CLA	CHC-C1C	2.41	1.41	1.35
25	3	308	CLA	CMB-C2B	-2.41	1.46	1.51
38	T	308	KC2	CMB-C2B	-2.41	1.45	1.50
25	V	302	CLA	C4B-CHC	-2.41	1.34	1.41
29	R	320	Q6L	C02-C03	2.41	1.37	1.34
38	W	308	KC2	C4D-ND	-2.41	1.33	1.35
29	S	316	Q6L	C12-C13	-2.41	1.46	1.51
25	V	309	CLA	C1C-C2C	2.41	1.49	1.44
25	S	309	CLA	CMB-C2B	-2.41	1.46	1.51
25	B	822	CLA	CMD-C2D	-2.41	1.45	1.50
25	P	310	CLA	CMB-C2B	-2.41	1.46	1.51
25	B	829	CLA	MG-ND	-2.41	2.01	2.05
25	B	809	CLA	CMD-C2D	-2.41	1.45	1.50
25	A	812	CLA	CAA-C2A	-2.40	1.49	1.54
38	S	308	KC2	CMC-C2C	-2.40	1.45	1.50
25	A	824	CLA	CHC-C1C	2.40	1.41	1.35
25	A	843	CLA	CHC-C1C	2.40	1.41	1.35
25	6	612	CLA	C4B-CHC	-2.40	1.34	1.41
25	K	204	CLA	C4B-CHC	-2.40	1.34	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	A	841	CLA	C3B-C2B	-2.40	1.37	1.40
38	P	308	KC2	CMB-C2B	-2.40	1.45	1.50
30	B	848	BCR	C16-C15	-2.40	1.29	1.36
24	T	314	CHL	CMB-C2B	-2.40	1.46	1.51
25	3	311	CLA	C4B-CHC	-2.40	1.34	1.41
38	X	309	KC2	C1B-NB	-2.40	1.34	1.37
24	S	305	CHL	CMD-C2D	-2.40	1.45	1.50
37	H	306	NEX	C38-C25	2.39	1.55	1.51
25	3	305	CLA	CMD-C2D	-2.39	1.45	1.50
25	U	308	CLA	C4B-CHC	-2.39	1.34	1.41
25	K	204	CLA	CMB-C2B	-2.39	1.46	1.51
25	A	829	CLA	CMD-C2D	-2.39	1.45	1.50
29	V	315	Q6L	C01-C02	2.39	1.54	1.50
38	T	308	KC2	CHD-C4C	2.39	1.41	1.35
25	A	828	CLA	CMD-C2D	-2.39	1.45	1.50
29	U	315	Q6L	C12-C13	-2.39	1.46	1.51
29	X	301	Q6L	C02-C03	2.39	1.37	1.34
25	T	312	CLA	CMD-C2D	-2.39	1.45	1.50
30	M	101	BCR	C8-C9	2.39	1.51	1.45
25	2	602	CLA	C2-C3	2.39	1.38	1.33
29	S	321	Q6L	C02-C03	2.39	1.37	1.34
25	B	808	CLA	CMD-C2D	-2.39	1.45	1.50
24	W	307	CHL	CMB-C2B	-2.39	1.46	1.51
25	6	612	CLA	CMD-C2D	-2.39	1.45	1.50
30	L	307	BCR	C17-C18	-2.39	1.32	1.35
25	V	302	CLA	CHC-C1C	2.39	1.41	1.35
25	B	818	CLA	C3B-CAB	-2.39	1.43	1.47
25	S	303	CLA	C3B-C2B	-2.39	1.37	1.40
24	V	306	CHL	CMB-C2B	-2.38	1.46	1.51
29	W	319	Q6L	C01-C02	2.38	1.54	1.50
25	6	608	CLA	CMB-C2B	-2.38	1.46	1.51
25	B	843	CLA	C3B-CAB	-2.38	1.43	1.47
25	S	312	CLA	CMC-C2C	-2.38	1.45	1.50
25	2	614	CLA	CHC-C1C	2.38	1.41	1.35
25	A	808	CLA	CHC-C1C	2.38	1.41	1.35
38	P	308	KC2	O2A-CGA	2.38	1.36	1.30
25	6	602	CLA	CHC-C1C	2.38	1.41	1.35
25	S	310	CLA	MG-NA	2.38	2.11	2.06
25	A	835	CLA	C3B-CAB	-2.38	1.43	1.47
25	H	304	CLA	C4B-CHC	-2.38	1.34	1.41
30	A	849	BCR	C12-C13	2.38	1.51	1.45
38	X	309	KC2	O2A-CGA	2.38	1.36	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B	824	CLA	CMD-C2D	-2.38	1.45	1.50
25	B	808	CLA	C4B-CHC	-2.38	1.34	1.41
25	W	312	CLA	C4B-CHC	-2.37	1.34	1.41
25	1	609	CLA	CMB-C2B	-2.37	1.46	1.51
24	P	306	CHL	CMD-C2D	-2.37	1.45	1.50
25	K	201	CLA	CMB-C2B	-2.37	1.46	1.51
29	P	319	Q6L	C01-C02	2.37	1.54	1.50
25	A	808	CLA	MG-ND	-2.37	2.01	2.05
25	A	842	CLA	C5-C3	-2.37	1.46	1.51
37	R	321	NEX	C28-C29	2.37	1.51	1.45
25	T	309	CLA	C3B-CAB	-2.37	1.43	1.47
24	U	304	CHL	CMB-C2B	-2.37	1.46	1.51
25	B	832	CLA	MG-ND	-2.37	2.01	2.05
29	T	319	Q6L	C02-C03	2.37	1.37	1.34
29	V	316	Q6L	C29-C27	2.37	1.51	1.45
29	P	316	Q6L	C33-C32	2.37	1.36	1.33
25	X	312	CLA	C3B-C2B	-2.37	1.37	1.40
29	U	317	Q6L	C12-C13	-2.37	1.46	1.51
25	B	823	CLA	MG-NC	2.37	2.11	2.06
25	S	302	CLA	C3B-CAB	-2.37	1.43	1.47
25	F	802	CLA	C4B-CHC	-2.37	1.34	1.41
38	S	308	KC2	O2A-CGA	2.37	1.36	1.30
38	R	312	KC2	MG-NB	-2.37	2.01	2.05
38	W	308	KC2	O2A-CGA	2.37	1.36	1.30
25	Q	315	CLA	CMB-C2B	-2.37	1.46	1.51
25	4	303	CLA	CMD-C2D	-2.37	1.45	1.50
25	O	2002	CLA	CMD-C2D	-2.37	1.45	1.50
29	V	321	Q6L	C02-C03	2.37	1.37	1.34
25	3	310	CLA	CMB-C2B	-2.36	1.46	1.51
25	A	835	CLA	C4B-CHC	-2.36	1.34	1.41
30	A	849	BCR	C14-C13	-2.36	1.32	1.35
25	2	602	CLA	CHC-C1C	2.36	1.41	1.35
29	X	317	Q6L	C12-C13	-2.36	1.46	1.51
25	L	302	CLA	C4B-CHC	-2.36	1.34	1.41
25	4	309	CLA	C3B-C2B	-2.36	1.37	1.40
25	P	303	CLA	CMB-C2B	-2.36	1.46	1.51
25	G	204	CLA	C4B-CHC	-2.36	1.34	1.41
24	R	318	CHL	CMD-C2D	-2.36	1.45	1.50
37	S	317	NEX	C35-C15	-2.36	1.29	1.36
29	R	319	Q6L	C01-C02	2.36	1.54	1.50
25	F	802	CLA	CHC-C1C	2.36	1.41	1.35
25	B	811	CLA	CAC-C3C	-2.36	1.45	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B	826	CLA	CMD-C2D	-2.36	1.45	1.50
25	U	310	CLA	CMB-C2B	-2.35	1.46	1.51
29	P	315	Q6L	C02-C03	2.35	1.37	1.34
24	1	604	CHL	CHC-C1C	2.35	1.41	1.35
25	4	312	CLA	CMB-C2B	-2.35	1.46	1.51
25	A	804	CLA	C3B-CAB	-2.35	1.43	1.47
25	A	808	CLA	CMD-C2D	-2.35	1.45	1.50
29	U	315	Q6L	C33-C32	2.35	1.36	1.33
25	A	812	CLA	CMB-C2B	-2.35	1.46	1.51
25	B	810	CLA	C3B-CAB	-2.35	1.43	1.47
25	B	830	CLA	CHC-C1C	2.35	1.41	1.35
25	X	303	CLA	C3B-CAB	-2.35	1.43	1.47
26	T	318	IWJ	C29-C35	-2.35	1.52	1.56
29	W	316	Q6L	C33-C32	2.35	1.36	1.33
24	U	304	CHL	C3B-C2B	-2.35	1.37	1.40
25	X	314	CLA	C3B-C2B	-2.35	1.37	1.40
25	B	816	CLA	CMB-C2B	-2.35	1.46	1.51
25	G	203	CLA	C3B-C2B	-2.35	1.37	1.40
38	S	308	KC2	C4D-ND	-2.35	1.33	1.35
25	4	303	CLA	MG-ND	-2.35	2.01	2.05
25	5	602	CLA	C3B-C2B	-2.35	1.37	1.40
25	V	309	CLA	CMB-C2B	-2.34	1.46	1.51
29	R	323	Q6L	C01-C02	2.34	1.54	1.50
26	Q	320	IWJ	C29-C35	-2.34	1.52	1.56
25	A	821	CLA	C4B-CHC	-2.34	1.34	1.41
25	A	810	CLA	C4B-CHC	-2.34	1.34	1.41
25	B	839	CLA	CMD-C2D	-2.34	1.45	1.50
24	4	302	CHL	CMD-C2D	-2.34	1.45	1.50
25	A	822	CLA	CMD-C2D	-2.34	1.45	1.50
24	2	607	CHL	CMA-C3A	-2.34	1.48	1.53
25	B	843	CLA	CMB-C2B	-2.34	1.46	1.51
27	4	318	XAT	C8-C9	2.34	1.51	1.45
30	K	202	BCR	C36-C18	2.34	1.55	1.50
25	T	301	CLA	CMD-C2D	-2.34	1.45	1.50
29	P	321	Q6L	C01-C02	2.33	1.54	1.50
29	R	304	Q6L	C01-C02	2.33	1.54	1.50
25	F	803	CLA	C4B-CHC	-2.33	1.34	1.41
25	R	307	CLA	C3B-C2B	-2.33	1.37	1.40
25	A	842	CLA	C4B-CHC	-2.33	1.34	1.41
25	B	815	CLA	CMD-C2D	-2.33	1.45	1.50
29	P	315	Q6L	C01-C02	2.33	1.54	1.50
25	T	313	CLA	C3B-C2B	-2.33	1.37	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	A	831	CLA	C3B-CAB	-2.33	1.43	1.47
29	S	321	Q6L	C29-C27	2.33	1.50	1.45
30	B	848	BCR	C19-C18	2.33	1.50	1.45
25	1	613	CLA	CMB-C2B	-2.33	1.46	1.51
25	A	816	CLA	CMB-C2B	-2.33	1.46	1.51
25	T	303	CLA	C3B-C2B	-2.33	1.37	1.40
25	R	306	CLA	C3B-C2B	-2.33	1.37	1.40
29	O	2007	Q6L	C12-C13	-2.33	1.46	1.51
38	R	312	KC2	O2A-CGA	2.33	1.36	1.30
30	3	318	BCR	C30-C25	-2.33	1.50	1.53
38	R	312	KC2	CMB-C2B	-2.33	1.45	1.50
24	6	605	CHL	CMB-C2B	-2.32	1.46	1.51
25	A	856	CLA	CHC-C1C	2.32	1.40	1.35
25	B	840	CLA	CHC-C1C	2.32	1.40	1.35
29	X	301	Q6L	C01-C02	2.32	1.54	1.50
29	T	319	Q6L	C12-C13	-2.32	1.46	1.51
25	H	302	CLA	C3B-C2B	-2.32	1.37	1.40
30	K	202	BCR	C12-C13	2.32	1.50	1.45
37	R	321	NEX	C32-C33	2.32	1.50	1.45
25	B	808	CLA	MG-ND	-2.32	2.01	2.05
25	B	823	CLA	C3B-C2B	-2.32	1.37	1.40
25	U	302	CLA	C3B-C2B	-2.32	1.37	1.40
25	P	312	CLA	CMB-C2B	-2.32	1.46	1.51
24	V	305	CHL	CMB-C2B	-2.32	1.46	1.51
25	B	818	CLA	CMB-C2B	-2.32	1.46	1.51
25	A	833	CLA	CMD-C2D	-2.32	1.45	1.50
25	B	821	CLA	C4B-CHC	-2.32	1.34	1.41
29	W	319	Q6L	C02-C03	2.32	1.37	1.34
25	B	808	CLA	C1D-ND	2.32	1.40	1.37
25	U	308	CLA	C1D-ND	2.32	1.40	1.37
25	W	303	CLA	O2D-CED	-2.32	1.39	1.45
25	F	803	CLA	CAC-C3C	-2.31	1.45	1.51
25	U	312	CLA	CMB-C2B	-2.31	1.46	1.51
24	U	306	CHL	C3B-C2B	-2.31	1.37	1.40
29	P	321	Q6L	C34-C33	2.31	1.53	1.50
29	T	316	Q6L	C33-C32	2.31	1.36	1.33
25	S	302	CLA	CMC-C2C	-2.31	1.45	1.50
30	B	846	BCR	C23-C22	2.31	1.50	1.45
30	F	801	BCR	C8-C9	2.31	1.50	1.45
25	B	832	CLA	C4B-CHC	-2.31	1.34	1.41
25	1	605	CLA	CMD-C2D	-2.31	1.45	1.50
38	V	308	KC2	CAA-C2A	2.31	1.53	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	6	607	CLA	C4B-CHC	-2.31	1.34	1.41
24	W	305	CHL	CMB-C2B	-2.31	1.46	1.51
25	U	308	CLA	CHC-C1C	2.31	1.40	1.35
25	4	313	CLA	C4B-CHC	-2.31	1.34	1.41
30	A	848	BCR	C23-C22	2.31	1.50	1.45
37	R	321	NEX	C12-C13	2.31	1.50	1.45
25	B	835	CLA	CMB-C2B	-2.30	1.46	1.51
25	B	834	CLA	CHC-C1C	2.30	1.40	1.35
25	S	313	CLA	CMB-C2B	-2.30	1.46	1.51
25	A	807	CLA	C4B-CHC	-2.30	1.34	1.41
25	B	815	CLA	CMC-C2C	-2.30	1.45	1.50
25	A	856	CLA	C3B-C2B	-2.30	1.37	1.40
25	1	603	CLA	CHC-C1C	2.30	1.40	1.35
30	K	207	BCR	C16-C15	-2.30	1.30	1.36
25	U	308	CLA	C3B-C2B	-2.30	1.37	1.40
30	J	101	BCR	C40-C30	-2.30	1.49	1.53
25	2	603	CLA	C3B-CAB	-2.30	1.43	1.47
26	R	303	IWJ	C29-C35	-2.30	1.52	1.56
24	Q	309	CHL	CMD-C2D	-2.30	1.45	1.50
25	B	838	CLA	CHC-C1C	2.30	1.40	1.35
24	T	306	CHL	C3B-CAB	-2.30	1.43	1.47
25	P	311	CLA	CMB-C2B	-2.30	1.46	1.51
30	K	205	BCR	C19-C18	2.30	1.50	1.45
25	A	805	CLA	CMB-C2B	-2.30	1.46	1.51
31	B	801	LMG	O1-C1	2.30	1.44	1.40
25	B	831	CLA	CMC-C2C	-2.30	1.45	1.50
37	P	317	NEX	C28-C29	2.30	1.50	1.45
25	V	301	CLA	CHC-C1C	2.30	1.40	1.35
25	A	807	CLA	C3B-C2B	-2.30	1.37	1.40
38	P	308	KC2	CHD-C4C	2.30	1.40	1.35
25	S	301	CLA	CMB-C2B	-2.30	1.46	1.51
24	R	311	CHL	CMC-C2C	2.30	1.50	1.45
25	B	842	CLA	C4D-ND	-2.29	1.34	1.37
29	V	319	Q6L	C01-C02	2.29	1.54	1.50
38	T	308	KC2	O2A-CGA	2.29	1.36	1.30
25	6	607	CLA	CHC-C1C	2.29	1.40	1.35
29	P	319	Q6L	C12-C13	-2.29	1.46	1.51
29	Q	317	Q6L	C02-C03	2.29	1.37	1.34
25	Q	304	CLA	C4B-CHC	-2.29	1.34	1.41
25	B	840	CLA	CMD-C2D	-2.29	1.45	1.50
33	A	802	CL0	CHC-C1C	2.29	1.40	1.35
29	T	319	Q6L	C33-C32	2.29	1.35	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	4	302	CHL	CMB-C2B	-2.29	1.46	1.51
25	A	807	CLA	CMD-C2D	-2.29	1.46	1.50
24	Q	308	CHL	MG-ND	-2.29	2.01	2.05
25	B	835	CLA	C3B-CAB	-2.28	1.43	1.47
25	B	841	CLA	CMC-C2C	-2.28	1.46	1.50
30	G	205	BCR	C10-C9	2.28	1.38	1.35
25	F	803	CLA	C3B-CAB	-2.28	1.43	1.47
34	A	844	PQN	C6-C5	2.28	1.43	1.39
27	2	617	XAT	C8-C9	2.28	1.50	1.45
30	G	201	BCR	C8-C9	2.28	1.50	1.45
25	A	808	CLA	CMB-C2B	-2.28	1.46	1.51
25	K	203	CLA	C4B-CHC	-2.28	1.34	1.41
38	U	307	KC2	MG-NB	-2.28	2.01	2.05
25	A	803	CLA	C1D-ND	2.28	1.40	1.37
24	4	302	CHL	CMA-C3A	-2.28	1.48	1.53
33	A	802	CL0	C3B-C2B	-2.28	1.37	1.40
24	S	305	CHL	MG-ND	-2.28	2.01	2.05
25	B	810	CLA	CMB-C2B	-2.28	1.46	1.51
27	3	316	XAT	O4-C5	-2.28	1.43	1.46
25	3	303	CLA	C4B-CHC	-2.28	1.34	1.41
25	B	802	CLA	CHC-C1C	2.28	1.40	1.35
30	B	846	BCR	C16-C15	-2.28	1.30	1.36
25	2	608	CLA	CMB-C2B	-2.28	1.46	1.51
24	R	302	CHL	CMB-C2B	-2.28	1.46	1.51
25	A	824	CLA	C3B-C2B	-2.28	1.37	1.40
29	S	320	Q6L	C01-C02	2.28	1.54	1.50
29	X	316	Q6L	C01-C02	2.28	1.54	1.50
25	S	311	CLA	CMB-C2B	-2.28	1.46	1.51
25	6	603	CLA	C4B-CHC	-2.28	1.34	1.41
25	1	608	CLA	C4B-CHC	-2.28	1.34	1.41
27	4	318	XAT	O4-C5	-2.27	1.43	1.46
24	3	306	CHL	C3B-CAB	-2.27	1.43	1.47
25	T	311	CLA	CMB-C2B	-2.27	1.46	1.51
25	V	310	CLA	CHC-C1C	2.27	1.40	1.35
24	U	306	CHL	CMD-C2D	-2.27	1.46	1.50
30	H	305	BCR	C12-C13	2.27	1.50	1.45
24	U	313	CHL	CMB-C2B	-2.27	1.46	1.51
38	W	308	KC2	CMB-C2B	-2.27	1.46	1.50
25	W	303	CLA	C3B-C2B	-2.27	1.37	1.40
25	2	611	CLA	CMB-C2B	-2.27	1.46	1.51
24	T	314	CHL	CMD-C2D	-2.27	1.46	1.50
25	Q	313	CLA	CMD-C2D	-2.27	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	M	101	BCR	C1-C6	-2.27	1.50	1.53
25	A	836	CLA	C3C-C2C	2.27	1.41	1.36
26	R	322	IWJ	C29-C35	-2.27	1.52	1.56
25	R	314	CLA	C3B-C2B	-2.27	1.37	1.40
29	T	315	Q6L	C33-C32	2.26	1.35	1.33
24	S	307	CHL	CMD-C2D	-2.26	1.46	1.50
38	U	307	KC2	CHD-C4C	2.26	1.40	1.35
25	R	313	CLA	CMB-C2B	-2.26	1.46	1.51
25	A	814	CLA	C4B-CHC	-2.26	1.34	1.41
24	X	307	CHL	CAC-C3C	-2.26	1.45	1.51
25	A	845	CLA	CMD-C2D	-2.26	1.46	1.50
30	B	845	BCR	C30-C25	-2.26	1.50	1.53
25	A	823	CLA	C4B-CHC	-2.26	1.34	1.41
25	B	834	CLA	C4B-CHC	-2.26	1.34	1.41
24	V	314	CHL	MG-ND	-2.26	2.01	2.05
25	A	838	CLA	CMD-C2D	-2.26	1.46	1.50
30	B	845	BCR	C19-C18	2.26	1.50	1.45
25	3	313	CLA	C3B-C2B	-2.26	1.37	1.40
25	B	820	CLA	CMD-C2D	-2.26	1.46	1.50
25	6	608	CLA	CMA-C3A	-2.26	1.48	1.53
24	2	615	CHL	C4B-CHC	-2.26	1.34	1.41
30	3	319	BCR	C16-C15	-2.26	1.30	1.36
25	U	301	CLA	CMB-C2B	-2.26	1.46	1.51
25	T	313	CLA	CMD-C2D	-2.26	1.46	1.50
25	3	311	CLA	C3B-C2B	-2.26	1.37	1.40
25	A	810	CLA	C3B-C2B	-2.26	1.37	1.40
29	O	2006	Q6L	C01-C02	2.26	1.54	1.50
30	F	804	BCR	C19-C18	2.26	1.50	1.45
37	P	317	NEX	C32-C33	2.26	1.50	1.45
25	K	204	CLA	C3B-C2B	-2.25	1.37	1.40
25	B	812	CLA	CMB-C2B	-2.25	1.47	1.51
25	1	608	CLA	MG-ND	-2.25	2.01	2.05
25	4	311	CLA	CHC-C1C	2.25	1.40	1.35
25	B	813	CLA	CAC-C3C	-2.25	1.45	1.51
25	B	820	CLA	C3B-C2B	-2.25	1.37	1.40
29	W	316	Q6L	C01-C02	2.25	1.54	1.50
25	J	102	CLA	MG-ND	-2.25	2.01	2.05
26	3	315	IWJ	O39-C29	-2.25	1.39	1.43
25	B	834	CLA	CMD-C2D	-2.25	1.46	1.50
25	B	812	CLA	MG-ND	-2.25	2.01	2.05
29	W	319	Q6L	C33-C32	2.25	1.35	1.33
24	W	314	CHL	CMB-C2B	-2.25	1.47	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	4	306	CHL	CAC-C3C	-2.25	1.46	1.50
29	P	316	Q6L	C01-C02	2.25	1.54	1.50
34	A	844	PQN	C9-C10	2.25	1.43	1.39
25	B	820	CLA	C4B-CHC	-2.25	1.34	1.41
25	Q	304	CLA	CMB-C2B	-2.25	1.47	1.51
24	R	310	CHL	CMB-C2B	-2.25	1.47	1.51
25	B	813	CLA	C4B-CHC	-2.25	1.34	1.41
25	B	817	CLA	C4B-CHC	-2.25	1.34	1.41
29	S	323	Q6L	C34-C33	2.25	1.53	1.50
24	V	304	CHL	CMB-C2B	-2.25	1.47	1.51
25	W	301	CLA	CMC-C2C	-2.24	1.46	1.50
25	J	102	CLA	C3B-C2B	-2.24	1.37	1.40
27	5	612	XAT	O4-C5	-2.24	1.43	1.46
25	P	301	CLA	C3B-C2B	-2.24	1.37	1.40
25	U	302	CLA	CMC-C2C	-2.24	1.46	1.50
25	Q	311	CLA	CMB-C2B	-2.24	1.47	1.51
24	S	305	CHL	CMB-C2B	-2.24	1.47	1.51
25	V	309	CLA	CMD-C2D	-2.24	1.46	1.50
30	A	849	BCR	C16-C15	-2.24	1.30	1.36
24	S	304	CHL	CMD-C2D	-2.24	1.46	1.50
25	B	832	CLA	CMD-C2D	-2.24	1.46	1.50
25	S	301	CLA	MG-ND	-2.24	2.01	2.05
37	H	306	NEX	C32-C33	2.24	1.50	1.45
24	P	314	CHL	CMB-C2B	-2.24	1.47	1.51
25	B	805	CLA	CMA-C3A	-2.24	1.48	1.53
25	O	2001	CLA	CMB-C2B	-2.24	1.47	1.51
25	3	310	CLA	CMD-C2D	-2.24	1.46	1.50
24	U	313	CHL	CMD-C2D	-2.24	1.46	1.50
29	U	314	Q6L	C01-C02	2.24	1.54	1.50
24	6	605	CHL	MG-ND	-2.24	2.01	2.05
25	B	824	CLA	CMC-C2C	-2.24	1.46	1.50
27	1	612	XAT	C8-C9	2.23	1.50	1.45
25	B	841	CLA	C4B-CHC	-2.23	1.34	1.41
25	B	814	CLA	CMD-C2D	-2.23	1.46	1.50
26	S	319	IWJ	C29-C35	-2.23	1.53	1.56
25	4	305	CLA	C4B-CHC	-2.23	1.34	1.41
26	V	320	IWJ	C29-C35	-2.23	1.53	1.56
30	H	305	BCR	C23-C22	2.23	1.50	1.45
30	I	101	BCR	C12-C13	2.23	1.50	1.45
25	V	303	CLA	C3B-CAB	-2.23	1.43	1.47
29	T	322	Q6L	C01-C02	2.23	1.54	1.50
29	P	321	Q6L	C33-C32	2.23	1.35	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	2	612	CLA	CMC-C2C	-2.23	1.46	1.50
30	3	318	BCR	C19-C18	2.23	1.50	1.45
29	T	315	Q6L	C02-C03	2.23	1.37	1.34
29	S	316	Q6L	C33-C32	2.23	1.35	1.33
25	S	311	CLA	CMD-C2D	-2.23	1.46	1.50
38	V	308	KC2	MG-NC	2.23	2.11	2.06
25	A	831	CLA	CHC-C1C	2.23	1.40	1.35
25	W	312	CLA	CHC-C1C	2.23	1.40	1.35
26	P	320	IWJ	C29-C35	-2.23	1.53	1.56
25	A	839	CLA	CMC-C2C	-2.23	1.46	1.50
25	B	810	CLA	C4B-CHC	-2.23	1.34	1.41
37	T	317	NEX	C35-C15	-2.23	1.30	1.36
24	4	307	CHL	CAC-C3C	-2.23	1.45	1.51
25	V	313	CLA	C3B-C2B	-2.23	1.37	1.40
24	U	305	CHL	CMD-C2D	-2.23	1.46	1.50
24	U	306	CHL	CMB-C2B	-2.23	1.47	1.51
30	B	847	BCR	C12-C13	2.23	1.50	1.45
25	Q	313	CLA	C3B-C2B	-2.23	1.37	1.40
29	Q	318	Q6L	C34-C33	2.23	1.53	1.50
25	A	834	CLA	C3B-CAB	-2.22	1.43	1.47
24	U	305	CHL	CMB-C2B	-2.22	1.47	1.51
25	2	614	CLA	MG-ND	-2.22	2.01	2.05
34	B	844	PQN	C5-C4	-2.22	1.43	1.48
25	5	609	CLA	CMD-C2D	-2.22	1.46	1.50
25	X	302	CLA	CMD-C2D	-2.22	1.46	1.50
24	4	308	CHL	CMB-C2B	-2.22	1.47	1.51
29	T	319	Q6L	C01-C02	2.22	1.54	1.50
25	N	202	CLA	CMD-C2D	-2.22	1.46	1.50
26	1	611	IWJ	C26-C24	-2.22	1.45	1.49
25	2	603	CLA	C4B-CHC	-2.22	1.34	1.41
25	T	302	CLA	CMD-C2D	-2.22	1.46	1.50
25	V	311	CLA	C3B-C2B	-2.22	1.37	1.40
24	V	314	CHL	CMB-C2B	-2.22	1.47	1.51
24	V	306	CHL	CMD-C2D	-2.22	1.46	1.50
25	A	828	CLA	MG-ND	-2.22	2.01	2.05
26	P	318	IWJ	C26-C24	-2.22	1.45	1.49
29	O	2007	Q6L	C01-C02	2.22	1.54	1.50
26	V	317	IWJ	C03-C02	2.22	1.35	1.33
25	T	312	CLA	CMC-C2C	-2.22	1.46	1.50
25	1	602	CLA	CMB-C2B	-2.22	1.47	1.51
25	B	825	CLA	CMB-C2B	-2.22	1.47	1.51
30	A	848	BCR	C16-C15	-2.22	1.30	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	O	2006	Q6L	C33-C32	2.21	1.35	1.33
38	S	308	KC2	CHD-C4C	2.21	1.40	1.35
24	2	607	CHL	OMC-CMC	-2.21	1.16	1.22
25	B	840	CLA	C3B-CAB	-2.21	1.43	1.47
25	B	842	CLA	CAC-C3C	-2.21	1.45	1.51
24	S	306	CHL	C4B-CHC	-2.21	1.34	1.41
29	T	315	Q6L	C01-C02	2.21	1.54	1.50
37	W	317	NEX	C35-C15	-2.21	1.30	1.36
25	1	608	CLA	C3B-CAB	-2.21	1.43	1.47
24	S	314	CHL	CMB-C2B	-2.21	1.47	1.51
29	T	316	Q6L	C12-C13	-2.21	1.46	1.51
24	X	315	CHL	CMD-C2D	-2.21	1.46	1.50
25	X	304	CLA	C4B-CHC	-2.21	1.34	1.41
24	4	302	CHL	MG-ND	-2.21	2.01	2.05
25	6	607	CLA	MG-ND	-2.21	2.01	2.05
25	Q	311	CLA	C3B-C2B	-2.21	1.37	1.40
29	U	317	Q6L	C01-C02	2.20	1.54	1.50
29	U	314	Q6L	C33-C32	2.20	1.35	1.33
25	3	313	CLA	C4B-CHC	-2.20	1.34	1.41
24	W	307	CHL	CMD-C2D	-2.20	1.46	1.50
25	W	302	CLA	C4B-CHC	-2.20	1.34	1.41
25	A	829	CLA	CMB-C2B	-2.20	1.47	1.51
25	3	305	CLA	CMC-C2C	-2.20	1.46	1.50
25	S	312	CLA	CMD-C2D	-2.20	1.46	1.50
37	P	317	NEX	C35-C15	-2.20	1.30	1.36
29	S	316	Q6L	C01-C02	2.20	1.54	1.50
25	K	203	CLA	C3B-C2B	-2.20	1.37	1.40
25	H	302	CLA	C4B-CHC	-2.20	1.34	1.41
24	X	307	CHL	CMD-C2D	-2.20	1.46	1.50
38	V	308	KC2	CMB-C2B	-2.20	1.46	1.50
25	3	304	CLA	C4B-CHC	-2.20	1.34	1.41
25	B	819	CLA	C4B-CHC	-2.20	1.34	1.41
29	S	321	Q6L	C01-C02	2.20	1.54	1.50
25	5	607	CLA	C4B-CHC	-2.20	1.34	1.41
24	W	306	CHL	CMD-C2D	-2.19	1.46	1.50
25	2	613	CLA	C1D-C2D	2.19	1.49	1.45
24	2	605	CHL	C3B-CAB	-2.19	1.43	1.47
30	J	101	BCR	C10-C9	2.19	1.38	1.35
38	X	309	KC2	MG-NB	-2.19	2.01	2.05
30	K	207	BCR	C8-C7	2.19	1.39	1.33
25	A	817	CLA	C3B-C2B	-2.19	1.37	1.40
38	S	308	KC2	MG-NB	-2.19	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	S	312	CLA	C3B-C2B	-2.19	1.37	1.40
25	4	314	CLA	C3B-C2B	-2.19	1.37	1.40
24	P	306	CHL	CHC-C1C	2.19	1.40	1.35
30	3	317	BCR	C12-C13	2.19	1.50	1.45
25	A	815	CLA	CMC-C2C	-2.19	1.46	1.50
25	A	821	CLA	CMC-C2C	-2.19	1.46	1.50
30	3	318	BCR	C23-C22	2.19	1.50	1.45
25	B	817	CLA	CMC-C2C	-2.19	1.46	1.50
25	B	843	CLA	C3B-C2B	-2.19	1.37	1.40
25	O	2001	CLA	CMD-C2D	-2.19	1.46	1.50
30	L	306	BCR	C16-C15	-2.18	1.30	1.36
25	X	312	CLA	C4B-CHC	-2.18	1.34	1.41
29	W	320	Q6L	C01-C02	2.18	1.54	1.50
26	T	321	IWJ	C29-C35	-2.18	1.53	1.56
38	X	309	KC2	C4D-ND	-2.18	1.33	1.35
25	Q	313	CLA	C4B-CHC	-2.18	1.34	1.41
25	6	612	CLA	C3B-CAB	-2.18	1.43	1.47
29	P	315	Q6L	C33-C32	2.18	1.35	1.33
25	R	307	CLA	CMD-C2D	-2.18	1.46	1.50
29	O	2007	Q6L	C29-C27	2.18	1.50	1.45
25	K	204	CLA	CMC-C2C	-2.18	1.46	1.50
24	Q	316	CHL	CMB-C2B	-2.18	1.47	1.51
30	B	848	BCR	C34-C9	2.18	1.55	1.50
25	W	301	CLA	C3B-CAB	-2.18	1.43	1.47
25	B	807	CLA	CMD-C2D	-2.18	1.46	1.50
29	X	317	Q6L	C01-C02	2.18	1.54	1.50
24	X	308	CHL	CMB-C2B	-2.18	1.47	1.51
30	K	205	BCR	C16-C15	-2.18	1.30	1.36
25	R	317	CLA	CMB-C2B	-2.18	1.47	1.51
24	6	601	CHL	MG-ND	-2.18	2.01	2.05
25	V	312	CLA	C4B-CHC	-2.18	1.34	1.41
29	R	323	Q6L	C33-C32	2.18	1.35	1.33
26	T	321	IWJ	O39-C29	-2.18	1.39	1.43
25	V	302	CLA	C3B-CAB	-2.18	1.43	1.47
25	A	810	CLA	CMD-C2D	-2.18	1.46	1.50
24	P	305	CHL	CMD-C2D	-2.18	1.46	1.50
25	A	804	CLA	C4B-CHC	-2.18	1.34	1.41
29	2	616	Q6L	C01-C02	2.18	1.54	1.50
29	P	321	Q6L	C02-C03	2.17	1.37	1.34
30	B	846	BCR	C12-C13	2.17	1.50	1.45
30	B	849	BCR	C8-C9	2.17	1.50	1.45
24	P	305	CHL	CMB-C2B	-2.17	1.47	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	A	844	PQN	C11-C3	2.17	1.55	1.51
26	V	318	IWJ	C29-C35	-2.17	1.53	1.56
25	V	309	CLA	C1B-NB	2.17	1.37	1.35
25	A	840	CLA	CMD-C2D	-2.17	1.46	1.50
30	G	201	BCR	C16-C15	-2.17	1.30	1.36
24	1	601	CHL	CMB-C2B	-2.17	1.47	1.51
25	B	809	CLA	C3B-CAB	-2.17	1.43	1.47
25	B	808	CLA	CMC-C2C	-2.17	1.46	1.50
29	W	315	Q6L	C01-C02	2.17	1.54	1.50
25	B	837	CLA	C4B-CHC	-2.17	1.35	1.41
25	H	304	CLA	CMD-C2D	-2.17	1.46	1.50
25	B	825	CLA	MG-ND	-2.17	2.01	2.05
25	O	2005	CLA	CMD-C2D	-2.16	1.46	1.50
25	A	809	CLA	C4B-CHC	-2.16	1.35	1.41
24	W	306	CHL	MG-ND	-2.16	2.01	2.05
29	R	320	Q6L	C33-C32	2.16	1.35	1.33
25	W	312	CLA	MG-NC	2.16	2.11	2.06
26	S	322	IWJ	C29-C35	-2.16	1.53	1.56
29	R	319	Q6L	C33-C32	2.16	1.35	1.33
27	2	617	XAT	O24-C25	-2.16	1.43	1.46
30	I	101	BCR	C16-C15	-2.16	1.30	1.36
25	X	302	CLA	CMC-C2C	-2.16	1.46	1.50
25	A	809	CLA	C3B-CAB	-2.16	1.43	1.47
25	N	202	CLA	CMB-C2B	-2.16	1.47	1.51
29	Q	319	Q6L	C01-C02	2.16	1.54	1.50
30	3	319	BCR	C1-C6	-2.16	1.50	1.53
24	4	302	CHL	C3B-C2B	-2.16	1.37	1.40
26	6	614	IWJ	C29-C35	-2.16	1.53	1.56
29	V	321	Q6L	C01-C02	2.16	1.54	1.50
25	Q	312	CLA	CMD-C2D	-2.16	1.46	1.50
25	A	819	CLA	CMB-C2B	-2.16	1.47	1.51
25	B	818	CLA	CMD-C2D	-2.16	1.46	1.50
29	Q	318	Q6L	C01-C02	2.16	1.54	1.50
25	B	812	CLA	C4B-CHC	-2.16	1.35	1.41
30	A	850	BCR	C8-C9	2.16	1.50	1.45
29	U	315	Q6L	C01-C02	2.16	1.54	1.50
25	B	829	CLA	C4B-CHC	-2.16	1.35	1.41
25	G	202	CLA	C4B-CHC	-2.15	1.35	1.41
25	U	308	CLA	CMB-C2B	-2.15	1.47	1.51
24	6	601	CHL	CMD-C2D	-2.15	1.46	1.50
25	Q	304	CLA	CMA-C3A	-2.15	1.48	1.53
25	W	301	CLA	CMB-C2B	-2.15	1.47	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	4	301	IWJ	C29-C35	-2.15	1.53	1.56
25	3	301	CLA	C3B-C2B	-2.15	1.37	1.40
25	B	828	CLA	C4B-CHC	-2.15	1.35	1.41
24	P	304	CHL	MG-ND	-2.15	2.01	2.05
25	Q	315	CLA	CMD-C2D	-2.15	1.46	1.50
25	S	301	CLA	C3B-CAB	-2.15	1.43	1.47
24	P	314	CHL	CMD-C2D	-2.15	1.46	1.50
24	V	304	CHL	CMD-C2D	-2.15	1.46	1.50
25	2	611	CLA	C4B-CHC	-2.15	1.35	1.41
24	V	307	CHL	CMB-C2B	-2.15	1.47	1.51
25	W	303	CLA	CMD-C2D	-2.15	1.46	1.50
26	S	322	IWJ	C26-C24	-2.15	1.45	1.49
24	4	307	CHL	CMA-C3A	-2.15	1.48	1.53
25	A	824	CLA	C4B-CHC	-2.15	1.35	1.41
25	A	832	CLA	C4B-CHC	-2.15	1.35	1.41
24	R	308	CHL	MG-ND	-2.15	2.01	2.05
29	T	316	Q6L	C01-C02	2.15	1.54	1.50
25	B	841	CLA	CMD-C2D	-2.14	1.46	1.50
29	V	319	Q6L	C33-C32	2.14	1.35	1.33
29	S	315	Q6L	C01-C02	2.14	1.54	1.50
25	6	607	CLA	CMC-C2C	-2.14	1.46	1.50
26	3	315	IWJ	C26-C24	-2.14	1.45	1.49
27	1	612	XAT	C18-C5	2.14	1.55	1.51
25	A	815	CLA	CMB-C2B	-2.14	1.47	1.51
26	X	318	IWJ	O39-C29	-2.14	1.39	1.43
26	Q	303	IWJ	O39-C29	-2.14	1.39	1.43
38	T	308	KC2	MG-NB	-2.14	2.01	2.05
25	B	839	CLA	CMC-C2C	-2.14	1.46	1.50
25	5	608	CLA	C3B-CAB	-2.14	1.43	1.47
25	B	843	CLA	CMC-C2C	-2.14	1.46	1.50
25	O	2004	CLA	C3B-C2B	-2.14	1.37	1.40
25	A	805	CLA	C4B-CHC	-2.14	1.35	1.41
24	U	304	CHL	CMD-C2D	-2.14	1.46	1.50
24	X	308	CHL	CMD-C2D	-2.14	1.46	1.50
25	X	313	CLA	CMC-C2C	-2.14	1.46	1.50
25	A	829	CLA	CHC-C1C	2.14	1.40	1.35
24	V	305	CHL	MG-ND	-2.13	2.01	2.05
25	H	304	CLA	C3B-C2B	-2.13	1.37	1.40
25	1	603	CLA	C4B-CHC	-2.13	1.35	1.41
30	A	852	BCR	C16-C15	-2.13	1.30	1.36
38	X	309	KC2	MG-NA	2.13	2.11	2.06
24	X	306	CHL	CMB-C2B	-2.13	1.47	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	3	308	CLA	CMD-C2D	-2.13	1.46	1.50
25	T	302	CLA	CMC-C2C	-2.13	1.46	1.50
26	S	318	IWJ	C29-C35	-2.13	1.53	1.56
25	1	602	CLA	C3B-C2B	-2.13	1.37	1.40
25	Q	306	CLA	MG-ND	-2.13	2.01	2.05
29	P	321	Q6L	C29-C27	2.13	1.50	1.45
30	K	202	BCR	C34-C9	2.13	1.55	1.50
25	U	311	CLA	C3B-C2B	-2.13	1.37	1.40
25	S	309	CLA	C1A-CHA	-2.13	1.34	1.43
25	B	826	CLA	MG-ND	-2.13	2.01	2.05
25	2	608	CLA	C4B-CHC	-2.13	1.35	1.41
25	2	612	CLA	C4B-CHC	-2.13	1.35	1.41
37	S	317	NEX	O24-C25	-2.13	1.43	1.46
25	X	303	CLA	C4B-CHC	-2.13	1.35	1.41
38	W	308	KC2	MG-NB	-2.13	2.01	2.05
25	A	834	CLA	C3B-C2B	-2.13	1.37	1.40
25	B	832	CLA	CMC-C2C	-2.13	1.46	1.50
27	3	316	XAT	C22-C21	-2.13	1.51	1.54
25	A	829	CLA	MG-ND	-2.13	2.01	2.05
25	B	819	CLA	CMD-C2D	-2.13	1.46	1.50
26	X	318	IWJ	C26-C24	-2.13	1.45	1.49
25	U	303	CLA	CMD-C2D	-2.12	1.46	1.50
25	2	606	CLA	C3B-CAB	-2.12	1.43	1.47
30	F	804	BCR	C5-C6	2.12	1.38	1.34
25	3	308	CLA	CHC-C1C	2.12	1.40	1.35
25	5	601	CLA	C4B-CHC	-2.12	1.35	1.41
25	O	2002	CLA	C4B-CHC	-2.12	1.35	1.41
25	Q	311	CLA	C3B-CAB	-2.12	1.43	1.47
38	W	308	KC2	MG-NA	2.12	2.11	2.06
25	4	310	CLA	CMB-C2B	-2.12	1.47	1.51
25	T	311	CLA	CMD-C2D	-2.12	1.46	1.50
24	P	306	CHL	C4B-CHC	-2.12	1.35	1.41
29	P	316	Q6L	C29-C27	2.12	1.50	1.45
37	W	317	NEX	O24-C25	-2.12	1.43	1.46
24	T	306	CHL	CMD-C2D	-2.12	1.46	1.50
25	L	304	CLA	CMC-C2C	-2.11	1.46	1.50
25	B	820	CLA	MG-ND	-2.11	2.01	2.05
24	R	318	CHL	CMB-C2B	-2.11	1.47	1.51
37	R	321	NEX	C35-C15	-2.11	1.30	1.36
26	S	319	IWJ	C26-C24	-2.11	1.45	1.49
25	X	313	CLA	C3B-C2B	-2.11	1.37	1.40
25	B	815	CLA	C4-C3	-2.11	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	T	320	CHL	C3B-CAB	-2.11	1.43	1.47
30	K	202	BCR	C37-C22	2.11	1.55	1.50
25	U	310	CLA	C3B-C2B	-2.11	1.37	1.40
25	A	827	CLA	MG-ND	-2.11	2.01	2.05
25	R	315	CLA	CMD-C2D	-2.11	1.46	1.50
24	X	306	CHL	CMD-C2D	-2.11	1.46	1.50
25	A	822	CLA	CMC-C2C	-2.11	1.46	1.50
30	L	306	BCR	C10-C9	2.11	1.38	1.35
25	H	304	CLA	C3C-C2C	2.11	1.41	1.36
26	S	318	IWJ	C32-C30	2.11	1.55	1.51
29	P	315	Q6L	C11-C03	-2.11	1.48	1.51
37	H	306	NEX	C35-C15	-2.11	1.30	1.36
24	U	304	CHL	C3B-CAB	-2.11	1.43	1.47
25	V	303	CLA	CMC-C2C	-2.11	1.46	1.50
24	S	306	CHL	CMD-C2D	-2.10	1.46	1.50
24	T	307	CHL	CMD-C2D	-2.10	1.46	1.50
25	4	309	CLA	CMD-C2D	-2.10	1.46	1.50
29	Q	317	Q6L	C01-C02	2.10	1.54	1.50
24	1	604	CHL	MG-ND	-2.10	2.01	2.05
25	U	301	CLA	MG-ND	-2.10	2.01	2.05
37	T	317	NEX	O24-C25	-2.10	1.43	1.46
25	A	826	CLA	C4B-CHC	-2.10	1.35	1.41
25	3	309	CLA	C3B-C2B	-2.10	1.37	1.40
25	A	820	CLA	CMD-C2D	-2.10	1.46	1.50
25	2	612	CLA	C3B-C2B	-2.10	1.37	1.40
24	1	604	CHL	CMB-C2B	-2.10	1.47	1.51
24	V	306	CHL	MG-ND	-2.10	2.01	2.05
37	R	321	NEX	C22-C21	-2.10	1.51	1.54
25	4	305	CLA	CMC-C2C	-2.10	1.46	1.50
24	4	308	CHL	CMD-C2D	-2.10	1.46	1.50
38	P	308	KC2	CHB-C1B	2.10	1.42	1.38
25	A	835	CLA	MG-ND	-2.10	2.01	2.05
26	R	303	IWJ	O39-C29	-2.10	1.39	1.43
25	T	302	CLA	C3B-C2B	-2.10	1.37	1.40
25	A	820	CLA	MG-ND	-2.10	2.01	2.05
25	4	312	CLA	CMD-C2D	-2.09	1.46	1.50
25	B	833	CLA	C4B-CHC	-2.09	1.35	1.41
37	P	317	NEX	C22-C21	-2.09	1.51	1.54
25	2	614	CLA	C4B-CHC	-2.09	1.35	1.41
25	6	604	CLA	C3B-CAB	-2.09	1.43	1.47
25	T	301	CLA	CMA-C3A	-2.09	1.48	1.53
25	N	202	CLA	CAC-C3C	-2.09	1.45	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	U	309	CLA	CMD-C2D	-2.09	1.46	1.50
24	R	310	CHL	MG-ND	-2.09	2.01	2.05
30	3	317	BCR	C8-C9	2.09	1.50	1.45
24	2	615	CHL	CMB-C2B	-2.09	1.47	1.51
25	L	301	CLA	C4B-CHC	-2.09	1.35	1.41
25	A	840	CLA	C4B-CHC	-2.09	1.35	1.41
25	3	307	CLA	CHC-C1C	2.09	1.40	1.35
30	B	849	BCR	C21-C22	2.09	1.38	1.35
25	G	202	CLA	CMD-C2D	-2.09	1.46	1.50
25	Q	305	CLA	C4B-CHC	-2.09	1.35	1.41
29	R	320	Q6L	C01-C02	2.09	1.54	1.50
25	U	308	CLA	CMD-C2D	-2.09	1.46	1.50
25	1	602	CLA	C3B-CAB	-2.09	1.43	1.47
29	R	301	Q6L	C02-C03	2.09	1.37	1.34
29	W	316	Q6L	C29-C27	2.09	1.50	1.45
37	H	306	NEX	C1-C6	-2.08	1.51	1.54
38	W	308	KC2	MG-NC	2.08	2.11	2.06
25	B	813	CLA	C3B-C2B	-2.08	1.37	1.40
30	A	852	BCR	C20-C19	-2.08	1.29	1.34
25	B	828	CLA	C3B-C2B	-2.08	1.37	1.40
29	U	317	Q6L	C33-C32	2.08	1.35	1.33
25	A	828	CLA	C4B-CHC	-2.08	1.35	1.41
30	F	801	BCR	C12-C13	2.08	1.50	1.45
26	3	315	IWJ	C28-C26	2.08	1.53	1.51
24	P	306	CHL	CMC-C2C	2.08	1.49	1.45
30	B	847	BCR	C16-C15	-2.08	1.30	1.36
25	X	312	CLA	CMD-C2D	-2.08	1.46	1.50
27	1	612	XAT	C38-C25	2.08	1.55	1.51
25	U	309	CLA	C3B-C2B	-2.08	1.37	1.40
25	3	304	CLA	C1D-C2D	2.08	1.49	1.45
25	A	810	CLA	CMC-C2C	-2.08	1.46	1.50
25	Q	306	CLA	C3B-C2B	-2.08	1.37	1.40
25	2	606	CLA	CMD-C2D	-2.08	1.46	1.50
25	B	822	CLA	C4-C3	-2.08	1.44	1.50
38	X	309	KC2	MG-NC	2.08	2.11	2.06
25	2	609	CLA	CMD-C2D	-2.08	1.46	1.50
24	1	604	CHL	CMC-C2C	2.08	1.49	1.45
25	Q	315	CLA	CMC-C2C	-2.08	1.46	1.50
24	P	307	CHL	CMC-C2C	2.08	1.49	1.45
25	B	816	CLA	CMD-C2D	-2.08	1.46	1.50
25	S	309	CLA	CMC-C2C	-2.08	1.46	1.50
25	O	2001	CLA	C3B-C2B	-2.08	1.37	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	T	310	CLA	C3B-C2B	-2.08	1.37	1.40
24	S	304	CHL	C1D-ND	2.08	1.40	1.37
25	B	817	CLA	C3B-C2B	-2.08	1.37	1.40
27	3	316	XAT	C2-C1	-2.08	1.51	1.54
25	A	833	CLA	MG-ND	-2.08	2.01	2.05
25	1	603	CLA	CAC-C3C	-2.07	1.45	1.51
24	S	305	CHL	C3B-CAB	-2.07	1.43	1.47
25	Q	312	CLA	C3B-C2B	-2.07	1.37	1.40
24	R	311	CHL	C2C-C3C	2.07	1.41	1.36
25	1	602	CLA	CMA-C3A	-2.07	1.48	1.53
29	X	317	Q6L	C33-C32	2.07	1.35	1.33
25	U	310	CLA	CMC-C2C	-2.07	1.46	1.50
25	K	203	CLA	CMD-C2D	-2.07	1.46	1.50
25	U	301	CLA	C3B-CAB	-2.07	1.43	1.47
25	B	815	CLA	MG-ND	-2.07	2.01	2.05
25	3	311	CLA	O2A-CGA	2.07	1.39	1.33
25	S	302	CLA	C4B-CHC	-2.07	1.35	1.41
25	A	815	CLA	CMA-C3A	-2.07	1.48	1.53
38	R	312	KC2	C1B-C2B	2.07	1.49	1.45
25	B	803	CLA	MG-ND	-2.07	2.01	2.05
25	L	304	CLA	C4B-CHC	-2.07	1.35	1.41
25	6	604	CLA	C3B-C2B	-2.07	1.37	1.40
30	K	202	BCR	C14-C13	-2.07	1.33	1.35
25	A	833	CLA	C4B-CHC	-2.07	1.35	1.41
29	2	616	Q6L	C33-C32	2.07	1.35	1.33
25	Q	301	CLA	CMC-C2C	-2.07	1.46	1.50
38	P	308	KC2	C1B-C2B	2.06	1.49	1.45
25	6	602	CLA	CMB-C2B	-2.06	1.47	1.51
30	G	205	BCR	C16-C15	-2.06	1.30	1.36
24	P	307	CHL	CMD-C2D	-2.06	1.46	1.50
30	M	101	BCR	C16-C15	-2.06	1.30	1.36
25	S	310	CLA	CMD-C2D	-2.06	1.46	1.50
30	M	101	BCR	C19-C18	2.06	1.50	1.45
30	G	205	BCR	C23-C22	2.06	1.50	1.45
25	W	302	CLA	C3B-CAB	-2.06	1.43	1.47
24	R	310	CHL	CMC-C2C	2.06	1.49	1.45
25	B	811	CLA	C4B-CHC	-2.06	1.35	1.41
24	2	601	CHL	C3B-C2B	-2.06	1.37	1.40
25	J	102	CLA	CMD-C2D	-2.06	1.46	1.50
37	R	321	NEX	O24-C25	-2.06	1.43	1.46
29	S	323	Q6L	C01-C02	2.06	1.54	1.50
25	B	818	CLA	C3B-C2B	-2.06	1.37	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	V	310	CLA	C3B-CAB	-2.06	1.43	1.47
25	U	311	CLA	CMD-C2D	-2.06	1.46	1.50
24	T	305	CHL	CMB-C2B	-2.06	1.47	1.51
25	6	611	CLA	C4B-CHC	-2.06	1.35	1.41
25	R	306	CLA	CMC-C2C	-2.06	1.46	1.50
27	6	615	XAT	C38-C25	2.06	1.55	1.51
25	5	610	CLA	CMD-C2D	-2.06	1.46	1.50
25	N	203	CLA	CHC-C1C	2.06	1.40	1.35
24	5	605	CHL	CMD-C2D	-2.06	1.46	1.50
25	A	806	CLA	CMB-C2B	-2.06	1.47	1.51
25	2	604	CLA	C3B-CAB	-2.06	1.43	1.47
25	R	313	CLA	CAA-C2A	-2.06	1.50	1.54
25	A	825	CLA	CAC-C3C	-2.05	1.45	1.51
25	B	813	CLA	C3B-CAB	-2.05	1.43	1.47
26	S	319	IWJ	O39-C29	-2.05	1.40	1.43
25	U	301	CLA	C3B-C2B	-2.05	1.37	1.40
25	2	614	CLA	CMD-C2D	-2.05	1.46	1.50
25	A	843	CLA	C4B-CHC	-2.05	1.35	1.41
24	R	309	CHL	CMB-C2B	-2.05	1.47	1.51
25	P	301	CLA	CMD-C2D	-2.05	1.46	1.50
25	V	313	CLA	C4B-CHC	-2.05	1.35	1.41
25	W	310	CLA	C3B-C2B	-2.05	1.37	1.40
29	W	316	Q6L	C11-C03	-2.05	1.48	1.51
25	W	311	CLA	C4B-CHC	-2.05	1.35	1.41
24	S	306	CHL	CHC-C1C	2.05	1.40	1.35
25	2	606	CLA	C4B-CHC	-2.05	1.35	1.41
25	U	311	CLA	CMC-C2C	-2.05	1.46	1.50
26	X	318	IWJ	C32-C30	2.05	1.55	1.51
25	L	304	CLA	CMD-C2D	-2.05	1.46	1.50
25	A	808	CLA	C4B-CHC	-2.05	1.35	1.41
25	X	311	CLA	C3B-C2B	-2.05	1.37	1.40
24	2	601	CHL	C2C-C3C	2.05	1.41	1.36
25	B	842	CLA	CMD-C2D	-2.05	1.46	1.50
25	A	807	CLA	C2-C3	2.05	1.37	1.33
25	A	806	CLA	CMC-C2C	-2.05	1.46	1.50
30	2	618	BCR	C8-C9	2.04	1.50	1.45
25	X	314	CLA	C4B-CHC	-2.04	1.35	1.41
30	J	103	BCR	C8-C9	2.04	1.50	1.45
29	V	321	Q6L	C33-C32	2.04	1.35	1.33
25	T	303	CLA	MG-ND	-2.04	2.01	2.05
30	M	101	BCR	C35-C13	2.04	1.55	1.50
25	S	310	CLA	C4B-CHC	-2.04	1.35	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	V	311	CLA	C4B-CHC	-2.04	1.35	1.41
25	X	311	CLA	C4B-CHC	-2.04	1.35	1.41
25	A	809	CLA	CMD-C2D	-2.04	1.46	1.50
25	A	827	CLA	C5-C3	-2.04	1.47	1.51
25	B	824	CLA	C3B-C2B	-2.04	1.37	1.40
25	B	812	CLA	CHC-C1C	2.04	1.40	1.35
29	T	322	Q6L	C29-C27	2.04	1.50	1.45
24	T	304	CHL	CMB-C2B	-2.04	1.47	1.51
25	V	309	CLA	C4D-ND	-2.04	1.34	1.37
25	3	307	CLA	C3B-CAB	-2.04	1.43	1.47
25	B	811	CLA	C3B-CAB	-2.04	1.43	1.47
30	B	847	BCR	C36-C18	2.04	1.55	1.50
25	B	811	CLA	CHC-C1C	2.04	1.40	1.35
25	A	819	CLA	CMA-C3A	-2.04	1.48	1.53
25	Q	304	CLA	CMD-C2D	-2.04	1.46	1.50
26	T	318	IWJ	O39-C29	-2.04	1.40	1.43
27	6	615	XAT	O24-C25	-2.04	1.43	1.46
25	2	602	CLA	C4B-CHC	-2.04	1.35	1.41
24	4	307	CHL	CMD-C2D	-2.04	1.46	1.50
33	A	802	CL0	C4B-CHC	-2.04	1.35	1.41
25	A	831	CLA	CMD-C2D	-2.04	1.46	1.50
25	X	302	CLA	CMA-C3A	-2.04	1.48	1.53
30	L	306	BCR	C19-C18	2.04	1.50	1.45
25	4	309	CLA	C3B-CAB	-2.03	1.43	1.47
25	Q	314	CLA	C3B-CAB	-2.03	1.43	1.47
37	W	317	NEX	C22-C21	-2.03	1.51	1.54
24	R	309	CHL	OBD-CAD	-2.03	1.19	1.22
30	B	848	BCR	C12-C13	2.03	1.50	1.45
24	U	304	CHL	MG-ND	-2.03	2.01	2.05
38	Q	310	KC2	CMB-C2B	-2.03	1.46	1.50
25	P	313	CLA	C3B-C2B	-2.03	1.37	1.40
30	3	318	BCR	C37-C22	2.03	1.55	1.50
30	I	101	BCR	C31-C1	-2.03	1.49	1.53
29	U	315	Q6L	C29-C27	2.03	1.50	1.45
25	R	317	CLA	C4B-CHC	-2.03	1.35	1.41
25	A	829	CLA	C4B-CHC	-2.03	1.35	1.41
38	W	308	KC2	C1A-NA	2.03	1.42	1.38
25	1	606	CLA	C4B-CHC	-2.03	1.35	1.41
26	P	320	IWJ	C26-C24	-2.03	1.45	1.49
24	2	601	CHL	CMB-C2B	-2.03	1.47	1.51
25	5	604	CLA	CMD-C2D	-2.03	1.46	1.50
25	B	804	CLA	CMD-C2D	-2.03	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	W	315	Q6L	C33-C32	2.03	1.35	1.33
25	A	829	CLA	CMA-C3A	-2.03	1.48	1.53
25	B	811	CLA	CMD-C2D	-2.03	1.46	1.50
38	P	308	KC2	MG-NB	-2.03	2.01	2.05
29	W	320	Q6L	C33-C32	2.03	1.35	1.33
38	S	308	KC2	MG-NC	2.03	2.11	2.06
25	A	825	CLA	CMD-C2D	-2.03	1.46	1.50
25	R	315	CLA	C3B-C2B	-2.03	1.37	1.40
25	U	302	CLA	C4B-CHC	-2.03	1.35	1.41
25	Q	305	CLA	C3B-C2B	-2.03	1.37	1.40
25	4	313	CLA	CMA-C3A	-2.03	1.48	1.53
25	B	806	CLA	CMC-C2C	-2.02	1.46	1.50
25	V	302	CLA	MG-NC	2.02	2.11	2.06
25	4	309	CLA	C4B-CHC	-2.02	1.35	1.41
25	B	823	CLA	C3B-CAB	-2.02	1.43	1.47
25	3	312	CLA	C4B-CHC	-2.02	1.35	1.41
25	T	309	CLA	C1A-CHA	-2.02	1.34	1.43
25	P	302	CLA	CMD-C2D	-2.02	1.46	1.50
34	A	844	PQN	C5-C4	-2.02	1.44	1.48
26	S	319	IWJ	C32-C30	2.02	1.55	1.51
26	U	316	IWJ	C32-C30	2.02	1.55	1.51
26	V	320	IWJ	C32-C30	2.02	1.55	1.51
25	A	808	CLA	CMC-C2C	-2.02	1.46	1.50
30	B	849	BCR	C16-C15	-2.02	1.30	1.36
25	U	308	CLA	C1A-CHA	-2.02	1.34	1.43
25	U	302	CLA	MG-ND	-2.02	2.01	2.05
24	6	606	CHL	CMB-C2B	-2.02	1.47	1.51
25	F	802	CLA	MG-ND	-2.02	2.01	2.05
25	P	310	CLA	C3B-C2B	-2.02	1.37	1.40
29	R	301	Q6L	C01-C02	2.02	1.54	1.50
25	W	301	CLA	CMD-C2D	-2.02	1.46	1.50
25	3	307	CLA	CMD-C2D	-2.02	1.46	1.50
30	A	850	BCR	C16-C15	-2.02	1.30	1.36
30	L	305	BCR	C19-C18	2.02	1.50	1.45
25	B	809	CLA	MG-ND	-2.02	2.01	2.05
24	S	306	CHL	MG-ND	-2.02	2.01	2.05
30	3	317	BCR	C19-C18	2.02	1.50	1.45
24	P	304	CHL	CMD-C2D	-2.02	1.46	1.50
30	A	850	BCR	C14-C13	-2.01	1.33	1.35
24	1	601	CHL	CMD-C2D	-2.01	1.46	1.50
25	W	313	CLA	C3B-C2B	-2.01	1.37	1.40
25	A	823	CLA	MG-ND	-2.01	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	A	838	CLA	C4B-CHC	-2.01	1.35	1.41
24	2	601	CHL	CMC-C2C	2.01	1.49	1.45
25	A	856	CLA	CMD-C2D	-2.01	1.46	1.50
24	X	307	CHL	O2A-CGA	2.01	1.39	1.33
25	B	805	CLA	CMC-C2C	-2.01	1.46	1.50
25	X	310	CLA	C3B-C2B	-2.01	1.37	1.40
25	B	807	CLA	C4B-CHC	-2.01	1.35	1.41
25	O	2002	CLA	CMC-C2C	-2.01	1.46	1.50
25	V	312	CLA	MG-ND	-2.01	2.01	2.05
24	X	307	CHL	C4C-C3C	2.01	1.48	1.45
25	4	303	CLA	C4B-CHC	-2.01	1.35	1.41
25	X	313	CLA	CMD-C2D	-2.01	1.46	1.50
25	R	313	CLA	MG-NA	2.01	2.11	2.06
25	4	313	CLA	C3B-C2B	-2.01	1.37	1.40
25	O	2001	CLA	C3B-CAB	-2.01	1.43	1.47
25	B	828	CLA	MG-ND	-2.01	2.01	2.05
25	2	613	CLA	CMB-C2B	-2.01	1.47	1.51
36	A	854	DGD	O5D-C1E	2.01	1.43	1.40
25	X	304	CLA	C3B-CAB	-2.01	1.43	1.47
30	A	850	BCR	C19-C18	2.01	1.50	1.45
25	T	313	CLA	CMC-C2C	-2.01	1.46	1.50
25	2	609	CLA	C4B-CHC	-2.00	1.35	1.41
25	R	305	CLA	CMB-C2B	-2.00	1.47	1.51
25	L	301	CLA	C3B-C2B	-2.00	1.37	1.40
25	B	816	CLA	CMC-C2C	-2.00	1.46	1.50
25	O	2004	CLA	C4B-CHC	-2.00	1.35	1.41
24	R	302	CHL	CMA-C3A	-2.00	1.48	1.53
25	4	316	CLA	C3B-C2B	-2.00	1.37	1.40
27	4	318	XAT	C30-C29	2.00	1.38	1.35
27	5	612	XAT	O24-C25	-2.00	1.43	1.46
25	5	607	CLA	C3B-CAB	-2.00	1.43	1.47
25	A	808	CLA	C3B-C2B	-2.00	1.37	1.40
25	2	613	CLA	C3B-C2B	-2.00	1.37	1.40
25	P	311	CLA	C3D-C4D	2.00	1.48	1.44

All (4503) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	4	318	XAT	O4-C5-C4	15.74	125.20	113.38
37	S	317	NEX	O24-C25-C24	13.84	123.78	113.38
37	R	321	NEX	O24-C25-C24	13.41	123.46	113.38
27	6	615	XAT	O4-C5-C4	13.30	123.38	113.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	W	317	NEX	O24-C25-C24	13.18	123.28	113.38
27	2	617	XAT	O4-C5-C4	12.64	122.88	113.38
27	1	612	XAT	O4-C5-C4	12.60	122.85	113.38
37	T	317	NEX	O24-C25-C24	11.34	121.90	113.38
37	H	306	NEX	O24-C25-C24	10.78	121.48	113.38
25	1	607	CLA	CHA-C4D-ND	10.41	134.35	125.21
37	P	317	NEX	O24-C25-C24	10.32	121.14	113.38
30	B	849	BCR	C24-C23-C22	-9.77	111.47	126.23
27	3	316	XAT	O24-C25-C24	9.75	120.70	113.38
27	3	316	XAT	O4-C5-C4	9.53	120.54	113.38
27	5	612	XAT	O4-C5-C4	9.28	120.36	113.38
25	1	607	CLA	CBD-CHA-C1A	9.27	129.04	117.85
30	B	846	BCR	C37-C22-C21	-9.07	110.22	122.92
38	P	308	KC2	C1A-NA-C4A	8.78	110.65	106.71
38	P	308	KC2	CMA-C3A-C2A	-8.68	107.06	128.30
38	X	309	KC2	CMA-C3A-C4A	-8.51	112.08	125.04
27	4	318	XAT	O24-C25-C24	8.46	119.74	113.38
27	5	612	XAT	O24-C25-C24	8.46	119.73	113.38
27	2	617	XAT	O24-C25-C24	8.44	119.72	113.38
38	R	312	KC2	C1A-NA-C4A	8.43	110.50	106.71
30	K	202	BCR	C36-C18-C19	8.35	131.23	118.08
27	5	612	XAT	O4-C5-C18	8.17	124.84	115.06
30	B	847	BCR	C31-C1-C6	-8.07	97.21	110.30
30	J	101	BCR	C36-C18-C19	8.06	130.78	118.08
25	Q	304	CLA	C4A-NA-C1A	8.05	110.32	106.71
25	3	301	CLA	C4A-NA-C1A	7.97	110.29	106.71
30	L	307	BCR	C36-C18-C17	-7.84	111.94	122.92
38	T	308	KC2	CMA-C3A-C4A	-7.80	113.16	125.04
24	X	307	CHL	C4A-NA-C1A	7.68	110.16	106.71
38	S	308	KC2	CMA-C3A-C4A	-7.60	113.47	125.04
38	W	308	KC2	C1A-C2A-C3A	-7.54	101.13	107.11
38	U	307	KC2	CMA-C3A-C4A	-7.45	113.70	125.04
38	P	308	KC2	CMA-C3A-C4A	-7.40	113.77	125.04
24	S	307	CHL	CMB-C2B-C1B	-7.31	117.22	128.46
38	Q	310	KC2	CMA-C3A-C4A	-7.30	113.92	125.04
25	A	842	CLA	C4A-NA-C1A	7.29	109.98	106.71
25	A	830	CLA	C4A-NA-C1A	7.26	109.97	106.71
30	L	307	BCR	C34-C9-C10	-7.25	112.77	122.92
30	K	207	BCR	C36-C18-C19	7.21	129.44	118.08
30	B	845	BCR	C33-C5-C6	7.20	132.61	124.53
24	T	304	CHL	CMB-C2B-C1B	-7.19	117.41	128.46
29	R	323	Q6L	C11-C12-C13	7.18	133.09	112.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	X	307	CHL	OMC-CMC-C2C	-7.18	109.46	125.69
25	A	815	CLA	C4A-NA-C1A	7.17	109.93	106.71
30	A	849	BCR	C36-C18-C19	7.16	129.36	118.08
38	Q	310	KC2	C1A-NA-C4A	7.11	109.90	106.71
29	R	301	Q6L	C11-C12-C13	7.10	132.87	112.69
37	P	317	NEX	C16-C1-C6	7.05	116.78	110.47
25	1	603	CLA	C4A-NA-C1A	7.03	109.87	106.71
25	A	811	CLA	CMB-C2B-C1B	-7.00	117.70	128.46
34	B	844	PQN	C11-C12-C13	-6.99	115.16	126.79
25	Q	301	CLA	C4A-NA-C1A	6.98	109.84	106.71
24	T	307	CHL	CMB-C2B-C1B	-6.92	117.82	128.46
24	4	307	CHL	OMC-CMC-C2C	-6.92	110.03	125.69
25	4	304	CLA	C4A-NA-C1A	6.90	109.81	106.71
24	4	302	CHL	C4A-NA-C1A	6.90	109.81	106.71
29	W	320	Q6L	C11-C12-C13	6.89	132.26	112.69
30	B	848	BCR	C36-C18-C19	6.81	128.81	118.08
25	B	824	CLA	CMB-C2B-C1B	-6.81	118.00	128.46
24	W	314	CHL	CMB-C2B-C1B	-6.79	118.03	128.46
38	Q	310	KC2	C2A-C3A-C4A	-6.78	101.45	106.49
30	3	318	BCR	C36-C18-C19	6.72	128.67	118.08
38	X	309	KC2	C1A-NA-C4A	6.72	109.73	106.71
29	X	319	Q6L	C11-C12-C13	6.72	131.77	112.69
25	6	607	CLA	CMB-C2B-C1B	-6.70	118.17	128.46
38	T	308	KC2	C1A-NA-C4A	6.69	109.71	106.71
30	F	804	BCR	C36-C18-C19	6.68	128.61	118.08
30	A	852	BCR	C37-C22-C23	6.68	128.60	118.08
34	B	844	PQN	C15-C13-C12	-6.68	107.60	121.12
25	A	815	CLA	CMB-C2B-C1B	-6.68	118.20	128.46
30	3	319	BCR	C36-C18-C19	6.67	128.59	118.08
30	J	103	BCR	C36-C18-C19	6.67	128.58	118.08
29	U	317	Q6L	C11-C12-C13	6.66	131.61	112.69
29	Q	317	Q6L	C11-C12-C13	6.65	131.59	112.69
25	B	838	CLA	CMB-C2B-C1B	-6.65	118.25	128.46
25	6	609	CLA	CMB-C2B-C1B	-6.64	118.25	128.46
25	K	204	CLA	C4A-NA-C1A	6.63	109.69	106.71
25	B	815	CLA	CMB-C2B-C1B	-6.61	118.30	128.46
27	3	316	XAT	C19-C9-C8	-6.61	107.67	118.08
34	A	844	PQN	C15-C13-C12	-6.60	107.77	121.12
29	P	321	Q6L	C11-C12-C13	6.59	131.41	112.69
30	I	101	BCR	C38-C26-C25	-6.59	117.13	124.53
25	3	311	CLA	C4A-NA-C1A	6.58	109.67	106.71
25	4	313	CLA	C4A-NA-C1A	6.58	109.67	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	843	CLA	C4A-NA-C1A	6.56	109.66	106.71
25	B	809	CLA	C4A-NA-C1A	6.56	109.66	106.71
25	S	303	CLA	CMB-C2B-C1B	-6.56	118.38	128.46
24	P	305	CHL	C4A-NA-C1A	6.56	109.65	106.71
25	A	818	CLA	CMB-C2B-C1B	-6.55	118.39	128.46
25	B	802	CLA	CMB-C2B-C1B	-6.54	118.42	128.46
25	A	816	CLA	C4A-NA-C1A	6.54	109.64	106.71
25	L	303	CLA	CMB-C2B-C1B	-6.53	118.43	128.46
29	V	316	Q6L	C11-C12-C13	6.53	131.23	112.69
30	L	305	BCR	C38-C26-C25	-6.52	117.20	124.53
30	L	307	BCR	C36-C18-C19	6.48	128.29	118.08
29	U	314	Q6L	C11-C12-C13	6.45	131.02	112.69
29	V	319	Q6L	C11-C12-C13	6.45	131.02	112.69
29	V	321	Q6L	C11-C12-C13	6.44	130.98	112.69
24	P	307	CHL	CMB-C2B-C1B	-6.43	118.58	128.46
25	A	811	CLA	CMB-C2B-C3B	6.43	136.71	124.68
25	B	815	CLA	C4A-NA-C1A	6.42	109.59	106.71
25	V	301	CLA	CMB-C2B-C1B	-6.40	118.63	128.46
30	B	845	BCR	C36-C18-C19	6.39	128.14	118.08
25	B	831	CLA	CMB-C2B-C1B	-6.39	118.65	128.46
38	S	308	KC2	CMA-C3A-C2A	-6.38	112.68	128.30
25	R	316	CLA	C4A-NA-C1A	6.37	109.57	106.71
25	B	807	CLA	C4A-NA-C1A	6.37	109.57	106.71
25	X	312	CLA	C4A-NA-C1A	6.37	109.57	106.71
25	B	843	CLA	C4A-NA-C1A	6.34	109.56	106.71
25	5	607	CLA	C4A-NA-C1A	6.33	109.55	106.71
24	W	306	CHL	C4A-NA-C1A	6.32	109.55	106.71
24	X	308	CHL	CMB-C2B-C1B	-6.32	118.75	128.46
30	B	847	BCR	C38-C26-C25	-6.31	117.44	124.53
25	W	303	CLA	CMB-C2B-C1B	-6.31	118.77	128.46
30	A	850	BCR	C36-C18-C19	6.29	127.98	118.08
38	R	312	KC2	CMA-C3A-C2A	-6.28	112.93	128.30
29	S	320	Q6L	C11-C12-C13	6.28	130.52	112.69
25	B	803	CLA	CMB-C2B-C1B	-6.27	118.83	128.46
25	A	841	CLA	C4A-NA-C1A	6.27	109.52	106.71
25	Q	313	CLA	C4A-NA-C1A	6.27	109.52	106.71
30	A	850	BCR	C38-C26-C25	-6.26	117.50	124.53
25	A	856	CLA	O2D-CGD-O1D	-6.25	111.61	123.84
30	F	804	BCR	C35-C13-C14	-6.25	114.17	122.92
29	R	319	Q6L	C11-C12-C13	6.24	130.41	112.69
29	S	323	Q6L	C11-C12-C13	6.24	130.41	112.69
38	U	307	KC2	C1A-NA-C4A	6.23	109.51	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	T	319	Q6L	C11-C12-C13	6.22	130.37	112.69
25	L	304	CLA	C4A-NA-C1A	6.22	109.50	106.71
38	S	308	KC2	C1A-NA-C4A	6.21	109.50	106.71
25	B	833	CLA	C4A-NA-C1A	6.21	109.50	106.71
30	L	307	BCR	C31-C1-C6	6.19	120.34	110.30
25	B	842	CLA	C4A-NA-C1A	6.19	109.49	106.71
25	5	603	CLA	CMB-C2B-C1B	-6.18	118.96	128.46
29	W	315	Q6L	C11-C12-C13	6.18	130.25	112.69
30	A	851	BCR	C24-C23-C22	-6.18	116.90	126.23
30	4	319	BCR	C38-C26-C25	-6.18	117.59	124.53
25	A	829	CLA	C4A-NA-C1A	6.16	109.48	106.71
24	T	305	CHL	CMB-C2B-C1B	-6.16	119.00	128.46
25	6	602	CLA	CMB-C2B-C1B	-6.15	119.01	128.46
25	A	819	CLA	C4A-NA-C1A	6.13	109.46	106.71
27	1	612	XAT	C19-C9-C8	-6.13	108.42	118.08
29	P	319	Q6L	C11-C12-C13	6.13	130.11	112.69
29	O	2006	Q6L	C11-C12-C13	6.10	130.03	112.69
25	A	827	CLA	CMB-C2B-C1B	-6.09	119.10	128.46
25	B	822	CLA	C4A-NA-C1A	6.09	109.44	106.71
25	B	840	CLA	C4A-NA-C1A	6.09	109.44	106.71
38	V	308	KC2	C1A-C2A-C3A	-6.09	102.28	107.11
25	G	203	CLA	C4A-NA-C1A	6.08	109.44	106.71
38	U	307	KC2	CMA-C3A-C2A	-6.07	113.43	128.30
25	B	812	CLA	C4A-NA-C1A	6.07	109.43	106.71
30	4	319	BCR	C36-C18-C19	6.06	127.62	118.08
25	K	201	CLA	CMB-C2B-C1B	-6.05	119.17	128.46
25	B	811	CLA	C4A-NA-C1A	6.04	109.42	106.71
25	2	602	CLA	CMB-C2B-C1B	-6.02	119.22	128.46
24	W	305	CHL	C4A-NA-C1A	6.01	109.41	106.71
24	S	314	CHL	CMB-C2B-C1B	-6.00	119.24	128.46
25	H	302	CLA	C4A-NA-C1A	6.00	109.40	106.71
30	F	801	BCR	C24-C23-C22	-6.00	117.17	126.23
25	A	840	CLA	C4A-NA-C1A	5.99	109.40	106.71
25	5	609	CLA	C4A-NA-C1A	5.98	109.40	106.71
30	G	205	BCR	C28-C27-C26	-5.98	103.39	114.08
25	W	312	CLA	C4A-NA-C1A	5.98	109.39	106.71
25	L	302	CLA	C4A-NA-C1A	5.98	109.39	106.71
30	L	307	BCR	C8-C7-C6	-5.97	110.45	127.20
25	B	826	CLA	C4A-NA-C1A	5.96	109.39	106.71
25	A	812	CLA	C4A-NA-C1A	5.95	109.38	106.71
25	X	304	CLA	CMB-C2B-C1B	-5.95	119.33	128.46
30	A	851	BCR	C8-C7-C6	-5.94	110.51	127.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	U	305	CHL	CMB-C2B-C1B	-5.94	119.33	128.46
25	O	2001	CLA	C4A-NA-C1A	5.93	109.37	106.71
25	K	203	CLA	C4A-NA-C1A	5.93	109.37	106.71
25	A	836	CLA	C4A-NA-C1A	5.92	109.37	106.71
38	W	308	KC2	C1A-NA-C4A	5.92	109.37	106.71
29	O	2007	Q6L	C11-C12-C13	5.90	129.47	112.69
29	T	315	Q6L	C11-C12-C13	5.90	129.46	112.69
29	Q	319	Q6L	C11-C12-C13	5.90	129.45	112.69
25	T	301	CLA	C4-C3-C5	5.89	125.18	115.27
25	B	834	CLA	C4A-NA-C1A	5.89	109.35	106.71
25	N	202	CLA	C4A-NA-C1A	5.89	109.35	106.71
24	W	306	CHL	CMB-C2B-C1B	-5.88	119.42	128.46
25	F	803	CLA	C4A-NA-C1A	5.88	109.35	106.71
30	M	101	BCR	C36-C18-C19	5.88	127.34	118.08
29	X	301	Q6L	C11-C12-C13	5.87	129.37	112.69
24	T	304	CHL	CMB-C2B-C3B	5.87	135.66	124.68
30	B	847	BCR	C36-C18-C19	5.86	127.31	118.08
25	T	303	CLA	CMB-C2B-C1B	-5.86	119.46	128.46
25	T	311	CLA	C4A-NA-C1A	5.86	109.34	106.71
27	3	316	XAT	C6-C7-C8	-5.86	113.61	125.99
30	4	319	BCR	C8-C7-C6	-5.86	110.75	127.20
24	Q	308	CHL	CMB-C2B-C1B	-5.86	119.46	128.46
25	A	830	CLA	CMB-C2B-C1B	-5.85	119.48	128.46
24	W	307	CHL	CMB-C2B-C1B	-5.85	119.48	128.46
24	T	305	CHL	C4A-NA-C1A	5.84	109.33	106.71
30	B	846	BCR	C37-C22-C23	5.82	127.25	118.08
30	K	205	BCR	C36-C18-C19	5.81	127.24	118.08
25	A	839	CLA	C4A-NA-C1A	5.81	109.32	106.71
25	B	829	CLA	C4A-NA-C1A	5.81	109.32	106.71
30	A	849	BCR	C3-C4-C5	-5.80	103.72	114.08
29	R	304	Q6L	C11-C12-C13	5.80	129.18	112.69
27	1	612	XAT	O24-C25-C24	5.80	117.74	113.38
30	B	846	BCR	C34-C9-C10	-5.79	114.81	122.92
30	3	317	BCR	C36-C18-C19	5.79	127.20	118.08
27	3	316	XAT	C19-C9-C10	5.78	131.03	122.92
24	6	605	CHL	CMB-C2B-C1B	-5.78	119.58	128.46
25	B	815	CLA	CMB-C2B-C3B	5.77	135.47	124.68
24	5	605	CHL	CMB-C2B-C1B	-5.76	119.61	128.46
30	L	305	BCR	C36-C18-C19	5.75	127.14	118.08
25	V	309	CLA	CMC-C2C-C1C	5.73	133.77	125.04
25	U	311	CLA	C4A-NA-C1A	5.73	109.28	106.71
25	A	810	CLA	C4A-NA-C1A	5.71	109.27	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	T	308	KC2	CMA-C3A-C2A	-5.71	114.33	128.30
29	T	316	Q6L	C11-C12-C13	5.70	128.89	112.69
25	B	807	CLA	CMB-C2B-C1B	-5.69	119.71	128.46
38	X	309	KC2	CMD-C2D-C1D	-5.69	119.72	128.46
29	U	315	Q6L	C11-C12-C13	5.68	128.82	112.69
25	A	808	CLA	C4A-NA-C1A	5.67	109.26	106.71
25	B	832	CLA	CBA-CAA-C2A	5.67	125.98	114.02
25	3	307	CLA	C4A-NA-C1A	5.67	109.25	106.71
24	3	306	CHL	CMB-C2B-C1B	-5.66	119.77	128.46
25	2	611	CLA	C4A-NA-C1A	5.66	109.25	106.71
30	J	101	BCR	C36-C18-C17	-5.65	115.01	122.92
24	U	304	CHL	C4A-NA-C1A	5.63	109.24	106.71
25	S	312	CLA	C4A-NA-C1A	5.63	109.23	106.71
30	3	318	BCR	C38-C26-C25	-5.62	118.21	124.53
38	U	307	KC2	C1A-C2A-C3A	-5.62	102.66	107.11
25	L	301	CLA	C4A-NA-C1A	5.61	109.23	106.71
27	1	612	XAT	C18-C5-C4	-5.61	107.97	114.28
34	A	844	PQN	C14-C13-C15	-5.61	105.84	115.27
25	A	827	CLA	C4A-NA-C1A	5.60	109.22	106.71
25	V	303	CLA	CMB-C2B-C1B	-5.60	119.86	128.46
25	4	309	CLA	O2D-CGD-CBD	5.59	121.21	111.27
25	A	805	CLA	CMB-C2B-C1B	-5.58	119.89	128.46
24	P	304	CHL	C4A-NA-C1A	5.57	109.21	106.71
25	O	2004	CLA	C4A-NA-C1A	5.57	109.21	106.71
25	B	829	CLA	CMB-C2B-C1B	-5.56	119.91	128.46
29	Q	318	Q6L	C11-C12-C13	5.56	128.48	112.69
25	O	2002	CLA	C4A-NA-C1A	5.55	109.20	106.71
25	3	314	CLA	CMB-C2B-C1B	-5.55	119.93	128.46
25	Q	306	CLA	CMB-C2B-C1B	-5.54	119.94	128.46
27	2	617	XAT	O4-C5-C18	5.53	121.69	115.06
25	V	303	CLA	CAC-C3C-C4C	5.53	131.98	124.81
30	2	618	BCR	C23-C24-C25	-5.52	111.69	127.20
25	4	310	CLA	CMB-C2B-C1B	-5.52	119.99	128.46
25	A	825	CLA	CMB-C2B-C1B	-5.51	119.99	128.46
25	A	807	CLA	C4A-NA-C1A	5.50	109.18	106.71
25	1	607	CLA	CMB-C2B-C1B	-5.50	120.01	128.46
25	4	309	CLA	O2D-CGD-O1D	-5.49	113.11	123.84
24	V	306	CHL	CMB-C2B-C1B	-5.49	120.03	128.46
25	R	316	CLA	C4-C3-C5	5.49	124.50	115.27
29	X	316	Q6L	C11-C12-C13	5.49	128.28	112.69
27	4	318	XAT	C39-C29-C30	5.48	130.60	122.92
25	4	311	CLA	CMB-C2B-C1B	-5.48	120.04	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	J	101	BCR	C34-C9-C10	5.46	130.57	122.92
27	1	612	XAT	C8-C9-C10	5.46	127.31	118.94
30	A	851	BCR	C36-C18-C19	5.45	126.67	118.08
38	R	312	KC2	CMA-C3A-C4A	-5.45	116.74	125.04
25	X	314	CLA	C4A-NA-C1A	5.45	109.16	106.71
25	S	303	CLA	CMB-C2B-C3B	5.44	134.86	124.68
29	P	315	Q6L	C11-C12-C13	5.44	128.15	112.69
30	A	852	BCR	C23-C22-C21	-5.43	110.61	118.94
29	S	321	Q6L	C11-C12-C13	5.41	128.07	112.69
25	A	824	CLA	CMB-C2B-C1B	-5.41	120.16	128.46
25	T	311	CLA	CMB-C2B-C1B	-5.39	120.18	128.46
25	A	831	CLA	C4-C3-C5	5.39	124.34	115.27
25	O	2005	CLA	C4A-NA-C1A	5.39	109.13	106.71
30	2	618	BCR	C36-C18-C19	5.39	126.57	118.08
30	B	845	BCR	C37-C22-C23	5.38	126.55	118.08
25	A	805	CLA	C4A-NA-C1A	5.37	109.12	106.71
24	V	314	CHL	CMB-C2B-C1B	-5.37	120.21	128.46
25	A	821	CLA	CMB-C2B-C1B	-5.37	120.21	128.46
30	B	845	BCR	C40-C30-C25	-5.37	101.59	110.30
25	B	838	CLA	CMB-C2B-C3B	5.37	134.72	124.68
25	2	603	CLA	C4A-NA-C1A	5.37	109.12	106.71
24	R	311	CHL	CMB-C2B-C1B	-5.36	120.22	128.46
25	R	315	CLA	C4A-NA-C1A	5.36	109.12	106.71
27	4	318	XAT	C27-C28-C29	-5.36	117.21	125.53
25	A	809	CLA	C4A-NA-C1A	5.36	109.12	106.71
30	H	305	BCR	C37-C22-C23	5.36	126.52	118.08
29	T	322	Q6L	C11-C12-C13	5.36	127.92	112.69
24	V	306	CHL	C4A-NA-C1A	5.35	109.11	106.71
25	B	810	CLA	C4A-NA-C1A	5.35	109.11	106.71
27	1	612	XAT	O4-C5-C18	5.34	121.45	115.06
24	S	305	CHL	CMB-C2B-C1B	-5.33	120.27	128.46
30	B	845	BCR	C4-C5-C6	-5.32	115.01	122.73
37	W	317	NEX	C26-C27-C28	-5.31	114.76	125.99
27	6	615	XAT	O4-C5-C18	5.31	121.42	115.06
30	I	101	BCR	C33-C5-C6	5.31	130.49	124.53
25	Q	314	CLA	C4A-NA-C1A	5.29	109.08	106.71
25	A	822	CLA	CMB-C2B-C1B	-5.28	120.34	128.46
25	6	609	CLA	C4A-NA-C1A	5.28	109.08	106.71
30	A	848	BCR	C36-C18-C19	5.28	126.40	118.08
25	Q	315	CLA	C4A-NA-C1A	5.27	109.08	106.71
25	3	312	CLA	CMB-C2B-C1B	-5.26	120.37	128.46
25	6	609	CLA	CMB-C2B-C3B	5.26	134.52	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	4	305	CLA	C4A-NA-C1A	5.26	109.07	106.71
25	3	302	CLA	CMB-C2B-C1B	-5.25	120.39	128.46
29	S	315	Q6L	C11-C12-C13	5.24	127.58	112.69
25	A	815	CLA	CMB-C2B-C3B	5.24	134.47	124.68
30	B	846	BCR	C8-C9-C10	5.23	126.97	118.94
30	I	101	BCR	C8-C7-C6	-5.22	112.54	127.20
38	W	308	KC2	CMA-C3A-C2A	-5.22	115.52	128.30
25	B	826	CLA	CMB-C2B-C1B	-5.22	120.44	128.46
25	W	311	CLA	C4A-NA-C1A	5.21	109.05	106.71
25	1	607	CLA	C4A-NA-C1A	5.21	109.05	106.71
25	J	102	CLA	C4A-NA-C1A	5.21	109.05	106.71
25	T	302	CLA	C4A-NA-C1A	5.21	109.05	106.71
24	Q	308	CHL	C4A-NA-C1A	5.21	109.05	106.71
24	T	320	CHL	C4A-NA-C1A	5.21	109.05	106.71
25	T	301	CLA	CMB-C2B-C1B	-5.20	120.47	128.46
29	S	316	Q6L	C11-C12-C13	5.20	127.46	112.69
30	L	306	BCR	C36-C18-C19	5.19	126.26	118.08
25	6	602	CLA	CMB-C2B-C3B	5.19	134.39	124.68
24	R	310	CHL	C4-C3-C5	5.19	121.91	115.98
24	6	601	CHL	CMB-C2B-C1B	-5.18	120.50	128.46
30	3	317	BCR	C23-C24-C25	-5.18	112.65	127.20
25	A	804	CLA	CMB-C2B-C1B	-5.18	120.51	128.46
25	B	814	CLA	CMB-C2B-C1B	-5.16	120.53	128.46
30	A	852	BCR	C34-C9-C10	-5.15	115.70	122.92
25	5	606	CLA	C4A-NA-C1A	5.15	109.02	106.71
25	G	204	CLA	C4A-NA-C1A	5.15	109.02	106.71
25	B	837	CLA	CMB-C2B-C1B	-5.15	120.55	128.46
25	A	835	CLA	C4A-NA-C1A	5.14	109.02	106.71
27	4	318	XAT	C39-C29-C28	-5.14	109.97	118.08
25	U	308	CLA	C1D-ND-C4D	-5.14	102.68	106.33
25	V	311	CLA	C4A-NA-C1A	5.14	109.02	106.71
25	A	804	CLA	CMB-C2B-C3B	5.14	134.29	124.68
25	A	839	CLA	CMB-C2B-C3B	5.13	134.28	124.68
24	4	306	CHL	CMB-C2B-C1B	-5.12	120.59	128.46
24	W	306	CHL	C2C-C3C-C4C	5.11	110.13	106.49
25	2	614	CLA	O2D-CGD-O1D	-5.11	113.85	123.84
24	6	606	CHL	CMB-C2B-C1B	-5.09	120.63	128.46
30	K	205	BCR	C36-C18-C17	-5.08	115.81	122.92
34	B	844	PQN	C14-C13-C15	-5.08	106.72	115.27
25	O	2002	CLA	CMB-C2B-C1B	-5.07	120.67	128.46
27	1	612	XAT	C7-C8-C9	-5.07	117.66	125.53
25	3	303	CLA	C4A-NA-C1A	5.07	108.98	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	6	613	CLA	CMB-C2B-C1B	-5.06	120.69	128.46
29	X	317	Q6L	C11-C12-C13	5.06	127.06	112.69
24	Q	307	CHL	CMB-C2B-C1B	-5.05	120.70	128.46
25	V	301	CLA	CMB-C2B-C3B	5.05	134.12	124.68
25	B	820	CLA	CMB-C2B-C1B	-5.05	120.70	128.46
25	P	312	CLA	C4A-NA-C1A	5.05	108.97	106.71
25	4	314	CLA	C4A-NA-C1A	5.04	108.97	106.71
24	W	314	CHL	CMB-C2B-C3B	5.04	134.12	124.68
34	A	844	PQN	C11-C12-C13	-5.04	118.40	126.79
30	A	850	BCR	C3-C4-C5	-5.04	105.07	114.08
37	H	306	NEX	C26-C27-C28	-5.04	115.33	125.99
25	W	312	CLA	CMB-C2B-C1B	-5.04	120.72	128.46
30	3	319	BCR	C36-C18-C17	-5.03	115.87	122.92
37	T	317	NEX	C26-C27-C28	-5.03	115.35	125.99
25	3	304	CLA	C4A-NA-C1A	5.03	108.97	106.71
25	A	826	CLA	C4A-NA-C1A	5.03	108.97	106.71
24	Q	309	CHL	CMB-C2B-C1B	-5.03	120.73	128.46
25	4	312	CLA	C4A-NA-C1A	5.03	108.97	106.71
25	V	312	CLA	C4A-NA-C1A	5.03	108.97	106.71
29	W	316	Q6L	C11-C12-C13	5.03	126.98	112.69
38	V	308	KC2	CMA-C3A-C2A	-5.03	115.99	128.30
25	W	303	CLA	CMB-C2B-C3B	5.02	134.08	124.68
25	P	309	CLA	C4A-NA-C1A	5.02	108.96	106.71
24	X	306	CHL	CMB-C2B-C1B	-5.01	120.76	128.46
25	A	823	CLA	CMB-C2B-C1B	-5.01	120.76	128.46
25	A	845	CLA	C4A-NA-C1A	5.01	108.96	106.71
25	B	818	CLA	C4A-NA-C1A	5.01	108.96	106.71
30	F	801	BCR	C40-C30-C25	5.00	118.42	110.30
30	B	845	BCR	C7-C8-C9	-5.00	118.68	126.23
25	B	831	CLA	CMB-C2B-C3B	5.00	134.04	124.68
24	4	306	CHL	C4A-NA-C1A	5.00	108.95	106.71
25	B	841	CLA	C4A-NA-C1A	5.00	108.95	106.71
25	W	309	CLA	O2D-CGD-O1D	-5.00	114.07	123.84
25	G	204	CLA	CMB-C2B-C1B	-4.99	120.80	128.46
30	A	849	BCR	C38-C26-C25	-4.98	118.94	124.53
24	T	314	CHL	CMB-C2B-C1B	-4.98	120.81	128.46
38	R	312	KC2	C1A-C2A-C3A	-4.97	103.17	107.11
25	3	302	CLA	C4A-NA-C1A	4.97	108.94	106.71
25	B	823	CLA	C4A-NA-C1A	4.97	108.94	106.71
29	P	316	Q6L	C40-C32-C33	-4.96	112.95	123.56
30	L	307	BCR	C8-C9-C10	4.96	126.55	118.94
25	R	313	CLA	CMB-C2B-C1B	-4.96	120.85	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	S	311	CLA	C4A-NA-C1A	4.95	108.93	106.71
25	P	301	CLA	C4A-NA-C1A	4.94	108.93	106.71
30	G	201	BCR	C36-C18-C19	4.93	125.84	118.08
30	B	848	BCR	C36-C18-C17	-4.93	116.02	122.92
38	X	309	KC2	CMA-C3A-C2A	-4.93	116.24	128.30
25	A	806	CLA	C4A-NA-C1A	4.92	108.92	106.71
24	T	305	CHL	CMB-C2B-C3B	4.92	133.89	124.68
25	A	808	CLA	CMB-C2B-C3B	4.92	133.88	124.68
25	P	311	CLA	C4A-NA-C1A	4.92	108.92	106.71
25	2	612	CLA	C4A-NA-C1A	4.91	108.91	106.71
24	4	307	CHL	CHB-C4A-NA	4.91	131.30	124.51
29	O	2007	Q6L	C40-C32-C33	-4.91	113.06	123.56
25	B	841	CLA	CMB-C2B-C1B	-4.90	120.93	128.46
38	Q	310	KC2	CMA-C3A-C2A	-4.90	116.31	128.30
24	V	305	CHL	CMB-C2B-C1B	-4.90	120.94	128.46
24	S	304	CHL	C4A-NA-C1A	-4.90	104.50	106.71
24	S	306	CHL	CMB-C2B-C1B	-4.90	120.94	128.46
25	A	825	CLA	C4-C3-C2	-4.90	111.12	123.68
24	S	307	CHL	CMB-C2B-C3B	4.89	133.83	124.68
25	A	814	CLA	CMB-C2B-C1B	-4.89	120.95	128.46
24	P	305	CHL	CMB-C2B-C1B	-4.88	120.96	128.46
25	B	802	CLA	CMB-C2B-C3B	4.88	133.81	124.68
30	M	101	BCR	C10-C11-C12	4.87	138.42	123.22
25	U	310	CLA	C4A-NA-C1A	4.86	108.89	106.71
38	R	312	KC2	CMD-C2D-C1D	-4.85	121.01	128.46
27	3	316	XAT	C39-C29-C30	4.85	129.72	122.92
30	K	207	BCR	C28-C27-C26	-4.85	105.42	114.08
25	U	309	CLA	C4A-NA-C1A	4.83	108.88	106.71
25	A	834	CLA	CMB-C2B-C1B	-4.83	121.04	128.46
27	5	612	XAT	C18-C5-C6	-4.83	114.17	122.26
25	T	303	CLA	CMB-C2B-C3B	4.83	133.71	124.68
25	W	301	CLA	C4A-NA-C1A	4.83	108.88	106.71
29	V	321	Q6L	C40-C32-C33	-4.82	113.25	123.56
37	R	321	NEX	C26-C27-C28	-4.82	115.81	125.99
27	4	318	XAT	C26-C27-C28	-4.82	115.81	125.99
25	S	311	CLA	CMB-C2B-C1B	-4.81	121.07	128.46
25	B	803	CLA	CMB-C2B-C3B	4.81	133.67	124.68
25	R	317	CLA	C4A-NA-C1A	4.80	108.87	106.71
38	Q	310	KC2	CHB-C4A-C3A	-4.80	117.48	124.98
25	A	811	CLA	C4A-NA-C1A	4.80	108.86	106.71
25	5	602	CLA	CMB-C2B-C1B	-4.80	121.09	128.46
27	6	615	XAT	C38-C25-C26	-4.79	114.22	122.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	806	CLA	CMB-C2B-C1B	-4.79	121.10	128.46
25	5	603	CLA	CMB-C2B-C3B	4.79	133.64	124.68
30	A	852	BCR	C36-C18-C17	-4.79	116.21	122.92
30	A	848	BCR	C8-C7-C6	-4.79	113.75	127.20
25	H	304	CLA	C4A-NA-C1A	4.79	108.86	106.71
25	T	310	CLA	C4A-NA-C1A	4.79	108.86	106.71
25	3	310	CLA	C4A-NA-C1A	4.78	108.86	106.71
25	B	838	CLA	C4A-NA-C1A	4.78	108.85	106.71
25	A	832	CLA	CMB-C2B-C1B	-4.77	121.13	128.46
25	K	203	CLA	O2D-CGD-O1D	-4.77	114.51	123.84
25	B	804	CLA	C4A-NA-C1A	4.77	108.85	106.71
25	A	839	CLA	CMB-C2B-C1B	-4.77	121.13	128.46
25	L	303	CLA	CMB-C2B-C3B	4.77	133.60	124.68
25	3	304	CLA	CMB-C2B-C1B	-4.77	121.14	128.46
37	S	317	NEX	C26-C27-C28	-4.77	115.92	125.99
25	A	818	CLA	CMB-C2B-C3B	4.77	133.59	124.68
30	K	205	BCR	C8-C7-C6	-4.76	113.82	127.20
30	2	618	BCR	C37-C22-C23	4.76	125.58	118.08
25	B	828	CLA	C4A-NA-C1A	4.76	108.84	106.71
24	X	308	CHL	CMB-C2B-C3B	4.74	133.54	124.68
25	V	313	CLA	C4A-NA-C1A	4.74	108.83	106.71
30	G	205	BCR	C36-C18-C19	4.73	125.54	118.08
30	A	850	BCR	C33-C5-C6	-4.73	119.21	124.53
25	B	816	CLA	CMB-C2B-C1B	-4.73	121.20	128.46
25	K	206	CLA	C4A-NA-C1A	4.72	108.83	106.71
24	T	307	CHL	CMB-C2B-C3B	4.72	133.51	124.68
25	3	305	CLA	C4A-NA-C1A	4.71	108.82	106.71
25	3	311	CLA	CMB-C2B-C1B	-4.71	121.23	128.46
30	K	205	BCR	C23-C24-C25	-4.71	113.99	127.20
24	V	305	CHL	C4A-NA-C1A	4.70	108.82	106.71
25	B	817	CLA	C4A-NA-C1A	4.70	108.82	106.71
24	6	601	CHL	CMB-C2B-C3B	4.69	133.46	124.68
25	A	842	CLA	CHD-C1D-ND	-4.69	120.15	124.45
24	X	306	CHL	CMA-C3A-C2A	-4.68	105.17	116.10
29	U	315	Q6L	C40-C32-C33	-4.68	113.55	123.56
25	K	201	CLA	CMB-C2B-C3B	4.68	133.43	124.68
27	3	316	XAT	C7-C8-C9	-4.67	118.28	125.53
38	S	308	KC2	C2A-C3A-C4A	-4.67	103.02	106.49
25	V	303	CLA	CMB-C2B-C3B	4.67	133.42	124.68
37	T	317	NEX	C28-C29-C30	4.67	126.11	118.94
29	U	314	Q6L	C40-C32-C33	-4.66	113.58	123.56
25	W	311	CLA	CMB-C2B-C1B	-4.66	121.30	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	P	319	Q6L	C40-C32-C33	-4.66	113.58	123.56
29	V	315	Q6L	C11-C12-C13	4.66	125.93	112.69
30	A	849	BCR	C36-C18-C17	-4.66	116.40	122.92
38	R	312	KC2	CMD-C2D-C3D	4.66	133.40	124.68
29	X	301	Q6L	C40-C32-C33	-4.66	113.60	123.56
25	U	302	CLA	C4A-NA-C1A	4.65	108.80	106.71
29	R	304	Q6L	C40-C32-C33	-4.65	113.61	123.56
25	R	305	CLA	C4A-NA-C1A	4.65	108.80	106.71
25	N	203	CLA	C2D-C1D-ND	-4.65	106.68	110.10
25	Q	306	CLA	CHD-C1D-ND	-4.65	120.18	124.45
24	W	305	CHL	CMB-C2B-C1B	-4.64	121.33	128.46
30	L	305	BCR	C28-C27-C26	-4.64	105.79	114.08
24	U	305	CHL	CMB-C2B-C3B	4.64	133.36	124.68
38	T	308	KC2	C1A-C2A-C3A	-4.64	103.43	107.11
30	B	849	BCR	C36-C18-C19	4.64	125.38	118.08
25	2	608	CLA	CMB-C2B-C1B	-4.64	121.34	128.46
24	S	306	CHL	C1C-C2C-C3C	-4.63	103.44	107.11
25	L	302	CLA	CHD-C1D-ND	-4.63	120.19	124.45
29	2	616	Q6L	C11-C12-C13	4.63	125.84	112.69
26	5	611	IWJ	C01-C02-C03	-4.63	113.66	123.56
37	H	306	NEX	C28-C29-C30	4.63	126.04	118.94
25	T	311	CLA	CMB-C2B-C3B	4.63	133.33	124.68
30	B	848	BCR	C8-C7-C6	-4.62	114.21	127.20
25	2	610	CLA	C4A-NA-C1A	4.62	108.78	106.71
25	A	837	CLA	CMB-C2B-C1B	-4.62	121.36	128.46
30	J	103	BCR	C27-C26-C25	-4.62	116.02	122.73
24	T	306	CHL	C4A-NA-C1A	4.62	108.78	106.71
25	2	604	CLA	CMB-C2B-C1B	-4.62	121.36	128.46
24	P	306	CHL	C1C-C2C-C3C	-4.62	103.45	107.11
30	A	848	BCR	C23-C24-C25	-4.62	114.24	127.20
25	R	317	CLA	CMB-C2B-C1B	-4.62	121.37	128.46
25	A	817	CLA	C4A-NA-C1A	4.61	108.78	106.71
25	A	817	CLA	CMB-C2B-C1B	-4.60	121.39	128.46
26	U	316	IWJ	C33-C32-C30	4.60	119.90	112.04
29	W	319	Q6L	C11-C12-C13	4.60	125.76	112.69
25	S	302	CLA	C4A-NA-C1A	4.60	108.77	106.71
25	A	829	CLA	CMB-C2B-C3B	4.60	133.28	124.68
25	A	805	CLA	CMB-C2B-C3B	4.60	133.28	124.68
24	R	309	CHL	CMB-C2B-C1B	-4.60	121.40	128.46
24	U	313	CHL	CMB-C2B-C1B	-4.60	121.40	128.46
25	1	607	CLA	CMB-C2B-C3B	4.59	133.27	124.68
25	R	316	CLA	CMB-C2B-C1B	-4.59	121.41	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	1	609	CLA	C4A-NA-C1A	4.59	108.77	106.71
25	3	314	CLA	CMB-C2B-C3B	4.59	133.26	124.68
25	T	312	CLA	C4A-NA-C1A	4.58	108.76	106.71
25	A	808	CLA	CMB-C2B-C1B	-4.58	121.43	128.46
25	B	807	CLA	CMB-C2B-C3B	4.58	133.24	124.68
29	W	316	Q6L	C40-C32-C33	-4.57	113.78	123.56
30	M	101	BCR	C24-C23-C22	-4.57	119.33	126.23
30	A	852	BCR	C36-C18-C19	4.56	125.27	118.08
27	2	617	XAT	C18-C5-C4	-4.56	109.15	114.28
25	B	813	CLA	C4A-NA-C1A	4.56	108.75	106.71
30	K	202	BCR	C37-C22-C23	4.56	125.25	118.08
24	S	306	CHL	CAC-C3C-C4C	4.55	130.72	124.81
25	B	817	CLA	CMB-C2B-C1B	-4.55	121.47	128.46
27	3	316	XAT	C18-C5-C6	-4.55	114.63	122.26
37	P	317	NEX	C28-C29-C30	4.55	125.92	118.94
25	A	825	CLA	C4A-NA-C1A	4.55	108.75	106.71
25	B	837	CLA	C4A-NA-C1A	4.54	108.75	106.71
25	Q	306	CLA	C4D-C3D-CAD	-4.54	102.75	108.10
24	S	305	CHL	CMB-C2B-C3B	4.53	133.16	124.68
38	S	308	KC2	CBA-CAA-C2A	-4.53	107.99	125.27
29	S	315	Q6L	C40-C32-C33	-4.53	113.86	123.56
25	A	803	CLA	CMB-C2B-C1B	-4.53	121.50	128.46
25	W	313	CLA	C4A-NA-C1A	4.53	108.74	106.71
30	J	103	BCR	C36-C18-C17	-4.53	116.58	122.92
25	U	311	CLA	CMB-C2B-C1B	-4.53	121.50	128.46
30	K	202	BCR	C36-C18-C17	-4.53	116.58	122.92
30	G	201	BCR	C33-C5-C6	4.53	129.61	124.53
37	P	317	NEX	C26-C27-C28	-4.53	116.42	125.99
25	5	601	CLA	CHB-C4A-NA	4.53	130.77	124.51
25	B	839	CLA	C4A-NA-C1A	4.52	108.74	106.71
30	J	103	BCR	C37-C22-C23	4.52	125.20	118.08
25	B	815	CLA	C1-C2-C3	4.52	133.85	126.04
25	K	206	CLA	CMB-C2B-C1B	-4.51	121.53	128.46
25	B	816	CLA	C4A-NA-C1A	4.51	108.73	106.71
25	6	608	CLA	CMB-C2B-C1B	-4.50	121.54	128.46
30	B	848	BCR	C23-C24-C25	-4.50	114.56	127.20
25	B	843	CLA	CMB-C2B-C1B	-4.50	121.54	128.46
25	A	809	CLA	CMB-C2B-C1B	-4.50	121.55	128.46
25	3	302	CLA	C4-C3-C2	-4.50	112.14	123.68
25	4	309	CLA	CMB-C2B-C1B	-4.50	121.55	128.46
25	Q	304	CLA	O2A-CGA-O1A	-4.49	112.25	123.59
38	W	308	KC2	CMA-C3A-C4A	-4.49	118.19	125.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	K	202	BCR	C19-C18-C17	-4.49	112.05	118.94
30	K	202	BCR	C23-C22-C21	-4.48	112.06	118.94
25	X	313	CLA	CMB-C2B-C1B	-4.48	121.58	128.46
30	M	101	BCR	C34-C9-C10	4.48	129.20	122.92
30	K	205	BCR	C33-C5-C6	4.48	129.56	124.53
25	R	307	CLA	CMB-C2B-C1B	-4.48	121.58	128.46
24	P	305	CHL	CED-O2D-CGD	4.47	126.05	115.94
25	T	301	CLA	CMB-C2B-C3B	4.47	133.04	124.68
25	6	608	CLA	C4A-NA-C1A	4.47	108.72	106.71
30	F	804	BCR	C7-C8-C9	-4.47	119.48	126.23
26	R	303	IWJ	C01-C02-C03	-4.46	114.03	123.56
25	B	803	CLA	C4A-NA-C1A	4.46	108.71	106.71
25	U	301	CLA	CMB-C2B-C3B	4.45	133.01	124.68
25	P	303	CLA	CMB-C2B-C1B	-4.44	121.64	128.46
24	P	304	CHL	CMB-C2B-C1B	-4.44	121.64	128.46
25	1	602	CLA	CMB-C2B-C1B	-4.44	121.64	128.46
30	J	101	BCR	C15-C14-C13	-4.44	120.98	127.31
25	U	301	CLA	CMB-C2B-C1B	-4.44	121.65	128.46
38	X	309	KC2	C1A-C2A-C3A	-4.43	103.59	107.11
38	V	308	KC2	CMD-C2D-C1D	-4.43	121.65	128.46
25	X	313	CLA	C4A-NA-C1A	4.43	108.70	106.71
25	A	837	CLA	C4A-NA-C1A	4.43	108.70	106.71
24	S	314	CHL	CMB-C2B-C3B	4.43	132.96	124.68
24	S	306	CHL	CHD-C1D-ND	-4.43	120.39	124.45
25	1	613	CLA	CMB-C2B-C1B	-4.42	121.67	128.46
25	3	311	CLA	C1-O2A-CGA	4.42	128.05	116.44
29	W	320	Q6L	C40-C32-C33	-4.42	114.10	123.56
29	S	323	Q6L	C40-C32-C33	-4.42	114.10	123.56
25	B	829	CLA	CMB-C2B-C3B	4.42	132.95	124.68
25	1	609	CLA	CHD-C1D-ND	-4.42	120.39	124.45
25	B	827	CLA	C4A-NA-C1A	4.41	108.69	106.71
25	K	201	CLA	C4A-NA-C1A	4.41	108.69	106.71
26	U	316	IWJ	C01-C02-C03	-4.41	114.13	123.56
29	O	2006	Q6L	C40-C32-C33	-4.41	114.13	123.56
25	5	608	CLA	C4A-NA-C1A	4.40	108.69	106.71
24	X	307	CHL	CHB-C4A-NA	4.40	130.59	124.51
25	K	206	CLA	C4-C3-C5	4.40	122.67	115.27
25	A	834	CLA	CMB-C2B-C3B	4.39	132.90	124.68
24	P	307	CHL	CMB-C2B-C3B	4.39	132.90	124.68
24	Q	308	CHL	CHB-C4A-NA	4.39	130.58	124.51
25	Q	315	CLA	CMB-C2B-C1B	-4.39	121.72	128.46
25	V	309	CLA	CMB-C2B-C1B	-4.39	121.72	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	5	612	XAT	C36-C21-C22	-4.38	101.36	108.98
30	M	101	BCR	C31-C1-C6	-4.38	103.19	110.30
27	2	617	XAT	C38-C25-C26	-4.38	114.91	122.26
24	2	601	CHL	C1B-CHB-C4A	-4.38	121.44	130.12
25	A	806	CLA	CMB-C2B-C3B	4.38	132.87	124.68
25	B	811	CLA	CMB-C2B-C1B	-4.38	121.73	128.46
25	P	302	CLA	C4A-NA-C1A	4.38	108.67	106.71
29	Q	319	Q6L	C05-C06-C07	4.38	116.30	110.30
24	Q	309	CHL	C4A-NA-C1A	4.37	108.67	106.71
24	X	307	CHL	C2C-C3C-C4C	4.37	109.61	106.49
25	X	304	CLA	CMB-C2B-C3B	4.36	132.83	124.68
25	A	810	CLA	CMB-C2B-C1B	-4.36	121.77	128.46
25	T	309	CLA	C4-C3-C5	4.35	122.60	115.27
25	P	301	CLA	C4-C3-C5	4.35	122.59	115.27
25	4	310	CLA	CMB-C2B-C3B	4.35	132.81	124.68
30	B	845	BCR	C34-C9-C10	4.35	129.01	122.92
38	T	308	KC2	C2A-C3A-C4A	-4.34	103.26	106.49
37	H	306	NEX	C19-C9-C10	4.34	129.01	122.92
29	P	321	Q6L	C40-C32-C33	-4.34	114.28	123.56
25	2	602	CLA	O2A-CGA-O1A	-4.34	112.65	123.59
26	V	317	IWJ	C01-C02-C03	-4.33	114.29	123.56
24	S	305	CHL	C4A-NA-C1A	4.33	108.65	106.71
25	B	814	CLA	C4A-NA-C1A	4.33	108.65	106.71
24	X	306	CHL	CMA-C3A-C4A	4.33	123.42	111.77
25	B	843	CLA	CMB-C2B-C3B	4.33	132.78	124.68
24	W	304	CHL	C4A-NA-C1A	4.33	108.65	106.71
25	2	606	CLA	CMB-C2B-C1B	-4.33	121.81	128.46
27	2	617	XAT	C18-C5-C6	-4.33	115.01	122.26
25	2	606	CLA	C4A-NA-C1A	4.33	108.65	106.71
24	X	307	CHL	C1-O2A-CGA	4.32	127.79	116.44
29	T	322	Q6L	C40-C32-C33	-4.32	114.31	123.56
38	V	308	KC2	C2A-C3A-C4A	-4.32	103.28	106.49
30	4	319	BCR	C23-C24-C25	-4.32	115.07	127.20
30	K	207	BCR	C36-C18-C17	-4.32	116.87	122.92
24	P	304	CHL	CMB-C2B-C3B	4.32	132.76	124.68
25	B	828	CLA	CMB-C2B-C1B	-4.32	121.83	128.46
29	V	316	Q6L	C40-C32-C33	-4.32	114.32	123.56
24	S	306	CHL	O2D-CGD-O1D	-4.30	115.42	123.84
25	U	303	CLA	C4A-NA-C1A	4.29	108.64	106.71
25	B	805	CLA	CHD-C1D-ND	-4.28	120.52	124.45
25	U	302	CLA	CMB-C2B-C1B	-4.28	121.88	128.46
27	6	615	XAT	C38-C25-C24	4.28	119.09	114.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	J	101	BCR	C23-C24-C25	-4.28	115.18	127.20
25	V	309	CLA	C1D-ND-C4D	-4.28	103.30	106.33
25	X	310	CLA	CMB-C2B-C1B	-4.27	121.90	128.46
25	3	307	CLA	CMB-C2B-C1B	-4.27	121.90	128.46
25	A	813	CLA	C4A-NA-C1A	4.27	108.62	106.71
26	6	614	IWJ	C01-C02-C03	-4.27	114.43	123.56
29	P	316	Q6L	C11-C12-C13	4.26	124.81	112.69
30	A	851	BCR	C33-C5-C6	4.26	129.31	124.53
30	B	847	BCR	C8-C7-C6	-4.26	115.23	127.20
26	Q	303	IWJ	C01-C02-C03	-4.26	114.44	123.56
25	S	311	CLA	CMB-C2B-C3B	4.26	132.65	124.68
25	6	612	CLA	CMB-C2B-C1B	-4.26	121.92	128.46
24	2	615	CHL	C4A-NA-C1A	4.26	108.62	106.71
37	R	321	NEX	C28-C29-C30	4.26	125.47	118.94
24	W	306	CHL	CMB-C2B-C3B	4.25	132.64	124.68
27	2	617	XAT	C26-C27-C28	-4.25	117.00	125.99
24	S	306	CHL	CHD-C4C-C3C	4.25	131.09	124.84
25	6	608	CLA	CMB-C2B-C3B	4.25	132.63	124.68
25	B	816	CLA	CMB-C2B-C3B	4.25	132.63	124.68
25	A	825	CLA	CMB-C2B-C3B	4.25	132.63	124.68
25	2	602	CLA	CMB-C2B-C3B	4.25	132.63	124.68
26	P	320	IWJ	C01-C02-C03	-4.25	114.47	123.56
26	1	611	IWJ	C01-C02-C03	-4.25	114.47	123.56
25	4	313	CLA	CHD-C1D-ND	-4.25	120.55	124.45
25	A	856	CLA	CMB-C2B-C1B	-4.24	121.95	128.46
25	F	802	CLA	C4A-NA-C1A	4.24	108.61	106.71
30	B	849	BCR	C36-C18-C17	-4.23	116.99	122.92
25	2	602	CLA	C4A-NA-C1A	4.23	108.61	106.71
25	Q	306	CLA	CMB-C2B-C3B	4.23	132.59	124.68
24	W	307	CHL	CMB-C2B-C3B	4.23	132.59	124.68
30	A	850	BCR	C36-C18-C17	-4.22	117.00	122.92
25	3	310	CLA	CMB-C2B-C1B	-4.22	121.98	128.46
27	4	318	XAT	C37-C21-C36	-4.22	101.15	107.37
25	4	312	CLA	CMB-C2B-C1B	-4.22	121.98	128.46
26	W	318	IWJ	C01-C02-C03	-4.22	114.54	123.56
37	R	321	NEX	C19-C9-C10	4.22	128.83	122.92
29	R	301	Q6L	C40-C32-C33	-4.21	114.54	123.56
27	3	316	XAT	C26-C27-C28	-4.21	117.08	125.99
25	B	820	CLA	CMB-C2B-C3B	4.21	132.56	124.68
27	2	617	XAT	C39-C29-C30	4.21	128.83	122.92
25	R	307	CLA	C4A-NA-C1A	4.21	108.60	106.71
27	5	612	XAT	C38-C25-C26	-4.21	115.20	122.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	4	301	IWJ	C01-C02-C03	-4.21	114.55	123.56
25	R	314	CLA	C4A-NA-C1A	4.21	108.60	106.71
38	P	308	KC2	C1A-C2A-C3A	-4.21	103.77	107.11
29	R	320	Q6L	C11-C12-C13	4.21	124.64	112.69
26	V	320	IWJ	C01-C02-C03	-4.20	114.56	123.56
25	B	806	CLA	C4A-NA-C1A	4.20	108.60	106.71
26	V	318	IWJ	C01-C02-C03	-4.20	114.57	123.56
24	V	306	CHL	CMB-C2B-C3B	4.20	132.54	124.68
27	2	617	XAT	C38-C25-C24	4.20	119.00	114.28
25	Q	304	CLA	CHB-C4A-NA	4.20	130.32	124.51
25	B	818	CLA	CMB-C2B-C3B	4.19	132.53	124.68
26	X	318	IWJ	C01-C02-C03	-4.19	114.59	123.56
30	3	318	BCR	C37-C22-C23	4.19	124.68	118.08
30	B	847	BCR	C36-C18-C17	-4.19	117.05	122.92
25	T	312	CLA	C4-C3-C5	4.19	122.32	115.27
25	K	201	CLA	O2D-CGD-CBD	4.19	118.71	111.27
25	6	611	CLA	CMB-C2B-C1B	-4.19	122.03	128.46
25	B	842	CLA	C1C-C2C-C3C	-4.19	102.55	106.96
30	J	101	BCR	C28-C27-C26	-4.18	106.61	114.08
30	G	205	BCR	C37-C22-C21	-4.18	117.06	122.92
25	V	309	CLA	CMB-C2B-C3B	4.18	132.50	124.68
30	I	101	BCR	C24-C23-C22	-4.18	119.92	126.23
25	B	821	CLA	CMB-C2B-C1B	-4.18	122.04	128.46
25	B	818	CLA	CMB-C2B-C1B	-4.18	122.04	128.46
25	A	823	CLA	O2A-C1-C2	-4.18	97.65	108.64
25	U	303	CLA	CMB-C2B-C1B	-4.18	122.04	128.46
38	Q	310	KC2	CBA-CAA-C2A	-4.17	109.36	125.27
25	2	609	CLA	C4A-NA-C1A	4.17	108.58	106.71
25	3	302	CLA	O2A-CGA-O1A	-4.17	113.07	123.59
27	5	612	XAT	C39-C29-C30	4.17	128.76	122.92
30	K	202	BCR	C28-C27-C26	-4.17	106.64	114.08
27	4	318	XAT	C18-C5-C4	-4.16	109.60	114.28
25	6	604	CLA	CMB-C2B-C1B	-4.16	122.07	128.46
25	U	301	CLA	C1B-CHB-C4A	-4.16	121.88	130.12
25	2	608	CLA	CMB-C2B-C3B	4.16	132.46	124.68
29	S	316	Q6L	C40-C32-C33	-4.16	114.67	123.56
25	A	827	CLA	C1-C2-C3	-4.16	118.85	126.04
25	U	311	CLA	O2D-CGD-O1D	-4.16	115.71	123.84
25	A	838	CLA	CMB-C2B-C1B	-4.15	122.08	128.46
38	X	309	KC2	C2A-C3A-C4A	-4.15	103.41	106.49
28	Q	302	LHG	O7-C7-C8	4.15	120.45	111.50
25	B	831	CLA	C4A-NA-C1A	4.15	108.57	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	6	605	CHL	CMB-C2B-C3B	4.15	132.44	124.68
24	6	606	CHL	O2D-CGD-O1D	-4.14	115.73	123.84
25	V	309	CLA	O2D-CGD-O1D	-4.14	115.74	123.84
25	A	807	CLA	CMB-C2B-C1B	-4.14	122.10	128.46
25	A	832	CLA	C4A-NA-C1A	4.14	108.57	106.71
37	H	306	NEX	C16-C1-C6	4.14	114.18	110.47
29	U	317	Q6L	C40-C32-C33	-4.14	114.70	123.56
25	R	313	CLA	CMB-C2B-C3B	4.14	132.42	124.68
25	W	301	CLA	C1B-CHB-C4A	-4.14	121.92	130.12
29	X	317	Q6L	C40-C32-C33	-4.13	114.72	123.56
24	Q	308	CHL	CMB-C2B-C3B	4.13	132.41	124.68
24	Q	307	CHL	CMB-C2B-C3B	4.13	132.41	124.68
30	I	101	BCR	C7-C8-C9	-4.13	119.99	126.23
25	A	830	CLA	CMB-C2B-C3B	4.13	132.41	124.68
25	U	308	CLA	CMB-C2B-C1B	-4.13	122.12	128.46
25	2	609	CLA	O2D-CGD-CBD	4.13	118.60	111.27
25	S	301	CLA	CMB-C2B-C1B	-4.12	122.13	128.46
24	4	306	CHL	CHB-C4A-NA	4.12	130.21	124.51
25	V	301	CLA	C4A-NA-C1A	4.12	108.56	106.71
27	5	612	XAT	C26-C27-C28	-4.12	117.28	125.99
30	G	201	BCR	C37-C22-C23	4.12	124.56	118.08
25	A	817	CLA	CHD-C1D-ND	-4.12	120.67	124.45
37	S	317	NEX	C28-C29-C30	4.11	125.25	118.94
25	B	822	CLA	CMB-C2B-C1B	-4.11	122.14	128.46
27	6	615	XAT	O24-C25-C24	4.11	116.47	113.38
27	6	615	XAT	C18-C5-C4	-4.11	109.66	114.28
25	A	821	CLA	CMB-C2B-C3B	4.11	132.37	124.68
38	V	308	KC2	CMA-C3A-C4A	-4.11	118.78	125.04
25	6	613	CLA	C4A-NA-C1A	4.11	108.55	106.71
30	2	618	BCR	C36-C18-C17	-4.11	117.17	122.92
26	5	611	IWJ	C37-C35-C34	-4.11	101.84	108.98
24	W	306	CHL	C1C-C2C-C3C	-4.11	103.85	107.11
25	K	206	CLA	CMB-C2B-C3B	4.11	132.36	124.68
26	T	318	IWJ	C01-C02-C03	-4.11	114.78	123.56
29	S	321	Q6L	C40-C32-C33	-4.10	114.78	123.56
30	B	849	BCR	C8-C7-C6	-4.10	115.68	127.20
30	K	202	BCR	C27-C26-C25	-4.10	116.78	122.73
25	N	203	CLA	CMB-C2B-C1B	-4.09	122.18	128.46
25	B	829	CLA	C4-C3-C5	4.09	122.15	115.27
30	A	850	BCR	C35-C13-C12	4.09	124.52	118.08
30	K	207	BCR	C8-C7-C6	-4.09	115.73	127.20
24	R	318	CHL	CMB-C2B-C1B	-4.08	122.19	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	S	318	IWJ	C01-C02-C03	-4.08	114.82	123.56
25	A	827	CLA	CMB-C2B-C3B	4.08	132.31	124.68
25	6	608	CLA	CHB-C4A-NA	4.08	130.16	124.51
25	R	315	CLA	O2D-CGD-O1D	-4.08	115.86	123.84
24	V	314	CHL	CMB-C2B-C3B	4.08	132.30	124.68
30	A	851	BCR	C36-C18-C17	-4.07	117.22	122.92
26	S	322	IWJ	C01-C02-C03	-4.07	114.84	123.56
30	F	801	BCR	C36-C18-C19	4.07	124.49	118.08
29	R	320	Q6L	C40-C32-C33	-4.07	114.85	123.56
27	6	615	XAT	C26-C27-C28	-4.07	117.39	125.99
25	1	606	CLA	C4A-NA-C1A	4.07	108.53	106.71
24	Q	308	CHL	C2D-C1D-ND	-4.07	107.11	110.10
26	T	321	IWJ	C01-C02-C03	-4.07	114.86	123.56
25	B	826	CLA	CMB-C2B-C3B	4.06	132.28	124.68
25	P	303	CLA	CMB-C2B-C3B	4.05	132.26	124.68
25	5	606	CLA	O2D-CGD-CBD	4.05	118.47	111.27
25	X	302	CLA	C1B-CHB-C4A	-4.05	122.09	130.12
25	A	829	CLA	CMB-C2B-C1B	-4.05	122.23	128.46
29	2	616	Q6L	C40-C32-C33	-4.05	114.89	123.56
26	Q	320	IWJ	C01-C02-C03	-4.05	114.89	123.56
24	6	606	CHL	CMB-C2B-C3B	4.05	132.25	124.68
25	U	311	CLA	CMB-C2B-C3B	4.05	132.25	124.68
30	F	801	BCR	C36-C18-C17	-4.05	117.25	122.92
30	I	101	BCR	C36-C18-C19	4.05	124.45	118.08
25	A	822	CLA	CMB-C2B-C3B	4.04	132.25	124.68
24	V	306	CHL	C1B-CHB-C4A	-4.04	122.11	130.12
30	3	319	BCR	C33-C5-C6	-4.04	119.99	124.53
30	K	202	BCR	C20-C21-C22	-4.04	121.54	127.31
25	B	830	CLA	CMB-C2B-C1B	-4.04	122.26	128.46
25	1	613	CLA	C4A-NA-C1A	4.04	108.52	106.71
25	3	309	CLA	C4A-NA-C1A	4.04	108.52	106.71
29	X	316	Q6L	C05-C04-C03	4.04	116.28	109.92
25	V	301	CLA	C4-C3-C5	4.04	122.06	115.27
37	P	317	NEX	O24-C25-C38	4.03	119.89	115.06
24	P	305	CHL	C1B-CHB-C4A	-4.03	122.13	130.12
25	U	308	CLA	C4A-NA-C1A	-4.03	104.89	106.71
25	W	311	CLA	CMB-C2B-C3B	4.03	132.22	124.68
25	R	314	CLA	O2D-CGD-O1D	-4.03	115.96	123.84
24	2	607	CHL	CMB-C2B-C1B	-4.03	122.27	128.46
30	4	319	BCR	C31-C1-C6	-4.03	103.77	110.30
24	4	307	CHL	C4A-NA-C1A	4.03	108.52	106.71
26	S	319	IWJ	C01-C02-C03	-4.03	114.95	123.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	B	849	BCR	C29-C30-C25	4.02	116.67	110.48
24	X	307	CHL	CMB-C2B-C1B	-4.02	122.29	128.46
25	H	304	CLA	CMB-C2B-C1B	-4.02	122.29	128.46
30	3	319	BCR	C37-C22-C23	4.02	124.41	118.08
30	L	306	BCR	C34-C9-C10	4.02	128.55	122.92
26	3	315	IWJ	C01-C02-C03	-4.02	114.97	123.56
30	G	201	BCR	C15-C16-C17	-4.02	115.25	123.47
30	A	852	BCR	C20-C21-C22	-4.02	121.58	127.31
30	4	319	BCR	C36-C18-C17	-4.02	117.30	122.92
37	S	317	NEX	C39-C29-C30	-4.02	117.30	122.92
30	A	848	BCR	C36-C18-C17	-4.01	117.30	122.92
25	B	824	CLA	CMB-C2B-C3B	4.01	132.19	124.68
30	2	618	BCR	C8-C7-C6	-4.01	115.93	127.20
25	2	604	CLA	C4A-NA-C1A	4.01	108.51	106.71
24	P	314	CHL	CMB-C2B-C1B	-4.00	122.31	128.46
25	6	607	CLA	C4A-NA-C1A	4.00	108.50	106.71
26	R	322	IWJ	C01-C02-C03	-4.00	115.00	123.56
25	A	856	CLA	CMB-C2B-C3B	4.00	132.16	124.68
25	V	312	CLA	CMB-C2B-C1B	-4.00	122.32	128.46
27	3	316	XAT	C11-C10-C9	-4.00	121.60	127.31
24	2	601	CHL	C4A-NA-C1A	4.00	108.50	106.71
25	1	608	CLA	C4A-NA-C1A	4.00	108.50	106.71
25	P	311	CLA	CMB-C2B-C1B	-4.00	122.32	128.46
37	P	317	NEX	C38-C25-C26	-4.00	115.56	122.26
25	K	201	CLA	O2D-CGD-O1D	-3.99	116.03	123.84
30	L	305	BCR	C36-C18-C17	-3.99	117.33	122.92
24	X	307	CHL	C1C-C2C-C3C	-3.99	103.94	107.11
25	3	302	CLA	CMB-C2B-C3B	3.99	132.15	124.68
30	L	306	BCR	C36-C18-C17	-3.99	117.33	122.92
25	6	604	CLA	C4A-NA-C1A	3.98	108.50	106.71
25	B	836	CLA	CHD-C1D-ND	-3.98	120.79	124.45
29	X	319	Q6L	C05-C06-C07	3.98	115.75	110.30
30	L	306	BCR	C24-C23-C22	-3.98	120.22	126.23
25	R	306	CLA	C4A-NA-C1A	3.98	108.50	106.71
30	A	852	BCR	C8-C9-C10	3.98	125.05	118.94
24	V	305	CHL	CMB-C2B-C3B	3.98	132.12	124.68
25	4	303	CLA	CMB-C2B-C1B	-3.98	122.35	128.46
25	5	602	CLA	CMB-C2B-C3B	3.98	132.12	124.68
38	X	309	KC2	CMD-C2D-C3D	3.97	132.11	124.68
30	A	851	BCR	C23-C22-C21	-3.97	112.84	118.94
30	I	101	BCR	C4-C5-C6	-3.97	116.96	122.73
30	A	848	BCR	C28-C27-C26	-3.97	106.99	114.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	3	312	CLA	CMB-C2B-C3B	3.97	132.10	124.68
25	6	610	CLA	C4A-NA-C1A	3.96	108.49	106.71
24	P	304	CHL	C1B-CHB-C4A	-3.96	122.28	130.12
25	B	843	CLA	C3A-C2A-C1A	3.96	107.27	101.34
25	F	802	CLA	CMB-C2B-C1B	-3.96	122.38	128.46
25	B	814	CLA	CMB-C2B-C3B	3.96	132.08	124.68
30	B	845	BCR	C38-C26-C25	-3.96	120.08	124.53
25	U	302	CLA	CMB-C2B-C3B	3.96	132.08	124.68
25	B	813	CLA	O2A-CGA-O1A	-3.96	113.61	123.59
29	V	316	Q6L	C38-C36-C31	-3.95	103.55	109.55
38	T	308	KC2	CBA-CAA-C2A	-3.95	110.20	125.27
30	3	318	BCR	C36-C18-C17	-3.95	117.39	122.92
28	3	320	LHG	O7-C7-C8	3.95	120.01	111.50
24	Q	307	CHL	CHB-C4A-NA	3.95	129.97	124.51
25	3	309	CLA	O2D-CGD-O1D	-3.95	116.12	123.84
25	A	845	CLA	C1-C2-C3	-3.94	120.37	126.75
25	A	831	CLA	C4-C3-C2	-3.94	113.56	123.68
25	S	301	CLA	CMB-C2B-C3B	3.94	132.05	124.68
29	T	316	Q6L	C40-C32-C33	-3.94	115.13	123.56
29	X	316	Q6L	C34-C33-C32	-3.94	121.07	124.85
25	A	826	CLA	C4-C3-C5	3.94	121.90	115.27
29	R	319	Q6L	C40-C32-C33	-3.94	115.13	123.56
30	2	618	BCR	C37-C22-C21	-3.94	117.41	122.92
25	Q	304	CLA	C1B-CHB-C4A	-3.94	122.32	130.12
30	B	845	BCR	C36-C18-C17	-3.93	117.42	122.92
30	L	306	BCR	C28-C27-C26	-3.93	107.06	114.08
30	A	852	BCR	C24-C23-C22	-3.93	120.30	126.23
24	W	304	CHL	CMB-C2B-C1B	-3.93	122.43	128.46
25	A	840	CLA	C4-C3-C2	-3.93	113.61	123.68
30	2	618	BCR	C15-C16-C17	-3.93	115.43	123.47
31	N	201	LMG	O7-C10-C11	3.92	119.95	111.50
25	W	301	CLA	CHB-C4A-NA	3.92	129.94	124.51
25	6	603	CLA	CMB-C2B-C1B	-3.92	122.44	128.46
24	U	304	CHL	C1B-CHB-C4A	-3.92	122.35	130.12
25	O	2003	CLA	C4A-NA-C1A	3.92	108.47	106.71
25	O	2005	CLA	CMB-C2B-C1B	-3.91	122.45	128.46
25	W	310	CLA	CMB-C2B-C1B	-3.91	122.45	128.46
25	5	601	CLA	C4A-NA-C1A	3.91	108.46	106.71
25	U	312	CLA	C4A-NA-C1A	3.91	108.46	106.71
25	X	311	CLA	CMB-C2B-C1B	-3.91	122.46	128.46
25	2	609	CLA	O2D-CGD-O1D	-3.90	116.21	123.84
25	1	602	CLA	CMB-C2B-C3B	3.90	131.98	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	W	312	CLA	CMB-C2B-C3B	3.90	131.97	124.68
25	S	313	CLA	C4A-NA-C1A	3.90	108.46	106.71
37	T	317	NEX	C39-C29-C30	-3.90	117.47	122.92
25	5	601	CLA	O2D-CGD-O1D	-3.90	116.22	123.84
25	B	830	CLA	CMB-C2B-C3B	3.89	131.96	124.68
25	Q	312	CLA	O2D-CGD-O1D	-3.89	116.23	123.84
25	O	2002	CLA	CMB-C2B-C3B	3.89	131.96	124.68
25	2	610	CLA	O2D-CGD-O1D	-3.89	116.23	123.84
25	A	815	CLA	C4-C3-C5	3.89	121.81	115.27
25	K	204	CLA	CBA-CAA-C2A	3.89	125.34	113.86
24	S	304	CHL	C2A-C3A-C4A	-3.89	96.82	101.78
25	R	317	CLA	CMB-C2B-C3B	3.89	131.95	124.68
30	K	205	BCR	C3-C4-C5	-3.88	107.14	114.08
25	O	2002	CLA	C4-C3-C5	3.88	121.80	115.27
29	T	319	Q6L	C40-C32-C33	-3.88	115.26	123.56
30	A	851	BCR	C28-C27-C26	-3.88	107.15	114.08
37	W	317	NEX	C38-C25-C26	-3.88	115.77	122.26
25	A	856	CLA	C1B-CHB-C4A	-3.87	122.44	130.12
24	5	605	CHL	CMB-C2B-C3B	3.87	131.92	124.68
25	V	301	CLA	C1B-CHB-C4A	-3.87	122.45	130.12
25	B	834	CLA	CHD-C1D-ND	-3.87	120.90	124.45
25	3	301	CLA	CMB-C2B-C1B	-3.87	122.52	128.46
25	W	309	CLA	O2D-CGD-CBD	3.87	118.14	111.27
26	S	318	IWJ	C33-C32-C30	3.87	118.65	112.04
24	P	314	CHL	C4A-NA-C1A	3.86	108.44	106.71
30	I	101	BCR	C28-C27-C26	-3.86	107.18	114.08
30	G	205	BCR	C23-C24-C25	-3.86	116.36	127.20
29	W	319	Q6L	C40-C32-C33	-3.86	115.30	123.56
25	3	313	CLA	CMB-C2B-C1B	-3.86	122.53	128.46
30	F	804	BCR	C11-C10-C9	-3.86	121.80	127.31
30	2	618	BCR	C3-C4-C5	-3.86	107.19	114.08
25	W	313	CLA	CMB-C2B-C1B	-3.86	122.53	128.46
25	6	602	CLA	C4A-NA-C1A	3.86	108.44	106.71
25	A	820	CLA	C1B-CHB-C4A	-3.86	122.48	130.12
25	B	837	CLA	CHD-C1D-ND	-3.86	120.91	124.45
25	1	609	CLA	CAB-C3B-C4B	-3.85	122.54	128.46
30	A	848	BCR	C35-C13-C12	3.85	124.15	118.08
25	W	310	CLA	C4A-NA-C1A	3.85	108.44	106.71
25	3	311	CLA	CHD-C1D-ND	-3.85	120.92	124.45
38	W	308	KC2	CMD-C2D-C1D	-3.85	122.55	128.46
25	A	809	CLA	CMB-C2B-C3B	3.85	131.88	124.68
25	Q	313	CLA	CHB-C4A-NA	3.85	129.83	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	4	307	CHL	CMB-C2B-C1B	-3.85	122.55	128.46
24	T	306	CHL	CMB-C2B-C1B	-3.84	122.56	128.46
25	4	309	CLA	CMB-C2B-C3B	3.84	131.85	124.68
24	4	306	CHL	C2C-C3C-C4C	3.83	109.33	106.49
25	A	816	CLA	CHD-C1D-ND	-3.83	120.94	124.45
26	P	318	IWJ	C01-C02-C03	-3.82	115.38	123.56
33	A	802	CL0	C2D-C1D-ND	-3.82	107.29	110.10
25	A	825	CLA	C4-C3-C5	3.82	121.70	115.27
25	K	203	CLA	O2D-CGD-CBD	3.82	118.06	111.27
25	S	310	CLA	O2D-CGD-O1D	-3.82	116.37	123.84
30	K	202	BCR	C11-C10-C9	-3.82	121.86	127.31
25	B	821	CLA	CBA-CAA-C2A	3.82	125.13	113.86
25	B	804	CLA	CMB-C2B-C1B	-3.81	122.60	128.46
24	X	307	CHL	C3C-C4C-NC	-3.81	106.30	110.57
29	W	315	Q6L	C40-C32-C33	-3.81	115.41	123.56
25	S	309	CLA	CMB-C2B-C1B	-3.81	122.61	128.46
30	I	101	BCR	C1-C6-C5	-3.80	117.25	122.61
25	W	309	CLA	C4-C3-C5	3.80	121.67	115.27
25	B	805	CLA	C1B-CHB-C4A	-3.80	122.58	130.12
29	Q	318	Q6L	C40-C32-C33	-3.80	115.42	123.56
24	V	304	CHL	C1B-CHB-C4A	-3.80	122.59	130.12
30	J	101	BCR	C8-C7-C6	-3.80	116.53	127.20
24	4	307	CHL	C1B-CHB-C4A	-3.80	122.60	130.12
24	6	601	CHL	C1B-CHB-C4A	-3.80	122.60	130.12
25	A	823	CLA	C6-C5-C3	3.80	123.41	113.45
29	R	323	Q6L	C40-C32-C33	-3.80	115.44	123.56
29	W	320	Q6L	C38-C36-C35	-3.79	102.26	109.44
25	1	605	CLA	CMB-C2B-C1B	-3.79	122.64	128.46
30	A	849	BCR	C28-C27-C26	-3.79	107.31	114.08
25	6	607	CLA	CMB-C2B-C3B	3.79	131.76	124.68
31	L	308	LMG	O7-C10-C11	3.78	119.66	111.50
25	P	312	CLA	CMB-C2B-C1B	-3.78	122.65	128.46
24	Q	316	CHL	CMB-C2B-C1B	-3.78	122.65	128.46
30	L	305	BCR	C11-C10-C9	-3.78	121.91	127.31
25	A	821	CLA	CHB-C4A-NA	3.78	129.74	124.51
24	X	306	CHL	CMB-C2B-C3B	3.78	131.75	124.68
25	1	606	CLA	CAB-C3B-C4B	-3.78	122.65	128.46
25	A	856	CLA	O1D-CGD-CBD	3.78	132.22	124.48
30	L	306	BCR	C37-C22-C23	3.77	124.02	118.08
25	3	313	CLA	C4A-NA-C1A	3.77	108.40	106.71
24	V	314	CHL	C1B-CHB-C4A	-3.77	122.65	130.12
25	A	824	CLA	CHD-C1D-ND	-3.77	120.99	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	1	612	XAT	C31-C30-C29	-3.77	121.93	127.31
24	X	315	CHL	CMB-C2B-C1B	-3.77	122.67	128.46
25	2	606	CLA	CHD-C1D-ND	-3.77	120.99	124.45
30	B	848	BCR	C34-C9-C10	3.77	128.20	122.92
24	4	302	CHL	C4-C3-C5	3.77	120.29	115.98
31	O	2008	LMG	O7-C10-C11	3.77	119.62	111.50
24	V	307	CHL	C4A-NA-C1A	3.76	108.40	106.71
25	Q	305	CLA	CMB-C2B-C1B	-3.76	122.68	128.46
24	R	302	CHL	CMB-C2B-C1B	-3.76	122.69	128.46
25	A	833	CLA	C4A-NA-C1A	3.76	108.39	106.71
26	4	317	IWJ	C01-C02-C03	-3.76	115.52	123.56
25	B	808	CLA	CHB-C4A-NA	3.76	129.71	124.51
25	1	613	CLA	CMB-C2B-C3B	3.75	131.70	124.68
25	S	311	CLA	CHB-C4A-NA	3.75	129.70	124.51
30	A	850	BCR	C31-C1-C6	-3.75	104.21	110.30
30	L	307	BCR	C2-C1-C6	-3.75	104.70	110.48
25	4	316	CLA	CMB-C2B-C1B	-3.75	122.70	128.46
26	X	318	IWJ	C16-C15-C14	-3.75	121.96	127.31
25	4	311	CLA	O2D-CGD-O1D	-3.75	116.50	123.84
25	1	602	CLA	O2D-CGD-O1D	-3.75	116.51	123.84
25	R	307	CLA	CMB-C2B-C3B	3.75	131.69	124.68
24	P	306	CHL	C2C-C3C-C4C	3.75	109.16	106.49
25	1	607	CLA	CHD-C1D-ND	-3.75	121.01	124.45
25	5	606	CLA	CAB-C3B-C4B	-3.74	122.71	128.46
30	B	847	BCR	C12-C13-C14	-3.74	113.20	118.94
38	S	308	KC2	O2D-CGD-O1D	-3.74	116.53	123.84
25	A	832	CLA	CMB-C2B-C3B	3.74	131.67	124.68
38	S	308	KC2	C1A-C2A-C3A	-3.74	104.15	107.11
25	O	2001	CLA	C4-C3-C2	-3.74	114.10	123.68
30	B	848	BCR	C12-C13-C14	-3.73	113.21	118.94
30	G	201	BCR	C20-C19-C18	-3.73	115.93	126.42
24	P	306	CHL	C4A-NA-C1A	3.73	108.38	106.71
25	A	803	CLA	CMB-C2B-C3B	3.73	131.66	124.68
25	6	604	CLA	CMB-C2B-C3B	3.73	131.66	124.68
25	T	312	CLA	CMB-C2B-C1B	-3.73	122.73	128.46
25	3	302	CLA	C4-C3-C5	3.73	121.54	115.27
24	W	306	CHL	C3C-C4C-NC	-3.73	106.39	110.57
25	P	310	CLA	CMB-C2B-C1B	-3.73	122.74	128.46
30	B	845	BCR	C10-C11-C12	3.72	134.83	123.22
33	A	802	CL0	C4A-NA-C1A	3.72	108.38	106.71
25	B	814	CLA	O2D-CGD-O1D	-3.72	116.56	123.84
37	P	317	NEX	C39-C29-C30	-3.72	117.71	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	G	201	BCR	C8-C9-C10	-3.72	113.23	118.94
25	S	310	CLA	CMB-C2B-C1B	-3.72	122.75	128.46
29	X	319	Q6L	C40-C32-C33	-3.72	115.61	123.56
30	M	101	BCR	C20-C21-C22	-3.71	122.01	127.31
25	A	806	CLA	CHB-C4A-NA	3.71	129.65	124.51
25	R	305	CLA	C1B-CHB-C4A	-3.71	122.77	130.12
27	5	612	XAT	C6-C7-C8	-3.71	118.15	125.99
25	B	815	CLA	CHB-C4A-NA	3.71	129.64	124.51
25	4	316	CLA	C4A-NA-C1A	3.71	108.37	106.71
25	A	819	CLA	C4-C3-C5	3.71	121.51	115.27
30	B	845	BCR	C37-C22-C21	-3.71	117.73	122.92
25	2	604	CLA	CMB-C2B-C3B	3.71	131.62	124.68
25	A	828	CLA	C4A-NA-C1A	3.71	108.37	106.71
25	5	607	CLA	CMB-C2B-C1B	-3.71	122.77	128.46
25	A	843	CLA	CMB-C2B-C1B	-3.71	122.77	128.46
24	1	604	CHL	C1B-CHB-C4A	-3.70	122.78	130.12
30	G	205	BCR	C36-C18-C17	-3.70	117.74	122.92
25	U	308	CLA	C1B-CHB-C4A	-3.70	122.79	130.12
30	L	305	BCR	C34-C9-C10	3.70	128.11	122.92
25	A	823	CLA	C4A-NA-C1A	3.70	108.37	106.71
24	S	306	CHL	CHB-C4A-NA	3.70	129.63	124.51
25	B	805	CLA	CHB-C4A-NA	3.70	129.63	124.51
30	G	201	BCR	C28-C27-C26	-3.70	107.47	114.08
25	B	827	CLA	CHB-C4A-NA	3.70	129.63	124.51
25	H	301	CLA	CHB-C4A-NA	3.70	129.63	124.51
29	Q	317	Q6L	C40-C32-C33	-3.70	115.65	123.56
37	S	317	NEX	C38-C25-C26	-3.70	116.06	122.26
30	K	202	BCR	C34-C9-C10	3.70	128.10	122.92
25	A	810	CLA	CMB-C2B-C3B	3.70	131.59	124.68
25	P	301	CLA	C1B-CHB-C4A	-3.70	122.80	130.12
25	B	828	CLA	CMB-C2B-C3B	3.70	131.59	124.68
25	A	838	CLA	O2D-CGD-O1D	-3.70	116.61	123.84
30	L	307	BCR	C37-C22-C23	3.69	123.90	118.08
37	W	317	NEX	C39-C29-C30	-3.69	117.75	122.92
25	B	843	CLA	C1-C2-C3	-3.69	119.66	126.04
25	6	612	CLA	C4A-NA-C1A	3.69	108.37	106.71
25	P	309	CLA	O2D-CGD-O1D	-3.69	116.62	123.84
30	A	848	BCR	C3-C4-C5	-3.69	107.49	114.08
25	1	610	CLA	C4A-NA-C1A	3.69	108.36	106.71
25	A	838	CLA	C4A-NA-C1A	3.69	108.36	106.71
25	L	304	CLA	CMB-C2B-C1B	-3.69	122.80	128.46
29	V	315	Q6L	C40-C32-C33	-3.68	115.68	123.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	R	318	CHL	O2D-CGD-O1D	-3.68	116.64	123.84
24	T	306	CHL	CHB-C4A-NA	3.68	129.60	124.51
27	6	615	XAT	C39-C29-C30	3.68	128.08	122.92
30	B	848	BCR	C11-C10-C9	-3.68	122.06	127.31
30	K	207	BCR	C3-C4-C5	-3.68	107.50	114.08
29	Q	319	Q6L	C40-C32-C33	-3.68	115.69	123.56
25	A	829	CLA	CHB-C4A-NA	3.68	129.60	124.51
25	A	856	CLA	C4A-NA-C1A	3.68	108.36	106.71
30	B	846	BCR	C1-C6-C5	-3.68	117.43	122.61
25	3	302	CLA	C6-C5-C3	3.68	123.10	113.45
37	R	321	NEX	C39-C29-C30	-3.68	117.78	122.92
25	A	838	CLA	C4-C3-C5	3.67	121.45	115.27
25	1	608	CLA	C2D-C1D-ND	-3.67	107.40	110.10
38	V	308	KC2	CBA-CAA-C2A	-3.67	111.26	125.27
25	A	827	CLA	O2D-CGD-O1D	-3.67	116.65	123.84
25	2	609	CLA	C1B-CHB-C4A	-3.67	122.84	130.12
25	P	309	CLA	CMB-C2B-C1B	-3.67	122.82	128.46
29	T	315	Q6L	C40-C32-C33	-3.67	115.70	123.56
25	B	841	CLA	C1B-CHB-C4A	-3.67	122.85	130.12
30	2	618	BCR	C15-C14-C13	-3.67	122.08	127.31
25	6	602	CLA	CHD-C1D-ND	-3.67	121.08	124.45
25	B	836	CLA	C1B-CHB-C4A	-3.66	122.86	130.12
27	5	612	XAT	C31-C30-C29	-3.66	122.08	127.31
25	S	302	CLA	CMB-C2B-C1B	-3.66	122.84	128.46
25	1	610	CLA	CAB-C3B-C4B	-3.66	122.84	128.46
25	B	834	CLA	O2D-CGD-O1D	-3.66	116.68	123.84
30	F	804	BCR	C19-C18-C17	-3.66	113.33	118.94
25	2	614	CLA	CMB-C2B-C1B	-3.66	122.84	128.46
32	6	617	SQD	O47-C7-C8	3.66	119.38	111.50
24	R	310	CHL	CHB-C4A-NA	3.66	129.57	124.51
25	P	309	CLA	O2D-CGD-CBD	3.66	117.77	111.27
25	A	825	CLA	CBA-CAA-C2A	3.66	124.66	113.86
25	A	805	CLA	O2D-CGD-O1D	-3.65	116.69	123.84
25	B	832	CLA	C2D-C1D-ND	-3.65	107.41	110.10
27	3	316	XAT	C31-C30-C29	-3.65	122.10	127.31
24	W	307	CHL	C4A-NA-C1A	3.65	108.35	106.71
25	T	301	CLA	C4A-NA-C1A	3.65	108.35	106.71
38	Q	310	KC2	CMD-C2D-C1D	-3.65	122.86	128.46
25	2	613	CLA	CBA-CAA-C2A	3.65	121.71	114.02
25	Q	301	CLA	CBA-CAA-C2A	3.64	124.61	113.86
30	B	848	BCR	C8-C9-C10	-3.64	113.36	118.94
30	J	103	BCR	C4-C5-C6	-3.63	117.45	122.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	4	302	CHL	C1C-C2C-C3C	-3.63	104.23	107.11
25	B	827	CLA	CMB-C2B-C1B	-3.63	122.88	128.46
29	X	317	Q6L	C19-C18-C17	-3.63	122.13	127.31
36	A	854	DGD	O2G-C1B-C2B	3.63	119.33	111.50
30	H	305	BCR	C38-C26-C25	-3.63	120.45	124.53
38	V	308	KC2	O2D-CGD-O1D	-3.63	116.74	123.84
24	S	306	CHL	C1B-CHB-C4A	-3.63	122.94	130.12
24	6	606	CHL	CHB-C4A-NA	3.62	129.52	124.51
30	B	848	BCR	C15-C16-C17	-3.62	116.05	123.47
25	2	614	CLA	O2D-CGD-CBD	3.62	117.70	111.27
30	L	305	BCR	C23-C22-C21	-3.62	113.39	118.94
25	6	611	CLA	CMB-C2B-C3B	3.62	131.45	124.68
25	5	608	CLA	O2D-CGD-O1D	-3.62	116.77	123.84
30	J	101	BCR	C15-C16-C17	-3.62	116.06	123.47
25	4	312	CLA	CMB-C2B-C3B	3.61	131.44	124.68
25	2	613	CLA	C4A-NA-C1A	3.61	108.33	106.71
25	B	842	CLA	C2C-C1C-NC	3.61	113.36	109.97
25	B	830	CLA	C1B-CHB-C4A	-3.61	122.96	130.12
25	P	302	CLA	O2D-CGD-O1D	-3.61	116.78	123.84
25	R	306	CLA	C1B-CHB-C4A	-3.61	122.97	130.12
25	R	305	CLA	C1D-ND-C4D	-3.61	103.77	106.33
25	T	302	CLA	CMB-C2B-C1B	-3.61	122.92	128.46
28	3	323	LHG	O7-C7-C8	3.61	119.27	111.50
25	1	610	CLA	CMB-C2B-C1B	-3.61	122.92	128.46
30	3	319	BCR	C3-C4-C5	-3.61	107.64	114.08
25	B	839	CLA	C1B-CHB-C4A	-3.60	122.98	130.12
25	B	805	CLA	C4A-NA-C1A	3.60	108.32	106.71
25	B	839	CLA	CBA-CAA-C2A	3.60	124.48	113.86
25	A	824	CLA	C4A-NA-C1A	3.60	108.32	106.71
30	A	849	BCR	C20-C21-C22	-3.60	122.18	127.31
24	P	306	CHL	CMB-C2B-C1B	-3.59	122.94	128.46
25	T	313	CLA	C4A-NA-C1A	3.59	108.32	106.71
24	T	320	CHL	O2D-CGD-CBD	3.59	117.66	111.27
25	A	820	CLA	O2A-CGA-O1A	-3.59	114.52	123.59
29	S	323	Q6L	C38-C36-C35	-3.59	102.63	109.44
30	3	317	BCR	C3-C4-C5	-3.59	107.66	114.08
25	2	614	CLA	C1B-CHB-C4A	-3.59	123.00	130.12
25	5	609	CLA	CHB-C4A-NA	3.59	129.48	124.51
27	4	318	XAT	C18-C5-C6	-3.59	116.24	122.26
25	O	2004	CLA	CHB-C4A-NA	3.59	129.47	124.51
24	R	318	CHL	C1B-CHB-C4A	-3.59	123.01	130.12
29	R	323	Q6L	C35-C34-C33	3.59	115.82	111.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	T	314	CHL	CMB-C2B-C3B	3.58	131.38	124.68
25	B	839	CLA	CHD-C1D-ND	-3.58	121.16	124.45
25	2	606	CLA	CMB-C2B-C3B	3.58	131.38	124.68
25	2	606	CLA	O2D-CGD-O1D	-3.58	116.83	123.84
30	G	201	BCR	C23-C22-C21	-3.58	113.44	118.94
30	L	305	BCR	C3-C4-C5	-3.58	107.68	114.08
25	4	314	CLA	CMB-C2B-C1B	-3.58	122.96	128.46
30	F	804	BCR	C34-C9-C10	3.58	127.94	122.92
30	B	846	BCR	C33-C5-C6	-3.58	120.51	124.53
27	6	615	XAT	O4-C5-C6	-3.58	56.00	58.96
25	X	313	CLA	CMB-C2B-C3B	3.58	131.37	124.68
25	3	304	CLA	CHD-C1D-ND	-3.57	121.17	124.45
25	6	611	CLA	CBA-CAA-C2A	3.57	121.56	114.02
25	A	822	CLA	C4A-NA-C1A	3.57	108.31	106.71
25	5	610	CLA	CMB-C2B-C1B	-3.57	122.97	128.46
25	5	601	CLA	C1B-CHB-C4A	-3.57	123.04	130.12
24	4	306	CHL	CMB-C2B-C3B	3.57	131.36	124.68
28	6	616	LHG	O7-C7-C8	3.57	119.20	111.50
25	A	803	CLA	C4A-NA-C1A	3.57	108.31	106.71
30	K	202	BCR	C15-C16-C17	-3.57	116.16	123.47
25	X	304	CLA	C4A-NA-C1A	3.57	108.31	106.71
24	U	305	CHL	C4A-NA-C1A	3.57	108.31	106.71
25	2	613	CLA	CHD-C1D-ND	-3.56	121.18	124.45
30	J	101	BCR	C40-C30-C25	3.56	116.08	110.30
24	R	308	CHL	C1B-CHB-C4A	-3.56	123.06	130.12
30	K	202	BCR	C8-C9-C10	-3.56	113.47	118.94
25	3	314	CLA	CHD-C1D-ND	-3.56	121.18	124.45
25	P	310	CLA	C4A-NA-C1A	3.56	108.31	106.71
25	H	304	CLA	CBA-CAA-C2A	3.56	124.36	113.86
25	3	310	CLA	CMB-C2B-C3B	3.56	131.33	124.68
25	A	841	CLA	CMB-C2B-C1B	-3.56	123.00	128.46
25	2	614	CLA	CMB-C2B-C3B	3.56	131.33	124.68
25	B	818	CLA	CHB-C4A-NA	3.56	129.43	124.51
25	4	304	CLA	CAB-C3B-C4B	-3.55	123.00	128.46
24	R	302	CHL	C2C-C3C-C4C	3.55	109.02	106.49
27	5	612	XAT	C18-C5-C4	-3.55	110.28	114.28
30	B	845	BCR	C15-C16-C17	-3.55	116.19	123.47
25	Q	315	CLA	CMB-C2B-C3B	3.55	131.33	124.68
24	R	310	CHL	CMB-C2B-C1B	-3.55	123.00	128.46
24	4	302	CHL	CHB-C4A-NA	3.55	129.42	124.51
25	B	806	CLA	C4-C3-C2	-3.55	114.57	123.68
27	1	612	XAT	C38-C25-C24	3.55	118.28	114.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	2	605	CHL	C4A-NA-C1A	3.55	108.30	106.71
24	R	309	CHL	C4A-NA-C1A	3.55	108.30	106.71
24	S	306	CHL	CMB-C2B-C3B	3.55	131.31	124.68
24	T	306	CHL	C1B-CHB-C4A	-3.55	123.09	130.12
25	X	310	CLA	CMB-C2B-C3B	3.55	131.31	124.68
25	A	831	CLA	C4A-NA-C1A	3.55	108.30	106.71
25	3	307	CLA	C4-C3-C2	-3.55	114.58	123.68
25	K	204	CLA	CHB-C4A-NA	3.54	129.41	124.51
24	2	601	CHL	C1C-C2C-C3C	-3.54	104.30	107.11
24	2	605	CHL	CMB-C2B-C1B	-3.54	123.02	128.46
25	A	840	CLA	CMB-C2B-C1B	-3.54	123.02	128.46
25	W	309	CLA	CMB-C2B-C1B	-3.54	123.02	128.46
38	X	309	KC2	O2D-CGD-O1D	-3.54	116.92	123.84
24	X	305	CHL	C1B-CHB-C4A	-3.54	123.11	130.12
30	3	319	BCR	C8-C7-C6	-3.54	117.27	127.20
24	P	306	CHL	CHB-C4A-NA	3.54	129.40	124.51
27	1	612	XAT	C38-C25-C26	-3.54	116.33	122.26
30	J	101	BCR	C33-C5-C6	3.53	128.50	124.53
24	1	604	CHL	CMB-C2B-C1B	-3.53	123.03	128.46
25	6	608	CLA	C1B-CHB-C4A	-3.53	123.12	130.12
37	W	317	NEX	C28-C29-C30	3.53	124.36	118.94
32	H	303	SQD	O47-C7-C8	3.53	119.10	111.50
25	B	806	CLA	CMC-C2C-C1C	3.53	130.41	125.04
25	O	2005	CLA	CHD-C1D-ND	-3.53	121.21	124.45
25	B	833	CLA	CMB-C2B-C1B	-3.52	123.05	128.46
24	W	306	CHL	C1B-CHB-C4A	-3.52	123.14	130.12
25	R	315	CLA	CMB-C2B-C1B	-3.52	123.05	128.46
24	X	307	CHL	O2D-CGD-O1D	-3.52	116.95	123.84
25	A	840	CLA	CBA-CAA-C2A	3.52	124.25	113.86
31	O	2008	LMG	O2-C2-C1	3.52	118.60	110.05
25	2	608	CLA	O2D-CGD-CBD	3.52	117.52	111.27
25	B	833	CLA	CHD-C1D-ND	-3.52	121.22	124.45
24	U	306	CHL	CMB-C2B-C1B	-3.52	123.06	128.46
25	U	309	CLA	CMB-C2B-C1B	-3.52	123.06	128.46
25	P	311	CLA	CMB-C2B-C3B	3.52	131.26	124.68
27	6	615	XAT	C36-C21-C22	-3.52	102.87	108.98
24	2	607	CHL	CHB-C4A-NA	3.51	129.37	124.51
24	S	304	CHL	C1B-CHB-C4A	-3.51	123.16	130.12
25	R	307	CLA	CHD-C1D-ND	-3.51	121.22	124.45
24	4	308	CHL	CMB-C2B-C1B	-3.51	123.07	128.46
25	4	315	CLA	C4A-NA-C1A	3.51	108.28	106.71
30	L	305	BCR	C39-C30-C25	3.51	115.99	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	812	CLA	C1B-CHB-C4A	-3.51	123.17	130.12
31	5	613	LMG	O7-C10-C11	3.51	119.06	111.50
30	M	101	BCR	C8-C7-C6	-3.50	117.36	127.20
31	F	805	LMG	O7-C10-C11	3.50	119.05	111.50
30	B	848	BCR	C20-C21-C22	-3.50	122.31	127.31
25	A	817	CLA	CMB-C2B-C3B	3.50	131.23	124.68
25	B	805	CLA	C4-C3-C5	3.50	121.16	115.27
25	4	314	CLA	O2D-CGD-O1D	-3.50	116.99	123.84
25	B	806	CLA	CMB-C2B-C3B	3.50	131.23	124.68
25	B	832	CLA	C1B-CHB-C4A	-3.50	123.18	130.12
25	H	302	CLA	C5-C3-C2	3.50	128.20	121.12
30	F	801	BCR	C23-C22-C21	-3.50	113.58	118.94
37	T	317	NEX	C38-C25-C26	-3.50	116.40	122.26
25	6	603	CLA	C2C-C1C-NC	3.49	113.25	109.97
25	A	819	CLA	CHB-C4A-NA	3.49	129.34	124.51
24	S	304	CHL	CMB-C2B-C1B	-3.49	123.10	128.46
24	R	302	CHL	C4A-NA-C1A	3.49	108.28	106.71
25	P	312	CLA	O2A-C1-C2	3.49	117.81	108.64
24	S	305	CHL	CHB-C4A-NA	3.49	129.34	124.51
25	P	309	CLA	CHB-C4A-NA	3.49	129.33	124.51
30	G	205	BCR	C15-C16-C17	-3.49	116.33	123.47
25	4	315	CLA	CMB-C2B-C1B	-3.48	123.11	128.46
25	2	602	CLA	O2A-C1-C2	3.48	117.79	108.64
24	R	318	CHL	C4A-NA-C1A	3.48	108.27	106.71
38	V	308	KC2	C3A-C4A-NA	3.48	114.37	110.57
25	B	820	CLA	O2D-CGD-O1D	-3.48	117.03	123.84
25	2	610	CLA	CMB-C2B-C1B	-3.48	123.12	128.46
27	6	615	XAT	C18-C5-C6	-3.48	116.43	122.26
24	4	306	CHL	C1B-CHB-C4A	-3.48	123.23	130.12
25	1	603	CLA	CMB-C2B-C1B	-3.48	123.12	128.46
25	B	802	CLA	C4A-NA-C1A	3.48	108.27	106.71
30	M	101	BCR	C15-C14-C13	-3.48	122.35	127.31
25	H	301	CLA	C1B-CHB-C4A	-3.48	123.23	130.12
25	4	316	CLA	C1B-CHB-C4A	-3.48	123.23	130.12
25	4	313	CLA	CMB-C2B-C1B	-3.47	123.12	128.46
38	P	308	KC2	CBA-CAA-C2A	-3.47	112.03	125.27
27	4	318	XAT	O24-C25-C38	3.47	119.22	115.06
30	F	804	BCR	C36-C18-C17	-3.47	118.06	122.92
30	A	851	BCR	C37-C22-C23	3.47	123.54	118.08
30	M	101	BCR	C34-C9-C8	-3.47	112.61	118.08
25	V	311	CLA	CMB-C2B-C1B	-3.47	123.13	128.46
25	P	310	CLA	CMB-C2B-C3B	3.47	131.17	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	2	618	BCR	C28-C27-C26	-3.47	107.88	114.08
30	B	846	BCR	C36-C18-C17	-3.47	118.06	122.92
25	2	611	CLA	CMB-C2B-C1B	-3.47	123.14	128.46
25	U	303	CLA	CMB-C2B-C3B	3.47	131.16	124.68
25	A	831	CLA	CMB-C2B-C1B	-3.47	123.14	128.46
30	F	801	BCR	C20-C21-C22	-3.46	122.36	127.31
27	1	612	XAT	C6-C7-C8	-3.46	118.67	125.99
24	6	605	CHL	C1B-CHB-C4A	-3.46	123.26	130.12
25	H	304	CLA	C1B-CHB-C4A	-3.46	123.26	130.12
25	B	825	CLA	CMB-C2B-C3B	3.46	131.15	124.68
30	L	305	BCR	C8-C9-C10	-3.46	113.63	118.94
25	B	819	CLA	C1B-CHB-C4A	-3.46	123.26	130.12
25	P	312	CLA	CHD-C1D-ND	-3.46	121.27	124.45
25	1	603	CLA	CHB-C4A-NA	3.46	129.30	124.51
25	B	820	CLA	C1B-CHB-C4A	-3.46	123.27	130.12
25	W	309	CLA	C4A-NA-C1A	3.46	108.26	106.71
30	H	305	BCR	C36-C18-C17	-3.46	118.08	122.92
30	J	103	BCR	C33-C5-C6	3.46	128.41	124.53
27	1	612	XAT	C15-C14-C13	-3.46	122.38	127.31
25	S	309	CLA	C1B-CHB-C4A	-3.45	123.28	130.12
25	L	303	CLA	CHB-C4A-NA	3.45	129.29	124.51
24	4	307	CHL	C2C-C3C-C4C	3.45	108.95	106.49
25	U	311	CLA	CHB-C4A-NA	3.45	129.29	124.51
25	R	316	CLA	CMB-C2B-C3B	3.45	131.14	124.68
25	A	819	CLA	CHD-C1D-ND	-3.45	121.28	124.45
25	B	836	CLA	C4A-NA-C1A	3.45	108.26	106.71
25	A	833	CLA	CMB-C2B-C1B	-3.45	123.17	128.46
25	P	301	CLA	CMB-C2B-C1B	-3.45	123.17	128.46
24	6	601	CHL	C4A-NA-C1A	3.44	108.25	106.71
25	H	304	CLA	CHD-C1D-ND	-3.44	121.29	124.45
24	T	320	CHL	C1B-CHB-C4A	-3.44	123.30	130.12
25	B	806	CLA	C4-C3-C5	3.44	121.06	115.27
25	Q	314	CLA	C4-C3-C5	3.44	121.06	115.27
25	2	603	CLA	CMB-C2B-C1B	-3.44	123.18	128.46
30	G	201	BCR	C36-C18-C17	-3.44	118.10	122.92
30	A	851	BCR	C3-C4-C5	-3.44	107.94	114.08
24	X	308	CHL	C4A-NA-C1A	3.44	108.25	106.71
25	A	838	CLA	CHD-C1D-ND	-3.44	121.30	124.45
25	B	806	CLA	C1B-CHB-C4A	-3.43	123.31	130.12
24	X	315	CHL	C1B-CHB-C4A	-3.43	123.32	130.12
25	A	818	CLA	C4A-NA-C1A	3.43	108.25	106.71
24	X	307	CHL	CAA-C2A-C3A	3.43	122.17	112.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	2	612	CLA	CAA-C2A-C3A	-3.43	103.38	112.78
25	B	842	CLA	CHB-C4A-NA	3.43	129.26	124.51
30	K	207	BCR	C19-C18-C17	-3.43	113.68	118.94
25	H	302	CLA	CHB-C4A-NA	3.43	129.25	124.51
25	A	840	CLA	C4-C3-C5	3.43	121.04	115.27
25	P	309	CLA	CHD-C1D-ND	-3.43	121.30	124.45
25	S	310	CLA	C1B-CHB-C4A	-3.43	123.33	130.12
24	R	310	CHL	C2D-C1D-ND	-3.43	107.58	110.10
24	R	308	CHL	CMB-C2B-C1B	-3.42	123.20	128.46
25	V	309	CLA	C1B-CHB-C4A	-3.42	123.33	130.12
27	3	316	XAT	C36-C21-C22	-3.42	103.03	108.98
30	J	103	BCR	C3-C4-C5	-3.42	107.97	114.08
25	B	811	CLA	CMC-C2C-C1C	3.42	130.25	125.04
24	R	309	CHL	CMB-C2B-C3B	3.42	131.08	124.68
25	A	834	CLA	C4A-NA-C1A	3.42	108.24	106.71
25	4	304	CLA	O2D-CGD-O1D	-3.42	117.15	123.84
24	W	304	CHL	C1B-CHB-C4A	-3.42	123.34	130.12
25	H	301	CLA	C4A-NA-C1A	3.42	108.24	106.71
25	A	803	CLA	CHB-C4A-NA	3.42	129.24	124.51
24	6	605	CHL	C2D-C1D-ND	-3.42	107.59	110.10
25	A	833	CLA	C1B-CHB-C4A	-3.41	123.36	130.12
30	3	318	BCR	C19-C18-C17	-3.41	113.70	118.94
30	A	851	BCR	C15-C16-C17	-3.41	116.48	123.47
30	A	850	BCR	C12-C13-C14	-3.41	113.71	118.94
30	G	201	BCR	C3-C4-C5	-3.41	107.99	114.08
25	B	842	CLA	CMB-C2B-C1B	-3.41	123.22	128.46
30	G	205	BCR	C11-C10-C9	-3.41	122.45	127.31
24	R	310	CHL	C1B-CHB-C4A	-3.41	123.37	130.12
27	3	316	XAT	C28-C29-C30	-3.41	113.71	118.94
25	K	203	CLA	CHB-C4A-NA	3.41	129.22	124.51
29	P	315	Q6L	C40-C32-C33	-3.41	116.27	123.56
25	K	201	CLA	CED-O2D-CGD	3.41	123.64	115.94
24	S	304	CHL	OMC-CMC-C2C	-3.40	117.99	125.69
25	A	806	CLA	C1-O2A-CGA	3.40	125.37	116.44
31	2	620	LMG	O7-C10-C11	3.40	118.83	111.50
30	J	101	BCR	C38-C26-C27	3.40	120.15	113.62
25	B	816	CLA	CHD-C1D-ND	-3.40	121.33	124.45
30	L	307	BCR	C15-C16-C17	-3.40	116.51	123.47
24	4	306	CHL	C1C-C2C-C3C	-3.40	104.42	107.11
25	P	312	CLA	CMB-C2B-C3B	3.40	131.04	124.68
25	A	820	CLA	CHB-C4A-NA	3.40	129.21	124.51
25	3	308	CLA	CMC-C2C-C1C	3.40	130.21	125.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	X	302	CLA	C4A-NA-C1A	3.40	108.23	106.71
38	V	308	KC2	O2D-CGD-CBD	3.40	117.30	111.27
25	B	842	CLA	O2D-CGD-O1D	-3.40	117.20	123.84
25	B	813	CLA	C3C-C4C-NC	-3.40	106.76	110.57
25	B	820	CLA	CHB-C4A-NA	3.40	129.21	124.51
25	A	836	CLA	O2D-CGD-O1D	-3.40	117.20	123.84
25	W	302	CLA	CMB-C2B-C1B	-3.39	123.25	128.46
25	L	301	CLA	CMB-C2B-C1B	-3.39	123.25	128.46
25	3	302	CLA	O2A-CGA-CBA	3.39	122.56	111.91
31	B	801	LMG	O7-C10-C11	3.39	118.81	111.50
25	A	823	CLA	CHD-C1D-ND	-3.39	121.34	124.45
25	4	309	CLA	C1B-CHB-C4A	-3.39	123.40	130.12
25	B	829	CLA	CHB-C4A-NA	3.39	129.20	124.51
25	V	302	CLA	CMB-C2B-C1B	-3.39	123.26	128.46
28	A	847	LHG	O7-C7-C8	3.39	118.80	111.50
30	I	101	BCR	C37-C22-C23	3.39	123.41	118.08
25	P	302	CLA	C1B-CHB-C4A	-3.39	123.41	130.12
25	O	2003	CLA	CMB-C2B-C1B	-3.38	123.26	128.46
25	X	312	CLA	CMB-C2B-C1B	-3.38	123.26	128.46
24	5	605	CHL	C1B-CHB-C4A	-3.38	123.42	130.12
30	B	845	BCR	C8-C7-C6	-3.38	117.71	127.20
31	A	855	LMG	O1-C1-C2	3.38	113.58	108.30
24	1	601	CHL	C4A-NA-C1A	3.38	108.22	106.71
27	3	316	XAT	O4-C5-C18	3.38	119.10	115.06
25	W	302	CLA	C4A-NA-C1A	3.37	108.22	106.71
25	A	808	CLA	CHB-C4A-NA	3.37	129.18	124.51
24	X	305	CHL	CMB-C2B-C1B	-3.37	123.28	128.46
24	1	604	CHL	C1C-C2C-C3C	-3.37	104.44	107.11
38	S	308	KC2	CAA-CBA-CGA	-3.37	109.93	127.26
29	S	316	Q6L	C05-C06-C07	3.37	114.92	110.30
24	U	306	CHL	C1B-CHB-C4A	-3.37	123.44	130.12
30	J	101	BCR	C3-C4-C5	-3.37	108.06	114.08
24	R	311	CHL	C1C-C2C-C3C	-3.37	104.44	107.11
25	4	304	CLA	CMB-C2B-C1B	-3.37	123.29	128.46
24	X	307	CHL	O2D-CGD-CBD	3.37	117.25	111.27
24	X	307	CHL	C1B-CHB-C4A	-3.37	123.45	130.12
28	A	846	LHG	O7-C7-C8	3.37	118.76	111.50
25	B	815	CLA	O2D-CGD-CBD	3.37	117.25	111.27
25	A	836	CLA	CHD-C1D-ND	-3.37	121.36	124.45
25	1	605	CLA	CHD-C1D-ND	-3.36	121.36	124.45
24	Q	307	CHL	O2D-CGD-O1D	-3.36	117.26	123.84
24	4	306	CHL	C3C-C4C-NC	-3.36	106.90	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	P	309	CLA	C4-C3-C5	3.36	120.93	115.27
30	B	846	BCR	C36-C18-C19	3.36	123.37	118.08
24	2	615	CHL	CMB-C2B-C1B	-3.36	123.30	128.46
25	B	825	CLA	O2A-CGA-O1A	-3.36	114.92	123.30
34	A	844	PQN	C14-C13-C12	-3.36	115.06	123.68
25	A	811	CLA	CHD-C1D-ND	-3.36	121.37	124.45
25	N	203	CLA	CMB-C2B-C3B	3.36	130.96	124.68
25	U	308	CLA	CMB-C2B-C3B	3.36	130.96	124.68
24	P	306	CHL	C1B-CHB-C4A	-3.36	123.47	130.12
25	A	820	CLA	CMB-C2B-C3B	3.36	130.96	124.68
25	6	610	CLA	C1B-CHB-C4A	-3.36	123.47	130.12
29	X	316	Q6L	C25-C26-C27	3.36	132.10	127.31
38	W	308	KC2	O2D-CGD-O1D	-3.36	117.28	123.84
25	B	803	CLA	O2D-CGD-CBD	3.36	117.23	111.27
25	1	603	CLA	C4-C3-C2	-3.36	115.07	123.68
25	O	2005	CLA	CMB-C2B-C3B	3.35	130.95	124.68
25	U	301	CLA	CHB-C4A-NA	3.35	129.15	124.51
24	V	307	CHL	CHB-C4A-NA	3.35	129.15	124.51
25	P	311	CLA	C4-C3-C2	-3.35	115.08	123.68
25	B	827	CLA	CMB-C2B-C3B	3.35	130.95	124.68
29	P	315	Q6L	C05-C06-C07	3.35	114.89	110.30
25	A	813	CLA	CHD-C1D-ND	-3.35	121.38	124.45
30	L	305	BCR	C37-C22-C23	3.35	123.35	118.08
25	S	309	CLA	CMB-C2B-C3B	3.34	130.94	124.68
27	3	316	XAT	O24-C25-C38	3.34	119.06	115.06
30	A	850	BCR	C20-C21-C22	-3.34	122.54	127.31
30	L	306	BCR	C11-C10-C9	-3.34	122.54	127.31
24	U	313	CHL	CMB-C2B-C3B	3.34	130.93	124.68
25	5	608	CLA	O2D-CGD-CBD	3.34	117.20	111.27
30	B	848	BCR	C31-C1-C6	-3.34	104.88	110.30
25	A	819	CLA	C4-C3-C2	-3.34	115.11	123.68
25	V	309	CLA	O2D-CGD-CBD	3.34	117.20	111.27
25	Q	312	CLA	CMB-C2B-C1B	-3.34	123.33	128.46
25	X	310	CLA	C4A-NA-C1A	3.34	108.21	106.71
25	O	2002	CLA	CHD-C1D-ND	-3.34	121.39	124.45
30	B	846	BCR	C3-C4-C5	-3.34	108.12	114.08
25	R	306	CLA	CMB-C2B-C1B	-3.34	123.34	128.46
25	L	303	CLA	CBA-CAA-C2A	3.34	123.71	113.86
25	W	303	CLA	C1B-CHB-C4A	-3.34	123.51	130.12
25	W	302	CLA	C1B-CHB-C4A	-3.33	123.51	130.12
27	1	612	XAT	C39-C29-C30	3.33	127.59	122.92
25	5	601	CLA	C2A-C1A-CHA	3.33	129.69	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	B	802	CLA	C1B-CHB-C4A	-3.33	123.52	130.12
24	T	320	CHL	CHB-C4A-NA	3.33	129.12	124.51
30	K	202	BCR	C12-C13-C14	-3.33	113.83	118.94
29	U	315	Q6L	C05-C06-C07	3.33	114.86	110.30
25	B	826	CLA	CHD-C1D-ND	-3.33	121.39	124.45
25	2	611	CLA	CMB-C2B-C3B	3.33	130.91	124.68
30	J	101	BCR	C20-C21-C22	-3.33	122.56	127.31
30	H	305	BCR	C8-C7-C6	-3.33	117.86	127.20
25	Q	305	CLA	C2D-C1D-ND	-3.33	107.65	110.10
25	3	303	CLA	C1B-CHB-C4A	-3.33	123.53	130.12
24	W	306	CHL	CHB-C4A-NA	3.32	129.11	124.51
25	P	303	CLA	C4A-NA-C1A	3.32	108.20	106.71
25	3	309	CLA	CMB-C2B-C1B	-3.32	123.36	128.46
29	S	315	Q6L	C35-C34-C33	3.32	115.52	111.74
25	B	841	CLA	CMB-C2B-C3B	3.32	130.89	124.68
25	P	303	CLA	CHD-C1D-ND	-3.32	121.40	124.45
25	T	313	CLA	CMB-C2B-C1B	-3.32	123.36	128.46
25	A	830	CLA	C1B-CHB-C4A	-3.32	123.55	130.12
27	4	318	XAT	C6-C7-C8	-3.32	118.98	125.99
24	T	305	CHL	CHB-C4A-NA	3.32	129.10	124.51
25	H	302	CLA	CHD-C1D-ND	-3.32	121.41	124.45
25	R	314	CLA	CMB-C2B-C1B	-3.31	123.37	128.46
25	5	601	CLA	CMB-C2B-C3B	3.31	130.88	124.68
25	X	310	CLA	O2D-CGD-O1D	-3.31	117.36	123.84
25	P	309	CLA	C1B-CHB-C4A	-3.31	123.56	130.12
24	T	304	CHL	C1B-CHB-C4A	-3.31	123.56	130.12
25	4	311	CLA	C1B-CHB-C4A	-3.31	123.56	130.12
25	B	804	CLA	CMB-C2B-C3B	3.31	130.87	124.68
29	W	320	Q6L	C35-C34-C33	3.31	115.51	111.74
25	A	803	CLA	C1B-CHB-C4A	-3.31	123.57	130.12
25	5	604	CLA	CMB-C2B-C1B	-3.31	123.38	128.46
38	P	308	KC2	O2D-CGD-O1D	-3.31	117.37	123.84
25	3	313	CLA	C1B-CHB-C4A	-3.31	123.57	130.12
25	A	821	CLA	C1B-CHB-C4A	-3.31	123.57	130.12
27	6	615	XAT	C37-C21-C36	-3.30	102.50	107.37
30	J	101	BCR	C7-C8-C9	-3.30	121.24	126.23
25	O	2002	CLA	C4-C3-C2	-3.30	115.20	123.68
30	B	847	BCR	C2-C1-C6	3.30	115.57	110.48
25	B	809	CLA	C6-C5-C3	-3.30	104.80	113.45
30	F	804	BCR	C20-C21-C22	-3.30	122.60	127.31
25	B	811	CLA	CMB-C2B-C3B	3.30	130.85	124.68
24	R	302	CHL	CHB-C4A-NA	3.30	129.08	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	4	308	CHL	CBC-CAC-C3C	-3.30	103.33	112.43
29	S	315	Q6L	C05-C06-C07	3.30	114.82	110.30
37	T	317	NEX	O24-C25-C38	3.30	119.01	115.06
30	G	205	BCR	C37-C22-C23	3.30	123.27	118.08
25	A	824	CLA	CMB-C2B-C3B	3.30	130.84	124.68
30	K	207	BCR	C38-C26-C25	-3.29	120.83	124.53
25	B	825	CLA	C4A-NA-C1A	3.29	108.19	106.71
25	W	310	CLA	CMB-C2B-C3B	3.29	130.84	124.68
24	P	307	CHL	CHB-C4A-NA	3.29	129.07	124.51
24	P	307	CHL	C2C-C3C-C4C	3.29	108.84	106.49
30	A	852	BCR	C30-C25-C26	3.29	127.25	122.61
37	T	317	NEX	C15-C35-C34	-3.29	116.73	123.47
25	A	815	CLA	CHB-C4A-NA	3.29	129.06	124.51
24	X	307	CHL	C2D-C1D-ND	-3.29	107.68	110.10
25	B	815	CLA	C4-C3-C5	3.29	120.81	115.27
24	Q	309	CHL	CMB-C2B-C3B	3.29	130.84	124.68
25	3	311	CLA	CMB-C2B-C3B	3.29	130.84	124.68
30	B	846	BCR	C8-C7-C6	-3.29	117.96	127.20
25	1	606	CLA	CHD-C1D-ND	-3.29	121.43	124.45
24	U	313	CHL	C1B-CHB-C4A	-3.29	123.61	130.12
25	B	806	CLA	CMB-C2B-C1B	-3.29	123.41	128.46
37	S	317	NEX	C17-C1-C6	3.29	113.41	110.47
24	3	306	CHL	C1B-CHB-C4A	-3.28	123.61	130.12
25	5	606	CLA	CHD-C1D-ND	-3.28	121.44	124.45
25	Q	315	CLA	C1-O2A-CGA	3.28	125.06	116.44
24	U	304	CHL	CMB-C2B-C1B	-3.28	123.42	128.46
25	H	304	CLA	CMB-C2B-C3B	3.28	130.82	124.68
25	A	811	CLA	CHB-C4A-NA	3.28	129.05	124.51
25	Q	313	CLA	CMB-C2B-C1B	-3.28	123.42	128.46
25	A	809	CLA	C1B-CHB-C4A	-3.28	123.62	130.12
25	J	102	CLA	CMB-C2B-C1B	-3.28	123.42	128.46
25	Q	304	CLA	CMB-C2B-C3B	3.28	130.82	124.68
25	4	303	CLA	O2D-CGD-O1D	-3.28	117.42	123.84
24	5	605	CHL	C4A-NA-C1A	3.28	108.18	106.71
25	A	812	CLA	O2D-CGD-CBD	3.28	117.10	111.27
24	S	314	CHL	C1B-CHB-C4A	-3.28	123.62	130.12
25	B	836	CLA	C1-C2-C3	3.28	131.72	126.04
25	B	807	CLA	CHB-C4A-NA	3.28	129.05	124.51
25	2	606	CLA	O2D-CGD-CBD	3.28	117.09	111.27
25	P	313	CLA	C4A-NA-C1A	3.28	108.18	106.71
25	X	303	CLA	C1B-CHB-C4A	-3.28	123.62	130.12
25	B	826	CLA	C4-C3-C5	3.28	120.78	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	W	304	CHL	O2D-CGD-O1D	-3.28	117.43	123.84
25	6	611	CLA	C4A-NA-C1A	3.28	108.18	106.71
24	2	601	CHL	C2C-C3C-C4C	3.28	108.82	106.49
38	Q	310	KC2	CMD-C2D-C3D	3.28	130.81	124.68
25	Q	311	CLA	C1B-CHB-C4A	-3.27	123.63	130.12
25	Q	301	CLA	CMB-C2B-C1B	-3.27	123.43	128.46
24	U	305	CHL	CBC-CAC-C3C	3.27	121.45	112.43
25	R	313	CLA	C1B-CHB-C4A	-3.27	123.64	130.12
25	P	309	CLA	CMB-C2B-C3B	3.27	130.80	124.68
27	4	318	XAT	C11-C10-C9	3.27	131.98	127.31
29	P	319	Q6L	C20-C21-C22	3.27	131.98	127.31
25	B	840	CLA	CMB-C2B-C1B	-3.27	123.44	128.46
38	U	307	KC2	CBA-CAA-C2A	-3.27	112.81	125.27
24	R	302	CHL	C1B-CHB-C4A	-3.27	123.64	130.12
25	V	310	CLA	CMB-C2B-C1B	-3.27	123.44	128.46
30	J	103	BCR	C23-C24-C25	-3.26	118.03	127.20
24	P	305	CHL	CMB-C2B-C3B	3.26	130.78	124.68
25	1	606	CLA	CMB-C2B-C1B	-3.26	123.45	128.46
25	U	301	CLA	C4A-NA-C1A	3.26	108.17	106.71
30	L	307	BCR	C16-C17-C18	3.26	131.97	127.31
38	R	312	KC2	CBA-CAA-C2A	-3.26	112.83	125.27
25	3	307	CLA	C1B-CHB-C4A	-3.26	123.66	130.12
25	B	808	CLA	CMB-C2B-C1B	-3.26	123.45	128.46
24	Q	316	CHL	C4A-NA-C1A	3.26	108.17	106.71
25	5	602	CLA	C4A-NA-C1A	3.26	108.17	106.71
24	S	304	CHL	CMA-C3A-C4A	3.26	120.53	111.77
25	A	828	CLA	C1B-CHB-C4A	-3.26	123.67	130.12
30	4	319	BCR	C28-C27-C26	-3.26	108.26	114.08
38	U	307	KC2	O2D-CGD-O1D	-3.26	117.47	123.84
29	R	301	Q6L	C42-C13-C12	3.26	120.75	115.27
25	1	605	CLA	CMB-C2B-C3B	3.25	130.77	124.68
30	L	305	BCR	C31-C1-C6	3.25	115.58	110.30
25	4	305	CLA	CMB-C2B-C1B	-3.25	123.46	128.46
25	X	311	CLA	CMB-C2B-C3B	3.25	130.76	124.68
25	B	835	CLA	C4A-NA-C1A	3.25	108.17	106.71
27	1	612	XAT	C32-C33-C34	-3.25	113.95	118.94
38	V	308	KC2	CHB-C4A-C3A	-3.25	119.90	124.98
25	P	310	CLA	O2D-CGD-O1D	-3.25	117.48	123.84
38	P	308	KC2	CHB-C1B-NB	3.25	127.44	124.45
25	B	841	CLA	CHD-C1D-ND	-3.25	121.47	124.45
32	6	617	SQD	O7-S-C6	3.25	110.80	106.94
24	Q	316	CHL	O2D-CGD-O1D	-3.25	117.49	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	B	830	CLA	C2D-C1D-ND	-3.24	107.71	110.10
24	T	314	CHL	C1B-CHB-C4A	-3.24	123.69	130.12
25	U	309	CLA	CMB-C2B-C3B	3.24	130.74	124.68
25	K	204	CLA	CMB-C2B-C1B	-3.24	123.49	128.46
25	2	610	CLA	C1B-CHB-C4A	-3.24	123.70	130.12
25	V	302	CLA	O2D-CGD-O1D	-3.24	117.51	123.84
25	B	827	CLA	CHD-C1D-ND	-3.24	121.48	124.45
25	6	613	CLA	C6-C5-C3	-3.24	104.97	113.45
25	3	305	CLA	CMB-C2B-C1B	-3.24	123.49	128.46
37	W	317	NEX	C15-C35-C34	-3.23	116.85	123.47
30	B	845	BCR	C11-C10-C9	-3.23	122.69	127.31
30	3	318	BCR	C28-C27-C26	-3.23	108.30	114.08
25	A	804	CLA	CHA-C1A-NA	-3.23	119.00	126.40
25	B	841	CLA	CHB-C4A-NA	3.23	128.98	124.51
25	J	102	CLA	CMB-C2B-C3B	3.23	130.72	124.68
30	A	851	BCR	C34-C9-C8	-3.23	112.99	118.08
25	L	302	CLA	C1B-CHB-C4A	-3.23	123.72	130.12
25	2	609	CLA	CHB-C4A-NA	3.23	128.98	124.51
24	6	606	CHL	C1B-CHB-C4A	-3.23	123.72	130.12
25	X	311	CLA	C4A-NA-C1A	3.23	108.16	106.71
25	S	302	CLA	CMB-C2B-C3B	3.23	130.71	124.68
25	V	301	CLA	O2D-CGD-O1D	-3.22	117.53	123.84
30	M	101	BCR	C36-C18-C17	-3.22	118.41	122.92
25	O	2004	CLA	C1B-CHB-C4A	-3.22	123.73	130.12
27	3	316	XAT	C4-C3-C2	-3.22	104.55	110.77
25	S	309	CLA	O2D-CGD-O1D	-3.22	117.54	123.84
25	A	806	CLA	C1B-CHB-C4A	-3.22	123.74	130.12
30	L	306	BCR	C20-C21-C22	-3.22	122.71	127.31
30	3	318	BCR	C39-C30-C25	-3.22	105.08	110.30
25	4	303	CLA	C1B-CHB-C4A	-3.22	123.74	130.12
30	B	847	BCR	C28-C27-C26	-3.22	108.33	114.08
25	A	836	CLA	CHB-C4A-NA	3.22	128.96	124.51
25	A	826	CLA	CHB-C4A-NA	3.22	128.96	124.51
25	W	303	CLA	O2D-CGD-O1D	-3.22	117.55	123.84
25	L	304	CLA	CMB-C2B-C3B	3.21	130.69	124.68
24	4	307	CHL	CMB-C2B-C3B	3.21	130.98	124.69
24	V	306	CHL	O2D-CGD-O1D	-3.21	117.56	123.84
25	A	843	CLA	C4-C3-C5	3.21	120.67	115.27
30	H	305	BCR	C37-C22-C21	-3.21	118.43	122.92
25	X	302	CLA	CMB-C2B-C3B	3.21	130.68	124.68
30	F	804	BCR	C37-C22-C23	3.21	123.13	118.08
25	T	301	CLA	O1D-CGD-CBD	3.21	131.05	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	834	CLA	C1B-CHB-C4A	-3.21	123.77	130.12
25	W	312	CLA	C1D-ND-C4D	-3.21	104.06	106.33
33	A	802	CL0	C1B-CHB-C4A	-3.21	123.77	130.12
24	T	314	CHL	O2D-CGD-O1D	-3.20	117.57	123.84
24	V	304	CHL	CHB-C4A-NA	3.20	128.94	124.51
25	A	806	CLA	CHD-C1D-ND	-3.20	121.51	124.45
25	H	301	CLA	CHD-C1D-ND	-3.20	121.51	124.45
25	B	834	CLA	CMB-C2B-C1B	-3.20	123.54	128.46
25	A	814	CLA	C4A-NA-C1A	3.20	108.15	106.71
25	4	314	CLA	CHD-C1D-ND	-3.20	121.51	124.45
25	B	821	CLA	CHD-C1D-ND	-3.20	121.51	124.45
25	U	311	CLA	C1B-CHB-C4A	-3.20	123.78	130.12
25	Q	311	CLA	O2D-CGD-O1D	-3.20	117.58	123.84
25	4	310	CLA	C4A-NA-C1A	3.20	108.14	106.71
25	A	808	CLA	C11-C12-C13	-3.20	105.57	115.92
30	3	319	BCR	C15-C16-C17	-3.20	116.92	123.47
24	P	314	CHL	C1B-CHB-C4A	-3.20	123.78	130.12
30	3	317	BCR	C19-C18-C17	-3.20	114.03	118.94
24	S	306	CHL	C2D-C1D-ND	-3.20	107.75	110.10
28	1	614	LHG	O8-C23-C24	3.20	121.95	111.91
30	A	850	BCR	C23-C24-C25	-3.20	118.22	127.20
25	B	833	CLA	CMB-C2B-C3B	3.20	130.66	124.68
24	S	306	CHL	O2D-CGD-CBD	3.20	116.95	111.27
26	S	318	IWJ	C17-C18-C19	-3.20	122.75	127.31
25	5	608	CLA	C1B-CHB-C4A	-3.19	123.79	130.12
25	5	607	CLA	O2D-CGD-O1D	-3.19	117.59	123.84
25	X	314	CLA	CMB-C2B-C1B	-3.19	123.56	128.46
25	B	821	CLA	C1B-CHB-C4A	-3.19	123.79	130.12
25	3	311	CLA	O2A-CGA-O1A	-3.19	115.53	123.59
25	3	302	CLA	O2A-C1-C2	3.19	117.03	108.64
25	J	102	CLA	C1B-CHB-C4A	-3.19	123.79	130.12
24	2	605	CHL	CHB-C4A-NA	3.19	128.93	124.51
24	R	309	CHL	O2D-CGD-O1D	-3.19	117.60	123.84
25	B	817	CLA	CMB-C2B-C3B	3.19	130.65	124.68
25	T	312	CLA	CMB-C2B-C3B	3.19	130.65	124.68
25	5	603	CLA	C4A-NA-C1A	3.19	108.14	106.71
37	T	317	NEX	C19-C9-C10	3.19	127.39	122.92
25	3	305	CLA	C1B-CHB-C4A	-3.19	123.80	130.12
24	2	607	CHL	CMB-C2B-C3B	3.19	130.64	124.68
25	1	608	CLA	C1B-CHB-C4A	-3.19	123.80	130.12
27	3	316	XAT	C38-C25-C26	-3.19	116.92	122.26
25	A	829	CLA	C1B-CHB-C4A	-3.19	123.81	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	P	301	CLA	CHB-C4A-NA	3.19	128.92	124.51
25	A	810	CLA	CBA-CAA-C2A	3.18	123.26	113.86
25	V	302	CLA	C1B-CHB-C4A	-3.18	123.81	130.12
24	T	307	CHL	C4A-NA-C1A	3.18	108.14	106.71
37	H	306	NEX	C11-C10-C9	-3.18	122.77	127.31
25	5	609	CLA	C1B-CHB-C4A	-3.18	123.82	130.12
25	1	602	CLA	C4A-NA-C1A	3.18	108.14	106.71
25	2	612	CLA	CMB-C2B-C1B	-3.18	123.58	128.46
25	5	604	CLA	C1B-CHB-C4A	-3.18	123.82	130.12
25	Q	305	CLA	C4A-NA-C1A	3.18	108.14	106.71
25	A	845	CLA	C1B-CHB-C4A	-3.18	123.82	130.12
27	1	612	XAT	C35-C15-C14	-3.18	116.97	123.47
25	2	612	CLA	C6-C5-C3	3.18	121.78	113.45
25	V	312	CLA	C1B-CHB-C4A	-3.18	123.83	130.12
30	3	318	BCR	C16-C15-C14	-3.18	116.97	123.47
25	1	603	CLA	C5-C3-C2	3.18	127.54	121.12
24	R	302	CHL	C1C-C2C-C3C	-3.18	104.59	107.11
25	A	807	CLA	CMB-C2B-C3B	3.17	130.62	124.68
38	Q	310	KC2	O2D-CGD-O1D	-3.17	117.63	123.84
30	2	618	BCR	C31-C1-C6	-3.17	105.15	110.30
25	W	309	CLA	C1B-CHB-C4A	-3.17	123.83	130.12
25	V	309	CLA	C3A-C2A-C1A	-3.17	96.59	101.34
30	J	103	BCR	C37-C22-C21	-3.17	118.48	122.92
25	B	822	CLA	CMB-C2B-C3B	3.17	130.61	124.68
29	R	301	Q6L	C12-C13-C14	-3.17	112.38	121.98
25	3	311	CLA	C1B-CHB-C4A	-3.17	123.84	130.12
25	P	301	CLA	CMB-C2B-C3B	3.17	130.60	124.68
24	1	604	CHL	C4A-NA-C1A	3.17	108.13	106.71
25	A	823	CLA	CMB-C2B-C3B	3.17	130.60	124.68
25	2	613	CLA	C1B-CHB-C4A	-3.16	123.85	130.12
25	Q	306	CLA	C1B-CHB-C4A	-3.16	123.85	130.12
25	L	303	CLA	CHD-C1D-ND	-3.16	121.55	124.45
25	V	309	CLA	CHD-C1D-ND	-3.16	121.55	124.45
25	A	830	CLA	CHB-C4A-NA	3.16	128.88	124.51
25	4	316	CLA	CHD-C1D-ND	-3.16	121.55	124.45
25	R	305	CLA	CBA-CAA-C2A	3.16	123.19	113.86
25	3	301	CLA	CMB-C2B-C3B	3.16	130.59	124.68
24	V	305	CHL	C1B-CHB-C4A	-3.16	123.86	130.12
30	G	201	BCR	C15-C14-C13	-3.16	122.80	127.31
25	A	841	CLA	O2D-CGD-O1D	-3.16	117.66	123.84
25	6	604	CLA	C1B-CHB-C4A	-3.16	123.86	130.12
25	P	313	CLA	CMB-C2B-C1B	-3.16	123.61	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	P	310	CLA	C1B-CHB-C4A	-3.16	123.86	130.12
25	B	817	CLA	CHB-C4A-NA	3.16	128.88	124.51
30	H	305	BCR	C3-C4-C5	-3.16	108.44	114.08
37	H	306	NEX	C39-C29-C30	-3.16	118.50	122.92
25	5	602	CLA	O2D-CGD-O1D	-3.16	117.67	123.84
24	W	306	CHL	O2D-CGD-O1D	-3.16	117.67	123.84
38	T	308	KC2	O2D-CGD-O1D	-3.16	117.67	123.84
25	3	304	CLA	CMB-C2B-C3B	3.16	130.58	124.68
24	X	307	CHL	CHD-C4C-C3C	3.16	129.48	124.84
31	A	801	LMG	O7-C10-C11	3.16	118.30	111.50
25	3	307	CLA	CMB-C2B-C3B	3.15	130.58	124.68
30	M	101	BCR	C11-C10-C9	-3.15	122.81	127.31
30	F	804	BCR	C34-C9-C8	-3.15	113.11	118.08
25	5	604	CLA	C4A-NA-C1A	3.15	108.12	106.71
25	S	310	CLA	CMB-C2B-C3B	3.15	130.57	124.68
25	5	606	CLA	O2D-CGD-O1D	-3.15	117.68	123.84
25	Q	306	CLA	O2D-CGD-O1D	-3.15	117.68	123.84
25	B	829	CLA	C2D-C1D-ND	-3.15	107.78	110.10
25	A	830	CLA	C1-O2A-CGA	3.15	124.71	116.44
25	6	609	CLA	O2D-CGD-O1D	-3.15	117.68	123.84
25	B	803	CLA	C1B-CHB-C4A	-3.15	123.88	130.12
25	T	303	CLA	C4A-NA-C1A	3.15	108.12	106.71
24	Q	309	CHL	C1B-CHB-C4A	-3.15	123.88	130.12
24	Q	309	CHL	CHB-C4A-NA	3.15	128.86	124.51
24	W	314	CHL	C4A-NA-C1A	3.15	108.12	106.71
31	A	855	LMG	O7-C10-C11	3.14	119.57	110.80
25	W	313	CLA	CMB-C2B-C3B	3.14	130.56	124.68
24	P	307	CHL	C1C-C2C-C3C	-3.14	104.62	107.11
25	A	826	CLA	C1B-CHB-C4A	-3.14	123.89	130.12
25	4	304	CLA	CHD-C1D-ND	-3.14	121.57	124.45
25	A	828	CLA	O2D-CGD-O1D	-3.14	117.70	123.84
25	1	610	CLA	O2D-CGD-O1D	-3.14	117.70	123.84
25	A	809	CLA	CHD-C1D-ND	-3.14	121.57	124.45
24	W	314	CHL	C1B-CHB-C4A	-3.14	123.91	130.12
25	3	305	CLA	CAB-C3B-C4B	-3.14	123.64	128.46
25	4	305	CLA	CAB-C3B-C4B	-3.14	123.64	128.46
25	H	304	CLA	CHB-C4A-NA	3.13	128.85	124.51
25	O	2004	CLA	CMB-C2B-C1B	-3.13	123.65	128.46
25	B	837	CLA	CMB-C2B-C3B	3.13	130.54	124.68
25	L	304	CLA	CHD-C1D-ND	-3.13	121.58	124.45
25	B	819	CLA	CHB-C4A-NA	3.13	128.84	124.51
25	A	816	CLA	CMB-C2B-C3B	3.13	130.54	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	1	614	LHG	O7-C7-C8	3.13	118.25	111.50
25	5	606	CLA	CMB-C2B-C1B	-3.13	123.65	128.46
29	T	322	Q6L	C19-C18-C17	-3.13	122.84	127.31
25	V	312	CLA	O2A-CGA-O1A	-3.13	115.69	123.59
25	Q	311	CLA	CMB-C2B-C3B	3.13	130.53	124.68
25	A	825	CLA	CHD-C1D-ND	-3.13	121.58	124.45
27	6	615	XAT	C8-C9-C10	-3.13	114.14	118.94
24	2	601	CHL	CHB-C4A-NA	3.13	128.84	124.51
30	I	101	BCR	C34-C9-C10	3.13	127.31	122.92
30	B	847	BCR	C38-C26-C27	3.12	119.62	113.62
25	A	821	CLA	O2D-CGD-O1D	-3.12	117.73	123.84
25	G	202	CLA	O2D-CGD-O1D	-3.12	117.73	123.84
25	K	206	CLA	CHD-C1D-ND	-3.12	121.58	124.45
25	2	606	CLA	C1B-CHB-C4A	-3.12	123.93	130.12
25	U	309	CLA	C1B-CHB-C4A	-3.12	123.93	130.12
25	A	843	CLA	CHB-C4A-NA	3.12	128.83	124.51
24	R	308	CHL	C1C-C2C-C3C	-3.12	104.64	107.11
25	1	606	CLA	CAB-C3B-C2B	3.12	130.80	124.69
25	Q	315	CLA	O2A-CGA-O1A	-3.12	115.72	123.59
25	B	839	CLA	CMB-C2B-C1B	-3.12	123.67	128.46
25	R	313	CLA	O2D-CGD-CBD	3.12	116.81	111.27
25	A	810	CLA	CHD-C1D-ND	-3.12	121.59	124.45
25	5	608	CLA	CHB-C4A-NA	3.12	128.83	124.51
30	A	852	BCR	C12-C13-C14	-3.12	114.15	118.94
37	S	317	NEX	C15-C35-C34	-3.12	117.08	123.47
24	R	311	CHL	CMB-C2B-C3B	3.12	130.51	124.68
25	1	606	CLA	C1B-CHB-C4A	-3.12	123.94	130.12
25	5	610	CLA	CHD-C1D-ND	-3.12	121.59	124.45
25	A	856	CLA	CMC-C2C-C1C	3.12	129.78	125.04
25	6	613	CLA	C4-C3-C2	-3.12	115.69	123.68
25	U	308	CLA	C2C-C1C-NC	3.11	112.89	109.97
30	B	849	BCR	C20-C21-C22	-3.11	122.86	127.31
24	T	306	CHL	CMB-C2B-C3B	3.11	130.50	124.68
24	P	307	CHL	C1B-CHB-C4A	-3.11	123.95	130.12
25	2	604	CLA	C1B-CHB-C4A	-3.11	123.95	130.12
28	3	321	LHG	O7-C7-C8	3.11	118.21	111.50
30	A	848	BCR	C12-C13-C14	-3.11	114.17	118.94
25	B	810	CLA	O2D-CGD-O1D	-3.11	117.75	123.84
25	P	303	CLA	CHB-C4A-NA	3.11	128.81	124.51
25	5	609	CLA	O2D-CGD-O1D	-3.11	117.03	124.09
25	B	828	CLA	CHB-C4A-NA	3.11	128.81	124.51
25	T	301	CLA	C1B-CHB-C4A	-3.11	123.96	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	825	CLA	CMC-C2C-C1C	3.11	129.78	125.04
25	O	2001	CLA	CMB-C2B-C3B	3.11	130.49	124.68
30	J	101	BCR	C37-C22-C23	3.11	122.97	118.08
25	3	309	CLA	CHD-C1D-ND	-3.11	121.60	124.45
25	1	603	CLA	CBC-CAC-C3C	-3.10	103.87	112.43
25	A	831	CLA	C6-C5-C3	3.10	121.59	113.45
24	Q	307	CHL	C1B-CHB-C4A	-3.10	123.97	130.12
24	P	307	CHL	CBA-CAA-C2A	3.10	120.57	114.02
25	U	312	CLA	CMB-C2B-C1B	-3.10	123.69	128.46
30	G	201	BCR	C12-C13-C14	-3.10	114.18	118.94
25	R	314	CLA	CMB-C2B-C3B	3.10	130.48	124.68
25	S	313	CLA	CMB-C2B-C1B	-3.10	123.70	128.46
30	K	207	BCR	C23-C24-C25	-3.10	118.49	127.20
24	X	306	CHL	O2D-CGD-O1D	-3.10	117.78	123.84
24	V	314	CHL	C4A-NA-C1A	3.10	108.10	106.71
25	H	302	CLA	CMB-C2B-C1B	-3.10	123.70	128.46
30	A	850	BCR	C16-C15-C14	-3.10	117.12	123.47
24	Q	316	CHL	C1B-CHB-C4A	-3.10	123.98	130.12
30	B	845	BCR	C30-C25-C26	-3.10	118.25	122.61
25	B	813	CLA	O2A-CGA-CBA	3.10	121.62	111.91
25	B	817	CLA	C1B-CHB-C4A	-3.09	123.99	130.12
29	Q	318	Q6L	C06-C07-C02	3.09	118.02	111.85
25	4	316	CLA	CMB-C2B-C3B	3.09	130.47	124.68
25	A	804	CLA	C2A-C1A-CHA	3.09	129.27	123.86
25	Q	313	CLA	CMB-C2B-C3B	3.09	130.46	124.68
30	B	847	BCR	C23-C24-C25	-3.09	118.52	127.20
25	B	803	CLA	O2D-CGD-O1D	-3.09	117.79	123.84
25	4	310	CLA	C1B-CHB-C4A	-3.09	124.00	130.12
25	A	826	CLA	CHD-C1D-ND	-3.09	121.61	124.45
25	V	310	CLA	C1B-CHB-C4A	-3.09	124.00	130.12
25	1	605	CLA	C4A-NA-C1A	3.09	108.09	106.71
30	J	101	BCR	C19-C18-C17	-3.09	114.20	118.94
25	1	603	CLA	C2A-C1A-CHA	3.09	129.26	123.86
24	R	308	CHL	CMB-C2B-C3B	3.09	130.45	124.68
25	K	204	CLA	CMB-C2B-C3B	3.09	130.45	124.68
27	6	615	XAT	C35-C15-C14	-3.09	117.15	123.47
25	P	303	CLA	C1B-CHB-C4A	-3.08	124.01	130.12
38	R	312	KC2	O2D-CGD-O1D	-3.08	117.81	123.84
25	R	314	CLA	C1B-CHB-C4A	-3.08	124.01	130.12
30	M	101	BCR	C3-C4-C5	-3.08	108.57	114.08
25	6	610	CLA	CHB-C4A-NA	3.08	128.78	124.51
30	L	306	BCR	C23-C22-C21	-3.08	114.21	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	5	608	CLA	CMB-C2B-C3B	3.08	130.44	124.68
38	P	308	KC2	CHB-C4A-NA	3.08	129.06	124.20
24	W	305	CHL	CMB-C2B-C3B	3.08	130.44	124.68
29	X	319	Q6L	C42-C13-C12	3.08	120.45	115.27
25	B	808	CLA	CMB-C2B-C3B	3.08	130.44	124.68
38	W	308	KC2	C3C-C2C-C1C	3.08	108.77	106.49
25	X	302	CLA	C4D-CHA-C1A	3.08	124.99	121.25
25	X	310	CLA	C1B-CHB-C4A	-3.08	124.02	130.12
25	P	302	CLA	CHB-C4A-NA	3.08	128.77	124.51
30	A	849	BCR	C19-C18-C17	-3.08	114.22	118.94
25	R	305	CLA	CHB-C4A-NA	3.08	128.76	124.51
25	A	838	CLA	O2D-CGD-CBD	3.07	116.73	111.27
25	1	608	CLA	CBA-CAA-C2A	3.07	122.94	113.86
25	W	301	CLA	CMB-C2B-C3B	3.07	130.43	124.68
29	Q	318	Q6L	C05-C06-C07	3.07	114.51	110.30
25	B	818	CLA	CBA-CAA-C2A	3.07	122.93	113.86
25	X	312	CLA	O2D-CGD-O1D	-3.07	117.83	123.84
25	6	613	CLA	C1B-CHB-C4A	-3.07	124.03	130.12
25	A	804	CLA	O2D-CGD-O1D	-3.07	117.83	123.84
38	T	308	KC2	CAA-CBA-CGA	-3.07	111.48	127.26
25	F	803	CLA	OBD-CAD-C3D	-3.07	121.13	128.52
25	A	828	CLA	CMB-C2B-C3B	3.07	130.42	124.68
24	W	314	CHL	CBD-CHA-C1A	3.07	132.12	128.50
25	B	843	CLA	C1B-CHB-C4A	-3.07	124.05	130.12
25	A	838	CLA	C1B-CHB-C4A	-3.06	124.05	130.12
25	B	808	CLA	CAC-C3C-C4C	3.06	128.78	124.81
29	V	319	Q6L	C28-C27-C26	3.06	127.21	122.92
25	B	807	CLA	CBA-CAA-C2A	3.06	122.91	113.86
25	O	2001	CLA	CMB-C2B-C1B	-3.06	123.76	128.46
25	5	601	CLA	O2D-CGD-CBD	3.06	116.71	111.27
25	5	608	CLA	CMB-C2B-C1B	-3.06	123.76	128.46
25	V	302	CLA	C1-C2-C3	-3.06	121.80	126.75
25	H	302	CLA	C1B-CHB-C4A	-3.06	124.06	130.12
25	V	311	CLA	CMB-C2B-C3B	3.06	130.40	124.68
24	2	601	CHL	CMB-C2B-C1B	-3.06	123.76	128.46
25	A	821	CLA	C4A-NA-C1A	3.06	108.08	106.71
25	A	856	CLA	CHB-C4A-NA	3.06	128.74	124.51
25	A	818	CLA	CHD-C1D-ND	-3.06	121.64	124.45
24	T	304	CHL	O2D-CGD-O1D	-3.06	117.86	123.84
25	V	303	CLA	O2D-CGD-O1D	-3.06	117.86	123.84
24	X	307	CHL	CAC-C3C-C4C	3.06	128.78	124.81
25	A	820	CLA	CBA-CAA-C2A	3.06	122.89	113.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	B	819	CLA	CMB-C2B-C1B	-3.06	123.77	128.46
25	4	313	CLA	CHB-C4A-NA	3.06	128.74	124.51
25	5	606	CLA	C1B-CHB-C4A	-3.05	124.07	130.12
25	Q	304	CLA	CMB-C2B-C1B	-3.05	123.77	128.46
25	3	311	CLA	CHB-C4A-NA	3.05	128.74	124.51
25	B	811	CLA	CHD-C1D-ND	-3.05	121.65	124.45
30	M	101	BCR	C19-C18-C17	-3.05	114.25	118.94
25	Q	305	CLA	CMB-C2B-C3B	3.05	130.39	124.68
25	P	313	CLA	C1B-CHB-C4A	-3.05	124.07	130.12
25	Q	301	CLA	CHB-C4A-NA	3.05	128.73	124.51
25	P	312	CLA	C1B-CHB-C4A	-3.05	124.08	130.12
25	V	303	CLA	CAC-C3C-C2C	-3.05	122.31	127.53
25	B	837	CLA	C1B-CHB-C4A	-3.05	124.08	130.12
30	F	804	BCR	C16-C15-C14	-3.05	117.23	123.47
25	R	314	CLA	CHB-C4A-NA	3.05	128.73	124.51
25	1	607	CLA	C1B-CHB-C4A	-3.05	124.08	130.12
30	B	847	BCR	C11-C10-C9	-3.05	122.96	127.31
24	4	302	CHL	C1-O2A-CGA	3.04	124.43	116.44
25	P	313	CLA	CHD-C1D-ND	-3.04	121.66	124.45
25	V	312	CLA	CMB-C2B-C3B	3.04	130.37	124.68
37	T	317	NEX	C31-C30-C29	-3.04	122.97	127.31
24	X	307	CHL	O2A-CGA-O1A	-3.04	115.92	123.59
37	T	317	NEX	C5-C4-C3	3.04	115.34	111.75
25	4	315	CLA	C1B-CHB-C4A	-3.04	124.10	130.12
25	B	802	CLA	O2D-CGD-O1D	-3.04	117.90	123.84
25	X	304	CLA	O2D-CGD-O1D	-3.04	117.90	123.84
25	B	814	CLA	O2D-CGD-CBD	3.04	116.67	111.27
25	A	842	CLA	CMB-C2B-C1B	-3.04	123.80	128.46
25	4	304	CLA	O2D-CGD-CBD	3.04	116.67	111.27
24	S	305	CHL	C1B-CHB-C4A	-3.04	124.10	130.12
25	1	610	CLA	C1B-CHB-C4A	-3.04	124.11	130.12
30	B	846	BCR	C12-C13-C14	-3.03	114.29	118.94
25	S	310	CLA	C4-C3-C5	3.03	120.37	115.27
24	X	308	CHL	C1B-CHB-C4A	-3.03	124.11	130.12
25	B	834	CLA	CHB-C4A-NA	3.03	128.71	124.51
25	A	837	CLA	C1B-CHB-C4A	-3.03	124.11	130.12
25	A	827	CLA	O2D-CGD-CBD	3.03	116.66	111.27
25	A	840	CLA	C1B-CHB-C4A	-3.03	124.11	130.12
30	B	849	BCR	C40-C30-C25	-3.03	105.38	110.30
25	R	317	CLA	CHD-C1D-ND	-3.03	121.67	124.45
30	M	101	BCR	C38-C26-C25	-3.03	121.13	124.53
25	A	828	CLA	CHB-C4A-NA	3.03	128.70	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	4	303	CLA	CHB-C4A-NA	3.03	128.70	124.51
29	Q	318	Q6L	C23-C22-C21	3.03	127.16	122.92
38	S	308	KC2	CHB-C4A-C3A	-3.03	120.25	124.98
29	Q	317	Q6L	C42-C13-C12	3.03	120.36	115.27
37	H	306	NEX	C12-C13-C14	-3.03	114.30	118.94
27	1	612	XAT	C12-C13-C14	-3.03	114.30	118.94
25	Q	311	CLA	C4A-NA-C1A	3.03	108.07	106.71
27	5	612	XAT	C8-C9-C10	-3.02	114.30	118.94
30	M	101	BCR	C15-C16-C17	-3.02	117.28	123.47
25	R	306	CLA	CHB-C4A-NA	3.02	128.69	124.51
25	5	610	CLA	C1B-CHB-C4A	-3.02	124.13	130.12
25	6	611	CLA	C1B-CHB-C4A	-3.02	124.13	130.12
25	Q	314	CLA	C1B-CHB-C4A	-3.02	124.13	130.12
25	O	2004	CLA	CHD-C1D-ND	-3.02	121.68	124.45
25	4	311	CLA	C4A-NA-C1A	3.02	108.06	106.71
38	Q	310	KC2	CBD-CHA-C1A	3.02	134.52	128.88
25	4	305	CLA	CAB-C3B-C2B	3.02	130.61	124.69
24	V	304	CHL	CMB-C2B-C1B	-3.02	123.82	128.46
30	B	845	BCR	C19-C18-C17	-3.02	114.30	118.94
24	2	607	CHL	C1B-CHB-C4A	-3.02	124.13	130.12
30	A	849	BCR	C8-C7-C6	-3.02	118.72	127.20
25	A	837	CLA	C4-C3-C2	-3.02	115.93	123.68
25	3	303	CLA	CAB-C3B-C4B	-3.02	123.82	128.46
30	K	207	BCR	C15-C14-C13	-3.02	123.00	127.31
25	W	312	CLA	CAC-C3C-C4C	3.02	128.72	124.81
25	5	602	CLA	C1B-CHB-C4A	-3.02	124.14	130.12
25	6	610	CLA	CMB-C2B-C3B	3.02	130.32	124.68
25	V	301	CLA	CAA-C2A-C1A	-3.02	102.09	111.97
25	3	308	CLA	C2C-C1C-NC	3.02	112.80	109.97
25	2	608	CLA	O2D-CGD-O1D	-3.01	117.94	123.84
25	V	313	CLA	CMB-C2B-C1B	-3.01	123.83	128.46
29	R	323	Q6L	C42-C13-C12	3.01	120.34	115.27
25	B	833	CLA	O2D-CGD-O1D	-3.01	117.95	123.84
24	R	308	CHL	CHB-C4A-NA	3.01	128.68	124.51
30	F	801	BCR	C33-C5-C6	-3.01	121.14	124.53
25	B	836	CLA	CHB-C4A-NA	3.01	128.68	124.51
25	T	311	CLA	CHB-C4A-NA	3.01	128.68	124.51
38	W	308	KC2	CMD-C2D-C3D	3.01	130.31	124.68
25	3	312	CLA	C4A-NA-C1A	3.01	108.06	106.71
30	G	201	BCR	C31-C1-C6	3.01	115.18	110.30
25	T	313	CLA	O2D-CGD-O1D	-3.01	117.95	123.84
30	F	804	BCR	C3-C4-C5	-3.01	108.70	114.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	G	203	CLA	O2D-CGD-O1D	-3.01	117.95	123.84
29	R	301	Q6L	C05-C06-C07	3.01	114.42	110.30
25	2	609	CLA	CMB-C2B-C3B	3.01	130.31	124.68
25	A	832	CLA	O2D-CGD-O1D	-3.01	117.96	123.84
25	B	806	CLA	O2D-CGD-O1D	-3.01	117.96	123.84
25	3	312	CLA	CHD-C1D-ND	-3.01	121.69	124.45
25	6	613	CLA	CMB-C2B-C3B	3.01	130.31	124.68
37	H	306	NEX	O24-C25-C38	3.01	118.66	115.06
37	S	317	NEX	C31-C30-C29	-3.01	123.02	127.31
25	K	203	CLA	CMB-C2B-C1B	-3.00	123.85	128.46
25	W	303	CLA	C1-C2-C3	-3.00	121.89	126.75
25	4	316	CLA	O2D-CGD-O1D	-3.00	117.97	123.84
25	B	813	CLA	O2D-CGD-O1D	-3.00	117.97	123.84
24	3	306	CHL	CMB-C2B-C3B	3.00	130.29	124.68
37	P	317	NEX	C11-C10-C9	-3.00	123.03	127.31
27	6	615	XAT	C28-C29-C30	-3.00	114.34	118.94
24	4	308	CHL	C1B-CHB-C4A	-3.00	124.18	130.12
38	X	309	KC2	CAA-C2A-C1A	-3.00	110.96	124.75
24	W	305	CHL	C1C-C2C-C3C	-3.00	104.73	107.11
24	4	307	CHL	C3C-C4C-NC	-3.00	107.21	110.57
25	B	816	CLA	C1B-CHB-C4A	-3.00	124.18	130.12
25	A	828	CLA	CMB-C2B-C1B	-3.00	123.86	128.46
25	W	309	CLA	CMB-C2B-C3B	3.00	130.29	124.68
25	S	312	CLA	C1B-CHB-C4A	-3.00	124.18	130.12
24	4	307	CHL	O2D-CGD-O1D	-3.00	117.98	123.84
27	6	615	XAT	C32-C33-C34	-2.99	114.35	118.94
30	3	318	BCR	C12-C13-C14	-2.99	114.35	118.94
30	K	202	BCR	C35-C13-C12	2.99	122.79	118.08
25	B	842	CLA	C1-C2-C3	-2.99	120.87	126.04
25	A	856	CLA	O2A-CGA-O1A	-2.99	116.04	123.59
25	Q	311	CLA	CMB-C2B-C1B	-2.99	123.87	128.46
24	U	305	CHL	CHB-C4A-NA	2.99	128.65	124.51
25	4	312	CLA	CHB-C4A-NA	2.99	128.65	124.51
25	V	302	CLA	C4A-NA-C1A	2.99	108.05	106.71
30	A	849	BCR	C11-C10-C9	-2.99	123.04	127.31
38	U	307	KC2	C2A-C3A-C4A	-2.99	104.27	106.49
25	H	302	CLA	CBA-CAA-C2A	2.99	122.68	113.86
25	1	613	CLA	C1B-CHB-C4A	-2.99	124.20	130.12
25	3	311	CLA	C5-C3-C2	2.99	127.16	121.12
24	2	601	CHL	CMB-C2B-C3B	2.99	130.26	124.68
25	T	309	CLA	CMB-C2B-C1B	-2.99	123.88	128.46
25	U	302	CLA	C1B-CHB-C4A	-2.98	124.21	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	6	601	CHL	C1C-C2C-C3C	-2.98	104.75	107.11
24	V	305	CHL	CHB-C4A-NA	2.98	128.64	124.51
30	L	306	BCR	C39-C30-C25	2.98	115.14	110.30
25	A	812	CLA	CMB-C2B-C3B	2.98	130.26	124.68
27	4	318	XAT	C31-C30-C29	-2.98	123.05	127.31
24	T	320	CHL	O2D-CGD-O1D	-2.98	118.01	123.84
30	K	207	BCR	C33-C5-C6	2.98	127.88	124.53
25	T	302	CLA	O2D-CGD-O1D	-2.98	118.01	123.84
25	L	302	CLA	CHB-C4A-NA	2.98	128.63	124.51
25	P	311	CLA	O2A-CGA-O1A	-2.98	116.07	123.59
24	S	306	CHL	C4-C3-C5	2.98	119.39	115.98
25	B	840	CLA	C1B-CHB-C4A	-2.98	124.22	130.12
24	P	314	CHL	CHB-C4A-NA	2.98	128.63	124.51
38	T	308	KC2	CHB-C4A-C3A	-2.98	120.33	124.98
25	W	310	CLA	C1B-CHB-C4A	-2.98	124.22	130.12
25	B	835	CLA	O2D-CGD-O1D	-2.98	118.02	123.84
25	O	2002	CLA	C1-C2-C3	2.98	131.19	126.04
25	R	314	CLA	O2D-CGD-CBD	2.97	116.55	111.27
28	2	619	LHG	O7-C7-C8	2.97	117.91	111.50
25	R	316	CLA	CBA-CAA-C2A	2.97	122.64	113.86
29	V	319	Q6L	C26-C25-C24	-2.97	113.94	123.22
25	A	821	CLA	CHD-C1D-ND	-2.97	121.72	124.45
30	F	804	BCR	C15-C16-C17	-2.97	117.38	123.47
25	3	308	CLA	C1C-C2C-C3C	-2.97	103.83	106.96
25	5	610	CLA	CMB-C2B-C3B	2.97	130.24	124.68
24	T	307	CHL	C1B-CHB-C4A	-2.97	124.23	130.12
25	B	803	CLA	CHD-C1D-ND	-2.97	121.72	124.45
24	R	318	CHL	CMB-C2B-C3B	2.97	130.24	124.68
25	S	303	CLA	O2D-CGD-O1D	-2.97	118.03	123.84
25	5	606	CLA	CAB-C3B-C2B	2.97	130.50	124.69
25	K	206	CLA	CHB-C4A-NA	2.97	128.62	124.51
30	3	317	BCR	C36-C18-C17	-2.97	118.77	122.92
30	G	205	BCR	C34-C9-C10	2.97	127.08	122.92
25	L	301	CLA	CMB-C2B-C3B	2.96	130.22	124.68
30	K	202	BCR	C38-C26-C25	2.96	127.86	124.53
25	R	306	CLA	CMB-C2B-C3B	2.96	130.22	124.68
25	F	802	CLA	CHD-C1D-ND	-2.96	121.73	124.45
27	2	617	XAT	C36-C21-C22	-2.96	103.83	108.98
30	K	202	BCR	C15-C14-C13	-2.96	123.08	127.31
28	1	614	LHG	C5-O7-C7	-2.96	110.50	117.79
25	A	845	CLA	CMB-C2B-C3B	2.96	130.22	124.68
25	6	608	CLA	O2D-CGD-O1D	-2.96	118.05	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	R	310	CHL	C1C-C2C-C3C	-2.96	104.76	107.11
25	2	612	CLA	CHB-C4A-NA	2.96	128.61	124.51
25	B	823	CLA	C1B-CHB-C4A	-2.96	124.25	130.12
24	V	307	CHL	C2C-C3C-C4C	2.96	108.60	106.49
27	5	612	XAT	C32-C33-C34	-2.96	114.40	118.94
25	2	612	CLA	C1B-CHB-C4A	-2.96	124.25	130.12
38	Q	310	KC2	CHB-C4A-NA	2.96	128.87	124.20
27	1	612	XAT	O24-C25-C38	2.96	118.60	115.06
25	H	301	CLA	CMB-C2B-C3B	2.96	130.22	124.68
24	S	306	CHL	CHD-C1D-C2D	2.96	131.69	125.48
25	4	315	CLA	CHD-C1D-ND	-2.96	121.73	124.45
27	2	617	XAT	C31-C30-C29	-2.96	123.09	127.31
25	A	819	CLA	O2D-CGD-O1D	-2.96	118.05	123.84
25	B	821	CLA	C4A-NA-C1A	2.96	108.04	106.71
29	R	320	Q6L	C35-C34-C33	2.96	115.11	111.74
37	R	321	NEX	C16-C1-C6	2.96	113.12	110.47
26	S	318	IWJ	C36-C35-C34	-2.96	103.84	108.98
25	A	835	CLA	C1B-CHB-C4A	-2.96	124.26	130.12
25	Q	313	CLA	C1B-CHB-C4A	-2.96	124.26	130.12
30	F	804	BCR	C35-C13-C12	2.96	122.73	118.08
25	R	316	CLA	C5-C3-C2	-2.95	115.14	121.12
25	L	301	CLA	C1B-CHB-C4A	-2.95	124.27	130.12
25	B	834	CLA	O2D-CGD-CBD	2.95	116.52	111.27
34	A	844	PQN	C16-C15-C13	2.95	121.20	113.45
25	3	313	CLA	CHD-C1D-ND	-2.95	121.74	124.45
25	4	309	CLA	CHD-C1D-ND	-2.95	121.74	124.45
25	A	809	CLA	C3A-C2A-C1A	2.95	105.76	101.34
30	3	318	BCR	C3-C4-C5	-2.95	108.81	114.08
25	W	312	CLA	C1B-CHB-C4A	-2.95	124.27	130.12
25	V	311	CLA	CHB-C4A-NA	2.95	128.59	124.51
25	A	837	CLA	CHD-C1D-ND	-2.95	121.74	124.45
25	A	825	CLA	CAC-C3C-C4C	2.95	128.64	124.81
25	Q	312	CLA	C1B-CHB-C4A	-2.95	124.27	130.12
25	G	203	CLA	CMB-C2B-C1B	-2.95	123.93	128.46
25	A	831	CLA	CMB-C2B-C3B	2.95	130.20	124.68
31	N	201	LMG	O6-C5-C6	2.95	113.77	106.44
25	B	832	CLA	CMB-C2B-C1B	-2.95	123.93	128.46
30	F	801	BCR	C12-C13-C14	-2.95	114.42	118.94
30	B	846	BCR	C35-C13-C12	2.95	122.72	118.08
25	6	612	CLA	C1B-CHB-C4A	-2.95	124.28	130.12
25	4	314	CLA	O2D-CGD-CBD	2.95	116.50	111.27
25	B	827	CLA	O2D-CGD-O1D	-2.95	118.08	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	X	303	CLA	O2D-CGD-O1D	-2.95	118.08	123.84
30	4	319	BCR	C3-C4-C5	-2.95	108.82	114.08
25	P	310	CLA	O2A-CGA-O1A	-2.95	116.16	123.59
25	A	825	CLA	C5-C3-C2	2.94	127.08	121.12
25	5	602	CLA	CHB-C4A-NA	2.94	128.58	124.51
25	Q	311	CLA	CHB-C4A-NA	2.94	128.58	124.51
37	P	317	NEX	C40-C33-C32	2.94	122.72	118.08
25	1	609	CLA	CAB-C3B-C2B	2.94	130.45	124.69
25	Q	305	CLA	C1B-CHB-C4A	-2.94	124.29	130.12
25	6	611	CLA	CHD-C1D-ND	-2.94	121.75	124.45
25	B	842	CLA	C1B-CHB-C4A	-2.94	124.30	130.12
30	A	851	BCR	C15-C14-C13	-2.94	123.11	127.31
25	3	311	CLA	O2A-CGA-CBA	2.94	121.13	111.91
25	V	303	CLA	CHD-C1D-ND	-2.94	121.75	124.45
25	P	302	CLA	CMB-C2B-C3B	2.94	130.17	124.68
25	G	204	CLA	O2D-CGD-O1D	-2.94	118.09	123.84
30	B	847	BCR	C20-C21-C22	-2.94	123.12	127.31
25	B	833	CLA	C1B-CHB-C4A	-2.94	124.30	130.12
25	4	313	CLA	C1B-CHB-C4A	-2.94	124.30	130.12
25	2	602	CLA	O2D-CGD-O1D	-2.94	118.10	123.84
29	S	315	Q6L	C06-C07-C02	2.93	117.70	111.85
30	B	846	BCR	C39-C30-C25	-2.93	105.54	110.30
25	3	307	CLA	CHB-C4A-NA	2.93	128.57	124.51
25	6	602	CLA	O2A-CGA-O1A	-2.93	116.19	123.59
25	3	303	CLA	CHB-C4A-NA	2.93	128.57	124.51
25	4	315	CLA	CMB-C2B-C3B	2.93	130.16	124.68
25	A	805	CLA	C1-C2-C3	-2.93	120.97	126.04
30	A	848	BCR	C16-C15-C14	-2.93	117.47	123.47
25	U	303	CLA	C1B-CHB-C4A	-2.93	124.31	130.12
25	3	307	CLA	C1-C2-C3	2.93	131.11	126.04
25	B	813	CLA	CMC-C2C-C1C	2.93	129.50	125.04
25	A	803	CLA	O2D-CGD-O1D	-2.93	118.11	123.84
25	6	612	CLA	CMB-C2B-C3B	2.93	130.16	124.68
30	J	101	BCR	C38-C26-C25	-2.93	121.24	124.53
25	S	301	CLA	C1B-CHB-C4A	-2.93	124.31	130.12
25	2	602	CLA	CMC-C2C-C1C	2.93	129.50	125.04
25	6	608	CLA	CHD-C1D-ND	-2.93	121.76	124.45
25	A	804	CLA	CHD-C1D-ND	-2.93	121.76	124.45
25	6	602	CLA	CED-O2D-CGD	2.93	122.56	115.94
25	1	610	CLA	CHD-C1D-ND	-2.93	121.76	124.45
25	1	613	CLA	CHD-C1D-ND	-2.93	121.76	124.45
30	3	318	BCR	C35-C13-C12	2.93	122.69	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	W	308	KC2	CAC-C3C-C2C	-2.93	118.96	128.60
24	P	304	CHL	CMA-C3A-C4A	2.93	119.64	111.77
25	V	311	CLA	O2D-CGD-O1D	-2.92	118.12	123.84
30	J	103	BCR	C19-C18-C17	-2.92	114.45	118.94
25	B	843	CLA	CHD-C1D-ND	-2.92	121.77	124.45
30	J	103	BCR	C8-C7-C6	-2.92	118.99	127.20
37	W	317	NEX	C16-C1-C6	2.92	113.09	110.47
25	L	302	CLA	CBA-CAA-C2A	2.92	122.49	113.86
25	1	613	CLA	C5-C3-C2	2.92	127.03	121.12
25	O	2002	CLA	C3C-C4C-NC	-2.92	107.30	110.57
25	R	317	CLA	O2D-CGD-O1D	-2.92	118.13	123.84
32	6	617	SQD	O48-C23-C24	2.92	121.07	111.91
25	T	309	CLA	CMB-C2B-C3B	2.92	130.14	124.68
24	U	305	CHL	C1B-CHB-C4A	-2.92	124.34	130.12
29	X	319	Q6L	C12-C13-C14	-2.92	113.14	121.98
25	A	808	CLA	C1B-CHB-C4A	-2.92	124.34	130.12
25	A	843	CLA	C1B-CHB-C4A	-2.92	124.34	130.12
25	A	832	CLA	C1B-CHB-C4A	-2.92	124.34	130.12
30	K	202	BCR	C2-C1-C6	2.92	114.97	110.48
25	P	302	CLA	CMB-C2B-C1B	-2.92	123.98	128.46
25	6	604	CLA	O2D-CGD-O1D	-2.92	118.14	123.84
25	Q	312	CLA	CMB-C2B-C3B	2.92	130.13	124.68
24	1	601	CHL	C1C-C2C-C3C	-2.92	104.80	107.11
24	R	309	CHL	C1C-C2C-C3C	-2.92	104.80	107.11
30	3	319	BCR	C11-C10-C9	-2.91	123.15	127.31
25	A	843	CLA	C1-C2-C3	2.91	131.08	126.04
24	5	605	CHL	CHB-C4A-NA	2.91	128.54	124.51
27	4	318	XAT	O23-C23-C22	2.91	115.59	109.80
24	6	606	CHL	C2A-C1A-CHA	2.91	128.95	123.86
27	2	617	XAT	C17-C1-C16	-2.91	103.07	107.37
25	4	304	CLA	CAB-C3B-C2B	2.91	130.39	124.69
25	4	303	CLA	CAC-C3C-C4C	2.91	128.59	124.81
24	R	302	CHL	O2D-CGD-O1D	-2.91	118.14	123.84
29	R	323	Q6L	C12-C13-C14	-2.91	113.16	121.98
25	R	317	CLA	C1B-CHB-C4A	-2.91	124.35	130.12
25	P	310	CLA	CHD-C1D-ND	-2.91	121.78	124.45
25	4	311	CLA	O2D-CGD-CBD	2.91	116.44	111.27
25	A	805	CLA	O2D-CGD-CBD	2.91	116.44	111.27
25	3	301	CLA	C1D-ND-C4D	-2.91	104.27	106.33
25	K	203	CLA	C1B-CHB-C4A	-2.91	124.36	130.12
24	V	304	CHL	O2A-CGA-O1A	-2.91	116.06	123.30
25	Q	305	CLA	O2D-CGD-O1D	-2.91	118.16	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	T	303	CLA	C1B-CHB-C4A	-2.90	124.37	130.12
25	A	817	CLA	CHB-C4A-NA	2.90	128.53	124.51
30	I	101	BCR	C30-C25-C26	-2.90	118.53	122.61
25	4	310	CLA	CHB-C4A-NA	2.90	128.52	124.51
25	A	839	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
24	X	306	CHL	C4A-NA-C1A	2.90	108.01	106.71
30	3	319	BCR	C20-C21-C22	-2.90	123.17	127.31
25	Q	301	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
25	V	303	CLA	C1B-CHB-C4A	-2.90	124.38	130.12
25	L	301	CLA	CHD-C1D-ND	-2.90	121.79	124.45
29	V	319	Q6L	C40-C32-C33	-2.90	117.36	123.56
25	1	603	CLA	CMB-C2B-C3B	2.90	130.10	124.68
25	A	805	CLA	CHB-C4A-NA	2.90	128.52	124.51
25	O	2003	CLA	C1B-CHB-C4A	-2.89	124.39	130.12
25	1	610	CLA	CAB-C3B-C2B	2.89	130.35	124.69
24	V	305	CHL	O2D-CGD-O1D	-2.89	118.18	123.84
25	X	313	CLA	C1B-CHB-C4A	-2.89	124.39	130.12
25	T	303	CLA	O2D-CGD-O1D	-2.89	118.18	123.84
29	2	616	Q6L	C28-C27-C26	2.89	126.97	122.92
25	B	833	CLA	CHB-C4A-NA	2.89	128.51	124.51
25	B	818	CLA	C1-O2A-CGA	2.89	124.03	116.44
38	W	308	KC2	CBA-CAA-C2A	-2.89	114.25	125.27
25	G	202	CLA	C4A-NA-C1A	2.89	108.00	106.71
30	L	307	BCR	C23-C24-C25	-2.89	119.09	127.20
24	6	601	CHL	CHB-C4A-NA	2.89	128.51	124.51
29	W	320	Q6L	C01-C02-C07	-2.89	109.00	114.36
25	2	602	CLA	C7-C6-C5	2.89	121.20	113.36
29	X	301	Q6L	C19-C18-C17	-2.89	123.19	127.31
30	F	804	BCR	C8-C7-C6	-2.89	119.09	127.20
37	P	317	NEX	C20-C13-C12	2.89	122.63	118.08
25	S	302	CLA	C1B-CHB-C4A	-2.89	124.40	130.12
31	2	620	LMG	C8-O7-C10	-2.89	110.69	117.79
25	A	814	CLA	CMB-C2B-C3B	2.89	130.08	124.68
25	B	826	CLA	CHA-C1A-NA	-2.89	119.79	126.40
25	1	603	CLA	CHD-C1D-ND	-2.88	121.80	124.45
37	H	306	NEX	C15-C35-C34	-2.88	117.56	123.47
24	T	314	CHL	O2D-CGD-CBD	2.88	116.39	111.27
25	G	204	CLA	CMB-C2B-C3B	2.88	130.07	124.68
25	W	302	CLA	CMB-C2B-C3B	2.88	130.07	124.68
25	P	301	CLA	CMC-C2C-C1C	2.88	129.43	125.04
25	4	311	CLA	CED-O2D-CGD	2.88	122.46	115.94
25	A	830	CLA	O2A-CGA-O1A	-2.88	116.31	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	L	305	BCR	C29-C30-C25	-2.88	106.04	110.48
25	B	813	CLA	CMB-C2B-C3B	2.88	130.07	124.68
30	F	804	BCR	C33-C5-C6	2.88	127.76	124.53
25	A	837	CLA	CMB-C2B-C3B	2.88	130.07	124.68
25	O	2005	CLA	O2D-CGD-O1D	-2.88	118.21	123.84
38	W	308	KC2	CMC-C2C-C1C	2.88	129.43	125.04
25	B	831	CLA	C1B-CHB-C4A	-2.88	124.42	130.12
24	V	307	CHL	C1B-CHB-C4A	-2.88	124.42	130.12
30	3	318	BCR	C32-C1-C6	2.88	114.97	110.30
25	3	302	CLA	CHB-C4A-NA	2.88	128.49	124.51
24	X	307	CHL	CMB-C2B-C3B	2.88	130.06	124.68
25	A	813	CLA	O2D-CGD-O1D	-2.88	118.21	123.84
25	Q	315	CLA	C1B-CHB-C4A	-2.88	124.42	130.12
38	S	308	KC2	CAA-C2A-C1A	-2.87	111.53	124.75
25	A	834	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
25	A	823	CLA	C1B-CHB-C4A	-2.87	124.42	130.12
30	M	101	BCR	C23-C22-C21	-2.87	114.53	118.94
25	B	814	CLA	C1B-CHB-C4A	-2.87	124.43	130.12
25	T	301	CLA	C1-C2-C3	-2.87	121.07	126.04
24	5	605	CHL	C1C-C2C-C3C	-2.87	104.83	107.11
30	A	851	BCR	C4-C5-C6	-2.87	118.56	122.73
37	R	321	NEX	C38-C25-C26	-2.87	117.45	122.26
25	6	613	CLA	C5-C3-C2	2.87	126.93	121.12
25	A	830	CLA	C1-C2-C3	-2.87	121.08	126.04
30	B	847	BCR	C35-C13-C12	2.87	122.60	118.08
25	A	830	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
25	Q	314	CLA	CMB-C2B-C3B	2.87	130.05	124.68
24	V	304	CHL	CMB-C2B-C3B	2.87	130.05	124.68
25	U	310	CLA	CMB-C2B-C1B	-2.87	124.05	128.46
25	O	2003	CLA	CHD-C1D-ND	-2.87	121.82	124.45
25	A	812	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
27	4	318	XAT	C8-C9-C10	-2.87	114.54	118.94
29	P	316	Q6L	C10-C04-C03	2.87	113.81	109.71
25	O	2003	CLA	CMB-C2B-C3B	2.87	130.04	124.68
25	A	803	CLA	C1-O2A-CGA	2.87	123.97	116.44
25	2	610	CLA	CHD-C1D-ND	-2.87	121.82	124.45
37	W	317	NEX	C19-C9-C10	2.87	126.94	122.92
25	A	840	CLA	CHD-C1D-ND	-2.87	121.82	124.45
38	U	307	KC2	CMD-C2D-C3D	2.87	130.04	124.68
24	T	305	CHL	O2D-CGD-O1D	-2.87	118.23	123.84
29	P	319	Q6L	C23-C22-C21	2.87	126.94	122.92
25	T	301	CLA	CHB-C4A-NA	2.87	128.47	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	B	813	CLA	CHD-C1D-ND	-2.87	121.82	124.45
25	G	203	CLA	CHB-C4A-NA	2.86	128.47	124.51
25	6	610	CLA	CMB-C2B-C1B	-2.86	124.06	128.46
25	U	302	CLA	C2D-C1D-ND	-2.86	107.99	110.10
25	B	811	CLA	C1B-CHB-C4A	-2.86	124.45	130.12
25	B	824	CLA	CHD-C1D-ND	-2.86	121.82	124.45
25	Q	313	CLA	CHD-C1D-ND	-2.86	121.82	124.45
25	X	311	CLA	C1B-CHB-C4A	-2.86	124.45	130.12
25	B	811	CLA	CHB-C4A-NA	2.86	128.47	124.51
25	6	611	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
24	W	314	CHL	O2D-CGD-O1D	-2.86	118.25	123.84
25	A	845	CLA	O2A-CGA-O1A	-2.86	116.37	123.59
25	B	807	CLA	CHD-C1D-ND	-2.86	121.83	124.45
24	R	310	CHL	CAC-C3C-C4C	2.86	128.52	124.81
25	R	313	CLA	CHD-C1D-ND	-2.86	121.83	124.45
30	3	318	BCR	C23-C22-C21	-2.86	114.56	118.94
25	V	312	CLA	CHB-C4A-NA	2.86	128.46	124.51
25	Q	311	CLA	CBA-CAA-C2A	2.86	122.30	113.86
24	W	307	CHL	CHB-C4A-NA	2.86	128.46	124.51
24	V	306	CHL	CHB-C4A-NA	2.86	128.46	124.51
25	4	303	CLA	CMB-C2B-C3B	2.86	130.02	124.68
25	B	821	CLA	O2D-CGD-O1D	-2.85	118.26	123.84
25	3	303	CLA	O1D-CGD-CBD	2.85	130.32	124.48
25	A	804	CLA	C1B-CHB-C4A	-2.85	124.47	130.12
25	A	833	CLA	CHD-C1D-ND	-2.85	121.83	124.45
25	B	804	CLA	C1B-CHB-C4A	-2.85	124.47	130.12
24	6	606	CHL	CAC-C3C-C4C	2.85	128.51	124.81
25	O	2001	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
25	1	605	CLA	C1B-CHB-C4A	-2.85	124.48	130.12
25	P	302	CLA	C4-C3-C5	2.85	120.06	115.27
29	V	319	Q6L	C29-C27-C26	-2.85	114.57	118.94
25	3	309	CLA	C1B-CHB-C4A	-2.85	124.48	130.12
25	B	816	CLA	CHB-C4A-NA	2.85	128.45	124.51
30	A	851	BCR	C7-C6-C5	-2.85	114.57	121.46
25	1	608	CLA	O2D-CGD-O1D	-2.85	118.28	123.84
25	6	607	CLA	C1B-CHB-C4A	-2.85	124.48	130.12
25	B	820	CLA	C2A-C1A-CHA	2.85	128.83	123.86
25	A	814	CLA	C2D-C1D-ND	-2.84	108.01	110.10
25	P	311	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
25	4	314	CLA	CMB-C2B-C3B	2.84	130.00	124.68
25	X	314	CLA	C1B-CHB-C4A	-2.84	124.49	130.12
25	B	806	CLA	C1-C2-C3	2.84	130.95	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	U	316	IWJ	C36-C35-C34	-2.84	104.05	108.98
30	J	101	BCR	C27-C26-C25	-2.84	118.61	122.73
24	S	306	CHL	CBC-CAC-C3C	2.84	120.26	112.43
25	5	607	CLA	C1B-CHB-C4A	-2.84	124.50	130.12
25	A	813	CLA	CMB-C2B-C1B	-2.84	124.10	128.46
25	S	301	CLA	O2D-CGD-O1D	-2.84	118.30	123.84
25	U	312	CLA	O2D-CGD-O1D	-2.84	118.30	123.84
25	B	818	CLA	C1B-CHB-C4A	-2.83	124.50	130.12
25	A	818	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
24	T	320	CHL	CMB-C2B-C1B	-2.83	124.11	128.46
25	B	836	CLA	CMB-C2B-C1B	-2.83	124.11	128.46
24	R	318	CHL	CHB-C4A-NA	2.83	128.43	124.51
25	Q	311	CLA	C1-C2-C3	-2.83	121.14	126.04
25	X	302	CLA	CMB-C2B-C1B	-2.83	124.11	128.46
25	5	610	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
30	4	319	BCR	C35-C13-C12	2.83	122.54	118.08
25	G	204	CLA	CHD-C1D-ND	-2.83	121.85	124.45
31	F	805	LMG	O8-C28-C29	2.83	120.79	111.91
24	2	615	CHL	C1C-C2C-C3C	-2.83	104.87	107.11
25	5	603	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
25	B	817	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
30	B	847	BCR	C32-C1-C6	2.83	114.89	110.30
24	2	601	CHL	CHD-C1D-ND	-2.83	121.85	124.45
32	6	617	SQD	O9-S-C6	2.83	110.30	106.94
25	B	802	CLA	CMC-C2C-C1C	2.83	129.35	125.04
25	4	314	CLA	C1B-CHB-C4A	-2.83	124.51	130.12
37	W	317	NEX	C15-C14-C13	-2.83	123.27	127.31
24	P	307	CHL	C3C-C4C-NC	-2.83	107.40	110.57
25	L	304	CLA	CHB-C4A-NA	2.83	128.42	124.51
25	A	819	CLA	C1B-CHB-C4A	-2.83	124.52	130.12
29	V	321	Q6L	C38-C36-C35	-2.83	104.08	109.44
30	G	201	BCR	C38-C26-C27	2.83	119.05	113.62
25	4	303	CLA	CBA-CAA-C2A	2.83	122.21	113.86
25	5	607	CLA	CHD-C1D-ND	-2.83	121.86	124.45
24	2	615	CHL	CHB-C4A-NA	2.83	128.42	124.51
27	5	612	XAT	C35-C15-C14	-2.83	117.68	123.47
25	A	812	CLA	CMB-C2B-C1B	-2.83	124.12	128.46
25	A	803	CLA	CHD-C1D-ND	-2.83	121.86	124.45
30	B	849	BCR	C2-C1-C6	2.83	114.83	110.48
25	B	804	CLA	CAC-C3C-C4C	2.83	128.48	124.81
25	R	316	CLA	CHB-C4A-NA	2.83	128.42	124.51
24	Q	309	CHL	OMC-CMC-C2C	-2.82	119.30	125.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	S	307	CHL	C1B-CHB-C4A	-2.82	124.52	130.12
25	V	313	CLA	CHD-C1D-ND	-2.82	121.86	124.45
24	Q	308	CHL	C1B-CHB-C4A	-2.82	124.53	130.12
38	P	308	KC2	CHC-C4B-NB	2.82	127.05	124.45
25	5	601	CLA	CBA-CAA-C2A	2.82	122.19	113.86
24	S	314	CHL	O2D-CGD-O1D	-2.82	118.32	123.84
25	O	2004	CLA	CMB-C2B-C3B	2.82	129.96	124.68
25	A	807	CLA	C1B-CHB-C4A	-2.82	124.53	130.12
25	T	313	CLA	C1B-CHB-C4A	-2.82	124.53	130.12
24	2	601	CHL	C3C-C4C-NC	-2.82	107.41	110.57
25	R	313	CLA	O2A-CGA-O1A	-2.82	116.47	123.59
25	U	309	CLA	CHB-C4A-NA	2.82	128.41	124.51
25	B	835	CLA	C1B-CHB-C4A	-2.82	124.53	130.12
25	A	818	CLA	C1B-CHB-C4A	-2.82	124.53	130.12
24	S	304	CHL	CAA-C2A-C3A	-2.82	109.52	116.10
38	X	309	KC2	CBD-CHA-C1A	2.82	134.14	128.88
33	A	802	CL0	CMB-C2B-C1B	-2.82	124.13	128.46
24	V	305	CHL	C2D-C1D-ND	-2.82	108.03	110.10
29	U	315	Q6L	C19-C20-C21	-2.82	117.70	123.47
24	X	308	CHL	O2D-CGD-O1D	-2.82	118.33	123.84
30	G	205	BCR	C8-C7-C6	-2.82	119.29	127.20
29	2	616	Q6L	C06-C07-C02	2.82	117.46	111.85
30	B	845	BCR	C35-C13-C12	2.81	122.51	118.08
24	2	615	CHL	C1B-CHB-C4A	-2.81	124.54	130.12
29	S	320	Q6L	C35-C34-C33	2.81	114.94	111.74
24	R	308	CHL	C4A-NA-C1A	2.81	107.97	106.71
25	B	815	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
27	2	617	XAT	C32-C33-C34	-2.81	114.63	118.94
24	R	310	CHL	CMB-C2B-C3B	2.81	129.94	124.68
25	6	611	CLA	CHB-C4A-NA	2.81	128.40	124.51
25	P	310	CLA	CHB-C4A-NA	2.81	128.40	124.51
25	A	820	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
25	B	843	CLA	CHB-C4A-NA	2.81	128.40	124.51
25	2	604	CLA	O2D-CGD-O1D	-2.81	118.35	123.84
38	U	307	KC2	CMD-C2D-C1D	-2.81	124.15	128.46
25	2	602	CLA	C5-C3-C2	-2.81	115.44	121.12
24	1	601	CHL	O2D-CGD-O1D	-2.81	117.72	124.09
37	R	321	NEX	C11-C10-C9	-2.81	123.30	127.31
25	T	312	CLA	C1B-CHB-C4A	-2.81	124.56	130.12
25	A	814	CLA	C1B-CHB-C4A	-2.81	124.56	130.12
25	6	610	CLA	O2D-CGD-O1D	-2.81	118.35	123.84
25	Q	311	CLA	O2D-CGD-CBD	2.80	116.25	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	3	308	CLA	CMB-C2B-C3B	2.80	129.92	124.68
25	A	815	CLA	CHD-C1D-ND	-2.80	121.88	124.45
25	B	803	CLA	C1-O2A-CGA	-2.80	109.09	116.44
25	6	602	CLA	CHB-C4A-NA	2.80	128.39	124.51
25	S	313	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
29	U	317	Q6L	C42-C13-C12	2.80	119.98	115.27
25	S	309	CLA	CHB-C4A-NA	2.80	128.38	124.51
29	S	320	Q6L	C40-C32-C33	-2.80	117.57	123.56
25	A	845	CLA	CHB-C4A-NA	2.80	128.38	124.51
25	B	806	CLA	CAC-C3C-C4C	2.80	128.44	124.81
24	U	313	CHL	O2D-CGD-O1D	-2.80	118.36	123.84
25	A	814	CLA	CBA-CAA-C2A	2.80	122.13	113.86
25	U	308	CLA	CMC-C2C-C1C	2.80	129.30	125.04
24	W	305	CHL	CHB-C4A-NA	2.80	128.38	124.51
30	L	305	BCR	C20-C21-C22	-2.80	123.32	127.31
30	L	306	BCR	C33-C5-C6	-2.80	121.39	124.53
25	A	820	CLA	CHA-C1A-NA	-2.80	119.99	126.40
25	B	825	CLA	CMB-C2B-C1B	-2.80	124.17	128.46
25	B	825	CLA	CHD-C1D-ND	-2.80	121.89	124.45
25	B	826	CLA	C2A-C1A-CHA	2.80	128.75	123.86
25	L	303	CLA	O2D-CGD-O1D	-2.80	118.37	123.84
38	V	308	KC2	CAC-C3C-C2C	-2.79	119.40	128.60
24	P	314	CHL	CMB-C2B-C3B	2.79	129.91	124.68
38	X	309	KC2	CBA-CAA-C2A	-2.79	114.62	125.27
25	G	202	CLA	CHD-C1D-ND	-2.79	121.89	124.45
30	L	307	BCR	C3-C4-C5	-2.79	109.09	114.08
24	X	308	CHL	C2A-C1A-CHA	2.79	128.74	123.86
25	A	843	CLA	CMC-C2C-C1C	2.79	129.29	125.04
25	6	603	CLA	C1C-C2C-C3C	-2.79	104.02	106.96
24	S	307	CHL	CHB-C4A-NA	2.79	128.37	124.51
30	G	201	BCR	C27-C26-C25	-2.79	118.68	122.73
25	W	313	CLA	C1B-CHB-C4A	-2.79	124.59	130.12
25	5	608	CLA	CHD-C1D-ND	-2.79	121.89	124.45
29	X	319	Q6L	C35-C34-C33	2.79	114.92	111.74
25	U	303	CLA	O2D-CGD-O1D	-2.79	118.39	123.84
29	X	301	Q6L	C19-C20-C21	-2.79	117.76	123.47
25	B	820	CLA	O2D-CGD-CBD	2.79	116.22	111.27
25	6	603	CLA	C2D-C1D-ND	-2.79	108.05	110.10
38	T	308	KC2	CAA-C2A-C1A	-2.79	111.93	124.75
25	Q	301	CLA	C2A-C1A-CHA	2.79	128.73	123.86
25	B	831	CLA	CMC-C2C-C1C	2.79	129.28	125.04
24	P	306	CHL	C4-C3-C5	2.79	119.17	115.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	6	609	CLA	CHB-C4A-NA	2.79	128.36	124.51
29	W	316	Q6L	C41-C17-C18	2.79	126.83	122.92
25	W	310	CLA	O2D-CGD-O1D	-2.79	118.39	123.84
25	A	838	CLA	CMB-C2B-C3B	2.78	129.89	124.68
25	Q	311	CLA	CHD-C1D-ND	-2.78	121.89	124.45
25	A	809	CLA	C1-C2-C3	-2.78	122.25	126.75
25	B	836	CLA	CMB-C2B-C3B	2.78	129.89	124.68
25	K	206	CLA	O2D-CGD-O1D	-2.78	118.39	123.84
24	W	305	CHL	C2C-C3C-C4C	2.78	108.47	106.49
25	3	314	CLA	C1B-CHB-C4A	-2.78	124.61	130.12
30	3	317	BCR	C12-C13-C14	-2.78	114.67	118.94
38	P	308	KC2	CAA-C2A-C1A	-2.78	111.96	124.75
25	H	302	CLA	C4-C3-C2	-2.78	116.54	123.68
38	Q	310	KC2	O2A-CGA-O1A	-2.78	116.89	122.67
25	A	828	CLA	C2D-C1D-ND	-2.78	108.06	110.10
25	B	831	CLA	O1D-CGD-CBD	2.78	130.17	124.48
24	6	605	CHL	O2D-CGD-O1D	-2.78	118.40	123.84
24	R	302	CHL	C3C-C4C-NC	-2.78	107.45	110.57
24	W	307	CHL	C1B-CHB-C4A	-2.78	124.61	130.12
25	U	308	CLA	O2D-CGD-O1D	-2.78	118.40	123.84
29	X	317	Q6L	C19-C20-C21	-2.78	117.78	123.47
25	3	307	CLA	C2A-C1A-CHA	2.78	128.72	123.86
25	T	310	CLA	CMB-C2B-C1B	-2.78	124.19	128.46
25	T	310	CLA	O2D-CGD-O1D	-2.78	118.41	123.84
30	L	306	BCR	C3-C4-C5	-2.78	109.12	114.08
29	W	316	Q6L	C19-C20-C21	-2.78	117.78	123.47
25	A	842	CLA	CHB-C4A-NA	2.78	128.35	124.51
25	4	315	CLA	O2D-CGD-O1D	-2.78	118.41	123.84
36	B	850	DGD	O1G-C1A-C2A	2.78	120.62	111.91
25	5	604	CLA	CAB-C3B-C4B	-2.78	124.20	128.46
25	2	612	CLA	CHD-C1D-ND	-2.78	121.90	124.45
30	L	306	BCR	C27-C26-C25	-2.78	118.70	122.73
25	1	609	CLA	CMB-C2B-C1B	-2.77	124.20	128.46
25	O	2001	CLA	C3A-C2A-C1A	2.77	105.50	101.34
25	P	302	CLA	O2D-CGD-CBD	2.77	116.20	111.27
24	4	307	CHL	CAB-C3B-C4B	-2.77	124.20	128.46
25	H	302	CLA	O2D-CGD-O1D	-2.77	118.41	123.84
24	Q	316	CHL	CMB-C2B-C3B	2.77	129.87	124.68
25	B	822	CLA	C1B-CHB-C4A	-2.77	124.62	130.12
25	W	311	CLA	CHB-C4A-NA	2.77	128.35	124.51
24	U	306	CHL	CHB-C4A-NA	2.77	128.34	124.51
25	V	303	CLA	CHB-C4A-NA	2.77	128.34	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	S	311	CLA	C1B-CHB-C4A	-2.77	124.63	130.12
31	B	801	LMG	O1-C1-C2	2.77	112.63	108.30
29	T	316	Q6L	C29-C27-C26	-2.77	114.69	118.94
25	1	609	CLA	C1B-CHB-C4A	-2.77	124.63	130.12
30	L	307	BCR	C28-C27-C26	-2.77	109.13	114.08
24	V	314	CHL	O2D-CGD-O1D	-2.77	118.42	123.84
25	3	301	CLA	CHB-C4A-NA	2.77	128.34	124.51
29	V	319	Q6L	C19-C20-C21	-2.77	117.80	123.47
25	A	828	CLA	CHD-C1D-ND	-2.77	121.91	124.45
30	M	101	BCR	C28-C27-C26	-2.77	109.14	114.08
25	A	812	CLA	CHB-C4A-NA	2.77	128.34	124.51
24	3	306	CHL	C4A-NA-C1A	2.77	107.95	106.71
25	V	302	CLA	O2D-CGD-CBD	2.77	116.18	111.27
25	3	314	CLA	O2D-CGD-O1D	-2.76	117.81	124.09
25	A	837	CLA	C4-C3-C5	2.76	119.92	115.27
25	B	823	CLA	CMB-C2B-C1B	-2.76	124.22	128.46
29	S	323	Q6L	C20-C21-C22	2.76	131.25	127.31
30	3	317	BCR	C8-C7-C6	-2.76	119.44	127.20
25	R	305	CLA	CAA-CBA-CGA	2.76	121.32	113.25
25	1	608	CLA	CHB-C4A-NA	2.76	128.33	124.51
25	1	609	CLA	CHB-C4A-NA	2.76	128.33	124.51
25	A	845	CLA	CHD-C1D-ND	-2.76	121.92	124.45
25	X	313	CLA	CHB-C4A-NA	2.76	128.33	124.51
29	V	319	Q6L	C42-C13-C12	2.76	119.91	115.27
25	X	312	CLA	CMB-C2B-C3B	2.76	129.84	124.68
24	T	304	CHL	CHB-C4A-NA	2.76	128.33	124.51
30	K	202	BCR	C33-C5-C6	2.76	127.62	124.53
25	V	310	CLA	O2D-CGD-O1D	-2.76	118.45	123.84
30	A	849	BCR	C1-C6-C5	-2.76	118.73	122.61
25	S	303	CLA	C1B-CHB-C4A	-2.76	124.66	130.12
37	R	321	NEX	C40-C33-C32	2.76	122.42	118.08
25	A	807	CLA	CHB-C4A-NA	2.75	128.32	124.51
29	P	321	Q6L	C19-C18-C17	-2.75	123.38	127.31
25	B	819	CLA	CHD-C1D-ND	-2.75	121.92	124.45
25	B	823	CLA	CHD-C1D-ND	-2.75	121.92	124.45
38	U	307	KC2	CHB-C4A-C3A	-2.75	120.68	124.98
25	1	606	CLA	O2D-CGD-O1D	-2.75	118.45	123.84
24	X	306	CHL	C1B-CHB-C4A	-2.75	124.66	130.12
25	A	807	CLA	CBC-CAC-C3C	2.75	120.02	112.43
25	3	303	CLA	CMB-C2B-C1B	-2.75	124.23	128.46
25	B	805	CLA	CMB-C2B-C1B	-2.75	124.23	128.46
25	A	804	CLA	O2D-CGD-CBD	2.75	116.16	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	L	302	CLA	C4-C3-C5	2.75	119.90	115.27
27	2	617	XAT	C28-C29-C30	-2.75	114.72	118.94
24	V	307	CHL	C3C-C4C-NC	-2.75	107.49	110.57
30	K	202	BCR	C20-C19-C18	-2.75	118.69	126.42
25	A	820	CLA	C2A-C1A-CHA	2.75	128.67	123.86
25	R	305	CLA	O2D-CGD-O1D	-2.75	118.47	123.84
25	B	813	CLA	C7-C6-C5	-2.75	105.90	113.36
30	B	847	BCR	C37-C22-C23	2.75	122.41	118.08
25	3	307	CLA	C4-C3-C5	2.75	119.89	115.27
24	4	306	CHL	O2D-CGD-O1D	-2.75	117.85	124.09
25	V	313	CLA	O2D-CGD-O1D	-2.75	118.47	123.84
28	3	322	LHG	O7-C7-C8	2.75	117.42	111.50
38	P	308	KC2	CMD-C2D-C3D	2.75	129.81	124.68
25	B	809	CLA	O2D-CGD-O1D	-2.75	118.47	123.84
29	S	323	Q6L	C09-C04-C03	2.75	113.63	109.71
30	A	850	BCR	C19-C18-C17	-2.74	114.73	118.94
24	R	310	CHL	C4A-NA-C1A	2.74	107.94	106.71
25	1	613	CLA	O2D-CGD-O1D	-2.74	118.47	123.84
25	U	301	CLA	C2A-C1A-CHA	2.74	128.66	123.86
30	M	101	BCR	C29-C30-C25	-2.74	106.26	110.48
25	F	803	CLA	C1C-C2C-C3C	-2.74	104.07	106.96
25	L	302	CLA	CMB-C2B-C1B	-2.74	124.25	128.46
25	A	837	CLA	CHB-C4A-NA	2.74	128.31	124.51
25	L	303	CLA	CAA-CBA-CGA	2.74	119.78	112.51
24	X	307	CHL	O2A-CGA-CBA	2.74	120.51	111.91
25	4	305	CLA	C1B-CHB-C4A	-2.74	124.69	130.12
25	V	313	CLA	C1B-CHB-C4A	-2.74	124.69	130.12
25	A	856	CLA	O2D-CGD-CBD	2.74	116.14	111.27
24	Q	309	CHL	O2D-CGD-O1D	-2.74	118.48	123.84
25	1	602	CLA	CAC-C3C-C4C	2.74	128.36	124.81
25	N	202	CLA	O2D-CGD-O1D	-2.74	117.87	124.09
30	A	851	BCR	C39-C30-C25	2.74	114.74	110.30
25	W	303	CLA	CHD-C1D-ND	-2.74	121.94	124.45
25	Q	306	CLA	CBA-CAA-C2A	2.74	121.94	113.86
24	W	305	CHL	C1B-CHB-C4A	-2.74	124.70	130.12
25	6	612	CLA	O2D-CGD-O1D	-2.74	118.49	123.84
25	B	819	CLA	C5-C3-C2	2.73	126.65	121.12
25	B	839	CLA	CMB-C2B-C3B	2.73	129.79	124.68
25	B	828	CLA	C1B-CHB-C4A	-2.73	124.70	130.12
25	F	803	CLA	CHD-C1D-ND	-2.73	121.94	124.45
25	W	301	CLA	CMB-C2B-C1B	-2.73	124.27	128.46
25	S	309	CLA	CBA-CAA-C2A	2.73	121.93	113.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	2	616	Q6L	C29-C27-C26	-2.73	114.75	118.94
38	X	309	KC2	CAA-CBA-CGA	-2.73	113.23	127.26
25	5	604	CLA	CHD-C1D-ND	-2.73	121.95	124.45
30	3	317	BCR	C20-C21-C22	-2.73	123.42	127.31
30	4	319	BCR	C39-C30-C25	-2.73	105.88	110.30
25	A	820	CLA	CMB-C2B-C1B	-2.73	124.27	128.46
37	P	317	NEX	C12-C13-C14	-2.73	114.76	118.94
25	X	311	CLA	O2D-CGD-O1D	-2.73	118.51	123.84
25	Q	314	CLA	CHB-C4A-NA	2.73	128.28	124.51
25	X	314	CLA	CHD-C1D-ND	-2.73	121.95	124.45
25	U	312	CLA	CMB-C2B-C3B	2.73	129.78	124.68
37	T	317	NEX	C11-C10-C9	-2.73	123.42	127.31
25	P	302	CLA	CHD-C1D-ND	-2.73	121.95	124.45
25	R	306	CLA	CHD-C1D-ND	-2.73	121.95	124.45
25	R	315	CLA	O2A-CGA-O1A	-2.73	116.71	123.59
25	L	303	CLA	C4A-NA-C1A	2.72	107.93	106.71
30	B	848	BCR	C3-C4-C5	-2.72	109.21	114.08
25	2	612	CLA	C4-C3-C5	2.72	119.85	115.27
25	A	804	CLA	C2D-C1D-ND	-2.72	108.10	110.10
25	A	836	CLA	O2A-C1-C2	-2.72	101.48	108.64
25	B	826	CLA	O2D-CGD-O1D	-2.72	118.52	123.84
25	3	307	CLA	CBA-CAA-C2A	2.72	121.89	113.86
24	1	604	CHL	C2D-C1D-ND	-2.72	108.10	110.10
25	3	313	CLA	CMB-C2B-C3B	2.72	129.77	124.68
25	B	813	CLA	C5-C3-C2	2.72	126.62	121.12
25	O	2001	CLA	C5-C3-C2	2.72	126.62	121.12
25	5	606	CLA	CHB-C4A-NA	2.72	128.27	124.51
25	S	310	CLA	O2D-CGD-CBD	2.72	116.10	111.27
30	K	205	BCR	C16-C15-C14	-2.72	117.90	123.47
25	V	302	CLA	CMB-C2B-C3B	2.72	129.76	124.68
24	2	615	CHL	O2D-CGD-O1D	-2.72	118.52	123.84
25	O	2004	CLA	O2D-CGD-O1D	-2.72	118.52	123.84
25	6	609	CLA	O2A-CGA-O1A	-2.72	116.52	123.30
24	S	314	CHL	C1C-C2C-C3C	-2.72	104.96	107.11
25	W	302	CLA	CHB-C4A-NA	2.72	128.27	124.51
30	L	307	BCR	C12-C13-C14	-2.72	114.77	118.94
30	I	101	BCR	C15-C16-C17	-2.72	117.91	123.47
25	R	307	CLA	CHB-C4A-NA	2.72	128.27	124.51
25	A	823	CLA	C5-C3-C2	2.72	126.61	121.12
25	2	604	CLA	CHD-C1D-ND	-2.72	121.96	124.45
25	2	608	CLA	C4A-NA-C1A	2.72	107.93	106.71
30	A	848	BCR	C33-C5-C4	-2.72	108.40	113.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	3	310	CLA	CHB-C4A-NA	2.72	128.27	124.51
25	X	313	CLA	O2D-CGD-O1D	-2.71	118.53	123.84
25	S	301	CLA	CMD-C2D-C3D	2.71	133.86	127.61
27	4	318	XAT	C20-C13-C14	2.71	126.72	122.92
24	T	307	CHL	CHB-C4A-NA	2.71	128.26	124.51
25	A	818	CLA	CHB-C4A-NA	2.71	128.26	124.51
27	1	612	XAT	C37-C21-C36	-2.71	103.37	107.37
25	F	803	CLA	CMB-C2B-C1B	-2.71	124.29	128.46
25	A	825	CLA	CAC-C3C-C2C	-2.71	122.89	127.53
25	A	835	CLA	O2D-CGD-O1D	-2.71	118.53	123.84
25	B	842	CLA	CHD-C1D-ND	-2.71	121.96	124.45
24	V	304	CHL	O2D-CGD-O1D	-2.71	118.54	123.84
25	A	811	CLA	C1B-CHB-C4A	-2.71	124.75	130.12
38	W	308	KC2	CAA-CBA-CGA	-2.71	113.34	127.26
25	B	807	CLA	O2D-CGD-O1D	-2.71	118.54	123.84
24	W	304	CHL	CHB-C4A-NA	2.71	128.26	124.51
24	1	604	CHL	CMB-C2B-C3B	2.71	129.75	124.68
25	B	831	CLA	CHB-C4A-NA	2.71	128.26	124.51
25	6	604	CLA	CHD-C1D-ND	-2.71	121.97	124.45
24	P	304	CHL	O2D-CGD-O1D	-2.71	118.55	123.84
24	P	314	CHL	O2D-CGD-O1D	-2.71	118.55	123.84
25	N	203	CLA	C2C-C1C-NC	2.70	112.51	109.97
24	4	302	CHL	C2C-C3C-C4C	2.70	108.42	106.49
30	A	849	BCR	C15-C16-C17	-2.70	117.93	123.47
25	4	305	CLA	CHD-C1D-ND	-2.70	121.97	124.45
25	B	826	CLA	CHB-C4A-NA	2.70	128.25	124.51
26	V	318	IWJ	O27-C26-C28	-2.70	116.17	121.66
25	W	311	CLA	O2D-CGD-O1D	-2.70	118.55	123.84
25	W	312	CLA	C4-C3-C5	2.70	119.82	115.27
30	G	205	BCR	C35-C13-C12	2.70	122.33	118.08
25	R	307	CLA	O2D-CGD-O1D	-2.70	118.56	123.84
25	S	311	CLA	CED-O2D-CGD	2.70	122.05	115.94
25	B	820	CLA	C2D-C1D-ND	-2.70	108.11	110.10
30	F	801	BCR	C16-C15-C14	-2.70	117.94	123.47
30	J	103	BCR	C8-C9-C10	-2.70	114.80	118.94
25	H	301	CLA	O2D-CGD-O1D	-2.70	118.56	123.84
24	P	304	CHL	CHB-C4A-NA	2.70	128.25	124.51
25	2	602	CLA	CHB-C4A-NA	2.70	128.25	124.51
26	1	611	IWJ	C32-C30-C31	2.70	126.44	121.10
30	K	207	BCR	C20-C21-C22	-2.70	123.46	127.31
30	F	804	BCR	C12-C13-C14	2.70	123.08	118.94
25	T	302	CLA	C1B-CHB-C4A	-2.70	124.77	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	4	319	BCR	C16-C15-C14	-2.70	117.94	123.47
25	1	610	CLA	CMB-C2B-C3B	2.70	129.97	124.69
24	V	306	CHL	C2D-C1D-ND	-2.70	108.11	110.10
25	2	606	CLA	CHB-C4A-NA	2.70	128.24	124.51
34	B	844	PQN	O1-C1-C2	-2.70	116.75	120.25
25	R	315	CLA	O2D-CGD-CBD	2.70	116.06	111.27
38	V	308	KC2	CMD-C2D-C3D	2.70	129.73	124.68
25	A	856	CLA	C3A-C2A-C1A	2.70	105.38	101.34
25	S	311	CLA	O2D-CGD-O1D	-2.70	118.56	123.84
25	T	310	CLA	C1B-CHB-C4A	-2.70	124.78	130.12
24	U	304	CHL	O2D-CGD-O1D	-2.70	118.56	123.84
24	Q	308	CHL	C1C-C2C-C3C	-2.70	104.97	107.11
25	R	313	CLA	O2D-CGD-O1D	-2.69	118.57	123.84
27	4	318	XAT	C38-C25-C26	-2.69	117.75	122.26
25	W	303	CLA	CED-O2D-CGD	-2.69	109.84	115.94
29	W	319	Q6L	C05-C06-C07	2.69	113.99	110.30
25	6	603	CLA	C1B-CHB-C4A	-2.69	124.78	130.12
25	1	603	CLA	CHA-C1A-NA	-2.69	120.23	126.40
25	6	603	CLA	C4A-NA-C1A	2.69	107.92	106.71
25	B	820	CLA	C4A-NA-C1A	2.69	107.92	106.71
25	B	804	CLA	O2D-CGD-O1D	-2.69	118.58	123.84
32	H	303	SQD	O7-S-C6	2.69	110.14	106.94
25	R	315	CLA	CMB-C2B-C3B	2.69	129.71	124.68
30	3	318	BCR	C33-C5-C4	-2.69	108.45	113.62
25	3	308	CLA	C1B-CHB-C4A	-2.69	124.79	130.12
25	R	305	CLA	CMC-C2C-C1C	2.69	129.13	125.04
25	O	2002	CLA	CHB-C4A-NA	2.69	128.23	124.51
27	5	612	XAT	C37-C21-C36	-2.69	103.41	107.37
25	R	305	CLA	CMB-C2B-C3B	2.69	129.70	124.68
25	B	805	CLA	O2D-CGD-O1D	-2.69	118.59	123.84
25	W	310	CLA	CHB-C4A-NA	2.69	128.22	124.51
30	4	319	BCR	C16-C17-C18	-2.69	123.48	127.31
25	3	313	CLA	CED-O2D-CGD	2.68	122.01	115.94
25	4	310	CLA	CHD-C1D-ND	-2.68	121.99	124.45
26	S	318	IWJ	C17-C16-C15	-2.68	117.97	123.47
29	W	319	Q6L	C42-C13-C12	2.68	119.79	115.27
24	Q	308	CHL	C2C-C3C-C4C	2.68	108.40	106.49
25	B	809	CLA	C6-C7-C8	2.68	124.59	115.92
25	2	610	CLA	CMB-C2B-C3B	2.68	129.70	124.68
25	1	609	CLA	CMA-C3A-C2A	-2.68	109.84	116.10
25	V	310	CLA	C4A-NA-C1A	2.68	107.91	106.71
25	B	827	CLA	C2A-C1A-CHA	2.68	128.55	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	V	308	KC2	O2A-CGA-O1A	-2.68	117.10	122.67
30	K	205	BCR	C4-C5-C6	-2.68	118.84	122.73
25	L	304	CLA	C1B-CHB-C4A	-2.68	124.81	130.12
25	B	826	CLA	C6-C5-C3	-2.68	106.43	113.45
24	P	306	CHL	O2D-CGD-O1D	-2.68	118.60	123.84
27	5	612	XAT	C38-C25-C24	2.68	117.29	114.28
24	4	302	CHL	C1B-CHB-C4A	-2.68	124.81	130.12
30	L	306	BCR	C15-C16-C17	-2.68	117.99	123.47
30	A	848	BCR	C40-C30-C39	-2.68	100.32	108.53
25	R	307	CLA	C1B-CHB-C4A	-2.67	124.82	130.12
37	S	317	NEX	C25-C24-C23	2.67	118.04	112.75
25	A	809	CLA	CHB-C4A-NA	2.67	128.21	124.51
24	R	311	CHL	C1B-CHB-C4A	-2.67	124.82	130.12
38	T	308	KC2	O1A-CGA-CBA	2.67	129.34	120.99
24	X	315	CHL	O2D-CGD-O1D	-2.67	118.61	123.84
25	B	829	CLA	O2D-CGD-O1D	-2.67	118.61	123.84
27	6	615	XAT	O24-C25-C38	2.67	118.26	115.06
25	B	826	CLA	C4D-CHA-C1A	2.67	124.50	121.25
25	3	303	CLA	CAB-C3B-C2B	2.67	129.92	124.69
30	3	317	BCR	C16-C15-C14	-2.67	118.00	123.47
24	W	305	CHL	CMA-C3A-C2A	-2.67	109.87	116.10
38	Q	310	KC2	C3A-C4A-NA	2.67	113.49	110.57
25	F	802	CLA	C1B-CHB-C4A	-2.67	124.83	130.12
25	5	604	CLA	O2D-CGD-O1D	-2.67	118.03	124.09
30	A	848	BCR	C11-C10-C9	-2.67	123.50	127.31
24	Q	307	CHL	O2D-CGD-CBD	2.67	116.00	111.27
25	U	312	CLA	C1B-CHB-C4A	-2.67	124.84	130.12
25	K	206	CLA	C1B-CHB-C4A	-2.66	124.84	130.12
24	R	309	CHL	O2A-CGA-O1A	-2.66	116.87	123.59
24	Q	316	CHL	CHB-C4A-NA	2.66	128.19	124.51
25	5	601	CLA	CMB-C2B-C1B	-2.66	124.37	128.46
25	R	314	CLA	CHD-C1D-ND	-2.66	122.01	124.45
25	W	302	CLA	CHD-C1D-ND	-2.66	122.01	124.45
30	J	101	BCR	C34-C9-C8	-2.66	113.89	118.08
36	A	854	DGD	O5E-C6E-C5E	-2.66	102.17	111.29
38	R	312	KC2	O1A-CGA-CBA	2.66	129.29	120.99
25	3	309	CLA	CMB-C2B-C3B	2.66	129.65	124.68
25	A	821	CLA	O2D-CGD-CBD	2.66	115.99	111.27
25	S	310	CLA	CHD-C1D-ND	-2.66	122.01	124.45
25	X	303	CLA	CHD-C1D-ND	-2.66	122.01	124.45
25	Q	312	CLA	C4A-NA-C1A	2.66	107.90	106.71
25	2	612	CLA	CMB-C2B-C3B	2.65	129.65	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	843	CLA	CMB-C2B-C3B	2.65	129.65	124.68
38	W	308	KC2	CMC-C2C-C3C	-2.65	121.80	128.30
25	W	301	CLA	C4-C3-C5	2.65	119.73	115.27
25	A	805	CLA	C2D-C1D-ND	-2.65	108.15	110.10
25	W	312	CLA	CBC-CAC-C3C	2.65	119.74	112.43
24	5	605	CHL	O2D-CGD-O1D	-2.65	118.07	124.09
26	W	318	IWJ	C21-C19-C18	-2.65	114.88	118.94
25	X	310	CLA	CHB-C4A-NA	2.65	128.18	124.51
24	V	306	CHL	O2D-CGD-CBD	2.65	115.97	111.27
25	S	312	CLA	CMB-C2B-C1B	-2.65	124.39	128.46
38	P	308	KC2	CMD-C2D-C1D	-2.65	124.39	128.46
24	T	305	CHL	C2A-C1A-CHA	2.65	128.49	123.86
30	4	319	BCR	C20-C21-C22	-2.65	123.53	127.31
29	P	316	Q6L	C01-C02-C07	-2.65	109.45	114.36
30	H	305	BCR	C36-C18-C19	2.65	122.25	118.08
25	P	311	CLA	C4-C3-C5	2.65	119.72	115.27
29	O	2006	Q6L	C35-C34-C33	2.65	114.75	111.74
29	W	315	Q6L	C42-C13-C12	2.65	119.72	115.27
38	X	309	KC2	CAC-C3C-C2C	-2.65	119.89	128.60
25	1	602	CLA	C1B-CHB-C4A	-2.65	124.88	130.12
27	6	615	XAT	C36-C21-C26	2.64	117.19	110.05
26	Q	320	IWJ	O27-C26-C28	-2.64	116.29	121.66
25	T	301	CLA	C5-C3-C2	-2.64	115.77	121.12
24	P	305	CHL	C1C-C2C-C3C	-2.64	105.02	107.11
25	2	611	CLA	O2A-CGA-O1A	-2.64	116.71	123.30
30	K	205	BCR	C20-C21-C22	-2.64	123.54	127.31
38	R	312	KC2	C4C-C3C-C2C	-2.64	105.02	107.11
38	R	312	KC2	CAA-C2A-C1A	-2.64	112.62	124.75
25	6	613	CLA	C2D-C1D-ND	-2.64	108.16	110.10
25	R	317	CLA	CHB-C4A-NA	2.64	128.16	124.51
27	4	318	XAT	C15-C35-C34	-2.64	118.07	123.47
25	B	803	CLA	C4D-C3D-CAD	-2.64	104.99	108.10
27	5	612	XAT	O24-C25-C38	2.64	118.22	115.06
25	O	2001	CLA	C1B-CHB-C4A	-2.64	124.90	130.12
30	K	205	BCR	C35-C13-C12	2.64	122.23	118.08
25	2	611	CLA	CHD-C1D-ND	-2.64	122.03	124.45
29	V	315	Q6L	C24-C22-C21	-2.64	114.90	118.94
31	2	620	LMG	O8-C28-C29	2.63	120.17	111.91
24	R	302	CHL	CMB-C2B-C3B	2.63	129.61	124.68
25	W	312	CLA	CHB-C4A-NA	2.63	128.15	124.51
25	1	606	CLA	CMB-C2B-C3B	2.63	129.84	124.69
25	P	313	CLA	O2D-CGD-O1D	-2.63	118.69	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	B	808	CLA	CHD-C1D-ND	-2.63	122.03	124.45
25	K	204	CLA	C1B-CHB-C4A	-2.63	124.90	130.12
25	P	313	CLA	CAA-C2A-C3A	-2.63	105.57	112.78
24	W	307	CHL	C4-C3-C2	-2.63	116.92	123.68
25	P	312	CLA	CHB-C4A-NA	2.63	128.15	124.51
25	B	805	CLA	O2D-CGD-CBD	2.63	115.94	111.27
29	S	320	Q6L	C37-C36-C35	-2.63	104.45	109.44
25	A	841	CLA	C1B-CHB-C4A	-2.63	124.91	130.12
29	T	316	Q6L	C01-C02-C07	-2.63	109.48	114.36
24	P	307	CHL	O2D-CGD-O1D	-2.63	118.70	123.84
24	V	307	CHL	CHD-C1D-ND	-2.63	122.04	124.45
30	B	846	BCR	C16-C15-C14	-2.63	118.09	123.47
24	T	306	CHL	C3A-C2A-C1A	2.63	105.28	101.34
25	V	309	CLA	CHB-C4A-NA	2.63	128.15	124.51
26	4	317	IWJ	C32-C30-C31	2.63	126.29	121.10
25	2	608	CLA	C1B-CHB-C4A	-2.63	124.91	130.12
25	A	805	CLA	O2A-CGA-O1A	-2.63	116.96	123.59
24	V	314	CHL	C1D-CHD-C4C	-2.63	120.39	126.06
27	3	316	XAT	C12-C13-C14	-2.63	114.91	118.94
30	B	849	BCR	C12-C13-C14	-2.63	114.91	118.94
24	U	313	CHL	CHB-C4A-NA	2.63	128.14	124.51
27	1	612	XAT	C35-C34-C33	-2.62	123.56	127.31
25	K	206	CLA	C6-C5-C3	2.62	120.33	113.45
25	T	312	CLA	CHB-C4A-NA	2.62	128.14	124.51
25	A	812	CLA	CHD-C1D-ND	-2.62	122.05	124.45
25	4	310	CLA	C1-C2-C3	2.62	130.58	126.04
25	A	839	CLA	C1-C2-C3	-2.62	121.51	126.04
25	6	607	CLA	O2D-CGD-O1D	-2.62	118.72	123.84
25	B	827	CLA	C1B-CHB-C4A	-2.62	124.93	130.12
24	S	305	CHL	O2D-CGD-O1D	-2.62	118.72	123.84
25	A	835	CLA	O2D-CGD-CBD	2.62	115.92	111.27
26	V	318	IWJ	C22-C21-C19	2.62	133.77	126.42
25	O	2004	CLA	CMA-C3A-C2A	-2.62	109.99	116.10
25	A	826	CLA	O2D-CGD-O1D	-2.62	118.72	123.84
29	S	323	Q6L	C04-C05-C06	-2.62	107.73	113.64
25	5	607	CLA	CMB-C2B-C3B	2.62	129.58	124.68
25	B	803	CLA	OBD-CAD-C3D	2.62	134.82	128.52
25	S	313	CLA	CMB-C2B-C3B	2.62	129.58	124.68
25	B	839	CLA	CHB-C4A-NA	2.62	128.13	124.51
30	B	847	BCR	C34-C9-C10	2.62	126.59	122.92
27	6	615	XAT	C31-C30-C29	-2.62	123.58	127.31
25	T	302	CLA	CMB-C2B-C3B	2.62	129.57	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	F	805	LMG	O1-C1-C2	2.62	112.39	108.30
25	X	303	CLA	C4A-NA-C1A	2.62	107.88	106.71
25	B	817	CLA	CHD-C1D-ND	-2.61	122.05	124.45
25	L	303	CLA	CHA-C1A-NA	-2.61	120.41	126.40
25	3	302	CLA	CMC-C2C-C1C	2.61	129.02	125.04
25	K	201	CLA	CHD-C1D-ND	-2.61	122.05	124.45
27	3	316	XAT	C15-C14-C13	-2.61	123.58	127.31
30	B	847	BCR	C8-C9-C10	-2.61	114.94	118.94
25	F	802	CLA	CBC-CAC-C3C	2.61	119.62	112.43
25	2	611	CLA	O2D-CGD-O1D	-2.61	118.17	124.09
25	W	309	CLA	CHB-C4A-NA	2.61	128.12	124.51
30	B	845	BCR	C8-C9-C10	-2.61	114.94	118.94
24	S	306	CHL	CMD-C2D-C1D	2.61	129.31	124.71
25	R	316	CLA	C1B-CHB-C4A	-2.61	124.95	130.12
24	X	305	CHL	O2D-CGD-O1D	-2.61	118.74	123.84
24	U	313	CHL	C1C-C2C-C3C	-2.61	105.05	107.11
25	Q	314	CLA	CMB-C2B-C1B	-2.61	124.46	128.46
25	T	309	CLA	CHB-C4A-NA	2.60	128.11	124.51
25	A	813	CLA	CMB-C2B-C3B	2.60	129.55	124.68
25	A	807	CLA	CHD-C1D-ND	-2.60	122.06	124.45
25	A	810	CLA	C4-C3-C5	2.60	119.65	115.27
30	H	305	BCR	C12-C13-C14	-2.60	114.95	118.94
25	Q	315	CLA	CHB-C4A-NA	2.60	128.11	124.51
25	Q	314	CLA	CBA-CAA-C2A	2.60	121.54	113.86
25	4	313	CLA	CMB-C2B-C3B	2.60	129.54	124.68
24	W	307	CHL	C1-C2-C3	-2.60	121.54	126.04
30	B	849	BCR	C30-C25-C26	-2.60	118.95	122.61
24	2	607	CHL	OMC-CMC-C2C	-2.60	119.81	125.69
25	3	301	CLA	CHD-C1D-ND	-2.60	122.06	124.45
25	2	613	CLA	O2D-CGD-O1D	-2.60	118.19	124.09
25	V	310	CLA	CMB-C2B-C3B	2.60	129.54	124.68
25	4	311	CLA	CHD-C1D-ND	-2.60	122.07	124.45
25	Q	301	CLA	C6-C5-C3	2.60	120.26	113.45
26	T	318	IWJ	C16-C17-C18	-2.60	118.16	123.47
24	U	306	CHL	CMB-C2B-C3B	2.60	129.53	124.68
25	5	602	CLA	CBC-CAC-C3C	2.60	119.59	112.43
25	2	603	CLA	CHD-C1D-ND	-2.60	122.07	124.45
25	4	304	CLA	CMB-C2B-C3B	2.59	129.77	124.69
25	X	302	CLA	CHB-C4A-NA	2.59	128.10	124.51
30	J	103	BCR	C15-C16-C17	-2.59	118.16	123.47
37	R	321	NEX	C20-C13-C12	2.59	122.17	118.08
30	M	101	BCR	C38-C26-C27	2.59	118.60	113.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	Q	315	CLA	CHD-C1D-ND	-2.59	122.07	124.45
25	B	813	CLA	C11-C10-C8	2.59	124.30	115.92
25	N	202	CLA	CHB-C4A-NA	2.59	128.10	124.51
38	R	312	KC2	C2A-C3A-C4A	-2.59	104.56	106.49
25	2	612	CLA	C2A-C1A-CHA	2.59	128.39	123.86
24	T	314	CHL	CHB-C4A-NA	2.59	128.10	124.51
25	A	830	CLA	C6-C5-C3	-2.59	106.66	113.45
25	W	303	CLA	C4A-NA-C1A	2.59	107.87	106.71
25	2	603	CLA	CMB-C2B-C3B	2.59	129.53	124.68
25	T	313	CLA	CMB-C2B-C3B	2.59	129.53	124.68
25	U	302	CLA	CHB-C4A-NA	2.59	128.09	124.51
24	X	306	CHL	CAA-C2A-C3A	-2.59	110.05	116.10
38	X	309	KC2	O1A-CGA-CBA	2.59	129.08	120.99
30	L	306	BCR	C8-C7-C6	-2.59	119.93	127.20
24	S	306	CHL	CHD-C4C-NC	-2.59	120.13	124.20
25	A	824	CLA	C1C-C2C-C3C	-2.59	104.23	106.96
25	A	807	CLA	O2D-CGD-O1D	-2.59	118.78	123.84
25	P	313	CLA	CMB-C2B-C3B	2.59	129.52	124.68
25	F	802	CLA	CMB-C2B-C3B	2.59	129.52	124.68
25	P	311	CLA	CHB-C4A-NA	2.59	128.09	124.51
25	B	840	CLA	CHD-C1D-ND	-2.59	122.08	124.45
25	N	202	CLA	C1B-CHB-C4A	-2.59	124.99	130.12
25	A	834	CLA	CHB-C4A-NA	2.59	128.09	124.51
33	A	802	CL0	C1C-C2C-C3C	-2.59	104.24	106.96
25	3	304	CLA	O2D-CGD-O1D	-2.59	118.22	124.09
24	P	305	CHL	CHB-C4A-NA	2.59	128.09	124.51
25	B	810	CLA	C1B-CHB-C4A	-2.59	125.00	130.12
24	T	314	CHL	C4A-NA-C1A	2.58	107.87	106.71
25	1	605	CLA	O2D-CGD-O1D	-2.58	118.22	124.09
25	B	828	CLA	O2D-CGD-O1D	-2.58	118.79	123.84
30	M	101	BCR	C37-C22-C23	2.58	122.15	118.08
25	A	834	CLA	CHD-C1D-ND	-2.58	122.08	124.45
25	R	313	CLA	C1D-ND-C4D	-2.58	104.50	106.33
25	X	304	CLA	C1B-CHB-C4A	-2.58	125.00	130.12
30	A	851	BCR	C32-C1-C6	2.58	114.48	110.30
25	R	315	CLA	CHB-C4A-NA	2.58	128.08	124.51
38	R	312	KC2	CAA-CBA-CGA	-2.58	114.01	127.26
38	U	307	KC2	CAA-CBA-CGA	-2.58	114.01	127.26
24	U	304	CHL	CHB-C4A-NA	2.58	128.08	124.51
25	U	301	CLA	O2D-CGD-O1D	-2.58	118.80	123.84
25	Q	306	CLA	CGD-CBD-CAD	-2.58	102.39	110.73
37	S	317	NEX	C15-C14-C13	-2.58	123.63	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	W	306	CHL	C1-C2-C3	-2.58	121.59	126.04
25	S	310	CLA	C1-C2-C3	-2.58	121.59	126.04
30	F	801	BCR	C35-C13-C12	2.57	122.13	118.08
25	2	608	CLA	CHD-C1D-ND	-2.57	122.09	124.45
38	P	308	KC2	CHB-C4A-C3A	-2.57	120.96	124.98
29	V	321	Q6L	C01-C02-C07	-2.57	109.59	114.36
25	J	102	CLA	CMC-C2C-C1C	2.57	128.96	125.04
29	W	315	Q6L	C12-C13-C14	-2.57	114.19	121.98
25	3	305	CLA	CAB-C3B-C2B	2.57	129.72	124.69
29	X	319	Q6L	C01-C02-C07	-2.57	109.59	114.36
32	H	303	SQD	O48-C23-C24	2.57	119.97	111.91
25	B	842	CLA	C2D-C1D-ND	-2.57	108.21	110.10
25	S	313	CLA	C1B-CHB-C4A	-2.57	125.03	130.12
30	4	319	BCR	C19-C18-C17	-2.57	115.00	118.94
24	P	314	CHL	C1C-C2C-C3C	-2.57	105.08	107.11
24	1	604	CHL	CAC-C3C-C4C	2.57	128.14	124.81
24	4	302	CHL	CMB-C2B-C1B	-2.57	124.52	128.46
24	1	601	CHL	CBA-CAA-C2A	2.57	121.44	113.86
29	S	316	Q6L	C19-C20-C21	-2.57	118.21	123.47
30	3	317	BCR	C2-C3-C4	-2.57	105.64	111.38
25	U	302	CLA	O2D-CGD-O1D	-2.57	118.82	123.84
27	5	612	XAT	C28-C29-C30	-2.57	115.00	118.94
30	I	101	BCR	C23-C22-C21	-2.57	115.00	118.94
31	A	855	LMG	O6-C5-C4	2.57	114.35	109.69
25	A	814	CLA	CHD-C1D-ND	-2.57	122.10	124.45
25	B	834	CLA	C1C-C2C-C3C	-2.57	104.26	106.96
25	B	837	CLA	C1C-C2C-C3C	-2.57	104.26	106.96
24	4	302	CHL	C2D-C1D-ND	-2.56	108.21	110.10
25	A	824	CLA	O2D-CGD-O1D	-2.56	118.83	123.84
25	B	821	CLA	C4-C3-C5	2.56	119.58	115.27
29	R	323	Q6L	C10-C04-C03	-2.56	106.05	109.71
25	3	302	CLA	C5-C3-C2	2.56	126.30	121.12
30	L	305	BCR	C38-C26-C27	2.56	118.54	113.62
36	B	850	DGD	O2G-C1B-C2B	2.56	117.02	111.50
30	L	305	BCR	C24-C23-C22	-2.56	122.36	126.23
25	A	835	CLA	CMB-C2B-C1B	-2.56	124.53	128.46
25	B	834	CLA	CMB-C2B-C3B	2.56	129.47	124.68
27	2	617	XAT	C35-C15-C14	-2.56	118.23	123.47
25	5	606	CLA	CMB-C2B-C3B	2.56	129.70	124.69
25	S	312	CLA	CHB-C4A-NA	2.56	128.05	124.51
25	R	316	CLA	O2D-CGD-O1D	-2.56	118.83	123.84
26	P	320	IWJ	C25-C24-C26	2.56	120.32	116.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	P	308	KC2	CAA-CBA-CGA	-2.56	114.11	127.26
38	X	309	KC2	C4C-C3C-C2C	-2.56	105.08	107.11
25	V	311	CLA	C1B-CHB-C4A	-2.56	125.05	130.12
25	5	607	CLA	CHB-C4A-NA	2.56	128.05	124.51
30	3	319	BCR	C15-C14-C13	-2.56	123.66	127.31
25	1	609	CLA	O2D-CGD-O1D	-2.56	118.28	124.09
25	J	102	CLA	O2D-CGD-O1D	-2.56	118.84	123.84
25	Q	301	CLA	CMB-C2B-C3B	2.56	129.46	124.68
37	W	317	NEX	C31-C30-C29	-2.55	123.66	127.31
38	W	308	KC2	O1A-CGA-CBA	2.55	128.97	120.99
24	3	306	CHL	C3C-C4C-NC	-2.55	107.71	110.57
25	R	305	CLA	CMB-C2B-C1B	-2.55	124.54	128.46
25	B	832	CLA	CAC-C3C-C4C	2.55	128.12	124.81
25	B	823	CLA	O1D-CGD-CBD	2.55	129.71	124.48
30	K	205	BCR	C1-C6-C5	2.55	126.21	122.61
25	2	609	CLA	CMB-C2B-C1B	-2.55	124.54	128.46
29	S	323	Q6L	C19-C18-C17	-2.55	123.67	127.31
25	1	608	CLA	CMB-C2B-C1B	-2.55	124.54	128.46
25	B	829	CLA	O2D-CGD-CBD	2.55	115.80	111.27
25	3	312	CLA	CAA-C2A-C3A	-2.55	110.15	116.10
30	K	205	BCR	C11-C10-C9	-2.55	123.67	127.31
25	B	818	CLA	C6-C5-C3	2.55	120.14	113.45
24	T	305	CHL	CAA-C2A-C1A	2.55	120.33	111.97
25	A	840	CLA	CHB-C4A-NA	2.55	128.04	124.51
38	R	312	KC2	C3C-C2C-C1C	2.55	108.38	106.49
25	W	312	CLA	C2C-C1C-NC	2.55	112.36	109.97
25	A	827	CLA	C2A-C1A-CHA	2.55	128.31	123.86
25	T	303	CLA	CHB-C4A-NA	2.55	128.03	124.51
25	K	203	CLA	CHD-C1D-ND	-2.55	122.11	124.45
25	2	603	CLA	O2D-CGD-O1D	-2.55	118.31	124.09
29	2	616	Q6L	C25-C26-C27	2.55	130.94	127.31
25	2	613	CLA	CHB-C4A-NA	2.55	128.03	124.51
25	X	310	CLA	CHD-C1D-ND	-2.55	122.11	124.45
25	R	314	CLA	O2A-CGA-O1A	-2.55	117.17	123.59
25	B	840	CLA	O2D-CGD-O1D	-2.55	118.86	123.84
30	H	305	BCR	C23-C22-C21	-2.55	115.03	118.94
25	B	802	CLA	CAC-C3C-C4C	2.54	128.11	124.81
30	A	851	BCR	C20-C21-C22	-2.54	123.68	127.31
25	3	305	CLA	CHD-C1D-ND	-2.54	122.12	124.45
34	B	844	PQN	C2M-C2-C3	2.54	128.55	124.40
25	T	309	CLA	C1B-CHB-C4A	-2.54	125.08	130.12
25	S	303	CLA	CHB-C4A-NA	2.54	128.03	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	X	302	CLA	O2A-CGA-O1A	-2.54	117.18	123.59
26	P	320	IWJ	C21-C19-C18	-2.54	115.04	118.94
25	W	313	CLA	CHD-C1D-ND	-2.54	122.12	124.45
25	S	310	CLA	CHB-C4A-NA	2.54	128.03	124.51
30	I	101	BCR	C16-C15-C14	-2.54	118.27	123.47
30	J	103	BCR	C40-C30-C25	2.54	114.42	110.30
24	V	307	CHL	C1C-C2C-C3C	-2.54	105.10	107.11
27	2	617	XAT	C6-C7-C8	-2.54	120.62	125.99
25	R	316	CLA	CHD-C1D-ND	-2.54	122.12	124.45
25	V	309	CLA	CMC-C2C-C3C	-2.54	119.23	126.12
33	A	802	CL0	C2C-C1C-NC	2.54	112.35	109.97
25	P	311	CLA	C1B-CHB-C4A	-2.54	125.09	130.12
30	2	618	BCR	C27-C26-C25	-2.54	119.05	122.73
25	4	304	CLA	C1B-CHB-C4A	-2.54	125.09	130.12
25	2	610	CLA	CHB-C4A-NA	2.54	128.02	124.51
25	V	310	CLA	CHB-C4A-NA	2.53	128.02	124.51
25	B	821	CLA	CMB-C2B-C3B	2.53	129.42	124.68
24	X	305	CHL	CHD-C1D-ND	-2.53	122.12	124.45
25	P	311	CLA	CHD-C1D-ND	-2.53	122.12	124.45
25	1	608	CLA	CAC-C3C-C4C	2.53	128.10	124.81
24	6	601	CHL	O2D-CGD-O1D	-2.53	118.88	123.84
25	A	806	CLA	O2A-CGA-CBA	-2.53	103.95	111.91
25	B	838	CLA	O2D-CGD-O1D	-2.53	118.89	123.84
24	1	601	CHL	CHB-C4A-NA	2.53	128.01	124.51
37	R	321	NEX	C12-C13-C14	-2.53	115.05	118.94
25	S	309	CLA	O2D-CGD-CBD	2.53	115.77	111.27
30	B	849	BCR	C23-C24-C25	-2.53	120.09	127.20
25	2	611	CLA	CHB-C4A-NA	2.53	128.01	124.51
24	S	307	CHL	O2D-CGD-O1D	-2.53	118.89	123.84
25	G	202	CLA	O2A-CGA-O1A	-2.53	116.99	123.30
29	V	315	Q6L	C35-C34-C33	2.53	114.62	111.74
29	T	316	Q6L	C26-C25-C24	-2.53	115.32	123.22
24	X	305	CHL	C4A-NA-C1A	2.53	107.84	106.71
30	A	848	BCR	C16-C17-C18	-2.53	123.70	127.31
25	A	837	CLA	C6-C7-C8	2.53	124.09	115.92
24	R	309	CHL	C1B-CHB-C4A	-2.53	125.11	130.12
30	G	205	BCR	C10-C11-C12	2.53	131.10	123.22
24	P	304	CHL	CBA-CAA-C2A	2.53	121.32	113.86
29	U	314	Q6L	C12-C13-C14	-2.53	114.33	121.98
25	B	832	CLA	CHA-C1A-NA	-2.53	120.61	126.40
29	S	320	Q6L	C42-C13-C12	2.53	119.52	115.27
25	3	312	CLA	O2D-CGD-O1D	-2.52	118.36	124.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	4	303	CLA	O1D-CGD-CBD	2.52	129.65	124.48
24	T	306	CHL	O2D-CGD-O1D	-2.52	118.90	123.84
25	F	802	CLA	O2D-CGD-O1D	-2.52	118.90	123.84
25	B	832	CLA	O2D-CGD-O1D	-2.52	118.90	123.84
25	B	836	CLA	CHD-C1D-C2D	2.52	130.77	125.48
24	2	607	CHL	C3C-C4C-NC	-2.52	107.74	110.57
25	Q	315	CLA	O2D-CGD-O1D	-2.52	118.91	123.84
25	T	309	CLA	C4A-NA-C1A	2.52	107.84	106.71
25	6	604	CLA	CHB-C4A-NA	2.52	128.00	124.51
24	W	305	CHL	O2D-CGD-O1D	-2.52	118.91	123.84
29	U	314	Q6L	C42-C13-C12	2.52	119.51	115.27
30	B	849	BCR	C4-C5-C6	-2.52	119.07	122.73
25	A	839	CLA	C1B-CHB-C4A	-2.52	125.13	130.12
25	A	806	CLA	O2D-CGD-O1D	-2.52	118.91	123.84
25	U	311	CLA	O2A-CGA-O1A	-2.52	117.24	123.59
25	3	308	CLA	C1D-ND-C4D	-2.52	104.55	106.33
25	L	301	CLA	O2D-CGD-O1D	-2.52	118.92	123.84
30	I	101	BCR	C29-C30-C25	-2.52	106.61	110.48
25	B	806	CLA	CHB-C4A-NA	2.52	127.99	124.51
30	B	847	BCR	C21-C20-C19	2.52	131.07	123.22
25	H	302	CLA	CMB-C2B-C3B	2.52	129.39	124.68
30	B	848	BCR	C15-C14-C13	-2.52	123.72	127.31
24	1	601	CHL	C2C-C3C-C4C	2.52	108.28	106.49
25	V	301	CLA	CHB-C4A-NA	2.52	127.99	124.51
25	B	812	CLA	CMB-C2B-C3B	2.51	129.38	124.68
38	U	307	KC2	CAA-C2A-C1A	-2.51	113.19	124.75
25	4	312	CLA	O2D-CGD-O1D	-2.51	118.38	124.09
25	A	836	CLA	O2D-CGD-CBD	2.51	115.73	111.27
25	B	802	CLA	CHD-C1D-ND	-2.51	122.14	124.45
25	B	822	CLA	O2D-CGD-O1D	-2.51	118.93	123.84
25	S	312	CLA	O2D-CGD-O1D	-2.51	118.93	123.84
24	P	306	CHL	C3C-C4C-NC	-2.51	107.75	110.57
25	H	304	CLA	C3A-C2A-C1A	2.51	105.10	101.34
25	P	312	CLA	O2D-CGD-O1D	-2.51	118.93	123.84
37	H	306	NEX	C15-C14-C13	-2.51	123.73	127.31
25	5	610	CLA	C4A-NA-C1A	2.51	107.83	106.71
38	V	308	KC2	CAA-CBA-CGA	-2.51	114.36	127.26
37	R	321	NEX	C15-C35-C34	-2.51	118.33	123.47
25	B	810	CLA	C1-C2-C3	2.51	130.38	126.04
25	K	203	CLA	CMB-C2B-C3B	2.51	129.38	124.68
29	T	316	Q6L	C24-C22-C21	-2.51	115.09	118.94
24	3	306	CHL	CHB-C4A-NA	2.51	127.98	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	1	601	CHL	C1B-CHB-C4A	-2.51	125.15	130.12
30	K	205	BCR	C38-C26-C25	-2.51	121.71	124.53
25	U	301	CLA	CAA-C2A-C1A	-2.51	103.76	111.97
24	R	302	CHL	CAC-C3C-C4C	2.51	128.06	124.81
25	B	819	CLA	CHA-C1A-NA	-2.51	120.66	126.40
25	L	301	CLA	CHB-C4A-NA	2.51	127.98	124.51
24	R	311	CHL	C2C-C3C-C4C	2.51	108.28	106.49
25	3	301	CLA	C1B-CHB-C4A	-2.51	125.15	130.12
25	U	302	CLA	C4-C3-C5	2.51	119.49	115.27
24	T	305	CHL	CMA-C3A-C4A	2.51	118.51	111.77
25	S	302	CLA	C2D-C1D-ND	-2.50	108.26	110.10
34	B	844	PQN	C21-C22-C23	-2.50	107.83	115.92
29	V	315	Q6L	C19-C20-C21	-2.50	118.35	123.47
25	B	805	CLA	CMB-C2B-C3B	2.50	129.36	124.68
29	V	316	Q6L	C01-C02-C07	-2.50	109.72	114.36
25	A	825	CLA	O2D-CGD-O1D	-2.50	118.94	123.84
25	A	805	CLA	CAC-C3C-C4C	2.50	128.06	124.81
38	X	309	KC2	O2D-CGD-CBD	2.50	115.71	111.27
25	A	810	CLA	C11-C12-C13	-2.50	107.83	115.92
30	A	850	BCR	C8-C7-C6	-2.50	120.18	127.20
25	P	309	CLA	CAA-C2A-C3A	2.50	119.62	112.78
25	B	808	CLA	C1B-CHB-C4A	-2.50	125.17	130.12
25	4	310	CLA	CBA-CAA-C2A	2.50	121.24	113.86
25	R	305	CLA	O2A-CGA-O1A	-2.50	117.28	123.59
25	B	820	CLA	CHD-C1D-ND	-2.50	122.16	124.45
25	G	204	CLA	CHB-C4A-NA	2.50	127.97	124.51
25	X	312	CLA	CHB-C4A-NA	2.50	127.97	124.51
28	6	616	LHG	O8-C23-C24	2.50	119.75	111.91
25	A	810	CLA	C1B-CHB-C4A	-2.50	125.17	130.12
25	N	203	CLA	O2D-CGD-O1D	-2.50	118.95	123.84
25	B	835	CLA	CHD-C1D-ND	-2.50	122.16	124.45
25	B	812	CLA	C1C-C2C-C3C	-2.50	104.33	106.96
25	4	309	CLA	CED-O2D-CGD	2.50	121.58	115.94
30	A	848	BCR	C27-C26-C25	-2.50	119.11	122.73
25	B	814	CLA	CHB-C4A-NA	2.50	127.96	124.51
38	P	308	KC2	C2B-C1B-NB	-2.50	108.27	110.10
30	I	101	BCR	C16-C17-C18	-2.50	123.75	127.31
25	B	819	CLA	O2D-CGD-O1D	-2.49	118.96	123.84
25	A	817	CLA	C1-C2-C3	-2.49	121.73	126.04
25	A	837	CLA	C6-C5-C3	2.49	120.00	113.45
30	4	319	BCR	C38-C26-C27	2.49	118.41	113.62
25	A	827	CLA	CAA-C2A-C3A	-2.49	105.95	112.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	F	803	CLA	CMA-C3A-C2A	-2.49	110.28	116.10
29	V	316	Q6L	C37-C36-C31	2.49	113.32	109.55
25	2	609	CLA	CMC-C2C-C1C	2.49	128.84	125.04
25	O	2002	CLA	C1-O2A-CGA	2.49	122.98	116.44
30	K	207	BCR	C15-C16-C17	-2.49	118.37	123.47
25	W	312	CLA	O2D-CGD-O1D	-2.49	118.97	123.84
24	4	308	CHL	O2D-CGD-O1D	-2.49	118.97	123.84
24	S	304	CHL	O2D-CGD-O1D	-2.49	118.97	123.84
25	6	610	CLA	CBA-CAA-C2A	2.49	121.21	113.86
24	W	304	CHL	CMB-C2B-C3B	2.49	129.34	124.68
30	A	849	BCR	C24-C23-C22	-2.49	122.47	126.23
25	2	602	CLA	C1B-CHB-C4A	-2.49	125.19	130.12
25	O	2005	CLA	C1B-CHB-C4A	-2.49	125.19	130.12
30	3	319	BCR	C19-C18-C17	-2.49	115.12	118.94
29	X	317	Q6L	C05-C06-C07	2.49	113.71	110.30
29	R	320	Q6L	C19-C20-C21	-2.49	118.38	123.47
29	Q	319	Q6L	C01-C02-C07	-2.49	109.75	114.36
25	4	312	CLA	C1B-CHB-C4A	-2.49	125.19	130.12
30	4	319	BCR	C4-C5-C6	-2.49	119.12	122.73
25	A	827	CLA	O2A-CGA-O1A	-2.48	117.32	123.59
25	X	302	CLA	O1D-CGD-CBD	2.48	129.57	124.48
30	A	850	BCR	C11-C10-C9	-2.48	123.76	127.31
25	A	811	CLA	CAA-CBA-CGA	-2.48	106.00	113.25
37	S	317	NEX	C19-C9-C10	2.48	126.40	122.92
30	3	317	BCR	C11-C10-C9	-2.48	123.77	127.31
25	4	304	CLA	CHB-C4A-NA	2.48	127.94	124.51
25	A	845	CLA	CMB-C2B-C1B	-2.48	124.65	128.46
25	W	302	CLA	O2D-CGD-O1D	-2.48	118.99	123.84
27	6	615	XAT	C12-C13-C14	-2.48	115.13	118.94
24	1	601	CHL	CMB-C2B-C1B	-2.48	124.65	128.46
25	3	302	CLA	C1B-CHB-C4A	-2.48	125.20	130.12
25	O	2001	CLA	CHB-C4A-NA	2.48	127.94	124.51
25	5	604	CLA	CMB-C2B-C3B	2.48	129.54	124.69
29	V	319	Q6L	C12-C13-C14	-2.48	114.48	121.98
30	B	848	BCR	C19-C18-C17	-2.48	115.14	118.94
30	A	850	BCR	C2-C1-C6	-2.48	106.67	110.48
26	T	321	IWJ	C25-C24-C26	2.48	120.18	116.02
30	2	618	BCR	C11-C10-C9	-2.48	123.78	127.31
25	4	313	CLA	CMC-C2C-C1C	2.48	128.81	125.04
24	Q	308	CHL	C3C-C4C-NC	-2.48	107.80	110.57
25	U	310	CLA	CMB-C2B-C3B	2.48	129.31	124.68
25	5	609	CLA	O2A-CGA-O1A	-2.47	117.35	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	5	602	CLA	CAC-C3C-C4C	2.47	128.02	124.81
25	A	856	CLA	CAC-C3C-C4C	2.47	128.02	124.81
26	4	317	IWJ	C36-C35-C34	-2.47	104.69	108.98
25	P	302	CLA	C11-C12-C13	2.47	123.91	115.92
25	5	607	CLA	O2D-CGD-CBD	2.47	115.66	111.27
30	A	848	BCR	C30-C25-C26	2.47	126.10	122.61
25	4	303	CLA	CHA-C1A-NA	-2.47	120.74	126.40
25	2	613	CLA	CMB-C2B-C1B	-2.47	124.66	128.46
26	W	318	IWJ	C17-C18-C19	2.47	130.84	127.31
25	G	203	CLA	C1B-CHB-C4A	-2.47	125.22	130.12
25	B	813	CLA	C14-C13-C15	2.47	120.24	111.29
25	6	603	CLA	CMC-C2C-C1C	2.47	128.80	125.04
25	U	303	CLA	CHB-C4A-NA	2.47	127.93	124.51
25	A	812	CLA	C3A-C2A-C1A	2.47	105.04	101.34
25	6	613	CLA	O1D-CGD-CBD	2.47	129.54	124.48
25	R	314	CLA	C1-O2A-CGA	2.47	122.92	116.44
25	6	603	CLA	CHA-C1A-NA	-2.47	120.74	126.40
24	2	605	CHL	C1B-CHB-C4A	-2.47	125.23	130.12
25	B	829	CLA	C1B-CHB-C4A	-2.47	125.23	130.12
25	F	803	CLA	C1B-CHB-C4A	-2.47	125.23	130.12
25	P	303	CLA	O2D-CGD-O1D	-2.47	119.01	123.84
29	U	314	Q6L	C16-C17-C18	-2.47	115.16	118.94
25	K	201	CLA	CAC-C3C-C4C	2.47	128.01	124.81
25	T	309	CLA	CHD-C1D-ND	-2.47	122.19	124.45
25	X	314	CLA	O2D-CGD-O1D	-2.47	119.02	123.84
25	B	841	CLA	O2D-CGD-O1D	-2.47	119.02	123.84
25	3	304	CLA	CMC-C2C-C1C	2.47	128.79	125.04
25	B	827	CLA	C1-C2-C3	-2.46	122.76	126.75
31	O	2008	LMG	O8-C28-C29	2.46	119.64	111.91
25	G	203	CLA	CHD-C1D-ND	-2.46	122.19	124.45
24	V	307	CHL	O2D-CGD-O1D	-2.46	119.02	123.84
25	P	309	CLA	CBA-CAA-C2A	2.46	121.13	113.86
27	3	316	XAT	C15-C35-C34	-2.46	118.43	123.47
25	B	807	CLA	C1B-CHB-C4A	-2.46	125.24	130.12
25	A	833	CLA	CHB-C4A-NA	2.46	127.92	124.51
24	R	311	CHL	C2D-C1D-ND	-2.46	108.29	110.10
25	6	610	CLA	C2D-C1D-ND	-2.46	108.29	110.10
25	U	308	CLA	CMA-C3A-C2A	-2.46	110.35	116.10
25	B	811	CLA	O2D-CGD-O1D	-2.46	119.03	123.84
25	B	820	CLA	CHA-C1A-NA	-2.46	120.77	126.40
30	K	205	BCR	C12-C13-C14	-2.46	115.17	118.94
25	B	838	CLA	CHB-C4A-NA	2.46	127.91	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	837	CLA	O2D-CGD-O1D	-2.46	119.03	123.84
25	B	818	CLA	CED-O2D-CGD	2.46	121.50	115.94
25	A	842	CLA	CHD-C1D-C2D	2.46	130.64	125.48
29	S	320	Q6L	C12-C13-C14	-2.46	114.54	121.98
25	G	203	CLA	CMB-C2B-C3B	2.46	129.28	124.68
37	P	317	NEX	C15-C35-C34	-2.46	118.44	123.47
24	P	304	CHL	C2A-C1A-CHA	2.46	128.16	123.86
38	R	312	KC2	CHC-C4B-NB	2.46	126.71	124.45
37	P	317	NEX	C32-C33-C34	-2.46	115.17	118.94
27	5	612	XAT	C17-C1-C16	-2.45	103.75	107.37
25	A	813	CLA	C1B-CHB-C4A	-2.45	125.26	130.12
25	B	810	CLA	C6-C7-C8	2.45	123.85	115.92
25	A	856	CLA	C2A-C1A-CHA	2.45	128.15	123.86
25	O	2002	CLA	O2D-CGD-O1D	-2.45	119.05	123.84
38	P	308	KC2	O2A-CGA-O1A	-2.45	117.58	122.67
24	P	306	CHL	CMB-C2B-C3B	2.45	129.26	124.68
25	A	816	CLA	O2A-CGA-O1A	-2.45	117.19	123.30
30	K	207	BCR	C37-C22-C23	2.45	121.94	118.08
25	B	810	CLA	CBA-CAA-C2A	2.45	121.09	113.86
37	P	317	NEX	C31-C30-C29	-2.45	123.81	127.31
24	P	314	CHL	CHD-C1D-ND	-2.45	122.20	124.45
25	6	607	CLA	CHB-C4A-NA	2.45	127.90	124.51
25	B	832	CLA	CHB-C4A-NA	2.45	127.90	124.51
25	A	819	CLA	CMB-C2B-C3B	2.45	129.26	124.68
30	3	318	BCR	C20-C21-C22	-2.45	123.82	127.31
24	1	601	CHL	CMB-C2B-C3B	2.45	129.26	124.68
24	W	307	CHL	O2D-CGD-O1D	-2.45	119.05	123.84
25	A	840	CLA	CMB-C2B-C3B	2.45	129.26	124.68
25	A	836	CLA	C1B-CHB-C4A	-2.45	125.27	130.12
30	L	307	BCR	C37-C22-C21	-2.45	119.50	122.92
25	A	823	CLA	CAC-C3C-C4C	2.45	127.98	124.81
30	L	305	BCR	C15-C16-C17	-2.45	118.47	123.47
25	J	102	CLA	CHB-C4A-NA	2.44	127.89	124.51
38	T	308	KC2	CAC-C3C-C2C	-2.44	120.55	128.60
25	V	311	CLA	C2A-C1A-CHA	2.44	128.13	123.86
30	G	201	BCR	C34-C9-C8	2.44	121.93	118.08
25	3	303	CLA	O2A-CGA-O1A	-2.44	117.21	123.30
29	S	323	Q6L	C36-C31-C32	2.44	115.80	111.42
29	V	319	Q6L	C24-C22-C21	-2.44	115.19	118.94
25	B	813	CLA	CMB-C2B-C1B	-2.44	124.71	128.46
25	Q	314	CLA	O2D-CGD-O1D	-2.44	119.06	123.84
25	6	613	CLA	O2D-CGD-O1D	-2.44	119.07	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	6	606	CHL	O2D-CGD-CBD	2.44	115.60	111.27
24	X	308	CHL	CHB-C4A-NA	2.44	127.89	124.51
29	T	322	Q6L	C38-C36-C35	-2.44	104.81	109.44
25	X	312	CLA	C1B-CHB-C4A	-2.44	125.29	130.12
25	A	828	CLA	O2D-CGD-CBD	2.44	115.60	111.27
31	A	855	LMG	O8-C28-C29	2.44	119.56	111.91
30	B	846	BCR	C15-C16-C17	-2.44	118.48	123.47
25	4	313	CLA	CBA-CAA-C2A	2.44	121.06	113.86
30	J	101	BCR	C20-C19-C18	-2.44	119.57	126.42
25	A	825	CLA	C3C-C4C-NC	-2.44	107.84	110.57
24	T	320	CHL	C3A-C2A-C1A	2.44	104.99	101.34
25	U	303	CLA	CHD-C1D-ND	-2.44	122.22	124.45
26	4	301	IWJ	C36-C35-C34	-2.44	104.75	108.98
25	4	303	CLA	C4A-NA-C1A	2.44	107.80	106.71
26	T	318	IWJ	C05-C04-C03	2.43	114.51	111.74
25	6	603	CLA	O2D-CGD-O1D	-2.43	118.56	124.09
26	V	318	IWJ	C36-C35-C34	-2.43	104.75	108.98
25	B	827	CLA	O2D-CGD-CBD	2.43	115.59	111.27
25	S	303	CLA	C2D-C1D-ND	-2.43	108.31	110.10
25	3	305	CLA	CHB-C4A-NA	2.43	127.88	124.51
25	A	833	CLA	CMB-C2B-C3B	2.43	129.23	124.68
25	P	301	CLA	C5-C3-C2	-2.43	116.20	121.12
25	2	608	CLA	CMC-C2C-C1C	2.43	128.74	125.04
29	W	319	Q6L	C06-C07-C02	2.43	116.70	111.85
25	O	2002	CLA	O2A-CGA-O1A	-2.43	117.46	123.59
29	R	304	Q6L	C19-C18-C17	-2.43	123.84	127.31
25	B	823	CLA	O2D-CGD-O1D	-2.43	119.09	123.84
30	G	205	BCR	C12-C13-C14	-2.43	115.21	118.94
24	2	607	CHL	CAC-C3C-C4C	2.43	127.96	124.81
25	4	309	CLA	CHA-C1A-NA	-2.43	120.84	126.40
25	X	313	CLA	CAA-C2A-C3A	-2.43	110.43	116.10
25	B	805	CLA	C4D-C3D-CAD	-2.43	105.23	108.10
31	A	857	LMG	O7-C10-C11	2.43	116.73	111.50
25	X	314	CLA	CMB-C2B-C3B	2.43	129.22	124.68
25	B	824	CLA	CAC-C3C-C4C	2.43	127.96	124.81
25	V	312	CLA	O2D-CGD-O1D	-2.43	119.09	123.84
30	A	852	BCR	C40-C30-C25	2.43	114.23	110.30
37	W	317	NEX	C11-C10-C9	-2.43	123.85	127.31
25	A	841	CLA	CAA-CBA-CGA	-2.42	106.17	113.25
24	4	302	CHL	O2D-CGD-O1D	-2.42	119.10	123.84
31	J	104	LMG	O1-C1-C2	2.42	112.09	108.30
25	B	815	CLA	CGD-CBD-CAD	-2.42	102.89	110.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	4	306	CHL	CHD-C1D-ND	-2.42	122.23	124.45
27	5	612	XAT	C35-C34-C33	-2.42	123.85	127.31
25	1	608	CLA	C4-C3-C5	2.42	119.34	115.27
25	A	805	CLA	CMC-C2C-C1C	2.42	128.73	125.04
25	H	301	CLA	CMB-C2B-C1B	-2.42	124.74	128.46
29	S	320	Q6L	C01-C02-C07	-2.42	109.87	114.36
25	K	201	CLA	CHB-C4A-NA	2.42	127.86	124.51
26	P	320	IWJ	C23-C22-C21	-2.42	115.67	123.22
30	B	846	BCR	C16-C17-C18	-2.42	123.86	127.31
25	B	822	CLA	CBA-CAA-C2A	2.42	121.00	113.86
25	U	311	CLA	O1D-CGD-CBD	2.42	129.43	124.48
24	Q	316	CHL	O2D-CGD-CBD	2.42	115.57	111.27
25	A	829	CLA	CBA-CAA-C2A	2.42	121.00	113.86
30	B	845	BCR	C31-C1-C6	2.42	114.22	110.30
36	A	854	DGD	O1G-C1A-C2A	2.42	119.49	111.91
25	1	603	CLA	C6-C5-C3	2.41	119.79	113.45
25	A	817	CLA	C14-C13-C12	-2.41	102.55	111.29
25	A	822	CLA	CHD-C1D-ND	-2.41	122.24	124.45
25	A	814	CLA	CAC-C3C-C4C	2.41	127.94	124.81
25	A	842	CLA	O2D-CGD-O1D	-2.41	119.12	123.84
25	3	304	CLA	C1B-CHB-C4A	-2.41	125.34	130.12
25	A	829	CLA	O2D-CGD-O1D	-2.41	119.12	123.84
25	5	601	CLA	CHD-C1D-ND	-2.41	122.24	124.45
25	A	817	CLA	C1B-CHB-C4A	-2.41	125.34	130.12
25	A	822	CLA	C1B-CHB-C4A	-2.41	125.34	130.12
38	W	308	KC2	CBD-CHA-C1A	2.41	133.38	128.88
25	A	828	CLA	C6-C5-C3	-2.41	107.14	113.45
25	L	303	CLA	C1B-CHB-C4A	-2.41	125.34	130.12
24	V	306	CHL	C3C-C4C-NC	-2.41	107.87	110.57
25	A	804	CLA	C4D-C3D-CAD	-2.41	105.26	108.10
25	B	826	CLA	CAA-C2A-C3A	-2.41	106.18	112.78
27	4	318	XAT	O4-C5-C18	2.41	117.94	115.06
29	W	319	Q6L	C12-C13-C14	-2.41	114.69	121.98
25	5	602	CLA	O2A-CGA-O1A	-2.41	117.52	123.59
38	T	308	KC2	CHB-C4A-NA	2.41	128.00	124.20
30	I	101	BCR	C36-C18-C17	-2.41	119.55	122.92
24	6	605	CHL	OMC-CMC-C2C	-2.41	120.25	125.69
27	3	316	XAT	C20-C13-C12	2.41	121.87	118.08
25	3	312	CLA	CMA-C3A-C2A	-2.41	110.48	116.10
25	5	609	CLA	CBA-CAA-C2A	2.41	120.96	113.86
30	J	103	BCR	C11-C10-C9	-2.40	123.88	127.31
28	3	322	LHG	O8-C23-C24	2.40	119.45	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	T	311	CLA	C1B-CHB-C4A	-2.40	125.36	130.12
29	S	320	Q6L	O39-C34-C35	-2.40	104.66	110.74
24	W	314	CHL	CHB-C4A-NA	2.40	127.84	124.51
25	U	308	CLA	CHD-C4C-C3C	-2.40	121.31	124.84
25	A	842	CLA	C1-C2-C3	-2.40	121.89	126.04
25	A	833	CLA	CMC-C2C-C1C	2.40	128.70	125.04
25	A	838	CLA	CHB-C4A-NA	2.40	127.83	124.51
38	W	308	KC2	CAC-C3C-C4C	2.40	135.66	124.47
25	K	204	CLA	CHD-C1D-ND	-2.40	122.25	124.45
25	A	823	CLA	O2D-CGD-O1D	-2.40	119.14	123.84
25	P	311	CLA	CAC-C3C-C4C	2.40	127.93	124.81
25	4	313	CLA	C5-C3-C2	2.40	125.97	121.12
27	1	612	XAT	O24-C25-C26	-2.40	56.97	58.96
38	W	308	KC2	C4C-C3C-C2C	-2.40	105.21	107.11
25	5	609	CLA	CMB-C2B-C3B	2.40	129.17	124.68
25	T	309	CLA	CBA-CAA-C2A	2.40	120.94	113.86
25	A	821	CLA	CBA-CAA-C2A	2.40	120.94	113.86
25	A	803	CLA	C11-C10-C8	-2.40	108.17	115.92
25	1	602	CLA	O1D-CGD-CBD	2.40	129.39	124.48
25	B	813	CLA	C1C-C2C-C3C	-2.40	104.44	106.96
25	4	309	CLA	CBC-CAC-C3C	-2.40	105.82	112.43
25	2	613	CLA	CMB-C2B-C3B	2.40	129.16	124.68
25	2	602	CLA	CBA-CAA-C2A	2.40	120.94	113.86
24	1	604	CHL	O2D-CGD-O1D	-2.40	118.65	124.09
25	4	313	CLA	O2A-CGA-O1A	-2.40	117.55	123.59
24	6	601	CHL	C2D-C1D-ND	-2.40	108.34	110.10
37	W	317	NEX	C32-C33-C34	-2.39	115.27	118.94
31	L	308	LMG	O8-C28-C29	2.39	119.42	111.91
25	4	311	CLA	C2C-C1C-NC	2.39	112.22	109.97
27	2	617	XAT	C12-C13-C14	-2.39	115.27	118.94
38	S	308	KC2	CAC-C3C-C2C	-2.39	120.72	128.60
24	1	604	CHL	CHB-C4A-NA	2.39	127.82	124.51
25	B	823	CLA	CMB-C2B-C3B	2.39	129.15	124.68
25	S	303	CLA	O2D-CGD-CBD	2.39	115.52	111.27
24	4	308	CHL	CHB-C4A-NA	2.39	127.82	124.51
25	1	606	CLA	CHB-C4A-NA	2.39	127.82	124.51
25	A	842	CLA	C1B-CHB-C4A	-2.39	125.38	130.12
38	U	307	KC2	CHC-C4B-NB	2.39	126.65	124.45
25	S	301	CLA	CMD-C2D-C1D	-2.39	120.50	124.71
25	R	314	CLA	C1-C2-C3	-2.39	121.91	126.04
30	B	845	BCR	C40-C30-C39	2.39	115.86	108.53
25	A	843	CLA	O2D-CGD-O1D	-2.39	119.17	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	1	612	XAT	C15-C35-C34	-2.39	118.58	123.47
25	S	301	CLA	C5-C3-C2	2.39	125.95	121.12
25	X	302	CLA	O2D-CGD-O1D	-2.39	119.17	123.84
27	4	318	XAT	C19-C9-C8	2.39	121.84	118.08
30	J	103	BCR	C35-C13-C12	2.39	121.84	118.08
24	Q	307	CHL	C4A-NA-C1A	2.39	107.78	106.71
25	U	310	CLA	C1B-CHB-C4A	-2.39	125.39	130.12
25	O	2001	CLA	CHD-C1D-ND	-2.39	122.26	124.45
27	5	612	XAT	C12-C13-C14	-2.38	115.28	118.94
30	I	101	BCR	C12-C13-C14	-2.38	115.28	118.94
25	W	301	CLA	CHD-C1D-ND	-2.38	122.26	124.45
25	A	827	CLA	C6-C5-C3	-2.38	107.20	113.45
37	T	317	NEX	C32-C33-C34	-2.38	115.28	118.94
38	W	308	KC2	O2D-CGD-CBD	2.38	115.50	111.27
30	3	317	BCR	C39-C30-C25	2.38	114.17	110.30
25	U	309	CLA	O2D-CGD-O1D	-2.38	119.18	123.84
24	S	307	CHL	C1C-C2C-C3C	-2.38	105.22	107.11
24	W	314	CHL	C2D-C1D-ND	-2.38	108.35	110.10
29	P	319	Q6L	C06-C07-C02	2.38	116.60	111.85
30	G	201	BCR	C38-C26-C25	-2.38	121.86	124.53
25	O	2001	CLA	C4-C3-C5	2.38	119.28	115.27
25	A	833	CLA	O2D-CGD-O1D	-2.38	119.19	123.84
24	S	314	CHL	CHB-C4A-NA	2.38	127.80	124.51
25	3	309	CLA	O2D-CGD-CBD	2.38	115.49	111.27
25	B	826	CLA	O2D-CGD-CBD	2.38	115.49	111.27
25	B	808	CLA	C3C-C4C-NC	-2.38	107.90	110.57
25	A	804	CLA	O2A-CGA-CBA	-2.38	104.44	111.91
24	R	318	CHL	C1C-C2C-C3C	-2.38	105.23	107.11
24	4	302	CHL	O2A-C1-C2	-2.38	102.39	108.64
29	P	319	Q6L	C19-C20-C21	-2.38	118.61	123.47
30	3	319	BCR	C23-C22-C21	-2.38	115.29	118.94
25	A	835	CLA	CHD-C1D-ND	-2.38	122.27	124.45
25	B	813	CLA	C2D-C1D-ND	-2.38	108.35	110.10
28	6	616	LHG	O8-C6-C5	2.38	115.35	108.43
25	T	312	CLA	O2A-CGA-O1A	-2.38	117.60	123.59
25	4	309	CLA	CHB-C4A-NA	2.37	127.80	124.51
38	T	308	KC2	CMD-C2D-C1D	-2.37	124.81	128.46
25	T	312	CLA	O2D-CGD-O1D	-2.37	119.19	123.84
25	X	311	CLA	CHD-C1D-ND	-2.37	122.27	124.45
37	T	317	NEX	C15-C14-C13	-2.37	123.92	127.31
25	1	610	CLA	O1D-CGD-CBD	2.37	129.34	124.48
30	G	201	BCR	C35-C13-C14	2.37	126.25	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	T	315	Q6L	C01-C02-C07	-2.37	109.96	114.36
25	U	310	CLA	O2D-CGD-O1D	-2.37	119.20	123.84
25	B	806	CLA	CHD-C1D-ND	-2.37	122.27	124.45
25	B	819	CLA	CMB-C2B-C3B	2.37	129.12	124.68
25	4	316	CLA	CED-O2D-CGD	2.37	121.30	115.94
30	K	202	BCR	C16-C17-C18	-2.37	123.92	127.31
25	A	808	CLA	CMC-C2C-C1C	2.37	128.65	125.04
28	A	846	LHG	O8-C23-C24	2.37	119.35	111.91
29	P	316	Q6L	C19-C20-C21	-2.37	118.62	123.47
27	5	612	XAT	C16-C1-C2	-2.37	104.86	108.98
30	3	318	BCR	C8-C7-C6	-2.37	120.55	127.20
25	P	312	CLA	O2D-CGD-CBD	2.37	115.48	111.27
30	4	319	BCR	C33-C5-C6	2.37	127.19	124.53
25	A	827	CLA	CBC-CAC-C3C	2.37	118.96	112.43
25	A	841	CLA	CHB-C4A-NA	2.37	127.79	124.51
30	A	848	BCR	C20-C21-C22	-2.37	123.93	127.31
25	4	310	CLA	C6-C5-C3	2.37	119.66	113.45
24	W	314	CHL	C2A-C1A-CHA	2.37	126.38	122.71
24	Q	308	CHL	CHA-C4D-ND	2.37	137.45	132.50
30	H	305	BCR	C11-C10-C9	-2.37	123.93	127.31
25	B	840	CLA	CMB-C2B-C3B	2.37	129.11	124.68
25	B	819	CLA	C2A-C1A-CHA	2.37	128.00	123.86
25	K	204	CLA	O2D-CGD-O1D	-2.37	119.21	123.84
24	X	305	CHL	CHB-C4A-NA	2.37	127.78	124.51
37	S	317	NEX	C32-C33-C34	-2.36	115.31	118.94
25	A	829	CLA	CED-O2D-CGD	2.36	121.29	115.94
25	6	613	CLA	CHB-C4A-NA	2.36	127.78	124.51
24	S	306	CHL	C4A-NA-C1A	2.36	107.77	106.71
38	V	308	KC2	O1A-CGA-CBA	2.36	128.37	120.99
25	V	313	CLA	CHB-C4A-NA	2.36	127.78	124.51
24	U	304	CHL	CMB-C2B-C3B	2.36	129.10	124.68
25	V	313	CLA	CMB-C2B-C3B	2.36	129.10	124.68
29	Q	317	Q6L	C12-C13-C14	-2.36	114.83	121.98
25	2	603	CLA	C1B-CHB-C4A	-2.36	125.44	130.12
30	J	103	BCR	C20-C21-C22	-2.36	123.94	127.31
25	A	829	CLA	C2C-C1C-NC	2.36	112.18	109.97
25	A	810	CLA	CHB-C4A-NA	2.36	127.78	124.51
38	S	308	KC2	O1A-CGA-CBA	2.36	128.36	120.99
27	2	617	XAT	O24-C25-C26	-2.36	57.00	58.96
25	B	809	CLA	CAA-C2A-C1A	2.36	119.71	111.97
30	F	804	BCR	C1-C6-C5	-2.36	119.29	122.61
30	K	205	BCR	C28-C27-C26	-2.36	109.86	114.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	V	308	KC2	CAA-C2A-C1A	-2.36	113.90	124.75
31	N	201	LMG	O6-C1-C2	-2.36	105.36	110.35
25	5	602	CLA	O2D-CGD-CBD	2.36	115.46	111.27
25	P	302	CLA	C14-C13-C15	2.36	119.83	111.29
30	A	852	BCR	C8-C7-C6	-2.36	120.58	127.20
25	B	813	CLA	C14-C13-C12	-2.36	102.75	111.29
30	K	207	BCR	C10-C11-C12	2.36	130.57	123.22
25	B	825	CLA	O2D-CGD-O1D	-2.36	119.23	123.84
25	B	806	CLA	CAC-C3C-C2C	-2.36	123.50	127.53
25	H	302	CLA	C1-C2-C3	2.36	130.12	126.04
25	A	839	CLA	CHB-C4A-NA	2.36	127.77	124.51
25	O	2005	CLA	CHB-C4A-NA	2.36	127.77	124.51
25	B	831	CLA	CBA-CAA-C2A	2.36	120.82	113.86
25	1	613	CLA	CHB-C4A-NA	2.36	127.77	124.51
26	6	614	IWJ	C36-C35-C34	-2.36	104.89	108.98
25	2	602	CLA	CHD-C1D-ND	-2.35	122.29	124.45
24	P	304	CHL	O2D-CGD-CBD	2.35	115.45	111.27
25	1	607	CLA	CAC-C3C-C4C	2.35	127.86	124.81
25	T	309	CLA	O2D-CGD-O1D	-2.35	119.23	123.84
26	Q	320	IWJ	C25-C24-C26	2.35	119.98	116.02
24	4	308	CHL	CMB-C2B-C3B	2.35	129.08	124.68
24	W	306	CHL	CHD-C1D-ND	-2.35	122.29	124.45
24	W	306	CHL	CAA-C2A-C3A	2.35	119.22	112.78
25	K	203	CLA	C2A-C1A-CHA	2.35	127.97	123.86
30	A	851	BCR	C7-C8-C9	-2.35	122.68	126.23
27	6	615	XAT	C35-C34-C33	-2.35	123.95	127.31
25	6	609	CLA	CMC-C2C-C1C	2.35	128.62	125.04
25	R	315	CLA	C5-C3-C2	2.35	125.88	121.12
24	X	315	CHL	CMB-C2B-C3B	2.35	129.08	124.68
25	B	813	CLA	O2D-CGD-CBD	2.35	115.44	111.27
30	J	101	BCR	C8-C9-C10	-2.35	115.33	118.94
30	K	202	BCR	C16-C15-C14	-2.35	118.66	123.47
25	F	802	CLA	C2D-C1D-ND	-2.35	108.37	110.10
25	P	313	CLA	CBA-CAA-C2A	2.35	120.80	113.86
25	V	310	CLA	C2C-C1C-NC	2.35	112.17	109.97
25	B	818	CLA	O2D-CGD-O1D	-2.35	119.25	123.84
29	W	319	Q6L	C19-C20-C21	-2.35	118.66	123.47
29	V	319	Q6L	C16-C17-C18	-2.35	115.34	118.94
26	Q	320	IWJ	C16-C17-C18	-2.35	118.67	123.47
25	B	830	CLA	CHB-C4A-NA	2.35	127.76	124.51
25	T	312	CLA	CBA-CAA-C2A	2.35	120.79	113.86
29	Q	318	Q6L	C10-C04-C03	2.35	113.06	109.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	X	312	CLA	O2A-CGA-O1A	-2.34	117.67	123.59
29	Q	317	Q6L	C36-C31-C32	2.34	115.62	111.42
30	B	846	BCR	C23-C22-C21	2.34	122.54	118.94
25	2	604	CLA	CHB-C4A-NA	2.34	127.75	124.51
37	R	321	NEX	C38-C25-C24	-2.34	111.64	114.28
26	S	319	IWJ	C21-C19-C18	-2.34	115.35	118.94
25	Q	301	CLA	CAA-CBA-CGA	-2.34	106.41	113.25
25	A	814	CLA	CHB-C4A-NA	2.34	127.75	124.51
25	A	816	CLA	CMB-C2B-C1B	-2.34	124.86	128.46
25	S	303	CLA	C4A-NA-C1A	2.34	107.76	106.71
25	6	602	CLA	CMC-C2C-C1C	2.34	128.60	125.04
37	H	306	NEX	C20-C13-C12	2.34	121.77	118.08
25	5	610	CLA	O2D-CGD-CBD	2.34	115.43	111.27
25	S	310	CLA	CED-O2D-CGD	2.34	121.23	115.94
30	L	305	BCR	C19-C18-C17	-2.34	115.35	118.94
25	S	301	CLA	CAC-C3C-C4C	2.34	127.85	124.81
24	U	304	CHL	CED-O2D-CGD	2.34	121.23	115.94
38	U	307	KC2	O2A-CGA-O1A	-2.34	117.81	122.67
25	B	831	CLA	CAA-CBA-CGA	-2.34	106.42	113.25
38	U	307	KC2	CHB-C4A-NA	2.34	127.89	124.20
25	X	314	CLA	CHB-C4A-NA	2.34	127.75	124.51
38	V	308	KC2	OBD-CAD-CBD	-2.34	122.56	125.89
29	R	320	Q6L	C24-C22-C21	-2.34	115.35	118.94
27	5	612	XAT	C36-C21-C26	2.34	116.35	110.05
29	V	319	Q6L	C23-C22-C21	2.34	126.20	122.92
25	S	301	CLA	CHB-C4A-NA	2.34	127.74	124.51
25	U	309	CLA	CED-O2D-CGD	2.34	121.22	115.94
37	H	306	NEX	C38-C25-C26	-2.34	118.35	122.26
25	A	817	CLA	O2D-CGD-O1D	-2.33	119.27	123.84
25	U	310	CLA	CHA-C1A-NA	-2.33	121.05	126.40
30	F	804	BCR	C11-C12-C13	-2.33	119.86	126.42
25	3	305	CLA	O2D-CGD-O1D	-2.33	119.27	123.84
26	V	318	IWJ	C21-C19-C18	-2.33	115.36	118.94
25	A	843	CLA	C2D-C1D-ND	-2.33	108.38	110.10
29	O	2006	Q6L	C01-C02-C07	-2.33	110.03	114.36
25	A	841	CLA	O2D-CGD-CBD	2.33	115.42	111.27
25	G	203	CLA	C2A-C1A-CHA	2.33	127.94	123.86
25	5	603	CLA	CHD-C1D-ND	-2.33	122.31	124.45
25	X	302	CLA	CHD-C1D-ND	-2.33	122.31	124.45
24	2	605	CHL	CMB-C2B-C3B	2.33	129.04	124.68
24	W	304	CHL	CHD-C1D-ND	-2.33	122.31	124.45
37	H	306	NEX	C32-C33-C34	-2.33	115.36	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	T	310	CLA	CMB-C2B-C3B	2.33	129.04	124.68
25	3	307	CLA	C3C-C4C-NC	-2.33	107.96	110.57
25	X	303	CLA	CHB-C4A-NA	2.33	127.73	124.51
25	3	311	CLA	CBA-CAA-C2A	2.33	120.73	113.86
25	3	310	CLA	O2D-CGD-O1D	-2.33	119.29	123.84
25	B	828	CLA	C2A-C1A-CHA	2.33	127.93	123.86
30	I	101	BCR	C2-C3-C4	-2.33	106.18	111.38
25	X	314	CLA	CAA-C2A-C3A	-2.33	110.67	116.10
25	A	829	CLA	C2A-C1A-CHA	2.33	127.92	123.86
25	B	830	CLA	O2D-CGD-O1D	-2.33	119.29	123.84
25	O	2003	CLA	CHB-C4A-NA	2.32	127.73	124.51
25	S	301	CLA	CHA-C1A-NA	-2.32	121.07	126.40
25	P	310	CLA	C11-C10-C8	2.32	123.43	115.92
25	P	309	CLA	C11-C12-C13	-2.32	108.41	115.92
25	B	821	CLA	CHB-C4A-NA	2.32	127.73	124.51
25	B	824	CLA	CMC-C2C-C1C	2.32	128.58	125.04
25	A	820	CLA	C2D-C1D-ND	-2.32	108.39	110.10
25	Q	314	CLA	CAC-C3C-C4C	2.32	127.82	124.81
25	U	309	CLA	CHD-C1D-ND	-2.32	122.32	124.45
25	X	310	CLA	O2D-CGD-CBD	2.32	115.39	111.27
25	W	311	CLA	C1B-CHB-C4A	-2.32	125.52	130.12
25	N	203	CLA	O2D-CGD-CBD	2.32	115.39	111.27
25	B	820	CLA	C3C-C4C-NC	-2.32	107.97	110.57
25	O	2003	CLA	O2D-CGD-O1D	-2.32	119.30	123.84
25	R	313	CLA	CAA-C2A-C1A	-2.32	104.37	111.97
26	W	318	IWJ	C25-C24-C26	2.32	119.92	116.02
30	A	850	BCR	C38-C26-C27	2.32	118.07	113.62
25	A	815	CLA	O2D-CGD-O1D	-2.32	119.30	123.84
25	A	842	CLA	CBA-CAA-C2A	2.32	120.71	113.86
28	A	847	LHG	O8-C23-C24	2.32	119.18	111.91
25	B	813	CLA	CAC-C3C-C2C	-2.32	123.56	127.53
38	P	308	KC2	CAC-C3C-C2C	-2.32	120.97	128.60
34	B	844	PQN	C14-C13-C12	-2.32	117.73	123.68
25	3	313	CLA	CHB-C4A-NA	2.32	127.72	124.51
24	T	304	CHL	CHD-C1D-ND	-2.32	122.33	124.45
25	6	609	CLA	CHD-C1D-ND	-2.32	122.33	124.45
25	B	813	CLA	CHD-C4C-C3C	2.32	128.25	124.84
25	S	302	CLA	O2D-CGD-O1D	-2.32	119.31	123.84
25	T	301	CLA	CHA-C1A-NA	-2.32	121.09	126.40
38	R	312	KC2	CAC-C3C-C2C	-2.32	120.98	128.60
25	B	837	CLA	O2D-CGD-O1D	-2.31	119.31	123.84
30	F	801	BCR	C8-C7-C6	-2.31	120.70	127.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	A	850	BCR	C15-C16-C17	-2.31	118.74	123.47
25	B	831	CLA	CHD-C1D-ND	-2.31	122.33	124.45
25	3	310	CLA	C1B-CHB-C4A	-2.31	125.54	130.12
25	A	804	CLA	CAC-C3C-C4C	2.31	127.81	124.81
25	T	313	CLA	CHD-C1D-ND	-2.31	122.33	124.45
27	1	612	XAT	C17-C1-C16	-2.31	103.96	107.37
25	B	836	CLA	C2D-C1D-ND	-2.31	108.40	110.10
25	3	307	CLA	CMC-C2C-C1C	2.31	128.56	125.04
25	B	814	CLA	CHD-C1D-ND	-2.31	122.33	124.45
25	1	607	CLA	CHB-C4A-NA	2.31	127.71	124.51
25	A	814	CLA	O2A-CGA-O1A	-2.31	117.76	123.59
25	3	312	CLA	C1B-CHB-C4A	-2.31	125.54	130.12
38	S	308	KC2	O2D-CGD-CBD	2.31	115.37	111.27
24	X	315	CHL	CHB-C4A-NA	2.31	127.70	124.51
29	U	315	Q6L	C29-C27-C26	-2.31	115.40	118.94
24	2	615	CHL	CMB-C2B-C3B	2.31	129.00	124.68
24	S	307	CHL	CMA-C3A-C2A	-2.31	110.71	116.10
25	B	842	CLA	C3C-C4C-NC	-2.31	107.98	110.57
30	H	305	BCR	C24-C23-C22	-2.31	122.75	126.23
25	B	825	CLA	CED-O2D-CGD	2.30	121.15	115.94
25	R	317	CLA	O2A-CGA-O1A	-2.30	117.78	123.59
25	K	201	CLA	C1B-CHB-C4A	-2.30	125.56	130.12
29	W	315	Q6L	C01-C02-C07	-2.30	110.09	114.36
24	R	311	CHL	CHB-C4A-NA	2.30	127.70	124.51
25	A	822	CLA	O2D-CGD-O1D	-2.30	119.34	123.84
25	B	820	CLA	CBA-CAA-C2A	2.30	120.66	113.86
24	2	601	CHL	O2D-CGD-O1D	-2.30	119.34	123.84
25	A	842	CLA	CMB-C2B-C3B	2.30	128.98	124.68
30	A	849	BCR	C38-C26-C27	2.30	118.04	113.62
25	B	841	CLA	C5-C3-C2	2.30	125.77	121.12
25	A	811	CLA	C2A-C1A-CHA	2.30	127.88	123.86
25	3	307	CLA	CAC-C3C-C4C	2.30	127.80	124.81
26	S	319	IWJ	C25-C24-C26	2.30	119.89	116.02
36	A	854	DGD	O3G-C1D-C2D	-2.30	104.71	108.30
37	H	306	NEX	C31-C30-C29	-2.30	124.03	127.31
38	U	307	KC2	CAC-C3C-C2C	-2.30	121.03	128.60
25	A	823	CLA	CHB-C4A-NA	2.30	127.69	124.51
25	B	802	CLA	CHB-C4A-NA	2.30	127.69	124.51
25	V	301	CLA	C4-C3-C2	-2.30	117.78	123.68
27	1	612	XAT	O23-C23-C22	-2.30	105.24	109.80
25	A	835	CLA	CHB-C4A-NA	2.30	127.69	124.51
30	M	101	BCR	C32-C1-C6	2.30	114.03	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	3	317	BCR	C15-C16-C17	-2.30	118.77	123.47
25	K	204	CLA	C2A-C1A-CHA	2.30	127.88	123.86
25	B	807	CLA	C2A-C1A-CHA	2.30	127.87	123.86
24	U	305	CHL	C1C-C2C-C3C	-2.30	105.29	107.11
25	U	310	CLA	CHB-C4A-NA	2.29	127.68	124.51
25	A	808	CLA	CHD-C1D-ND	-2.29	122.35	124.45
25	A	841	CLA	CMB-C2B-C3B	2.29	128.97	124.68
25	3	308	CLA	CMB-C2B-C1B	-2.29	124.94	128.46
25	5	602	CLA	CHD-C1D-ND	-2.29	122.35	124.45
24	W	306	CHL	O2D-CGD-CBD	2.29	115.34	111.27
30	G	205	BCR	C27-C26-C25	-2.29	119.40	122.73
27	3	316	XAT	O3-C3-C4	2.29	114.36	109.80
38	R	312	KC2	CBD-CHA-C1A	2.29	133.15	128.88
25	W	310	CLA	O2A-CGA-O1A	-2.29	117.81	123.59
25	B	835	CLA	C2D-C1D-ND	-2.29	108.42	110.10
24	T	320	CHL	CMB-C2B-C3B	2.29	128.96	124.68
33	A	802	CL0	CHB-C4A-NA	2.29	127.68	124.51
30	3	317	BCR	C37-C22-C23	2.29	121.68	118.08
25	1	609	CLA	CMC-C2C-C1C	2.29	128.52	125.04
30	3	317	BCR	C38-C26-C25	-2.29	121.96	124.53
25	1	609	CLA	CMB-C2B-C3B	2.29	129.17	124.69
38	U	307	KC2	O1A-CGA-CBA	2.29	128.13	120.99
25	6	607	CLA	O2A-CGA-O1A	-2.29	117.60	123.30
30	B	847	BCR	C15-C16-C17	-2.29	118.79	123.47
30	A	851	BCR	C1-C6-C7	2.29	122.24	115.78
25	B	803	CLA	O2A-CGA-O1A	-2.29	117.83	123.59
25	A	830	CLA	C2A-C1A-CHA	2.28	127.85	123.86
38	S	308	KC2	CHC-C4B-NB	2.28	126.55	124.45
25	W	310	CLA	CHD-C1D-ND	-2.28	122.36	124.45
25	B	835	CLA	O2A-CGA-O1A	-2.28	117.61	123.30
29	U	315	Q6L	C35-C34-C33	2.28	114.34	111.74
37	H	306	NEX	C24-C23-C22	-2.28	106.36	110.77
25	B	832	CLA	C2A-C1A-CHA	2.28	127.85	123.86
25	A	841	CLA	CHD-C1D-ND	-2.28	122.36	124.45
25	A	823	CLA	O2A-CGA-O1A	-2.28	117.83	123.59
27	2	617	XAT	C36-C21-C26	2.28	116.20	110.05
25	B	812	CLA	CHB-C4A-NA	2.28	127.67	124.51
25	G	204	CLA	C1B-CHB-C4A	-2.28	125.60	130.12
24	2	615	CHL	C2C-C3C-C4C	2.28	108.11	106.49
29	X	316	Q6L	C29-C27-C26	-2.28	115.44	118.94
38	T	308	KC2	O2D-CGD-CBD	2.28	115.32	111.27
29	S	321	Q6L	C19-C18-C17	-2.28	124.06	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	S	316	Q6L	C24-C22-C21	-2.28	115.44	118.94
24	R	302	CHL	C2A-C1A-CHA	2.28	127.85	123.86
25	S	301	CLA	C4A-NA-C1A	2.28	107.73	106.71
25	W	309	CLA	CHD-C1D-ND	-2.28	122.36	124.45
30	J	101	BCR	C37-C22-C21	-2.28	119.73	122.92
24	6	605	CHL	CHB-C4A-NA	2.28	127.66	124.51
26	S	322	IWJ	C36-C35-C34	-2.28	105.02	108.98
30	K	205	BCR	C24-C25-C26	-2.28	115.94	121.46
25	B	808	CLA	CBA-CAA-C2A	2.28	120.59	113.86
25	1	606	CLA	CAC-C3C-C4C	2.28	127.76	124.81
25	A	839	CLA	CAA-CBA-CGA	-2.28	106.60	113.25
28	Q	302	LHG	O8-C23-C24	2.28	119.05	111.91
25	G	202	CLA	CBA-CAA-C2A	2.28	120.58	113.86
25	2	603	CLA	O1A-CGA-CBA	2.28	130.39	123.08
24	R	302	CHL	CHA-C1A-NA	-2.27	121.19	126.40
24	2	615	CHL	C3C-C4C-NC	-2.27	108.02	110.57
25	Q	301	CLA	C4-C3-C2	-2.27	117.84	123.68
30	4	319	BCR	C2-C1-C6	2.27	113.98	110.48
25	2	603	CLA	CMC-C2C-C1C	2.27	128.50	125.04
25	V	302	CLA	CAC-C3C-C4C	2.27	127.76	124.81
24	P	305	CHL	C2C-C3C-C4C	2.27	108.11	106.49
25	B	832	CLA	CMB-C2B-C3B	2.27	128.93	124.68
29	P	316	Q6L	C24-C22-C21	-2.27	115.46	118.94
25	S	302	CLA	CHB-C4A-NA	2.27	127.65	124.51
25	X	304	CLA	CHD-C1D-ND	-2.27	122.37	124.45
25	4	313	CLA	O2D-CGD-O1D	-2.27	119.40	123.84
25	A	843	CLA	C3C-C4C-NC	-2.27	108.03	110.57
25	T	311	CLA	O2A-CGA-O1A	-2.27	117.87	123.59
25	F	803	CLA	CMB-C2B-C3B	2.27	128.92	124.68
29	U	315	Q6L	C20-C19-C18	2.27	128.12	123.47
25	B	824	CLA	C4A-NA-C1A	2.27	107.72	106.71
27	6	615	XAT	C6-C7-C8	-2.27	121.20	125.99
38	Q	310	KC2	CAA-CBA-CGA	-2.27	115.62	127.26
29	S	315	Q6L	C42-C13-C12	2.26	119.08	115.27
24	T	304	CHL	C2D-C1D-ND	-2.26	108.44	110.10
24	4	307	CHL	C1C-C2C-C3C	-2.26	105.32	107.11
25	B	808	CLA	CHD-C4C-C3C	2.26	128.17	124.84
25	B	812	CLA	CHD-C1D-ND	-2.26	122.37	124.45
25	B	822	CLA	CHD-C1D-ND	-2.26	122.37	124.45
25	B	803	CLA	C5-C3-C2	2.26	125.69	121.12
30	2	618	BCR	C34-C9-C10	2.26	126.09	122.92
38	X	309	KC2	CAC-C3C-C4C	2.26	135.01	124.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	R	315	CLA	CHD-C1D-ND	-2.26	122.38	124.45
25	T	301	CLA	CBA-CAA-C2A	2.26	120.53	113.86
38	R	312	KC2	O2A-CGA-O1A	-2.26	117.98	122.67
30	B	847	BCR	C19-C18-C17	-2.26	115.47	118.94
30	F	801	BCR	C20-C19-C18	-2.26	120.07	126.42
24	4	307	CHL	CMA-C3A-C4A	-2.26	105.70	111.77
24	R	310	CHL	O2D-CGD-O1D	-2.26	119.42	123.84
25	P	303	CLA	CBA-CAA-C2A	2.26	120.52	113.86
31	2	620	LMG	O6-C1-C2	-2.26	105.57	110.35
25	A	807	CLA	O2A-CGA-O1A	-2.26	117.90	123.59
24	V	306	CHL	C2C-C3C-C4C	2.26	108.10	106.49
38	T	308	KC2	CMD-C2D-C3D	2.26	128.90	124.68
26	V	318	IWJ	C37-C35-C34	-2.26	105.06	108.98
25	B	840	CLA	C1C-C2C-C3C	-2.26	104.58	106.96
25	2	603	CLA	O2A-CGA-O1A	-2.26	117.68	123.30
29	Q	319	Q6L	C06-C07-C02	2.25	116.35	111.85
25	Q	306	CLA	O2D-CGD-CBD	2.25	115.28	111.27
26	Q	303	IWJ	C12-C11-C10	2.25	130.53	127.31
25	B	838	CLA	CHD-C1D-ND	-2.25	122.38	124.45
25	W	301	CLA	O2A-C1-C2	-2.25	102.71	108.64
25	B	834	CLA	C1B-CHB-C4A	-2.25	125.65	130.12
30	B	845	BCR	C38-C26-C27	2.25	117.94	113.62
24	T	314	CHL	C1C-C2C-C3C	-2.25	105.33	107.11
30	B	849	BCR	C31-C1-C6	-2.25	106.64	110.30
26	S	322	IWJ	C25-C24-C26	2.25	119.81	116.02
38	T	308	KC2	O2A-CGA-O1A	-2.25	117.99	122.67
37	P	317	NEX	C35-C15-C14	-2.25	118.86	123.47
25	N	203	CLA	C3D-C2D-C1D	2.25	108.90	105.83
30	H	305	BCR	C16-C17-C18	-2.25	124.10	127.31
25	S	309	CLA	C3A-C2A-C1A	-2.25	97.97	101.34
25	P	313	CLA	CHB-C4A-NA	2.25	127.62	124.51
25	H	304	CLA	O2D-CGD-O1D	-2.25	119.44	123.84
25	L	302	CLA	CAC-C3C-C4C	2.25	127.73	124.81
30	A	850	BCR	C24-C23-C22	-2.25	122.84	126.23
24	S	305	CHL	CBC-CAC-C3C	2.25	118.63	112.43
25	V	310	CLA	CHD-C1D-ND	-2.25	122.39	124.45
25	B	815	CLA	CMA-C3A-C4A	2.25	117.82	111.77
25	A	838	CLA	O2A-C1-C2	-2.25	102.72	108.64
24	P	305	CHL	CMA-C3A-C4A	2.25	117.81	111.77
37	R	321	NEX	O24-C25-C38	2.25	117.75	115.06
25	5	601	CLA	CMA-C3A-C4A	2.25	117.81	111.77
24	4	302	CHL	C2A-C1A-CHA	2.25	127.79	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	2	617	XAT	C4-C3-C2	-2.25	106.43	110.77
25	A	822	CLA	CHB-C4A-NA	2.25	127.62	124.51
27	3	316	XAT	C24-C23-C22	-2.25	106.44	110.77
25	5	603	CLA	CHA-C1A-NA	-2.24	121.26	126.40
25	B	808	CLA	O2D-CGD-O1D	-2.24	119.45	123.84
24	6	606	CHL	C4A-NA-C1A	2.24	107.72	106.71
30	B	849	BCR	C33-C5-C6	2.24	127.05	124.53
25	A	821	CLA	C16-C15-C13	-2.24	108.67	115.92
29	U	317	Q6L	C12-C13-C14	-2.24	115.19	121.98
25	5	604	CLA	CHB-C4A-NA	2.24	127.61	124.51
25	W	312	CLA	O2D-CGD-CBD	2.24	115.25	111.27
25	1	603	CLA	C1C-C2C-C3C	-2.24	104.60	106.96
30	A	851	BCR	C2-C3-C4	-2.24	106.36	111.38
24	4	306	CHL	OMC-CMC-C2C	-2.24	120.62	125.69
33	A	802	CL0	CMB-C2B-C3B	2.24	128.87	124.68
24	V	314	CHL	CHB-C4A-NA	2.24	127.61	124.51
30	I	101	BCR	C35-C13-C12	2.24	121.61	118.08
25	R	314	CLA	CMA-C3A-C4A	2.24	117.80	111.77
25	X	312	CLA	C5-C3-C2	2.24	126.04	120.50
25	A	819	CLA	O2A-CGA-O1A	-2.24	117.94	123.59
25	T	309	CLA	C1D-ND-C4D	-2.24	104.75	106.33
25	A	825	CLA	CHB-C4A-NA	2.24	127.61	124.51
30	A	850	BCR	C29-C30-C25	-2.24	107.04	110.48
25	U	310	CLA	C2A-C1A-CHA	2.24	127.77	123.86
25	4	309	CLA	C4D-CHA-C1A	2.24	123.97	121.25
30	H	305	BCR	C16-C15-C14	-2.24	118.89	123.47
24	Q	308	CHL	C3D-C2D-C1D	2.24	108.88	105.83
25	B	831	CLA	C2D-C1D-ND	-2.24	108.46	110.10
25	3	301	CLA	C3B-C4B-NB	2.24	112.10	109.21
25	T	301	CLA	C6-C5-C3	2.24	119.32	113.45
25	L	303	CLA	O2A-CGA-O1A	-2.24	117.73	123.30
25	B	821	CLA	C1-O2A-CGA	-2.24	110.58	116.44
37	R	321	NEX	C31-C30-C29	-2.24	124.12	127.31
30	A	851	BCR	C20-C19-C18	-2.24	120.14	126.42
26	R	303	IWJ	C21-C19-C18	-2.23	115.51	118.94
25	V	310	CLA	CAC-C3C-C4C	2.23	127.71	124.81
30	G	201	BCR	C20-C21-C22	-2.23	124.12	127.31
25	L	303	CLA	C2A-C1A-CHA	2.23	127.76	123.86
25	A	839	CLA	CHD-C1D-ND	-2.23	122.40	124.45
25	W	309	CLA	C6-C5-C3	2.23	119.31	113.45
24	P	304	CHL	CED-O2D-CGD	2.23	120.99	115.94
30	B	848	BCR	C40-C30-C25	2.23	113.92	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	X	313	CLA	CHD-C1D-ND	-2.23	122.40	124.45
25	A	845	CLA	O2D-CGD-O1D	-2.23	119.47	123.84
25	S	313	CLA	CMA-C3A-C2A	-2.23	110.89	116.10
24	T	306	CHL	CAC-C3C-C4C	2.23	127.70	124.81
25	V	302	CLA	CHB-C4A-NA	2.23	127.60	124.51
24	P	304	CHL	C1D-CHD-C4C	-2.23	121.25	126.06
25	B	809	CLA	CHD-C1D-ND	-2.23	122.40	124.45
36	A	854	DGD	C4D-C3D-C2D	-2.23	106.93	110.82
30	F	801	BCR	C16-C17-C18	-2.23	124.13	127.31
25	3	304	CLA	CHB-C4A-NA	2.23	127.59	124.51
36	A	854	DGD	O2E-C2E-C1E	-2.23	104.63	110.05
30	3	317	BCR	C24-C23-C22	-2.23	122.87	126.23
25	B	809	CLA	CBA-CAA-C2A	2.23	120.44	113.86
25	L	303	CLA	CMC-C2C-C1C	2.23	128.43	125.04
24	R	310	CHL	O2A-CGA-O1A	-2.23	117.97	123.59
25	B	828	CLA	CAA-C2A-C3A	-2.23	106.68	112.78
30	F	801	BCR	C37-C22-C23	2.23	121.59	118.08
25	P	311	CLA	CBA-CAA-C2A	2.23	120.44	113.86
25	1	602	CLA	CMC-C2C-C1C	2.23	128.43	125.04
25	S	309	CLA	CHD-C1D-ND	-2.23	122.41	124.45
29	T	319	Q6L	C42-C13-C12	2.23	119.02	115.27
30	K	207	BCR	C34-C9-C10	-2.23	119.81	122.92
30	A	849	BCR	C16-C15-C14	-2.23	118.92	123.47
30	4	319	BCR	C11-C10-C9	-2.22	124.14	127.31
38	V	308	KC2	C2A-C1A-NA	2.22	112.97	109.40
25	B	814	CLA	CMC-C2C-C1C	2.22	128.43	125.04
27	1	612	XAT	C40-C33-C32	2.22	121.58	118.08
25	4	303	CLA	CMC-C2C-C1C	2.22	128.42	125.04
25	4	310	CLA	C4-C3-C2	-2.22	117.98	123.68
25	P	301	CLA	CAC-C3C-C4C	2.22	127.69	124.81
38	T	308	KC2	CHC-C4B-NB	2.22	126.49	124.45
25	B	840	CLA	O1D-CGD-CBD	2.22	129.03	124.48
25	S	313	CLA	C2D-C1D-ND	-2.22	108.47	110.10
38	S	308	KC2	CMD-C2D-C1D	-2.22	125.05	128.46
24	P	304	CHL	C3B-C4B-NB	-2.22	106.34	109.21
30	A	850	BCR	C37-C22-C23	2.22	121.57	118.08
25	6	602	CLA	CAC-C3C-C4C	2.22	127.69	124.81
30	3	317	BCR	C35-C13-C12	2.22	121.57	118.08
25	B	818	CLA	CHD-C1D-ND	-2.22	122.42	124.45
25	S	312	CLA	CMB-C2B-C3B	2.22	128.82	124.68
25	B	809	CLA	C4-C3-C2	-2.22	117.99	123.68
27	4	318	XAT	C12-C13-C14	-2.22	115.54	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	X	316	Q6L	C28-C27-C26	2.22	126.03	122.92
25	B	810	CLA	O2D-CGD-CBD	2.21	115.20	111.27
25	3	305	CLA	CMC-C2C-C1C	2.21	128.41	125.04
37	T	317	NEX	C16-C1-C6	2.21	112.45	110.47
25	A	830	CLA	CAC-C3C-C4C	2.21	127.68	124.81
25	B	821	CLA	C6-C5-C3	2.21	119.26	113.45
25	1	602	CLA	CHB-C4A-NA	2.21	127.57	124.51
25	B	822	CLA	CHB-C4A-NA	2.21	127.57	124.51
25	S	303	CLA	CHD-C1D-ND	-2.21	122.42	124.45
27	1	612	XAT	O4-C5-C6	-2.21	57.13	58.96
25	L	304	CLA	O2D-CGD-O1D	-2.21	119.51	123.84
25	3	310	CLA	CED-O2D-CGD	2.21	120.94	115.94
26	W	318	IWJ	C32-C30-C31	2.21	125.47	121.10
25	U	310	CLA	C4D-CHA-C1A	2.21	123.94	121.25
26	U	316	IWJ	C05-C04-C03	2.21	114.26	111.74
25	V	309	CLA	C4A-NA-C1A	2.21	107.70	106.71
25	V	302	CLA	C2C-C1C-NC	2.21	112.04	109.97
26	Q	303	IWJ	C36-C35-C34	-2.21	105.14	108.98
25	3	302	CLA	O1D-CGD-CBD	2.21	129.01	124.48
25	3	311	CLA	O2D-CGD-O1D	-2.21	119.07	124.09
25	P	301	CLA	O2A-CGA-O1A	-2.21	118.02	123.59
25	A	833	CLA	CBA-CAA-C2A	2.21	120.39	113.86
25	N	202	CLA	C3A-C2A-C1A	2.21	104.65	101.34
25	B	802	CLA	CBA-CAA-C2A	2.21	120.38	113.86
24	1	604	CHL	C1D-CHD-C4C	-2.21	121.29	126.06
25	Q	312	CLA	O1D-CGD-CBD	2.21	129.00	124.48
25	P	302	CLA	O2A-CGA-O1A	-2.21	118.02	123.59
24	U	304	CHL	CAC-C3C-C4C	2.21	127.67	124.81
27	2	617	XAT	C35-C34-C33	-2.21	124.16	127.31
26	W	318	IWJ	C36-C35-C34	-2.21	105.15	108.98
25	A	809	CLA	O2D-CGD-O1D	-2.21	119.52	123.84
25	Q	315	CLA	O2A-CGA-CBA	2.21	118.83	111.91
25	A	825	CLA	O2A-C1-C2	2.21	114.44	108.64
25	4	312	CLA	CHD-C1D-ND	-2.21	122.43	124.45
30	L	307	BCR	C30-C25-C26	2.21	125.72	122.61
25	3	311	CLA	C3A-C2A-C1A	2.21	104.64	101.34
25	B	842	CLA	CMC-C2C-C1C	2.21	128.40	125.04
25	5	609	CLA	CHD-C1D-ND	-2.20	122.43	124.45
25	Q	301	CLA	CHD-C1D-ND	-2.20	122.43	124.45
25	W	311	CLA	CHA-C1A-NA	-2.20	121.35	126.40
25	F	802	CLA	CHB-C4A-NA	2.20	127.56	124.51
25	A	827	CLA	CMA-C3A-C4A	2.20	117.70	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	5	603	CLA	CMC-C2C-C1C	2.20	128.39	125.04
25	V	310	CLA	CMC-C2C-C1C	2.20	128.39	125.04
24	R	309	CHL	CHB-C4A-NA	2.20	127.56	124.51
25	2	603	CLA	CHB-C4A-NA	2.20	127.56	124.51
29	V	319	Q6L	C01-C02-C07	-2.20	110.28	114.36
25	3	309	CLA	CHB-C4A-NA	2.20	127.56	124.51
26	Q	303	IWJ	C21-C19-C18	-2.20	115.56	118.94
25	P	301	CLA	C6-C5-C3	2.20	119.23	113.45
25	B	841	CLA	O2A-CGA-O1A	-2.20	118.03	123.59
30	3	319	BCR	C34-C9-C10	2.20	126.01	122.92
24	U	305	CHL	O2D-CGD-CBD	2.20	115.18	111.27
25	B	827	CLA	C1C-C2C-C3C	-2.20	104.64	106.96
25	A	842	CLA	C1C-C2C-C3C	-2.20	104.64	106.96
25	B	826	CLA	C1B-CHB-C4A	-2.20	125.76	130.12
25	O	2005	CLA	CMA-C3A-C2A	-2.20	110.97	116.10
25	Q	304	CLA	O2A-CGA-CBA	2.20	118.81	111.91
26	V	318	IWJ	C23-C22-C21	-2.20	116.35	123.22
25	W	313	CLA	O2D-CGD-O1D	-2.20	119.54	123.84
25	T	312	CLA	O2D-CGD-CBD	2.20	115.17	111.27
24	4	302	CHL	CMB-C2B-C3B	2.20	128.79	124.68
25	A	834	CLA	C6-C5-C3	2.20	119.22	113.45
25	A	835	CLA	C5-C3-C2	2.20	125.56	121.12
25	Q	306	CLA	CHA-C1A-NA	-2.20	121.37	126.40
25	A	804	CLA	C3C-C4C-NC	-2.20	108.11	110.57
29	W	315	Q6L	C05-C06-C07	2.20	113.31	110.30
25	B	841	CLA	CAA-C2A-C3A	-2.20	106.77	112.78
24	Q	316	CHL	C1C-C2C-C3C	-2.19	105.37	107.11
25	V	311	CLA	CHD-C1D-ND	-2.19	122.44	124.45
26	X	318	IWJ	C23-C22-C21	-2.19	116.37	123.22
25	B	808	CLA	CAC-C3C-C2C	-2.19	123.78	127.53
29	S	321	Q6L	C19-C20-C21	-2.19	118.98	123.47
33	A	802	CL0	O2A-CGA-O1A	-2.19	118.06	123.59
25	B	809	CLA	CMB-C2B-C1B	-2.19	125.09	128.46
29	S	323	Q6L	C24-C22-C21	-2.19	115.58	118.94
25	S	302	CLA	CHD-C1D-ND	-2.19	122.44	124.45
25	A	821	CLA	C2A-C1A-CHA	2.19	127.69	123.86
30	K	202	BCR	C40-C30-C25	2.19	113.85	110.30
25	B	812	CLA	C2C-C1C-NC	2.19	112.02	109.97
27	4	318	XAT	O23-C23-C24	-2.19	105.45	109.80
29	T	315	Q6L	C12-C13-C14	-2.19	115.35	121.98
38	S	308	KC2	CHB-C1B-NB	2.19	126.47	124.45
25	V	301	CLA	CHD-C1D-ND	-2.19	122.44	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	B	828	CLA	CHA-C1A-NA	-2.19	121.39	126.40
25	K	203	CLA	C1-O2A-CGA	2.19	122.18	116.44
25	B	813	CLA	O2A-C1-C2	2.19	114.38	108.64
25	O	2002	CLA	CAA-CBA-CGA	2.19	119.64	113.25
38	Q	310	KC2	CAC-C3C-C2C	-2.19	121.40	128.60
25	K	203	CLA	C1C-C2C-C3C	-2.19	104.66	106.96
25	A	843	CLA	CBA-CAA-C2A	2.19	120.31	113.86
25	P	303	CLA	C1-C2-C3	-2.19	123.22	126.75
37	S	317	NEX	C35-C34-C33	-2.18	124.19	127.31
25	Q	305	CLA	CHB-C4A-NA	2.18	127.53	124.51
25	T	301	CLA	O2A-CGA-O1A	-2.18	118.08	123.59
30	B	847	BCR	C33-C5-C6	-2.18	122.08	124.53
25	3	308	CLA	O2D-CGD-O1D	-2.18	119.57	123.84
24	T	306	CHL	O2A-CGA-O1A	-2.18	118.08	123.59
25	5	610	CLA	CHB-C4A-NA	2.18	127.53	124.51
25	1	610	CLA	C4D-C3D-CAD	-2.18	105.52	108.10
38	P	308	KC2	O1A-CGA-CBA	2.18	127.81	120.99
25	2	614	CLA	CHB-C4A-NA	2.18	127.53	124.51
25	L	302	CLA	O2D-CGD-O1D	-2.18	119.57	123.84
25	B	831	CLA	C1-O2A-CGA	2.18	122.17	116.44
29	S	323	Q6L	C35-C34-C33	2.18	114.22	111.74
25	1	603	CLA	CBA-CAA-C2A	2.18	120.30	113.86
25	B	835	CLA	CMB-C2B-C3B	2.18	128.76	124.68
25	A	829	CLA	O1D-CGD-CBD	2.18	128.95	124.48
25	W	302	CLA	CAC-C3C-C4C	2.18	127.64	124.81
25	A	822	CLA	O1D-CGD-CBD	2.18	128.94	124.48
30	2	618	BCR	C38-C26-C27	2.18	117.80	113.62
25	X	303	CLA	O2A-CGA-O1A	-2.18	118.09	123.59
24	T	305	CHL	OMC-CMC-C2C	-2.18	120.76	125.69
25	3	307	CLA	C5-C3-C2	2.18	125.53	121.12
25	A	806	CLA	O2D-CGD-CBD	2.18	115.14	111.27
25	T	301	CLA	C2A-C1A-CHA	2.18	127.67	123.86
24	T	306	CHL	C4-C3-C2	-2.18	118.09	123.68
25	N	203	CLA	C1B-CHB-C4A	-2.18	125.81	130.12
30	3	318	BCR	C21-C20-C19	2.18	130.01	123.22
25	A	804	CLA	C1D-ND-C4D	2.17	107.88	106.33
24	T	320	CHL	C4-C3-C5	-2.17	113.50	115.98
25	B	832	CLA	CHD-C1D-C2D	2.17	130.04	125.48
28	3	322	LHG	C25-C24-C23	-2.17	105.71	113.62
25	A	830	CLA	O2A-CGA-CBA	2.17	118.73	111.91
25	B	812	CLA	C1B-CHB-C4A	-2.17	125.81	130.12
25	4	314	CLA	CMC-C2C-C1C	2.17	128.35	125.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	T	311	CLA	O2D-CGD-O1D	-2.17	119.59	123.84
25	1	610	CLA	CHB-C4A-NA	2.17	127.52	124.51
30	M	101	BCR	C11-C12-C13	-2.17	120.31	126.42
25	B	828	CLA	CHD-C1D-ND	-2.17	122.46	124.45
30	A	849	BCR	C35-C13-C12	2.17	121.50	118.08
25	B	802	CLA	C15-C13-C12	2.17	123.54	112.13
25	B	809	CLA	C11-C10-C8	-2.17	108.90	115.92
24	R	308	CHL	O2A-CGA-O1A	-2.17	117.89	123.30
25	4	312	CLA	CAC-C3C-C4C	2.17	127.63	124.81
25	V	311	CLA	C1-C2-C3	-2.17	122.29	126.04
25	K	204	CLA	CAC-C3C-C4C	2.17	127.62	124.81
25	1	610	CLA	CMC-C2C-C1C	2.17	128.34	125.04
27	6	615	XAT	C19-C9-C8	2.17	121.50	118.08
25	A	828	CLA	CHD-C1D-C2D	2.17	130.03	125.48
25	A	817	CLA	CHA-C1A-NA	-2.17	121.43	126.40
29	U	314	Q6L	C01-C02-C03	2.17	127.34	124.49
25	N	203	CLA	CHA-C4D-ND	2.17	137.03	132.50
25	Q	312	CLA	CHD-C1D-ND	-2.17	122.46	124.45
30	I	101	BCR	C38-C26-C27	2.17	117.78	113.62
24	6	601	CHL	C2C-C3C-C4C	2.17	108.09	106.49
25	O	2002	CLA	C11-C12-C13	-2.17	108.91	115.92
24	U	306	CHL	CAC-C3C-C4C	2.17	127.62	124.81
29	2	616	Q6L	C01-C02-C07	-2.17	110.34	114.36
25	B	827	CLA	CMC-C2C-C1C	2.17	128.34	125.04
38	W	308	KC2	O2A-CGA-O1A	-2.17	118.17	122.67
25	3	302	CLA	CHA-C1A-NA	-2.17	121.44	126.40
25	V	309	CLA	CAA-C2A-C3A	2.17	119.67	114.26
25	Q	313	CLA	O2D-CGD-O1D	-2.17	119.60	123.84
25	A	831	CLA	C2C-C1C-NC	2.17	112.00	109.97
24	T	320	CHL	C2A-C1A-CHA	2.17	127.65	123.86
30	L	306	BCR	C35-C13-C12	2.17	121.49	118.08
30	L	305	BCR	C12-C13-C14	-2.17	115.62	118.94
25	A	808	CLA	CHA-C4D-ND	2.17	137.03	132.50
24	V	304	CHL	C4A-NA-C1A	2.16	107.68	106.71
25	B	804	CLA	O2A-CGA-O1A	-2.16	118.13	123.59
38	P	308	KC2	C3C-C2C-C1C	2.16	108.09	106.49
25	1	613	CLA	C4-C3-C2	-2.16	118.13	123.68
25	A	804	CLA	CHD-C1D-C2D	2.16	130.02	125.48
25	2	610	CLA	O1D-CGD-CBD	2.16	128.91	124.48
38	P	308	KC2	C4C-C3C-C2C	-2.16	105.40	107.11
25	A	815	CLA	C1B-CHB-C4A	-2.16	125.83	130.12
31	N	201	LMG	O8-C28-C29	2.16	118.69	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	B	842	CLA	C1-O2A-CGA	-2.16	110.78	116.44
25	A	821	CLA	CAC-C3C-C4C	2.16	127.61	124.81
25	A	829	CLA	CBC-CAC-C3C	2.16	118.39	112.43
25	A	815	CLA	O1A-CGA-CBA	2.16	132.16	123.73
24	V	314	CHL	C2D-C1D-ND	-2.16	108.51	110.10
25	B	843	CLA	CAA-C2A-C3A	-2.16	106.87	112.78
30	B	845	BCR	C24-C23-C22	-2.16	122.97	126.23
38	X	309	KC2	C3C-C2C-C1C	2.16	108.09	106.49
25	2	612	CLA	CHA-C1A-NA	-2.16	121.46	126.40
25	3	303	CLA	C4C-C3C-C2C	-2.16	105.09	107.07
25	V	311	CLA	O2A-CGA-O1A	-2.16	118.15	123.59
25	A	842	CLA	CED-O2D-CGD	2.16	120.81	115.94
25	2	608	CLA	CHB-C4A-NA	2.16	127.49	124.51
25	2	604	CLA	CMC-C2C-C1C	2.16	128.32	125.04
25	H	301	CLA	CHA-C1A-NA	-2.16	121.46	126.40
27	2	617	XAT	C25-C24-C23	-2.16	108.48	112.75
24	P	306	CHL	CAA-C2A-C3A	2.16	118.68	112.78
25	B	840	CLA	CHB-C4A-NA	2.16	127.49	124.51
38	W	308	KC2	CAA-C2A-C1A	-2.15	114.84	124.75
25	4	311	CLA	CHA-C1A-NA	-2.15	121.46	126.40
25	B	808	CLA	O1D-CGD-CBD	2.15	128.89	124.48
24	T	320	CHL	CAC-C3C-C4C	2.15	127.60	124.81
30	K	202	BCR	C8-C7-C6	-2.15	121.16	127.20
25	R	314	CLA	CHA-C1A-NA	-2.15	121.47	126.40
25	2	602	CLA	O2A-CGA-CBA	2.15	118.66	111.91
25	F	802	CLA	C1C-C2C-C3C	-2.15	104.69	106.96
24	X	308	CHL	OMC-CMC-C2C	-2.15	120.82	125.69
25	B	818	CLA	CAC-C3C-C4C	2.15	127.60	124.81
25	F	803	CLA	CHB-C4A-NA	2.15	127.48	124.51
25	B	831	CLA	C3C-C4C-NC	-2.15	108.16	110.57
27	1	612	XAT	C11-C12-C13	-2.15	120.38	126.42
25	A	843	CLA	C7-C6-C5	-2.15	107.52	113.36
25	W	312	CLA	C3A-C2A-C1A	2.15	104.56	101.34
29	R	319	Q6L	C01-C02-C07	-2.15	110.38	114.36
25	2	612	CLA	CMC-C2C-C1C	2.15	128.31	125.04
26	T	318	IWJ	C36-C35-C34	-2.15	105.25	108.98
24	V	314	CHL	C1C-C2C-C3C	-2.15	105.41	107.11
25	A	816	CLA	CAA-CBA-CGA	2.15	118.20	112.51
25	4	305	CLA	CMB-C2B-C3B	2.15	128.89	124.69
25	5	601	CLA	C3A-C2A-C1A	2.15	104.55	101.34
25	4	314	CLA	CHB-C4A-NA	2.15	127.48	124.51
25	A	838	CLA	CHA-C1A-NA	-2.15	121.48	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	4	309	CLA	C4A-NA-C1A	2.14	107.67	106.71
25	U	303	CLA	C1-C2-C3	-2.14	123.28	126.75
25	Q	304	CLA	C1D-ND-C4D	-2.14	104.81	106.33
29	Q	319	Q6L	C35-C34-C33	2.14	114.18	111.74
24	2	607	CHL	CHD-C1D-ND	-2.14	122.48	124.45
24	T	305	CHL	C1B-CHB-C4A	-2.14	125.87	130.12
24	W	307	CHL	CBA-CAA-C2A	2.14	120.19	113.86
25	A	832	CLA	CHB-C4A-NA	2.14	127.48	124.51
37	T	317	NEX	C36-C21-C22	-2.14	105.26	108.98
30	A	848	BCR	C32-C1-C6	2.14	113.78	110.30
25	3	308	CLA	CED-O2D-CGD	2.14	120.78	115.94
25	U	308	CLA	CHB-C4A-NA	2.14	127.47	124.51
30	4	319	BCR	C7-C6-C5	-2.14	116.27	121.46
25	Q	301	CLA	C3A-C2A-C1A	2.14	104.55	101.34
25	A	819	CLA	CMB-C2B-C1B	-2.14	125.17	128.46
29	V	315	Q6L	C05-C06-C07	2.14	113.23	110.30
24	R	302	CHL	O2D-CGD-CBD	2.14	115.07	111.27
25	P	309	CLA	C1-C2-C3	-2.14	122.34	126.04
31	B	801	LMG	C3-C4-C5	2.14	114.06	110.24
25	2	613	CLA	OBD-CAD-C3D	2.14	133.67	128.52
25	B	810	CLA	CHB-C4A-NA	2.14	127.47	124.51
25	A	825	CLA	C6-C5-C3	2.14	119.06	113.45
30	H	305	BCR	C34-C9-C8	-2.14	114.71	118.08
25	X	304	CLA	CAC-C3C-C4C	2.14	127.58	124.81
25	R	316	CLA	O2A-CGA-O1A	-2.14	118.19	123.59
25	B	837	CLA	CHB-C4A-NA	2.14	127.47	124.51
26	R	303	IWJ	C36-C35-C34	-2.14	105.27	108.98
25	W	303	CLA	C3A-C2A-C1A	2.14	104.54	101.34
25	A	803	CLA	C4-C3-C5	2.14	118.87	115.27
30	H	305	BCR	C35-C13-C12	2.14	121.44	118.08
25	4	311	CLA	CMB-C2B-C3B	2.14	128.68	124.68
26	U	316	IWJ	C17-C16-C15	-2.14	119.10	123.47
25	2	611	CLA	C1B-CHB-C4A	-2.14	125.89	130.12
25	B	816	CLA	CBA-CAA-C2A	2.14	120.17	113.86
29	S	323	Q6L	C01-C02-C07	-2.14	110.40	114.36
25	A	805	CLA	C1B-CHB-C4A	-2.14	125.89	130.12
25	A	829	CLA	O2A-CGA-O1A	-2.13	118.20	123.59
27	5	612	XAT	C15-C35-C34	-2.13	119.10	123.47
25	B	822	CLA	O1D-CGD-CBD	2.13	128.85	124.48
25	X	304	CLA	CMA-C3A-C4A	-2.13	106.04	111.77
24	R	308	CHL	C2A-C1A-CHA	2.13	127.59	123.86
24	3	306	CHL	O1D-CGD-CBD	2.13	128.85	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	4	315	CLA	CMA-C3A-C2A	-2.13	111.12	116.10
26	3	315	IWJ	C21-C19-C18	-2.13	115.67	118.94
36	B	850	DGD	O4D-C4D-C3D	2.13	115.28	110.35
25	3	305	CLA	CMB-C2B-C3B	2.13	128.86	124.69
38	X	309	KC2	CHB-C4A-C3A	-2.13	121.65	124.98
37	R	321	NEX	C35-C15-C14	-2.13	119.11	123.47
25	X	302	CLA	CMC-C2C-C1C	2.13	128.29	125.04
24	X	305	CHL	CAA-C2A-C3A	-2.13	111.12	116.10
25	T	310	CLA	CHB-C4A-NA	2.13	127.46	124.51
25	B	834	CLA	C2C-C1C-NC	2.13	111.97	109.97
29	T	315	Q6L	C05-C06-C07	2.13	113.22	110.30
25	T	311	CLA	CAA-C2A-C3A	-2.13	106.94	112.78
26	T	321	IWJ	C36-C35-C34	-2.13	105.28	108.98
25	B	812	CLA	O2A-CGA-O1A	-2.13	118.22	123.59
30	A	849	BCR	C20-C19-C18	-2.13	120.43	126.42
25	3	302	CLA	O2D-CGD-O1D	-2.13	119.67	123.84
25	3	312	CLA	CMC-C2C-C1C	2.13	128.28	125.04
25	P	311	CLA	CMC-C2C-C1C	2.13	128.28	125.04
30	B	848	BCR	C33-C5-C6	-2.13	122.14	124.53
25	6	602	CLA	C1B-CHB-C4A	-2.13	125.90	130.12
25	B	803	CLA	CMD-C2D-C3D	2.13	132.51	127.61
25	4	311	CLA	CAC-C3C-C4C	2.13	127.57	124.81
25	A	839	CLA	C3A-C2A-C1A	2.13	104.53	101.34
25	A	831	CLA	C1B-CHB-C4A	-2.13	125.90	130.12
25	B	832	CLA	CHD-C1D-ND	-2.13	122.50	124.45
25	B	826	CLA	C1-O2A-CGA	2.13	122.03	116.44
25	2	608	CLA	CBA-CAA-C2A	2.13	120.14	113.86
25	4	316	CLA	CGD-CBD-CAD	2.13	117.63	110.73
25	G	202	CLA	C1B-CHB-C4A	-2.13	125.90	130.12
25	A	827	CLA	CHA-C1A-NA	-2.13	121.53	126.40
26	1	611	IWJ	C36-C35-C34	-2.13	105.29	108.98
25	W	309	CLA	C2D-C1D-ND	-2.13	108.54	110.10
28	2	619	LHG	O8-C6-C5	-2.13	102.24	108.43
25	W	309	CLA	C1-C2-C3	-2.13	122.36	126.04
24	T	307	CHL	O2D-CGD-O1D	-2.13	119.68	123.84
25	B	806	CLA	C1-O2A-CGA	-2.13	110.86	116.44
26	V	320	IWJ	C22-C21-C19	2.13	132.39	126.42
25	3	314	CLA	CBC-CAC-C3C	-2.13	106.57	112.43
30	L	306	BCR	C16-C17-C18	-2.13	124.28	127.31
24	W	307	CHL	C5-C3-C2	2.12	125.42	121.12
25	B	819	CLA	C2D-C1D-ND	-2.12	108.54	110.10
25	3	305	CLA	CBA-CAA-C2A	2.12	118.19	113.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	S	310	CLA	CHA-C1A-NA	-2.12	121.53	126.40
25	4	315	CLA	CHB-C4A-NA	2.12	127.45	124.51
25	W	311	CLA	C2A-C1A-CHA	2.12	127.57	123.86
25	B	808	CLA	CHA-C1A-NA	-2.12	121.54	126.40
25	G	204	CLA	CAC-C3C-C4C	2.12	127.56	124.81
29	T	316	Q6L	C25-C26-C27	2.12	130.34	127.31
38	V	308	KC2	CAC-C3C-C4C	2.12	134.35	124.47
25	A	838	CLA	O1A-CGA-CBA	2.12	132.01	123.73
25	T	302	CLA	CAC-C3C-C4C	2.12	127.56	124.81
25	V	312	CLA	O1D-CGD-CBD	2.12	128.82	124.48
30	A	849	BCR	C12-C13-C14	-2.12	115.69	118.94
25	W	303	CLA	CHB-C4A-NA	2.12	127.44	124.51
25	B	820	CLA	C1C-C2C-C3C	-2.12	104.73	106.96
25	Q	301	CLA	CHA-C1A-NA	-2.12	121.55	126.40
25	W	313	CLA	CHB-C4A-NA	2.12	127.44	124.51
24	1	601	CHL	C2A-C1A-CHA	2.12	127.56	123.86
30	L	305	BCR	C2-C1-C6	-2.12	107.22	110.48
25	W	301	CLA	CAA-C2A-C1A	-2.12	105.04	111.97
25	X	302	CLA	CHA-C1A-NA	-2.12	121.55	126.40
24	1	601	CHL	C3C-C4C-NC	-2.12	108.20	110.57
29	U	315	Q6L	C20-C21-C22	2.12	130.33	127.31
25	B	812	CLA	O2D-CGD-O1D	-2.12	119.70	123.84
25	U	312	CLA	CMA-C3A-C2A	-2.12	111.16	116.10
24	S	304	CHL	CAC-C3C-C4C	2.11	127.55	124.81
30	A	848	BCR	C37-C22-C23	2.11	121.41	118.08
26	5	611	IWJ	C12-C11-C10	-2.11	124.29	127.31
30	A	849	BCR	C11-C12-C13	-2.11	120.48	126.42
25	1	602	CLA	C1D-ND-C4D	-2.11	104.83	106.33
25	A	832	CLA	CHD-C1D-ND	-2.11	122.51	124.45
25	V	301	CLA	C4D-CHA-C1A	2.11	123.82	121.25
24	R	311	CHL	CHA-C4D-ND	2.11	136.92	132.50
25	S	311	CLA	O2A-CGA-O1A	-2.11	118.26	123.59
24	Q	309	CHL	O2D-CGD-CBD	2.11	115.02	111.27
25	K	206	CLA	CAA-C2A-C3A	2.11	118.56	112.78
26	S	319	IWJ	C36-C35-C34	-2.11	105.31	108.98
29	O	2007	Q6L	C42-C13-C12	2.11	118.83	115.27
25	A	830	CLA	O1D-CGD-CBD	2.11	128.81	124.48
25	A	809	CLA	CBA-CAA-C2A	2.11	120.10	113.86
37	S	317	NEX	C36-C21-C22	-2.11	105.31	108.98
25	B	829	CLA	CBA-CAA-C2A	2.11	120.10	113.86
26	Q	320	IWJ	C21-C19-C18	-2.11	115.70	118.94
38	T	308	KC2	CBD-CHA-C1A	2.11	132.82	128.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	P	321	Q6L	C01-C02-C03	2.11	127.27	124.49
25	X	312	CLA	CHD-C1D-ND	-2.11	122.52	124.45
25	Q	313	CLA	C2A-C1A-CHA	2.11	127.55	123.86
25	S	302	CLA	C3A-C2A-C1A	2.11	104.50	101.34
30	B	845	BCR	C23-C22-C21	-2.11	115.71	118.94
26	R	322	IWJ	C36-C35-C34	-2.11	105.32	108.98
29	T	316	Q6L	C19-C20-C21	-2.11	119.16	123.47
29	S	315	Q6L	C01-C02-C07	-2.11	110.45	114.36
29	Q	319	Q6L	C25-C26-C27	-2.11	124.30	127.31
25	B	802	CLA	C11-C10-C8	-2.11	109.11	115.92
24	X	308	CHL	C2A-C3A-C4A	-2.11	98.47	101.87
25	S	311	CLA	C2A-C3A-C4A	2.11	105.27	101.87
25	S	312	CLA	C4-C3-C5	2.10	118.81	115.27
30	J	103	BCR	C12-C13-C14	-2.10	115.71	118.94
25	S	303	CLA	O2A-CGA-O1A	-2.10	118.28	123.59
29	T	319	Q6L	C05-C06-C07	2.10	113.18	110.30
30	F	804	BCR	C29-C30-C25	-2.10	107.24	110.48
26	V	318	IWJ	C34-C33-C32	2.10	113.18	110.30
24	R	311	CHL	O2D-CGD-O1D	-2.10	119.73	123.84
24	T	305	CHL	CHA-C4D-ND	2.10	136.90	132.50
25	B	819	CLA	C4A-NA-C1A	2.10	107.65	106.71
25	B	841	CLA	C6-C5-C3	2.10	118.97	113.45
25	A	814	CLA	CHD-C1D-C2D	2.10	129.89	125.48
24	Q	316	CHL	CMA-C3A-C4A	2.10	117.42	111.77
25	R	305	CLA	C2C-C1C-NC	2.10	111.94	109.97
38	Q	310	KC2	O1A-CGA-CBA	2.10	127.55	120.99
24	X	305	CHL	CMB-C2B-C3B	2.10	128.61	124.68
25	B	808	CLA	CMA-C3A-C2A	-2.10	105.36	113.83
25	3	311	CLA	C6-C5-C3	-2.10	107.95	113.45
26	X	318	IWJ	C25-C24-C26	2.10	119.55	116.02
25	F	802	CLA	CHD-C1D-C2D	2.10	129.88	125.48
25	V	309	CLA	C3D-C4D-ND	2.10	113.63	110.24
25	A	835	CLA	CAA-CBA-CGA	-2.10	107.12	113.25
24	U	304	CHL	C3C-C4C-NC	-2.10	108.22	110.57
25	F	803	CLA	CAA-C2A-C3A	-2.10	111.20	116.10
38	X	309	KC2	C1B-CHB-C4A	2.10	130.58	126.06
24	P	304	CHL	C3A-C2A-C1A	2.10	104.48	101.34
25	A	842	CLA	O1D-CGD-CBD	2.10	128.78	124.48
25	S	313	CLA	CAA-C2A-C3A	-2.10	111.20	116.10
25	B	835	CLA	O1A-CGA-CBA	2.10	129.82	123.08
31	A	857	LMG	O8-C28-C29	2.10	118.49	111.91
25	F	803	CLA	O2D-CGD-O1D	-2.10	119.74	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	842	CLA	O2A-CGA-O1A	-2.10	118.30	123.59
25	X	312	CLA	C2A-C1A-CHA	2.10	127.52	123.86
25	B	809	CLA	C5-C3-C2	2.10	125.36	121.12
24	W	314	CHL	OMC-CMC-C2C	-2.10	120.95	125.69
30	J	101	BCR	C11-C12-C13	-2.10	120.53	126.42
38	P	308	KC2	CBD-CHA-C1A	2.09	132.79	128.88
25	B	834	CLA	CHD-C1D-C2D	2.09	129.87	125.48
25	A	813	CLA	O2D-CGD-CBD	2.09	114.99	111.27
25	A	838	CLA	CAA-C2A-C3A	2.09	118.51	112.78
28	3	323	LHG	O8-C23-C24	2.09	118.48	111.91
25	F	803	CLA	O2D-CGD-CBD	2.09	114.99	111.27
25	U	311	CLA	O2A-CGA-CBA	2.09	118.47	111.91
25	6	603	CLA	C2A-C1A-CHA	2.09	127.52	123.86
25	6	603	CLA	CMB-C2B-C3B	2.09	128.59	124.68
24	P	306	CHL	C2D-C1D-ND	-2.09	108.56	110.10
30	3	318	BCR	C11-C10-C9	-2.09	124.32	127.31
24	Q	307	CHL	O2A-CGA-O1A	-2.09	118.08	123.30
25	V	313	CLA	O2A-CGA-O1A	-2.09	118.31	123.59
25	H	301	CLA	C2A-C1A-CHA	2.09	127.52	123.86
25	A	830	CLA	O2A-C1-C2	2.09	114.13	108.64
25	1	608	CLA	CMC-C2C-C1C	2.09	128.22	125.04
25	X	313	CLA	CMA-C3A-C2A	-2.09	111.22	116.10
24	V	306	CHL	C2A-C1A-CHA	2.09	127.51	123.86
25	A	807	CLA	C1-C2-C3	2.09	129.66	126.04
25	R	315	CLA	C1B-CHB-C4A	-2.09	125.98	130.12
25	1	610	CLA	CBA-CAA-C2A	2.09	118.12	113.47
25	Q	306	CLA	C3D-C2D-C1D	-2.09	102.98	105.83
25	S	309	CLA	C2D-C1D-ND	-2.09	108.56	110.10
25	4	310	CLA	O2A-CGA-O1A	-2.09	118.32	123.59
25	S	301	CLA	O1D-CGD-CBD	2.09	128.76	124.48
33	A	802	CL0	CHA-C4D-ND	2.09	136.87	132.50
25	G	203	CLA	O2D-CGD-CBD	2.09	114.98	111.27
27	2	617	XAT	O23-C23-C24	2.09	113.95	109.80
31	J	104	LMG	O7-C10-C11	2.09	116.00	111.50
25	P	309	CLA	C6-C5-C3	2.09	118.93	113.45
25	3	302	CLA	CHA-C4D-ND	2.09	136.86	132.50
26	Q	320	IWJ	C05-C04-C03	2.09	114.11	111.74
24	6	601	CHL	CAA-C2A-C3A	2.09	119.47	114.26
29	O	2007	Q6L	C01-C02-C07	-2.09	110.49	114.36
25	K	206	CLA	C14-C13-C15	-2.09	103.74	111.29
25	A	840	CLA	C5-C3-C2	2.08	125.34	121.12
25	B	829	CLA	CHA-C4D-ND	2.08	136.86	132.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	3	323	LHG	C5-O7-C7	-2.08	112.66	117.79
25	B	809	CLA	CMB-C2B-C3B	2.08	128.58	124.68
25	W	309	CLA	CAA-CBA-CGA	-2.08	107.16	113.25
25	V	311	CLA	CHA-C1A-NA	-2.08	121.63	126.40
25	B	812	CLA	O1D-CGD-CBD	2.08	128.75	124.48
25	2	612	CLA	C11-C10-C8	2.08	122.65	115.92
25	A	816	CLA	CHD-C1D-C2D	2.08	129.85	125.48
29	R	319	Q6L	C12-C13-C14	-2.08	115.67	121.98
25	1	607	CLA	CMC-C2C-C1C	2.08	128.21	125.04
25	2	609	CLA	CBA-CAA-C2A	2.08	120.01	113.86
29	W	315	Q6L	C19-C20-C21	-2.08	119.21	123.47
29	Q	319	Q6L	C42-C13-C12	2.08	118.77	115.27
24	Q	307	CHL	CAC-C3C-C4C	2.08	127.51	124.81
25	R	313	CLA	CAA-C2A-C3A	2.08	118.48	112.78
29	P	321	Q6L	C05-C06-C07	2.08	113.15	110.30
25	4	305	CLA	CHB-C4A-NA	2.08	127.39	124.51
30	A	851	BCR	C27-C26-C25	-2.08	119.71	122.73
27	2	617	XAT	C24-C23-C22	-2.08	106.76	110.77
24	P	305	CHL	C3C-C4C-NC	-2.08	108.24	110.57
25	B	833	CLA	C1C-C2C-C3C	-2.08	104.77	106.96
31	N	201	LMG	C7-O1-C1	-2.08	109.68	113.74
25	P	301	CLA	CHD-C1D-ND	-2.08	122.55	124.45
29	Q	319	Q6L	C38-C36-C35	-2.08	105.50	109.44
27	3	316	XAT	C5-C4-C3	-2.07	108.64	112.75
24	4	302	CHL	O2A-CGA-O1A	-2.07	118.36	123.59
29	2	616	Q6L	C19-C20-C21	-2.07	119.22	123.47
25	X	311	CLA	CHB-C4A-NA	2.07	127.38	124.51
29	T	316	Q6L	C23-C22-C21	2.07	125.83	122.92
25	2	608	CLA	C2A-C1A-CHA	2.07	127.48	123.86
24	S	305	CHL	CHA-C4D-ND	2.07	136.84	132.50
25	R	315	CLA	CBA-CAA-C2A	2.07	119.98	113.86
29	U	317	Q6L	C01-C02-C07	-2.07	110.51	114.36
30	3	319	BCR	C27-C26-C25	-2.07	119.72	122.73
25	R	313	CLA	CMC-C2C-C1C	2.07	128.20	125.04
27	2	617	XAT	C15-C35-C34	-2.07	119.23	123.47
25	A	822	CLA	CHA-C1A-NA	-2.07	121.65	126.40
38	Q	310	KC2	CHB-C1B-NB	2.07	126.36	124.45
25	5	601	CLA	CHA-C1A-NA	-2.07	121.65	126.40
25	B	841	CLA	C3A-C2A-C1A	2.07	104.44	101.34
25	6	603	CLA	CHA-C4D-ND	2.07	136.83	132.50
25	R	315	CLA	CAC-C3C-C4C	2.07	127.50	124.81
25	2	602	CLA	C2C-C1C-NC	2.07	111.91	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	2	619	LHG	O8-C23-C24	2.07	118.41	111.91
38	Q	310	KC2	CHC-C4B-NB	2.07	126.36	124.45
24	U	313	CHL	C2D-C1D-ND	-2.07	108.58	110.10
26	S	319	IWJ	C23-C22-C21	-2.07	116.75	123.22
27	6	615	XAT	C40-C33-C34	2.07	125.82	122.92
25	B	838	CLA	C1B-CHB-C4A	-2.07	126.02	130.12
25	A	810	CLA	O2D-CGD-O1D	-2.07	119.79	123.84
25	K	201	CLA	O1A-CGA-CBA	2.07	129.73	123.08
25	U	310	CLA	CAA-C2A-C3A	-2.07	107.11	112.78
25	B	803	CLA	CMD-C2D-C1D	-2.07	121.07	124.71
27	1	612	XAT	C26-C27-C28	-2.07	121.62	125.99
25	U	303	CLA	O2A-CGA-O1A	-2.07	118.37	123.59
25	P	312	CLA	CBA-CAA-C2A	2.07	119.97	113.86
24	4	302	CHL	CHA-C1A-NA	-2.07	121.66	126.40
25	U	301	CLA	CHA-C1A-NA	-2.07	121.66	126.40
38	R	312	KC2	O1D-CGD-CBD	2.07	128.72	124.48
25	B	813	CLA	CHD-C1D-C2D	2.07	129.82	125.48
25	B	810	CLA	O2A-CGA-O1A	-2.07	118.37	123.59
24	T	306	CHL	C2A-C1A-CHA	2.07	127.47	123.86
25	1	606	CLA	CMC-C2C-C1C	2.07	128.19	125.04
27	2	617	XAT	C8-C9-C10	-2.07	115.77	118.94
25	X	312	CLA	C4-C3-C2	-2.07	118.38	123.68
38	S	308	KC2	O2A-CGA-O1A	-2.07	118.38	122.67
34	A	844	PQN	C19-C18-C17	-2.07	103.81	111.29
30	B	845	BCR	C12-C13-C14	-2.07	115.77	118.94
25	A	845	CLA	O1D-CGD-CBD	2.07	128.71	124.48
25	B	842	CLA	CHD-C1D-C2D	2.07	129.81	125.48
29	P	315	Q6L	C19-C20-C21	-2.07	119.24	123.47
38	R	312	KC2	CHB-C4A-NA	2.07	127.46	124.20
25	Q	313	CLA	CMC-C2C-C1C	2.07	128.18	125.04
38	U	307	KC2	CHB-C1B-NB	2.06	126.35	124.45
25	2	612	CLA	O2D-CGD-CBD	2.06	114.94	111.27
29	T	315	Q6L	C42-C13-C12	2.06	118.74	115.27
25	B	809	CLA	CMC-C2C-C1C	2.06	128.18	125.04
37	R	321	NEX	C15-C14-C13	-2.06	124.37	127.31
37	S	317	NEX	C40-C33-C32	2.06	121.33	118.08
24	W	306	CHL	CHD-C4C-C3C	2.06	127.87	124.84
37	W	317	NEX	C40-C33-C32	2.06	121.33	118.08
25	6	609	CLA	O2D-CGD-CBD	2.06	114.93	111.27
30	B	848	BCR	C29-C28-C27	-2.06	106.77	111.38
24	Q	316	CHL	CHA-C1A-NA	-2.06	121.68	126.40
25	3	314	CLA	CMC-C2C-C1C	2.06	128.18	125.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	K	204	CLA	CHA-C4D-ND	2.06	136.81	132.50
25	P	310	CLA	CHA-C1A-NA	-2.06	121.68	126.40
29	S	320	Q6L	C16-C17-C18	-2.06	115.78	118.94
26	P	320	IWJ	C36-C35-C34	-2.06	105.41	108.98
27	1	612	XAT	C4-C3-C2	-2.06	106.80	110.77
30	L	307	BCR	C7-C6-C5	-2.06	116.48	121.46
25	2	602	CLA	CAC-C3C-C4C	2.06	127.48	124.81
25	B	802	CLA	O2A-CGA-O1A	-2.06	118.40	123.59
29	Q	319	Q6L	C16-C17-C18	-2.06	115.79	118.94
30	K	202	BCR	C11-C12-C13	-2.06	120.64	126.42
24	T	320	CHL	CAA-CBA-CGA	-2.06	107.25	113.25
25	W	309	CLA	C5-C3-C2	-2.06	116.96	121.12
27	6	615	XAT	C37-C21-C22	2.06	112.55	108.98
25	B	809	CLA	C1C-C2C-C3C	-2.05	104.80	106.96
25	N	203	CLA	C4A-NA-C1A	2.05	107.63	106.71
25	X	303	CLA	C2C-C1C-NC	2.05	111.89	109.97
25	4	310	CLA	O2D-CGD-O1D	-2.05	119.83	123.84
26	6	614	IWJ	C17-C16-C15	-2.05	119.27	123.47
30	A	850	BCR	C31-C1-C2	2.05	117.11	108.91
30	3	319	BCR	C12-C13-C14	-2.05	115.79	118.94
32	6	617	SQD	C26-C25-C24	-2.05	105.82	113.19
29	P	315	Q6L	C01-C02-C07	-2.05	110.56	114.36
25	5	602	CLA	CBA-CAA-C2A	2.05	119.92	113.86
30	F	801	BCR	C40-C30-C39	-2.05	102.23	108.53
37	P	317	NEX	C36-C21-C22	-2.05	105.42	108.98
24	6	601	CHL	CHA-C1A-NA	-2.05	121.70	126.40
26	Q	303	IWJ	C25-C24-C26	2.05	119.47	116.02
25	X	302	CLA	C4-C3-C2	-2.05	118.42	123.68
25	A	804	CLA	CHB-C4A-NA	2.05	127.35	124.51
30	L	306	BCR	C12-C13-C14	-2.05	115.80	118.94
25	U	311	CLA	C1-C2-C3	-2.05	122.50	126.04
25	A	836	CLA	C5-C3-C2	2.05	125.26	121.12
26	X	318	IWJ	C36-C35-C34	-2.05	105.42	108.98
25	A	820	CLA	CHA-C4D-ND	2.05	136.78	132.50
25	6	612	CLA	CHB-C4A-NA	2.05	127.34	124.51
25	6	610	CLA	CHD-C1D-ND	-2.05	122.57	124.45
25	4	311	CLA	CMC-C2C-C1C	2.05	128.16	125.04
27	2	617	XAT	C37-C21-C36	-2.05	104.35	107.37
30	4	319	BCR	C12-C13-C14	-2.05	115.80	118.94
30	B	846	BCR	C11-C10-C9	-2.05	124.39	127.31
26	Q	320	IWJ	C36-C35-C34	-2.05	105.43	108.98
25	1	603	CLA	O2A-CGA-O1A	-2.05	118.43	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	B	845	BCR	C28-C27-C26	-2.04	110.43	114.08
30	B	849	BCR	C28-C27-C26	-2.04	110.43	114.08
25	B	805	CLA	O2A-CGA-O1A	-2.04	118.43	123.59
25	T	309	CLA	CAA-C2A-C3A	2.04	118.38	112.78
30	L	307	BCR	C27-C26-C25	-2.04	119.76	122.73
30	K	207	BCR	C38-C26-C27	2.04	117.54	113.62
25	T	302	CLA	C5-C3-C2	2.04	125.25	121.12
25	6	609	CLA	C2A-C1A-CHA	2.04	127.43	123.86
26	X	318	IWJ	C22-C23-C24	2.04	132.61	126.61
30	A	850	BCR	C8-C9-C10	-2.04	115.81	118.94
25	B	806	CLA	C2D-C1D-ND	-2.04	108.60	110.10
25	U	308	CLA	CBC-CAC-C3C	2.04	118.06	112.43
25	2	612	CLA	O2D-CGD-O1D	-2.04	119.85	123.84
26	X	318	IWJ	C33-C32-C30	2.04	115.53	112.04
25	B	807	CLA	O2A-CGA-O1A	-2.04	118.44	123.59
25	L	304	CLA	O1D-CGD-CBD	2.04	128.66	124.48
24	R	309	CHL	CHA-C4D-ND	2.04	136.77	132.50
25	O	2002	CLA	CHD-C1D-C2D	2.04	129.76	125.48
25	1	610	CLA	CHA-C1A-NA	-2.04	121.73	126.40
29	T	319	Q6L	C19-C20-C21	-2.04	119.30	123.47
26	S	319	IWJ	C33-C32-C30	2.04	115.52	112.04
25	B	804	CLA	C1-C2-C3	-2.04	122.52	126.04
30	H	305	BCR	C7-C8-C9	-2.04	123.16	126.23
29	P	321	Q6L	C19-C20-C21	-2.04	119.30	123.47
25	H	304	CLA	O2A-CGA-O1A	-2.04	118.22	123.30
25	G	204	CLA	O1A-CGA-CBA	2.04	129.63	123.08
25	1	606	CLA	CAA-C2A-C3A	-2.04	111.34	116.10
25	A	827	CLA	CHA-C4D-ND	2.04	136.76	132.50
25	K	201	CLA	CMC-C2C-C1C	2.04	128.14	125.04
25	A	831	CLA	CHA-C1A-NA	-2.04	121.73	126.40
29	X	301	Q6L	C24-C22-C21	-2.04	115.82	118.94
25	4	310	CLA	C5-C3-C2	2.03	125.23	121.12
29	S	321	Q6L	C38-C36-C35	-2.03	105.58	109.44
25	3	314	CLA	CHB-C4A-NA	2.03	127.33	124.51
30	A	848	BCR	C21-C20-C19	2.03	129.56	123.22
30	L	306	BCR	C16-C15-C14	-2.03	119.31	123.47
25	B	805	CLA	O2A-C1-C2	2.03	113.98	108.64
37	S	317	NEX	C11-C12-C13	-2.03	120.70	126.42
25	3	301	CLA	O1D-CGD-CBD	2.03	128.64	124.48
25	4	303	CLA	C2A-C1A-CHA	2.03	127.41	123.86
25	P	301	CLA	C1D-ND-C4D	-2.03	104.89	106.33
24	U	304	CHL	O2D-CGD-CBD	2.03	114.88	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	T	302	CLA	CHB-C4A-NA	2.03	127.32	124.51
25	A	831	CLA	O1D-CGD-CBD	2.03	128.64	124.48
25	B	814	CLA	CAC-C3C-C4C	2.03	127.45	124.81
25	1	603	CLA	C1B-CHB-C4A	-2.03	126.09	130.12
38	S	308	KC2	CBD-CHA-C1A	2.03	132.67	128.88
25	A	856	CLA	C2C-C1C-NC	2.03	111.88	109.97
25	B	832	CLA	C1D-ND-C4D	2.03	107.78	106.33
24	4	302	CHL	C3C-C4C-NC	-2.03	108.29	110.57
25	3	304	CLA	CHD-C1D-C2D	2.03	129.74	125.48
26	Q	303	IWJ	C33-C32-C30	2.03	115.51	112.04
25	A	831	CLA	CMC-C2C-C1C	2.03	128.13	125.04
30	B	849	BCR	C15-C16-C17	-2.03	119.31	123.47
25	A	827	CLA	C2D-C1D-ND	-2.03	108.61	110.10
25	X	304	CLA	O2D-CGD-CBD	2.03	114.88	111.27
30	J	103	BCR	C16-C15-C14	-2.03	119.32	123.47
29	T	316	Q6L	C35-C34-C33	2.03	114.05	111.74
24	P	305	CHL	O1A-CGA-CBA	2.03	129.60	123.08
30	4	319	BCR	C15-C16-C17	-2.03	119.32	123.47
24	6	606	CHL	O1D-CGD-CBD	2.03	128.64	124.48
25	H	302	CLA	C1C-C2C-C3C	-2.03	104.82	106.96
24	V	307	CHL	CMB-C2B-C1B	-2.03	125.35	128.46
25	3	309	CLA	CAC-C3C-C4C	2.03	127.44	124.81
25	A	838	CLA	C6-C7-C8	-2.03	109.36	115.92
25	6	610	CLA	O2A-CGA-O1A	-2.03	118.47	123.59
29	R	301	Q6L	C19-C20-C21	-2.03	119.32	123.47
25	1	607	CLA	CMD-C2D-C1D	2.03	129.24	125.36
25	5	607	CLA	C4-C3-C2	-2.03	118.48	123.68
29	S	315	Q6L	C12-C13-C14	-2.03	115.84	121.98
25	X	311	CLA	O2A-CGA-O1A	-2.03	118.48	123.59
24	Q	307	CHL	C1C-C2C-C3C	-2.03	105.51	107.11
25	T	311	CLA	CHA-C1A-NA	-2.03	121.76	126.40
26	S	318	IWJ	C05-C04-C03	2.03	114.05	111.74
30	J	101	BCR	C33-C5-C4	-2.03	109.72	113.62
30	J	103	BCR	C34-C9-C10	2.03	125.76	122.92
25	B	842	CLA	CMB-C2B-C3B	2.03	128.47	124.68
25	A	834	CLA	C3A-C2A-C1A	2.03	104.37	101.34
25	A	816	CLA	CHB-C4A-NA	2.03	127.31	124.51
30	4	319	BCR	C20-C19-C18	-2.03	120.73	126.42
25	2	613	CLA	CHD-C1D-C2D	2.02	129.72	125.48
29	W	316	Q6L	C41-C17-C16	-2.02	114.89	118.08
25	B	824	CLA	C6-C5-C3	-2.02	108.15	113.45
25	3	313	CLA	O2D-CGD-O1D	-2.02	119.88	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	B	803	CLA	CHB-C4A-NA	2.02	127.31	124.51
25	S	302	CLA	CMC-C2C-C1C	-2.02	121.96	125.04
24	U	304	CHL	CHD-C1D-ND	-2.02	122.60	124.45
25	A	829	CLA	CHA-C1A-NA	-2.02	121.77	126.40
26	V	317	IWJ	C33-C32-C30	2.02	115.49	112.04
38	R	312	KC2	CAC-C3C-C4C	2.02	133.89	124.47
25	A	825	CLA	C1B-CHB-C4A	-2.02	126.11	130.12
29	R	323	Q6L	C19-C20-C21	-2.02	119.33	123.47
25	B	812	CLA	C3A-C2A-C1A	2.02	104.37	101.34
29	Q	317	Q6L	C16-C17-C18	-2.02	115.84	118.94
25	2	602	CLA	C1C-C2C-C3C	-2.02	104.83	106.96
25	T	302	CLA	O2A-C1-C2	-2.02	103.33	108.64
29	P	319	Q6L	C01-C02-C07	-2.02	110.61	114.36
25	4	316	CLA	CHB-C4A-NA	2.02	127.31	124.51
24	P	304	CHL	CHA-C1A-NA	-2.02	121.77	126.40
25	B	820	CLA	CHD-C1D-C2D	2.02	129.72	125.48
29	U	315	Q6L	C41-C17-C16	-2.02	114.90	118.08
25	A	814	CLA	O2D-CGD-O1D	-2.02	119.89	123.84
26	4	317	IWJ	C17-C16-C15	-2.02	119.34	123.47
29	S	321	Q6L	C01-C02-C07	-2.02	110.62	114.36
30	3	317	BCR	C34-C9-C10	2.02	125.75	122.92
30	F	804	BCR	C2-C1-C6	2.02	113.59	110.48
25	V	312	CLA	CBA-CAA-C2A	2.02	119.82	113.86
24	4	307	CHL	O1D-CGD-CBD	2.02	128.61	124.48
25	B	820	CLA	O2A-CGA-O1A	-2.02	118.50	123.59
25	V	302	CLA	O2A-CGA-O1A	-2.02	118.50	123.59
37	P	317	NEX	C19-C9-C10	2.02	125.75	122.92
30	B	847	BCR	C16-C17-C18	-2.02	124.43	127.31
25	3	308	CLA	CHA-C4D-ND	2.02	136.72	132.50
25	A	826	CLA	O2D-CGD-CBD	2.02	114.85	111.27
36	B	850	DGD	C2G-O2G-C1B	-2.02	112.83	117.79
24	V	306	CHL	C1D-CHD-C4C	-2.02	121.71	126.06
24	U	313	CHL	C4A-NA-C1A	2.02	107.61	106.71
25	S	312	CLA	CBA-CAA-C2A	2.02	119.81	113.86
25	4	315	CLA	CAA-C2A-C3A	-2.01	111.40	116.10
37	H	306	NEX	C35-C15-C14	-2.01	119.35	123.47
25	A	831	CLA	C1D-ND-C4D	2.01	107.77	106.33
29	S	315	Q6L	C19-C20-C21	-2.01	119.35	123.47
25	B	804	CLA	C11-C10-C8	2.01	122.43	115.92
24	Q	308	CHL	C2A-C3A-C4A	2.01	105.12	101.87
27	5	612	XAT	C19-C9-C10	2.01	125.74	122.92
25	3	310	CLA	CHA-C1A-NA	-2.01	121.79	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	P	311	CLA	C5-C3-C2	2.01	125.19	121.12
24	R	311	CHL	C4A-NA-C1A	2.01	107.61	106.71
30	H	305	BCR	C39-C30-C25	2.01	113.56	110.30
25	N	203	CLA	CHA-C1A-NA	-2.01	121.79	126.40
24	6	601	CHL	C1D-CHD-C4C	-2.01	121.72	126.06
25	4	310	CLA	CMC-C2C-C1C	2.01	128.10	125.04
30	B	848	BCR	C24-C23-C22	-2.01	123.19	126.23
25	U	308	CLA	C3C-C4C-NC	2.01	112.83	110.57
24	6	601	CHL	C2A-C1A-CHA	2.01	127.38	123.86
25	B	843	CLA	O2D-CGD-O1D	-2.01	119.91	123.84
25	X	310	CLA	C2D-C1D-ND	-2.01	108.62	110.10
26	5	611	IWJ	C37-C35-C36	2.01	110.34	107.37
25	6	602	CLA	CHA-C1A-NA	-2.01	121.79	126.40
24	R	318	CHL	O1D-CGD-CBD	2.01	128.60	124.48
25	T	309	CLA	C6-C5-C3	2.01	118.72	113.45
24	P	304	CHL	O1A-CGA-CBA	2.01	129.54	123.08
25	A	823	CLA	O1D-CGD-CBD	2.01	128.59	124.48
25	P	310	CLA	C1-C2-C3	-2.01	122.57	126.04
25	R	317	CLA	CAC-C3C-C4C	2.01	127.42	124.81
30	3	318	BCR	C20-C19-C18	-2.01	120.78	126.42
25	S	312	CLA	CHD-C1D-ND	-2.01	122.61	124.45
24	P	307	CHL	O2D-CGD-CBD	2.01	114.83	111.27
33	A	802	CL0	CMC-C2C-C1C	2.01	128.09	125.04
27	4	318	XAT	C4-C3-C2	-2.01	106.90	110.77
24	Q	316	CHL	C1D-CHD-C4C	-2.01	121.73	126.06
38	X	309	KC2	O2A-CGA-O1A	-2.01	118.50	122.67
29	O	2006	Q6L	C42-C13-C12	2.01	118.64	115.27
30	F	801	BCR	C27-C26-C25	-2.01	119.82	122.73
25	B	825	CLA	CHA-C1A-NA	-2.01	121.81	126.40
24	V	314	CHL	CHA-C1A-NA	-2.00	121.81	126.40
24	R	309	CHL	O2D-CGD-CBD	2.00	114.83	111.27
25	2	609	CLA	C2A-C1A-CHA	2.00	127.36	123.86
24	X	308	CHL	O1D-CGD-CBD	2.00	128.59	124.48
36	A	854	DGD	O2D-C2D-C3D	-2.00	105.72	110.35
25	4	304	CLA	C3A-C2A-C1A	2.00	104.34	101.34
25	W	303	CLA	O2A-CGA-O1A	-2.00	118.54	123.59
25	Q	304	CLA	CHD-C1D-ND	-2.00	122.61	124.45
25	B	818	CLA	CHA-C4D-ND	2.00	136.69	132.50
29	W	316	Q6L	C29-C27-C26	-2.00	115.87	118.94
31	N	201	LMG	O3-C3-C4	-2.00	105.72	110.35
25	S	301	CLA	O2A-CGA-O1A	-2.00	118.54	123.59
25	G	202	CLA	CAC-C3C-C4C	2.00	127.41	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	824	CLA	C1B-CHB-C4A	-2.00	126.15	130.12
37	H	306	NEX	C40-C33-C32	2.00	121.23	118.08
25	A	821	CLA	CHA-C1A-NA	-2.00	121.82	126.40
24	V	304	CHL	C2D-C1D-ND	-2.00	108.63	110.10
24	W	305	CHL	C3C-C4C-NC	-2.00	108.33	110.57

All (413) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
24	1	601	CHL	NA
24	1	601	CHL	NC
24	1	601	CHL	ND
24	1	604	CHL	NA
24	1	604	CHL	NC
24	1	604	CHL	ND
24	2	601	CHL	NA
24	2	601	CHL	NC
24	2	601	CHL	ND
24	2	605	CHL	NA
24	2	605	CHL	NC
24	2	605	CHL	ND
24	2	607	CHL	NA
24	2	607	CHL	NC
24	2	607	CHL	ND
24	2	615	CHL	NA
24	2	615	CHL	NC
24	2	615	CHL	ND
24	3	306	CHL	NA
24	3	306	CHL	NC
24	3	306	CHL	ND
24	4	302	CHL	NA
24	4	302	CHL	NC
24	4	302	CHL	ND
24	4	306	CHL	NA
24	4	306	CHL	NC
24	4	306	CHL	ND
24	4	307	CHL	NA
24	4	307	CHL	NC
24	4	307	CHL	ND
24	4	308	CHL	NA
24	4	308	CHL	NC
24	4	308	CHL	ND

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Mol	Chain	Res	Type	Atom
24	5	605	CHL	NA
24	5	605	CHL	NC
24	5	605	CHL	ND
24	6	601	CHL	NA
24	6	601	CHL	NC
24	6	601	CHL	ND
24	6	605	CHL	NA
24	6	605	CHL	NC
24	6	605	CHL	ND
24	6	606	CHL	NA
24	6	606	CHL	NC
24	6	606	CHL	ND
24	P	304	CHL	NA
24	P	304	CHL	NC
24	P	304	CHL	ND
24	P	305	CHL	NA
24	P	305	CHL	NC
24	P	305	CHL	ND
24	P	306	CHL	NA
24	P	306	CHL	NC
24	P	306	CHL	ND
24	P	307	CHL	NA
24	P	307	CHL	NC
24	P	307	CHL	ND
24	P	314	CHL	NA
24	P	314	CHL	NC
24	P	314	CHL	ND
24	Q	307	CHL	NA
24	Q	307	CHL	NC
24	Q	307	CHL	ND
24	Q	308	CHL	NA
24	Q	308	CHL	NC
24	Q	308	CHL	ND
24	Q	309	CHL	NA
24	Q	309	CHL	NC
24	Q	309	CHL	ND
24	Q	316	CHL	NA
24	Q	316	CHL	NC
24	Q	316	CHL	ND
24	R	302	CHL	NA
24	R	302	CHL	NC
24	R	302	CHL	ND

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Mol	Chain	Res	Type	Atom
24	R	308	CHL	NA
24	R	308	CHL	NC
24	R	308	CHL	ND
24	R	309	CHL	NA
24	R	309	CHL	NC
24	R	309	CHL	ND
24	R	310	CHL	NA
24	R	310	CHL	NC
24	R	310	CHL	ND
24	R	311	CHL	NA
24	R	311	CHL	NC
24	R	311	CHL	ND
24	R	318	CHL	NA
24	R	318	CHL	NC
24	R	318	CHL	ND
24	S	304	CHL	NA
24	S	304	CHL	NC
24	S	304	CHL	ND
24	S	305	CHL	NA
24	S	305	CHL	NC
24	S	305	CHL	ND
24	S	306	CHL	NA
24	S	306	CHL	NC
24	S	306	CHL	ND
24	S	307	CHL	NA
24	S	307	CHL	NC
24	S	307	CHL	ND
24	S	314	CHL	NA
24	S	314	CHL	NC
24	S	314	CHL	ND
24	T	304	CHL	NA
24	T	304	CHL	NC
24	T	304	CHL	ND
24	T	305	CHL	NA
24	T	305	CHL	NC
24	T	305	CHL	ND
24	T	306	CHL	NA
24	T	306	CHL	NC
24	T	306	CHL	ND
24	T	307	CHL	NA
24	T	307	CHL	NC
24	T	307	CHL	ND

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Mol	Chain	Res	Type	Atom
24	T	314	CHL	NA
24	T	314	CHL	NC
24	T	314	CHL	ND
24	T	320	CHL	NA
24	T	320	CHL	NC
24	T	320	CHL	ND
24	U	304	CHL	NA
24	U	304	CHL	NC
24	U	304	CHL	ND
24	U	305	CHL	NA
24	U	305	CHL	NC
24	U	305	CHL	ND
24	U	306	CHL	NA
24	U	306	CHL	NC
24	U	306	CHL	ND
24	U	313	CHL	NA
24	U	313	CHL	NC
24	U	313	CHL	ND
24	V	304	CHL	NA
24	V	304	CHL	NC
24	V	304	CHL	ND
24	V	305	CHL	NA
24	V	305	CHL	NC
24	V	305	CHL	ND
24	V	306	CHL	NA
24	V	306	CHL	NC
24	V	306	CHL	ND
24	V	307	CHL	NA
24	V	307	CHL	NC
24	V	307	CHL	ND
24	V	314	CHL	NA
24	V	314	CHL	NC
24	V	314	CHL	ND
24	W	304	CHL	NA
24	W	304	CHL	NC
24	W	304	CHL	ND
24	W	305	CHL	NA
24	W	305	CHL	NC
24	W	305	CHL	ND
24	W	306	CHL	NA
24	W	306	CHL	NC
24	W	306	CHL	ND

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Mol	Chain	Res	Type	Atom
24	W	307	CHL	NA
24	W	307	CHL	NC
24	W	307	CHL	ND
24	W	314	CHL	NA
24	W	314	CHL	NC
24	W	314	CHL	ND
24	X	305	CHL	NA
24	X	305	CHL	NC
24	X	305	CHL	ND
24	X	306	CHL	NA
24	X	306	CHL	NC
24	X	306	CHL	ND
24	X	307	CHL	NA
24	X	307	CHL	NC
24	X	307	CHL	ND
24	X	308	CHL	NA
24	X	308	CHL	NC
24	X	308	CHL	ND
24	X	315	CHL	NA
24	X	315	CHL	NC
24	X	315	CHL	ND
25	1	602	CLA	ND
25	1	603	CLA	ND
25	1	605	CLA	ND
25	1	606	CLA	ND
25	1	607	CLA	ND
25	1	608	CLA	ND
25	1	609	CLA	ND
25	1	613	CLA	ND
25	2	602	CLA	ND
25	2	603	CLA	ND
25	2	604	CLA	ND
25	2	606	CLA	ND
25	2	608	CLA	ND
25	2	609	CLA	ND
25	2	610	CLA	ND
25	2	611	CLA	ND
25	2	612	CLA	ND
25	2	613	CLA	ND
25	2	614	CLA	ND
25	3	301	CLA	ND
25	3	302	CLA	ND

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Mol	Chain	Res	Type	Atom
25	3	303	CLA	ND
25	3	304	CLA	ND
25	3	305	CLA	ND
25	3	307	CLA	ND
25	3	308	CLA	ND
25	3	309	CLA	ND
25	3	310	CLA	ND
25	3	311	CLA	ND
25	3	312	CLA	ND
25	3	313	CLA	ND
25	4	303	CLA	ND
25	4	304	CLA	ND
25	4	305	CLA	ND
25	4	309	CLA	ND
25	4	310	CLA	ND
25	4	311	CLA	ND
25	4	312	CLA	ND
25	4	314	CLA	ND
25	4	315	CLA	ND
25	4	316	CLA	ND
25	5	601	CLA	ND
25	5	602	CLA	ND
25	5	603	CLA	ND
25	5	604	CLA	ND
25	5	606	CLA	ND
25	5	607	CLA	ND
25	5	608	CLA	ND
25	5	609	CLA	ND
25	5	610	CLA	ND
25	6	602	CLA	ND
25	6	603	CLA	ND
25	6	604	CLA	ND
25	6	607	CLA	ND
25	6	608	CLA	ND
25	6	609	CLA	ND
25	6	610	CLA	ND
25	6	611	CLA	ND
25	6	612	CLA	ND
25	A	803	CLA	ND
25	A	804	CLA	ND
25	A	805	CLA	ND
25	A	806	CLA	ND

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Mol	Chain	Res	Type	Atom
25	A	807	CLA	ND
25	A	808	CLA	ND
25	A	809	CLA	ND
25	A	810	CLA	ND
25	A	811	CLA	ND
25	A	812	CLA	ND
25	A	813	CLA	ND
25	A	814	CLA	ND
25	A	815	CLA	ND
25	A	816	CLA	ND
25	A	818	CLA	ND
25	A	819	CLA	ND
25	A	820	CLA	ND
25	A	821	CLA	ND
25	A	822	CLA	ND
25	A	823	CLA	ND
25	A	824	CLA	ND
25	A	825	CLA	ND
25	A	826	CLA	ND
25	A	827	CLA	ND
25	A	829	CLA	ND
25	A	830	CLA	ND
25	A	831	CLA	ND
25	A	832	CLA	ND
25	A	834	CLA	ND
25	A	835	CLA	ND
25	A	836	CLA	ND
25	A	837	CLA	ND
25	A	839	CLA	ND
25	A	841	CLA	ND
25	A	842	CLA	ND
25	A	843	CLA	ND
25	A	845	CLA	ND
25	A	856	CLA	ND
25	B	802	CLA	ND
25	B	803	CLA	ND
25	B	804	CLA	ND
25	B	805	CLA	ND
25	B	806	CLA	ND
25	B	807	CLA	ND
25	B	808	CLA	ND
25	B	809	CLA	ND

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Mol	Chain	Res	Type	Atom
25	B	810	CLA	ND
25	B	811	CLA	ND
25	B	812	CLA	ND
25	B	813	CLA	ND
25	B	814	CLA	ND
25	B	815	CLA	ND
25	B	816	CLA	ND
25	B	817	CLA	ND
25	B	818	CLA	ND
25	B	819	CLA	ND
25	B	820	CLA	ND
25	B	821	CLA	ND
25	B	822	CLA	ND
25	B	823	CLA	ND
25	B	824	CLA	ND
25	B	825	CLA	ND
25	B	826	CLA	ND
25	B	827	CLA	ND
25	B	828	CLA	ND
25	B	829	CLA	ND
25	B	830	CLA	ND
25	B	831	CLA	ND
25	B	832	CLA	ND
25	B	833	CLA	ND
25	B	834	CLA	ND
25	B	835	CLA	ND
25	B	837	CLA	ND
25	B	838	CLA	ND
25	B	839	CLA	ND
25	B	841	CLA	ND
25	B	842	CLA	ND
25	B	843	CLA	ND
25	F	802	CLA	ND
25	F	803	CLA	ND
25	G	202	CLA	ND
25	G	203	CLA	ND
25	G	204	CLA	ND
25	H	301	CLA	ND
25	H	302	CLA	ND
25	H	304	CLA	ND
25	J	102	CLA	ND
25	K	201	CLA	ND

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Mol	Chain	Res	Type	Atom
25	K	203	CLA	ND
25	K	204	CLA	ND
25	K	206	CLA	ND
25	L	301	CLA	ND
25	L	303	CLA	ND
25	L	304	CLA	ND
25	N	202	CLA	ND
25	N	203	CLA	ND
25	O	2001	CLA	ND
25	O	2002	CLA	ND
25	O	2003	CLA	ND
25	O	2004	CLA	ND
25	O	2005	CLA	ND
25	P	301	CLA	ND
25	P	302	CLA	ND
25	P	303	CLA	ND
25	P	309	CLA	ND
25	P	310	CLA	ND
25	P	311	CLA	ND
25	P	312	CLA	ND
25	Q	301	CLA	ND
25	Q	304	CLA	ND
25	Q	305	CLA	ND
25	Q	306	CLA	ND
25	Q	311	CLA	ND
25	Q	312	CLA	ND
25	Q	313	CLA	ND
25	Q	314	CLA	ND
25	Q	315	CLA	ND
25	R	305	CLA	ND
25	R	306	CLA	ND
25	R	307	CLA	ND
25	R	313	CLA	ND
25	R	314	CLA	ND
25	R	315	CLA	ND
25	R	316	CLA	ND
25	S	301	CLA	ND
25	S	302	CLA	ND
25	S	303	CLA	ND
25	S	309	CLA	ND
25	S	310	CLA	ND
25	S	311	CLA	ND

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Mol	Chain	Res	Type	Atom
25	S	312	CLA	ND
25	S	313	CLA	ND
25	T	301	CLA	ND
25	T	302	CLA	ND
25	T	303	CLA	ND
25	T	309	CLA	ND
25	T	310	CLA	ND
25	T	311	CLA	ND
25	T	312	CLA	ND
25	T	313	CLA	ND
25	U	301	CLA	ND
25	U	302	CLA	ND
25	U	303	CLA	ND
25	U	308	CLA	ND
25	U	309	CLA	ND
25	U	310	CLA	ND
25	U	311	CLA	ND
25	U	312	CLA	ND
25	V	301	CLA	ND
25	V	302	CLA	ND
25	V	303	CLA	ND
25	V	309	CLA	ND
25	V	310	CLA	ND
25	V	311	CLA	ND
25	V	313	CLA	ND
25	W	301	CLA	ND
25	W	302	CLA	ND
25	W	303	CLA	ND
25	W	309	CLA	ND
25	W	310	CLA	ND
25	W	311	CLA	ND
25	W	312	CLA	ND
25	W	313	CLA	ND
25	X	302	CLA	ND
25	X	303	CLA	ND
25	X	304	CLA	ND
25	X	310	CLA	ND
25	X	311	CLA	ND
25	X	312	CLA	ND
25	X	313	CLA	ND
25	X	314	CLA	ND
33	A	802	CL0	NA

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Mol	Chain	Res	Type	Atom
33	A	802	CL0	NC
33	A	802	CL0	ND

All (2988) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	1	601	CHL	C1A-C2A-CAA-CBA
24	2	605	CHL	C1A-C2A-CAA-CBA
24	2	605	CHL	C3A-C2A-CAA-CBA
24	2	605	CHL	CHA-CBD-CGD-O1D
24	2	605	CHL	CHA-CBD-CGD-O2D
24	2	605	CHL	CAD-CBD-CGD-O1D
24	2	605	CHL	CBD-CGD-O2D-CED
24	2	607	CHL	C3C-C2C-CMC-OMC
24	4	307	CHL	C1A-C2A-CAA-CBA
24	4	307	CHL	C1C-C2C-CMC-OMC
24	4	307	CHL	C3C-C2C-CMC-OMC
24	4	307	CHL	CBD-CGD-O2D-CED
24	6	606	CHL	C1A-C2A-CAA-CBA
24	6	606	CHL	C3A-C2A-CAA-CBA
24	6	606	CHL	CAD-CBD-CGD-O1D
24	6	606	CHL	CAD-CBD-CGD-O2D
24	6	606	CHL	CBD-CGD-O2D-CED
24	P	304	CHL	C1A-C2A-CAA-CBA
24	P	304	CHL	C3A-C2A-CAA-CBA
24	P	304	CHL	C1C-C2C-CMC-OMC
24	P	304	CHL	C3C-C2C-CMC-OMC
24	P	304	CHL	CBD-CGD-O2D-CED
24	P	314	CHL	C1A-C2A-CAA-CBA
24	P	314	CHL	CHA-CBD-CGD-O1D
24	P	314	CHL	CHA-CBD-CGD-O2D
24	R	302	CHL	CBA-CGA-O2A-C1
24	R	308	CHL	CHA-CBD-CGD-O1D
24	R	308	CHL	CHA-CBD-CGD-O2D
24	R	309	CHL	CBD-CGD-O2D-CED
24	R	310	CHL	C2-C3-C5-C6
24	R	310	CHL	C4-C3-C5-C6
24	R	311	CHL	CBD-CGD-O2D-CED
24	R	318	CHL	CBD-CGD-O2D-CED
24	S	304	CHL	C3C-C2C-CMC-OMC
24	S	306	CHL	CAD-CBD-CGD-O1D
24	S	306	CHL	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
24	S	307	CHL	CBD-CGD-O2D-CED
24	S	314	CHL	CHA-CBD-CGD-O1D
24	S	314	CHL	CHA-CBD-CGD-O2D
24	T	304	CHL	CBD-CGD-O2D-CED
24	T	320	CHL	CHA-CBD-CGD-O2D
24	U	304	CHL	CHA-CBD-CGD-O1D
24	U	304	CHL	CHA-CBD-CGD-O2D
24	U	304	CHL	CBD-CGD-O2D-CED
24	V	304	CHL	CHA-CBD-CGD-O1D
24	V	304	CHL	CHA-CBD-CGD-O2D
24	V	304	CHL	CBD-CGD-O2D-CED
24	V	305	CHL	C3C-C2C-CMC-OMC
24	W	307	CHL	C1A-C2A-CAA-CBA
24	W	314	CHL	C3C-C2C-CMC-OMC
24	W	314	CHL	CHA-CBD-CGD-O1D
24	W	314	CHL	CHA-CBD-CGD-O2D
24	X	307	CHL	C3A-C2A-CAA-CBA
24	X	307	CHL	CBA-CGA-O2A-C1
24	X	307	CHL	O1A-CGA-O2A-C1
24	X	307	CHL	C1C-C2C-CMC-OMC
24	X	307	CHL	C3C-C2C-CMC-OMC
24	X	307	CHL	O2A-C1-C2-C3
24	X	308	CHL	C1A-C2A-CAA-CBA
24	X	308	CHL	CHA-CBD-CGD-O1D
24	X	308	CHL	CHA-CBD-CGD-O2D
24	X	308	CHL	CAD-CBD-CGD-O1D
24	X	308	CHL	CBD-CGD-O2D-CED
24	X	315	CHL	CBD-CGD-O2D-CED
25	1	602	CLA	CHA-CBD-CGD-O1D
25	1	602	CLA	CAD-CBD-CGD-O1D
25	1	605	CLA	C1A-C2A-CAA-CBA
25	1	605	CLA	C3A-C2A-CAA-CBA
25	1	606	CLA	CBD-CGD-O2D-CED
25	1	608	CLA	C1A-C2A-CAA-CBA
25	1	608	CLA	C3A-C2A-CAA-CBA
25	1	608	CLA	CBD-CGD-O2D-CED
25	1	610	CLA	C1A-C2A-CAA-CBA
25	1	610	CLA	C3A-C2A-CAA-CBA
25	1	610	CLA	CBD-CGD-O2D-CED
25	2	602	CLA	C1A-C2A-CAA-CBA
25	2	602	CLA	C3A-C2A-CAA-CBA
25	2	603	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
25	2	606	CLA	C1A-C2A-CAA-CBA
25	2	606	CLA	C3A-C2A-CAA-CBA
25	2	608	CLA	C1A-C2A-CAA-CBA
25	2	608	CLA	C3A-C2A-CAA-CBA
25	2	608	CLA	CBD-CGD-O2D-CED
25	2	610	CLA	CBD-CGD-O2D-CED
25	2	611	CLA	C1A-C2A-CAA-CBA
25	2	611	CLA	C3A-C2A-CAA-CBA
25	2	611	CLA	CHA-CBD-CGD-O2D
25	2	612	CLA	C4-C3-C5-C6
25	2	614	CLA	C1A-C2A-CAA-CBA
25	3	302	CLA	CBA-CGA-O2A-C1
25	3	304	CLA	C1A-C2A-CAA-CBA
25	3	304	CLA	C3A-C2A-CAA-CBA
25	3	307	CLA	C1A-C2A-CAA-CBA
25	3	307	CLA	C3A-C2A-CAA-CBA
25	3	310	CLA	CBD-CGD-O2D-CED
25	3	311	CLA	CBA-CGA-O2A-C1
25	3	311	CLA	O1A-CGA-O2A-C1
25	3	313	CLA	CHA-CBD-CGD-O1D
25	3	313	CLA	CHA-CBD-CGD-O2D
25	4	303	CLA	C3A-C2A-CAA-CBA
25	4	303	CLA	CBD-CGD-O2D-CED
25	4	304	CLA	CBD-CGD-O2D-CED
25	4	304	CLA	O1D-CGD-O2D-CED
25	4	305	CLA	CHA-CBD-CGD-O1D
25	4	305	CLA	CHA-CBD-CGD-O2D
25	4	309	CLA	CBD-CGD-O2D-CED
25	4	310	CLA	CHA-CBD-CGD-O1D
25	4	310	CLA	CHA-CBD-CGD-O2D
25	4	311	CLA	C1A-C2A-CAA-CBA
25	4	311	CLA	C3A-C2A-CAA-CBA
25	4	311	CLA	CBD-CGD-O2D-CED
25	4	312	CLA	C1A-C2A-CAA-CBA
25	4	312	CLA	C3A-C2A-CAA-CBA
25	4	313	CLA	CHA-CBD-CGD-O1D
25	4	313	CLA	CHA-CBD-CGD-O2D
25	4	314	CLA	CHA-CBD-CGD-O1D
25	4	314	CLA	CHA-CBD-CGD-O2D
25	4	315	CLA	CBD-CGD-O2D-CED
25	4	316	CLA	C1A-C2A-CAA-CBA
25	4	316	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
25	5	601	CLA	C3A-C2A-CAA-CBA
25	5	601	CLA	CBA-CGA-O2A-C1
25	5	602	CLA	C1A-C2A-CAA-CBA
25	5	602	CLA	C3A-C2A-CAA-CBA
25	5	602	CLA	CHA-CBD-CGD-O1D
25	5	602	CLA	CHA-CBD-CGD-O2D
25	5	608	CLA	CHA-CBD-CGD-O1D
25	5	608	CLA	CHA-CBD-CGD-O2D
25	5	609	CLA	C1A-C2A-CAA-CBA
25	5	609	CLA	C3A-C2A-CAA-CBA
25	6	602	CLA	C1A-C2A-CAA-CBA
25	6	602	CLA	C3A-C2A-CAA-CBA
25	6	607	CLA	C1A-C2A-CAA-CBA
25	6	608	CLA	C1A-C2A-CAA-CBA
25	6	608	CLA	C3A-C2A-CAA-CBA
25	6	608	CLA	CBD-CGD-O2D-CED
25	6	610	CLA	C1A-C2A-CAA-CBA
25	6	610	CLA	CHA-CBD-CGD-O1D
25	6	610	CLA	CHA-CBD-CGD-O2D
25	6	611	CLA	C1A-C2A-CAA-CBA
25	6	611	CLA	C3A-C2A-CAA-CBA
25	A	804	CLA	CBD-CGD-O2D-CED
25	A	806	CLA	C1A-C2A-CAA-CBA
25	A	807	CLA	CHA-CBD-CGD-O1D
25	A	807	CLA	CHA-CBD-CGD-O2D
25	A	814	CLA	C1A-C2A-CAA-CBA
25	A	814	CLA	C3A-C2A-CAA-CBA
25	A	817	CLA	C3A-C2A-CAA-CBA
25	A	819	CLA	CBD-CGD-O2D-CED
25	A	820	CLA	C3A-C2A-CAA-CBA
25	A	821	CLA	C3A-C2A-CAA-CBA
25	A	821	CLA	CHA-CBD-CGD-O1D
25	A	821	CLA	CHA-CBD-CGD-O2D
25	A	821	CLA	CAD-CBD-CGD-O1D
25	A	824	CLA	C1A-C2A-CAA-CBA
25	A	824	CLA	CBD-CGD-O2D-CED
25	A	825	CLA	C1A-C2A-CAA-CBA
25	A	830	CLA	C1A-C2A-CAA-CBA
25	A	830	CLA	C3A-C2A-CAA-CBA
25	A	835	CLA	CBD-CGD-O2D-CED
25	A	836	CLA	CBD-CGD-O2D-CED
25	A	840	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
25	A	841	CLA	CHA-CBD-CGD-O1D
25	A	841	CLA	CHA-CBD-CGD-O2D
25	A	842	CLA	C1A-C2A-CAA-CBA
25	A	842	CLA	CHA-CBD-CGD-O1D
25	A	842	CLA	CHA-CBD-CGD-O2D
25	A	843	CLA	C1A-C2A-CAA-CBA
25	A	843	CLA	C3A-C2A-CAA-CBA
25	A	856	CLA	CAD-CBD-CGD-O1D
25	A	856	CLA	CAD-CBD-CGD-O2D
25	B	803	CLA	CBD-CGD-O2D-CED
25	B	804	CLA	CHA-CBD-CGD-O1D
25	B	804	CLA	CHA-CBD-CGD-O2D
25	B	805	CLA	CBD-CGD-O2D-CED
25	B	807	CLA	C1A-C2A-CAA-CBA
25	B	807	CLA	C3A-C2A-CAA-CBA
25	B	809	CLA	C1A-C2A-CAA-CBA
25	B	809	CLA	C6-C7-C8-C9
25	B	810	CLA	C1A-C2A-CAA-CBA
25	B	810	CLA	CHA-CBD-CGD-O2D
25	B	811	CLA	C2A-CAA-CBA-CGA
25	B	814	CLA	CHA-CBD-CGD-O1D
25	B	814	CLA	CHA-CBD-CGD-O2D
25	B	814	CLA	CAD-CBD-CGD-O1D
25	B	816	CLA	C2-C3-C5-C6
25	B	817	CLA	CBD-CGD-O2D-CED
25	B	818	CLA	C1A-C2A-CAA-CBA
25	B	820	CLA	C3A-C2A-CAA-CBA
25	B	821	CLA	C1A-C2A-CAA-CBA
25	B	823	CLA	CBD-CGD-O2D-CED
25	B	825	CLA	CHA-CBD-CGD-O1D
25	B	825	CLA	CHA-CBD-CGD-O2D
25	B	829	CLA	C1A-C2A-CAA-CBA
25	B	829	CLA	C3A-C2A-CAA-CBA
25	B	829	CLA	CBD-CGD-O2D-CED
25	B	830	CLA	C1A-C2A-CAA-CBA
25	B	832	CLA	C1A-C2A-CAA-CBA
25	B	832	CLA	C3A-C2A-CAA-CBA
25	B	834	CLA	CAD-CBD-CGD-O1D
25	B	834	CLA	CAD-CBD-CGD-O2D
25	B	839	CLA	C1A-C2A-CAA-CBA
25	B	842	CLA	C1A-C2A-CAA-CBA
25	B	842	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
25	B	842	CLA	CHA-CBD-CGD-O1D
25	B	842	CLA	CHA-CBD-CGD-O2D
25	B	842	CLA	CAD-CBD-CGD-O1D
25	F	803	CLA	CHA-CBD-CGD-O1D
25	F	803	CLA	CHA-CBD-CGD-O2D
25	G	202	CLA	CHA-CBD-CGD-O1D
25	G	202	CLA	CHA-CBD-CGD-O2D
25	G	204	CLA	C1A-C2A-CAA-CBA
25	G	204	CLA	C3A-C2A-CAA-CBA
25	G	204	CLA	CAD-CBD-CGD-O1D
25	G	204	CLA	CAD-CBD-CGD-O2D
25	H	301	CLA	C1A-C2A-CAA-CBA
25	H	301	CLA	C3A-C2A-CAA-CBA
25	H	302	CLA	C1A-C2A-CAA-CBA
25	H	302	CLA	CHA-CBD-CGD-O1D
25	H	302	CLA	CHA-CBD-CGD-O2D
25	J	102	CLA	C1A-C2A-CAA-CBA
25	J	102	CLA	C3A-C2A-CAA-CBA
25	K	201	CLA	CBD-CGD-O2D-CED
25	K	203	CLA	C1A-C2A-CAA-CBA
25	K	204	CLA	C1A-C2A-CAA-CBA
25	K	204	CLA	CBD-CGD-O2D-CED
25	K	206	CLA	C1A-C2A-CAA-CBA
25	K	206	CLA	C3A-C2A-CAA-CBA
25	K	206	CLA	CBD-CGD-O2D-CED
25	K	206	CLA	C2-C3-C5-C6
25	K	206	CLA	C4-C3-C5-C6
25	L	302	CLA	C1A-C2A-CAA-CBA
25	L	302	CLA	C3A-C2A-CAA-CBA
25	L	303	CLA	C1A-C2A-CAA-CBA
25	L	303	CLA	C3A-C2A-CAA-CBA
25	L	304	CLA	C1A-C2A-CAA-CBA
25	L	304	CLA	C3A-C2A-CAA-CBA
25	N	202	CLA	C1A-C2A-CAA-CBA
25	N	202	CLA	C3A-C2A-CAA-CBA
25	O	2002	CLA	C1A-C2A-CAA-CBA
25	O	2002	CLA	C3A-C2A-CAA-CBA
25	O	2005	CLA	CHA-CBD-CGD-O1D
25	O	2005	CLA	CHA-CBD-CGD-O2D
25	P	301	CLA	C3A-C2A-CAA-CBA
25	P	301	CLA	C2-C3-C5-C6
25	P	301	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
25	P	302	CLA	CHA-CBD-CGD-O1D
25	P	302	CLA	CHA-CBD-CGD-O2D
25	P	302	CLA	CAD-CBD-CGD-O1D
25	P	302	CLA	CAD-CBD-CGD-O2D
25	P	303	CLA	C1A-C2A-CAA-CBA
25	P	303	CLA	C3A-C2A-CAA-CBA
25	P	303	CLA	CBD-CGD-O2D-CED
25	P	309	CLA	C3A-C2A-CAA-CBA
25	P	310	CLA	CHA-CBD-CGD-O1D
25	P	310	CLA	CHA-CBD-CGD-O2D
25	P	312	CLA	CHA-CBD-CGD-O1D
25	P	312	CLA	CHA-CBD-CGD-O2D
25	Q	301	CLA	C1A-C2A-CAA-CBA
25	Q	301	CLA	C3A-C2A-CAA-CBA
25	Q	301	CLA	CHA-CBD-CGD-O1D
25	Q	301	CLA	CHA-CBD-CGD-O2D
25	Q	306	CLA	C1A-C2A-CAA-CBA
25	Q	311	CLA	C1A-C2A-CAA-CBA
25	Q	312	CLA	C1A-C2A-CAA-CBA
25	Q	312	CLA	CHA-CBD-CGD-O1D
25	Q	313	CLA	CBA-CGA-O2A-C1
25	Q	314	CLA	CHA-CBD-CGD-O1D
25	Q	314	CLA	CHA-CBD-CGD-O2D
25	R	305	CLA	C1A-C2A-CAA-CBA
25	R	313	CLA	C1A-C2A-CAA-CBA
25	R	313	CLA	C3A-C2A-CAA-CBA
25	R	314	CLA	C3A-C2A-CAA-CBA
25	R	315	CLA	CHA-CBD-CGD-O1D
25	R	315	CLA	CHA-CBD-CGD-O2D
25	R	315	CLA	CAD-CBD-CGD-O1D
25	R	316	CLA	C1A-C2A-CAA-CBA
25	R	316	CLA	C3A-C2A-CAA-CBA
25	R	316	CLA	C4-C3-C5-C6
25	R	317	CLA	O1A-CGA-O2A-C1
25	S	301	CLA	C3A-C2A-CAA-CBA
25	S	302	CLA	C6-C7-C8-C9
25	S	303	CLA	CHA-CBD-CGD-O1D
25	S	303	CLA	CHA-CBD-CGD-O2D
25	S	309	CLA	C1A-C2A-CAA-CBA
25	S	309	CLA	C3A-C2A-CAA-CBA
25	S	310	CLA	C1A-C2A-CAA-CBA
25	S	311	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
25	S	312	CLA	CHA-CBD-CGD-O1D
25	S	312	CLA	CHA-CBD-CGD-O2D
25	T	301	CLA	C3A-C2A-CAA-CBA
25	T	301	CLA	C4-C3-C5-C6
25	T	302	CLA	C1A-C2A-CAA-CBA
25	T	302	CLA	C3A-C2A-CAA-CBA
25	T	303	CLA	CHA-CBD-CGD-O1D
25	T	303	CLA	CHA-CBD-CGD-O2D
25	T	303	CLA	CBD-CGD-O2D-CED
25	T	309	CLA	C1A-C2A-CAA-CBA
25	T	309	CLA	C3A-C2A-CAA-CBA
25	T	309	CLA	C2-C3-C5-C6
25	T	309	CLA	C4-C3-C5-C6
25	T	310	CLA	C1A-C2A-CAA-CBA
25	T	310	CLA	CHA-CBD-CGD-O1D
25	T	310	CLA	CHA-CBD-CGD-O2D
25	T	311	CLA	CBD-CGD-O2D-CED
25	T	312	CLA	C1A-C2A-CAA-CBA
25	T	313	CLA	C1A-C2A-CAA-CBA
25	U	301	CLA	C1A-C2A-CAA-CBA
25	U	301	CLA	C3A-C2A-CAA-CBA
25	U	301	CLA	CBD-CGD-O2D-CED
25	U	303	CLA	CHA-CBD-CGD-O1D
25	U	303	CLA	CHA-CBD-CGD-O2D
25	U	311	CLA	CBD-CGD-O2D-CED
25	V	302	CLA	CHA-CBD-CGD-O1D
25	V	302	CLA	CHA-CBD-CGD-O2D
25	V	303	CLA	CBD-CGD-O2D-CED
25	V	312	CLA	C1A-C2A-CAA-CBA
25	V	312	CLA	C3A-C2A-CAA-CBA
25	V	312	CLA	CHA-CBD-CGD-O1D
25	V	312	CLA	CHA-CBD-CGD-O2D
25	W	301	CLA	C1A-C2A-CAA-CBA
25	X	303	CLA	C1A-C2A-CAA-CBA
25	X	303	CLA	C3A-C2A-CAA-CBA
25	X	304	CLA	CHA-CBD-CGD-O1D
25	X	304	CLA	CHA-CBD-CGD-O2D
25	X	311	CLA	C1A-C2A-CAA-CBA
25	X	311	CLA	C3A-C2A-CAA-CBA
25	X	311	CLA	CBD-CGD-O2D-CED
25	X	312	CLA	CBD-CGD-O2D-CED
25	X	313	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
25	X	314	CLA	CHA-CBD-CGD-O1D
25	X	314	CLA	CHA-CBD-CGD-O2D
25	X	314	CLA	CAD-CBD-CGD-O1D
25	X	314	CLA	CBD-CGD-O2D-CED
26	1	611	IWJ	C18-C19-C21-C22
26	1	611	IWJ	C20-C19-C21-C22
26	3	315	IWJ	C26-C28-C29-C35
26	4	301	IWJ	C02-C07-C08-C09
26	4	301	IWJ	C06-C07-C08-C09
26	4	301	IWJ	C26-C28-C29-C30
26	4	301	IWJ	C26-C28-C29-C35
26	4	301	IWJ	C26-C28-C29-O39
26	4	317	IWJ	C26-C28-C29-O39
26	5	611	IWJ	C26-C28-C29-C30
26	5	611	IWJ	C26-C28-C29-C35
26	5	611	IWJ	C26-C28-C29-O39
26	6	614	IWJ	C26-C28-C29-C30
26	6	614	IWJ	C26-C28-C29-O39
26	P	318	IWJ	C18-C19-C21-C22
26	P	318	IWJ	C20-C19-C21-C22
26	P	320	IWJ	C26-C28-C29-C30
26	P	320	IWJ	C26-C28-C29-O39
26	Q	303	IWJ	C26-C28-C29-C30
26	Q	303	IWJ	C26-C28-C29-O39
26	Q	320	IWJ	C18-C19-C21-C22
26	Q	320	IWJ	C20-C19-C21-C22
26	Q	320	IWJ	C26-C28-C29-C30
26	Q	320	IWJ	C26-C28-C29-C35
26	Q	320	IWJ	C26-C28-C29-O39
26	R	303	IWJ	C26-C28-C29-C30
26	R	303	IWJ	C26-C28-C29-C35
26	R	303	IWJ	C26-C28-C29-O39
26	R	322	IWJ	C18-C19-C21-C22
26	R	322	IWJ	C20-C19-C21-C22
26	R	322	IWJ	C26-C28-C29-C30
26	R	322	IWJ	C26-C28-C29-C35
26	R	322	IWJ	C26-C28-C29-O39
26	S	319	IWJ	C18-C19-C21-C22
26	S	319	IWJ	C20-C19-C21-C22
26	S	319	IWJ	C26-C28-C29-C30
26	S	319	IWJ	C26-C28-C29-O39
26	S	322	IWJ	C26-C28-C29-C30

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Mol	Chain	Res	Type	Atoms
26	S	322	IWJ	C26-C28-C29-C35
26	S	322	IWJ	C26-C28-C29-O39
26	T	318	IWJ	C18-C19-C21-C22
26	T	318	IWJ	C20-C19-C21-C22
26	T	318	IWJ	C26-C28-C29-C30
26	T	318	IWJ	C26-C28-C29-O39
26	T	321	IWJ	C26-C28-C29-C30
26	T	321	IWJ	C26-C28-C29-O39
26	V	317	IWJ	C18-C19-C21-C22
26	V	317	IWJ	C20-C19-C21-C22
26	V	317	IWJ	C26-C28-C29-C30
26	V	317	IWJ	C26-C28-C29-C35
26	V	317	IWJ	C26-C28-C29-O39
26	V	318	IWJ	C26-C28-C29-C30
26	V	318	IWJ	C26-C28-C29-C35
26	V	318	IWJ	C26-C28-C29-O39
26	V	320	IWJ	C26-C28-C29-C30
26	V	320	IWJ	C26-C28-C29-C35
26	V	320	IWJ	C26-C28-C29-O39
26	W	318	IWJ	C18-C19-C21-C22
26	W	318	IWJ	C20-C19-C21-C22
26	W	318	IWJ	C26-C28-C29-C30
26	W	318	IWJ	C26-C28-C29-C35
26	W	318	IWJ	C26-C28-C29-O39
26	X	318	IWJ	C18-C19-C21-C22
26	X	318	IWJ	C20-C19-C21-C22
26	X	318	IWJ	C26-C28-C29-C30
26	X	318	IWJ	C26-C28-C29-O39
27	1	612	XAT	O4-C6-C7-C8
27	1	612	XAT	C11-C12-C13-C14
27	1	612	XAT	C11-C12-C13-C20
27	1	612	XAT	O24-C26-C27-C28
27	3	316	XAT	O4-C6-C7-C8
27	3	316	XAT	C7-C8-C9-C19
27	4	318	XAT	O4-C6-C7-C8
27	4	318	XAT	C27-C28-C29-C39
28	1	614	LHG	C3-O3-P-O5
28	1	614	LHG	C4-O6-P-O4
28	3	320	LHG	C4-O6-P-O3
28	3	320	LHG	C4-O6-P-O5
28	3	321	LHG	C3-O3-P-O5
28	3	321	LHG	C3-O3-P-O6

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Mol	Chain	Res	Type	Atoms
28	3	322	LHG	C3-O3-P-O5
28	3	322	LHG	C4-O6-P-O5
28	3	323	LHG	C1-C2-C3-O3
28	6	616	LHG	C3-O3-P-O4
28	6	616	LHG	C4-O6-P-O5
28	A	846	LHG	C3-O3-P-O5
28	Q	302	LHG	C4-O6-P-O4
29	2	616	Q6L	C02-C03-C11-C12
29	2	616	Q6L	C11-C12-C13-C14
29	2	616	Q6L	C11-C12-C13-C42
29	O	2006	Q6L	C21-C22-C24-C25
29	O	2006	Q6L	C23-C22-C24-C25
29	O	2006	Q6L	C29-C30-C31-C36
29	O	2007	Q6L	C27-C29-C30-C31
29	P	315	Q6L	C28-C27-C29-C30
29	P	315	Q6L	C26-C27-C29-C30
29	P	315	Q6L	C15-C16-C17-C18
29	P	315	Q6L	C15-C16-C17-C41
29	P	319	Q6L	C11-C12-C13-C14
29	P	319	Q6L	C11-C12-C13-C42
29	Q	317	Q6L	C02-C03-C11-C12
29	Q	317	Q6L	C11-C12-C13-C14
29	Q	317	Q6L	C11-C12-C13-C42
29	Q	317	Q6L	C28-C27-C29-C30
29	Q	317	Q6L	C26-C27-C29-C30
29	Q	317	Q6L	C27-C29-C30-C31
29	Q	318	Q6L	C28-C27-C29-C30
29	Q	318	Q6L	C26-C27-C29-C30
29	R	301	Q6L	C04-C03-C11-C12
29	R	301	Q6L	C11-C12-C13-C42
29	R	301	Q6L	C21-C22-C24-C25
29	R	301	Q6L	C23-C22-C24-C25
29	R	301	Q6L	C28-C27-C29-C30
29	R	301	Q6L	C26-C27-C29-C30
29	R	301	Q6L	C29-C30-C31-C32
29	R	301	Q6L	C27-C29-C30-C31
29	R	319	Q6L	C11-C12-C13-C14
29	R	319	Q6L	C11-C12-C13-C42
29	R	319	Q6L	C21-C22-C24-C25
29	R	319	Q6L	C23-C22-C24-C25
29	R	319	Q6L	C29-C30-C31-C36
29	R	319	Q6L	C29-C30-C31-C32

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Mol	Chain	Res	Type	Atoms
29	R	323	Q6L	C11-C12-C13-C42
29	R	323	Q6L	C28-C27-C29-C30
29	R	323	Q6L	C27-C29-C30-C31
29	S	315	Q6L	C28-C27-C29-C30
29	S	315	Q6L	C26-C27-C29-C30
29	S	320	Q6L	C11-C12-C13-C42
29	S	320	Q6L	C21-C22-C24-C25
29	S	320	Q6L	C23-C22-C24-C25
29	S	320	Q6L	C27-C29-C30-C31
29	S	321	Q6L	C02-C03-C11-C12
29	S	321	Q6L	C29-C30-C31-C36
29	S	321	Q6L	C29-C30-C31-C32
29	S	321	Q6L	C15-C16-C17-C18
29	S	321	Q6L	C15-C16-C17-C41
29	S	323	Q6L	C02-C03-C11-C12
29	S	323	Q6L	C29-C30-C31-C36
29	S	323	Q6L	C29-C30-C31-C32
29	T	315	Q6L	C28-C27-C29-C30
29	T	315	Q6L	C15-C16-C17-C18
29	T	315	Q6L	C15-C16-C17-C41
29	T	316	Q6L	C13-C14-C15-C16
29	T	319	Q6L	C11-C12-C13-C42
29	T	319	Q6L	C27-C29-C30-C31
29	T	322	Q6L	C02-C03-C11-C12
29	T	322	Q6L	C11-C12-C13-C14
29	T	322	Q6L	C11-C12-C13-C42
29	T	322	Q6L	C28-C27-C29-C30
29	T	322	Q6L	C29-C30-C31-C36
29	T	322	Q6L	C29-C30-C31-C32
29	U	314	Q6L	C11-C12-C13-C14
29	U	314	Q6L	C11-C12-C13-C42
29	U	314	Q6L	C28-C27-C29-C30
29	U	314	Q6L	C26-C27-C29-C30
29	U	314	Q6L	C15-C16-C17-C41
29	U	317	Q6L	C29-C30-C31-C36
29	U	317	Q6L	C29-C30-C31-C32
29	V	315	Q6L	C02-C03-C11-C12
29	V	315	Q6L	C21-C22-C24-C25
29	V	315	Q6L	C23-C22-C24-C25
29	V	315	Q6L	C29-C30-C31-C32
29	V	315	Q6L	C27-C29-C30-C31
29	V	315	Q6L	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
29	V	315	Q6L	C15-C16-C17-C41
29	V	316	Q6L	C04-C03-C11-C12
29	V	316	Q6L	C29-C30-C31-C36
29	V	316	Q6L	C29-C30-C31-C32
29	V	316	Q6L	C27-C29-C30-C31
29	V	316	Q6L	C19-C20-C21-C22
29	V	319	Q6L	C02-C03-C11-C12
29	V	319	Q6L	C28-C27-C29-C30
29	V	319	Q6L	C26-C27-C29-C30
29	V	321	Q6L	C04-C03-C11-C12
29	W	315	Q6L	C15-C16-C17-C18
29	W	315	Q6L	C15-C16-C17-C41
29	W	319	Q6L	C28-C27-C29-C30
29	W	319	Q6L	C26-C27-C29-C30
29	W	320	Q6L	C02-C03-C11-C12
29	W	320	Q6L	C11-C12-C13-C14
29	W	320	Q6L	C11-C12-C13-C42
29	W	320	Q6L	C28-C27-C29-C30
29	W	320	Q6L	C29-C30-C31-C36
29	W	320	Q6L	C29-C30-C31-C32
29	X	301	Q6L	C29-C30-C31-C32
29	X	301	Q6L	C27-C29-C30-C31
29	X	317	Q6L	C04-C03-C11-C12
29	X	319	Q6L	C11-C12-C13-C14
29	X	319	Q6L	C11-C12-C13-C42
29	X	319	Q6L	C21-C22-C24-C25
29	X	319	Q6L	C23-C22-C24-C25
29	X	319	Q6L	C28-C27-C29-C30
29	X	319	Q6L	C26-C27-C29-C30
29	X	319	Q6L	C29-C30-C31-C36
29	X	319	Q6L	C29-C30-C31-C32
29	X	319	Q6L	C27-C29-C30-C31
29	X	319	Q6L	C24-C25-C26-C27
30	3	317	BCR	C21-C22-C23-C24
30	3	317	BCR	C37-C22-C23-C24
30	4	319	BCR	C21-C22-C23-C24
30	4	319	BCR	C37-C22-C23-C24
30	A	848	BCR	C7-C8-C9-C34
30	A	849	BCR	C11-C12-C13-C35
30	A	851	BCR	C1-C6-C7-C8
30	A	851	BCR	C37-C22-C23-C24
30	B	848	BCR	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
30	B	848	BCR	C37-C22-C23-C24
30	B	849	BCR	C21-C22-C23-C24
30	B	849	BCR	C37-C22-C23-C24
30	F	804	BCR	C7-C8-C9-C10
30	F	804	BCR	C11-C12-C13-C14
30	F	804	BCR	C11-C12-C13-C35
30	G	201	BCR	C17-C18-C19-C20
30	G	201	BCR	C36-C18-C19-C20
30	H	305	BCR	C7-C8-C9-C10
30	H	305	BCR	C7-C8-C9-C34
30	H	305	BCR	C11-C12-C13-C14
30	H	305	BCR	C36-C18-C19-C20
30	I	101	BCR	C1-C6-C7-C8
30	I	101	BCR	C7-C8-C9-C34
30	I	101	BCR	C21-C22-C23-C24
30	I	101	BCR	C37-C22-C23-C24
30	K	205	BCR	C21-C22-C23-C24
30	K	205	BCR	C37-C22-C23-C24
30	L	305	BCR	C21-C22-C23-C24
30	L	305	BCR	C37-C22-C23-C24
30	L	306	BCR	C21-C22-C23-C24
30	L	306	BCR	C37-C22-C23-C24
30	M	101	BCR	C21-C22-C23-C24
30	M	101	BCR	C37-C22-C23-C24
32	6	617	SQD	C2-C1-O6-C44
32	6	617	SQD	O5-C1-O6-C44
32	6	617	SQD	O5-C5-C6-S
32	H	303	SQD	C2-C1-O6-C44
32	H	303	SQD	O5-C1-O6-C44
36	B	850	DGD	O6D-C1D-O3G-C3G
37	H	306	NEX	O24-C26-C27-C28
38	P	308	KC2	C1A-C2A-CAA-CBA
38	P	308	KC2	C2A-CAA-CBA-CGA
38	Q	310	KC2	C1A-C2A-CAA-CBA
38	Q	310	KC2	C3A-C2A-CAA-CBA
38	Q	310	KC2	C2A-CAA-CBA-CGA
38	R	312	KC2	C1A-C2A-CAA-CBA
38	R	312	KC2	C2A-CAA-CBA-CGA
38	S	308	KC2	C3A-C2A-CAA-CBA
38	S	308	KC2	C2A-CAA-CBA-CGA
38	S	308	KC2	CHA-CBD-CGD-O1D
38	S	308	KC2	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
38	T	308	KC2	C3A-C2A-CAA-CBA
38	T	308	KC2	C2A-CAA-CBA-CGA
38	U	307	KC2	C1A-C2A-CAA-CBA
38	U	307	KC2	C3A-C2A-CAA-CBA
38	U	307	KC2	C2A-CAA-CBA-CGA
38	U	307	KC2	CAA-CBA-CGA-O1A
38	U	307	KC2	CAA-CBA-CGA-O2A
38	V	308	KC2	C3A-C2A-CAA-CBA
38	V	308	KC2	C2A-CAA-CBA-CGA
38	V	308	KC2	CHA-CBD-CGD-O1D
38	V	308	KC2	CHA-CBD-CGD-O2D
38	W	308	KC2	C3A-C2A-CAA-CBA
38	W	308	KC2	C2A-CAA-CBA-CGA
38	X	309	KC2	C1A-C2A-CAA-CBA
38	X	309	KC2	C3A-C2A-CAA-CBA
38	X	309	KC2	C2A-CAA-CBA-CGA
24	P	304	CHL	O1D-CGD-O2D-CED
24	S	307	CHL	O1D-CGD-O2D-CED
24	U	304	CHL	O1D-CGD-O2D-CED
24	V	307	CHL	O1D-CGD-O2D-CED
24	X	308	CHL	O1D-CGD-O2D-CED
24	X	315	CHL	O1D-CGD-O2D-CED
25	4	311	CLA	O1D-CGD-O2D-CED
25	6	609	CLA	O1D-CGD-O2D-CED
25	A	830	CLA	O1D-CGD-O2D-CED
25	B	804	CLA	O1D-CGD-O2D-CED
25	B	805	CLA	O1D-CGD-O2D-CED
25	K	201	CLA	O1D-CGD-O2D-CED
25	U	311	CLA	O1D-CGD-O2D-CED
25	V	310	CLA	O1D-CGD-O2D-CED
25	W	303	CLA	O1D-CGD-O2D-CED
25	1	608	CLA	O1D-CGD-O2D-CED
25	5	603	CLA	O1D-CGD-O2D-CED
25	O	2005	CLA	O1D-CGD-O2D-CED
25	S	311	CLA	O1D-CGD-O2D-CED
25	W	311	CLA	O1D-CGD-O2D-CED
25	X	312	CLA	O1D-CGD-O2D-CED
24	3	306	CHL	CBD-CGD-O2D-CED
24	4	302	CHL	CBD-CGD-O2D-CED
24	S	305	CHL	CBD-CGD-O2D-CED
24	T	305	CHL	CBD-CGD-O2D-CED
24	V	307	CHL	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
24	W	307	CHL	CBD-CGD-O2D-CED
25	1	602	CLA	CBD-CGD-O2D-CED
25	3	301	CLA	CBD-CGD-O2D-CED
25	4	314	CLA	CBD-CGD-O2D-CED
25	5	601	CLA	CBD-CGD-O2D-CED
25	5	603	CLA	CBD-CGD-O2D-CED
25	6	604	CLA	CBD-CGD-O2D-CED
25	6	609	CLA	CBD-CGD-O2D-CED
25	A	830	CLA	CBD-CGD-O2D-CED
25	A	838	CLA	CBD-CGD-O2D-CED
25	B	804	CLA	CBD-CGD-O2D-CED
25	B	808	CLA	CBD-CGD-O2D-CED
25	B	812	CLA	CBD-CGD-O2D-CED
25	B	834	CLA	CBD-CGD-O2D-CED
25	B	840	CLA	CBD-CGD-O2D-CED
25	G	204	CLA	CBD-CGD-O2D-CED
25	L	304	CLA	CBD-CGD-O2D-CED
25	O	2004	CLA	CBD-CGD-O2D-CED
25	O	2005	CLA	CBD-CGD-O2D-CED
25	P	311	CLA	CBD-CGD-O2D-CED
25	Q	314	CLA	CBD-CGD-O2D-CED
25	R	306	CLA	CBD-CGD-O2D-CED
25	R	316	CLA	CBD-CGD-O2D-CED
25	S	309	CLA	CBD-CGD-O2D-CED
25	T	302	CLA	CBD-CGD-O2D-CED
25	T	312	CLA	CBD-CGD-O2D-CED
25	T	313	CLA	CBD-CGD-O2D-CED
25	U	302	CLA	CBD-CGD-O2D-CED
25	U	310	CLA	CBD-CGD-O2D-CED
25	V	301	CLA	CBD-CGD-O2D-CED
25	V	310	CLA	CBD-CGD-O2D-CED
25	W	301	CLA	CBD-CGD-O2D-CED
25	W	303	CLA	CBD-CGD-O2D-CED
25	W	311	CLA	CBD-CGD-O2D-CED
25	W	313	CLA	CBD-CGD-O2D-CED
25	X	303	CLA	CBD-CGD-O2D-CED
25	X	304	CLA	CBD-CGD-O2D-CED
38	U	307	KC2	CBD-CGD-O2D-CED
38	X	309	KC2	CBD-CGD-O2D-CED
25	1	603	CLA	O1A-CGA-O2A-C1
25	1	613	CLA	O1A-CGA-O2A-C1
25	3	302	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
25	A	830	CLA	O1A-CGA-O2A-C1
25	A	856	CLA	O1A-CGA-O2A-C1
25	B	813	CLA	O1A-CGA-O2A-C1
25	O	2002	CLA	O1A-CGA-O2A-C1
25	Q	315	CLA	O1A-CGA-O2A-C1
25	R	314	CLA	O1A-CGA-O2A-C1
25	U	311	CLA	O1A-CGA-O2A-C1
25	V	302	CLA	O1A-CGA-O2A-C1
25	5	601	CLA	O1A-CGA-O2A-C1
25	Q	313	CLA	O1A-CGA-O2A-C1
24	V	304	CHL	O1D-CGD-O2D-CED
24	W	307	CHL	O1D-CGD-O2D-CED
25	1	610	CLA	O1D-CGD-O2D-CED
25	3	310	CLA	O1D-CGD-O2D-CED
25	4	303	CLA	O1D-CGD-O2D-CED
25	5	601	CLA	O1D-CGD-O2D-CED
25	B	817	CLA	O1D-CGD-O2D-CED
25	T	302	CLA	O1D-CGD-O2D-CED
25	T	303	CLA	O1D-CGD-O2D-CED
25	V	303	CLA	O1D-CGD-O2D-CED
25	W	313	CLA	O1D-CGD-O2D-CED
25	X	313	CLA	O1D-CGD-O2D-CED
25	X	314	CLA	O1D-CGD-O2D-CED
24	2	605	CHL	O1D-CGD-O2D-CED
24	4	307	CHL	O1D-CGD-O2D-CED
24	R	309	CHL	O1D-CGD-O2D-CED
24	T	304	CHL	O1D-CGD-O2D-CED
25	2	608	CLA	O1D-CGD-O2D-CED
25	4	309	CLA	O1D-CGD-O2D-CED
25	6	604	CLA	O1D-CGD-O2D-CED
25	A	819	CLA	O1D-CGD-O2D-CED
25	A	824	CLA	O1D-CGD-O2D-CED
25	K	204	CLA	O1D-CGD-O2D-CED
25	P	303	CLA	O1D-CGD-O2D-CED
25	R	306	CLA	O1D-CGD-O2D-CED
25	X	303	CLA	O1D-CGD-O2D-CED
25	A	827	CLA	CBA-CGA-O2A-C1
25	A	830	CLA	CBA-CGA-O2A-C1
25	B	813	CLA	CBA-CGA-O2A-C1
25	O	2002	CLA	CBA-CGA-O2A-C1
25	Q	315	CLA	CBA-CGA-O2A-C1
25	R	317	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
25	U	311	CLA	CBA-CGA-O2A-C1
25	V	302	CLA	CBA-CGA-O2A-C1
24	2	615	CHL	CBD-CGD-O2D-CED
24	Q	307	CHL	CBD-CGD-O2D-CED
24	U	306	CHL	CBD-CGD-O2D-CED
24	X	306	CHL	CBD-CGD-O2D-CED
25	1	613	CLA	CBD-CGD-O2D-CED
25	2	609	CLA	CBD-CGD-O2D-CED
25	5	607	CLA	CBD-CGD-O2D-CED
25	5	608	CLA	CBD-CGD-O2D-CED
25	6	610	CLA	CBD-CGD-O2D-CED
25	6	612	CLA	CBD-CGD-O2D-CED
25	A	812	CLA	CBD-CGD-O2D-CED
25	A	815	CLA	CBD-CGD-O2D-CED
25	A	825	CLA	CBD-CGD-O2D-CED
25	A	839	CLA	CBD-CGD-O2D-CED
25	B	811	CLA	CBD-CGD-O2D-CED
25	B	818	CLA	CBD-CGD-O2D-CED
25	B	820	CLA	CBD-CGD-O2D-CED
25	B	835	CLA	CBD-CGD-O2D-CED
25	O	2002	CLA	CBD-CGD-O2D-CED
25	Q	311	CLA	CBD-CGD-O2D-CED
25	V	302	CLA	CBD-CGD-O2D-CED
25	V	309	CLA	CBD-CGD-O2D-CED
38	P	308	KC2	CBD-CGD-O2D-CED
38	W	308	KC2	CBD-CGD-O2D-CED
24	P	306	CHL	O1A-CGA-O2A-C1
24	R	310	CHL	O1A-CGA-O2A-C1
24	S	306	CHL	O1A-CGA-O2A-C1
24	W	306	CHL	O1A-CGA-O2A-C1
24	W	307	CHL	O1A-CGA-O2A-C1
25	2	602	CLA	O1A-CGA-O2A-C1
25	A	805	CLA	O1A-CGA-O2A-C1
25	A	807	CLA	O1A-CGA-O2A-C1
25	A	808	CLA	O1A-CGA-O2A-C1
25	A	814	CLA	O1A-CGA-O2A-C1
25	A	819	CLA	O1A-CGA-O2A-C1
25	A	827	CLA	O1A-CGA-O2A-C1
25	A	829	CLA	O1A-CGA-O2A-C1
25	A	835	CLA	O1A-CGA-O2A-C1
25	A	837	CLA	O1A-CGA-O2A-C1
25	A	845	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
25	B	812	CLA	O1A-CGA-O2A-C1
25	B	819	CLA	O1A-CGA-O2A-C1
25	B	831	CLA	O1A-CGA-O2A-C1
25	B	839	CLA	O1A-CGA-O2A-C1
25	P	302	CLA	O1A-CGA-O2A-C1
25	P	311	CLA	O1A-CGA-O2A-C1
25	Q	304	CLA	O1A-CGA-O2A-C1
25	R	305	CLA	O1A-CGA-O2A-C1
25	R	315	CLA	O1A-CGA-O2A-C1
25	S	311	CLA	O1A-CGA-O2A-C1
25	T	309	CLA	O1A-CGA-O2A-C1
25	V	313	CLA	O1A-CGA-O2A-C1
25	X	302	CLA	O1A-CGA-O2A-C1
25	X	311	CLA	O1A-CGA-O2A-C1
25	X	312	CLA	O1A-CGA-O2A-C1
24	R	302	CHL	O1A-CGA-O2A-C1
24	6	606	CHL	O1D-CGD-O2D-CED
24	R	311	CHL	O1D-CGD-O2D-CED
24	R	318	CHL	O1D-CGD-O2D-CED
25	1	602	CLA	O1D-CGD-O2D-CED
25	2	610	CLA	O1D-CGD-O2D-CED
25	4	315	CLA	O1D-CGD-O2D-CED
25	A	835	CLA	O1D-CGD-O2D-CED
25	B	823	CLA	O1D-CGD-O2D-CED
25	T	311	CLA	O1D-CGD-O2D-CED
25	U	301	CLA	O1D-CGD-O2D-CED
24	3	306	CHL	O1D-CGD-O2D-CED
25	1	606	CLA	O1D-CGD-O2D-CED
25	A	836	CLA	O1D-CGD-O2D-CED
25	B	803	CLA	O1D-CGD-O2D-CED
25	B	829	CLA	O1D-CGD-O2D-CED
25	K	206	CLA	O1D-CGD-O2D-CED
25	X	311	CLA	O1D-CGD-O2D-CED
24	U	305	CHL	CBD-CGD-O2D-CED
25	A	814	CLA	CBD-CGD-O2D-CED
25	A	816	CLA	CBD-CGD-O2D-CED
25	A	821	CLA	CBD-CGD-O2D-CED
25	B	815	CLA	CBD-CGD-O2D-CED
25	P	309	CLA	CBD-CGD-O2D-CED
25	S	312	CLA	CBD-CGD-O2D-CED
24	T	305	CHL	O1D-CGD-O2D-CED
25	6	608	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
25	A	804	CLA	O1D-CGD-O2D-CED
25	B	808	CLA	O1D-CGD-O2D-CED
25	B	840	CLA	O1D-CGD-O2D-CED
25	P	311	CLA	O1D-CGD-O2D-CED
25	U	302	CLA	O1D-CGD-O2D-CED
25	A	823	CLA	C3-C5-C6-C7
25	A	830	CLA	C3-C5-C6-C7
25	A	839	CLA	C3-C5-C6-C7
25	B	808	CLA	C3-C5-C6-C7
25	B	813	CLA	C3-C5-C6-C7
25	B	814	CLA	C3-C5-C6-C7
25	B	815	CLA	C3-C5-C6-C7
25	B	836	CLA	C3-C5-C6-C7
25	K	206	CLA	C3-C5-C6-C7
25	R	315	CLA	C3-C5-C6-C7
25	S	301	CLA	C3-C5-C6-C7
25	T	309	CLA	C3-C5-C6-C7
25	V	312	CLA	C3-C5-C6-C7
25	W	302	CLA	C3-C5-C6-C7
25	W	312	CLA	C3-C5-C6-C7
24	P	306	CHL	CBA-CGA-O2A-C1
24	S	306	CHL	CBA-CGA-O2A-C1
24	W	307	CHL	CBA-CGA-O2A-C1
25	1	603	CLA	CBA-CGA-O2A-C1
25	1	613	CLA	CBA-CGA-O2A-C1
25	A	807	CLA	CBA-CGA-O2A-C1
25	A	820	CLA	CBA-CGA-O2A-C1
25	A	845	CLA	CBA-CGA-O2A-C1
25	A	856	CLA	CBA-CGA-O2A-C1
25	B	818	CLA	CBA-CGA-O2A-C1
25	B	819	CLA	CBA-CGA-O2A-C1
25	B	831	CLA	CBA-CGA-O2A-C1
25	B	839	CLA	CBA-CGA-O2A-C1
25	P	302	CLA	CBA-CGA-O2A-C1
25	Q	304	CLA	CBA-CGA-O2A-C1
25	R	305	CLA	CBA-CGA-O2A-C1
25	R	314	CLA	CBA-CGA-O2A-C1
25	R	316	CLA	CBA-CGA-O2A-C1
25	S	311	CLA	CBA-CGA-O2A-C1
25	X	302	CLA	CBA-CGA-O2A-C1
25	X	311	CLA	CBA-CGA-O2A-C1
25	O	2004	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
24	T	307	CHL	CBD-CGD-O2D-CED
25	A	818	CLA	CBD-CGD-O2D-CED
25	A	833	CLA	CBD-CGD-O2D-CED
25	A	841	CLA	CBD-CGD-O2D-CED
25	N	203	CLA	CBD-CGD-O2D-CED
25	1	613	CLA	C3-C5-C6-C7
25	B	808	CLA	C2C-C3C-CAC-CBC
25	A	819	CLA	C4-C3-C5-C6
25	A	831	CLA	C4-C3-C5-C6
29	U	317	Q6L	C11-C12-C13-C42
25	2	612	CLA	C2-C3-C5-C6
25	R	316	CLA	C2-C3-C5-C6
25	T	301	CLA	C2-C3-C5-C6
29	R	301	Q6L	C11-C12-C13-C14
29	R	323	Q6L	C11-C12-C13-C14
29	S	320	Q6L	C11-C12-C13-C14
29	T	319	Q6L	C11-C12-C13-C14
25	Q	304	CLA	CBD-CGD-O2D-CED
25	T	301	CLA	CBD-CGD-O2D-CED
25	V	311	CLA	CBD-CGD-O2D-CED
24	Q	308	CHL	C2A-CAA-CBA-CGA
24	V	304	CHL	C2A-CAA-CBA-CGA
25	A	810	CLA	C2A-CAA-CBA-CGA
25	B	806	CLA	C2A-CAA-CBA-CGA
25	B	816	CLA	C2A-CAA-CBA-CGA
25	B	841	CLA	C2A-CAA-CBA-CGA
25	K	204	CLA	C2A-CAA-CBA-CGA
25	O	2001	CLA	C2A-CAA-CBA-CGA
25	Q	314	CLA	C2A-CAA-CBA-CGA
25	V	313	CLA	C2A-CAA-CBA-CGA
25	W	301	CLA	C2A-CAA-CBA-CGA
25	W	301	CLA	O1D-CGD-O2D-CED
25	5	607	CLA	C3-C5-C6-C7
25	6	613	CLA	C3-C5-C6-C7
25	A	820	CLA	C3-C5-C6-C7
25	A	837	CLA	C3-C5-C6-C7
25	B	824	CLA	C3-C5-C6-C7
25	B	842	CLA	C3-C5-C6-C7
25	T	301	CLA	C3-C5-C6-C7
25	W	301	CLA	C3-C5-C6-C7
24	R	310	CHL	CBA-CGA-O2A-C1
24	W	306	CHL	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
25	1	608	CLA	CBA-CGA-O2A-C1
25	2	602	CLA	CBA-CGA-O2A-C1
25	4	303	CLA	CBA-CGA-O2A-C1
25	A	805	CLA	CBA-CGA-O2A-C1
25	A	808	CLA	CBA-CGA-O2A-C1
25	A	809	CLA	CBA-CGA-O2A-C1
25	A	812	CLA	CBA-CGA-O2A-C1
25	A	814	CLA	CBA-CGA-O2A-C1
25	A	819	CLA	CBA-CGA-O2A-C1
25	A	823	CLA	CBA-CGA-O2A-C1
25	A	829	CLA	CBA-CGA-O2A-C1
25	A	835	CLA	CBA-CGA-O2A-C1
25	A	837	CLA	CBA-CGA-O2A-C1
25	B	802	CLA	CBA-CGA-O2A-C1
25	B	812	CLA	CBA-CGA-O2A-C1
25	B	821	CLA	CBA-CGA-O2A-C1
25	B	823	CLA	CBA-CGA-O2A-C1
25	B	829	CLA	CBA-CGA-O2A-C1
25	P	311	CLA	CBA-CGA-O2A-C1
25	Q	314	CLA	CBA-CGA-O2A-C1
25	R	315	CLA	CBA-CGA-O2A-C1
25	T	309	CLA	CBA-CGA-O2A-C1
25	V	313	CLA	CBA-CGA-O2A-C1
25	X	312	CLA	CBA-CGA-O2A-C1
25	A	838	CLA	O1D-CGD-O2D-CED
25	B	834	CLA	O1D-CGD-O2D-CED
34	A	844	PQN	C11-C12-C13-C14
34	B	844	PQN	C11-C12-C13-C14
25	B	842	CLA	CBD-CGD-O2D-CED
24	S	305	CHL	O1D-CGD-O2D-CED
25	3	301	CLA	O1D-CGD-O2D-CED
25	4	314	CLA	O1D-CGD-O2D-CED
25	T	313	CLA	O1D-CGD-O2D-CED
25	U	310	CLA	O1D-CGD-O2D-CED
25	V	301	CLA	O1D-CGD-O2D-CED
25	6	602	CLA	O1A-CGA-O2A-C1
25	A	809	CLA	O1A-CGA-O2A-C1
25	A	820	CLA	O1A-CGA-O2A-C1
25	A	823	CLA	O1A-CGA-O2A-C1
25	B	802	CLA	O1A-CGA-O2A-C1
25	B	804	CLA	O1A-CGA-O2A-C1
25	B	805	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
25	B	823	CLA	O1A-CGA-O2A-C1
25	B	829	CLA	O1A-CGA-O2A-C1
25	Q	314	CLA	O1A-CGA-O2A-C1
33	A	802	CL0	O1A-CGA-O2A-C1
25	T	312	CLA	O1D-CGD-O2D-CED
26	V	320	IWJ	C10-C11-C12-C13
29	P	321	Q6L	C13-C14-C15-C16
29	R	323	Q6L	C24-C25-C26-C27
29	S	320	Q6L	C24-C25-C26-C27
29	U	315	Q6L	C13-C14-C15-C16
29	V	315	Q6L	C17-C18-C19-C20
24	2	607	CHL	CBD-CGD-O2D-CED
24	P	306	CHL	CBD-CGD-O2D-CED
24	X	307	CHL	CBD-CGD-O2D-CED
25	2	606	CLA	CBD-CGD-O2D-CED
25	2	614	CLA	CBD-CGD-O2D-CED
25	3	308	CLA	CBD-CGD-O2D-CED
25	6	611	CLA	CBD-CGD-O2D-CED
25	A	805	CLA	CBD-CGD-O2D-CED
25	A	823	CLA	CBD-CGD-O2D-CED
25	F	802	CLA	CBD-CGD-O2D-CED
25	F	803	CLA	CBD-CGD-O2D-CED
25	J	102	CLA	CBD-CGD-O2D-CED
25	L	301	CLA	CBD-CGD-O2D-CED
25	L	302	CLA	CBD-CGD-O2D-CED
25	Q	301	CLA	CBD-CGD-O2D-CED
25	Q	306	CLA	CBD-CGD-O2D-CED
25	R	307	CLA	CBD-CGD-O2D-CED
25	W	310	CLA	CBD-CGD-O2D-CED
25	G	204	CLA	O1D-CGD-O2D-CED
38	X	309	KC2	O1D-CGD-O2D-CED
28	3	323	LHG	O2-C2-C3-O3
25	A	817	CLA	C3-C5-C6-C7
25	B	834	CLA	C3-C5-C6-C7
25	Q	304	CLA	C3-C5-C6-C7
25	5	607	CLA	CBA-CGA-O2A-C1
25	A	843	CLA	CBA-CGA-O2A-C1
25	B	805	CLA	CBA-CGA-O2A-C1
25	W	303	CLA	CBA-CGA-O2A-C1
25	W	310	CLA	CBA-CGA-O2A-C1
25	X	303	CLA	CBA-CGA-O2A-C1
33	A	802	CL0	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
25	4	303	CLA	O1A-CGA-O2A-C1
25	5	602	CLA	O1A-CGA-O2A-C1
25	B	818	CLA	O1A-CGA-O2A-C1
25	O	2001	CLA	O1A-CGA-O2A-C1
28	6	616	LHG	O10-C23-O8-C6
25	Q	314	CLA	O1D-CGD-O2D-CED
38	U	307	KC2	O1D-CGD-O2D-CED
28	3	322	LHG	C8-C7-O7-C5
24	T	314	CHL	CBD-CGD-O2D-CED
25	5	602	CLA	CBD-CGD-O2D-CED
25	B	843	CLA	CBD-CGD-O2D-CED
25	S	303	CLA	CBD-CGD-O2D-CED
25	U	309	CLA	CBD-CGD-O2D-CED
25	L	304	CLA	O1D-CGD-O2D-CED
24	W	314	CHL	CBD-CGD-O2D-CED
25	B	820	CLA	C3-C5-C6-C7
25	V	311	CLA	C3-C5-C6-C7
25	W	309	CLA	C3-C5-C6-C7
25	X	302	CLA	C3-C5-C6-C7
25	5	602	CLA	CBA-CGA-O2A-C1
25	6	602	CLA	CBA-CGA-O2A-C1
25	B	804	CLA	CBA-CGA-O2A-C1
25	B	820	CLA	CBA-CGA-O2A-C1
25	O	2001	CLA	CBA-CGA-O2A-C1
28	6	616	LHG	C24-C23-O8-C6
25	S	309	CLA	O1D-CGD-O2D-CED
38	S	308	KC2	CAA-CBA-CGA-O2A
25	1	608	CLA	O1A-CGA-O2A-C1
25	A	843	CLA	O1A-CGA-O2A-C1
25	B	820	CLA	O1A-CGA-O2A-C1
25	B	821	CLA	O1A-CGA-O2A-C1
25	R	316	CLA	O1A-CGA-O2A-C1
25	3	302	CLA	C4-C3-C5-C6
25	V	301	CLA	C4-C3-C5-C6
29	O	2006	Q6L	C11-C12-C13-C42
29	Q	319	Q6L	C11-C12-C13-C42
29	S	321	Q6L	C11-C12-C13-C42
29	S	323	Q6L	C11-C12-C13-C42
29	V	315	Q6L	C11-C12-C13-C42
29	V	319	Q6L	C11-C12-C13-C42
25	A	819	CLA	C2-C3-C5-C6
25	V	301	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
29	O	2006	Q6L	C11-C12-C13-C14
29	Q	319	Q6L	C11-C12-C13-C14
29	S	321	Q6L	C11-C12-C13-C14
29	S	323	Q6L	C11-C12-C13-C14
29	V	315	Q6L	C11-C12-C13-C14
29	V	319	Q6L	C11-C12-C13-C14
25	1	603	CLA	C2A-CAA-CBA-CGA
25	A	819	CLA	C2A-CAA-CBA-CGA
25	A	829	CLA	C2A-CAA-CBA-CGA
25	A	845	CLA	C2A-CAA-CBA-CGA
25	A	856	CLA	C2A-CAA-CBA-CGA
25	B	830	CLA	C2A-CAA-CBA-CGA
25	H	304	CLA	C2A-CAA-CBA-CGA
25	L	303	CLA	C2A-CAA-CBA-CGA
25	Q	301	CLA	C2A-CAA-CBA-CGA
25	V	311	CLA	C2A-CAA-CBA-CGA
24	4	302	CHL	O1D-CGD-O2D-CED
25	5	607	CLA	O1A-CGA-O2A-C1
25	A	812	CLA	O1A-CGA-O2A-C1
25	A	821	CLA	O1A-CGA-O2A-C1
25	W	303	CLA	O1A-CGA-O2A-C1
25	W	310	CLA	O1A-CGA-O2A-C1
25	X	303	CLA	O1A-CGA-O2A-C1
25	A	826	CLA	CBA-CGA-O2A-C1
25	T	312	CLA	CBA-CGA-O2A-C1
25	V	311	CLA	CBA-CGA-O2A-C1
25	H	301	CLA	CBD-CGD-O2D-CED
24	Q	307	CHL	O1D-CGD-O2D-CED
25	2	609	CLA	O1D-CGD-O2D-CED
25	A	839	CLA	O1D-CGD-O2D-CED
25	B	811	CLA	O1D-CGD-O2D-CED
25	B	812	CLA	O1D-CGD-O2D-CED
25	R	316	CLA	O1D-CGD-O2D-CED
25	X	304	CLA	O1D-CGD-O2D-CED
38	R	312	KC2	CAA-CBA-CGA-O1A
24	X	306	CHL	O1D-CGD-O2D-CED
25	V	309	CLA	O1D-CGD-O2D-CED
38	W	308	KC2	O1D-CGD-O2D-CED
25	A	826	CLA	O1A-CGA-O2A-C1
25	B	842	CLA	O1A-CGA-O2A-C1
25	V	311	CLA	O1A-CGA-O2A-C1
34	A	844	PQN	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
25	6	612	CLA	O1D-CGD-O2D-CED
25	B	818	CLA	O1D-CGD-O2D-CED
25	B	835	CLA	O1D-CGD-O2D-CED
24	T	306	CHL	CBA-CGA-O2A-C1
25	4	310	CLA	CBA-CGA-O2A-C1
25	6	610	CLA	CBA-CGA-O2A-C1
25	A	813	CLA	CBA-CGA-O2A-C1
25	A	821	CLA	CBA-CGA-O2A-C1
25	A	831	CLA	CBA-CGA-O2A-C1
25	B	806	CLA	CBA-CGA-O2A-C1
25	B	827	CLA	CBA-CGA-O2A-C1
25	B	830	CLA	CBA-CGA-O2A-C1
25	B	842	CLA	CBA-CGA-O2A-C1
25	P	301	CLA	CBA-CGA-O2A-C1
25	W	301	CLA	CBA-CGA-O2A-C1
25	W	302	CLA	CBA-CGA-O2A-C1
25	2	604	CLA	CBD-CGD-O2D-CED
29	P	319	Q6L	C13-C14-C15-C16
25	W	310	CLA	C8-C10-C11-C12
38	S	308	KC2	CAA-CBA-CGA-O1A
38	V	308	KC2	CAA-CBA-CGA-O1A
38	V	308	KC2	CAA-CBA-CGA-O2A
38	W	308	KC2	CAA-CBA-CGA-O1A
24	W	307	CHL	C5-C6-C7-C8
25	A	830	CLA	C10-C11-C12-C13
25	A	838	CLA	C13-C15-C16-C17
25	B	807	CLA	C13-C15-C16-C17
25	B	813	CLA	C8-C10-C11-C12
25	B	834	CLA	C10-C11-C12-C13
25	T	311	CLA	C5-C6-C7-C8
25	T	312	CLA	O1A-CGA-O2A-C1
25	3	302	CLA	C2-C3-C5-C6
25	A	831	CLA	C2-C3-C5-C6
25	Q	314	CLA	C2-C3-C5-C6
29	U	317	Q6L	C11-C12-C13-C14
24	W	307	CHL	C6-C7-C8-C9
25	2	612	CLA	C11-C10-C8-C9
25	A	819	CLA	C11-C10-C8-C9
25	A	828	CLA	C11-C10-C8-C9
25	B	813	CLA	C14-C13-C15-C16
25	B	815	CLA	C6-C7-C8-C9
25	B	834	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
25	L	302	CLA	C11-C10-C8-C9
25	P	310	CLA	C11-C10-C8-C9
25	R	315	CLA	C11-C10-C8-C9
25	V	301	CLA	C11-C10-C8-C9
34	A	844	PQN	C24-C23-C25-C26
25	5	607	CLA	O1D-CGD-O2D-CED
25	V	302	CLA	O1D-CGD-O2D-CED
38	P	308	KC2	O1D-CGD-O2D-CED
24	P	314	CHL	CBD-CGD-O2D-CED
25	O	2002	CLA	C15-C16-C17-C18
24	T	306	CHL	C2A-CAA-CBA-CGA
25	5	601	CLA	C2A-CAA-CBA-CGA
25	A	833	CLA	C2A-CAA-CBA-CGA
26	S	318	IWJ	C20-C19-C21-C22
27	1	612	XAT	C7-C8-C9-C19
29	2	616	Q6L	C23-C22-C24-C25
29	2	616	Q6L	C28-C27-C29-C30
29	O	2006	Q6L	C28-C27-C29-C30
29	P	321	Q6L	C28-C27-C29-C30
29	Q	319	Q6L	C28-C27-C29-C30
29	R	304	Q6L	C28-C27-C29-C30
29	R	319	Q6L	C15-C16-C17-C41
29	R	323	Q6L	C23-C22-C24-C25
29	S	321	Q6L	C28-C27-C29-C30
29	S	323	Q6L	C28-C27-C29-C30
29	T	319	Q6L	C28-C27-C29-C30
29	V	321	Q6L	C28-C27-C29-C30
29	W	319	Q6L	C23-C22-C24-C25
29	X	316	Q6L	C15-C16-C17-C41
30	3	318	BCR	C11-C12-C13-C35
30	A	849	BCR	C37-C22-C23-C24
30	F	801	BCR	C37-C22-C23-C24
30	F	804	BCR	C7-C8-C9-C34
30	H	305	BCR	C11-C12-C13-C35
30	M	101	BCR	C7-C8-C9-C34
29	2	616	Q6L	C26-C27-C29-C30
29	O	2006	Q6L	C26-C27-C29-C30
29	P	319	Q6L	C26-C27-C29-C30
29	P	321	Q6L	C26-C27-C29-C30
29	Q	319	Q6L	C26-C27-C29-C30
29	R	304	Q6L	C26-C27-C29-C30
29	R	323	Q6L	C26-C27-C29-C30

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Mol	Chain	Res	Type	Atoms
29	S	321	Q6L	C26-C27-C29-C30
29	S	323	Q6L	C26-C27-C29-C30
29	T	319	Q6L	C26-C27-C29-C30
29	T	322	Q6L	C26-C27-C29-C30
29	V	321	Q6L	C26-C27-C29-C30
29	W	319	Q6L	C21-C22-C24-C25
29	W	320	Q6L	C26-C27-C29-C30
30	B	845	BCR	C7-C8-C9-C10
30	F	801	BCR	C21-C22-C23-C24
24	U	306	CHL	O1D-CGD-O2D-CED
25	4	310	CLA	O1A-CGA-O2A-C1
25	A	831	CLA	O1A-CGA-O2A-C1
25	B	827	CLA	O1A-CGA-O2A-C1
25	B	830	CLA	O1A-CGA-O2A-C1
25	H	302	CLA	C15-C16-C17-C18
25	5	608	CLA	O1D-CGD-O2D-CED
25	A	825	CLA	O1D-CGD-O2D-CED
25	K	204	CLA	CBA-CGA-O2A-C1
25	U	309	CLA	CBA-CGA-O2A-C1
38	R	312	KC2	CAA-CBA-CGA-O2A
38	T	308	KC2	CAA-CBA-CGA-O1A
38	W	308	KC2	CAA-CBA-CGA-O2A
25	B	820	CLA	O1D-CGD-O2D-CED
25	O	2002	CLA	O1D-CGD-O2D-CED
25	A	832	CLA	CBA-CGA-O2A-C1
25	A	838	CLA	CBA-CGA-O2A-C1
25	S	309	CLA	CBA-CGA-O2A-C1
25	A	821	CLA	C15-C16-C17-C18
25	A	835	CLA	C5-C6-C7-C8
25	A	842	CLA	C5-C6-C7-C8
25	B	814	CLA	C10-C11-C12-C13
25	B	826	CLA	C10-C11-C12-C13
25	R	305	CLA	C13-C15-C16-C17
25	S	302	CLA	C5-C6-C7-C8
34	A	844	PQN	C18-C20-C21-C22
25	Q	311	CLA	O1D-CGD-O2D-CED
25	A	804	CLA	C15-C16-C17-C18
25	A	825	CLA	C15-C16-C17-C18
25	A	837	CLA	C5-C6-C7-C8
25	B	805	CLA	C13-C15-C16-C17
25	B	807	CLA	C15-C16-C17-C18
25	B	809	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
25	B	834	CLA	C8-C10-C11-C12
25	P	301	CLA	C10-C11-C12-C13
25	R	306	CLA	C10-C11-C12-C13
25	T	301	CLA	C8-C10-C11-C12
25	W	310	CLA	C5-C6-C7-C8
25	Q	304	CLA	O1D-CGD-O2D-CED
28	2	619	LHG	C7-C8-C9-C10
28	A	846	LHG	C23-C24-C25-C26
36	B	850	DGD	C1B-C2B-C3B-C4B
25	U	303	CLA	CBD-CGD-O2D-CED
25	A	812	CLA	O1D-CGD-O2D-CED
25	A	815	CLA	O1D-CGD-O2D-CED
25	2	612	CLA	C5-C6-C7-C8
25	A	815	CLA	C8-C10-C11-C12
25	B	809	CLA	C5-C6-C7-C8
25	B	829	CLA	C15-C16-C17-C18
25	S	301	CLA	C8-C10-C11-C12
25	B	804	CLA	C3-C5-C6-C7
25	A	839	CLA	CBA-CGA-O2A-C1
25	W	312	CLA	CBA-CGA-O2A-C1
25	1	613	CLA	O1D-CGD-O2D-CED
38	T	308	KC2	CAA-CBA-CGA-O2A
25	A	830	CLA	C2-C1-O2A-CGA
25	B	805	CLA	C2-C1-O2A-CGA
33	A	802	CL0	C2-C1-O2A-CGA
25	B	810	CLA	C8-C10-C11-C12
28	2	619	LHG	C23-C24-C25-C26
25	X	310	CLA	CBD-CGD-O2D-CED
25	K	203	CLA	C13-C15-C16-C17
25	A	817	CLA	C13-C15-C16-C17
25	A	831	CLA	C15-C16-C17-C18
24	2	615	CHL	O1D-CGD-O2D-CED
25	A	830	CLA	C11-C10-C8-C7
25	B	808	CLA	C11-C12-C13-C15
25	B	810	CLA	C6-C7-C8-C10
25	B	813	CLA	C11-C10-C8-C7
25	T	302	CLA	C6-C7-C8-C10
25	A	842	CLA	C3-C5-C6-C7
25	6	610	CLA	O1A-CGA-O2A-C1
25	A	813	CLA	O1A-CGA-O2A-C1
25	A	838	CLA	O1A-CGA-O2A-C1
25	W	301	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
26	V	318	IWJ	C10-C11-C12-C13
29	S	316	Q6L	C13-C14-C15-C16
29	W	319	Q6L	C24-C25-C26-C27
25	B	843	CLA	C2A-CAA-CBA-CGA
25	U	309	CLA	C2A-CAA-CBA-CGA
25	6	610	CLA	O1D-CGD-O2D-CED
25	A	814	CLA	O1D-CGD-O2D-CED
25	A	833	CLA	O1D-CGD-O2D-CED
25	3	307	CLA	C5-C6-C7-C8
25	4	313	CLA	C5-C6-C7-C8
25	B	824	CLA	C10-C11-C12-C13
25	R	306	CLA	C15-C16-C17-C18
24	T	306	CHL	O1A-CGA-O2A-C1
25	W	302	CLA	O1A-CGA-O2A-C1
25	B	806	CLA	CBD-CGD-O2D-CED
25	B	813	CLA	C10-C11-C12-C13
25	N	203	CLA	O1D-CGD-O2D-CED
25	S	312	CLA	O1D-CGD-O2D-CED
28	3	322	LHG	O9-C7-O7-C5
25	2	613	CLA	C2A-CAA-CBA-CGA
25	B	832	CLA	C2A-CAA-CBA-CGA
25	1	603	CLA	C5-C6-C7-C8
25	B	802	CLA	C15-C16-C17-C18
25	B	819	CLA	C5-C6-C7-C8
25	P	310	CLA	C8-C10-C11-C12
25	P	311	CLA	C8-C10-C11-C12
25	V	301	CLA	C10-C11-C12-C13
25	P	309	CLA	O1D-CGD-O2D-CED
25	B	806	CLA	O1A-CGA-O2A-C1
25	P	301	CLA	O1A-CGA-O2A-C1
25	S	309	CLA	O1A-CGA-O2A-C1
25	W	312	CLA	O1A-CGA-O2A-C1
25	A	819	CLA	C10-C11-C12-C13
25	A	827	CLA	C5-C6-C7-C8
25	A	839	CLA	C13-C15-C16-C17
25	A	842	CLA	C13-C15-C16-C17
25	B	804	CLA	C10-C11-C12-C13
25	B	810	CLA	C5-C6-C7-C8
25	R	314	CLA	C5-C6-C7-C8
24	T	307	CHL	O1D-CGD-O2D-CED
24	U	305	CHL	O1D-CGD-O2D-CED
25	A	818	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
25	T	301	CLA	O1D-CGD-O2D-CED
25	A	832	CLA	O1A-CGA-O2A-C1
25	A	839	CLA	O1A-CGA-O2A-C1
31	2	620	LMG	C11-C10-O7-C8
25	A	807	CLA	C13-C15-C16-C17
25	B	802	CLA	C13-C15-C16-C17
25	B	814	CLA	C15-C16-C17-C18
25	R	313	CLA	C8-C10-C11-C12
25	U	302	CLA	C5-C6-C7-C8
28	1	614	LHG	C4-O6-P-O3
28	2	619	LHG	C4-O6-P-O3
28	3	321	LHG	C4-O6-P-O3
28	6	616	LHG	C3-O3-P-O6
28	6	616	LHG	C4-O6-P-O3
28	Q	302	LHG	C4-O6-P-O3
25	R	314	CLA	C3-C5-C6-C7
24	T	305	CHL	CBA-CGA-O2A-C1
25	6	613	CLA	CBA-CGA-O2A-C1
25	P	310	CLA	CBA-CGA-O2A-C1
25	A	841	CLA	O1D-CGD-O2D-CED
25	Q	306	CLA	O1D-CGD-O2D-CED
25	R	314	CLA	CBD-CGD-O2D-CED
25	B	839	CLA	C5-C6-C7-C8
25	P	309	CLA	C13-C15-C16-C17
34	A	844	PQN	C25-C26-C27-C28
25	A	816	CLA	O1D-CGD-O2D-CED
25	B	815	CLA	O1D-CGD-O2D-CED
31	2	620	LMG	O9-C10-O7-C8
29	P	315	Q6L	C11-C12-C13-C42
29	W	315	Q6L	C11-C12-C13-C42
25	A	825	CLA	C2-C3-C5-C6
25	B	839	CLA	C15-C16-C17-C18
25	B	843	CLA	C15-C16-C17-C18
24	3	306	CHL	C2A-CAA-CBA-CGA
25	2	612	CLA	C2A-CAA-CBA-CGA
25	3	311	CLA	C2A-CAA-CBA-CGA
25	B	821	CLA	C2A-CAA-CBA-CGA
25	A	803	CLA	C16-C17-C18-C20
25	A	819	CLA	C11-C12-C13-C14
25	2	609	CLA	C3-C5-C6-C7
25	V	311	CLA	O1D-CGD-O2D-CED
24	Q	308	CHL	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
24	R	309	CHL	CBA-CGA-O2A-C1
25	A	817	CLA	CBA-CGA-O2A-C1
25	B	803	CLA	CBA-CGA-O2A-C1
25	2	609	CLA	C6-C7-C8-C10
25	A	832	CLA	C16-C17-C18-C19
25	B	811	CLA	C16-C17-C18-C19
25	T	312	CLA	C6-C7-C8-C9
25	A	804	CLA	CBA-CGA-O2A-C1
25	Q	301	CLA	CBA-CGA-O2A-C1
25	3	308	CLA	O1D-CGD-O2D-CED
25	K	206	CLA	C15-C16-C17-C18
25	A	805	CLA	O1D-CGD-O2D-CED
25	A	821	CLA	O1D-CGD-O2D-CED
25	A	819	CLA	C3-C5-C6-C7
25	2	606	CLA	O1D-CGD-O2D-CED
25	B	842	CLA	O1D-CGD-O2D-CED
25	W	310	CLA	O1D-CGD-O2D-CED
25	P	310	CLA	O1A-CGA-O2A-C1
25	3	311	CLA	C6-C7-C8-C9
25	B	818	CLA	C6-C7-C8-C9
34	A	844	PQN	C26-C27-C28-C30
25	F	802	CLA	O1D-CGD-O2D-CED
25	6	602	CLA	C11-C12-C13-C14
25	B	810	CLA	C6-C7-C8-C9
25	B	812	CLA	C14-C13-C15-C16
25	B	841	CLA	C6-C7-C8-C9
25	B	842	CLA	C6-C7-C8-C9
25	S	309	CLA	C6-C7-C8-C9
25	U	302	CLA	C6-C7-C8-C9
36	A	854	DGD	O6D-C5D-C6D-O5D
28	3	321	LHG	C34-C35-C36-C37
31	5	613	LMG	C16-C17-C18-C19
25	A	830	CLA	C15-C16-C17-C18
25	A	838	CLA	C15-C16-C17-C18
25	2	606	CLA	C2A-CAA-CBA-CGA
25	2	611	CLA	C2A-CAA-CBA-CGA
25	4	313	CLA	C2A-CAA-CBA-CGA
25	B	840	CLA	C2A-CAA-CBA-CGA
24	R	309	CHL	O1A-CGA-O2A-C1
29	P	319	Q6L	C28-C27-C29-C30
29	R	319	Q6L	C28-C27-C29-C30
29	W	316	Q6L	C28-C27-C29-C30

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Mol	Chain	Res	Type	Atoms
29	X	301	Q6L	C28-C27-C29-C30
30	B	845	BCR	C7-C8-C9-C34
26	S	318	IWJ	C18-C19-C21-C22
27	1	612	XAT	C7-C8-C9-C10
27	4	318	XAT	C27-C28-C29-C30
29	R	319	Q6L	C26-C27-C29-C30
29	R	323	Q6L	C21-C22-C24-C25
29	T	315	Q6L	C26-C27-C29-C30
29	U	314	Q6L	C15-C16-C17-C18
29	X	301	Q6L	C26-C27-C29-C30
30	A	851	BCR	C21-C22-C23-C24
30	I	101	BCR	C7-C8-C9-C10
25	B	810	CLA	C15-C16-C17-C18
25	B	813	CLA	C13-C15-C16-C17
25	B	828	CLA	C13-C15-C16-C17
25	F	803	CLA	O1D-CGD-O2D-CED
25	L	301	CLA	O1D-CGD-O2D-CED
25	R	307	CLA	O1D-CGD-O2D-CED
32	6	617	SQD	C29-C30-C31-C32
25	3	301	CLA	C11-C12-C13-C14
25	3	301	CLA	C11-C12-C13-C15
25	B	810	CLA	C16-C17-C18-C20
25	Q	311	CLA	C6-C7-C8-C10
25	T	312	CLA	C6-C7-C8-C10
25	W	312	CLA	C6-C7-C8-C9
34	A	844	PQN	C26-C27-C28-C29
25	X	302	CLA	C5-C6-C7-C8
36	A	854	DGD	C4D-C5D-C6D-O5D
25	A	826	CLA	CBD-CGD-O2D-CED
24	P	306	CHL	O1D-CGD-O2D-CED
31	A	857	LMG	C28-C29-C30-C31
25	6	613	CLA	O1A-CGA-O2A-C1
25	B	803	CLA	O1A-CGA-O2A-C1
28	1	614	LHG	C30-C31-C32-C33
25	6	611	CLA	O1D-CGD-O2D-CED
25	A	823	CLA	O1D-CGD-O2D-CED
25	V	312	CLA	CBA-CGA-O2A-C1
24	2	601	CHL	C3A-C2A-CAA-CBA
24	P	305	CHL	C3A-C2A-CAA-CBA
24	P	314	CHL	C3A-C2A-CAA-CBA
24	Q	307	CHL	C3A-C2A-CAA-CBA
24	R	302	CHL	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
24	V	314	CHL	C3A-C2A-CAA-CBA
24	W	307	CHL	C3A-C2A-CAA-CBA
25	2	603	CLA	C3A-C2A-CAA-CBA
25	2	614	CLA	C3A-C2A-CAA-CBA
25	3	302	CLA	C3A-C2A-CAA-CBA
25	3	310	CLA	C3A-C2A-CAA-CBA
25	6	610	CLA	C3A-C2A-CAA-CBA
25	6	613	CLA	C3A-C2A-CAA-CBA
25	A	805	CLA	C3A-C2A-CAA-CBA
25	A	811	CLA	C3A-C2A-CAA-CBA
25	A	840	CLA	C3A-C2A-CAA-CBA
25	A	842	CLA	C3A-C2A-CAA-CBA
25	B	809	CLA	C3A-C2A-CAA-CBA
25	B	818	CLA	C3A-C2A-CAA-CBA
25	B	821	CLA	C3A-C2A-CAA-CBA
25	B	839	CLA	C3A-C2A-CAA-CBA
25	H	302	CLA	C3A-C2A-CAA-CBA
25	Q	306	CLA	C3A-C2A-CAA-CBA
25	Q	311	CLA	C3A-C2A-CAA-CBA
25	Q	313	CLA	C3A-C2A-CAA-CBA
25	R	305	CLA	C3A-C2A-CAA-CBA
25	S	310	CLA	C3A-C2A-CAA-CBA
25	S	311	CLA	C3A-C2A-CAA-CBA
25	T	312	CLA	C3A-C2A-CAA-CBA
25	Q	301	CLA	C5-C6-C7-C8
32	6	617	SQD	C31-C32-C33-C34
24	2	607	CHL	O1D-CGD-O2D-CED
25	J	102	CLA	O1D-CGD-O2D-CED
25	Q	301	CLA	O1D-CGD-O2D-CED
25	A	817	CLA	O1A-CGA-O2A-C1
25	3	311	CLA	C6-C7-C8-C10
25	A	803	CLA	C16-C17-C18-C19
25	Q	311	CLA	C6-C7-C8-C9
25	W	312	CLA	C6-C7-C8-C10
25	H	301	CLA	C2A-CAA-CBA-CGA
25	B	837	CLA	CBD-CGD-O2D-CED
36	A	854	DGD	C2B-C3B-C4B-C5B
25	4	313	CLA	C3-C5-C6-C7
25	B	808	CLA	C4-C3-C5-C6
29	S	315	Q6L	C11-C12-C13-C42
25	B	807	CLA	CBA-CGA-O2A-C1
25	Q	306	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
25	B	808	CLA	C2-C3-C5-C6
29	Q	318	Q6L	C11-C12-C13-C14
29	S	315	Q6L	C11-C12-C13-C14
29	V	316	Q6L	C11-C12-C13-C14
28	1	614	LHG	C8-C7-O7-C5
25	2	602	CLA	C8-C10-C11-C12
25	B	811	CLA	C16-C17-C18-C20
25	B	806	CLA	C5-C6-C7-C8
25	R	306	CLA	C3-C5-C6-C7
24	T	305	CHL	O1A-CGA-O2A-C1
24	P	306	CHL	C2-C1-O2A-CGA
24	S	306	CHL	C2-C1-O2A-CGA
25	A	827	CLA	C2-C1-O2A-CGA
25	B	819	CLA	C2-C1-O2A-CGA
25	B	831	CLA	C2-C1-O2A-CGA
25	P	302	CLA	C2-C1-O2A-CGA
25	Q	315	CLA	C2-C1-O2A-CGA
25	P	311	CLA	C5-C6-C7-C8
25	3	307	CLA	O1A-CGA-O2A-C1
25	A	804	CLA	O1A-CGA-O2A-C1
25	Q	301	CLA	O1A-CGA-O2A-C1
25	B	808	CLA	C4C-C3C-CAC-CBC
28	1	614	LHG	C28-C29-C30-C31
31	B	801	LMG	C12-C13-C14-C15
30	2	618	BCR	C23-C24-C25-C30
30	I	101	BCR	C23-C24-C25-C26
30	I	101	BCR	C23-C24-C25-C30
30	J	101	BCR	C23-C24-C25-C26
30	J	101	BCR	C23-C24-C25-C30
30	K	207	BCR	C1-C6-C7-C8
30	L	305	BCR	C5-C6-C7-C8
30	L	307	BCR	C1-C6-C7-C8
30	L	307	BCR	C5-C6-C7-C8
30	M	101	BCR	C23-C24-C25-C26
30	M	101	BCR	C23-C24-C25-C30
25	L	302	CLA	O1D-CGD-O2D-CED
25	S	303	CLA	O1D-CGD-O2D-CED
25	A	815	CLA	CBA-CGA-O2A-C1
25	P	313	CLA	CBA-CGA-O2A-C1
25	A	837	CLA	C15-C16-C17-C18
25	T	302	CLA	C8-C10-C11-C12
25	P	313	CLA	O2A-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
25	V	312	CLA	O1A-CGA-O2A-C1
25	6	610	CLA	C14-C13-C15-C16
25	K	204	CLA	O1A-CGA-O2A-C1
25	A	805	CLA	C15-C16-C17-C18
28	3	323	LHG	C15-C16-C17-C18
25	Q	314	CLA	C4-C3-C5-C6
25	W	309	CLA	C4-C3-C5-C6
29	Q	318	Q6L	C11-C12-C13-C42
34	B	844	PQN	C14-C13-C15-C16
24	T	314	CHL	O1D-CGD-O2D-CED
24	W	314	CHL	O1D-CGD-O2D-CED
25	3	301	CLA	C11-C10-C8-C7
25	4	303	CLA	C11-C10-C8-C7
25	A	821	CLA	C11-C10-C8-C7
25	A	839	CLA	C12-C13-C15-C16
25	B	814	CLA	C11-C10-C8-C7
25	B	815	CLA	C6-C7-C8-C10
25	B	842	CLA	C11-C12-C13-C15
25	Q	304	CLA	C6-C7-C8-C10
25	R	306	CLA	C11-C12-C13-C15
25	S	309	CLA	C6-C7-C8-C10
25	S	310	CLA	C6-C7-C8-C10
25	U	302	CLA	C6-C7-C8-C10
29	P	321	Q6L	C11-C12-C13-C14
29	W	319	Q6L	C11-C12-C13-C14
33	A	802	CL0	C12-C13-C15-C16
34	A	844	PQN	C22-C23-C25-C26
34	B	844	PQN	C16-C17-C18-C20
25	B	830	CLA	C3-C5-C6-C7
25	L	302	CLA	C2C-C3C-CAC-CBC
25	A	813	CLA	C15-C16-C17-C18
25	B	810	CLA	C10-C11-C12-C13
25	S	310	CLA	C10-C11-C12-C13
26	1	611	IWJ	C10-C11-C12-C13
29	V	319	Q6L	C24-C25-C26-C27
29	X	301	Q6L	C24-C25-C26-C27
25	A	825	CLA	C16-C17-C18-C19
25	B	810	CLA	C16-C17-C18-C19
25	B	843	CLA	C16-C17-C18-C19
24	X	307	CHL	O1D-CGD-O2D-CED
28	1	614	LHG	O9-C7-O7-C5
25	3	307	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
25	4	313	CLA	CBA-CGA-O2A-C1
25	A	842	CLA	CBA-CGA-O2A-C1
25	B	809	CLA	CBA-CGA-O2A-C1
25	P	312	CLA	CBA-CGA-O2A-C1
25	R	313	CLA	CBA-CGA-O2A-C1
25	4	303	CLA	C2A-CAA-CBA-CGA
25	A	808	CLA	C2A-CAA-CBA-CGA
25	B	813	CLA	C2A-CAA-CBA-CGA
25	B	814	CLA	C2A-CAA-CBA-CGA
25	B	815	CLA	C2A-CAA-CBA-CGA
25	R	315	CLA	C2A-CAA-CBA-CGA
25	Q	304	CLA	C10-C11-C12-C13
31	J	104	LMG	C10-C11-C12-C13
25	H	301	CLA	O1D-CGD-O2D-CED
25	U	309	CLA	O1D-CGD-O2D-CED
25	A	819	CLA	C8-C10-C11-C12
25	A	834	CLA	C5-C6-C7-C8
25	A	843	CLA	C13-C15-C16-C17
25	R	306	CLA	C8-C10-C11-C12
25	3	301	CLA	C3-C5-C6-C7
25	5	602	CLA	O1D-CGD-O2D-CED
24	Q	308	CHL	O1A-CGA-O2A-C1
25	A	832	CLA	CBD-CGD-O2D-CED
25	A	834	CLA	CBA-CGA-O2A-C1
25	A	835	CLA	C13-C15-C16-C17
25	2	614	CLA	O1D-CGD-O2D-CED
25	B	843	CLA	O1D-CGD-O2D-CED
28	6	616	LHG	C8-C7-O7-C5
25	A	807	CLA	C15-C16-C17-C18
38	P	308	KC2	C4C-C3C-CAC-CBC
38	Q	310	KC2	C4C-C3C-CAC-CBC
38	T	308	KC2	C4C-C3C-CAC-CBC
38	U	307	KC2	C4C-C3C-CAC-CBC
38	X	309	KC2	C4C-C3C-CAC-CBC
25	H	302	CLA	C8-C10-C11-C12
25	O	2002	CLA	C8-C10-C11-C12
25	S	302	CLA	CBD-CGD-O2D-CED
25	R	314	CLA	O1D-CGD-O2D-CED
36	B	850	DGD	O2G-C2G-C3G-O3G
31	F	805	LMG	O6-C5-C6-O5
25	A	813	CLA	C16-C17-C18-C19
25	A	819	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
31	J	104	LMG	C11-C12-C13-C14
25	B	811	CLA	C5-C6-C7-C8
29	P	321	Q6L	C11-C12-C13-C42
29	V	316	Q6L	C11-C12-C13-C42
29	W	319	Q6L	C11-C12-C13-C42
29	X	301	Q6L	C11-C12-C13-C42
29	P	315	Q6L	C11-C12-C13-C14
29	R	304	Q6L	C11-C12-C13-C14
29	W	315	Q6L	C11-C12-C13-C14
25	4	310	CLA	C5-C6-C7-C8
25	3	301	CLA	C11-C10-C8-C9
25	4	303	CLA	C11-C10-C8-C9
25	A	825	CLA	C11-C12-C13-C14
25	B	808	CLA	C11-C12-C13-C14
25	B	814	CLA	C11-C10-C8-C9
25	B	826	CLA	C11-C10-C8-C9
25	B	842	CLA	C11-C12-C13-C14
25	Q	304	CLA	C6-C7-C8-C9
25	S	310	CLA	C6-C7-C8-C9
34	B	844	PQN	C16-C17-C18-C19
25	B	819	CLA	C3-C5-C6-C7
25	2	603	CLA	C2A-CAA-CBA-CGA
25	3	307	CLA	C2A-CAA-CBA-CGA
25	B	803	CLA	C2A-CAA-CBA-CGA
25	P	312	CLA	C2A-CAA-CBA-CGA
25	R	313	CLA	C2A-CAA-CBA-CGA
25	T	311	CLA	C2A-CAA-CBA-CGA
25	W	311	CLA	C2A-CAA-CBA-CGA
31	A	855	LMG	O6-C5-C6-O5
31	O	2008	LMG	O6-C5-C6-O5
26	4	317	IWJ	C20-C19-C21-C22
24	P	314	CHL	O1D-CGD-O2D-CED
25	2	604	CLA	O1D-CGD-O2D-CED
25	A	803	CLA	C15-C16-C17-C18
25	A	815	CLA	O1A-CGA-O2A-C1
25	A	842	CLA	O1A-CGA-O2A-C1
25	B	807	CLA	O1A-CGA-O2A-C1
25	B	809	CLA	O1A-CGA-O2A-C1
25	Q	306	CLA	O1A-CGA-O2A-C1
25	R	313	CLA	O1A-CGA-O2A-C1
24	2	601	CHL	C1A-C2A-CAA-CBA
24	P	305	CHL	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
24	P	307	CHL	C1A-C2A-CAA-CBA
24	Q	307	CHL	C1A-C2A-CAA-CBA
24	R	302	CHL	C1A-C2A-CAA-CBA
24	U	306	CHL	C1A-C2A-CAA-CBA
24	V	314	CHL	C1A-C2A-CAA-CBA
24	X	307	CHL	C1A-C2A-CAA-CBA
24	X	315	CHL	C1A-C2A-CAA-CBA
25	3	302	CLA	C1A-C2A-CAA-CBA
25	3	310	CLA	C1A-C2A-CAA-CBA
25	4	303	CLA	C1A-C2A-CAA-CBA
25	4	310	CLA	C1A-C2A-CAA-CBA
25	5	601	CLA	C1A-C2A-CAA-CBA
25	A	805	CLA	C1A-C2A-CAA-CBA
25	A	811	CLA	C1A-C2A-CAA-CBA
25	A	813	CLA	C1A-C2A-CAA-CBA
25	A	817	CLA	C1A-C2A-CAA-CBA
25	A	820	CLA	C1A-C2A-CAA-CBA
25	A	821	CLA	C1A-C2A-CAA-CBA
25	A	834	CLA	C1A-C2A-CAA-CBA
25	B	811	CLA	C1A-C2A-CAA-CBA
25	B	813	CLA	C1A-C2A-CAA-CBA
25	B	820	CLA	C1A-C2A-CAA-CBA
25	P	301	CLA	C1A-C2A-CAA-CBA
25	P	309	CLA	C1A-C2A-CAA-CBA
25	Q	313	CLA	C1A-C2A-CAA-CBA
25	R	306	CLA	C1A-C2A-CAA-CBA
25	R	314	CLA	C1A-C2A-CAA-CBA
25	S	301	CLA	C1A-C2A-CAA-CBA
25	S	311	CLA	C1A-C2A-CAA-CBA
25	T	301	CLA	C1A-C2A-CAA-CBA
25	2	609	CLA	C6-C7-C8-C9
25	A	813	CLA	C16-C17-C18-C20
25	A	821	CLA	C16-C17-C18-C19
25	B	818	CLA	C6-C7-C8-C10
25	B	839	CLA	C16-C17-C18-C19
28	6	616	LHG	O9-C7-O7-C5
28	A	847	LHG	C8-C7-O7-C5
31	L	308	LMG	C11-C10-O7-C8
29	O	2007	Q6L	C24-C25-C26-C27
29	X	316	Q6L	C17-C18-C19-C20
24	W	307	CHL	C15-C16-C17-C18
25	B	831	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
25	K	203	CLA	C10-C11-C12-C13
25	P	312	CLA	O1A-CGA-O2A-C1
32	6	617	SQD	C24-C23-O48-C46
25	X	310	CLA	O1D-CGD-O2D-CED
25	A	825	CLA	C16-C17-C18-C20
25	B	808	CLA	C8-C10-C11-C12
28	A	847	LHG	O9-C7-O7-C5
25	A	825	CLA	C4-C3-C5-C6
24	4	307	CHL	C3A-C2A-CAA-CBA
25	3	305	CLA	C3A-C2A-CAA-CBA
25	U	309	CLA	O1A-CGA-O2A-C1
25	X	311	CLA	C4C-C3C-CAC-CBC
28	A	846	LHG	C27-C28-C29-C30
25	P	313	CLA	O1A-CGA-O2A-C1
25	A	831	CLA	C16-C17-C18-C19
25	B	839	CLA	C16-C17-C18-C20
25	B	843	CLA	C16-C17-C18-C20
25	U	303	CLA	O1D-CGD-O2D-CED
28	Q	302	LHG	C4-C5-C6-O8
31	A	857	LMG	O1-C7-C8-C9
31	F	805	LMG	C10-C11-C12-C13
25	4	313	CLA	O1A-CGA-O2A-C1
25	T	301	CLA	O1A-CGA-O2A-C1
32	H	303	SQD	C45-C44-O6-C1
24	U	313	CHL	CBD-CGD-O2D-CED
28	Q	302	LHG	C29-C30-C31-C32
32	6	617	SQD	O10-C23-O48-C46
25	R	305	CLA	CBD-CGD-O2D-CED
25	R	317	CLA	O2A-C1-C2-C3
25	A	808	CLA	C13-C15-C16-C17
31	L	308	LMG	O6-C5-C6-O5
29	R	304	Q6L	C11-C12-C13-C42
25	A	821	CLA	C16-C17-C18-C20
25	A	832	CLA	C16-C17-C18-C20
25	P	311	CLA	C11-C12-C13-C14
24	T	320	CHL	CBA-CGA-O2A-C1
25	B	840	CLA	CBA-CGA-O2A-C1
25	P	309	CLA	CBA-CGA-O2A-C1
25	S	310	CLA	CBA-CGA-O2A-C1
25	T	301	CLA	CBA-CGA-O2A-C1
25	A	856	CLA	CBD-CGD-O2D-CED
25	2	612	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
36	B	850	DGD	O6E-C5E-C6E-O5E
25	U	301	CLA	C2A-CAA-CBA-CGA
25	W	312	CLA	C2A-CAA-CBA-CGA
25	B	842	CLA	C5-C6-C7-C8
25	A	807	CLA	C2-C1-O2A-CGA
25	B	826	CLA	C3-C5-C6-C7
25	5	609	CLA	CBA-CGA-O2A-C1
25	B	810	CLA	CBA-CGA-O2A-C1
25	V	310	CLA	CBA-CGA-O2A-C1
28	3	322	LHG	C24-C23-O8-C6
28	3	323	LHG	O6-C4-C5-O7
25	A	813	CLA	C8-C10-C11-C12
28	Q	302	LHG	O7-C5-C6-O8
32	6	617	SQD	O6-C44-C45-O47
25	P	309	CLA	C15-C16-C17-C18
25	A	806	CLA	C4-C3-C5-C6
25	A	829	CLA	C4-C3-C5-C6
24	W	307	CHL	C11-C12-C13-C15
25	2	612	CLA	C11-C10-C8-C7
25	2	612	CLA	C11-C12-C13-C15
25	5	607	CLA	C6-C7-C8-C10
25	A	804	CLA	C11-C12-C13-C15
25	A	812	CLA	C6-C7-C8-C10
25	A	812	CLA	C12-C13-C15-C16
25	A	815	CLA	C12-C13-C15-C16
25	A	821	CLA	C12-C13-C15-C16
25	A	823	CLA	C12-C13-C15-C16
25	A	825	CLA	C11-C12-C13-C15
25	A	827	CLA	C11-C10-C8-C7
25	A	828	CLA	C11-C10-C8-C7
25	A	829	CLA	C2-C3-C5-C6
25	A	830	CLA	C6-C7-C8-C10
25	A	830	CLA	C12-C13-C15-C16
25	A	831	CLA	C12-C13-C15-C16
25	B	803	CLA	C12-C13-C15-C16
25	B	804	CLA	C11-C10-C8-C7
25	B	813	CLA	C12-C13-C15-C16
25	B	826	CLA	C11-C10-C8-C7
25	B	834	CLA	C11-C12-C13-C15
25	B	842	CLA	C12-C13-C15-C16
25	P	310	CLA	C11-C10-C8-C7
25	R	305	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
25	S	302	CLA	C11-C12-C13-C15
25	T	309	CLA	C11-C10-C8-C7
34	A	844	PQN	C16-C17-C18-C20
25	P	312	CLA	C3-C5-C6-C7
25	P	309	CLA	O1A-CGA-O2A-C1
24	W	307	CHL	C11-C12-C13-C14
25	2	612	CLA	C11-C12-C13-C14
25	5	602	CLA	C11-C10-C8-C9
25	A	804	CLA	C11-C12-C13-C14
25	A	810	CLA	C11-C12-C13-C14
25	A	812	CLA	C6-C7-C8-C9
25	A	812	CLA	C14-C13-C15-C16
25	A	813	CLA	C11-C10-C8-C9
25	A	815	CLA	C14-C13-C15-C16
25	A	821	CLA	C14-C13-C15-C16
25	A	823	CLA	C14-C13-C15-C16
25	A	827	CLA	C11-C10-C8-C9
25	A	830	CLA	C6-C7-C8-C9
25	A	830	CLA	C11-C10-C8-C9
25	A	830	CLA	C14-C13-C15-C16
25	B	803	CLA	C14-C13-C15-C16
25	B	807	CLA	C6-C7-C8-C9
25	B	807	CLA	C14-C13-C15-C16
25	B	811	CLA	C11-C12-C13-C14
25	B	813	CLA	C11-C10-C8-C9
25	B	831	CLA	C11-C12-C13-C14
25	R	305	CLA	C11-C12-C13-C14
25	R	306	CLA	C11-C12-C13-C14
25	S	301	CLA	C6-C7-C8-C9
25	S	302	CLA	C11-C12-C13-C14
25	S	309	CLA	C11-C10-C8-C9
34	A	844	PQN	C16-C17-C18-C19
29	U	314	Q6L	C24-C25-C26-C27
24	V	314	CHL	C2A-CAA-CBA-CGA
25	B	808	CLA	C2A-CAA-CBA-CGA
30	2	618	BCR	C7-C8-C9-C34
30	A	851	BCR	C7-C8-C9-C34
30	G	205	BCR	C36-C18-C19-C20
30	J	101	BCR	C7-C8-C9-C34
27	3	316	XAT	C7-C8-C9-C10
29	2	616	Q6L	C21-C22-C24-C25
31	L	308	LMG	O9-C10-O7-C8

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Mol	Chain	Res	Type	Atoms
25	A	817	CLA	C8-C10-C11-C12
25	A	839	CLA	C5-C6-C7-C8
25	B	802	CLA	C10-C11-C12-C13
25	B	836	CLA	C10-C11-C12-C13
31	B	801	LMG	C4-C5-C6-O5
25	K	206	CLA	CBA-CGA-O2A-C1
25	P	303	CLA	CBA-CGA-O2A-C1
25	S	301	CLA	CBA-CGA-O2A-C1
31	5	613	LMG	C35-C36-C37-C38
25	V	313	CLA	O2A-C1-C2-C3
24	S	314	CHL	CBD-CGD-O2D-CED
25	A	829	CLA	CBD-CGD-O2D-CED
25	A	831	CLA	C16-C17-C18-C20
25	H	302	CLA	CBA-CGA-O2A-C1
25	2	612	CLA	C13-C15-C16-C17
25	A	810	CLA	C13-C15-C16-C17
25	A	838	CLA	C4-C3-C5-C6
25	A	806	CLA	C2-C3-C5-C6
29	X	301	Q6L	C11-C12-C13-C14
25	B	840	CLA	O1A-CGA-O2A-C1
34	B	844	PQN	C26-C27-C28-C29
25	P	311	CLA	C2A-CAA-CBA-CGA
25	A	825	CLA	CBA-CGA-O2A-C1
25	B	808	CLA	CBA-CGA-O2A-C1
25	B	806	CLA	O1D-CGD-O2D-CED
25	B	837	CLA	O1D-CGD-O2D-CED
24	1	601	CHL	C3A-C2A-CAA-CBA
25	4	309	CLA	C3A-C2A-CAA-CBA
25	6	607	CLA	C3A-C2A-CAA-CBA
25	A	806	CLA	C3A-C2A-CAA-CBA
25	A	813	CLA	C3A-C2A-CAA-CBA
25	A	825	CLA	C3A-C2A-CAA-CBA
25	A	826	CLA	C3A-C2A-CAA-CBA
25	B	810	CLA	C3A-C2A-CAA-CBA
25	B	811	CLA	C3A-C2A-CAA-CBA
25	B	830	CLA	C3A-C2A-CAA-CBA
25	K	204	CLA	C3A-C2A-CAA-CBA
25	W	301	CLA	C3A-C2A-CAA-CBA
25	B	808	CLA	C15-C16-C17-C18
34	A	844	PQN	C23-C25-C26-C27
26	X	318	IWJ	C21-C22-C23-C24
26	5	611	IWJ	O27-C26-C28-C29

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Mol	Chain	Res	Type	Atoms
26	Q	303	IWJ	O27-C26-C28-C29
26	Q	320	IWJ	O27-C26-C28-C29
26	R	322	IWJ	O27-C26-C28-C29
26	S	318	IWJ	O27-C26-C28-C29
26	S	319	IWJ	O27-C26-C28-C29
26	S	322	IWJ	O27-C26-C28-C29
26	T	321	IWJ	O27-C26-C28-C29
26	U	316	IWJ	O27-C26-C28-C29
26	V	317	IWJ	O27-C26-C28-C29
26	V	320	IWJ	O27-C26-C28-C29
26	X	318	IWJ	O27-C26-C28-C29
25	A	826	CLA	O1D-CGD-O2D-CED
25	2	602	CLA	C10-C11-C12-C13
25	P	311	CLA	C11-C12-C13-C15
25	A	812	CLA	C5-C6-C7-C8
25	H	302	CLA	C10-C11-C12-C13
28	A	847	LHG	C4-C5-C6-O8
29	V	319	Q6L	C29-C30-C31-C36
32	6	617	SQD	C44-C45-C46-O48
36	B	850	DGD	C1G-C2G-C3G-O3G
28	A	847	LHG	C7-C8-C9-C10
25	A	834	CLA	O1A-CGA-O2A-C1
25	V	310	CLA	O1A-CGA-O2A-C1
25	B	805	CLA	O2A-C1-C2-C3
25	B	814	CLA	O2A-C1-C2-C3
25	U	302	CLA	C3-C5-C6-C7
25	A	825	CLA	O1A-CGA-O2A-C1
25	S	310	CLA	O1A-CGA-O2A-C1
25	X	302	CLA	C6-C7-C8-C10
25	W	309	CLA	C2-C3-C5-C6
24	Q	316	CHL	C3C-C2C-CMC-OMC
24	R	302	CHL	C3C-C2C-CMC-OMC
24	U	304	CHL	C3C-C2C-CMC-OMC
24	U	306	CHL	C3C-C2C-CMC-OMC
24	V	304	CHL	C3C-C2C-CMC-OMC
28	1	614	LHG	C3-O3-P-O6
24	T	320	CHL	O1A-CGA-O2A-C1
25	T	311	CLA	C3-C5-C6-C7
25	3	307	CLA	C10-C11-C12-C13
25	A	832	CLA	O1D-CGD-O2D-CED
38	P	308	KC2	C3A-C2A-CAA-CBA
24	4	302	CHL	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
31	N	201	LMG	C18-C19-C20-C21
25	A	804	CLA	C8-C10-C11-C12
25	B	805	CLA	C10-C11-C12-C13
25	B	808	CLA	O1A-CGA-O2A-C1
25	H	302	CLA	O1A-CGA-O2A-C1
28	A	847	LHG	O7-C5-C6-O8
32	6	617	SQD	O47-C45-C46-O48
25	P	312	CLA	O1D-CGD-O2D-CED
25	T	302	CLA	C5-C6-C7-C8
26	Q	320	IWJ	C23-C24-C26-C28
26	W	318	IWJ	C23-C24-C26-C28
25	Q	301	CLA	C3-C5-C6-C7
25	4	303	CLA	C4-C3-C5-C6
25	A	806	CLA	C2-C1-O2A-CGA
25	A	838	CLA	C2-C1-O2A-CGA
25	S	302	CLA	C2-C1-O2A-CGA
25	A	837	CLA	C2-C3-C5-C6
25	A	831	CLA	C6-C7-C8-C9
25	A	831	CLA	C14-C13-C15-C16
25	B	814	CLA	C6-C7-C8-C9
25	B	830	CLA	C6-C7-C8-C9
25	O	2001	CLA	C6-C7-C8-C9
25	S	310	CLA	C11-C10-C8-C9
25	T	301	CLA	C11-C12-C13-C14
25	T	302	CLA	C6-C7-C8-C9
25	T	311	CLA	C11-C10-C8-C9
25	B	815	CLA	CBA-CGA-O2A-C1
25	B	816	CLA	C4-C3-C5-C6
38	W	308	KC2	C1A-C2A-CAA-CBA
25	B	810	CLA	O1A-CGA-O2A-C1
28	3	323	LHG	C9-C10-C11-C12
25	U	311	CLA	C2A-CAA-CBA-CGA
25	A	838	CLA	C16-C17-C18-C19
25	A	838	CLA	C16-C17-C18-C20
25	A	839	CLA	C16-C17-C18-C19
30	2	618	BCR	C23-C24-C25-C26
30	A	849	BCR	C23-C24-C25-C26
30	K	207	BCR	C5-C6-C7-C8
24	4	306	CHL	C1A-C2A-CAA-CBA
25	2	610	CLA	C1A-C2A-CAA-CBA
25	V	309	CLA	C1A-C2A-CAA-CBA
25	X	304	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
29	X	316	Q6L	C15-C16-C17-C18
30	A	848	BCR	C7-C8-C9-C10
30	A	849	BCR	C21-C22-C23-C24
30	G	205	BCR	C17-C18-C19-C20
30	H	305	BCR	C17-C18-C19-C20
30	I	101	BCR	C17-C18-C19-C20
30	J	103	BCR	C17-C18-C19-C20
30	M	101	BCR	C7-C8-C9-C10
25	B	839	CLA	C13-C15-C16-C17
25	X	302	CLA	C6-C7-C8-C9
25	2	602	CLA	C14-C13-C15-C16
25	U	302	CLA	C11-C10-C8-C9
25	B	830	CLA	C8-C10-C11-C12
34	A	844	PQN	C15-C16-C17-C18
25	3	309	CLA	O1D-CGD-O2D-CED
25	S	301	CLA	O1A-CGA-O2A-C1
28	3	322	LHG	O10-C23-O8-C6
28	3	321	LHG	O6-C4-C5-C6
28	A	847	LHG	O2-C2-C3-O3
25	2	612	CLA	C6-C7-C8-C10
25	5	602	CLA	C11-C10-C8-C7
25	6	602	CLA	C11-C12-C13-C15
25	6	613	CLA	C11-C12-C13-C15
25	A	803	CLA	C11-C10-C8-C7
25	A	805	CLA	C11-C12-C13-C15
25	A	805	CLA	C12-C13-C15-C16
25	A	807	CLA	C11-C10-C8-C7
25	A	807	CLA	C12-C13-C15-C16
25	A	810	CLA	C11-C12-C13-C15
25	A	813	CLA	C11-C10-C8-C7
25	A	817	CLA	C11-C12-C13-C15
25	A	825	CLA	C11-C10-C8-C7
25	A	831	CLA	C6-C7-C8-C10
25	A	832	CLA	C11-C12-C13-C15
25	A	832	CLA	C12-C13-C15-C16
25	A	838	CLA	C12-C13-C15-C16
25	A	842	CLA	C11-C12-C13-C15
25	B	803	CLA	C11-C10-C8-C7
25	B	805	CLA	C11-C12-C13-C15
25	B	807	CLA	C6-C7-C8-C10
25	B	807	CLA	C12-C13-C15-C16
25	B	809	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
25	B	810	CLA	C11-C12-C13-C15
25	B	811	CLA	C11-C12-C13-C15
25	B	813	CLA	C11-C12-C13-C15
25	B	814	CLA	C6-C7-C8-C10
25	B	828	CLA	C12-C13-C15-C16
25	B	829	CLA	C11-C10-C8-C7
25	B	830	CLA	C6-C7-C8-C10
25	B	836	CLA	C11-C10-C8-C7
25	O	2001	CLA	C6-C7-C8-C10
25	R	313	CLA	C12-C13-C15-C16
25	R	314	CLA	C6-C7-C8-C10
25	S	302	CLA	C6-C7-C8-C10
25	S	309	CLA	C11-C10-C8-C7
25	S	310	CLA	C11-C10-C8-C7
25	W	309	CLA	C11-C10-C8-C7
26	S	318	IWJ	C14-C15-C16-C17
29	2	616	Q6L	C13-C14-C15-C16
29	S	321	Q6L	C17-C18-C19-C20
29	T	319	Q6L	C24-C25-C26-C27
29	V	316	Q6L	C24-C25-C26-C27
29	W	316	Q6L	C13-C14-C15-C16
29	X	317	Q6L	C13-C14-C15-C16
25	S	302	CLA	C10-C11-C12-C13
25	B	812	CLA	C2A-CAA-CBA-CGA
25	Q	313	CLA	C2A-CAA-CBA-CGA
28	A	846	LHG	C15-C16-C17-C18
32	6	617	SQD	C14-C15-C16-C17
25	B	803	CLA	C3-C5-C6-C7
31	A	801	LMG	O7-C10-C11-C12
25	2	602	CLA	C12-C13-C15-C16
24	S	314	CHL	O1D-CGD-O2D-CED
25	R	316	CLA	C5-C6-C7-C8
25	G	202	CLA	CBD-CGD-O2D-CED
24	P	307	CHL	CAD-CBD-CGD-O2D
24	Q	309	CHL	CAD-CBD-CGD-O2D
24	S	305	CHL	CAD-CBD-CGD-O2D
24	T	305	CHL	CAD-CBD-CGD-O2D
24	T	314	CHL	CAD-CBD-CGD-O2D
24	U	306	CHL	CAD-CBD-CGD-O2D
24	V	307	CHL	CAD-CBD-CGD-O2D
24	V	314	CHL	CAD-CBD-CGD-O2D
24	W	306	CHL	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
24	X	308	CHL	CAD-CBD-CGD-O2D
25	3	310	CLA	CAD-CBD-CGD-O2D
25	4	311	CLA	CAD-CBD-CGD-O2D
25	6	608	CLA	CAD-CBD-CGD-O2D
25	A	818	CLA	CAD-CBD-CGD-O2D
25	A	821	CLA	CAD-CBD-CGD-O2D
25	A	822	CLA	CAD-CBD-CGD-O2D
25	A	828	CLA	CAD-CBD-CGD-O2D
25	A	836	CLA	CAD-CBD-CGD-O2D
25	B	807	CLA	CAD-CBD-CGD-O2D
25	B	815	CLA	CAD-CBD-CGD-O2D
25	B	833	CLA	CAD-CBD-CGD-O2D
25	B	835	CLA	CAD-CBD-CGD-O2D
25	B	836	CLA	CAD-CBD-CGD-O2D
25	B	842	CLA	CAD-CBD-CGD-O2D
25	O	2001	CLA	CAD-CBD-CGD-O2D
25	P	303	CLA	CAD-CBD-CGD-O2D
25	R	315	CLA	CAD-CBD-CGD-O2D
25	R	317	CLA	CAD-CBD-CGD-O2D
25	S	309	CLA	CAD-CBD-CGD-O2D
25	T	301	CLA	CAD-CBD-CGD-O2D
25	T	302	CLA	CAD-CBD-CGD-O2D
25	T	312	CLA	CAD-CBD-CGD-O2D
25	U	308	CLA	CAD-CBD-CGD-O2D
25	U	312	CLA	CAD-CBD-CGD-O2D
25	V	309	CLA	CAD-CBD-CGD-O2D
25	W	302	CLA	CAD-CBD-CGD-O2D
25	X	310	CLA	CAD-CBD-CGD-O2D
38	R	312	KC2	CAD-CBD-CGD-O2D
38	T	308	KC2	C2B-C3B-CAB-CBB
38	V	308	KC2	C2B-C3B-CAB-CBB
38	X	309	KC2	C2B-C3B-CAB-CBB
36	B	850	DGD	O1B-C1B-O2G-C2G
25	A	805	CLA	C13-C15-C16-C17
25	B	820	CLA	C8-C10-C11-C12
25	R	315	CLA	C10-C11-C12-C13
25	5	609	CLA	O1A-CGA-O2A-C1
25	L	302	CLA	CBA-CGA-O2A-C1
31	J	104	LMG	C29-C28-O8-C9
25	A	837	CLA	C4-C3-C5-C6
25	T	311	CLA	C8-C10-C11-C12
25	4	303	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
29	X	316	Q6L	C11-C12-C13-C14
34	A	844	PQN	C12-C13-C15-C16
26	Q	320	IWJ	C25-C24-C26-O27
26	W	318	IWJ	C25-C24-C26-O27
31	J	104	LMG	C7-C8-C9-O8
36	B	850	DGD	O1G-C1G-C2G-C3G
25	O	2001	CLA	CBD-CGD-O2D-CED
25	P	312	CLA	CBD-CGD-O2D-CED
25	B	836	CLA	C5-C6-C7-C8
25	A	828	CLA	C3-C5-C6-C7
24	Q	308	CHL	O2A-C1-C2-C3
38	R	312	KC2	C4C-C3C-CAC-CBC
38	S	308	KC2	C4C-C3C-CAC-CBC
38	V	308	KC2	C4C-C3C-CAC-CBC
38	W	308	KC2	C4C-C3C-CAC-CBC
24	T	320	CHL	C2A-CAA-CBA-CGA
25	A	823	CLA	C2A-CAA-CBA-CGA
25	B	824	CLA	C11-C12-C13-C14
24	2	615	CHL	CHA-CBD-CGD-O1D
24	2	615	CHL	CHA-CBD-CGD-O2D
24	S	307	CHL	CHA-CBD-CGD-O1D
24	T	304	CHL	CHA-CBD-CGD-O1D
24	T	304	CHL	CHA-CBD-CGD-O2D
24	T	320	CHL	CHA-CBD-CGD-O1D
25	1	602	CLA	CHA-CBD-CGD-O2D
25	2	606	CLA	CHA-CBD-CGD-O1D
25	5	610	CLA	CHA-CBD-CGD-O1D
25	6	609	CLA	CHA-CBD-CGD-O1D
25	6	609	CLA	CHA-CBD-CGD-O2D
25	A	810	CLA	CHA-CBD-CGD-O1D
25	A	810	CLA	CHA-CBD-CGD-O2D
25	A	813	CLA	CHA-CBD-CGD-O1D
25	A	813	CLA	CHA-CBD-CGD-O2D
25	A	815	CLA	CHA-CBD-CGD-O1D
25	A	815	CLA	CHA-CBD-CGD-O2D
25	A	816	CLA	CHA-CBD-CGD-O1D
25	A	816	CLA	CHA-CBD-CGD-O2D
25	A	824	CLA	CHA-CBD-CGD-O1D
25	A	832	CLA	CHA-CBD-CGD-O1D
25	A	832	CLA	CHA-CBD-CGD-O2D
25	A	838	CLA	CHA-CBD-CGD-O1D
25	A	838	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
25	A	839	CLA	CHA-CBD-CGD-O1D
25	A	839	CLA	CHA-CBD-CGD-O2D
25	B	810	CLA	CHA-CBD-CGD-O1D
25	B	827	CLA	CHA-CBD-CGD-O1D
25	B	827	CLA	CHA-CBD-CGD-O2D
25	B	839	CLA	CHA-CBD-CGD-O1D
25	B	839	CLA	CHA-CBD-CGD-O2D
25	G	203	CLA	CHA-CBD-CGD-O1D
25	N	203	CLA	CHA-CBD-CGD-O1D
25	N	203	CLA	CHA-CBD-CGD-O2D
25	O	2004	CLA	CHA-CBD-CGD-O1D
25	O	2004	CLA	CHA-CBD-CGD-O2D
25	Q	312	CLA	CHA-CBD-CGD-O2D
25	R	313	CLA	CHA-CBD-CGD-O1D
25	R	313	CLA	CHA-CBD-CGD-O2D
25	R	314	CLA	CHA-CBD-CGD-O1D
25	R	314	CLA	CHA-CBD-CGD-O2D
25	S	310	CLA	CHA-CBD-CGD-O1D
25	U	309	CLA	CHA-CBD-CGD-O1D
25	V	310	CLA	CHA-CBD-CGD-O1D
25	K	206	CLA	O1A-CGA-O2A-C1
25	P	303	CLA	O1A-CGA-O2A-C1
31	A	857	LMG	O1-C7-C8-O7
31	J	104	LMG	O7-C8-C9-O8
25	5	607	CLA	C16-C17-C18-C20
25	B	808	CLA	C16-C17-C18-C19
26	Q	320	IWJ	C23-C24-C26-O27
26	W	318	IWJ	C23-C24-C26-O27
29	O	2006	Q6L	C02-C03-C11-C12
29	R	301	Q6L	C02-C03-C11-C12
29	T	319	Q6L	C02-C03-C11-C12
29	U	317	Q6L	C02-C03-C11-C12
25	R	305	CLA	O1D-CGD-O2D-CED
25	X	311	CLA	C2C-C3C-CAC-CBC
25	3	313	CLA	CBD-CGD-O2D-CED
25	B	815	CLA	C4-C3-C5-C6
29	X	316	Q6L	C11-C12-C13-C42
25	L	302	CLA	O1A-CGA-O2A-C1
31	J	104	LMG	O10-C28-O8-C9
25	5	607	CLA	C6-C7-C8-C9
25	A	804	CLA	C6-C7-C8-C9
25	A	807	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
25	A	807	CLA	C14-C13-C15-C16
25	A	808	CLA	C11-C12-C13-C14
25	A	817	CLA	C11-C12-C13-C14
25	A	832	CLA	C11-C12-C13-C14
25	A	832	CLA	C14-C13-C15-C16
25	A	838	CLA	C14-C13-C15-C16
25	B	803	CLA	C11-C10-C8-C9
25	B	806	CLA	C14-C13-C15-C16
25	B	836	CLA	C11-C10-C8-C9
25	B	843	CLA	C14-C13-C15-C16
25	T	309	CLA	C11-C10-C8-C9
25	3	309	CLA	CBD-CGD-O2D-CED
25	A	829	CLA	O1D-CGD-O2D-CED
25	3	302	CLA	C3-C5-C6-C7
25	A	825	CLA	C2A-CAA-CBA-CGA
25	L	302	CLA	C2A-CAA-CBA-CGA
25	Q	306	CLA	C2A-CAA-CBA-CGA
26	Q	320	IWJ	C08-C09-C10-C41
29	X	316	Q6L	C23-C22-C24-C25
30	F	801	BCR	C36-C18-C19-C20
29	R	319	Q6L	C15-C16-C17-C18
30	3	318	BCR	C11-C12-C13-C14
30	A	851	BCR	C7-C8-C9-C10
30	J	101	BCR	C7-C8-C9-C10
25	1	605	CLA	CHA-CBD-CGD-O2D
25	3	311	CLA	CHA-CBD-CGD-O2D
25	4	309	CLA	C1A-C2A-CAA-CBA
25	6	613	CLA	C1A-C2A-CAA-CBA
25	A	845	CLA	C1A-C2A-CAA-CBA
25	A	856	CLA	C1A-C2A-CAA-CBA
25	B	834	CLA	C1A-C2A-CAA-CBA
25	B	843	CLA	C1A-C2A-CAA-CBA
29	P	319	Q6L	C04-C03-C11-C12
29	Q	318	Q6L	C04-C03-C11-C12
29	S	316	Q6L	C04-C03-C11-C12
29	S	323	Q6L	C04-C03-C11-C12
29	T	322	Q6L	C04-C03-C11-C12
24	R	310	CHL	C2-C1-O2A-CGA
25	A	804	CLA	C2-C1-O2A-CGA
25	K	206	CLA	C2-C1-O2A-CGA
25	T	311	CLA	C2-C1-O2A-CGA
25	B	825	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
25	B	843	CLA	C13-C15-C16-C17
25	T	311	CLA	C10-C11-C12-C13
28	3	322	LHG	C3-O3-P-O6
28	A	846	LHG	C3-O3-P-O6
28	A	847	LHG	C3-O3-P-O6
25	6	602	CLA	CBD-CGD-O2D-CED
25	6	602	CLA	O1D-CGD-O2D-CED
28	2	619	LHG	C4-O6-P-O5
28	3	321	LHG	C4-O6-P-O5
28	6	616	LHG	C4-O6-P-O4
25	B	826	CLA	C16-C17-C18-C20
31	2	620	LMG	O6-C1-O1-C7
25	A	842	CLA	C10-C11-C12-C13
25	B	830	CLA	C10-C11-C12-C13
28	3	323	LHG	O6-C4-C5-C6
25	3	313	CLA	O1D-CGD-O2D-CED
25	P	310	CLA	CAA-CBA-CGA-O2A
25	2	602	CLA	C3-C5-C6-C7
25	T	312	CLA	C3-C5-C6-C7
24	U	305	CHL	C2C-C3C-CAC-CBC
25	S	302	CLA	O1D-CGD-O2D-CED
25	A	828	CLA	C11-C12-C13-C14
25	5	609	CLA	C6-C7-C8-C9
24	2	615	CHL	CAD-CBD-CGD-O1D
24	R	308	CHL	CAD-CBD-CGD-O1D
24	S	306	CHL	C2-C3-C5-C6
24	T	304	CHL	CAD-CBD-CGD-O1D
24	T	306	CHL	C2-C3-C5-C6
25	1	608	CLA	CAD-CBD-CGD-O1D
25	1	610	CLA	CAD-CBD-CGD-O1D
25	4	314	CLA	CAD-CBD-CGD-O1D
25	6	610	CLA	CAD-CBD-CGD-O1D
25	A	807	CLA	CAD-CBD-CGD-O1D
25	A	815	CLA	CAD-CBD-CGD-O1D
25	A	816	CLA	CAD-CBD-CGD-O1D
25	A	824	CLA	CAD-CBD-CGD-O1D
25	B	839	CLA	CAD-CBD-CGD-O1D
25	G	202	CLA	CAD-CBD-CGD-O1D
25	G	203	CLA	CAD-CBD-CGD-O1D
25	H	302	CLA	CAD-CBD-CGD-O1D
25	O	2004	CLA	CAD-CBD-CGD-O1D
25	U	310	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
25	V	302	CLA	CAD-CBD-CGD-O1D
25	V	311	CLA	CAD-CBD-CGD-O1D
25	X	303	CLA	C2-C3-C5-C6
25	A	805	CLA	C3-C5-C6-C7
25	S	312	CLA	CBA-CGA-O2A-C1
25	A	835	CLA	C16-C17-C18-C20
25	T	312	CLA	C4-C3-C5-C6
29	O	2007	Q6L	C11-C12-C13-C42
24	6	601	CHL	C3A-C2A-CAA-CBA
24	W	307	CHL	C6-C7-C8-C10
25	1	608	CLA	C6-C7-C8-C10
25	2	602	CLA	C6-C7-C8-C10
25	2	613	CLA	CAD-CBD-CGD-O2D
25	A	804	CLA	C6-C7-C8-C10
25	B	808	CLA	C12-C13-C15-C16
25	B	830	CLA	C11-C12-C13-C15
25	B	831	CLA	C6-C7-C8-C10
25	B	843	CLA	C12-C13-C15-C16
25	K	203	CLA	C3A-C2A-CAA-CBA
25	L	302	CLA	C11-C10-C8-C7
25	P	309	CLA	C6-C7-C8-C10
25	P	309	CLA	C11-C12-C13-C15
26	5	611	IWJ	C02-C07-C08-C09
26	U	316	IWJ	C02-C07-C08-C09
28	3	321	LHG	O6-C4-C5-O7
29	2	616	Q6L	C29-C30-C31-C32
29	O	2006	Q6L	C29-C30-C31-C32
29	O	2007	Q6L	C29-C30-C31-C32
29	P	321	Q6L	C29-C30-C31-C32
29	S	316	Q6L	C29-C30-C31-C32
29	T	319	Q6L	C29-C30-C31-C32
29	V	319	Q6L	C29-C30-C31-C32
29	W	319	Q6L	C29-C30-C31-C32
25	B	829	CLA	C2C-C3C-CAC-CBC
25	W	310	CLA	CAA-CBA-CGA-O2A
25	A	810	CLA	C15-C16-C17-C18
25	T	311	CLA	O1A-CGA-O2A-C1
25	B	805	CLA	C5-C6-C7-C8
24	U	305	CHL	C2A-CAA-CBA-CGA
25	A	826	CLA	C2A-CAA-CBA-CGA
24	V	307	CHL	C2C-C3C-CAC-CBC
36	A	854	DGD	C2A-C3A-C4A-C5A

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Mol	Chain	Res	Type	Atoms
24	1	601	CHL	CAD-CBD-CGD-O1D
24	2	607	CHL	C1C-C2C-CMC-OMC
24	5	605	CHL	CAD-CBD-CGD-O1D
24	Q	309	CHL	C1C-C2C-CMC-OMC
24	S	304	CHL	C1C-C2C-CMC-OMC
24	V	305	CHL	C1C-C2C-CMC-OMC
25	1	609	CLA	CAD-CBD-CGD-O1D
26	3	315	IWJ	C26-C28-C29-O39
26	4	317	IWJ	C26-C28-C29-C30
26	6	614	IWJ	C26-C28-C29-C35
26	S	319	IWJ	C26-C28-C29-C35
26	T	318	IWJ	C26-C28-C29-C35
26	T	321	IWJ	C26-C28-C29-C35
32	6	617	SQD	O6-C44-C45-C46
28	1	614	LHG	O7-C5-C6-O8
24	U	313	CHL	O1D-CGD-O2D-CED
25	B	822	CLA	O2A-C1-C2-C3
25	S	312	CLA	O1A-CGA-O2A-C1
25	T	311	CLA	CBA-CGA-O2A-C1
25	5	607	CLA	C10-C11-C12-C13
25	B	804	CLA	C8-C10-C11-C12
25	2	612	CLA	C6-C7-C8-C9
25	A	803	CLA	C11-C10-C8-C9
25	A	805	CLA	C11-C12-C13-C14
25	A	805	CLA	C14-C13-C15-C16
25	A	825	CLA	C11-C10-C8-C9
25	A	842	CLA	C11-C12-C13-C14
25	B	802	CLA	C11-C10-C8-C9
25	B	806	CLA	C11-C10-C8-C9
25	B	810	CLA	C11-C12-C13-C14
25	B	829	CLA	C11-C10-C8-C9
25	B	839	CLA	C11-C10-C8-C9
25	R	313	CLA	C14-C13-C15-C16
25	R	314	CLA	C6-C7-C8-C9
25	W	309	CLA	C11-C10-C8-C9
25	A	839	CLA	C16-C17-C18-C20
25	T	309	CLA	C11-C12-C13-C14
25	A	825	CLA	C10-C11-C12-C13
24	S	307	CHL	C2C-C3C-CAC-CBC
26	3	315	IWJ	C16-C17-C18-C19
30	I	101	BCR	C36-C18-C19-C20
25	A	807	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
28	A	846	LHG	C12-C13-C14-C15
26	4	317	IWJ	C18-C19-C21-C22
26	Q	320	IWJ	C08-C09-C10-C11
30	2	618	BCR	C7-C8-C9-C10
36	B	850	DGD	C2A-C3A-C4A-C5A
25	A	839	CLA	C8-C10-C11-C12
25	A	808	CLA	C4-C3-C5-C6
25	A	820	CLA	C5-C6-C7-C8
25	A	831	CLA	C5-C6-C7-C8
28	3	321	LHG	C25-C26-C27-C28
25	A	830	CLA	C5-C6-C7-C8
25	B	812	CLA	C10-C11-C12-C13
28	3	322	LHG	C4-C5-O7-C7
25	A	815	CLA	C2A-CAA-CBA-CGA
25	S	312	CLA	C2A-CAA-CBA-CGA
25	V	311	CLA	C2-C1-O2A-CGA
25	A	807	CLA	C4C-C3C-CAC-CBC
34	B	844	PQN	C26-C27-C28-C30
25	A	807	CLA	C2C-C3C-CAC-CBC
25	2	612	CLA	CAA-CBA-CGA-O2A
26	4	317	IWJ	C25-C24-C26-C28
26	Q	320	IWJ	C25-C24-C26-C28
26	W	318	IWJ	C25-C24-C26-C28
29	2	616	Q6L	C27-C29-C30-C31
29	W	319	Q6L	C27-C29-C30-C31
28	A	846	LHG	O6-C4-C5-O7
25	A	815	CLA	C13-C15-C16-C17
25	B	805	CLA	C4-C3-C5-C6
24	W	305	CHL	O1D-CGD-O2D-CED
25	B	815	CLA	C2-C3-C5-C6
25	T	312	CLA	C2-C3-C5-C6
28	2	619	LHG	O9-C7-O7-C5
25	B	834	CLA	CAA-CBA-CGA-O2A
31	L	308	LMG	O7-C10-C11-C12
25	A	807	CLA	C10-C11-C12-C13
28	2	619	LHG	C3-O3-P-O6
28	3	320	LHG	C3-O3-P-O6
28	3	322	LHG	C4-O6-P-O3
28	3	323	LHG	C3-O3-P-O6
28	3	323	LHG	C4-O6-P-O3
28	A	846	LHG	C4-O6-P-O3
28	A	847	LHG	C4-O6-P-O3

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Mol	Chain	Res	Type	Atoms
28	Q	302	LHG	C3-O3-P-O6
25	O	2001	CLA	O1D-CGD-O2D-CED
25	G	202	CLA	O1D-CGD-O2D-CED
25	A	808	CLA	C11-C12-C13-C15
25	A	808	CLA	C12-C13-C15-C16
25	B	802	CLA	C11-C10-C8-C7
25	B	841	CLA	C2-C3-C5-C6
29	O	2007	Q6L	C11-C12-C13-C14
25	B	843	CLA	CAA-CBA-CGA-O2A
25	2	602	CLA	C6-C7-C8-C9
25	6	613	CLA	C11-C12-C13-C14
25	A	837	CLA	C11-C12-C13-C14
25	A	839	CLA	C14-C13-C15-C16
25	B	808	CLA	C14-C13-C15-C16
25	B	842	CLA	C14-C13-C15-C16
25	P	309	CLA	C11-C12-C13-C14
33	A	802	CL0	C14-C13-C15-C16
27	4	318	XAT	C33-C34-C35-C15
29	S	323	Q6L	C17-C18-C19-C20
25	5	609	CLA	C6-C7-C8-C10
25	A	843	CLA	C16-C17-C18-C19
25	P	302	CLA	C13-C15-C16-C17
25	Q	315	CLA	O2A-C1-C2-C3
25	1	607	CLA	CHA-CBD-CGD-O1D
25	P	301	CLA	C8-C10-C11-C12
30	3	319	BCR	C7-C8-C9-C34
25	1	608	CLA	C5-C6-C7-C8
25	B	808	CLA	C16-C17-C18-C20
28	3	323	LHG	C24-C23-O8-C6
36	B	850	DGD	C6B-C7B-C8B-C9B
30	F	801	BCR	C17-C18-C19-C20
25	6	610	CLA	C12-C13-C15-C16
25	U	302	CLA	C11-C10-C8-C7
25	A	838	CLA	C2-C3-C5-C6
25	A	820	CLA	C10-C11-C12-C13
25	R	306	CLA	C5-C6-C7-C8
25	A	807	CLA	C2A-CAA-CBA-CGA
26	T	318	IWJ	C16-C17-C18-C19
26	W	318	IWJ	C16-C17-C18-C19
29	Q	318	Q6L	C24-C25-C26-C27
29	Q	319	Q6L	C24-C25-C26-C27
29	S	321	Q6L	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
31	N	201	LMG	C37-C38-C39-C40
25	B	828	CLA	C2C-C3C-CAC-CBC
38	T	308	KC2	C4B-C3B-CAB-CBB
38	V	308	KC2	C4B-C3B-CAB-CBB
38	X	309	KC2	C4B-C3B-CAB-CBB
25	B	819	CLA	C4-C3-C5-C6
25	R	313	CLA	C4-C3-C5-C6
29	T	315	Q6L	C11-C12-C13-C42
25	H	302	CLA	C5-C6-C7-C8
25	4	313	CLA	C2-C3-C5-C6
25	B	819	CLA	C2-C3-C5-C6
24	T	306	CHL	CAA-CBA-CGA-O2A
24	R	309	CHL	C2-C1-O2A-CGA
25	T	302	CLA	C2-C1-O2A-CGA
25	T	311	CLA	C11-C12-C13-C15
25	3	310	CLA	C2A-CAA-CBA-CGA
25	A	803	CLA	C2A-CAA-CBA-CGA
25	B	805	CLA	C2A-CAA-CBA-CGA
24	Q	316	CHL	C3A-C2A-CAA-CBA
25	5	607	CLA	C3A-C2A-CAA-CBA
25	A	804	CLA	C3A-C2A-CAA-CBA
25	G	202	CLA	C3A-C2A-CAA-CBA
25	P	312	CLA	C3A-C2A-CAA-CBA
25	P	313	CLA	C3A-C2A-CAA-CBA
25	Q	314	CLA	C3A-C2A-CAA-CBA
25	U	309	CLA	C3A-C2A-CAA-CBA
24	R	309	CHL	O2A-C1-C2-C3
29	V	321	Q6L	C24-C25-C26-C27
25	B	815	CLA	O1A-CGA-O2A-C1
26	1	611	IWJ	O27-C26-C28-C29
25	4	313	CLA	C4-C3-C5-C6
25	A	808	CLA	C2-C3-C5-C6
25	4	303	CLA	C6-C7-C8-C9
25	A	807	CLA	C6-C7-C8-C9
25	A	808	CLA	C6-C7-C8-C9
25	A	808	CLA	C14-C13-C15-C16
25	A	828	CLA	C6-C7-C8-C9
25	A	837	CLA	C6-C7-C8-C9
25	A	856	CLA	C6-C7-C8-C9
25	B	805	CLA	C11-C10-C8-C9
25	B	806	CLA	C11-C12-C13-C14
25	B	828	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
25	B	839	CLA	C11-C12-C13-C14
25	B	839	CLA	C14-C13-C15-C16
25	P	302	CLA	C11-C12-C13-C14
25	B	808	CLA	C5-C6-C7-C8
25	W	312	CLA	C5-C6-C7-C8
29	2	616	Q6L	C29-C30-C31-C36
29	O	2007	Q6L	C29-C30-C31-C36
30	A	852	BCR	C11-C10-C9-C34
30	A	852	BCR	C16-C17-C18-C36
30	B	846	BCR	C11-C10-C9-C34
30	B	846	BCR	C20-C21-C22-C37
30	F	804	BCR	C35-C13-C14-C15
30	L	307	BCR	C11-C10-C9-C34
37	H	306	NEX	C39-C29-C30-C31
37	P	317	NEX	C39-C29-C30-C31
37	R	321	NEX	C39-C29-C30-C31
37	S	317	NEX	C39-C29-C30-C31
37	T	317	NEX	C39-C29-C30-C31
37	W	317	NEX	C39-C29-C30-C31
25	B	821	CLA	CBD-CGD-O2D-CED
25	B	804	CLA	C2A-CAA-CBA-CGA
25	R	317	CLA	C2A-CAA-CBA-CGA
25	A	843	CLA	C16-C17-C18-C20
25	B	826	CLA	C16-C17-C18-C19
25	B	802	CLA	O2A-C1-C2-C3
25	B	819	CLA	O2A-C1-C2-C3
25	4	309	CLA	CAA-CBA-CGA-O1A
25	4	309	CLA	CAA-CBA-CGA-O2A
30	B	849	BCR	C7-C8-C9-C34
28	3	322	LHG	C14-C15-C16-C17
30	A	849	BCR	C11-C12-C13-C14
24	4	308	CHL	C1A-C2A-CAA-CBA
24	R	318	CHL	C1A-C2A-CAA-CBA
24	T	307	CHL	C1A-C2A-CAA-CBA
25	4	304	CLA	C1A-C2A-CAA-CBA
25	5	607	CLA	C1A-C2A-CAA-CBA
25	6	612	CLA	C1A-C2A-CAA-CBA
25	A	804	CLA	C1A-C2A-CAA-CBA
25	A	826	CLA	C1A-C2A-CAA-CBA
25	A	829	CLA	C1A-C2A-CAA-CBA
25	A	839	CLA	C1A-C2A-CAA-CBA
25	B	804	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
25	G	202	CLA	C1A-C2A-CAA-CBA
25	H	304	CLA	C1A-C2A-CAA-CBA
25	P	312	CLA	C1A-C2A-CAA-CBA
25	Q	314	CLA	C1A-C2A-CAA-CBA
25	U	310	CLA	C1A-C2A-CAA-CBA
25	2	602	CLA	C11-C12-C13-C15
25	6	602	CLA	C6-C7-C8-C10
25	6	602	CLA	C11-C10-C8-C7
25	A	835	CLA	C11-C12-C13-C15
25	A	838	CLA	C6-C7-C8-C10
25	A	842	CLA	C11-C10-C8-C7
25	B	802	CLA	C6-C7-C8-C10
25	B	831	CLA	C12-C13-C15-C16
25	P	302	CLA	C11-C12-C13-C15
25	V	311	CLA	C6-C7-C8-C10
25	5	602	CLA	C8-C10-C11-C12
29	R	301	Q6L	C17-C18-C19-C20
29	X	301	Q6L	C19-C20-C21-C22
38	Q	310	KC2	O1D-CGD-O2D-CED
24	Q	309	CHL	C3C-C2C-CMC-OMC
31	O	2008	LMG	O7-C10-C11-C12
25	2	606	CLA	CAA-CBA-CGA-O2A
25	Q	314	CLA	C5-C6-C7-C8
31	5	613	LMG	C41-C42-C43-C44
25	B	843	CLA	C3-C5-C6-C7
25	Q	304	CLA	C2A-CAA-CBA-CGA
28	2	619	LHG	C10-C11-C12-C13
32	H	303	SQD	C28-C29-C30-C31
38	R	312	KC2	C3A-C2A-CAA-CBA
36	B	850	DGD	C2B-C1B-O2G-C2G
25	V	301	CLA	C5-C6-C7-C8
33	A	802	CL0	C8-C10-C11-C12
25	A	818	CLA	CAA-CBA-CGA-O2A
25	A	827	CLA	C13-C15-C16-C17
25	B	806	CLA	C8-C10-C11-C12
25	B	820	CLA	C5-C6-C7-C8
24	1	601	CHL	C3-C5-C6-C7
32	H	303	SQD	O49-C7-O47-C45
28	A	846	LHG	C14-C15-C16-C17
30	A	852	BCR	C11-C10-C9-C8
30	A	852	BCR	C16-C17-C18-C19
30	B	846	BCR	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
30	B	846	BCR	C20-C21-C22-C23
30	F	804	BCR	C12-C13-C14-C15
30	L	307	BCR	C11-C10-C9-C8
37	H	306	NEX	C28-C29-C30-C31
37	P	317	NEX	C28-C29-C30-C31
37	R	321	NEX	C28-C29-C30-C31
37	S	317	NEX	C28-C29-C30-C31
37	T	317	NEX	C28-C29-C30-C31
37	W	317	NEX	C28-C29-C30-C31
25	2	606	CLA	CAA-CBA-CGA-O1A
31	A	855	LMG	O7-C8-C9-O8
32	H	303	SQD	O47-C45-C46-O48
26	4	301	IWJ	C10-C11-C12-C13
24	U	305	CHL	CAA-CBA-CGA-O1A
25	4	316	CLA	O1D-CGD-O2D-CED
25	B	807	CLA	C10-C11-C12-C13
28	3	320	LHG	C9-C10-C11-C12
25	5	610	CLA	O1D-CGD-O2D-CED
38	P	308	KC2	CAA-CBA-CGA-O2A
25	4	303	CLA	C2-C1-O2A-CGA
25	A	820	CLA	C2-C1-O2A-CGA
25	R	317	CLA	C2-C1-O2A-CGA
25	F	802	CLA	C3A-C2A-CAA-CBA
25	3	307	CLA	C11-C10-C8-C9
25	A	804	CLA	C11-C10-C8-C9
25	P	310	CLA	C6-C7-C8-C9
25	5	603	CLA	CAA-CBA-CGA-O2A
24	S	306	CHL	C4-C3-C5-C6
24	T	306	CHL	C4-C3-C5-C6
38	T	308	KC2	C1A-C2A-CAA-CBA
25	B	802	CLA	C2A-CAA-CBA-CGA
24	V	304	CHL	CAA-CBA-CGA-O2A
30	4	319	BCR	C1-C6-C7-C8
30	A	848	BCR	C23-C24-C25-C30
30	B	845	BCR	C1-C6-C7-C8
30	J	103	BCR	C23-C24-C25-C30
30	K	205	BCR	C1-C6-C7-C8
30	L	305	BCR	C1-C6-C7-C8
25	S	302	CLA	C13-C15-C16-C17
30	K	207	BCR	C7-C8-C9-C34
28	1	614	LHG	C4-C5-C6-O8
28	6	616	LHG	C34-C35-C36-C37

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Mol	Chain	Res	Type	Atoms
32	6	617	SQD	C9-C10-C11-C12
26	S	319	IWJ	C21-C22-C23-C24
29	P	316	Q6L	C24-C25-C26-C27
29	P	321	Q6L	C24-C25-C26-C27
31	A	857	LMG	C22-C23-C24-C25
25	A	830	CLA	C4-C3-C5-C6
25	A	840	CLA	C4-C3-C5-C6
25	B	829	CLA	C4-C3-C5-C6
29	V	321	Q6L	C11-C12-C13-C42
29	W	316	Q6L	C26-C27-C29-C30
25	B	815	CLA	C13-C15-C16-C17
25	T	302	CLA	C2-C3-C5-C6
24	P	305	CHL	CAA-CBA-CGA-O2A
31	5	613	LMG	C14-C15-C16-C17
25	A	823	CLA	C15-C16-C17-C18
31	L	308	LMG	C8-C7-O1-C1
24	V	307	CHL	C4C-C3C-CAC-CBC
28	3	323	LHG	C11-C10-C9-C8
24	1	601	CHL	CBA-CGA-O2A-C1
25	6	603	CLA	CAA-CBA-CGA-O2A
25	W	311	CLA	CAA-CBA-CGA-O2A
25	A	840	CLA	C6-C7-C8-C9
25	B	829	CLA	C16-C17-C18-C19
25	5	607	CLA	C5-C6-C7-C8
33	A	802	CL0	C13-C15-C16-C17
24	U	305	CHL	CAA-CBA-CGA-O2A
25	6	610	CLA	C3-C5-C6-C7
25	5	603	CLA	CAA-CBA-CGA-O1A
25	6	603	CLA	CAA-CBA-CGA-O1A
25	W	311	CLA	CAA-CBA-CGA-O1A
25	P	302	CLA	C5-C6-C7-C8
25	A	856	CLA	C11-C10-C8-C7
25	B	805	CLA	C2-C3-C5-C6
25	B	841	CLA	C11-C12-C13-C15
25	R	313	CLA	C6-C7-C8-C10
25	T	311	CLA	C11-C10-C8-C7
24	3	306	CHL	CAA-CBA-CGA-O2A
25	B	825	CLA	CAA-CBA-CGA-O2A
25	K	201	CLA	CAA-CBA-CGA-O2A
31	A	855	LMG	O7-C10-C11-C12
25	P	302	CLA	CAA-CBA-CGA-O2A
38	P	308	KC2	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
36	B	850	DGD	C3A-C4A-C5A-C6A
25	A	856	CLA	O1D-CGD-O2D-CED
25	B	821	CLA	O1D-CGD-O2D-CED
28	A	846	LHG	O8-C23-C24-C25
25	P	302	CLA	C8-C10-C11-C12
24	V	314	CHL	O1D-CGD-O2D-CED
25	A	835	CLA	C15-C16-C17-C18
25	B	839	CLA	CAA-CBA-CGA-O2A
25	B	840	CLA	CAA-CBA-CGA-O2A
25	2	602	CLA	C4-C3-C5-C6
25	B	826	CLA	C4-C3-C5-C6
25	5	602	CLA	C10-C11-C12-C13
25	H	304	CLA	CAA-CBA-CGA-O1A
38	V	308	KC2	CBD-CGD-O2D-CED
31	N	201	LMG	C19-C20-C21-C22
25	A	835	CLA	C16-C17-C18-C19
25	3	311	CLA	CAA-CBA-CGA-O2A
25	V	301	CLA	CAA-CBA-CGA-O2A
25	1	608	CLA	C6-C7-C8-C9
25	A	835	CLA	C11-C12-C13-C14
25	A	842	CLA	C11-C10-C8-C9
25	B	811	CLA	C6-C7-C8-C9
25	B	813	CLA	C11-C12-C13-C14
25	B	830	CLA	C11-C12-C13-C14
25	B	831	CLA	C6-C7-C8-C9
25	B	839	CLA	C6-C7-C8-C9
25	P	309	CLA	C6-C7-C8-C9
25	B	831	CLA	C3-C5-C6-C7
24	W	306	CHL	C3A-C2A-CAA-CBA
25	1	603	CLA	C3A-C2A-CAA-CBA
25	A	829	CLA	C3A-C2A-CAA-CBA
25	A	837	CLA	C3A-C2A-CAA-CBA
25	A	845	CLA	C3A-C2A-CAA-CBA
25	B	804	CLA	C3A-C2A-CAA-CBA
25	T	303	CLA	C3A-C2A-CAA-CBA
25	A	829	CLA	CAA-CBA-CGA-O2A
24	R	309	CHL	CAD-CBD-CGD-O2D
24	R	311	CHL	CAD-CBD-CGD-O2D
24	S	304	CHL	CAD-CBD-CGD-O2D
24	U	313	CHL	CAD-CBD-CGD-O2D
24	X	305	CHL	CAD-CBD-CGD-O2D
24	X	307	CHL	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
25	3	305	CLA	CAD-CBD-CGD-O2D
25	3	307	CLA	CAD-CBD-CGD-O2D
25	4	315	CLA	CAD-CBD-CGD-O2D
25	5	603	CLA	CAD-CBD-CGD-O2D
25	5	610	CLA	CAD-CBD-CGD-O2D
25	A	806	CLA	CAD-CBD-CGD-O2D
25	A	809	CLA	CAD-CBD-CGD-O2D
25	A	814	CLA	CAD-CBD-CGD-O2D
25	A	817	CLA	CAD-CBD-CGD-O2D
25	A	820	CLA	CAD-CBD-CGD-O2D
25	A	825	CLA	CAD-CBD-CGD-O2D
25	A	843	CLA	CAD-CBD-CGD-O2D
25	B	816	CLA	CAD-CBD-CGD-O2D
25	B	819	CLA	CAD-CBD-CGD-O2D
25	B	822	CLA	CAD-CBD-CGD-O2D
25	B	823	CLA	CAD-CBD-CGD-O2D
25	B	841	CLA	CAD-CBD-CGD-O2D
25	F	802	CLA	CAD-CBD-CGD-O2D
25	H	301	CLA	CAD-CBD-CGD-O2D
25	L	301	CLA	CAD-CBD-CGD-O2D
25	P	309	CLA	CAD-CBD-CGD-O2D
25	P	311	CLA	CAD-CBD-CGD-O2D
25	Q	311	CLA	CAD-CBD-CGD-O2D
25	Q	315	CLA	CAD-CBD-CGD-O2D
25	S	301	CLA	CAD-CBD-CGD-O2D
25	S	310	CLA	CAD-CBD-CGD-O2D
25	S	313	CLA	CAD-CBD-CGD-O2D
25	T	313	CLA	CAD-CBD-CGD-O2D
25	U	302	CLA	CAD-CBD-CGD-O2D
25	X	302	CLA	CAD-CBD-CGD-O2D
25	X	313	CLA	CAD-CBD-CGD-O2D
38	U	307	KC2	C2B-C3B-CAB-CBB
38	U	307	KC2	CAD-CBD-CGD-O2D
25	A	836	CLA	C16-C17-C18-C19
25	A	809	CLA	C2A-CAA-CBA-CGA
25	3	311	CLA	C3-C5-C6-C7
25	U	303	CLA	O1A-CGA-O2A-C1
24	P	305	CHL	CAA-CBA-CGA-O1A
24	Q	307	CHL	CAA-CBA-CGA-O2A
25	A	822	CLA	CAA-CBA-CGA-O2A
28	3	323	LHG	C11-C12-C13-C14
25	V	310	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
24	W	305	CHL	CBD-CGD-O2D-CED
25	B	839	CLA	C3-C5-C6-C7
24	V	304	CHL	CAA-CBA-CGA-O1A
25	L	303	CLA	CAA-CBA-CGA-O2A
25	A	813	CLA	C13-C15-C16-C17
25	B	826	CLA	C2-C3-C5-C6
25	B	829	CLA	C2-C3-C5-C6
25	A	831	CLA	CAA-CBA-CGA-O2A
25	B	806	CLA	CAA-CBA-CGA-O2A
25	Q	313	CLA	CAA-CBA-CGA-O2A
25	R	313	CLA	CAA-CBA-CGA-O2A
29	X	316	Q6L	C21-C22-C24-C25
30	A	850	BCR	C21-C22-C23-C24
25	1	607	CLA	CHA-CBD-CGD-O2D
26	4	317	IWJ	C25-C24-C26-O27
27	4	318	XAT	O24-C26-C27-C28
37	R	321	NEX	O24-C26-C27-C28
37	S	317	NEX	O24-C26-C27-C28
37	T	317	NEX	O24-C26-C27-C28
25	A	818	CLA	CAA-CBA-CGA-O1A
25	U	301	CLA	CAA-CBA-CGA-O2A
38	Q	310	KC2	CBD-CGD-O2D-CED
25	P	303	CLA	CAA-CBA-CGA-O2A
24	4	302	CHL	CAA-CBA-CGA-O1A
25	L	303	CLA	CAA-CBA-CGA-O1A
32	H	303	SQD	C24-C25-C26-C27
24	1	601	CHL	O2A-C1-C2-C3
25	A	812	CLA	O2A-C1-C2-C3
25	A	826	CLA	O2A-C1-C2-C3
25	A	828	CLA	O2A-C1-C2-C3
25	B	829	CLA	O2A-C1-C2-C3
25	P	301	CLA	O2A-C1-C2-C3
25	Q	301	CLA	O2A-C1-C2-C3
25	S	302	CLA	O2A-C1-C2-C3
25	T	311	CLA	O2A-C1-C2-C3
25	V	303	CLA	O2A-C1-C2-C3
25	W	302	CLA	O2A-C1-C2-C3
38	R	312	KC2	C4B-C3B-CAB-CBB
38	U	307	KC2	C4B-C3B-CAB-CBB
38	W	308	KC2	C4B-C3B-CAB-CBB
25	P	303	CLA	C2A-CAA-CBA-CGA
25	X	302	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
25	K	206	CLA	CAA-CBA-CGA-O2A
25	Q	301	CLA	CAA-CBA-CGA-O2A
24	Q	307	CHL	CAA-CBA-CGA-O1A
25	B	825	CLA	CAA-CBA-CGA-O1A
25	K	201	CLA	CAA-CBA-CGA-O1A
25	U	301	CLA	CAA-CBA-CGA-O1A
25	A	829	CLA	C16-C17-C18-C20
25	A	840	CLA	C6-C7-C8-C10
25	T	311	CLA	C11-C12-C13-C14
24	6	601	CHL	CHA-CBD-CGD-O1D
24	6	606	CHL	CHA-CBD-CGD-O1D
24	6	606	CHL	CHA-CBD-CGD-O2D
24	S	307	CHL	CHA-CBD-CGD-O2D
25	1	606	CLA	CHA-CBD-CGD-O1D
25	1	606	CLA	CHA-CBD-CGD-O2D
25	1	613	CLA	CHA-CBD-CGD-O2D
25	2	602	CLA	CHA-CBD-CGD-O1D
25	2	602	CLA	CHA-CBD-CGD-O2D
25	2	604	CLA	CHA-CBD-CGD-O1D
25	2	606	CLA	CHA-CBD-CGD-O2D
25	2	609	CLA	CHA-CBD-CGD-O1D
25	2	609	CLA	CHA-CBD-CGD-O2D
25	2	614	CLA	CHA-CBD-CGD-O1D
25	2	614	CLA	CHA-CBD-CGD-O2D
25	4	304	CLA	CHA-CBD-CGD-O1D
25	4	304	CLA	CHA-CBD-CGD-O2D
25	4	309	CLA	CHA-CBD-CGD-O2D
25	6	602	CLA	CHA-CBD-CGD-O2D
25	6	611	CLA	CHA-CBD-CGD-O1D
25	6	611	CLA	CHA-CBD-CGD-O2D
25	6	612	CLA	CHA-CBD-CGD-O1D
25	A	803	CLA	CHA-CBD-CGD-O1D
25	A	803	CLA	CHA-CBD-CGD-O2D
25	A	824	CLA	CHA-CBD-CGD-O2D
25	A	827	CLA	CHA-CBD-CGD-O1D
25	A	827	CLA	CHA-CBD-CGD-O2D
25	A	829	CLA	CHA-CBD-CGD-O1D
25	A	829	CLA	CHA-CBD-CGD-O2D
25	A	830	CLA	CHA-CBD-CGD-O1D
25	A	830	CLA	CHA-CBD-CGD-O2D
25	A	845	CLA	CHA-CBD-CGD-O1D
25	A	845	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
25	B	802	CLA	CHA-CBD-CGD-O1D
25	B	802	CLA	CHA-CBD-CGD-O2D
25	B	806	CLA	CHA-CBD-CGD-O1D
25	B	806	CLA	CHA-CBD-CGD-O2D
25	B	812	CLA	CHA-CBD-CGD-O1D
25	B	812	CLA	CHA-CBD-CGD-O2D
25	B	817	CLA	CHA-CBD-CGD-O1D
25	B	818	CLA	CHA-CBD-CGD-O2D
25	B	831	CLA	CHA-CBD-CGD-O2D
25	B	840	CLA	CHA-CBD-CGD-O2D
25	B	843	CLA	CHA-CBD-CGD-O1D
25	B	843	CLA	CHA-CBD-CGD-O2D
25	G	203	CLA	CHA-CBD-CGD-O2D
25	G	204	CLA	CHA-CBD-CGD-O1D
25	G	204	CLA	CHA-CBD-CGD-O2D
25	K	201	CLA	CHA-CBD-CGD-O1D
25	K	201	CLA	CHA-CBD-CGD-O2D
25	O	2001	CLA	CHA-CBD-CGD-O2D
25	P	303	CLA	CHA-CBD-CGD-O2D
25	Q	306	CLA	CHA-CBD-CGD-O1D
25	Q	306	CLA	CHA-CBD-CGD-O2D
25	U	309	CLA	CHA-CBD-CGD-O2D
25	V	303	CLA	CHA-CBD-CGD-O1D
25	V	303	CLA	CHA-CBD-CGD-O2D
25	V	310	CLA	CHA-CBD-CGD-O2D
25	W	301	CLA	CHA-CBD-CGD-O1D
25	W	301	CLA	CHA-CBD-CGD-O2D
25	W	310	CLA	CHA-CBD-CGD-O1D
25	W	310	CLA	CHA-CBD-CGD-O2D
25	W	312	CLA	CHA-CBD-CGD-O1D
25	W	312	CLA	CHA-CBD-CGD-O2D
26	S	322	IWJ	C16-C17-C18-C19
24	3	306	CHL	CAA-CBA-CGA-O1A
25	A	822	CLA	CAA-CBA-CGA-O1A
25	B	811	CLA	CAA-CBA-CGA-O2A
31	A	857	LMG	O7-C10-C11-C12
25	A	829	CLA	C2C-C3C-CAC-CBC
25	B	816	CLA	CBA-CGA-O2A-C1
28	3	321	LHG	C9-C10-C11-C12
31	B	801	LMG	O6-C5-C6-O5
25	A	829	CLA	C16-C17-C18-C19
25	5	609	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
25	A	809	CLA	CAA-CBA-CGA-O2A
25	B	808	CLA	CAA-CBA-CGA-O2A
25	B	812	CLA	CAA-CBA-CGA-O2A
25	P	312	CLA	CAA-CBA-CGA-O2A
25	R	313	CLA	C15-C16-C17-C18
32	H	303	SQD	O6-C44-C45-O47
31	A	857	LMG	O10-C28-O8-C9
38	X	309	KC2	CAA-CBA-CGA-O1A
25	A	831	CLA	C13-C15-C16-C17
25	A	817	CLA	CAA-CBA-CGA-O2A
25	5	607	CLA	C16-C17-C18-C19
25	2	608	CLA	CAA-CBA-CGA-O1A
26	4	317	IWJ	C23-C24-C26-O27
25	A	821	CLA	C5-C6-C7-C8
25	A	838	CLA	C8-C10-C11-C12
25	G	204	CLA	CAA-CBA-CGA-O2A
28	1	614	LHG	C29-C30-C31-C32
25	A	828	CLA	C6-C7-C8-C10
25	A	830	CLA	C2-C3-C5-C6
25	B	804	CLA	C6-C7-C8-C10
25	B	805	CLA	C11-C10-C8-C7
25	B	812	CLA	C12-C13-C15-C16
25	O	2001	CLA	C11-C10-C8-C7
28	3	323	LHG	O8-C23-C24-C25
25	A	838	CLA	C6-C7-C8-C9
25	A	838	CLA	C11-C10-C8-C9
25	A	856	CLA	C11-C10-C8-C9
25	B	802	CLA	C6-C7-C8-C9
25	B	805	CLA	C11-C12-C13-C14
25	B	809	CLA	C11-C10-C8-C9
25	B	828	CLA	C11-C12-C13-C14
25	B	829	CLA	C6-C7-C8-C9
25	O	2001	CLA	C11-C10-C8-C9
25	R	313	CLA	C6-C7-C8-C9
26	R	322	IWJ	C14-C15-C16-C17
25	H	304	CLA	CAA-CBA-CGA-O2A
25	U	303	CLA	CBA-CGA-O2A-C1
31	A	857	LMG	C29-C28-O8-C9
33	A	802	CL0	C16-C17-C18-C19
28	2	619	LHG	C8-C7-O7-C5
25	A	820	CLA	C2A-CAA-CBA-CGA
31	L	308	LMG	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
32	H	303	SQD	O48-C23-C24-C25
25	3	311	CLA	CAA-CBA-CGA-O1A
25	B	811	CLA	CAA-CBA-CGA-O1A
25	T	302	CLA	C4-C3-C5-C6
25	U	302	CLA	C4-C3-C5-C6
25	A	840	CLA	C2-C3-C5-C6
25	A	829	CLA	CAA-CBA-CGA-O1A
25	A	831	CLA	CAA-CBA-CGA-O1A
25	B	808	CLA	CAA-CBA-CGA-O1A
25	B	840	CLA	CAA-CBA-CGA-O1A
25	P	312	CLA	CAA-CBA-CGA-O1A
24	4	306	CHL	CHA-CBD-CGD-O2D
24	P	306	CHL	C1A-C2A-CAA-CBA
24	Q	316	CHL	C1A-C2A-CAA-CBA
24	S	314	CHL	C1A-C2A-CAA-CBA
24	W	306	CHL	C1A-C2A-CAA-CBA
25	1	603	CLA	C1A-C2A-CAA-CBA
25	2	612	CLA	C1A-C2A-CAA-CBA
25	4	312	CLA	CHA-CBD-CGD-O2D
25	A	833	CLA	C1A-C2A-CAA-CBA
25	A	837	CLA	C1A-C2A-CAA-CBA
25	B	806	CLA	C1A-C2A-CAA-CBA
25	B	808	CLA	C1A-C2A-CAA-CBA
25	B	823	CLA	C1A-C2A-CAA-CBA
25	B	831	CLA	C1A-C2A-CAA-CBA
25	S	303	CLA	C1A-C2A-CAA-CBA
25	T	303	CLA	C1A-C2A-CAA-CBA
25	U	302	CLA	C1A-C2A-CAA-CBA
25	U	309	CLA	C1A-C2A-CAA-CBA
29	S	315	Q6L	C04-C03-C11-C12
29	V	315	Q6L	C04-C03-C11-C12
29	W	316	Q6L	C04-C03-C11-C12
25	T	302	CLA	C16-C17-C18-C19
32	H	303	SQD	C8-C7-O47-C45
25	P	309	CLA	C2-C1-O2A-CGA
25	Q	311	CLA	C5-C6-C7-C8
25	K	206	CLA	CAA-CBA-CGA-O1A
25	P	302	CLA	CAA-CBA-CGA-O1A
25	P	303	CLA	CAA-CBA-CGA-O1A
25	V	301	CLA	CAA-CBA-CGA-O1A
28	A	846	LHG	O10-C23-C24-C25
29	W	316	Q6L	C19-C20-C21-C22

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Mol	Chain	Res	Type	Atoms
25	R	313	CLA	C16-C17-C18-C19
25	Q	313	CLA	CAA-CBA-CGA-O1A
25	4	303	CLA	C8-C10-C11-C12
25	B	842	CLA	C10-C11-C12-C13
25	B	825	CLA	O1D-CGD-O2D-CED
25	W	309	CLA	C16-C17-C18-C19
28	3	323	LHG	C25-C26-C27-C28
25	B	806	CLA	CAA-CBA-CGA-O1A
28	3	323	LHG	C3-O3-P-O5
28	A	846	LHG	C4-O6-P-O5
28	A	847	LHG	C4-O6-P-O5
25	B	839	CLA	CAA-CBA-CGA-O1A
25	R	313	CLA	CAA-CBA-CGA-O1A
31	A	857	LMG	O9-C10-C11-C12
25	5	601	CLA	CAA-CBA-CGA-O2A
25	A	809	CLA	CAA-CBA-CGA-O1A
25	A	817	CLA	CAA-CBA-CGA-O1A
25	B	812	CLA	CAA-CBA-CGA-O1A
25	Q	301	CLA	CAA-CBA-CGA-O1A
25	V	310	CLA	CAA-CBA-CGA-O1A
25	3	307	CLA	CAA-CBA-CGA-O2A
25	A	841	CLA	CAA-CBA-CGA-O2A
25	B	819	CLA	CAA-CBA-CGA-O2A
28	1	614	LHG	O8-C23-C24-C25
24	R	310	CHL	C4C-C3C-CAC-CBC
25	G	204	CLA	CAA-CBA-CGA-O1A
25	B	820	CLA	C11-C12-C13-C14
25	B	822	CLA	C2A-CAA-CBA-CGA
25	T	301	CLA	C2A-CAA-CBA-CGA
25	4	303	CLA	CAA-CBA-CGA-O2A
25	A	820	CLA	CAA-CBA-CGA-O2A
25	O	2001	CLA	CAA-CBA-CGA-O2A
25	H	302	CLA	C13-C15-C16-C17
29	U	315	Q6L	C17-C18-C19-C20
29	T	315	Q6L	C11-C12-C13-C14
25	B	824	CLA	C11-C12-C13-C15
24	6	601	CHL	CAD-CBD-CGD-O1D
24	P	306	CHL	C2-C3-C5-C6
24	R	318	CHL	CAD-CBD-CGD-O1D
24	T	320	CHL	CAD-CBD-CGD-O1D
24	X	315	CHL	CAD-CBD-CGD-O1D
25	1	606	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
25	2	606	CLA	CAD-CBD-CGD-O1D
25	3	309	CLA	CAD-CBD-CGD-O1D
25	4	309	CLA	CAD-CBD-CGD-O1D
25	6	612	CLA	CAD-CBD-CGD-O1D
25	A	833	CLA	CAD-CBD-CGD-O1D
25	B	815	CLA	CAD-CBD-CGD-O1D
25	B	817	CLA	CAD-CBD-CGD-O1D
25	U	311	CLA	CAD-CBD-CGD-O1D
38	P	308	KC2	CAD-CBD-CGD-O1D
38	W	308	KC2	CAD-CBD-CGD-O1D
24	1	601	CHL	O1A-CGA-O2A-C1
28	3	323	LHG	O10-C23-O8-C6
24	T	320	CHL	CAA-CBA-CGA-O2A
25	B	815	CLA	C8-C10-C11-C12
25	6	602	CLA	C6-C7-C8-C9
25	6	602	CLA	C11-C10-C8-C9
25	A	810	CLA	C14-C13-C15-C16
25	A	821	CLA	C11-C10-C8-C9
25	A	823	CLA	C11-C10-C8-C9
25	A	839	CLA	C11-C12-C13-C14
25	B	804	CLA	C6-C7-C8-C9
25	S	301	CLA	C14-C13-C15-C16
25	V	311	CLA	C6-C7-C8-C9
38	X	309	KC2	CAA-CBA-CGA-O2A
25	5	610	CLA	CBD-CGD-O2D-CED
25	2	608	CLA	CAA-CBA-CGA-O2A
31	5	613	LMG	C32-C33-C34-C35
25	A	806	CLA	CAA-CBA-CGA-O2A
25	A	837	CLA	CAA-CBA-CGA-O2A
25	X	303	CLA	CAA-CBA-CGA-O2A
25	A	816	CLA	CAA-CBA-CGA-O2A
25	B	808	CLA	C10-C11-C12-C13
25	P	302	CLA	C10-C11-C12-C13
25	6	613	CLA	CAA-CBA-CGA-O2A
25	A	840	CLA	CAA-CBA-CGA-O2A
25	B	824	CLA	CAA-CBA-CGA-O2A
25	R	314	CLA	CAA-CBA-CGA-O2A
25	V	302	CLA	CAA-CBA-CGA-O2A
24	4	308	CHL	CAA-CBA-CGA-O2A
24	S	305	CHL	C4C-C3C-CAC-CBC
24	W	307	CHL	C3-C5-C6-C7
25	B	841	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
25	P	309	CLA	C4-C3-C5-C6
25	B	831	CLA	C13-C15-C16-C17
24	1	601	CHL	CAD-CBD-CGD-O2D
24	4	306	CHL	CHA-CBD-CGD-O1D
24	5	605	CHL	CAD-CBD-CGD-O2D
24	P	307	CHL	C3A-C2A-CAA-CBA
24	X	308	CHL	C3A-C2A-CAA-CBA
25	1	609	CLA	CAD-CBD-CGD-O2D
25	2	611	CLA	CHA-CBD-CGD-O1D
25	2	613	CLA	CHA-CBD-CGD-O1D
25	3	311	CLA	CAD-CBD-CGD-O2D
25	4	304	CLA	C3A-C2A-CAA-CBA
25	6	610	CLA	C11-C10-C8-C7
25	A	839	CLA	C3A-C2A-CAA-CBA
25	A	856	CLA	C3A-C2A-CAA-CBA
25	B	806	CLA	C11-C10-C8-C7
25	B	806	CLA	C12-C13-C15-C16
25	B	829	CLA	C6-C7-C8-C10
25	B	839	CLA	C11-C10-C8-C7
25	R	306	CLA	C12-C13-C15-C16
25	U	310	CLA	C3A-C2A-CAA-CBA
25	V	301	CLA	C11-C10-C8-C7
29	R	304	Q6L	C29-C30-C31-C32
29	R	323	Q6L	C29-C30-C31-C32
29	S	320	Q6L	C29-C30-C31-C32
29	V	321	Q6L	C29-C30-C31-C32
25	V	302	CLA	CAA-CBA-CGA-O1A
25	A	835	CLA	CAA-CBA-CGA-O2A
26	4	301	IWJ	C08-C09-C10-C11
29	P	316	Q6L	C15-C16-C17-C18
30	3	319	BCR	C7-C8-C9-C10
30	A	851	BCR	C17-C18-C19-C20
30	A	852	BCR	C17-C18-C19-C20
30	L	306	BCR	C17-C18-C19-C20
24	T	320	CHL	CAA-CBA-CGA-O1A
25	5	601	CLA	CAA-CBA-CGA-O1A
25	O	2001	CLA	CAA-CBA-CGA-O1A
29	V	319	Q6L	C19-C20-C21-C22
26	R	303	IWJ	O27-C26-C28-C29
25	N	202	CLA	CAA-CBA-CGA-O2A
31	B	801	LMG	C33-C34-C35-C36
25	X	303	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
31	A	855	LMG	C29-C28-O8-C9
31	A	857	LMG	C11-C10-O7-C8
25	B	830	CLA	CAA-CBA-CGA-O2A
25	S	309	CLA	CAA-CBA-CGA-O2A
25	A	841	CLA	CAA-CBA-CGA-O1A
25	5	603	CLA	C2A-CAA-CBA-CGA
25	P	310	CLA	C2A-CAA-CBA-CGA
25	T	302	CLA	C2A-CAA-CBA-CGA
25	W	309	CLA	O1A-CGA-O2A-C1
36	B	850	DGD	C4A-C5A-C6A-C7A
25	B	824	CLA	CAA-CBA-CGA-O1A
24	4	308	CHL	CAA-CBA-CGA-O1A

All (7) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
26	3	315	IWJ	C29-C30-C32-C33-C34-C35
26	X	318	IWJ	C29-C30-C32-C33-C34-C35
26	T	321	IWJ	C29-C30-C32-C33-C34-C35
26	S	319	IWJ	C29-C30-C32-C33-C34-C35
26	V	320	IWJ	C29-C30-C32-C33-C34-C35
26	R	322	IWJ	C29-C30-C32-C33-C34-C35
26	5	611	IWJ	C29-C30-C32-C33-C34-C35

201 monomers are involved in 301 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	F	805	LMG	1	0
25	V	301	CLA	5	0
25	W	312	CLA	2	0
25	A	813	CLA	3	0
25	B	803	CLA	1	0
24	T	307	CHL	1	0
25	R	316	CLA	1	0
25	R	313	CLA	1	0
25	Q	315	CLA	1	0
24	2	607	CHL	1	0
30	4	319	BCR	2	0
25	V	309	CLA	4	0
25	N	202	CLA	1	0
25	A	826	CLA	1	0
25	K	201	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	J	101	BCR	3	0
30	L	305	BCR	3	0
25	S	309	CLA	4	0
30	B	848	BCR	1	0
25	R	307	CLA	1	0
25	B	826	CLA	1	0
25	2	609	CLA	5	0
25	5	609	CLA	3	0
25	B	824	CLA	3	0
25	B	835	CLA	2	0
25	L	303	CLA	1	0
30	G	201	BCR	5	0
26	V	320	IWJ	1	0
29	R	320	Q6L	1	0
30	B	845	BCR	1	0
25	V	302	CLA	1	0
25	6	610	CLA	2	0
25	B	808	CLA	5	0
25	X	310	CLA	1	0
24	Q	307	CHL	1	0
36	A	854	DGD	1	0
25	W	303	CLA	1	0
25	R	305	CLA	4	0
25	A	824	CLA	1	0
24	V	314	CHL	1	0
32	H	303	SQD	1	0
26	4	301	IWJ	1	0
25	B	809	CLA	1	0
25	L	302	CLA	1	0
24	S	304	CHL	2	0
25	F	802	CLA	1	0
24	V	307	CHL	1	0
29	R	319	Q6L	1	0
25	P	309	CLA	2	0
25	B	829	CLA	2	0
26	Q	320	IWJ	1	0
24	W	314	CHL	1	0
29	2	616	Q6L	2	0
38	V	308	KC2	1	0
25	6	602	CLA	2	0
25	5	610	CLA	1	0
25	1	609	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	V	311	CLA	3	0
25	B	843	CLA	1	0
27	6	615	XAT	2	0
25	6	612	CLA	2	0
26	R	322	IWJ	1	0
24	R	308	CHL	7	0
24	P	307	CHL	1	0
25	H	301	CLA	1	0
25	A	830	CLA	3	0
30	B	847	BCR	1	0
25	A	820	CLA	1	0
28	2	619	LHG	1	0
25	B	810	CLA	1	0
38	R	312	KC2	2	0
25	4	309	CLA	1	0
25	O	2001	CLA	1	0
25	G	203	CLA	1	0
25	S	310	CLA	3	0
29	Q	319	Q6L	1	0
26	6	614	IWJ	2	0
26	W	318	IWJ	2	0
25	B	841	CLA	1	0
25	B	830	CLA	2	0
24	4	306	CHL	2	0
25	R	306	CLA	1	0
25	X	302	CLA	3	0
25	F	803	CLA	1	0
25	S	301	CLA	6	0
25	1	610	CLA	1	0
25	6	611	CLA	1	0
25	A	822	CLA	1	0
25	1	605	CLA	2	0
38	T	308	KC2	1	0
38	P	308	KC2	1	0
26	T	321	IWJ	1	0
25	B	832	CLA	1	0
25	B	815	CLA	4	0
29	V	321	Q6L	1	0
25	A	832	CLA	1	0
30	J	103	BCR	1	0
26	S	319	IWJ	1	0
25	5	602	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	1	607	CLA	3	0
25	B	819	CLA	2	0
26	V	317	IWJ	1	0
25	3	301	CLA	3	0
25	B	818	CLA	2	0
25	A	825	CLA	1	0
25	T	311	CLA	1	0
24	1	601	CHL	1	0
26	T	318	IWJ	1	0
25	A	856	CLA	1	0
25	2	602	CLA	1	0
25	B	840	CLA	1	0
26	P	318	IWJ	1	0
25	B	842	CLA	5	0
24	2	601	CHL	1	0
24	X	306	CHL	1	0
25	G	204	CLA	1	0
28	6	616	LHG	1	0
30	A	850	BCR	1	0
25	A	814	CLA	1	0
25	X	311	CLA	3	0
30	A	849	BCR	1	0
24	S	307	CHL	5	0
25	A	807	CLA	2	0
25	W	309	CLA	5	0
24	R	311	CHL	2	0
25	6	607	CLA	3	0
26	4	317	IWJ	2	0
25	A	803	CLA	1	0
29	X	319	Q6L	1	0
25	3	308	CLA	3	0
25	3	303	CLA	1	0
29	U	314	Q6L	2	0
36	B	850	DGD	1	0
25	B	813	CLA	1	0
30	A	852	BCR	3	0
25	B	806	CLA	1	0
34	A	844	PQN	1	0
25	Q	314	CLA	2	0
29	T	316	Q6L	1	0
24	3	306	CHL	1	0
29	P	316	Q6L	1	0

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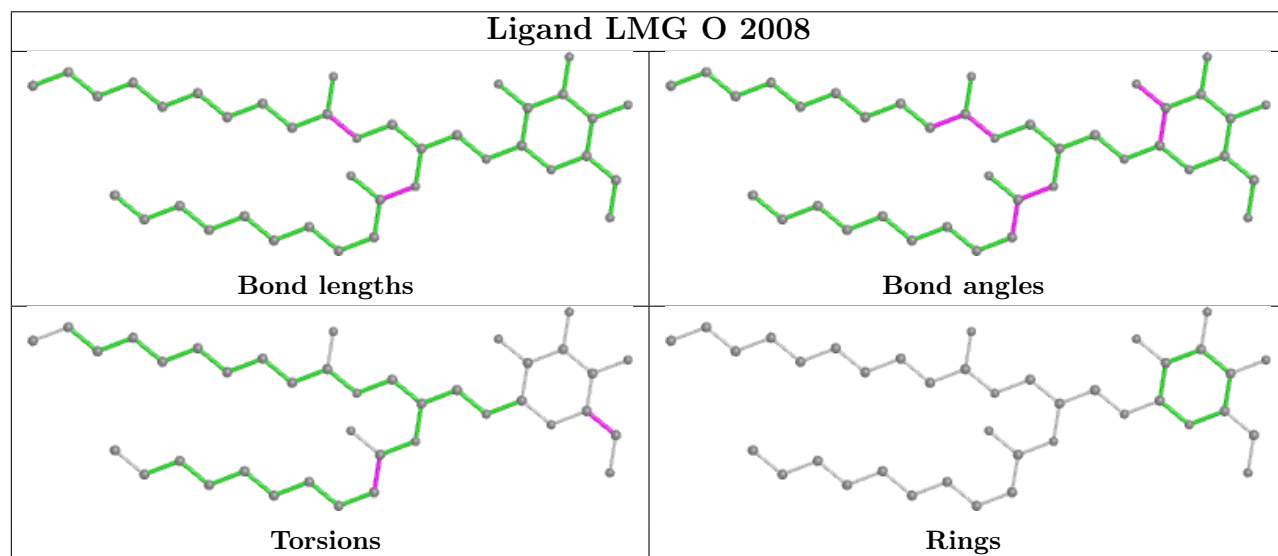
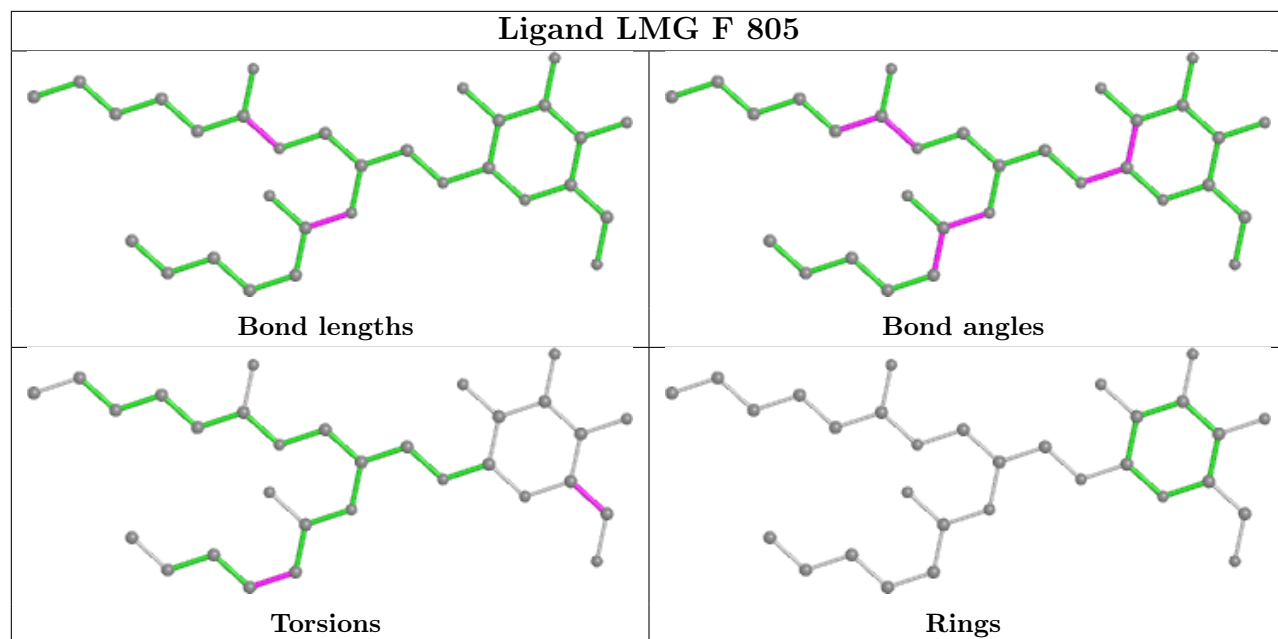
Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	K	206	CLA	2	0
25	Q	306	CLA	1	0
25	5	607	CLA	2	0
25	A	833	CLA	1	0
27	2	617	XAT	1	0
28	1	614	LHG	1	0
30	K	207	BCR	2	0
26	P	320	IWJ	1	0
25	2	613	CLA	2	0
25	A	836	CLA	1	0
25	J	102	CLA	1	0
29	W	315	Q6L	2	0
25	X	313	CLA	1	0
25	1	606	CLA	2	0
25	X	304	CLA	1	0
25	U	301	CLA	1	0
25	B	827	CLA	1	0
30	M	101	BCR	1	0
25	B	823	CLA	1	0
24	V	305	CHL	1	0
38	S	308	KC2	1	0
26	3	315	IWJ	2	0
25	4	310	CLA	2	0
24	X	308	CHL	1	0
25	A	809	CLA	1	0
25	3	307	CLA	4	0
37	P	317	NEX	1	0
25	T	312	CLA	1	0
25	A	815	CLA	3	0
31	A	857	LMG	1	0
26	S	322	IWJ	1	0
25	A	808	CLA	2	0
25	B	825	CLA	2	0
29	O	2006	Q6L	1	0
25	W	301	CLA	3	0
30	3	317	BCR	1	0
25	G	202	CLA	1	0
25	B	807	CLA	1	0
25	P	301	CLA	3	0
25	V	303	CLA	1	0
25	4	303	CLA	3	0
29	S	315	Q6L	1	0

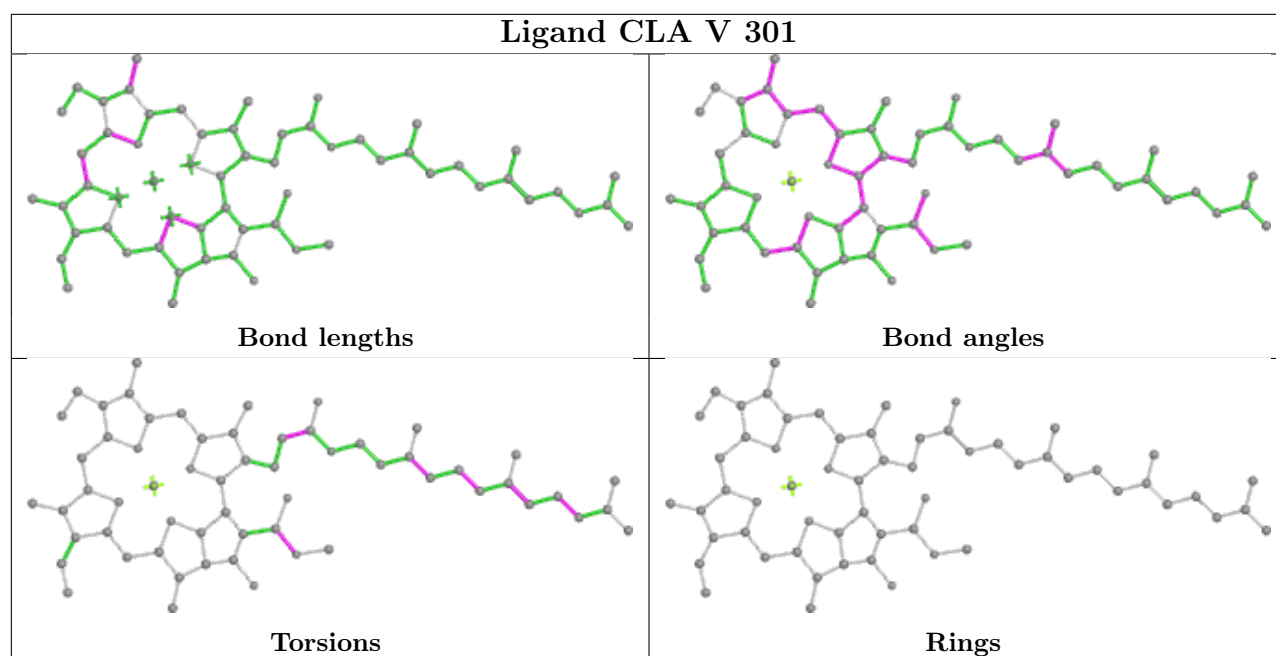
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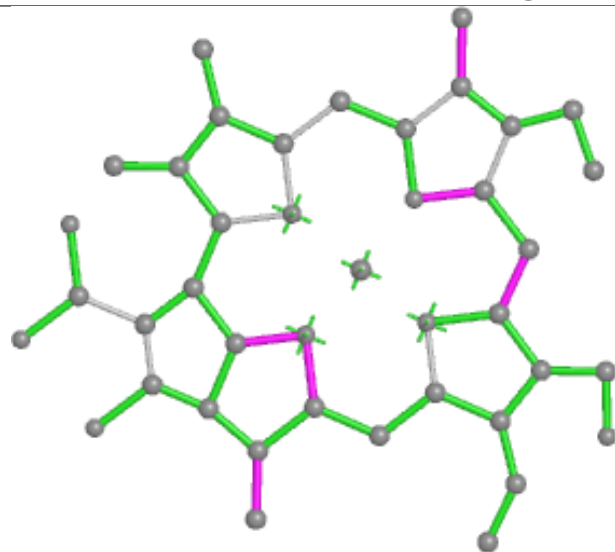
Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	T	310	CLA	1	0
30	F	801	BCR	1	0
25	A	810	CLA	1	0
25	3	304	CLA	3	0
25	A	812	CLA	1	0
25	Q	304	CLA	6	0
27	5	612	XAT	1	0
25	V	312	CLA	2	0
27	3	316	XAT	2	0
25	Q	312	CLA	1	0
25	3	313	CLA	1	0
25	O	2002	CLA	1	0
25	A	811	CLA	2	0
24	4	308	CHL	1	0
25	B	834	CLA	2	0
25	2	608	CLA	3	0
27	4	318	XAT	1	0
24	U	304	CHL	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.

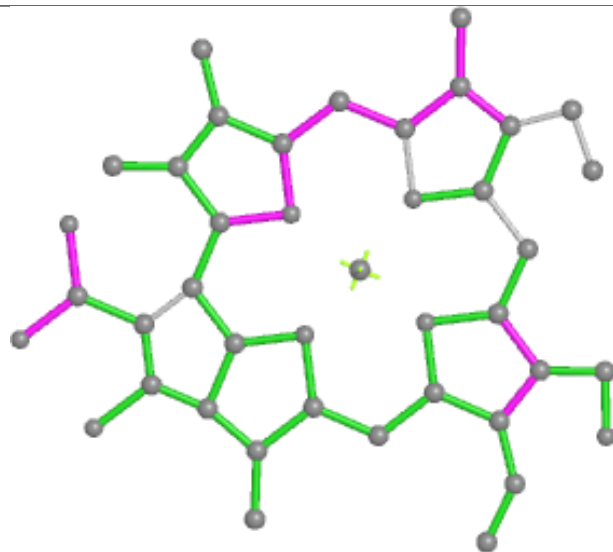




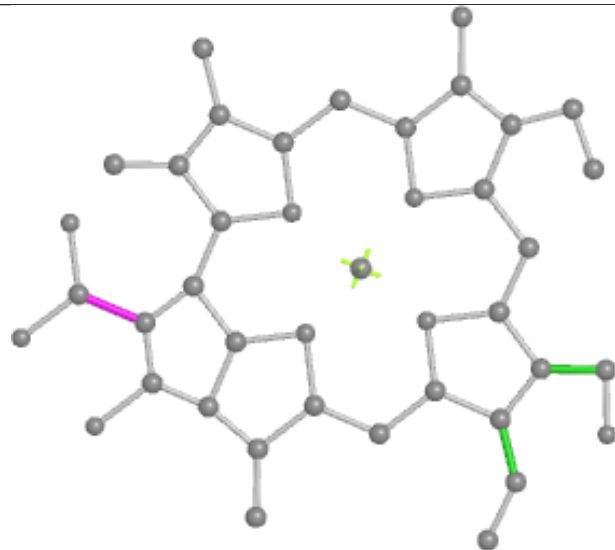
Ligand CHL 5 605



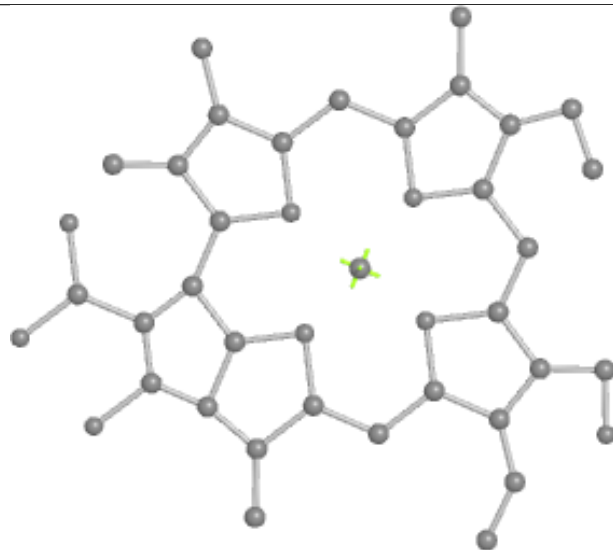
Bond lengths



Bond angles

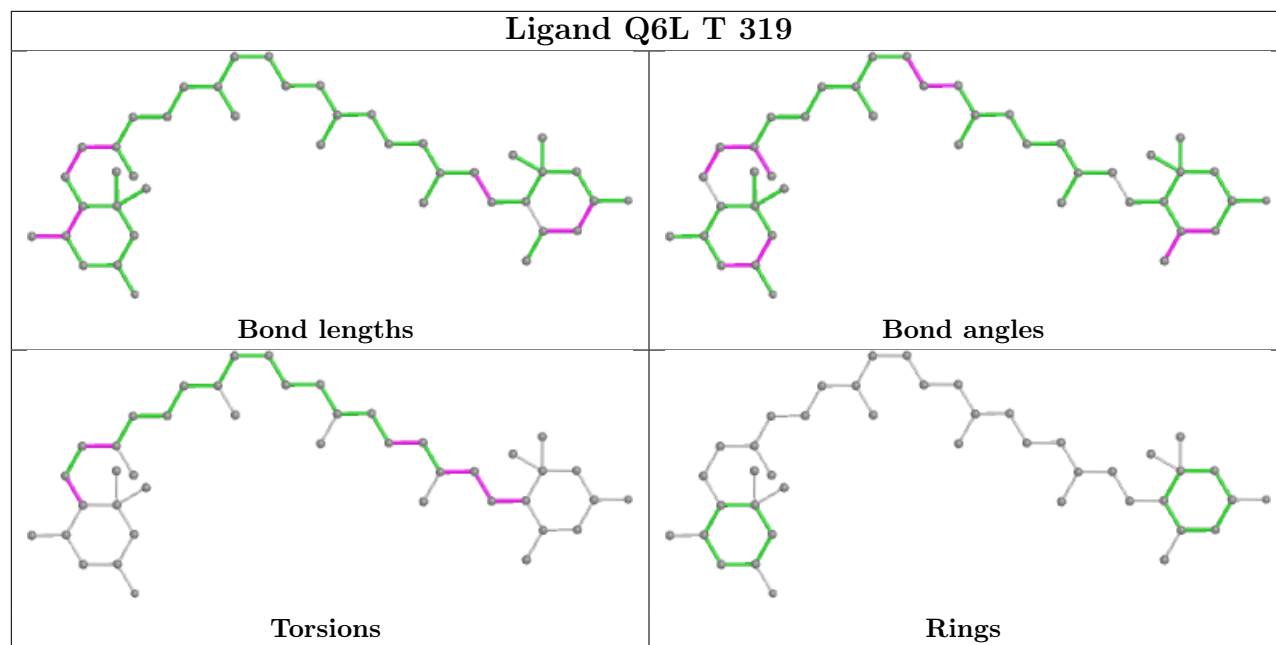


Torsions

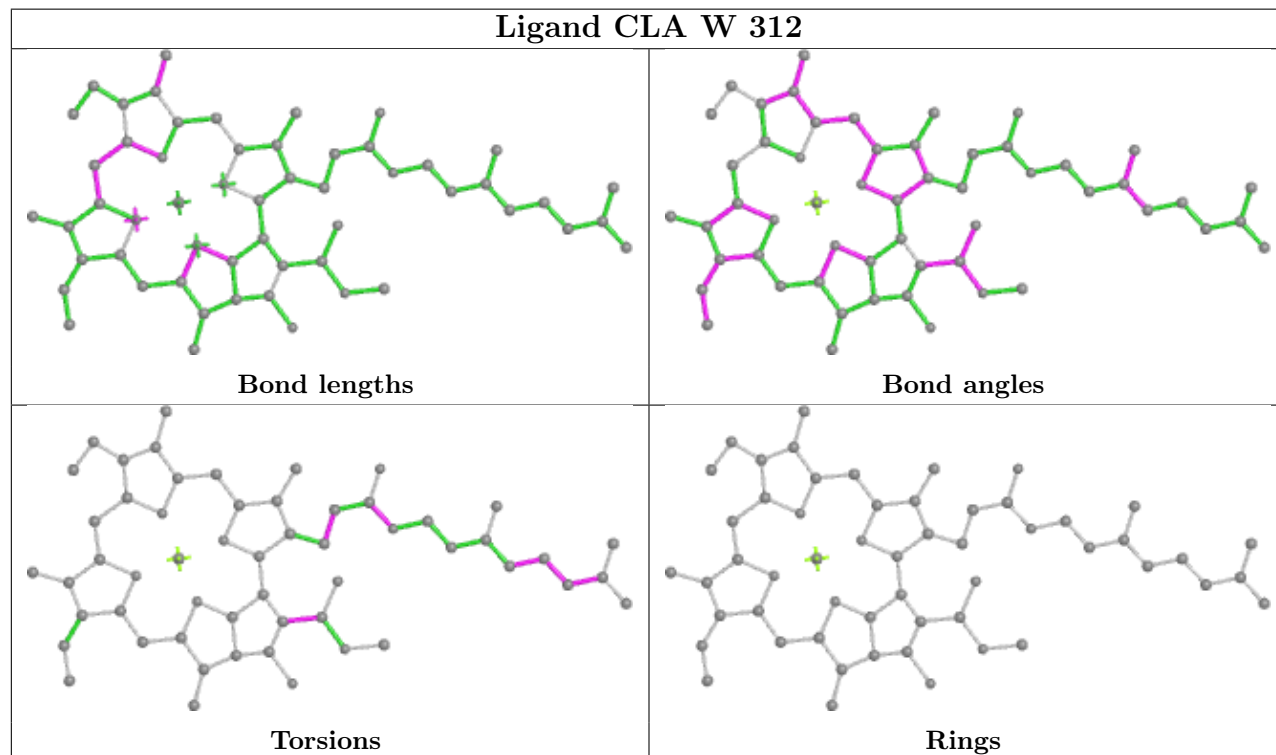


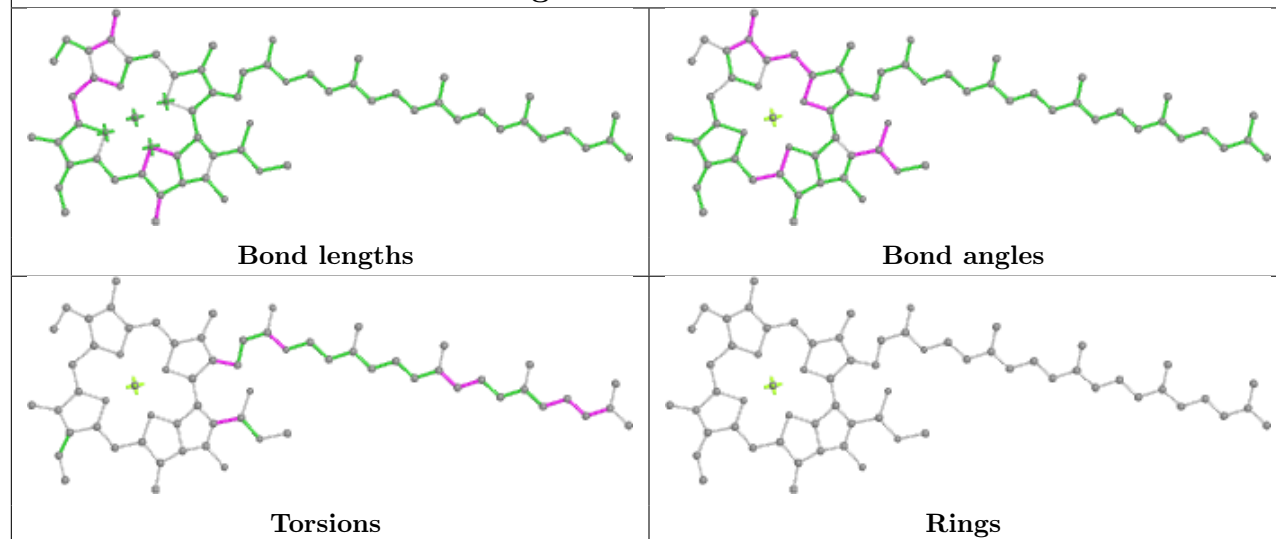
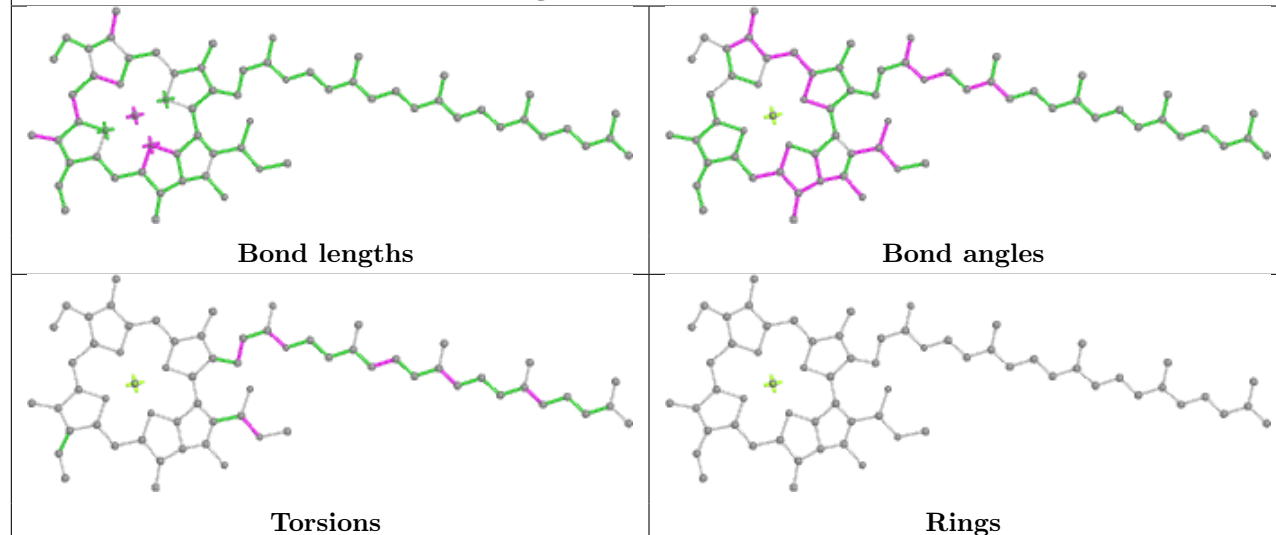
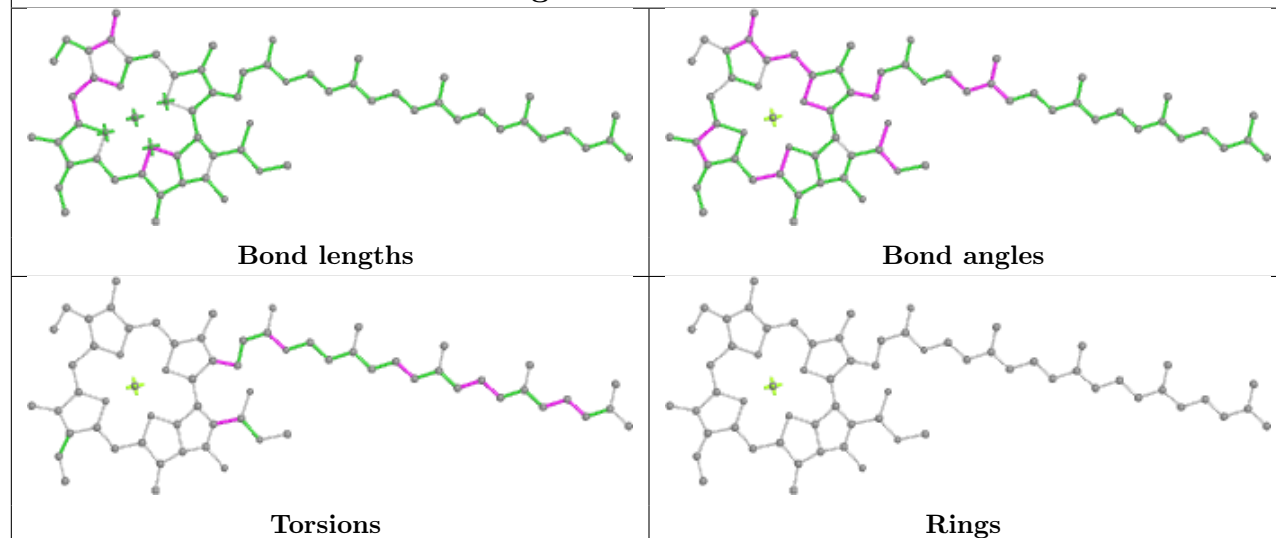
Rings

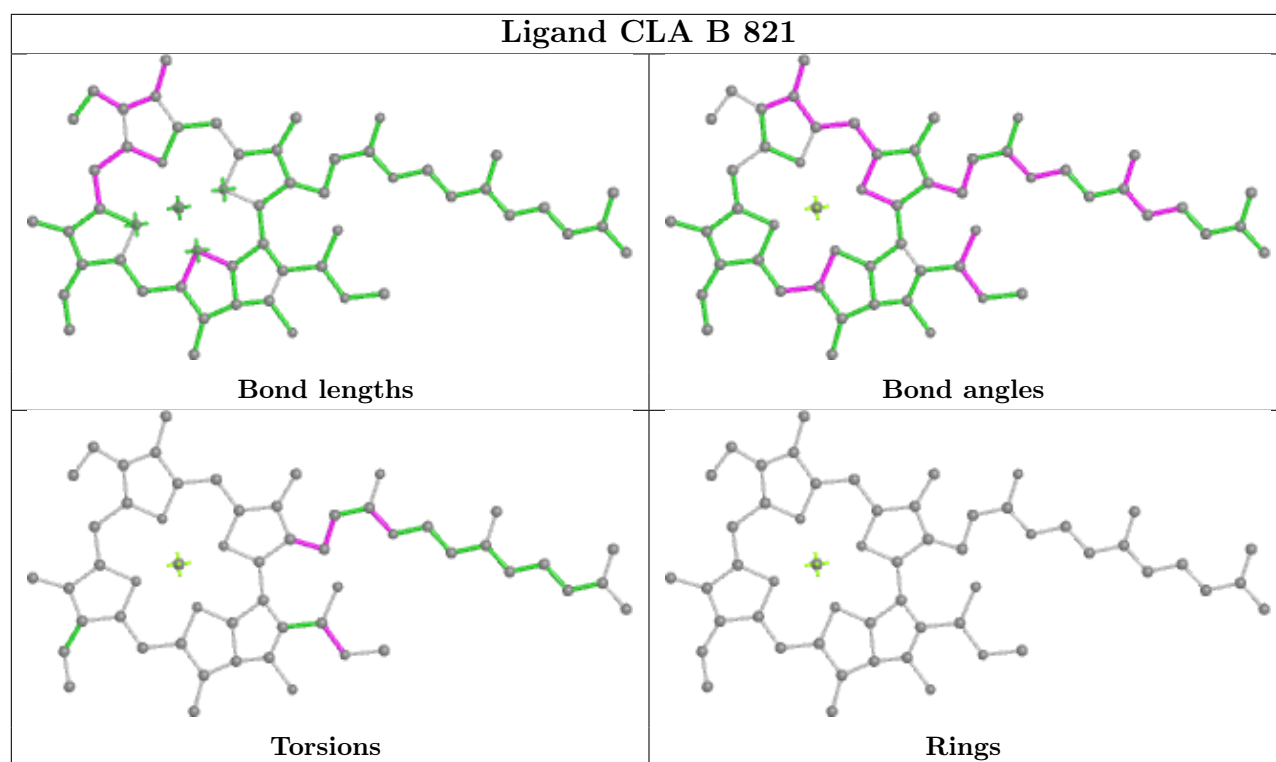
Ligand Q6L T 319



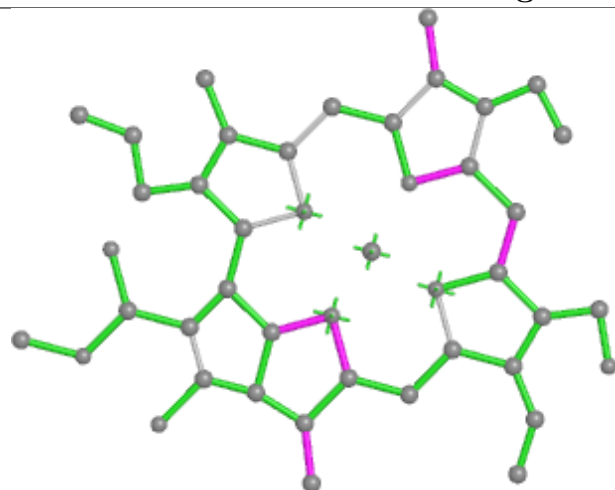
Ligand CLA W 312



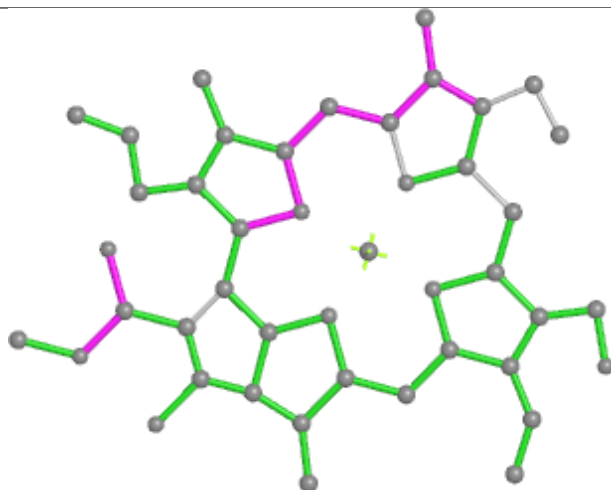
Ligand CLA A 813**Ligand CLA B 803****Ligand CLA H 302**



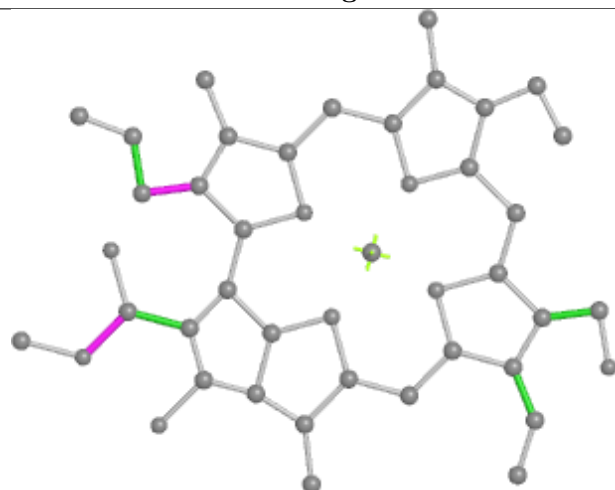
Ligand CHL T 307



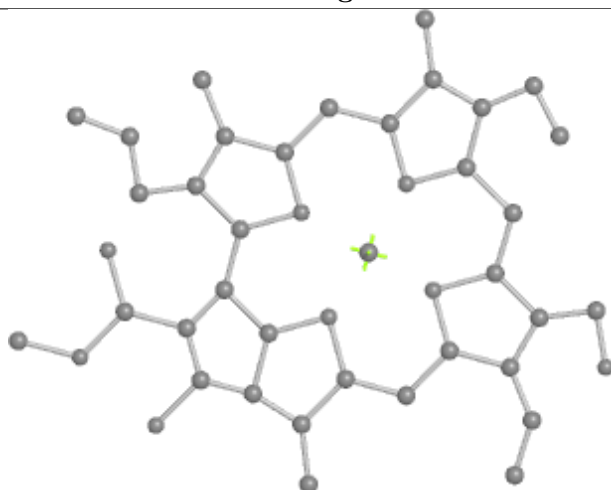
Bond lengths



Bond angles

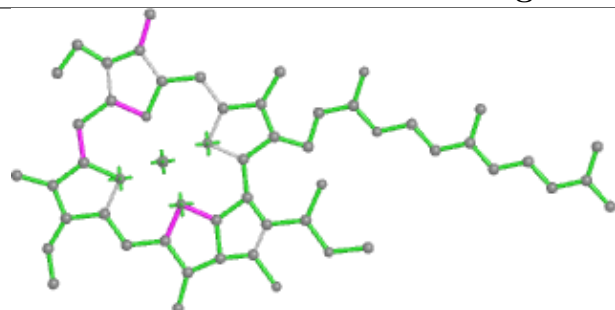


Torsions

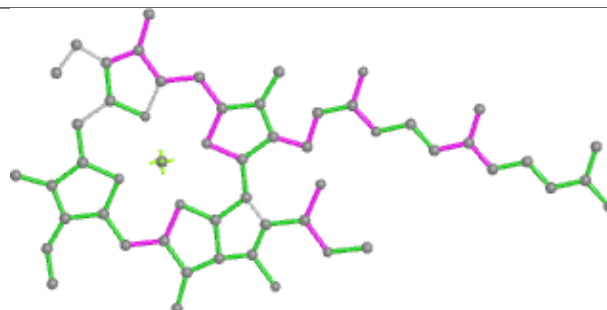


Rings

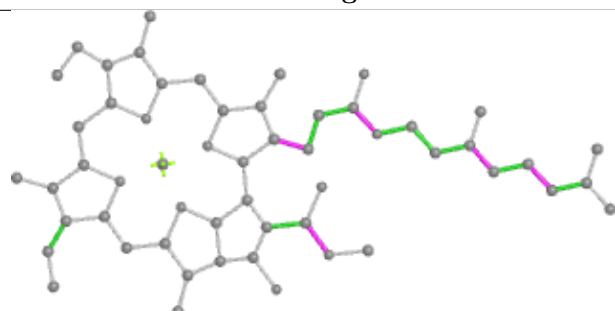
Ligand CLA R 316



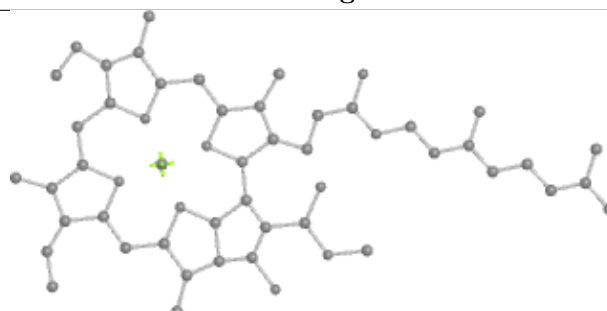
Bond lengths



Bond angles

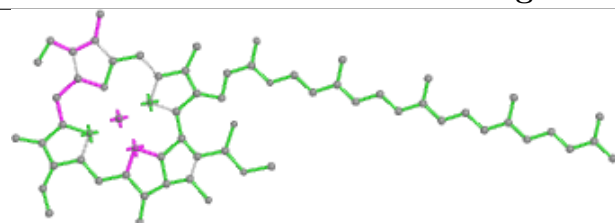


Torsions

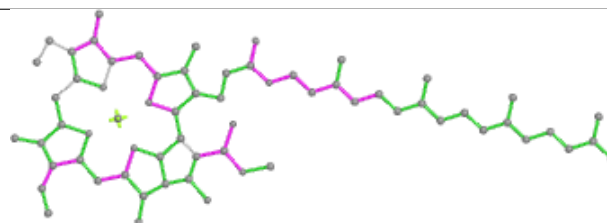


Rings

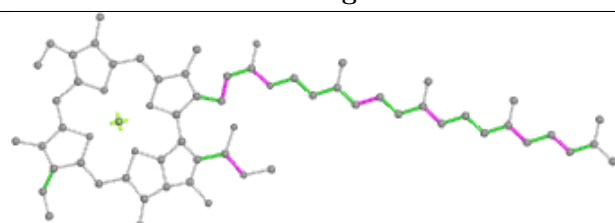
Ligand CLA A 823



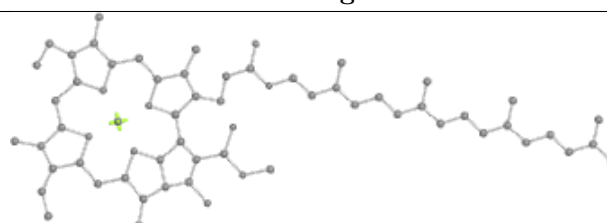
Bond lengths



Bond angles

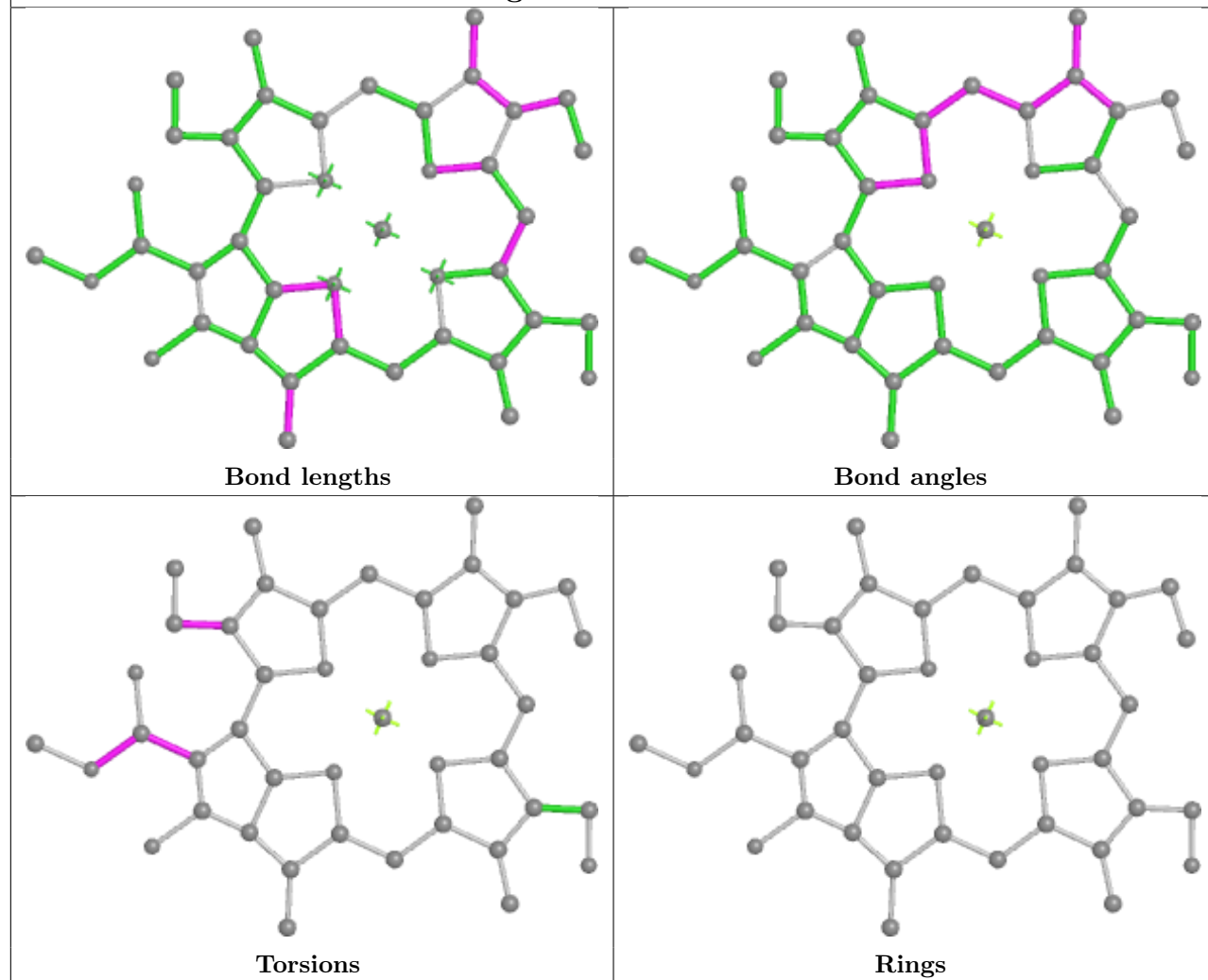


Torsions

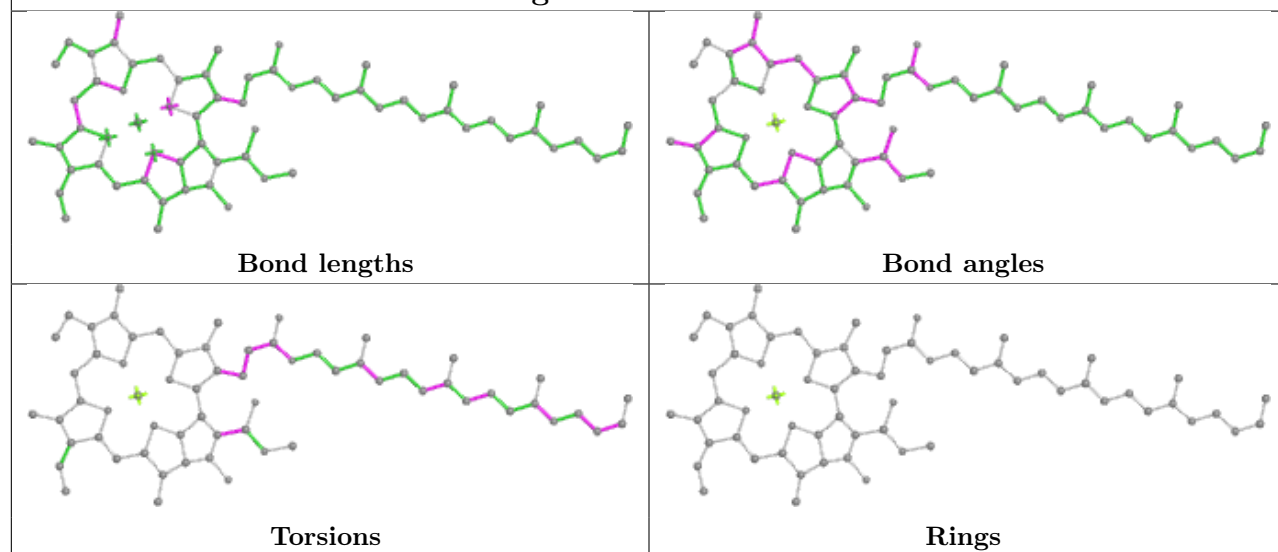


Rings

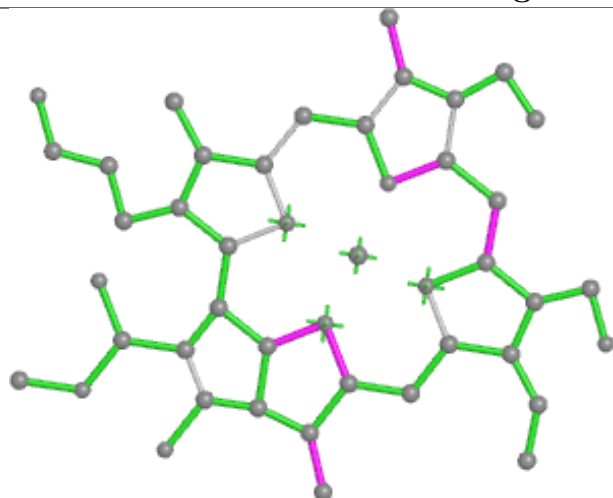
Ligand CHL 2 605



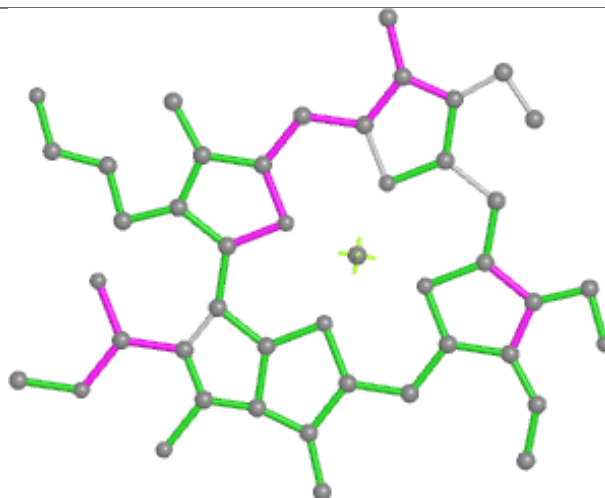
Ligand CLA R 313



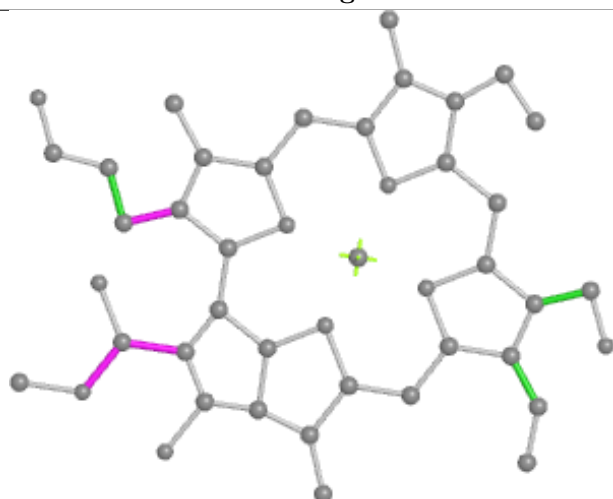
Ligand CHL R 318



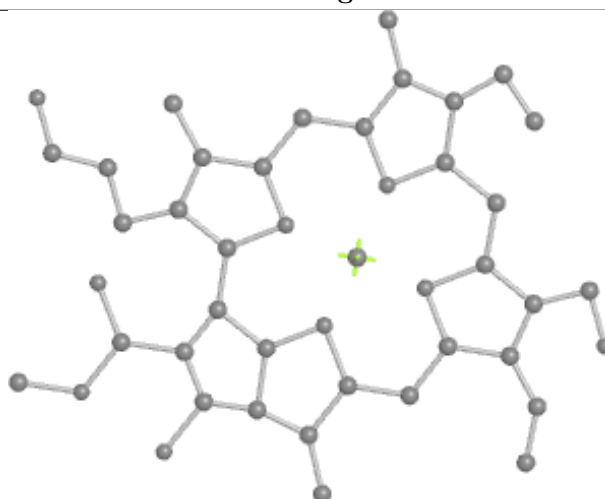
Bond lengths



Bond angles

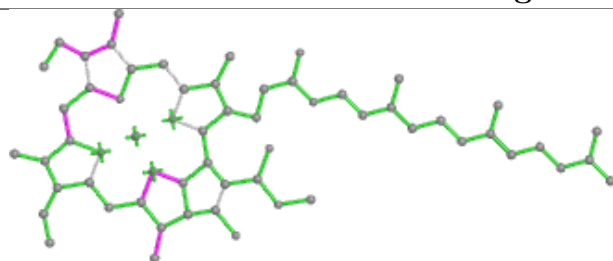


Torsions

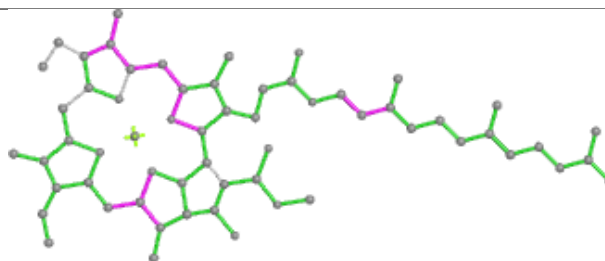


Rings

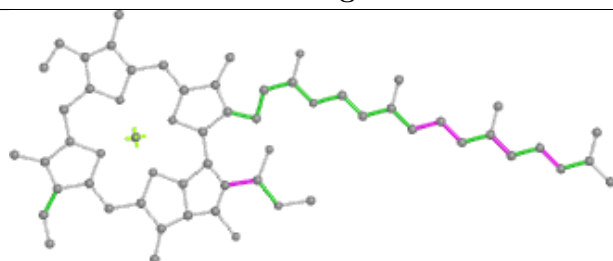
Ligand CLA B 836



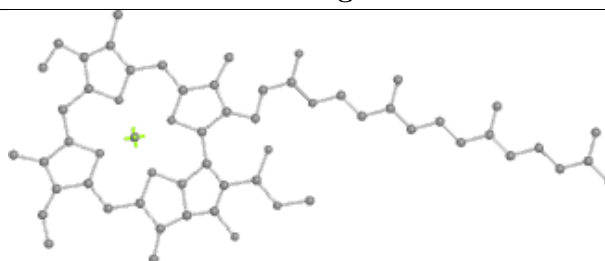
Bond lengths



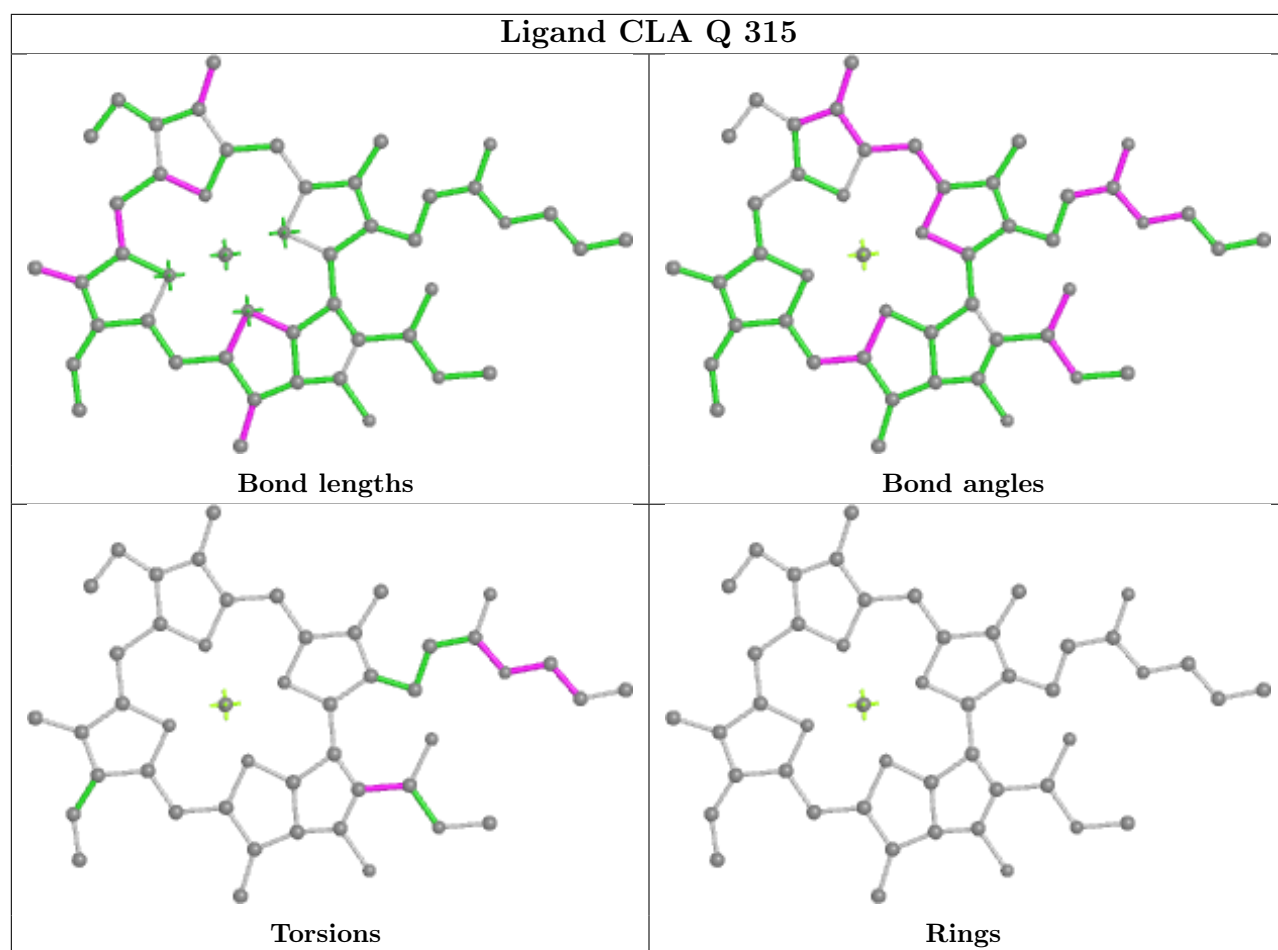
Bond angles



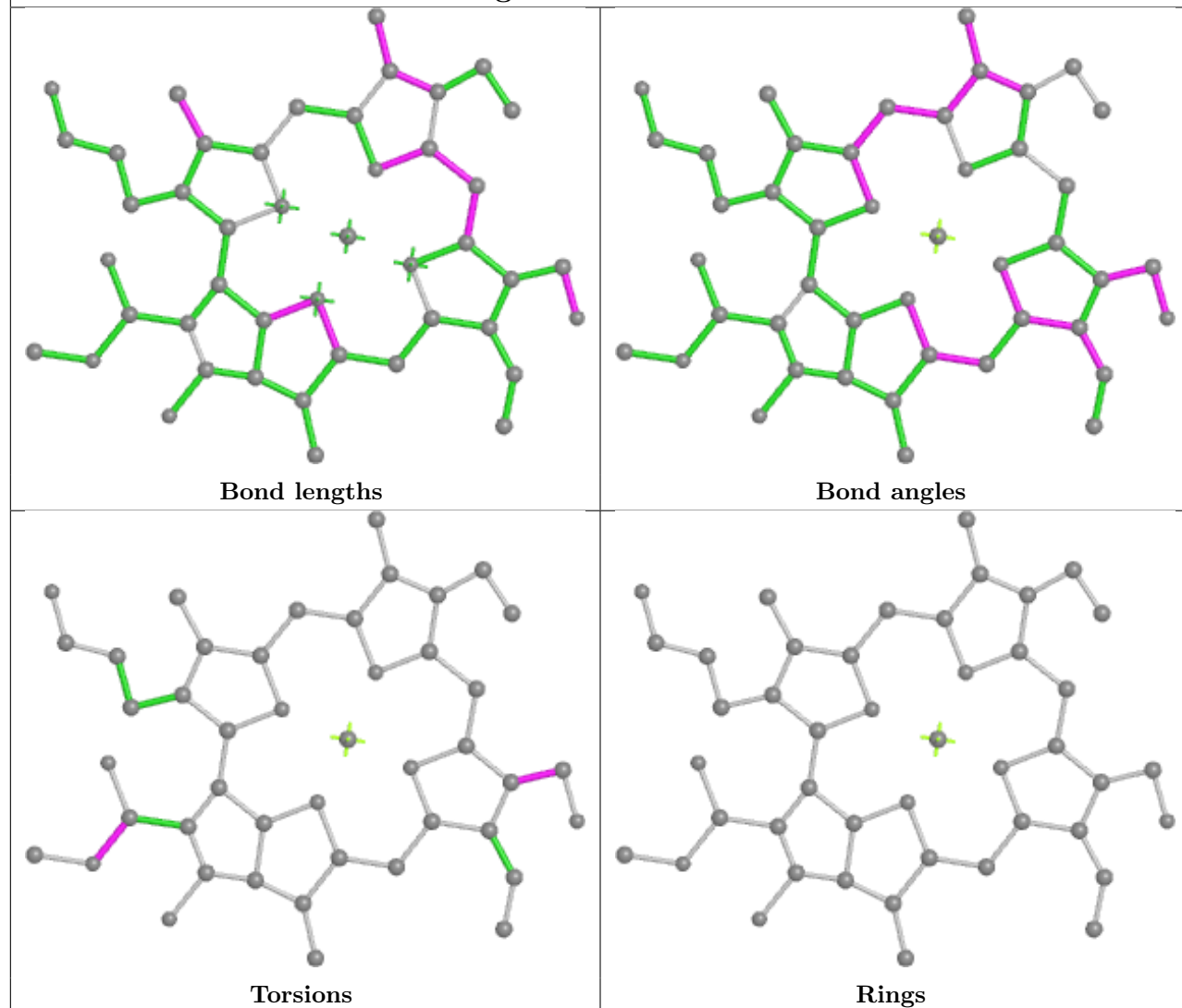
Torsions



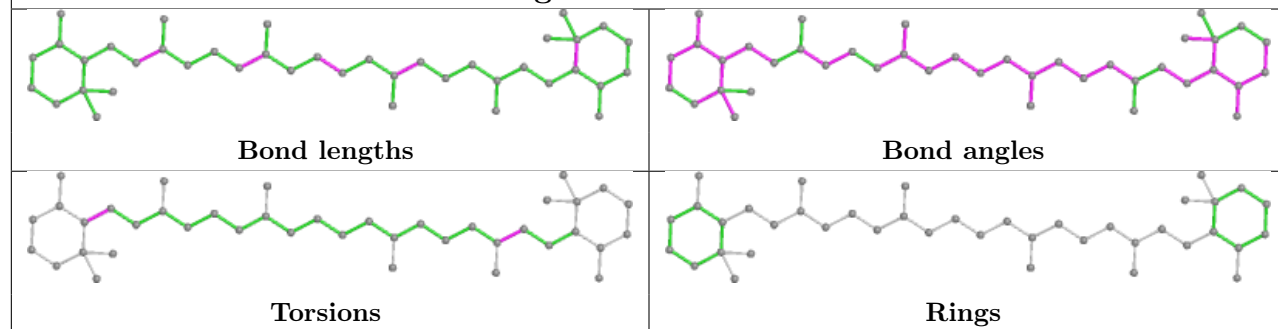
Rings



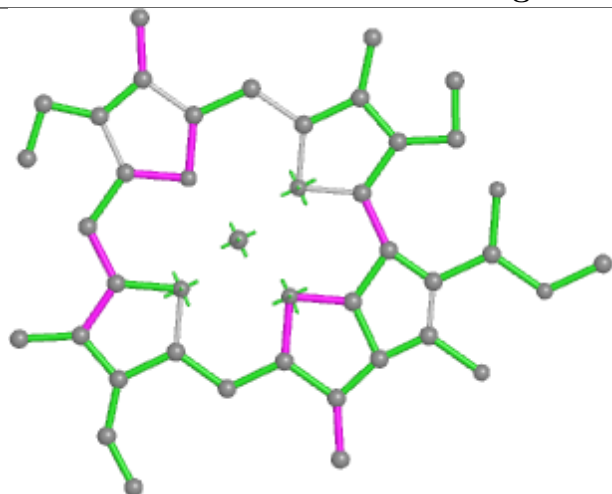
Ligand CHL 2 607



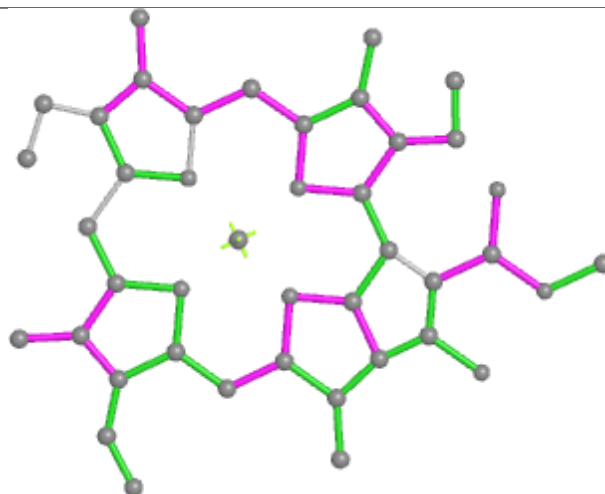
Ligand BCR 4 319



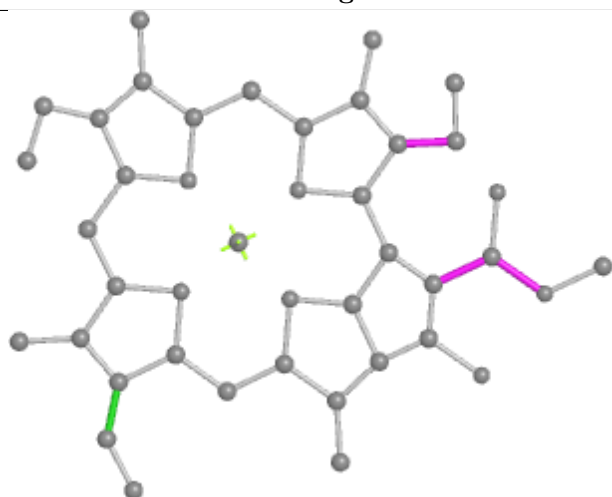
Ligand CLA V 309



Bond lengths



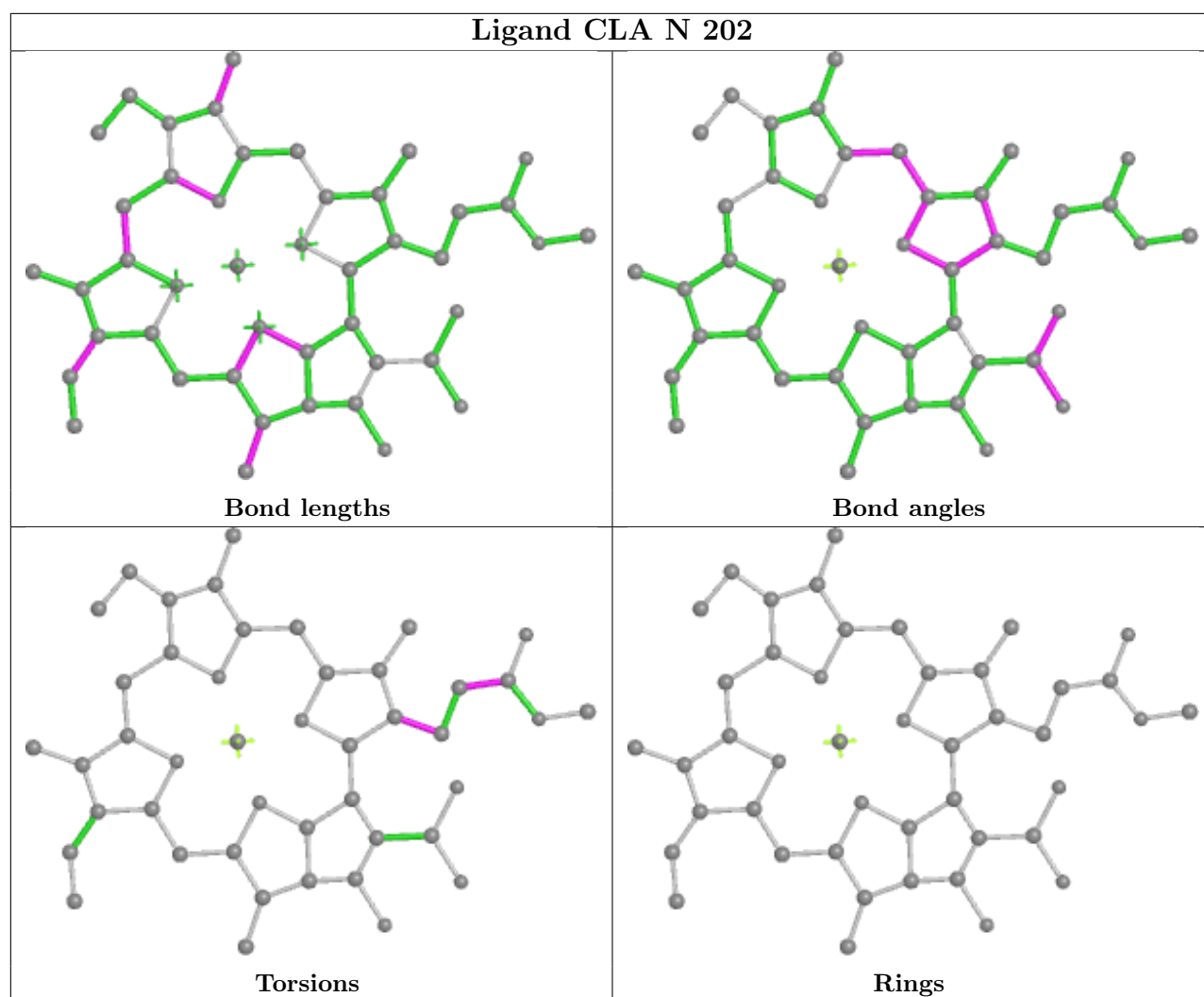
Bond angles



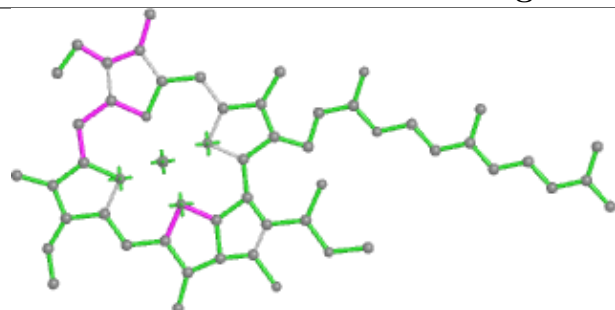
Torsions



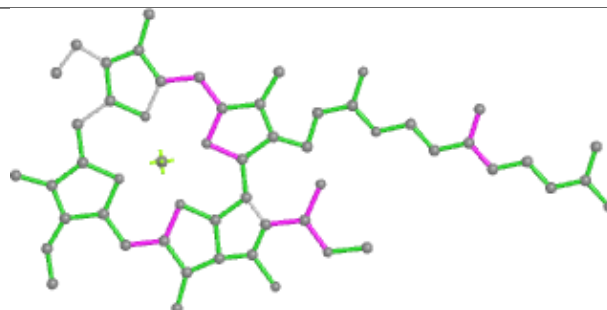
Rings



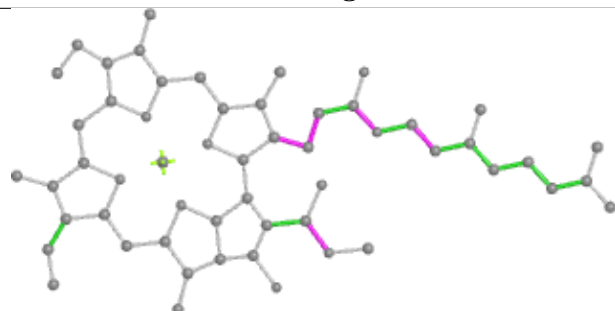
Ligand CLA A 826



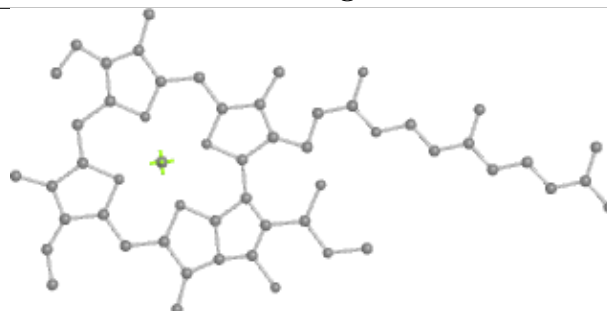
Bond lengths



Bond angles

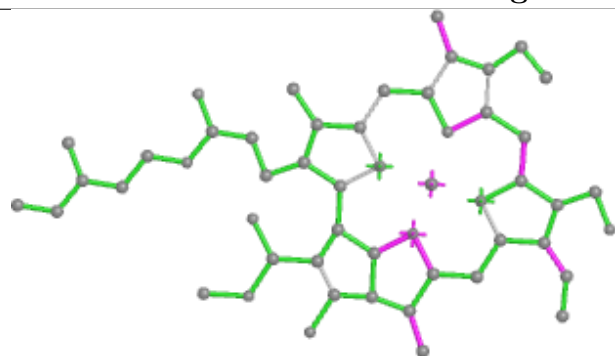


Torsions

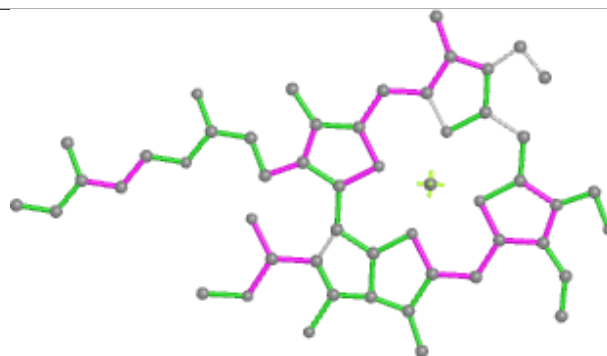


Rings

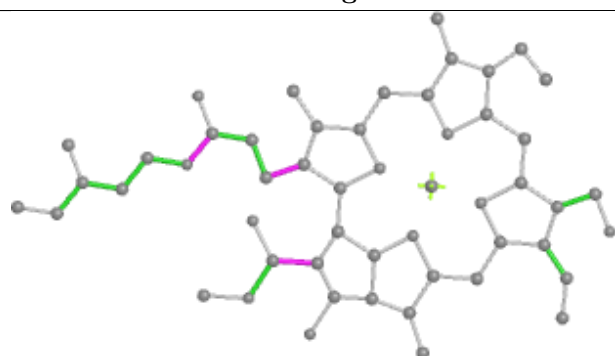
Ligand CHL W 306



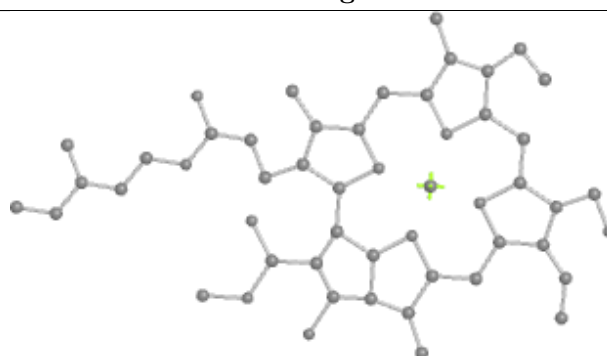
Bond lengths



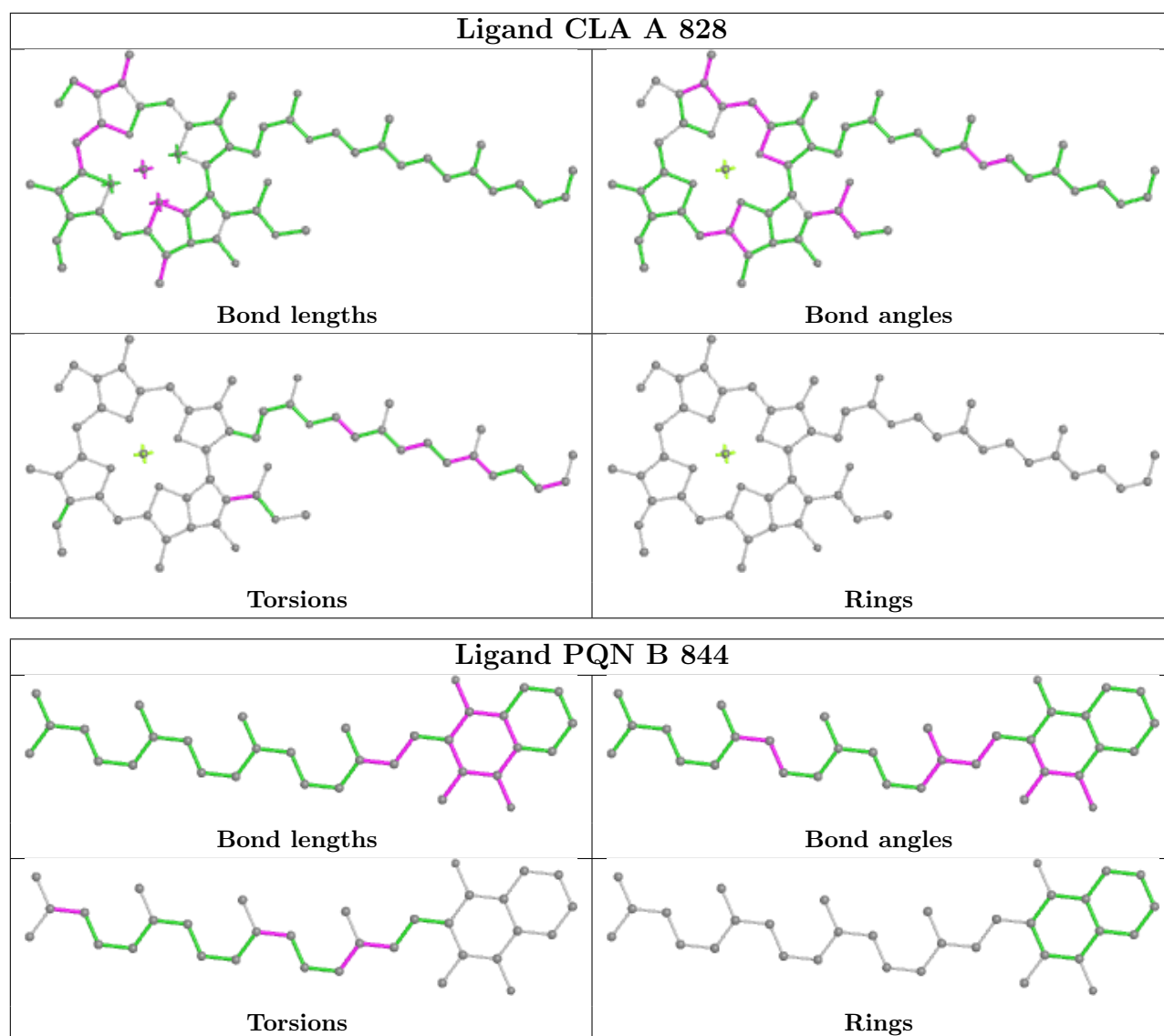
Bond angles

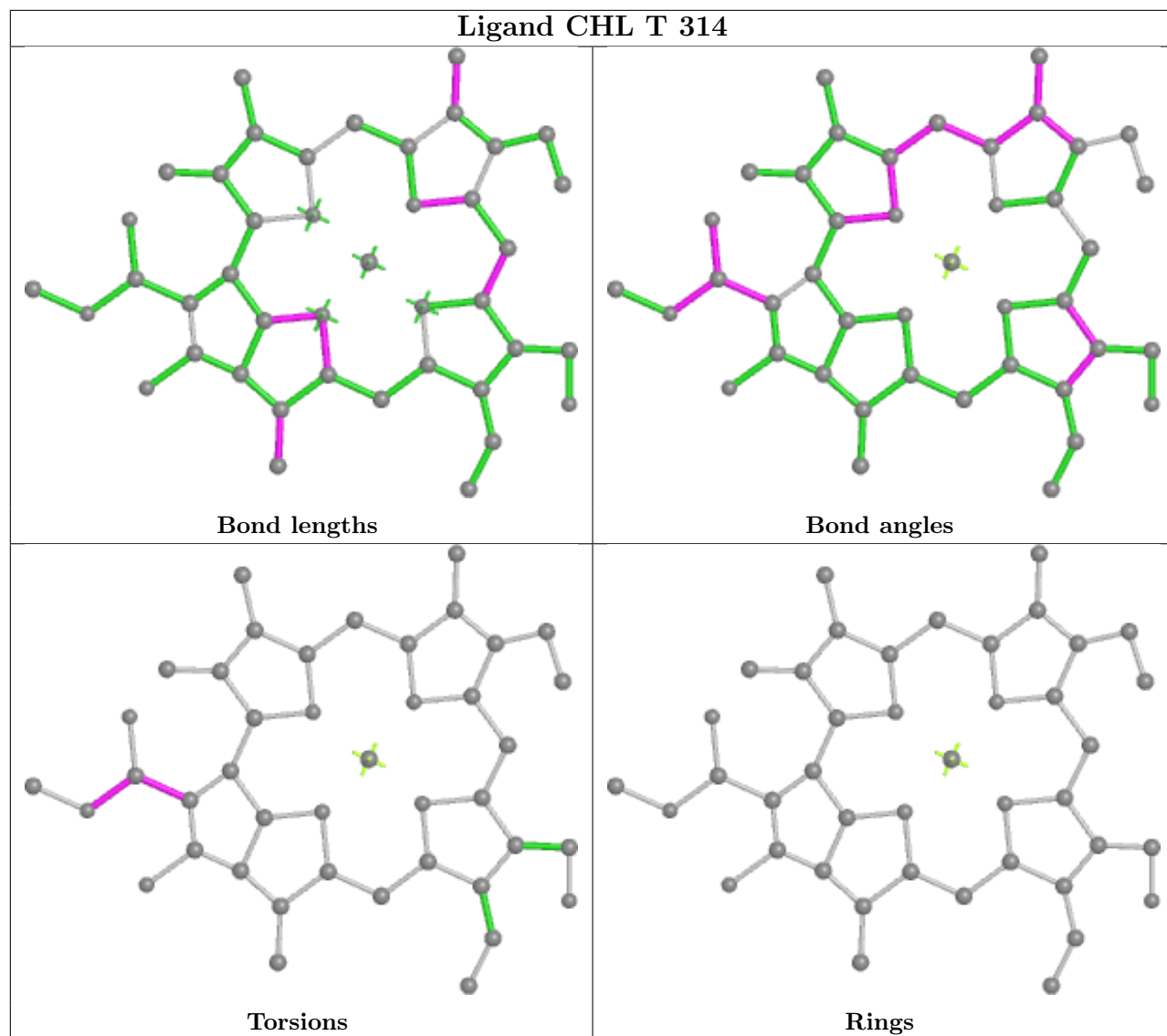


Torsions

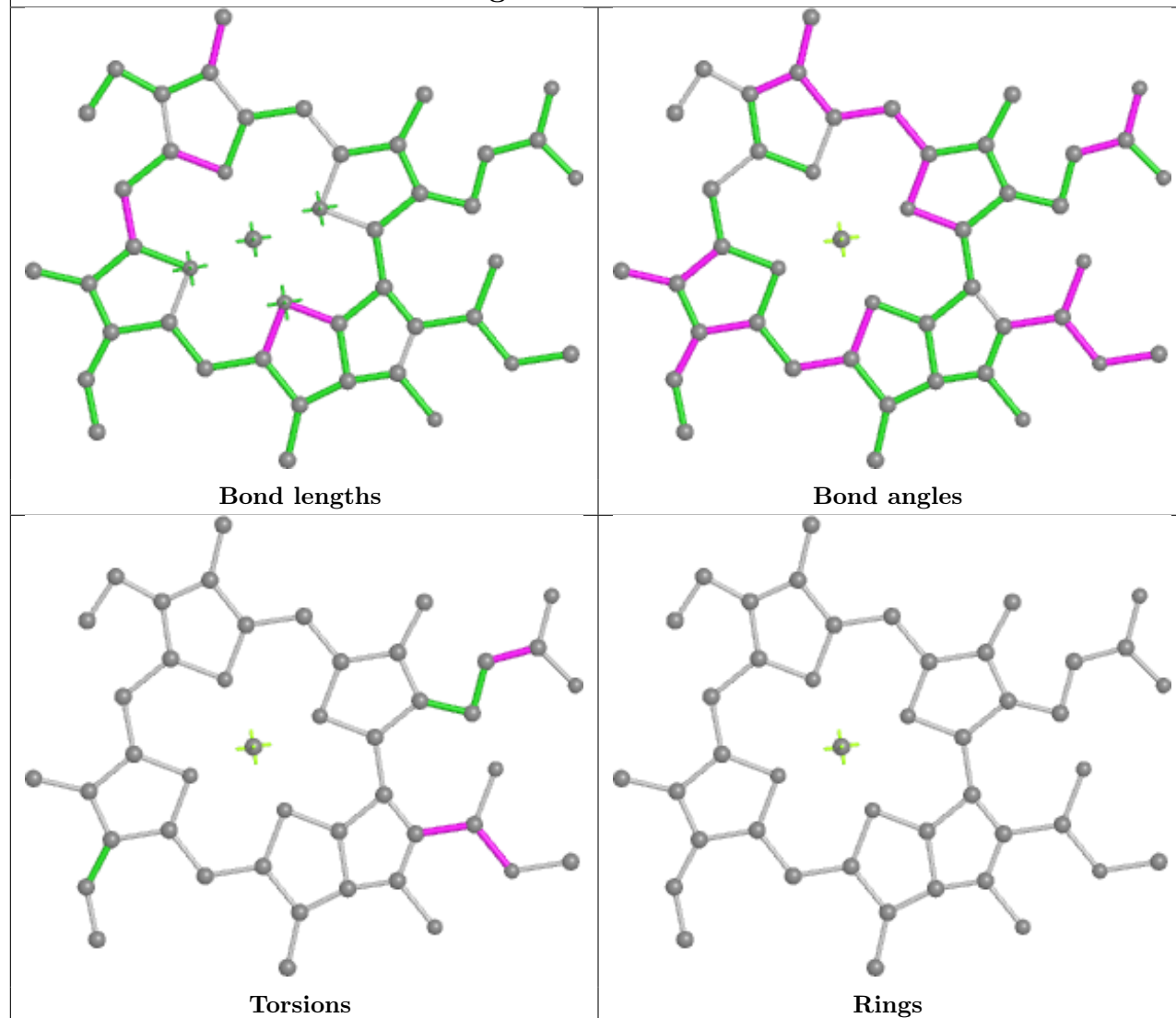


Rings

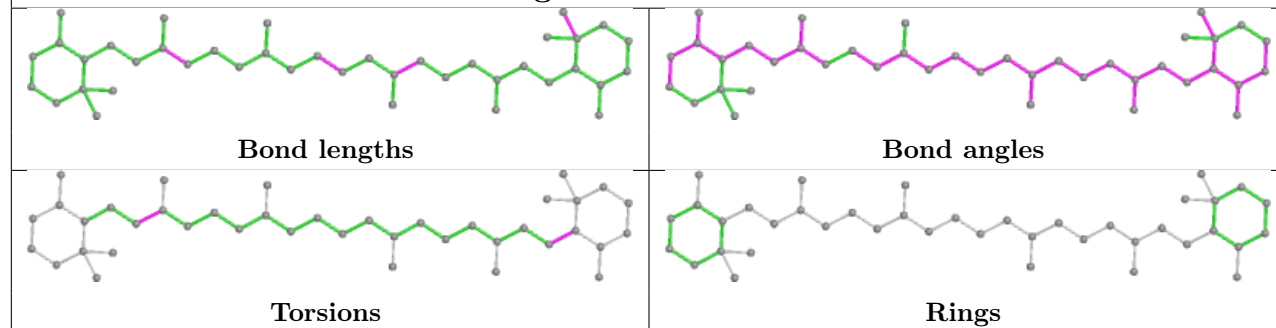


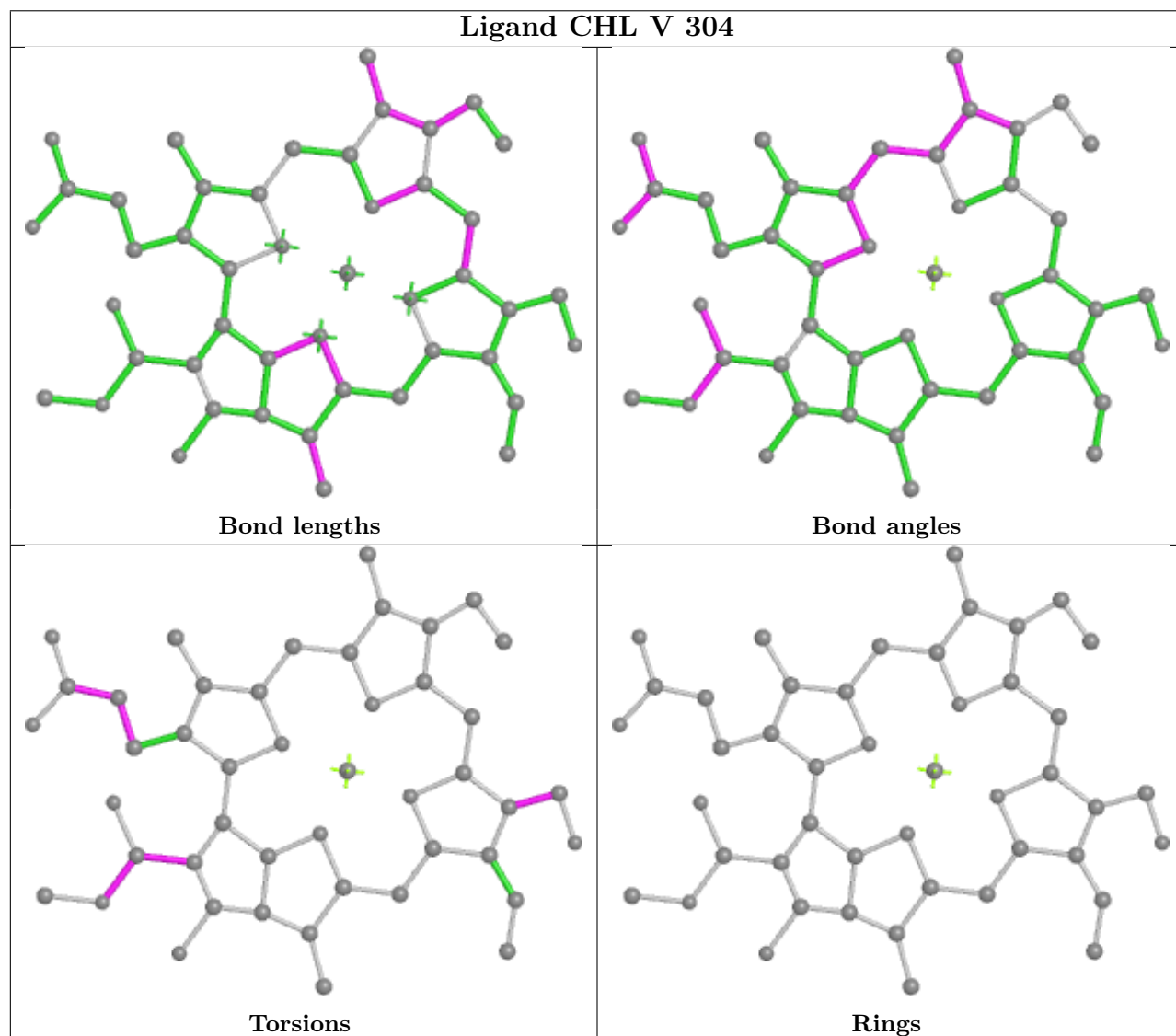
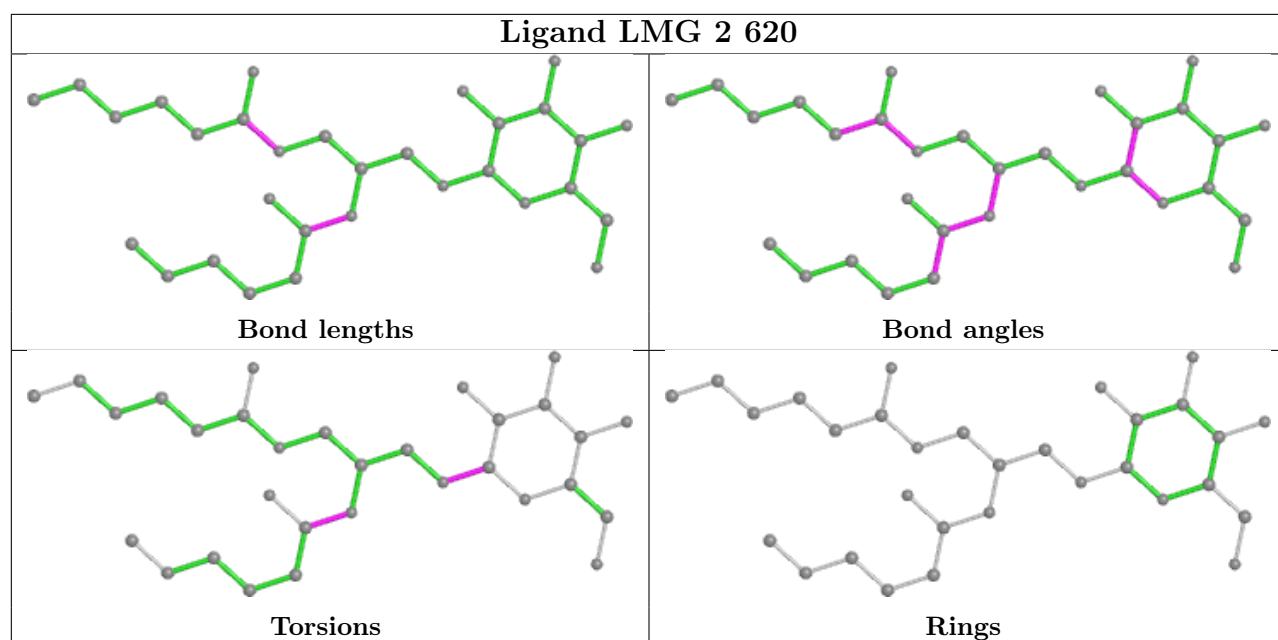


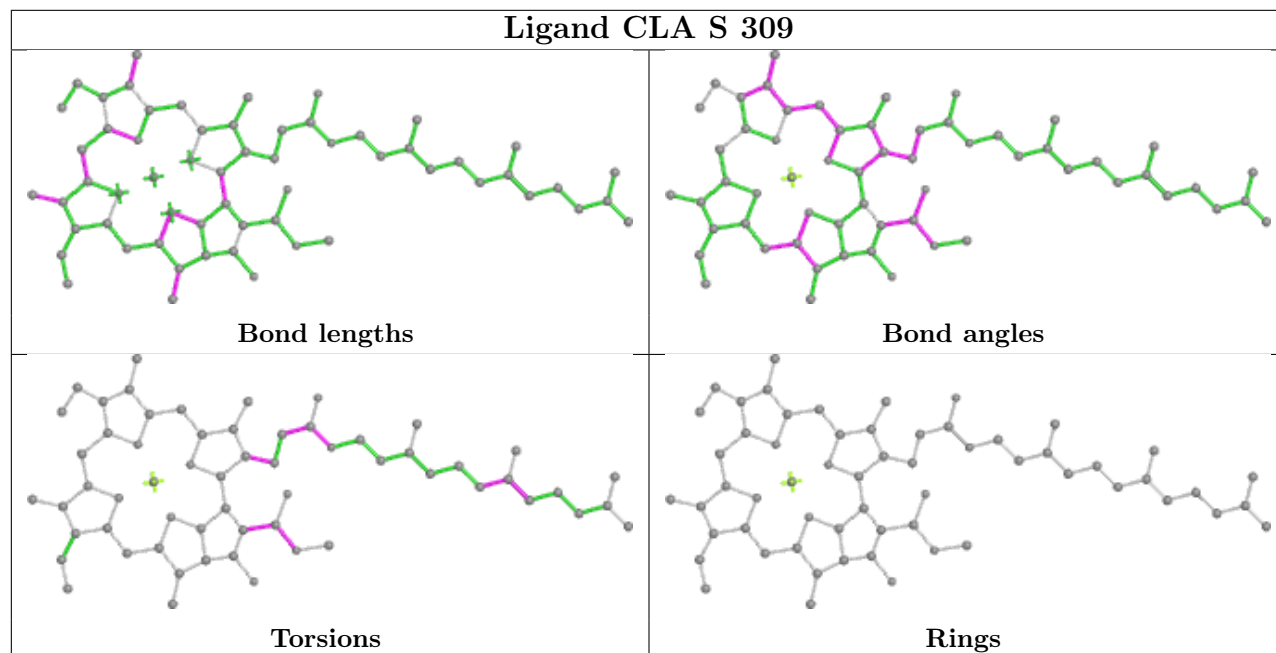
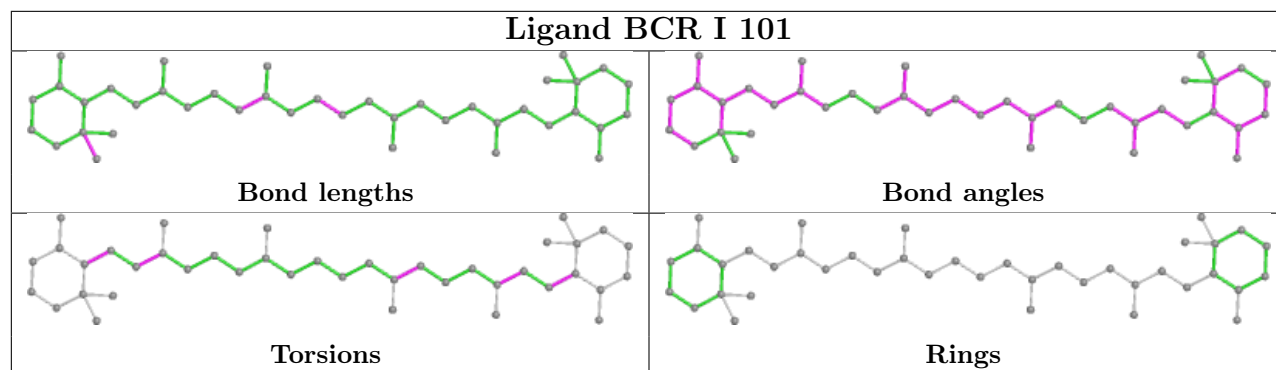
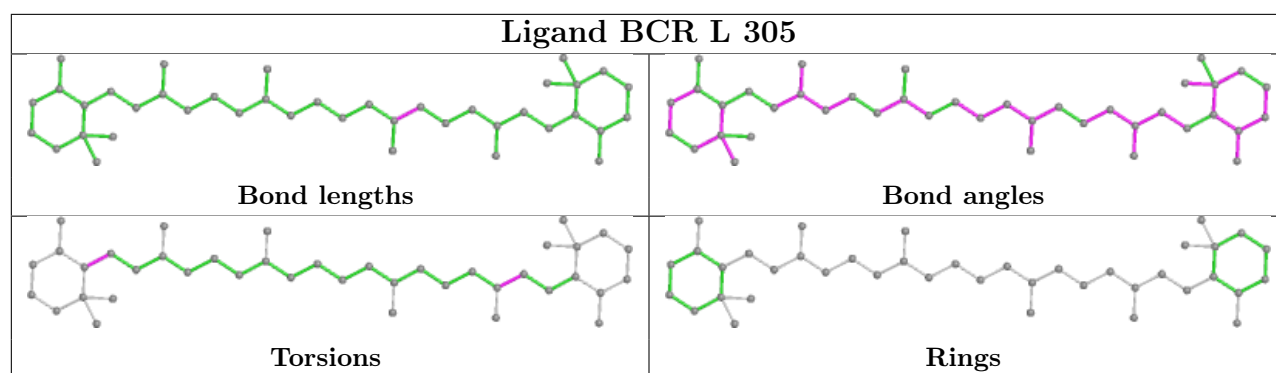
Ligand CLA K 201



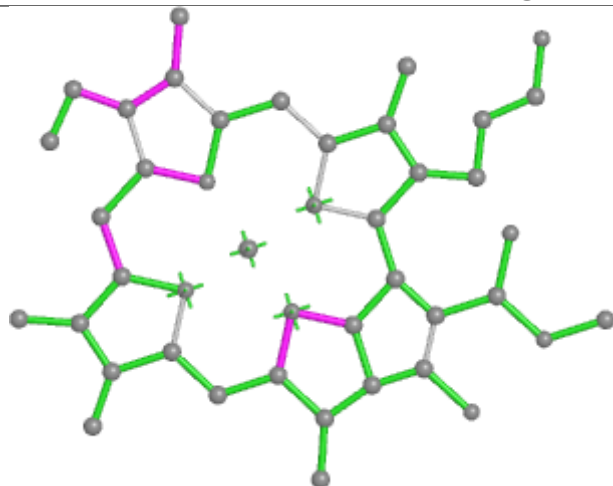
Ligand BCR J 101



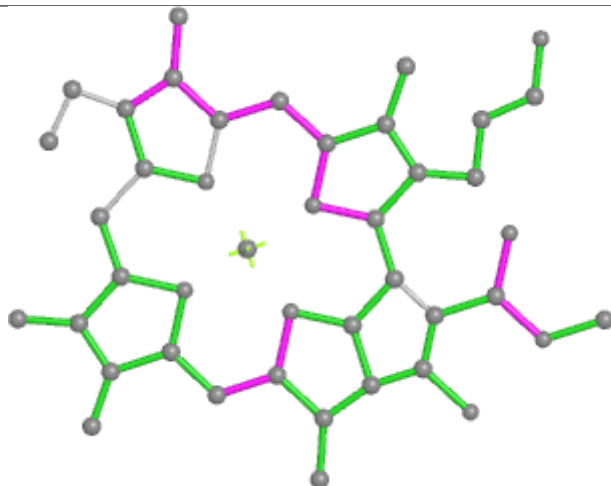




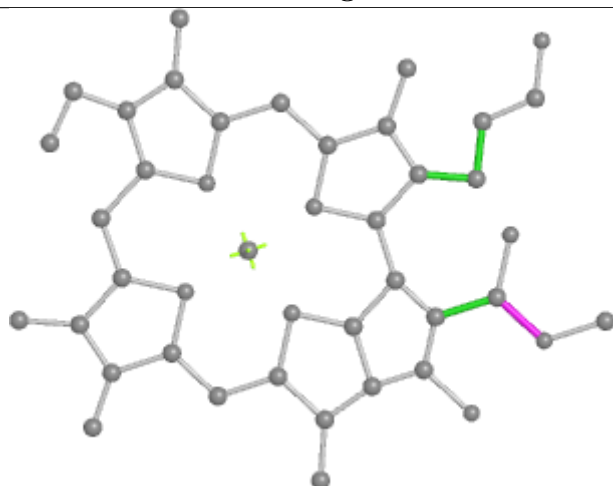
Ligand CLA 6 604



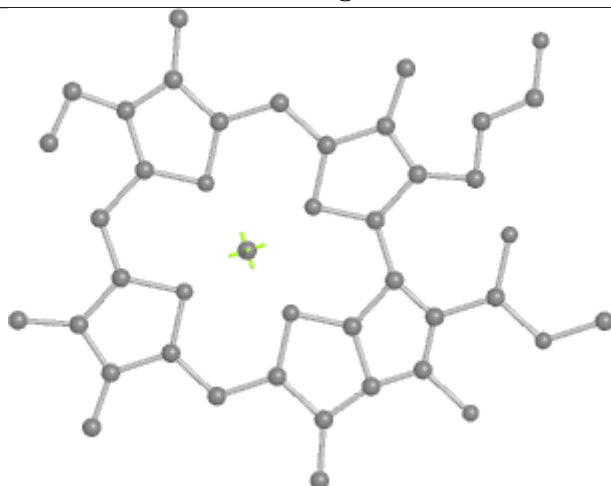
Bond lengths



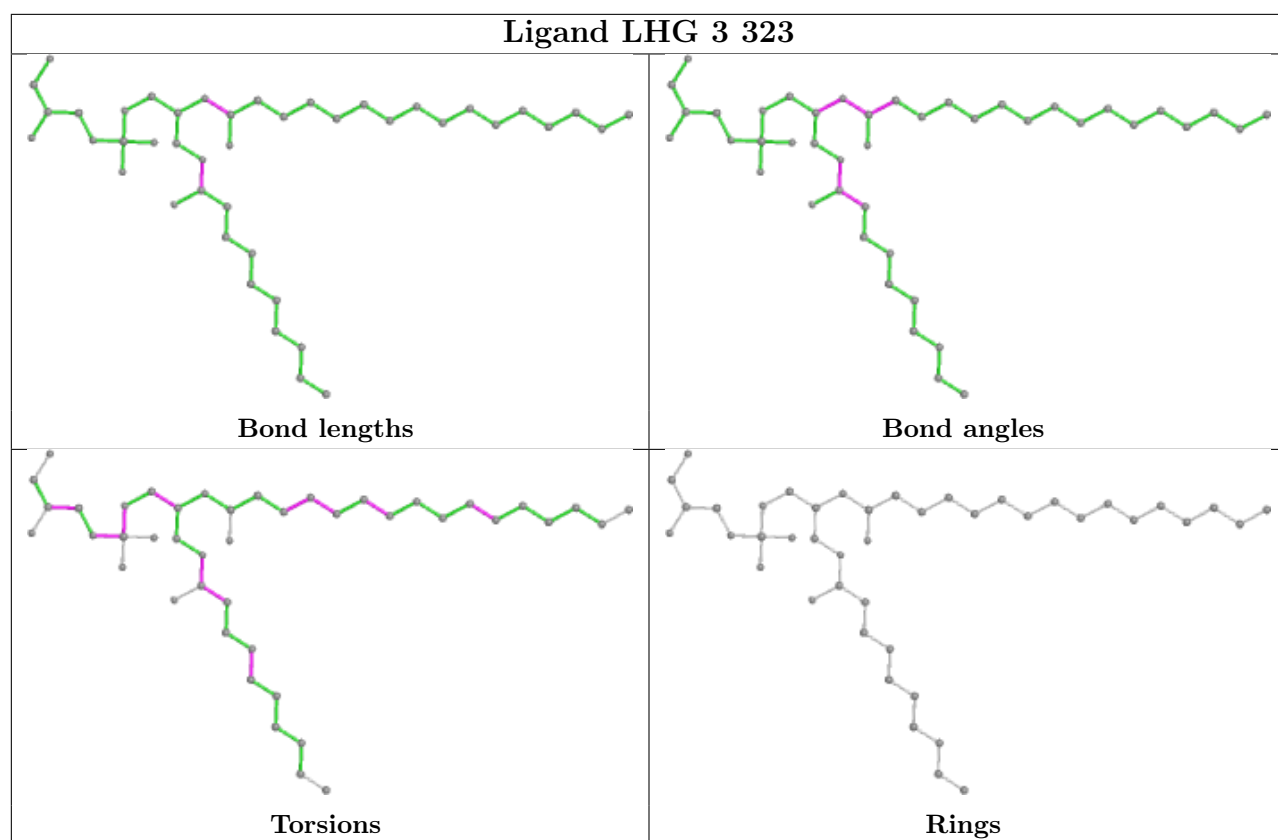
Bond angles

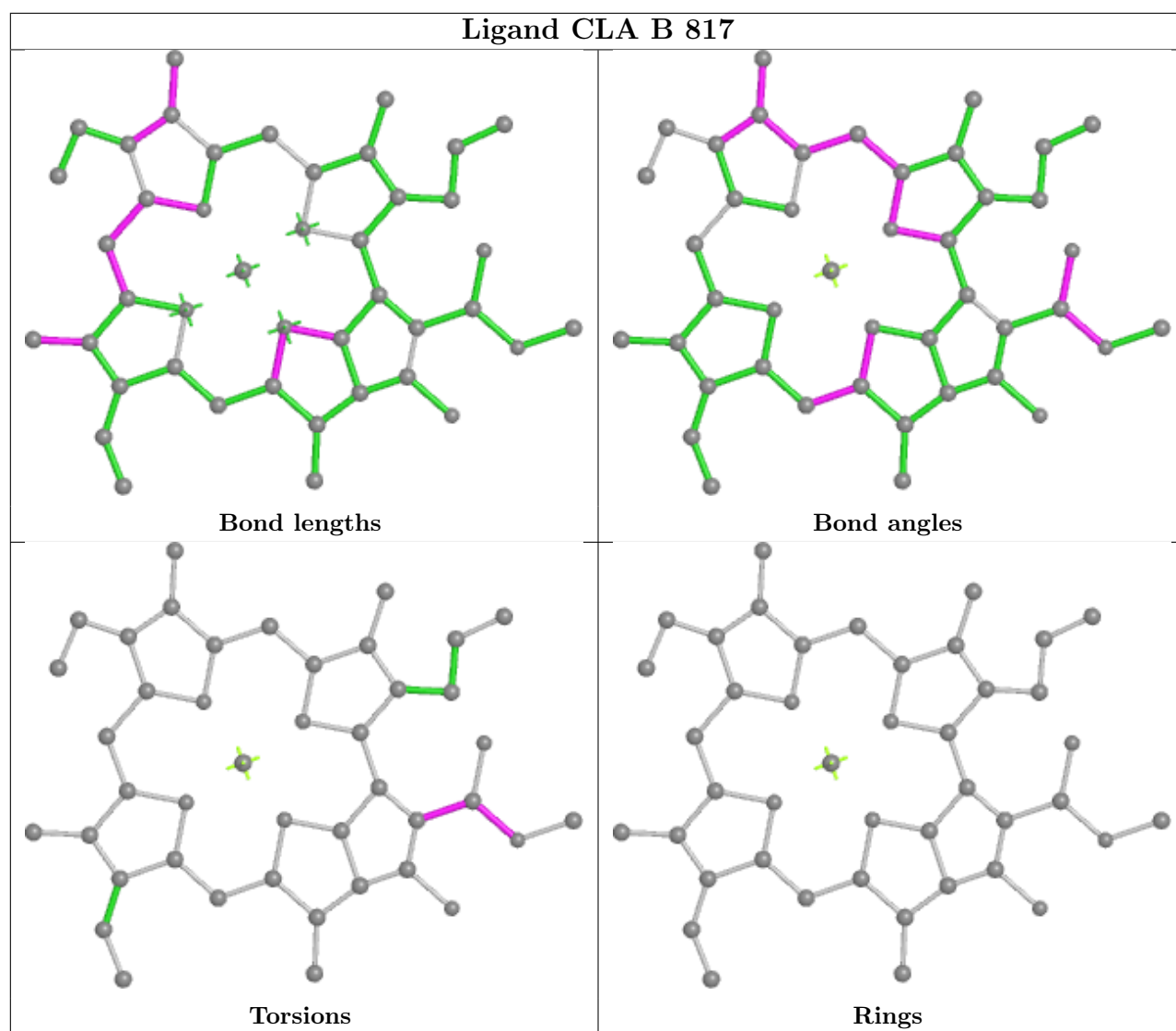


Torsions

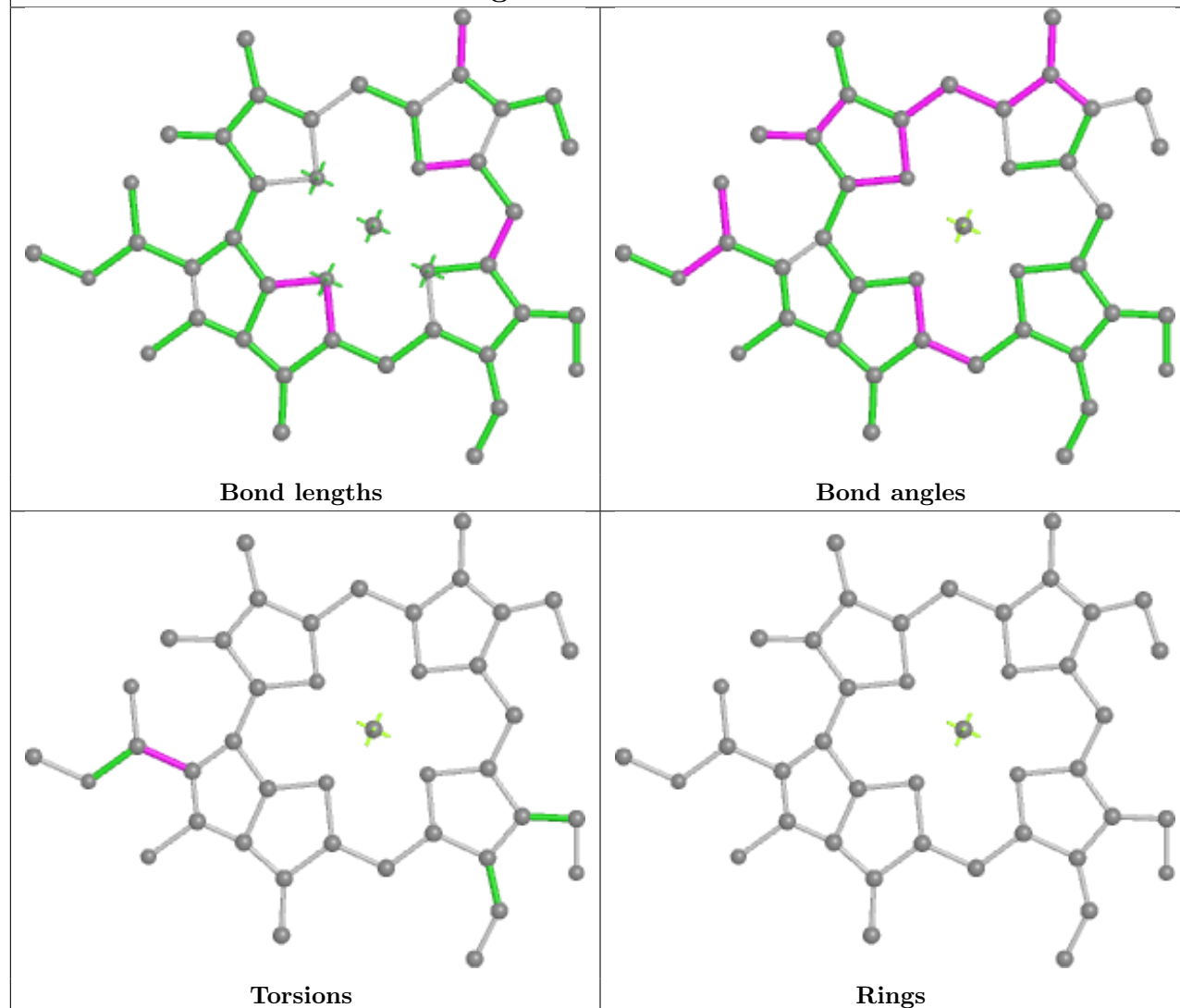


Rings

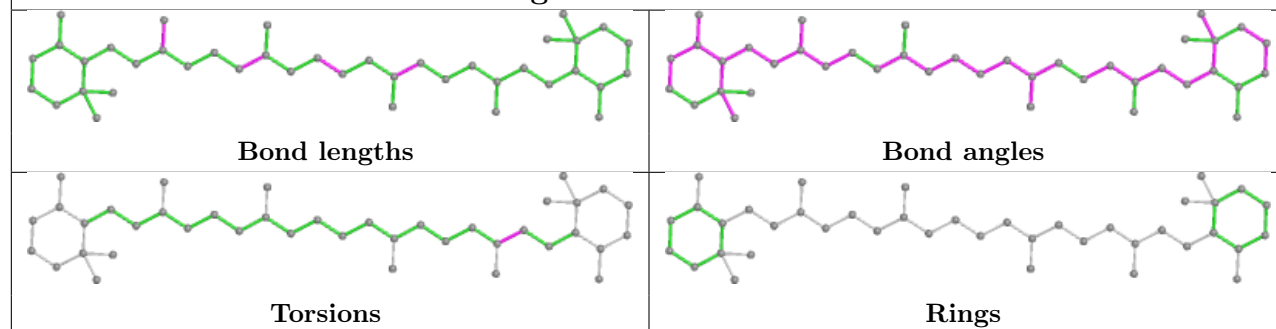


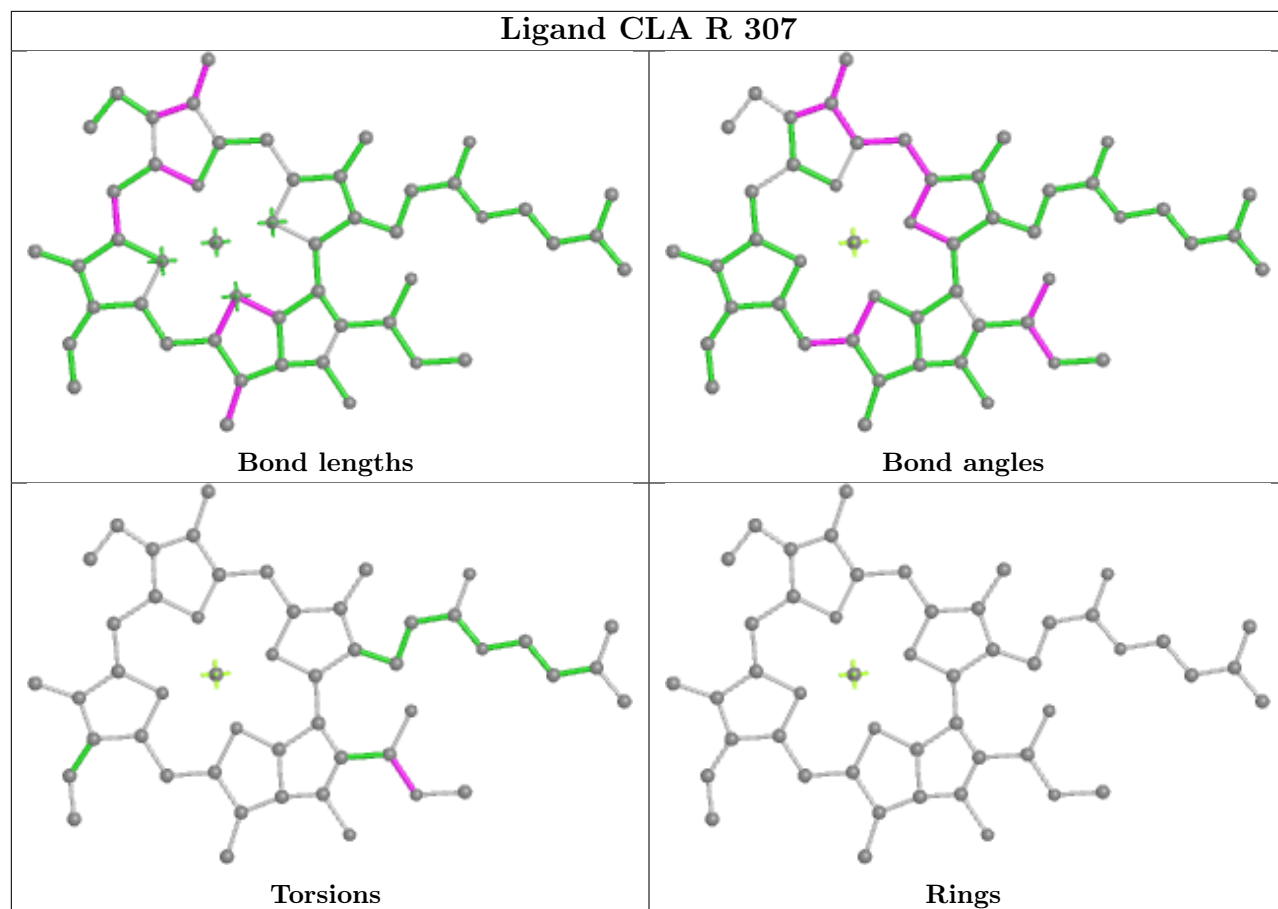


Ligand CHL X 305

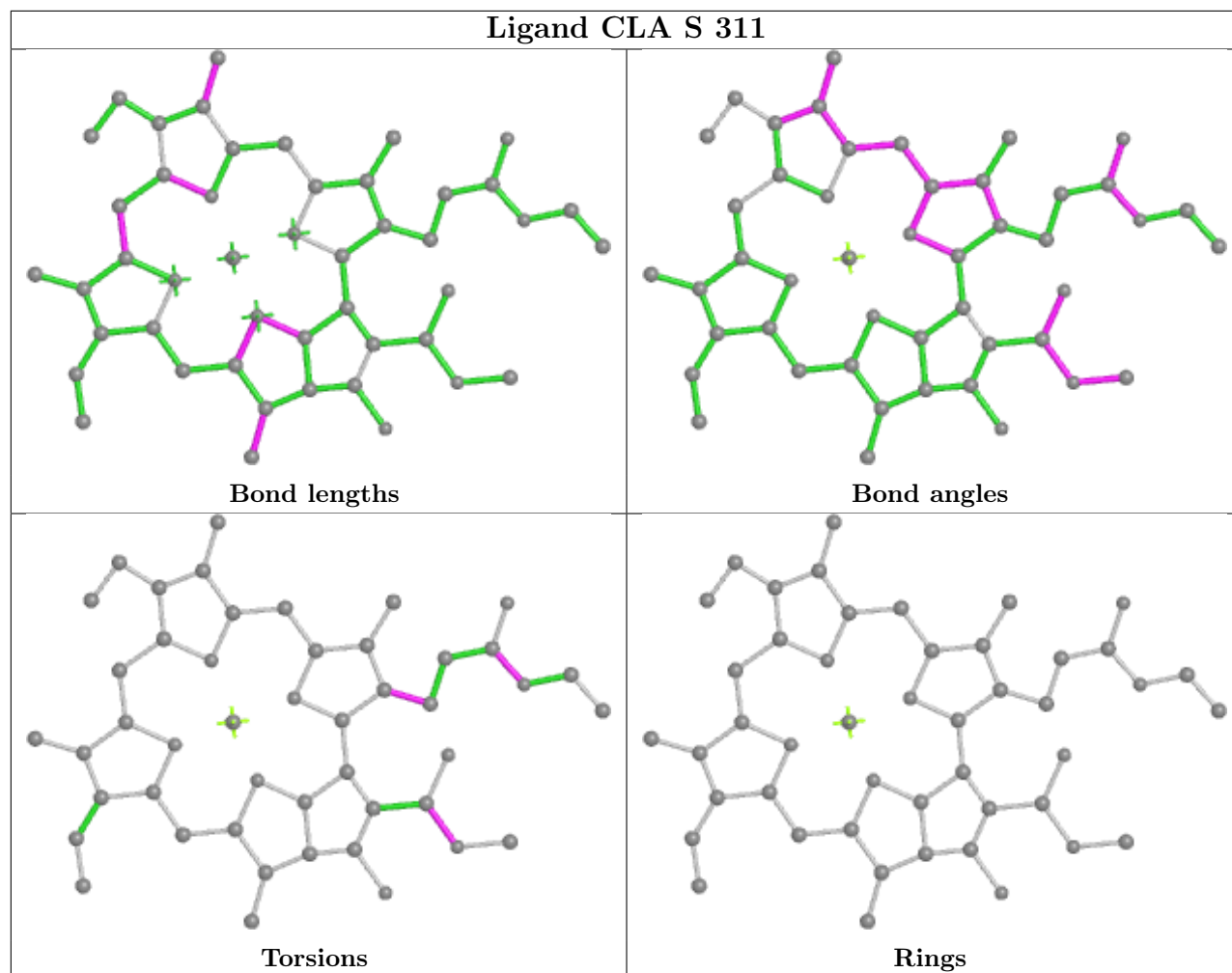


Ligand BCR B 848

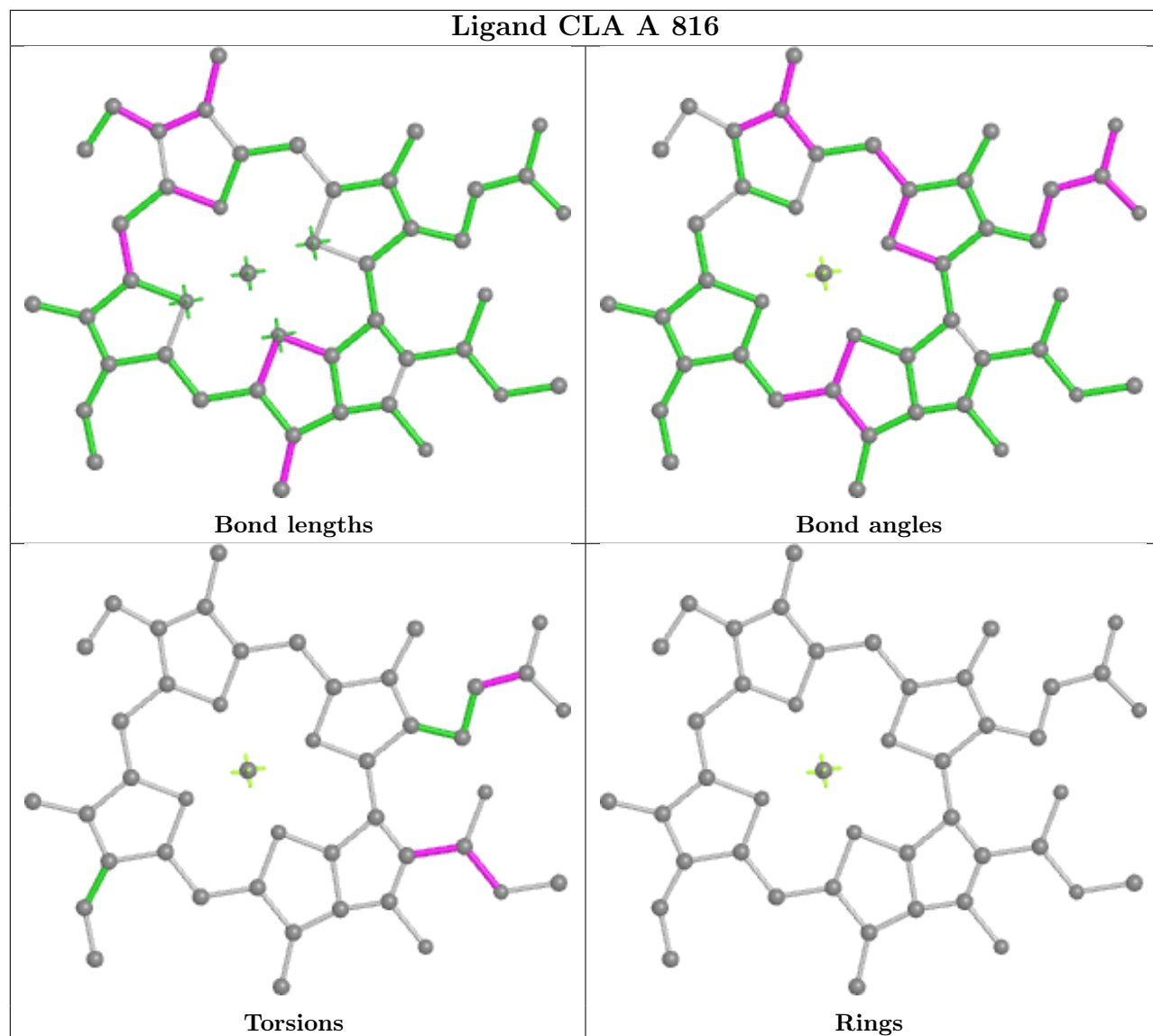




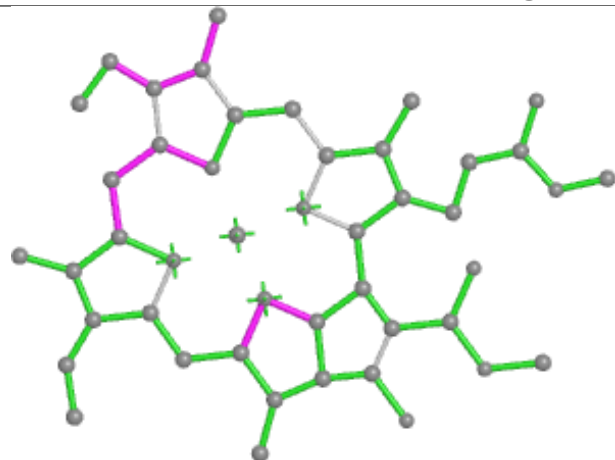
Ligand CLA S 311



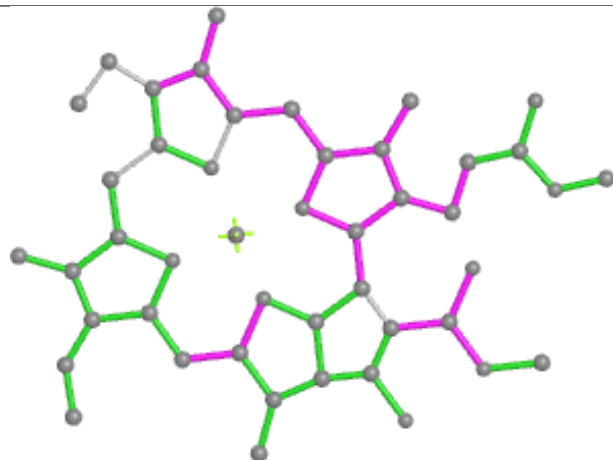
Ligand CLA A 816



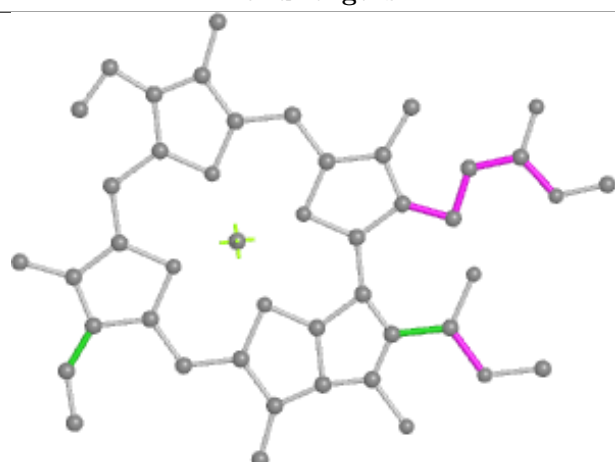
Ligand CLA 5 601



Bond lengths



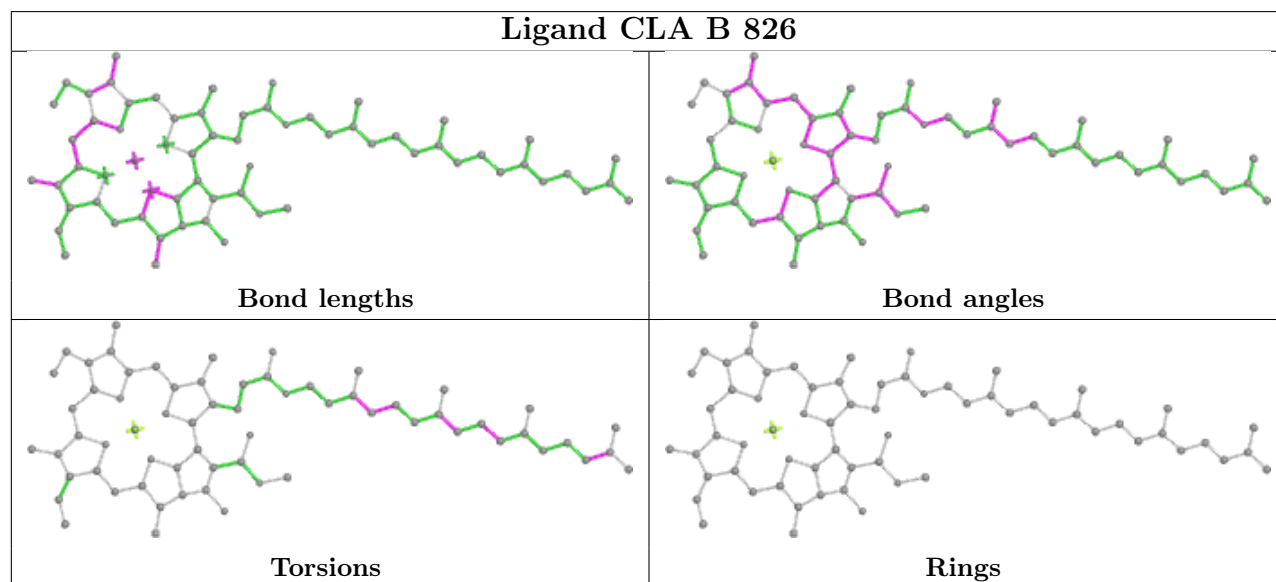
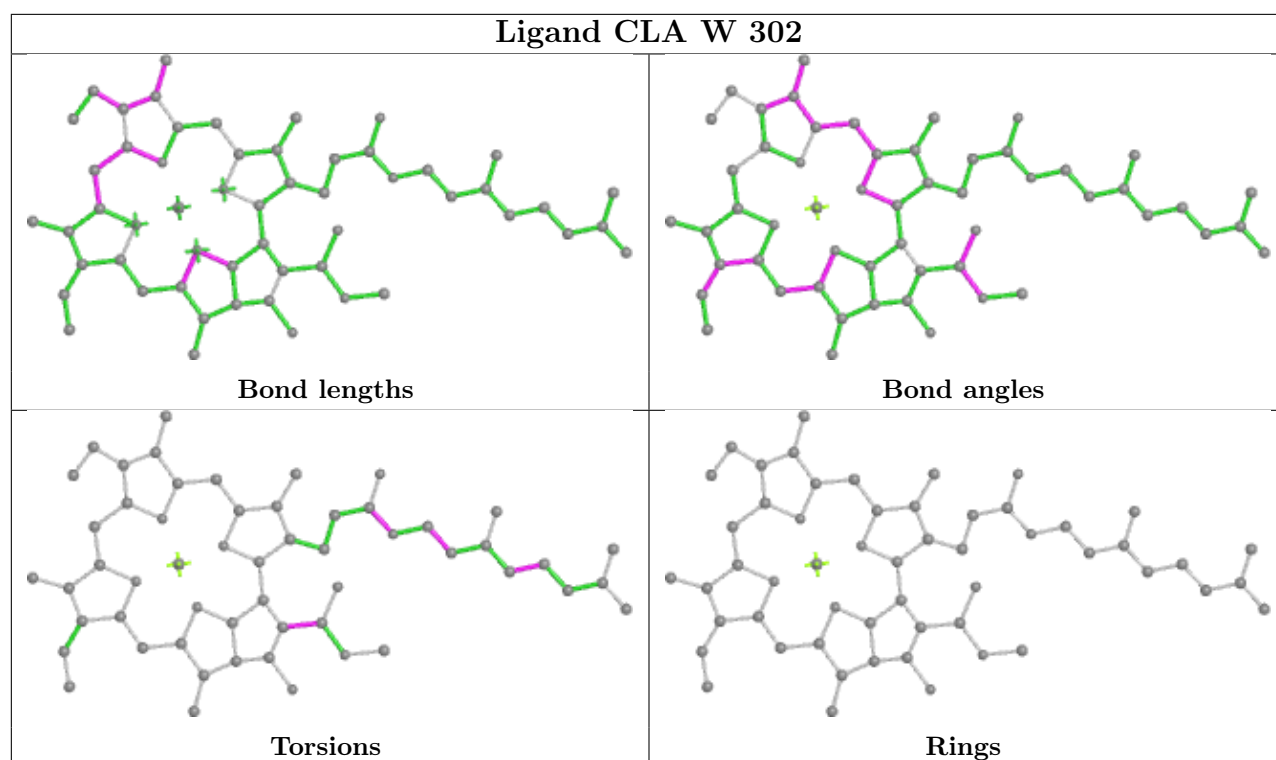
Bond angles



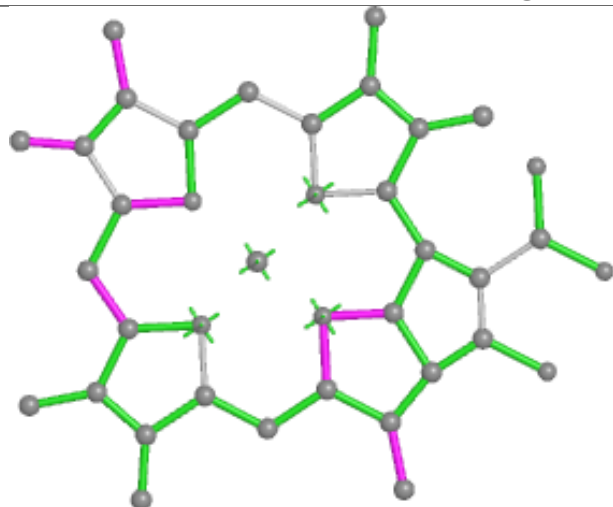
Torsions



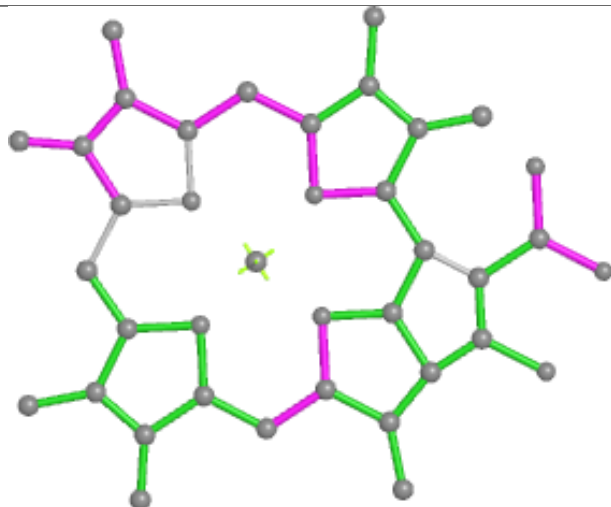
Rings



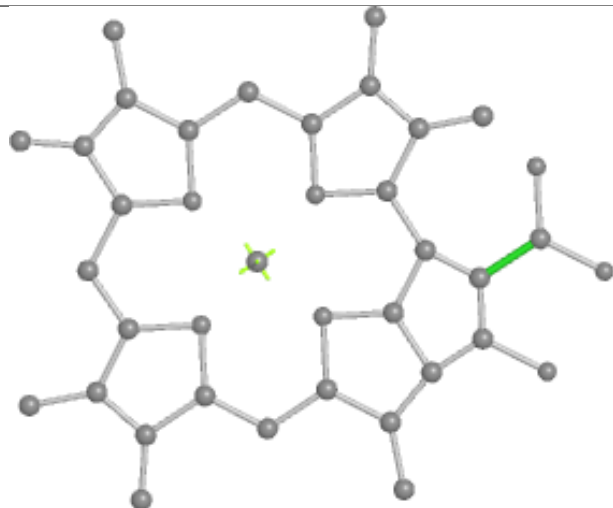
Ligand CLA 5 604



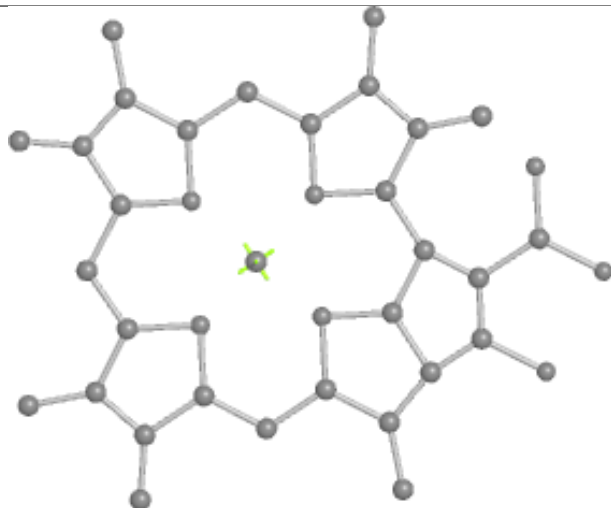
Bond lengths



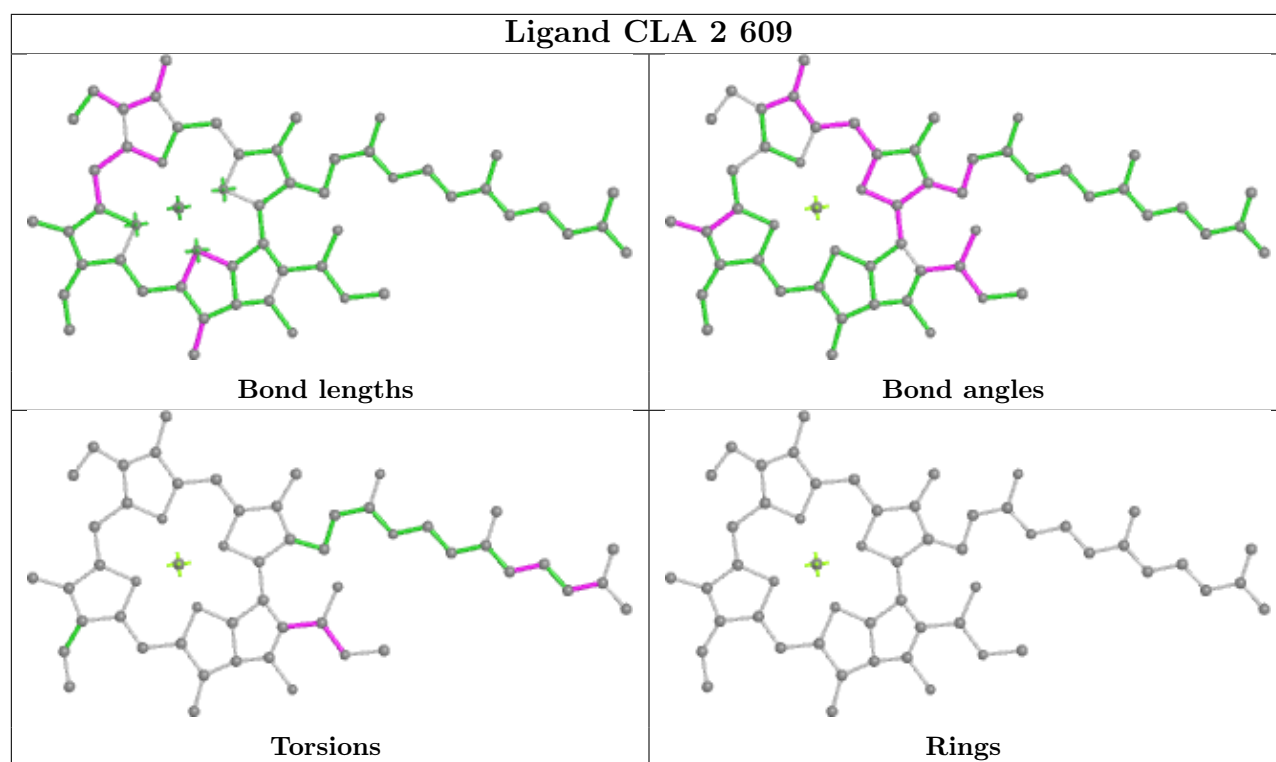
Bond angles



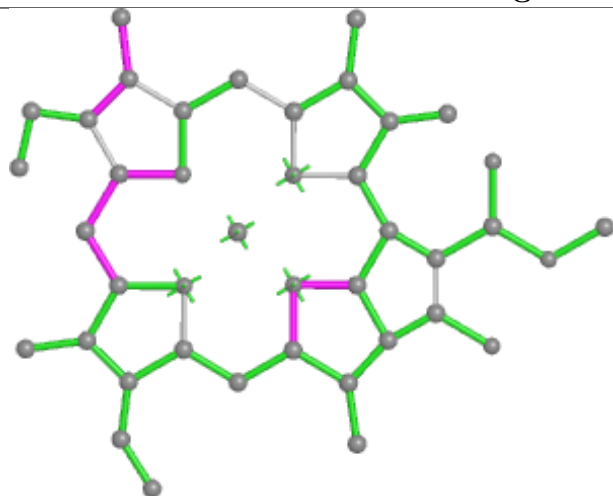
Torsions



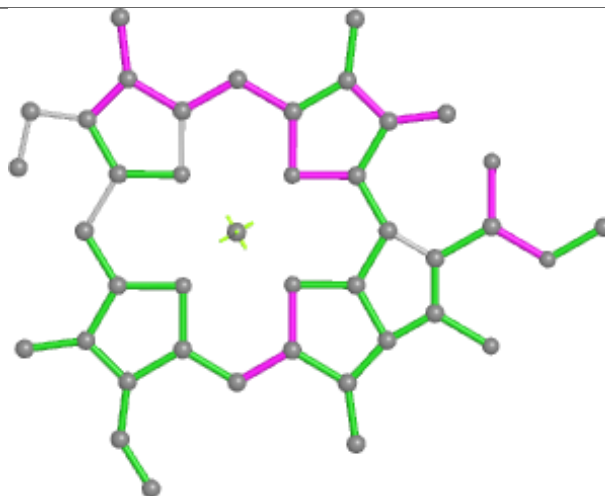
Rings



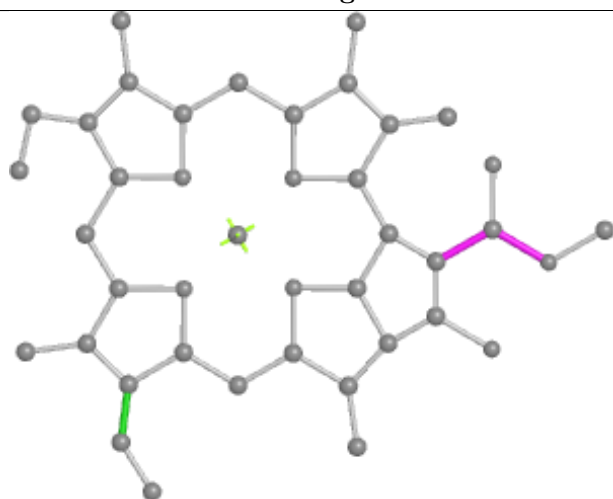
Ligand CLA X 314



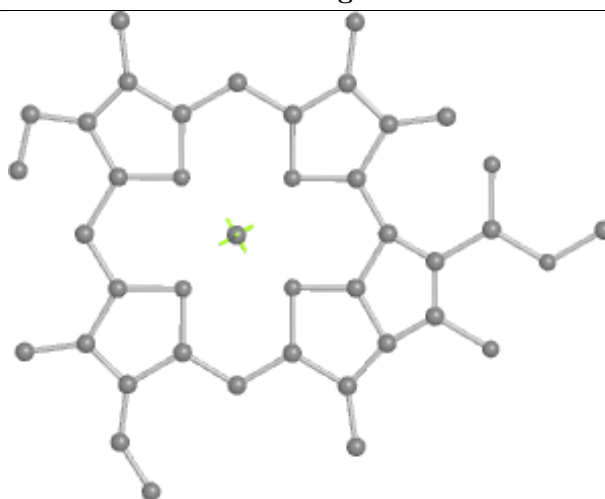
Bond lengths



Bond angles

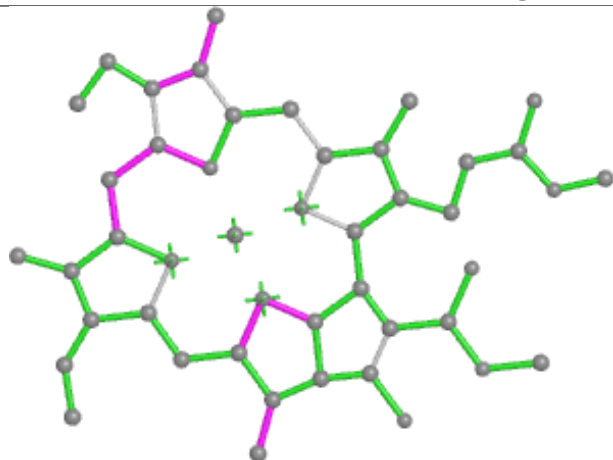


Torsions

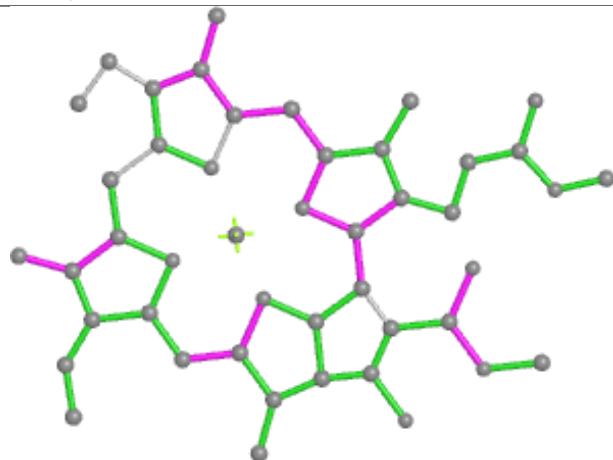


Rings

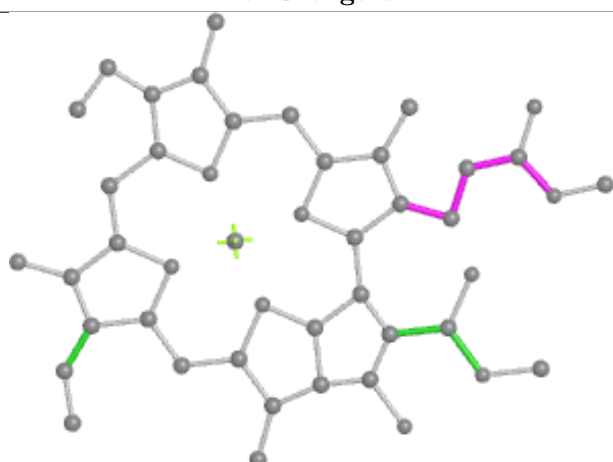
Ligand CLA Q 313



Bond lengths



Bond angles

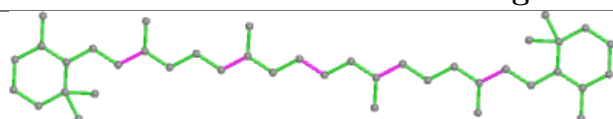


Torsions

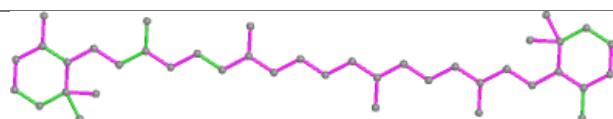


Rings

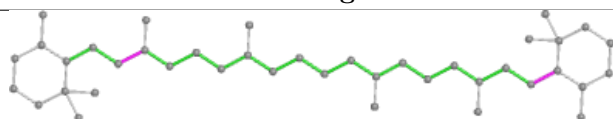
Ligand BCR A 848



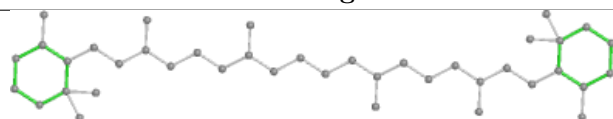
Bond lengths



Bond angles

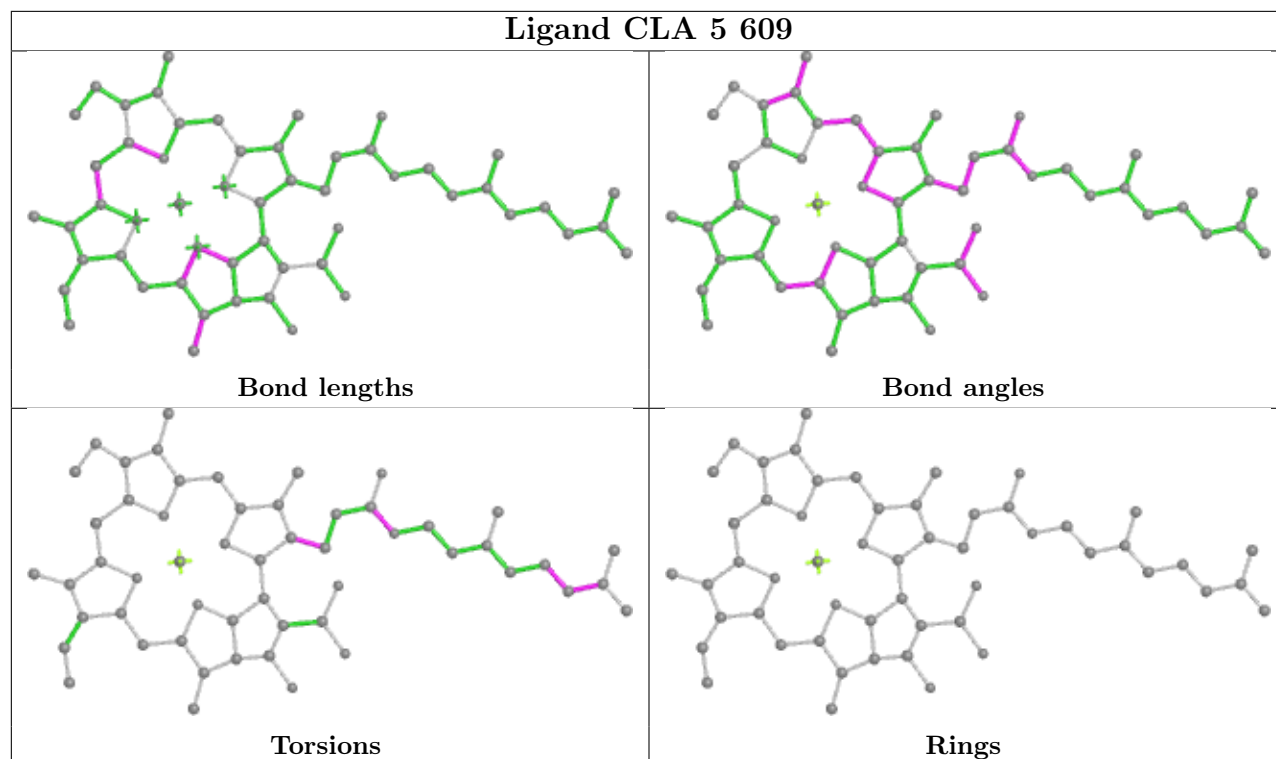


Torsions

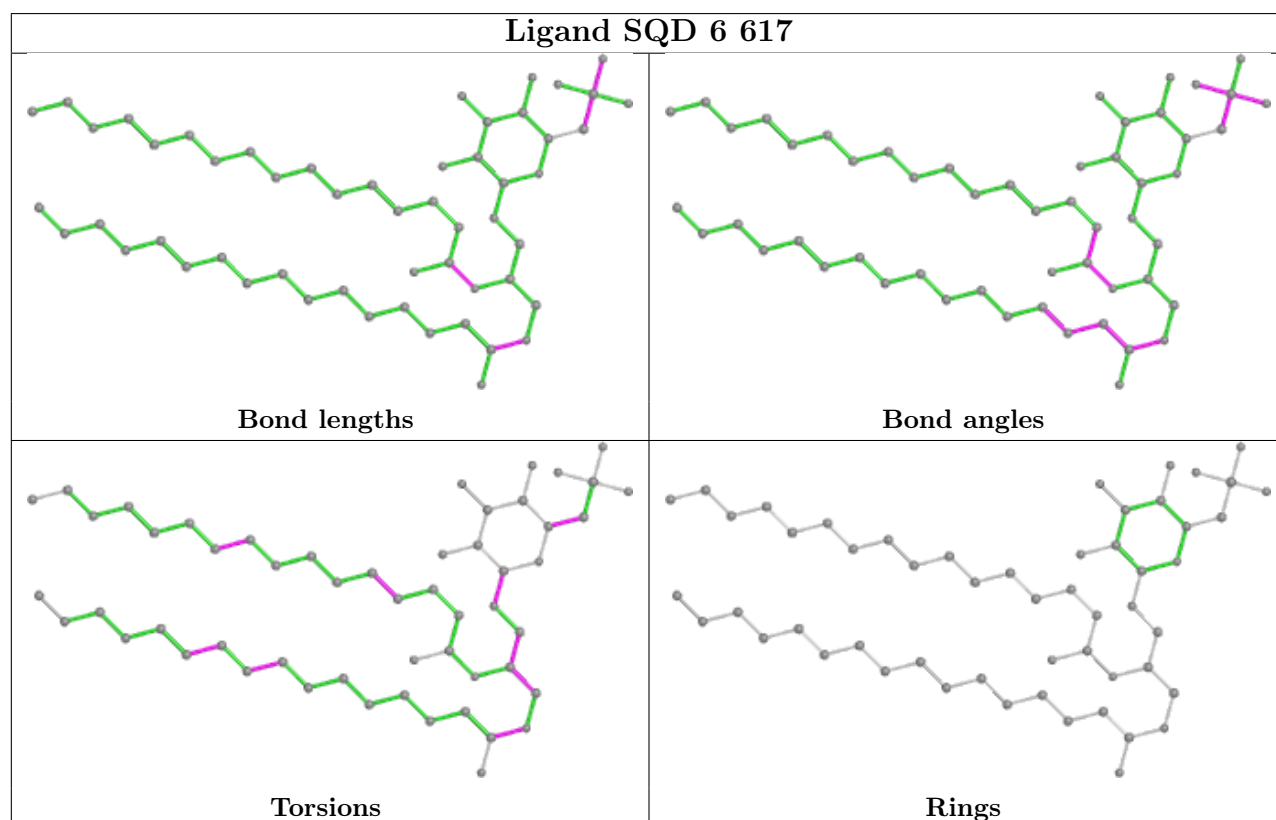


Rings

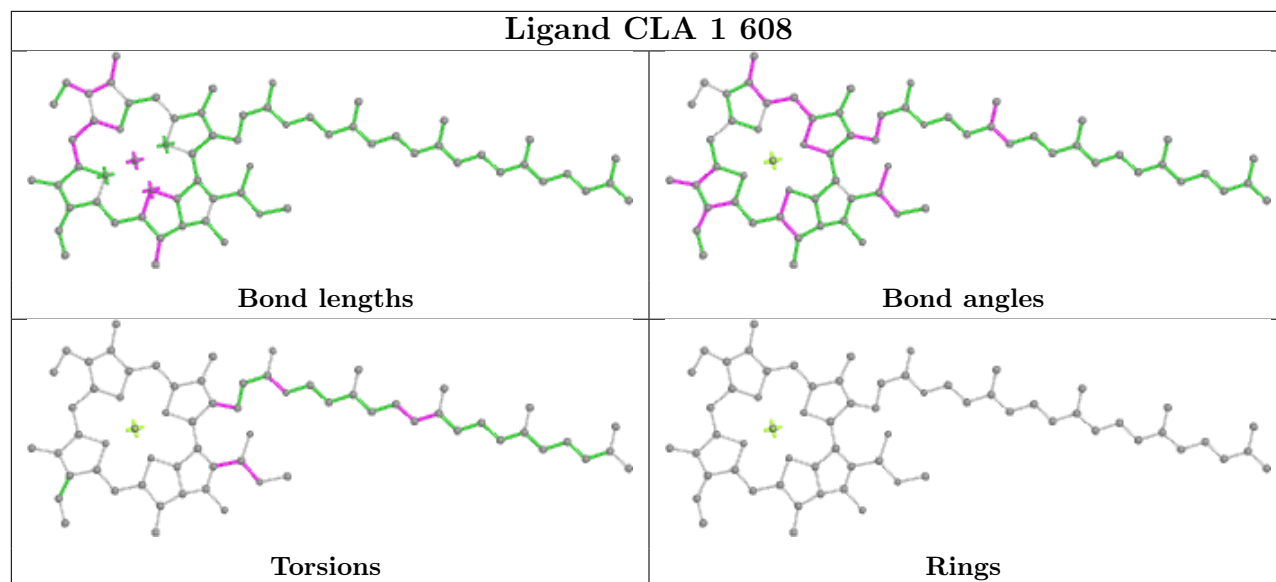
Ligand CLA 5 609



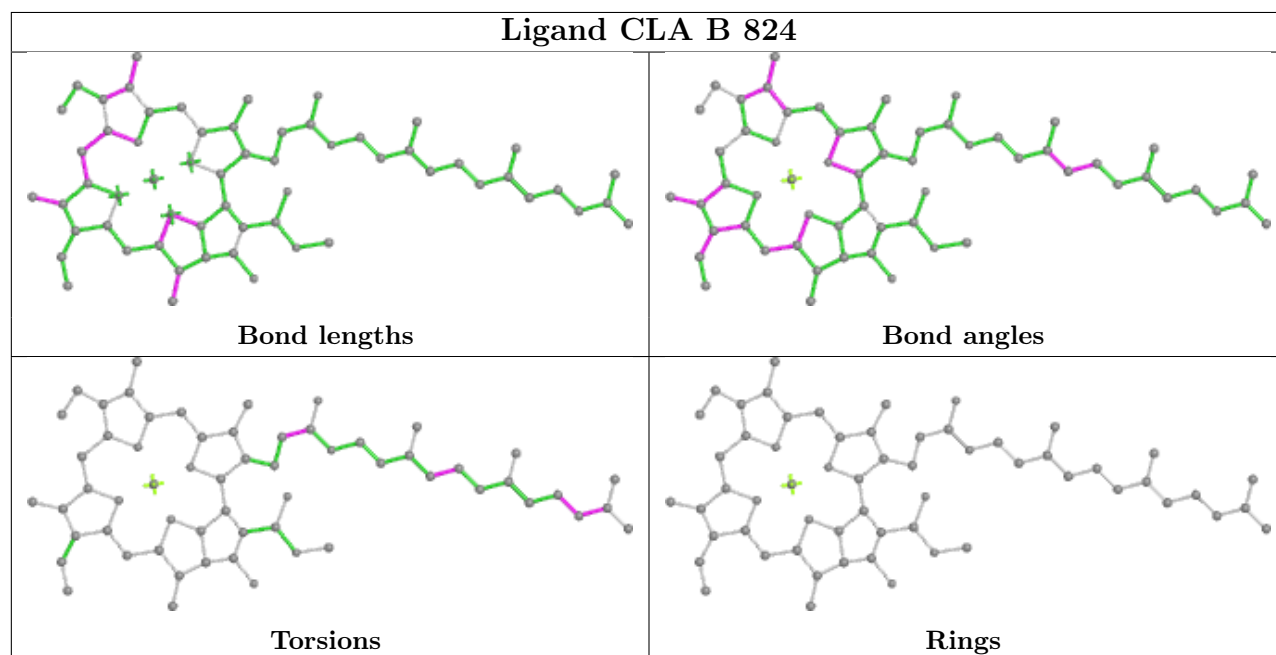
Ligand SQD 6 617



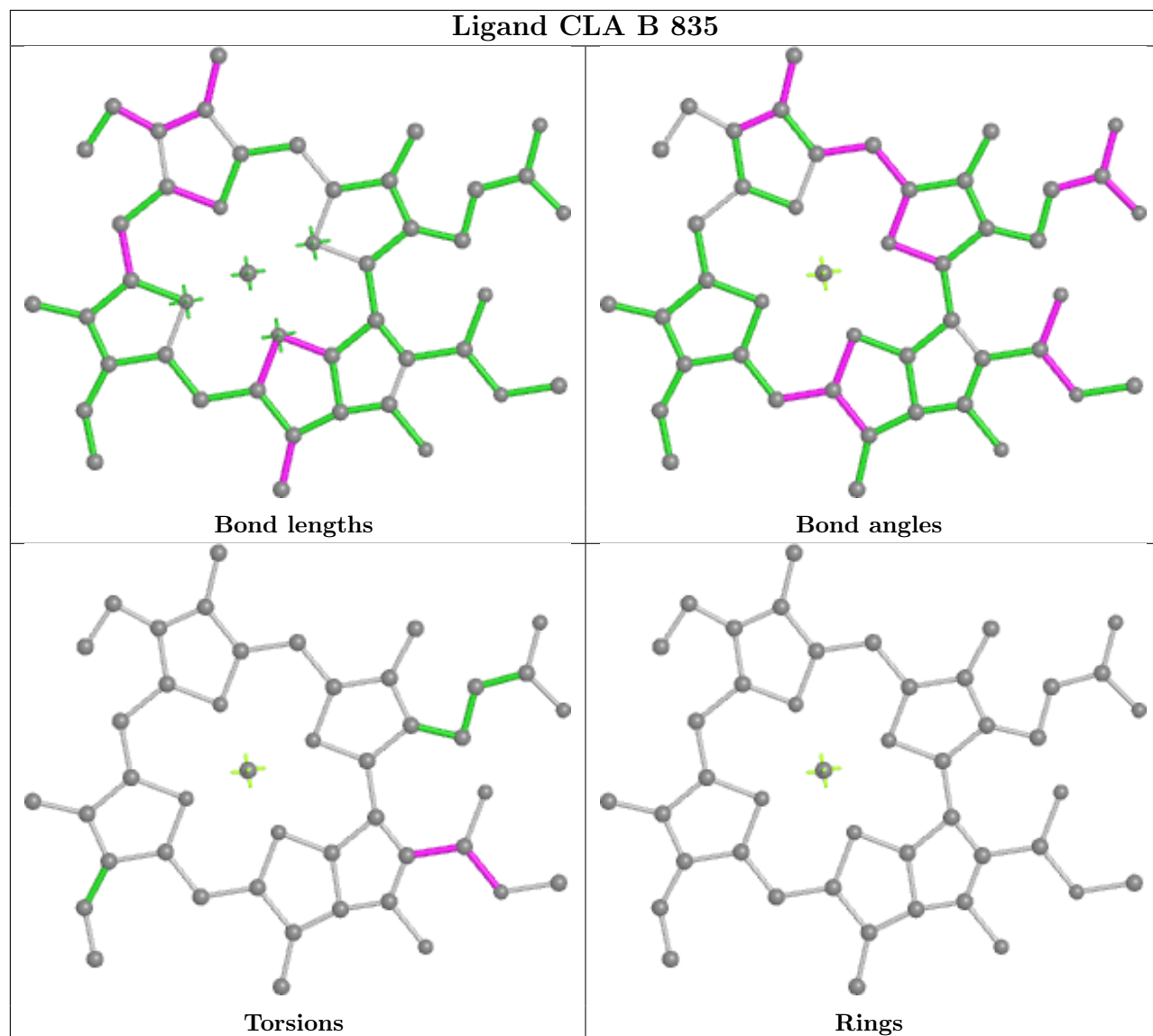
Ligand CLA 1 608



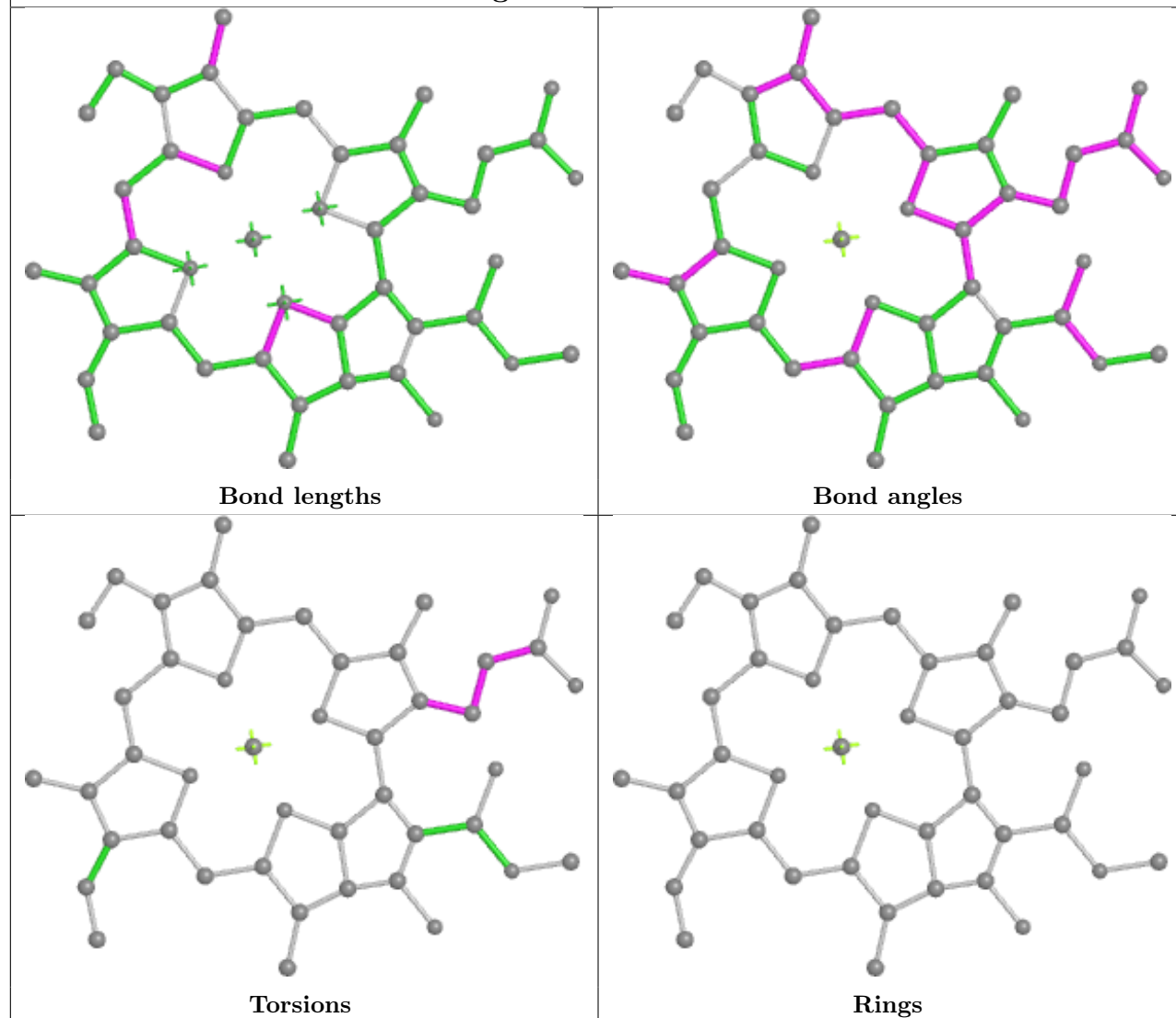
Ligand CLA B 824



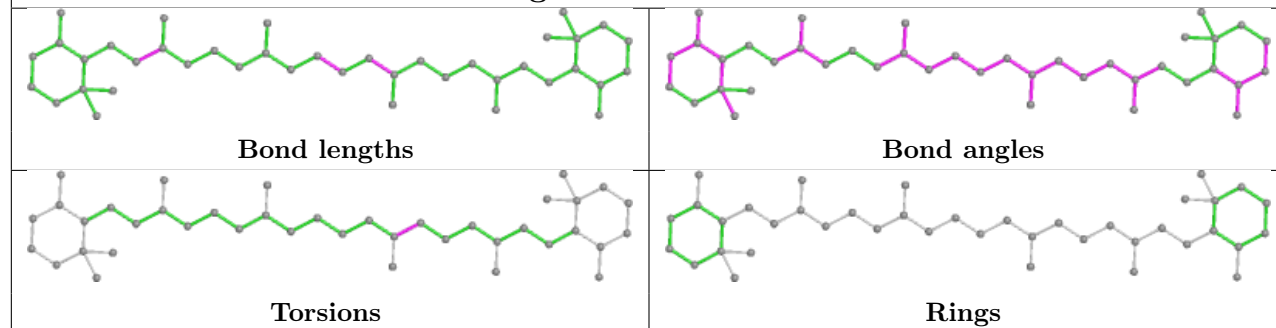
Ligand CLA B 835



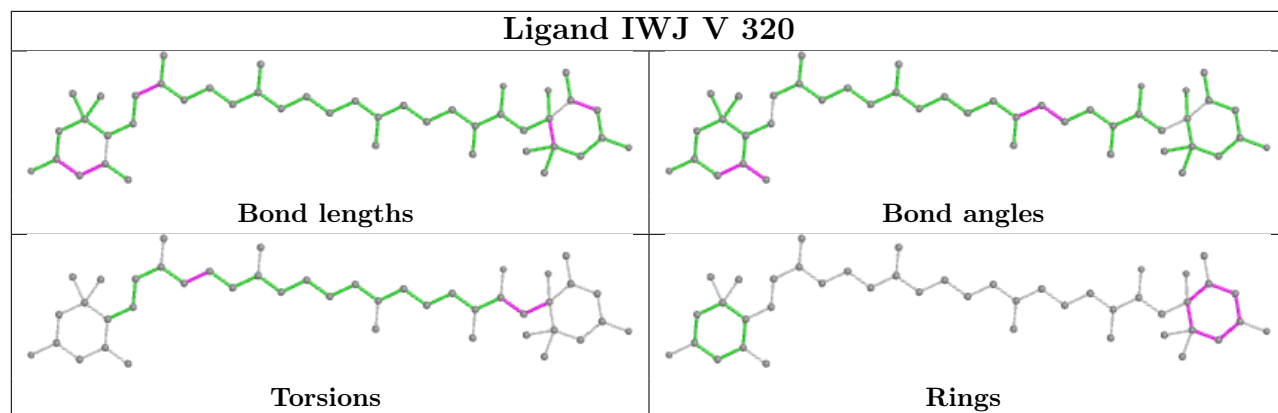
Ligand CLA L 303



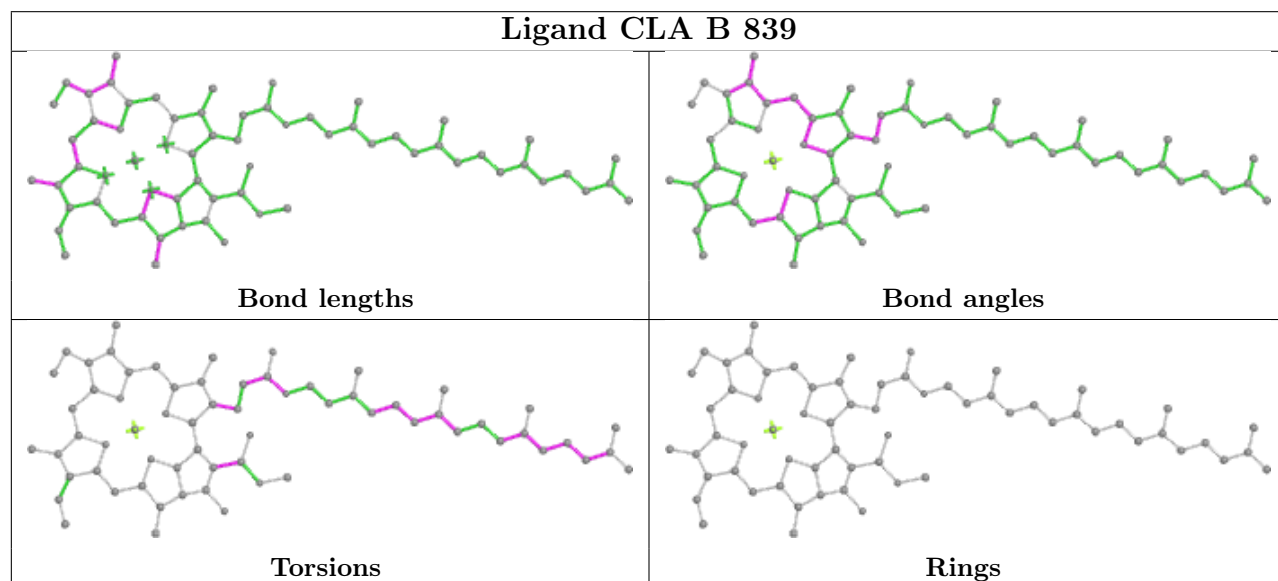
Ligand BCR G 201



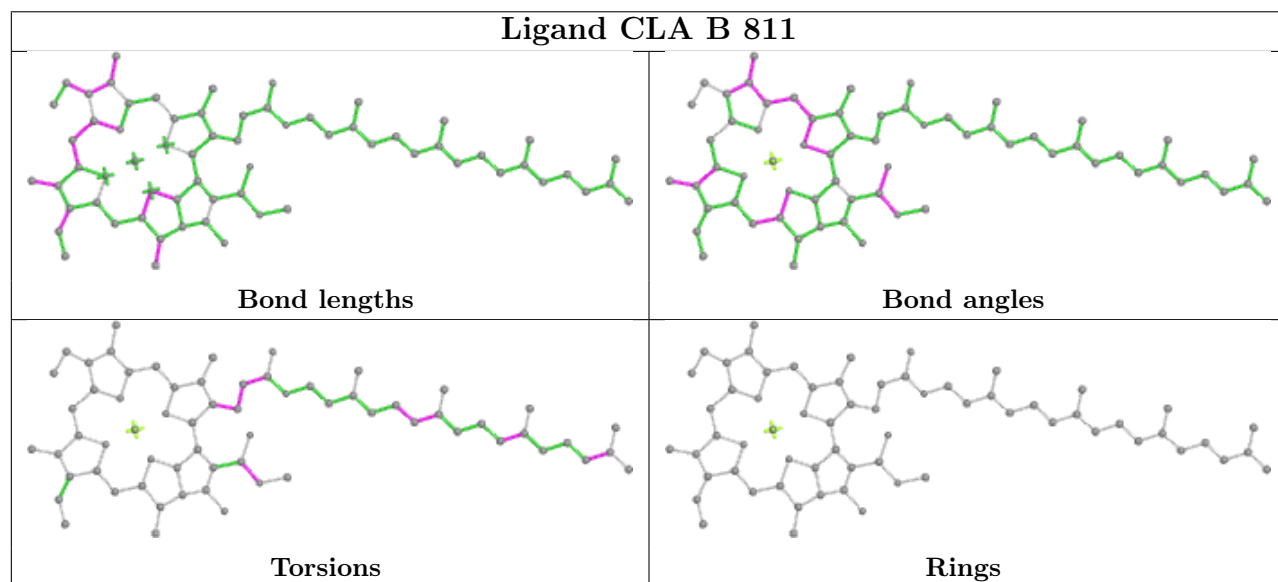
Ligand IWJ V 320



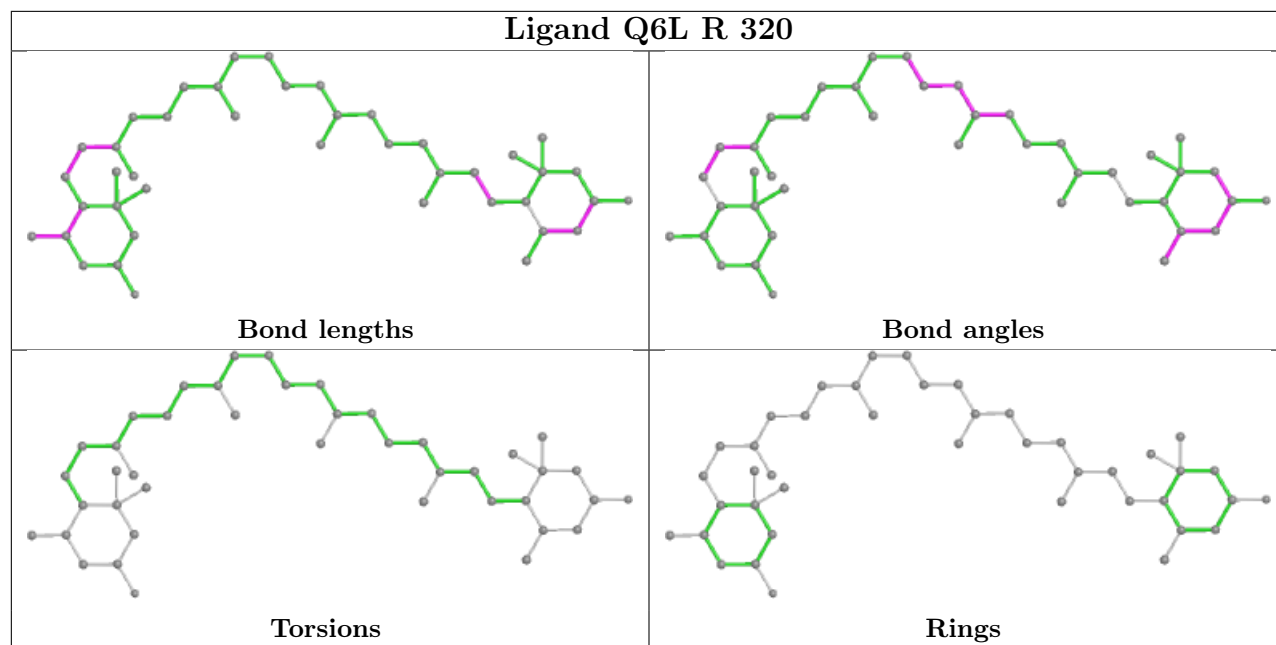
Ligand CLA B 839



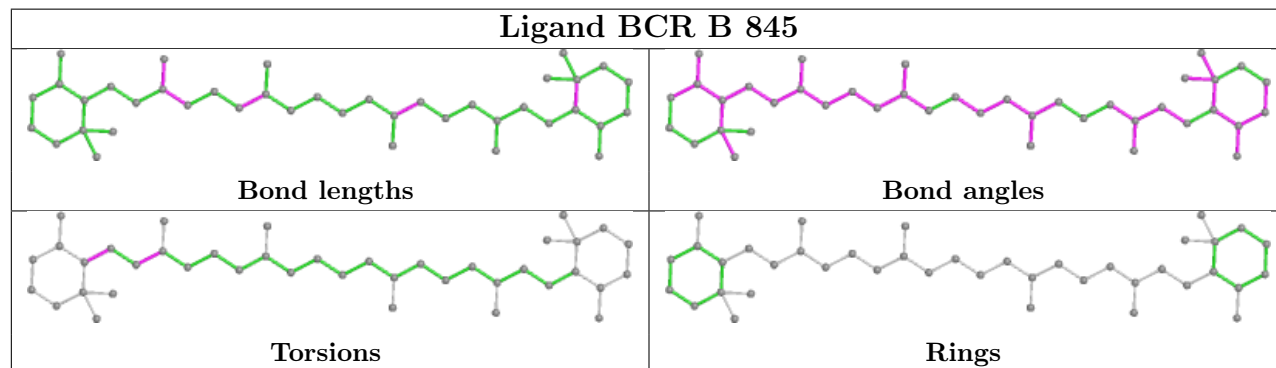
Ligand CLA B 811



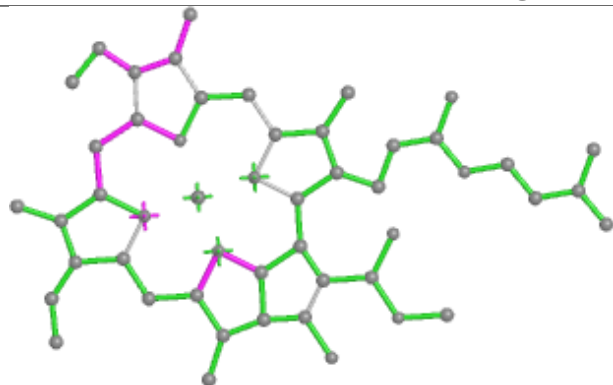
Ligand Q6L R 320



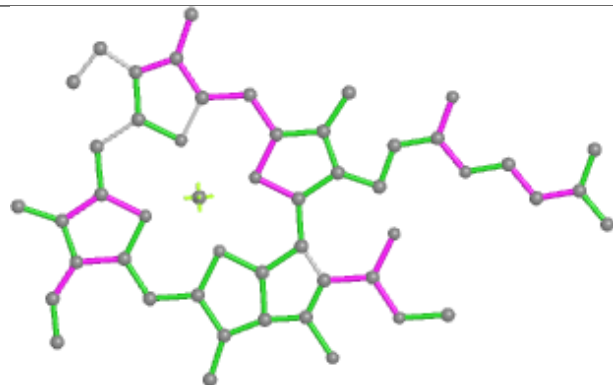
Ligand BCR B 845



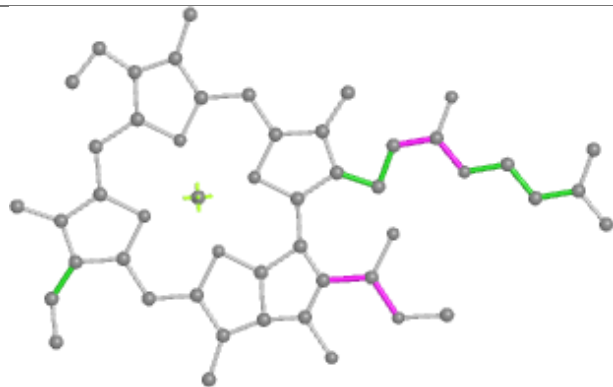
Ligand CLA V 302



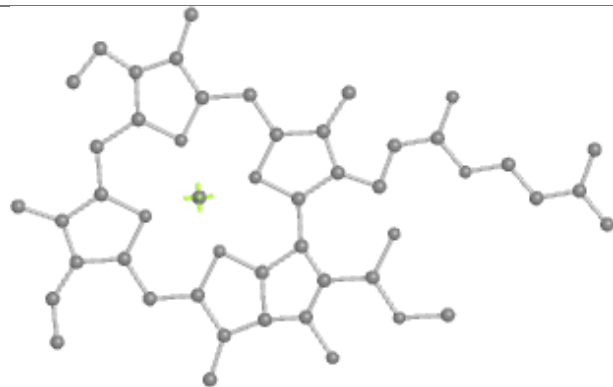
Bond lengths



Bond angles

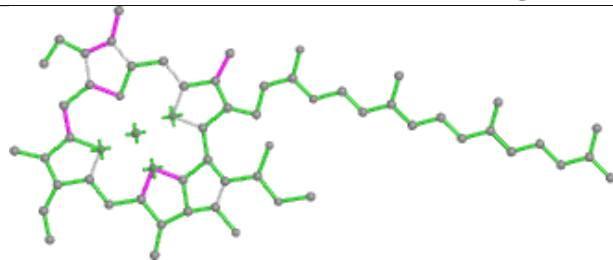


Torsions

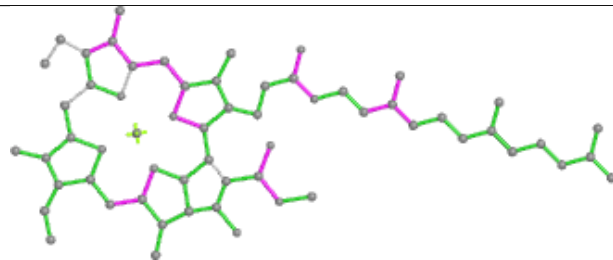


Rings

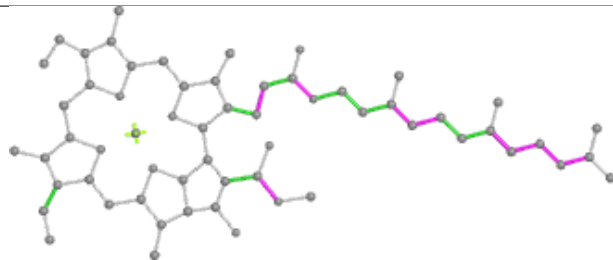
Ligand CLA A 819



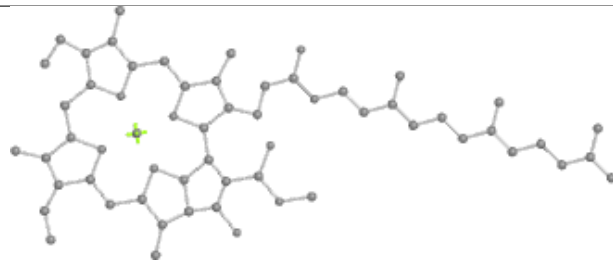
Bond lengths



Bond angles

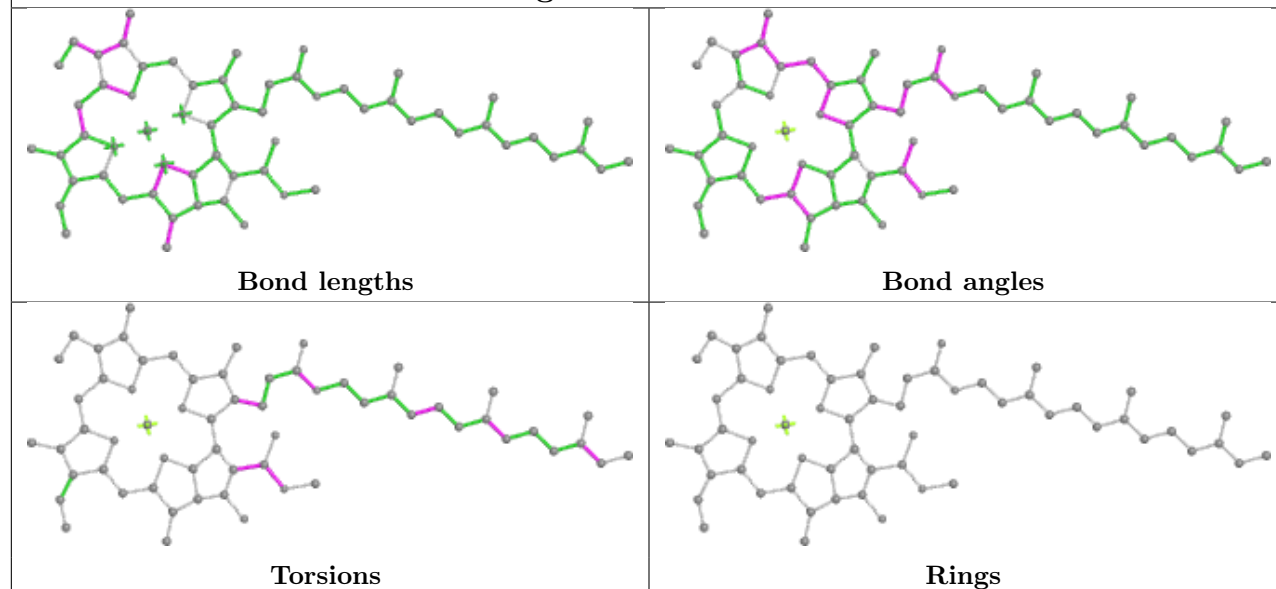


Torsions

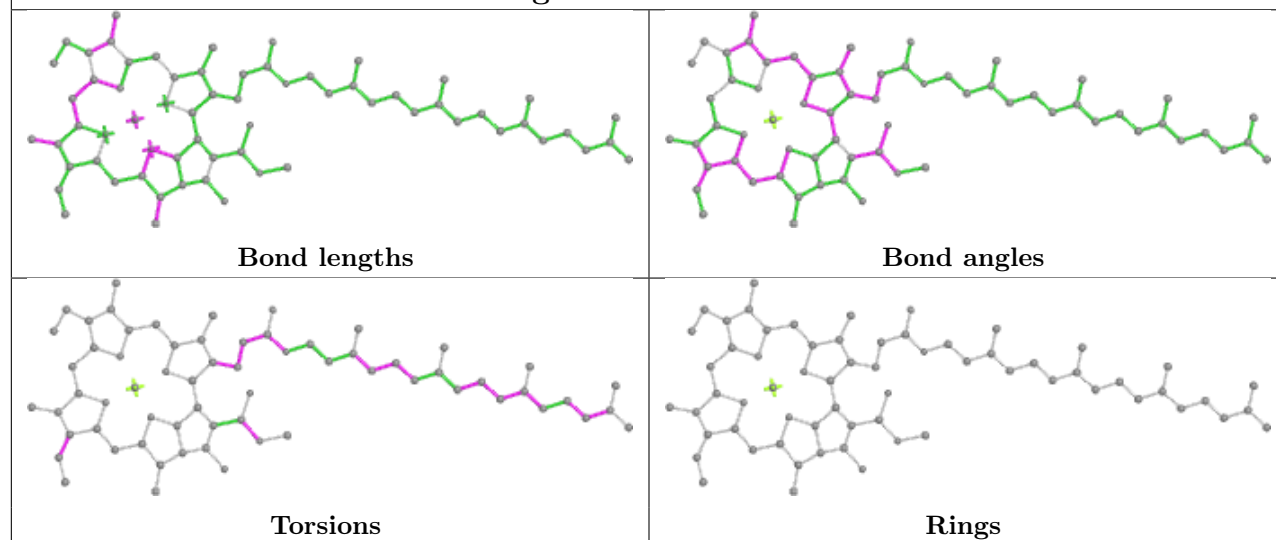


Rings

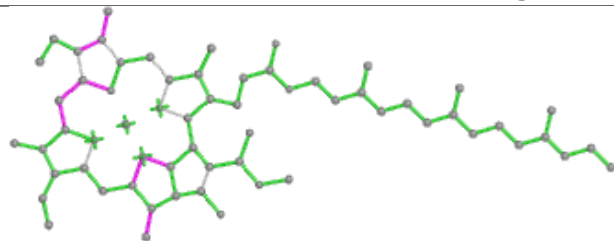
Ligand CLA 6 610



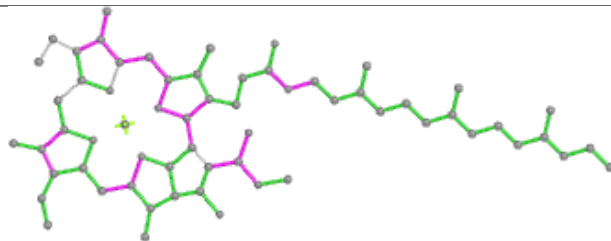
Ligand CLA B 808



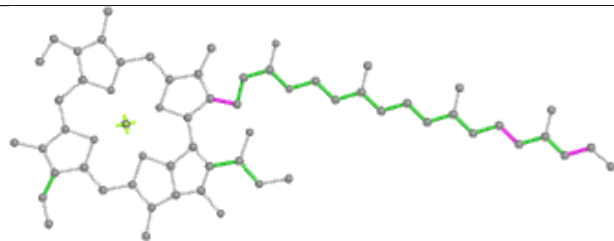
Ligand CLA K 203



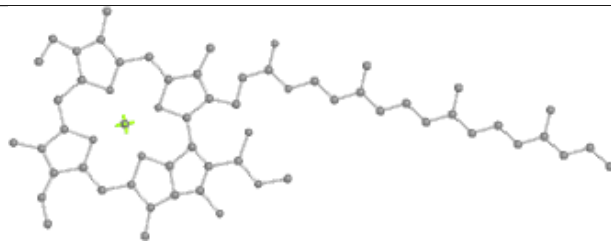
Bond lengths



Bond angles

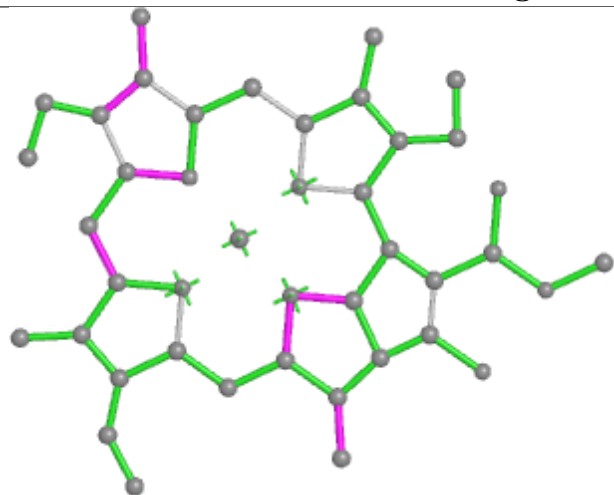


Torsions

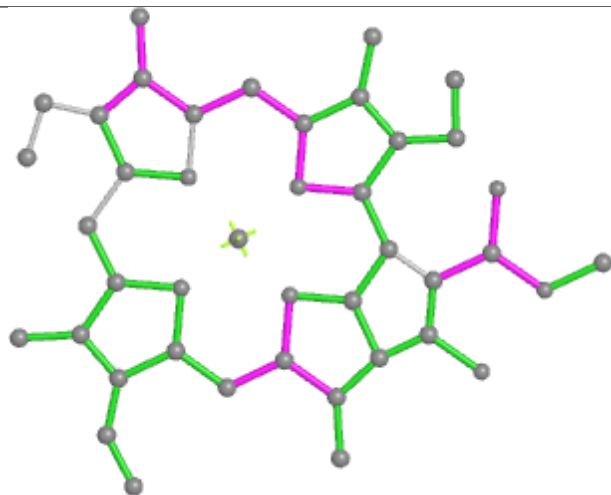


Rings

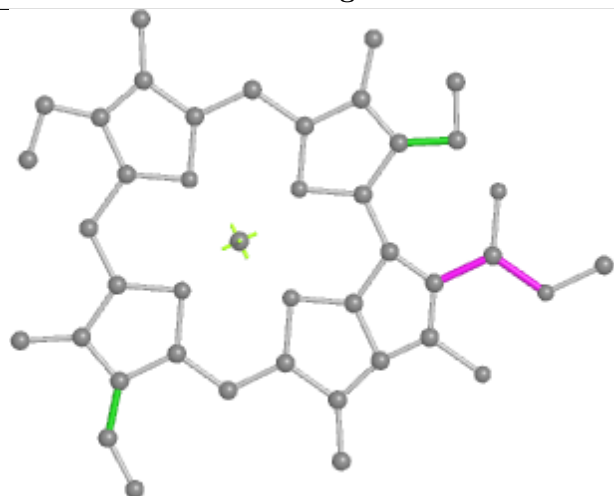
Ligand CLA X 310



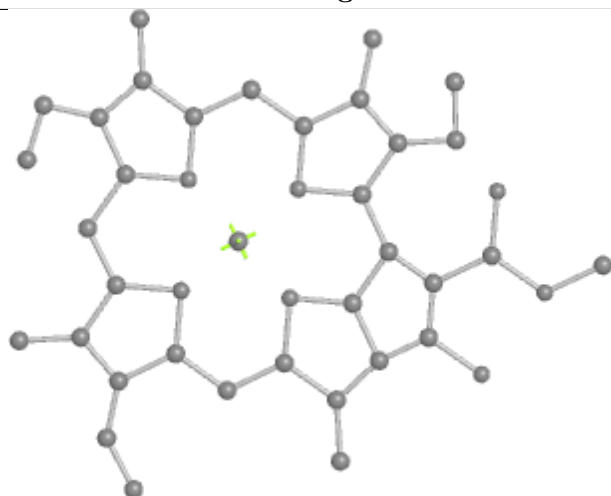
Bond lengths



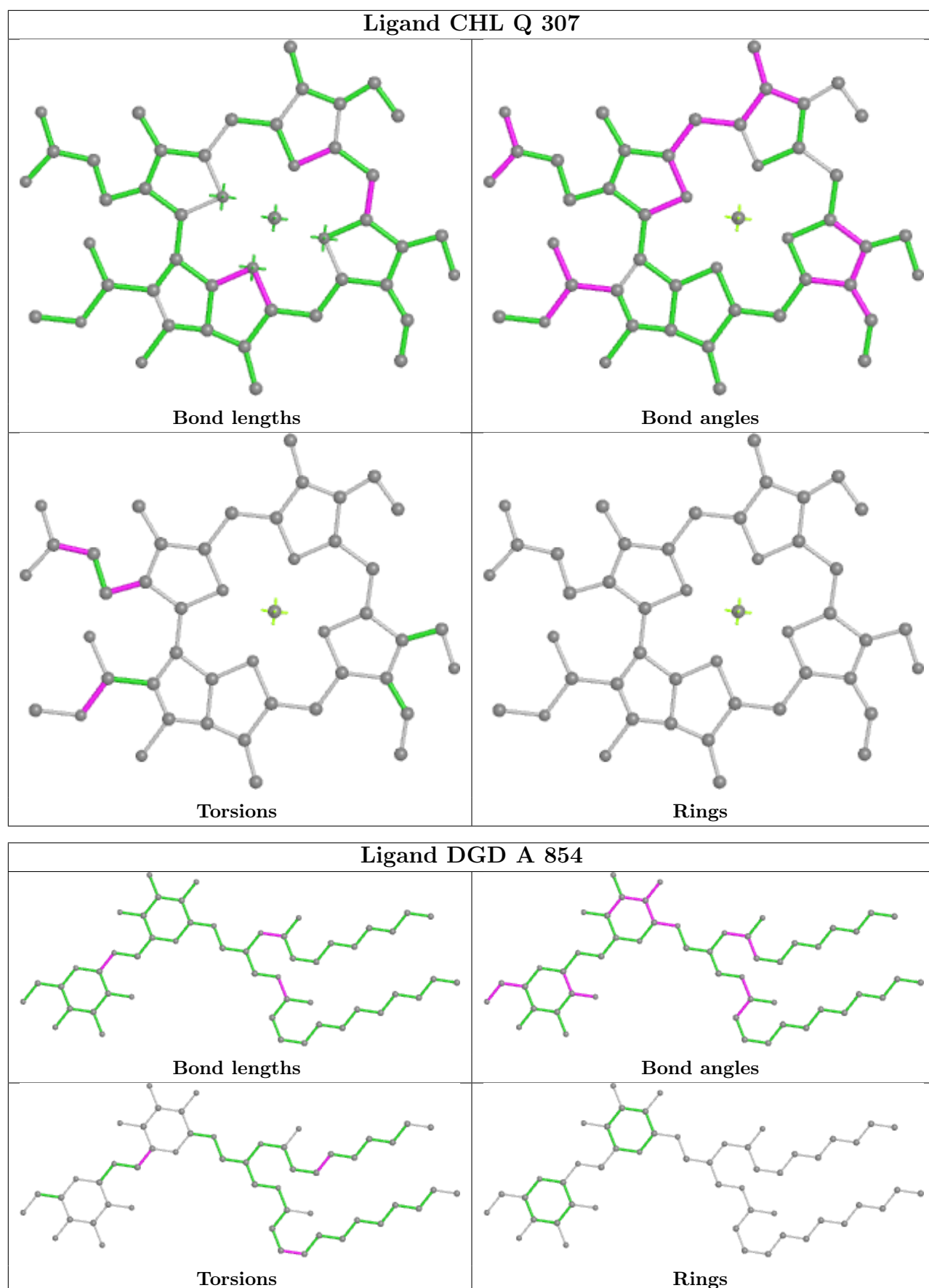
Bond angles



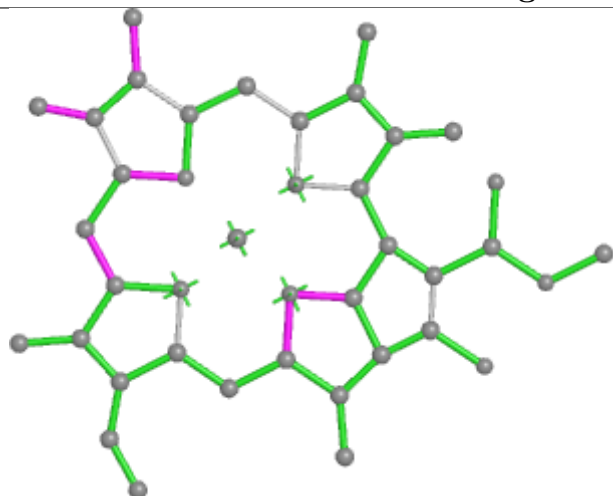
Torsions



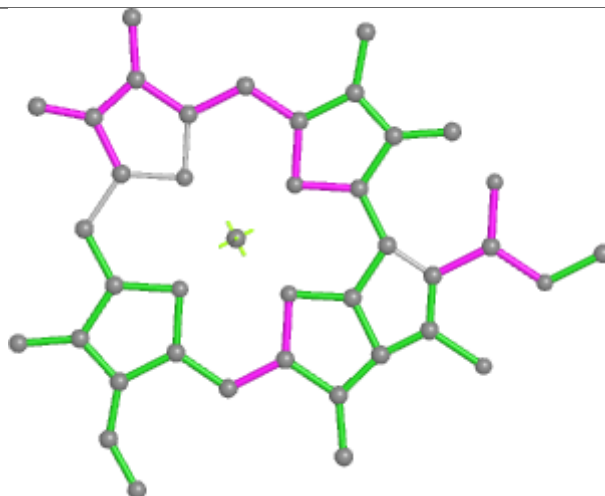
Rings



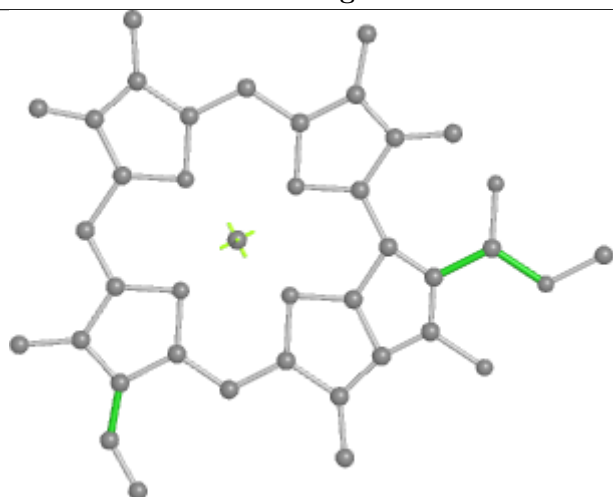
Ligand CLA 5 606



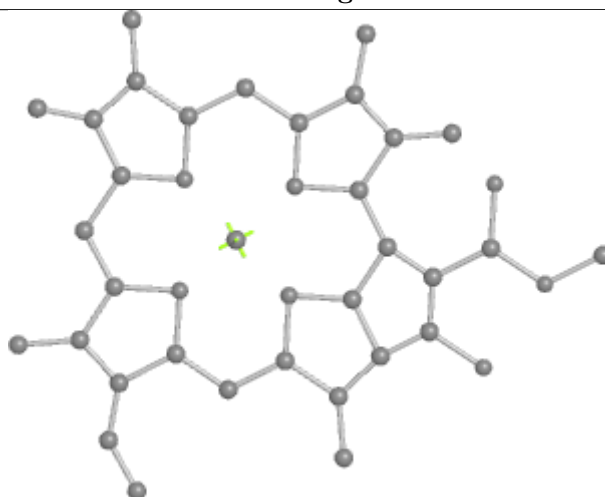
Bond lengths



Bond angles

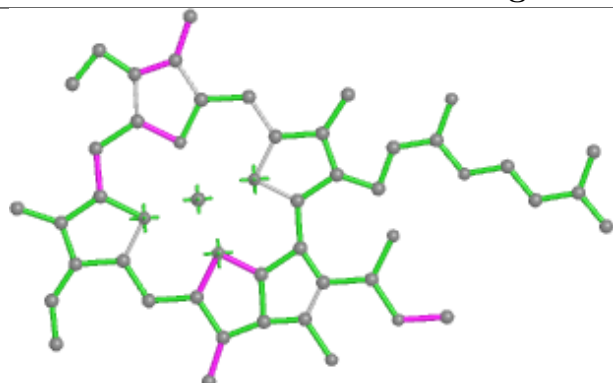


Torsions

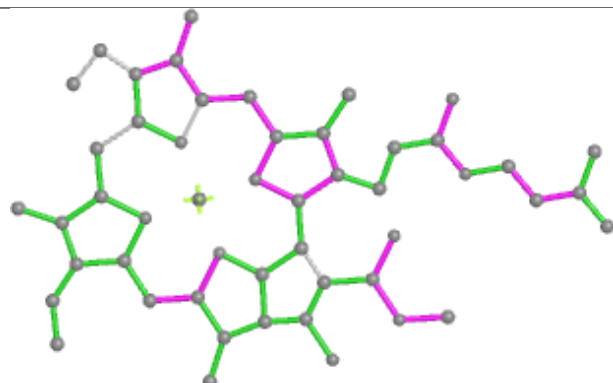


Rings

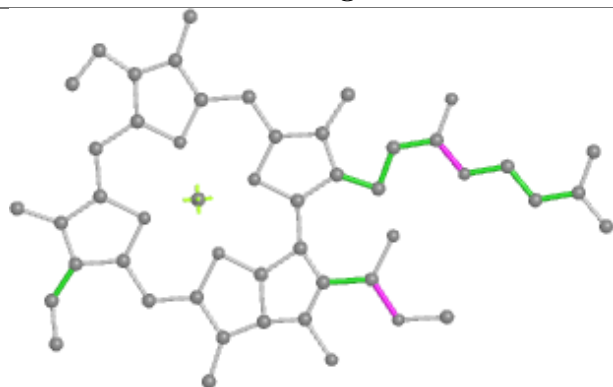
Ligand CLA W 303



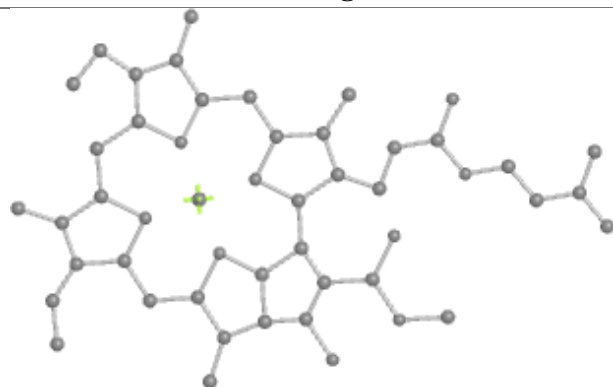
Bond lengths



Bond angles

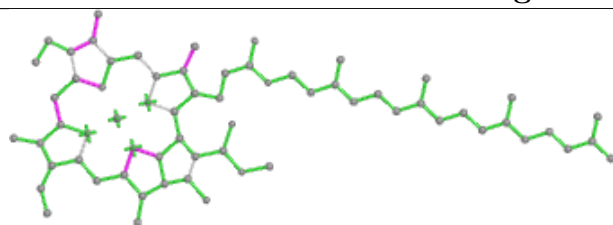


Torsions

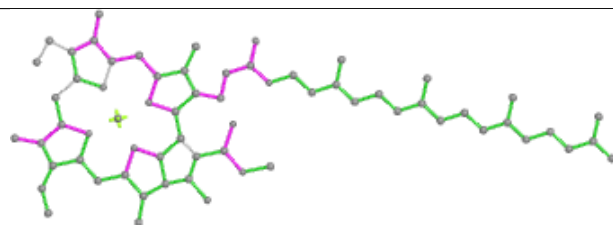


Rings

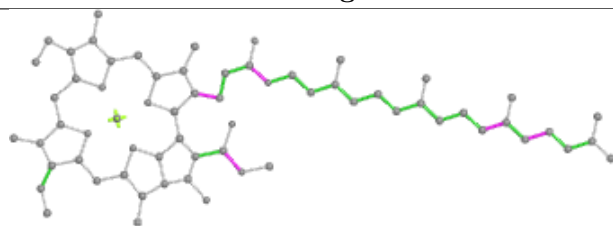
Ligand CLA R 305



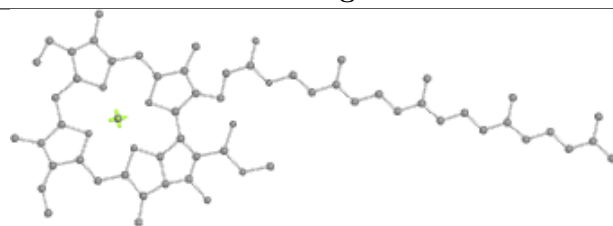
Bond lengths



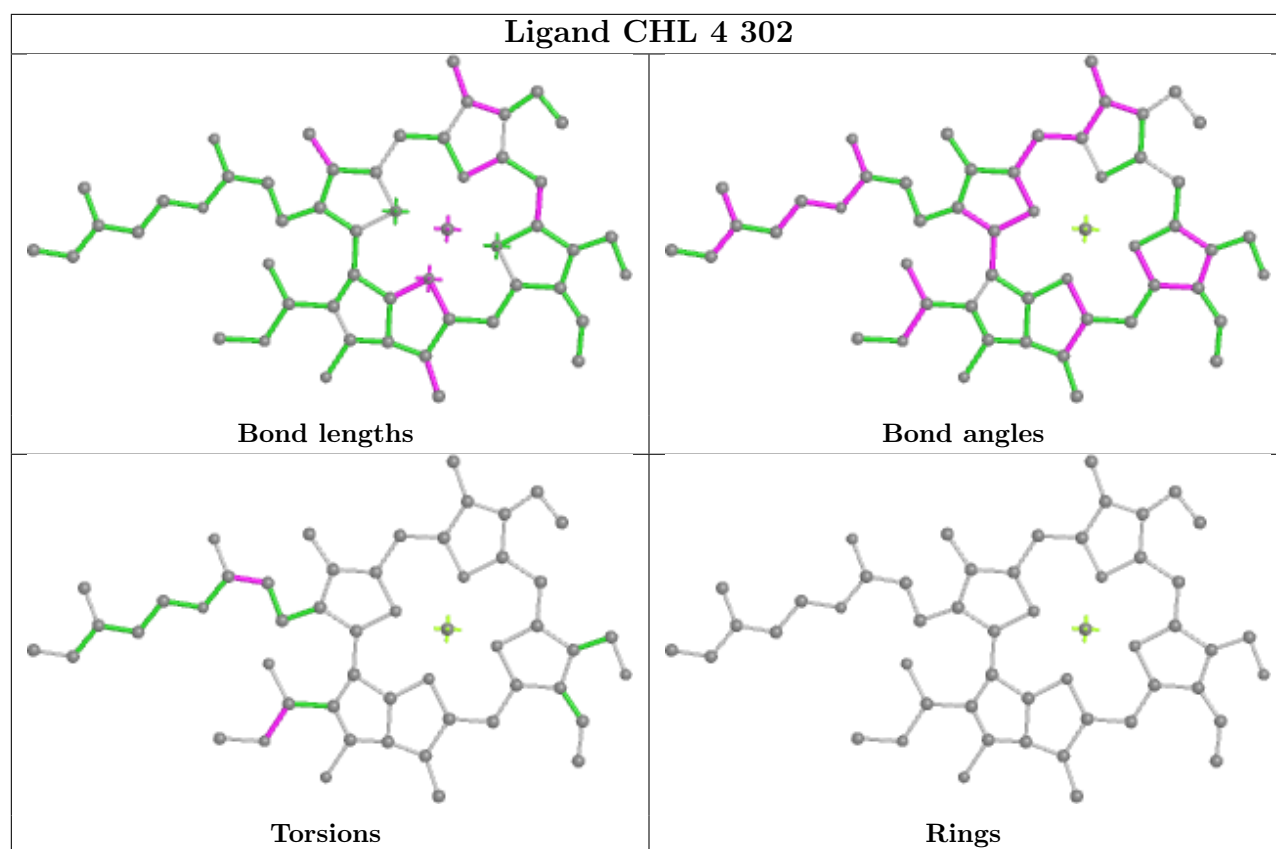
Bond angles



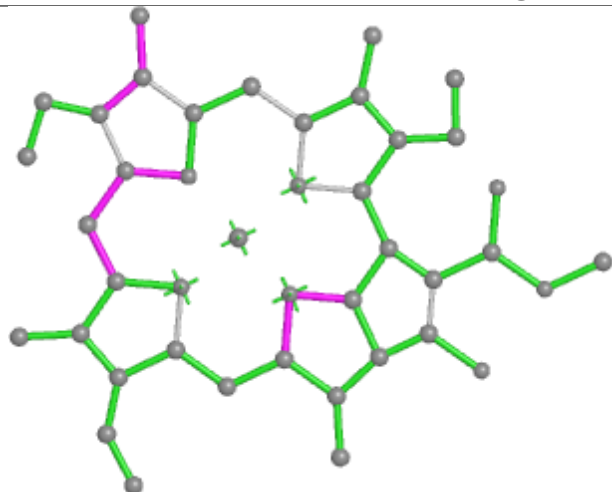
Torsions



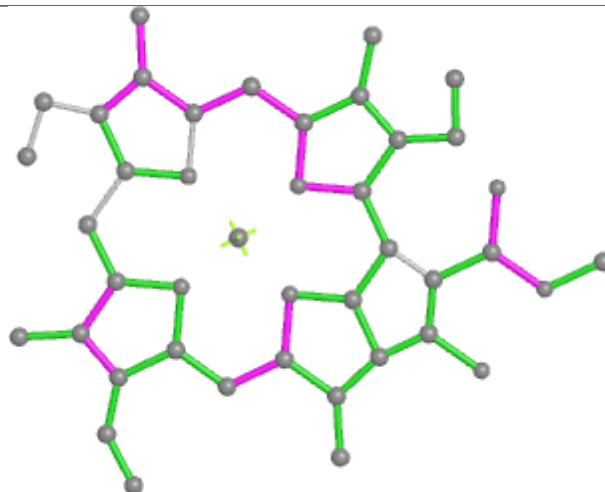
Rings



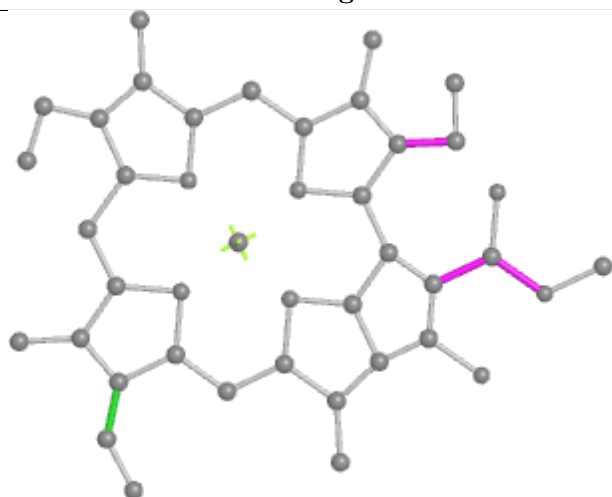
Ligand CLA A 824



Bond lengths



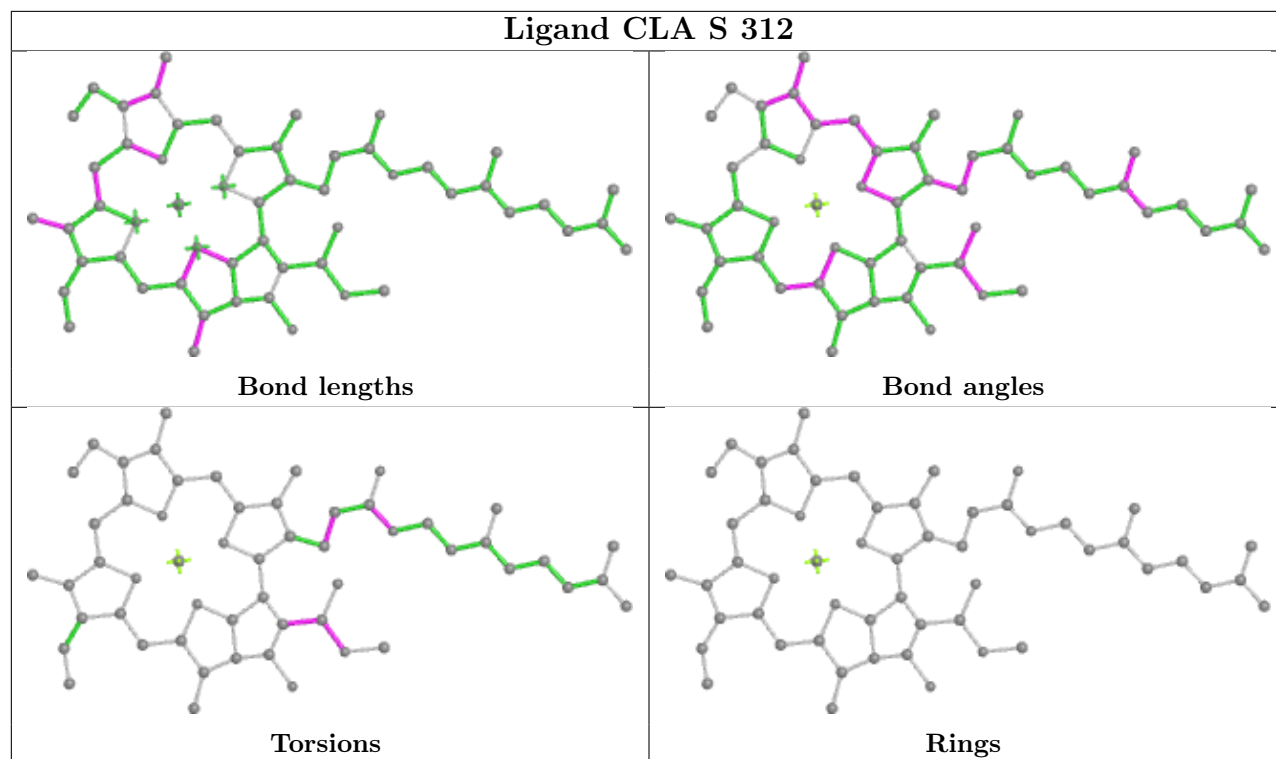
Bond angles



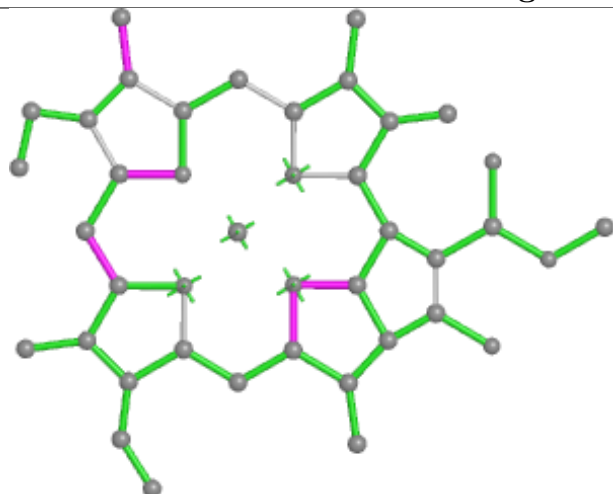
Torsions



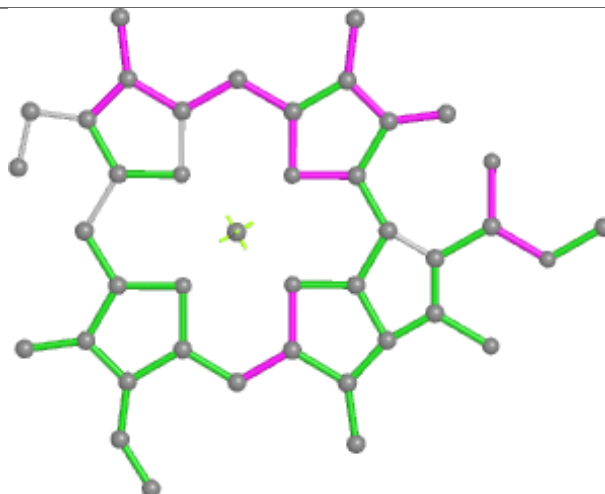
Rings



Ligand CLA 4 315



Bond lengths



Bond angles

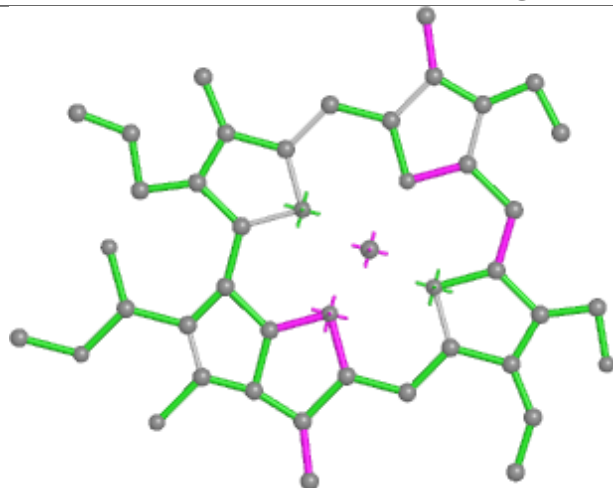


Torsions

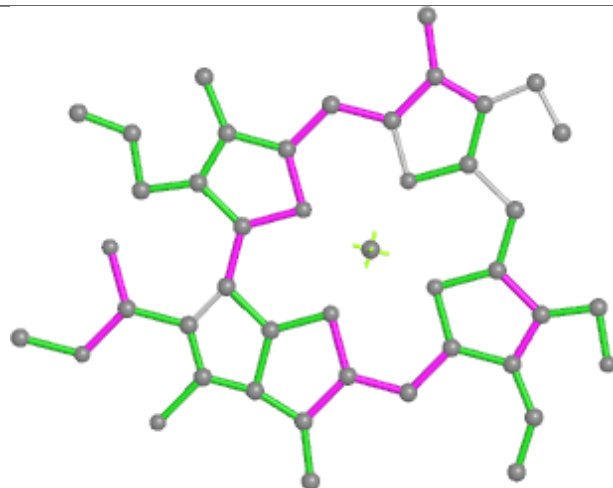


Rings

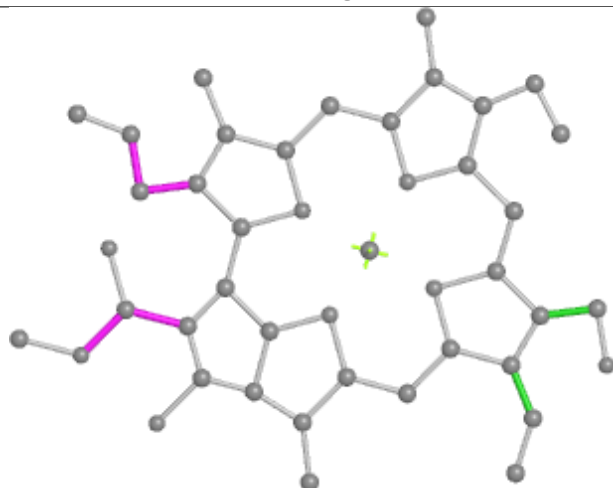
Ligand CHL V 314



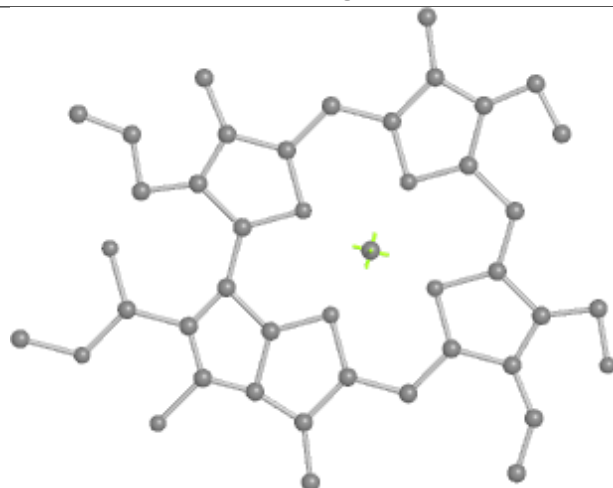
Bond lengths



Bond angles

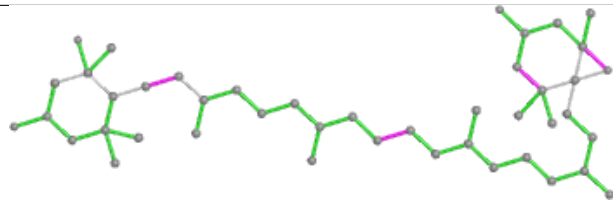


Torsions

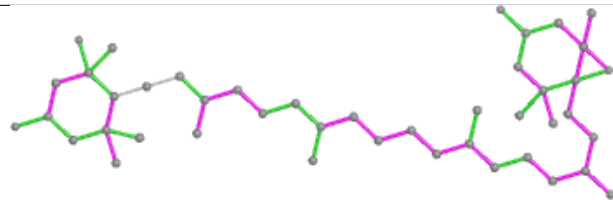


Rings

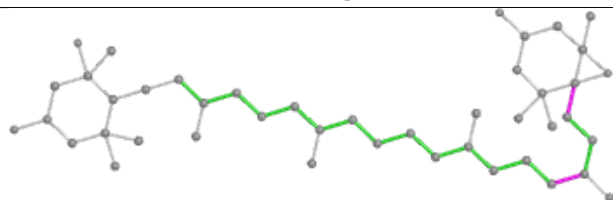
Ligand NEX T 317



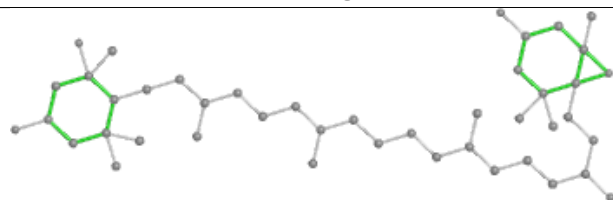
Bond lengths



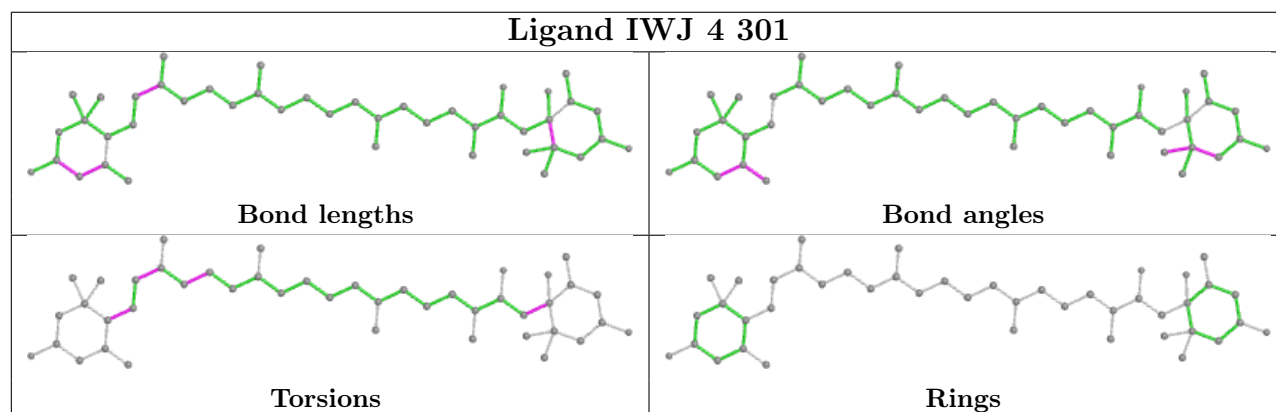
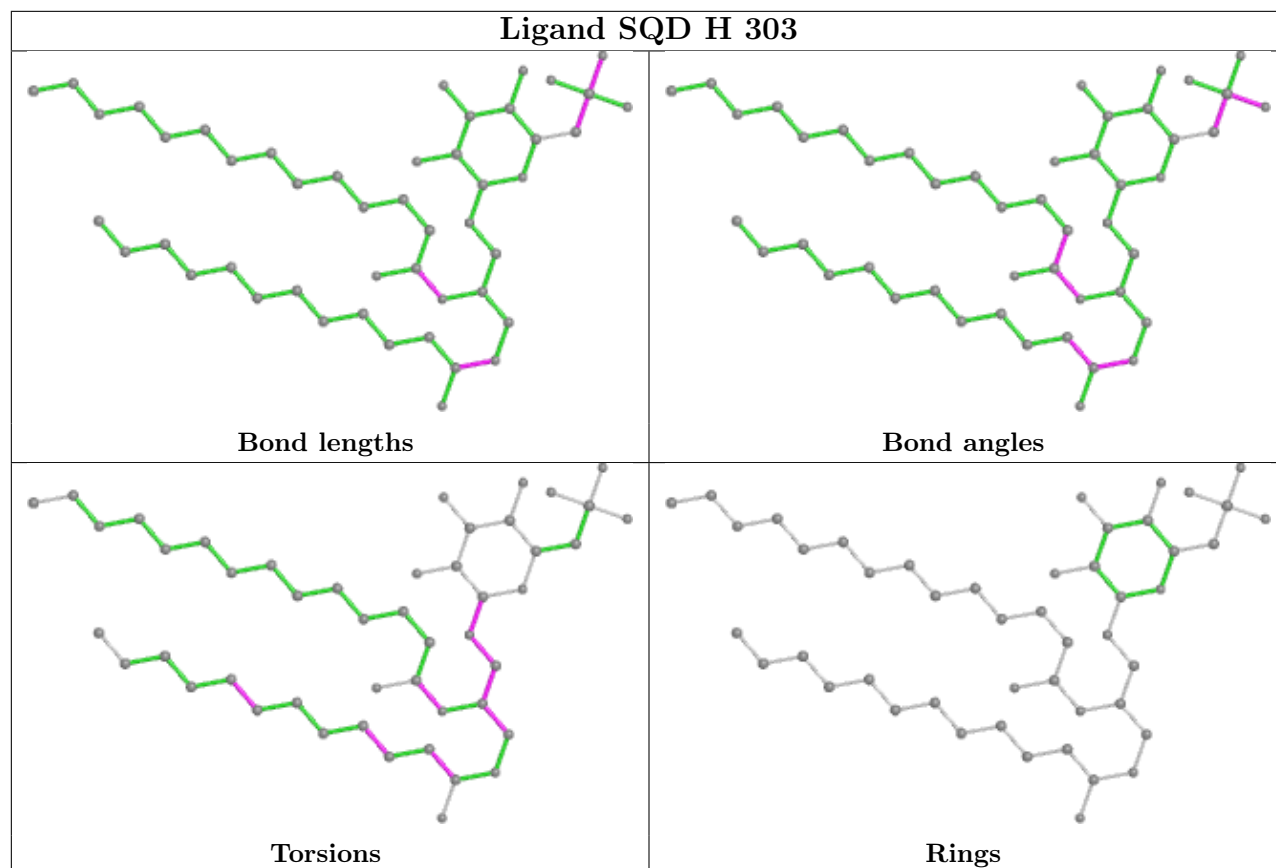
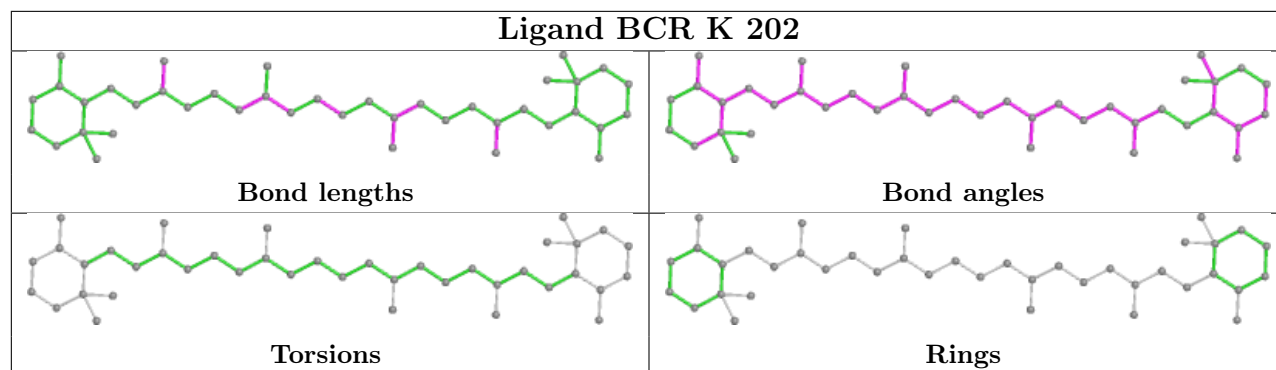
Bond angles

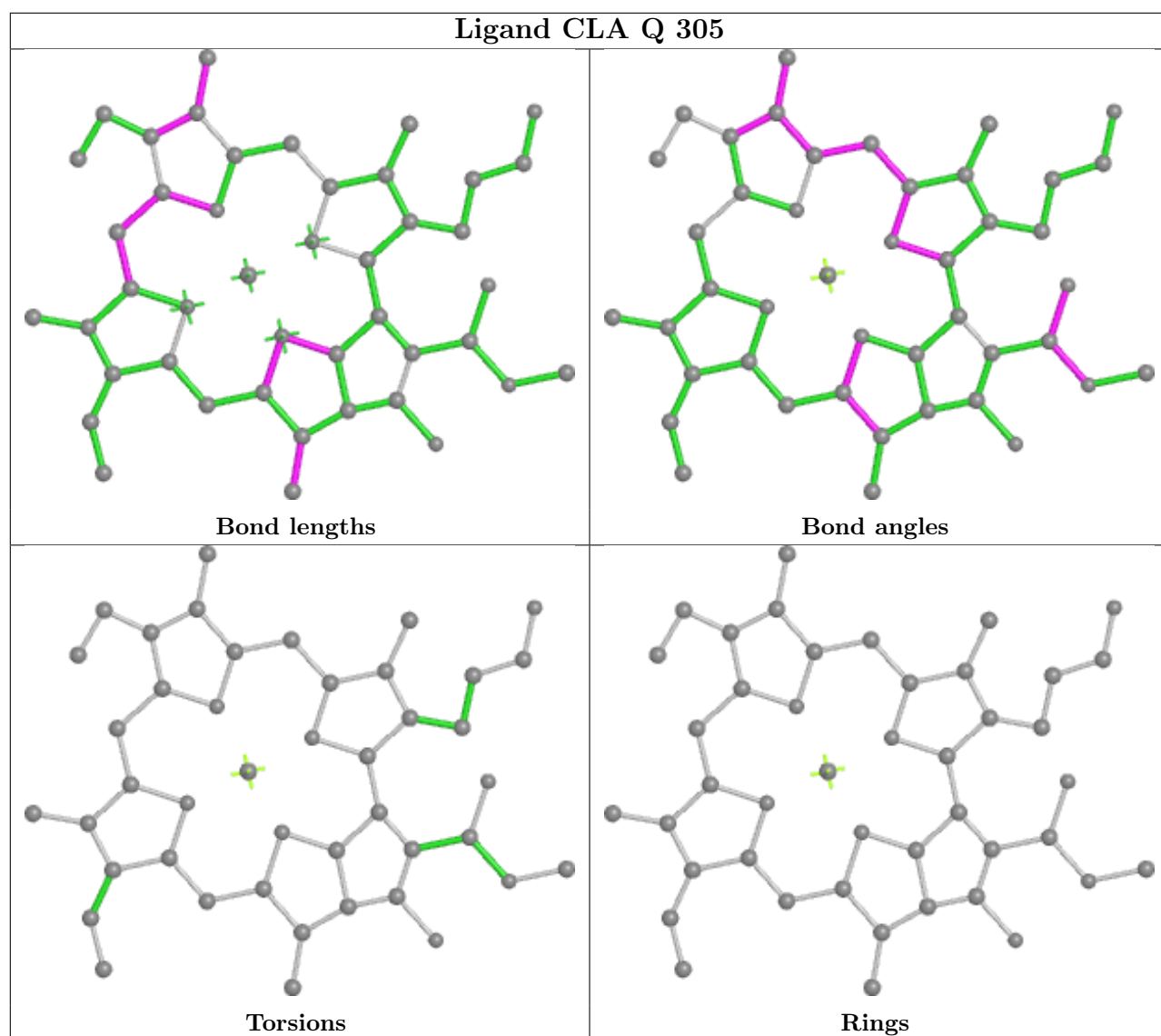


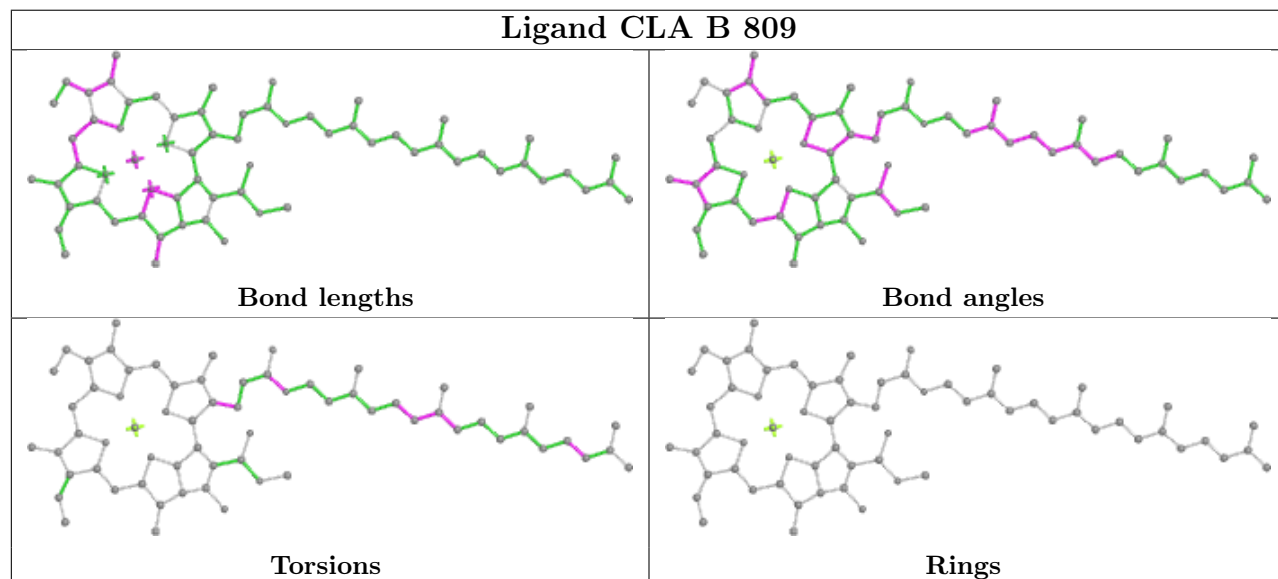
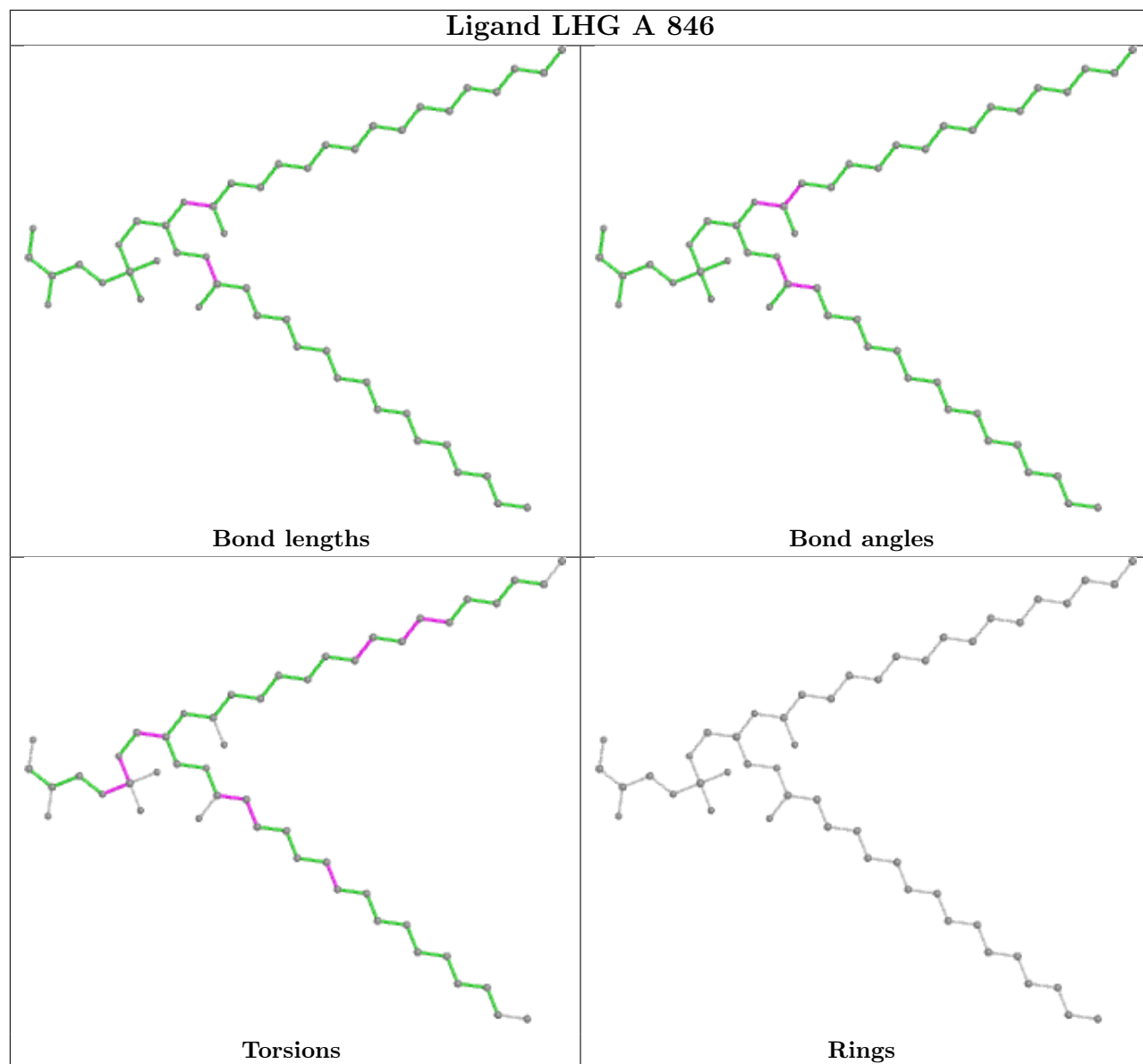
Torsions



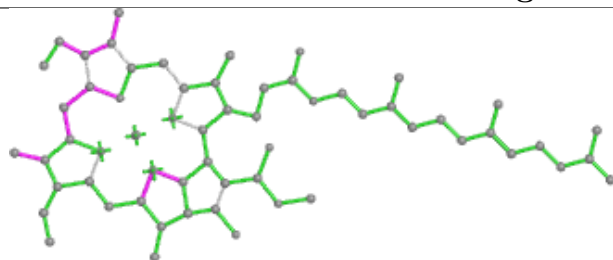
Rings



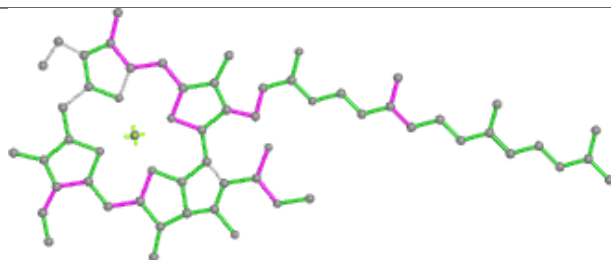




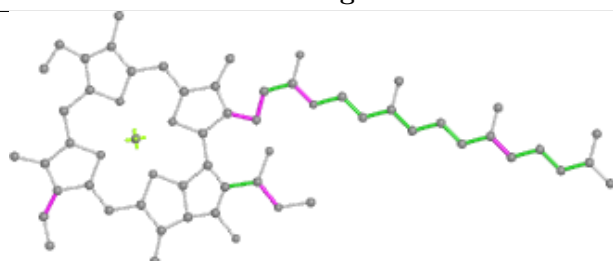
Ligand CLA L 302



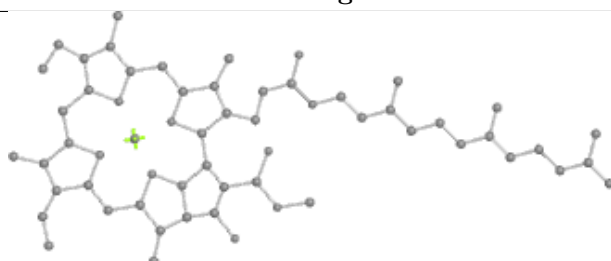
Bond lengths



Bond angles

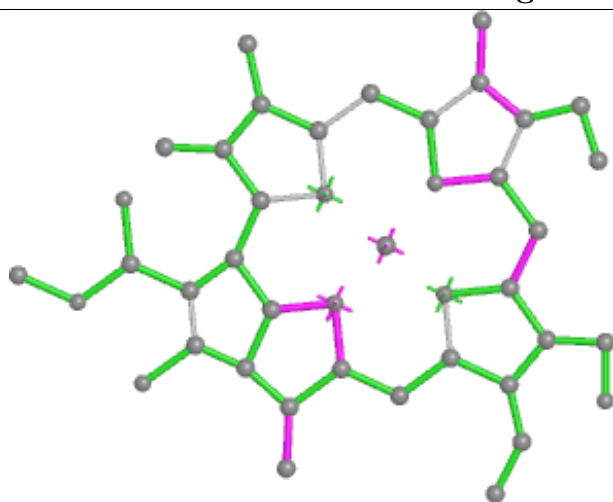


Torsions

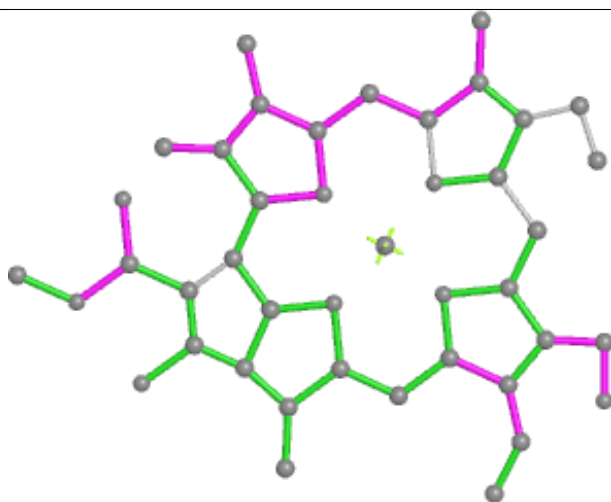


Rings

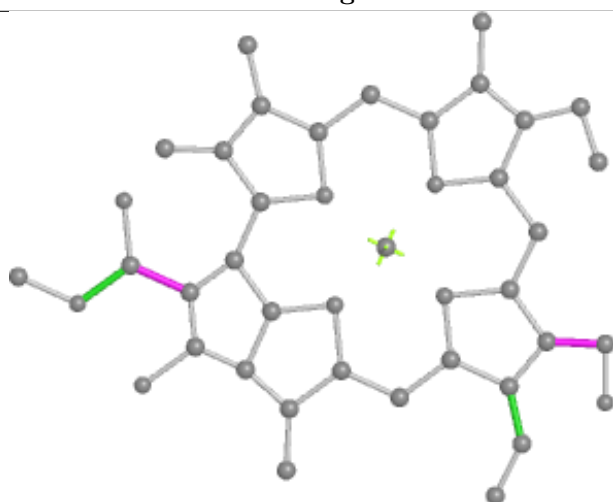
Ligand CHL S 304



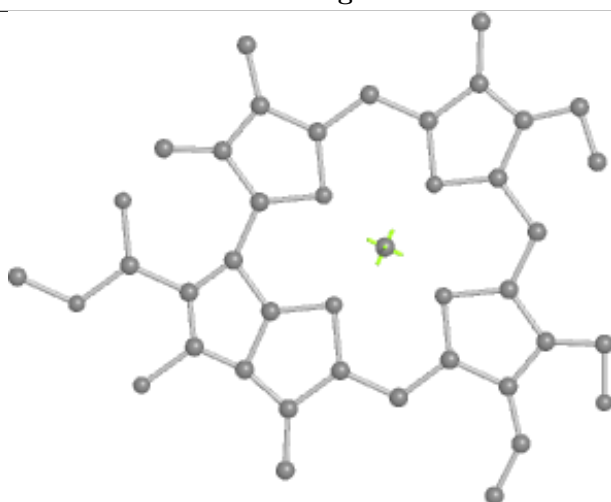
Bond lengths



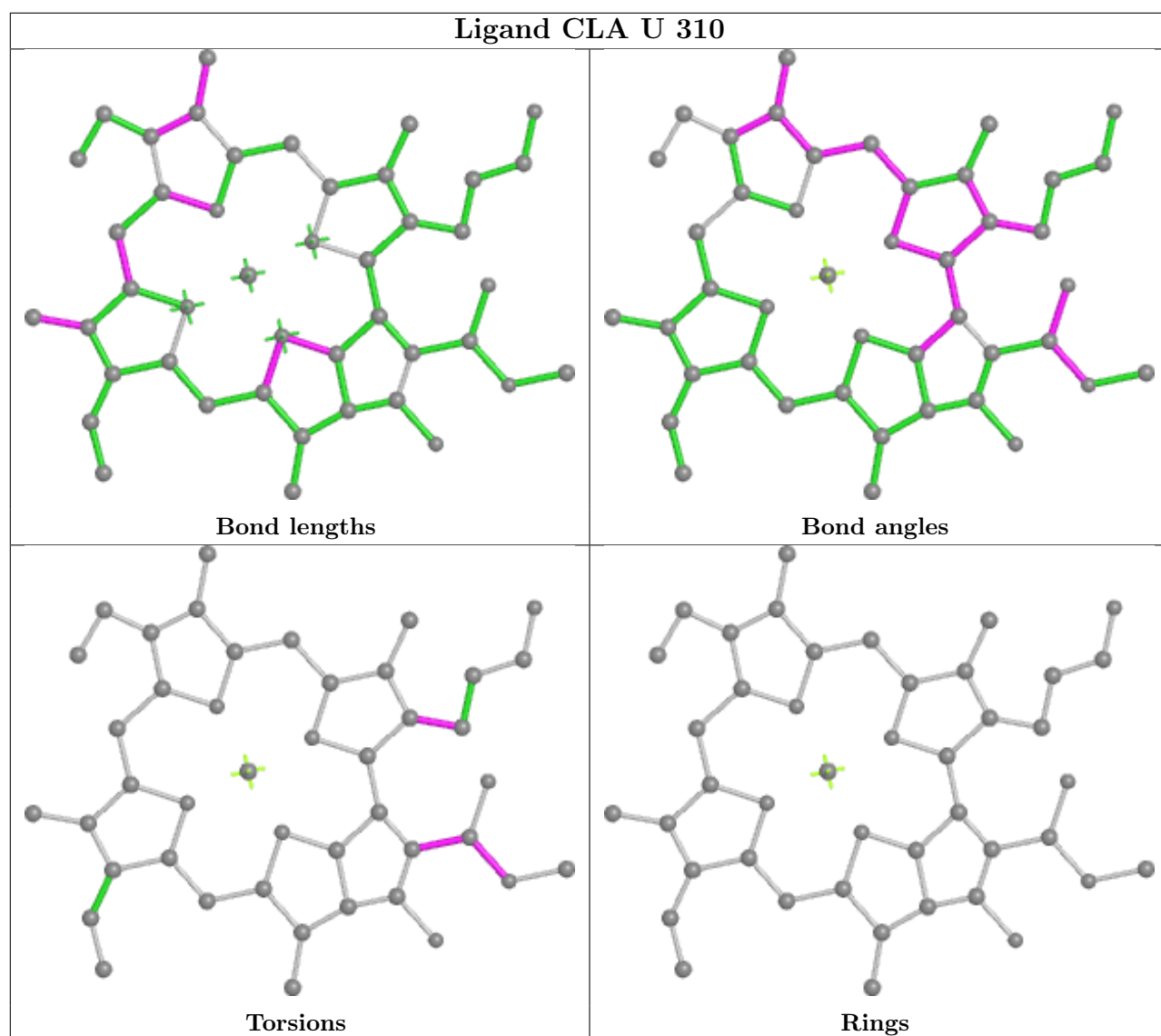
Bond angles



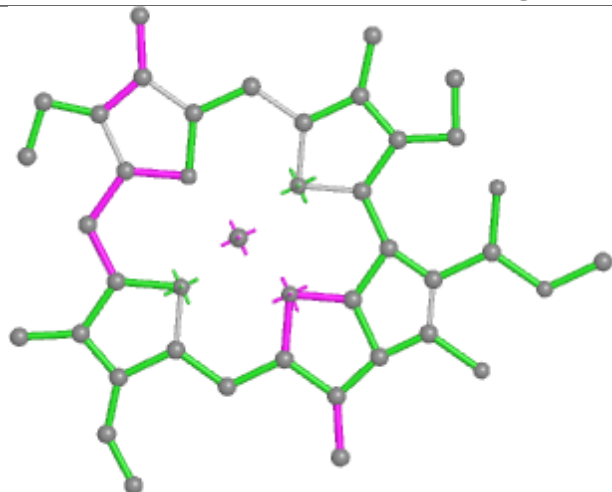
Torsions



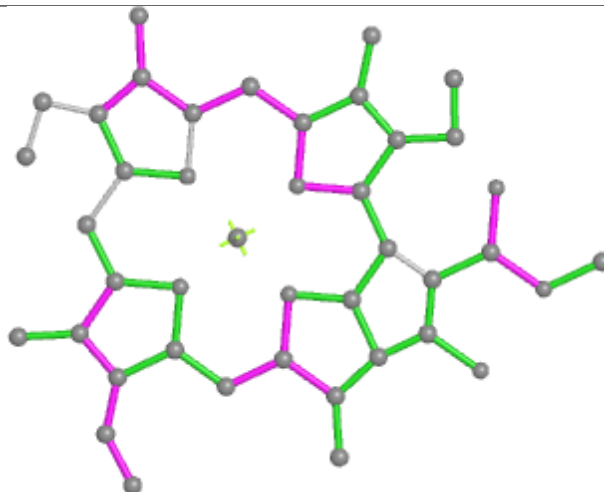
Rings



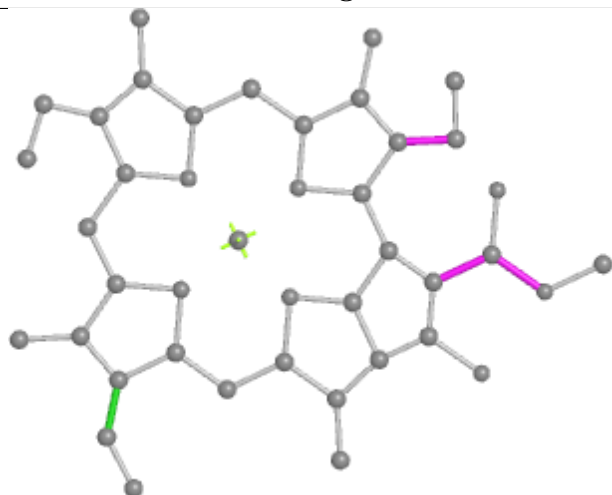
Ligand CLA F 802



Bond lengths



Bond angles

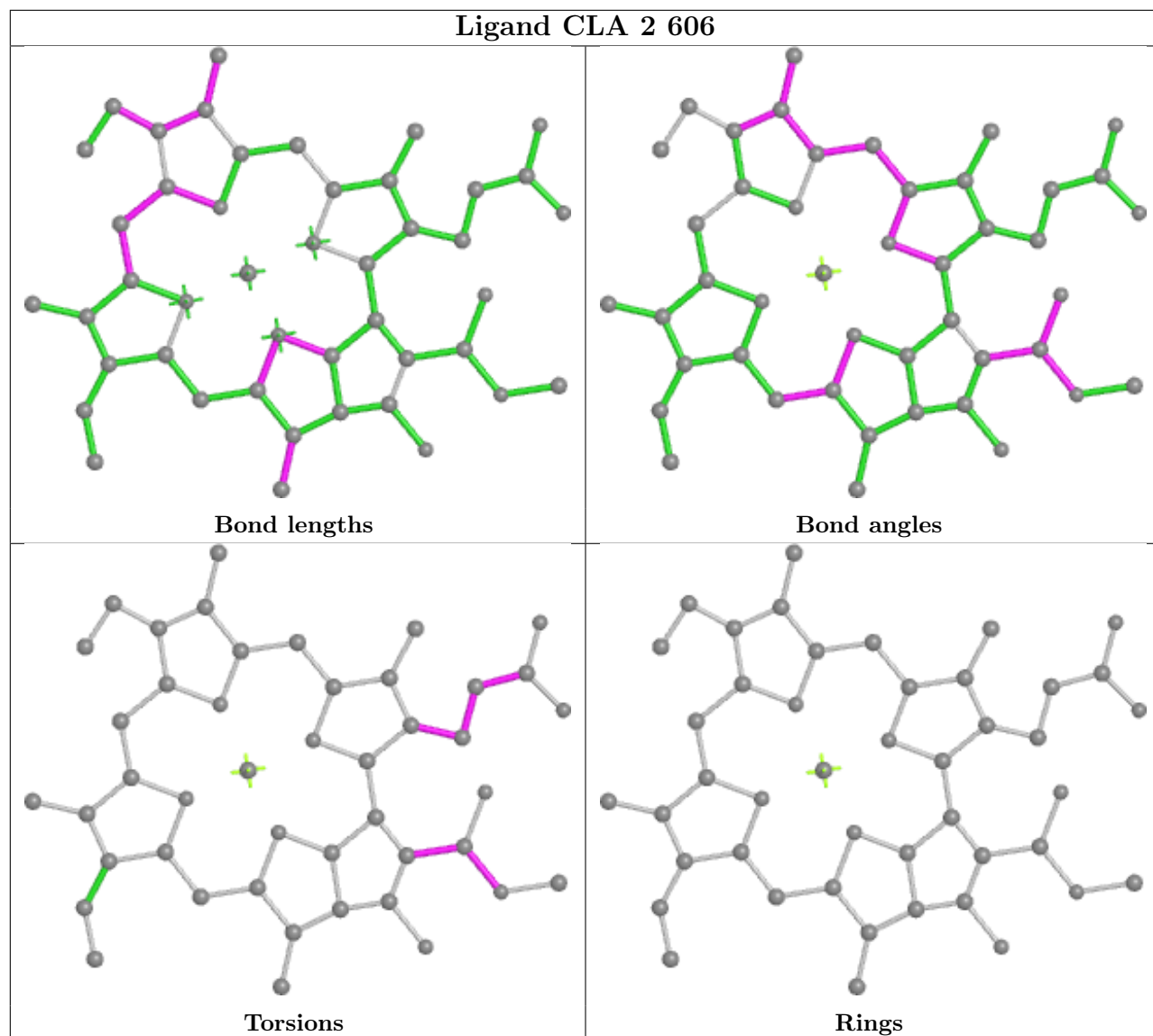


Torsions

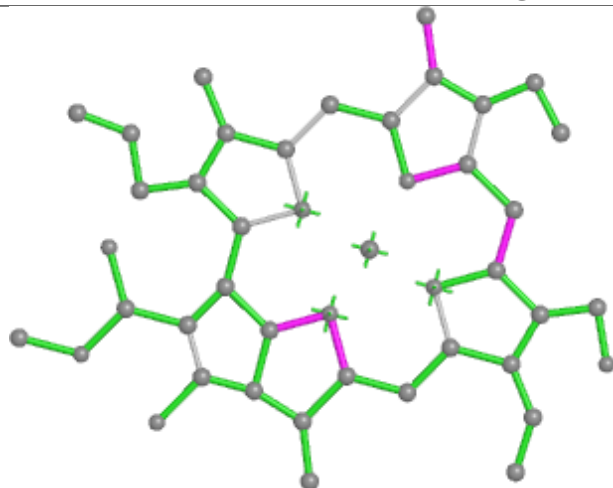


Rings

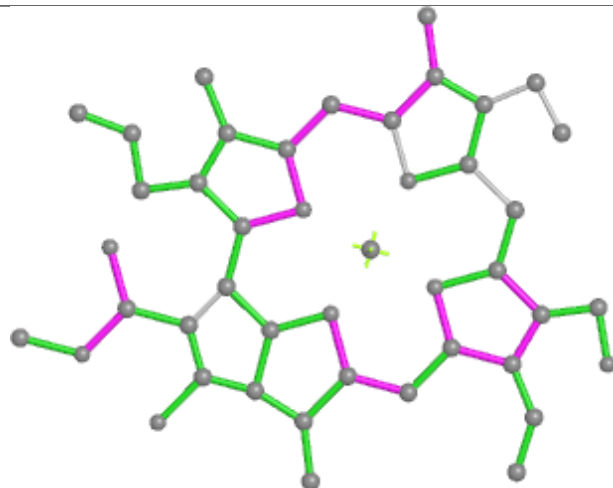
Ligand CLA 2 606



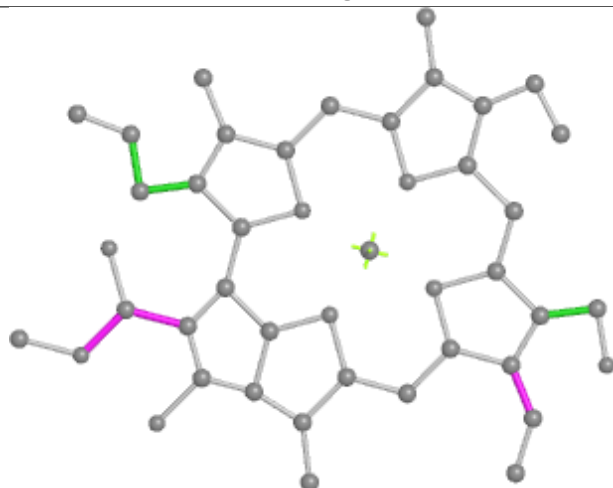
Ligand CHL V 307



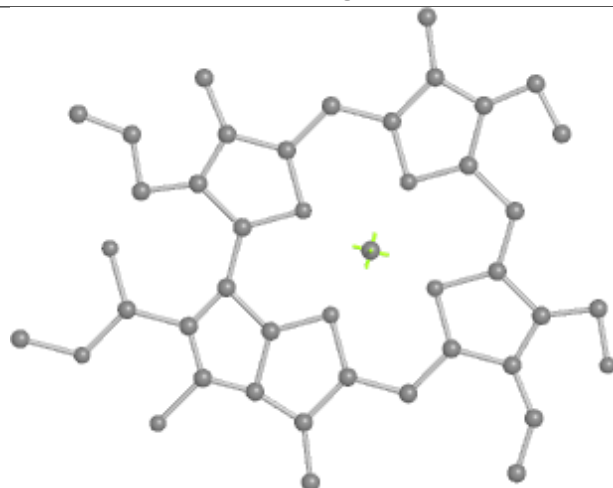
Bond lengths



Bond angles

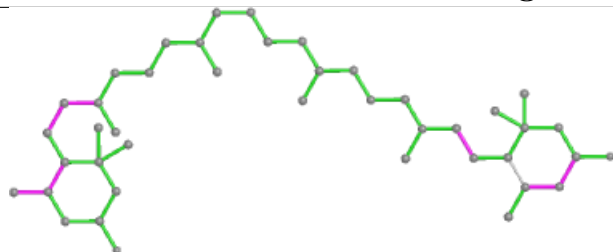


Torsions

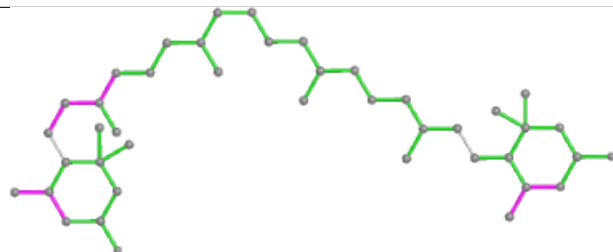


Rings

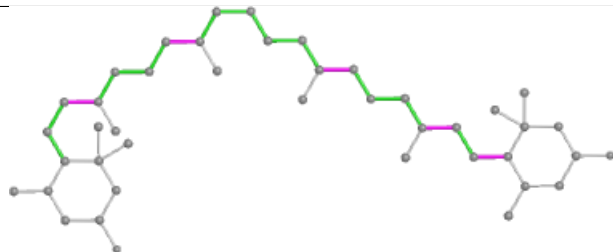
Ligand Q6L R 319



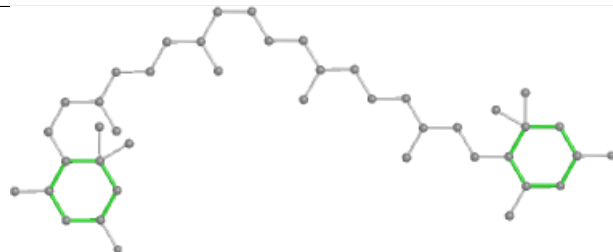
Bond lengths



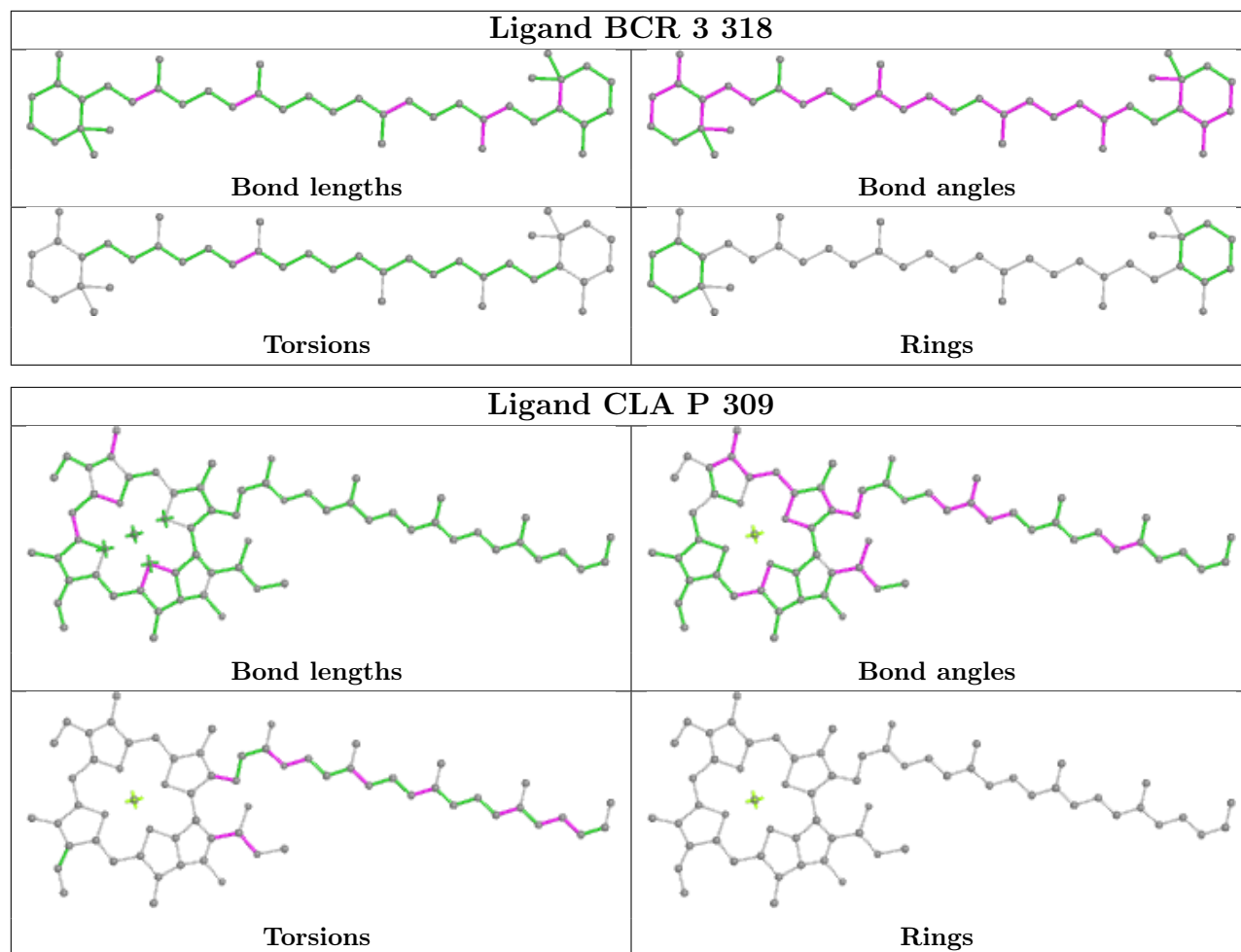
Bond angles



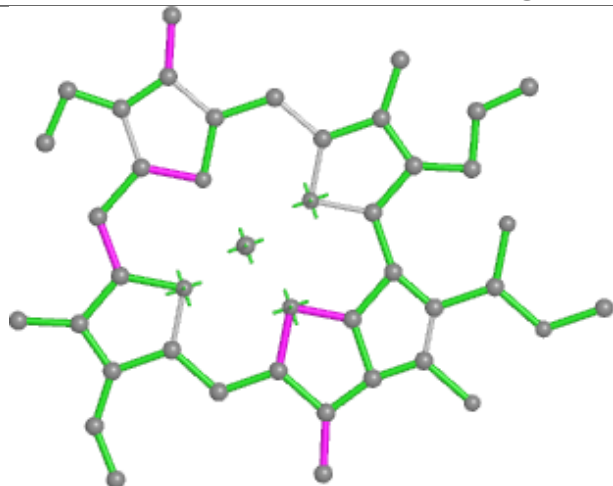
Torsions



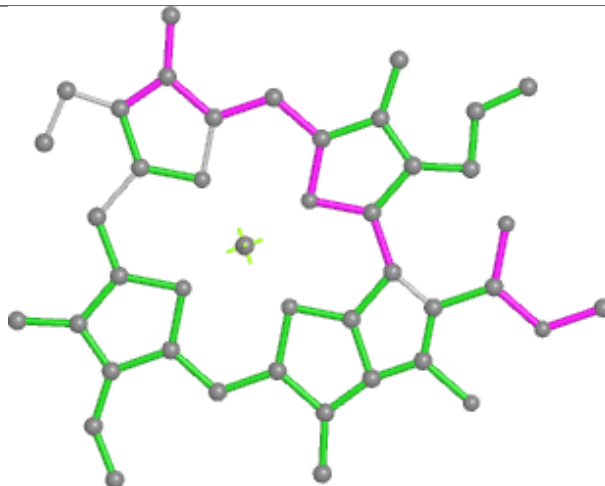
Rings



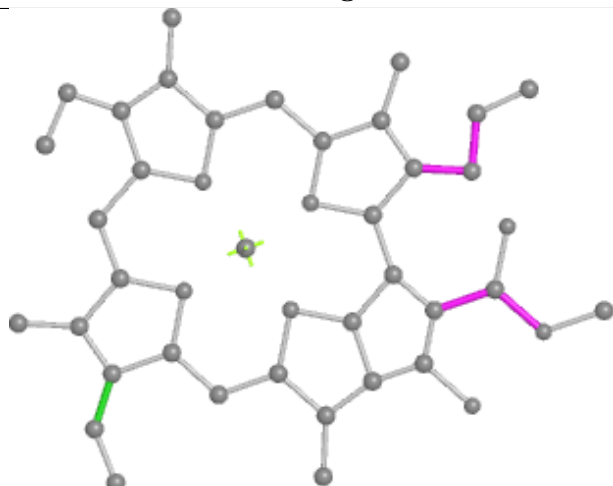
Ligand CLA 3 310



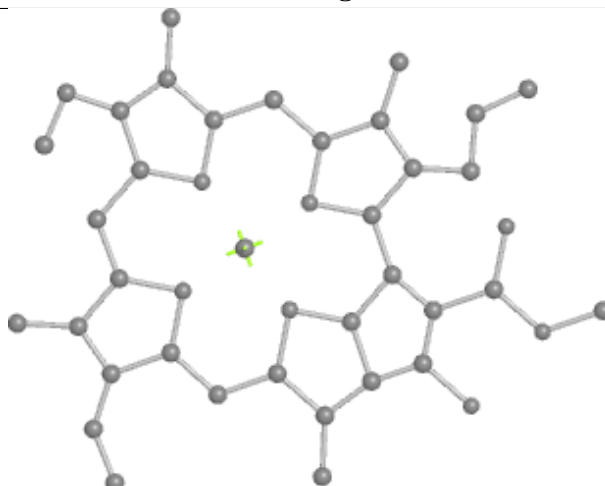
Bond lengths



Bond angles

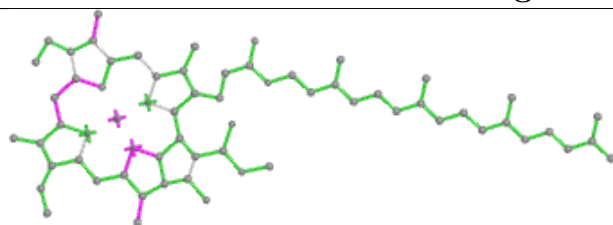


Torsions

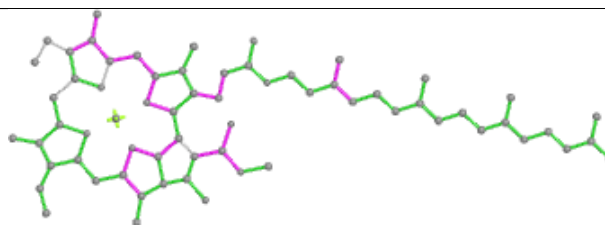


Rings

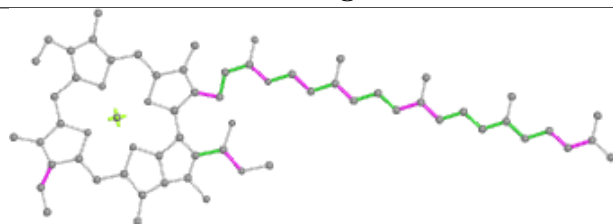
Ligand CLA B 829



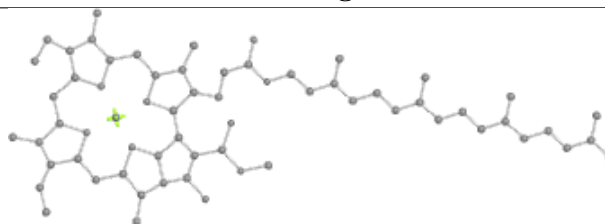
Bond lengths



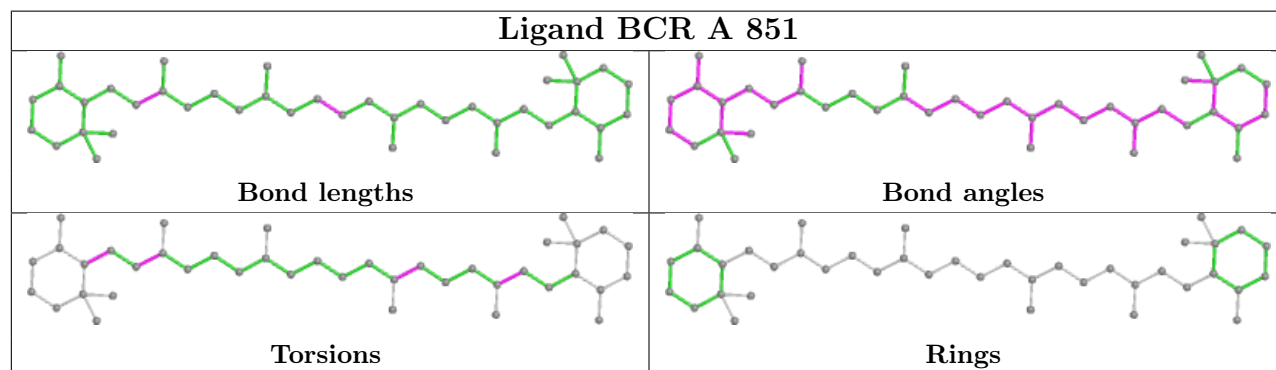
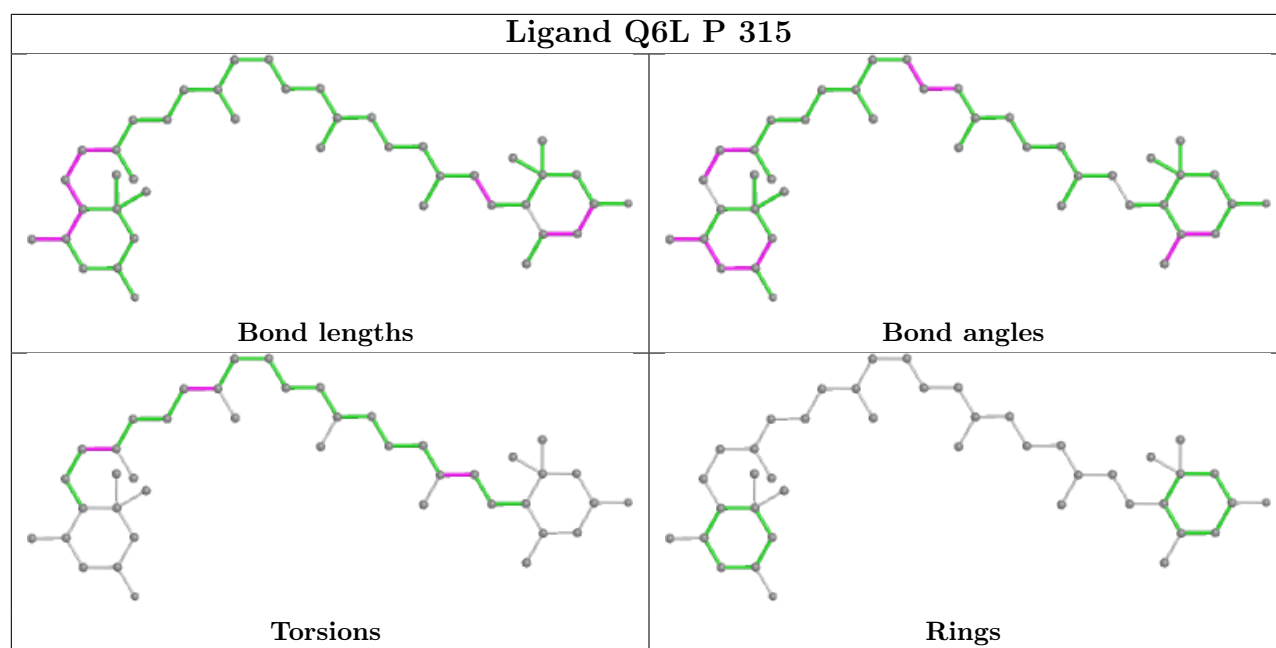
Bond angles



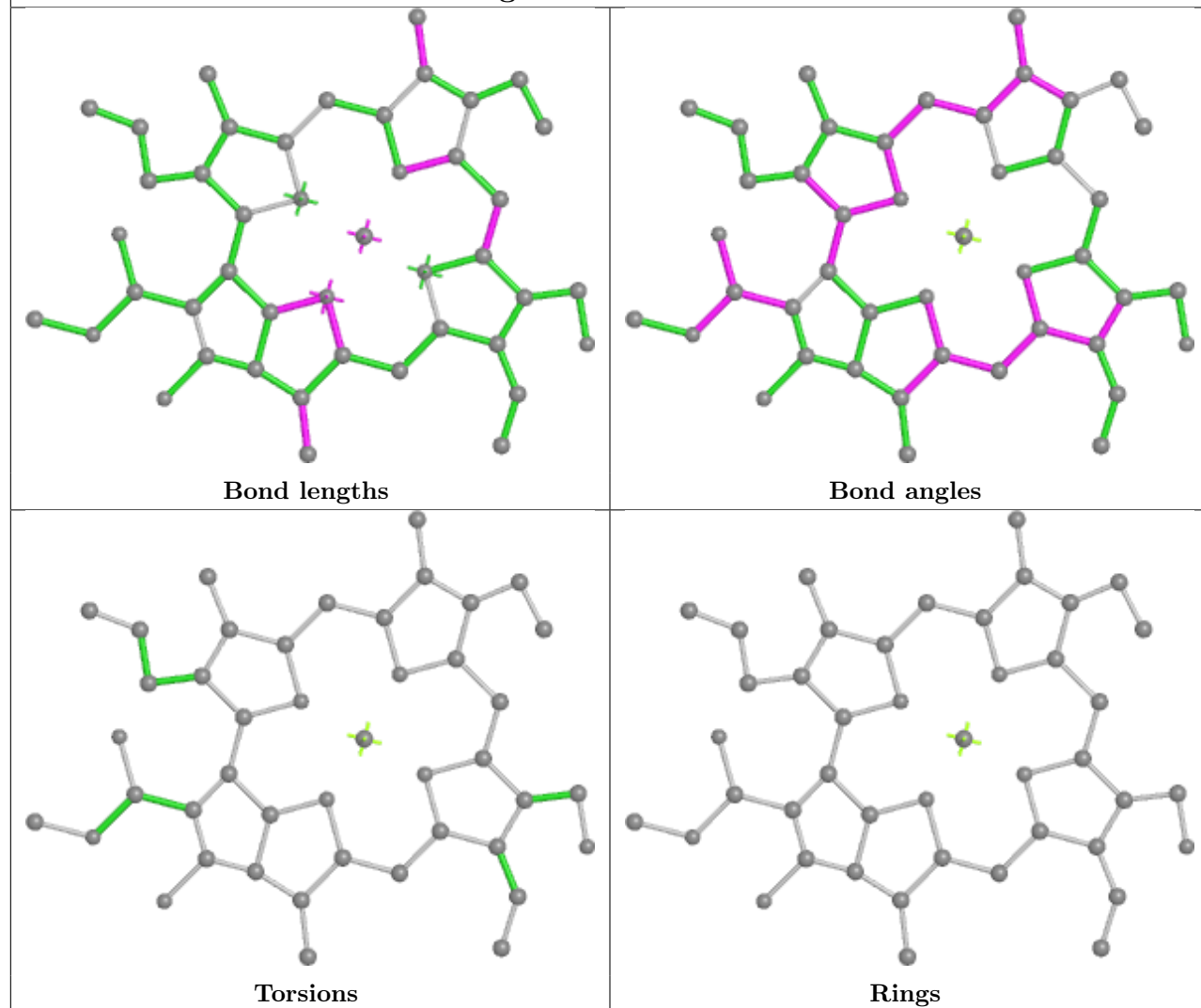
Torsions



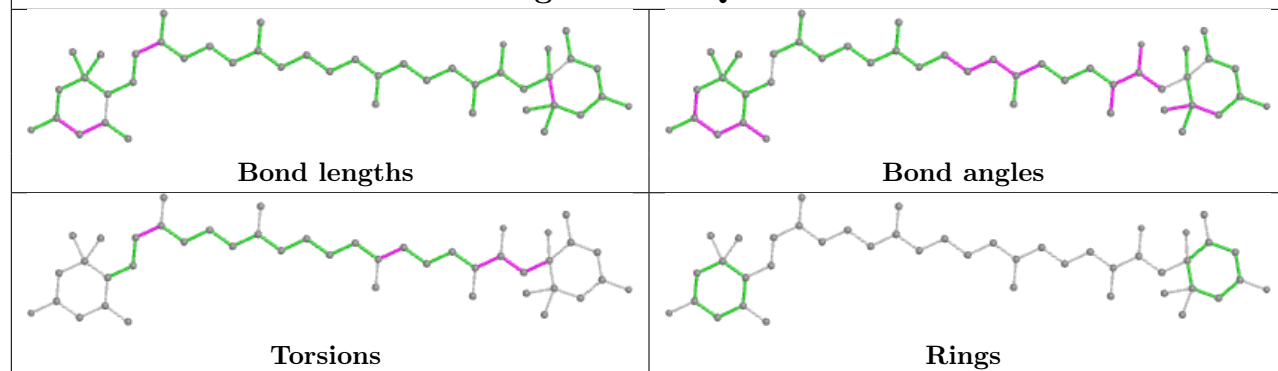
Rings



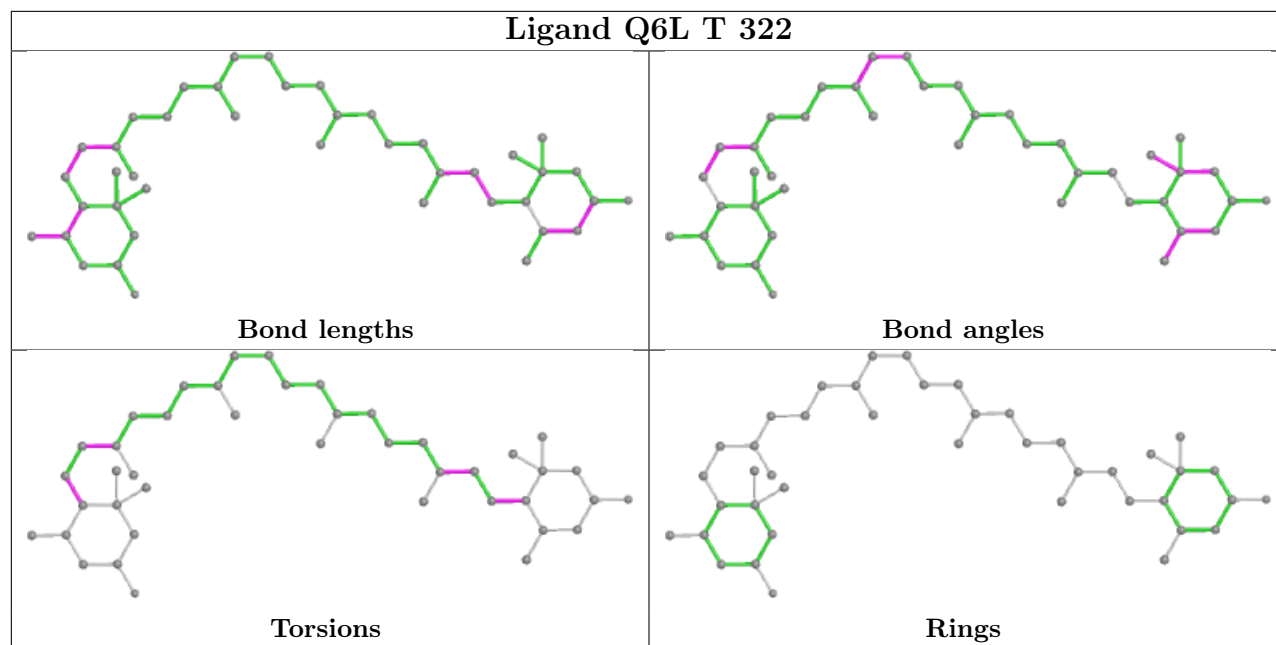
Ligand CHL V 306



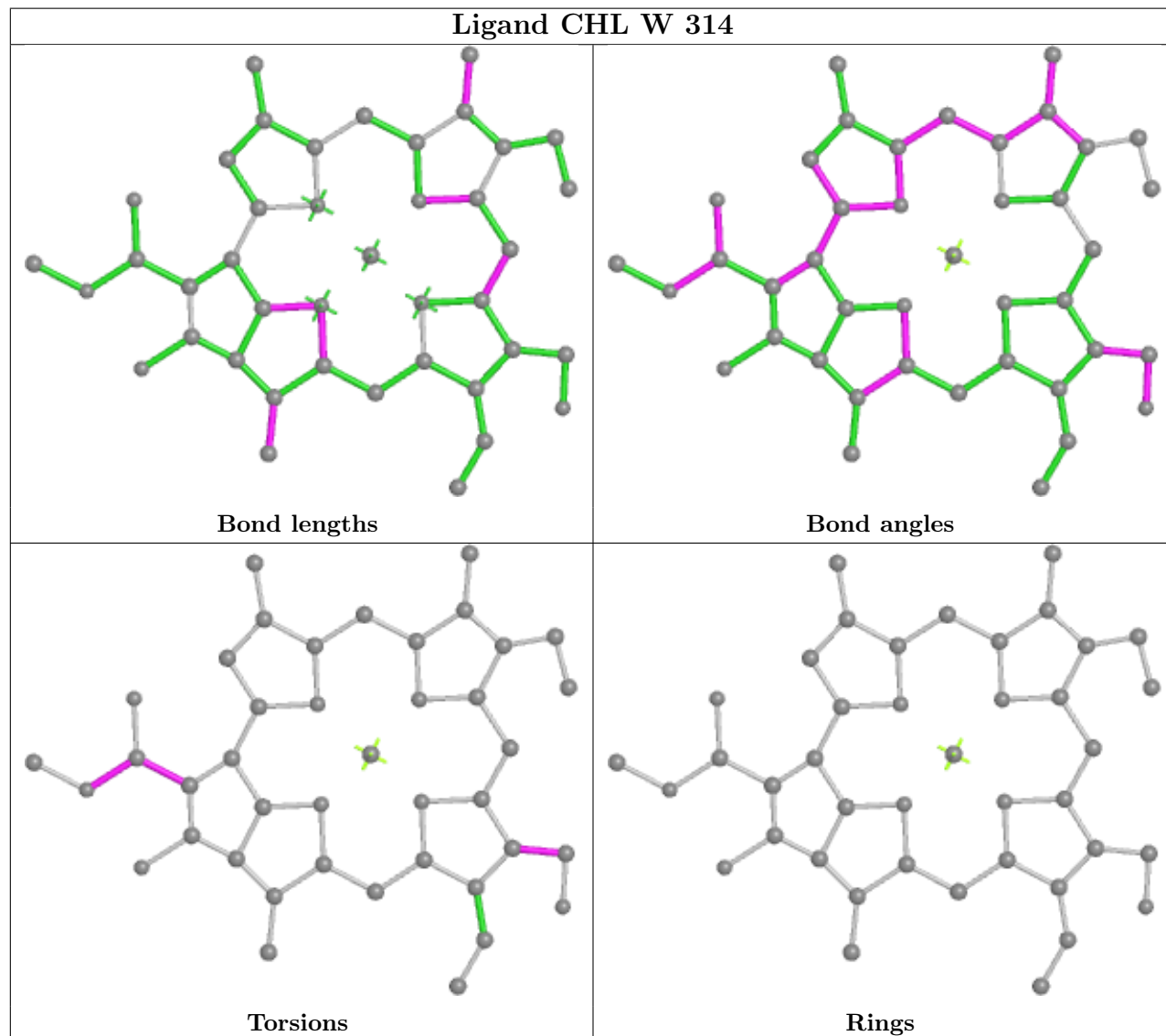
Ligand IWJ Q 320



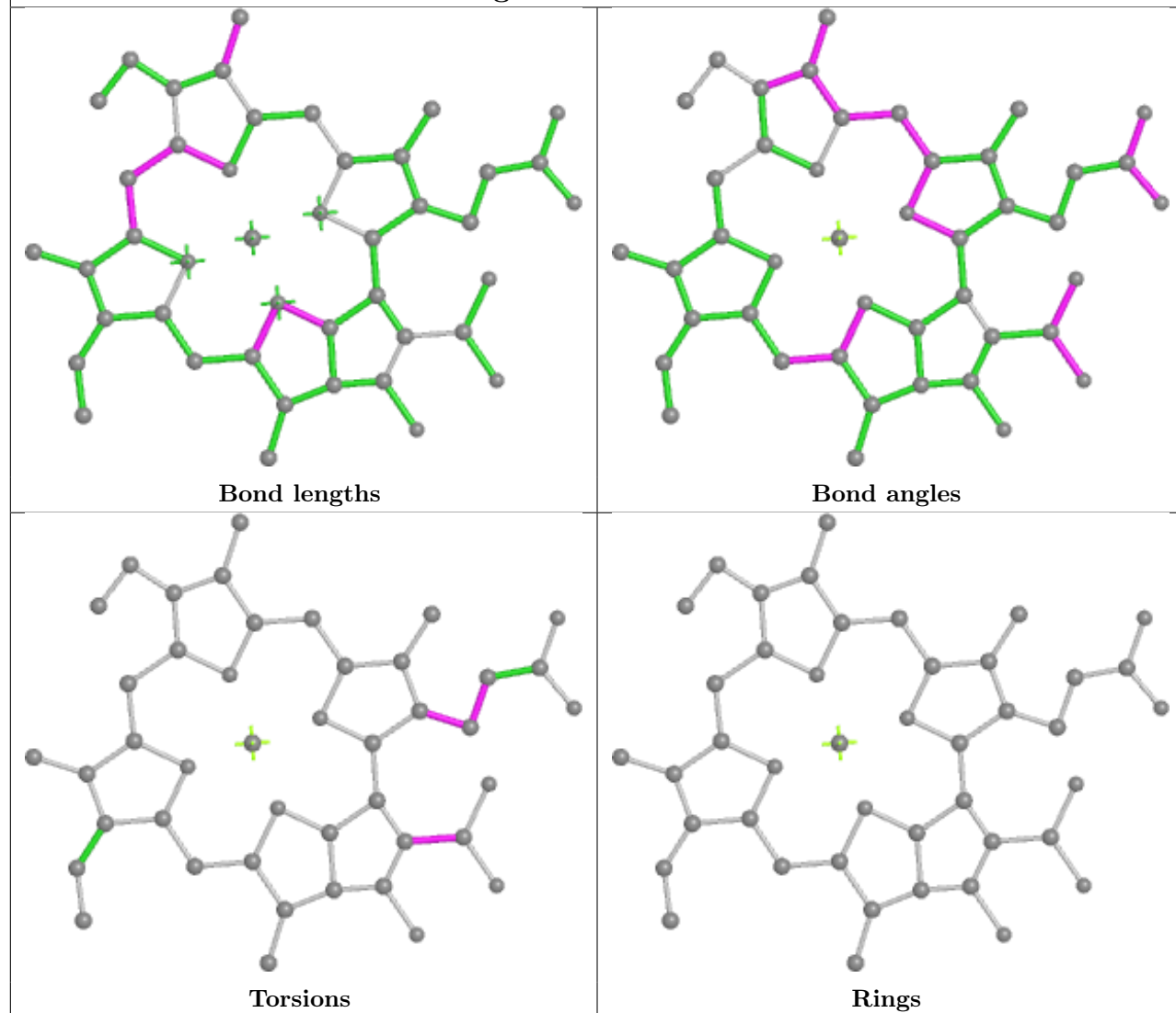
Ligand Q6L T 322



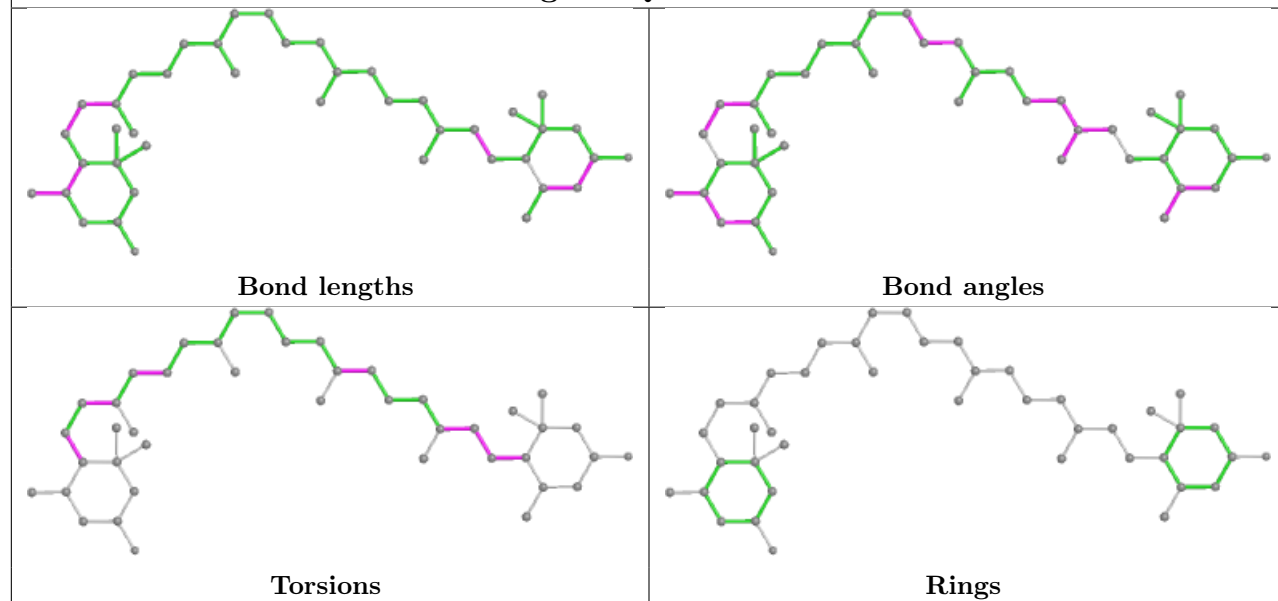
Ligand CHL W 314

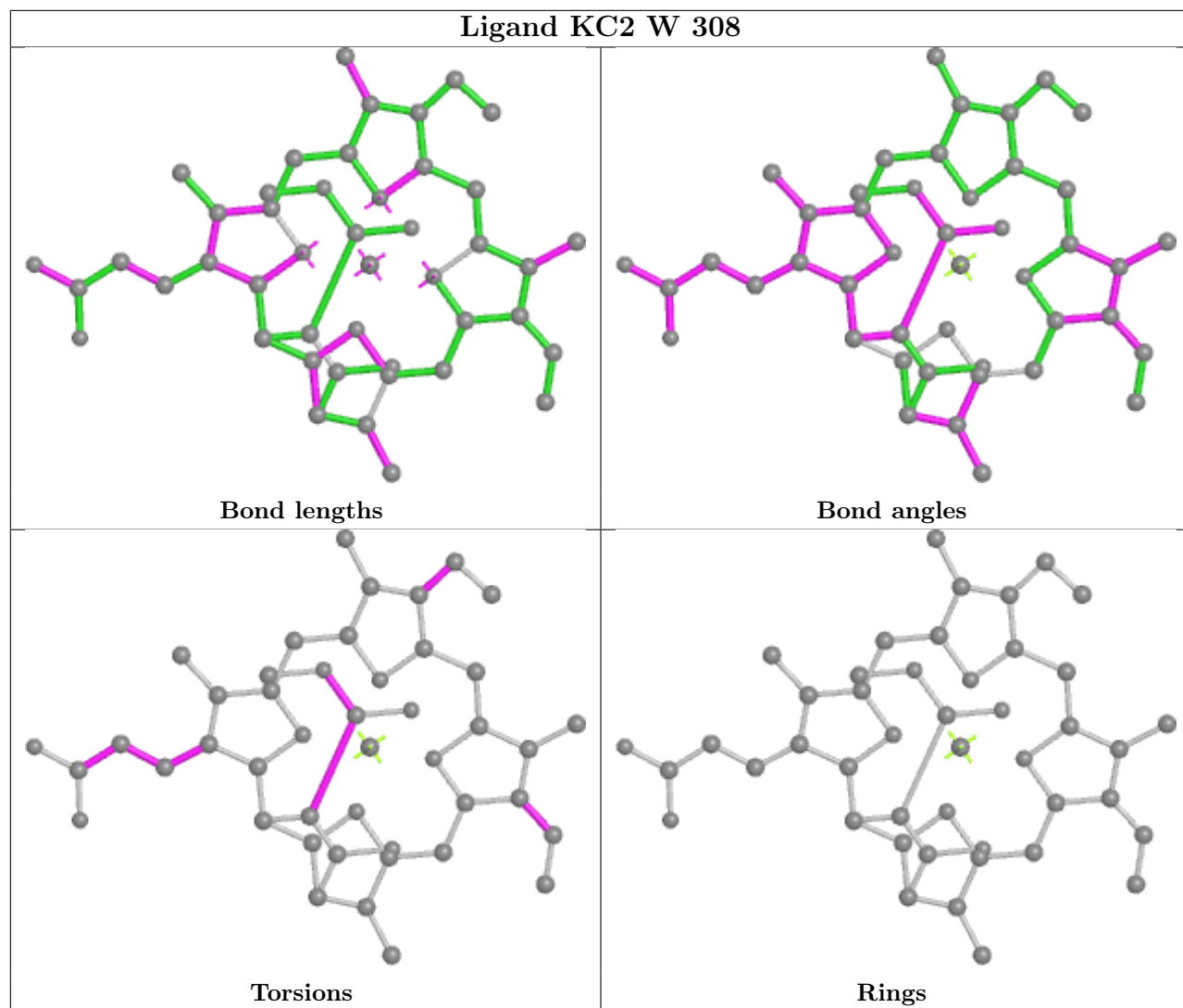


Ligand CLA 2 611

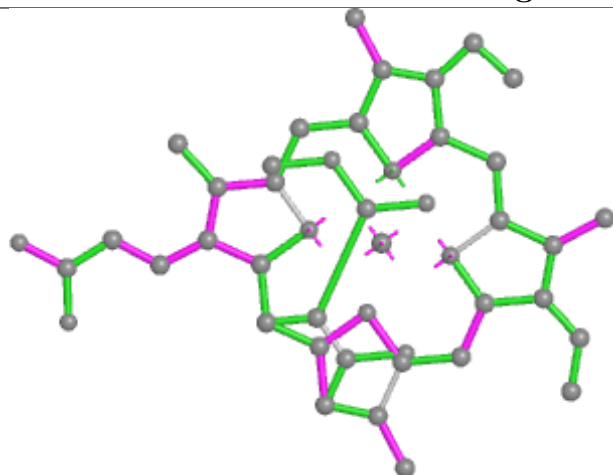


Ligand Q6L 2 616

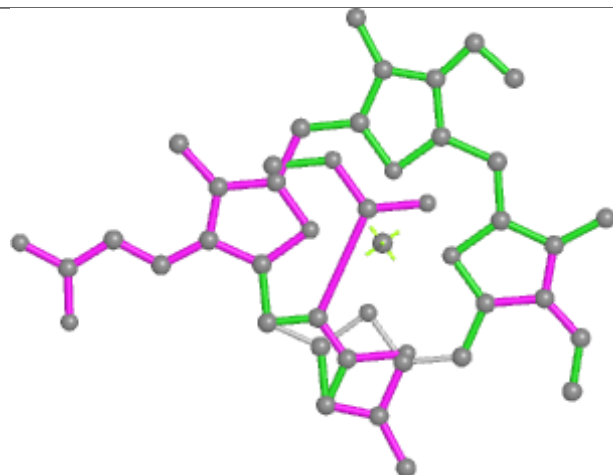




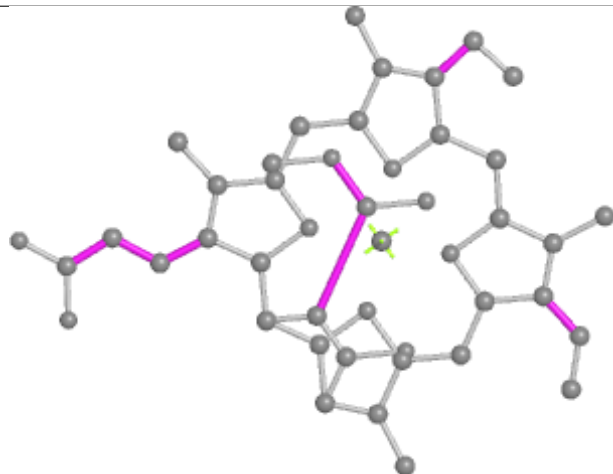
Ligand KC2 V 308



Bond lengths



Bond angles

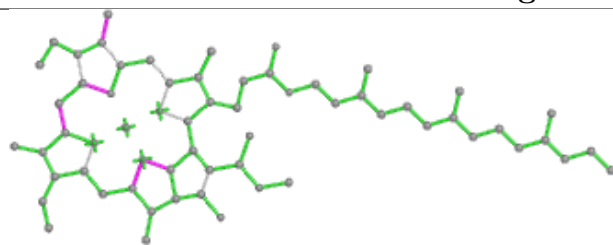


Torsions

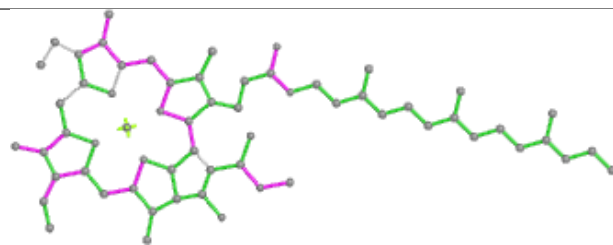


Rings

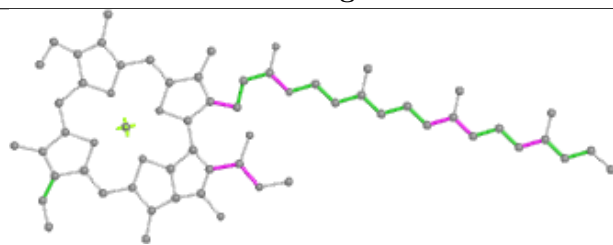
Ligand CLA 6 602



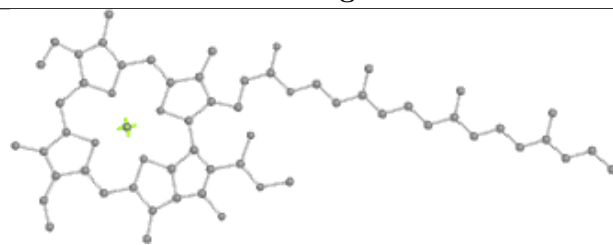
Bond lengths



Bond angles

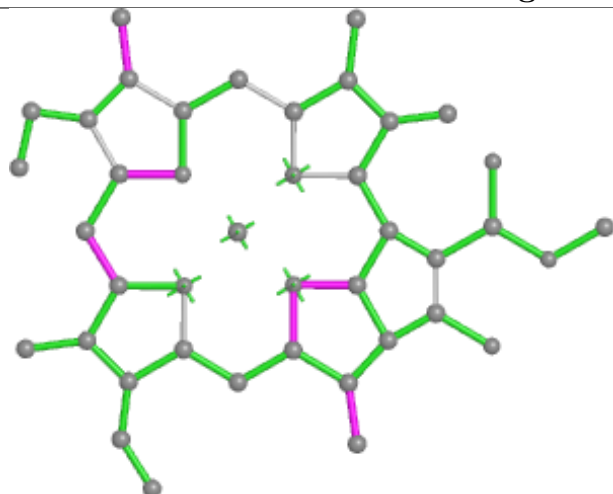


Torsions

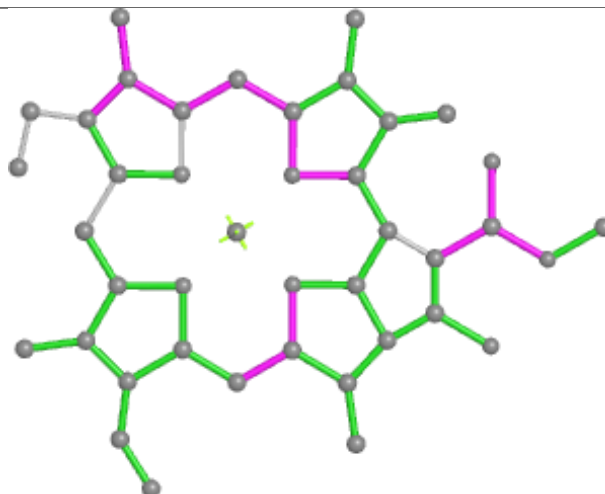


Rings

Ligand CLA 5 610



Bond lengths



Bond angles

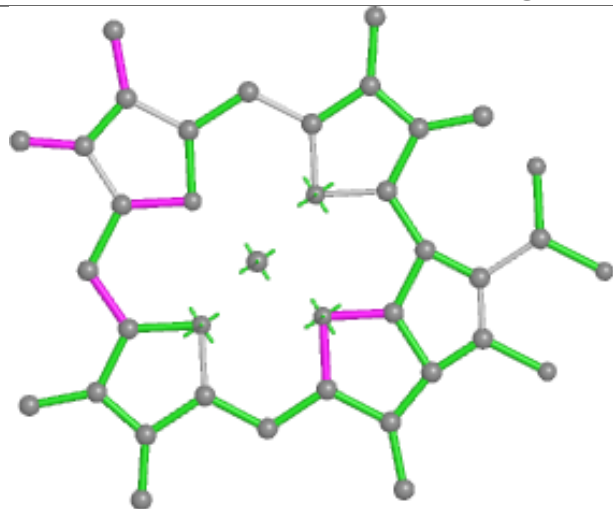


Torsions

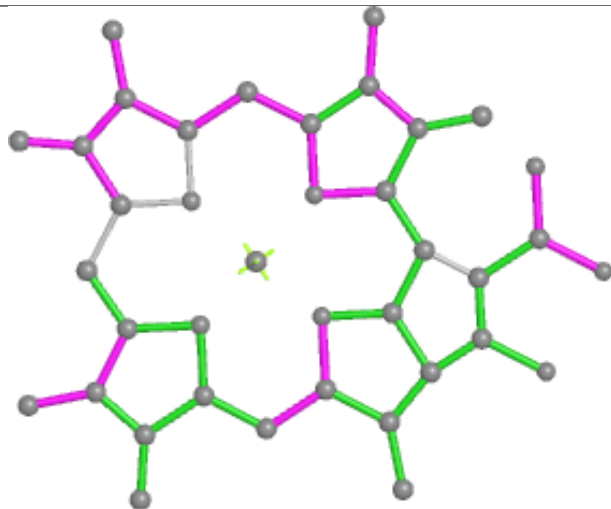


Rings

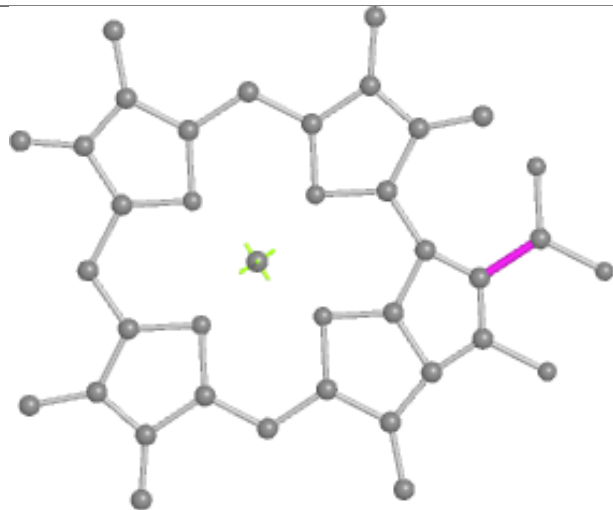
Ligand CLA 1 609



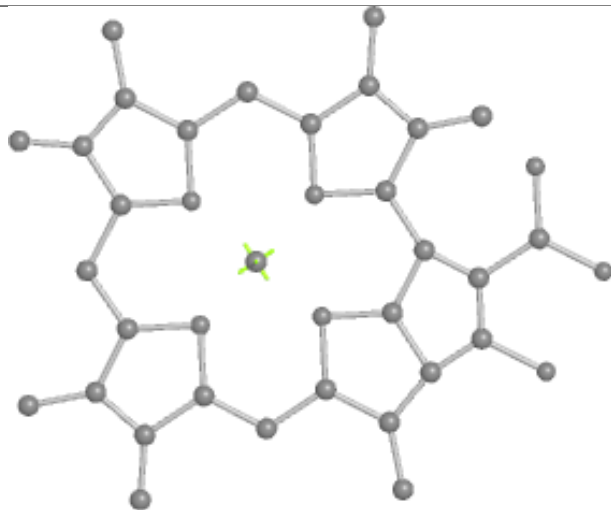
Bond lengths



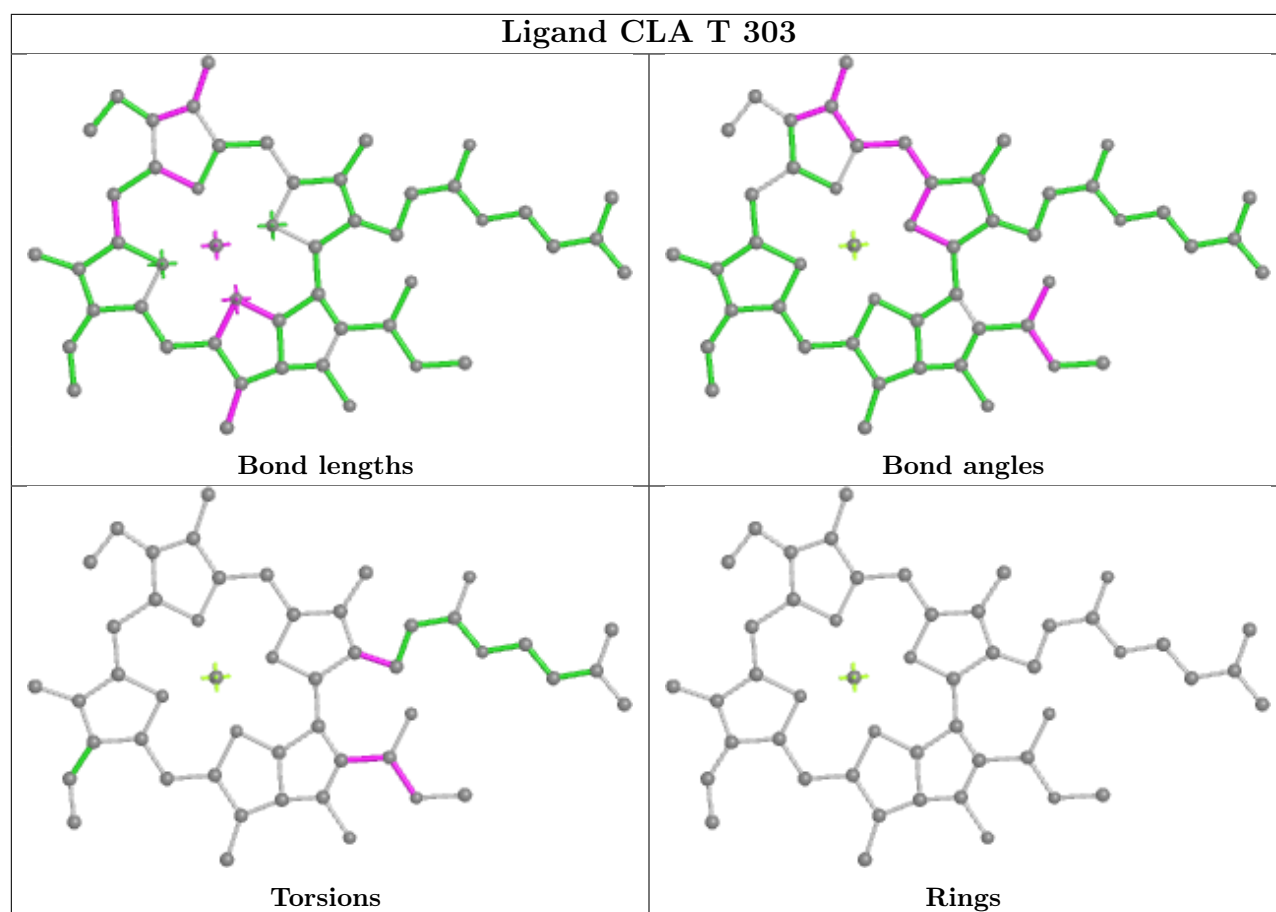
Bond angles

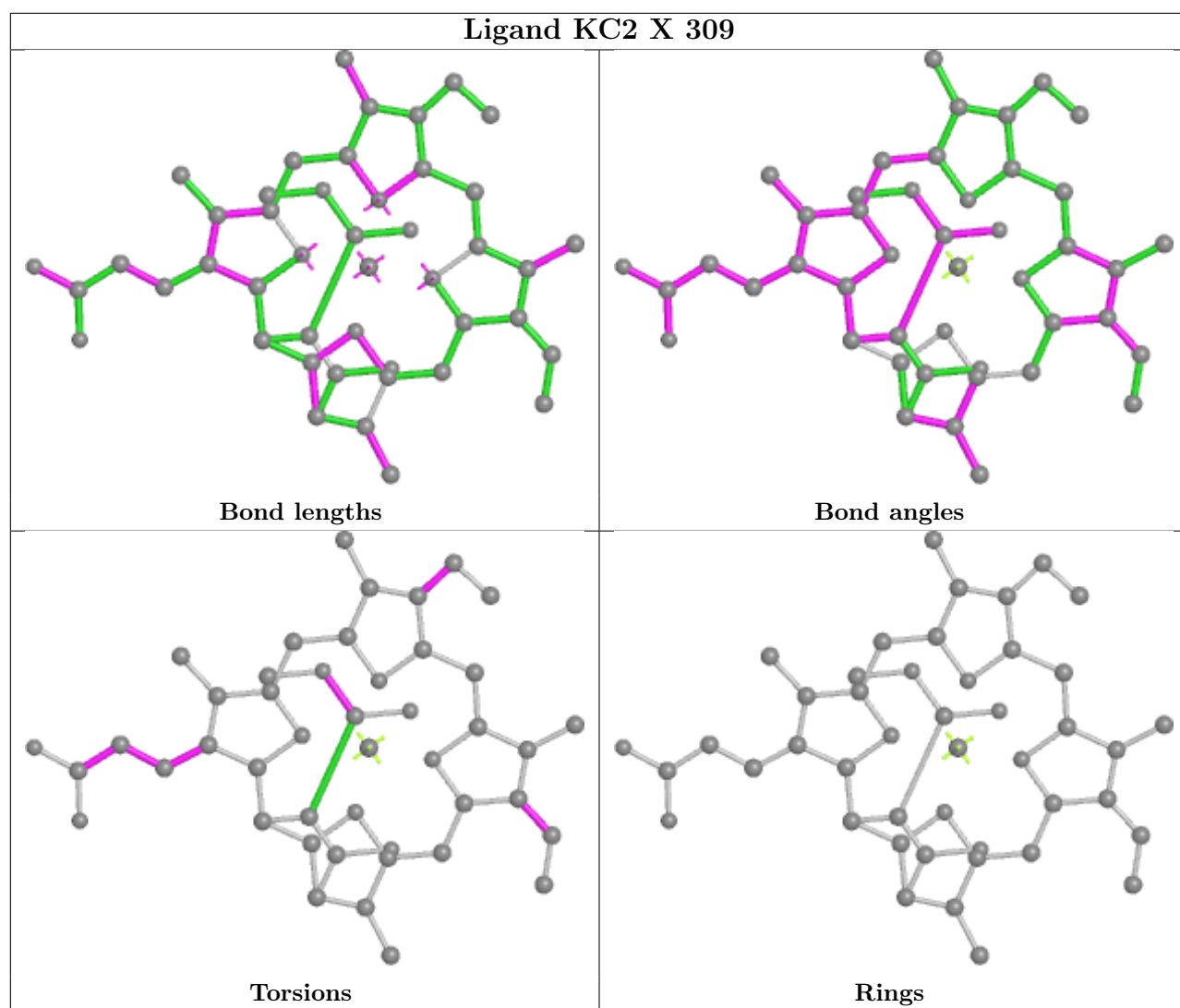


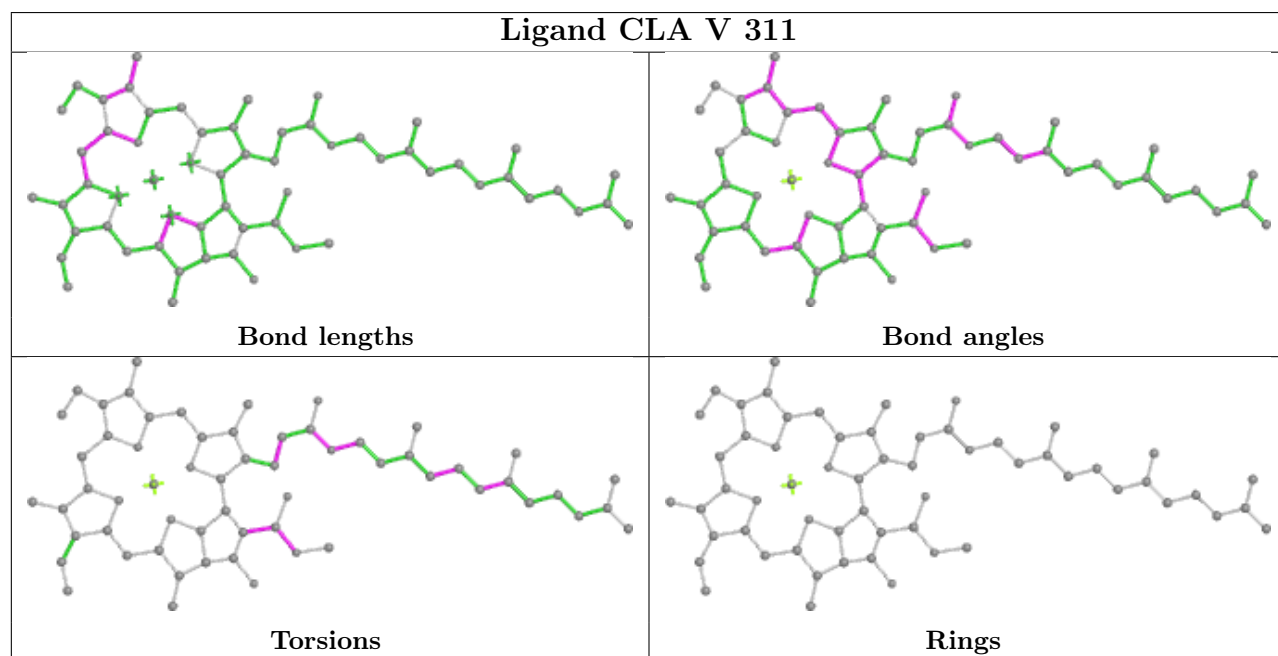
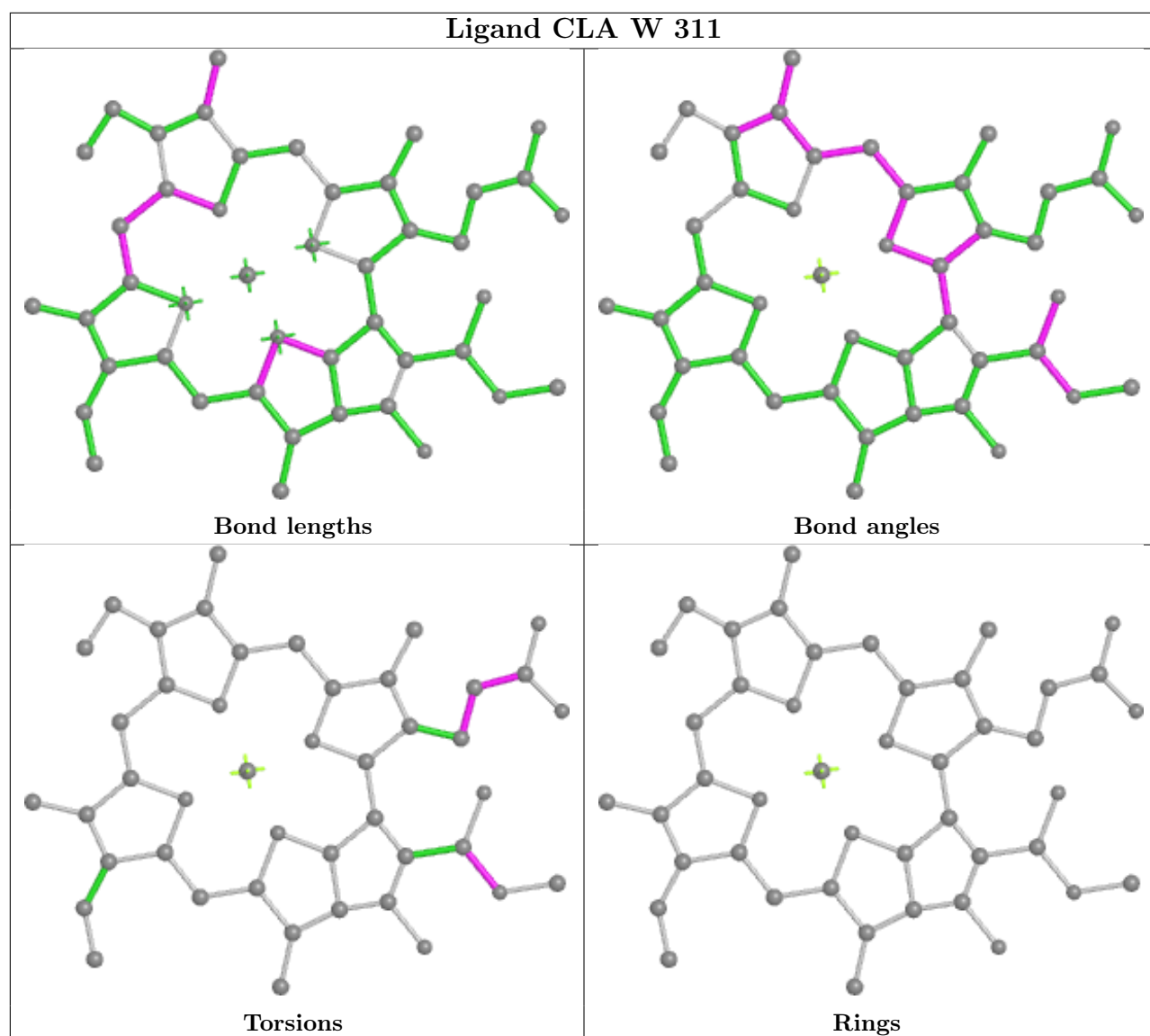
Torsions



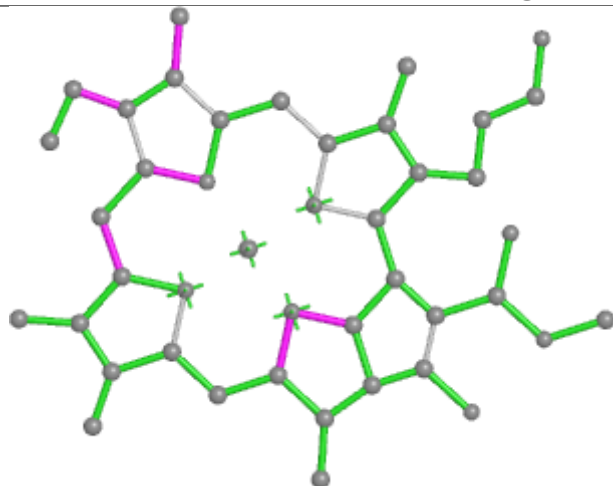
Rings



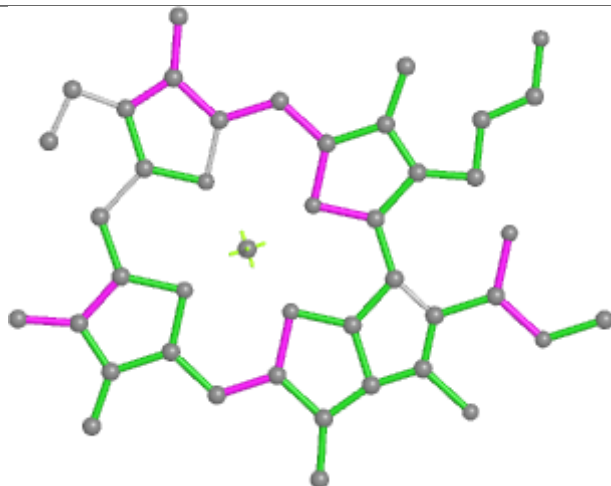




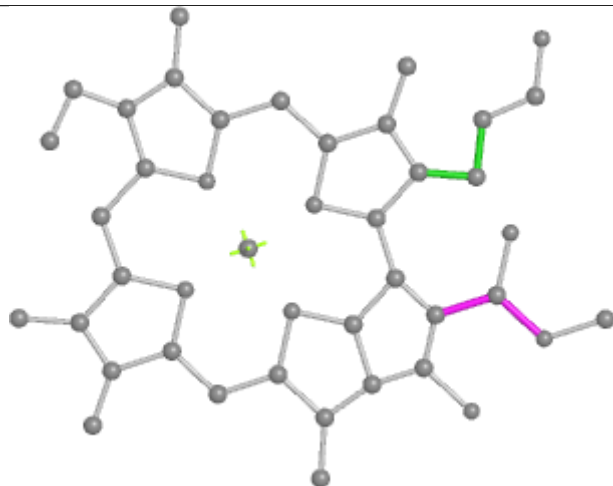
Ligand CLA 2 604



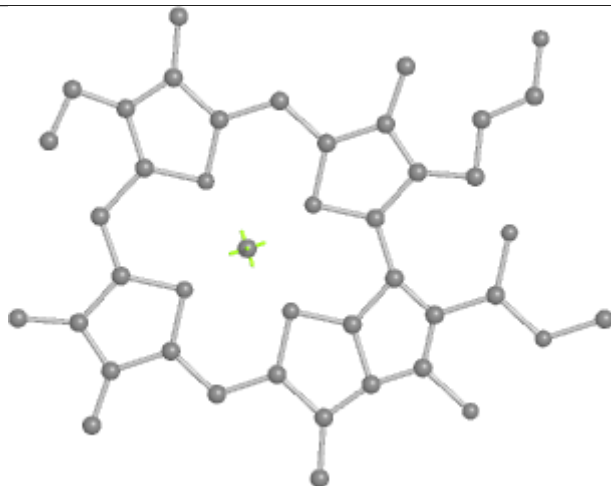
Bond lengths



Bond angles

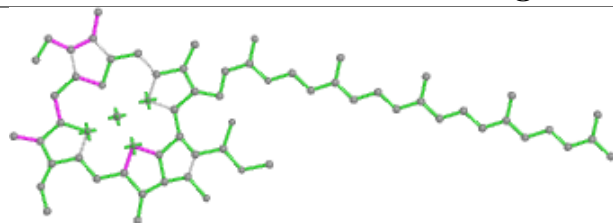


Torsions

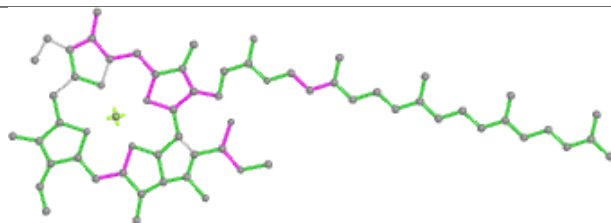


Rings

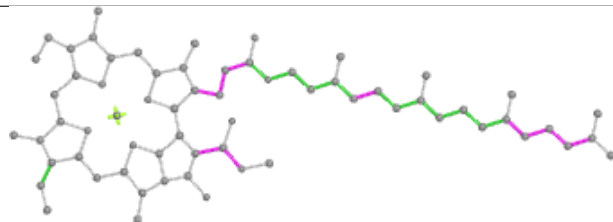
Ligand CLA B 843



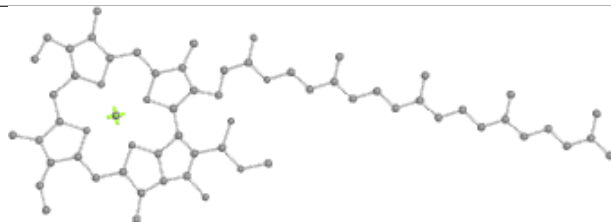
Bond lengths



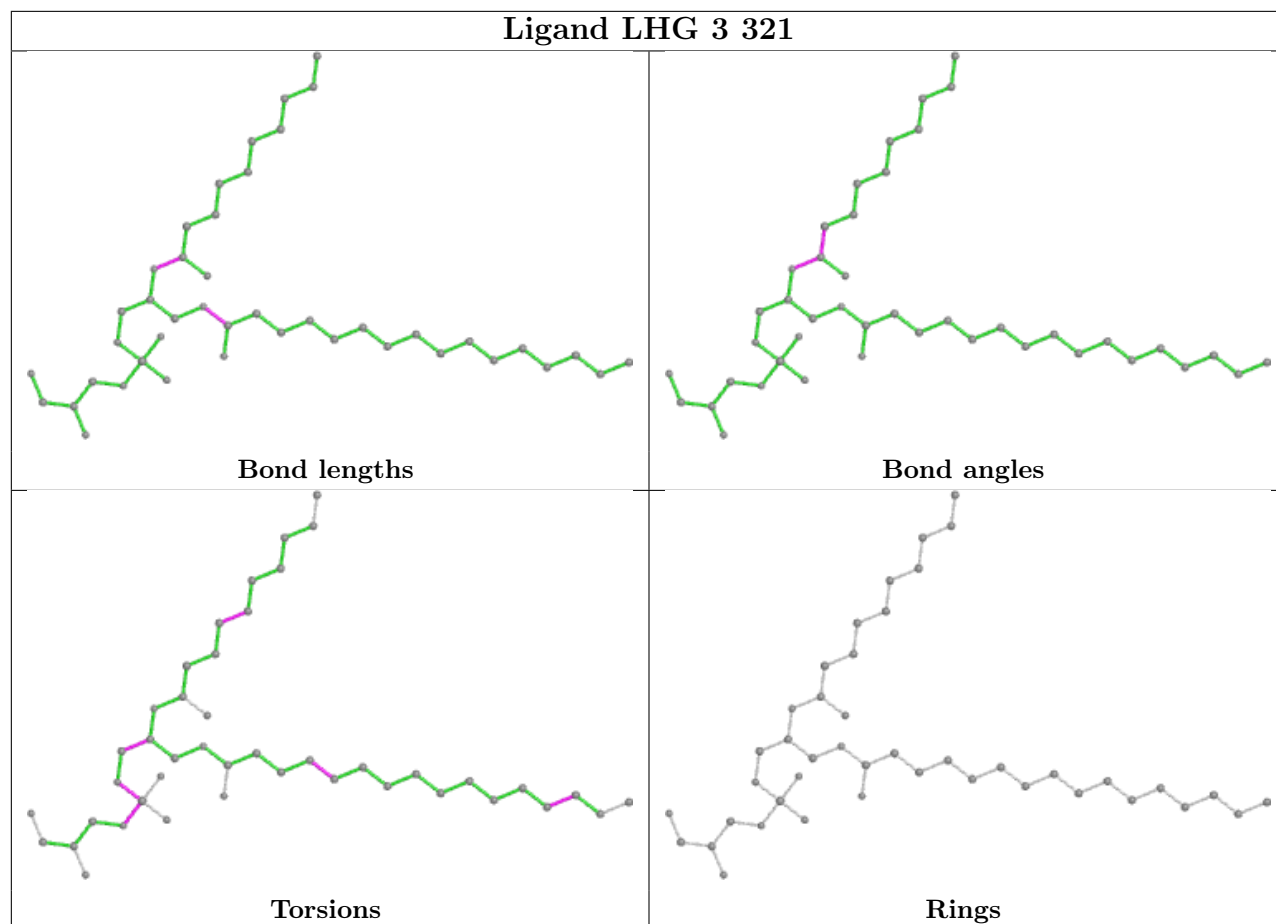
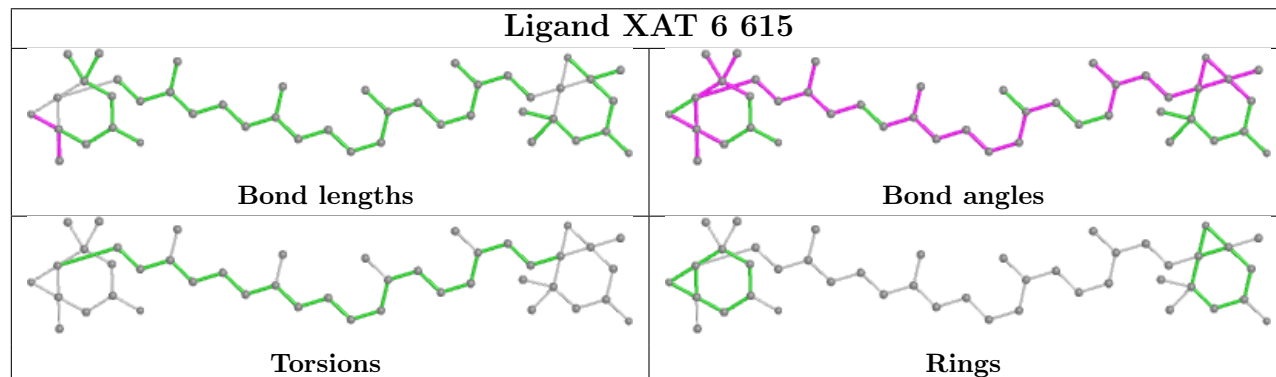
Bond angles



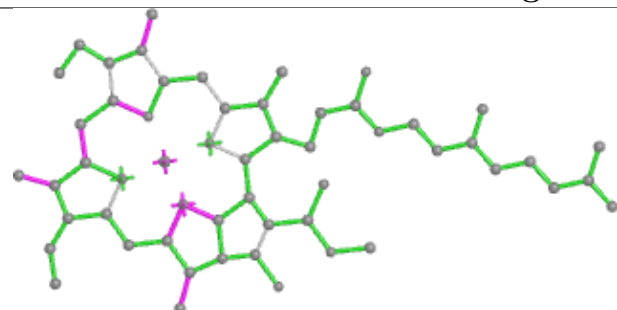
Torsions



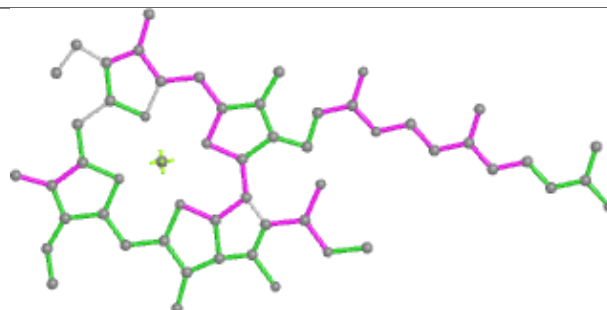
Rings

Ligand LHG 3 321**Ligand XAT 6 615**

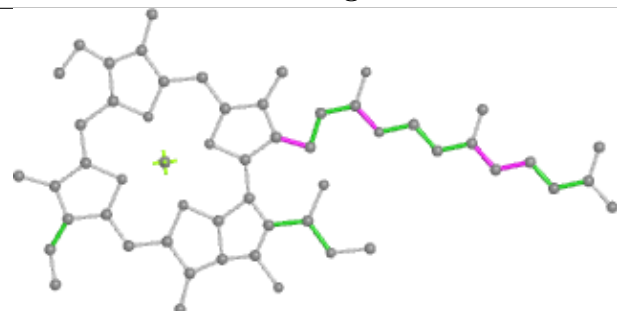
Ligand CLA 3 302



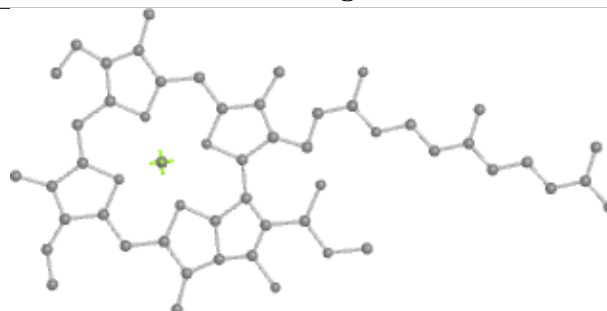
Bond lengths



Bond angles

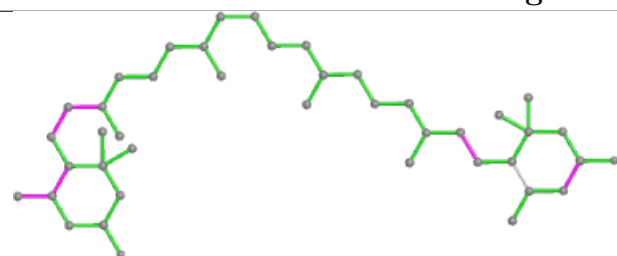


Torsions

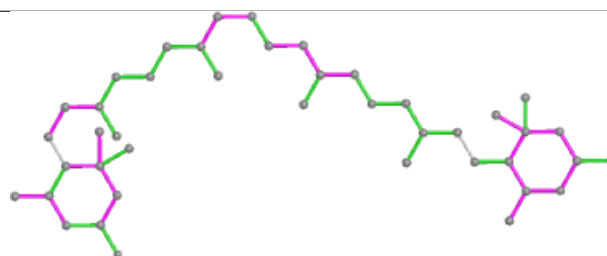


Rings

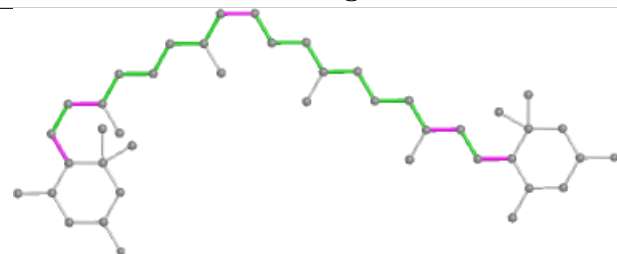
Ligand Q6L S 323



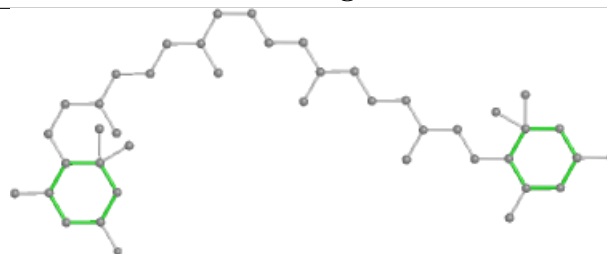
Bond lengths



Bond angles

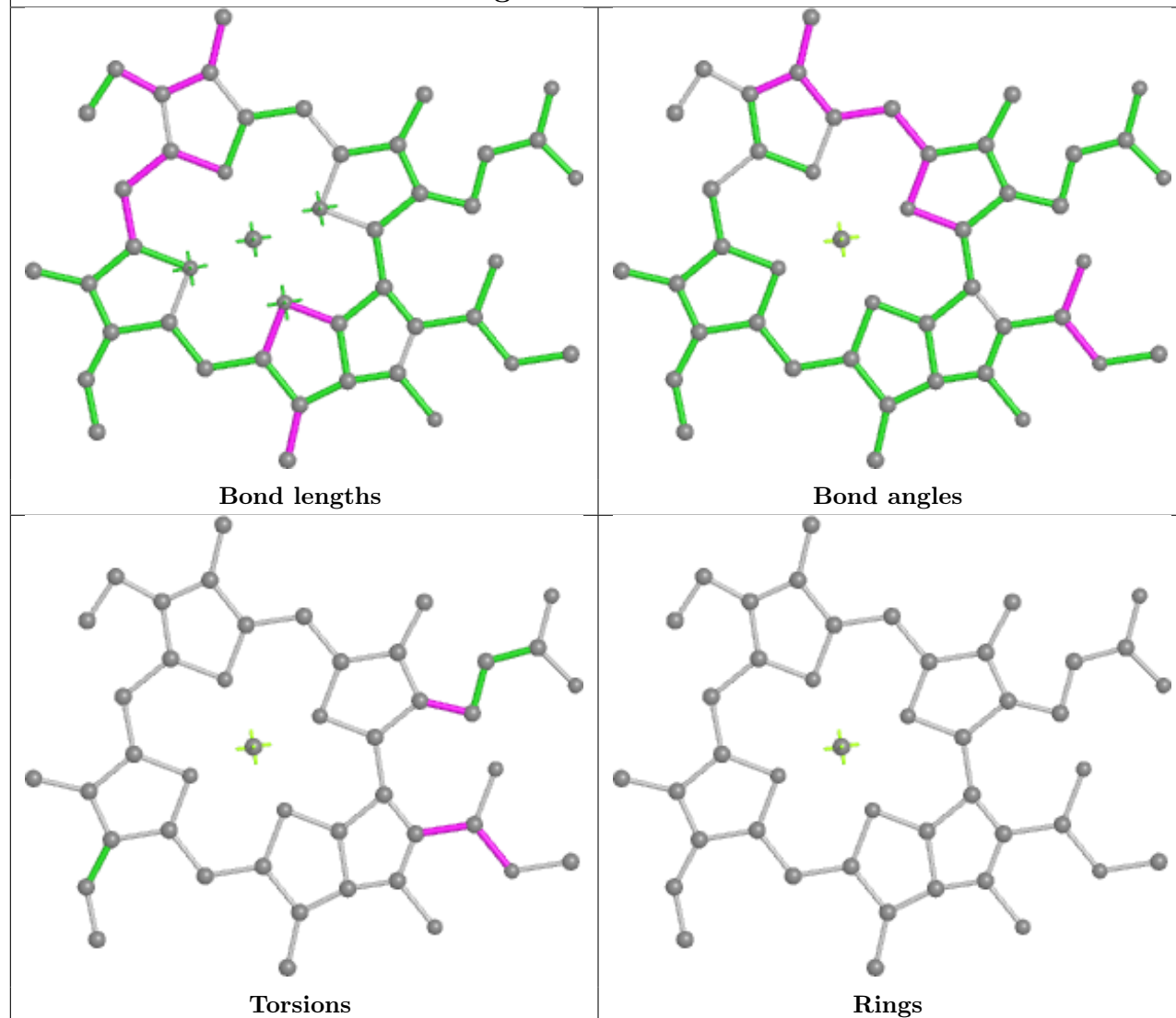


Torsions

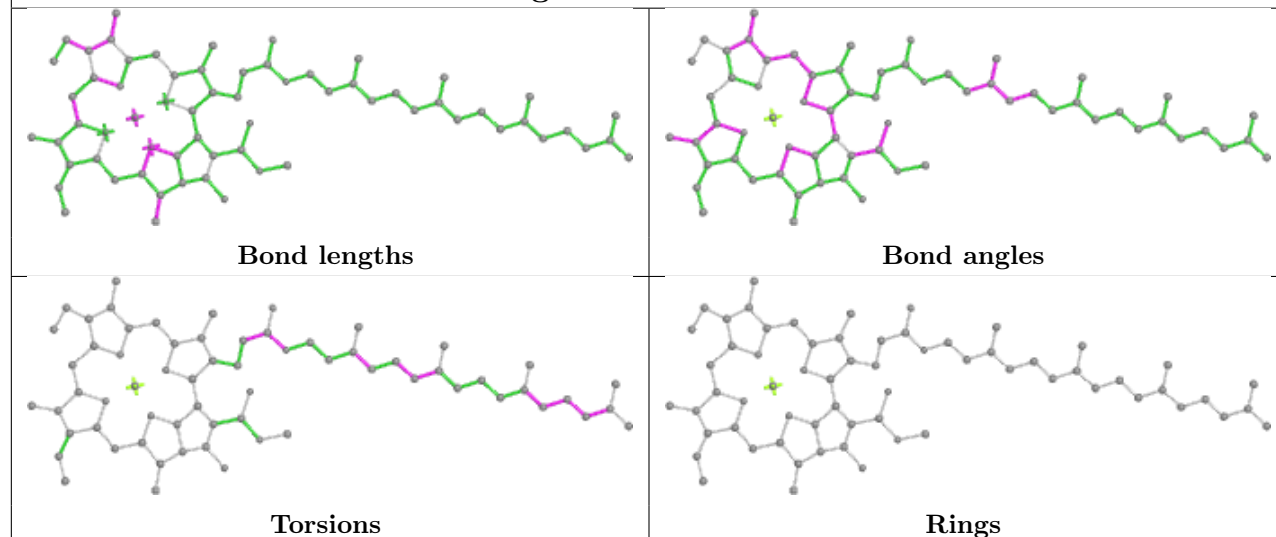


Rings

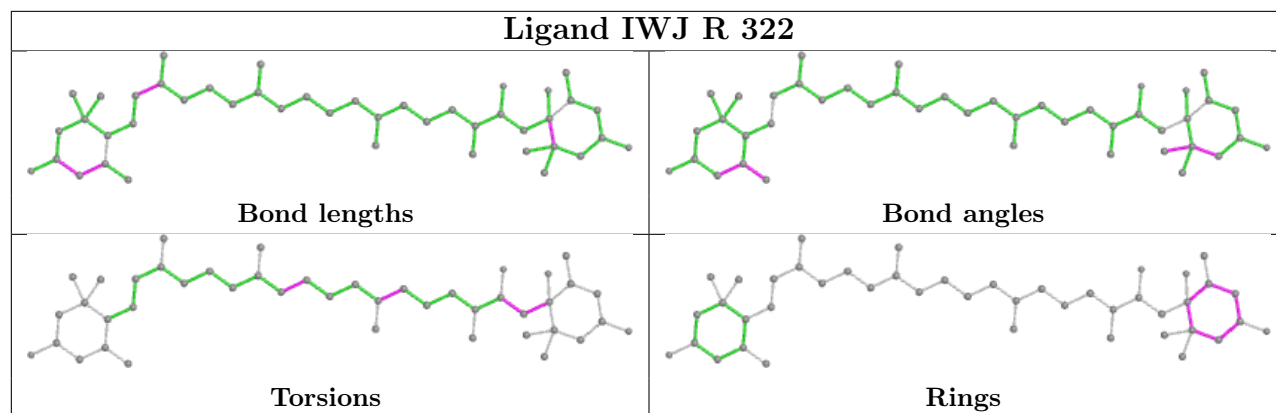
Ligand CLA 6 612



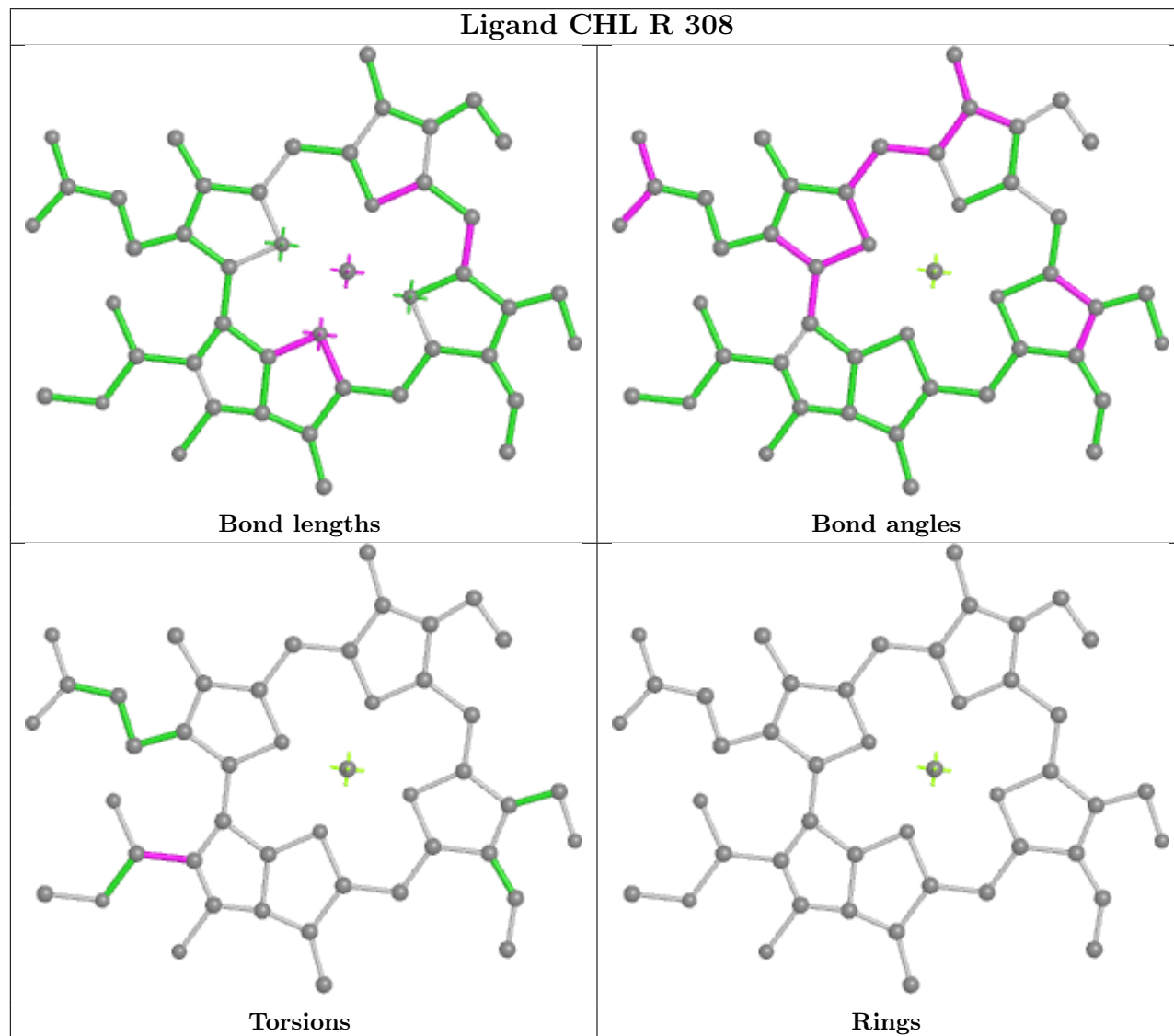
Ligand CLA A 831

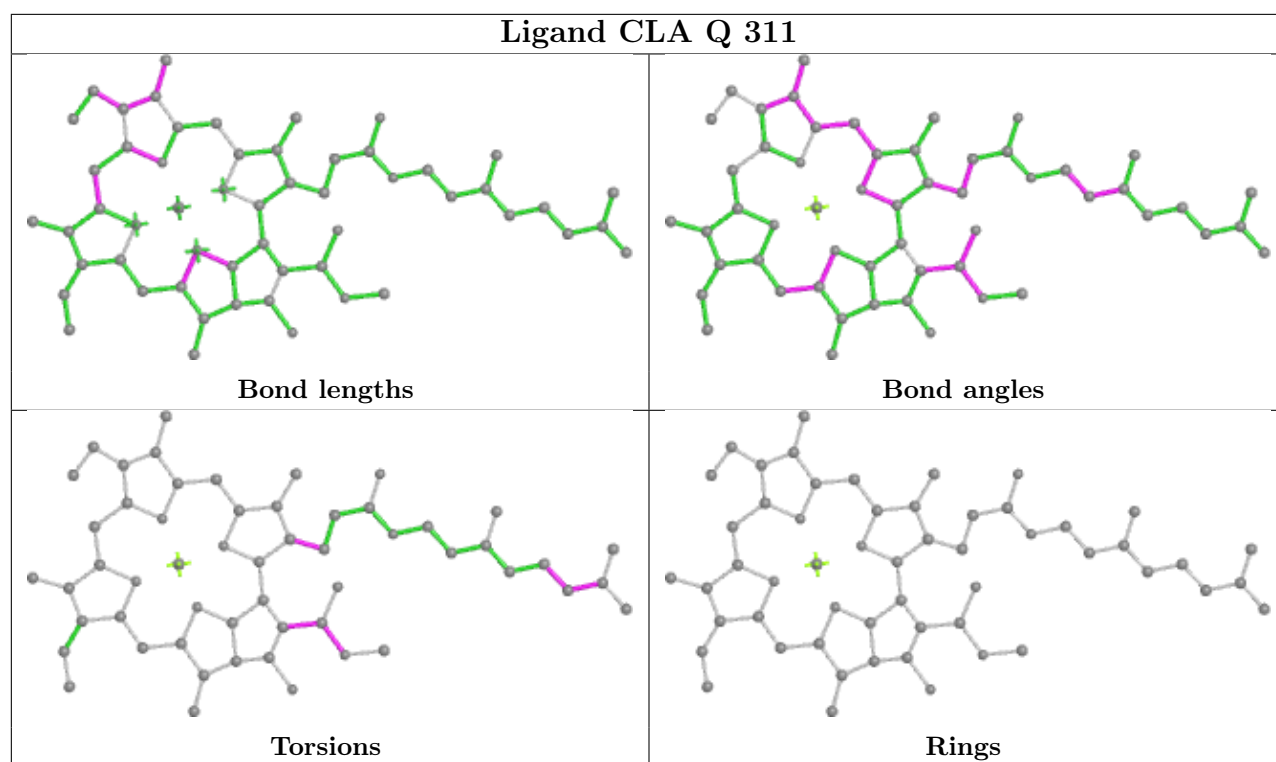


Ligand IWJ R 322

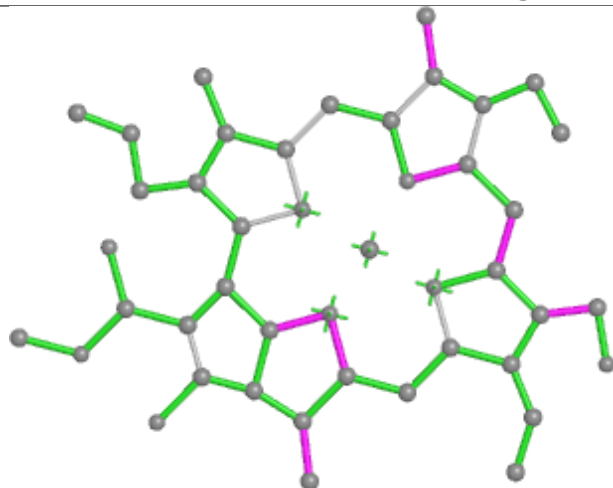


Ligand CHL R 308

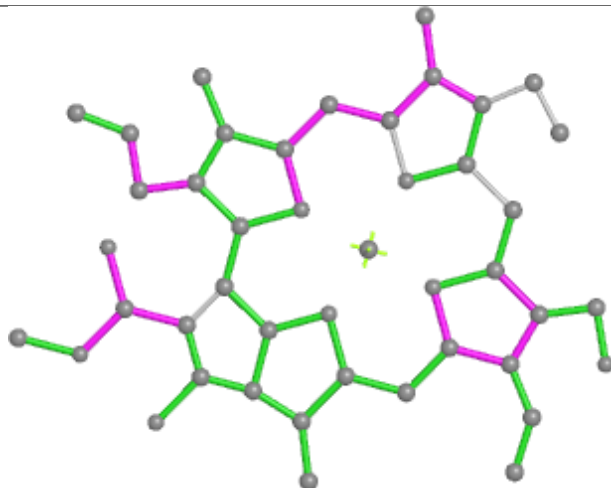




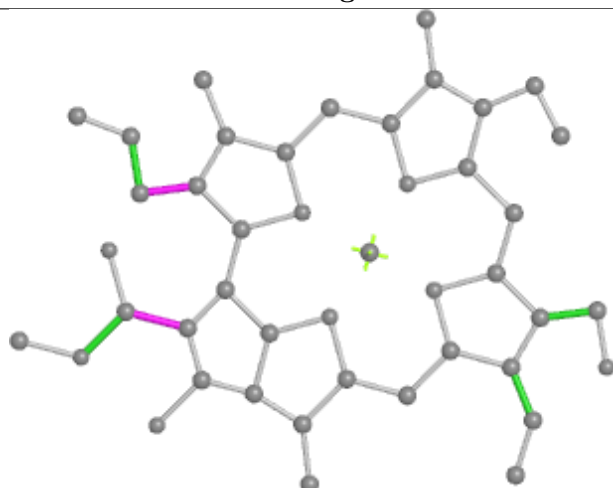
Ligand CHL P 307



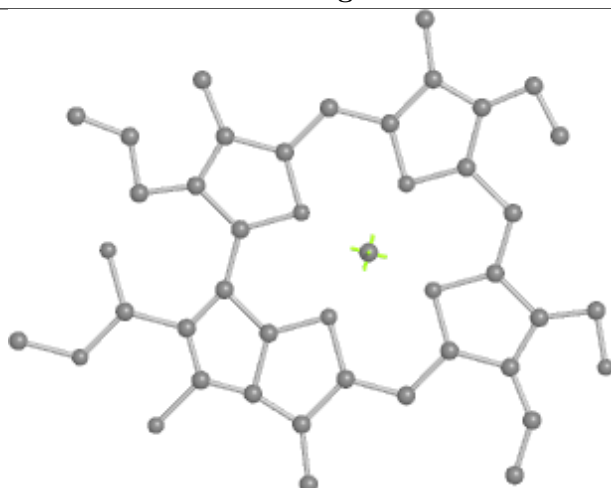
Bond lengths



Bond angles

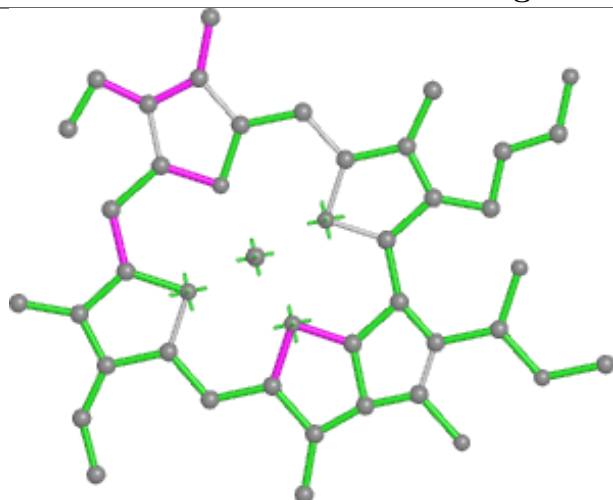


Torsions

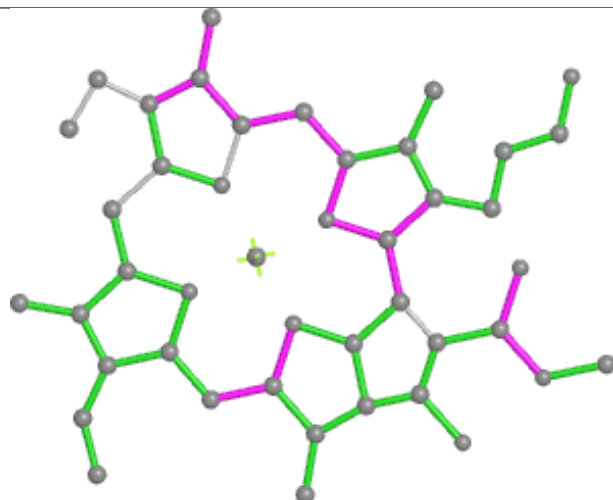


Rings

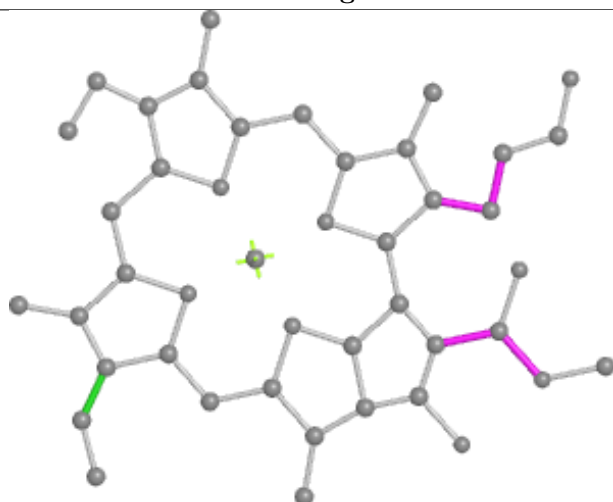
Ligand CLA H 301



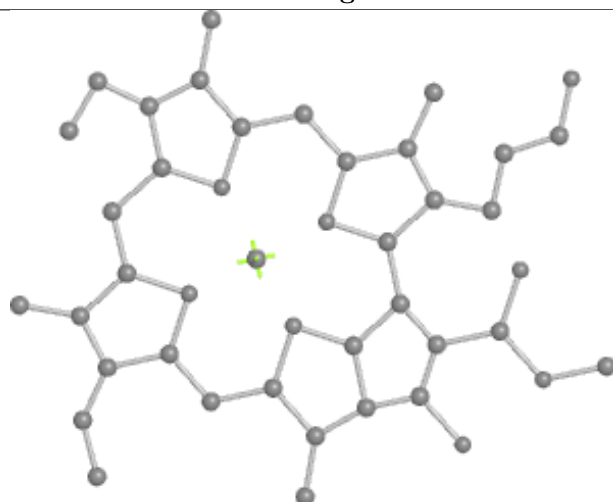
Bond lengths



Bond angles

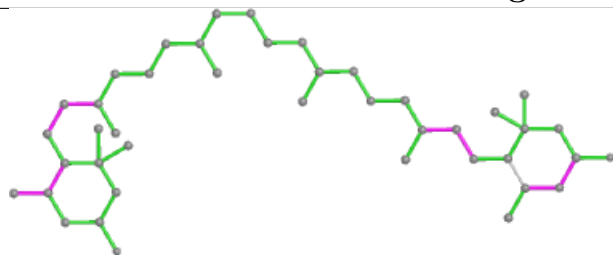


Torsions

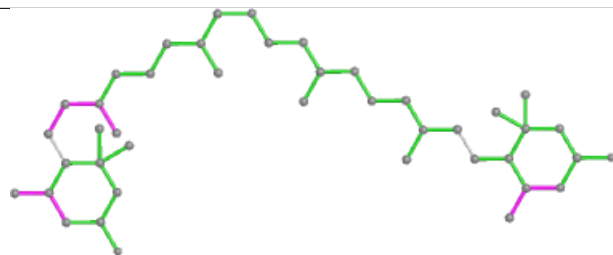


Rings

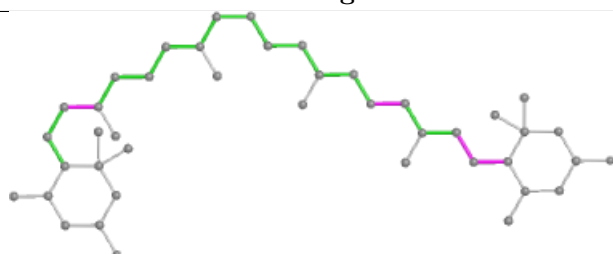
Ligand Q6L O 2007



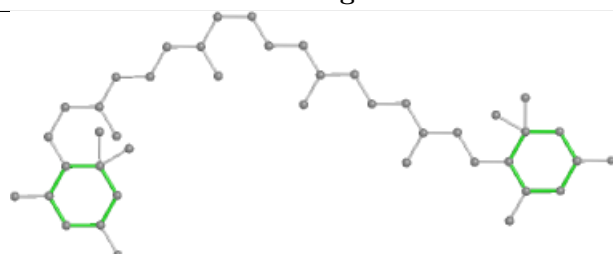
Bond lengths



Bond angles

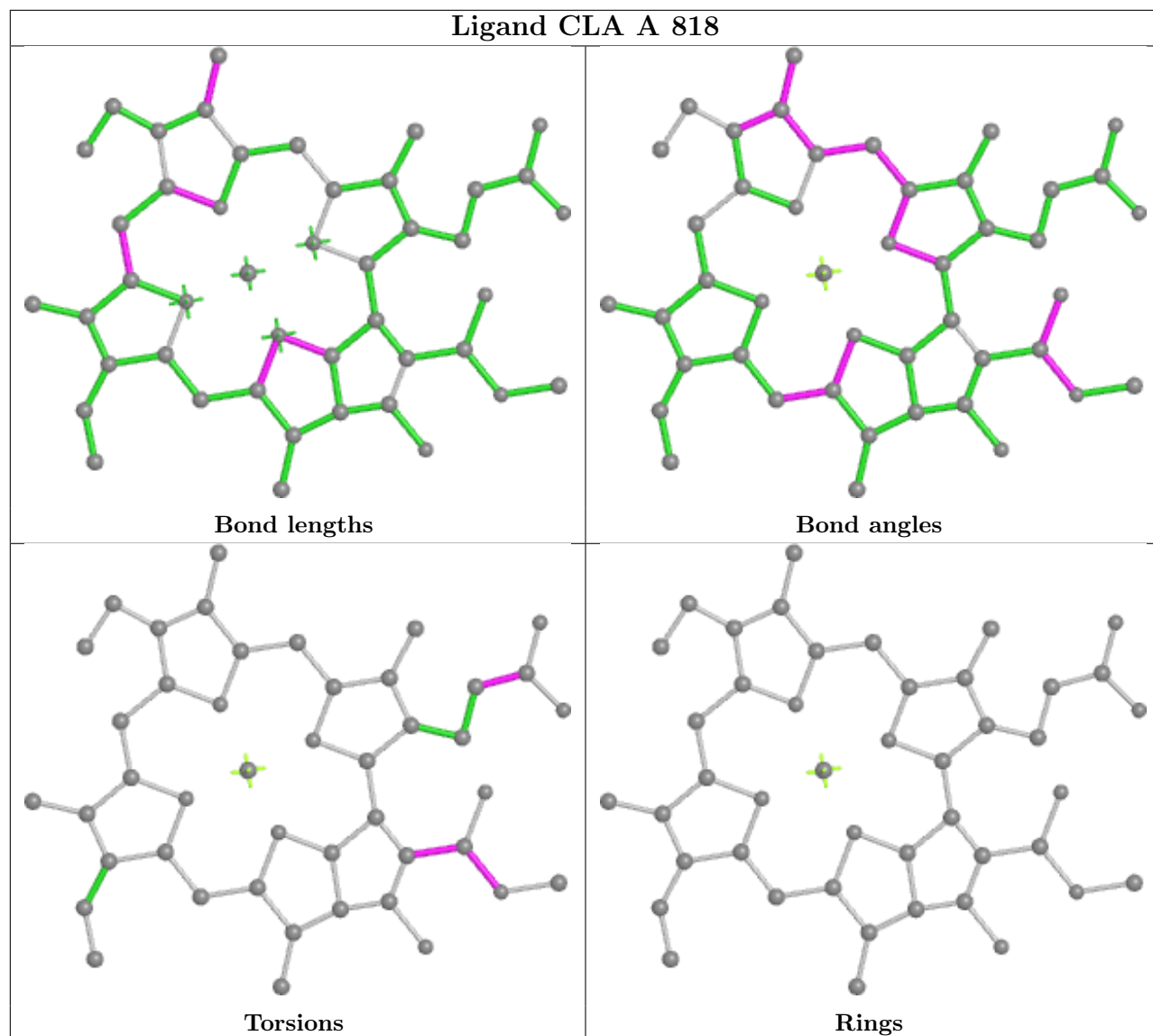


Torsions

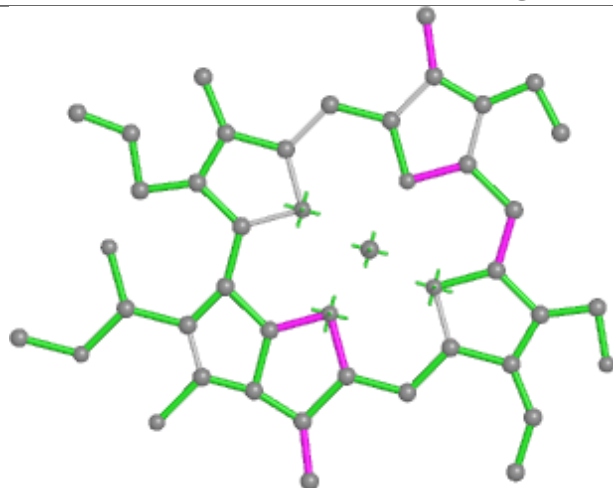


Rings

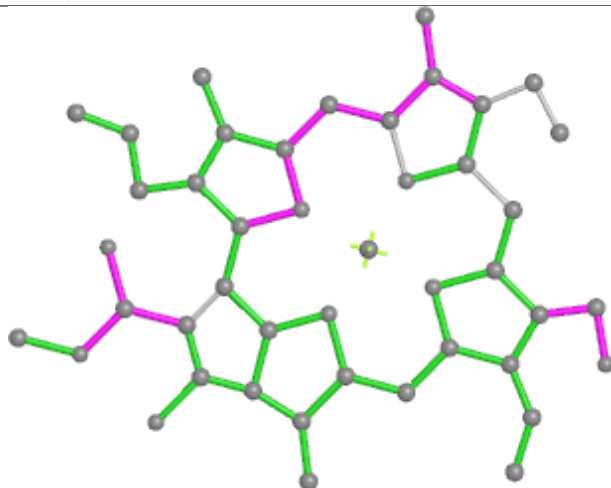
Ligand CLA A 818



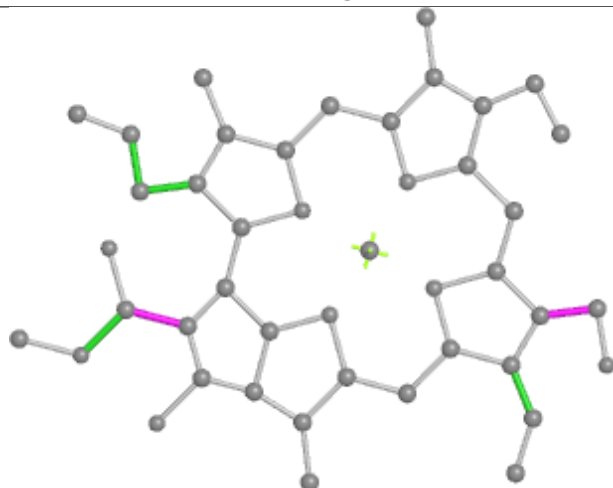
Ligand CHL Q 309



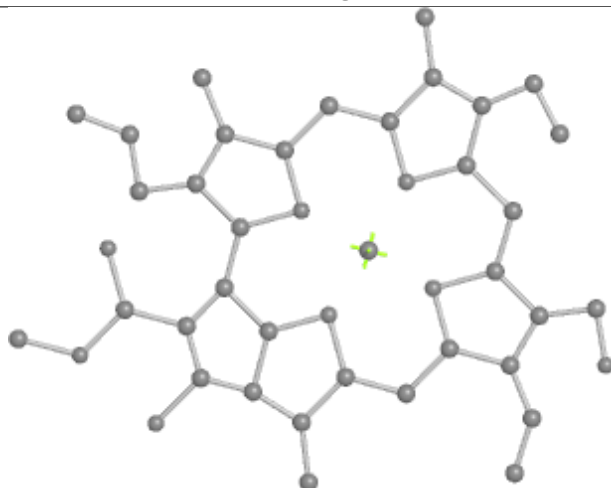
Bond lengths



Bond angles

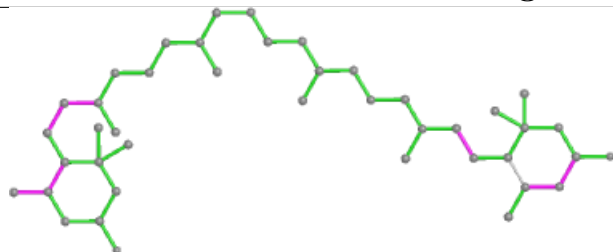


Torsions

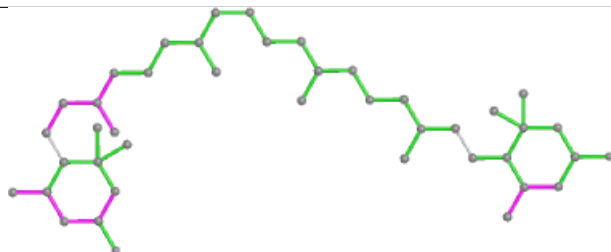


Rings

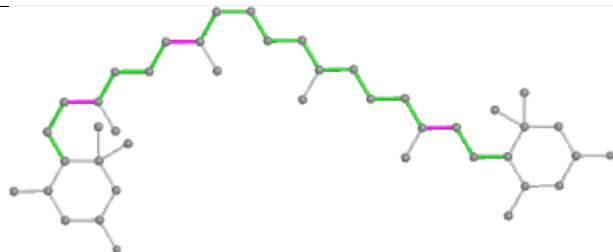
Ligand Q6L T 315



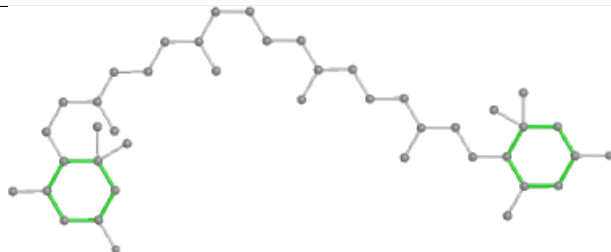
Bond lengths



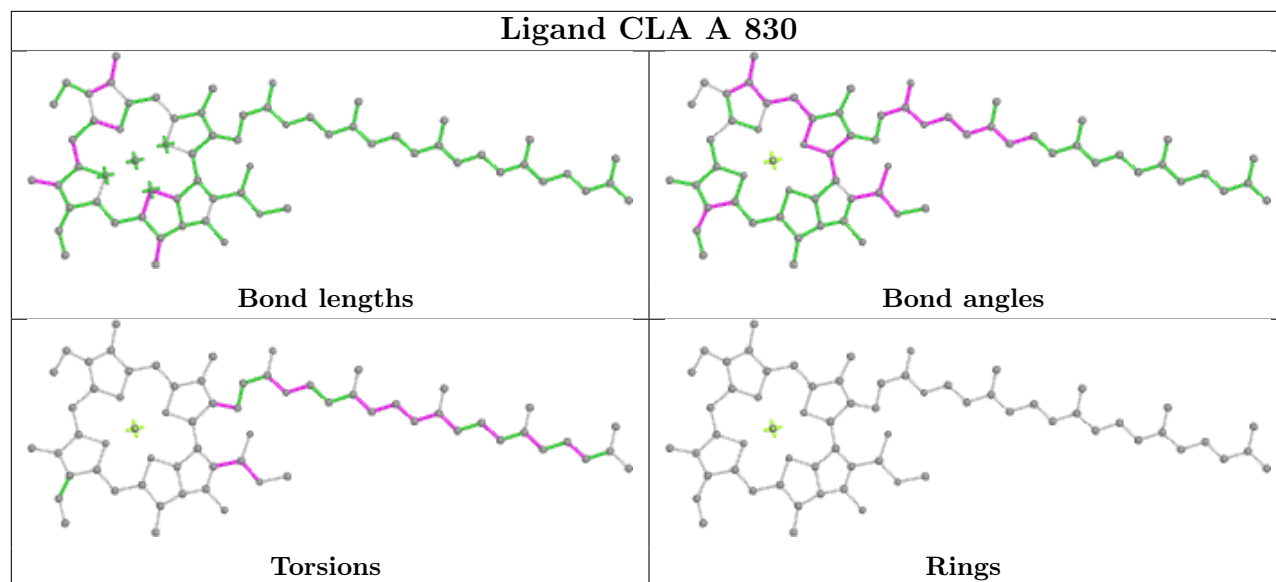
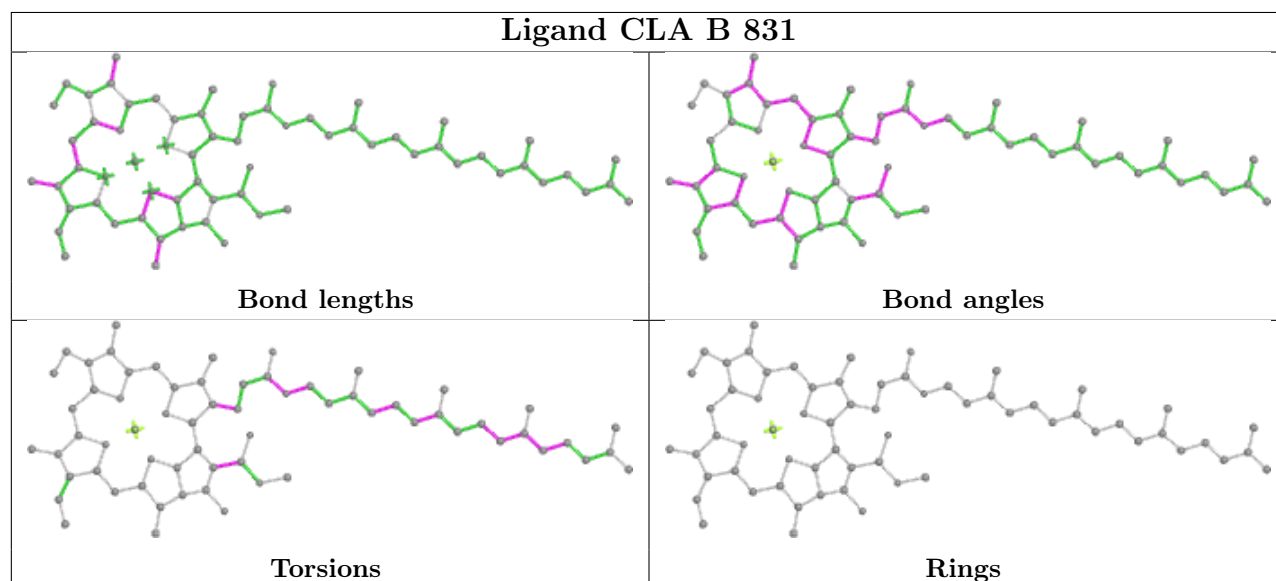
Bond angles



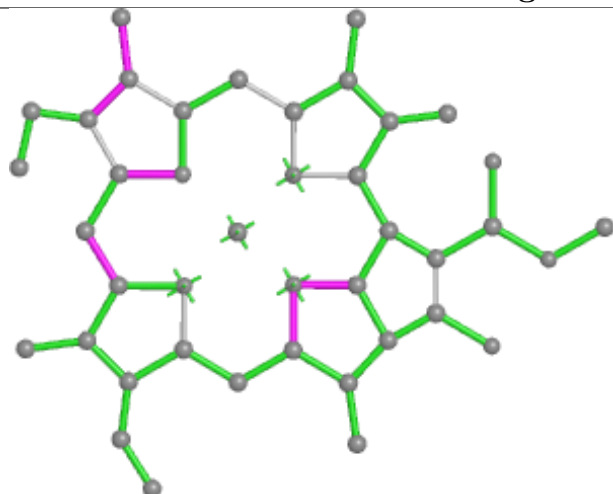
Torsions



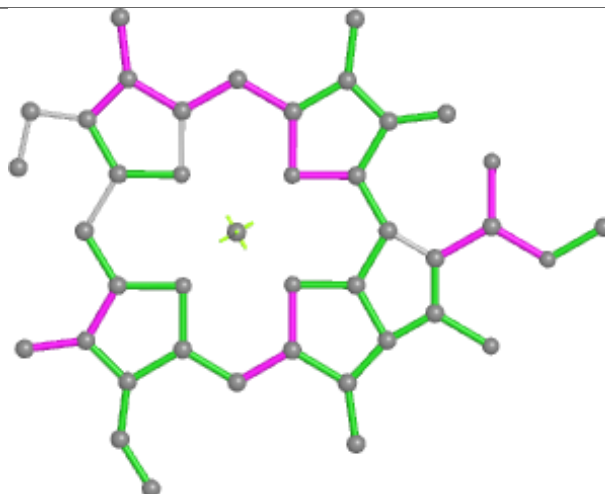
Rings

Ligand CLA A 830**Ligand CLA B 831**

Ligand CLA 4 314



Bond lengths



Bond angles

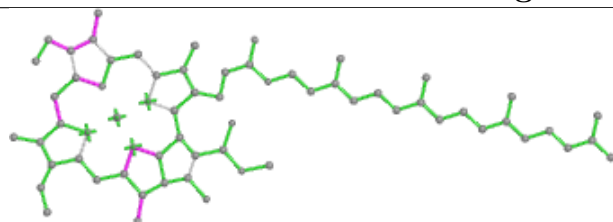


Torsions

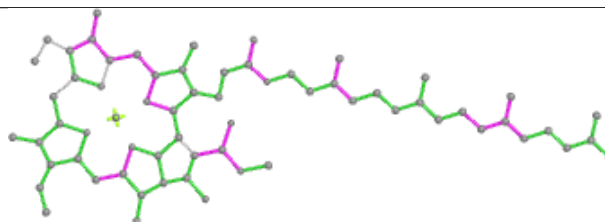


Rings

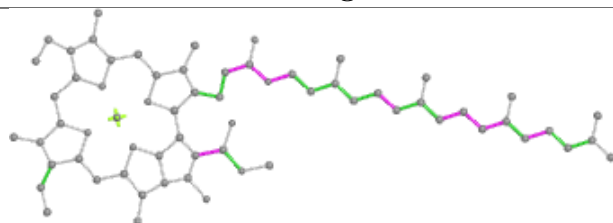
Ligand CLA P 302



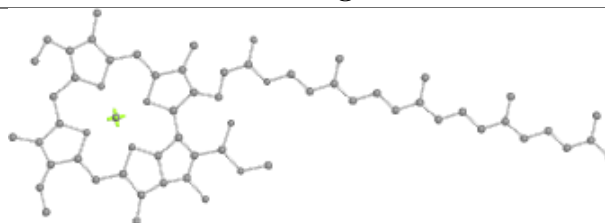
Bond lengths



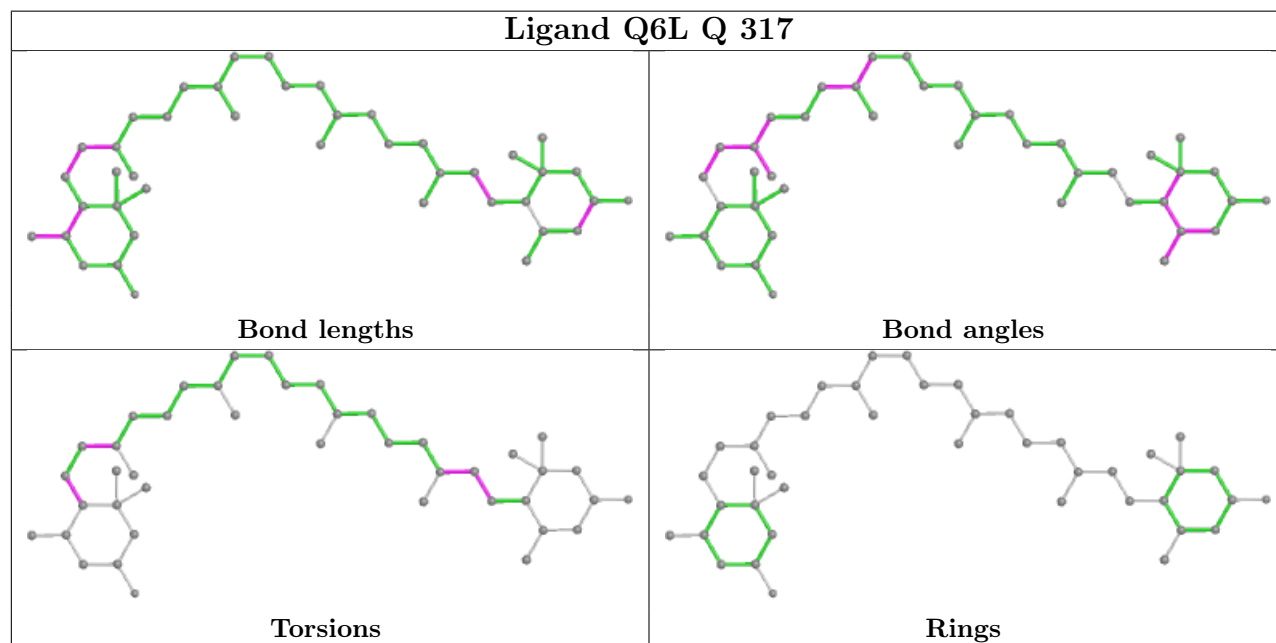
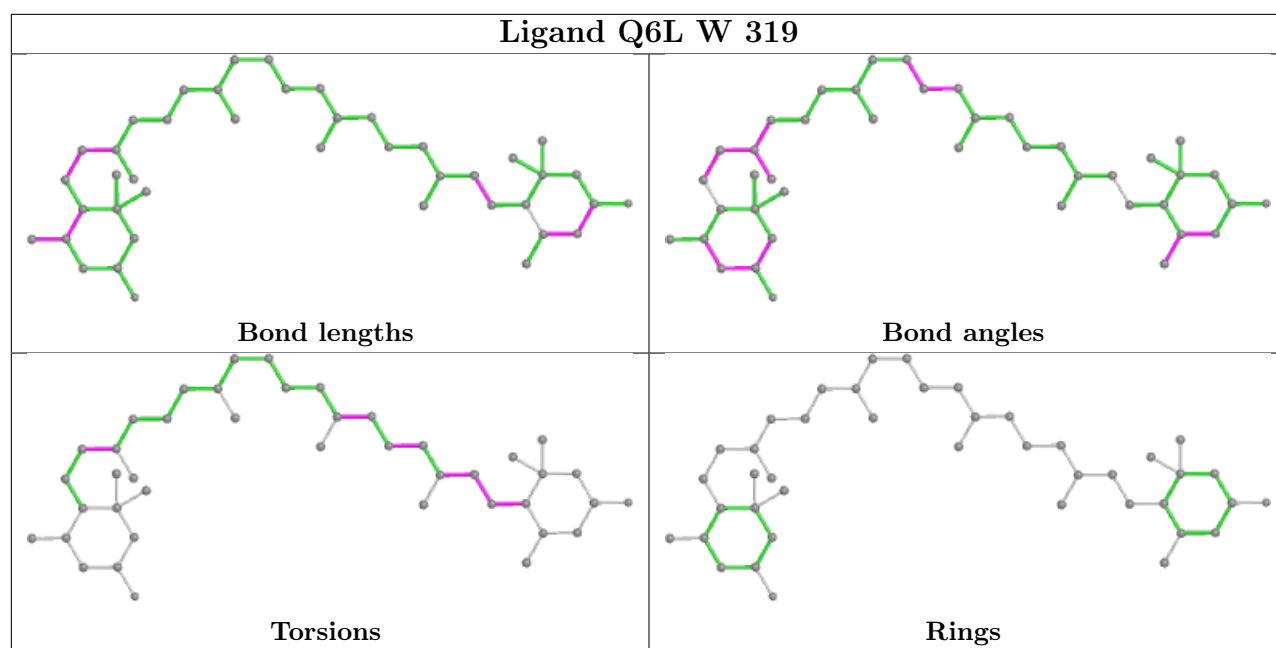
Bond angles

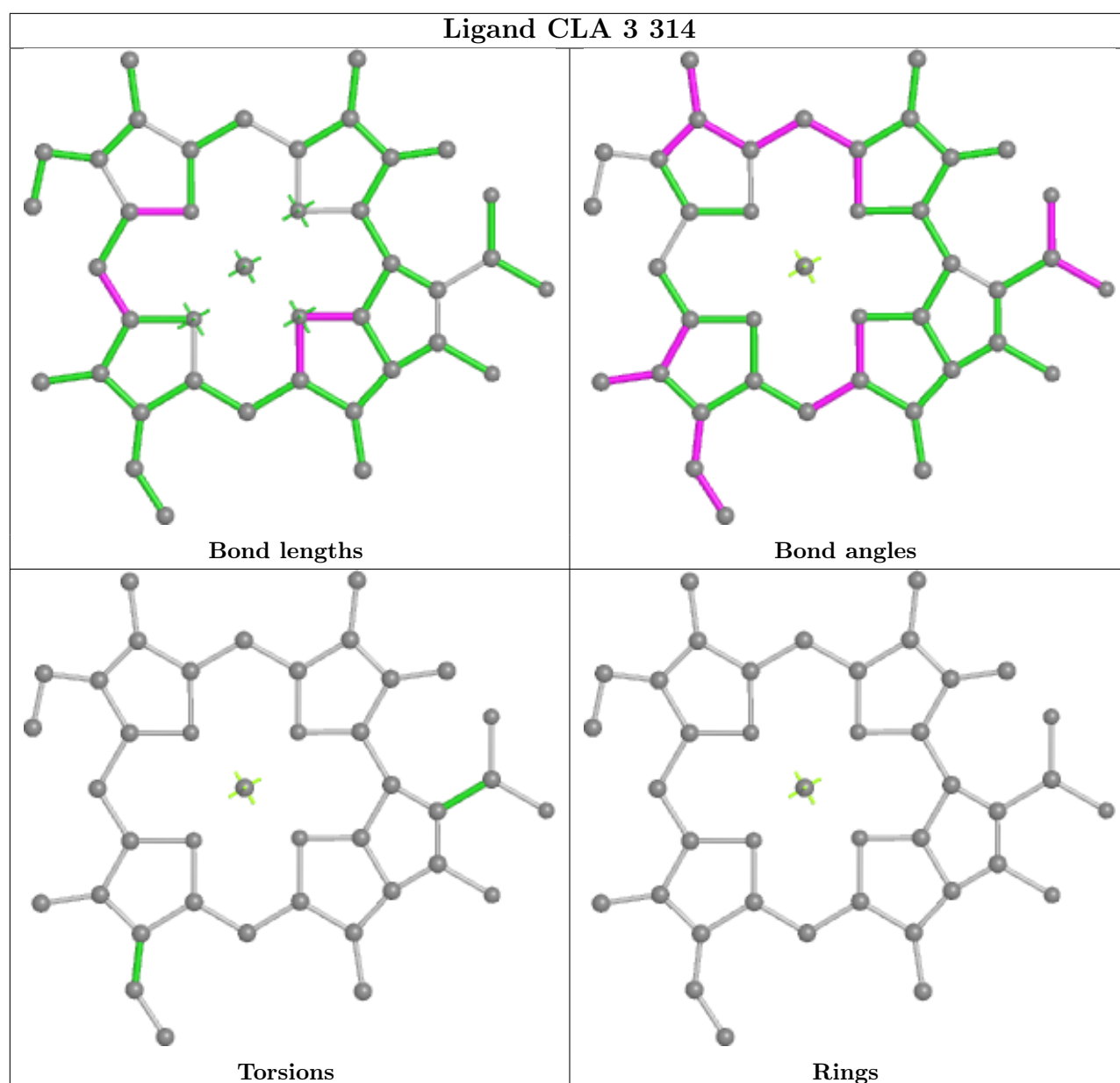
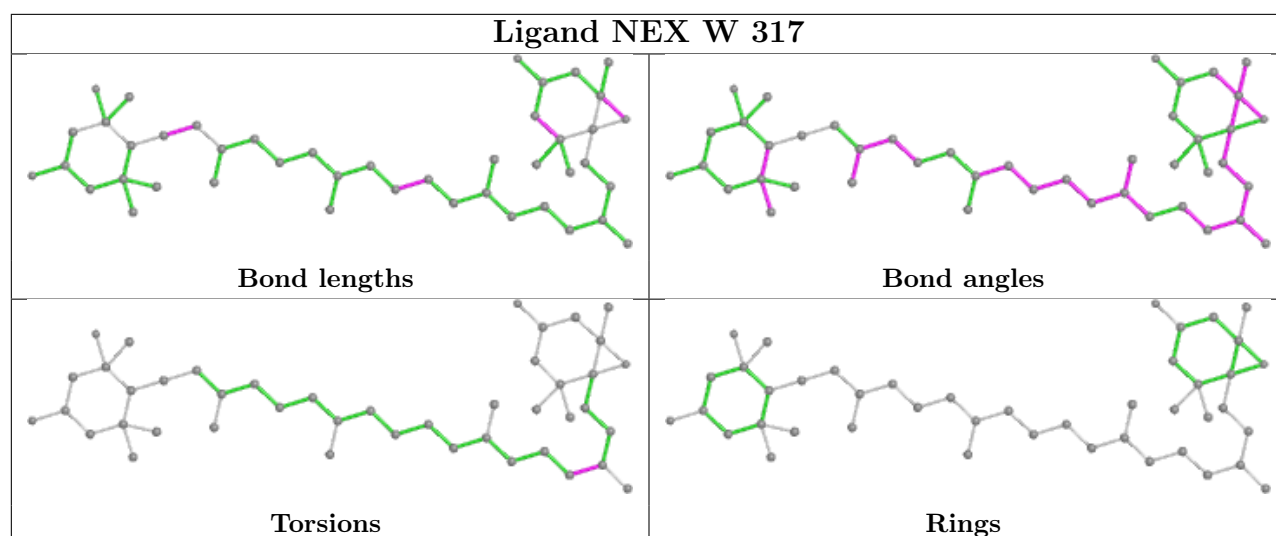


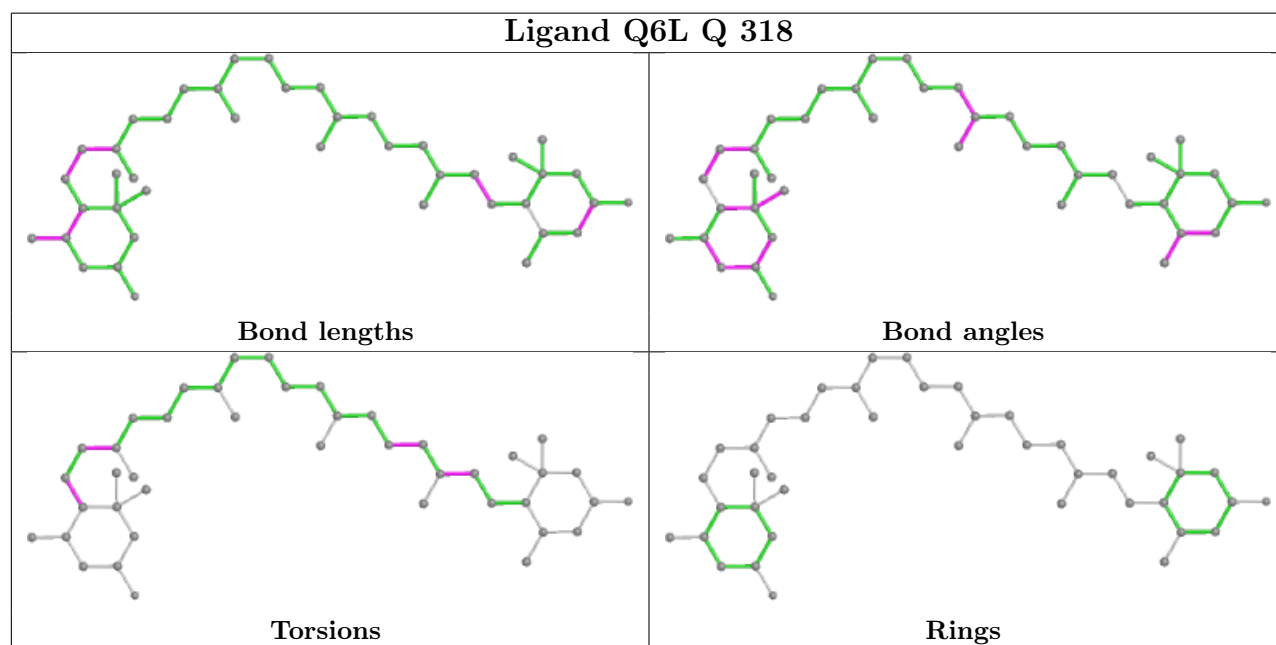
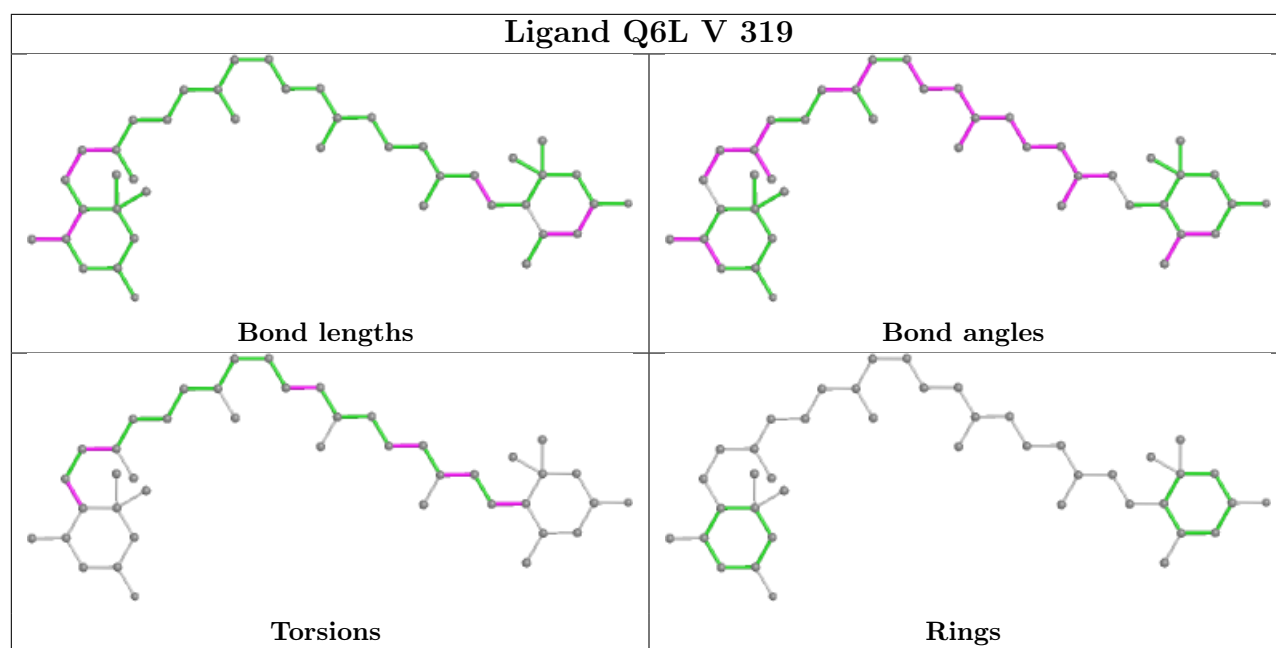
Torsions

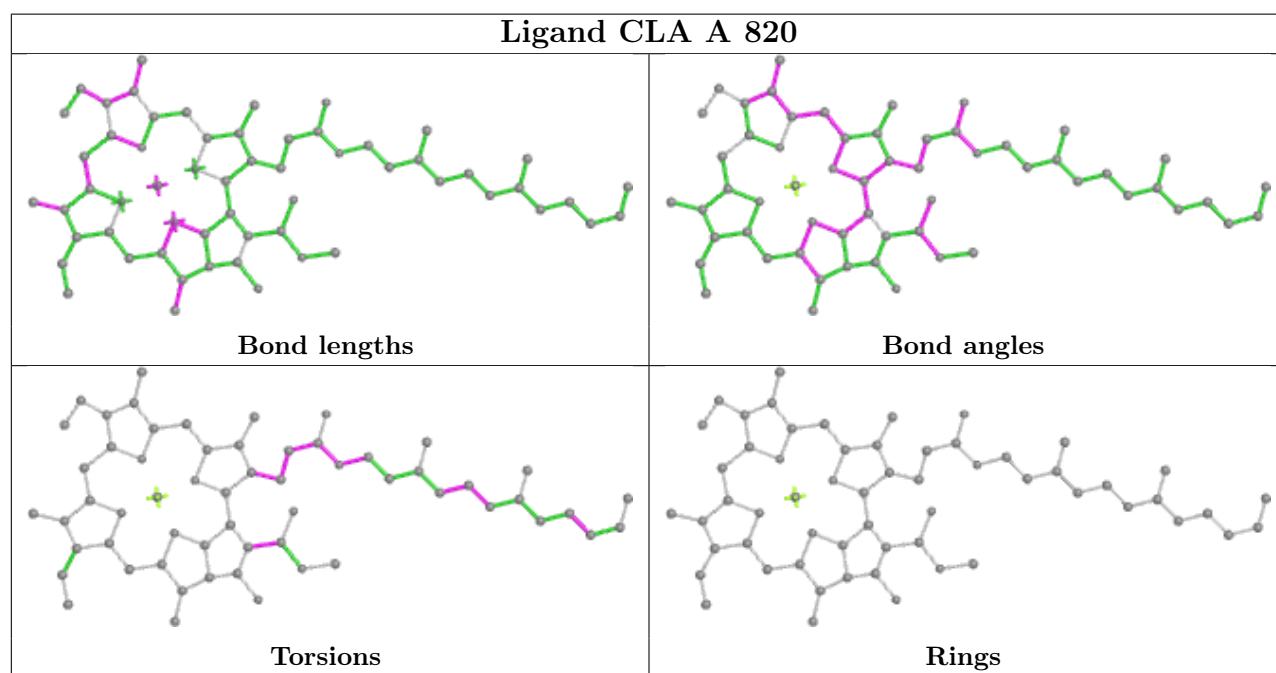
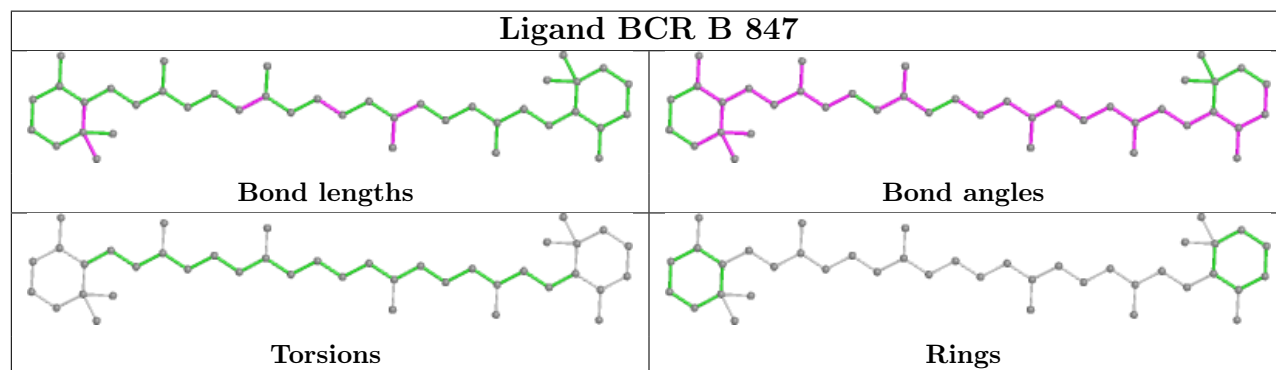
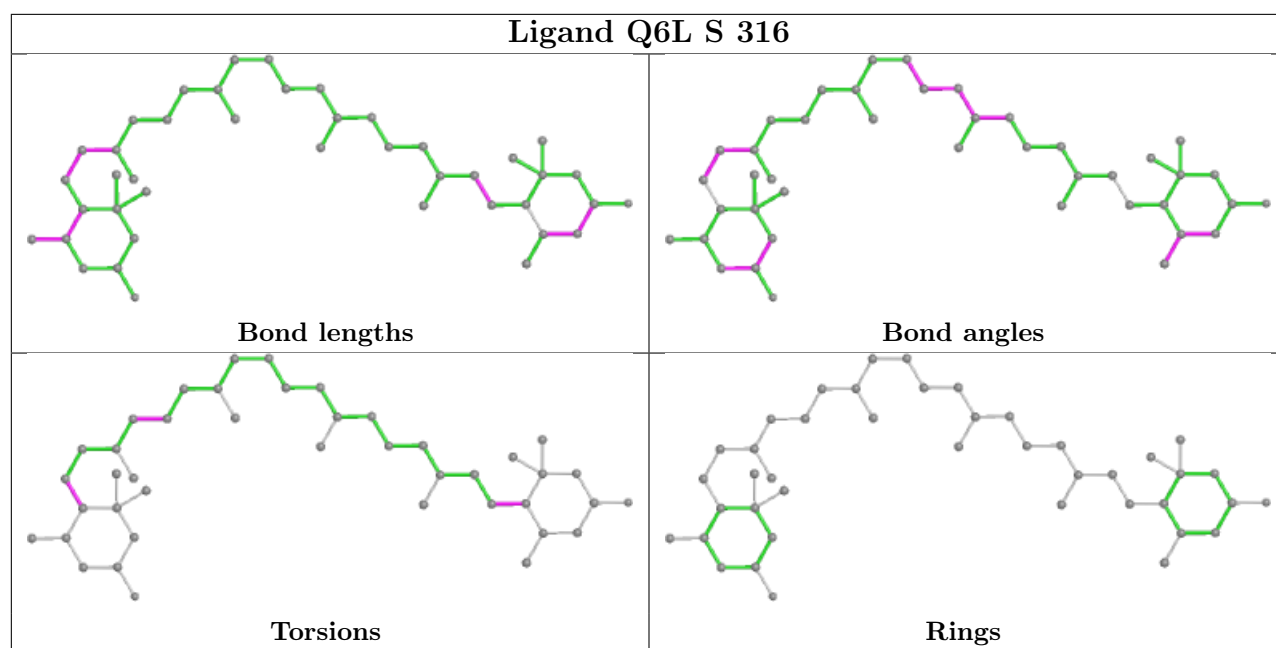


Rings

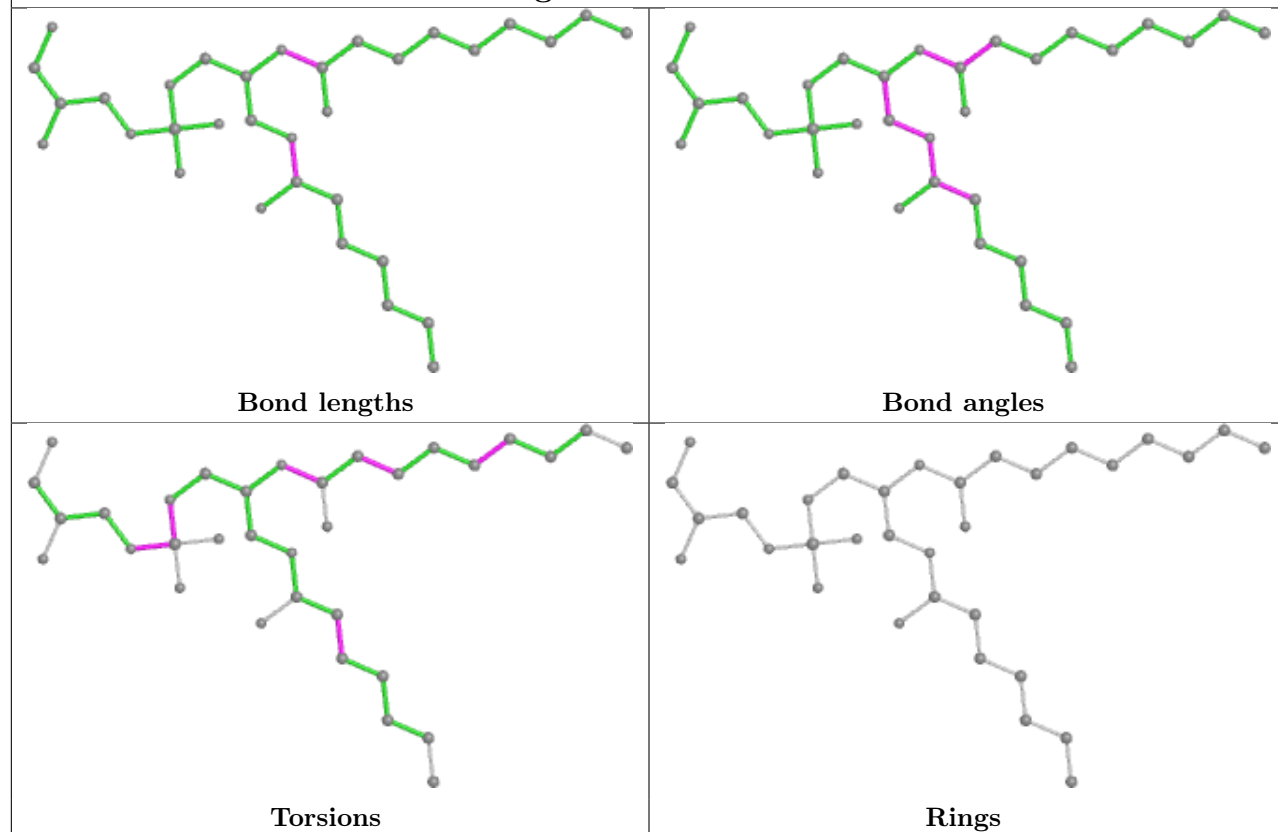




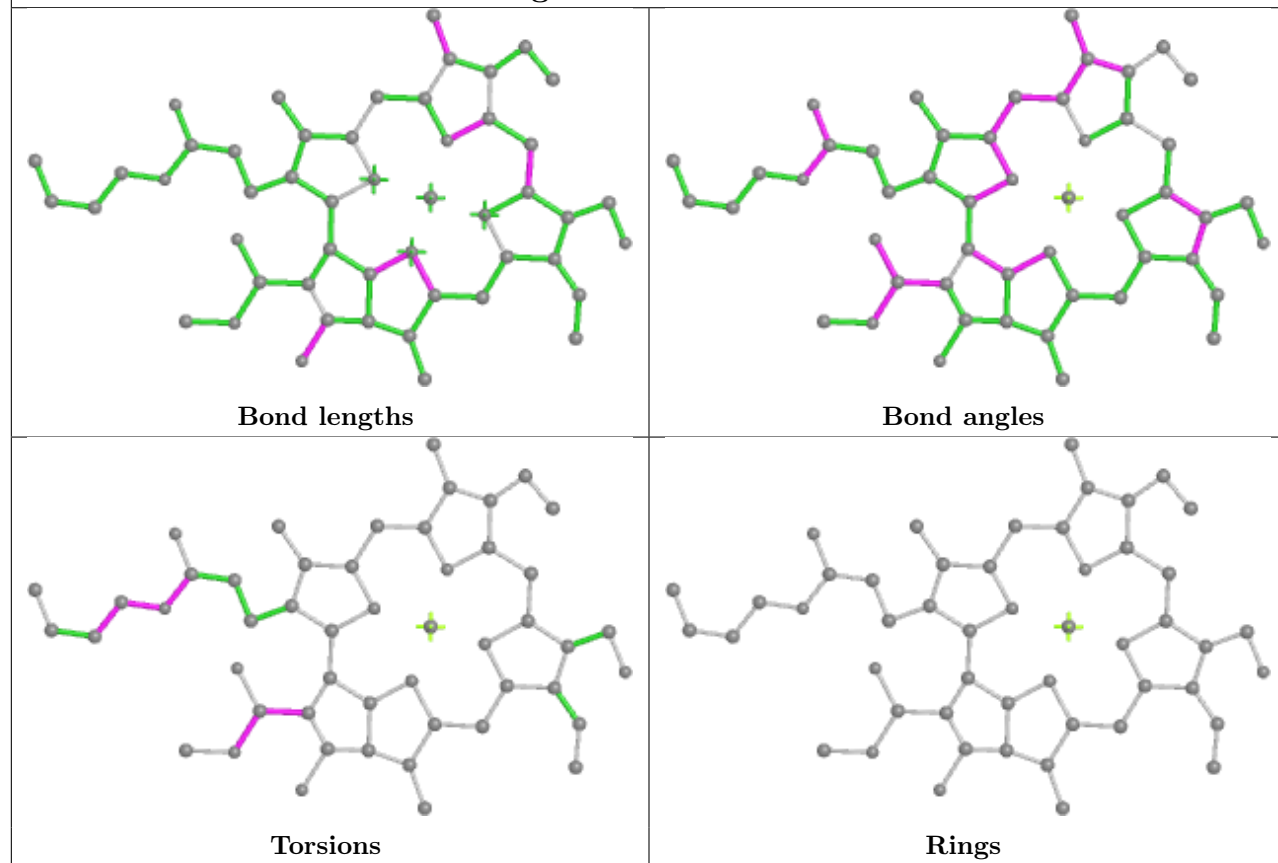




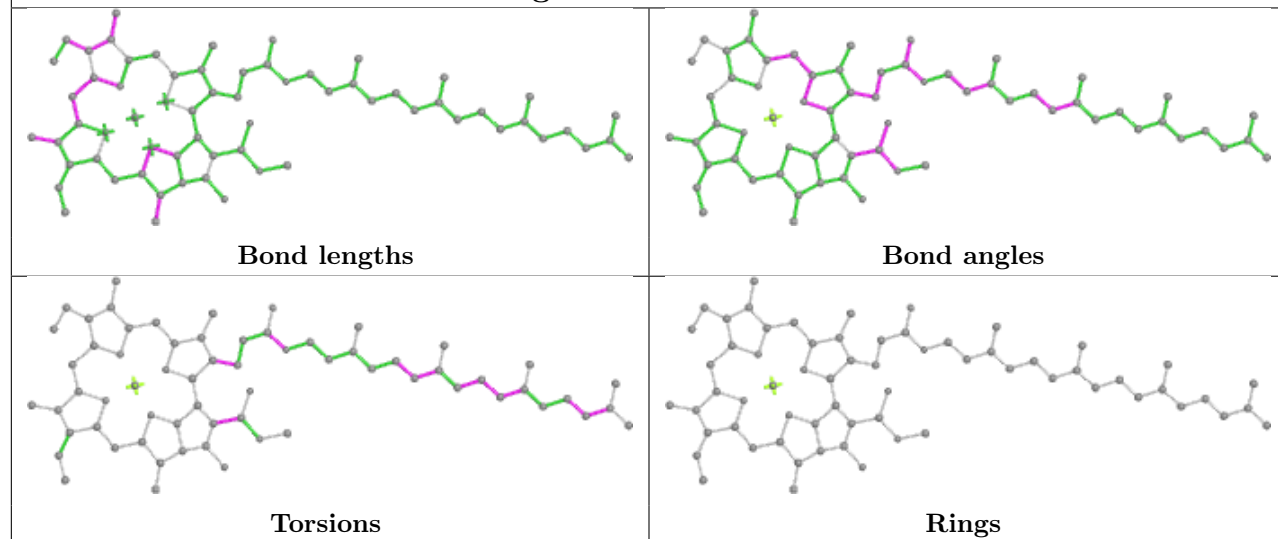
Ligand LHG 2 619



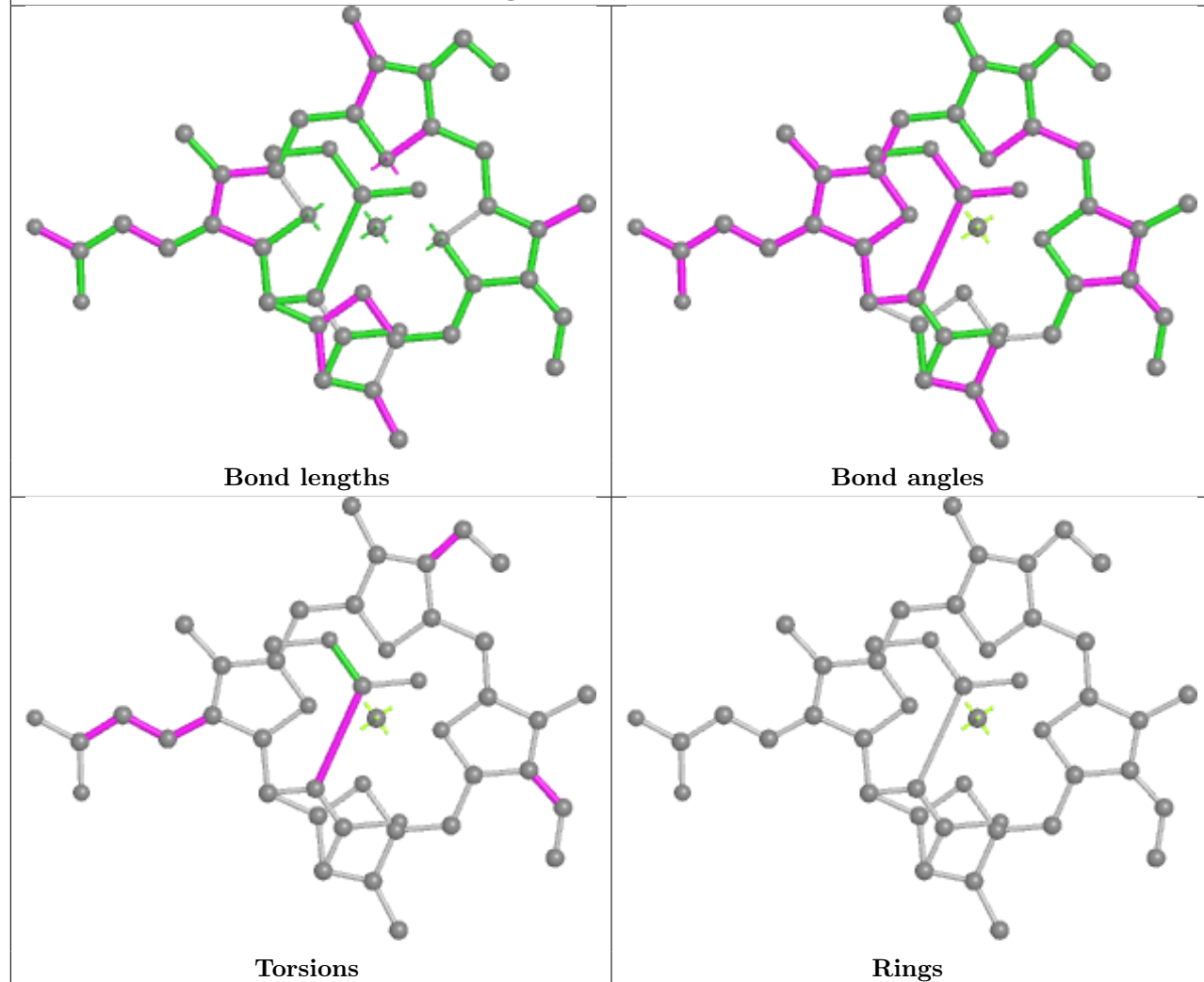
Ligand CHL R 309



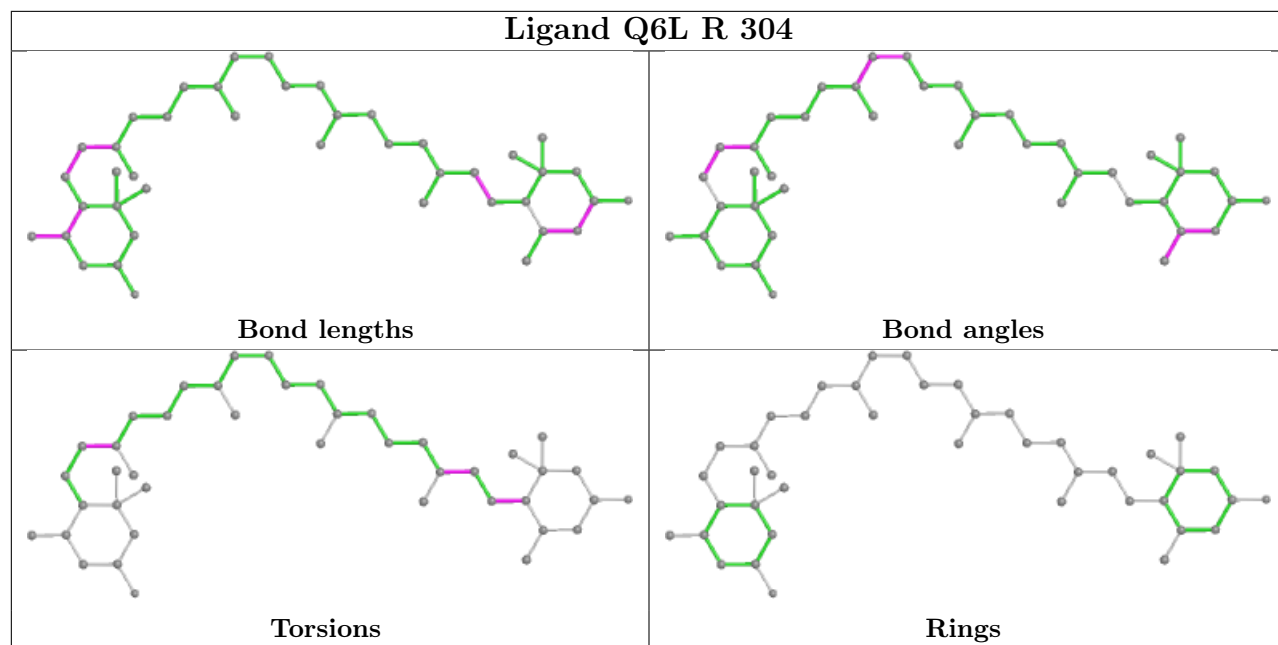
Ligand CLA B 810



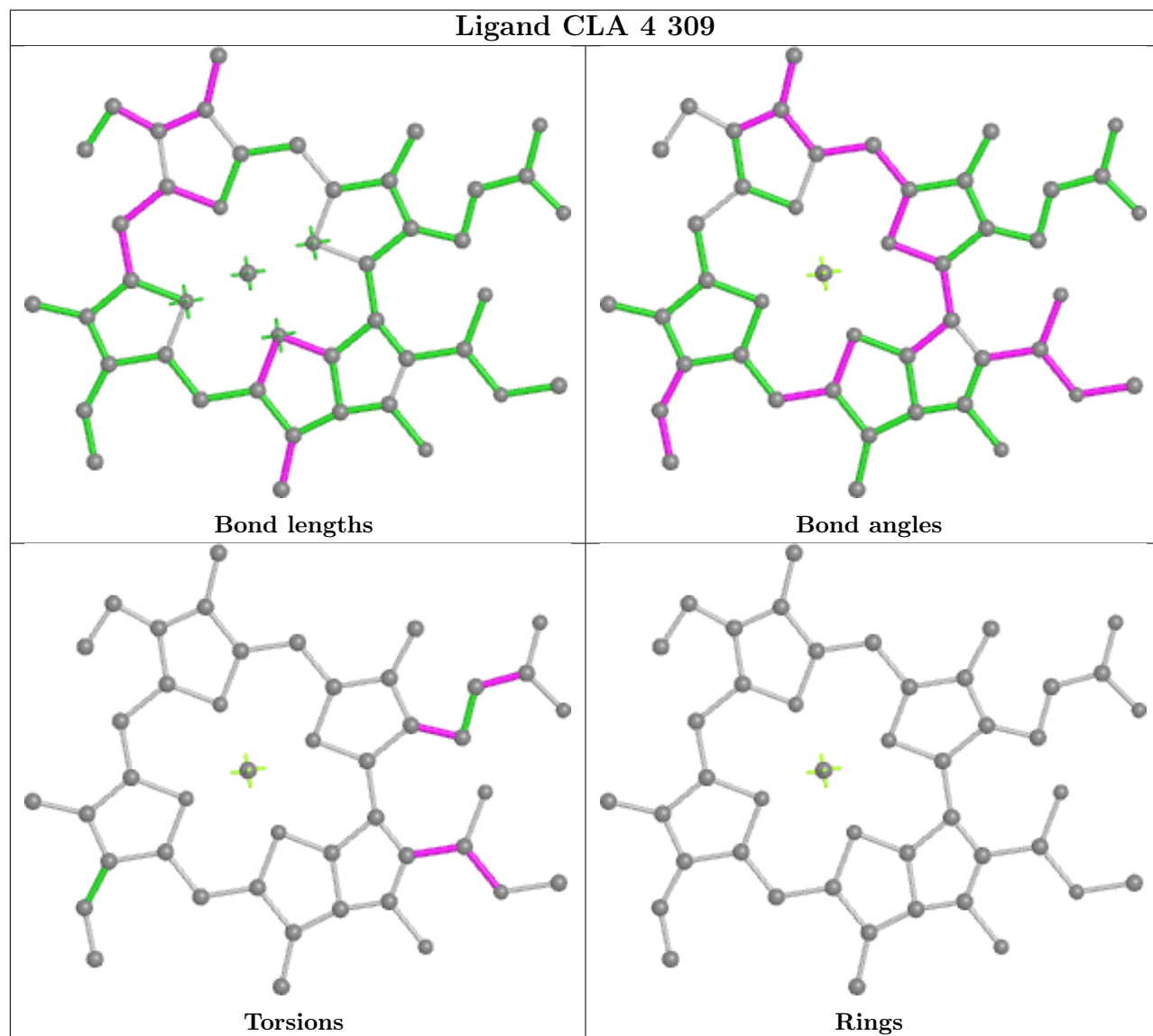
Ligand KC2 R 312



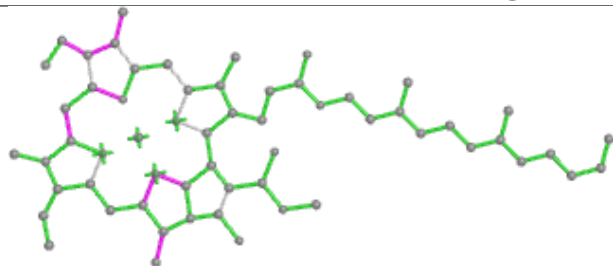
Ligand Q6L R 304



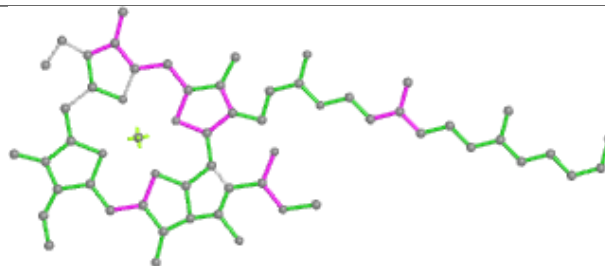
Ligand CLA 4 309



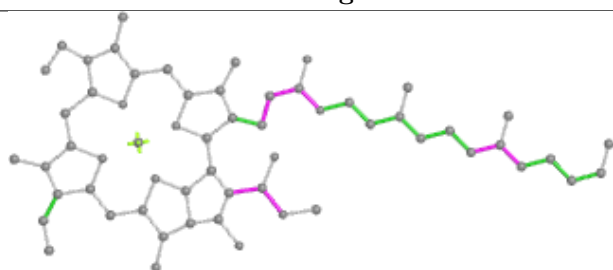
Ligand CLA O 2001



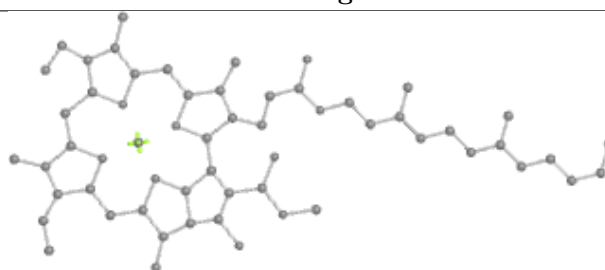
Bond lengths



Bond angles

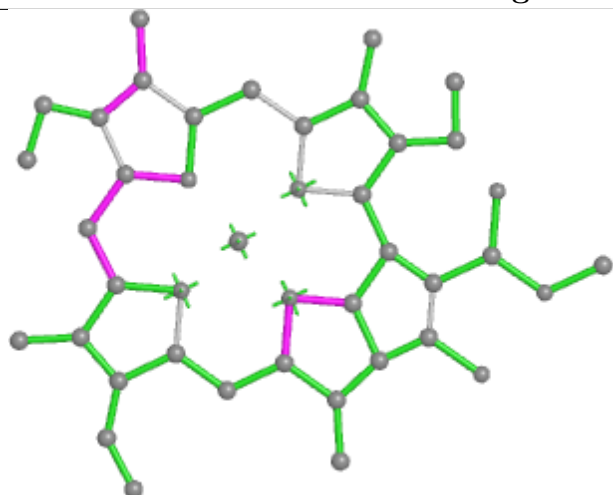


Torsions

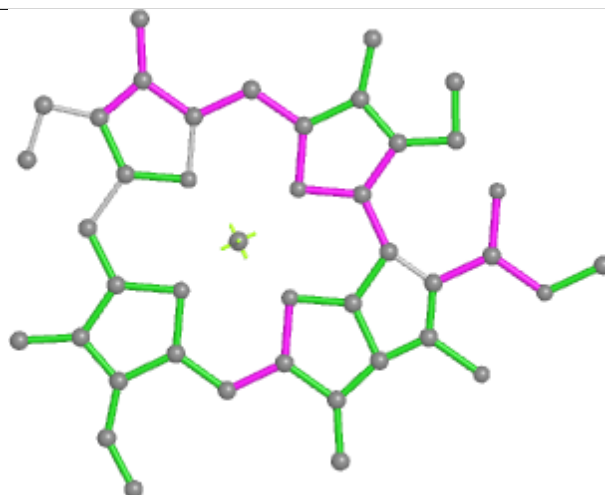


Rings

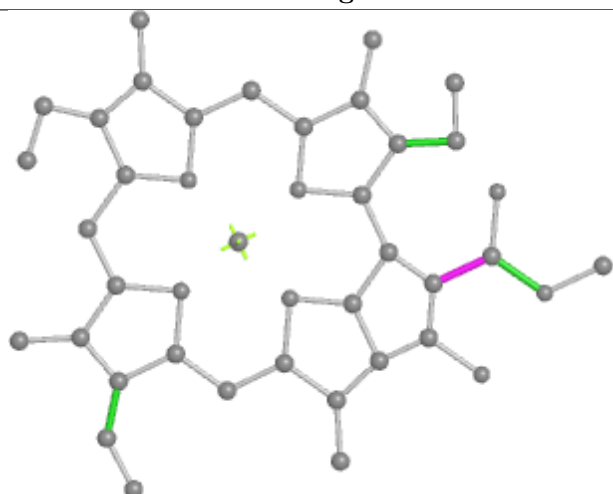
Ligand CLA G 203



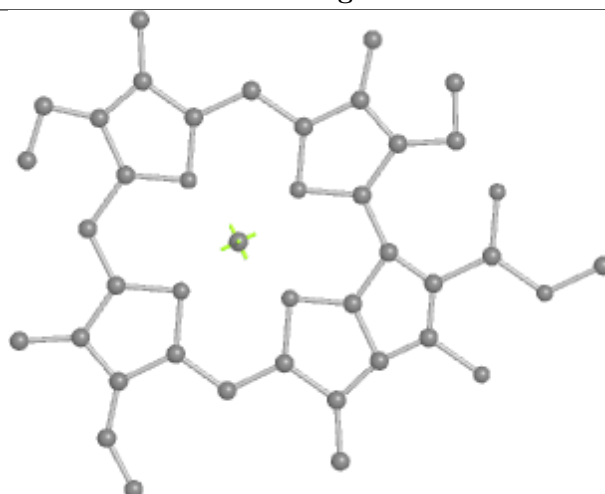
Bond lengths



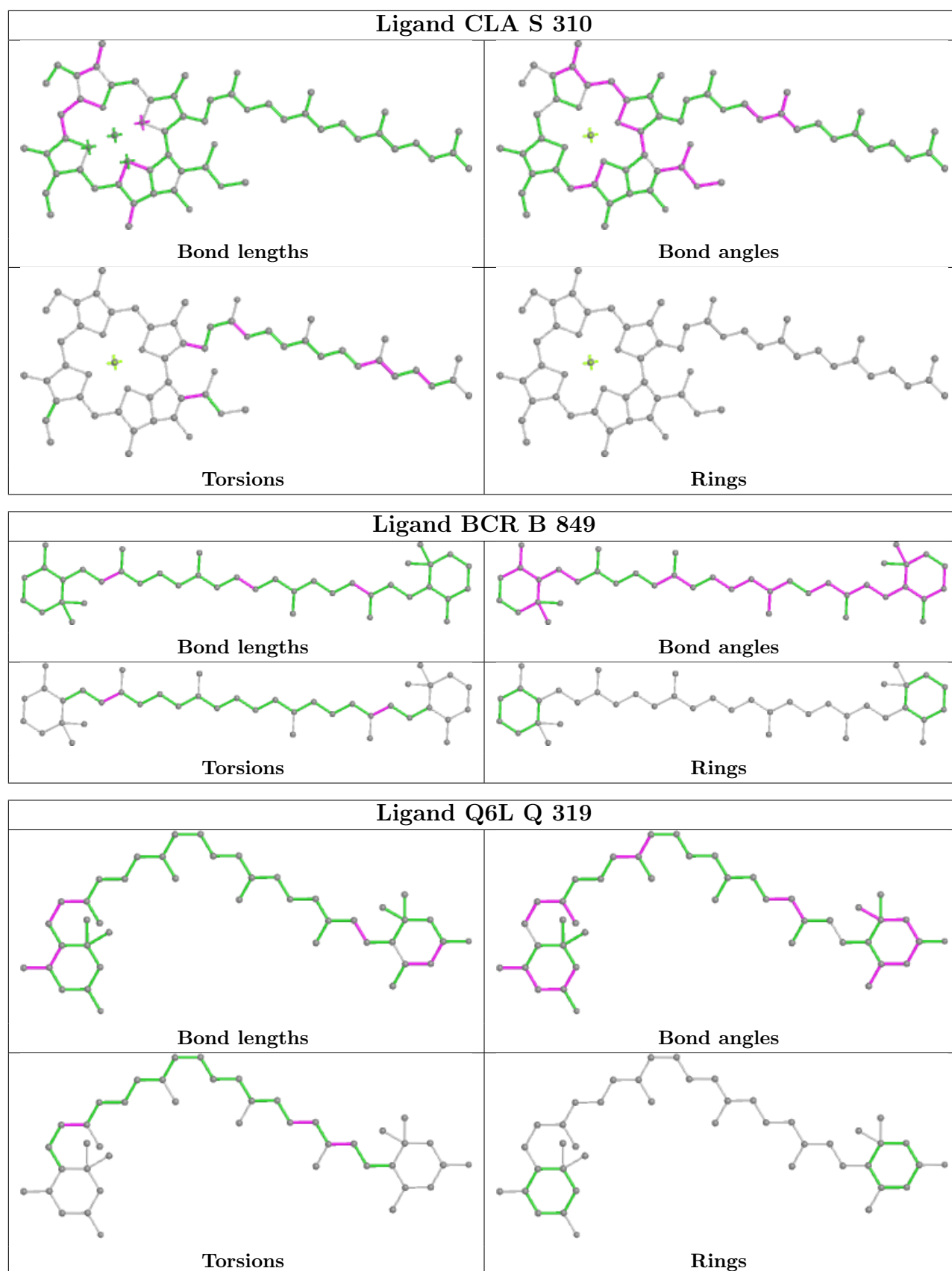
Bond angles



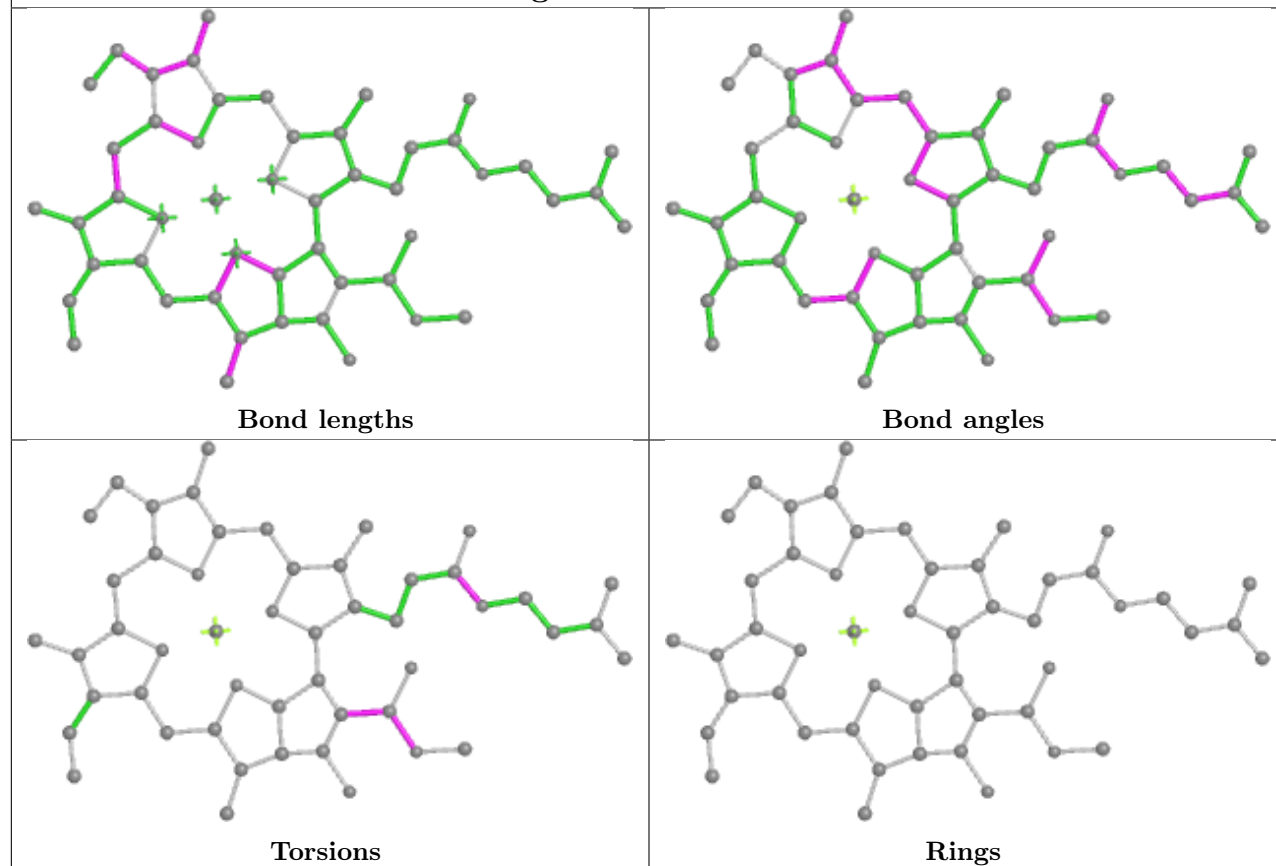
Torsions



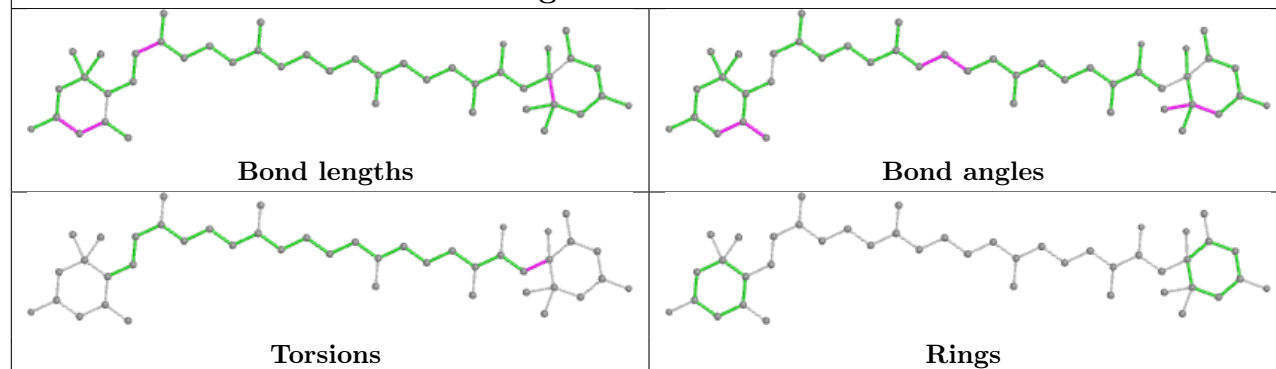
Rings



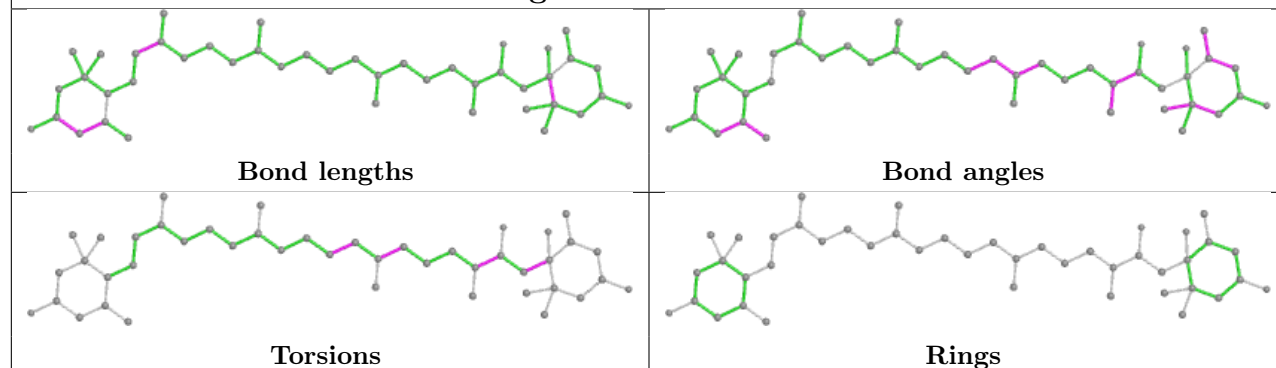
Ligand CLA U 303

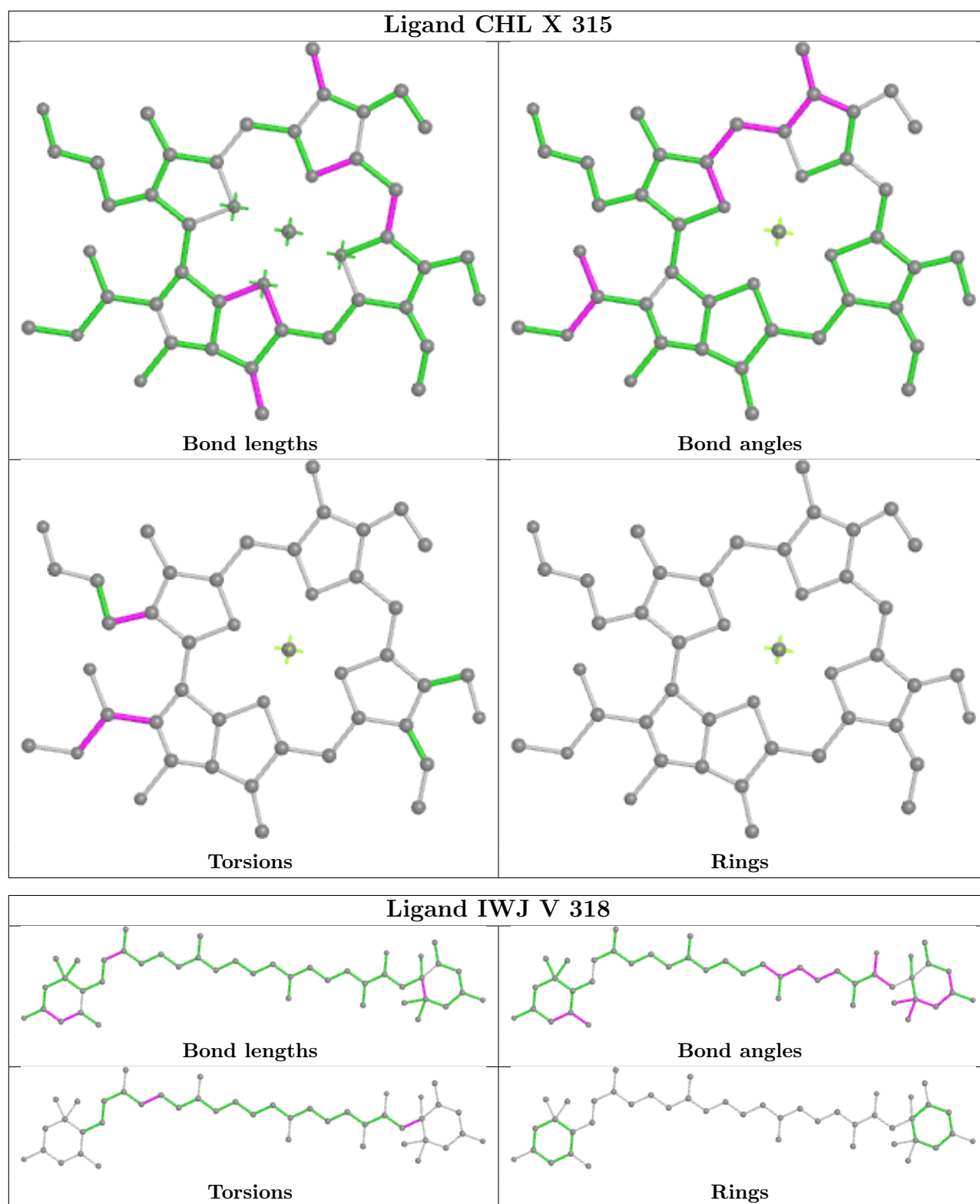


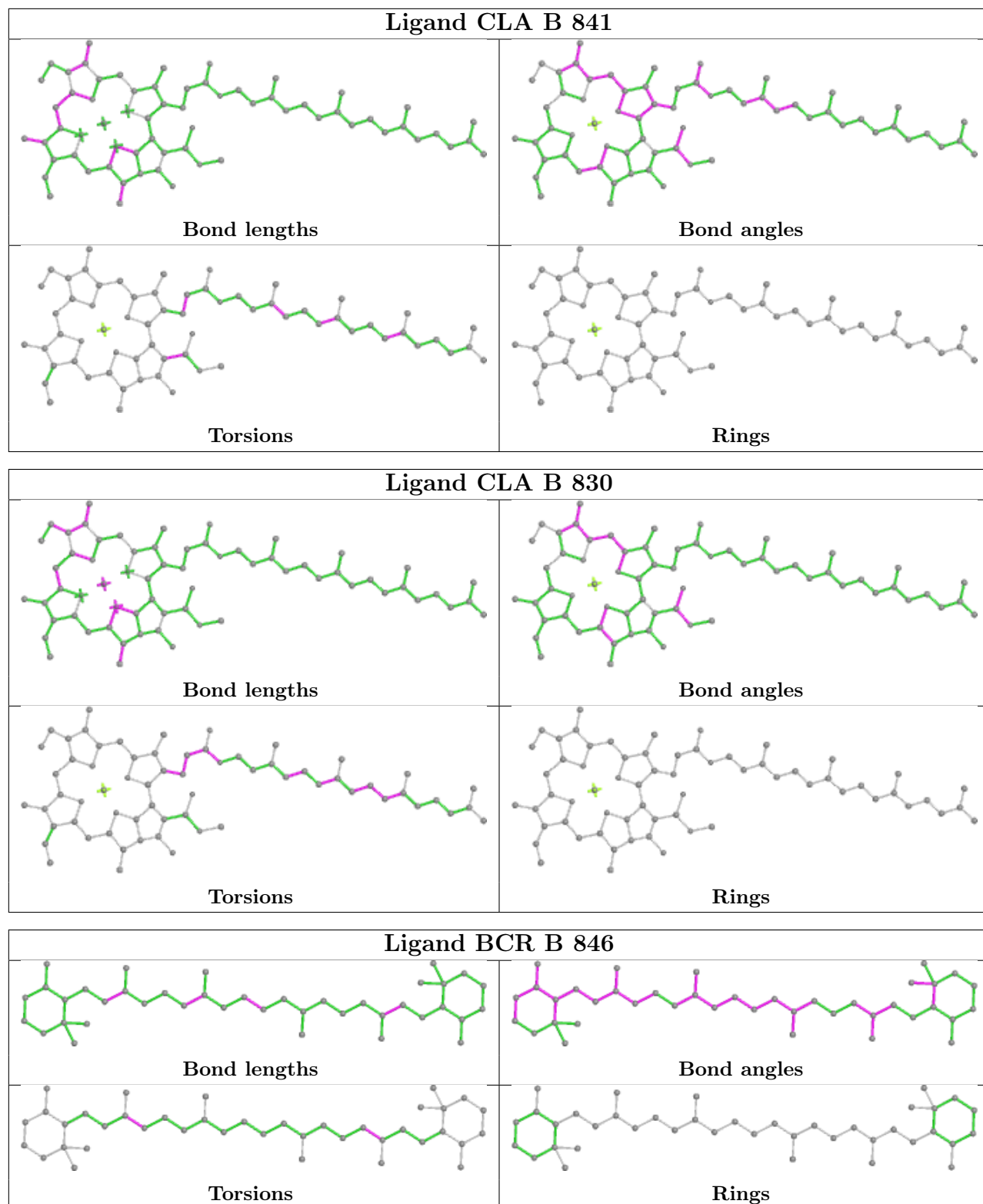
Ligand IWJ 6 614



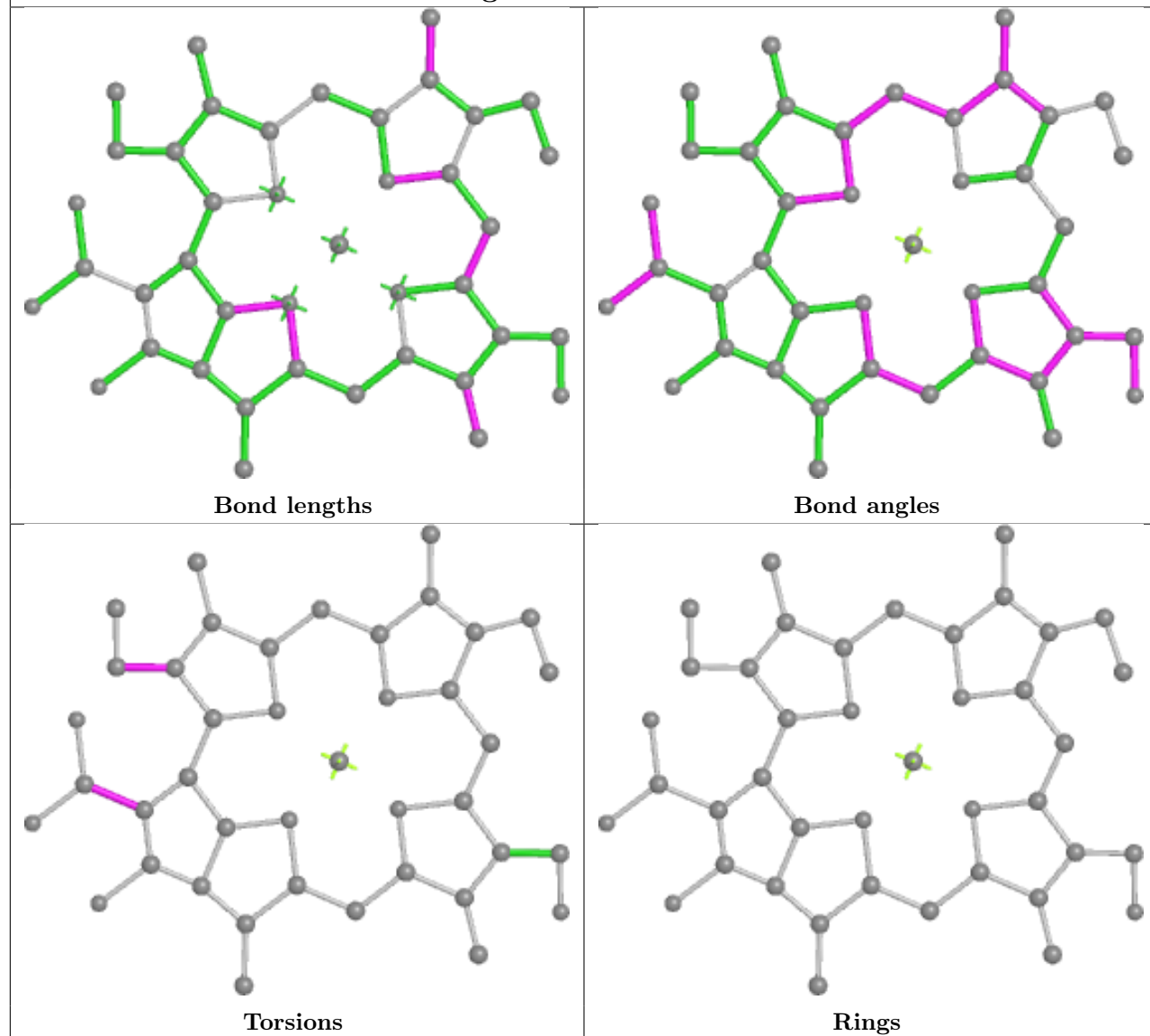
Ligand IWJ W 318



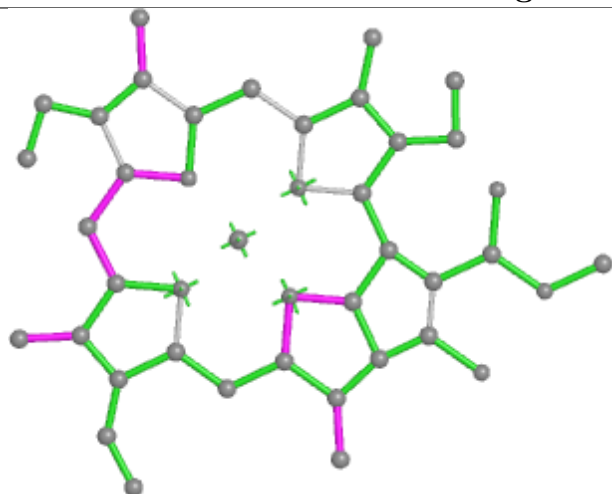




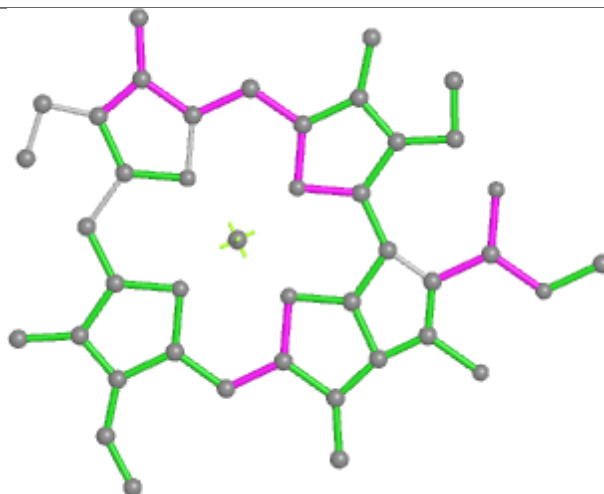
Ligand CHL 4 306



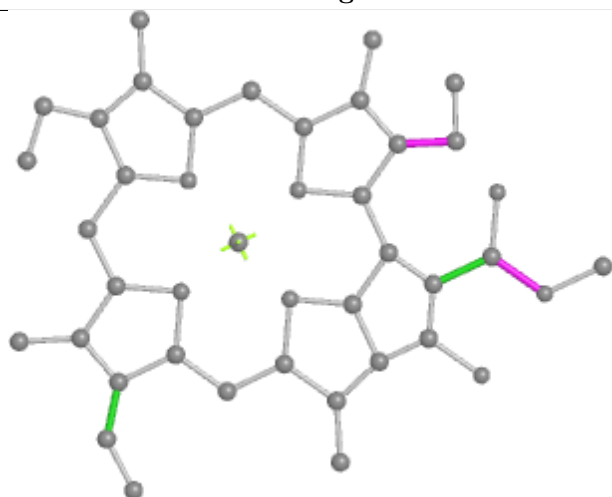
Ligand CLA L 304



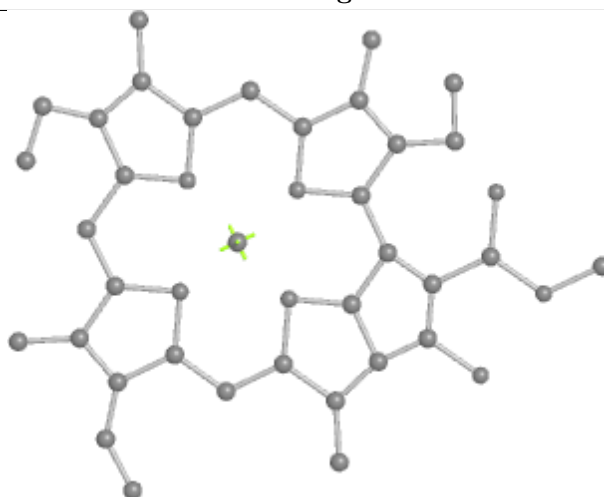
Bond lengths



Bond angles

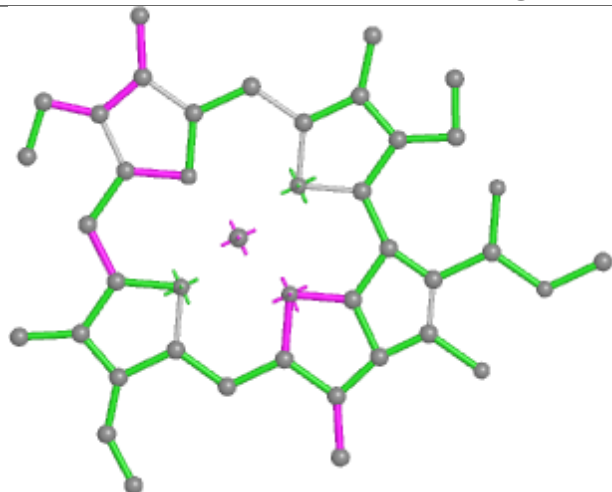


Torsions

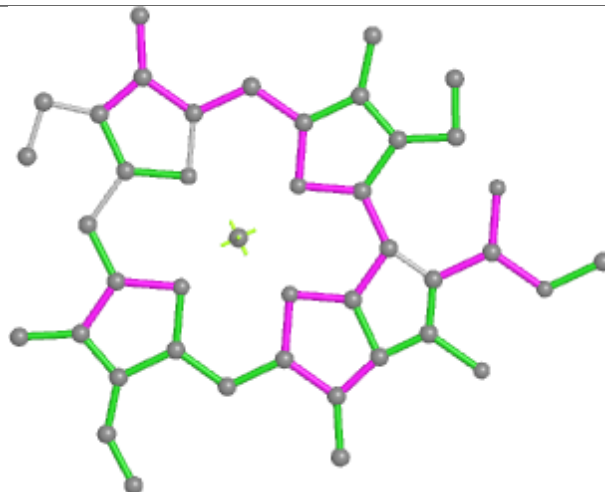


Rings

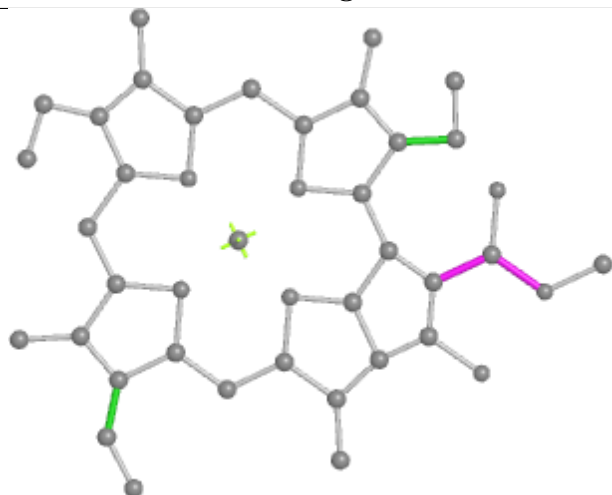
Ligand CLA N 203



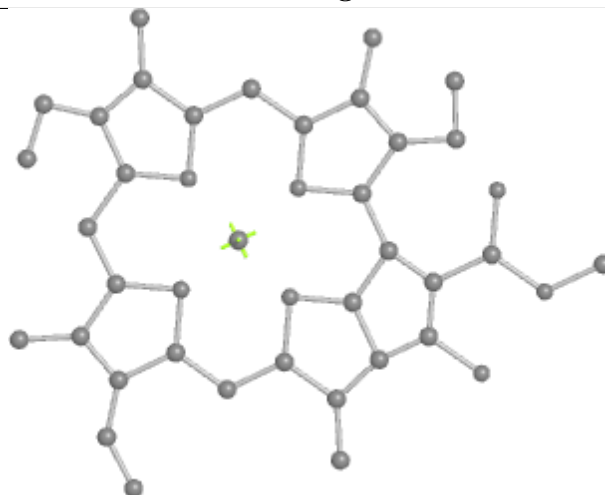
Bond lengths



Bond angles

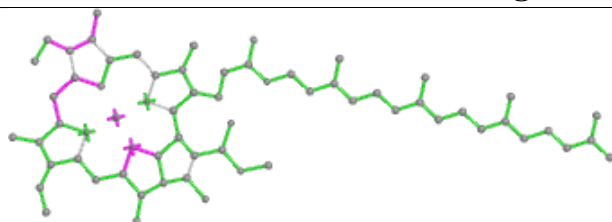


Torsions

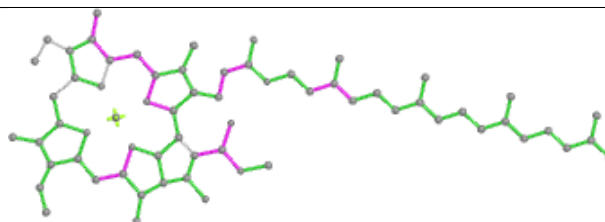


Rings

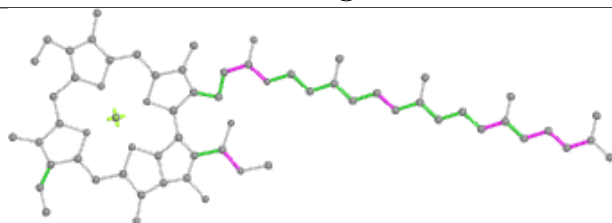
Ligand CLA A 835



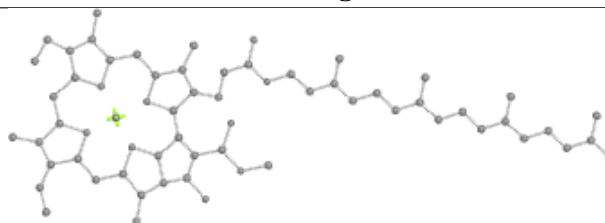
Bond lengths



Bond angles

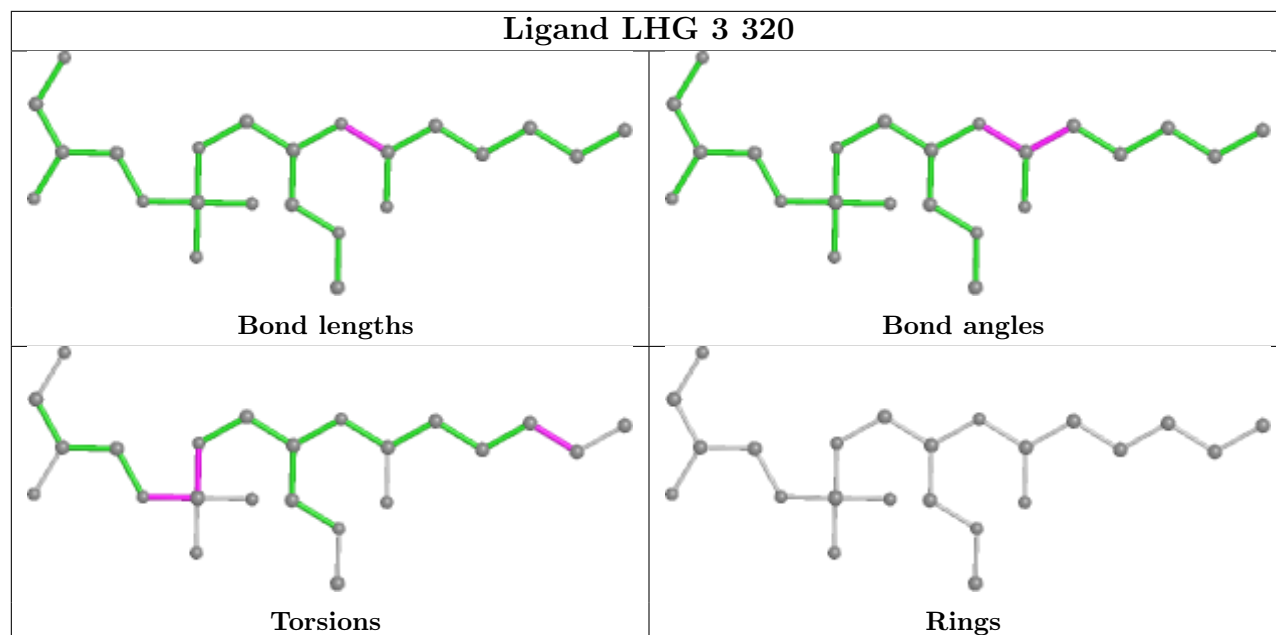


Torsions

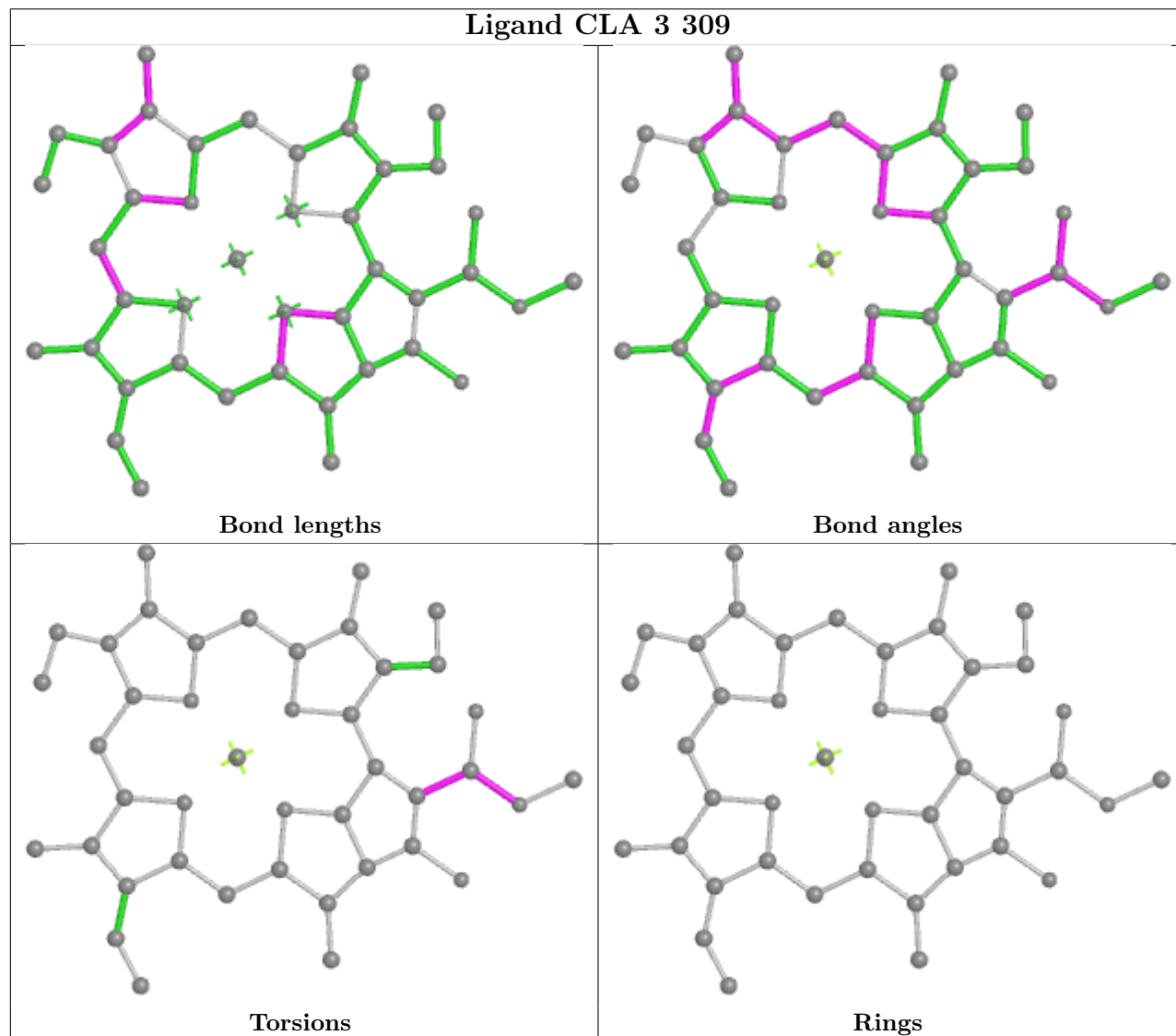


Rings

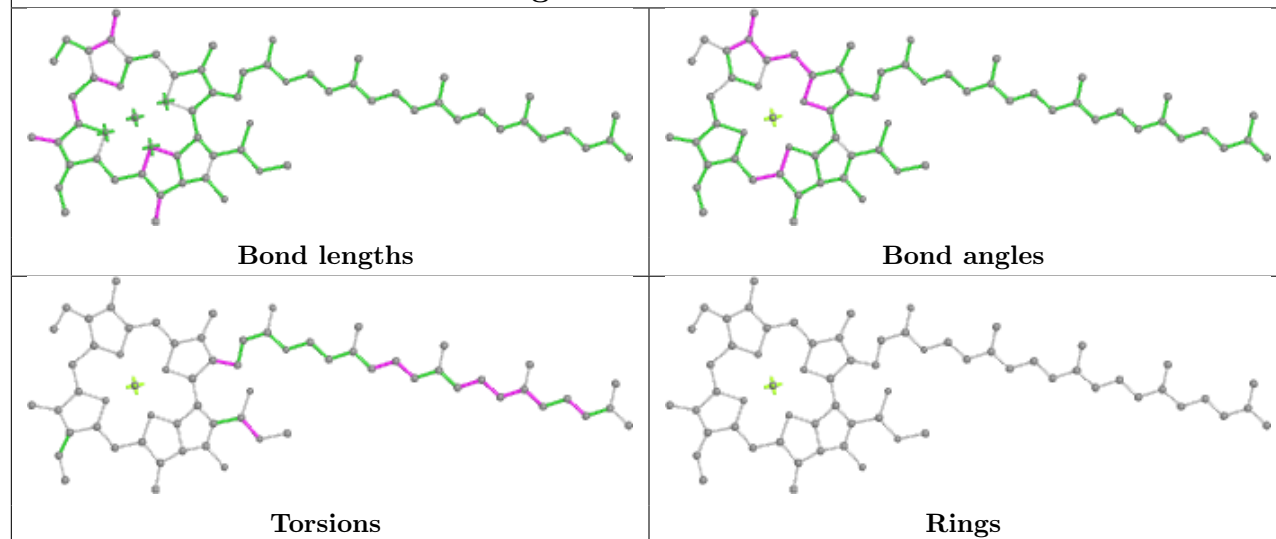
Ligand LHG 3 320



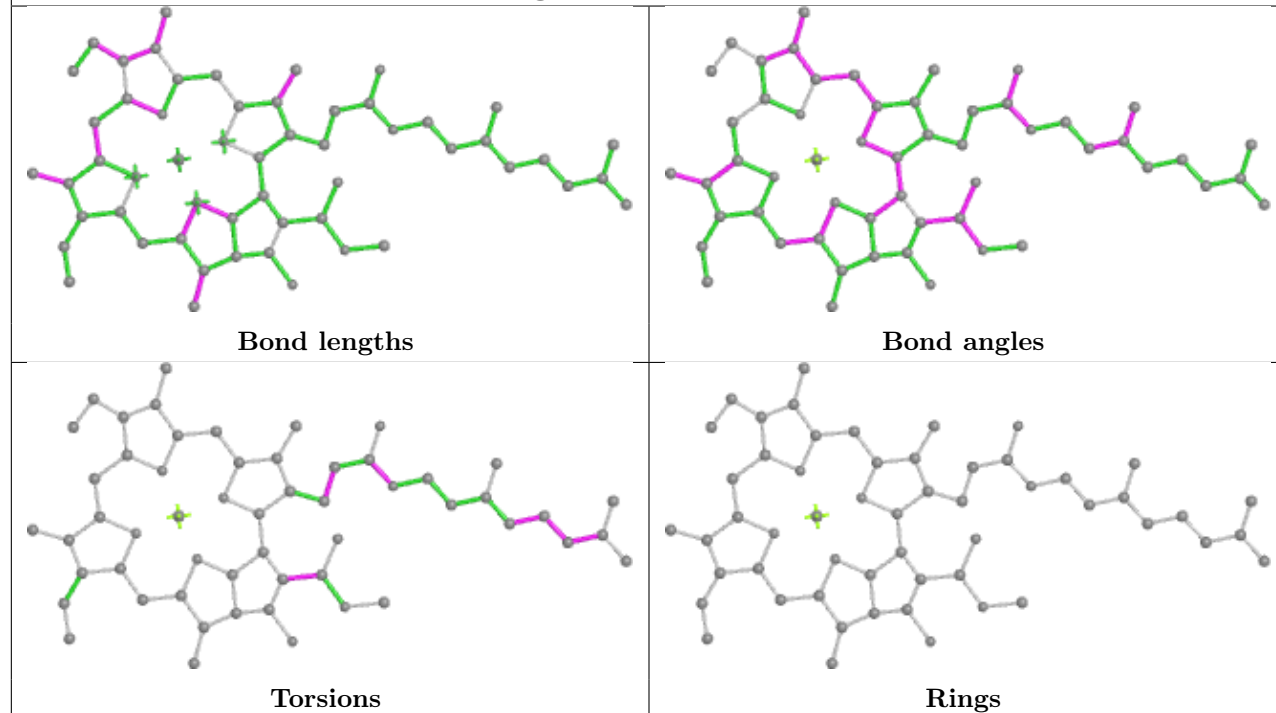
Ligand CLA 3 309



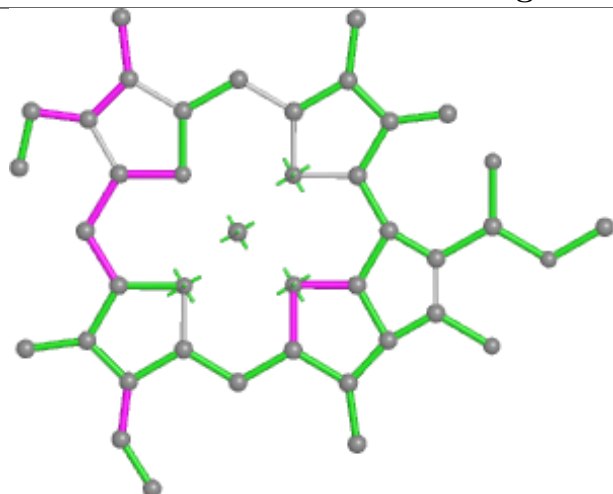
Ligand CLA R 306



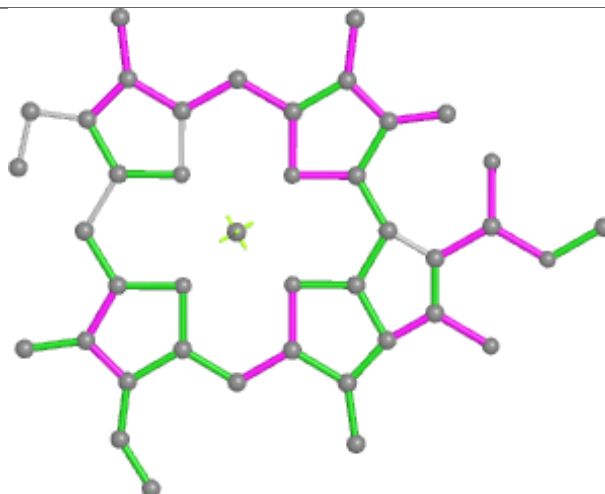
Ligand CLA X 302



Ligand CLA F 803



Bond lengths



Bond angles

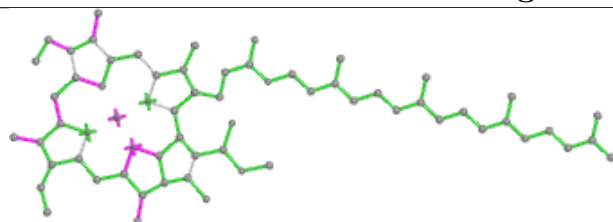


Torsions

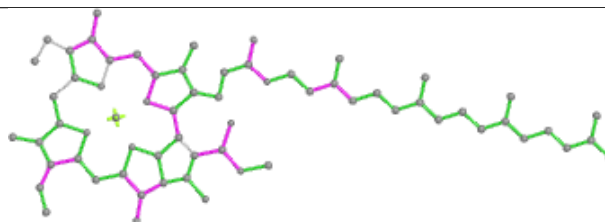


Rings

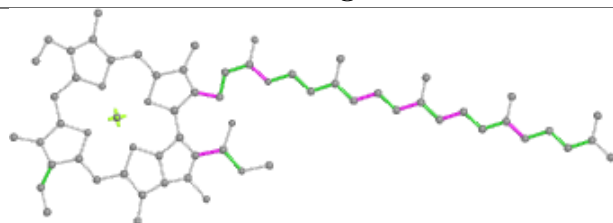
Ligand CLA S 301



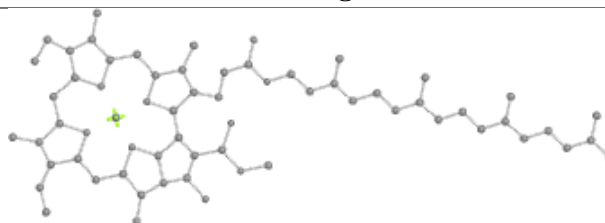
Bond lengths



Bond angles

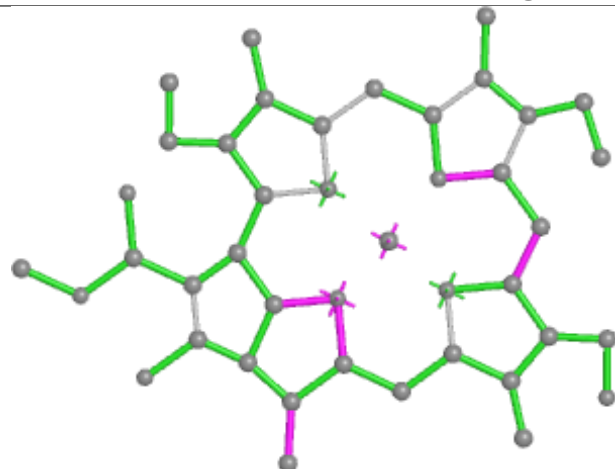


Torsions

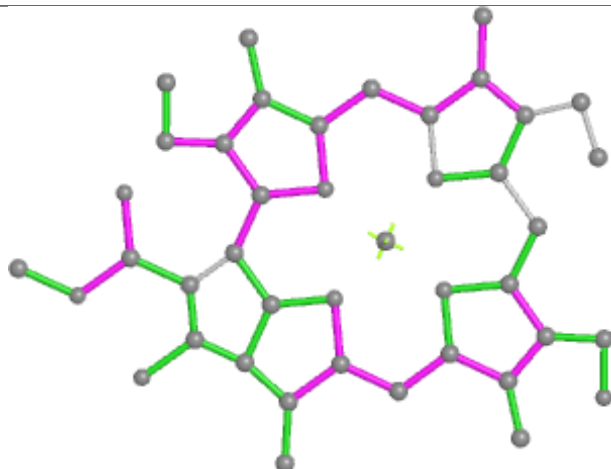


Rings

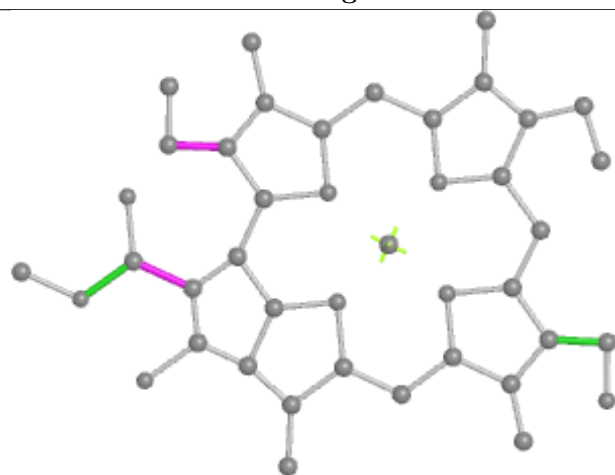
Ligand CHL 6 601



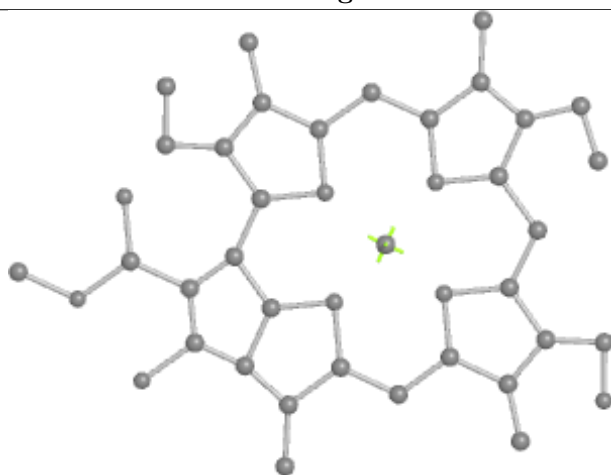
Bond lengths



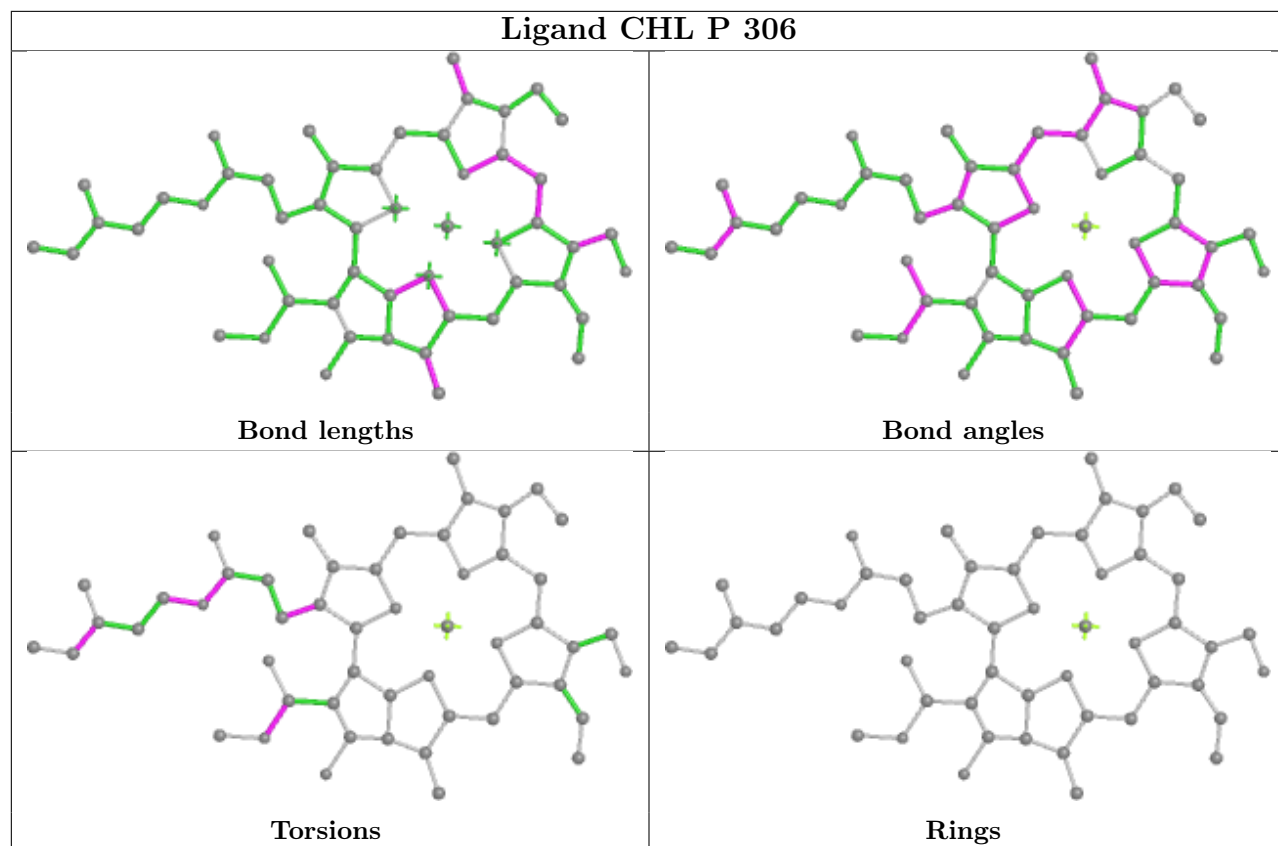
Bond angles



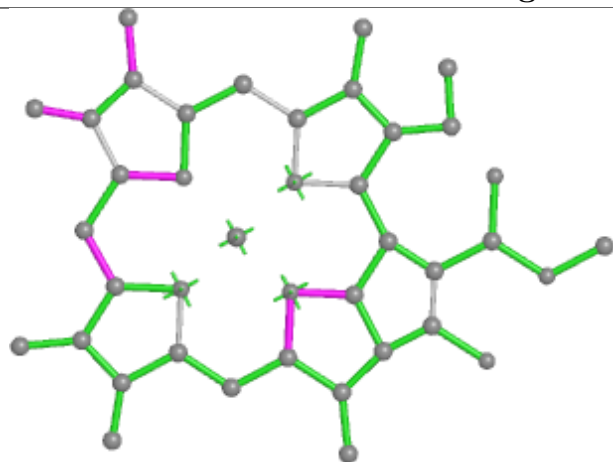
Torsions



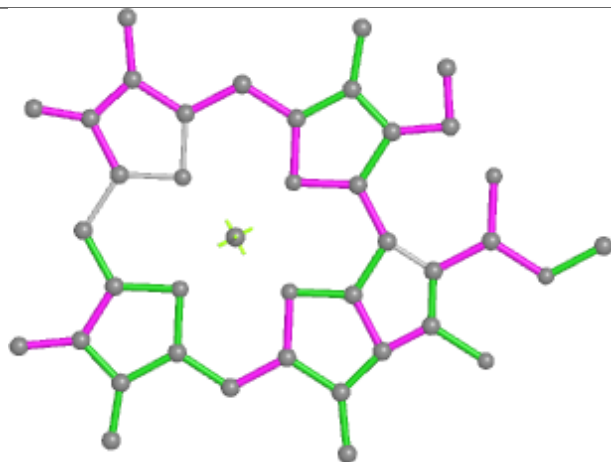
Rings



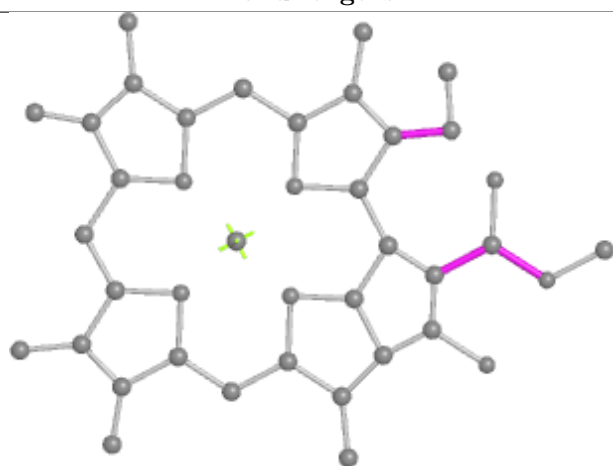
Ligand CLA 1 610



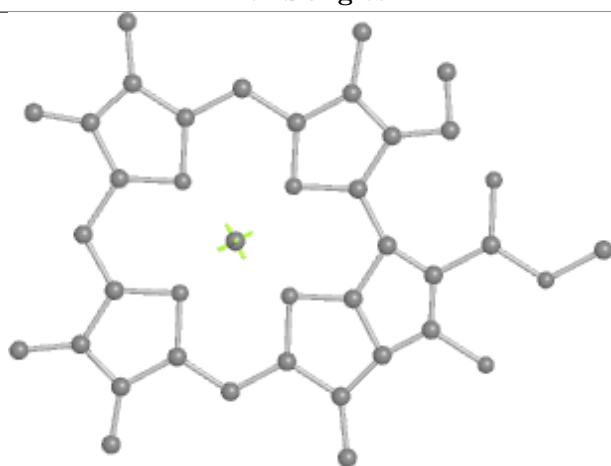
Bond lengths



Bond angles

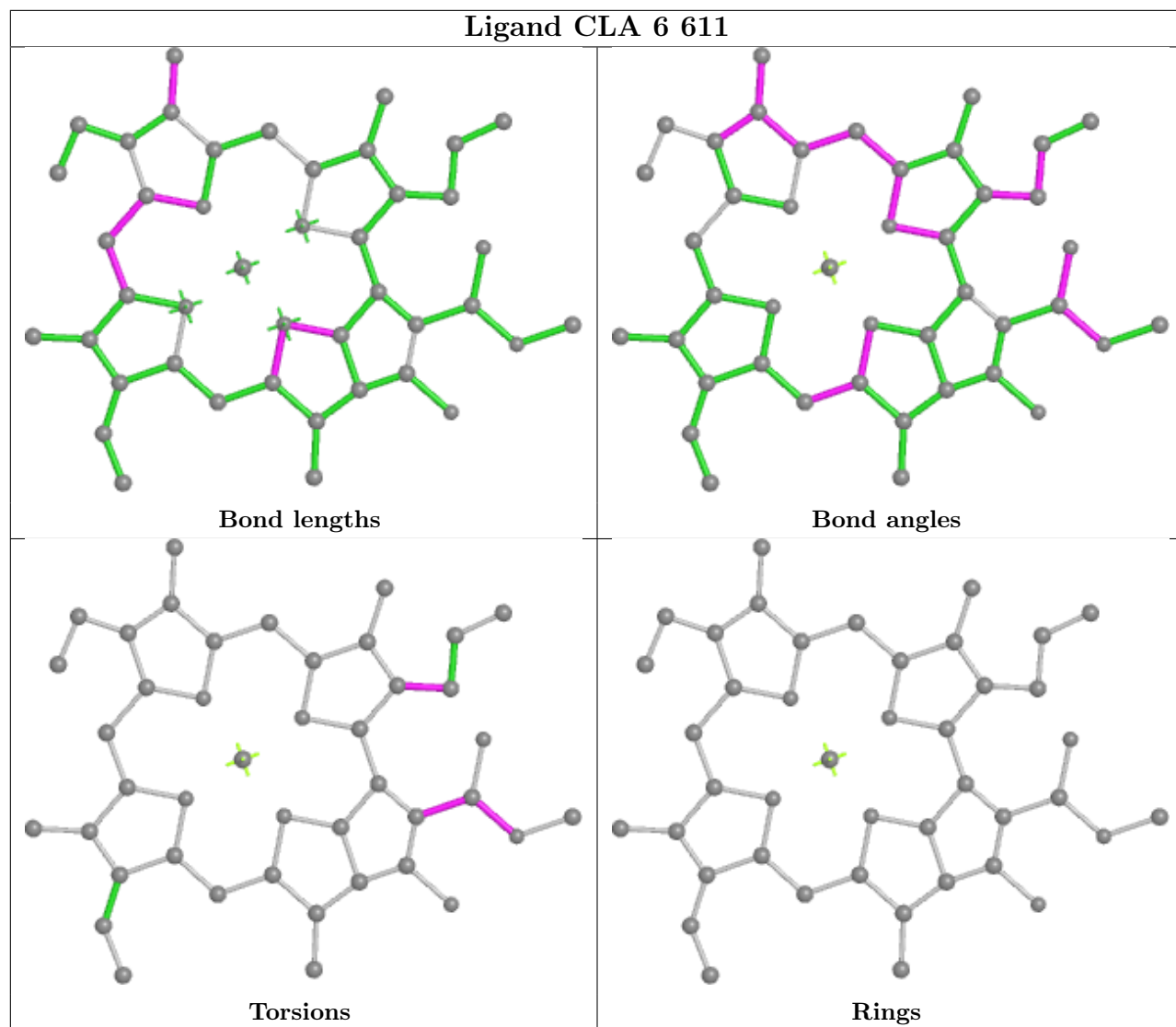


Torsions

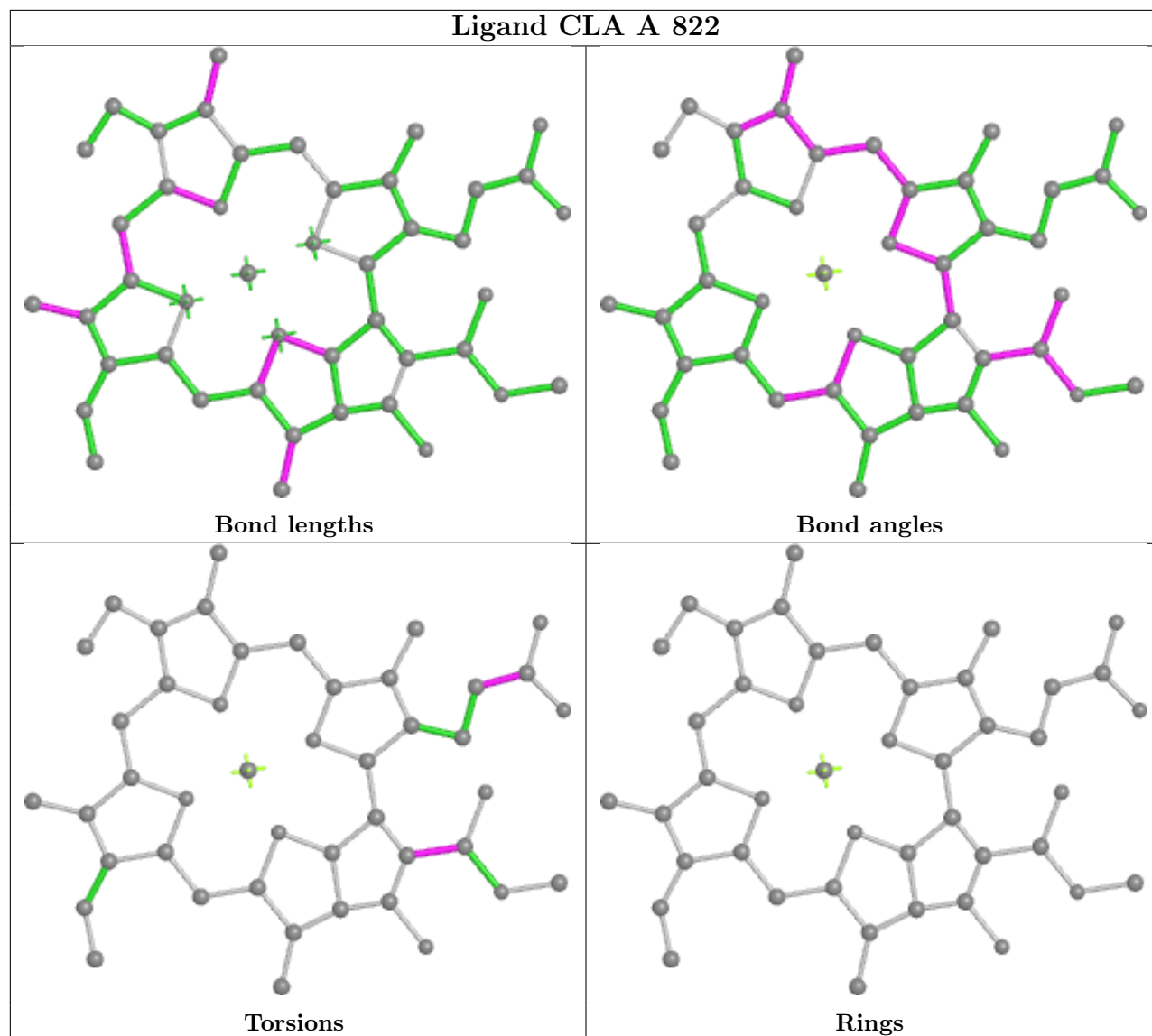


Rings

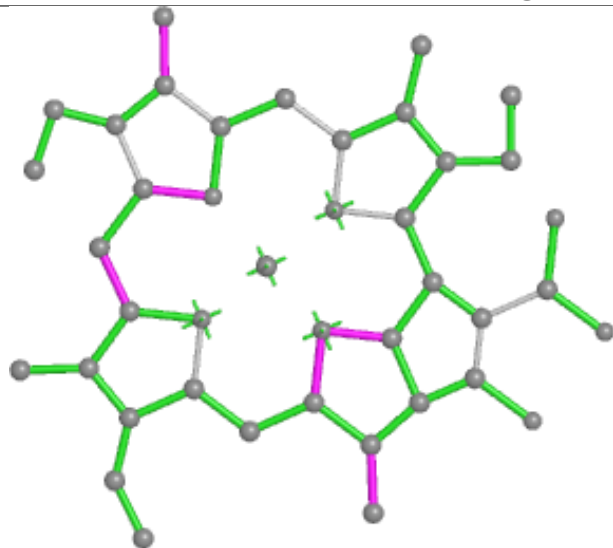
Ligand CLA 6 611



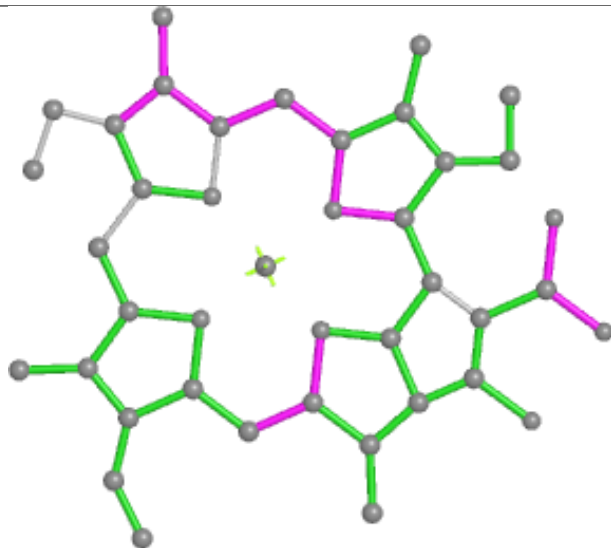
Ligand CLA A 822



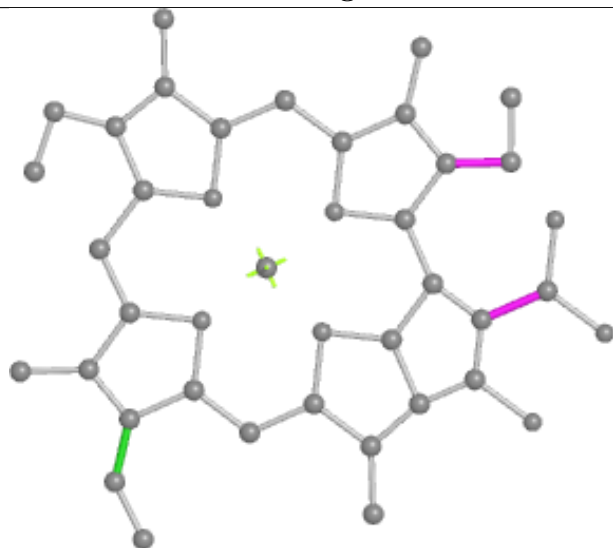
Ligand CLA 1 605



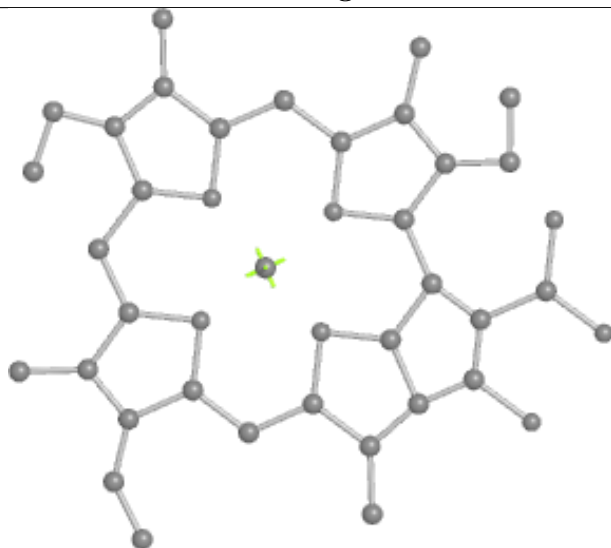
Bond lengths



Bond angles

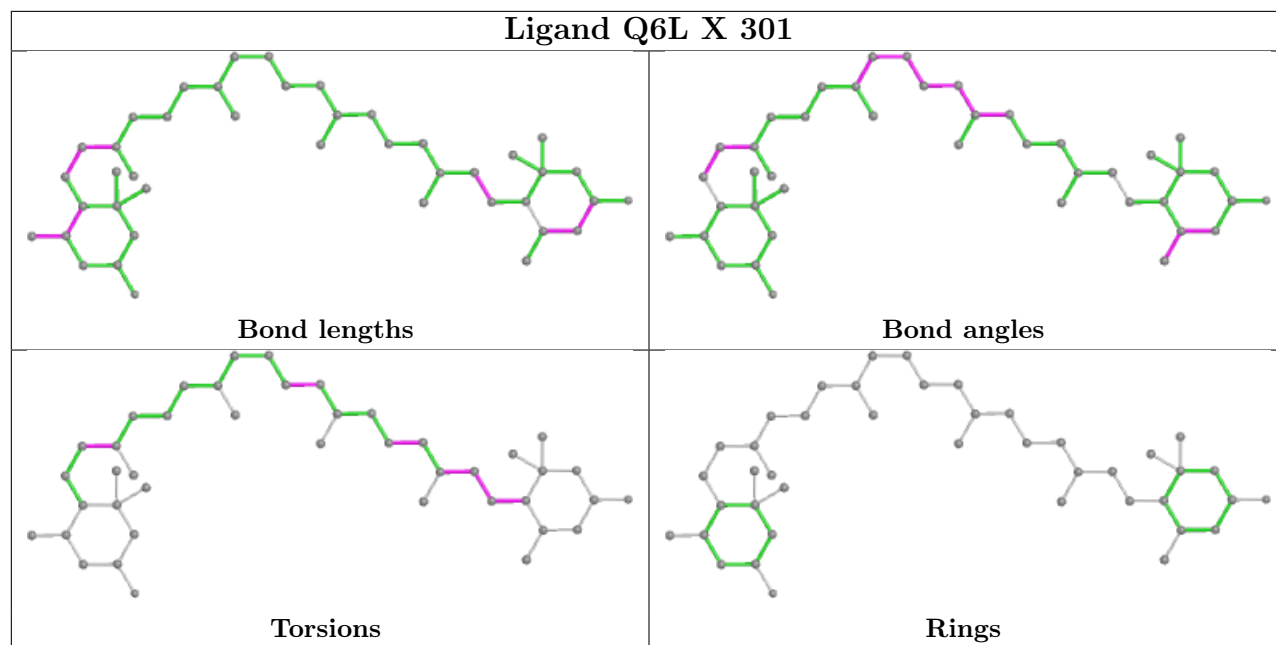


Torsions

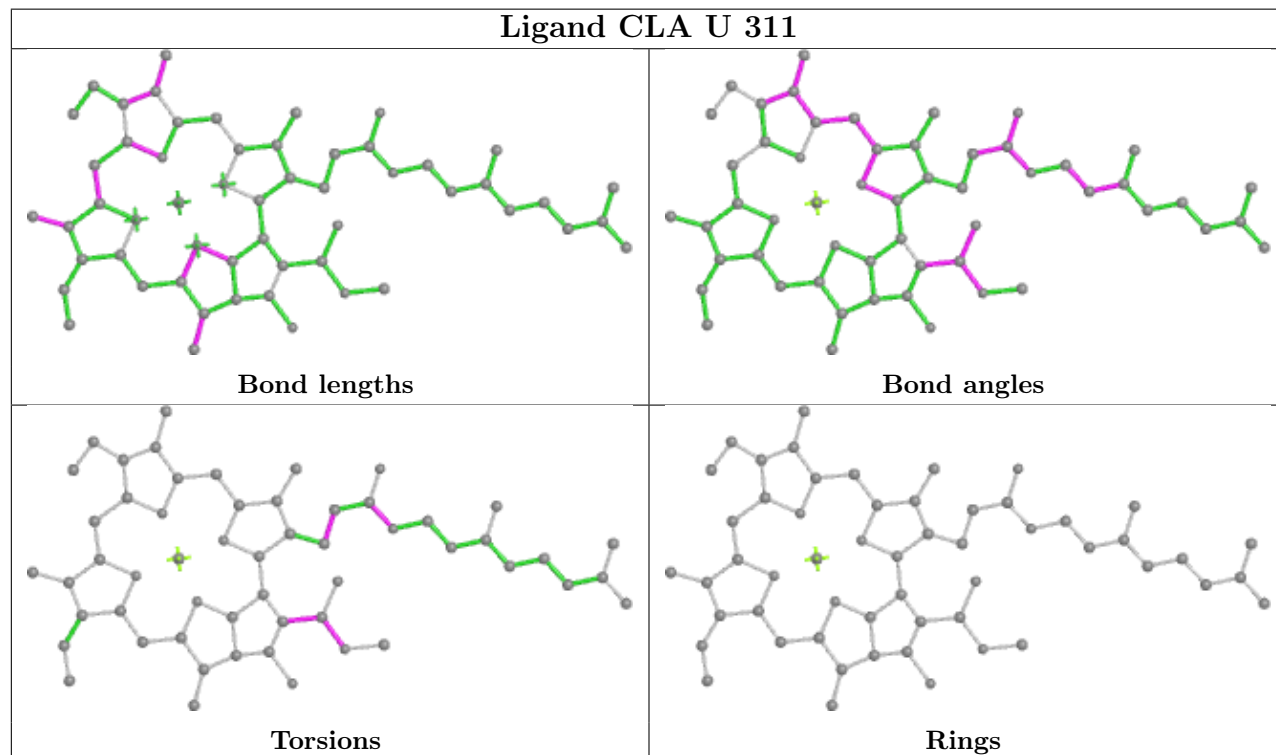


Rings

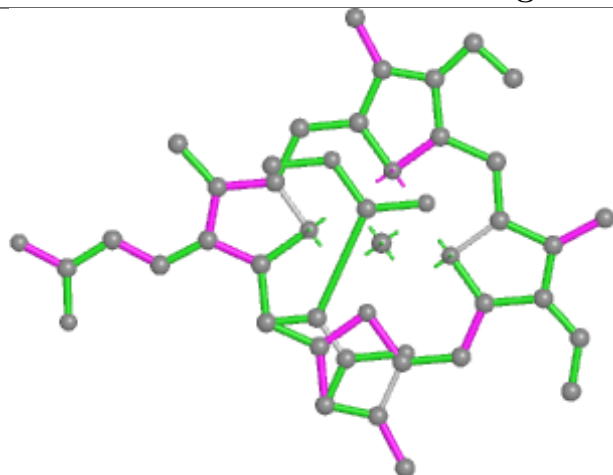
Ligand Q6L X 301



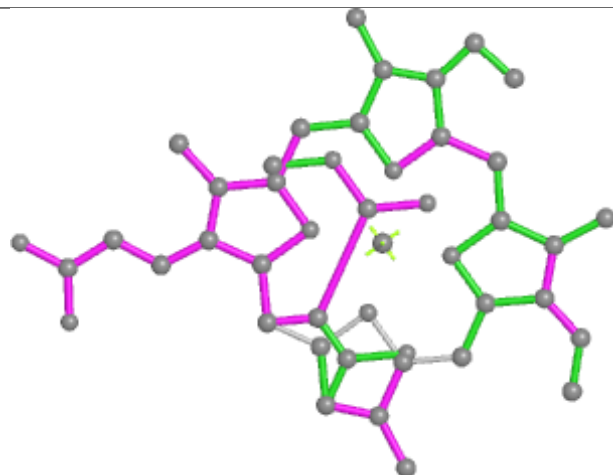
Ligand CLA U 311



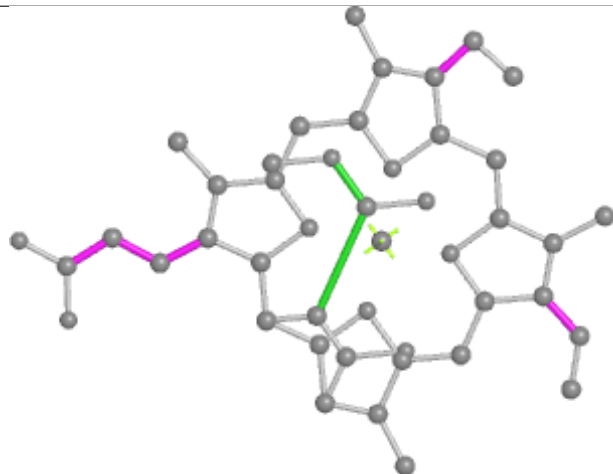
Ligand KC2 T 308



Bond lengths



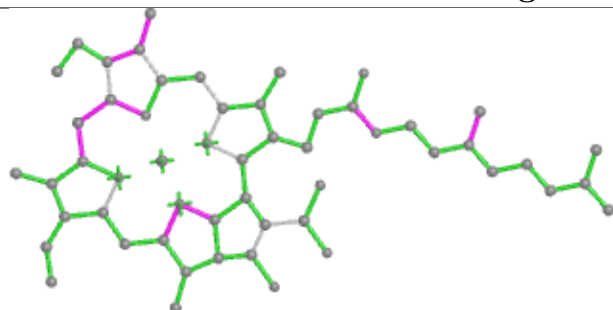
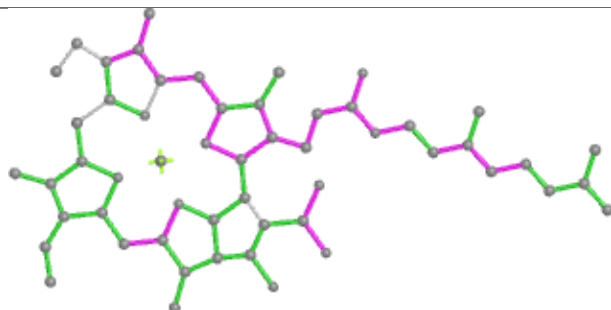
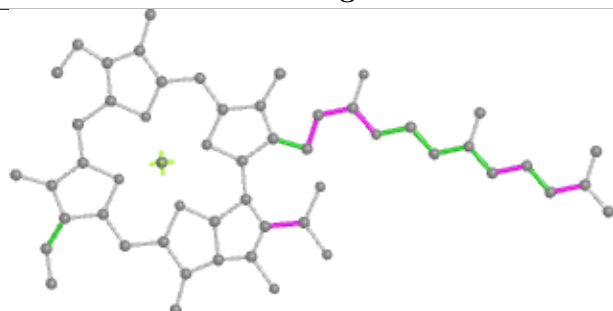
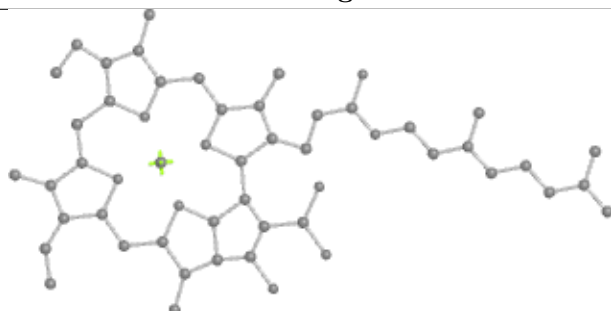
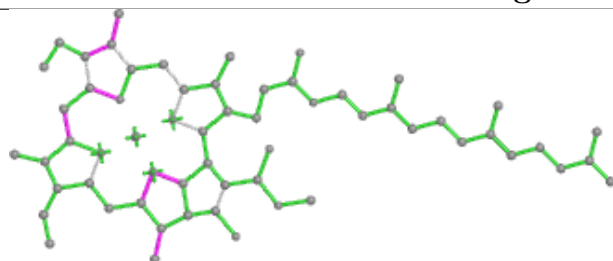
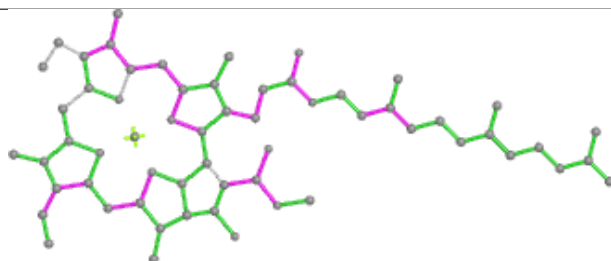
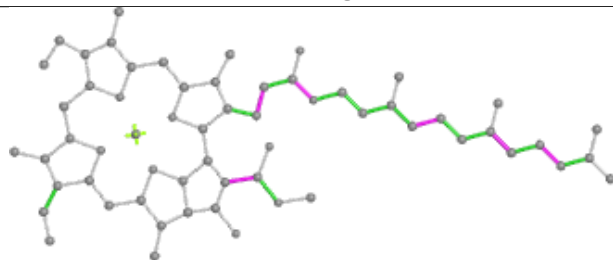
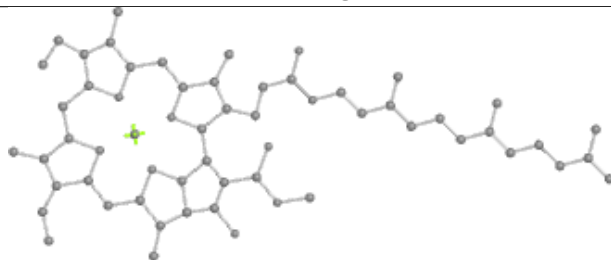
Bond angles



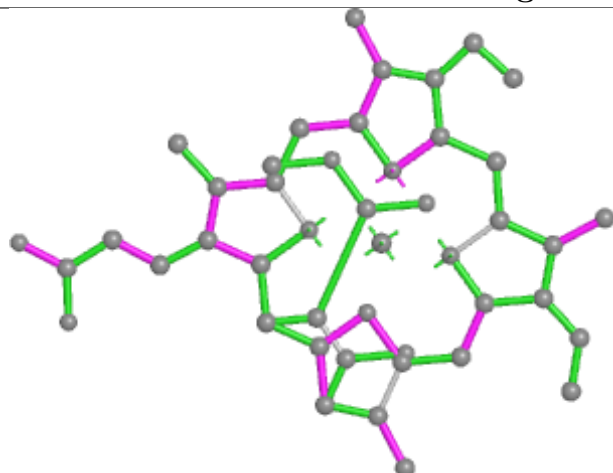
Torsions



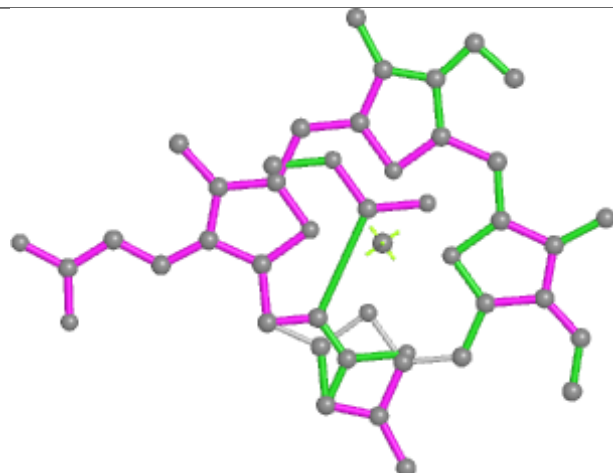
Rings

Ligand CLA 3 311**Bond lengths****Bond angles****Torsions****Rings****Ligand CLA R 315****Bond lengths****Bond angles****Torsions****Rings**

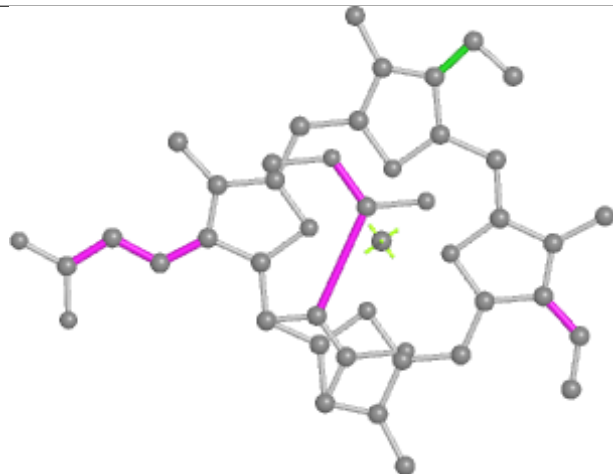
Ligand KC2 P 308



Bond lengths



Bond angles

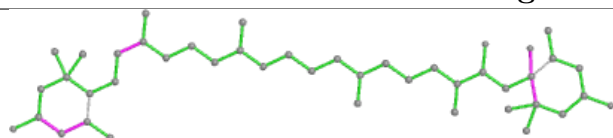


Torsions

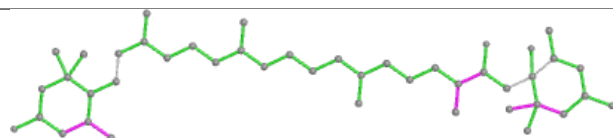


Rings

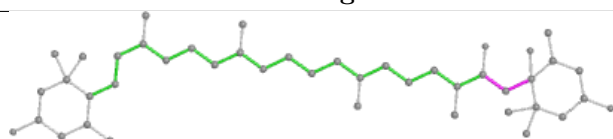
Ligand IWJ T 321



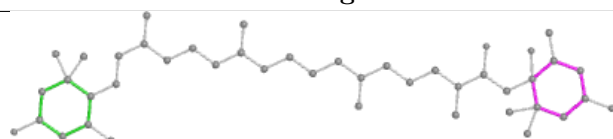
Bond lengths



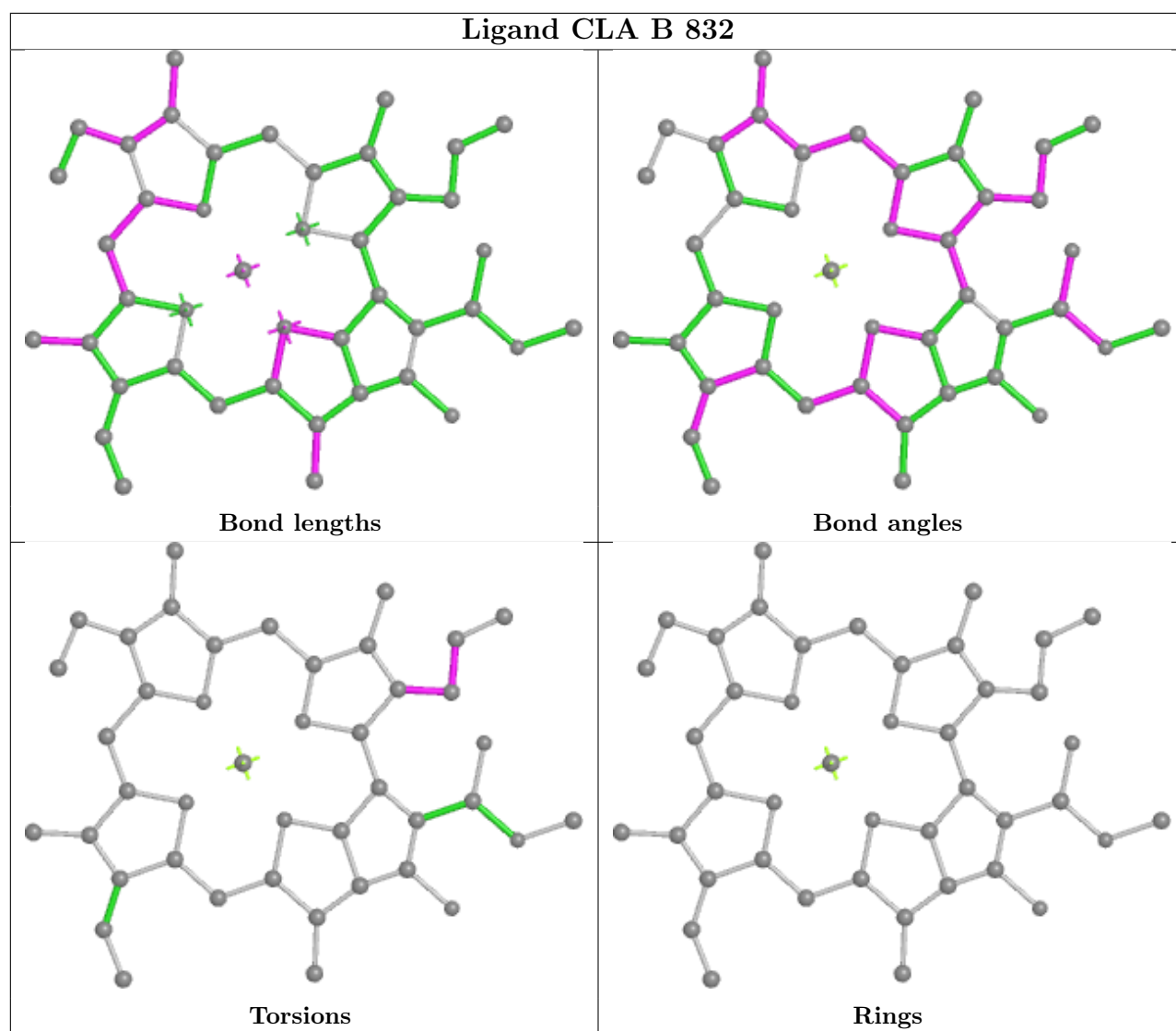
Bond angles

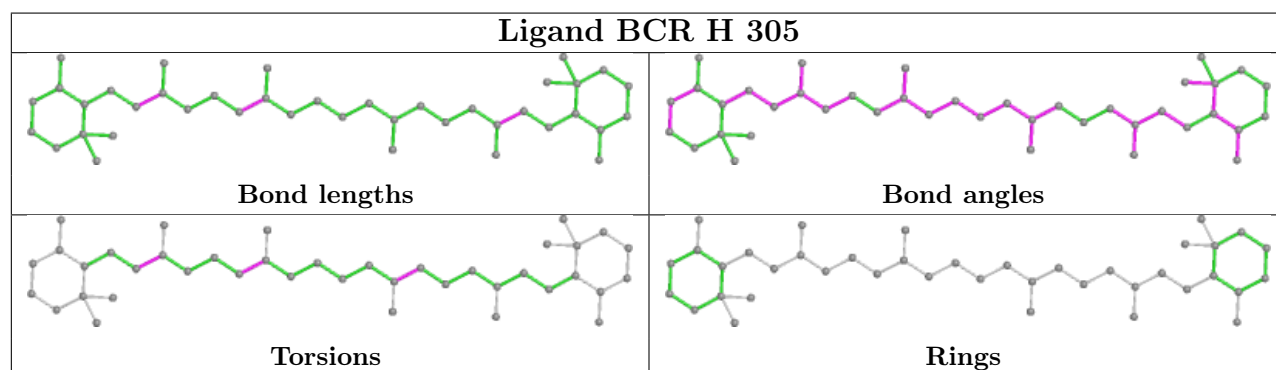
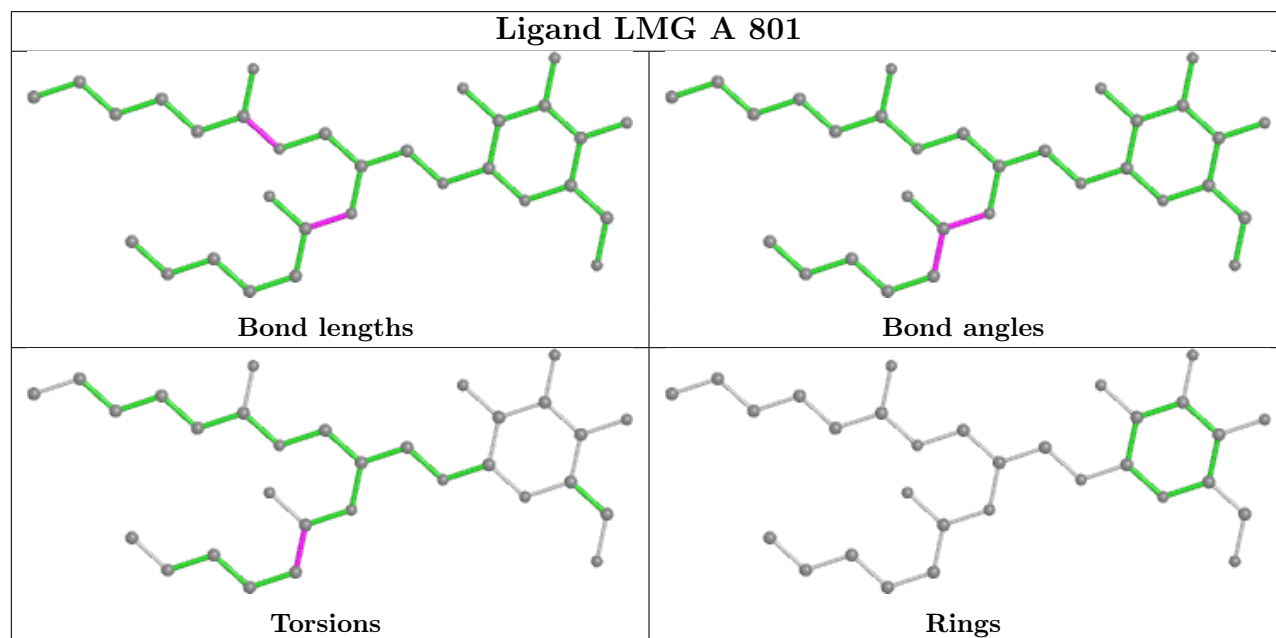
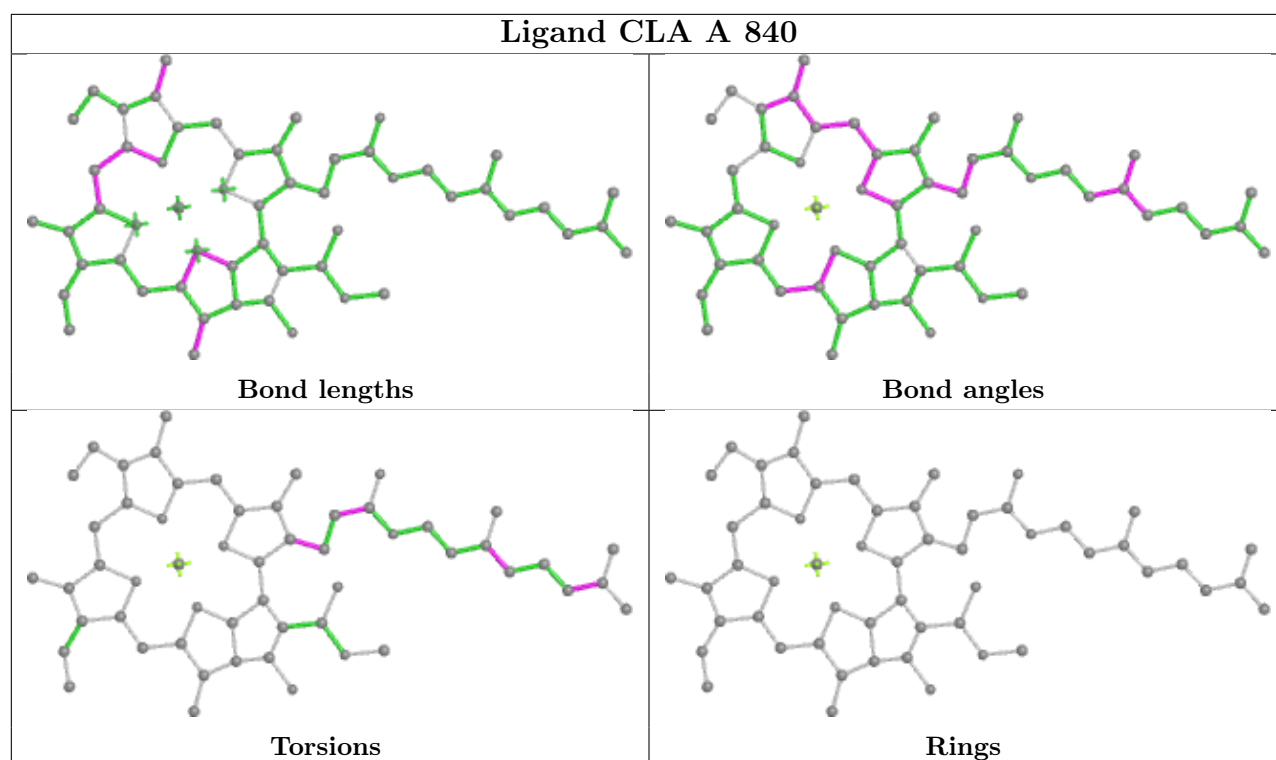


Torsions

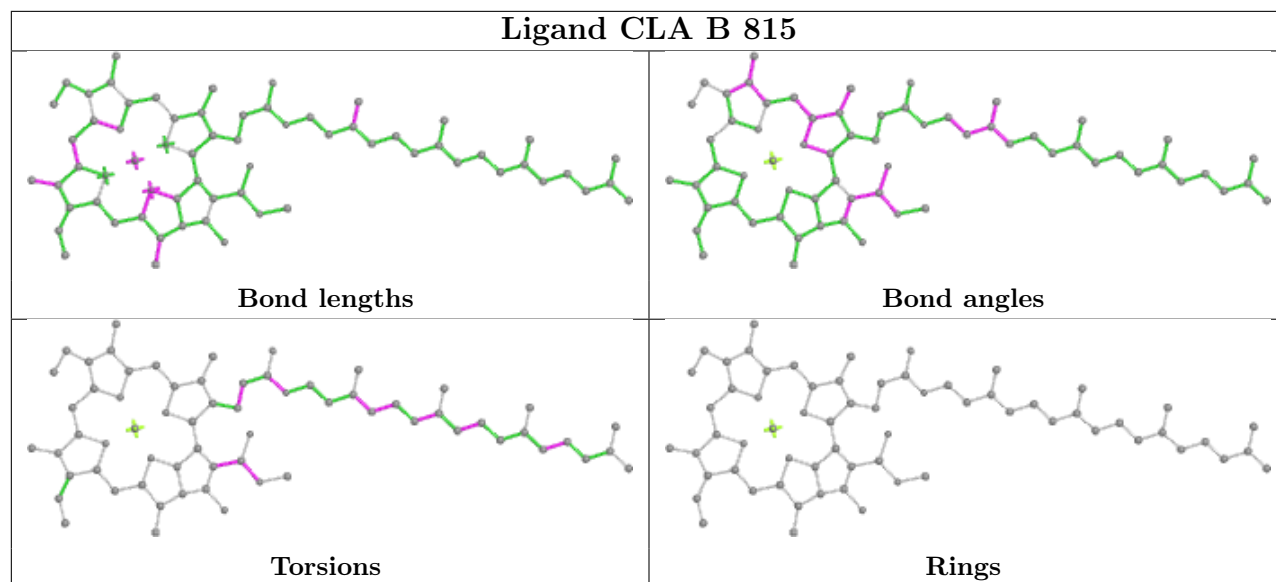


Rings

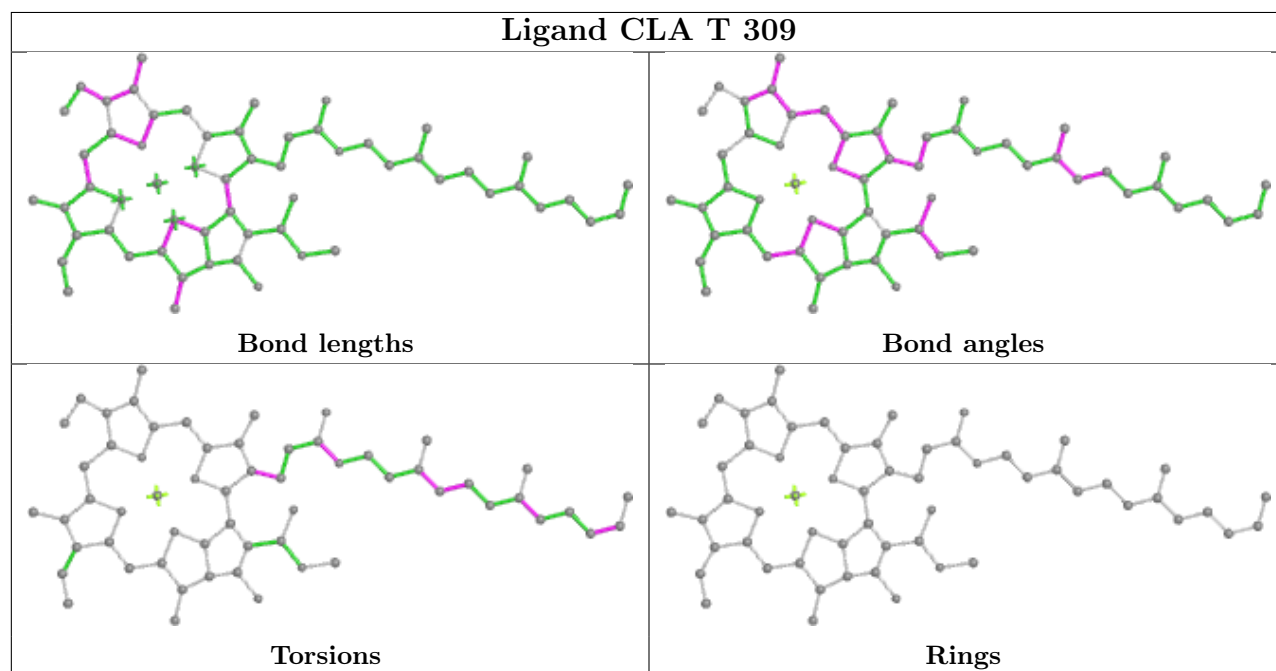




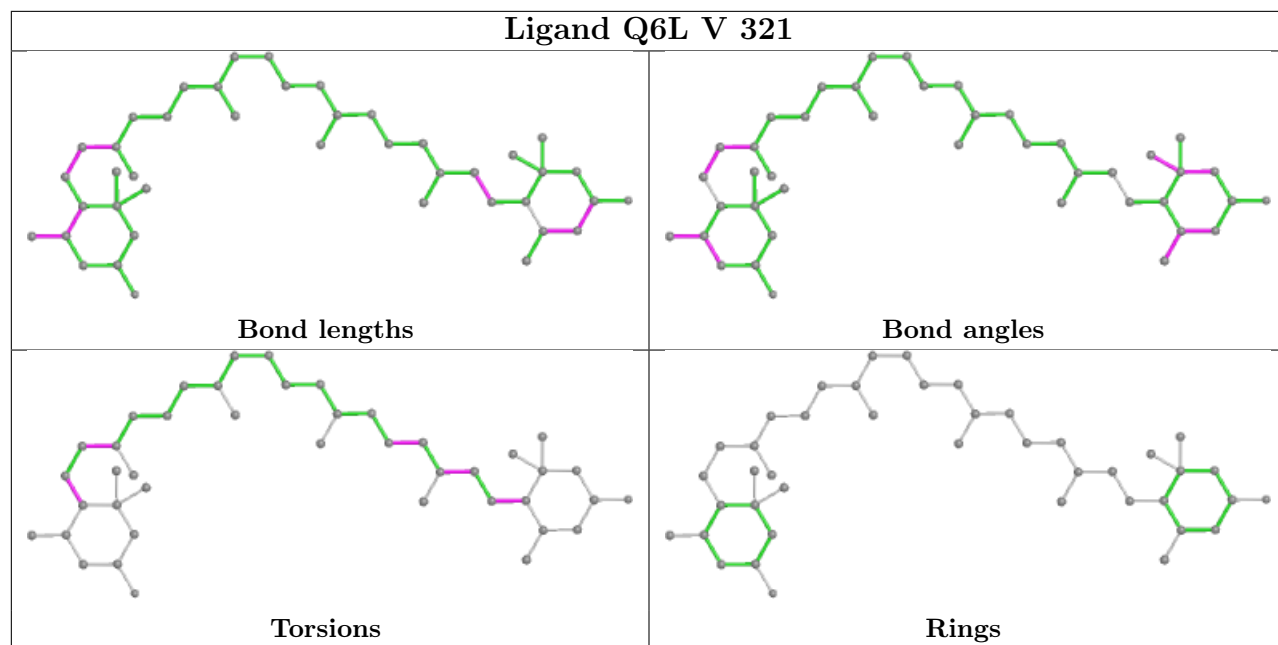
Ligand CLA B 815



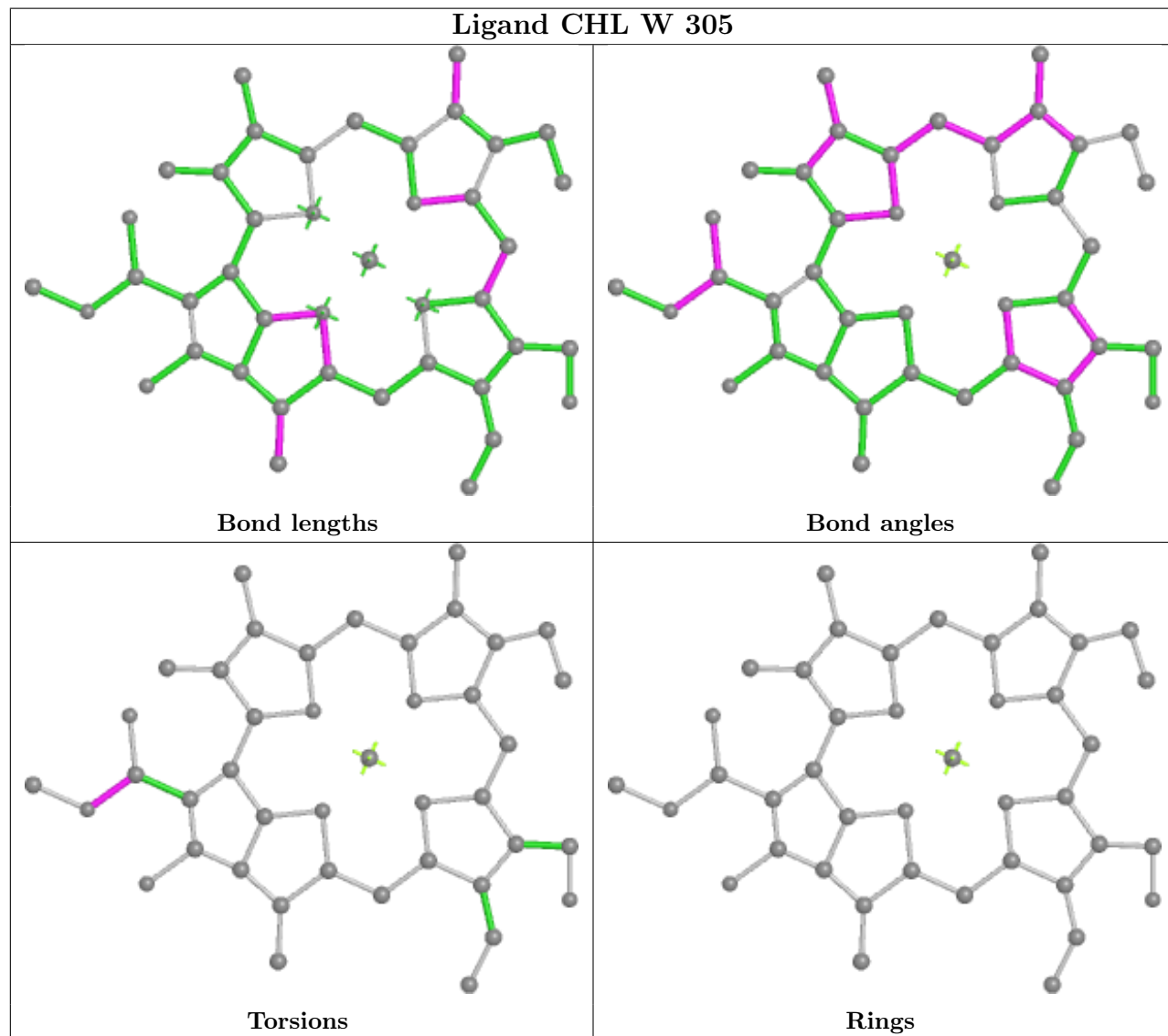
Ligand CLA T 309

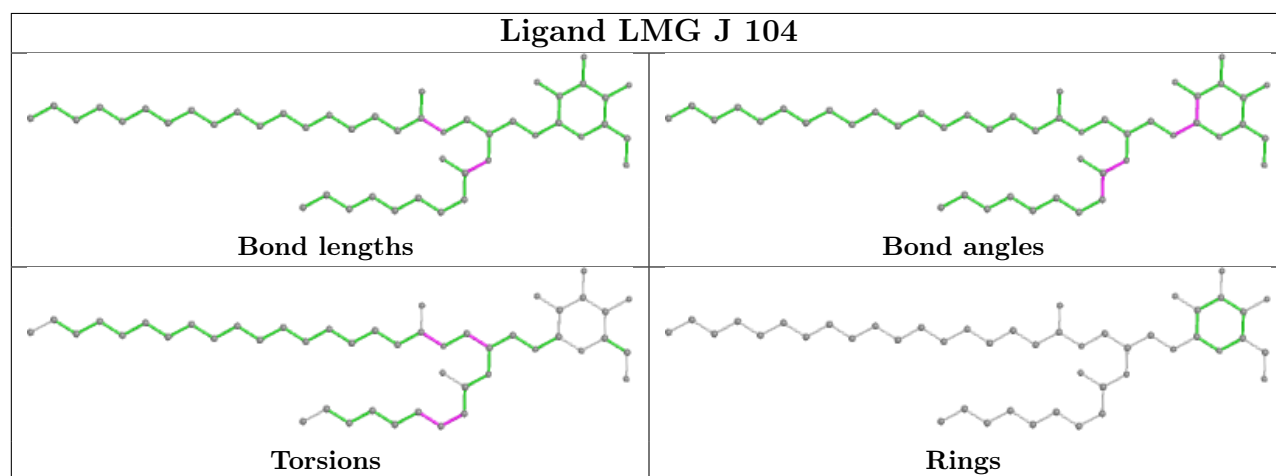
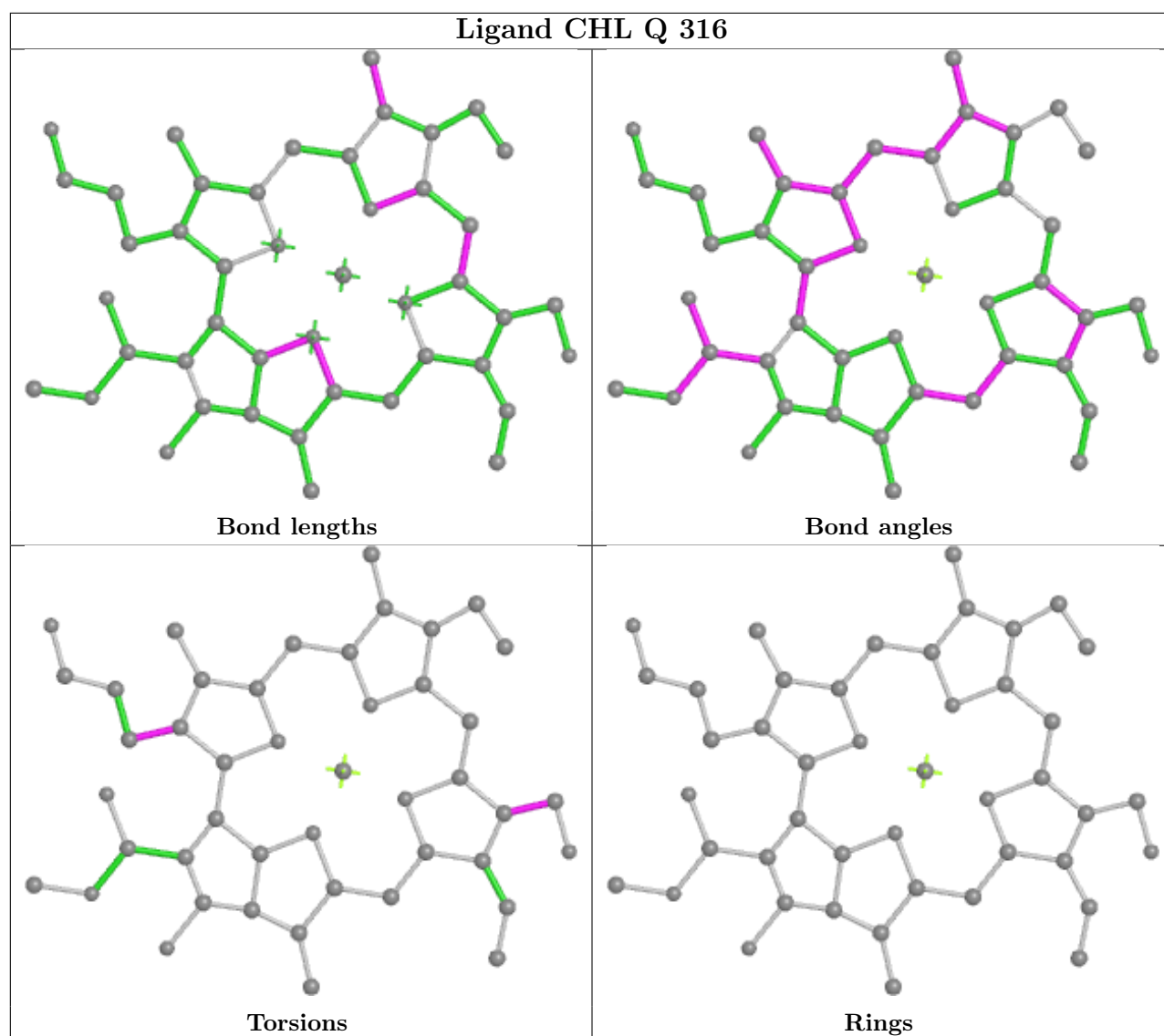


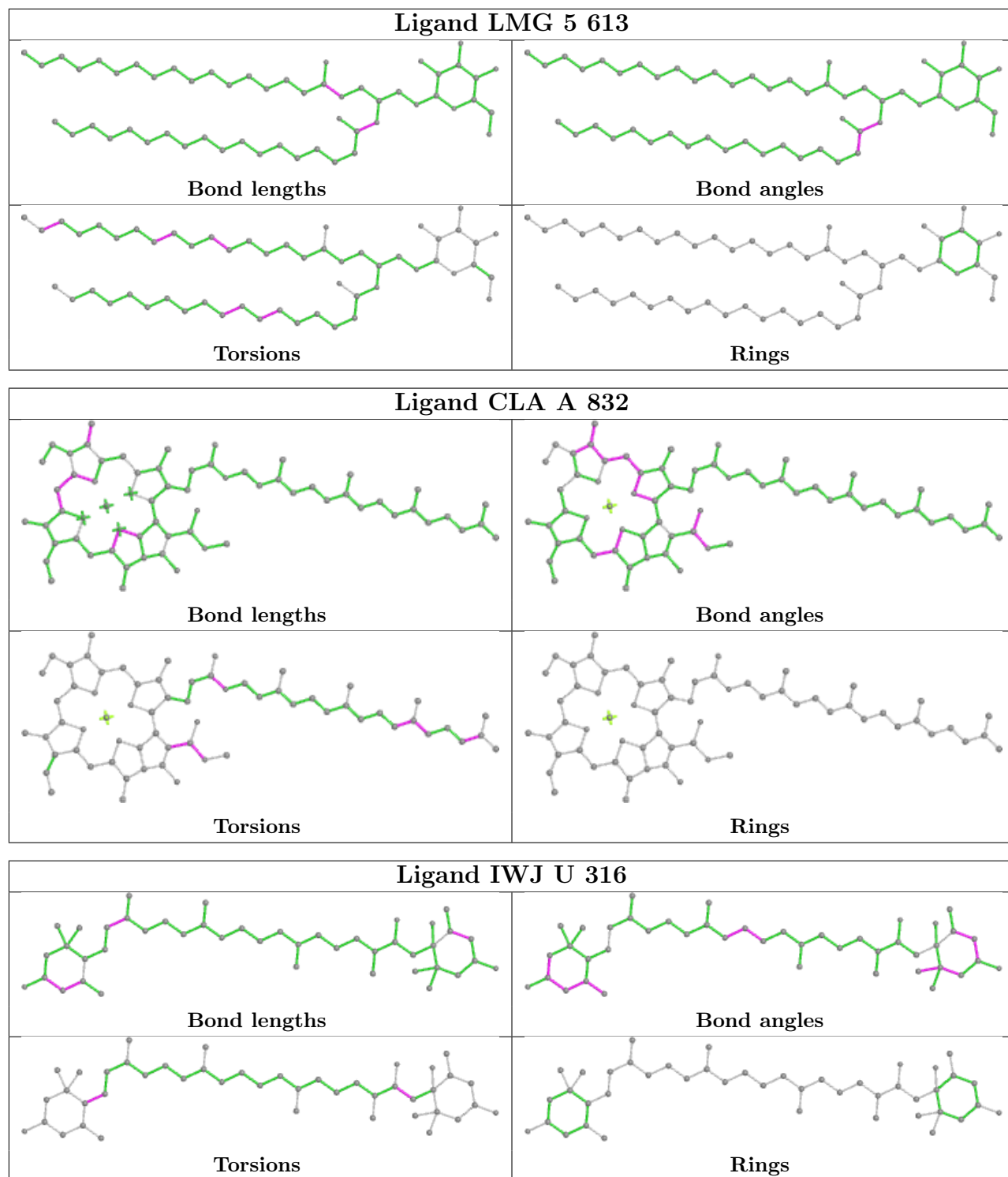
Ligand Q6L V 321

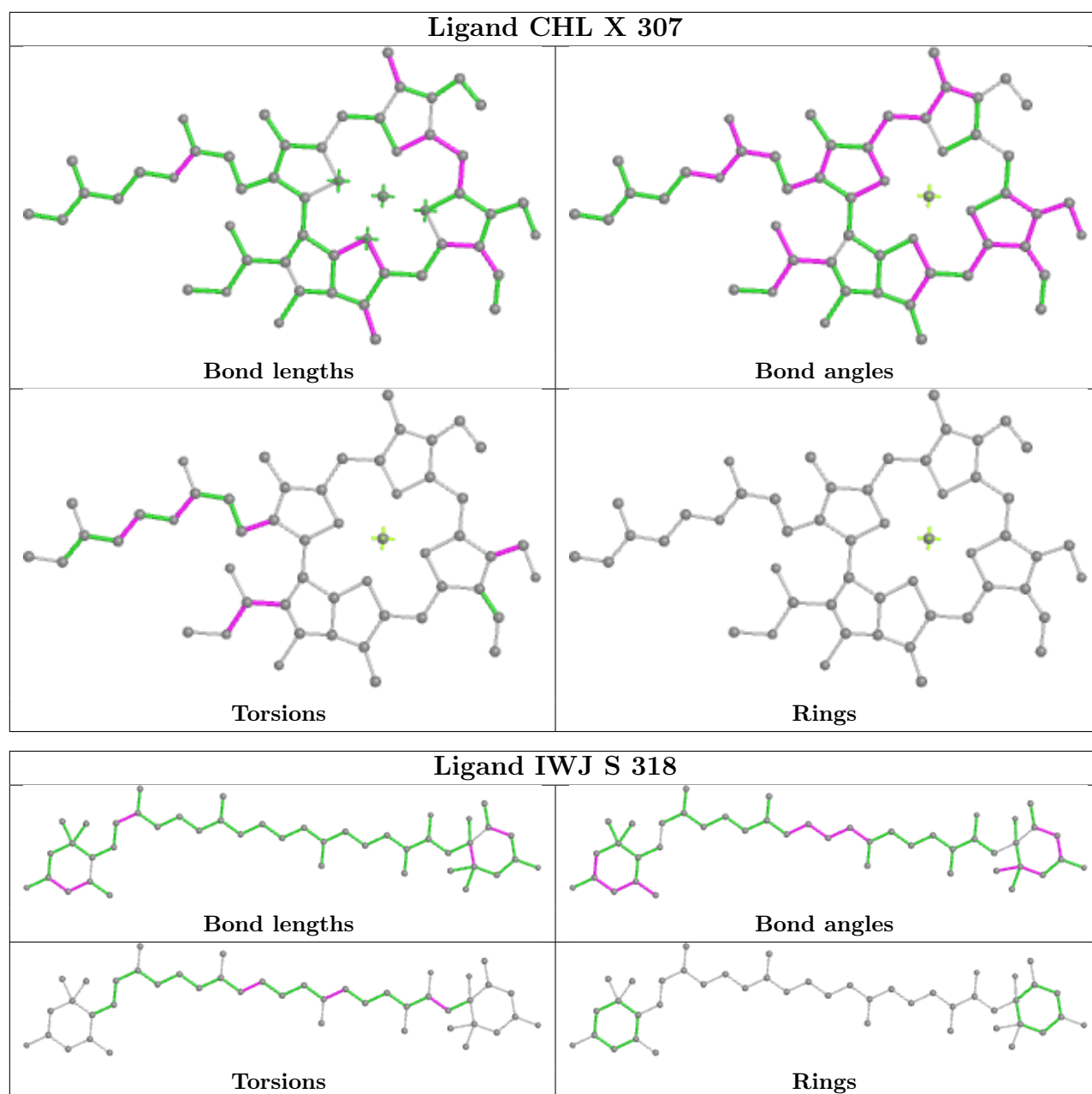


Ligand CHL W 305

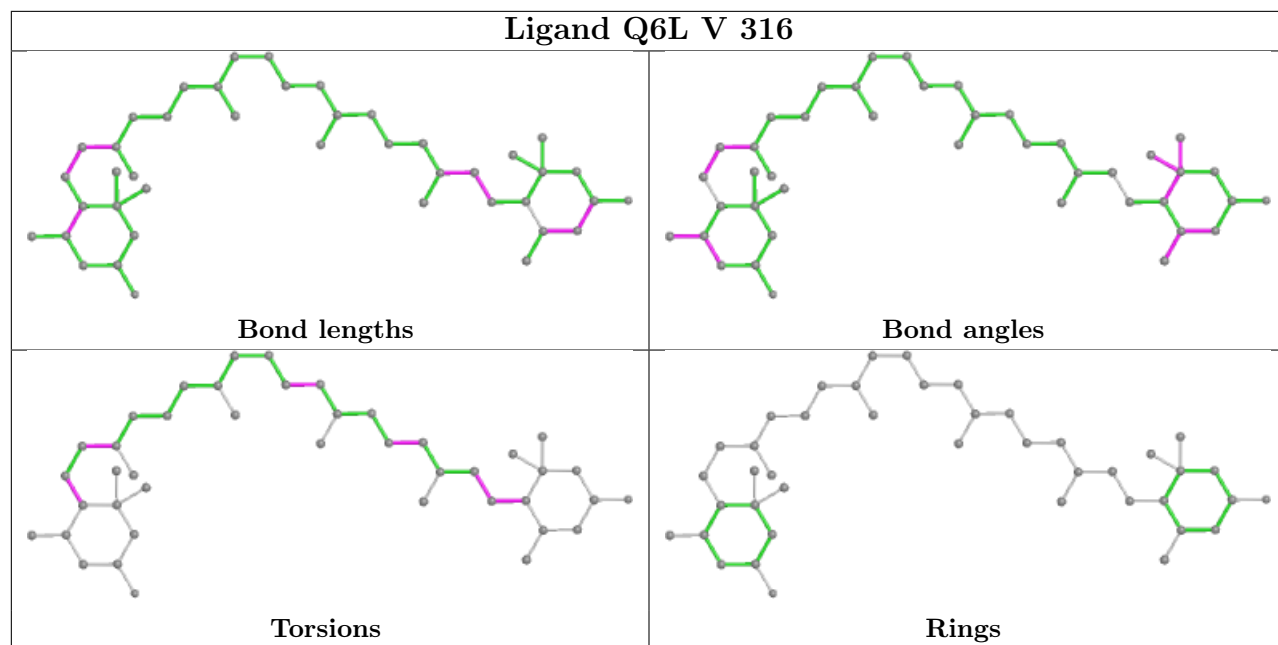




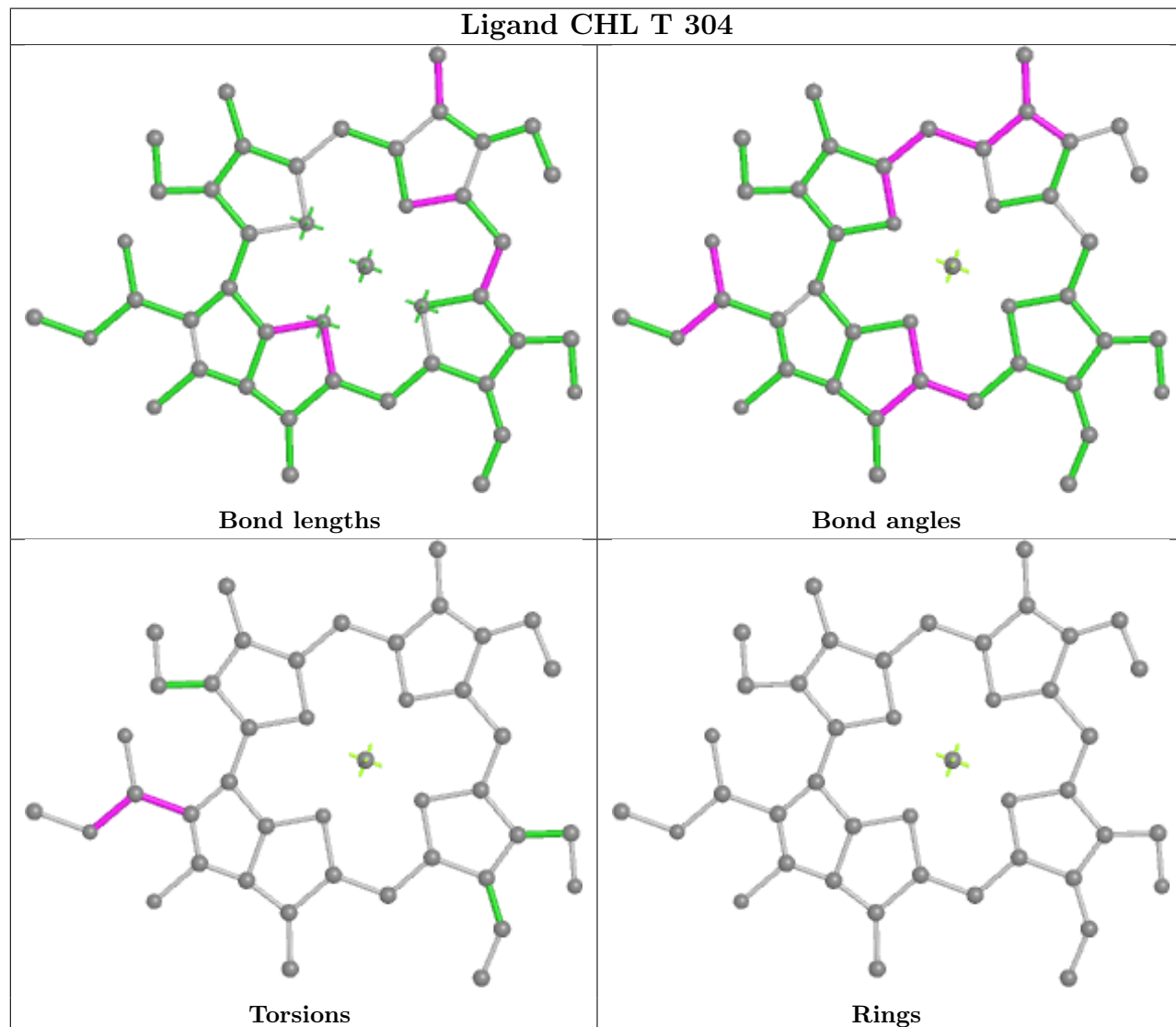


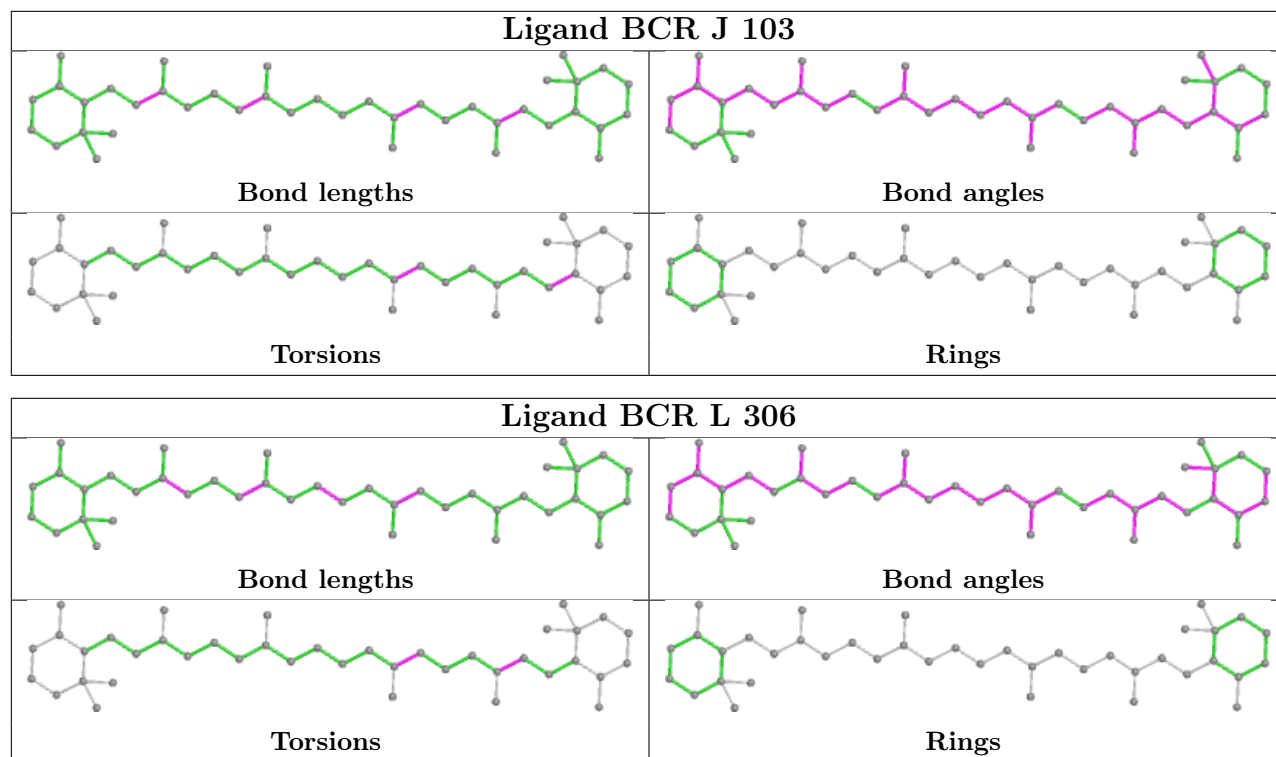


Ligand Q6L V 316

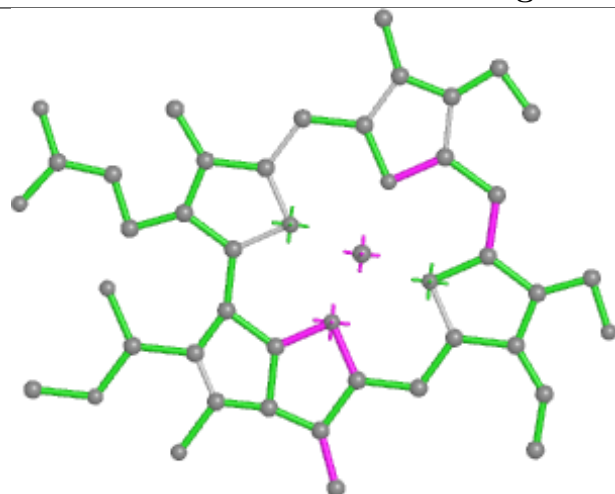


Ligand CHL T 304

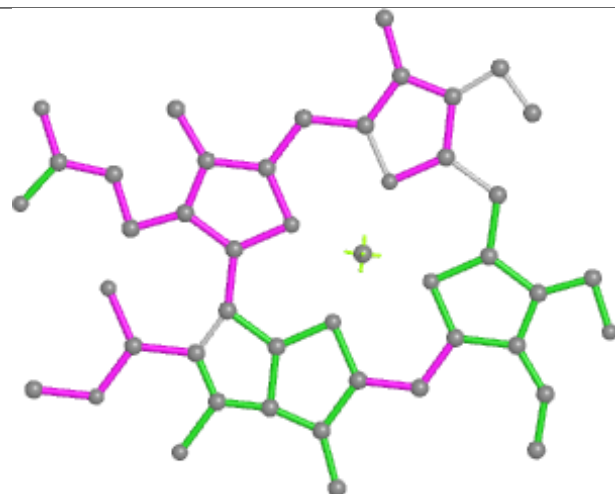




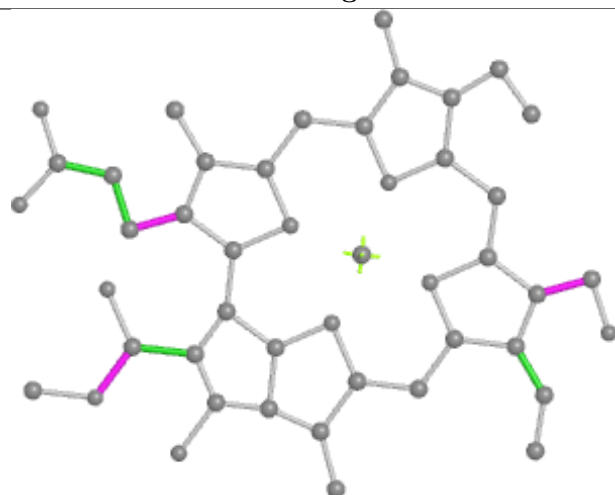
Ligand CHL P 304



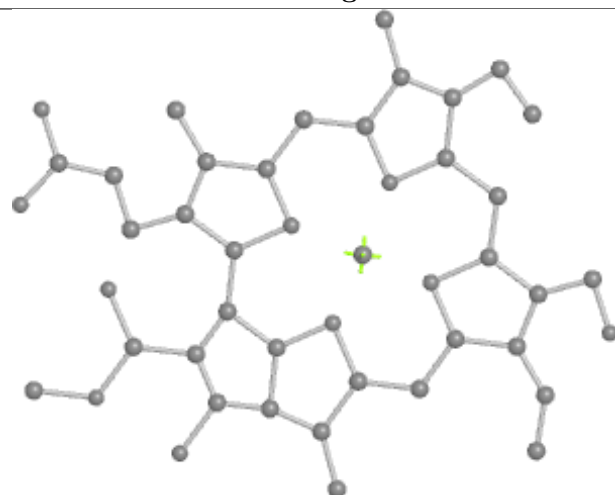
Bond lengths



Bond angles

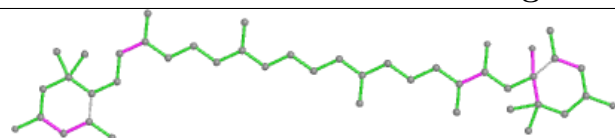


Torsions

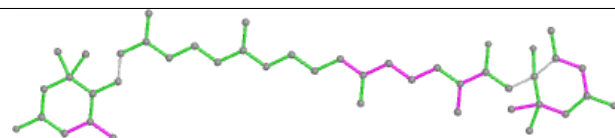


Rings

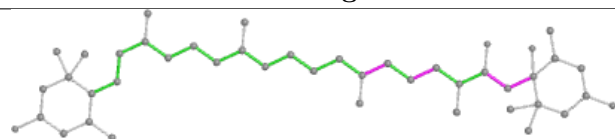
Ligand IWJ S 319



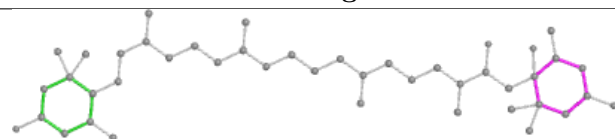
Bond lengths



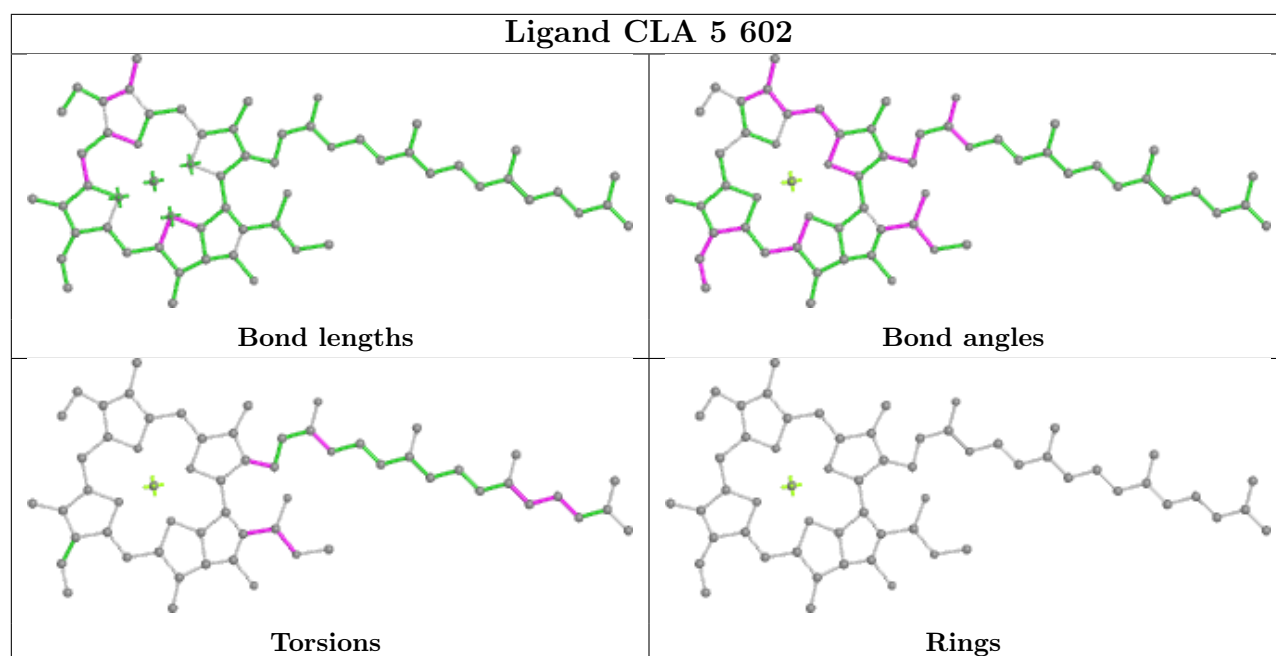
Bond angles



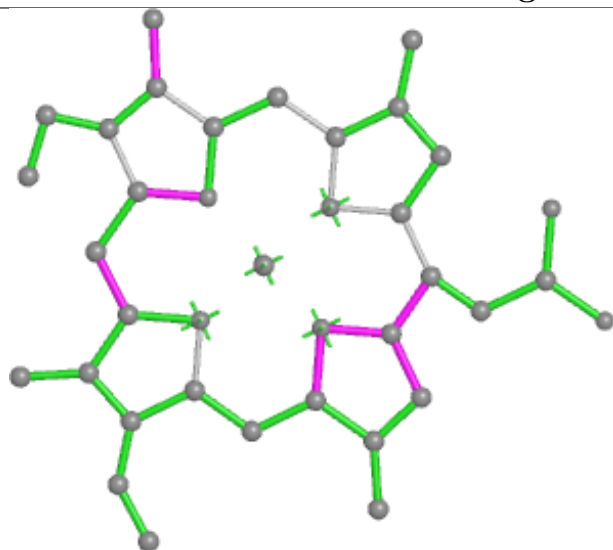
Torsions



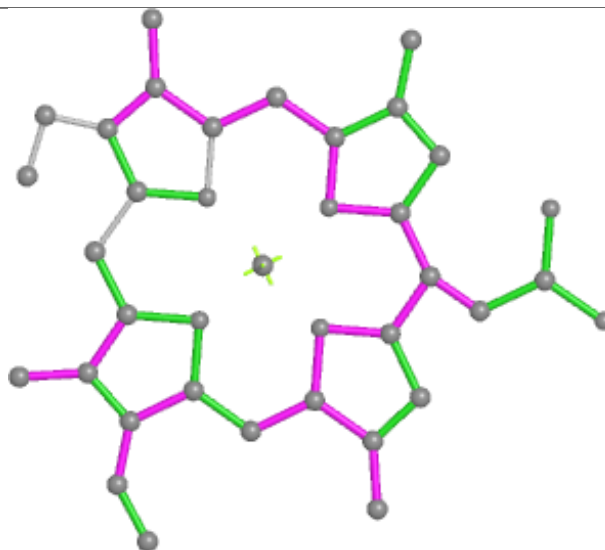
Rings



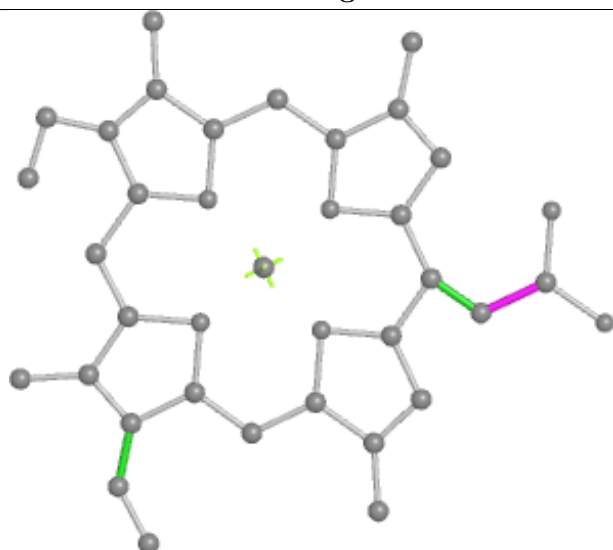
Ligand CLA 1 607



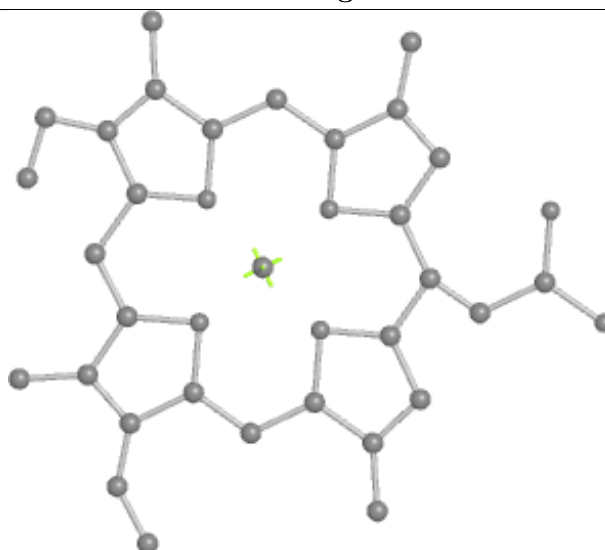
Bond lengths



Bond angles

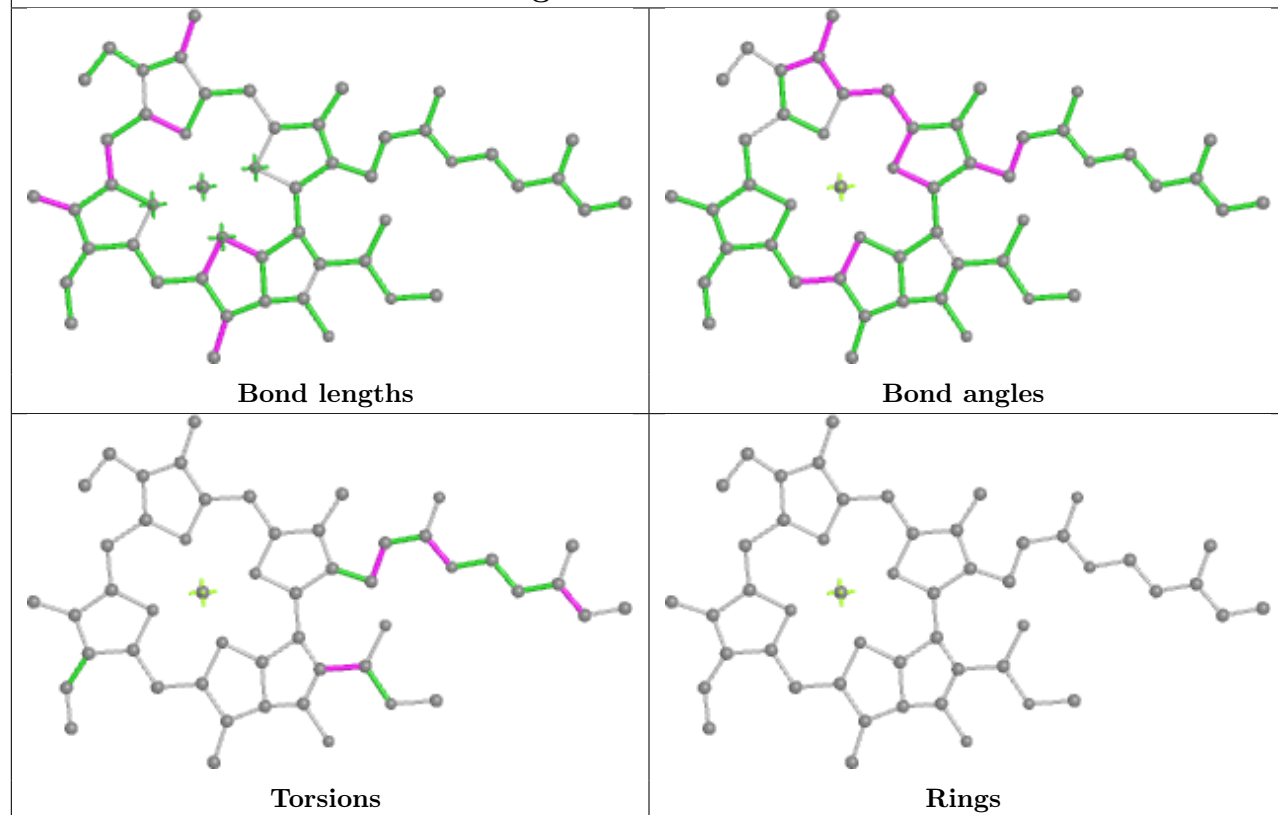


Torsions

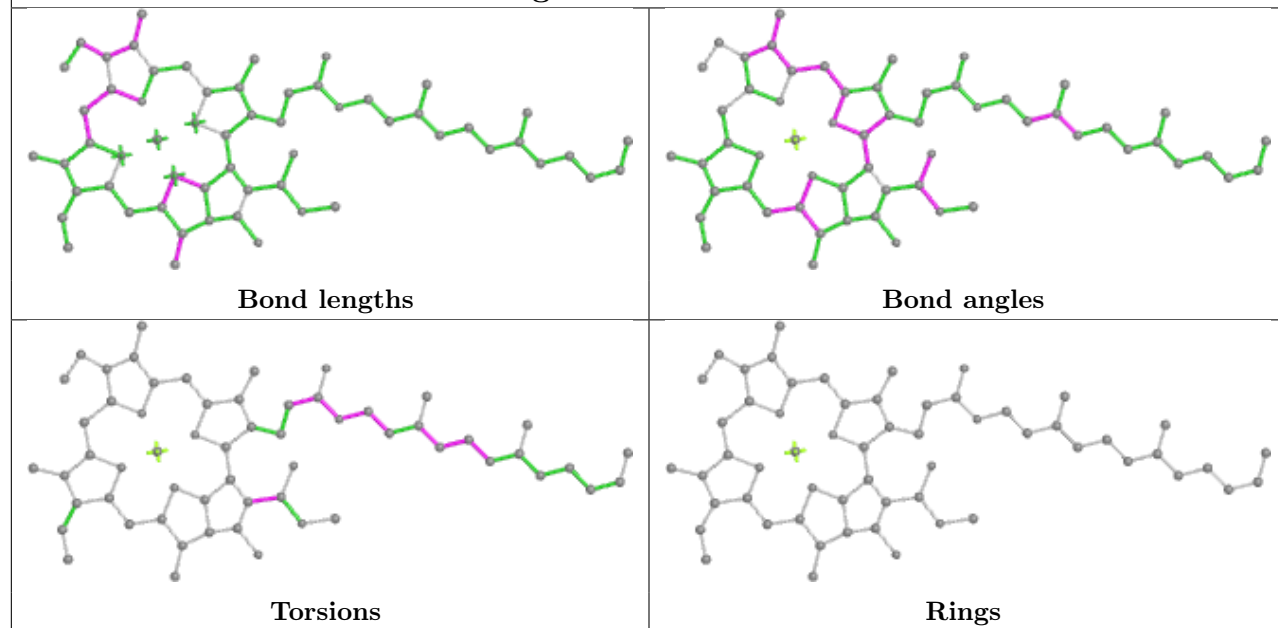


Rings

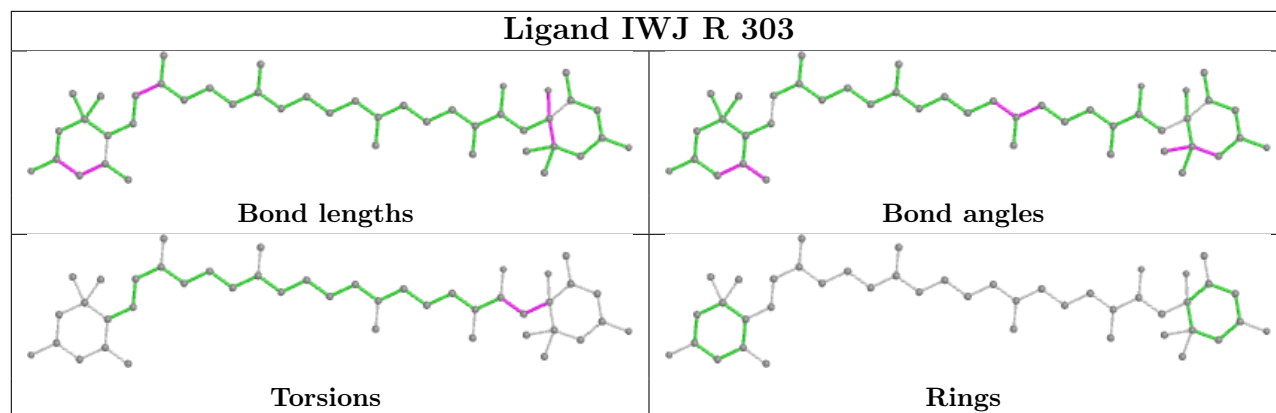
Ligand CLA B 816



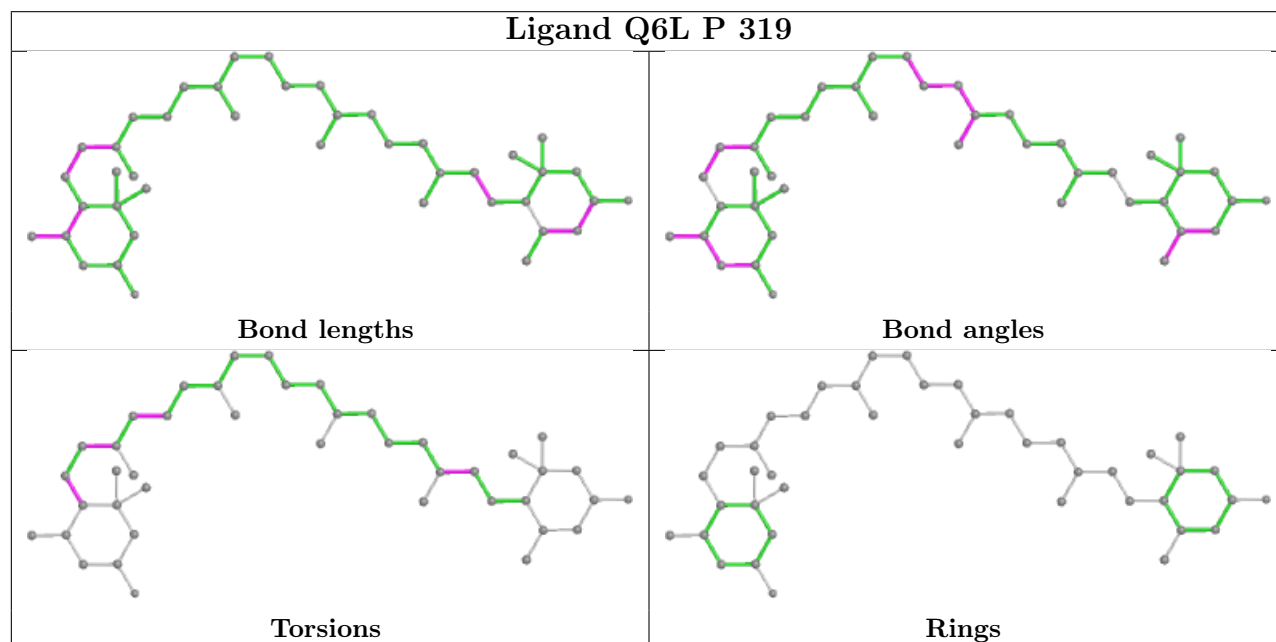
Ligand CLA B 819



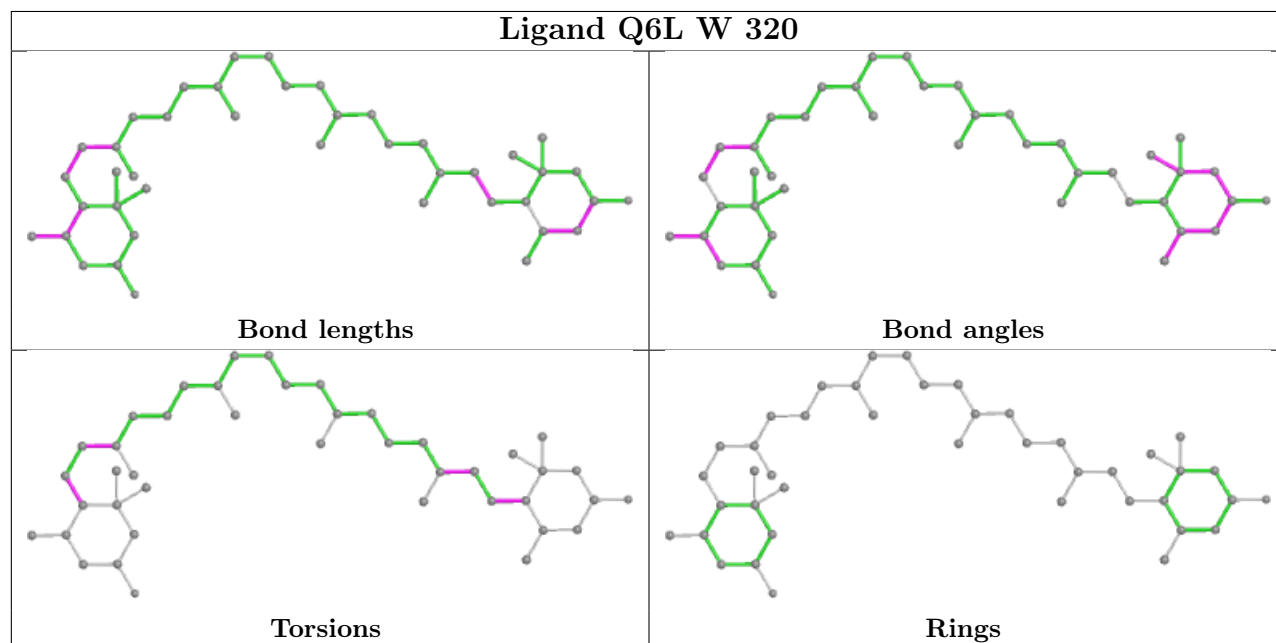
Ligand IWJ R 303

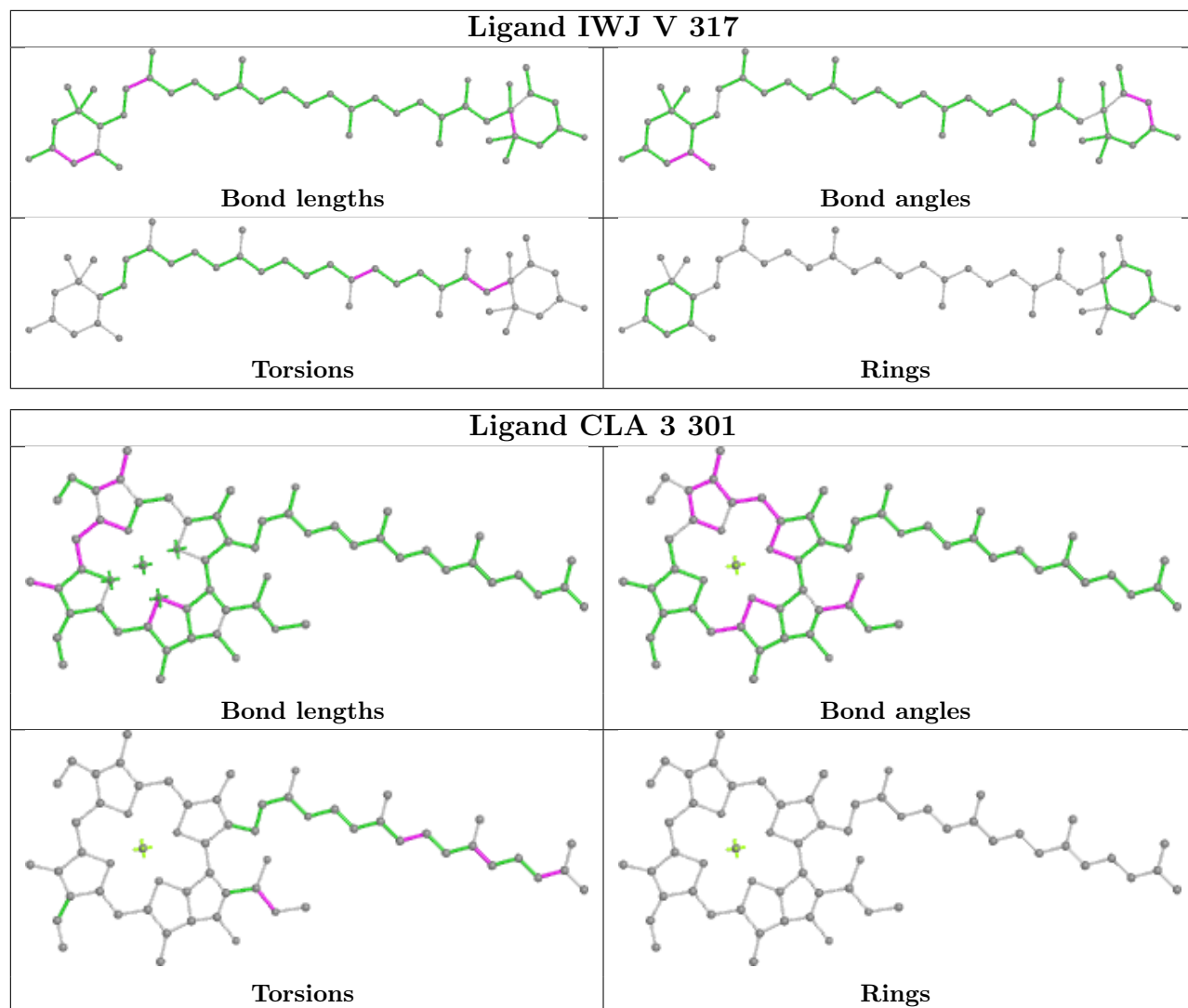


Ligand Q6L P 319

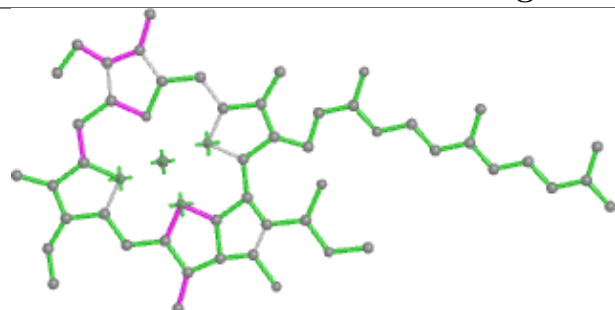


Ligand Q6L W 320

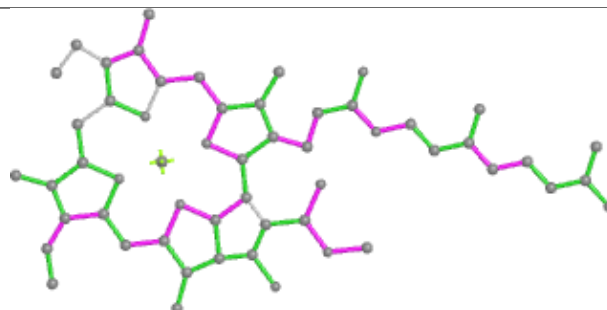




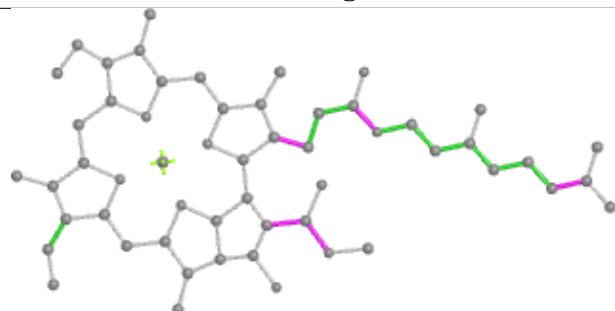
Ligand CLA B 818



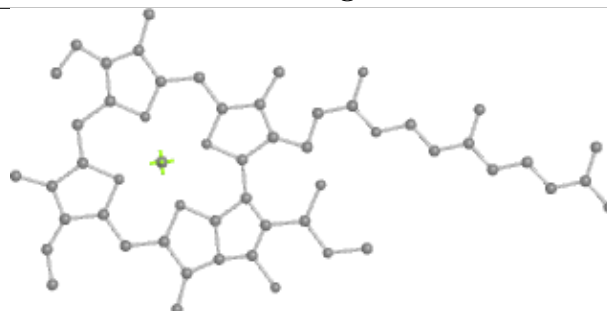
Bond lengths



Bond angles

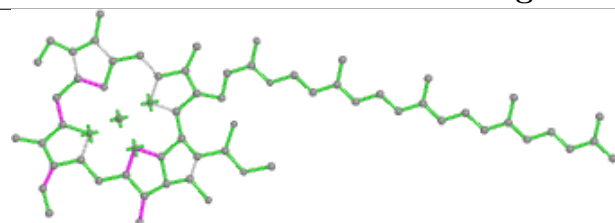


Torsions

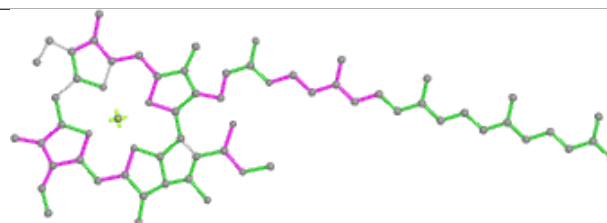


Rings

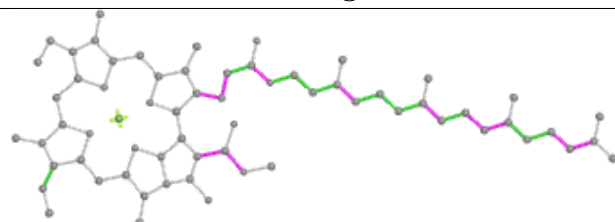
Ligand CLA A 825



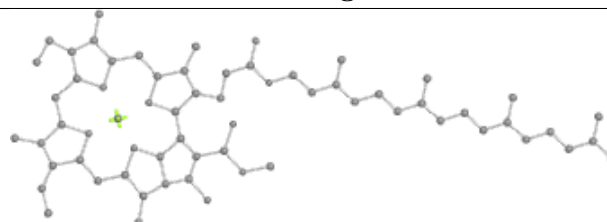
Bond lengths



Bond angles

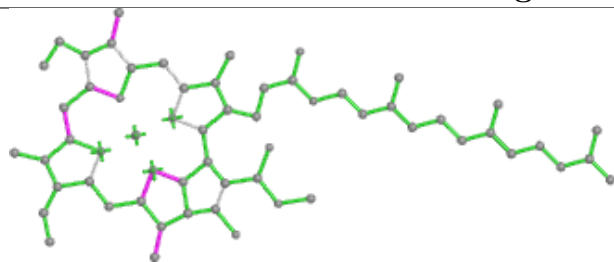


Torsions

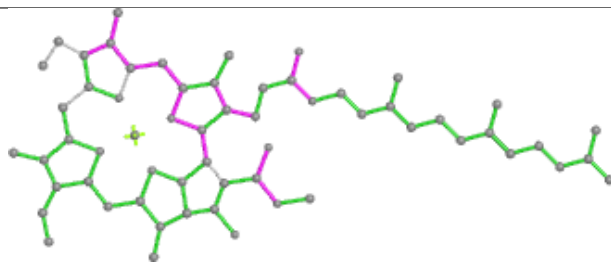


Rings

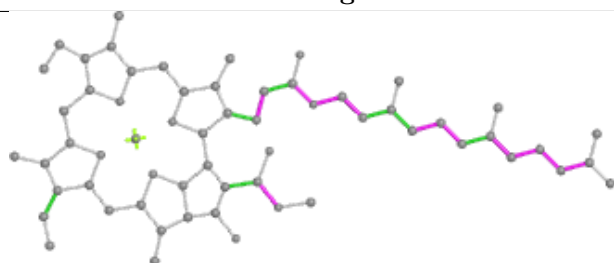
Ligand CLA T 311



Bond lengths



Bond angles

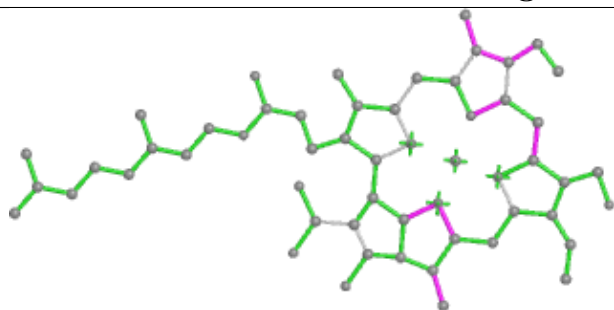


Torsions

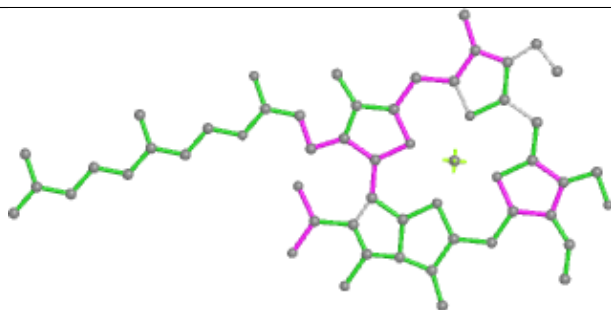


Rings

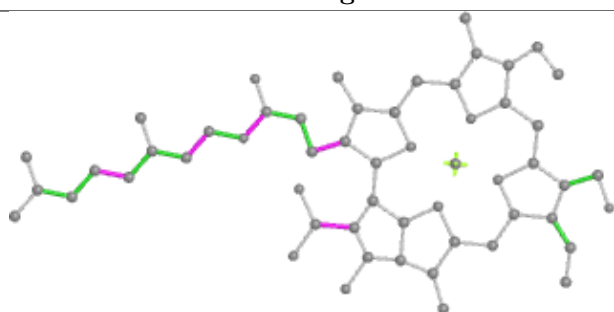
Ligand CHL 1 601



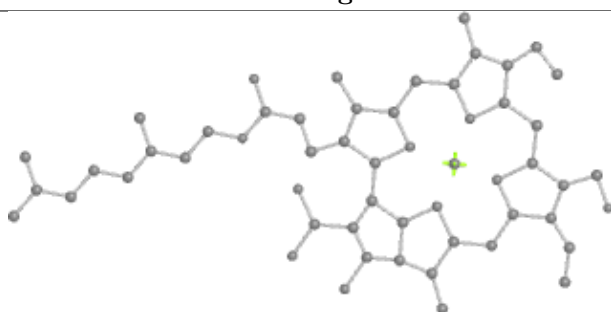
Bond lengths



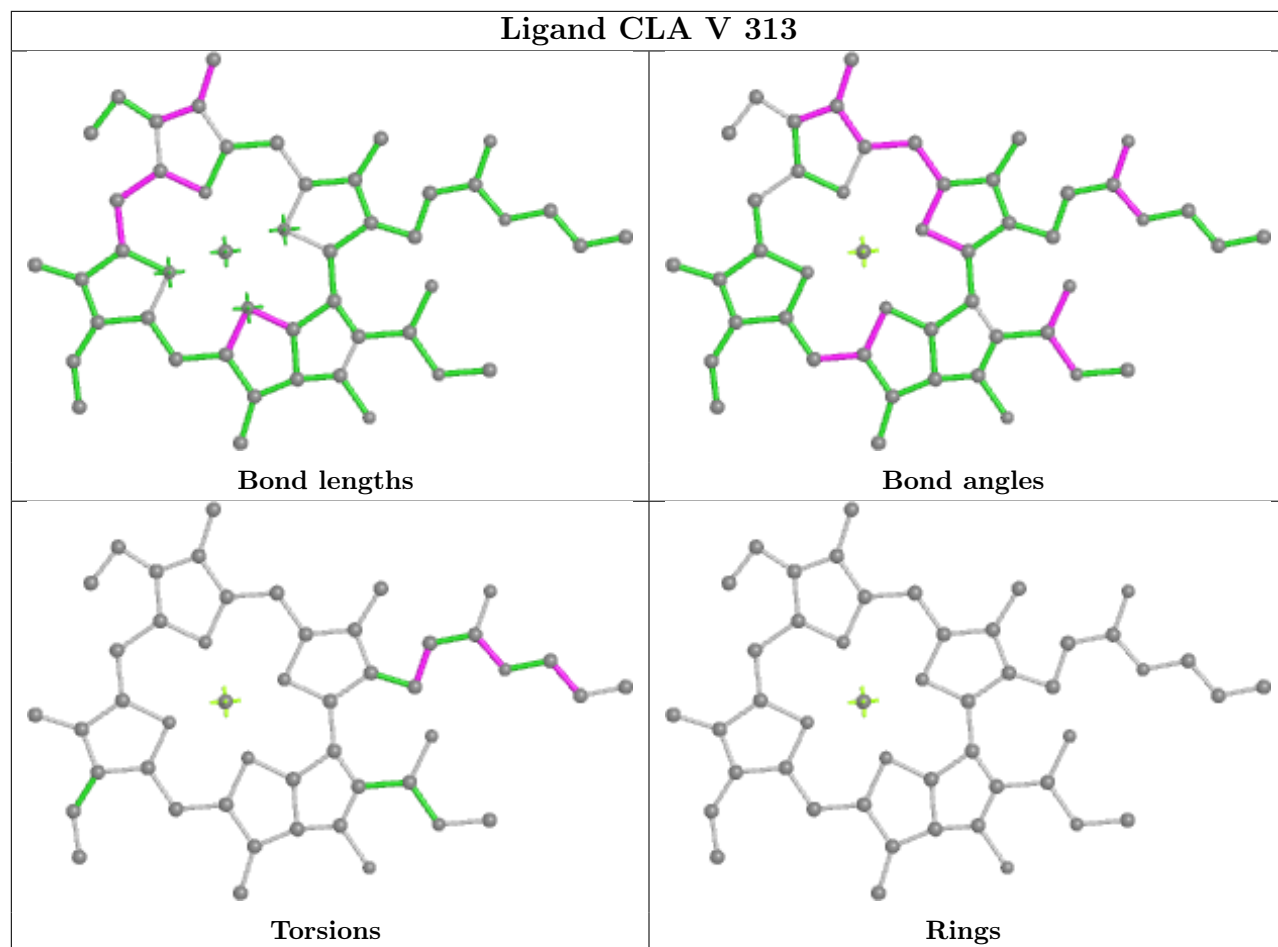
Bond angles



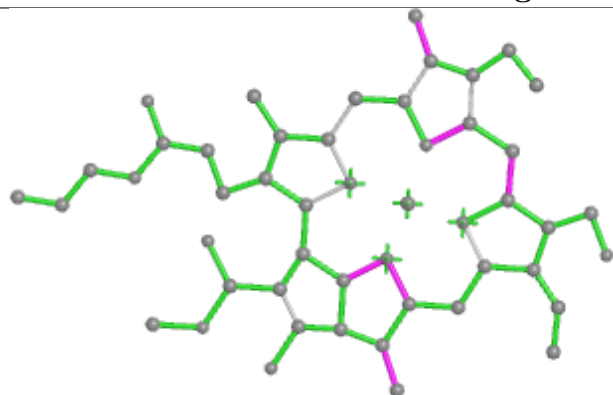
Torsions



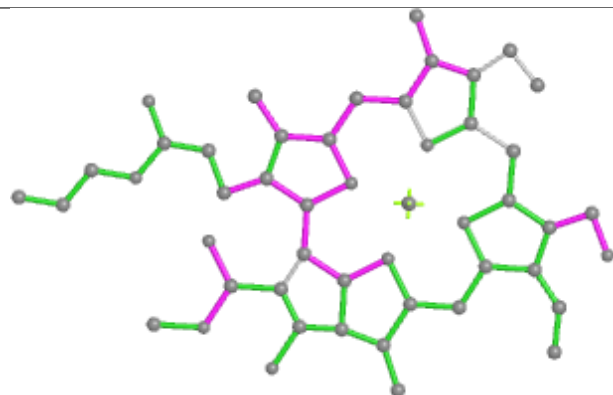
Rings



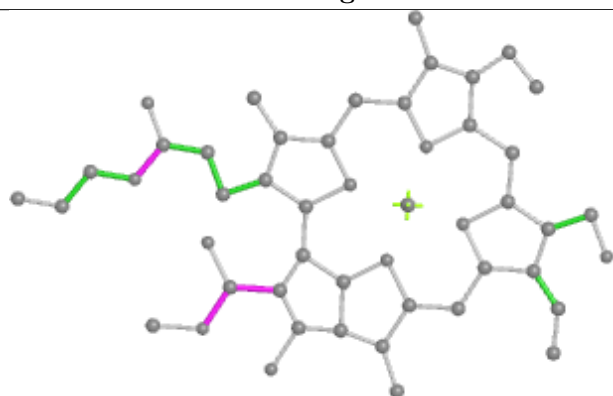
Ligand CHL T 305



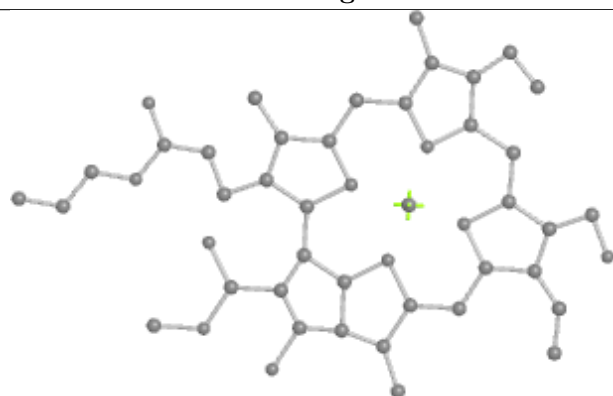
Bond lengths



Bond angles

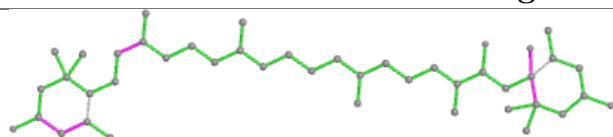


Torsions

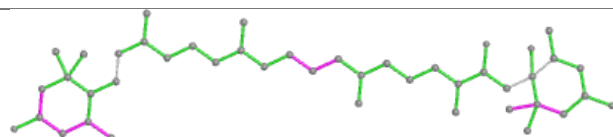


Rings

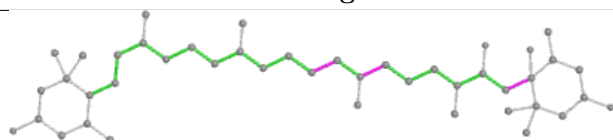
Ligand IWJ T 318



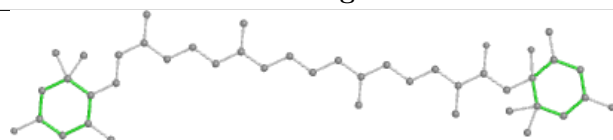
Bond lengths



Bond angles

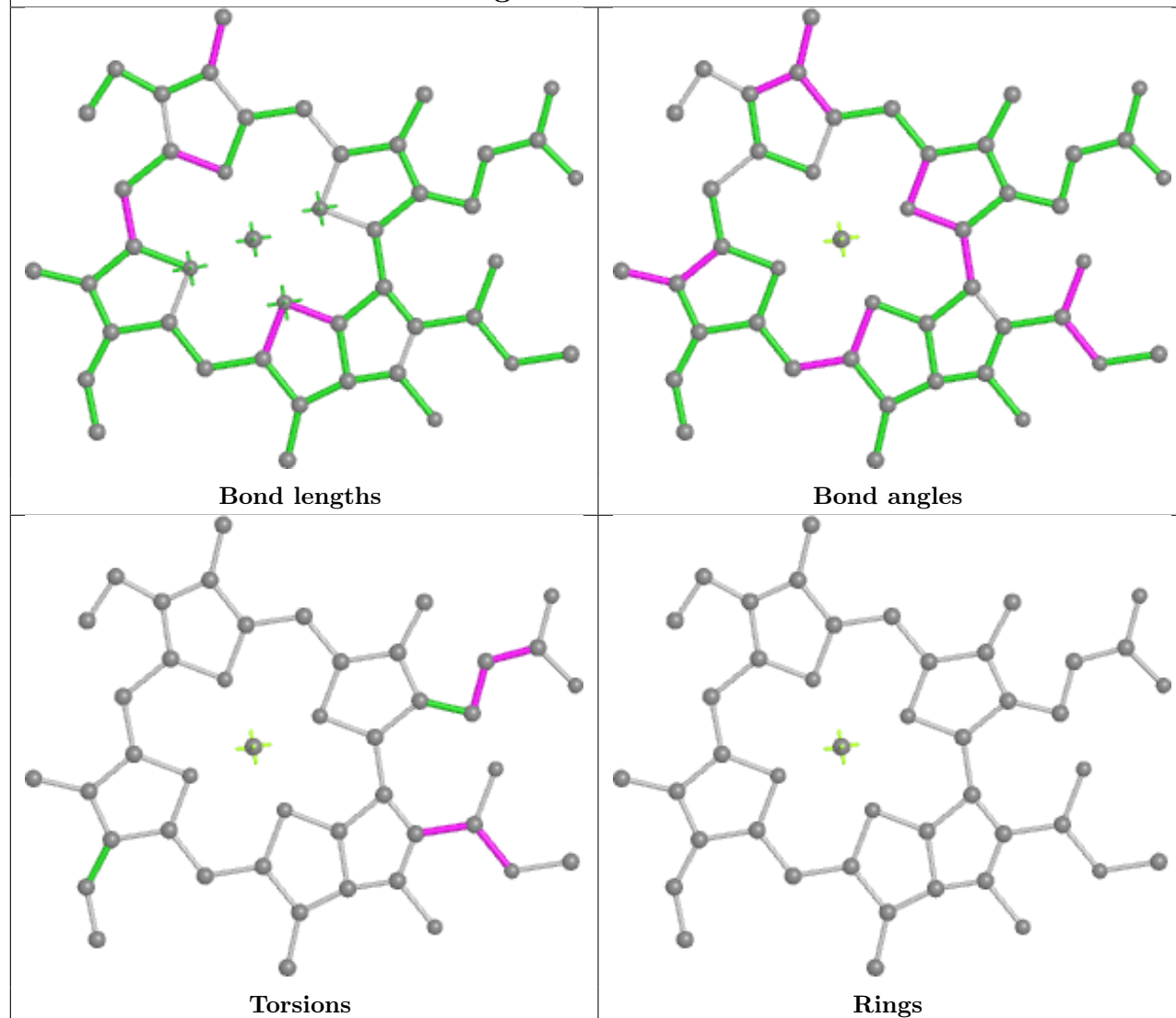


Torsions

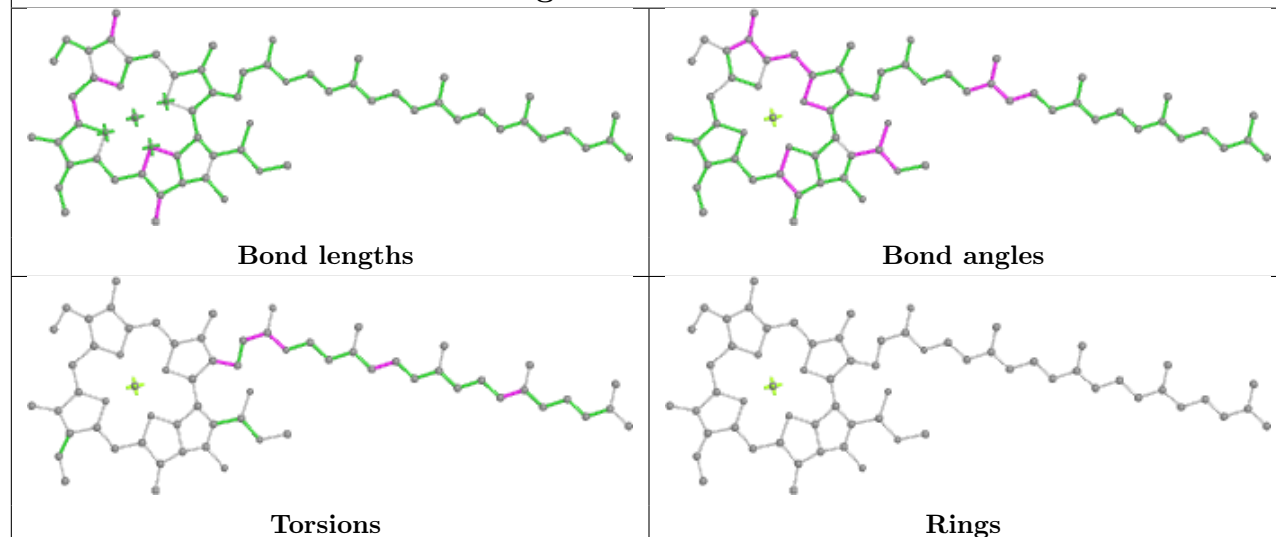


Rings

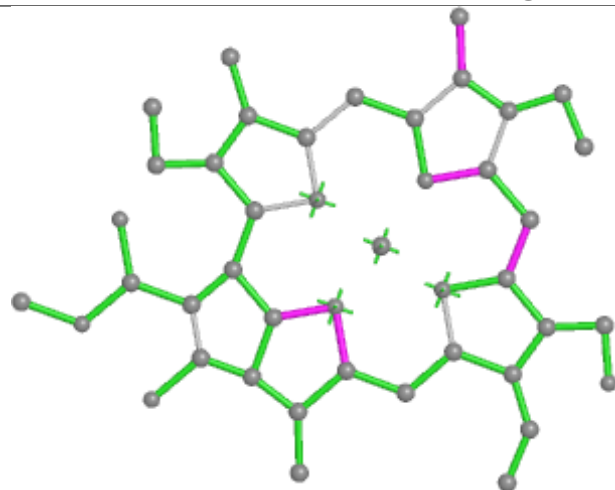
Ligand CLA 5 603



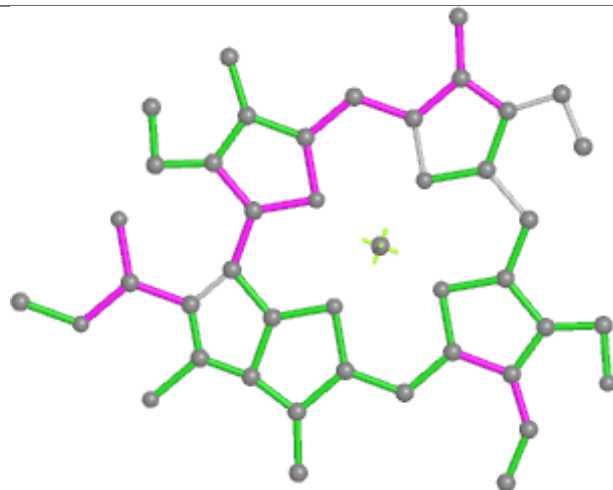
Ligand CLA 6 613



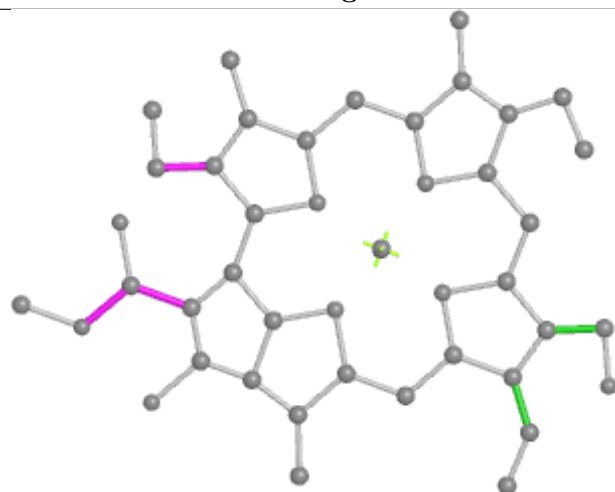
Ligand CHL 6 606



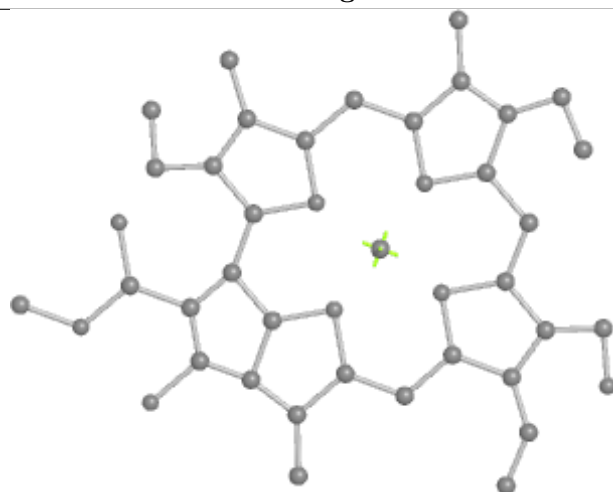
Bond lengths



Bond angles

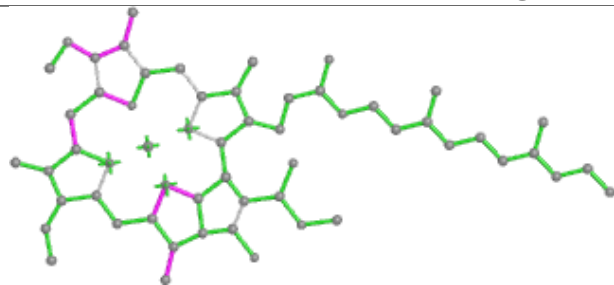


Torsions

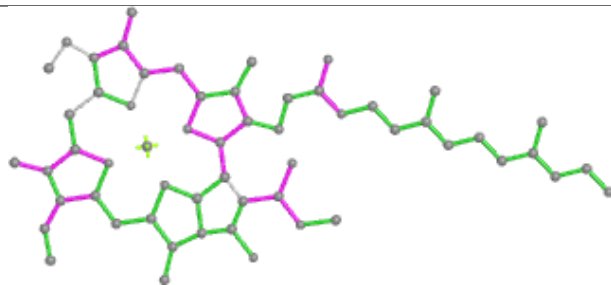


Rings

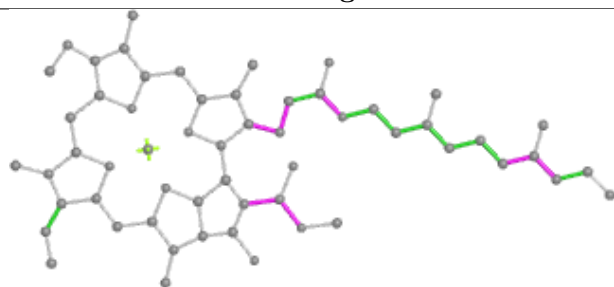
Ligand CLA A 856



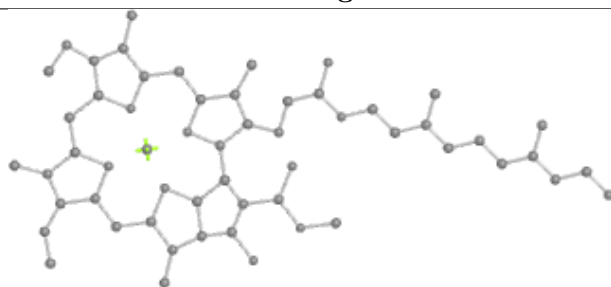
Bond lengths



Bond angles

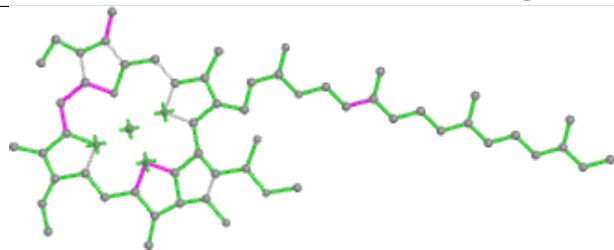


Torsions

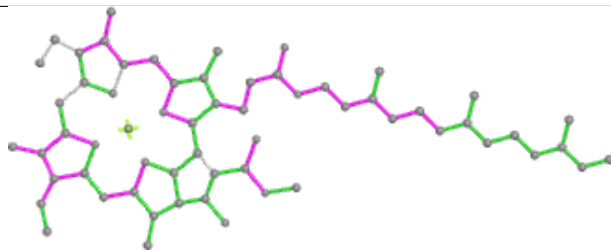


Rings

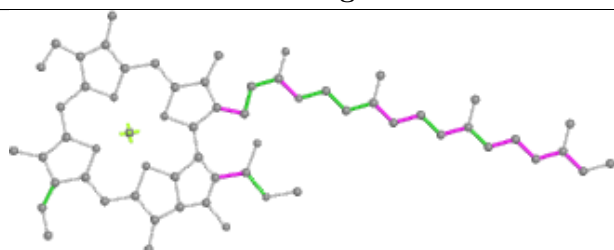
Ligand CLA 2 602



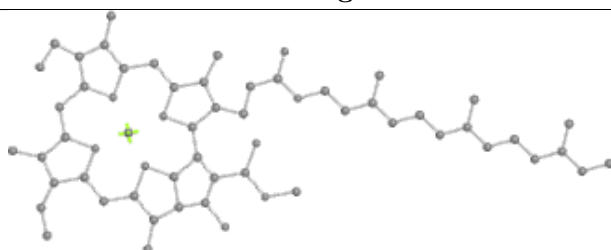
Bond lengths



Bond angles

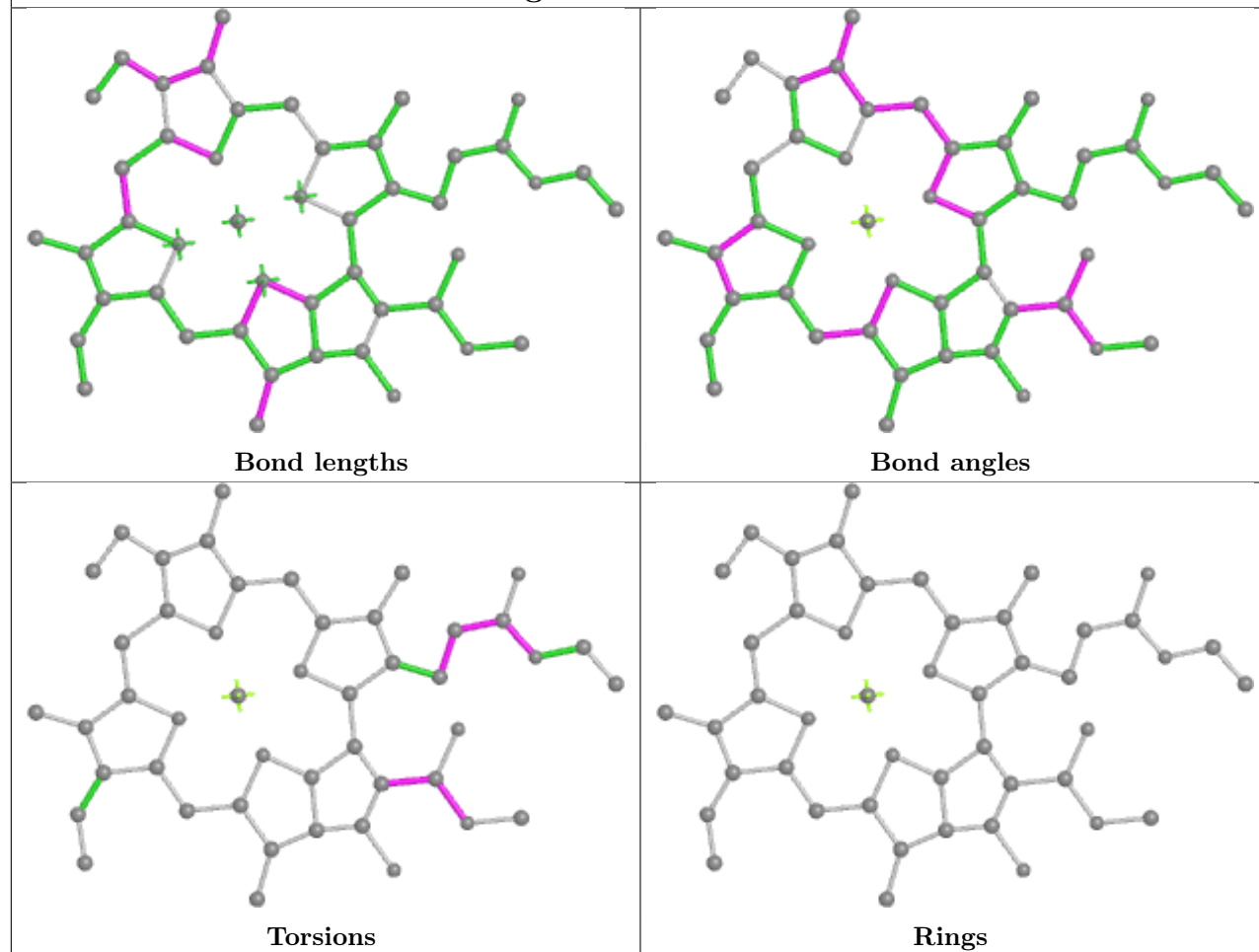


Torsions

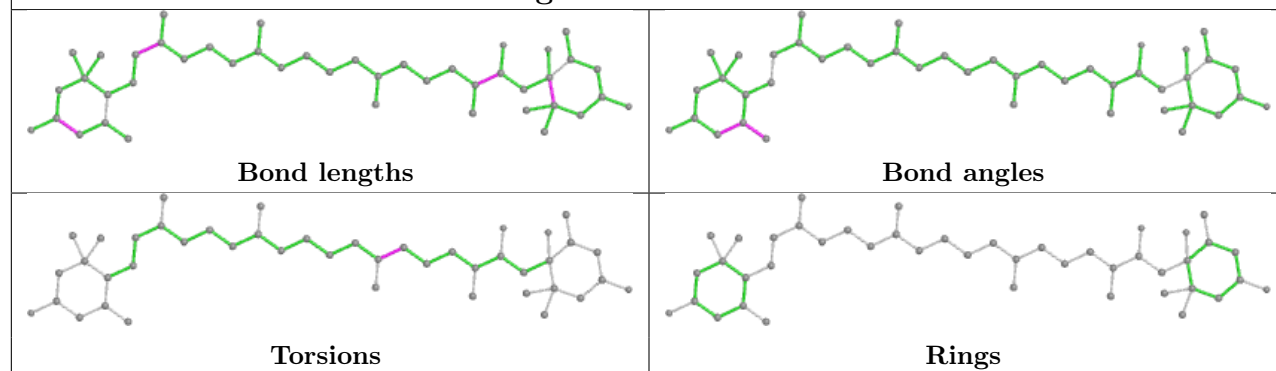


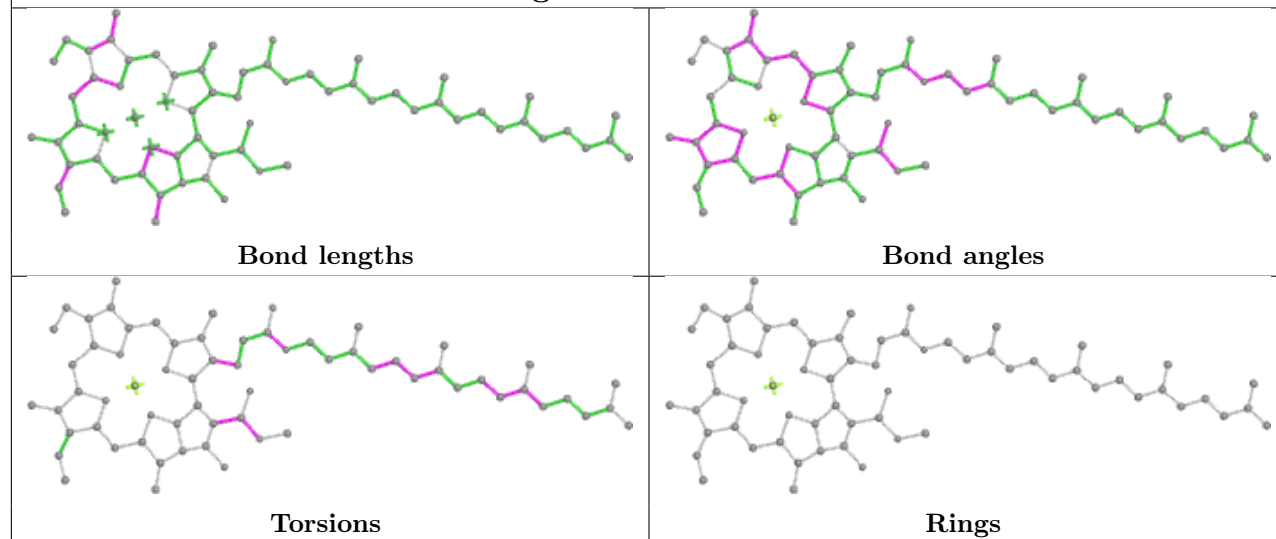
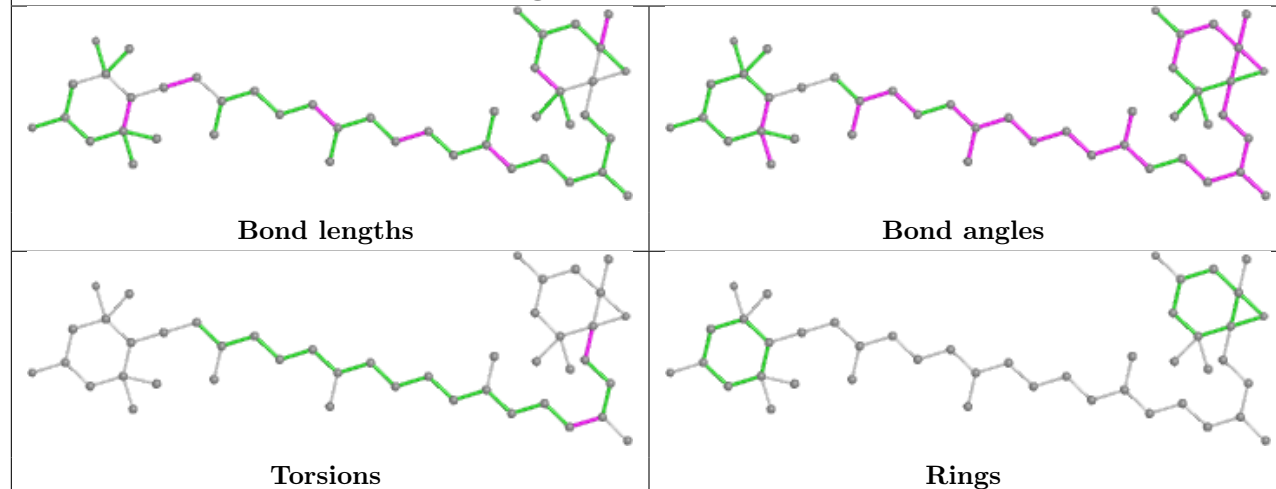
Rings

Ligand CLA B 840

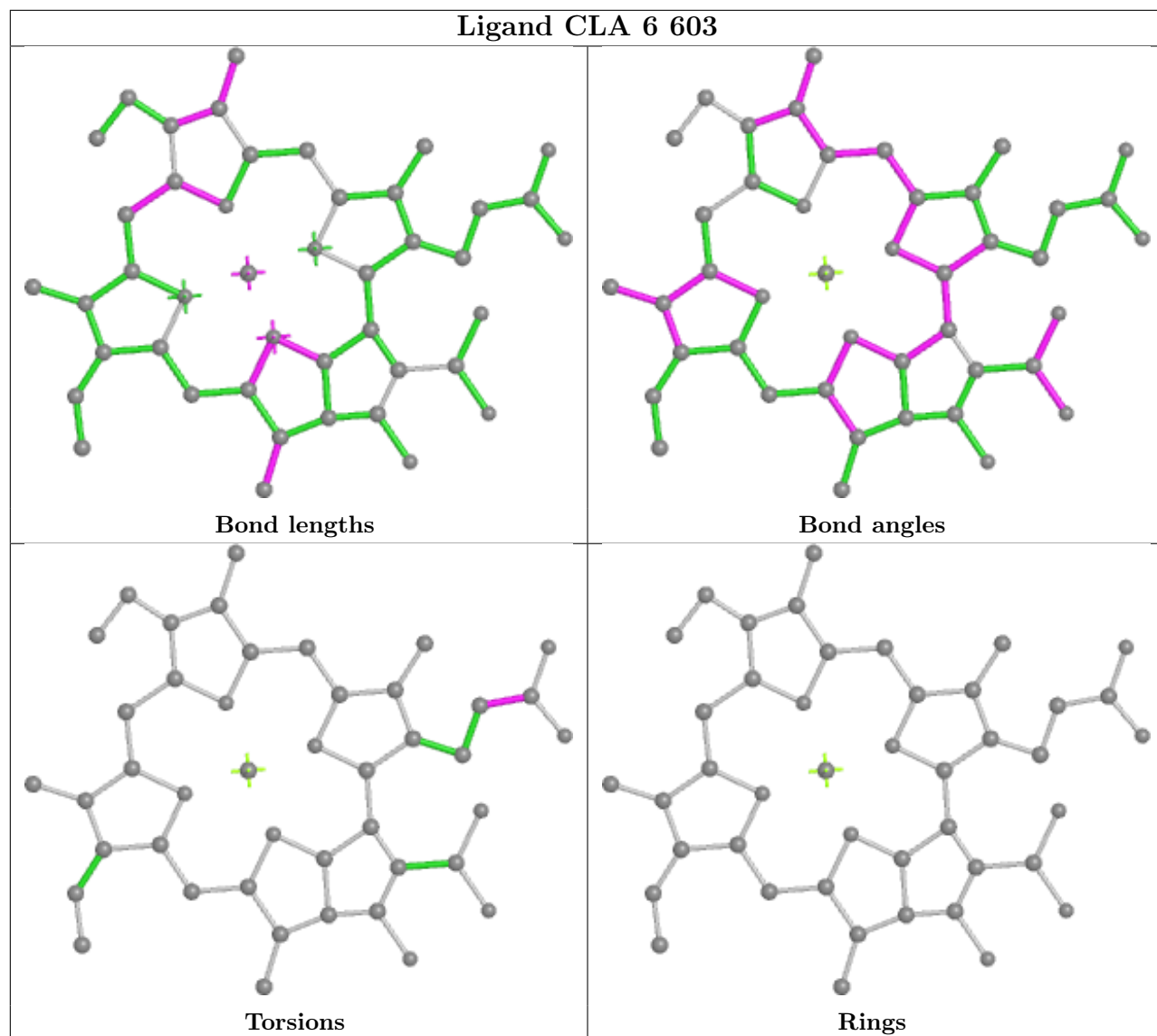


Ligand IWJ P 318

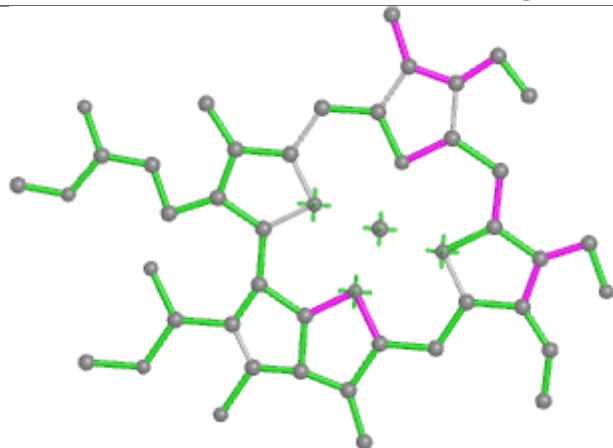


Ligand CLA B 842**Ligand NEX H 306**

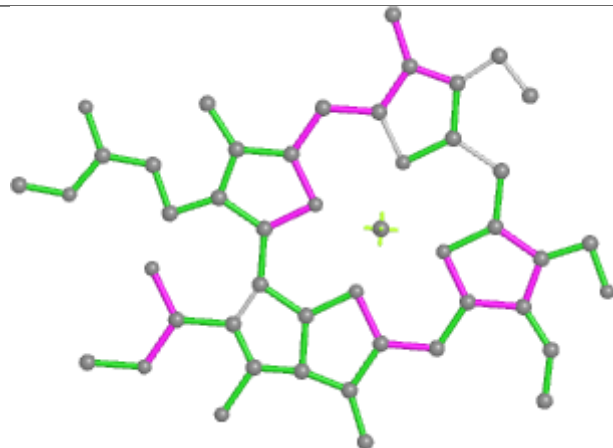
Ligand CLA 6 603



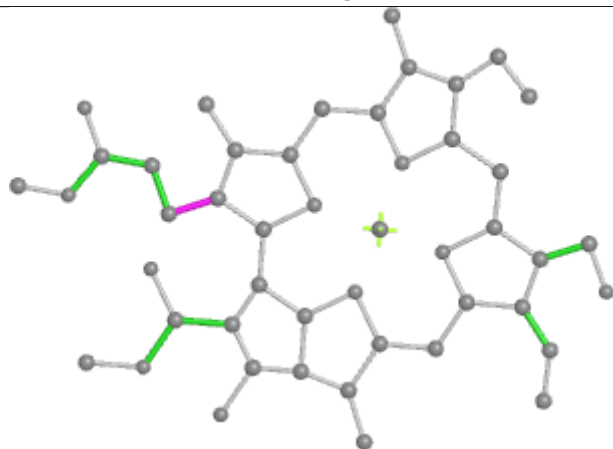
Ligand CHL 2 601



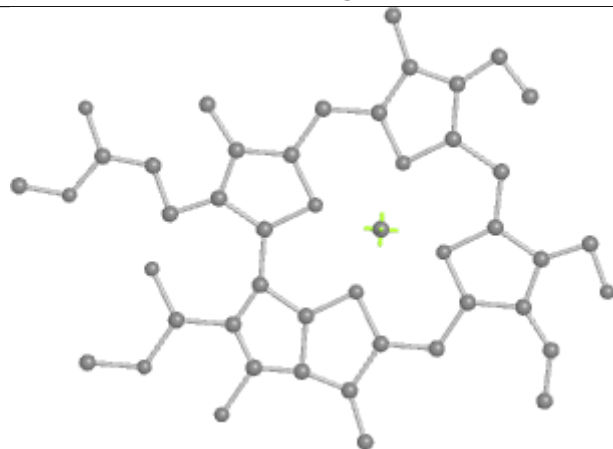
Bond lengths



Bond angles

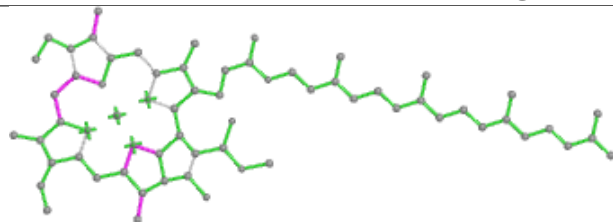


Torsions

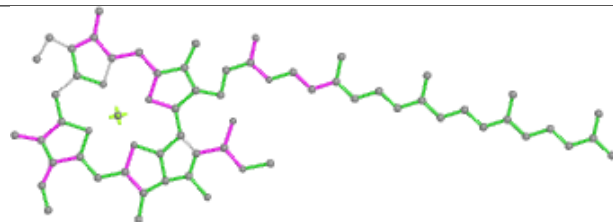


Rings

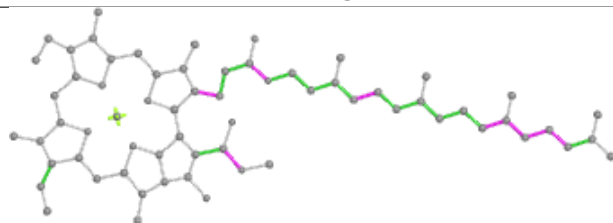
Ligand CLA A 805



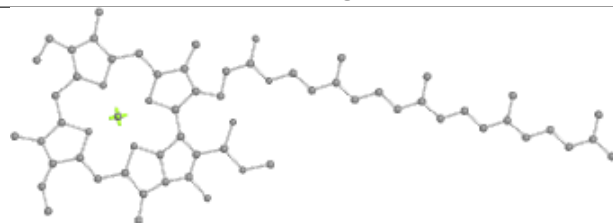
Bond lengths



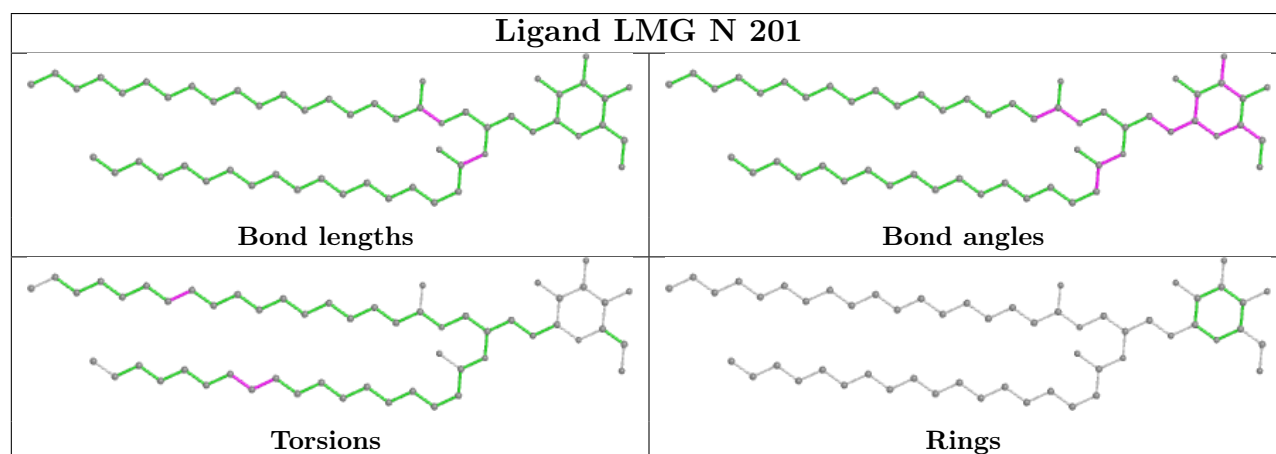
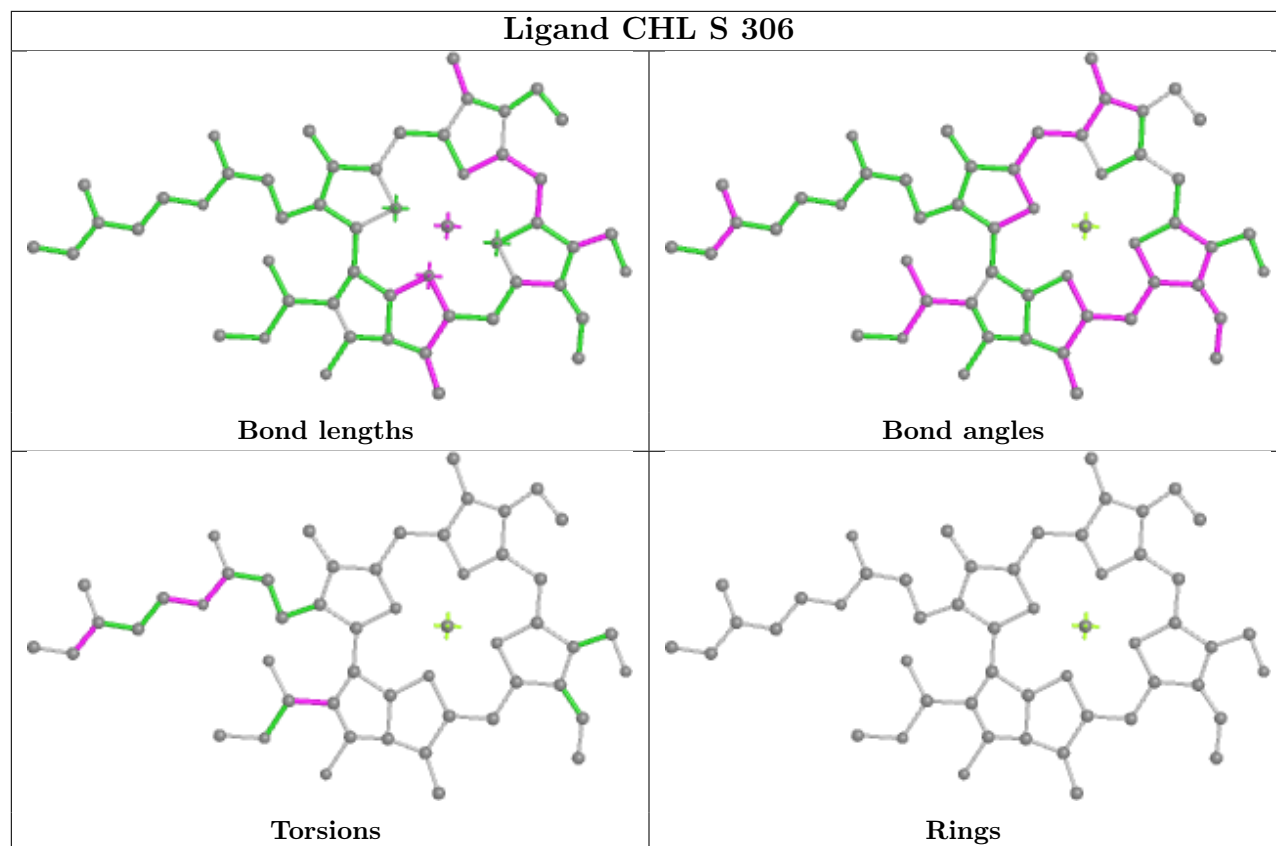
Bond angles



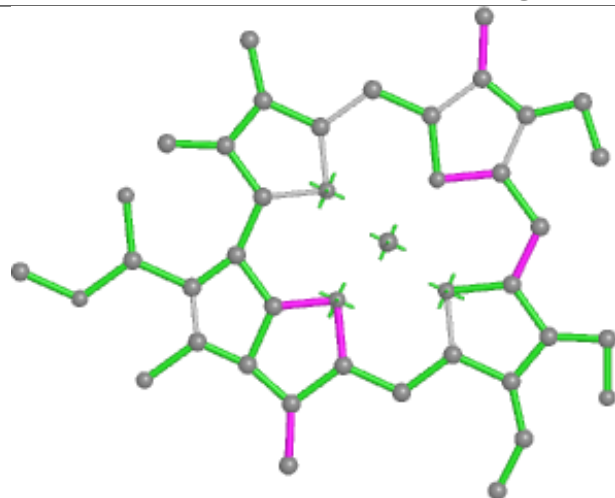
Torsions



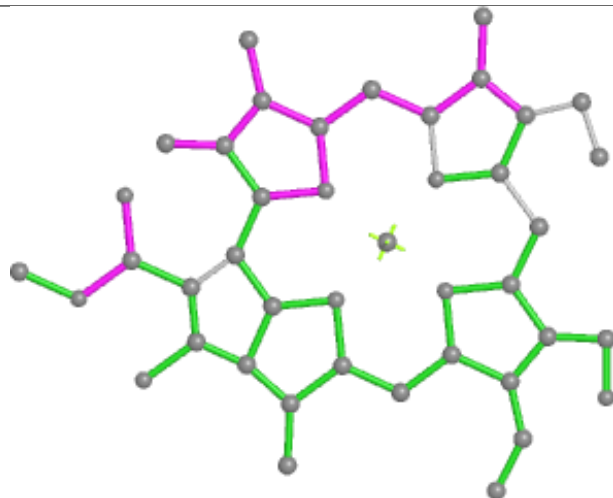
Rings



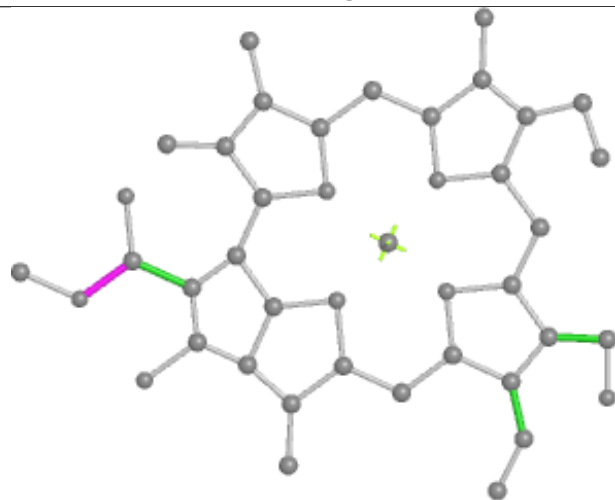
Ligand CHL X 306



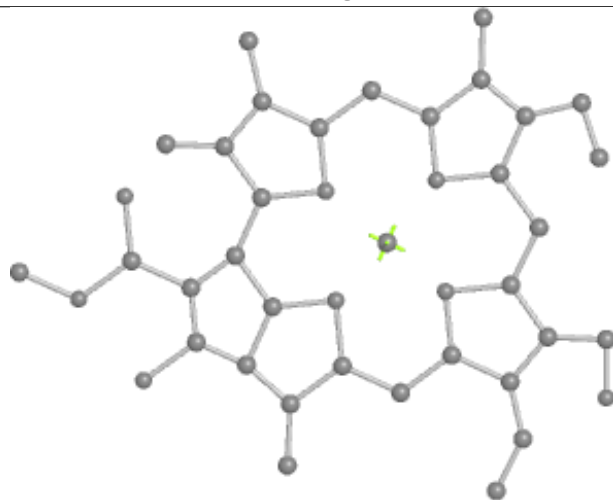
Bond lengths



Bond angles

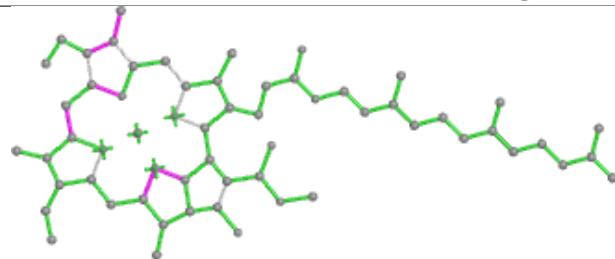


Torsions

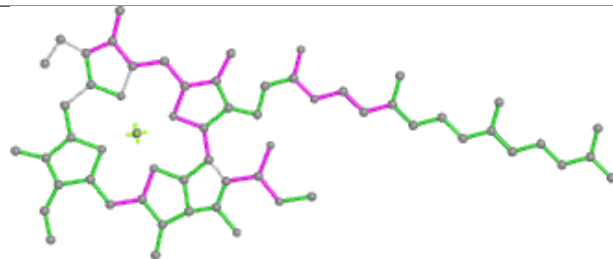


Rings

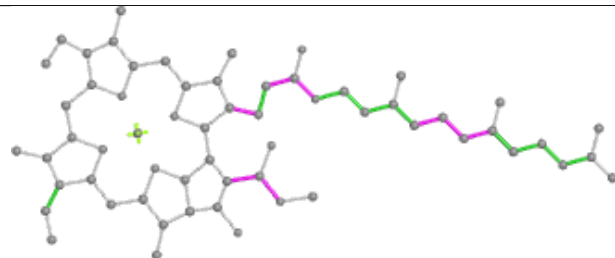
Ligand CLA R 314



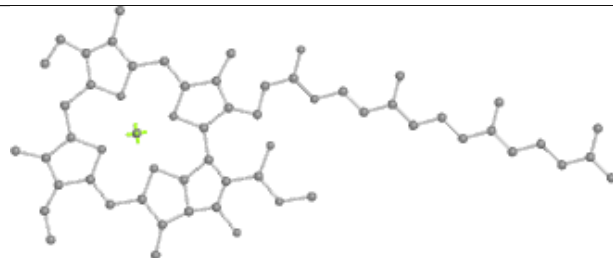
Bond lengths



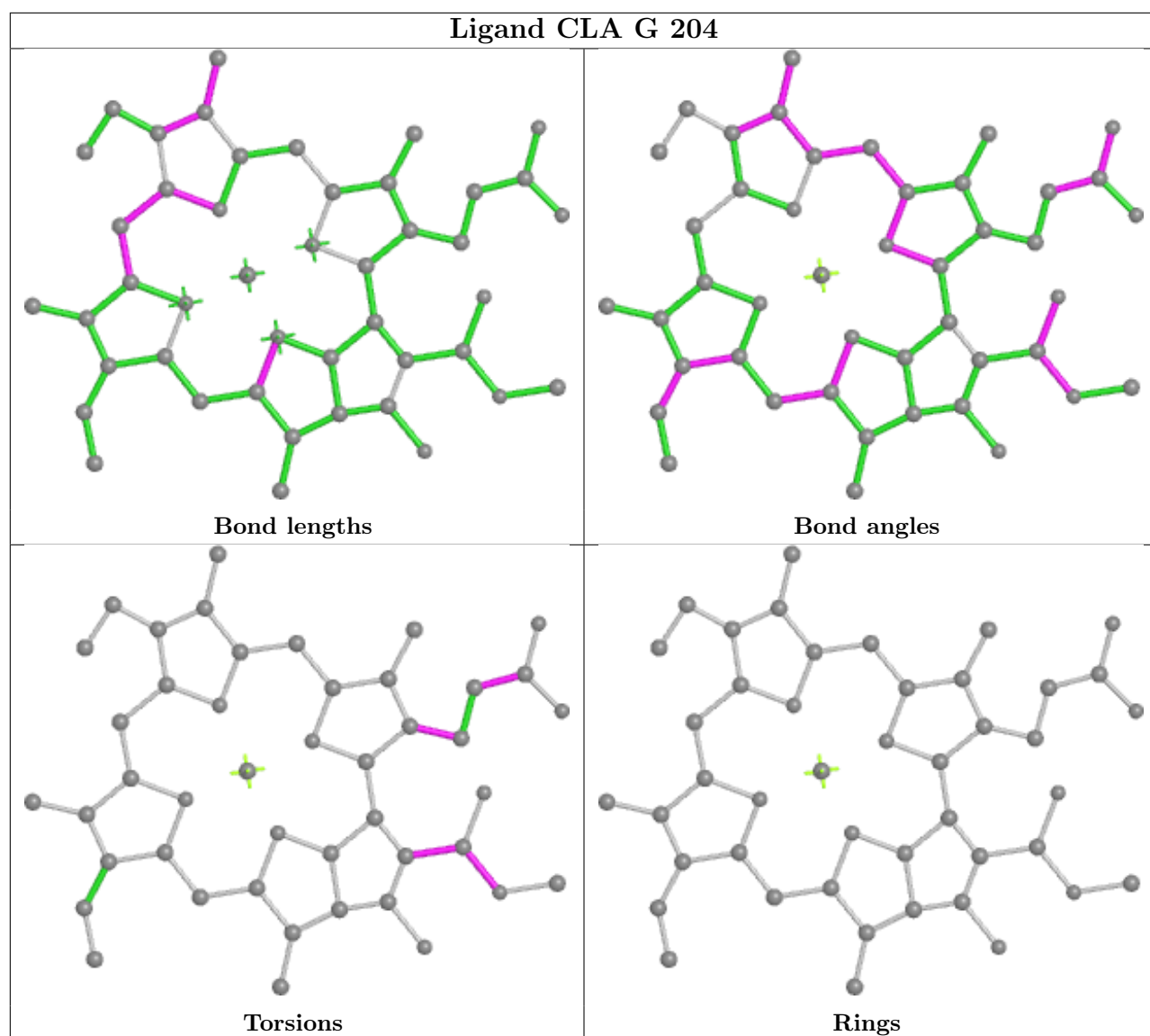
Bond angles



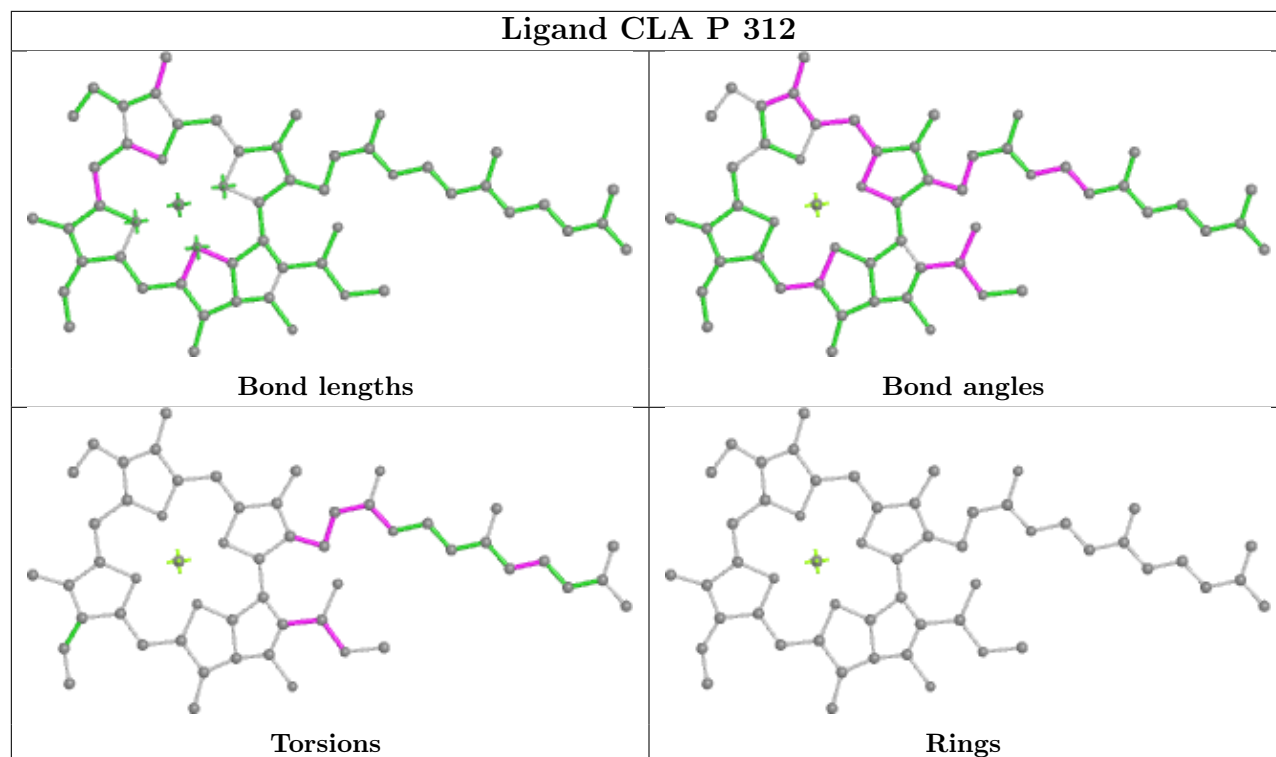
Torsions



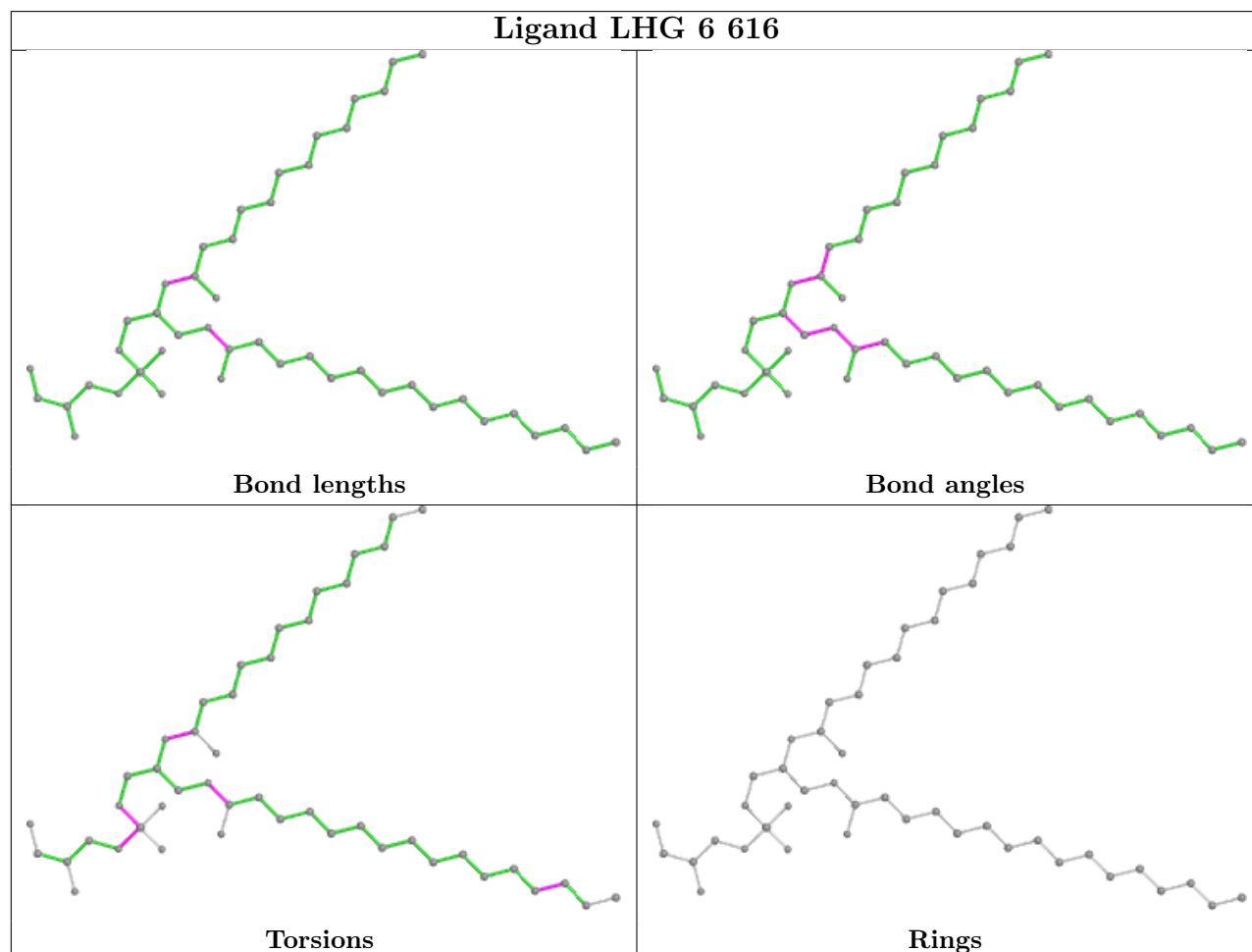
Rings

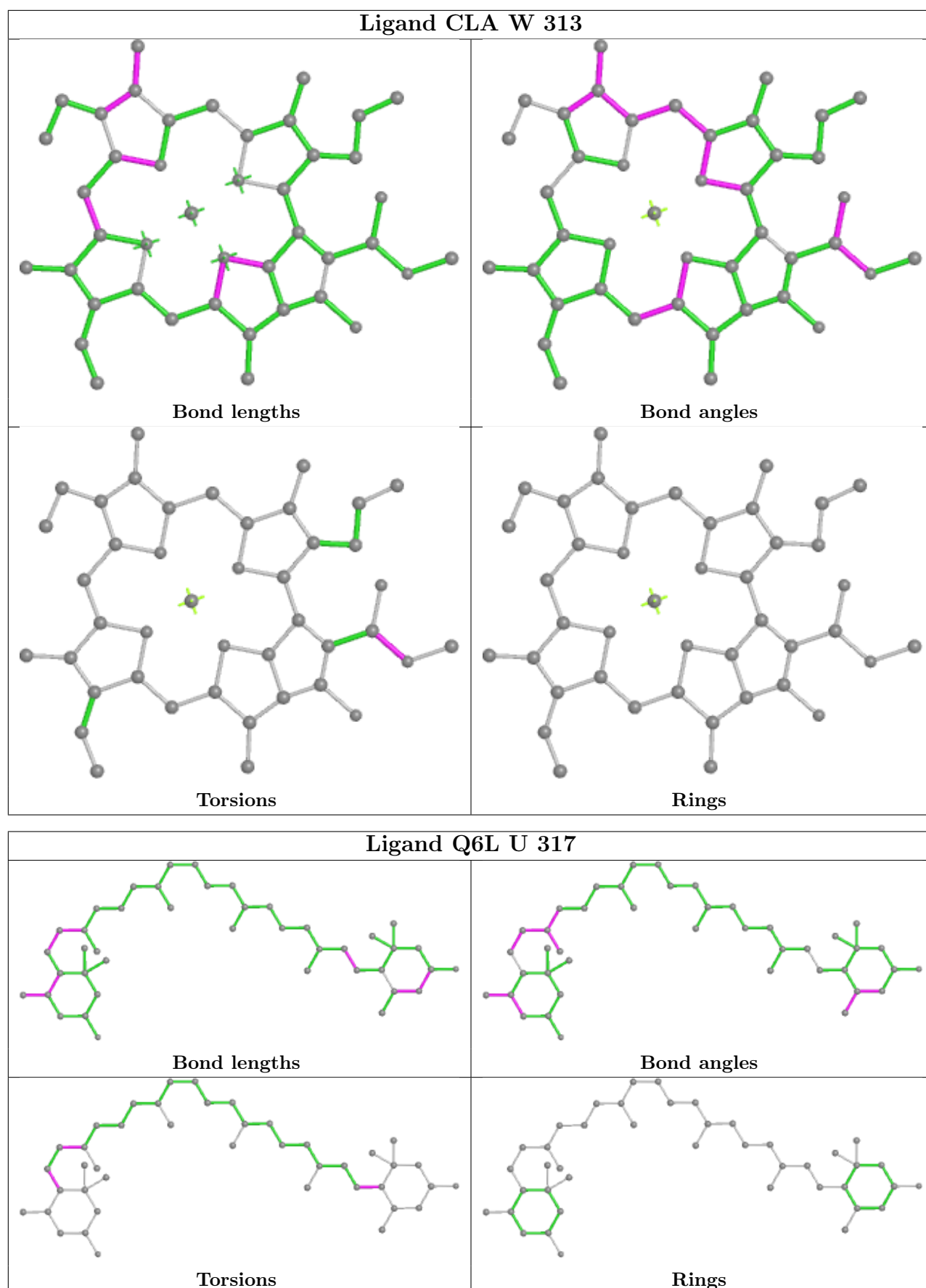


Ligand CLA P 312

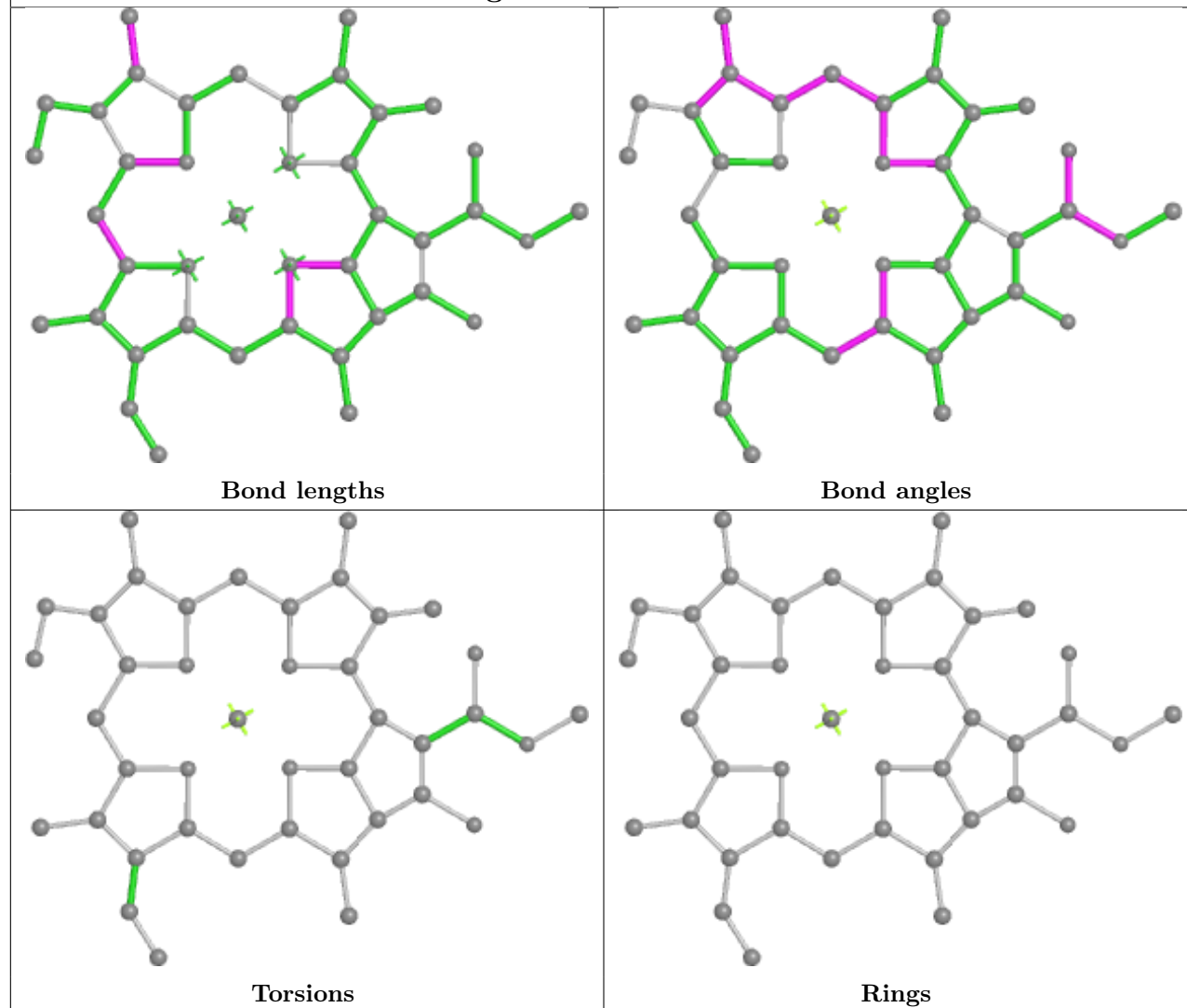


Ligand LHG 6 616

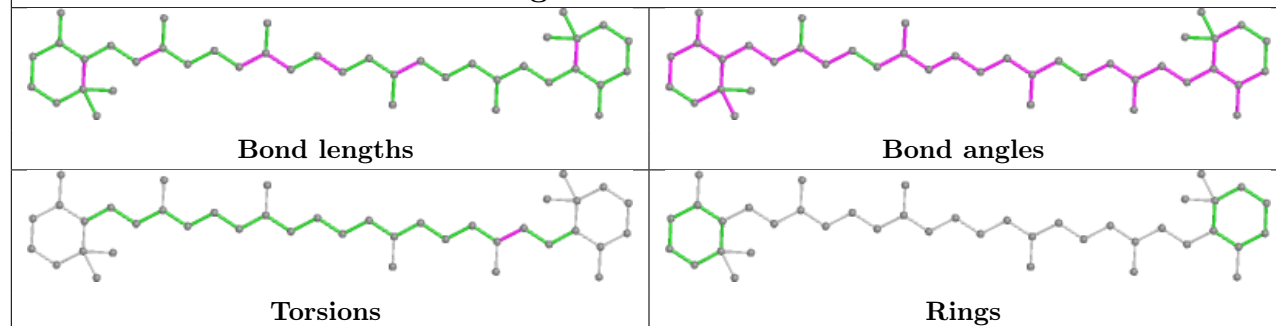


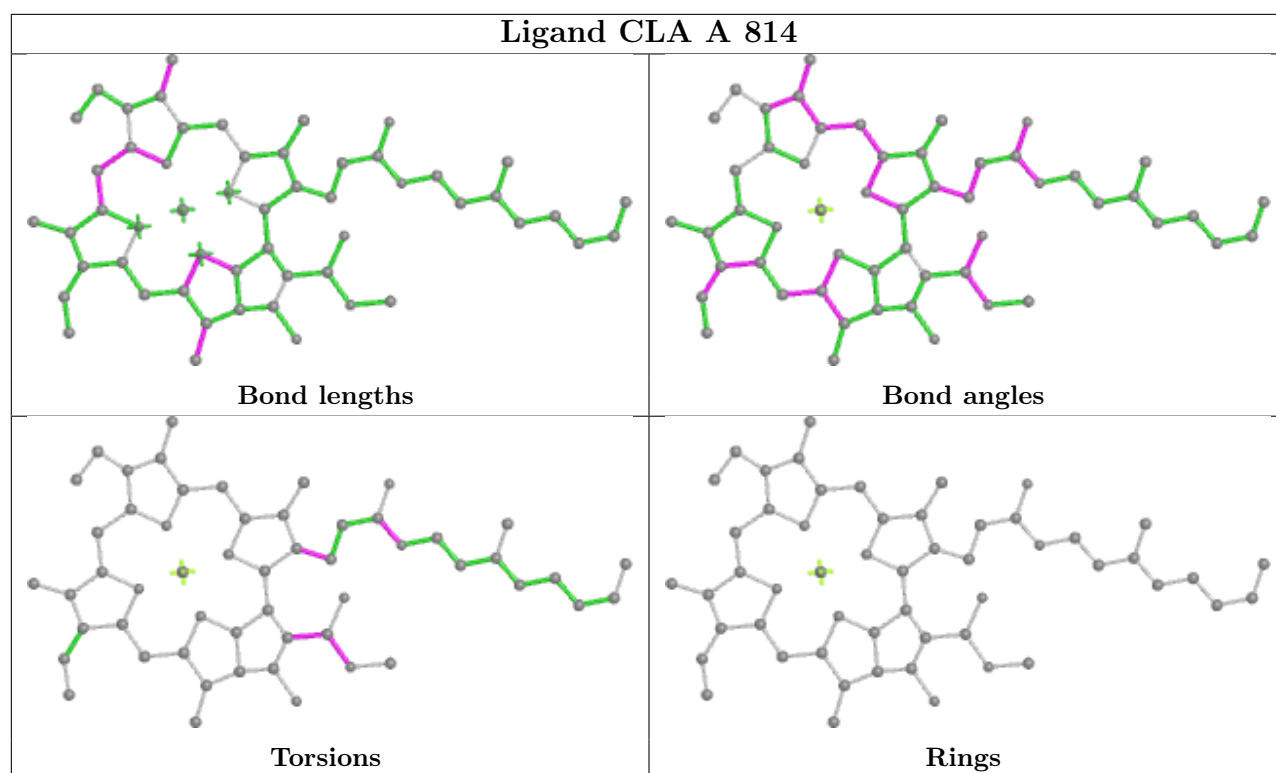


Ligand CLA O 2003

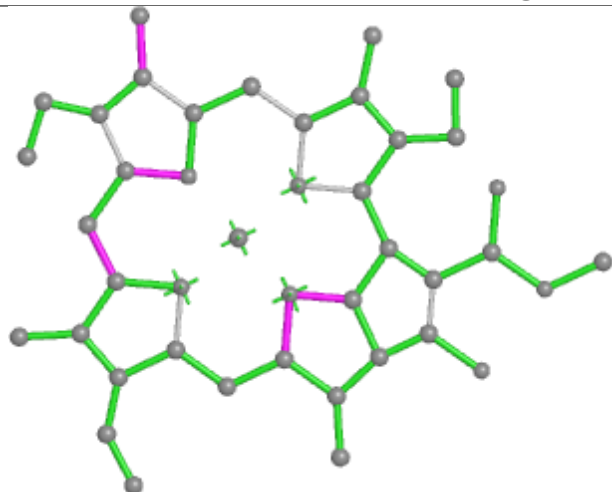


Ligand BCR A 850

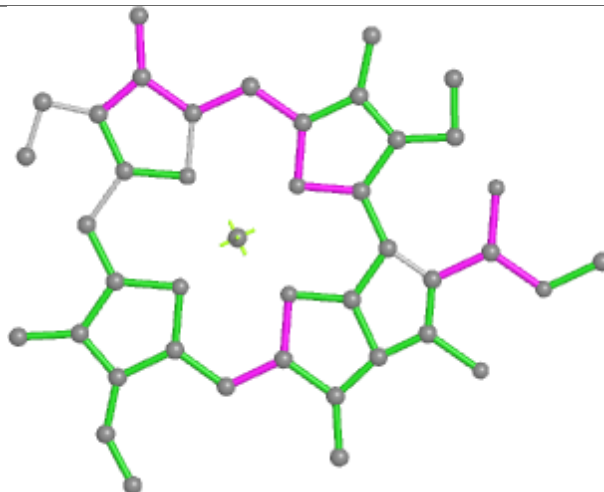




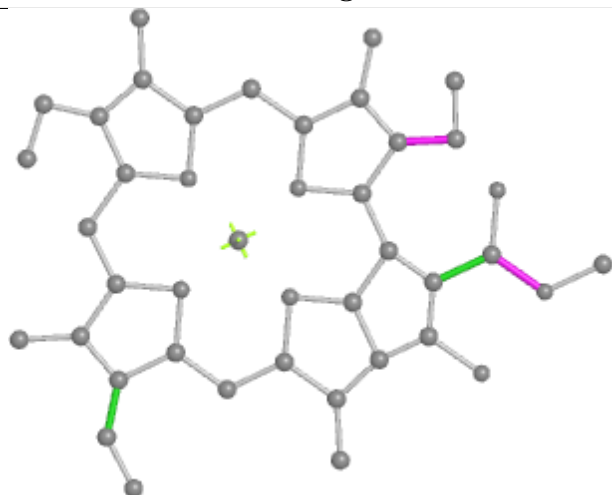
Ligand CLA 2 610



Bond lengths



Bond angles

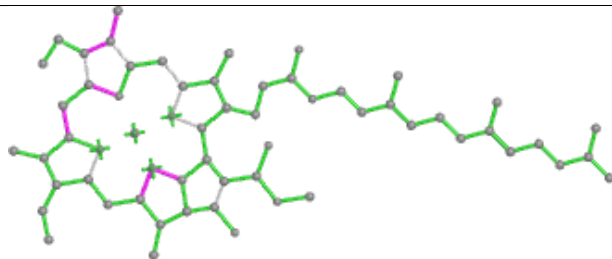


Torsions

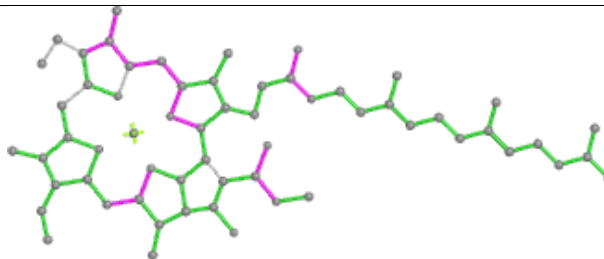


Rings

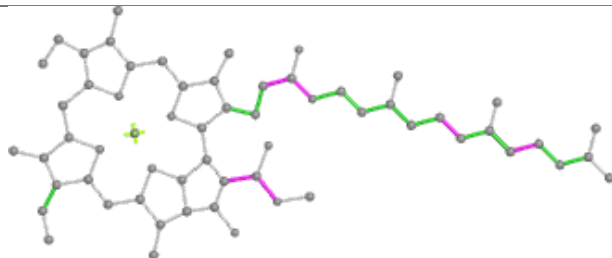
Ligand CLA W 310



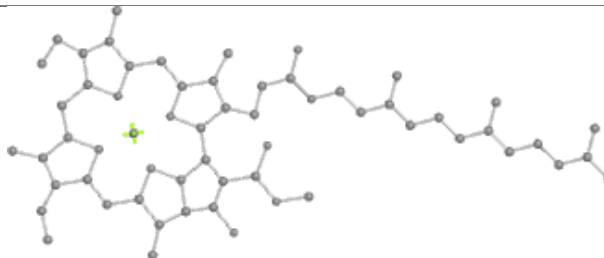
Bond lengths



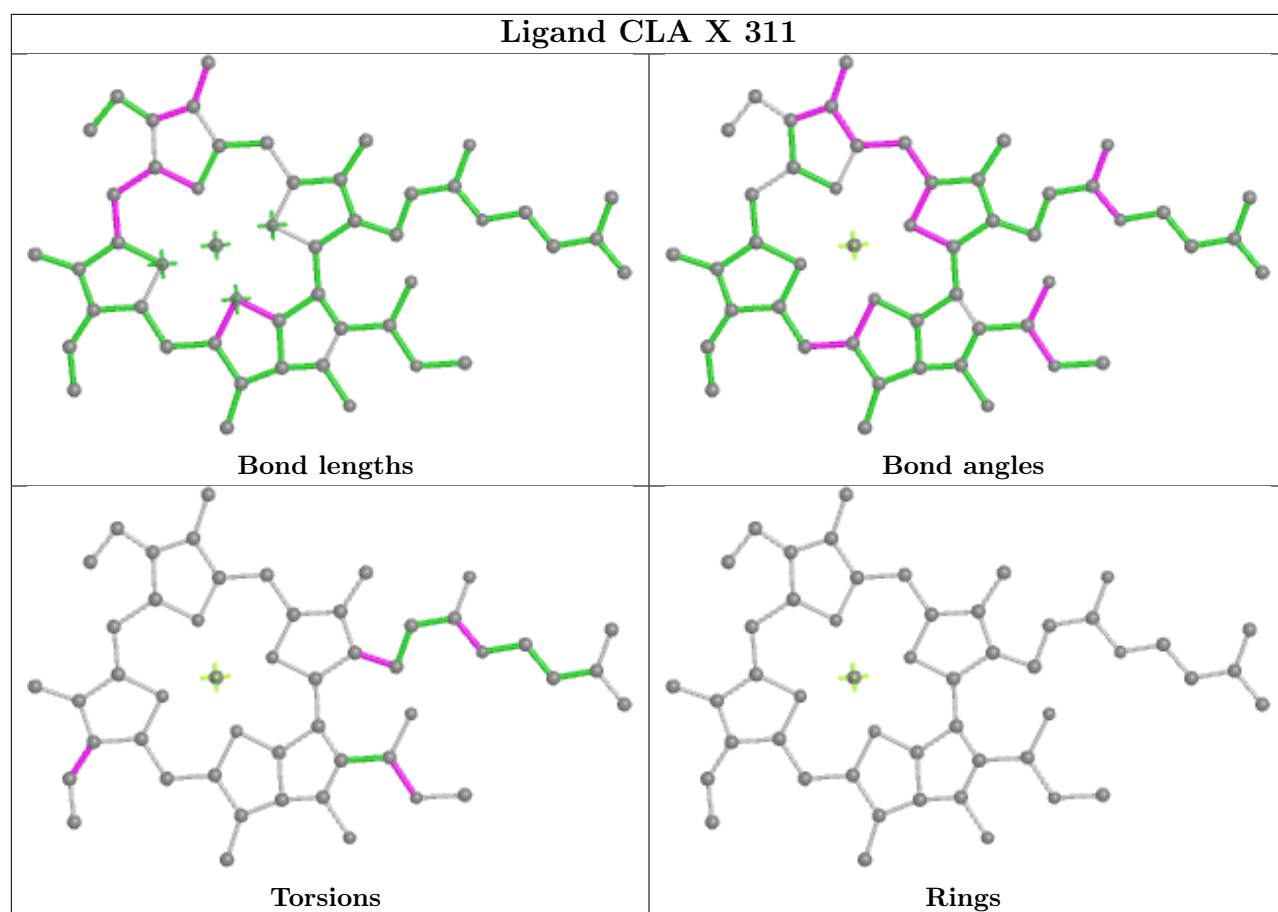
Bond angles



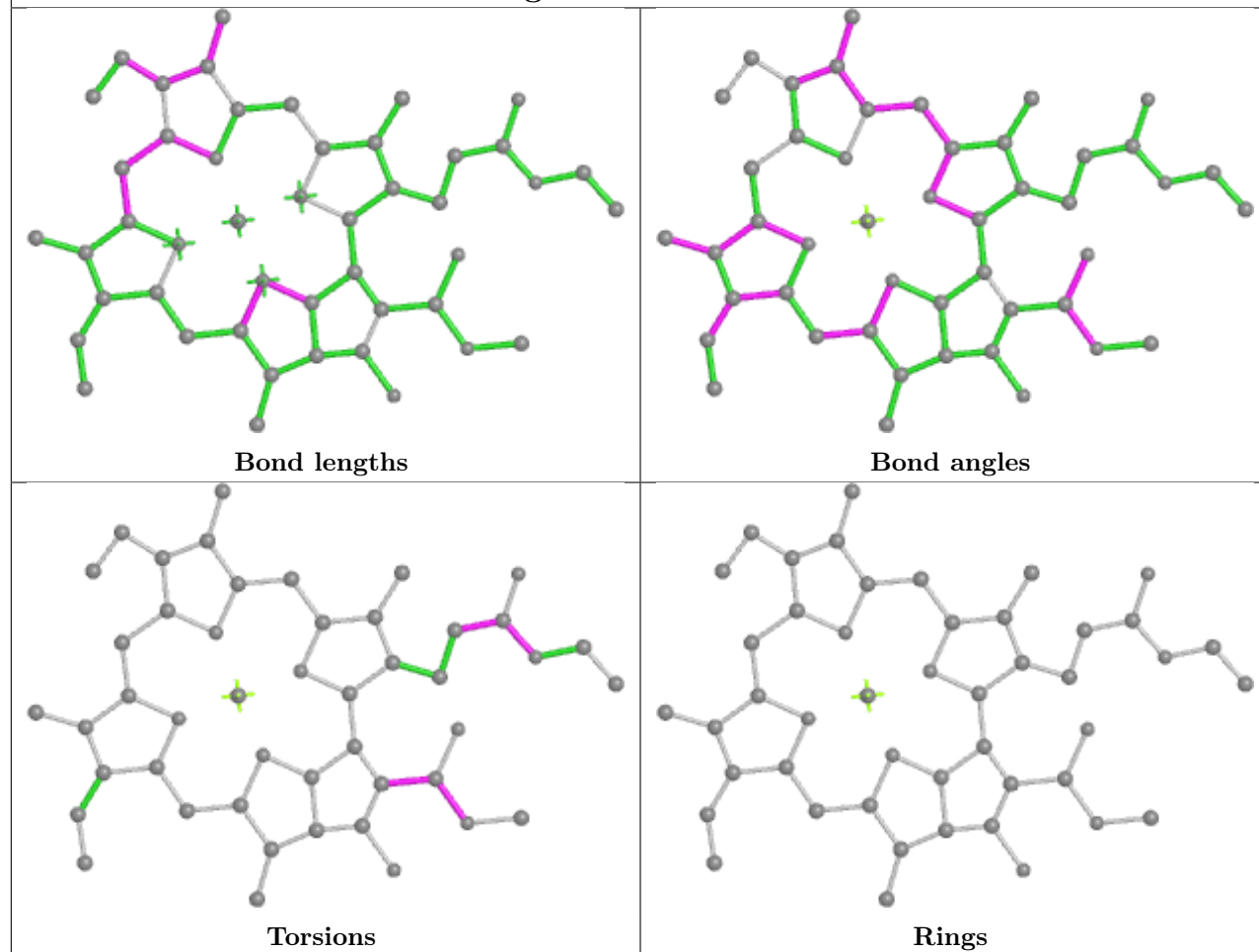
Torsions



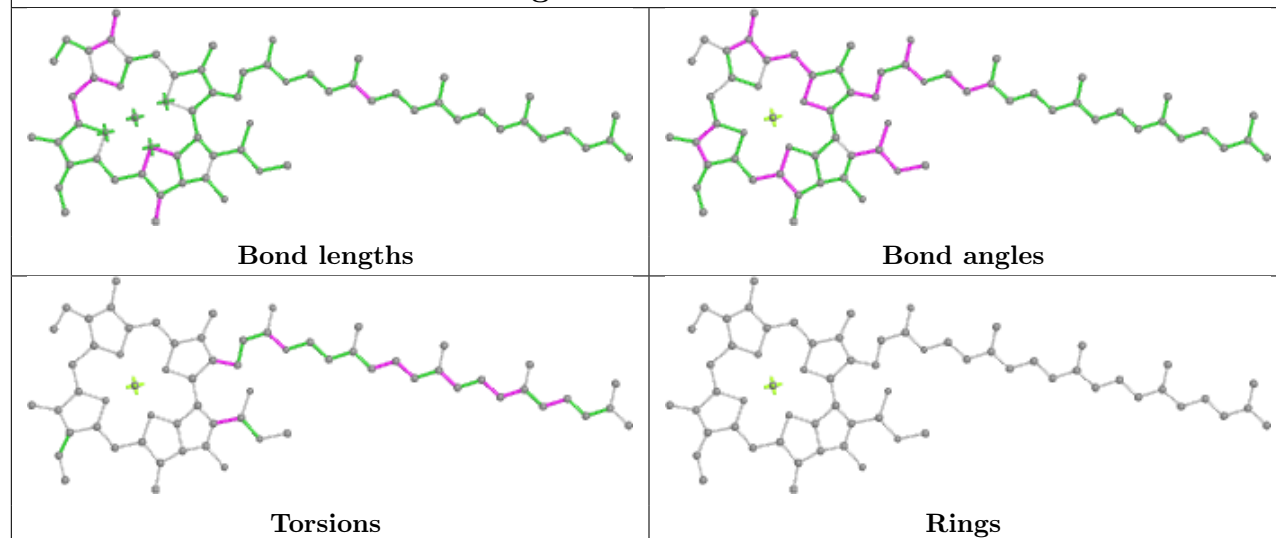
Rings

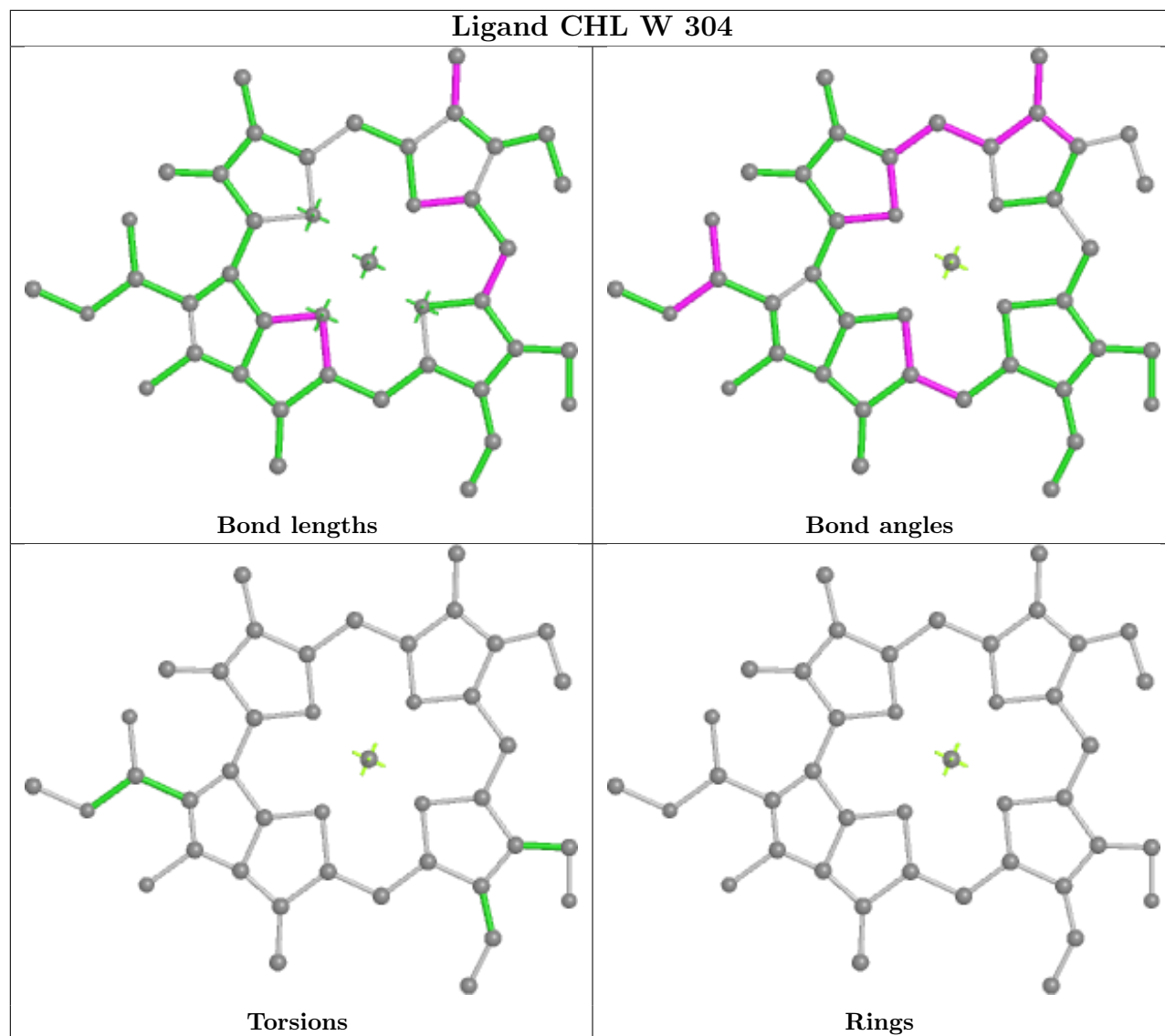
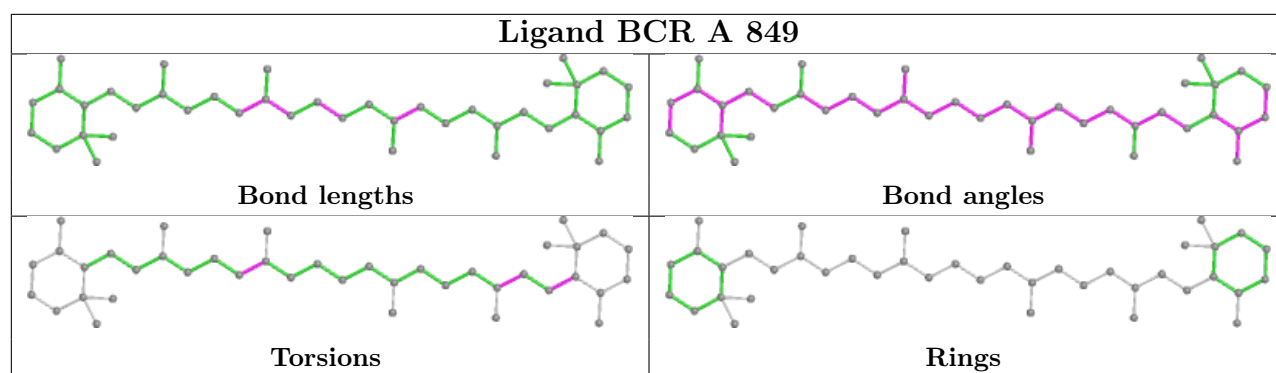


Ligand CLA V 310

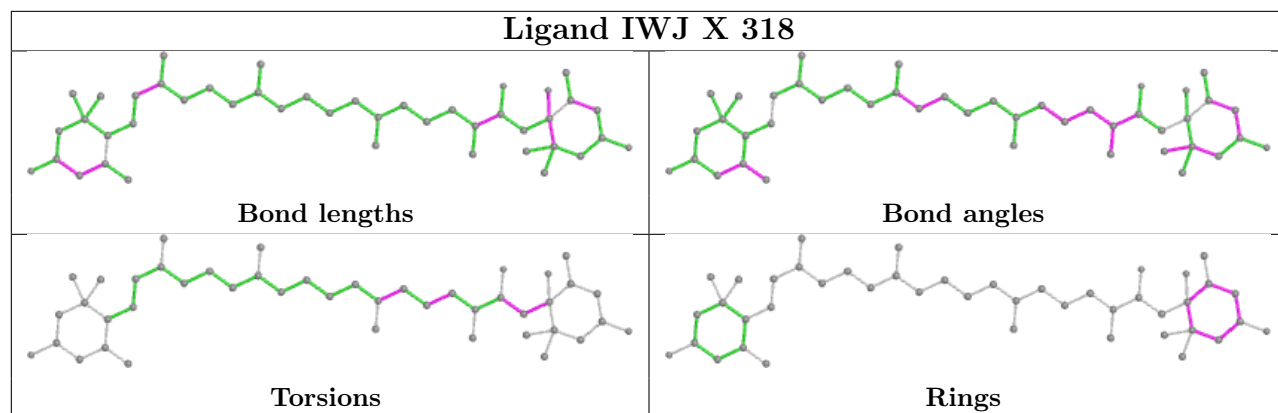


Ligand CLA A 842

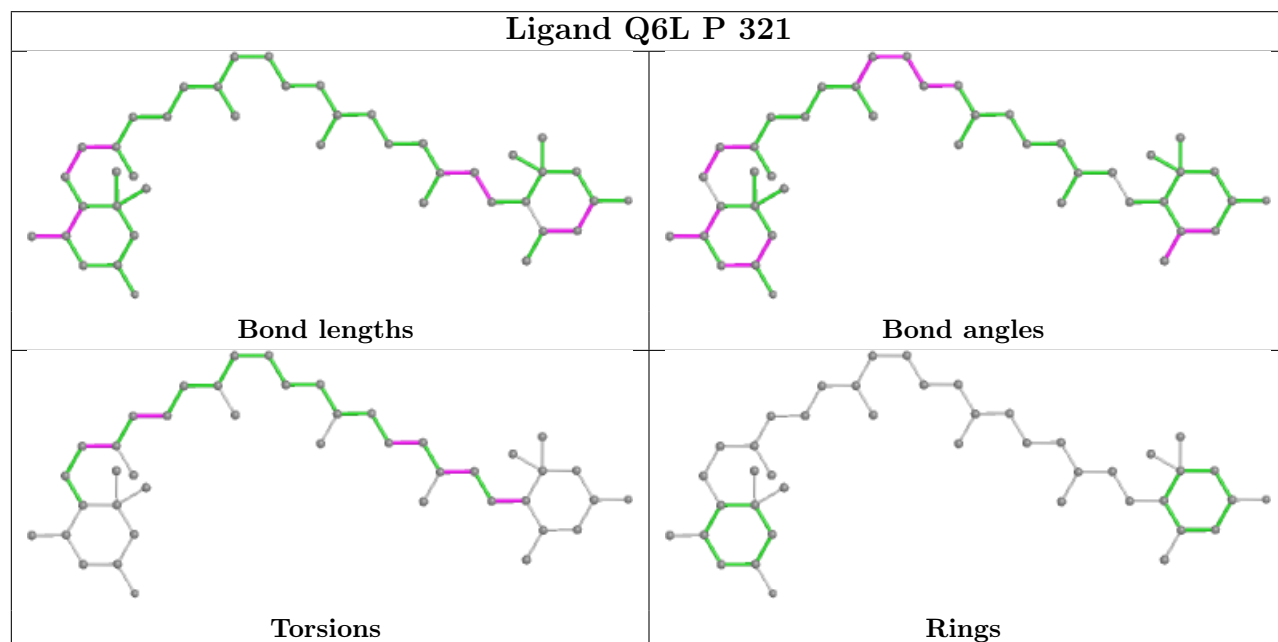




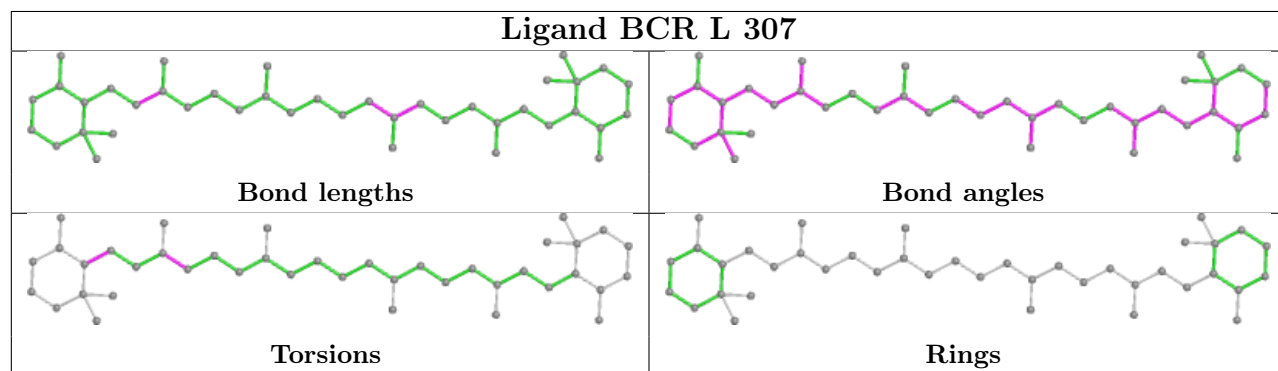
Ligand IWJ X 318



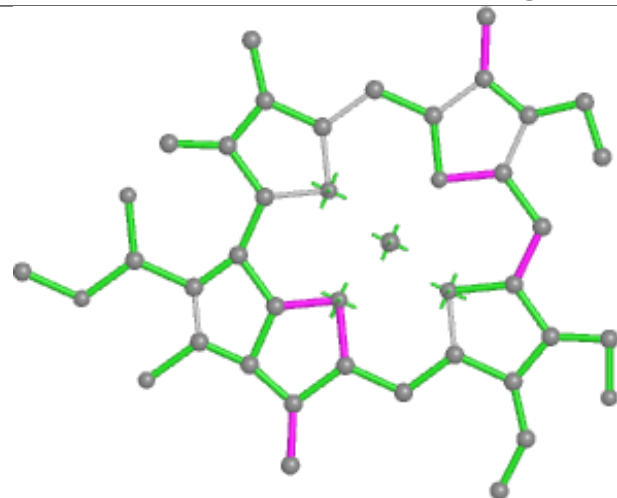
Ligand Q6L P 321



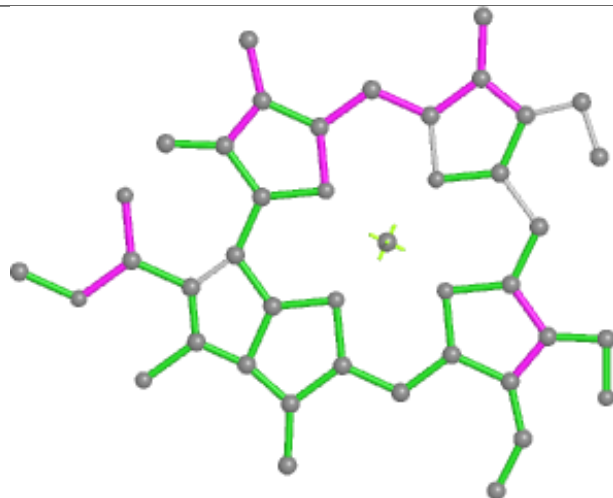
Ligand BCR L 307



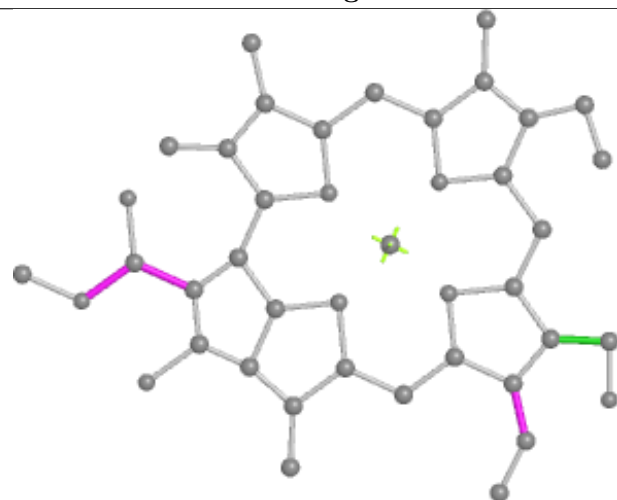
Ligand CHL S 307



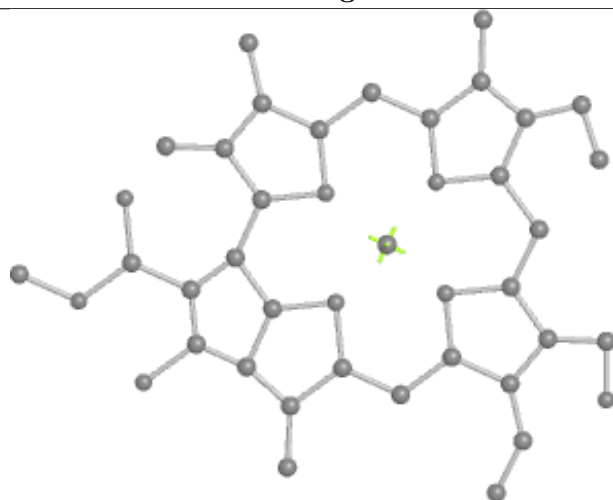
Bond lengths



Bond angles

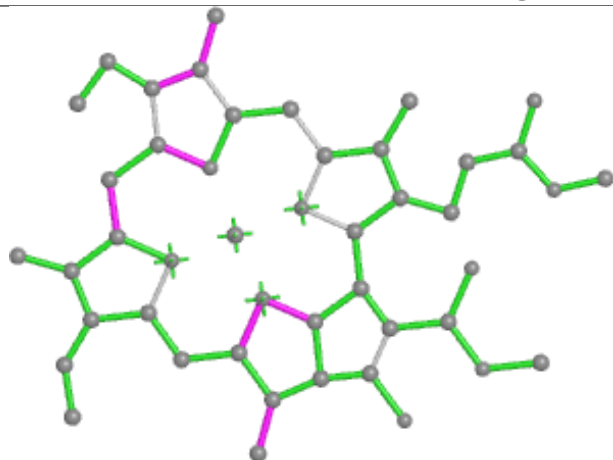


Torsions

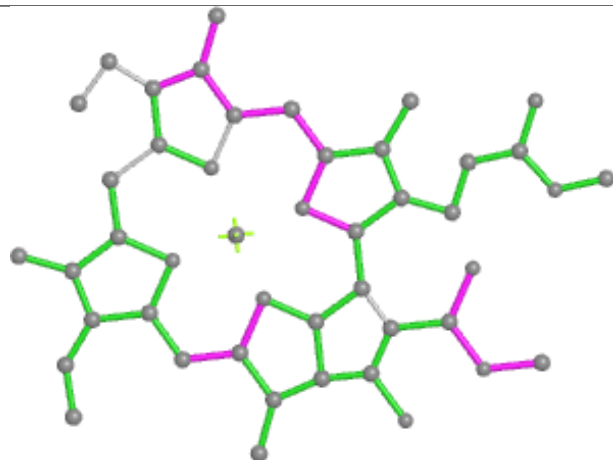


Rings

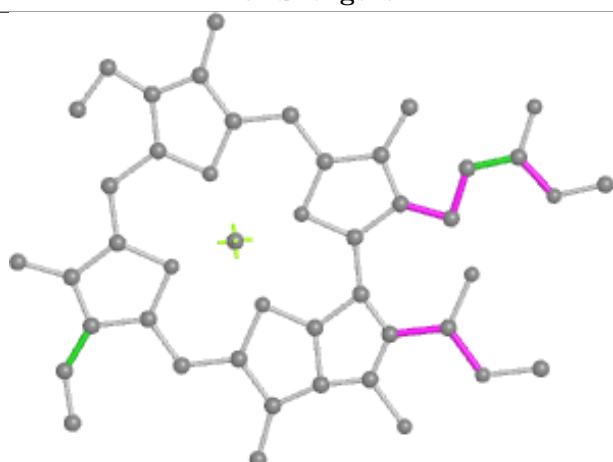
Ligand CLA U 309



Bond lengths



Bond angles

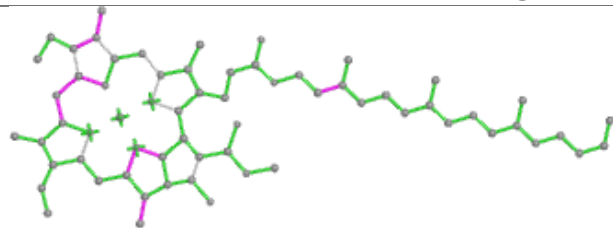


Torsions

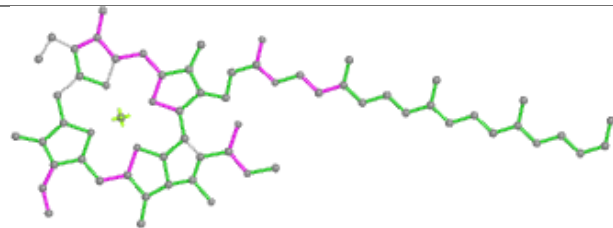


Rings

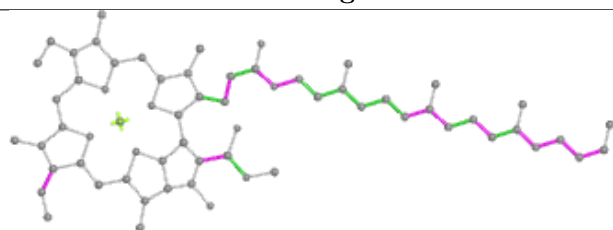
Ligand CLA A 807



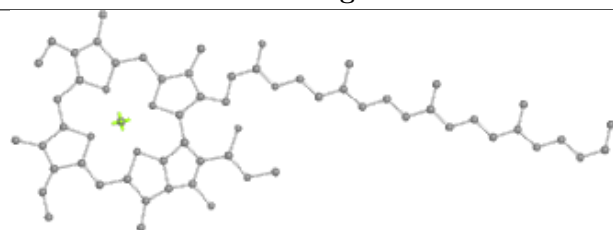
Bond lengths



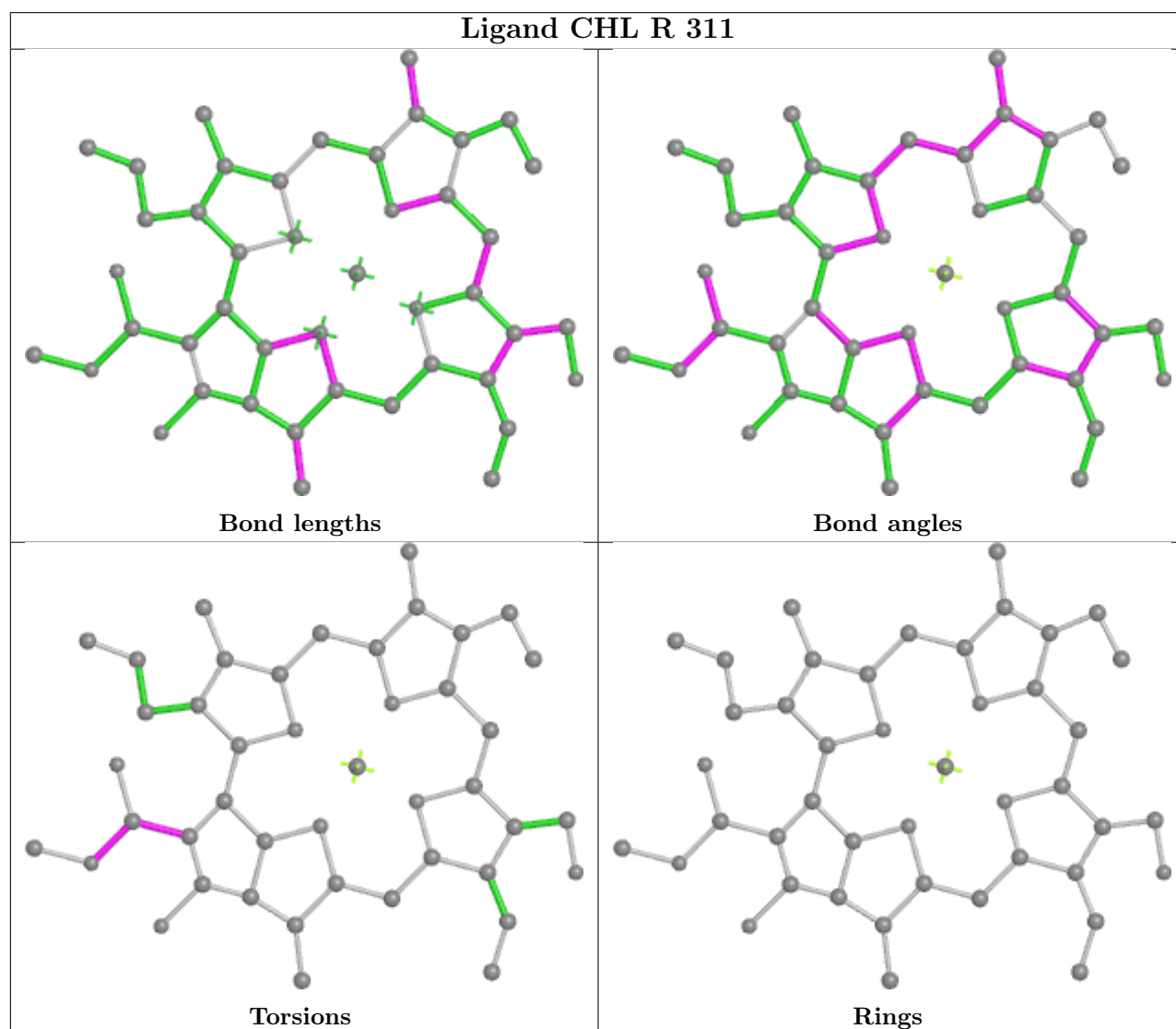
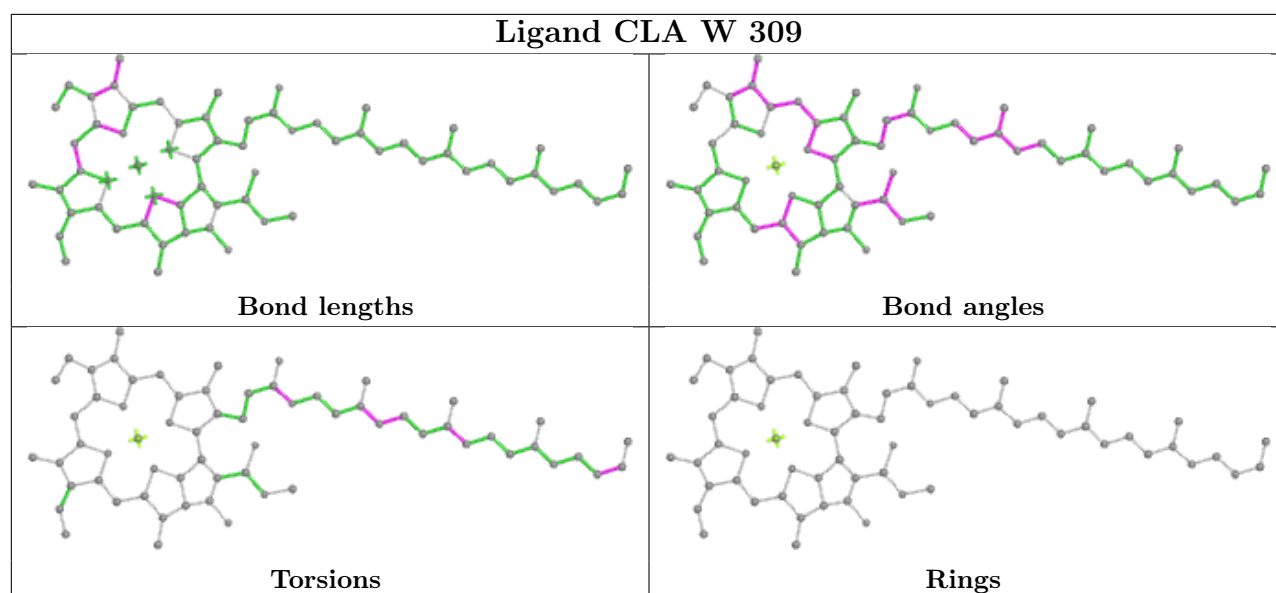
Bond angles



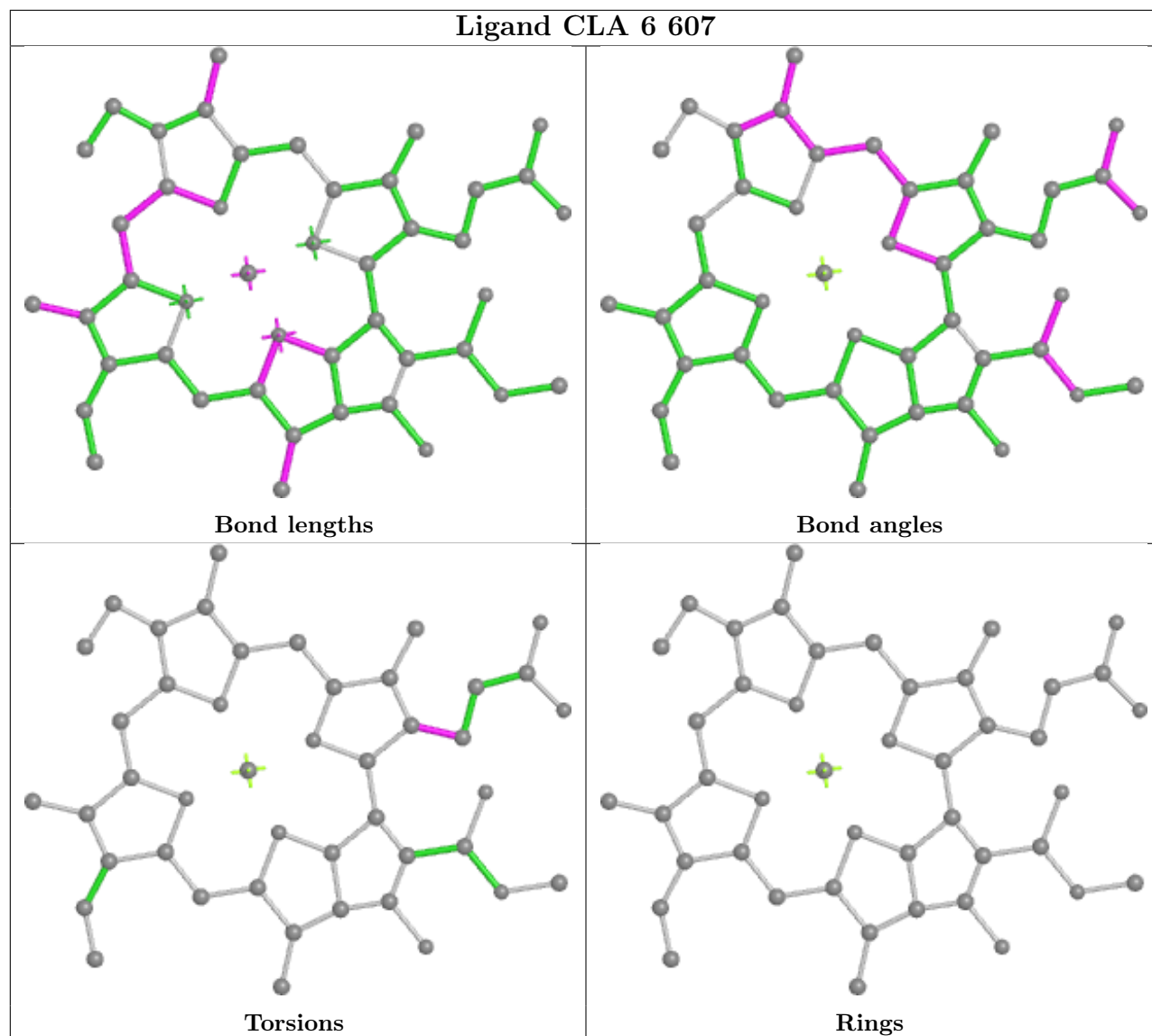
Torsions



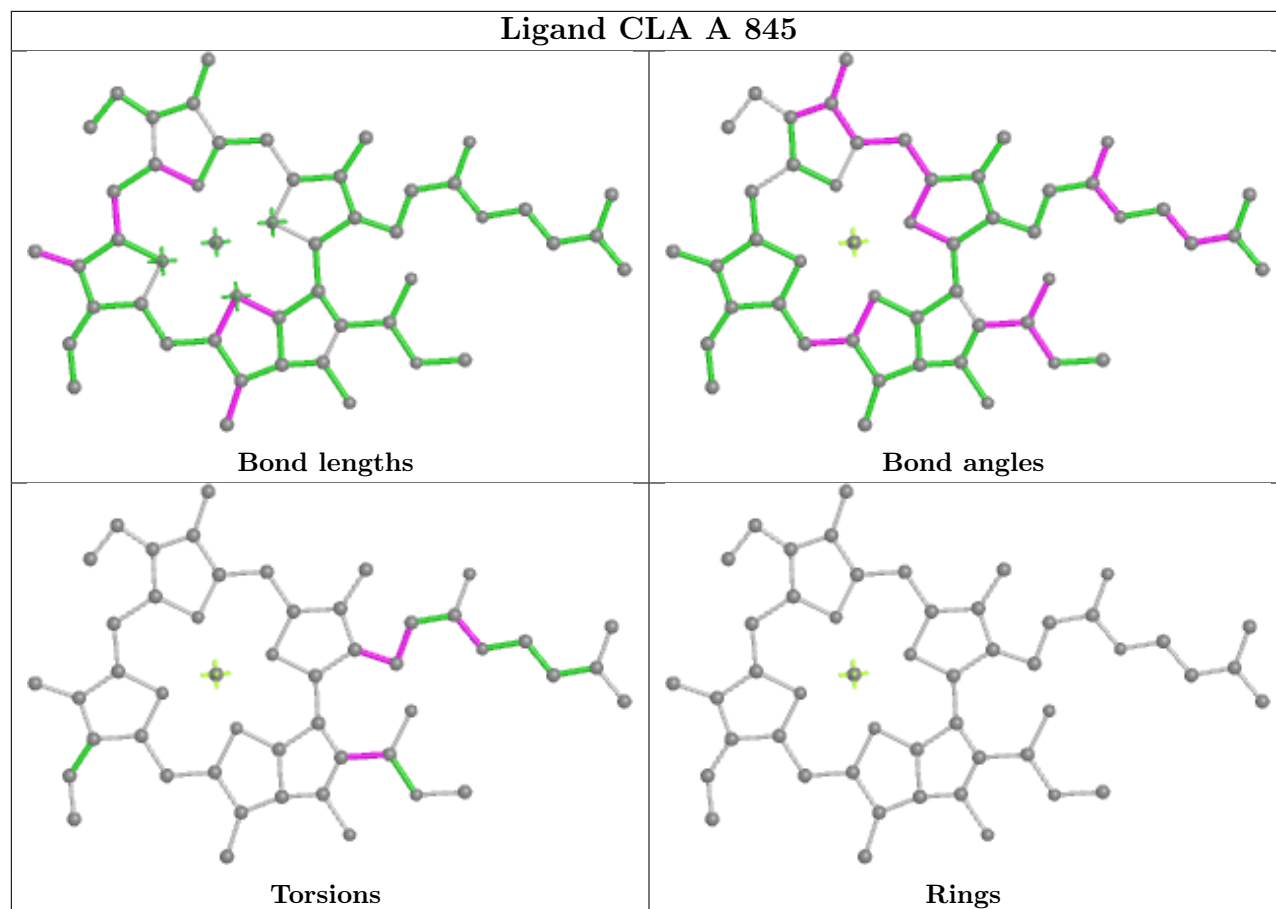
Rings



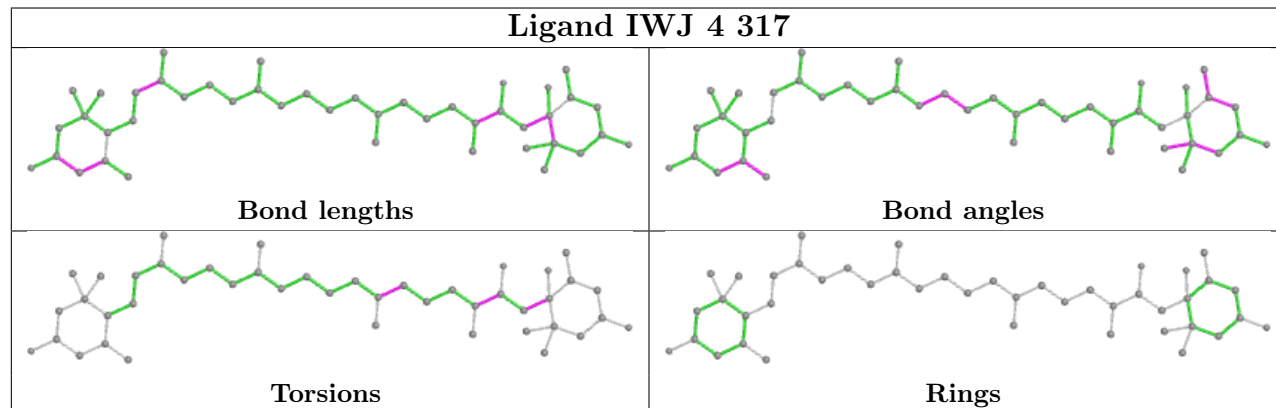
Ligand CLA 6 607

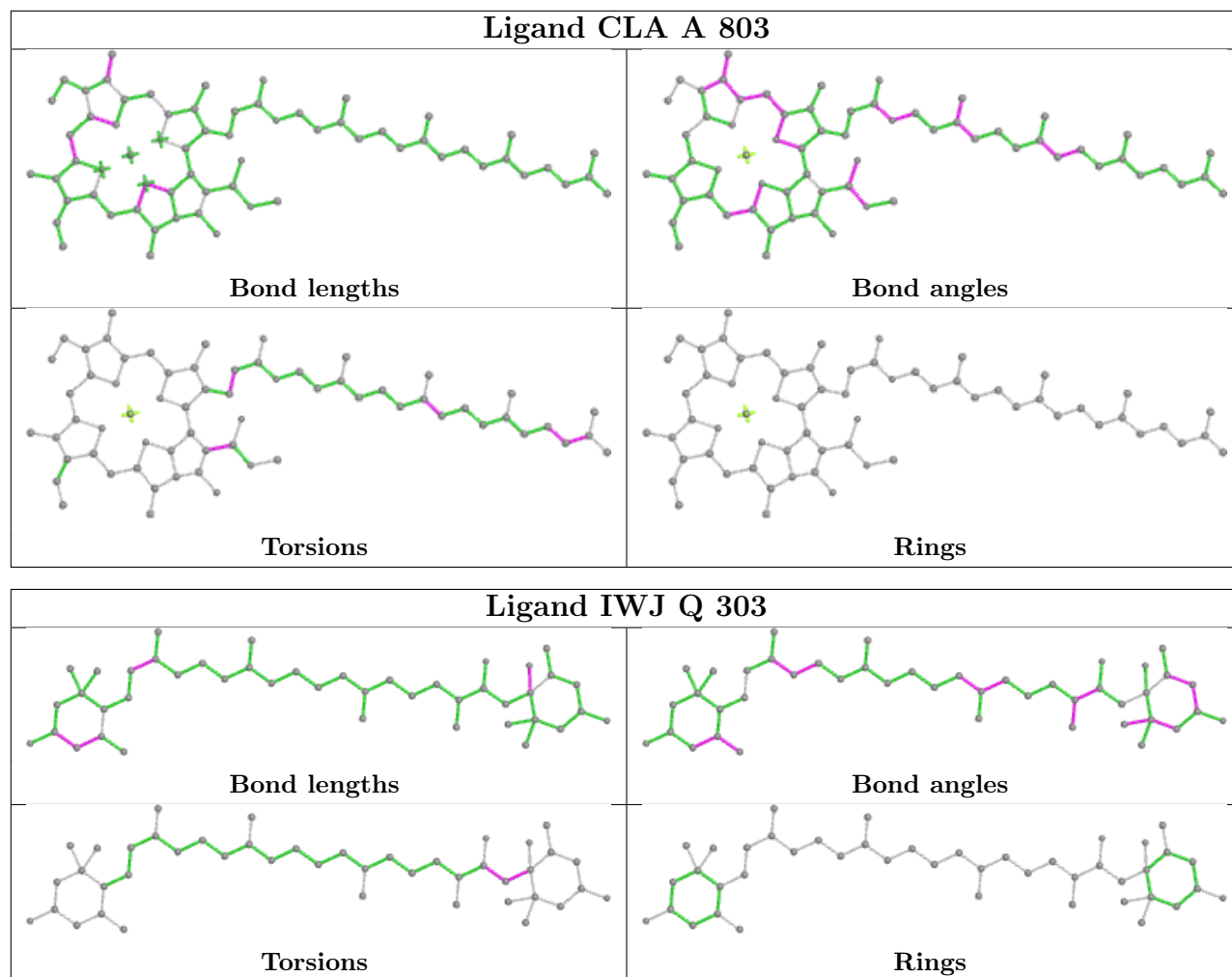


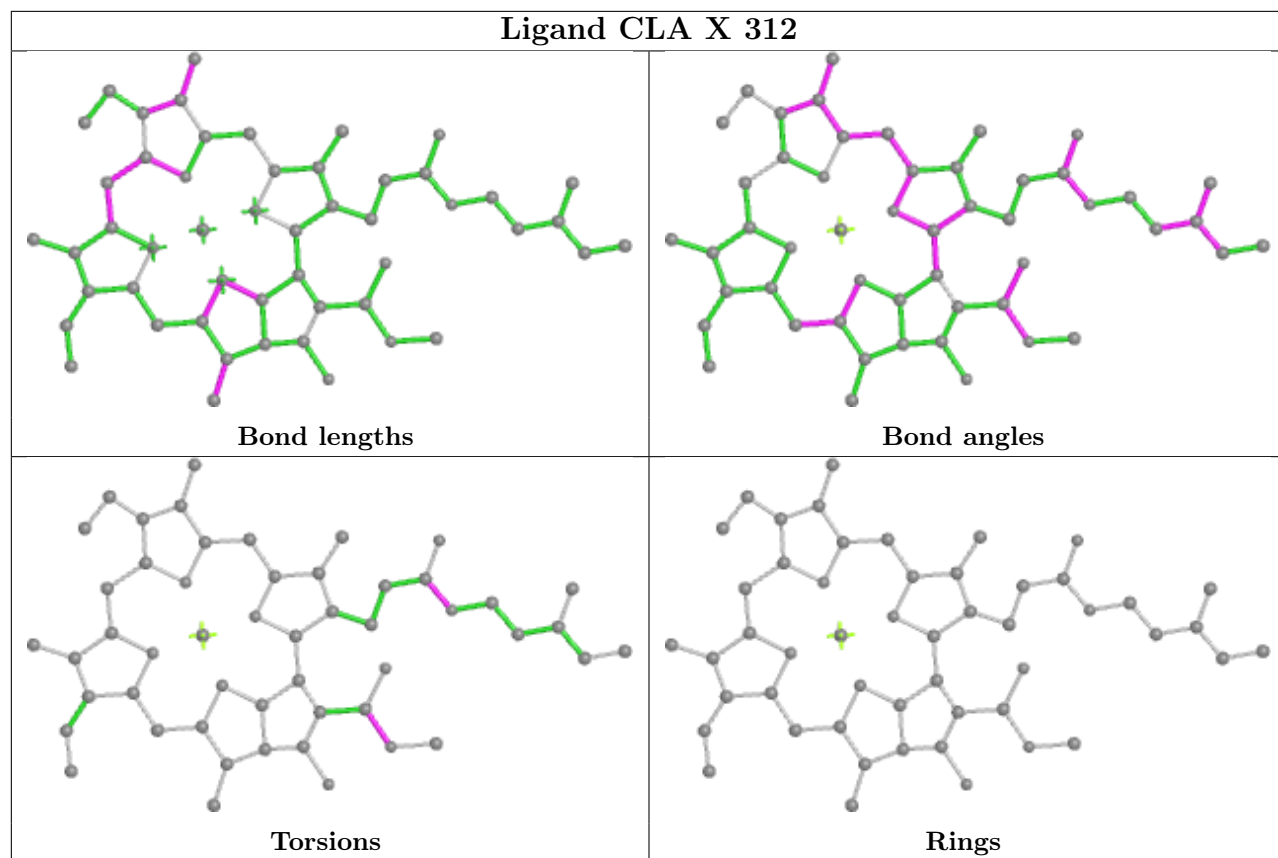
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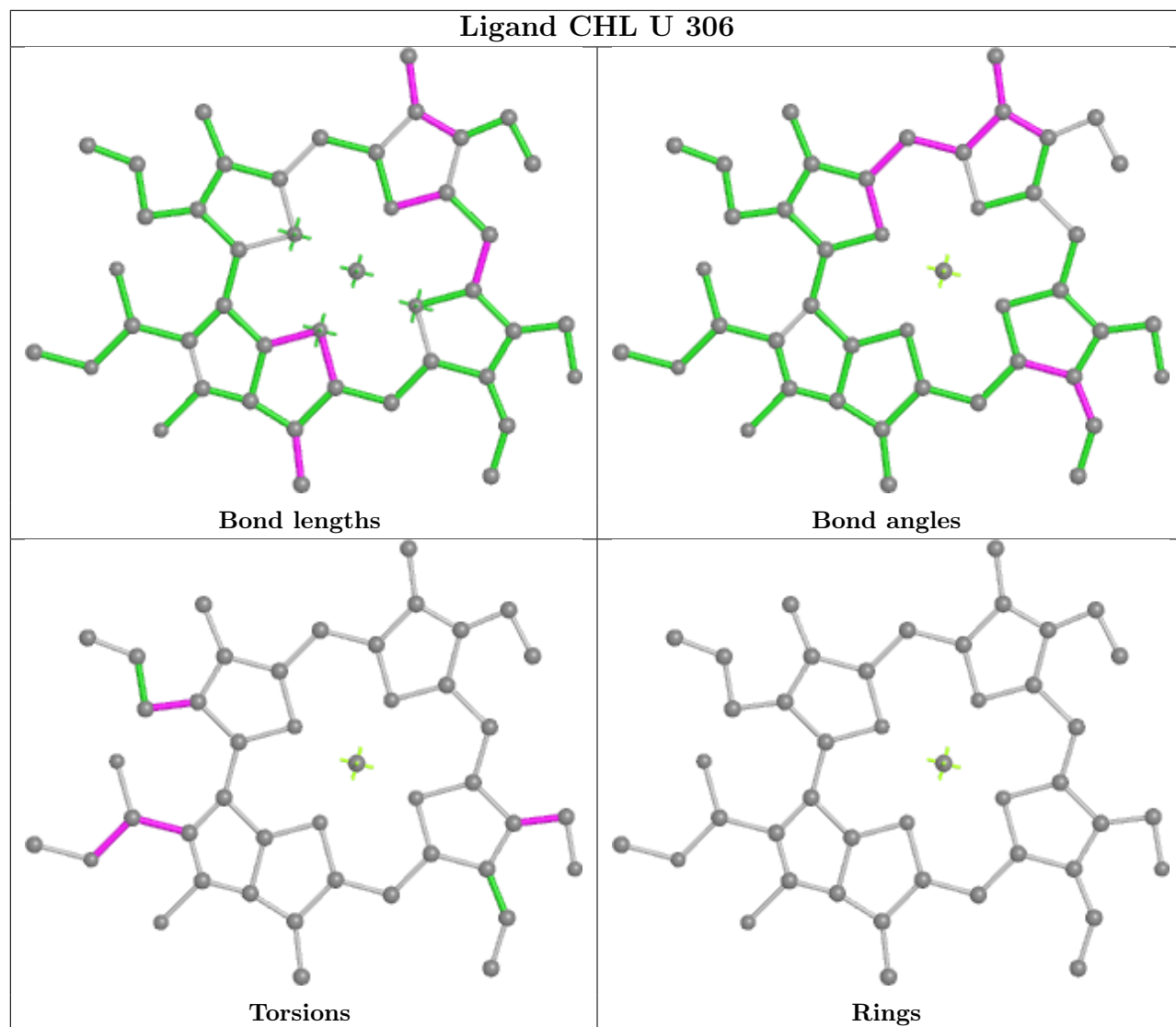


Ligand IWJ 4 317

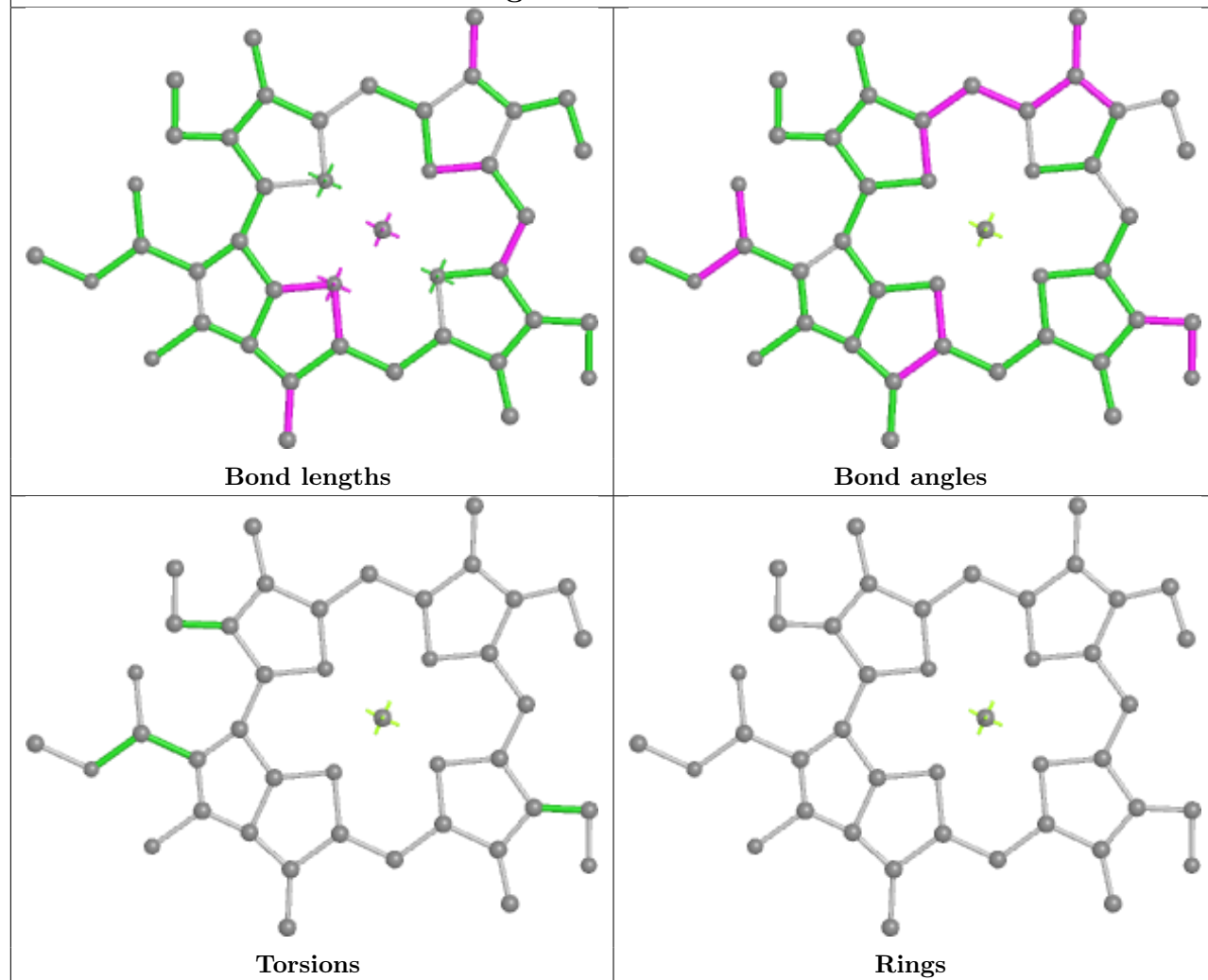




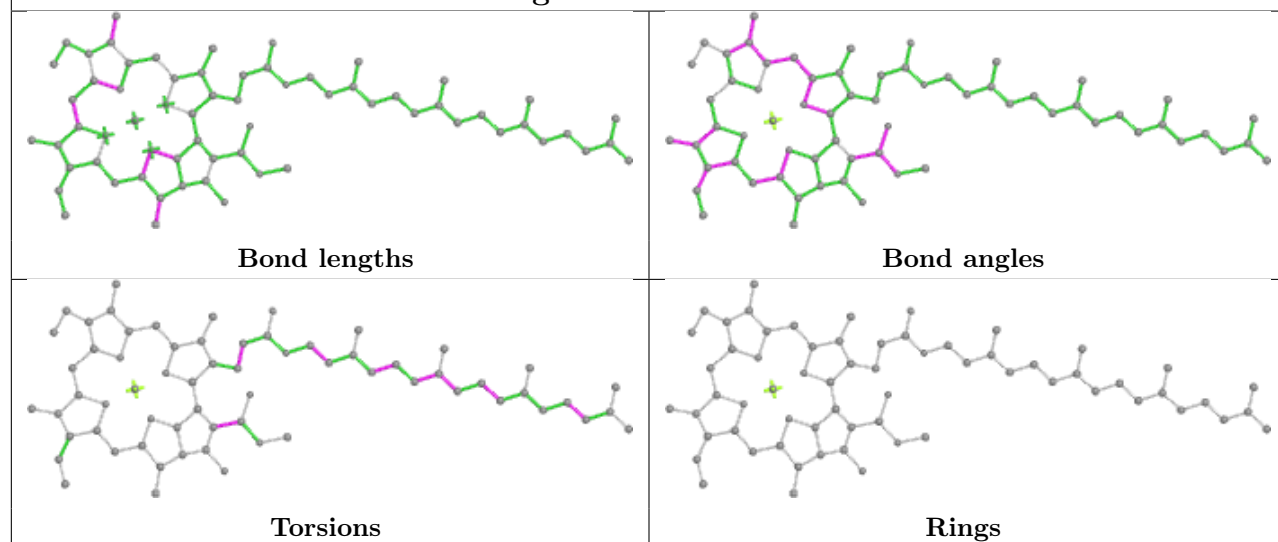




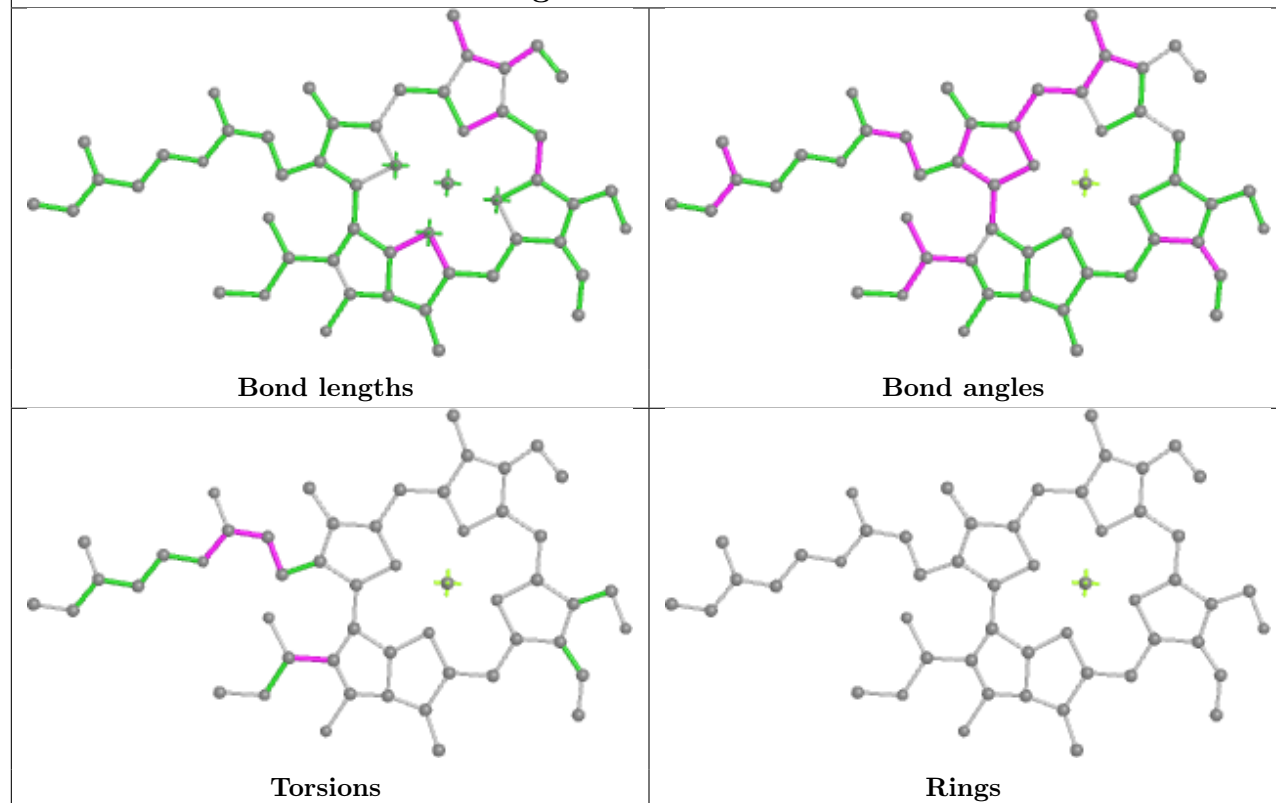
Ligand CHL 6 605



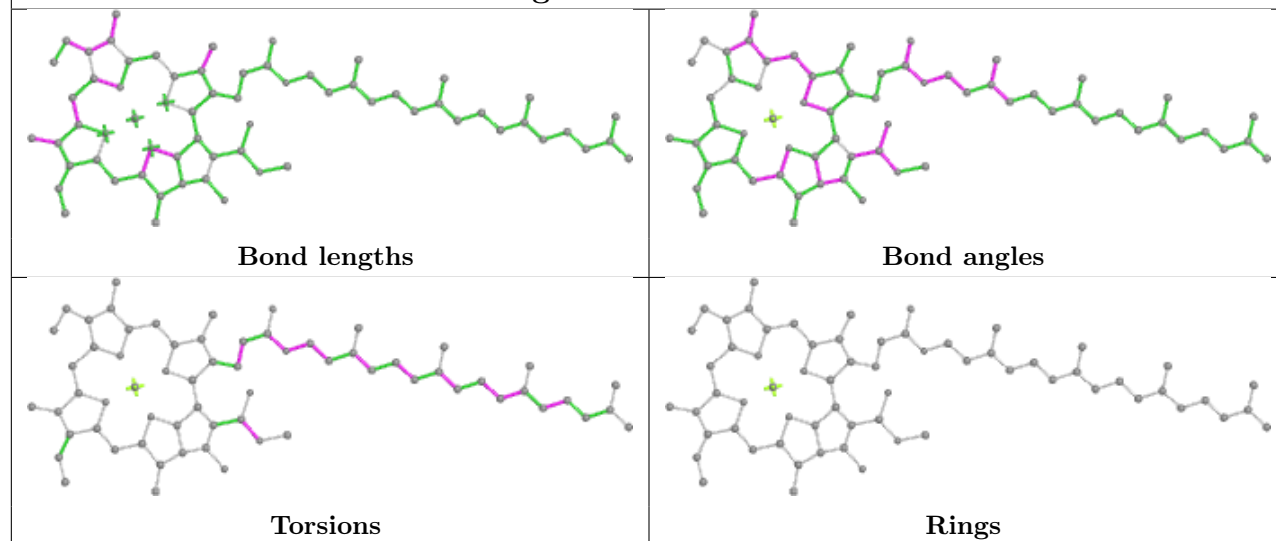
Ligand CLA B 814



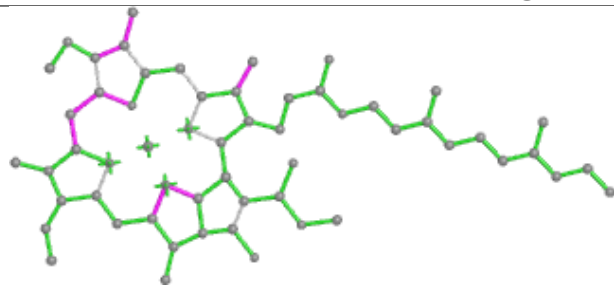
Ligand CHL T 320



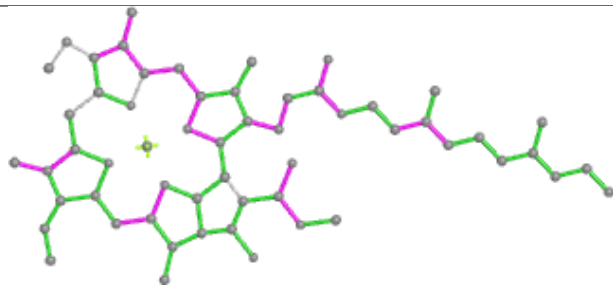
Ligand CLA B 805



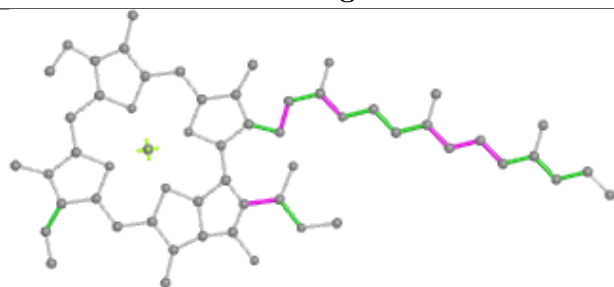
Ligand CLA 4 313



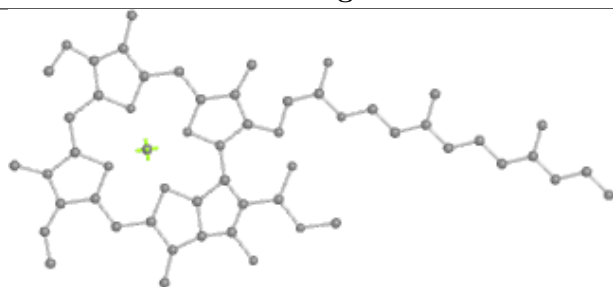
Bond lengths



Bond angles

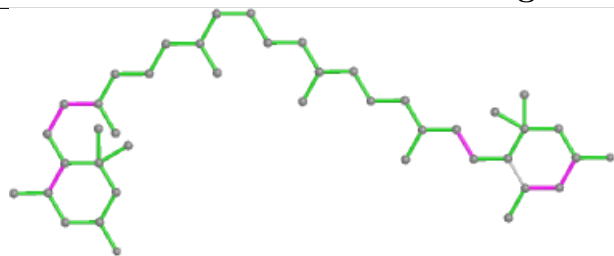


Torsions

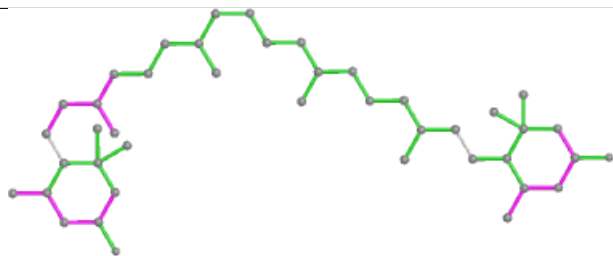


Rings

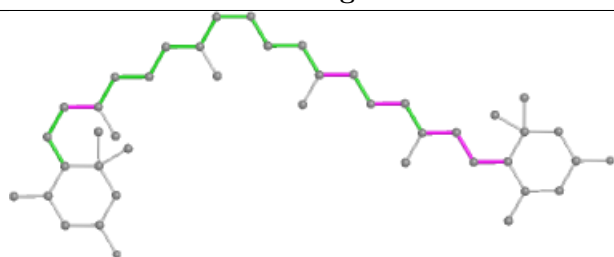
Ligand Q6L X 319



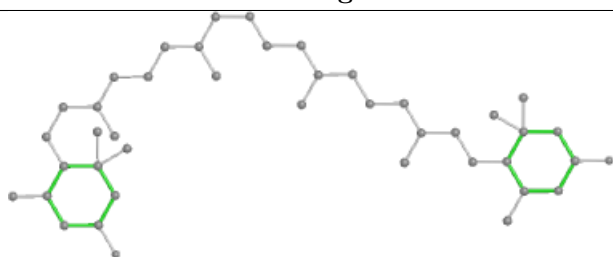
Bond lengths



Bond angles

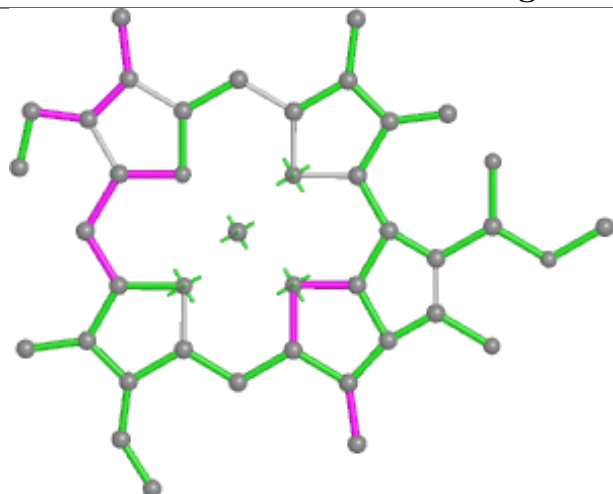


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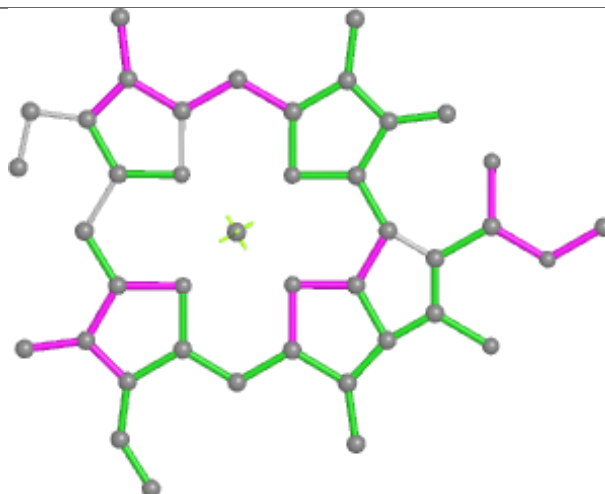


Rings

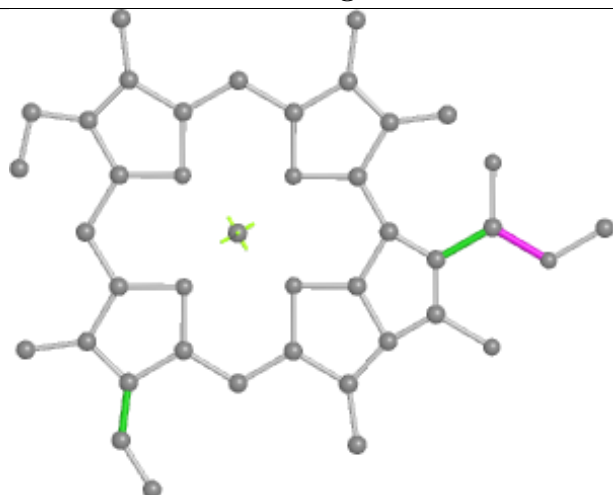
Ligand CLA 3 308



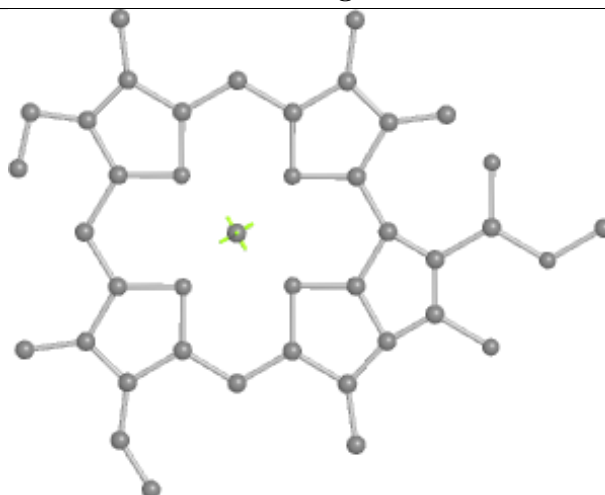
Bond lengths



Bond angles

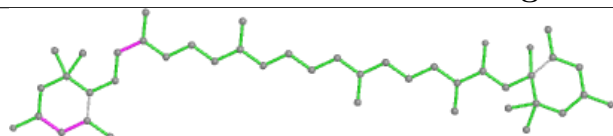


Torsions

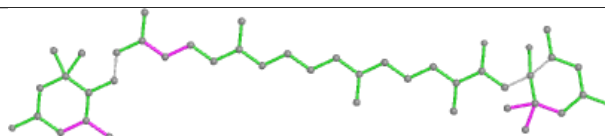


Rings

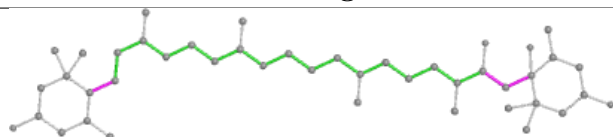
Ligand IWJ 5 611



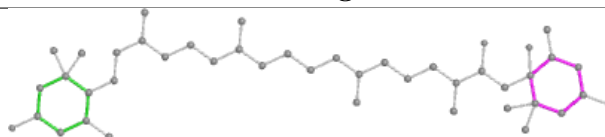
Bond lengths



Bond angles

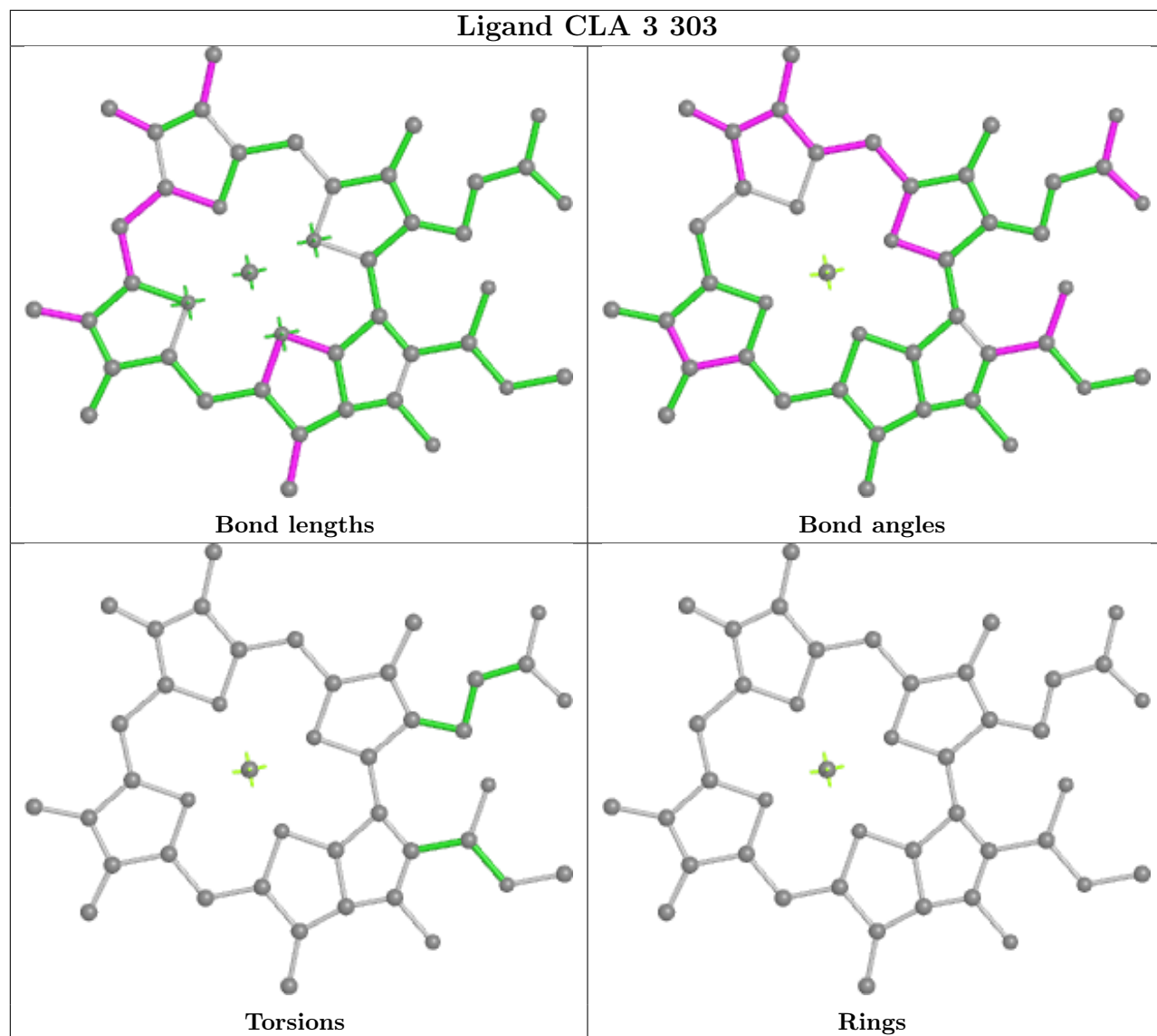


Torsions

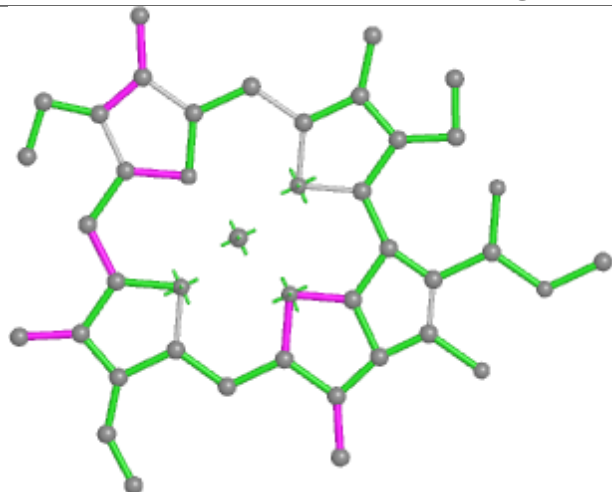


Rings

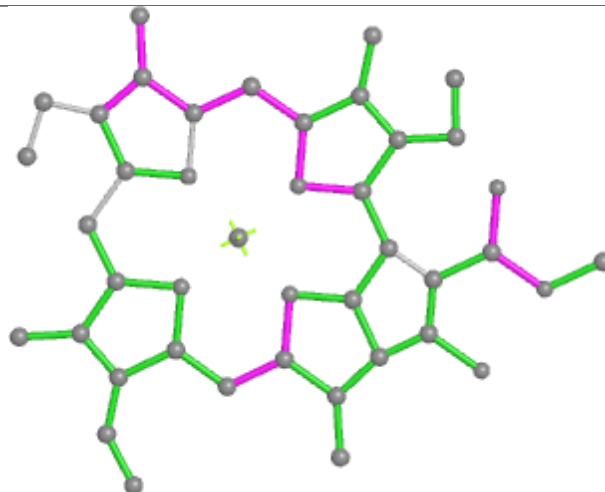
Ligand CLA 3 303



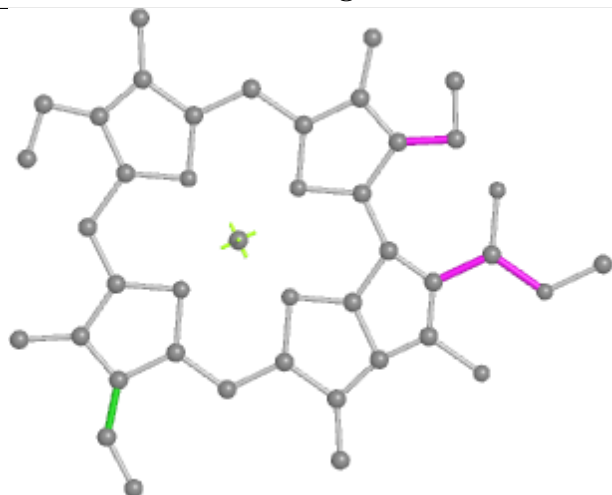
Ligand CLA T 313



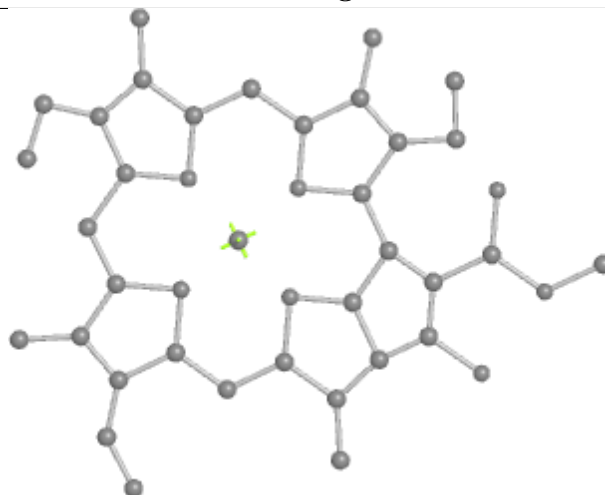
Bond lengths



Bond angles

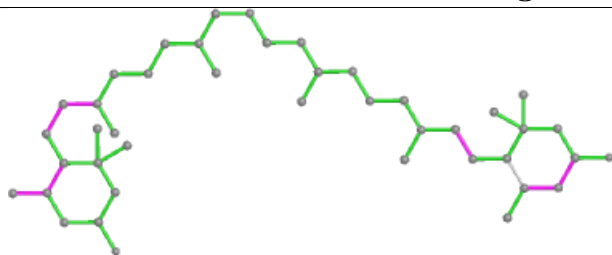


Torsions

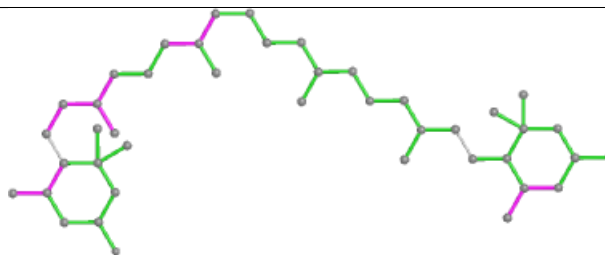


Rings

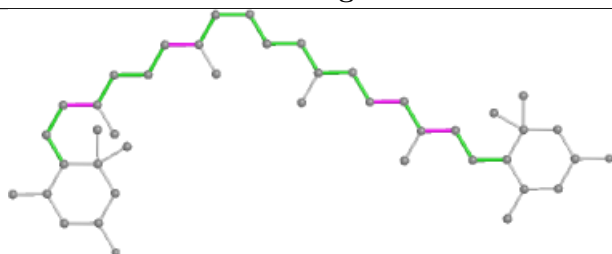
Ligand Q6L U 314



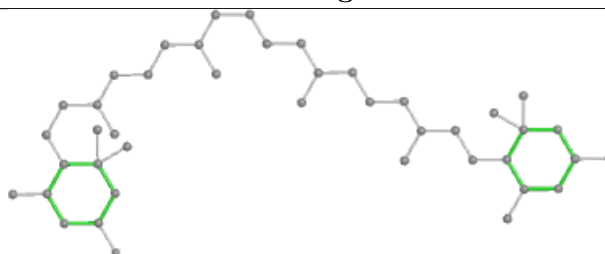
Bond lengths



Bond angles

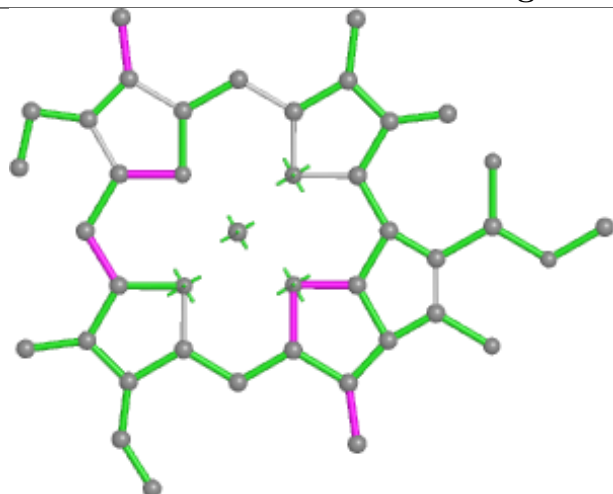


Torsions

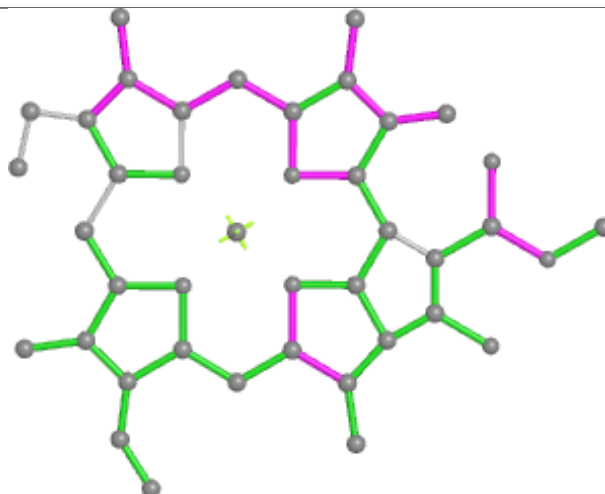


Rings

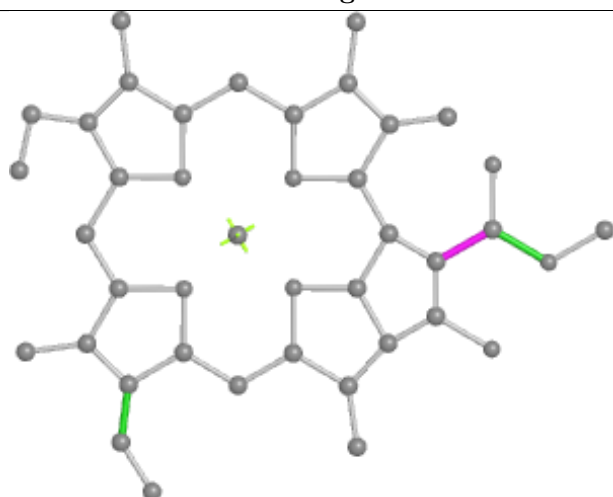
Ligand CLA S 313



Bond lengths



Bond angles

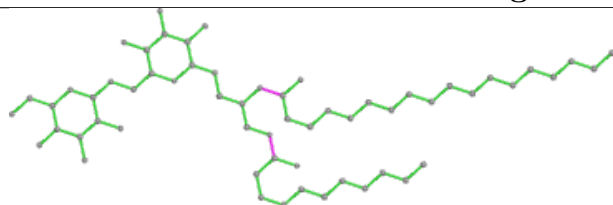


Torsions

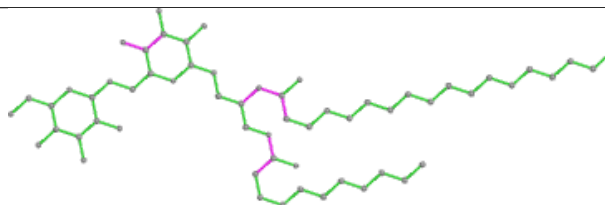


Rings

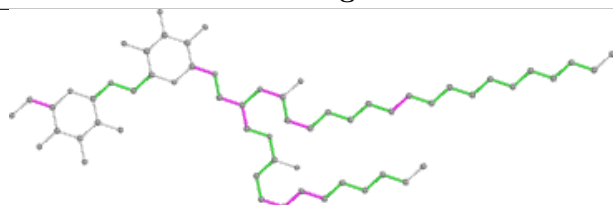
Ligand DGD B 850



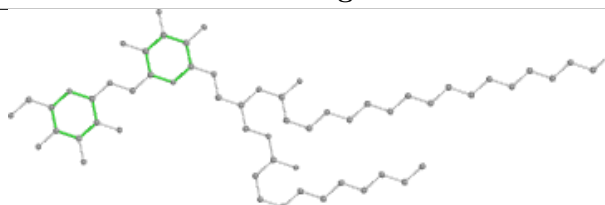
Bond lengths



Bond angles

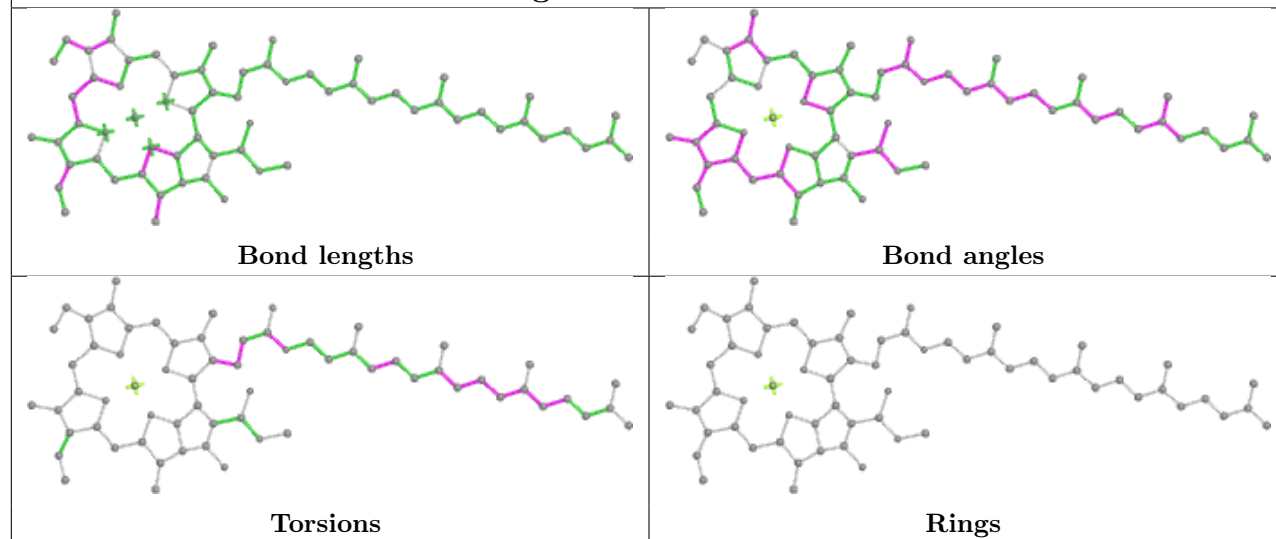


Torsions

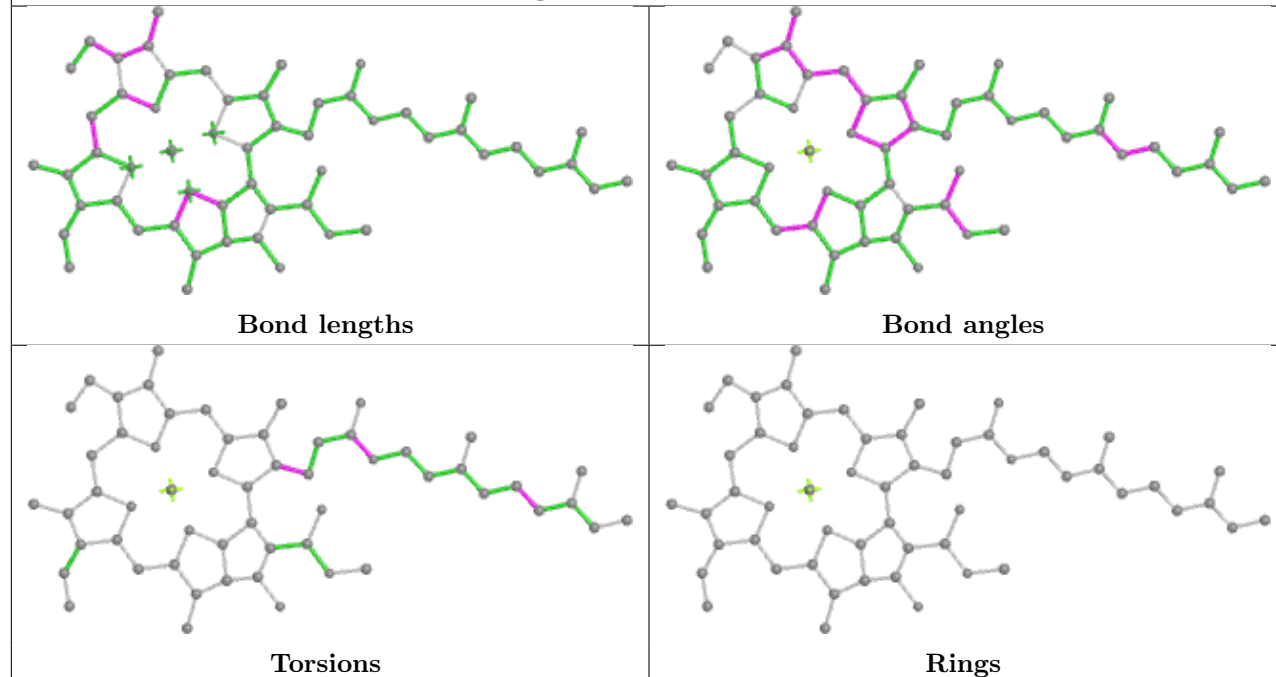


Rings

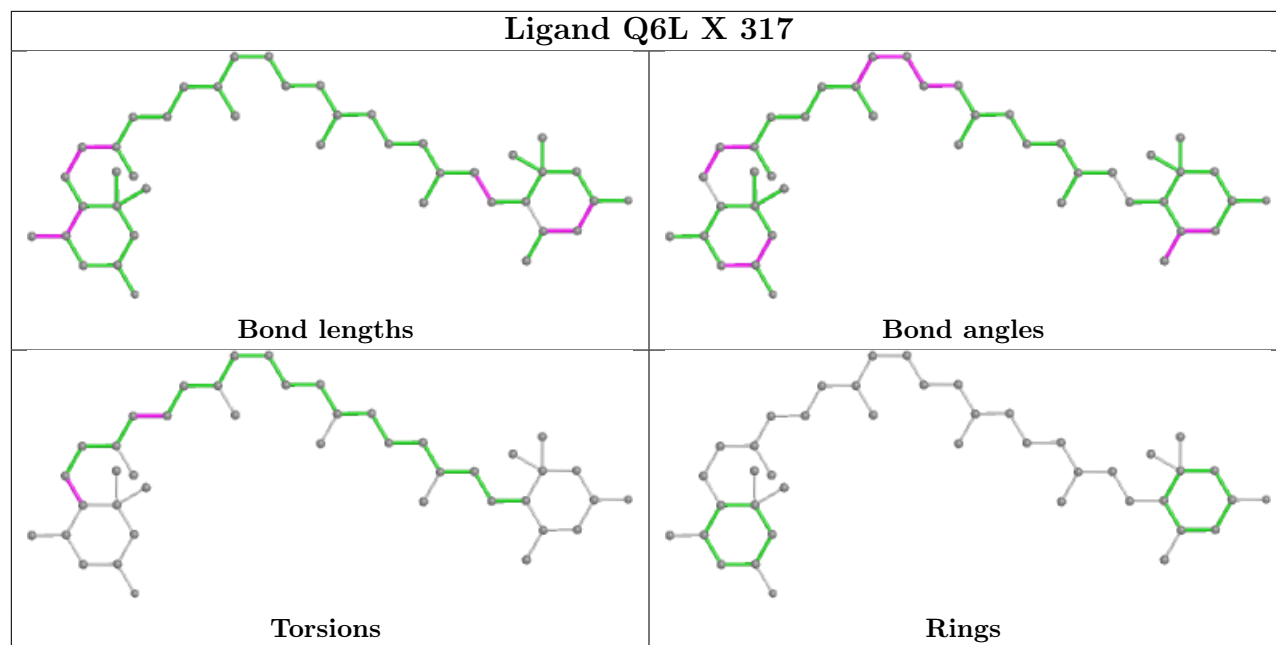
Ligand CLA B 813



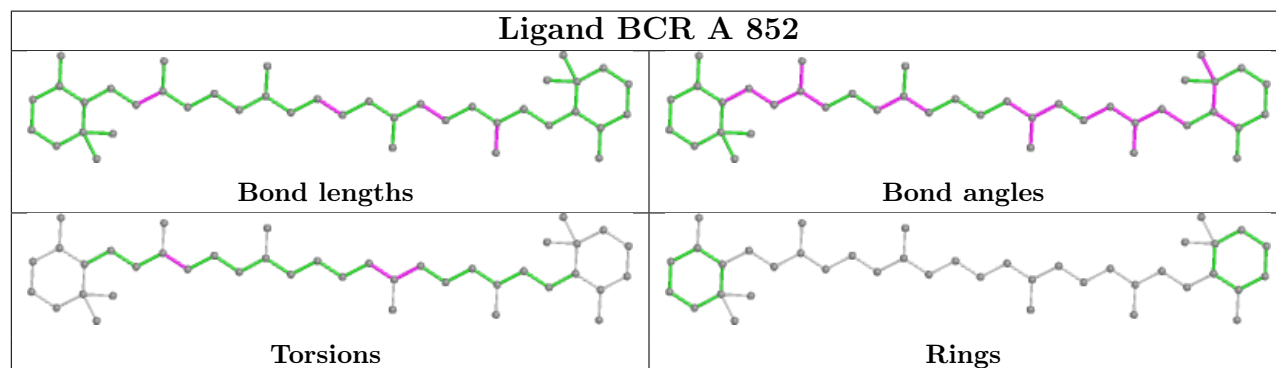
Ligand CLA A 834



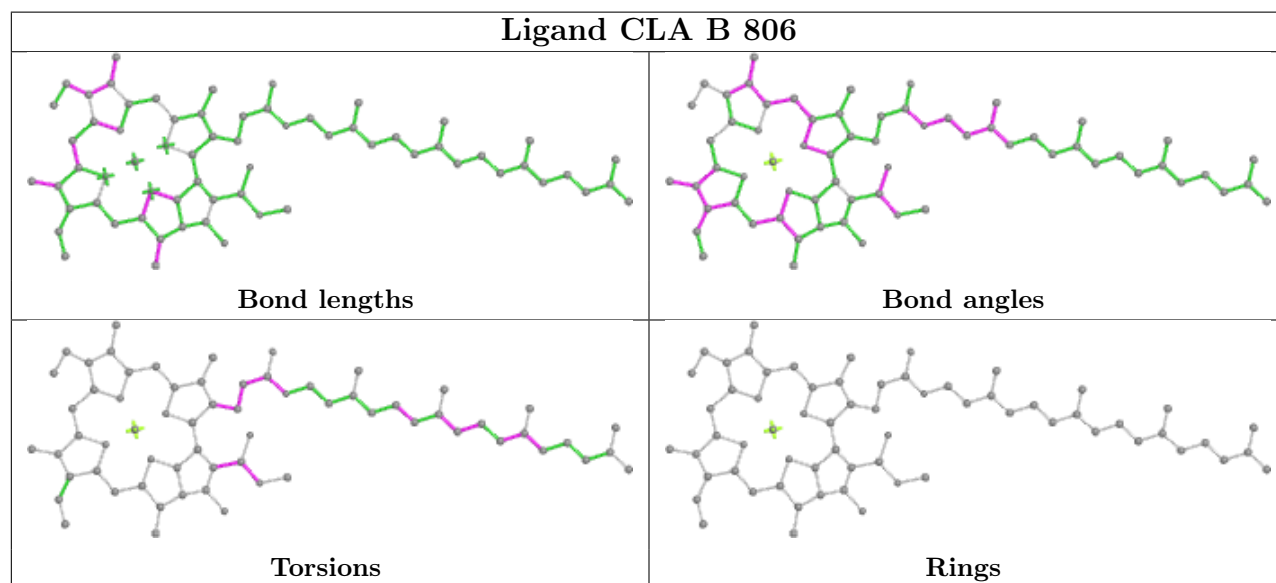
Ligand Q6L X 317

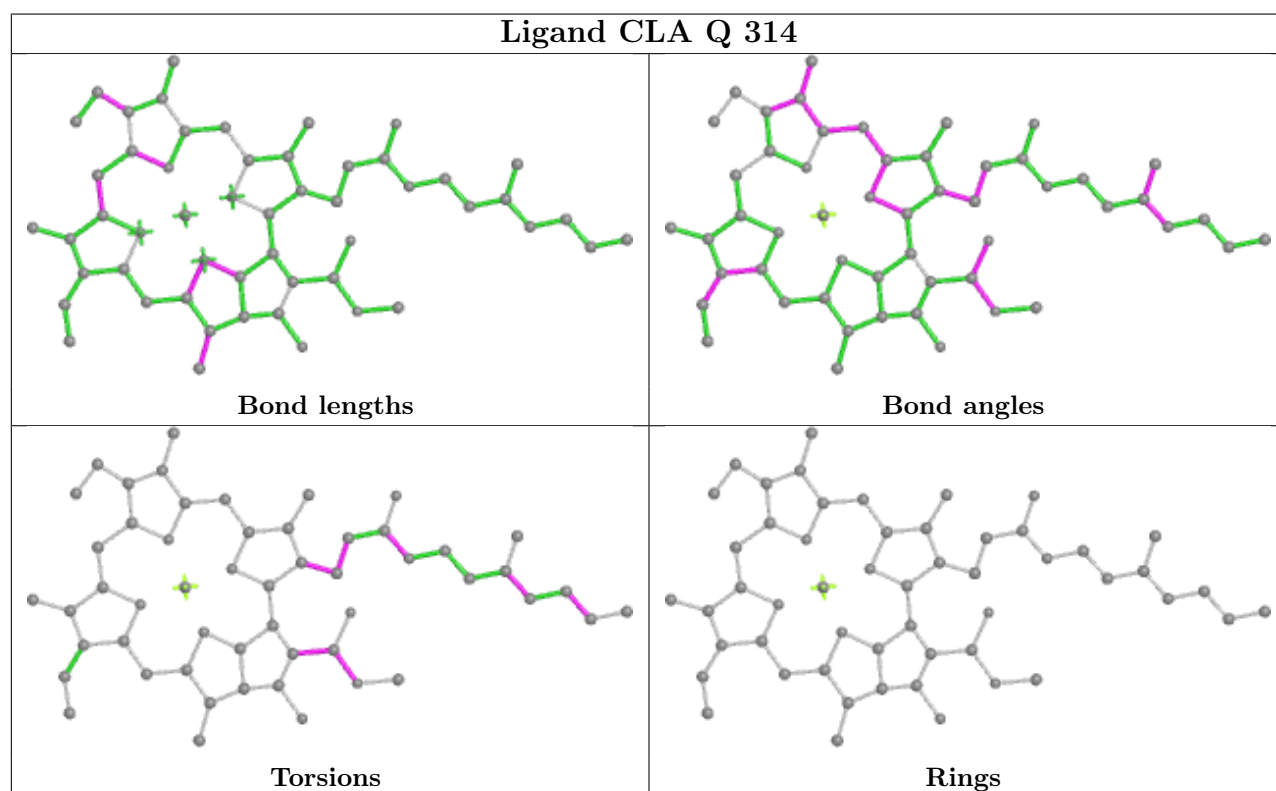
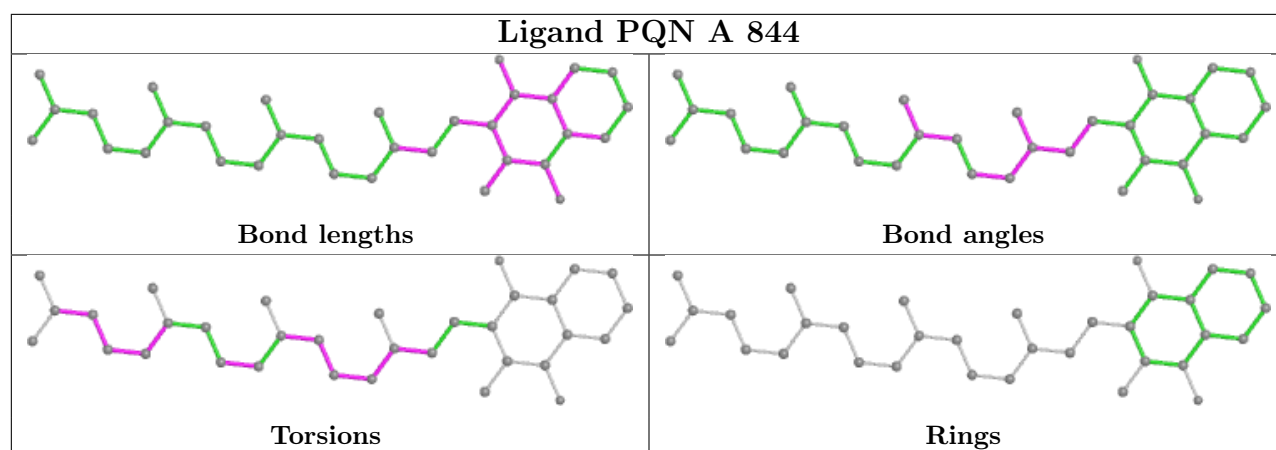


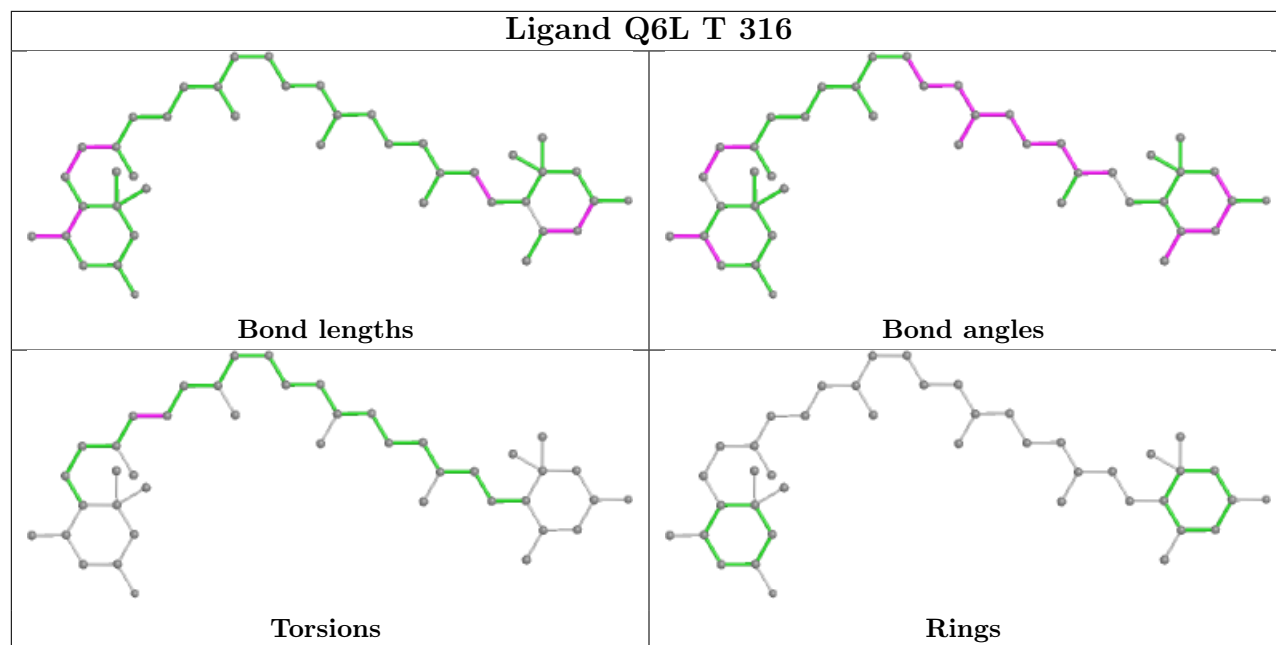
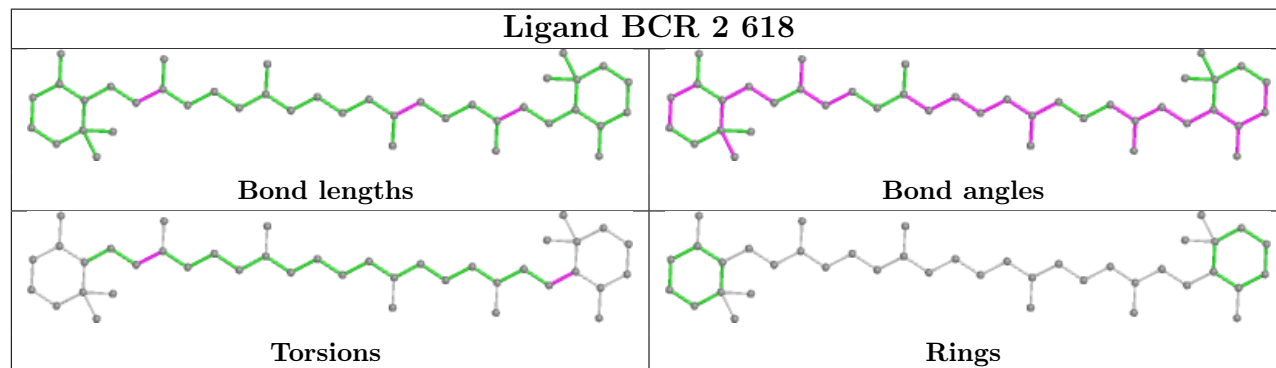
Ligand BCR A 852



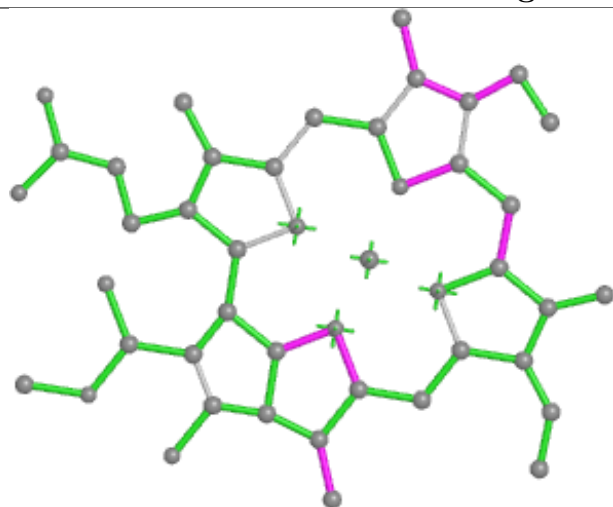
Ligand CLA B 806



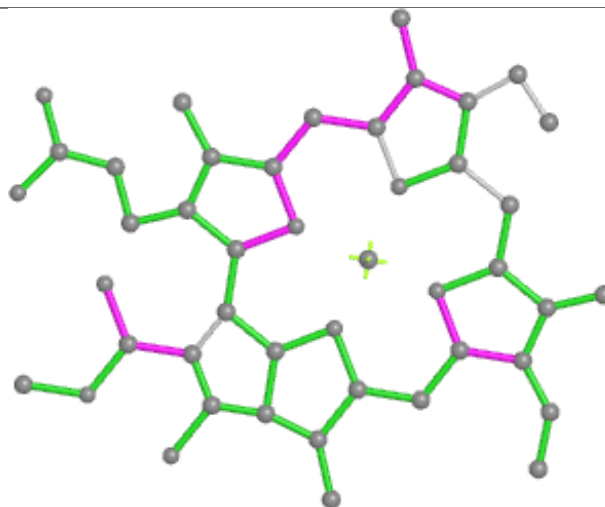


Ligand Q6L T 316**Ligand BCR 2 618**

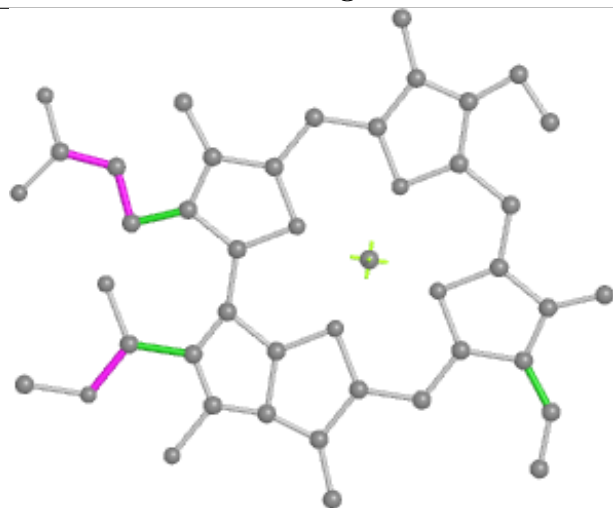
Ligand CHL 3 306



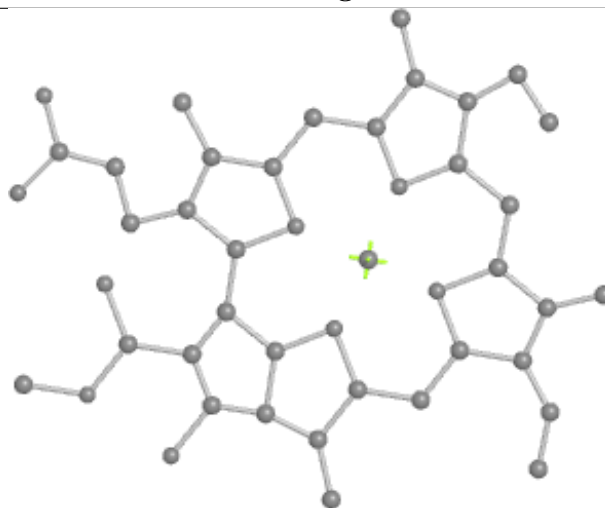
Bond lengths



Bond angles

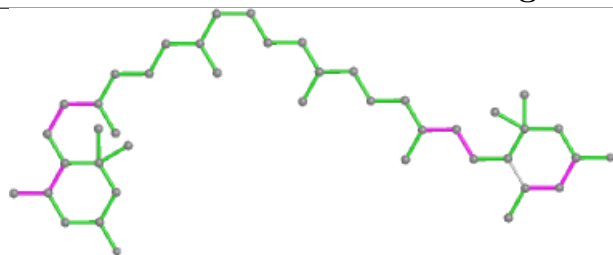


Torsions

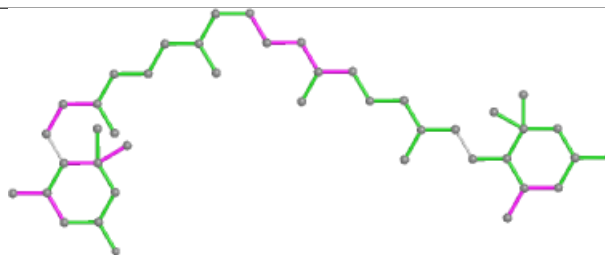


Rings

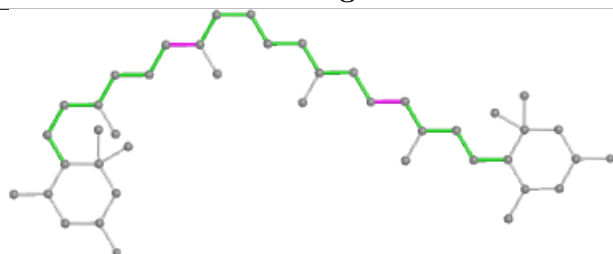
Ligand Q6L P 316



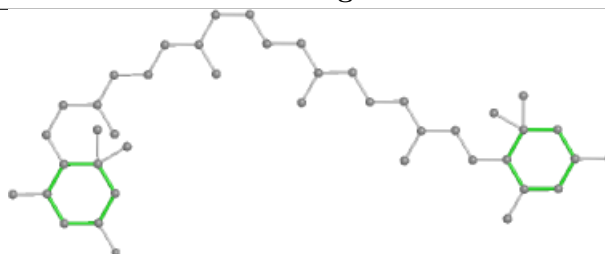
Bond lengths



Bond angles

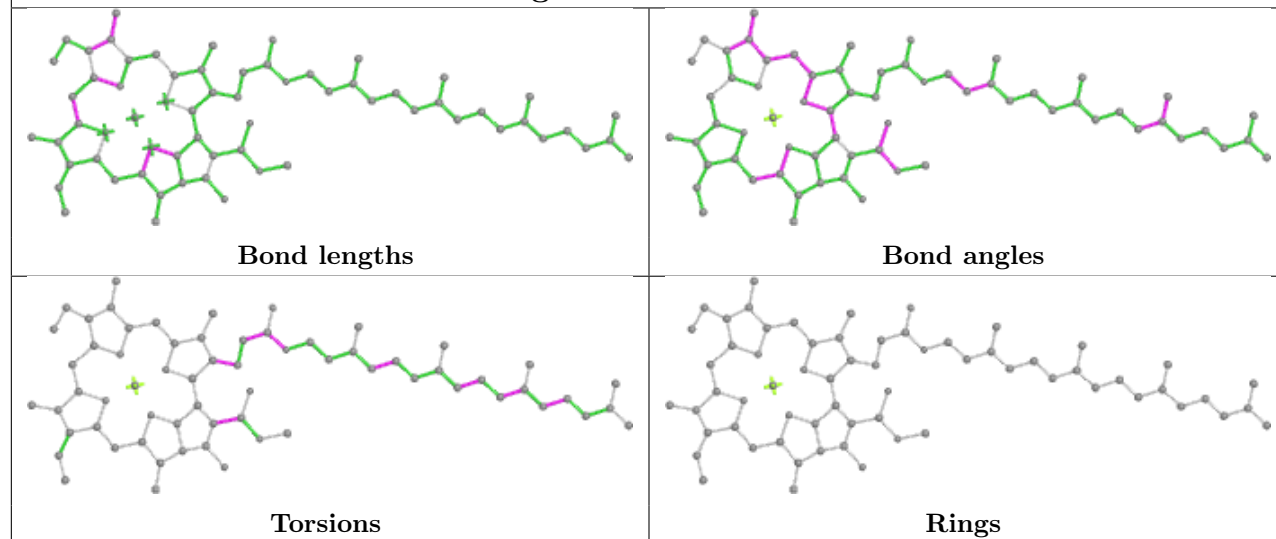


Torsions

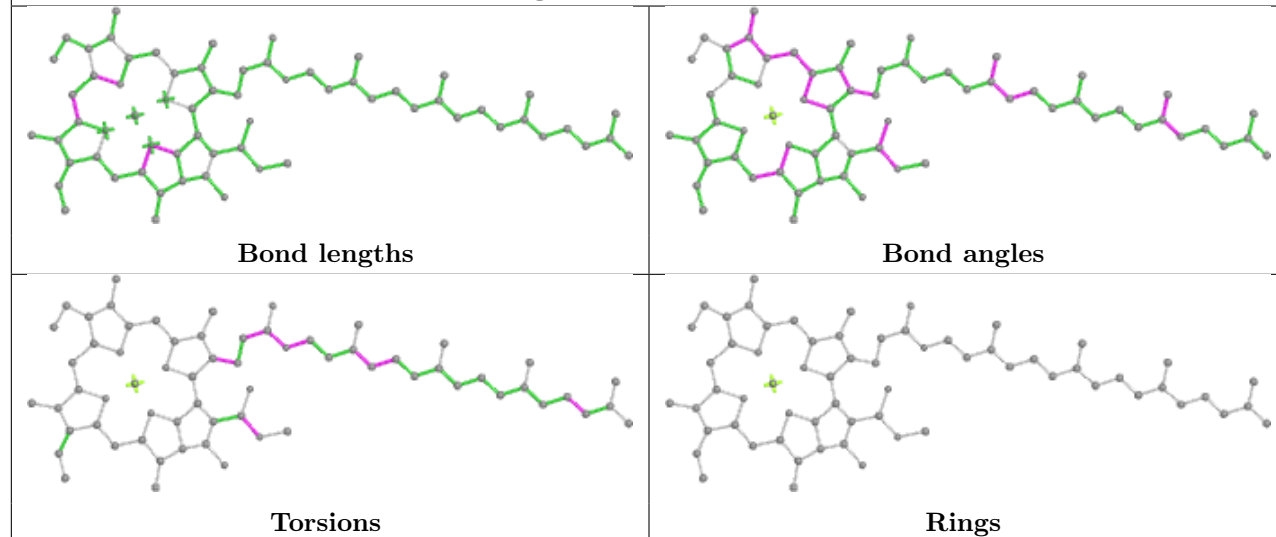


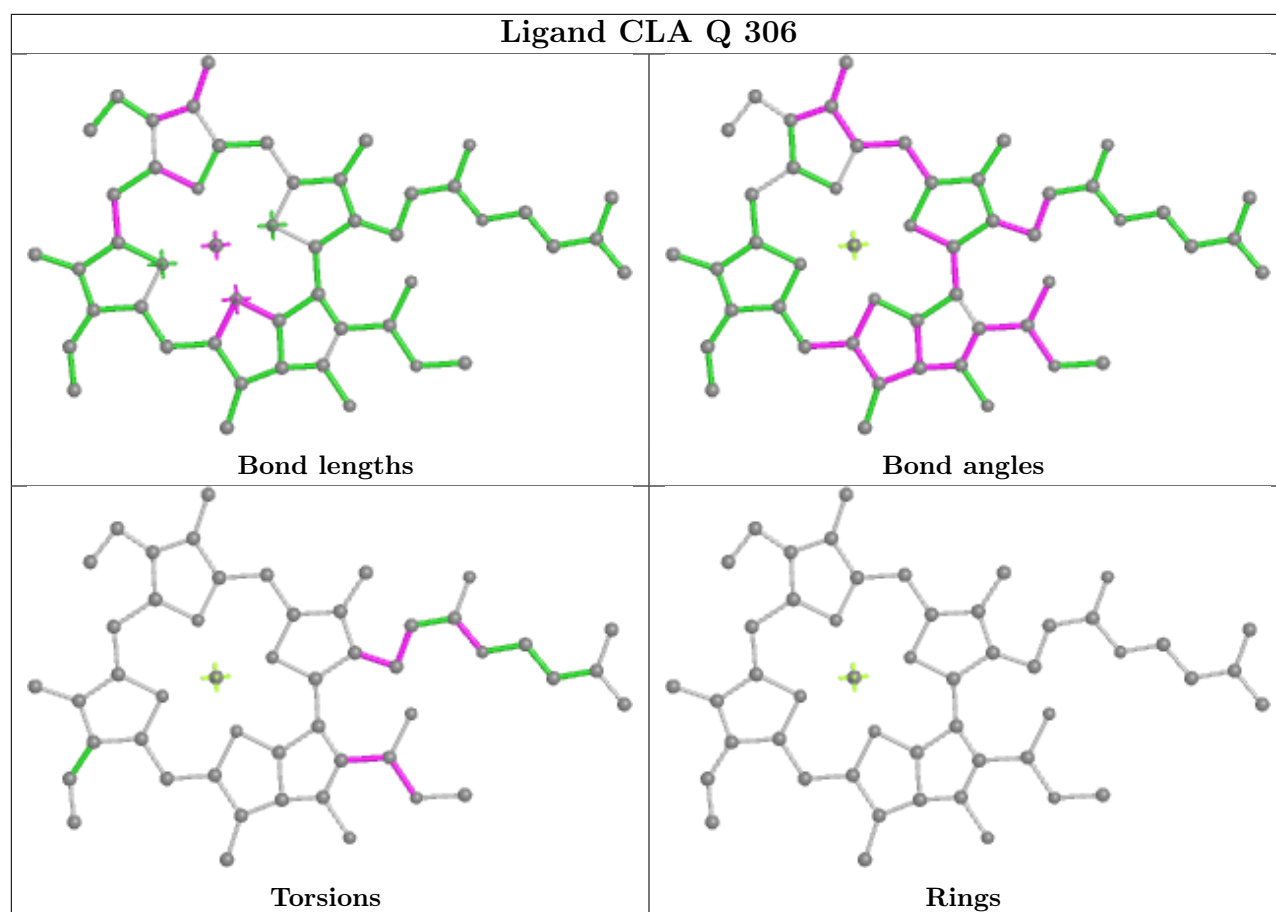
Rings

Ligand CLA A 817

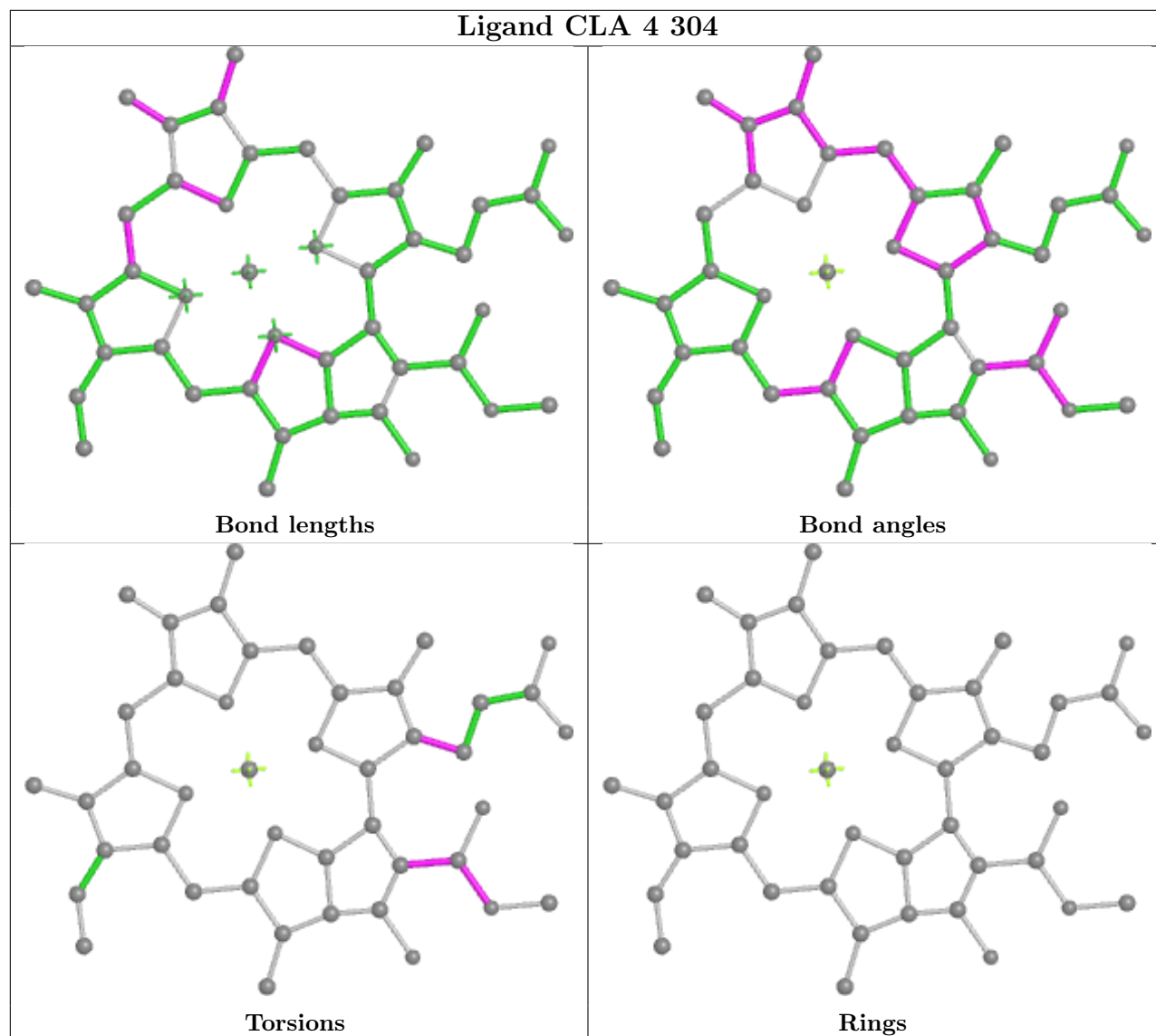


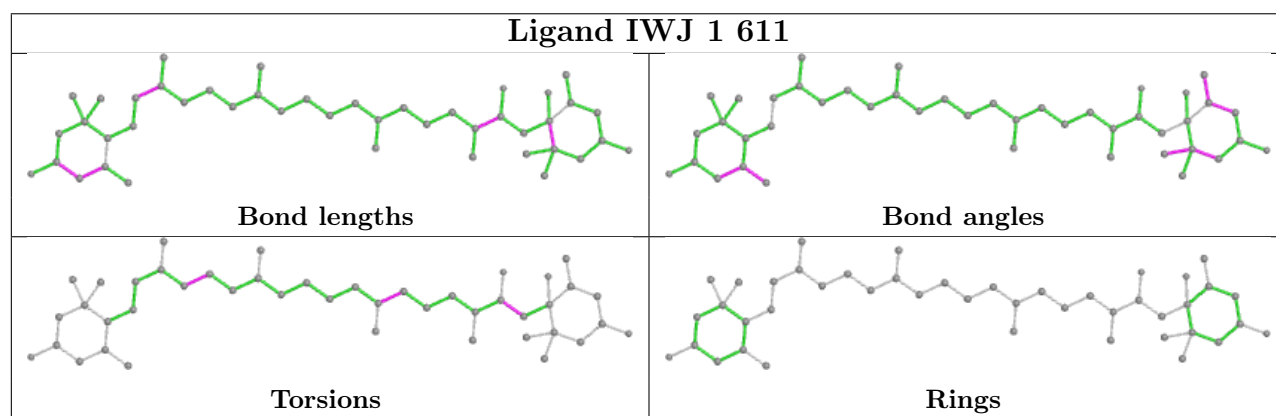
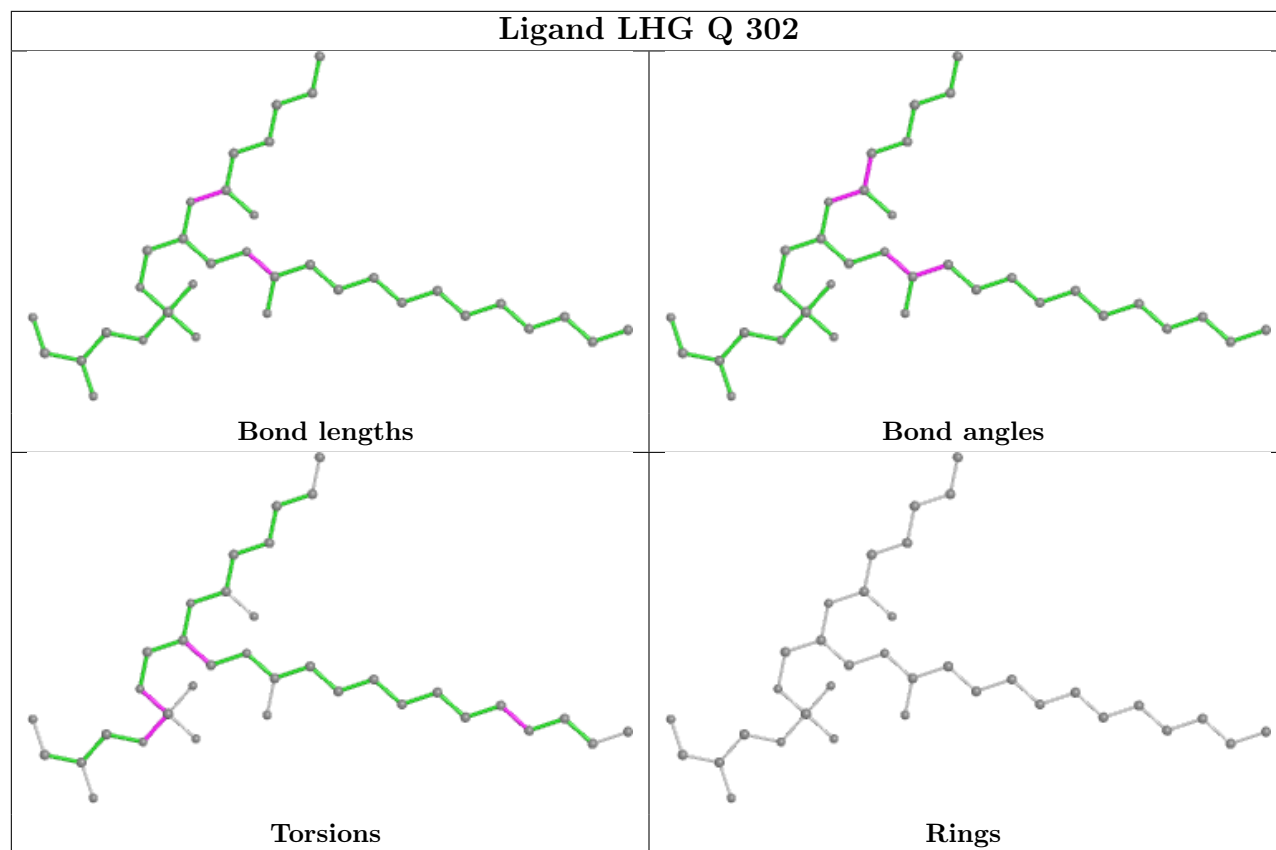
Ligand CLA K 206

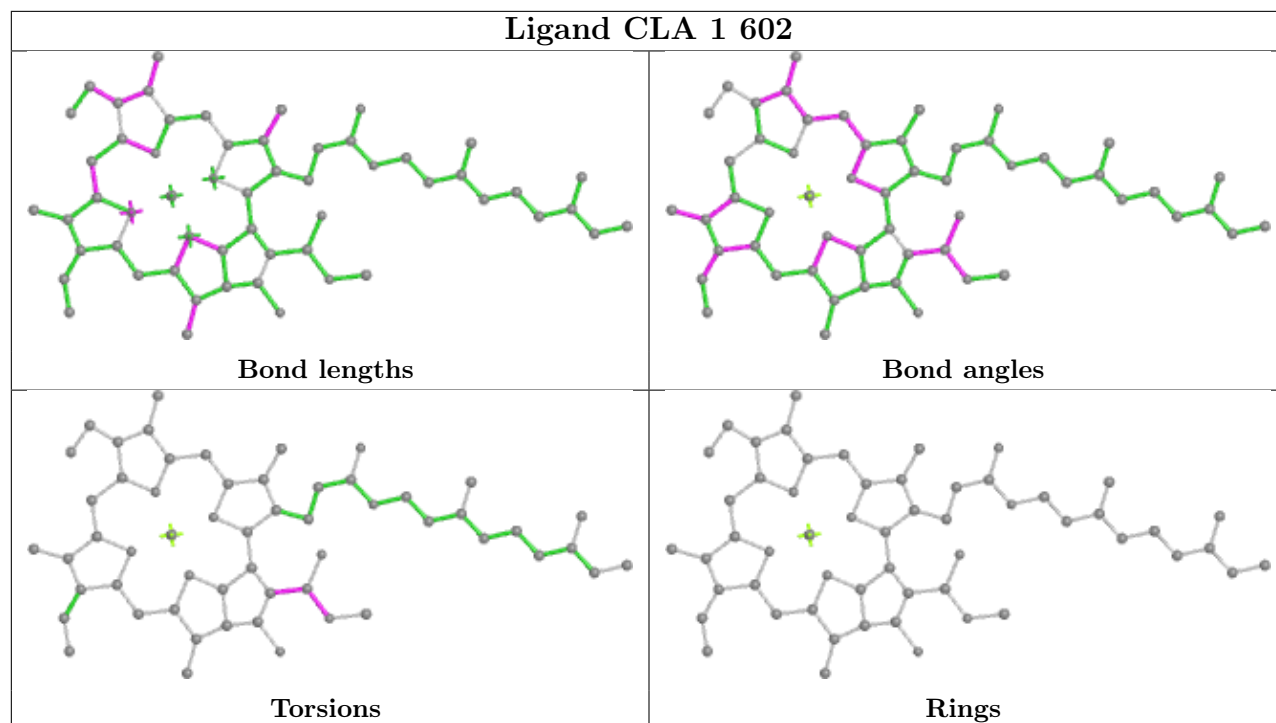
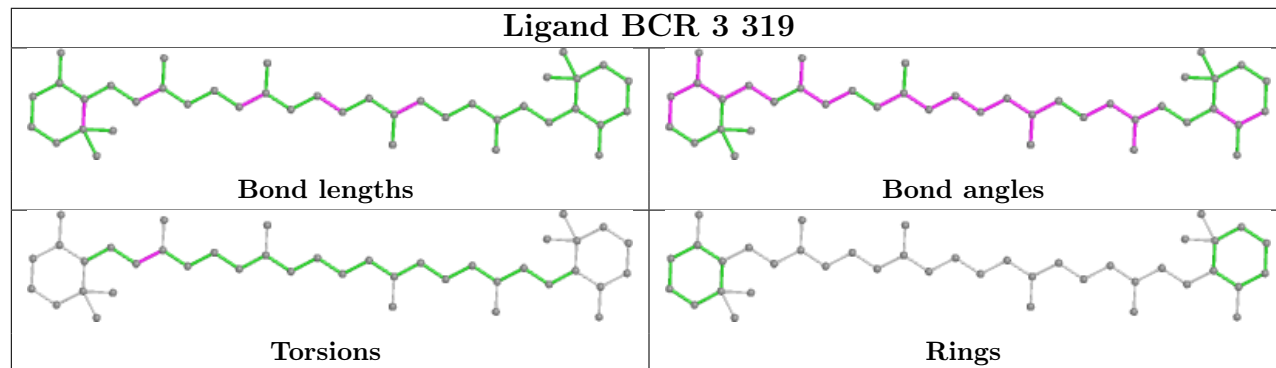


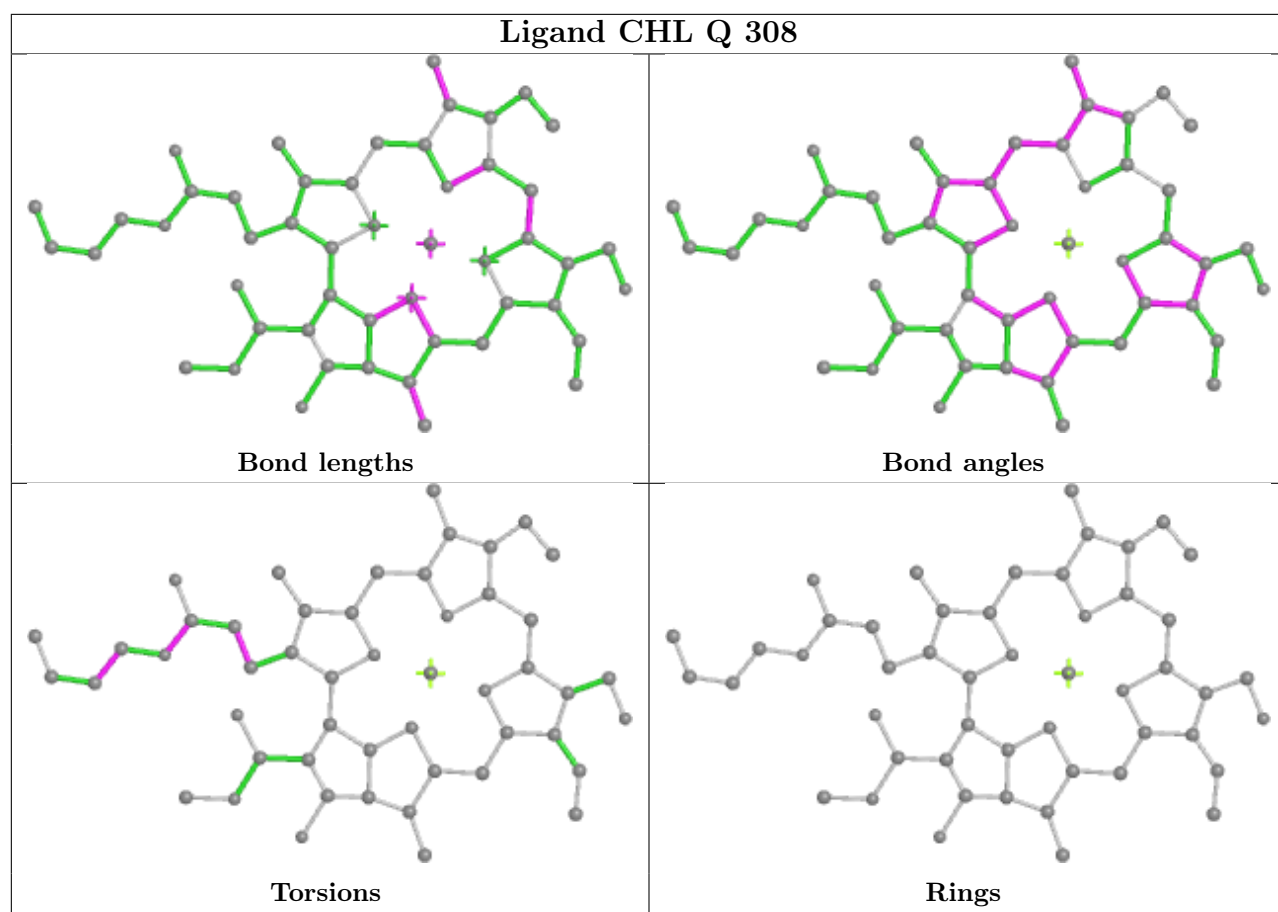


Ligand CLA 4 304

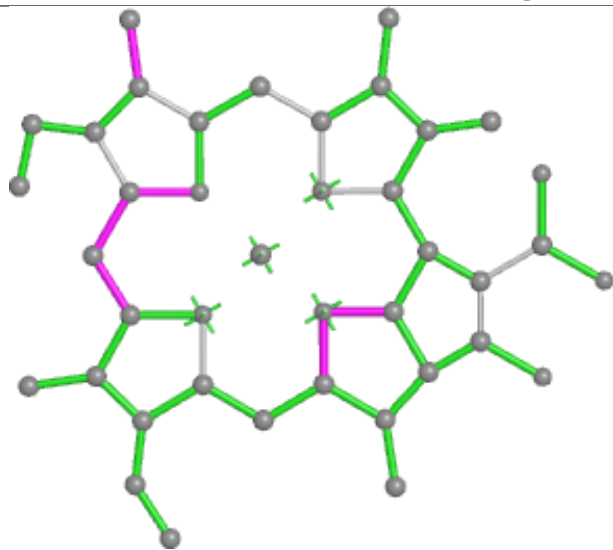




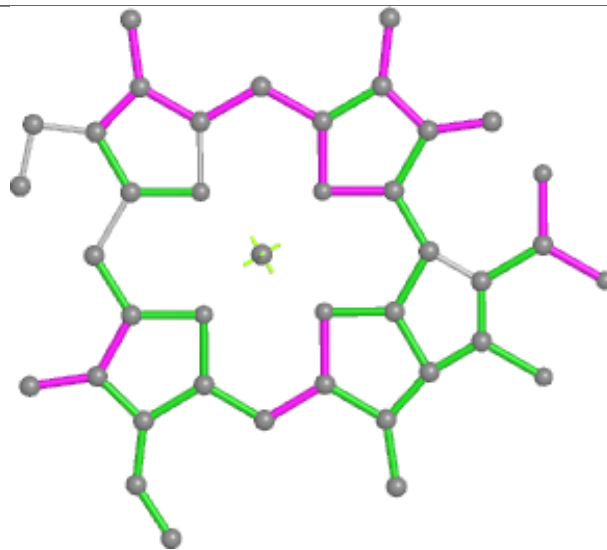
Ligand CLA 1 602**Ligand BCR 3 319**



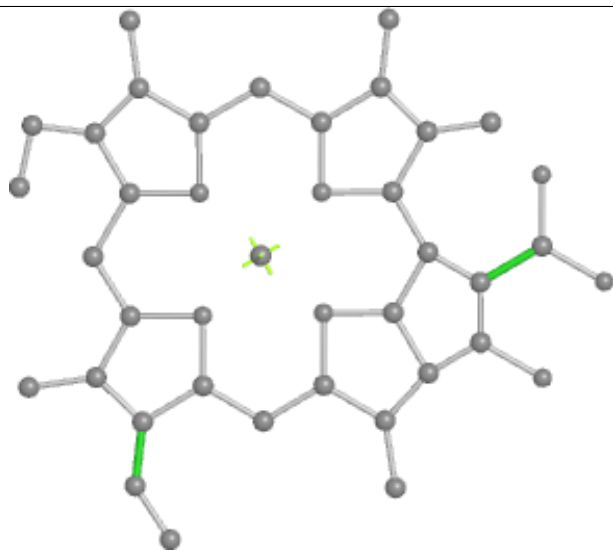
Ligand CLA 3 312



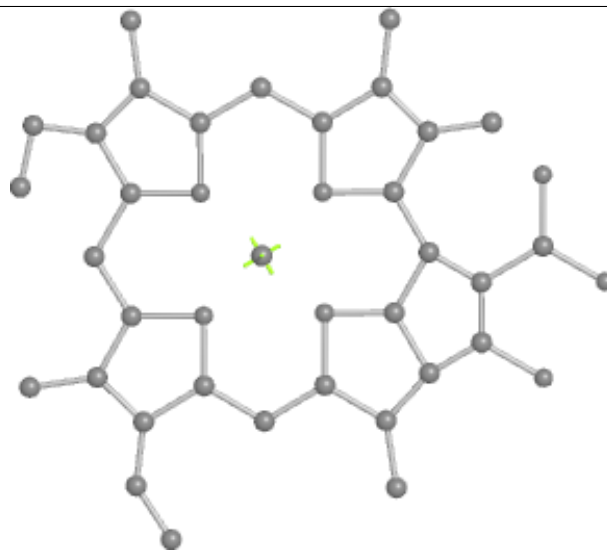
Bond lengths



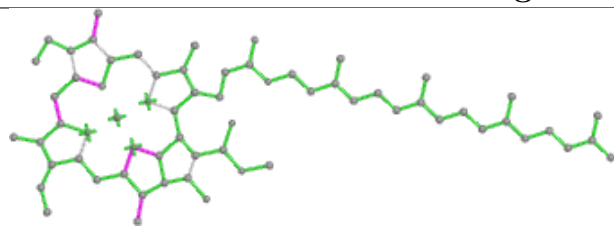
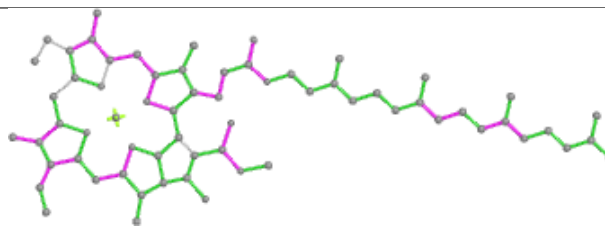
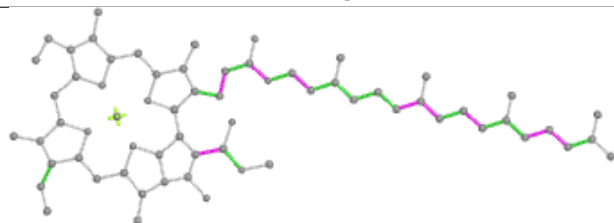
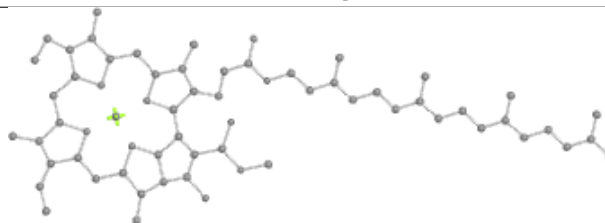
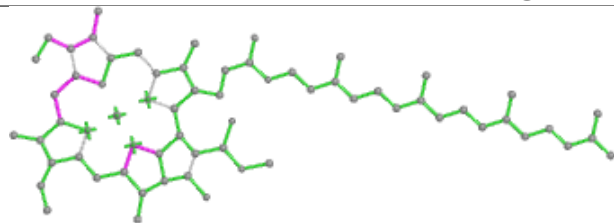
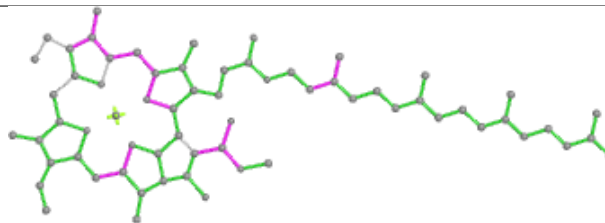
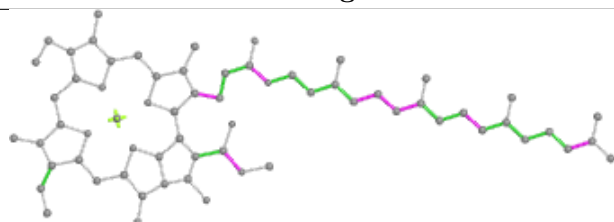
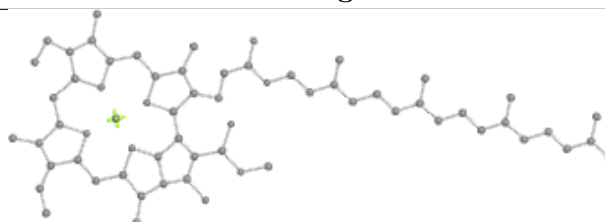
Bond angles



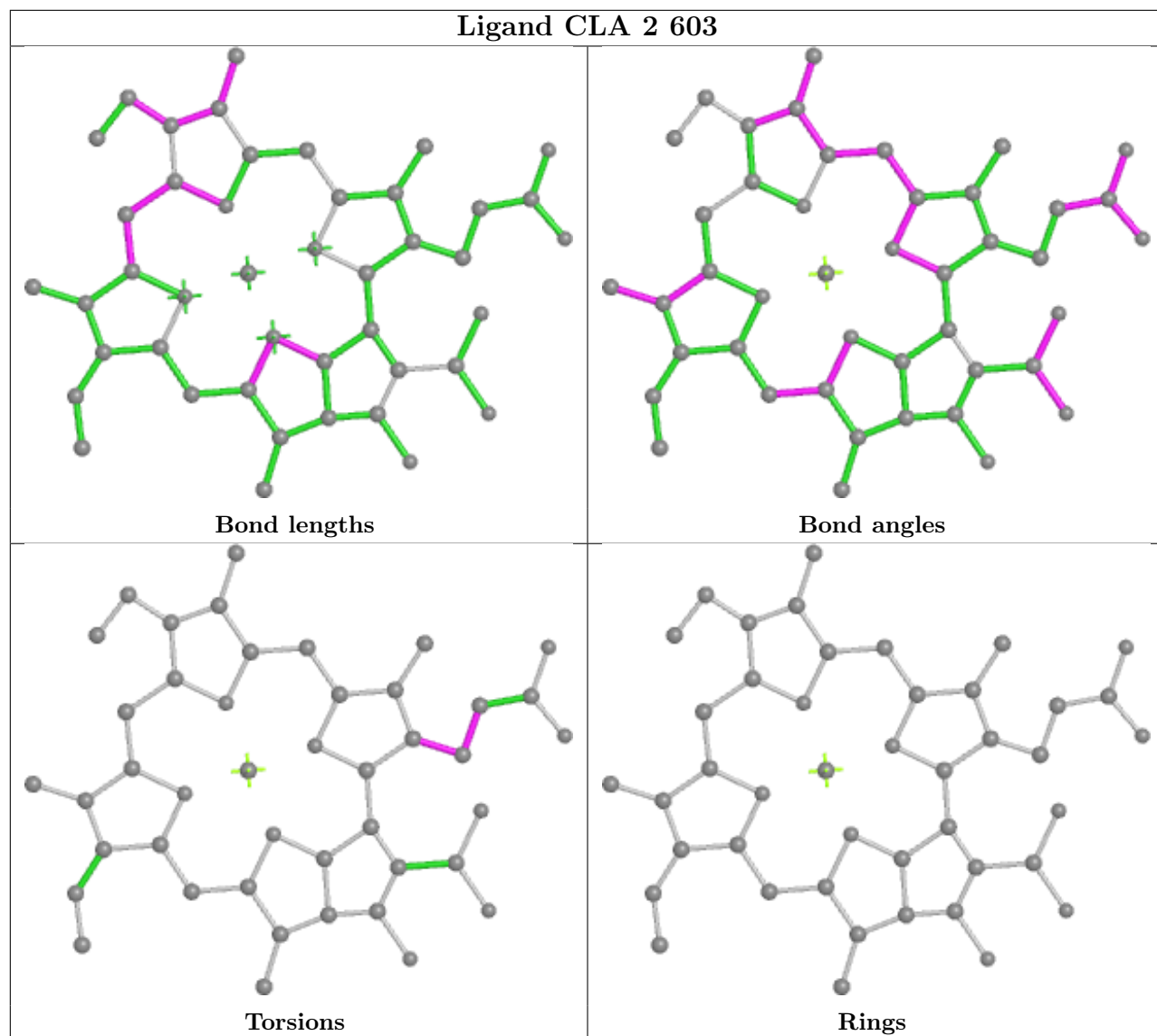
Torsions



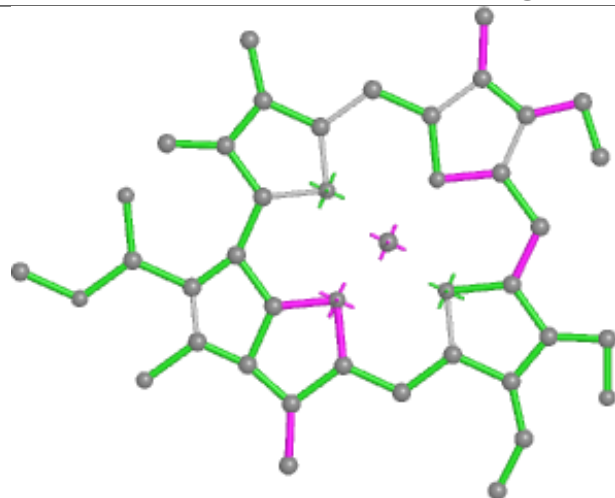
Rings

Ligand CLA B 802**Bond lengths****Bond angles****Torsions****Rings****Ligand CLA 5 607****Bond lengths****Bond angles****Torsions****Rings**

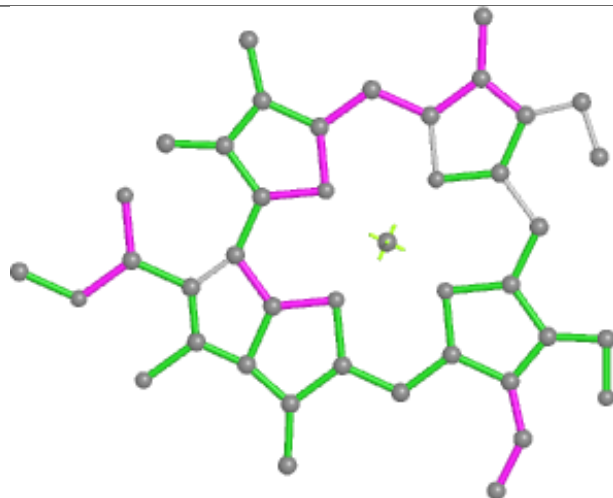
Ligand CLA 2 603



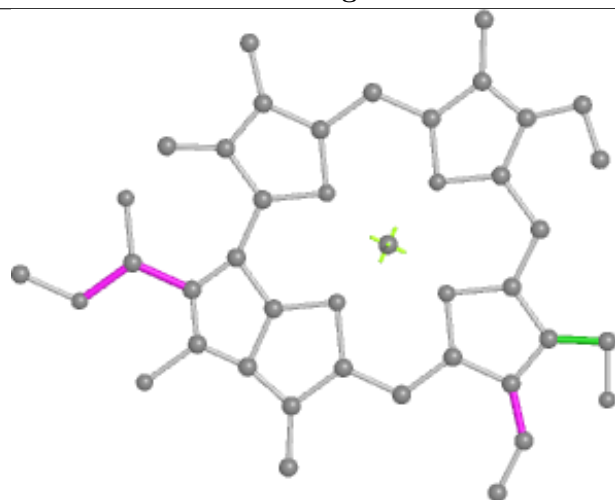
Ligand CHL S 305



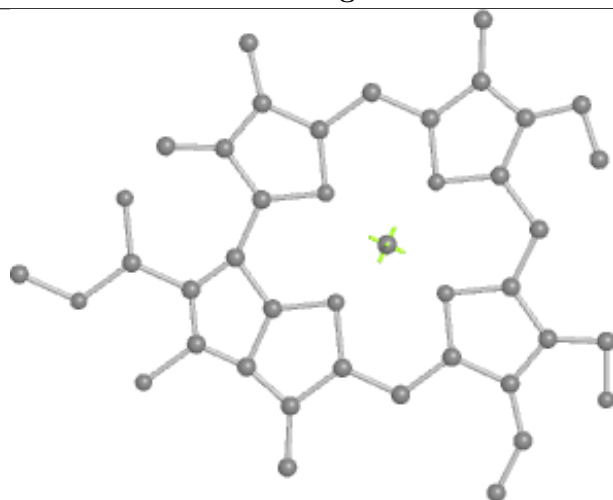
Bond lengths



Bond angles

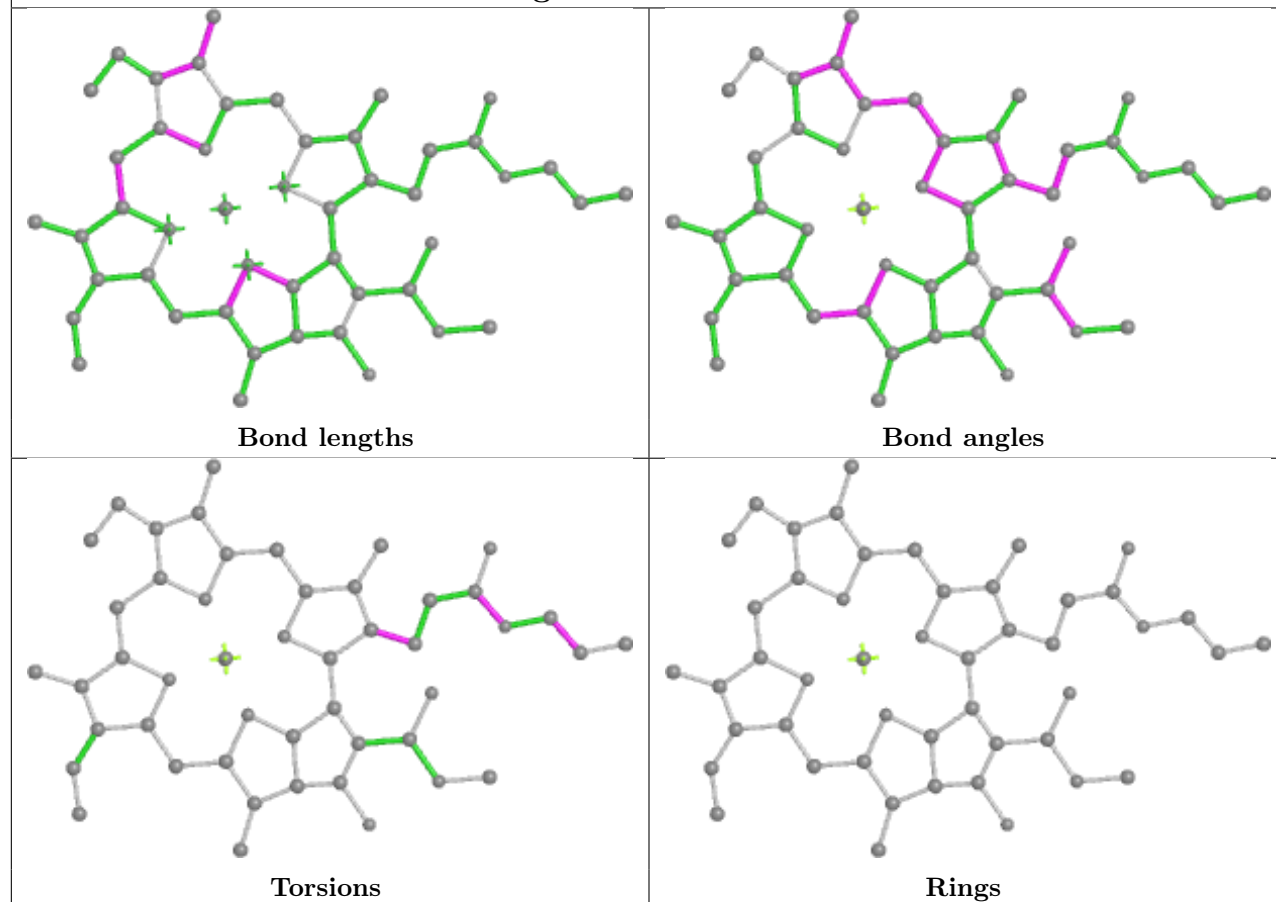


Torsions

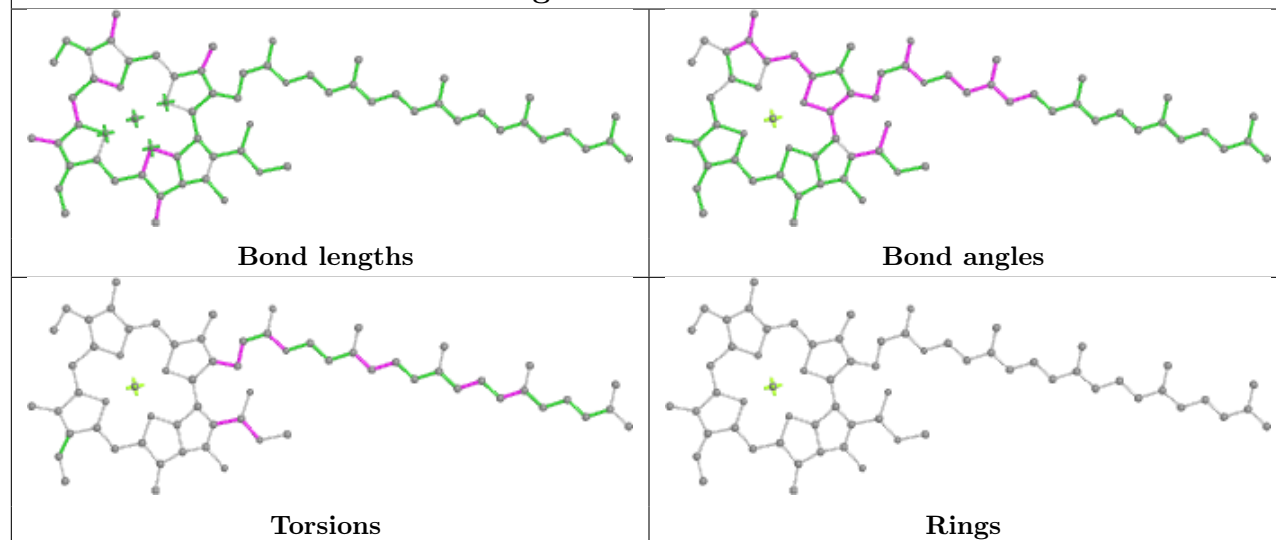


Rings

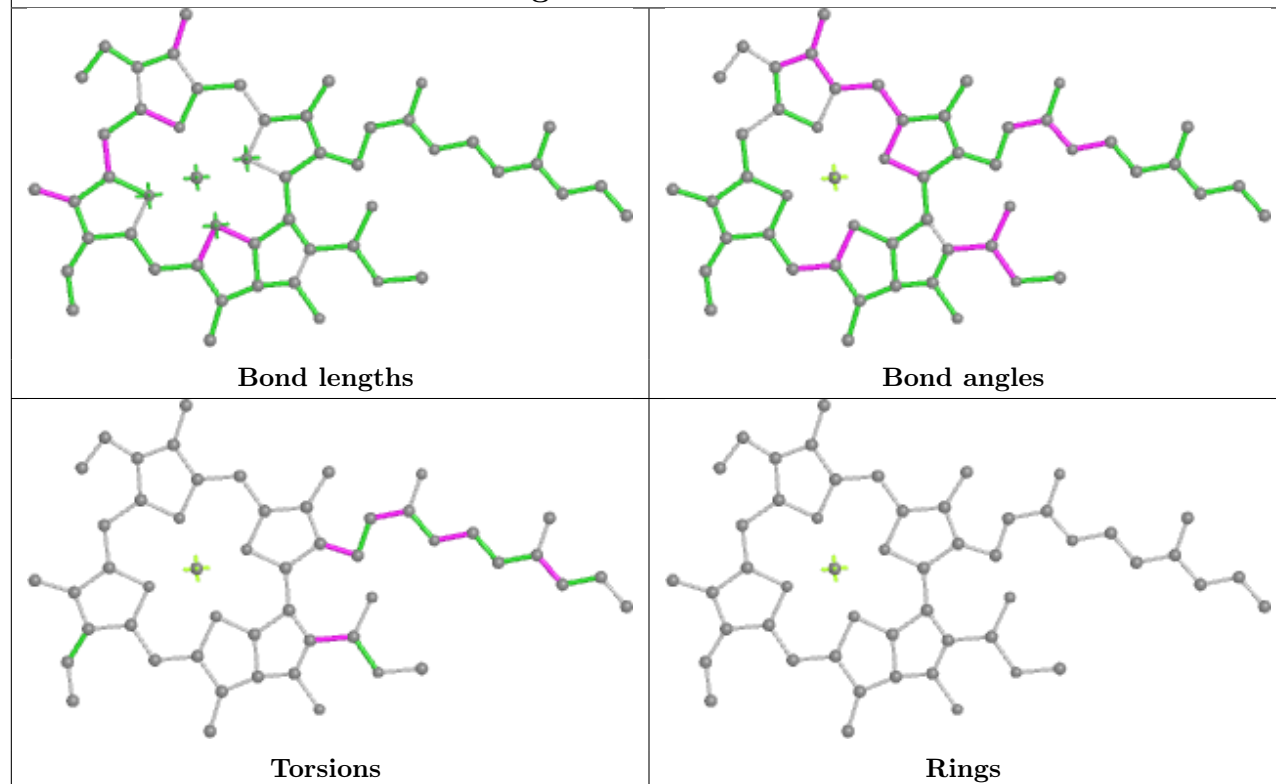
Ligand CLA P 313



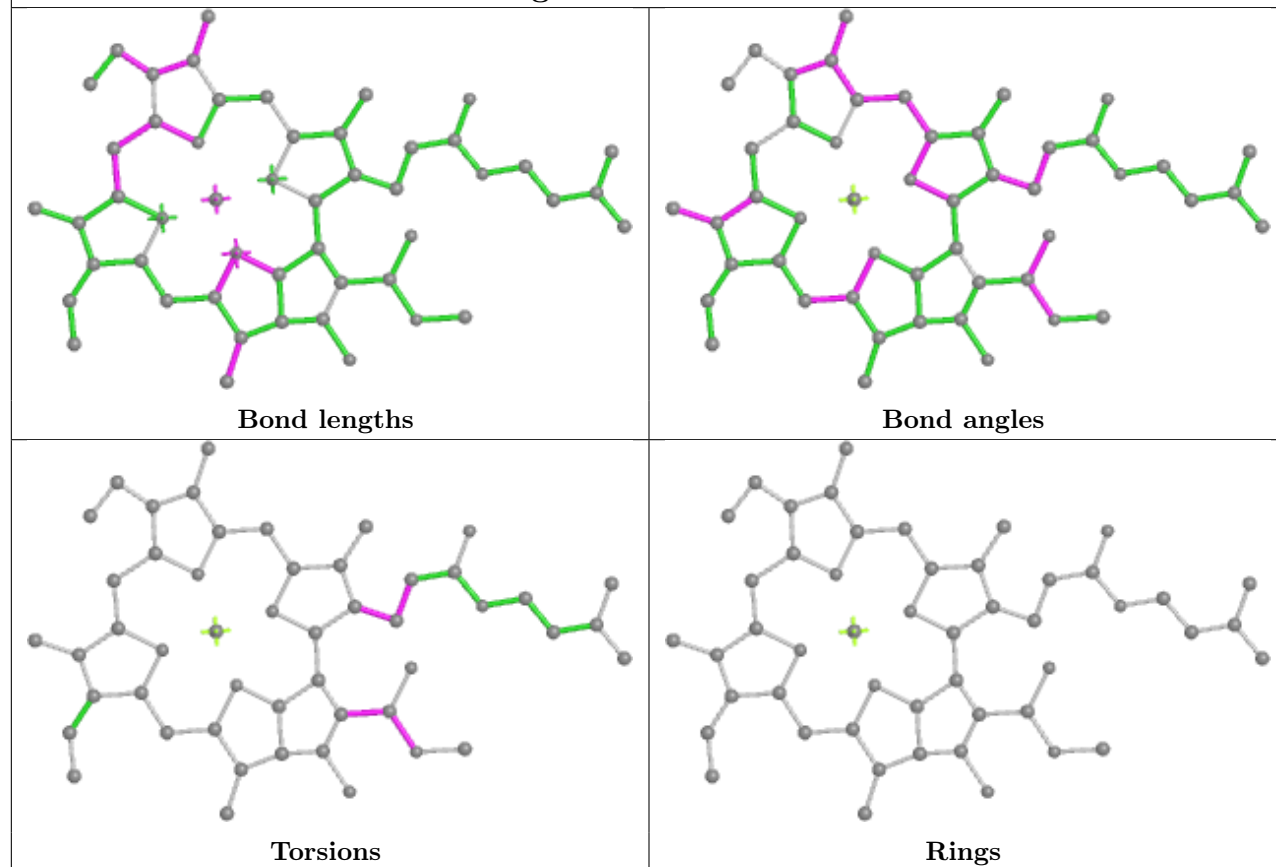
Ligand CLA T 301

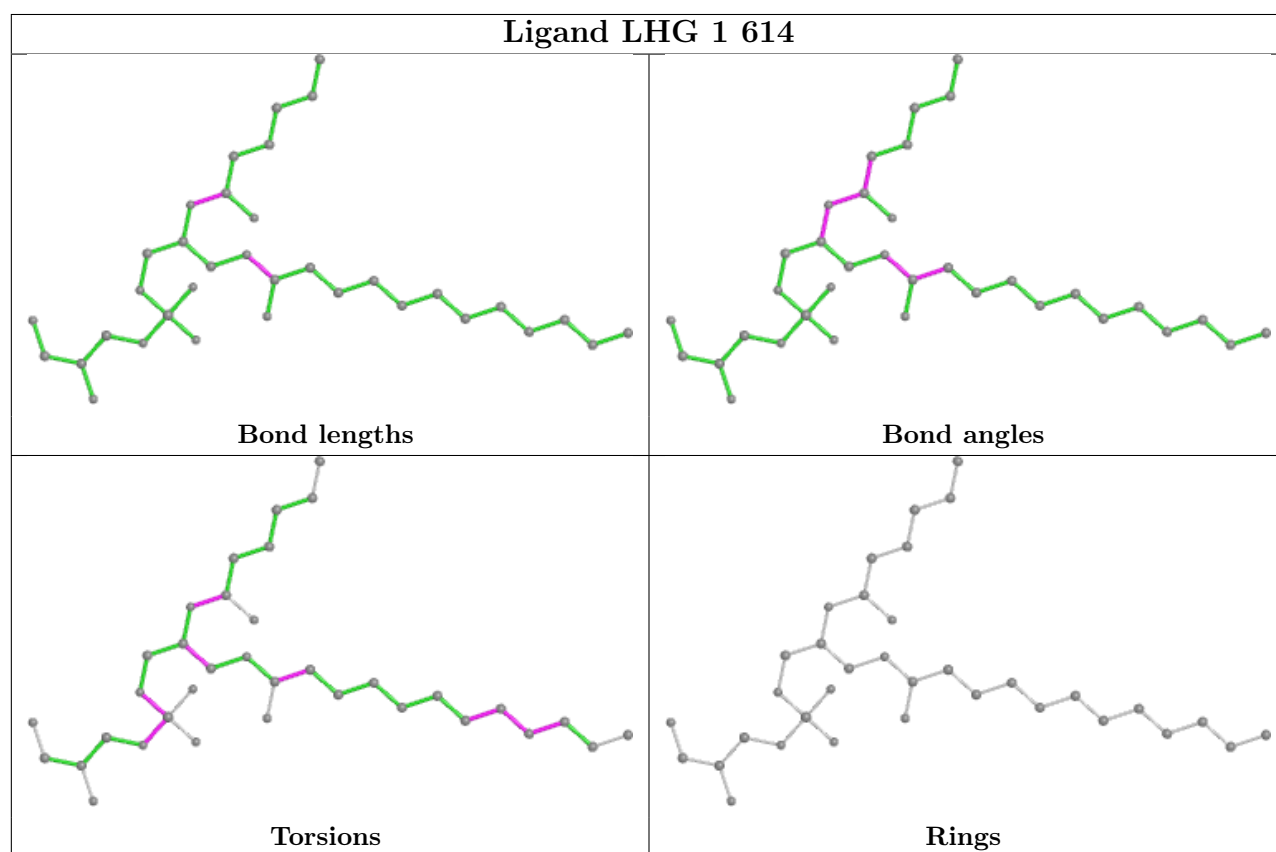
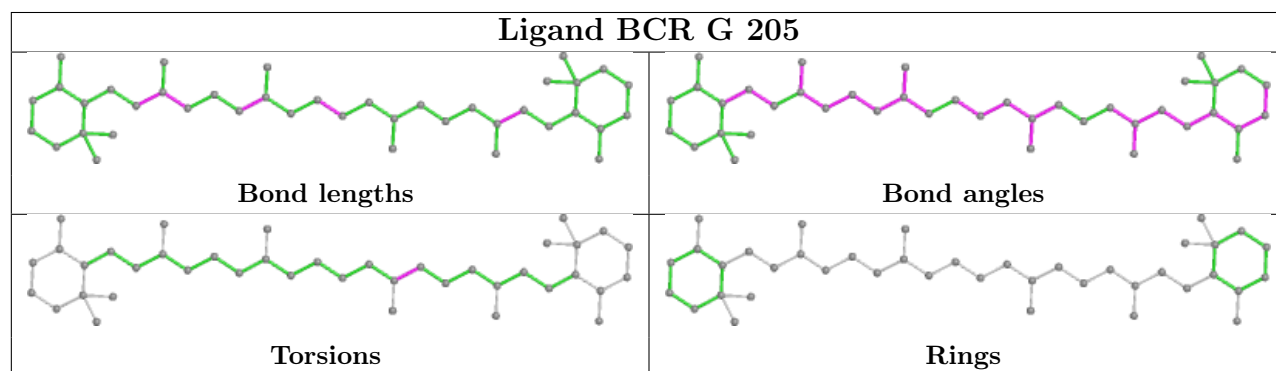
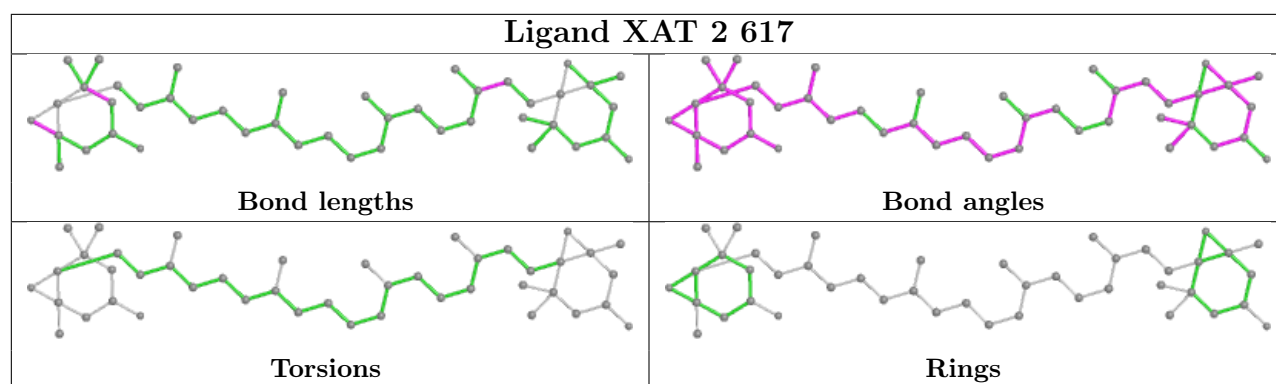


Ligand CLA A 806

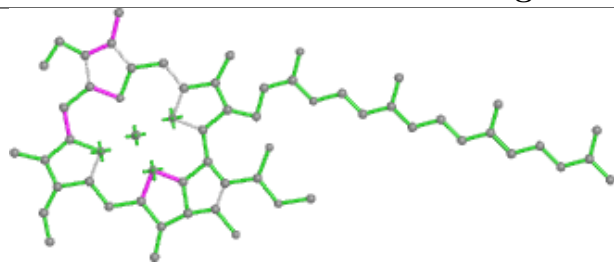


Ligand CLA A 833

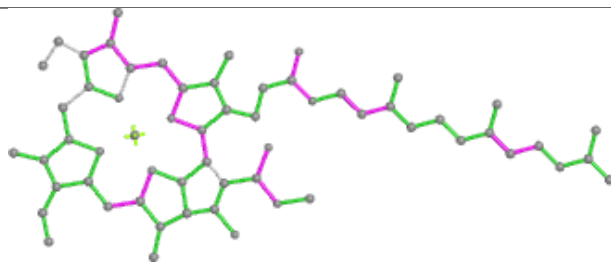




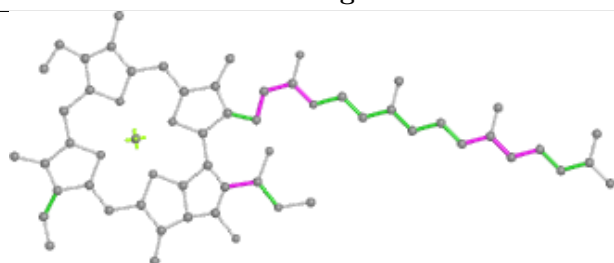
Ligand CLA P 310



Bond lengths



Bond angles

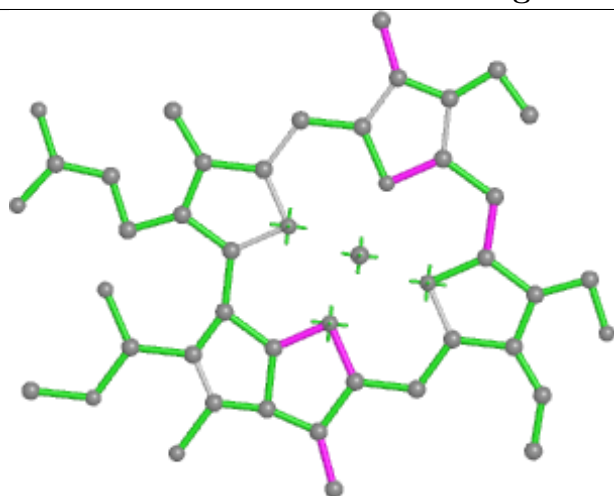


Torsions

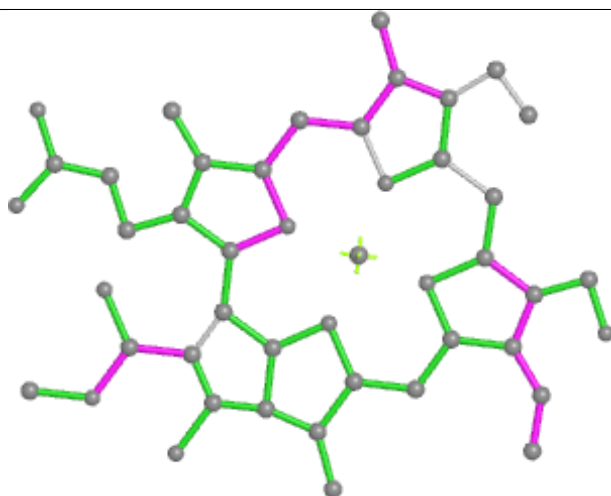


Rings

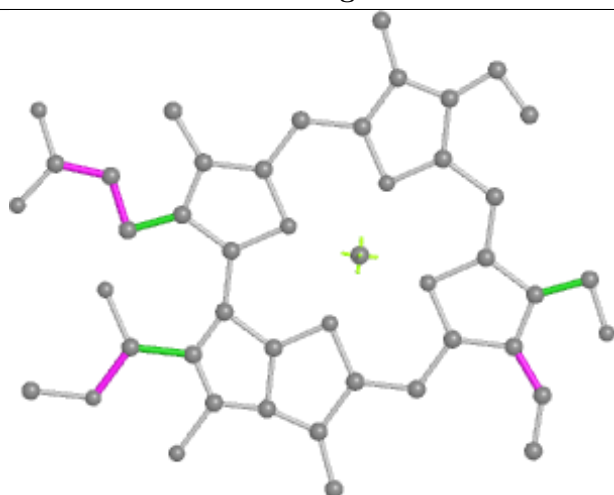
Ligand CHL U 305



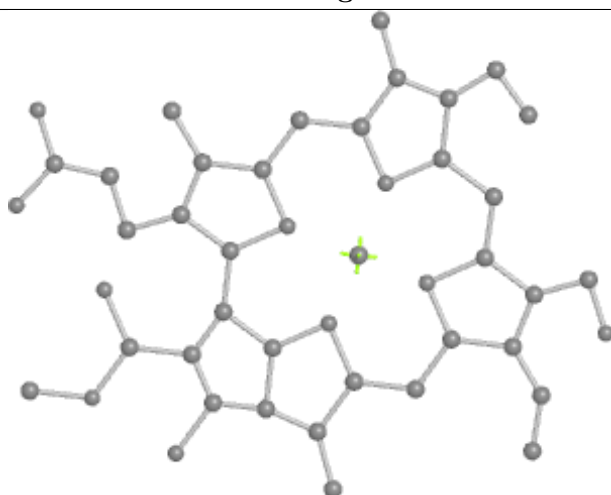
Bond lengths



Bond angles

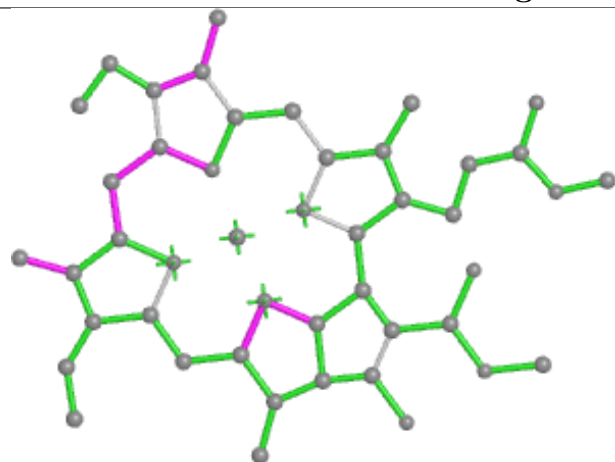


Torsions

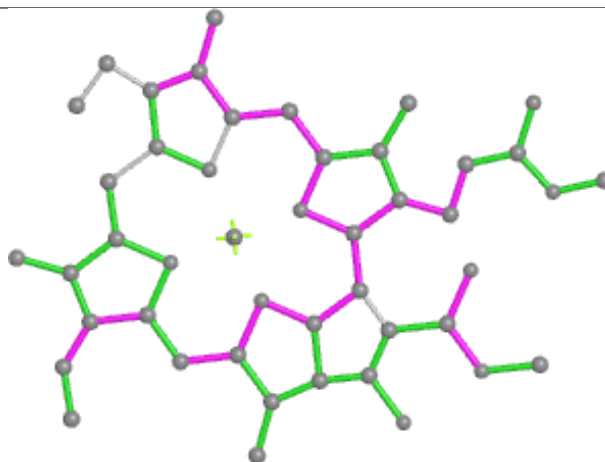


Rings

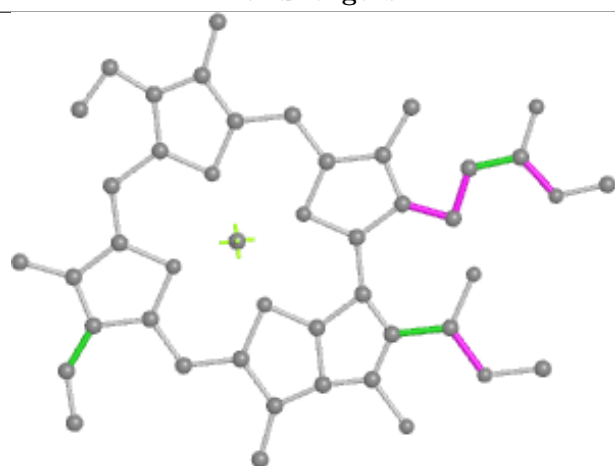
Ligand CLA K 204



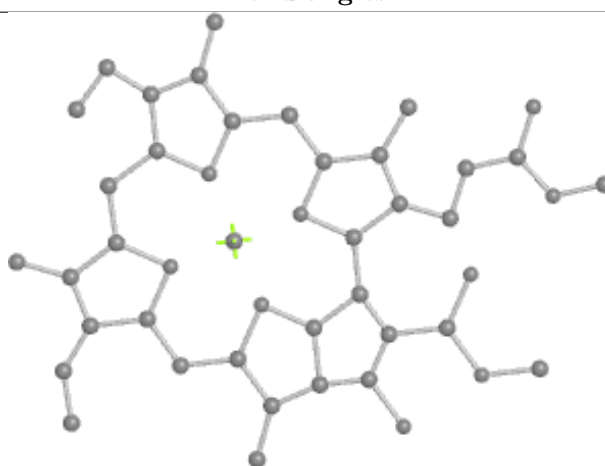
Bond lengths



Bond angles

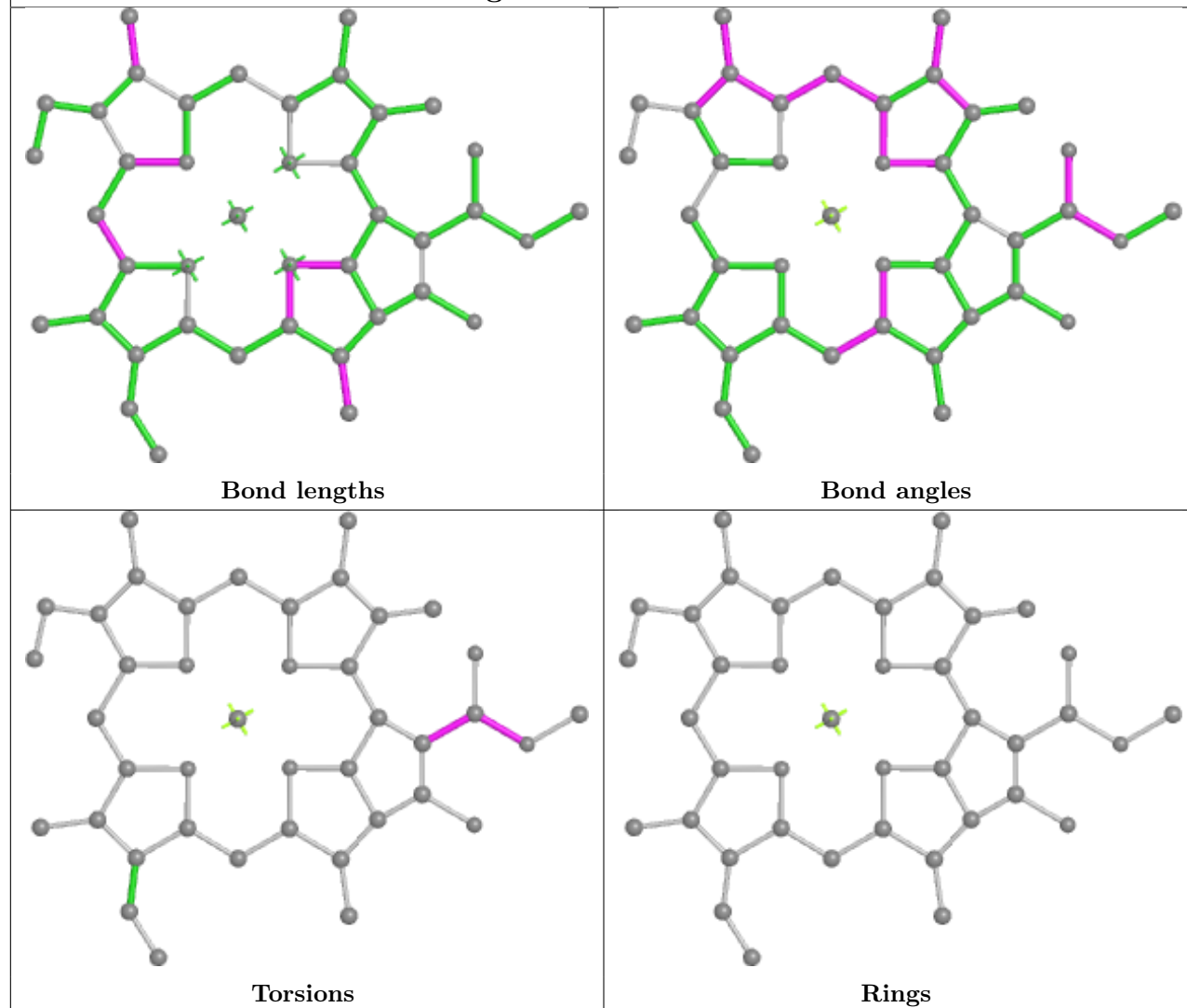


Torsions

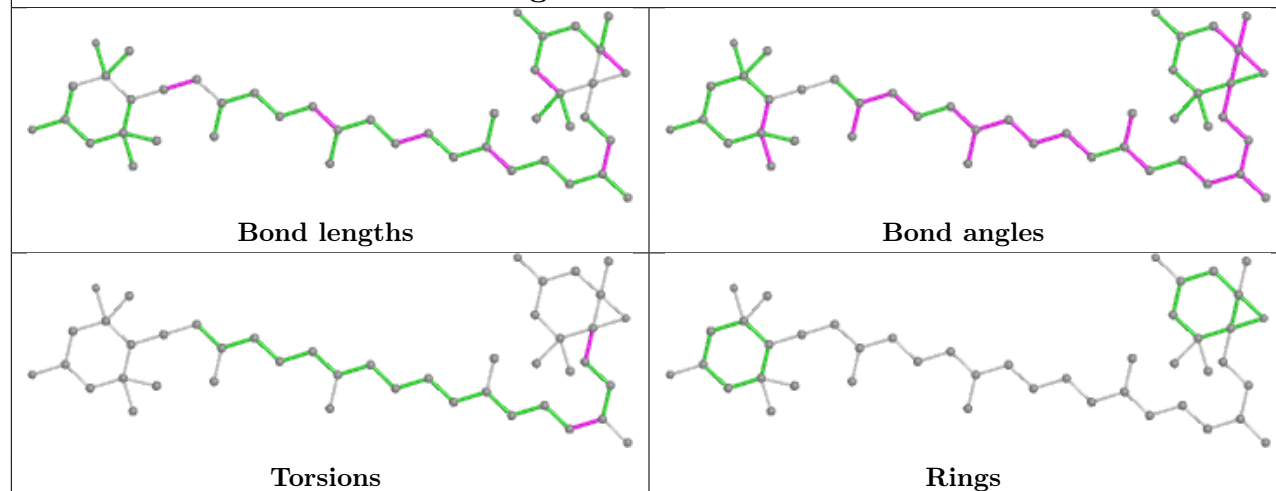


Rings

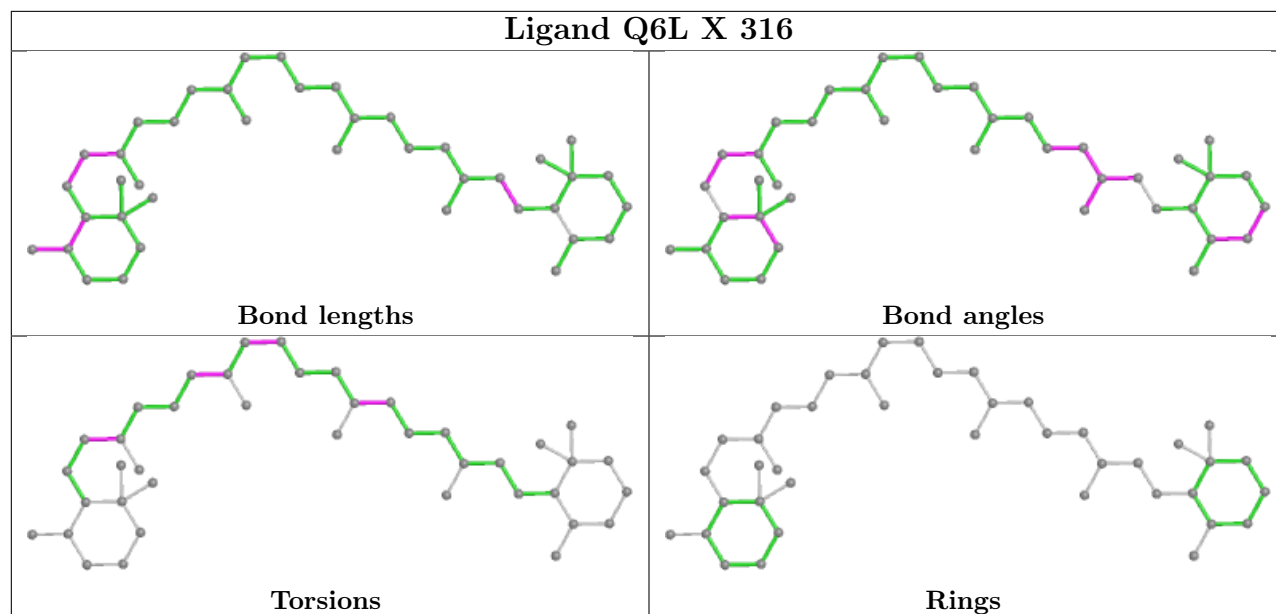
Ligand CLA O 2005



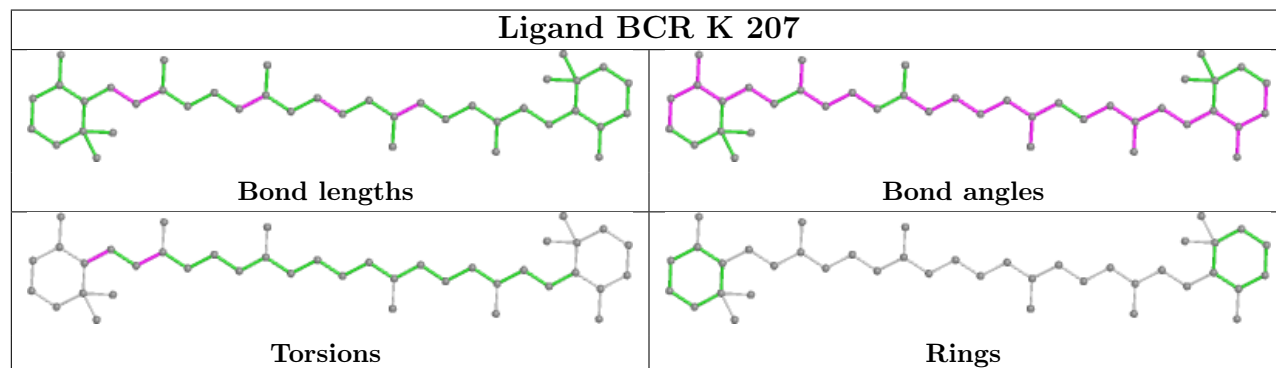
Ligand NEX R 321



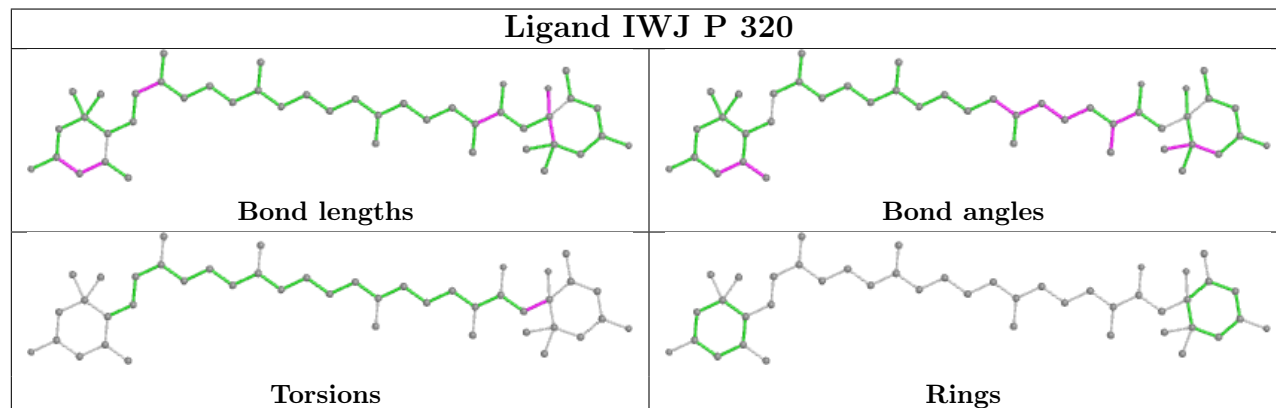
Ligand Q6L X 316



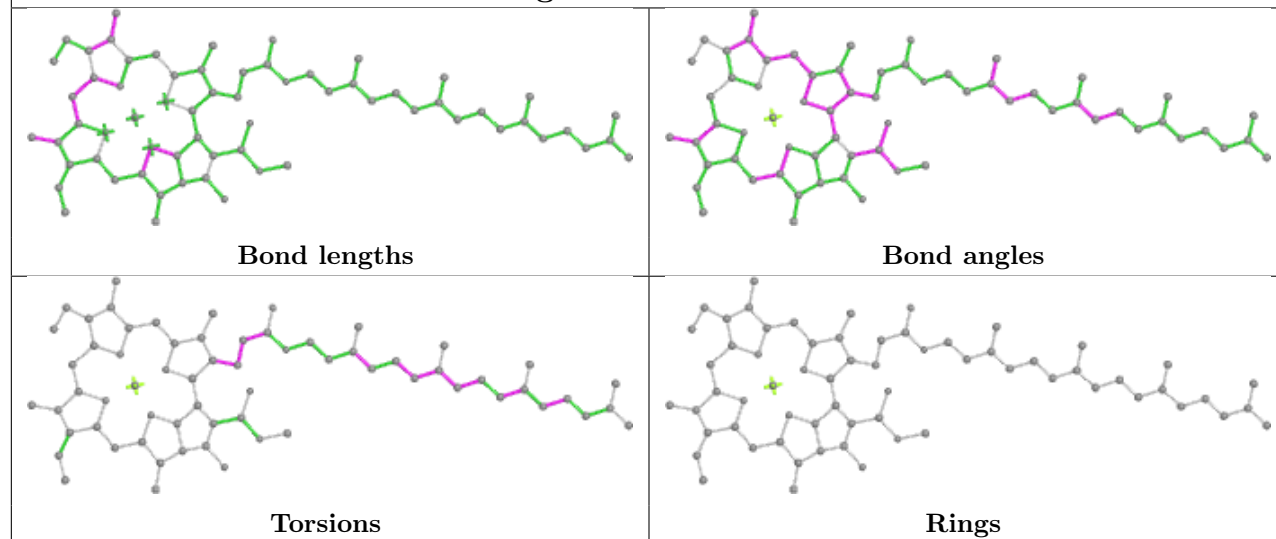
Ligand BCR K 207



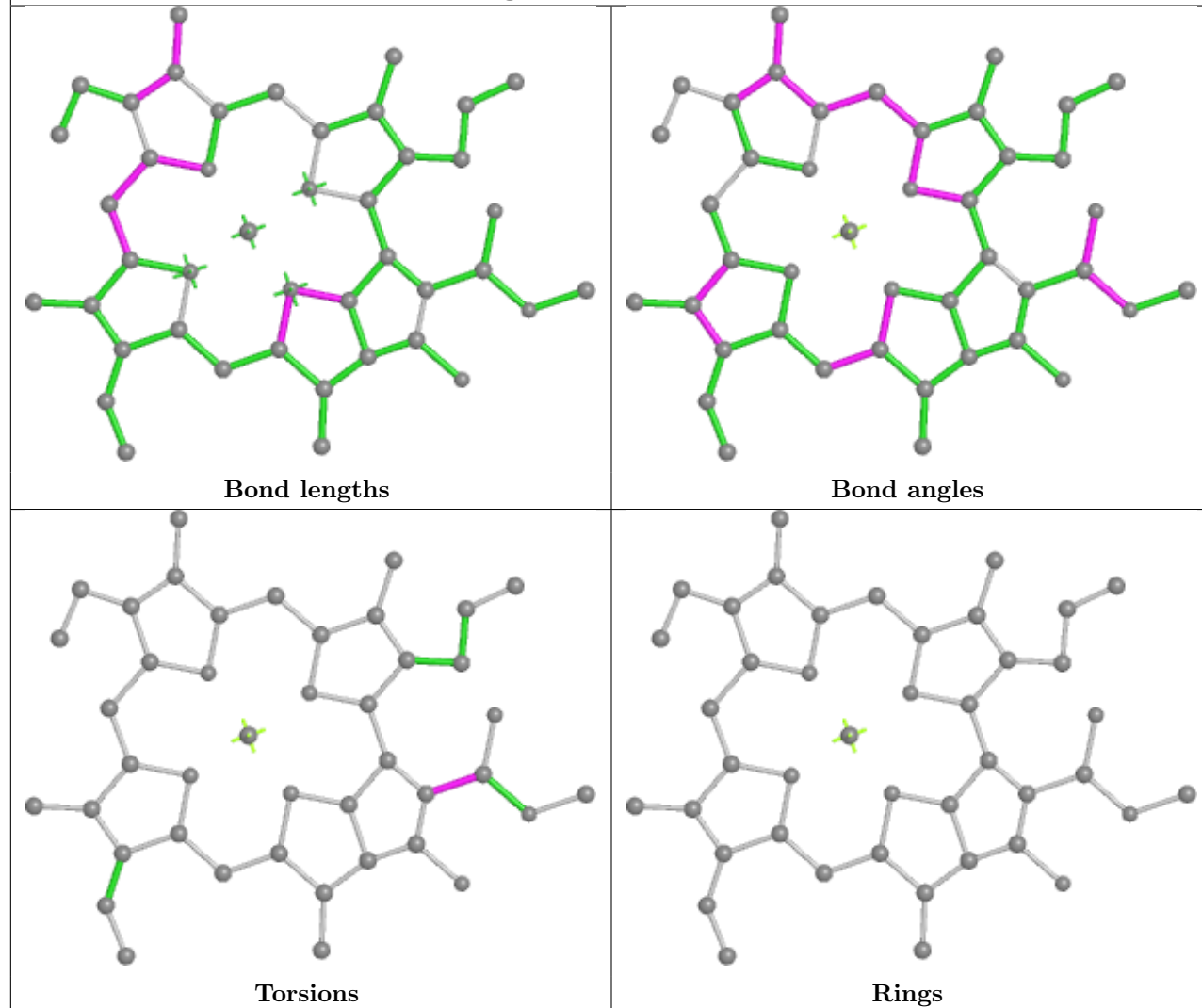
Ligand IWJ P 320

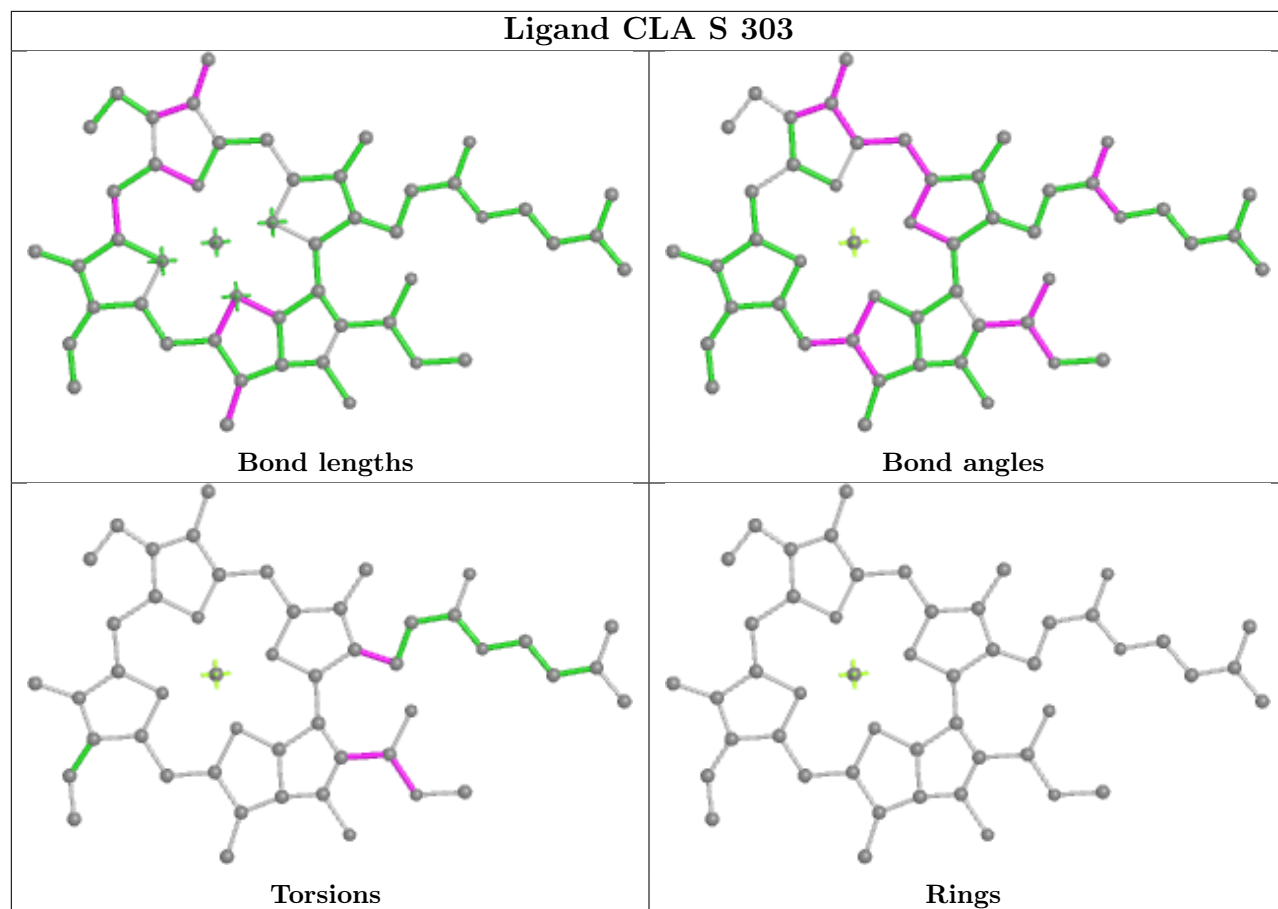


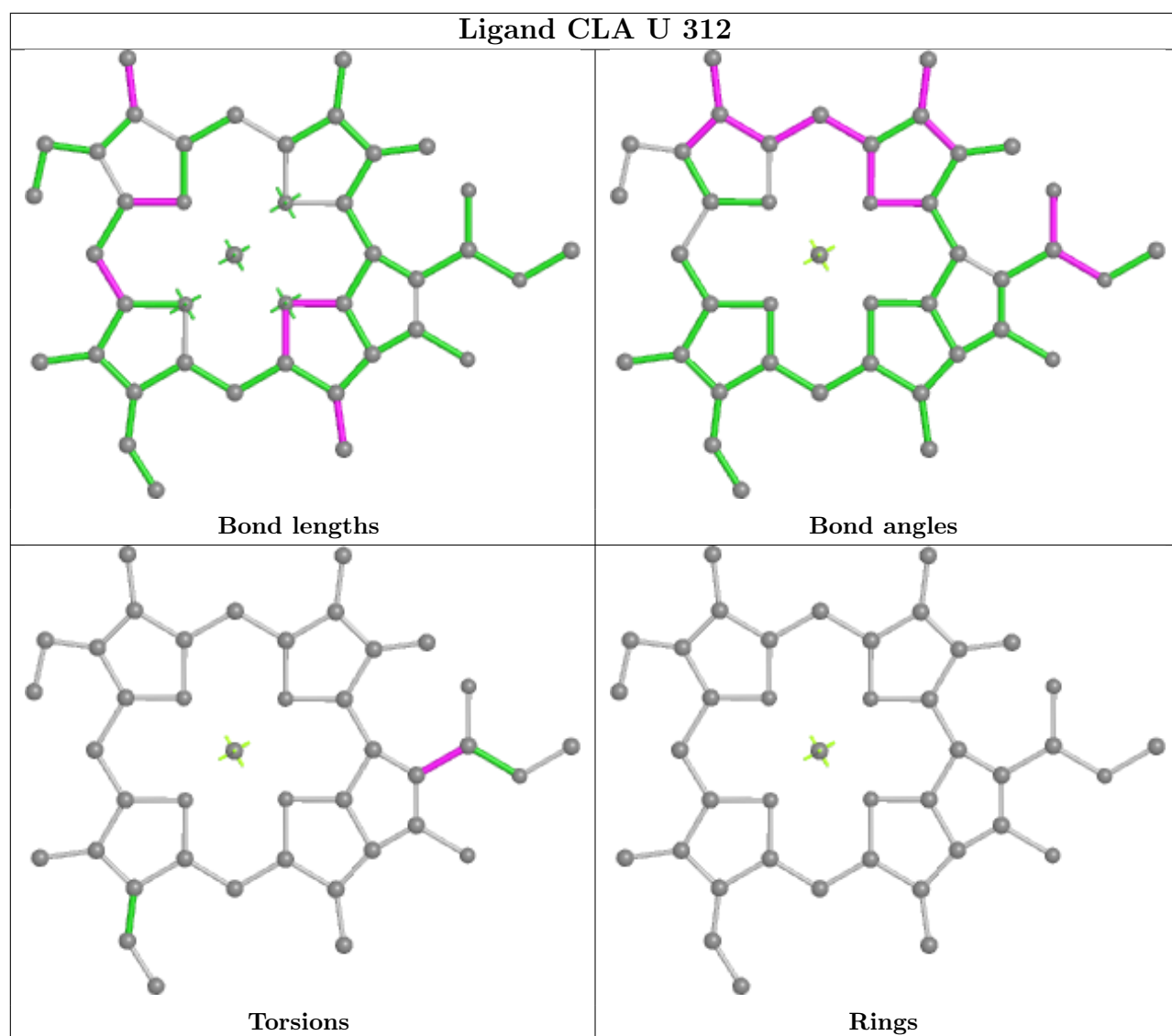
Ligand CLA 2 612



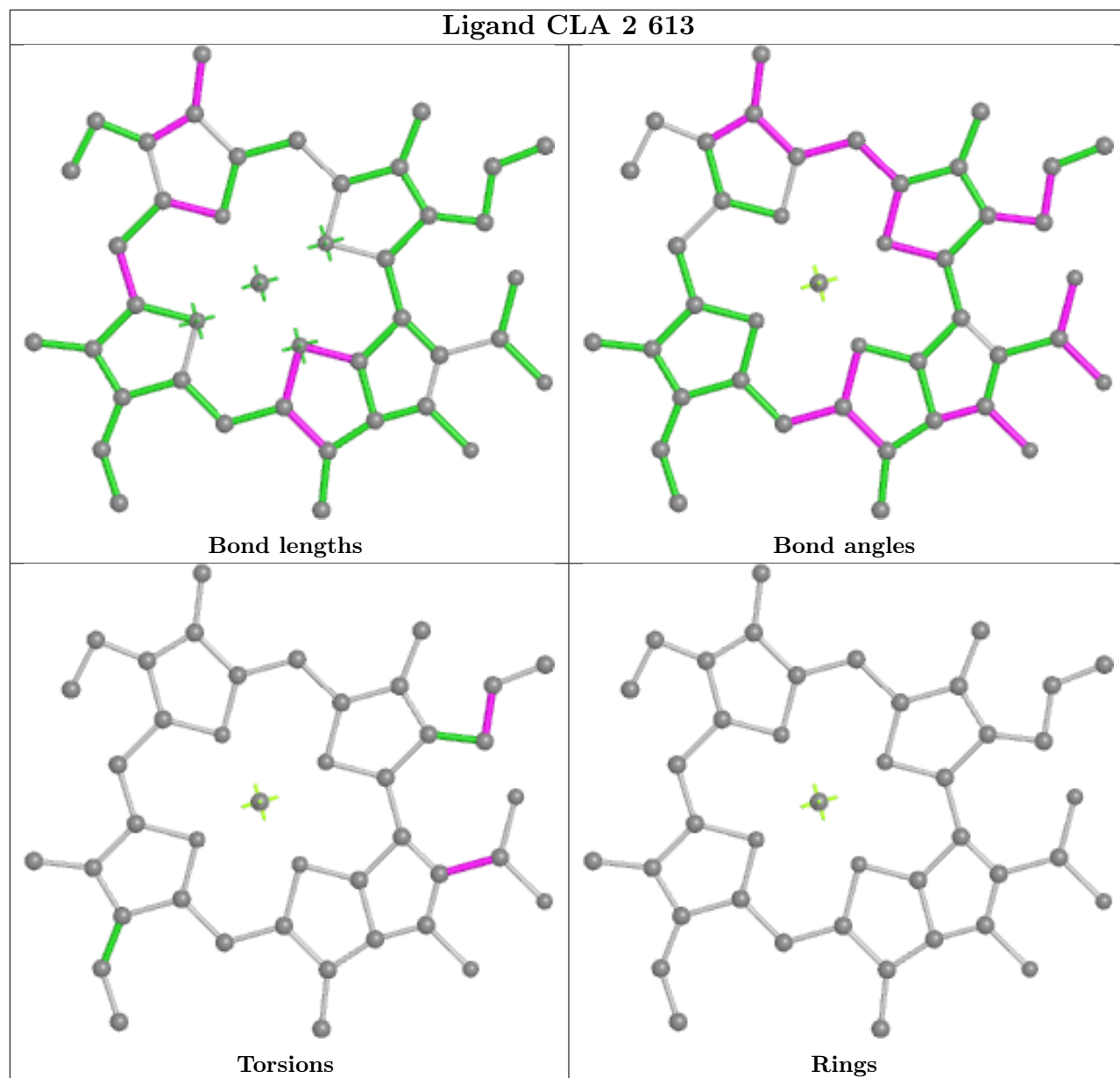
Ligand CLA B 833



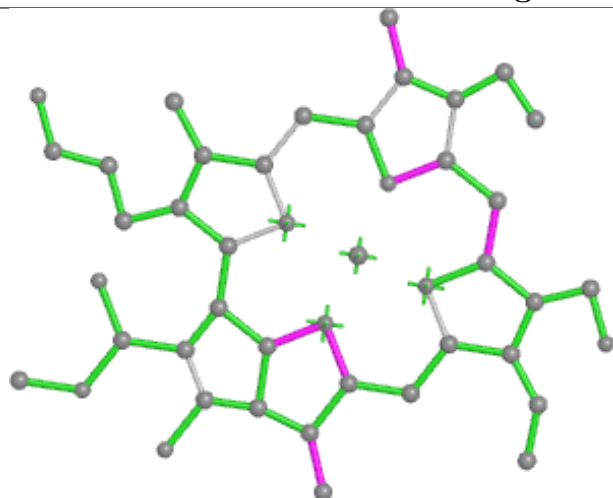




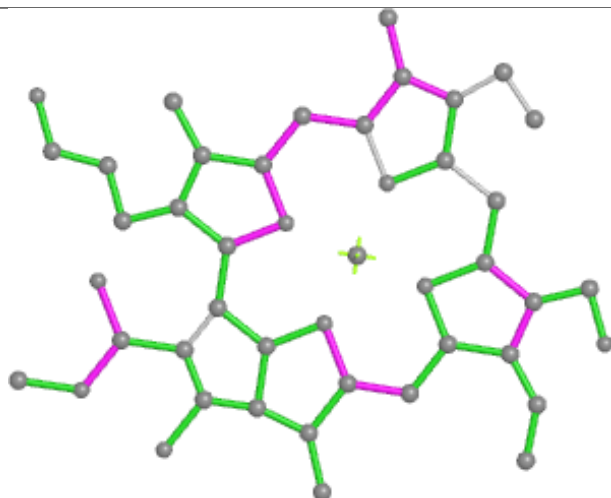
Ligand CLA 2 613



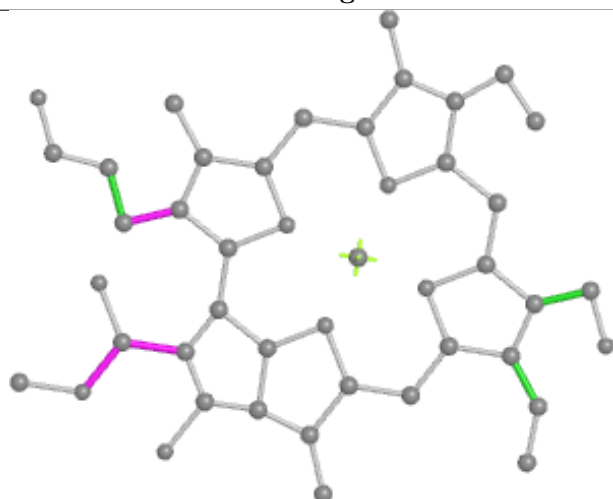
Ligand CHL P 314



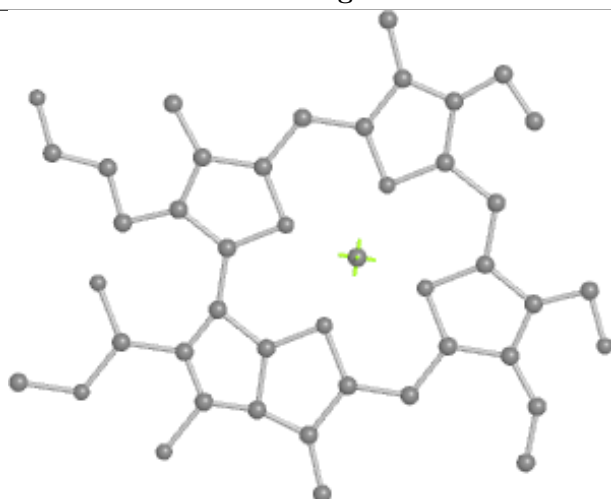
Bond lengths



Bond angles

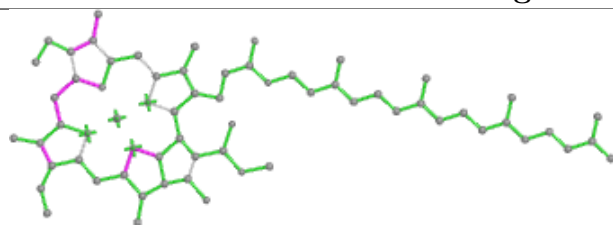


Torsions

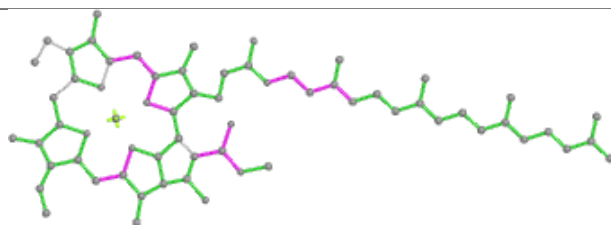


Rings

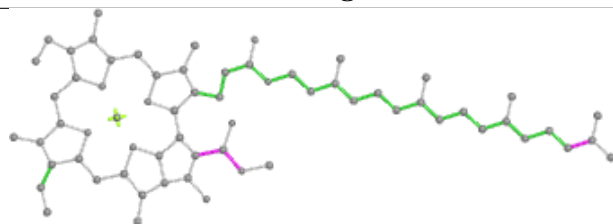
Ligand CLA A 836



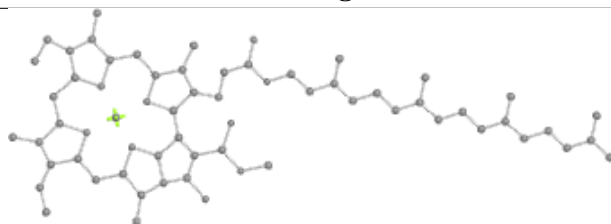
Bond lengths



Bond angles

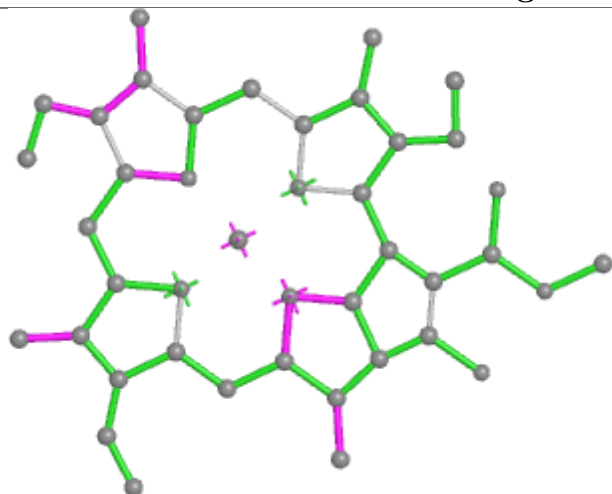


Torsions

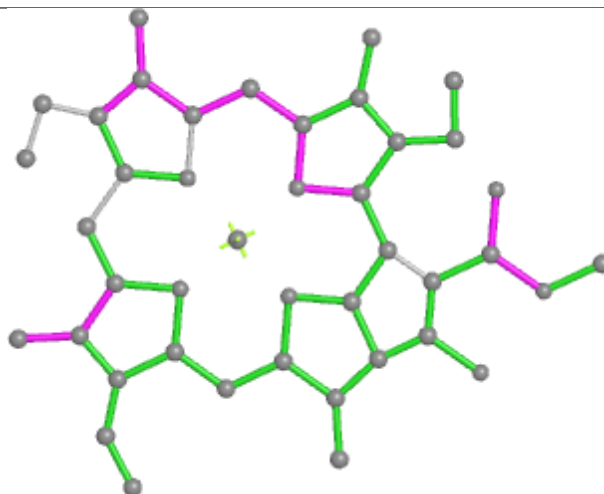


Rings

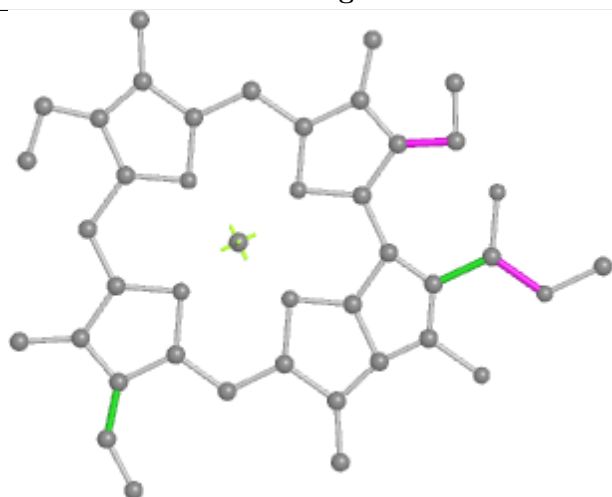
Ligand CLA J 102



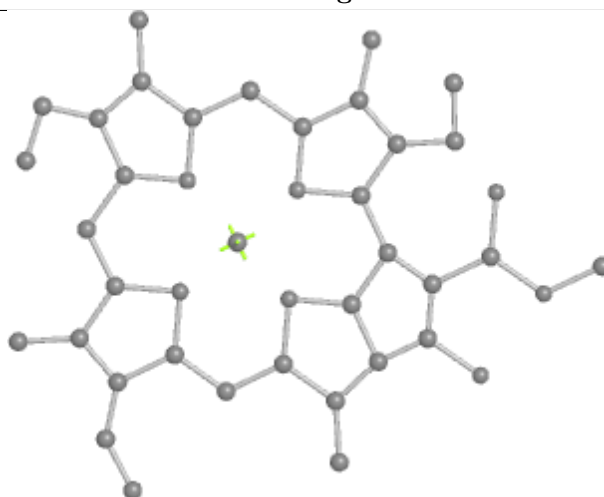
Bond lengths



Bond angles

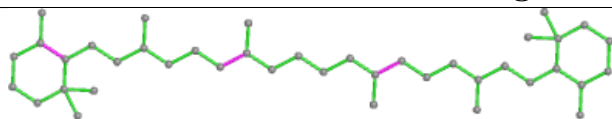


Torsions

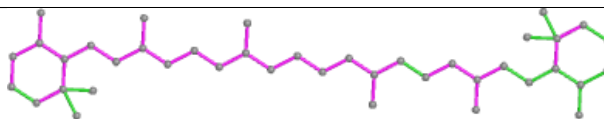


Rings

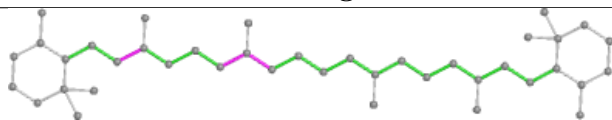
Ligand BCR F 804



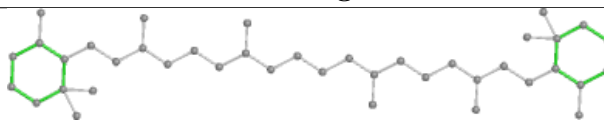
Bond lengths



Bond angles

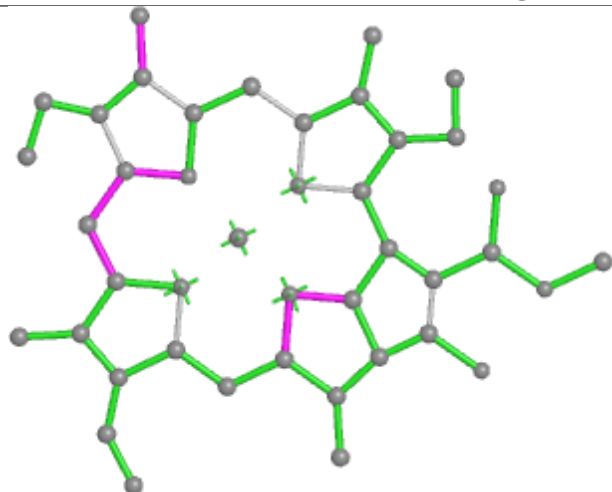


Torsions

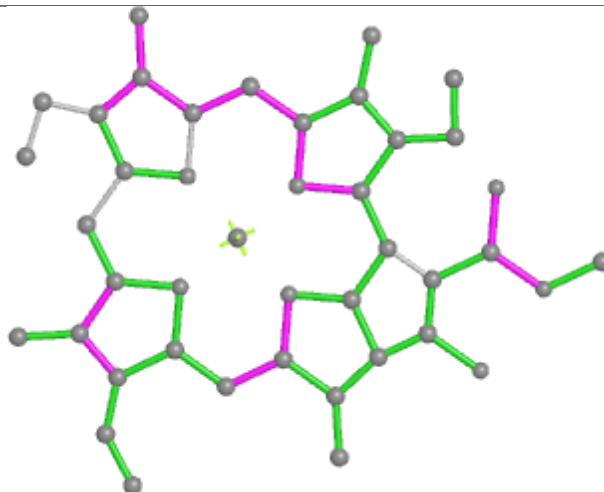


Rings

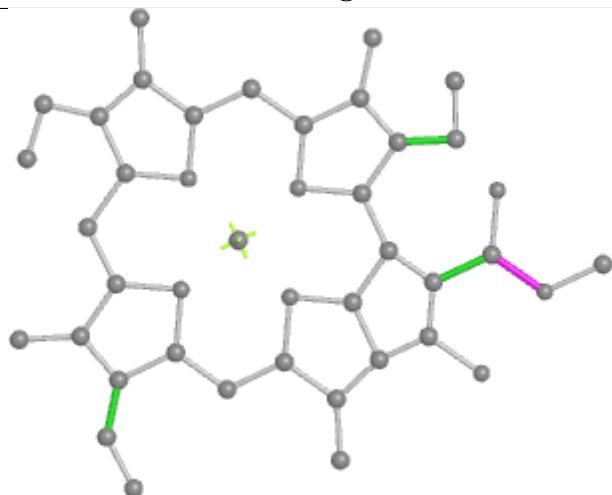
Ligand CLA B 837



Bond lengths



Bond angles

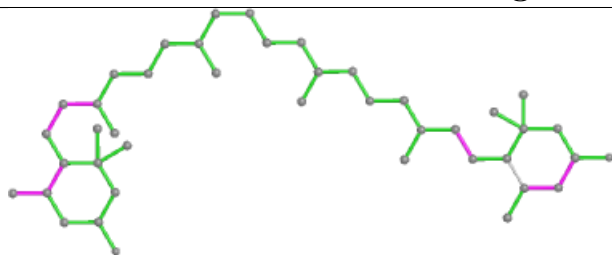


Torsions

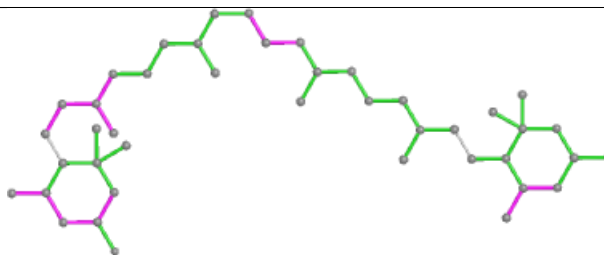


Rings

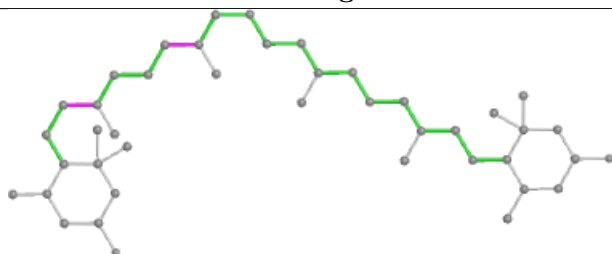
Ligand Q6L W 315



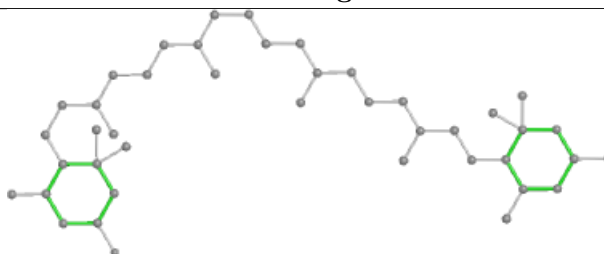
Bond lengths



Bond angles

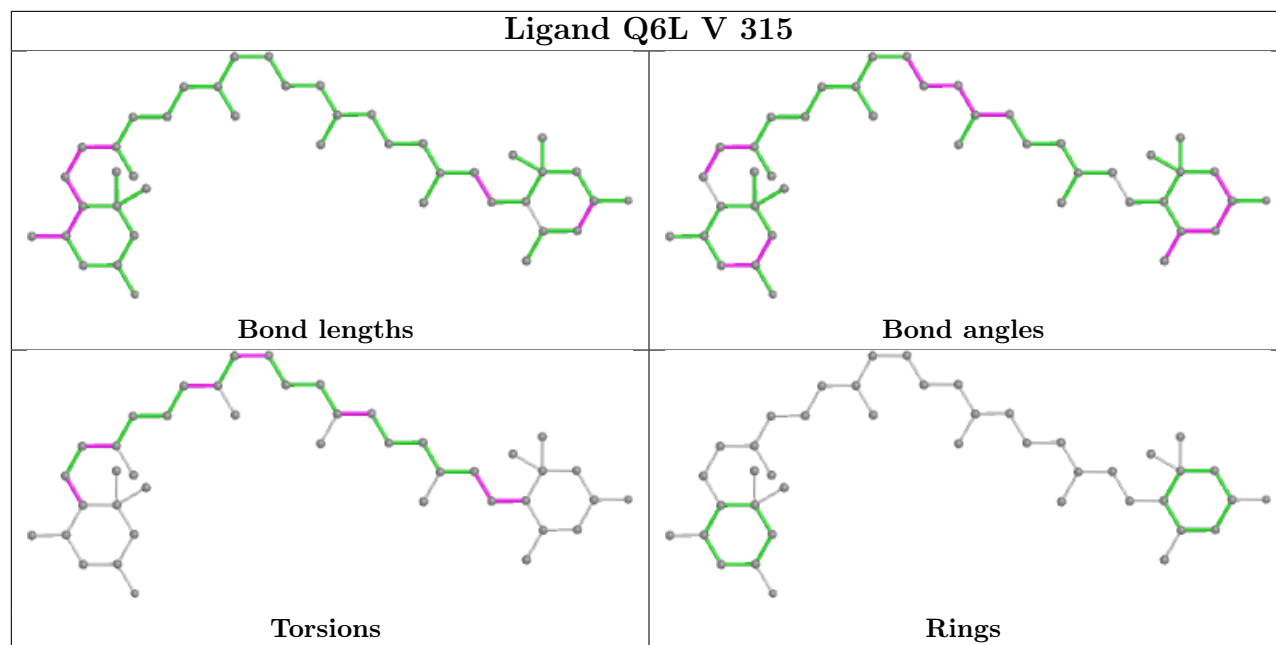


Torsions

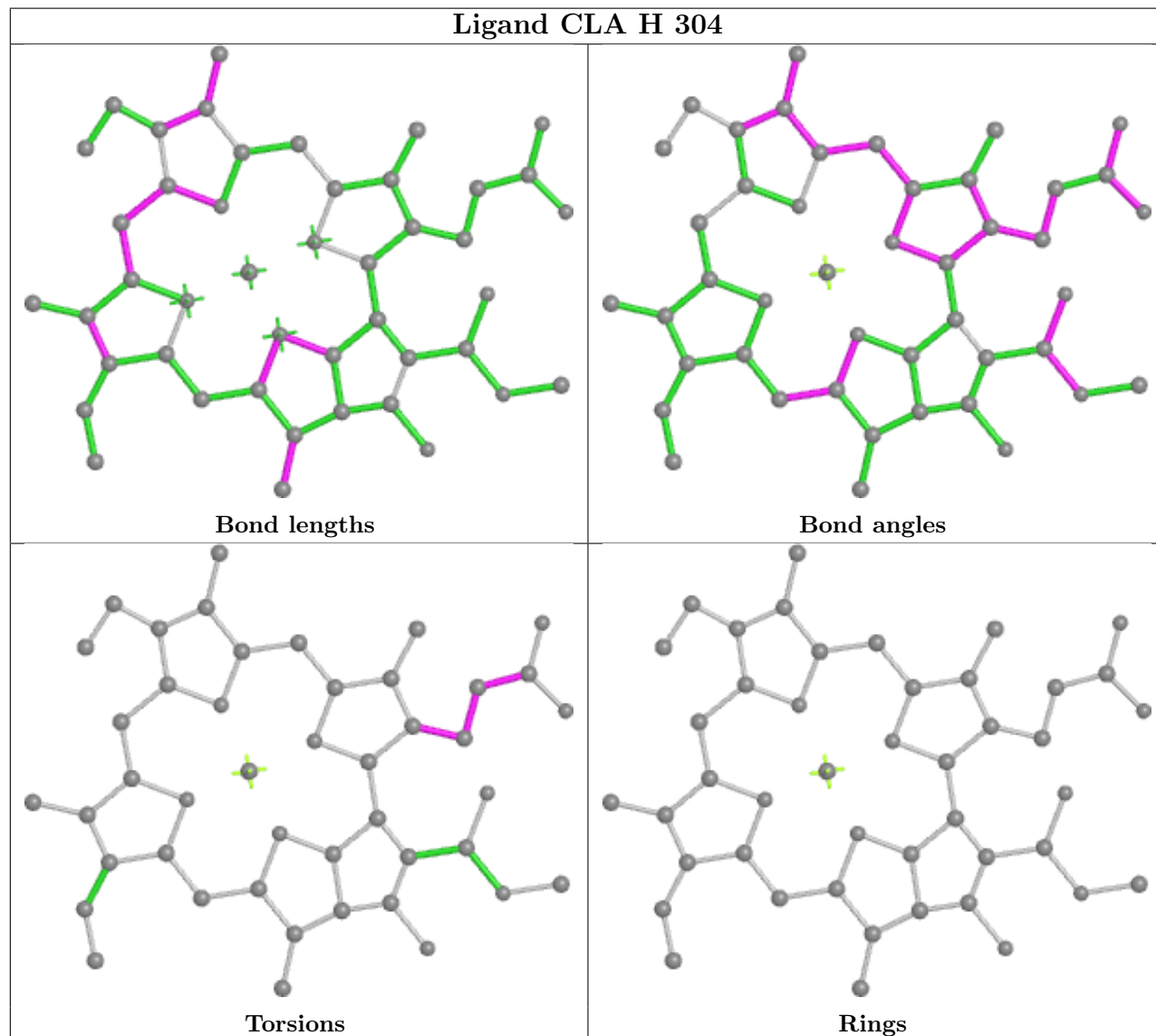


Rings

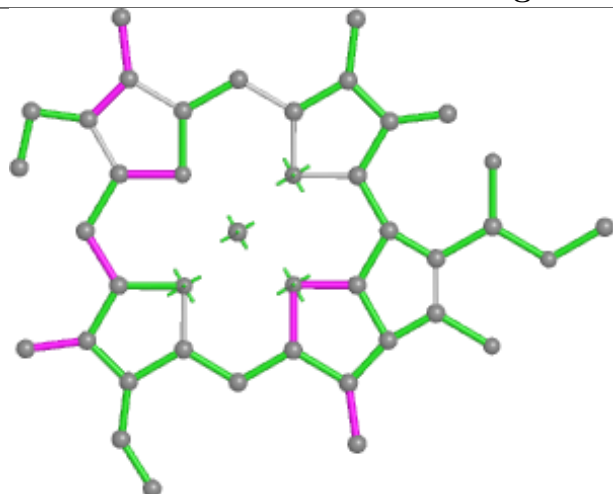
Ligand Q6L V 315



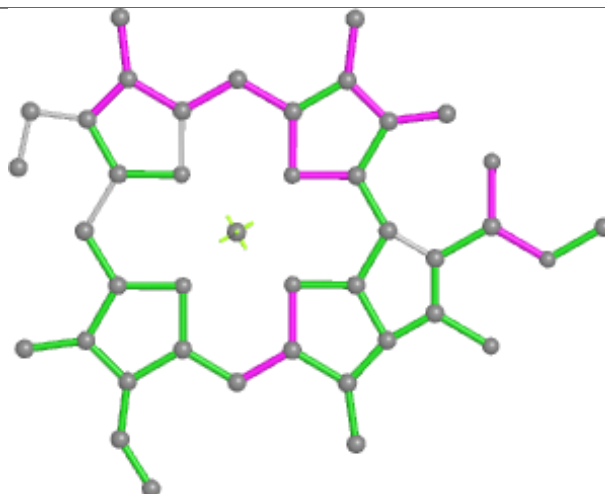
Ligand CLA H 304



Ligand CLA X 313



Bond lengths



Bond angles

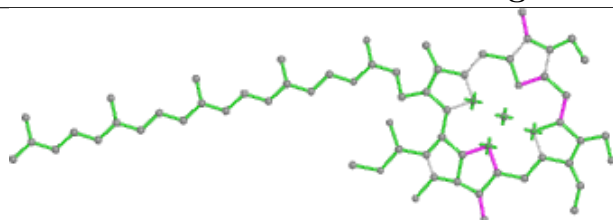


Torsions

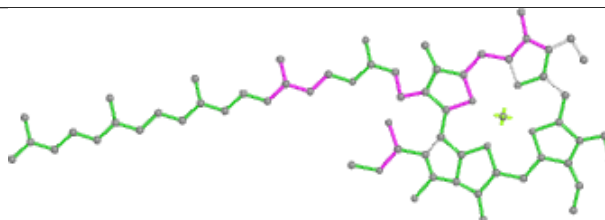


Rings

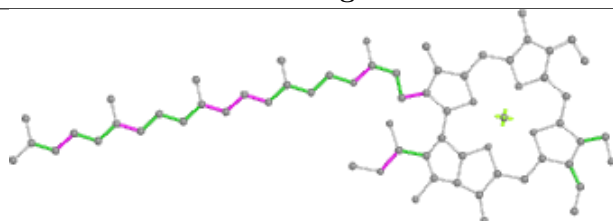
Ligand CHL W 307



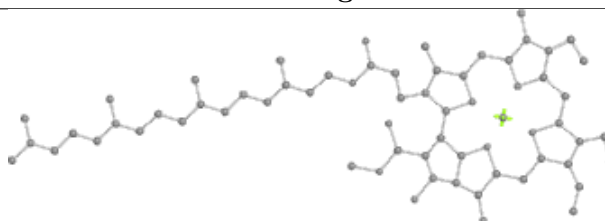
Bond lengths



Bond angles

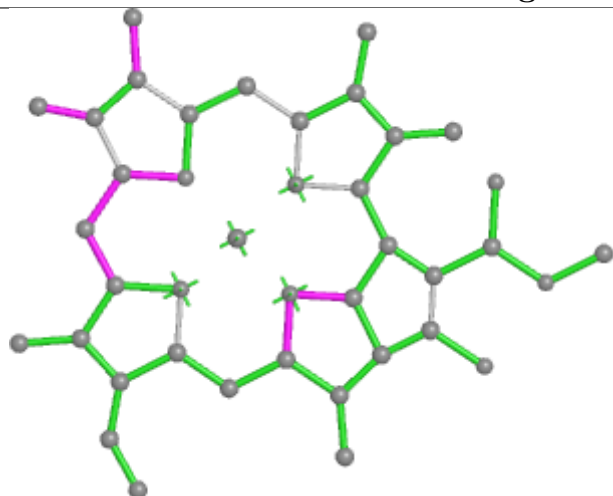


Torsions

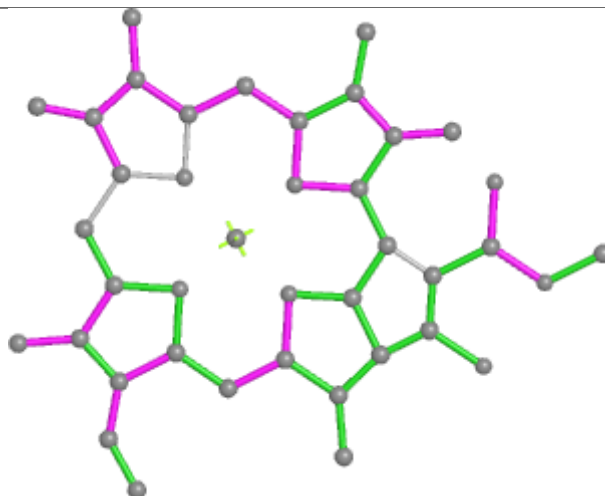


Rings

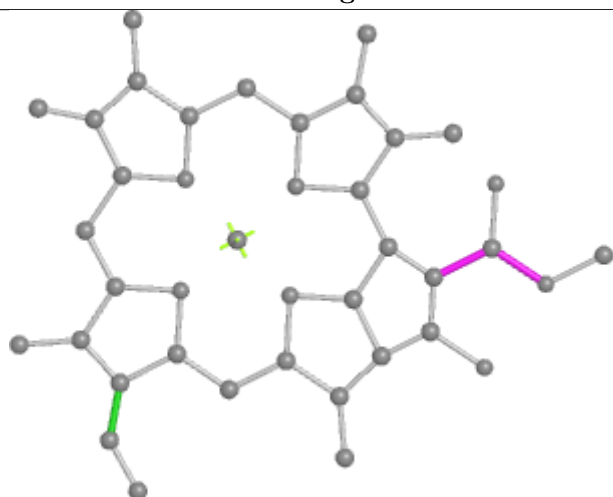
Ligand CLA 1 606



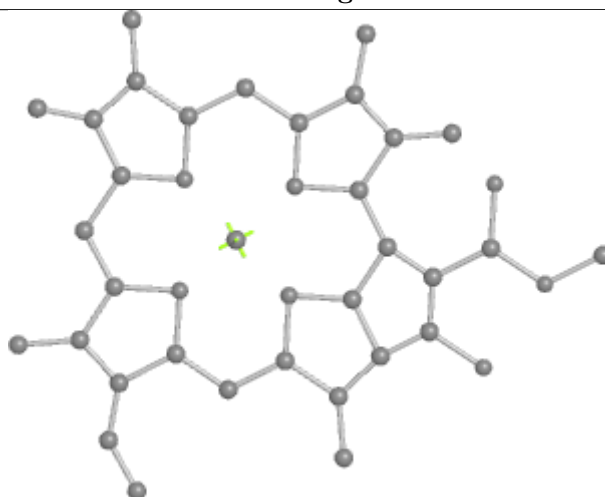
Bond lengths



Bond angles

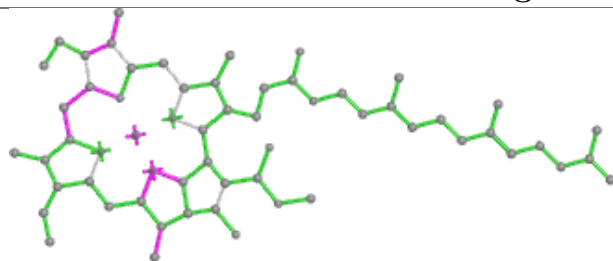


Torsions

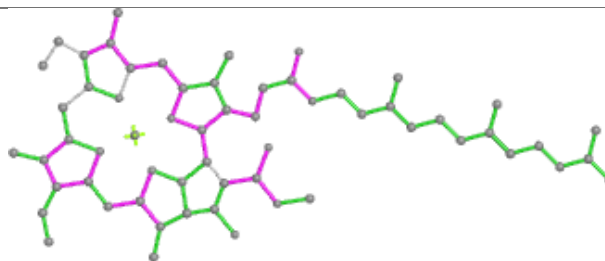


Rings

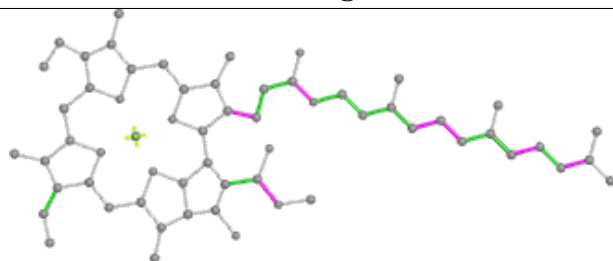
Ligand CLA B 820



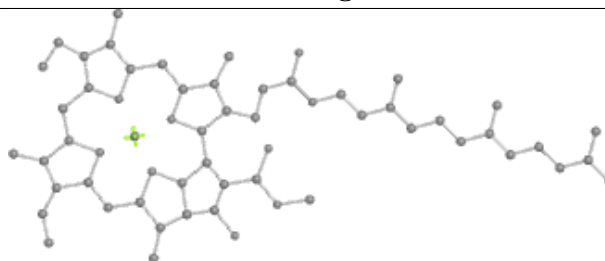
Bond lengths



Bond angles

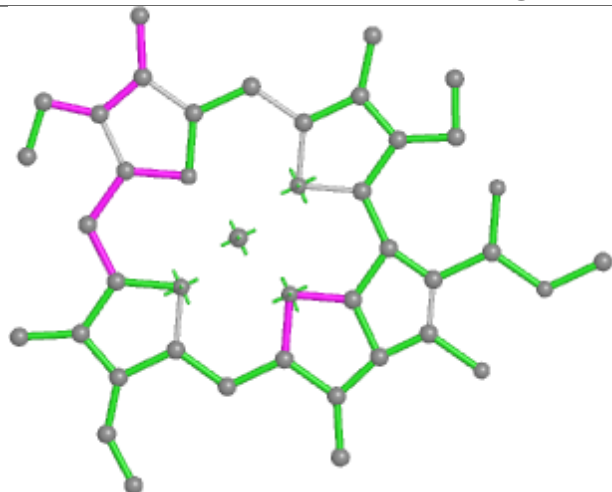


Torsions

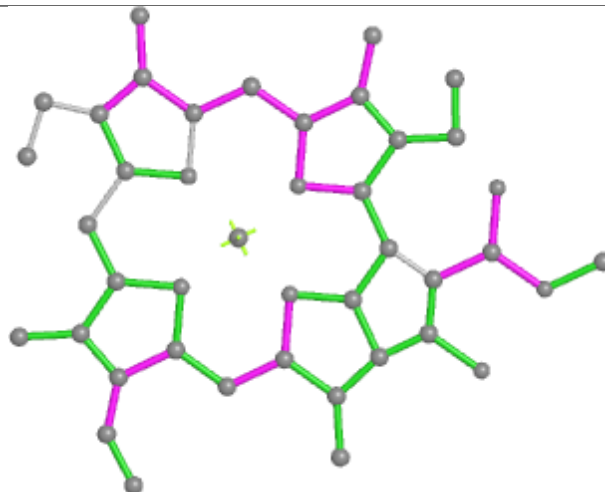


Rings

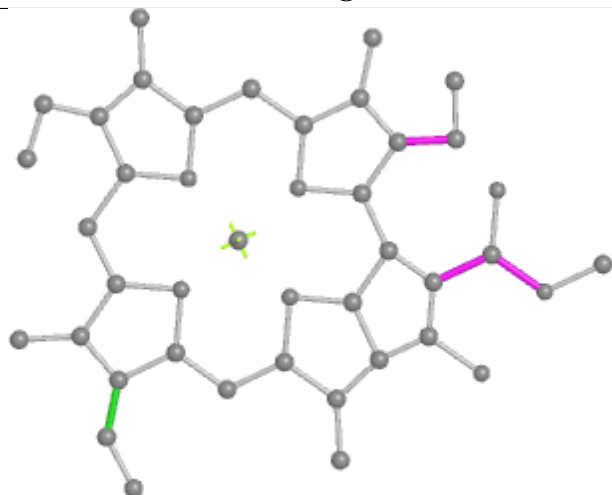
Ligand CLA X 304



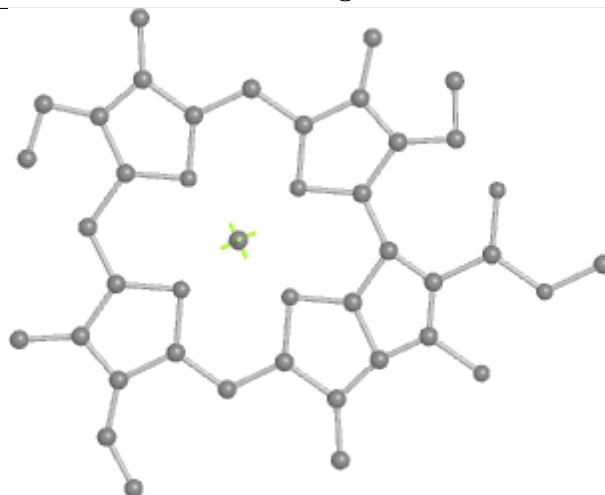
Bond lengths



Bond angles

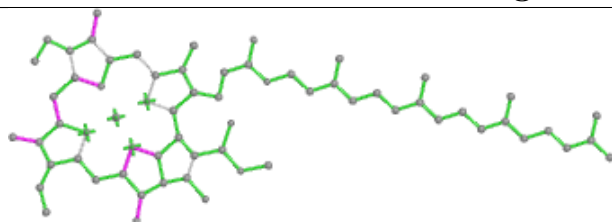


Torsions

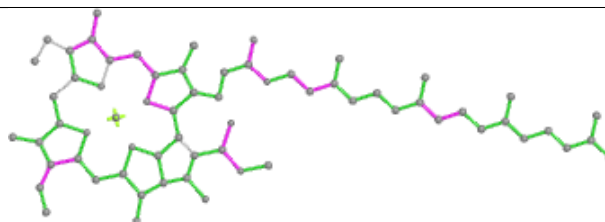


Rings

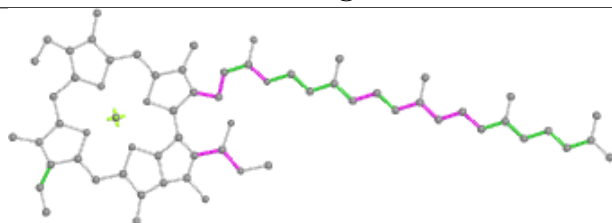
Ligand CLA B 804



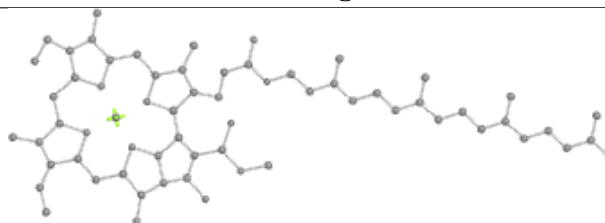
Bond lengths



Bond angles

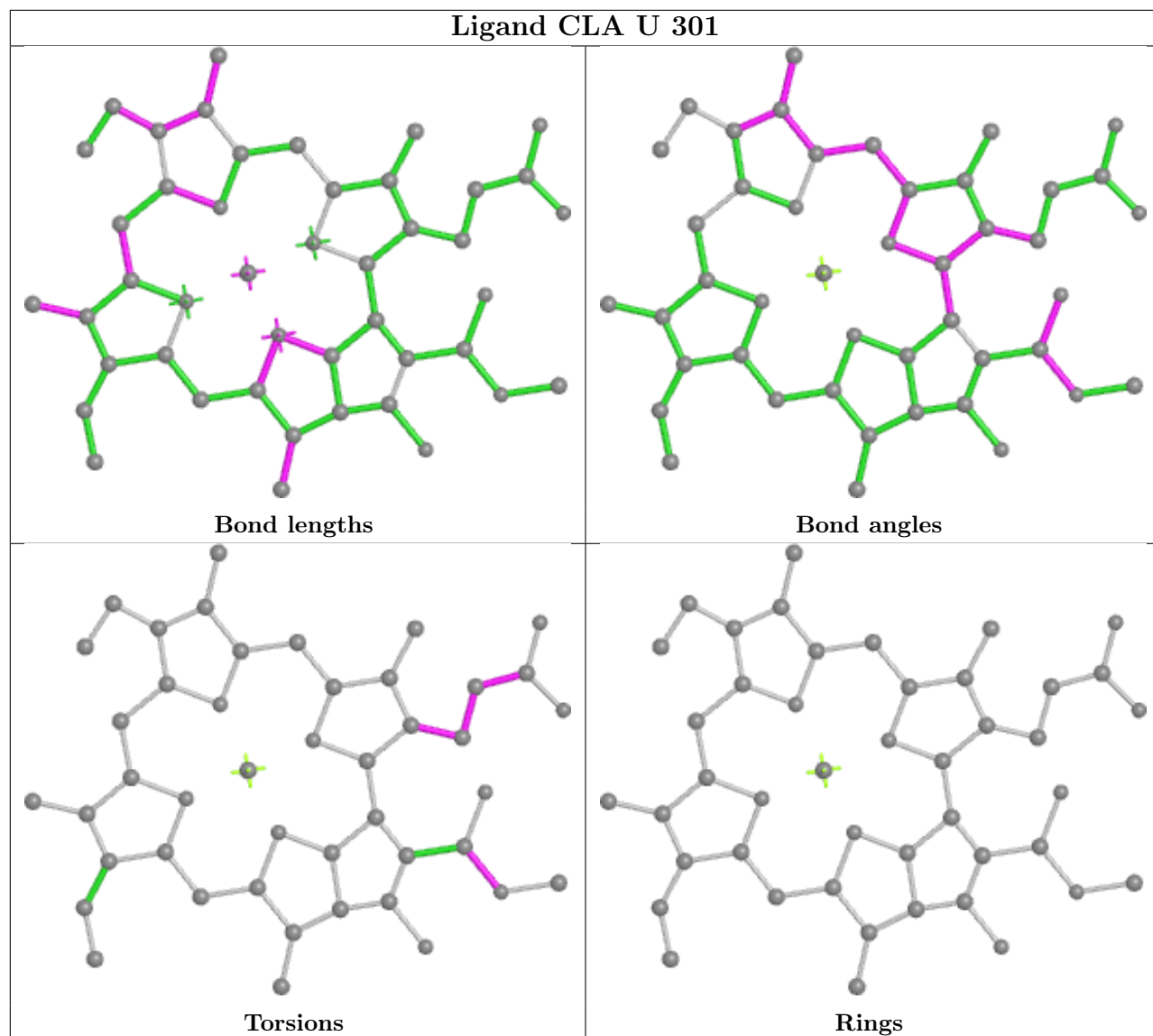


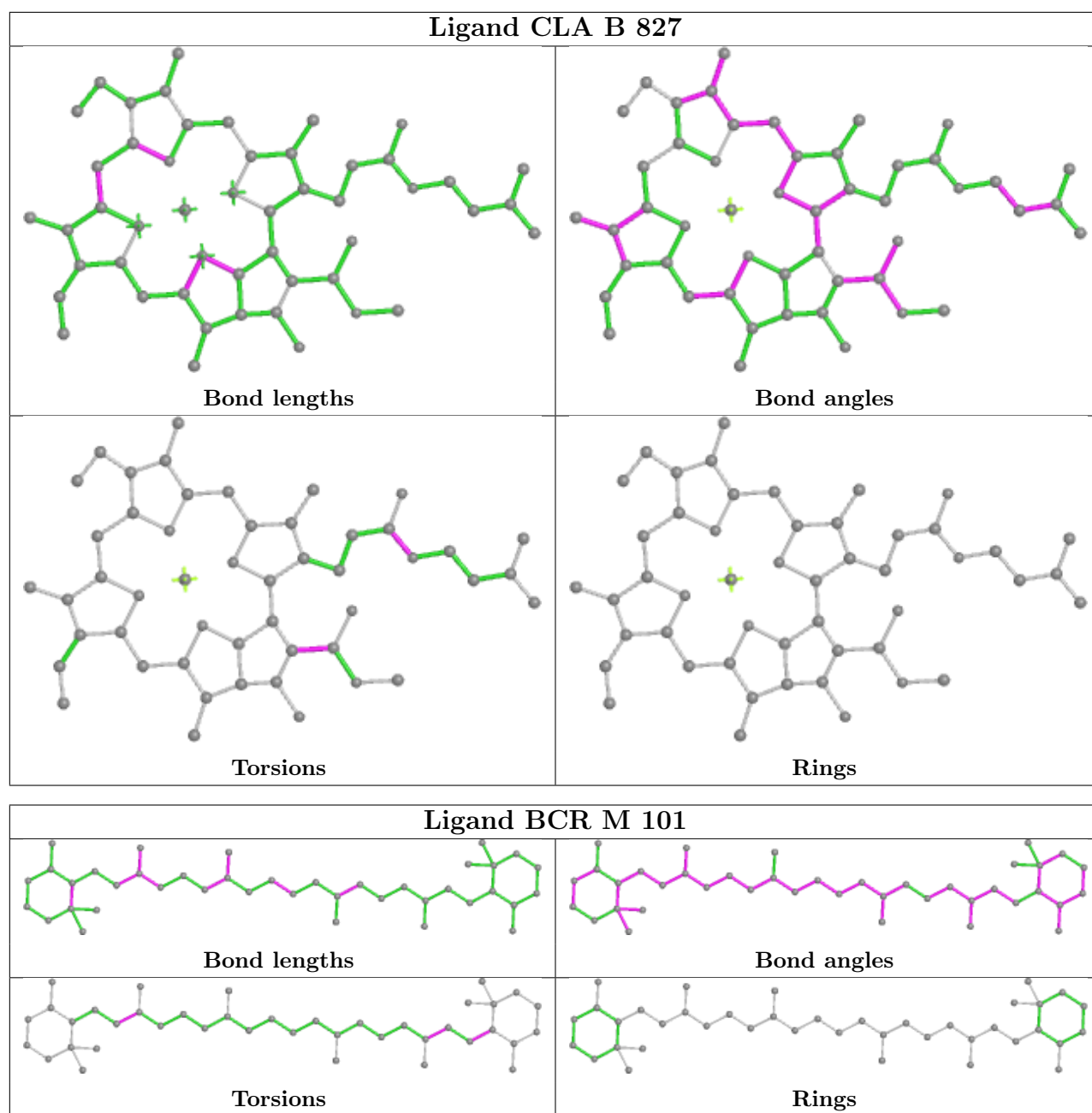
Torsions



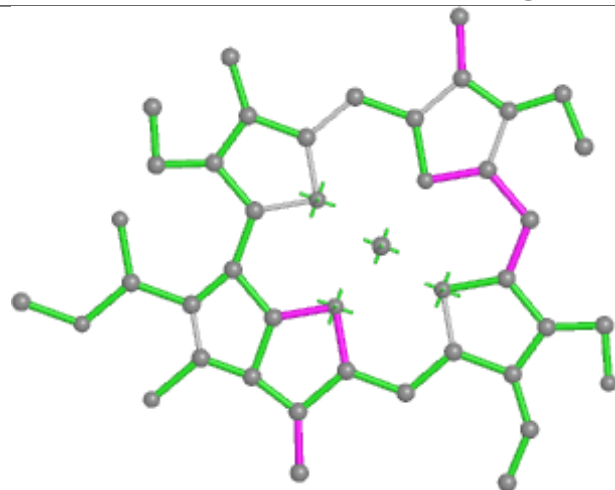
Rings

Ligand CLA U 301

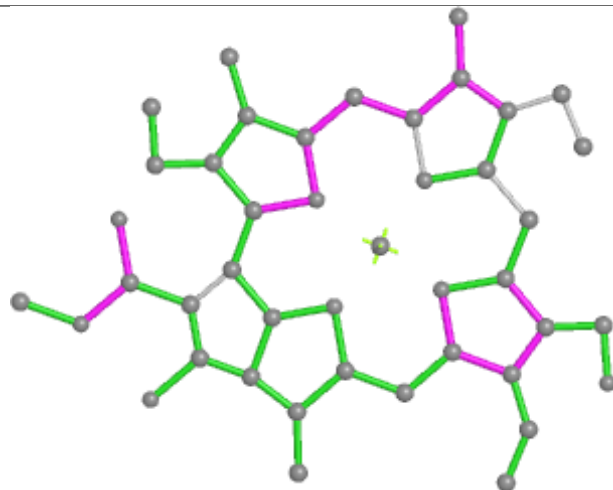




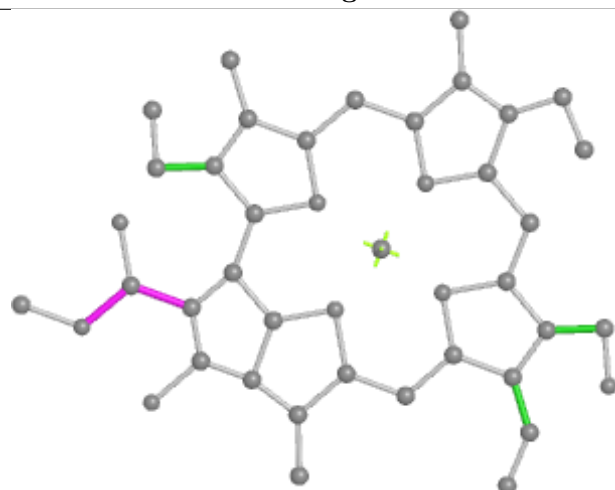
Ligand CHL 2 615



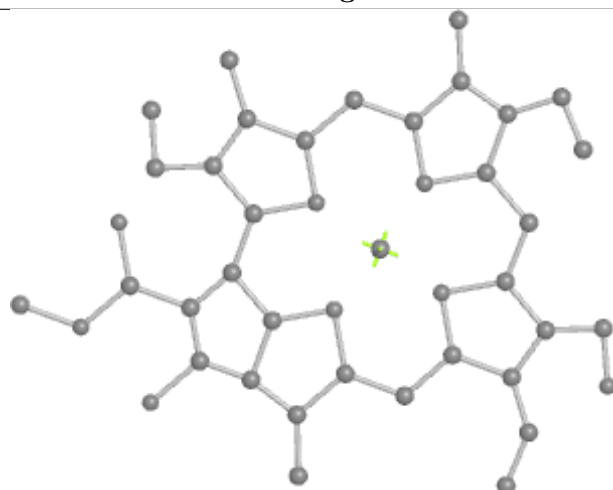
Bond lengths



Bond angles

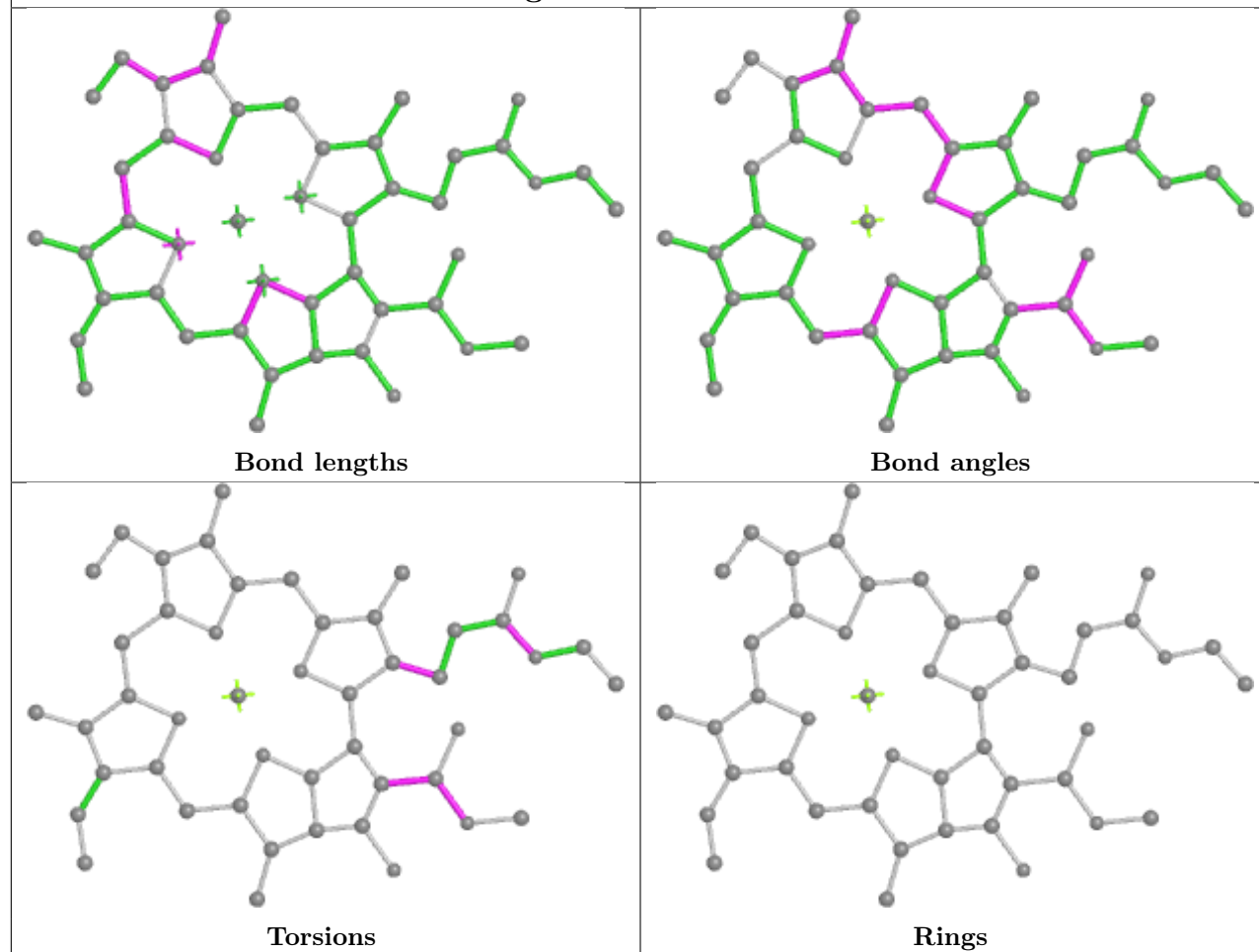


Torsions

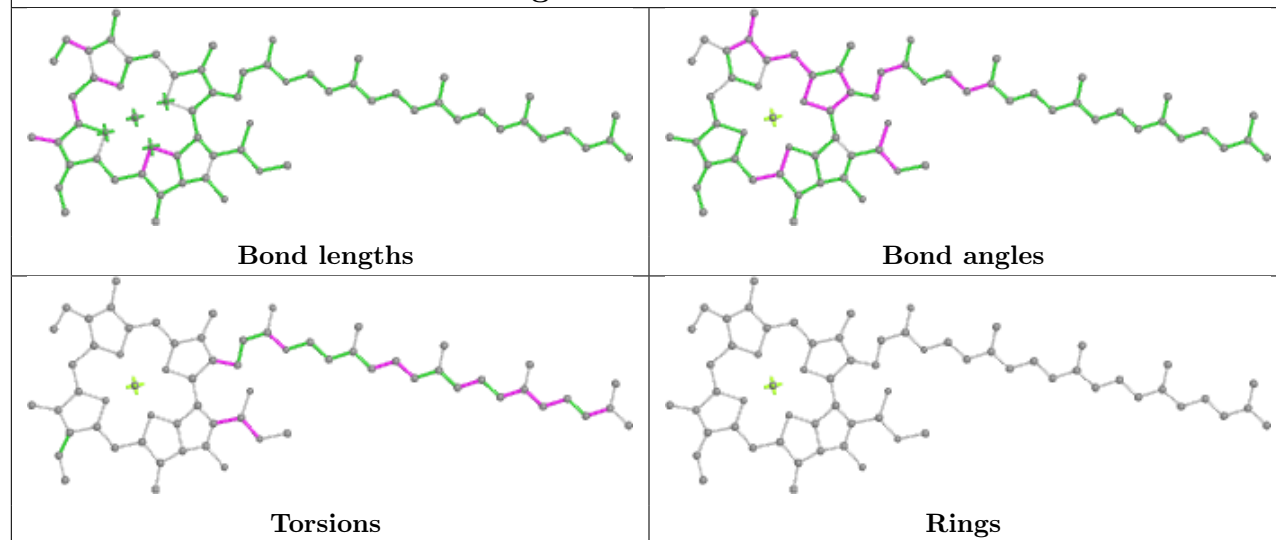


Rings

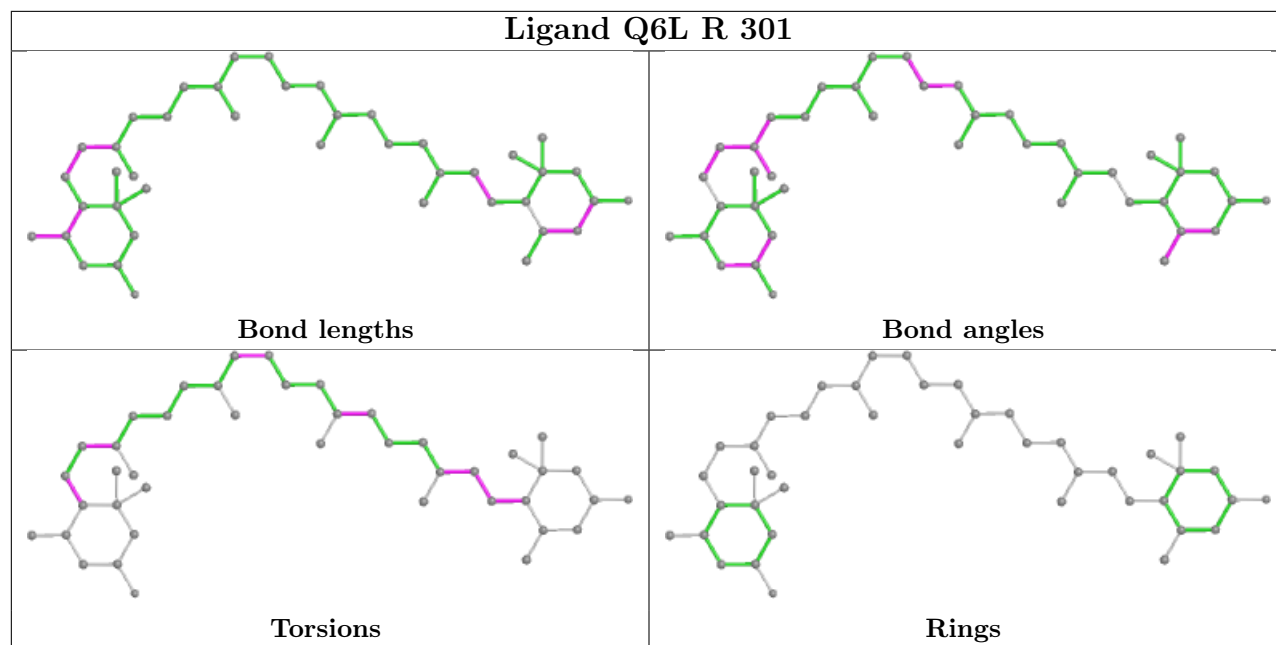
Ligand CLA B 823



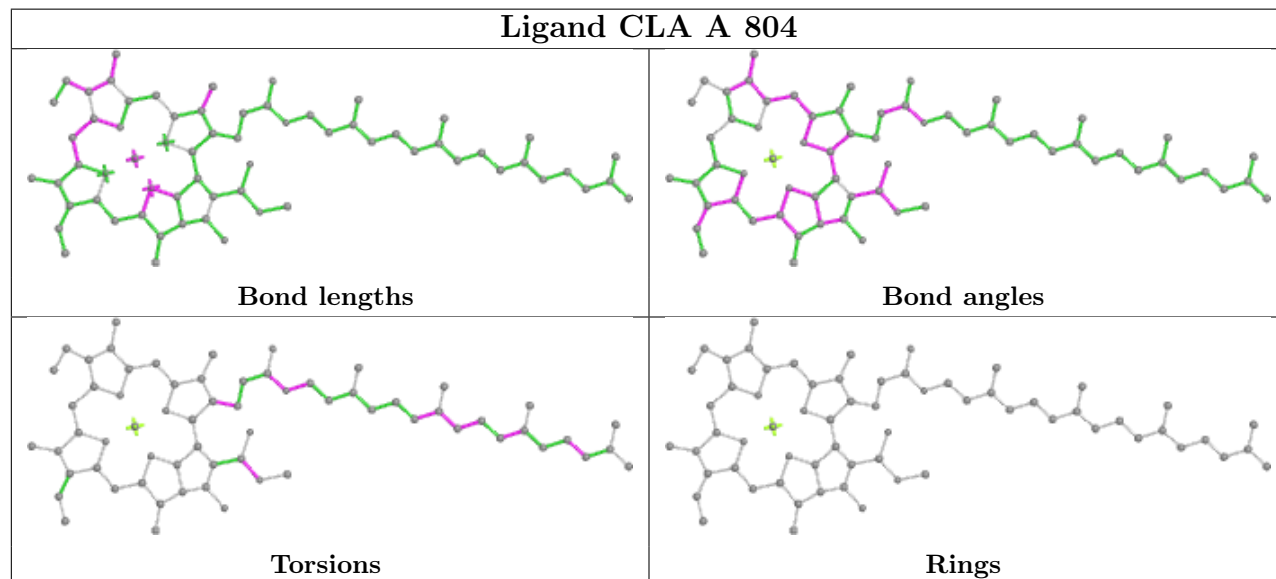
Ligand CLA A 839



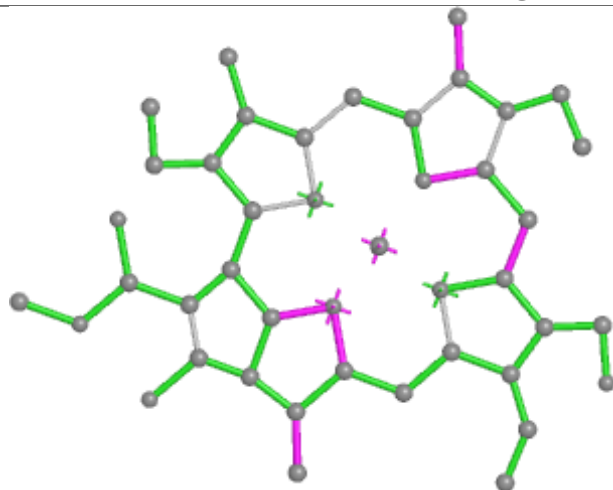
Ligand Q6L R 301



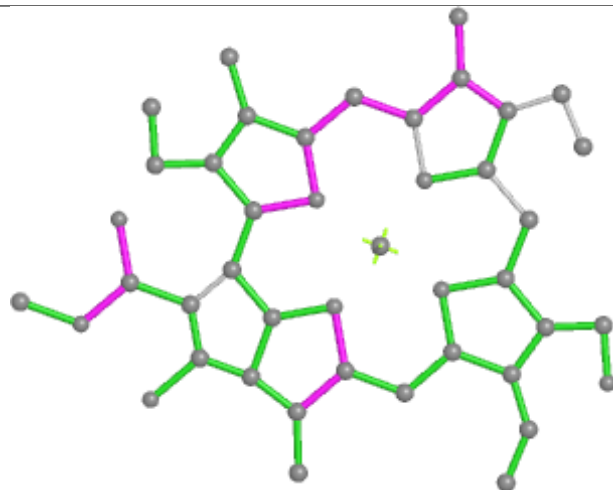
Ligand CLA A 804



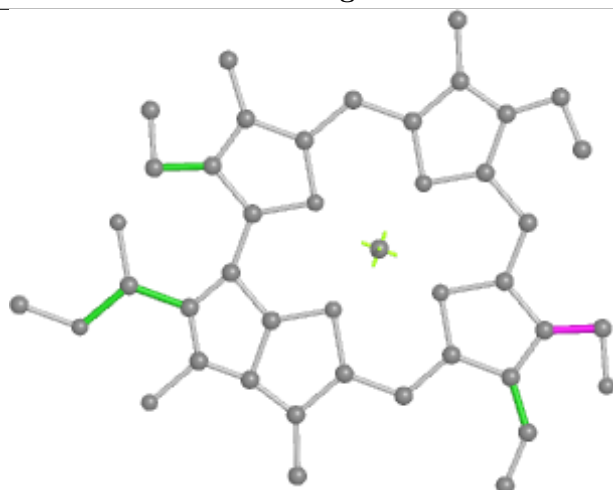
Ligand CHL V 305



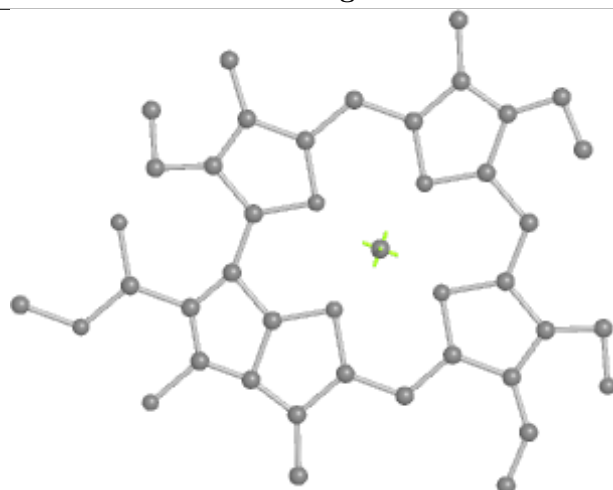
Bond lengths



Bond angles

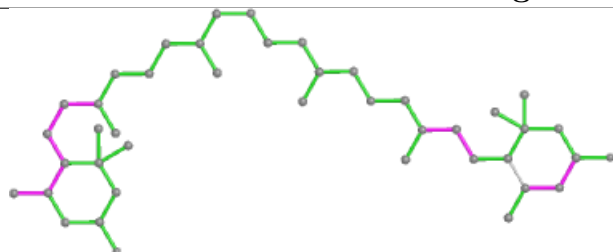


Torsions

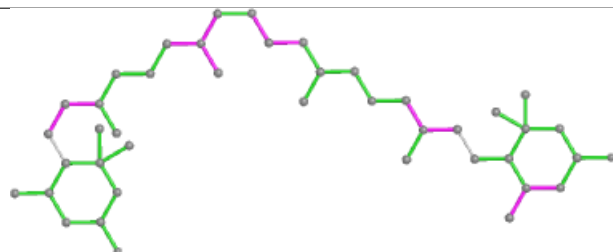


Rings

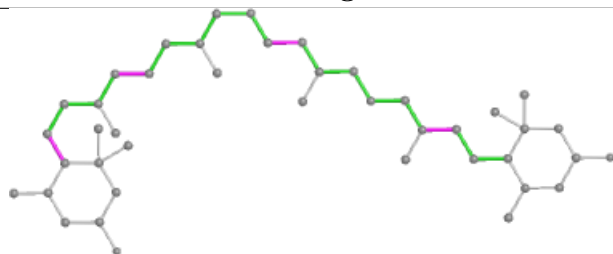
Ligand Q6L W 316



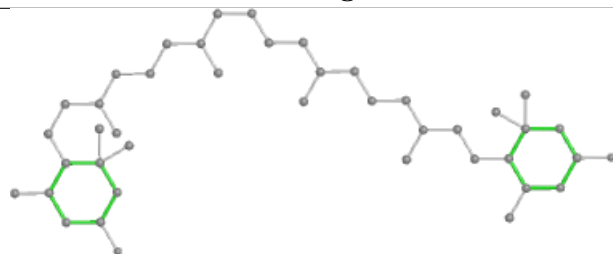
Bond lengths



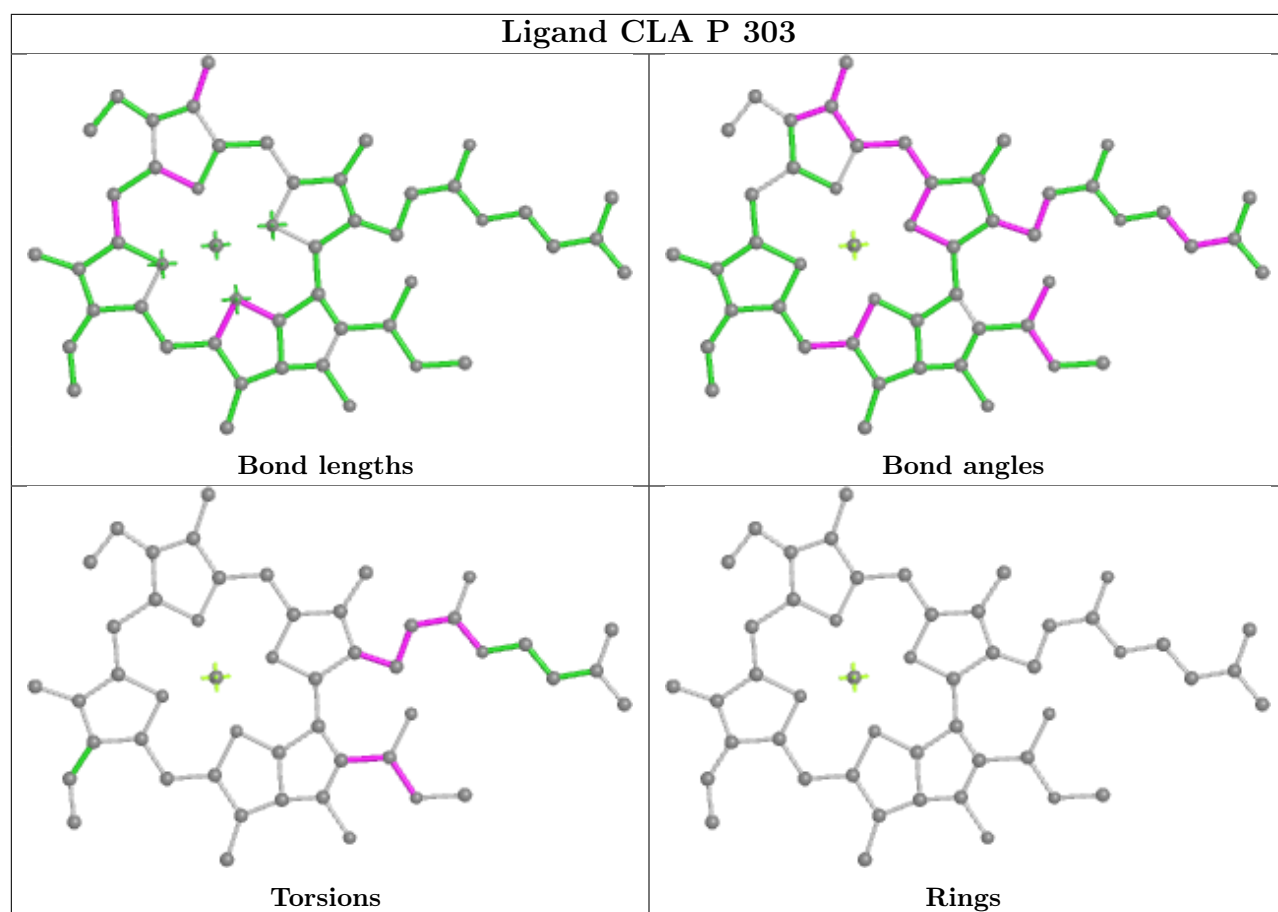
Bond angles



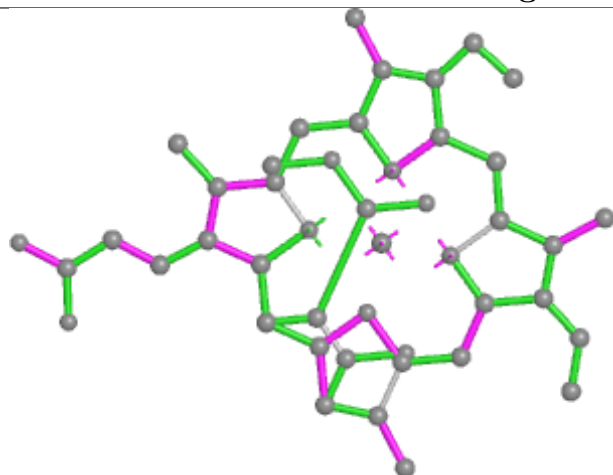
Torsions



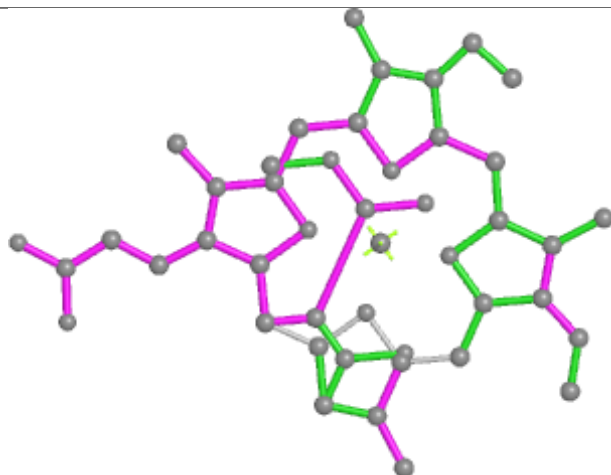
Rings



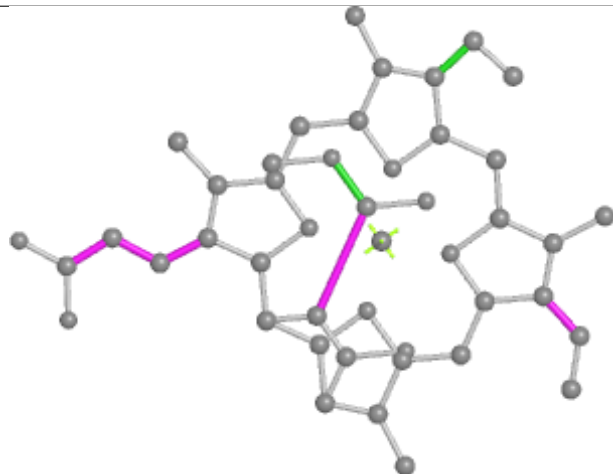
Ligand KC2 S 308



Bond lengths



Bond angles

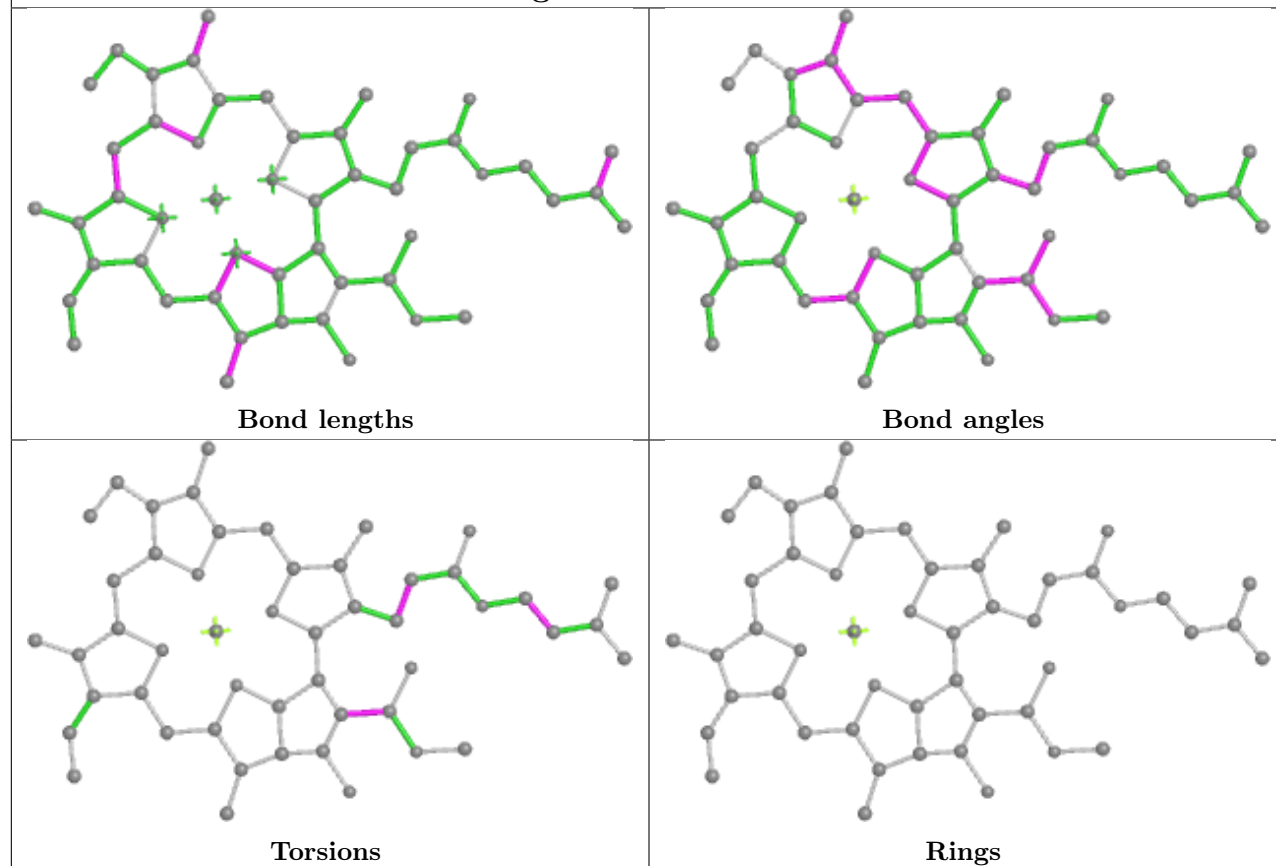


Torsions

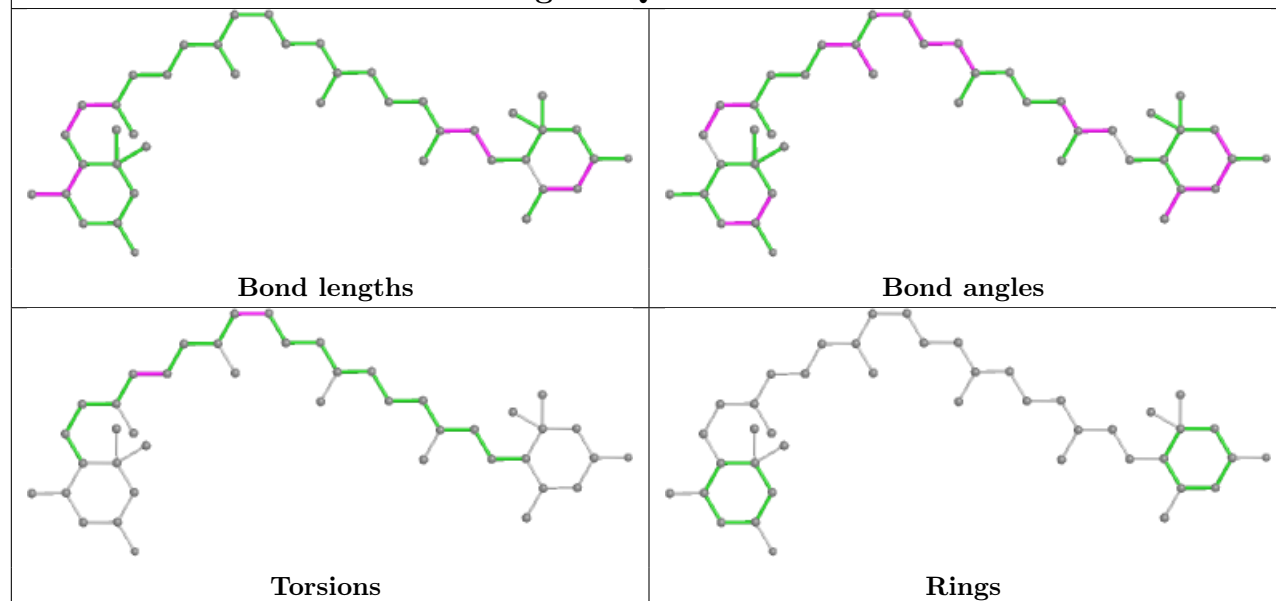


Rings

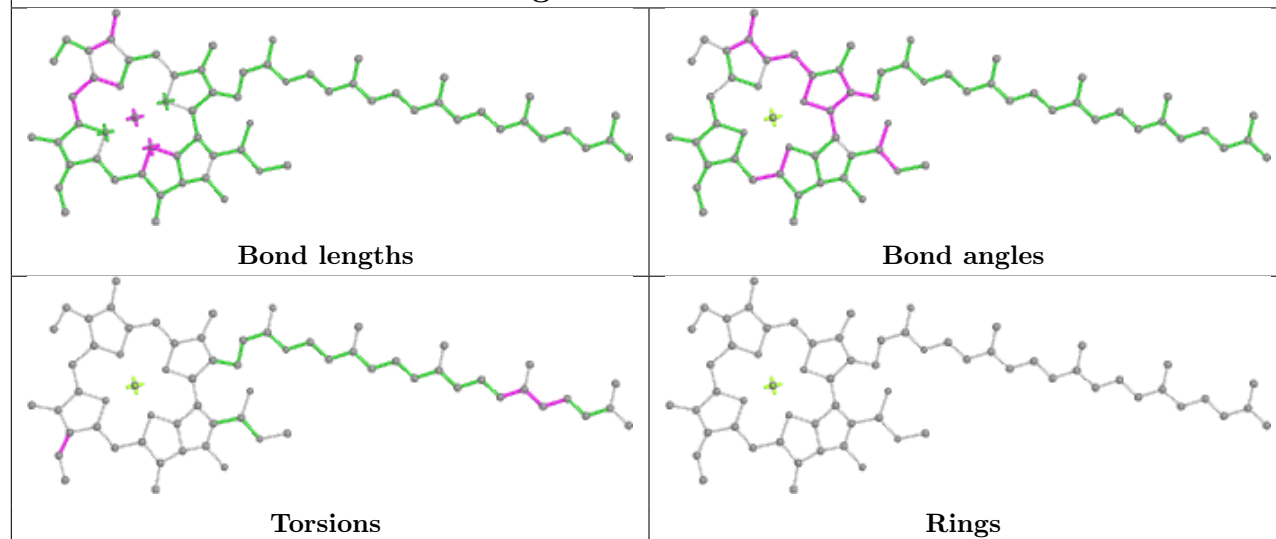
Ligand CLA B 822



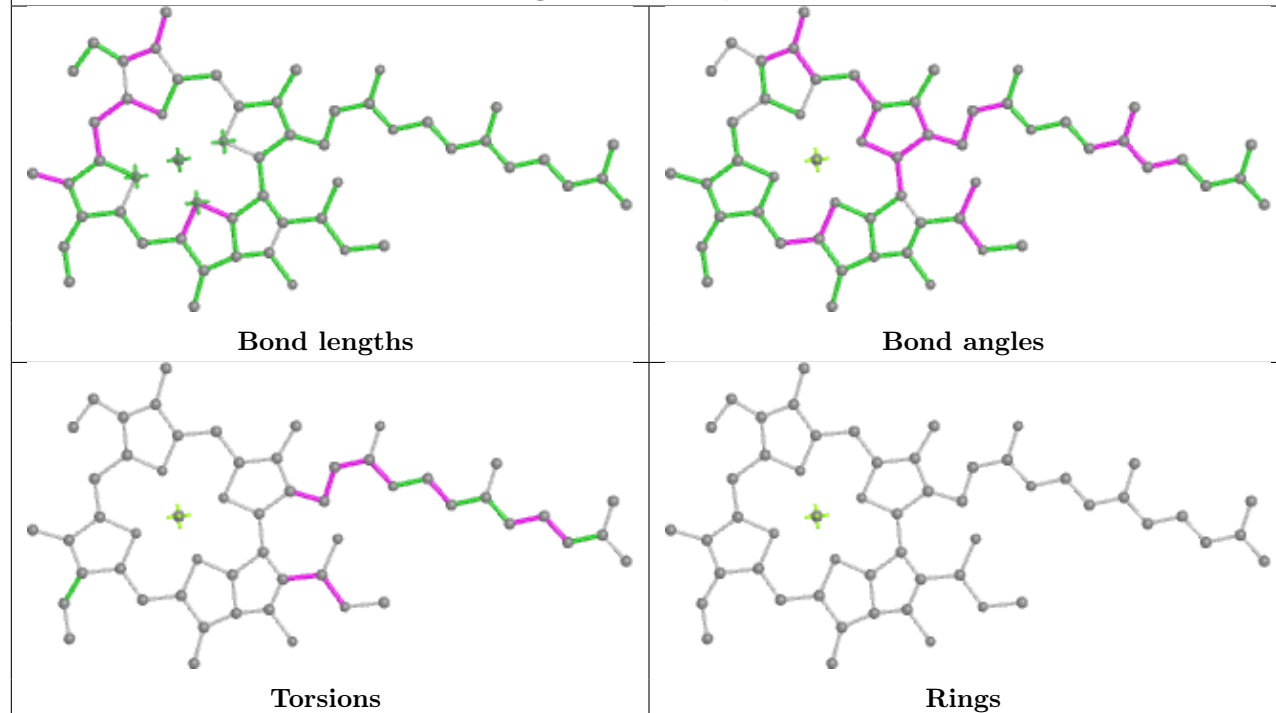
Ligand Q6L U 315



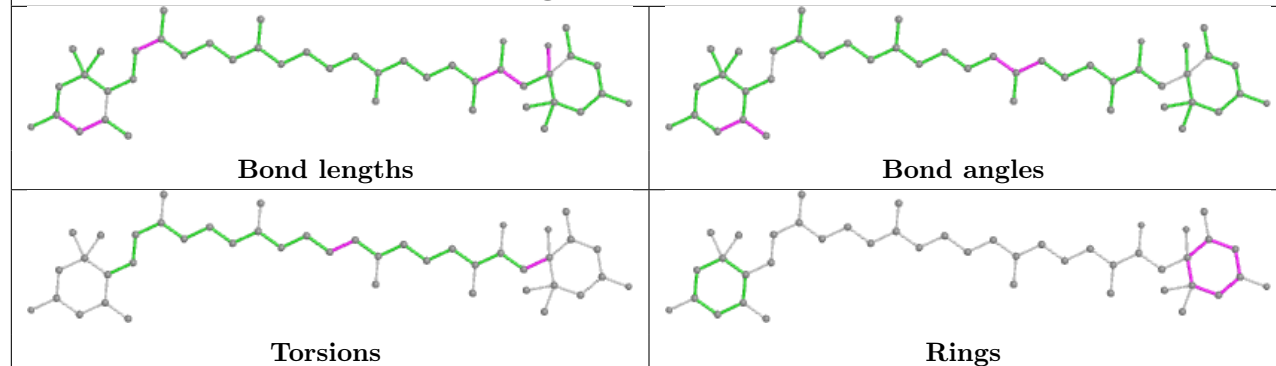
Ligand CLA B 828



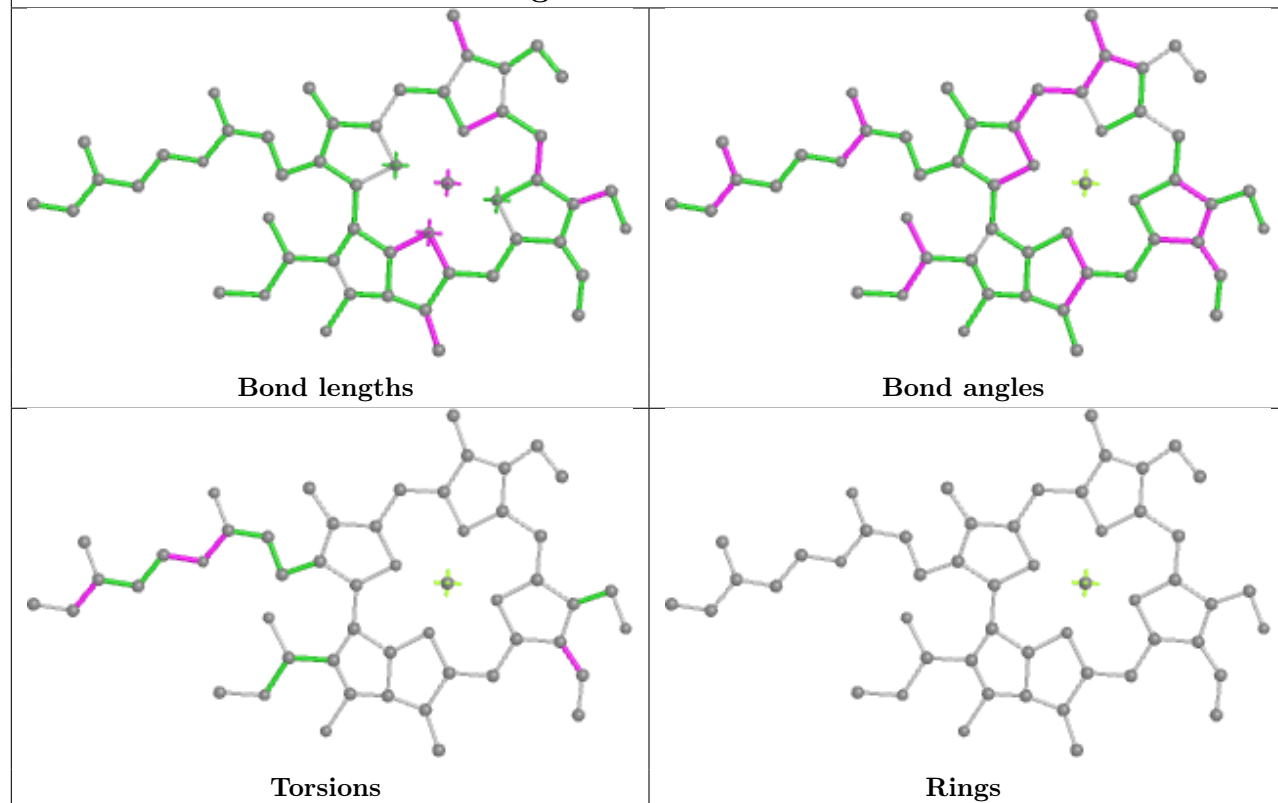
Ligand CLA Q 301



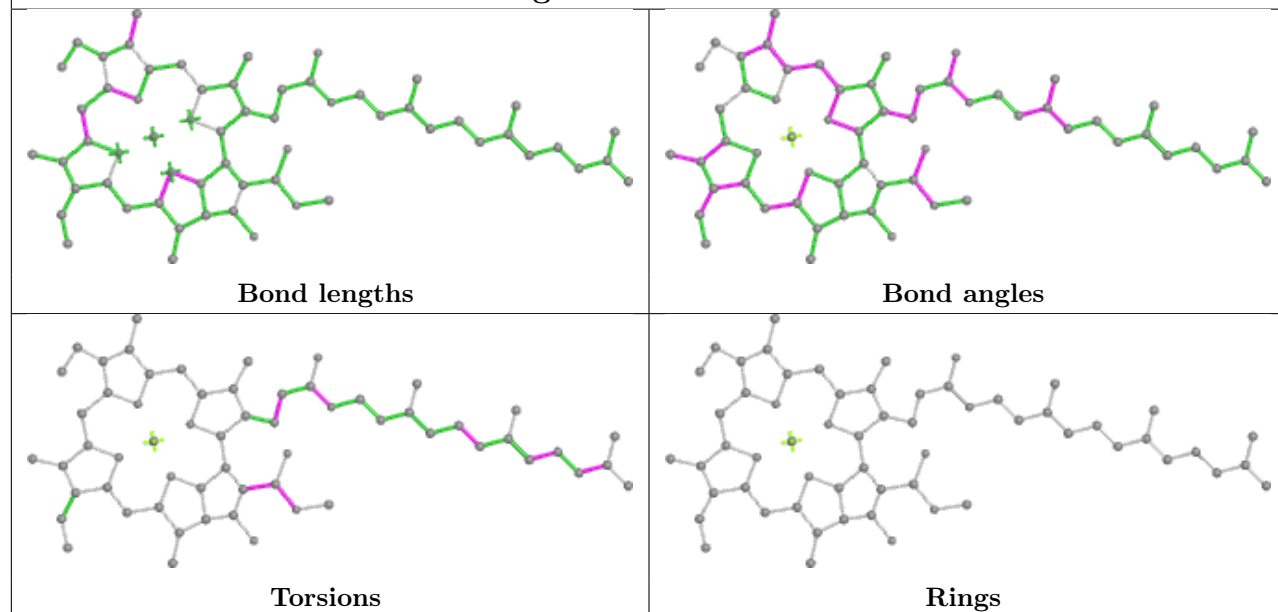
Ligand IWJ 3 315

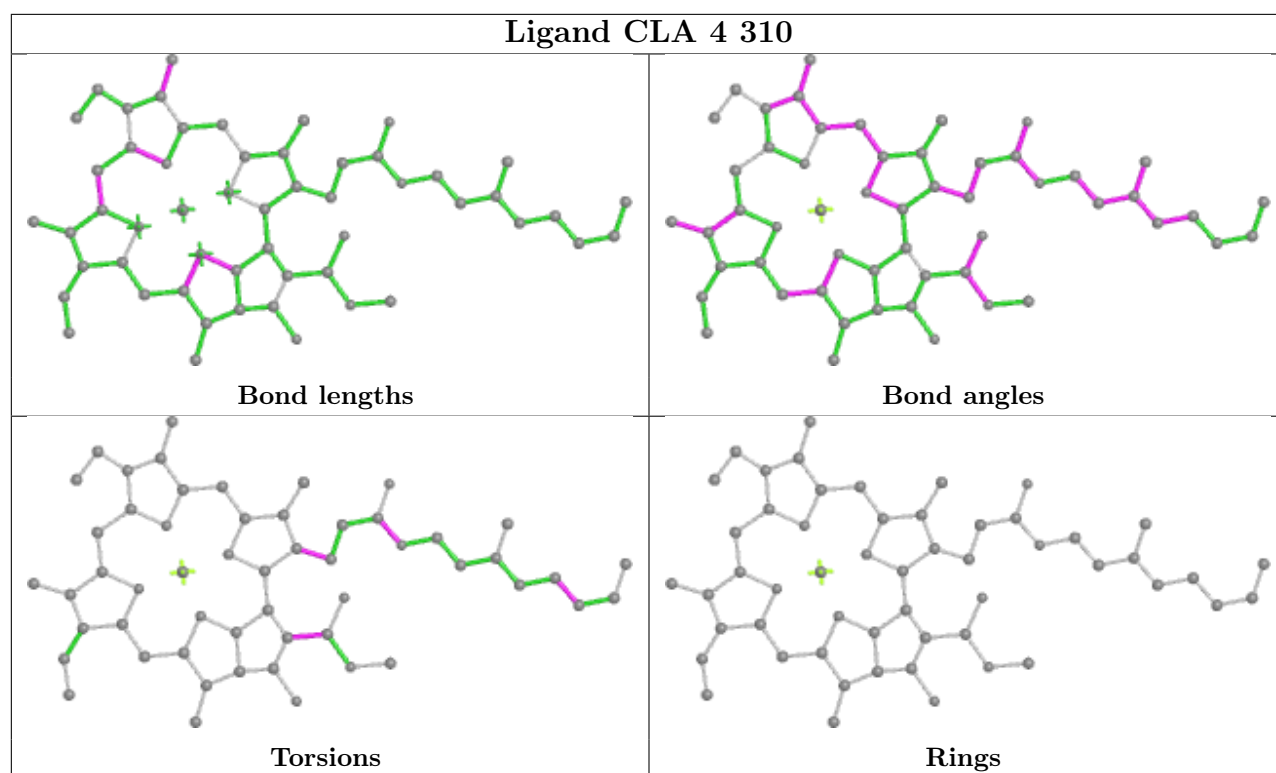


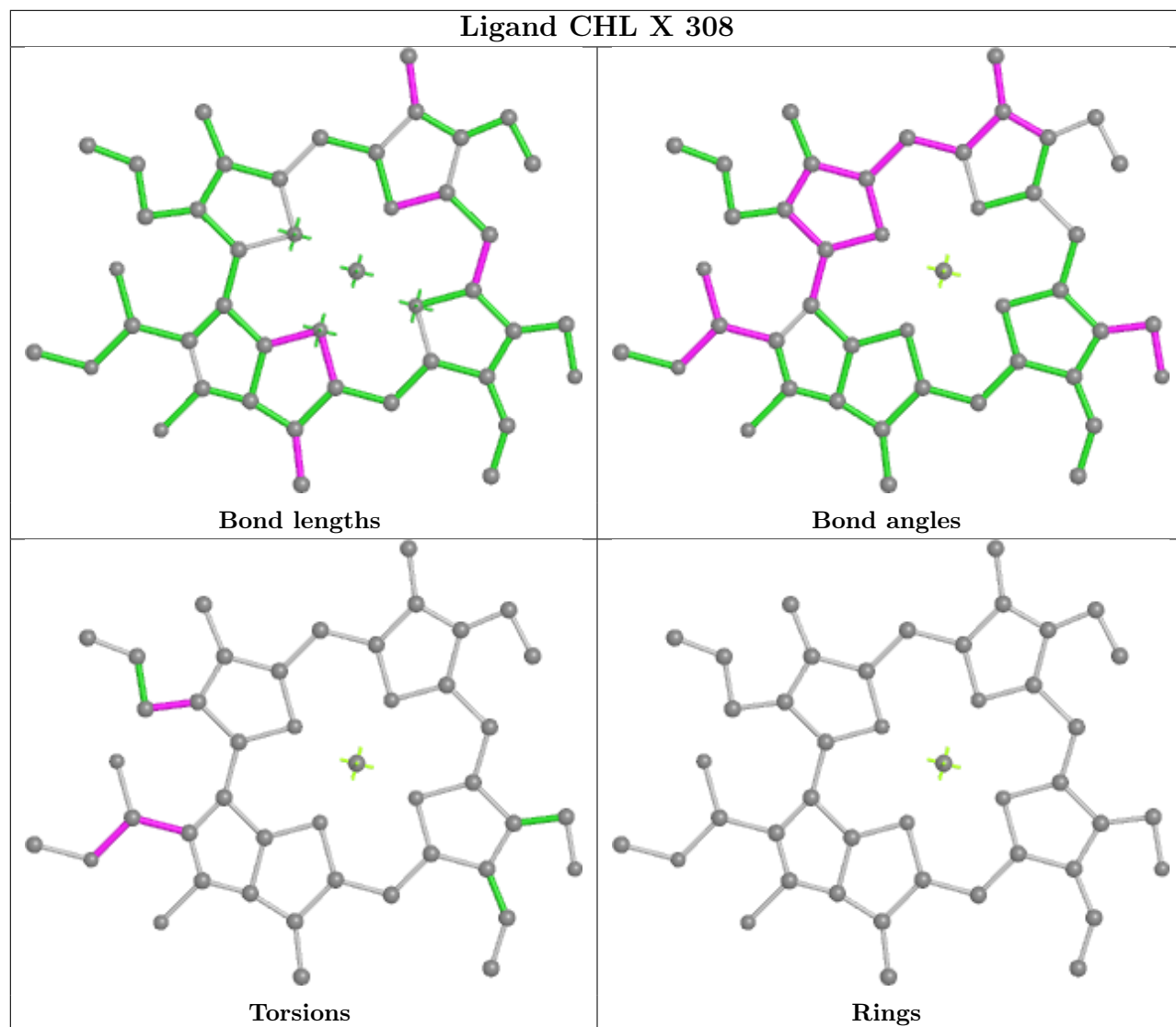
Ligand CHL R 310



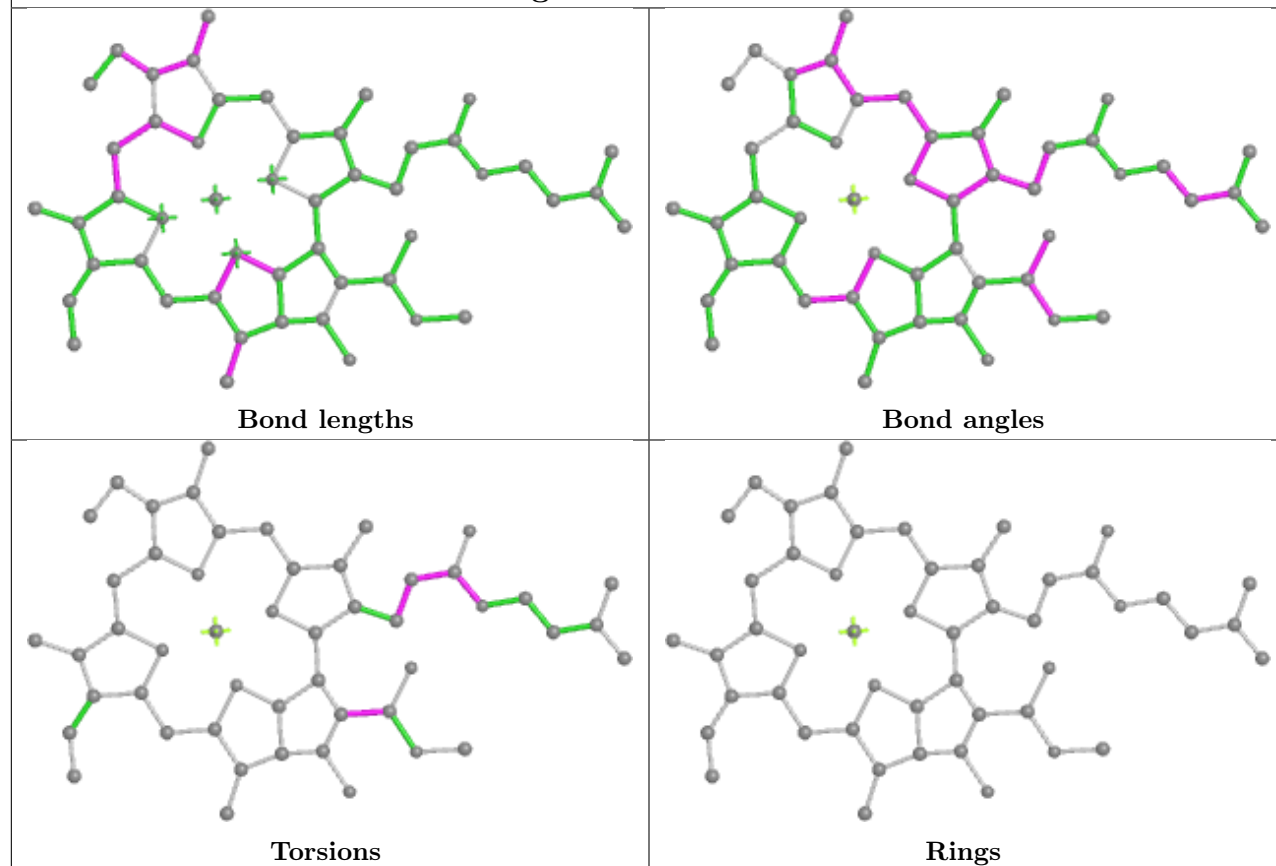
Ligand CLA P 311



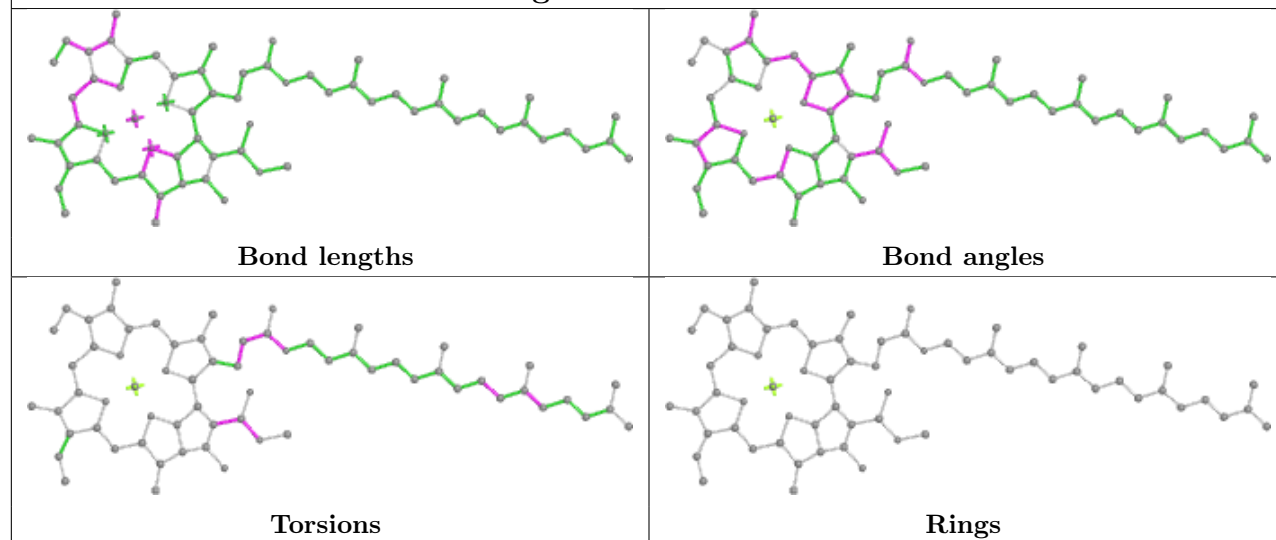


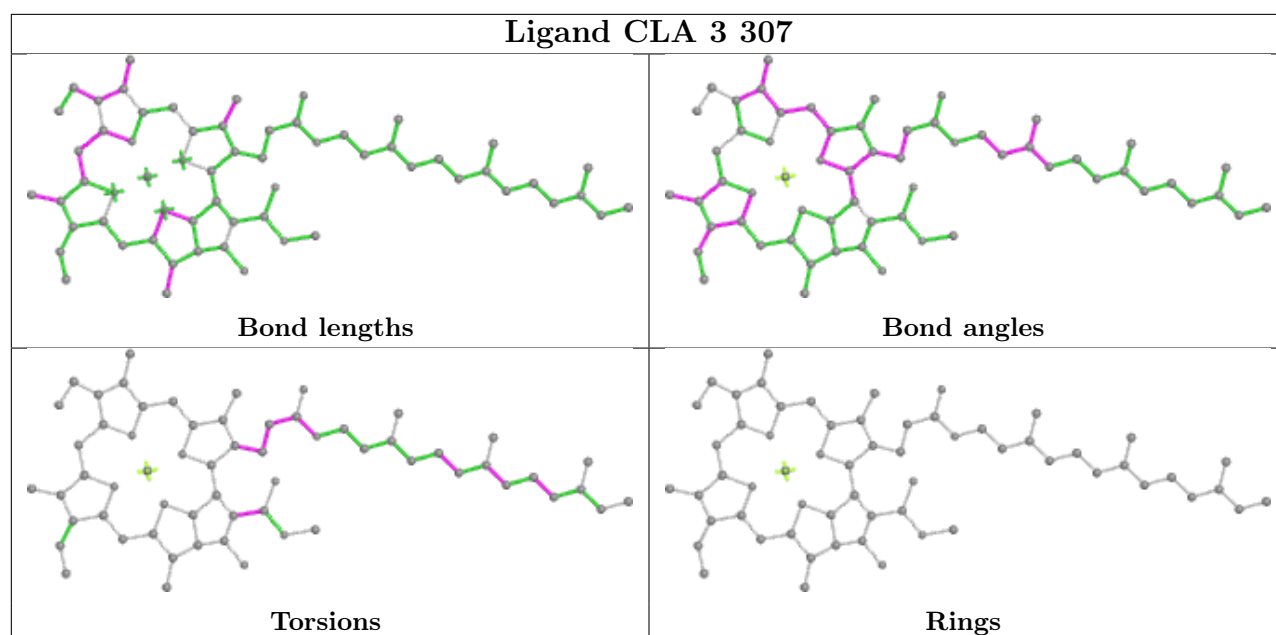


Ligand CLA A 809

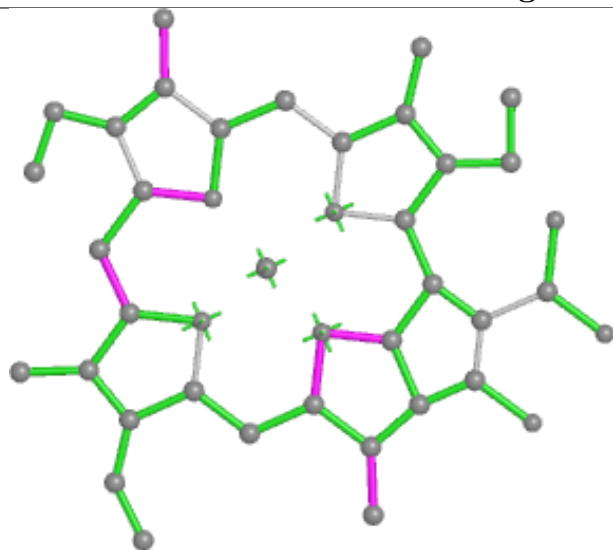


Ligand CLA B 812

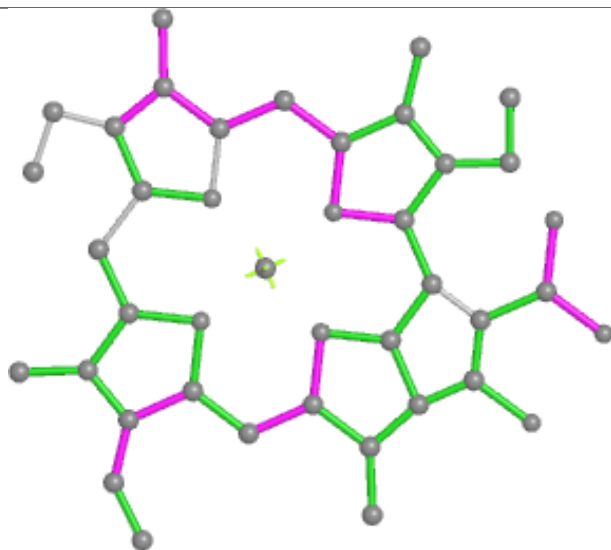




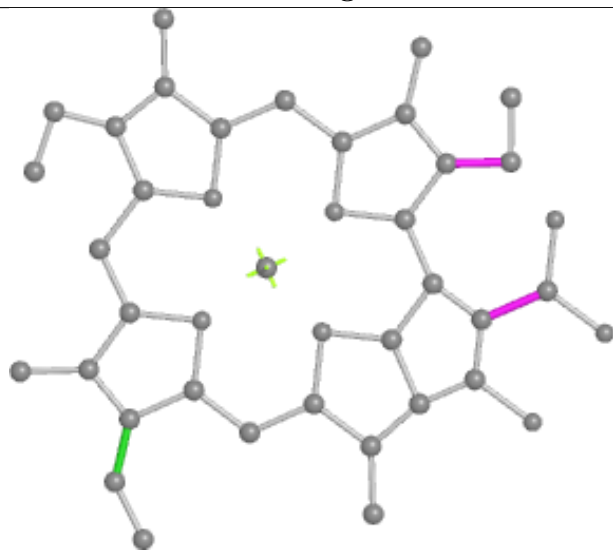
Ligand CLA 4 312



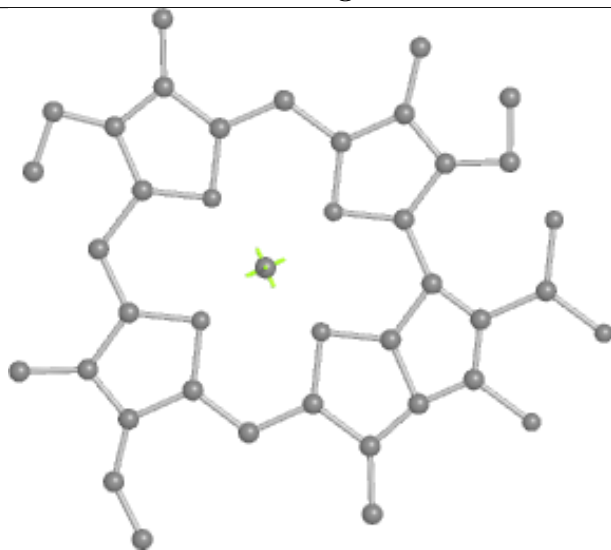
Bond lengths



Bond angles

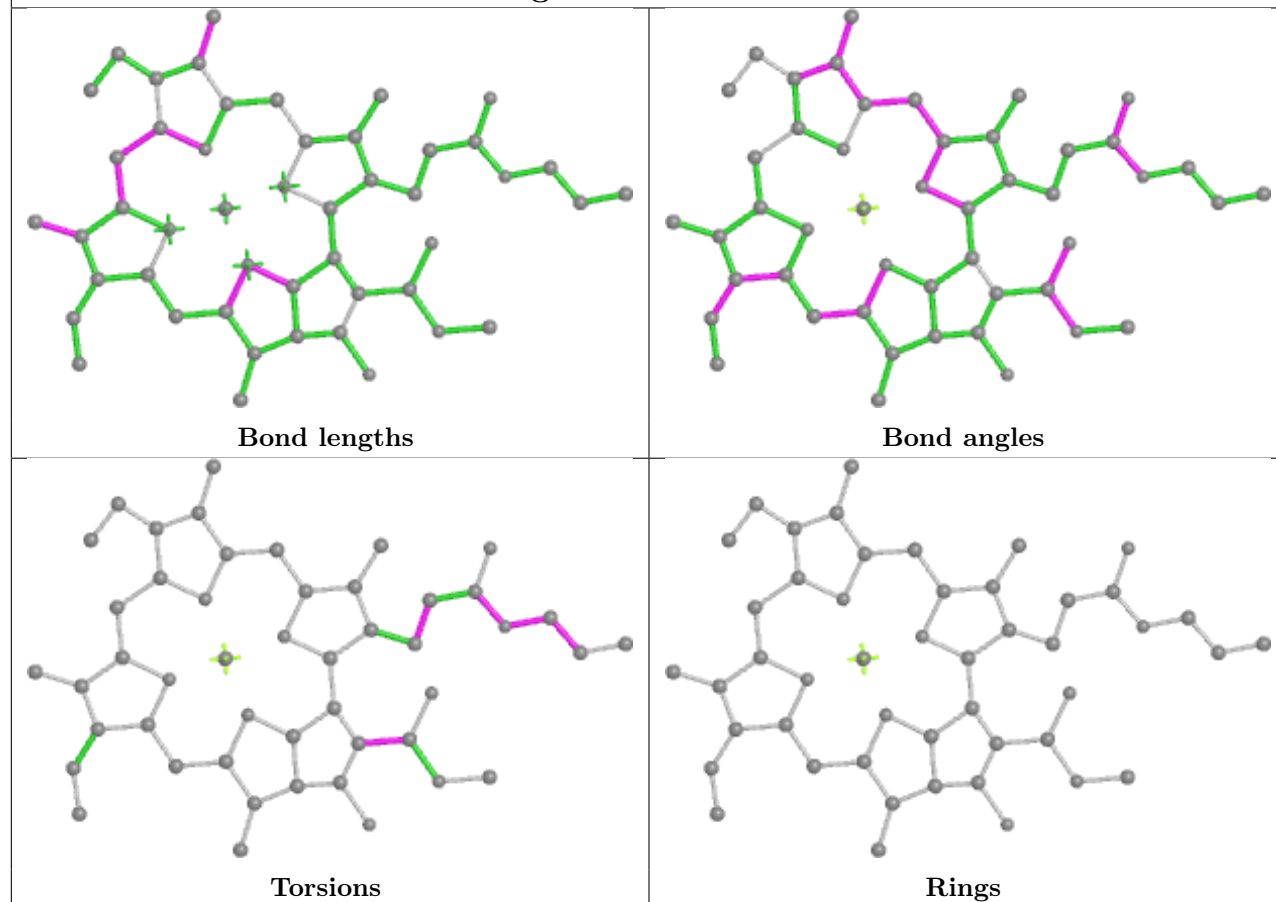


Torsions

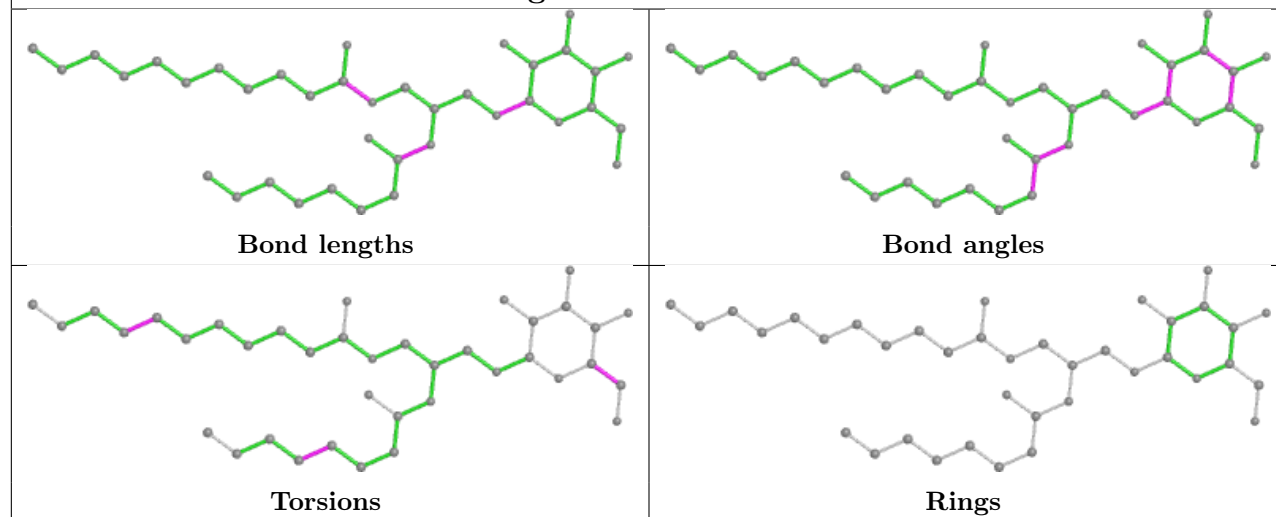


Rings

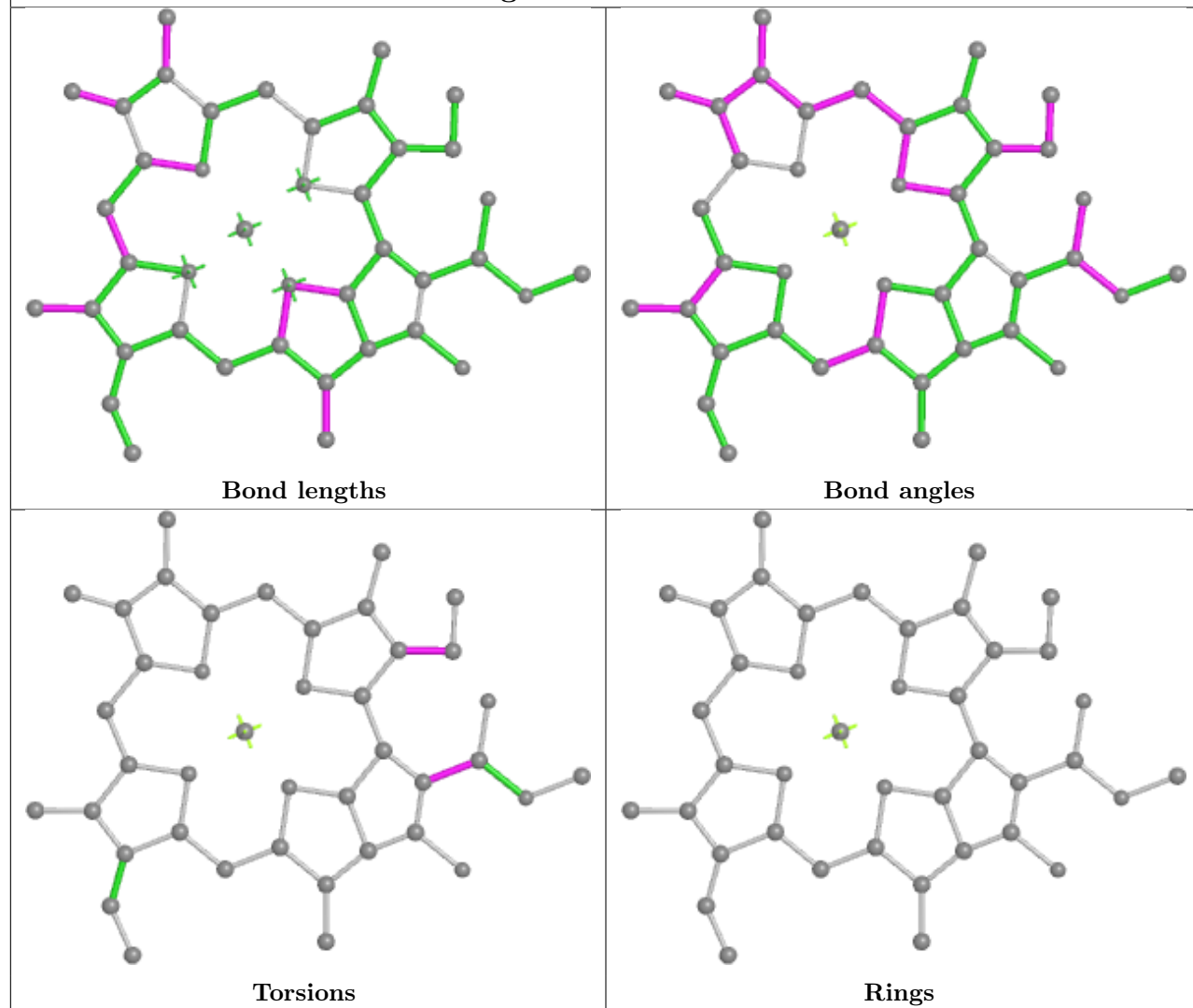
Ligand CLA R 317



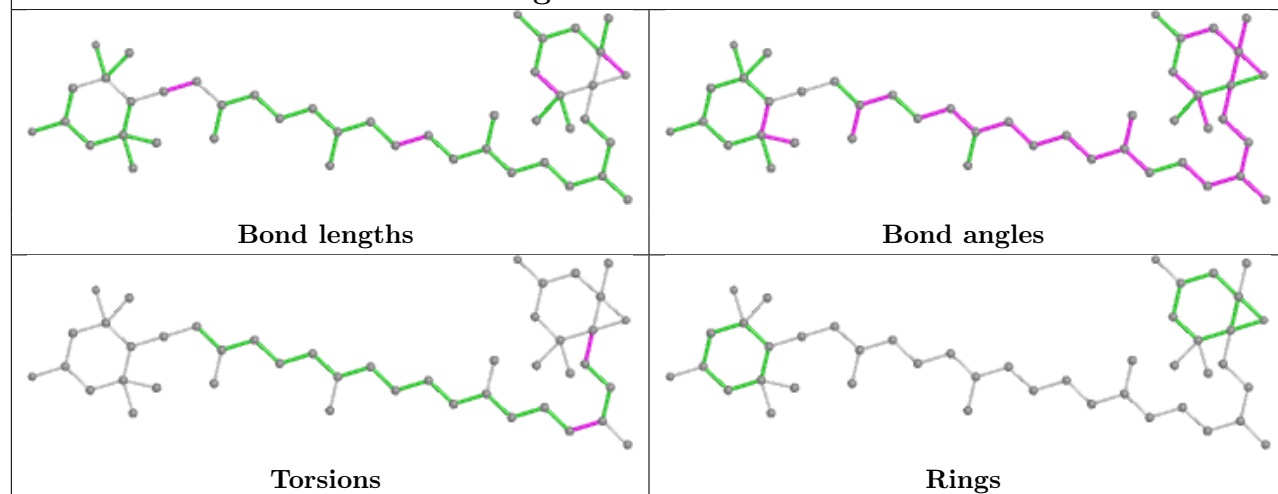
Ligand LMG B 801



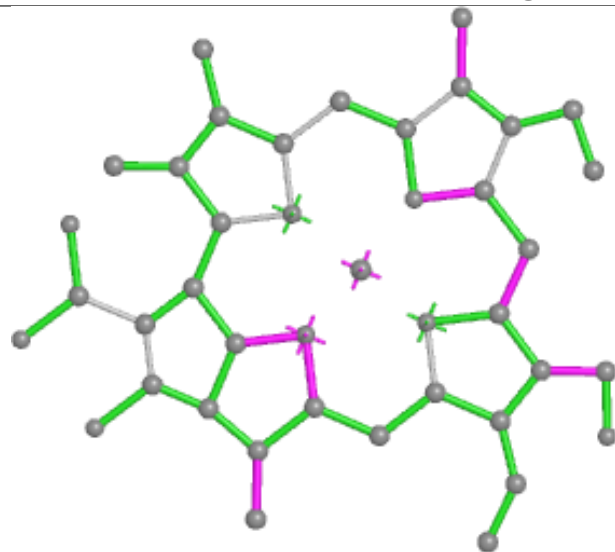
Ligand CLA 3 305



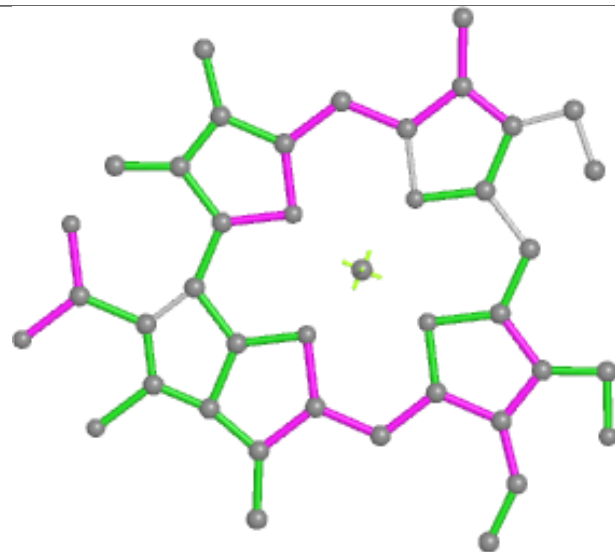
Ligand NEX S 317



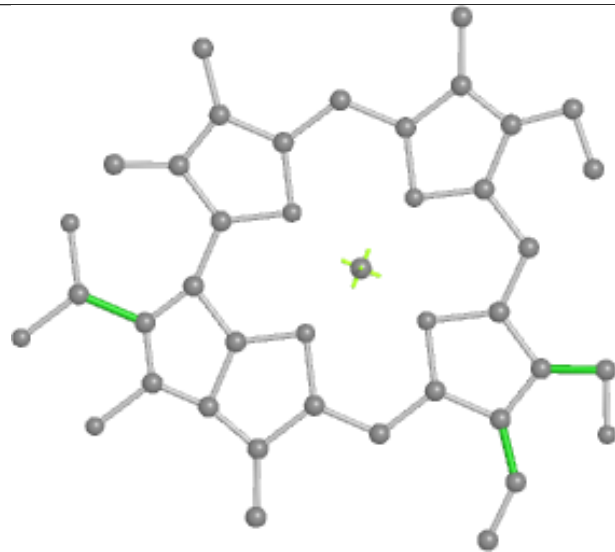
Ligand CHL 1 604



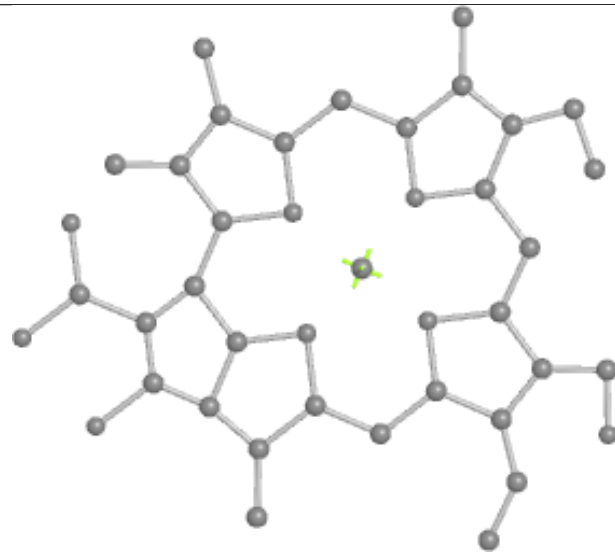
Bond lengths



Bond angles

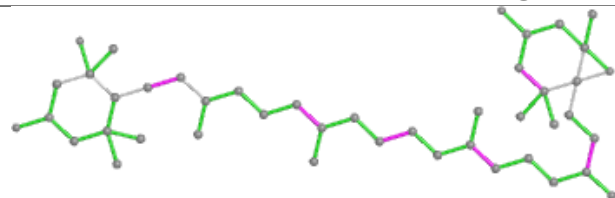


Torsions

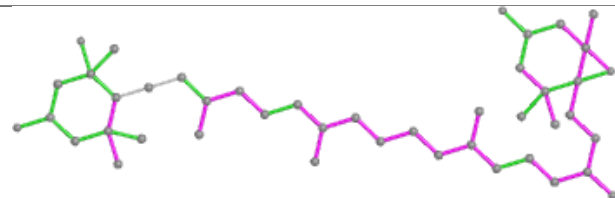


Rings

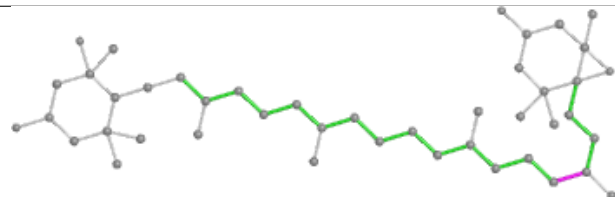
Ligand NEX P 317



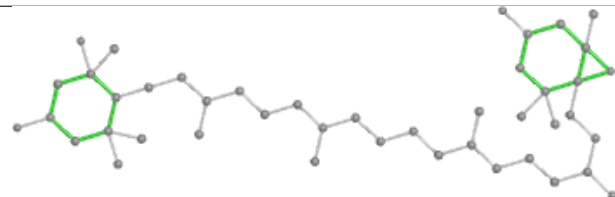
Bond lengths



Bond angles

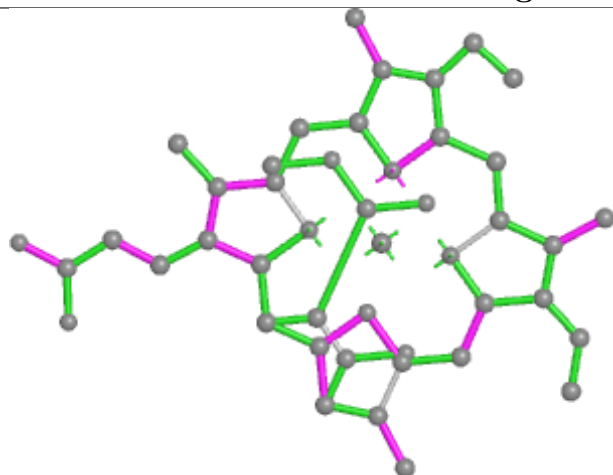


Torsions

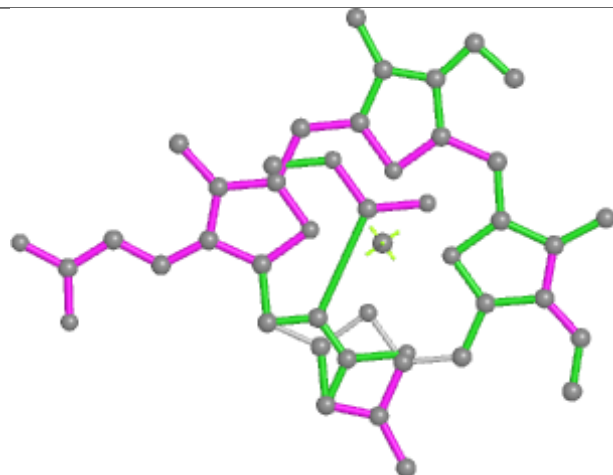


Rings

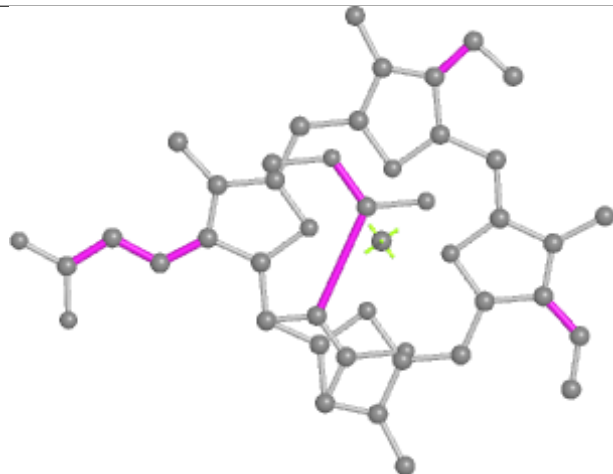
Ligand KC2 U 307



Bond lengths



Bond angles

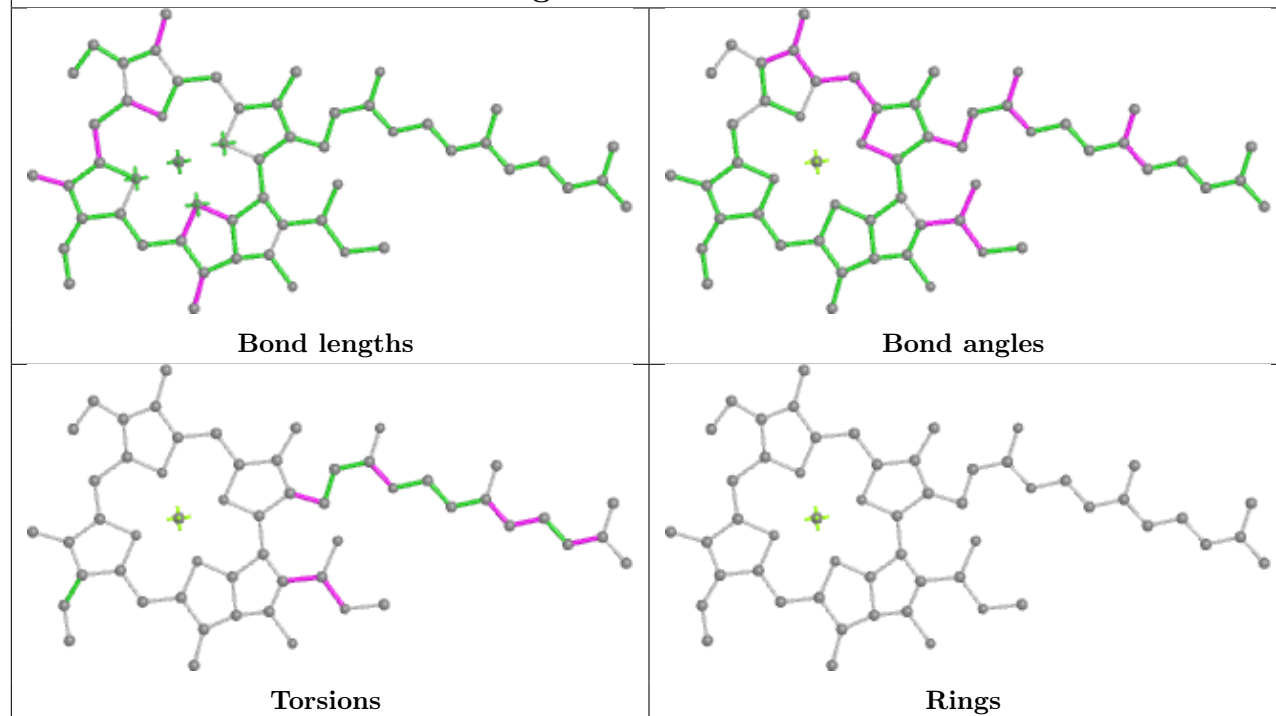


Torsions

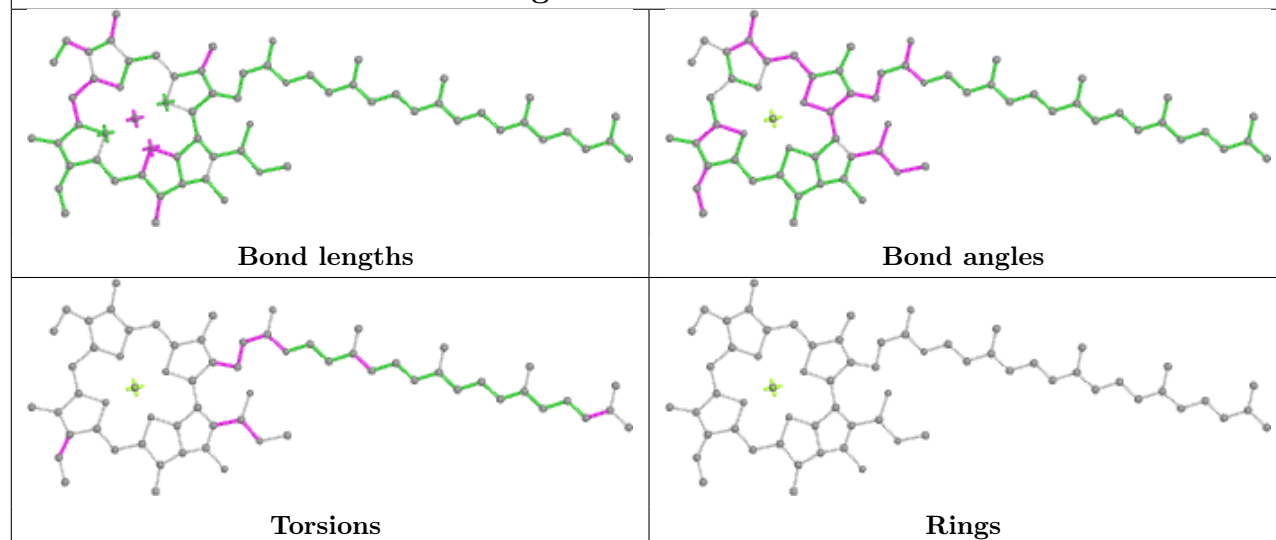


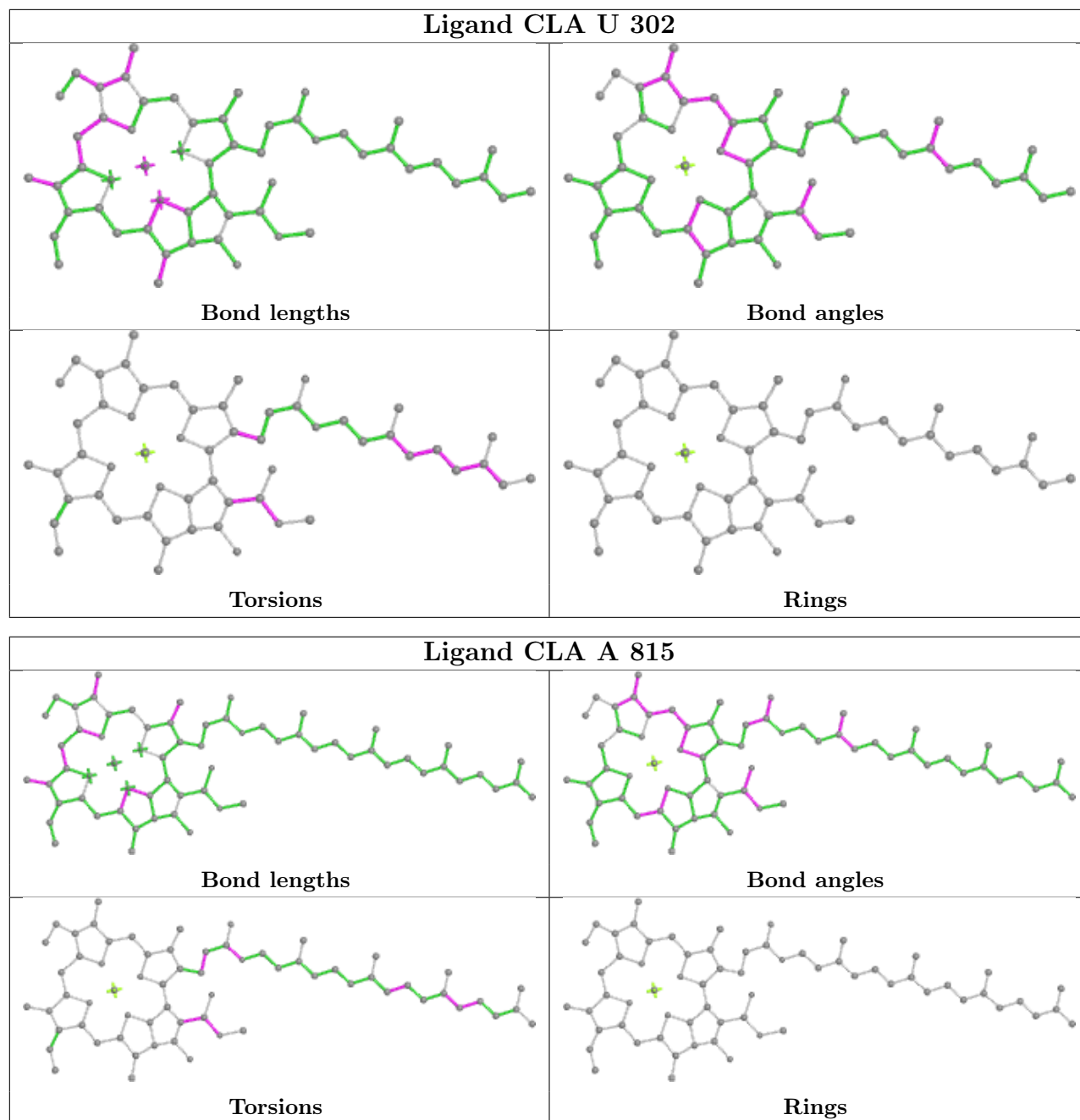
Rings

Ligand CLA T 312

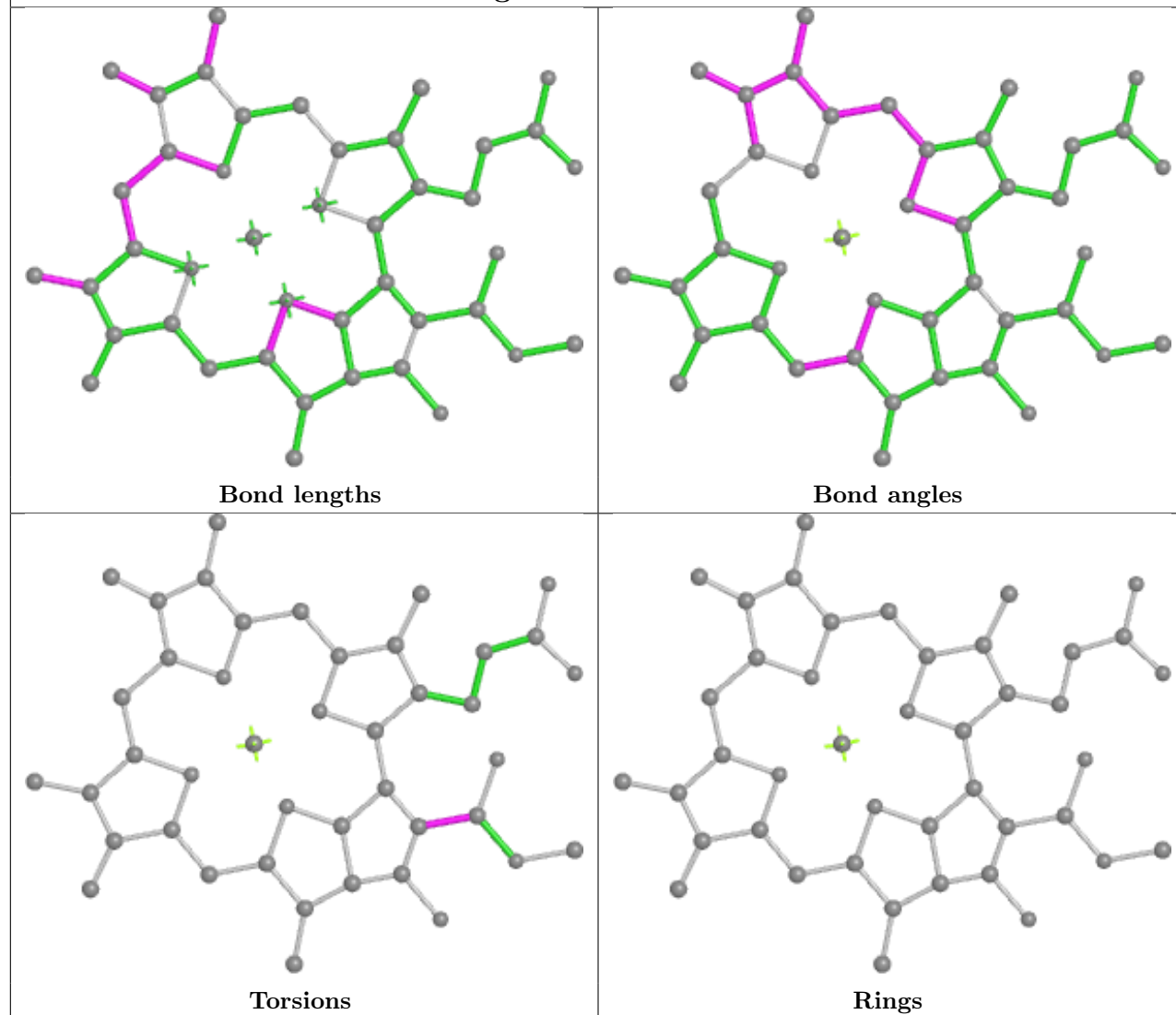


Ligand CLA A 829

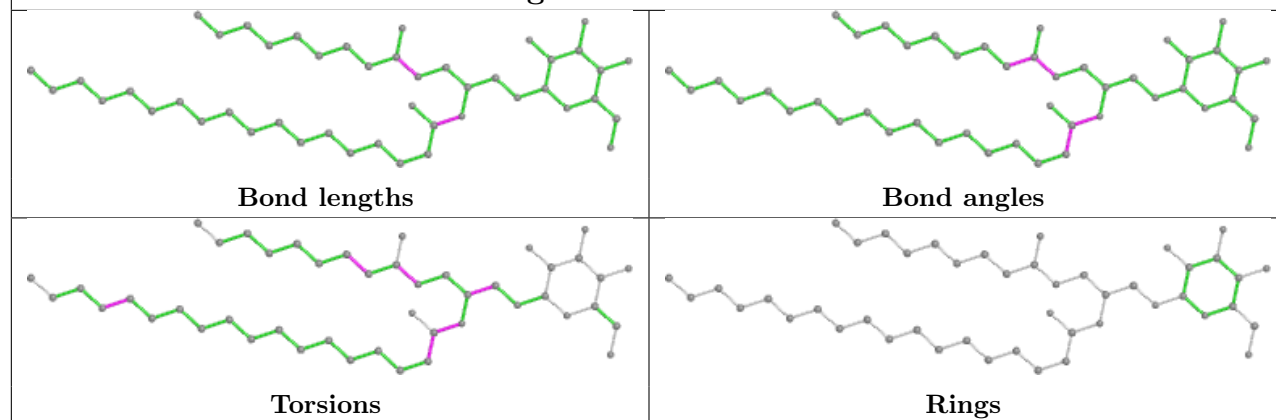




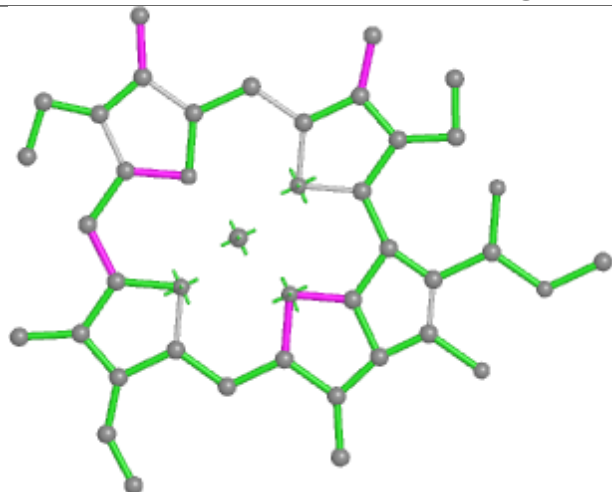
Ligand CLA 4 305



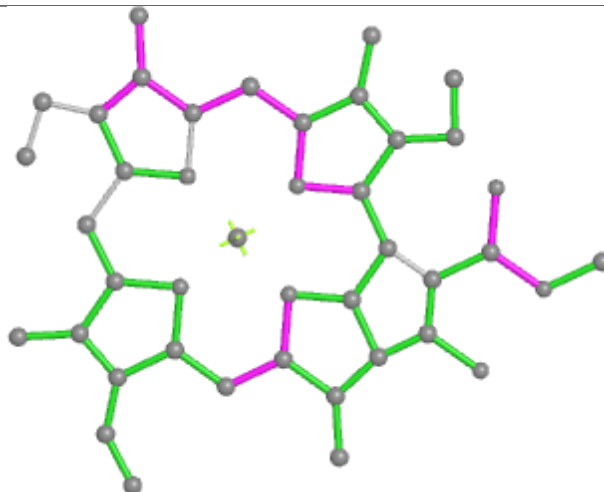
Ligand LMG A 857



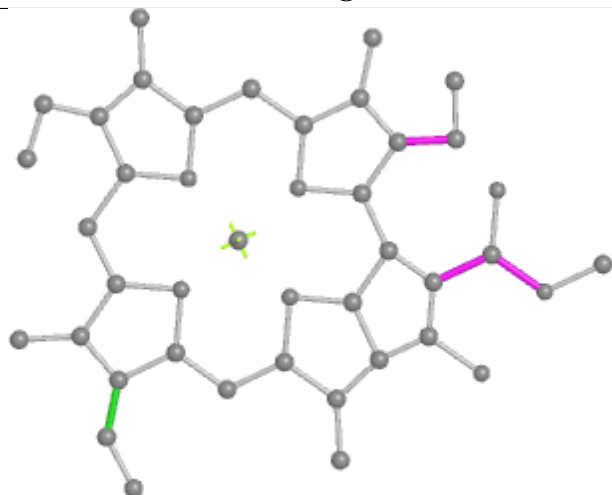
Ligand CLA 6 608



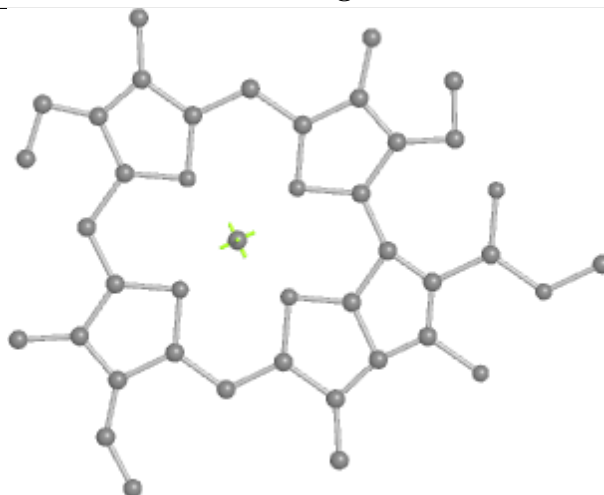
Bond lengths



Bond angles

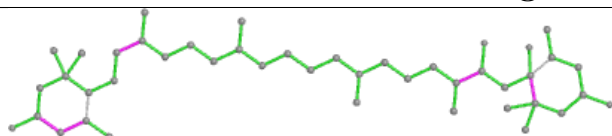


Torsions

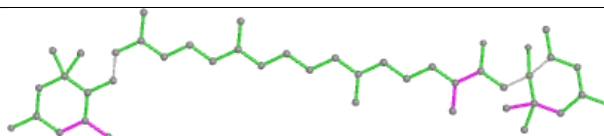


Rings

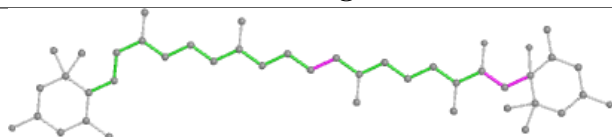
Ligand IWJ S 322



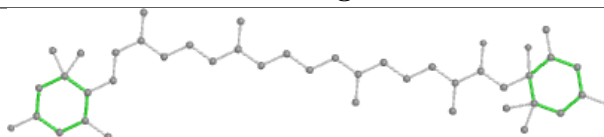
Bond lengths



Bond angles

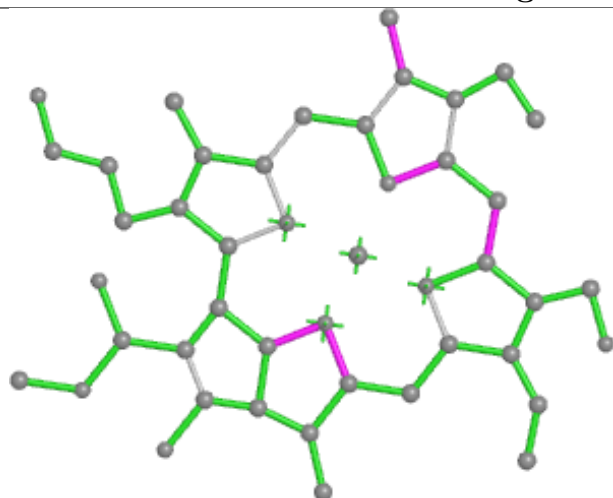


Torsions

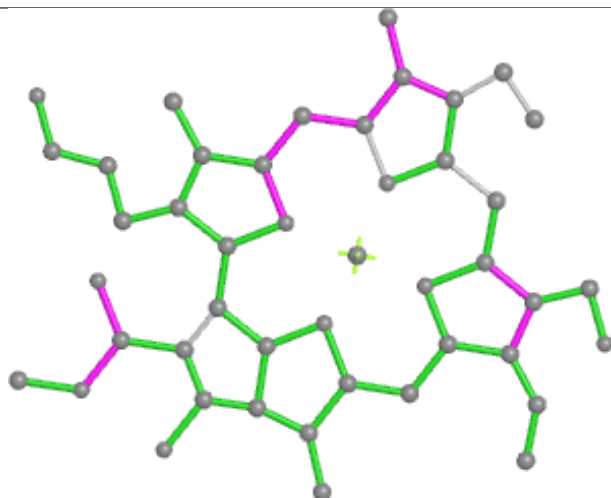


Rings

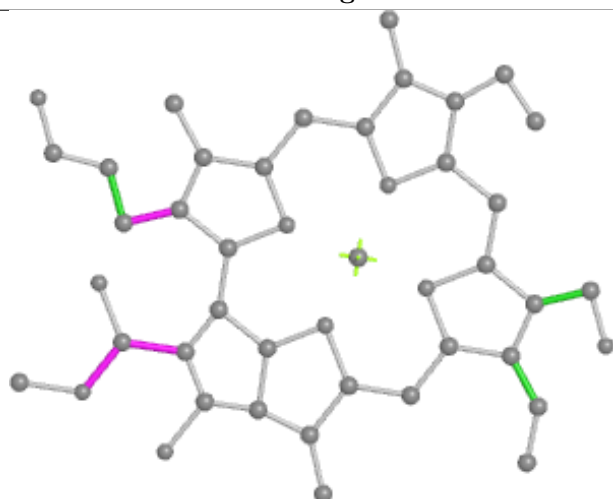
Ligand CHL S 314



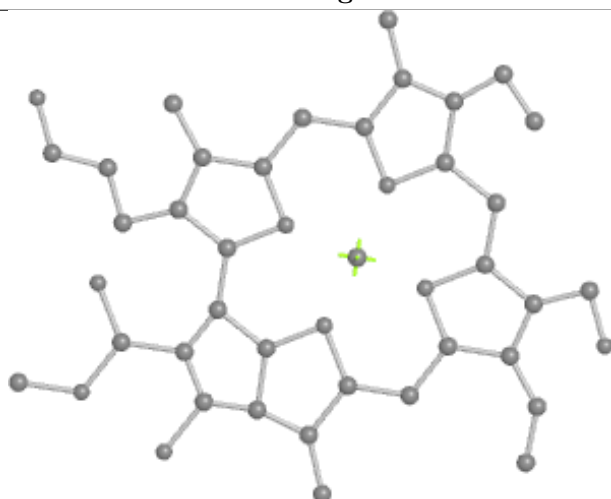
Bond lengths



Bond angles

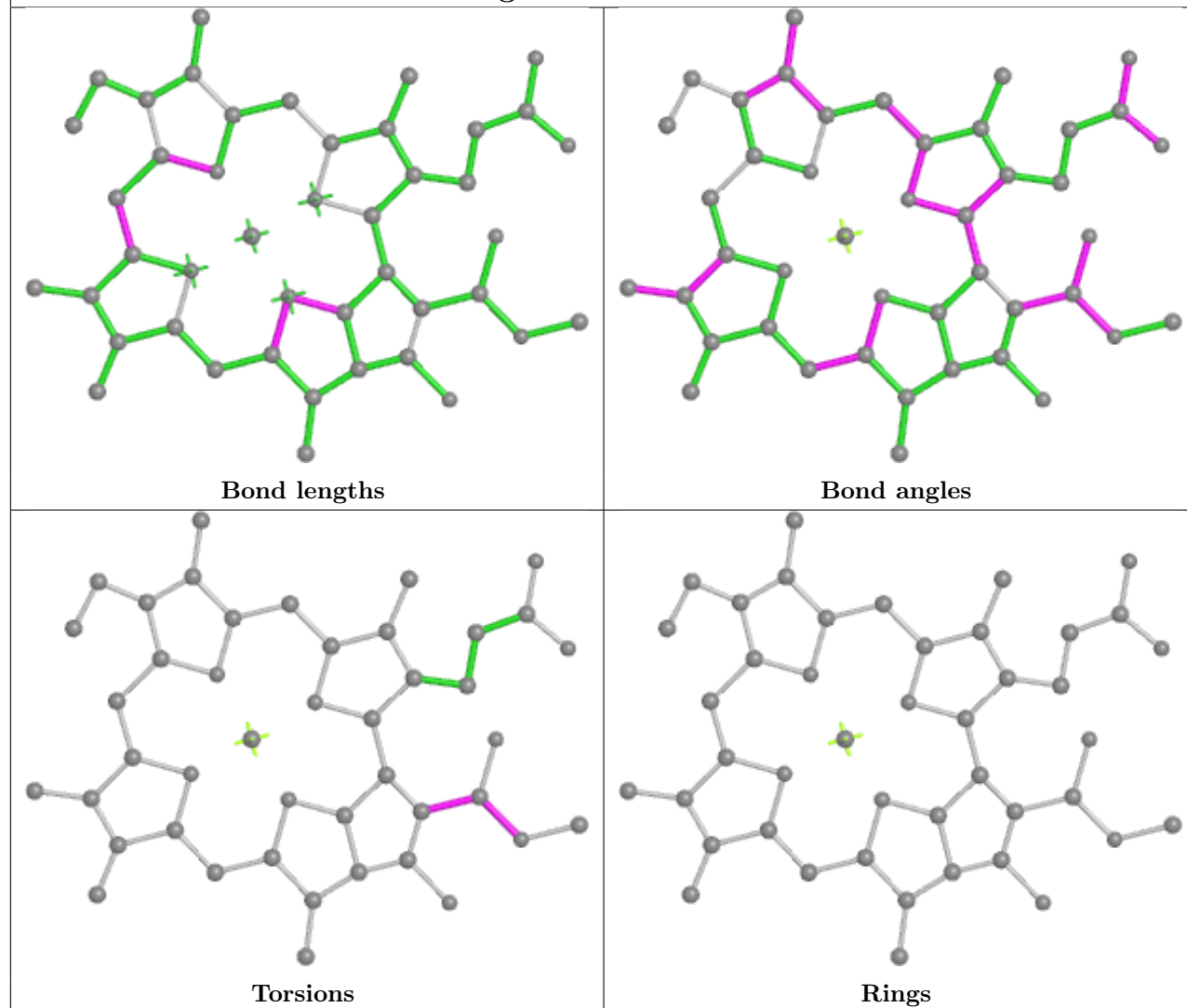


Torsions

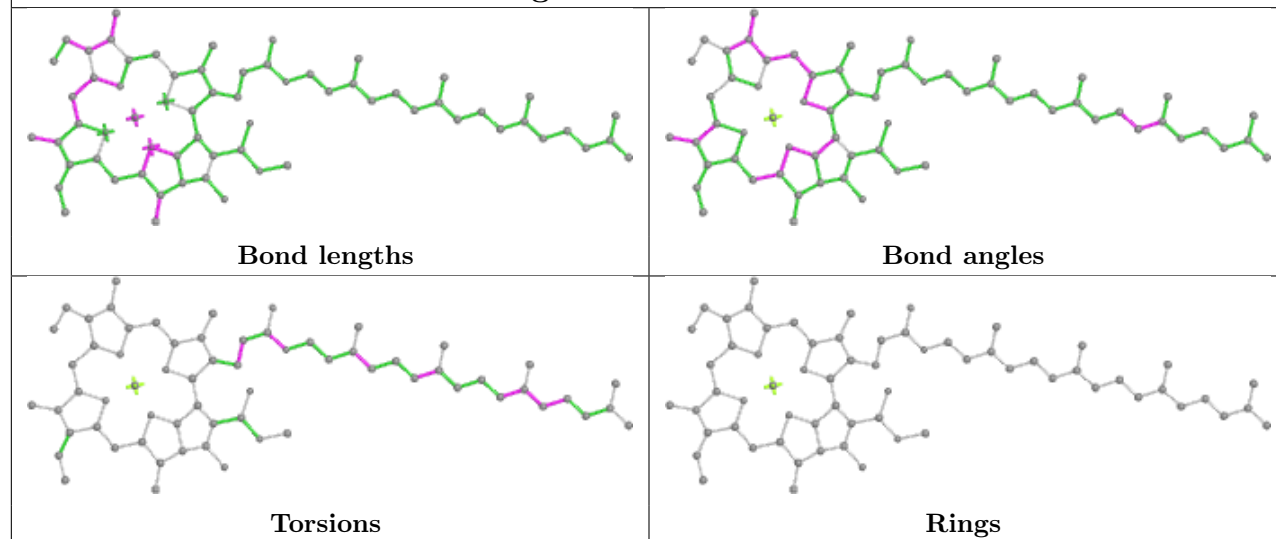


Rings

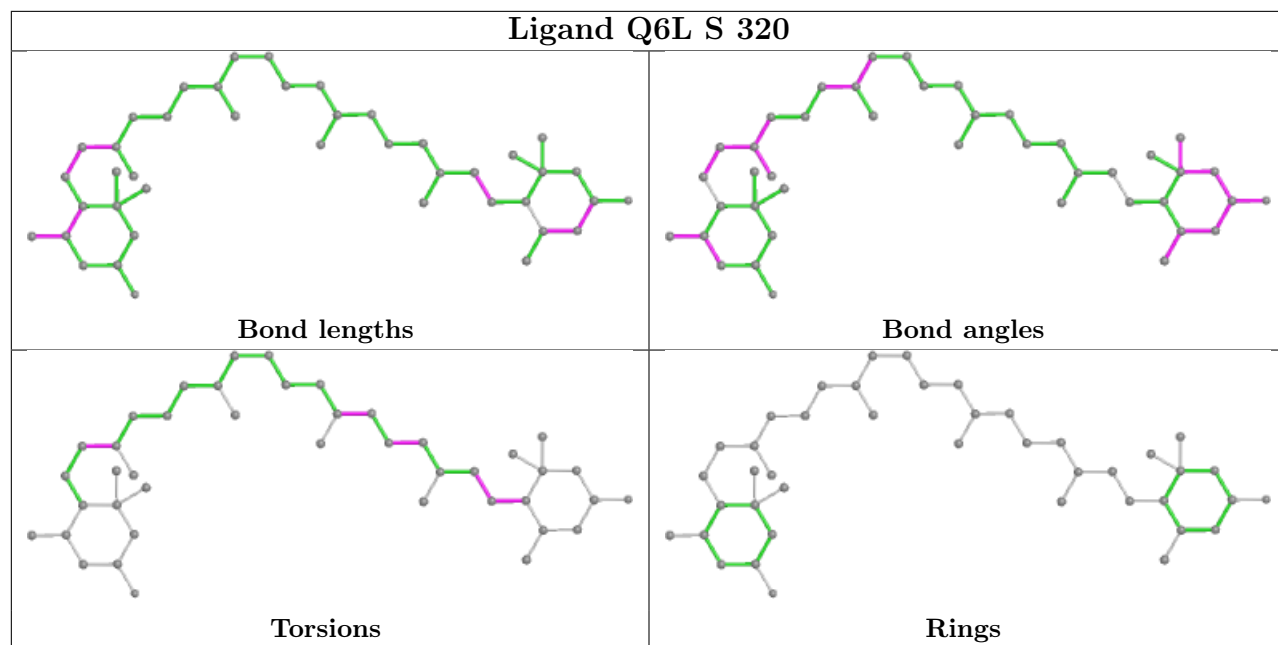
Ligand CLA 6 609



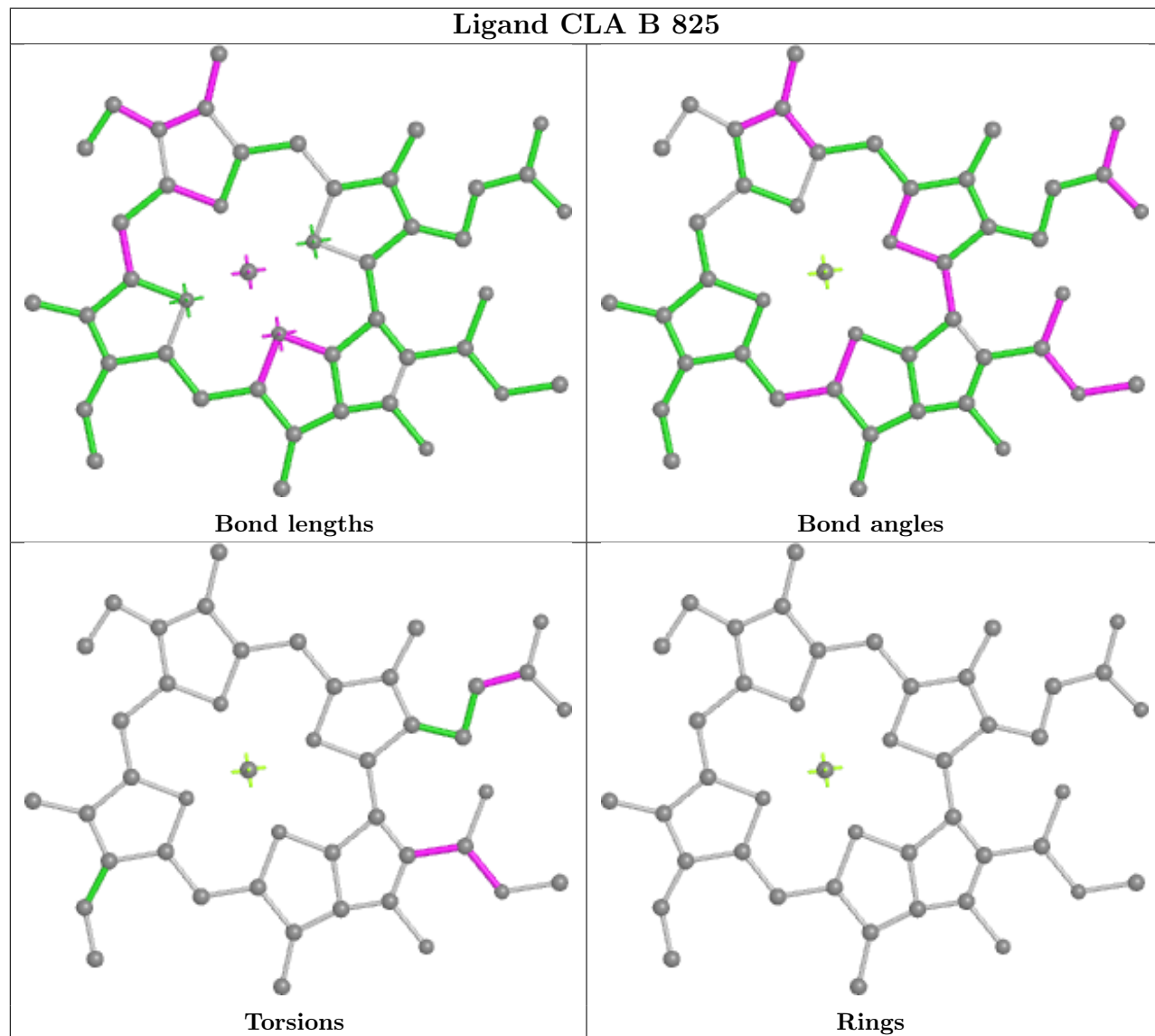
Ligand CLA A 808

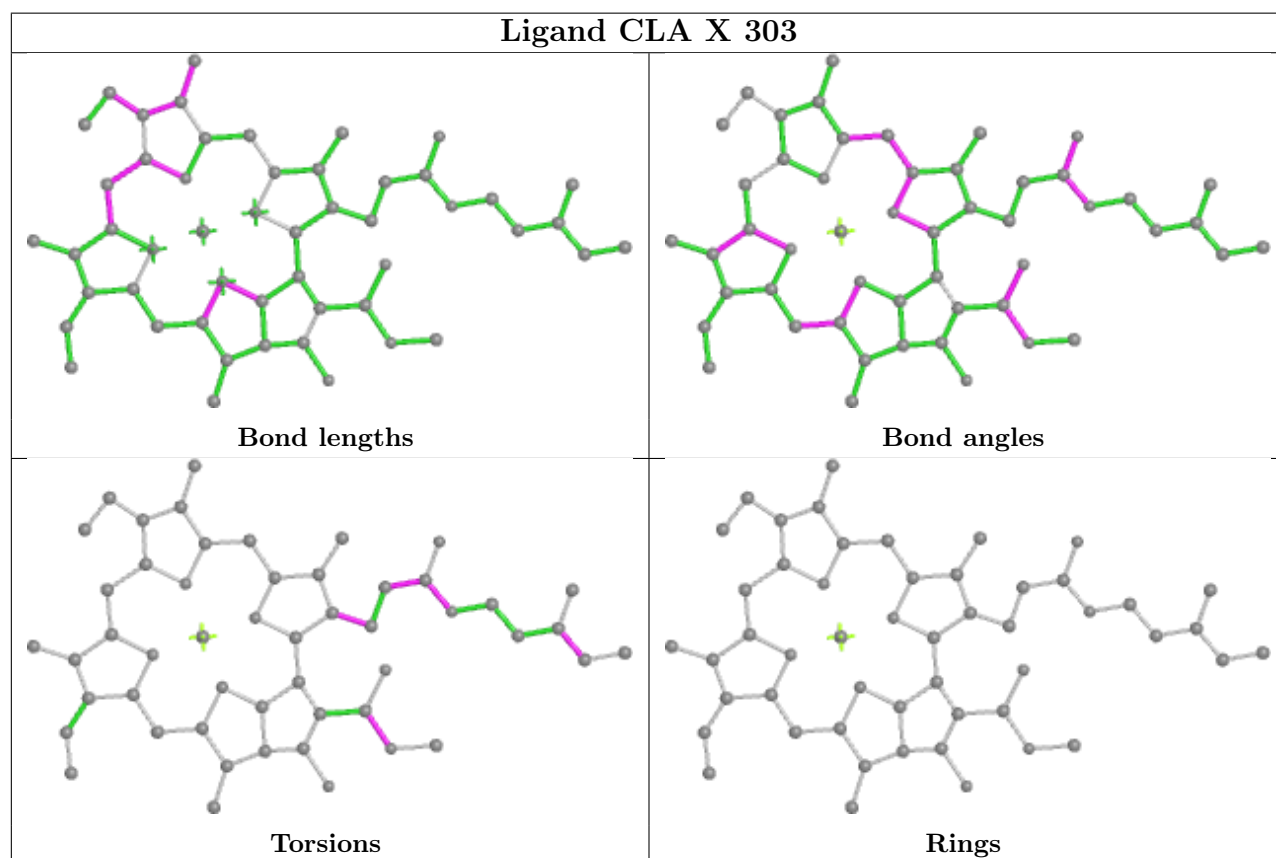
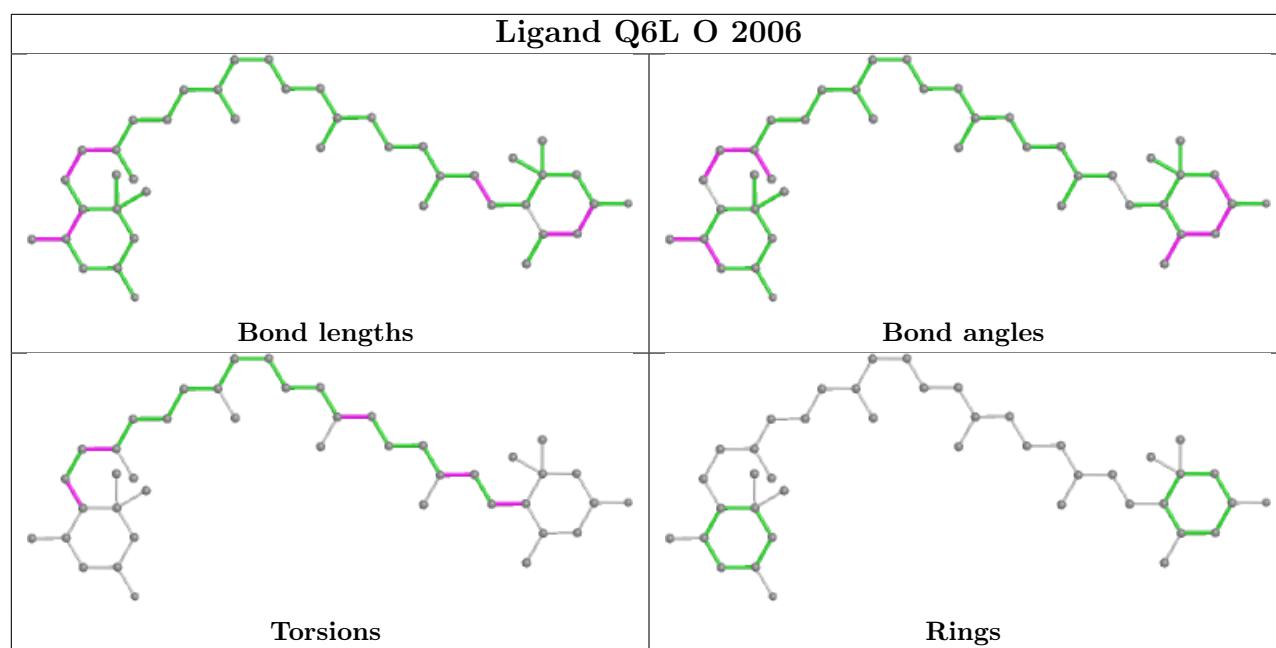


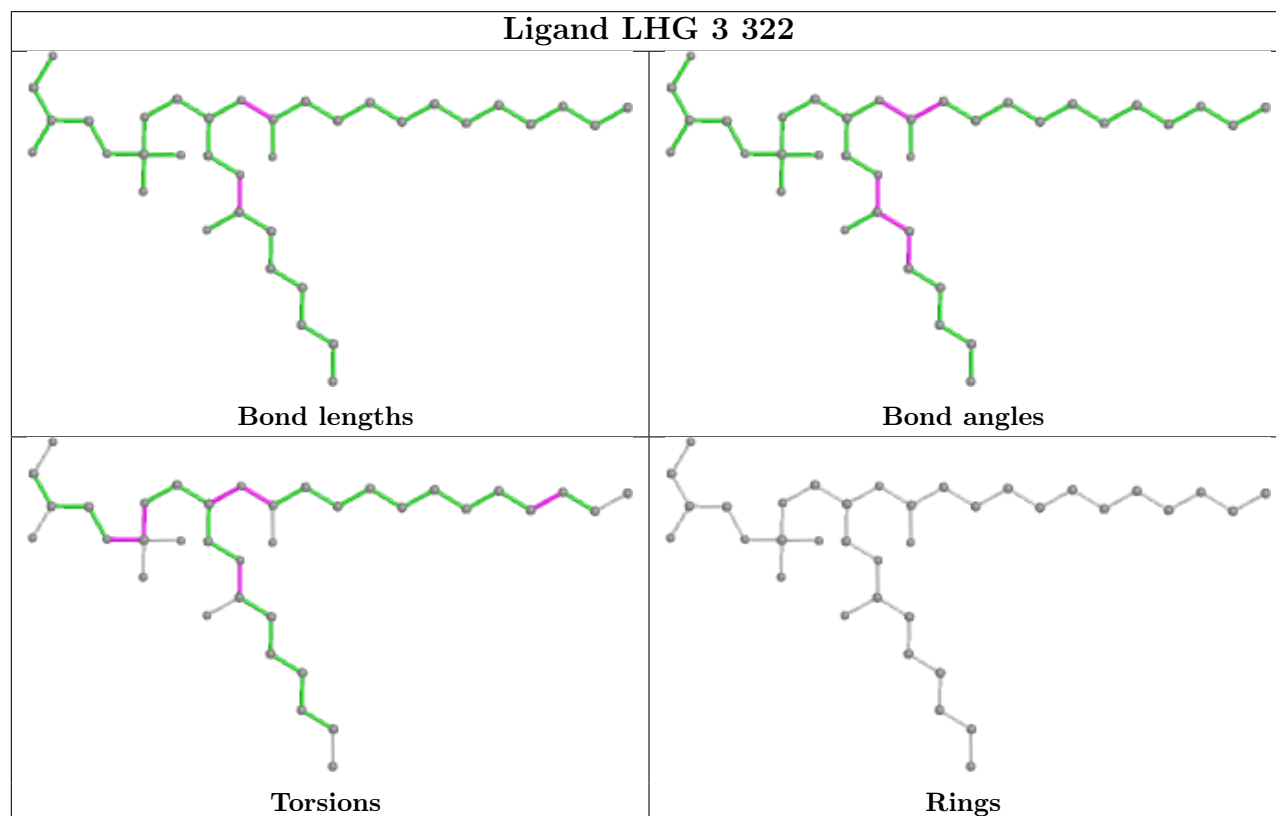
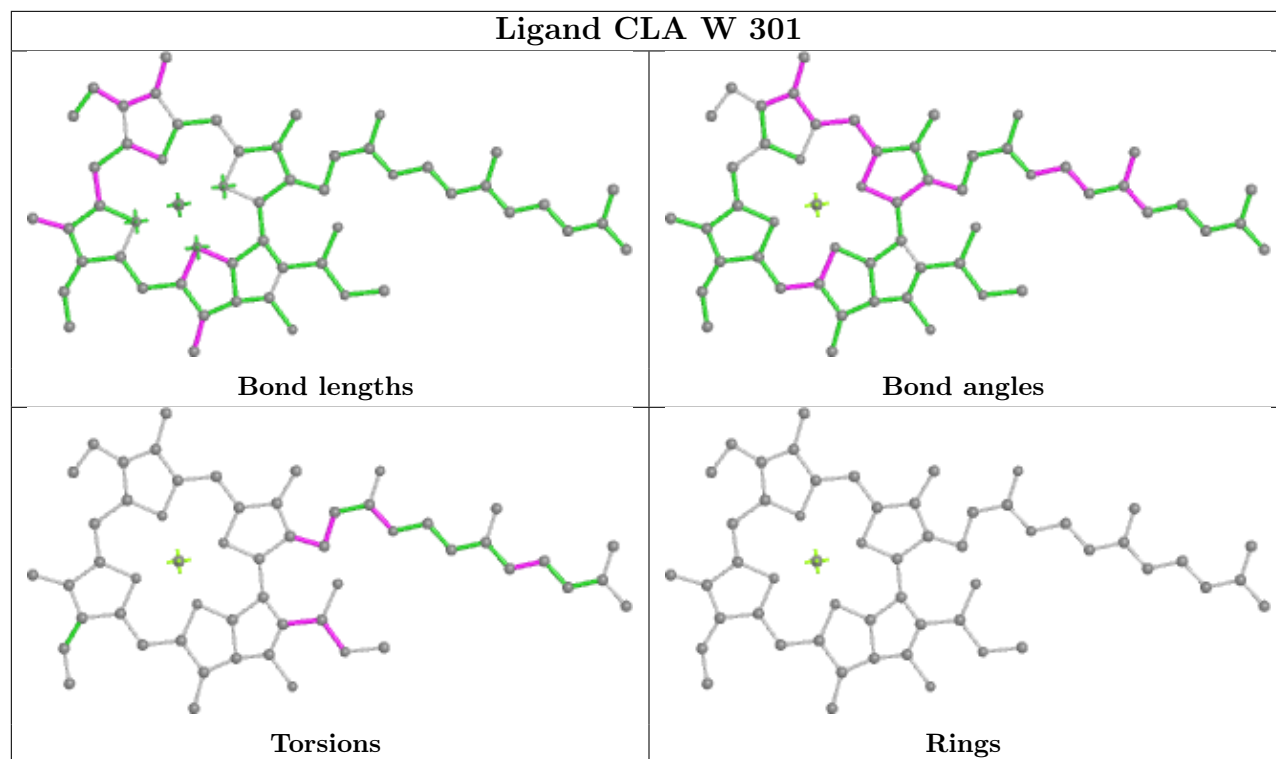
Ligand Q6L S 320

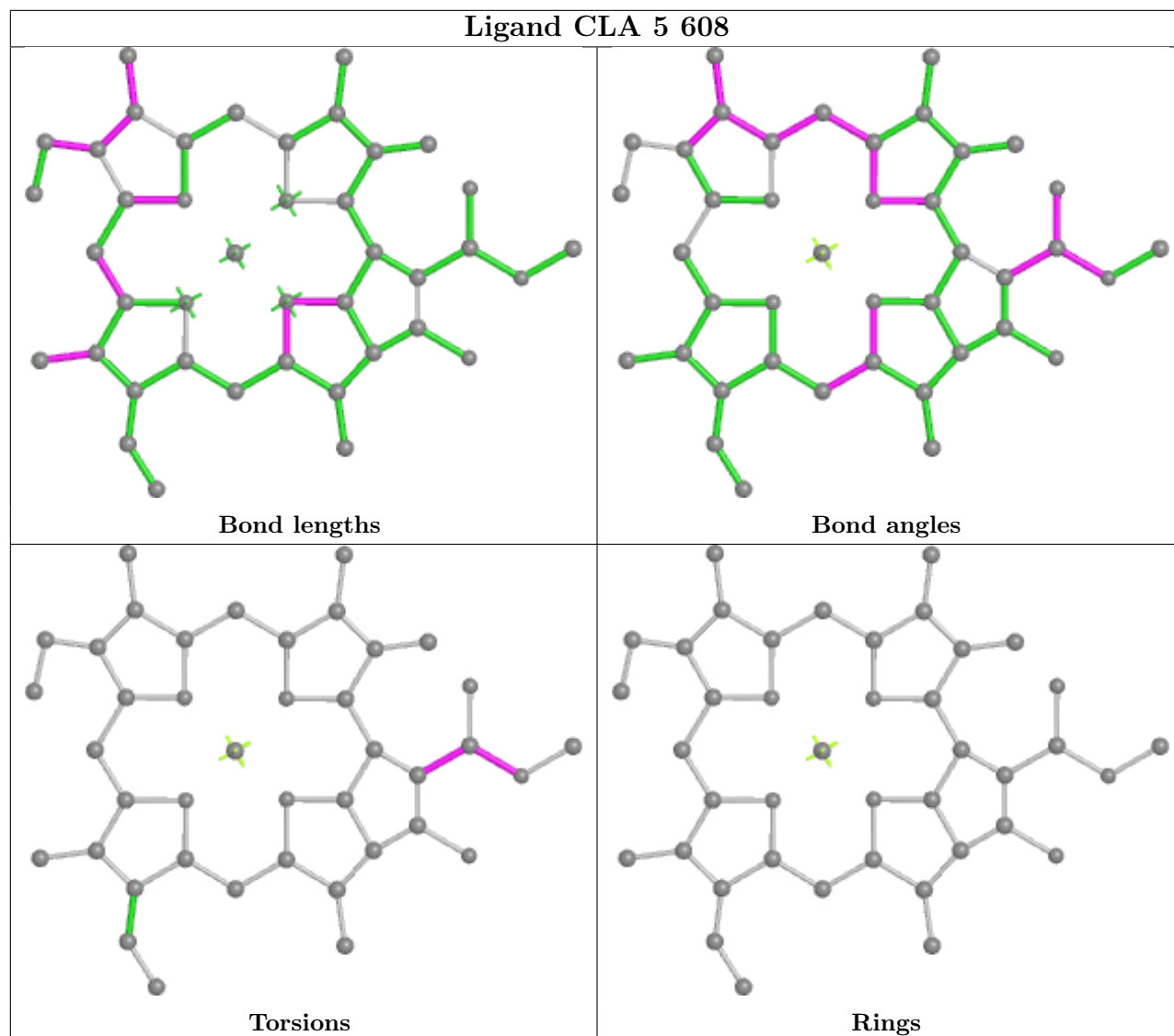
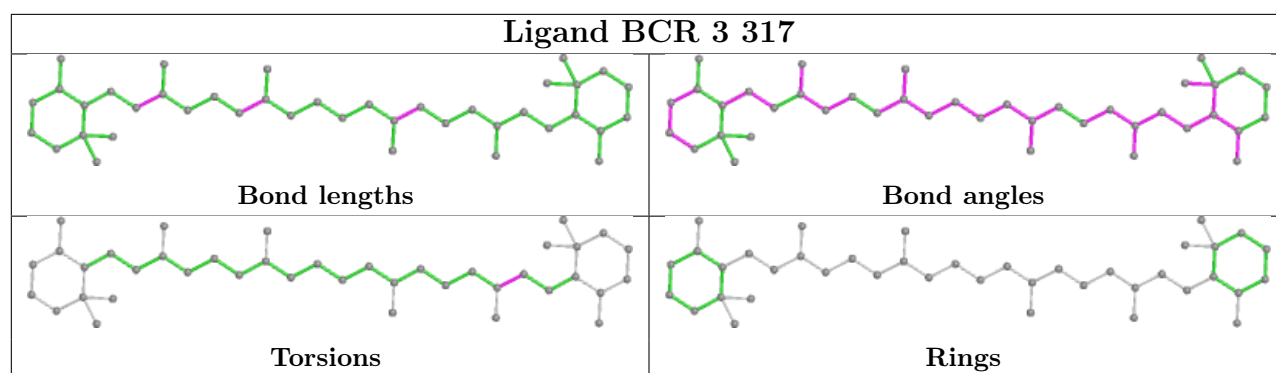


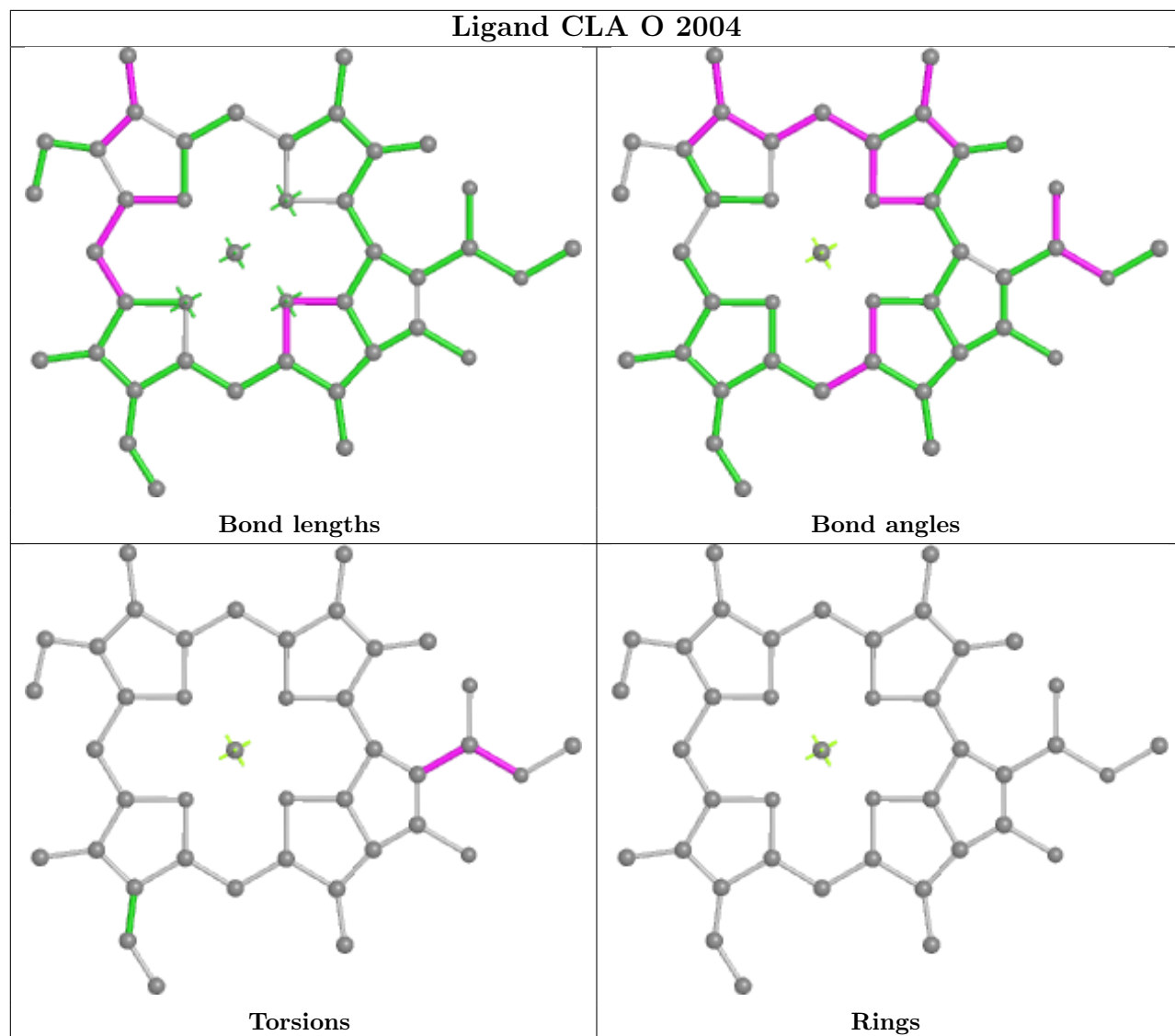
Ligand CLA B 825

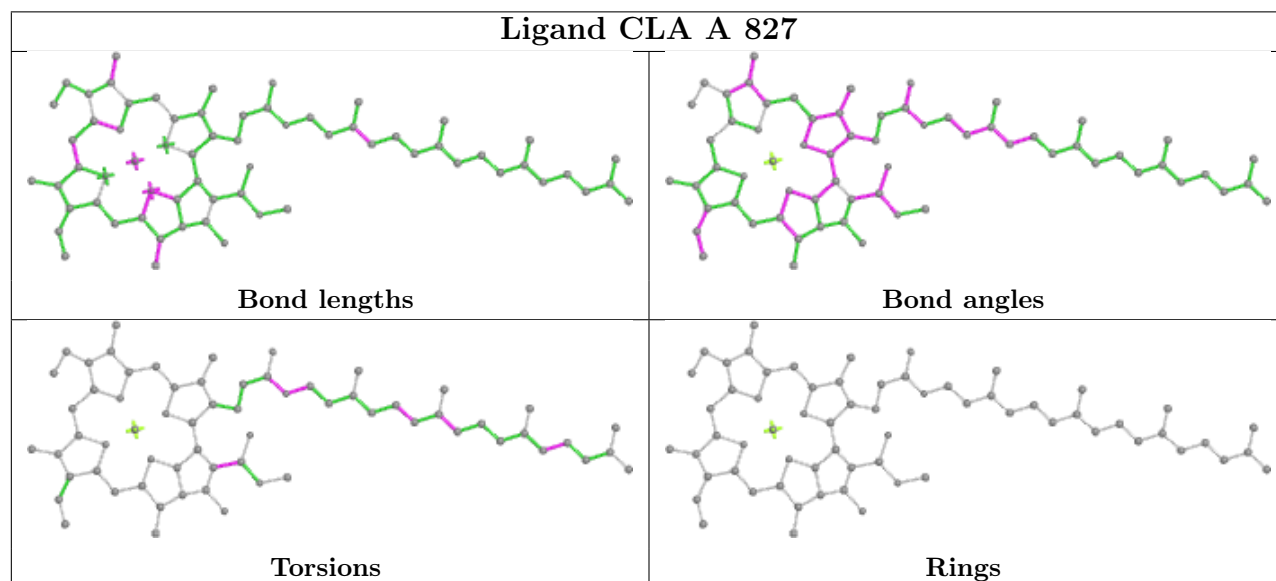
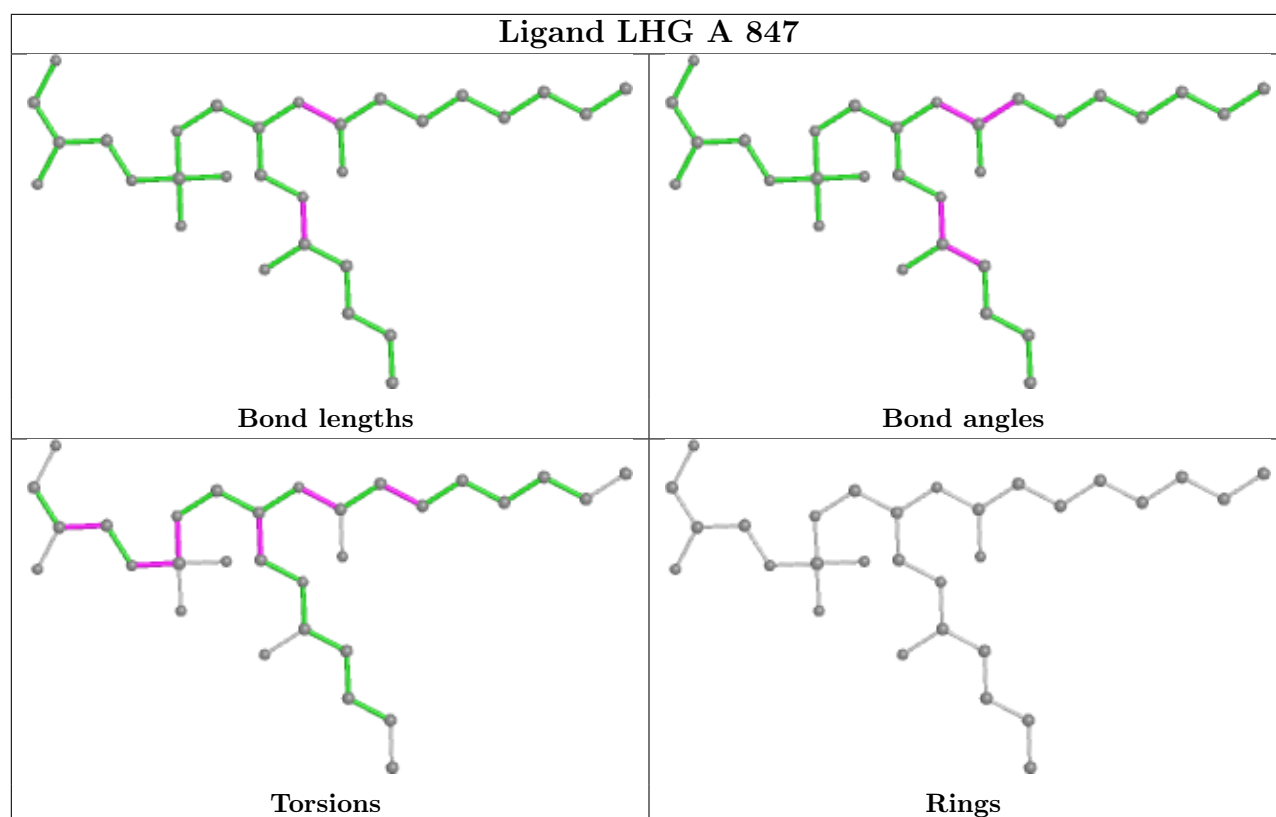




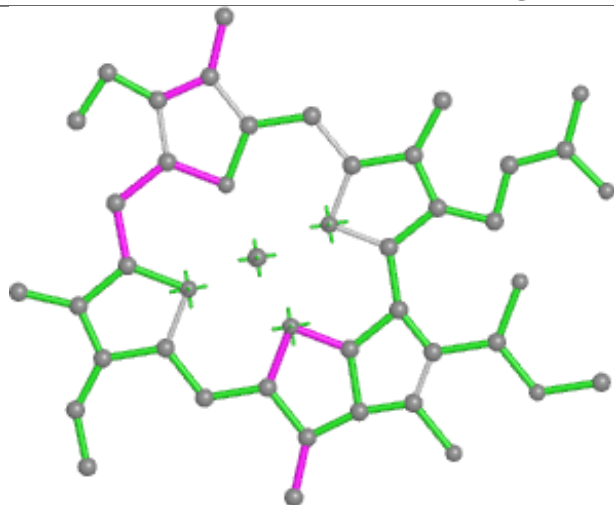




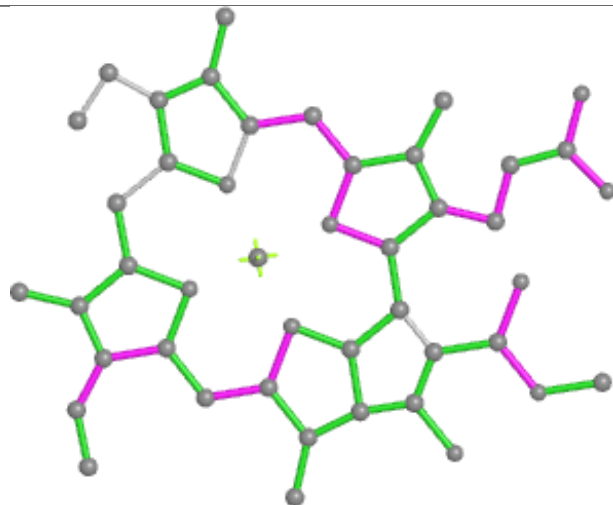




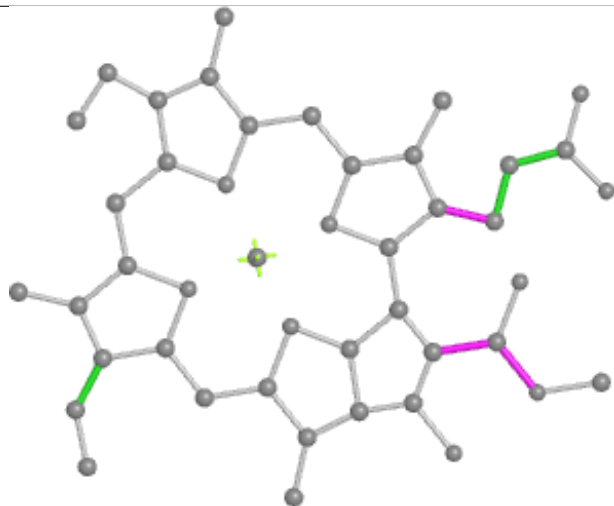
Ligand CLA G 202



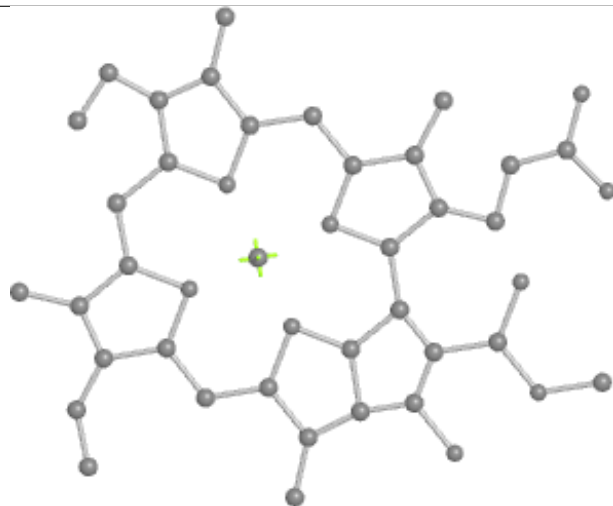
Bond lengths



Bond angles

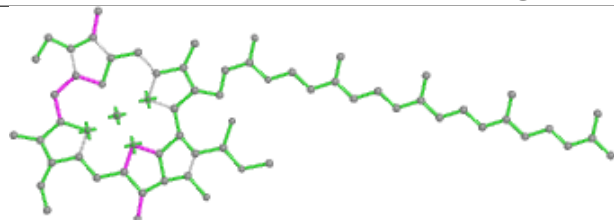


Torsions

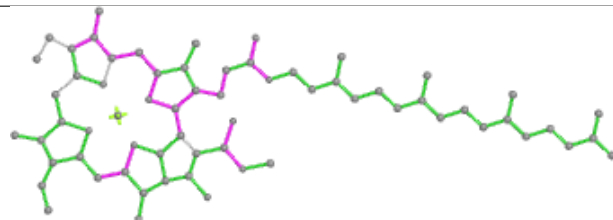


Rings

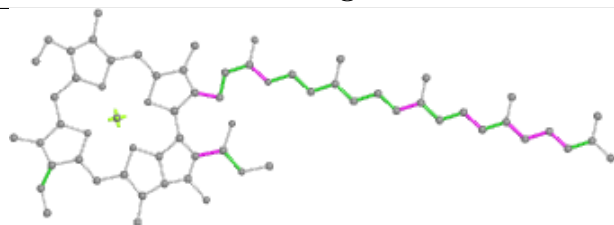
Ligand CLA B 807



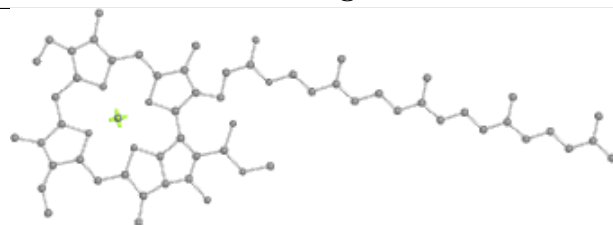
Bond lengths



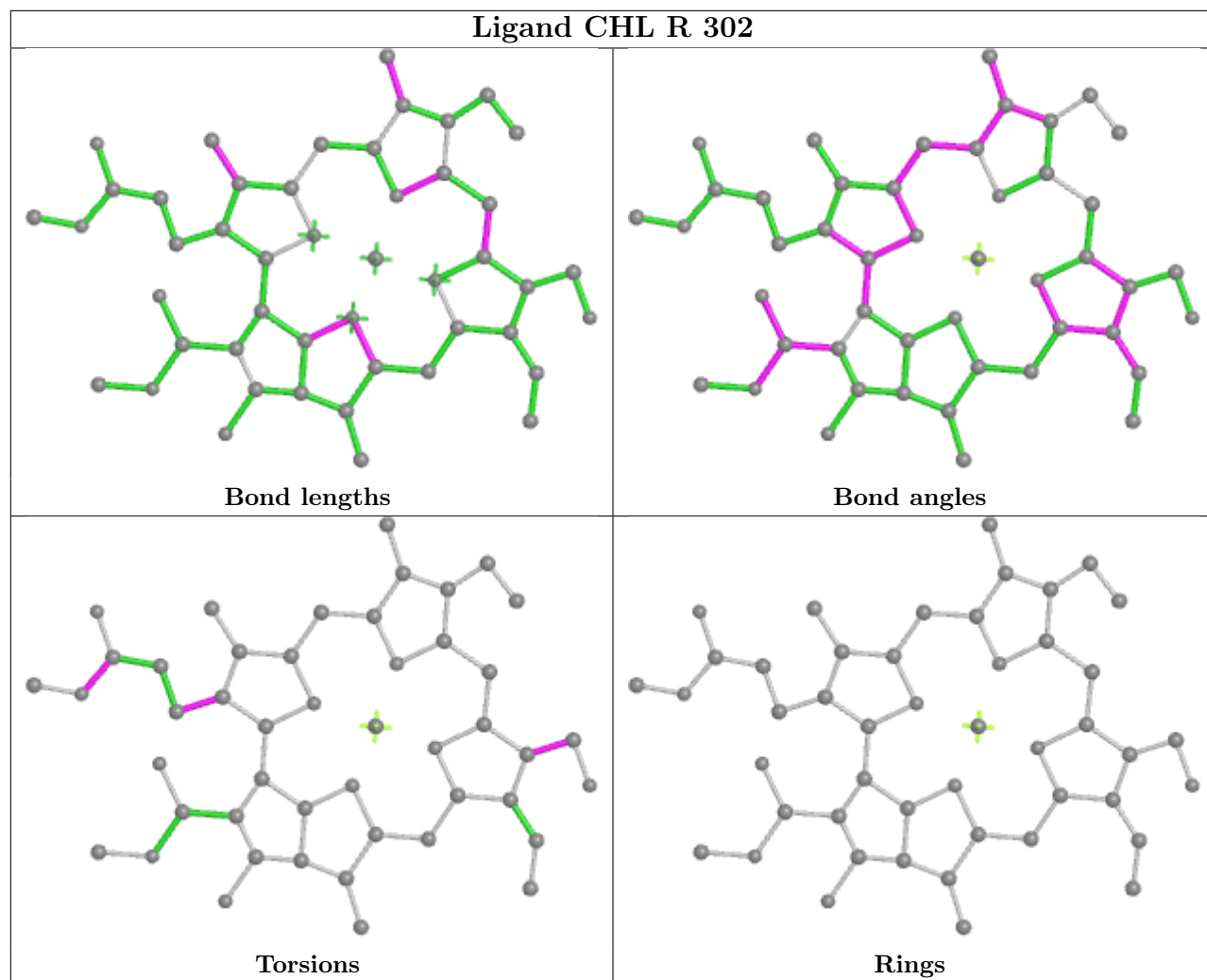
Bond angles

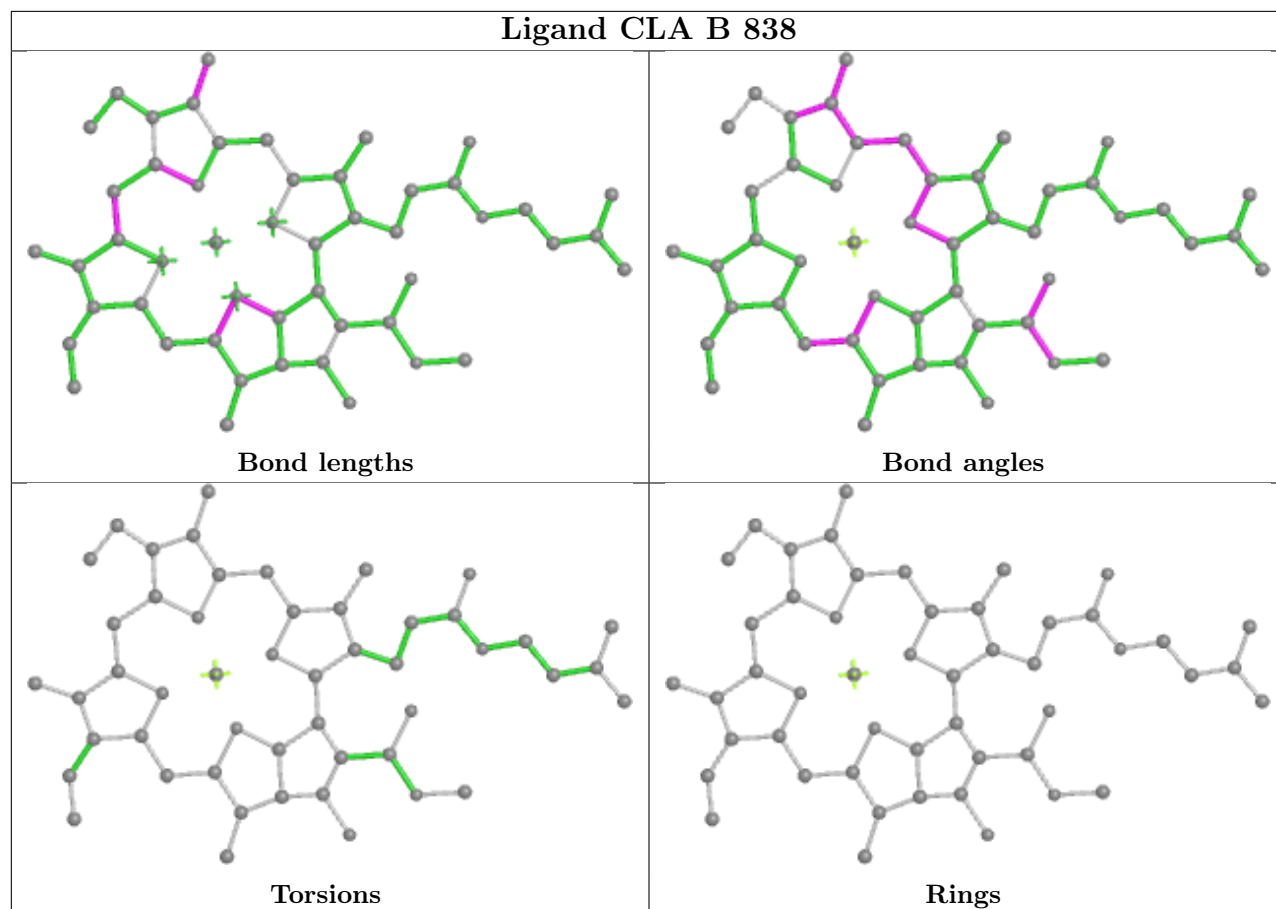


Torsions

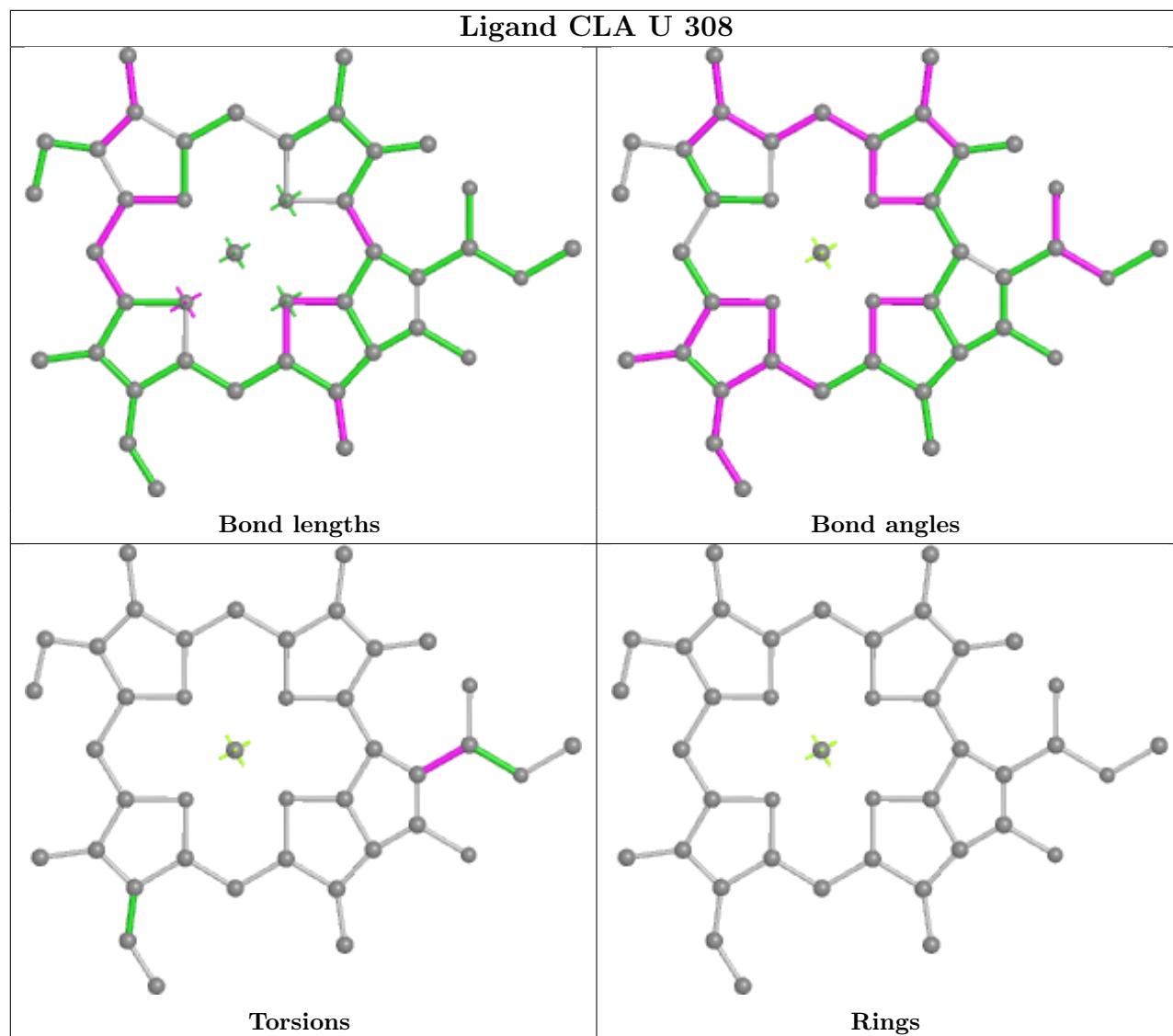


Rings

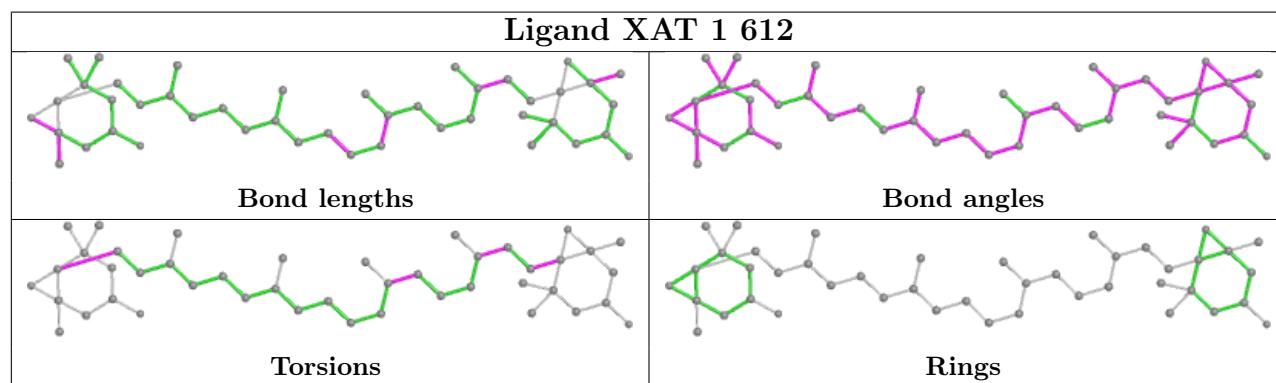




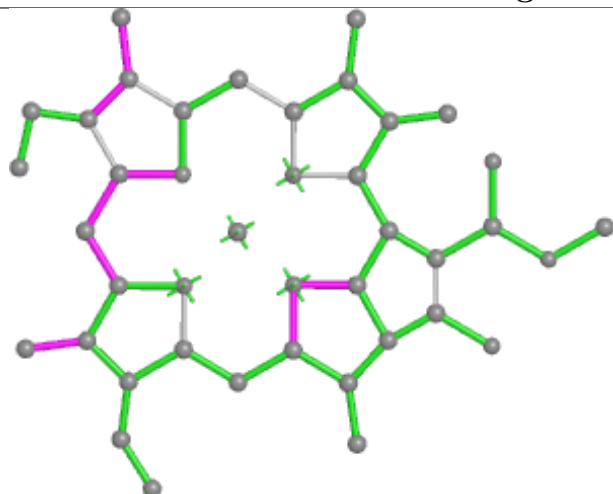
Ligand CLA U 308



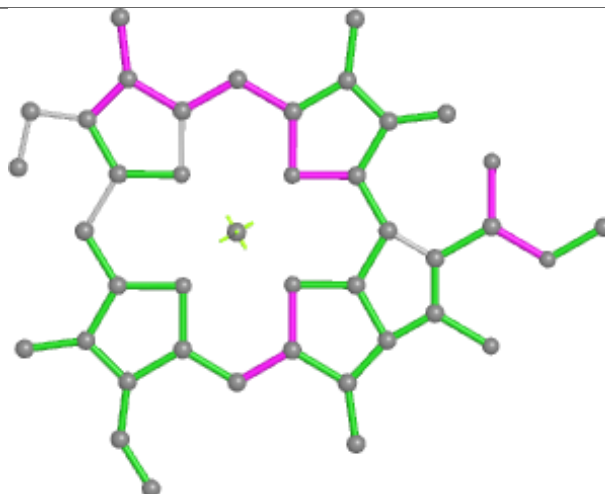
Ligand XAT 1 612



Ligand CLA L 301



Bond lengths



Bond angles

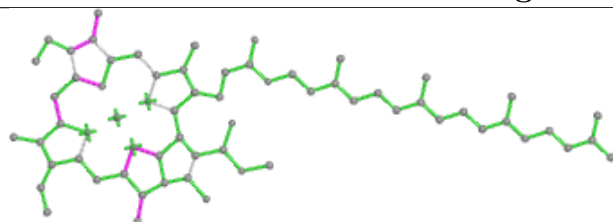


Torsions

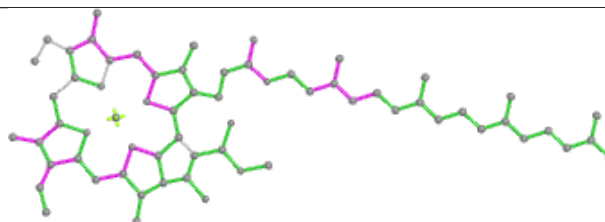


Rings

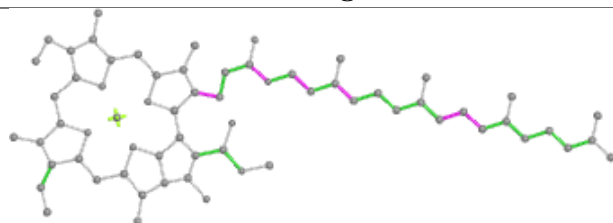
Ligand CLA P 301



Bond lengths



Bond angles

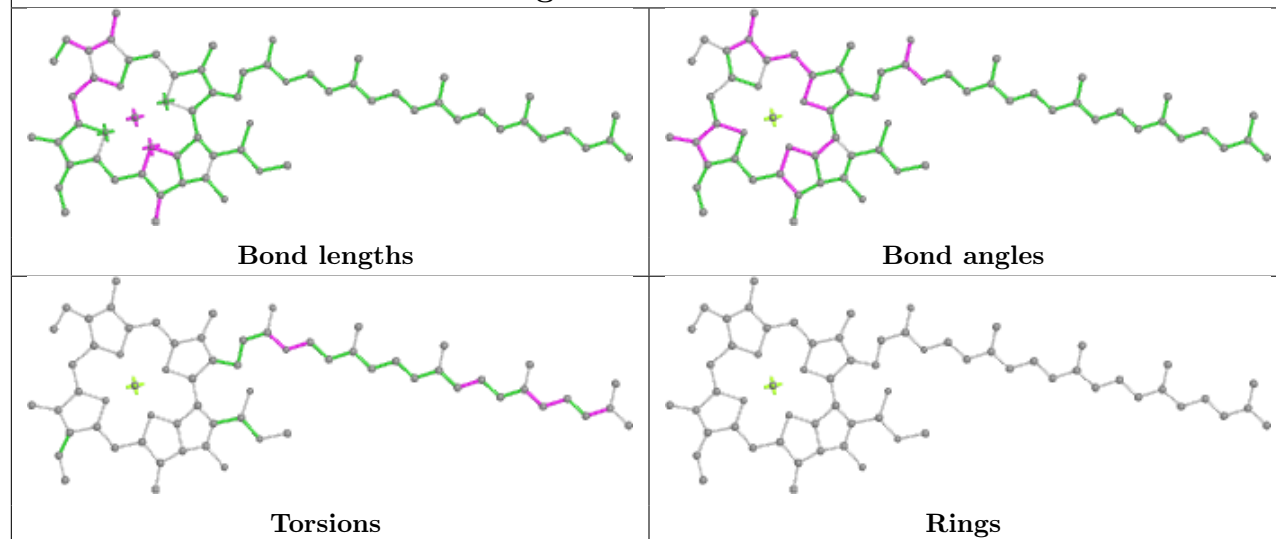


Torsions

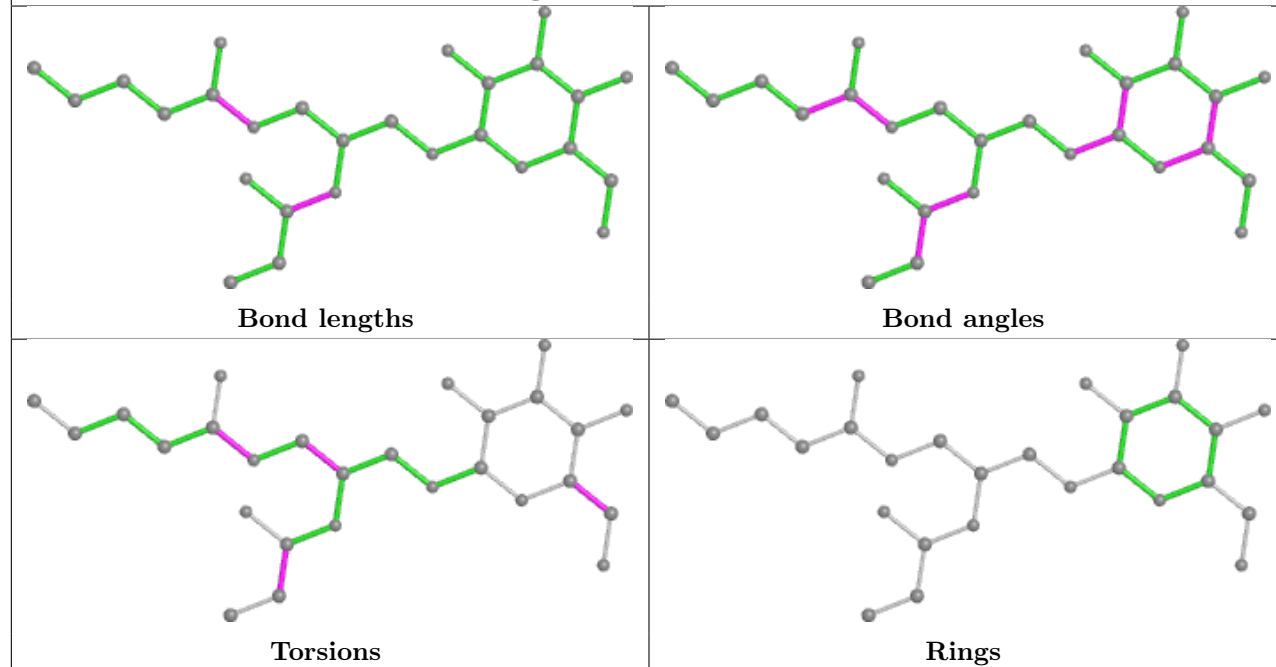


Rings

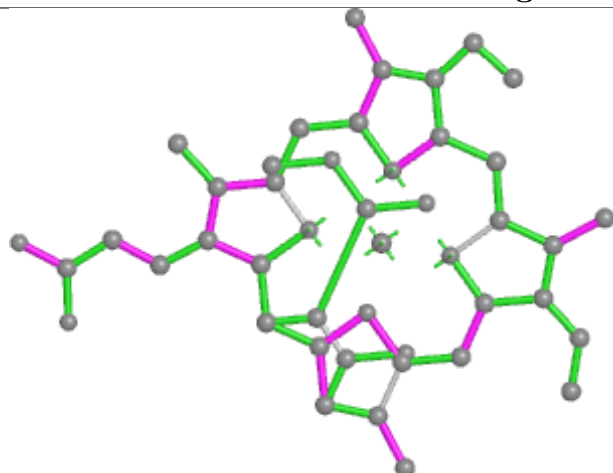
Ligand CL0 A 802



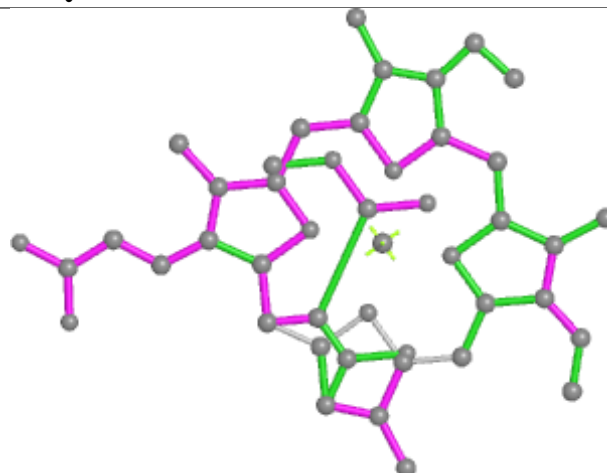
Ligand LMG A 855



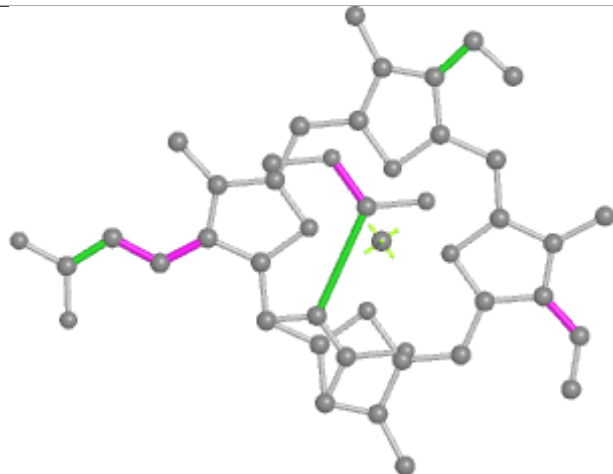
Ligand KC2 Q 310



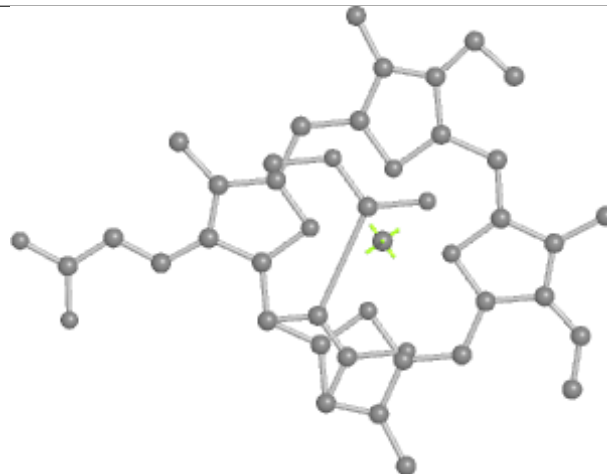
Bond lengths



Bond angles

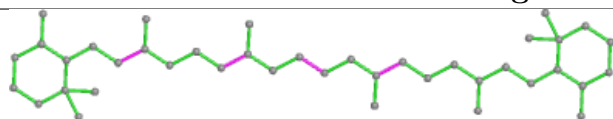


Torsions

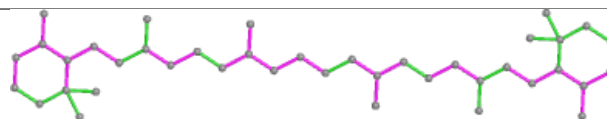


Rings

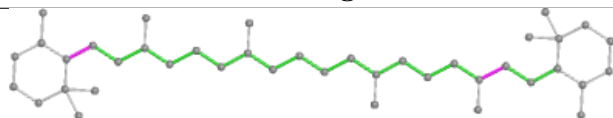
Ligand BCR K 205



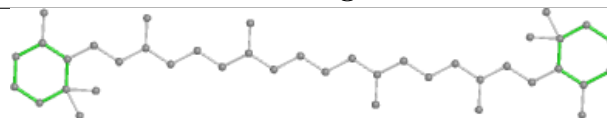
Bond lengths



Bond angles

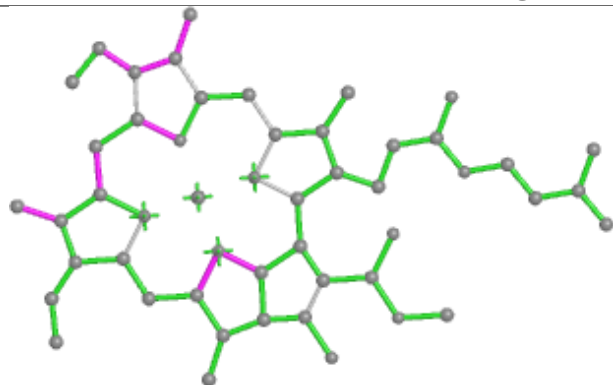


Torsions

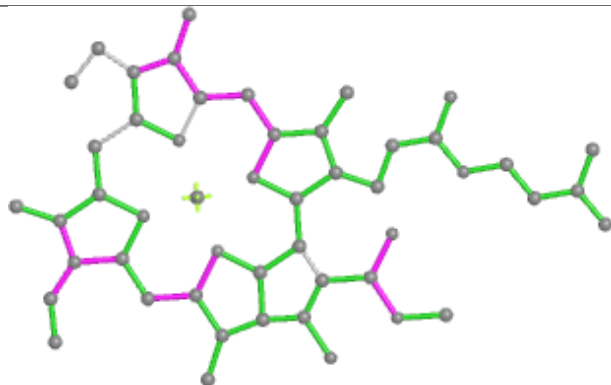


Rings

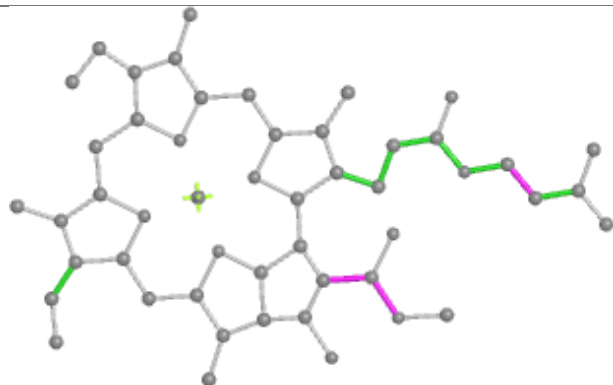
Ligand CLA V 303



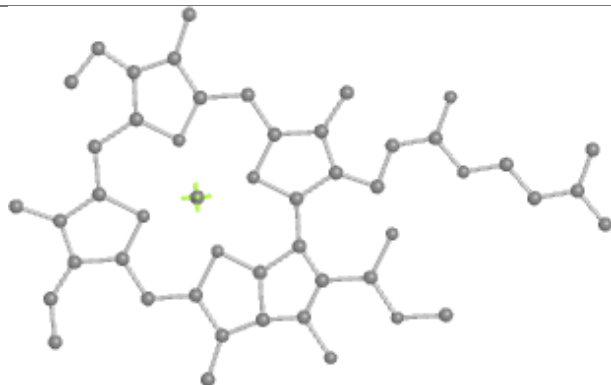
Bond lengths



Bond angles

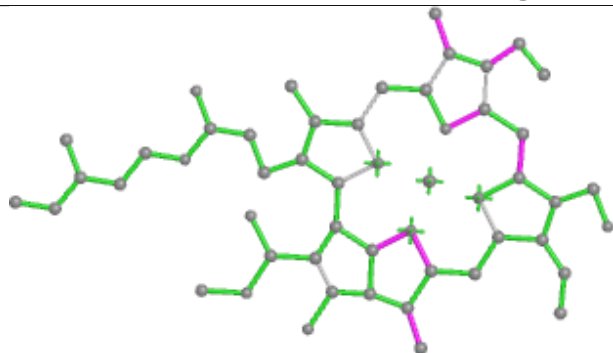


Torsions

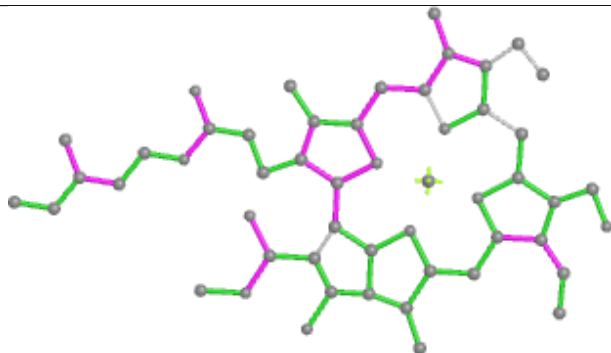


Rings

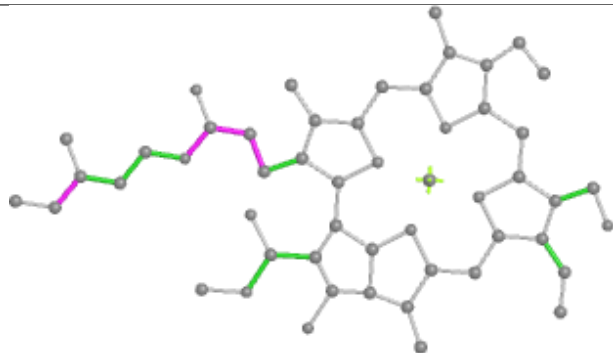
Ligand CHL T 306



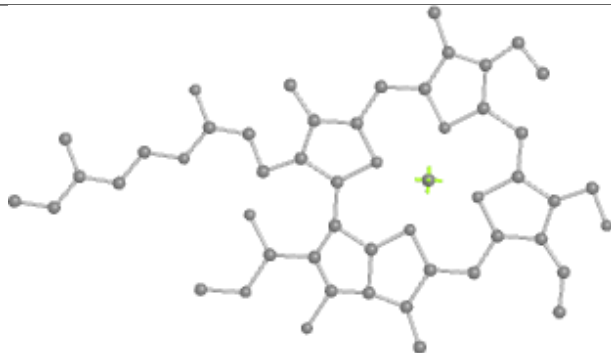
Bond lengths



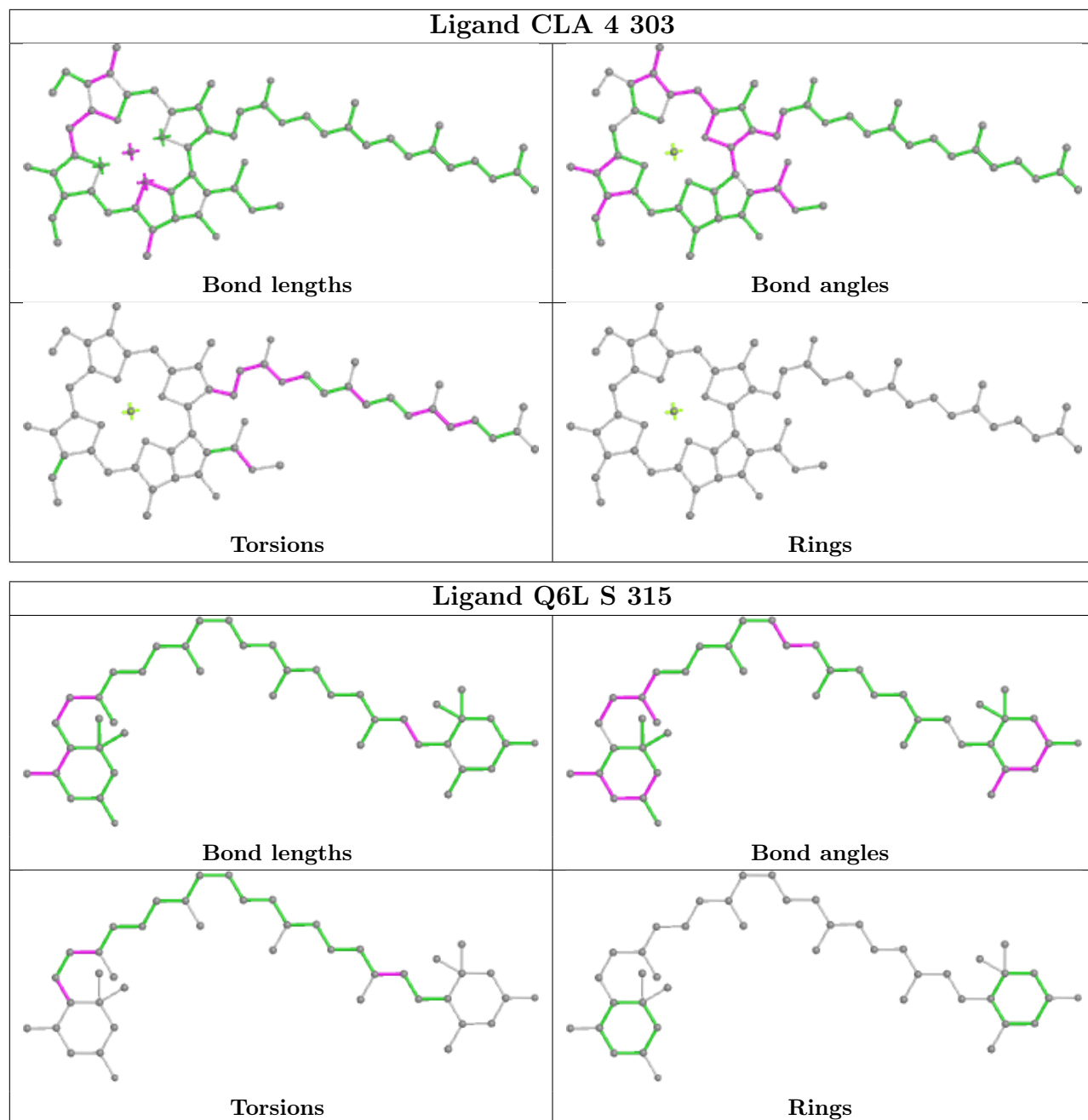
Bond angles



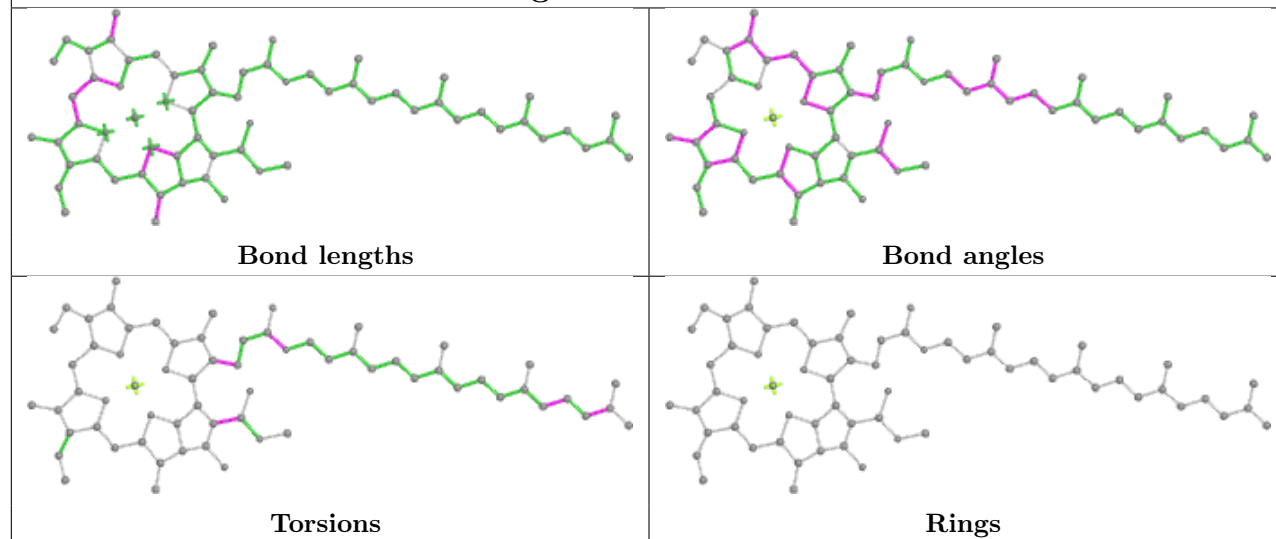
Torsions



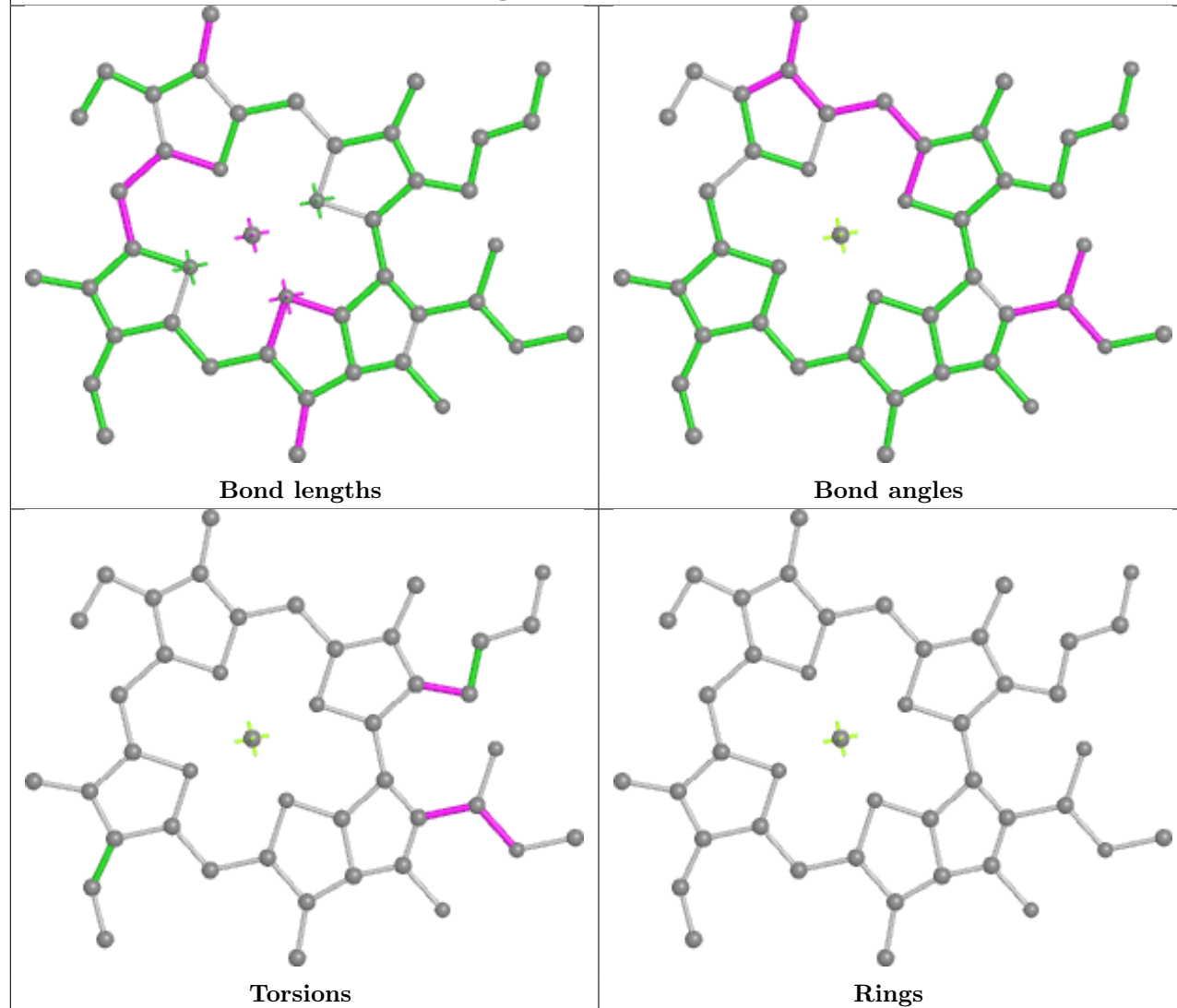
Rings



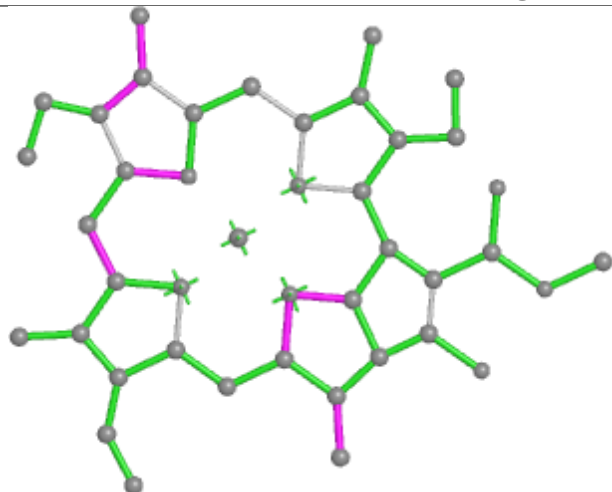
Ligand CLA A 843



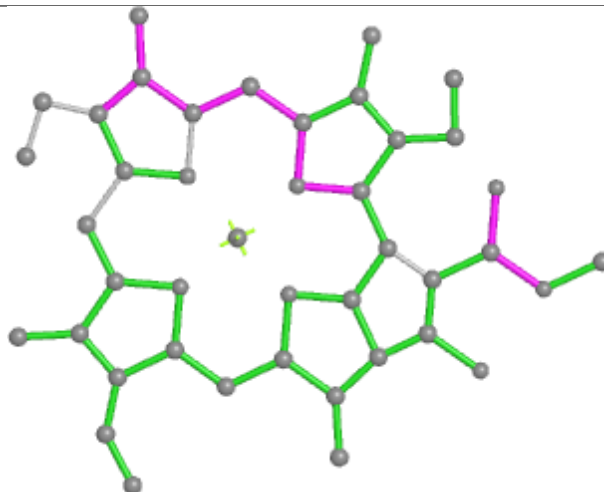
Ligand CLA 2 614



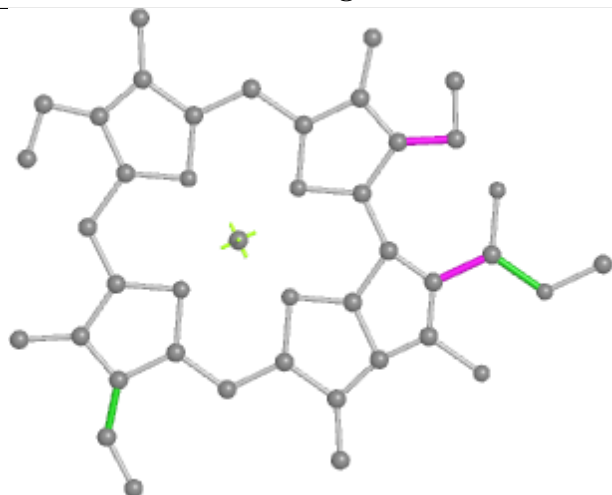
Ligand CLA T 310



Bond lengths



Bond angles

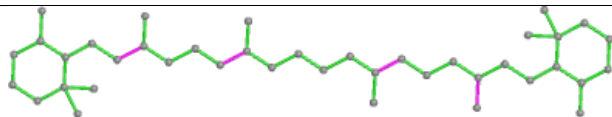


Torsions

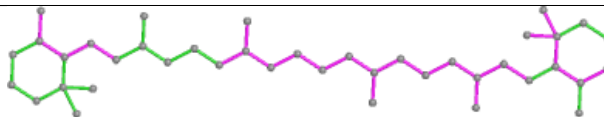


Rings

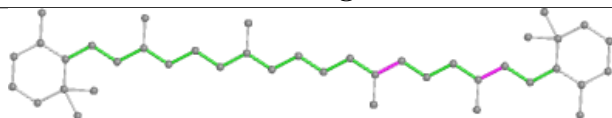
Ligand BCR F 801



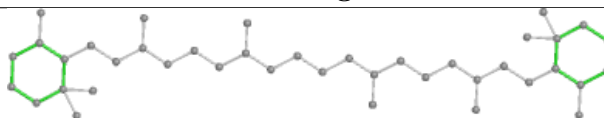
Bond lengths



Bond angles

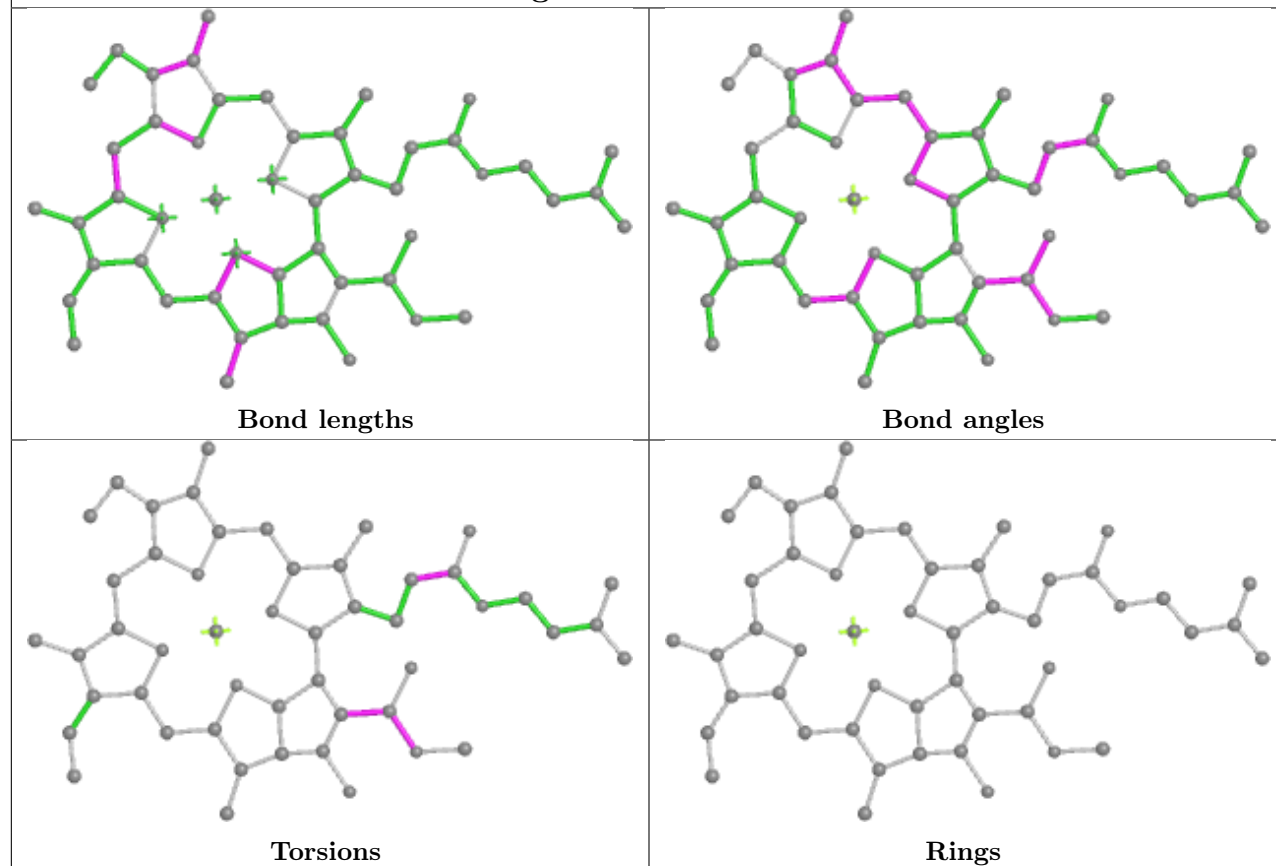


Torsions

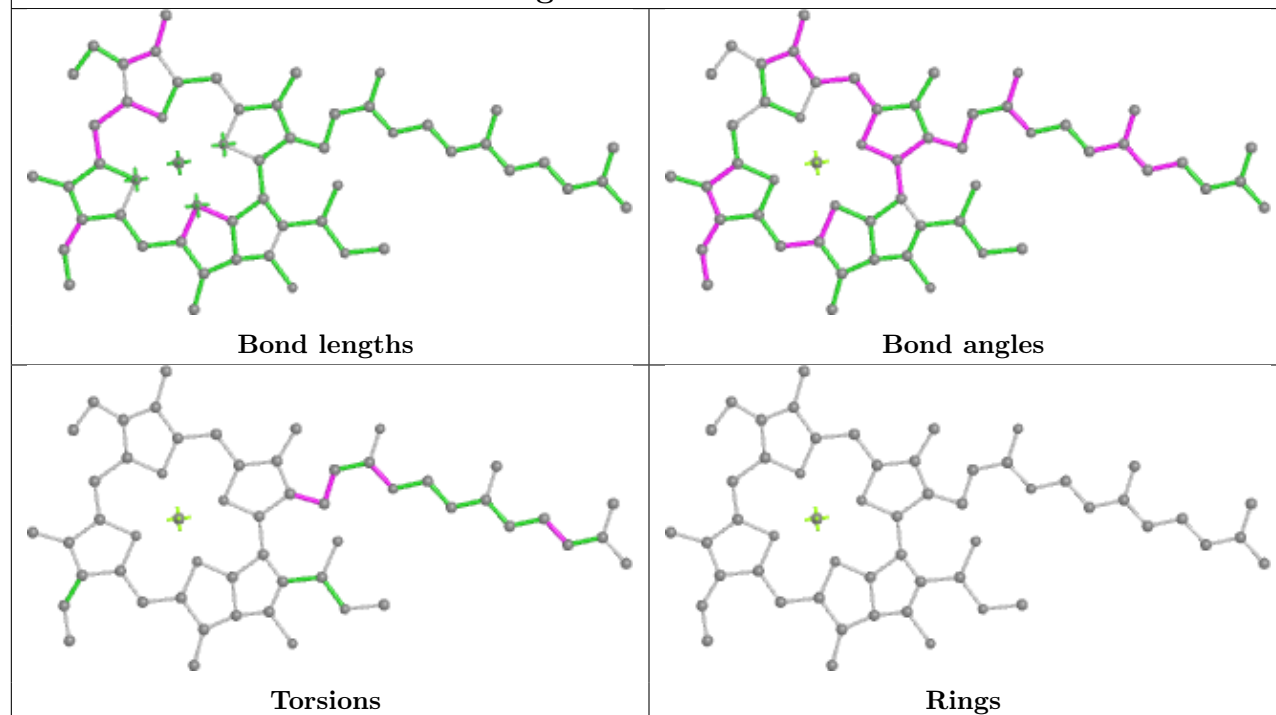


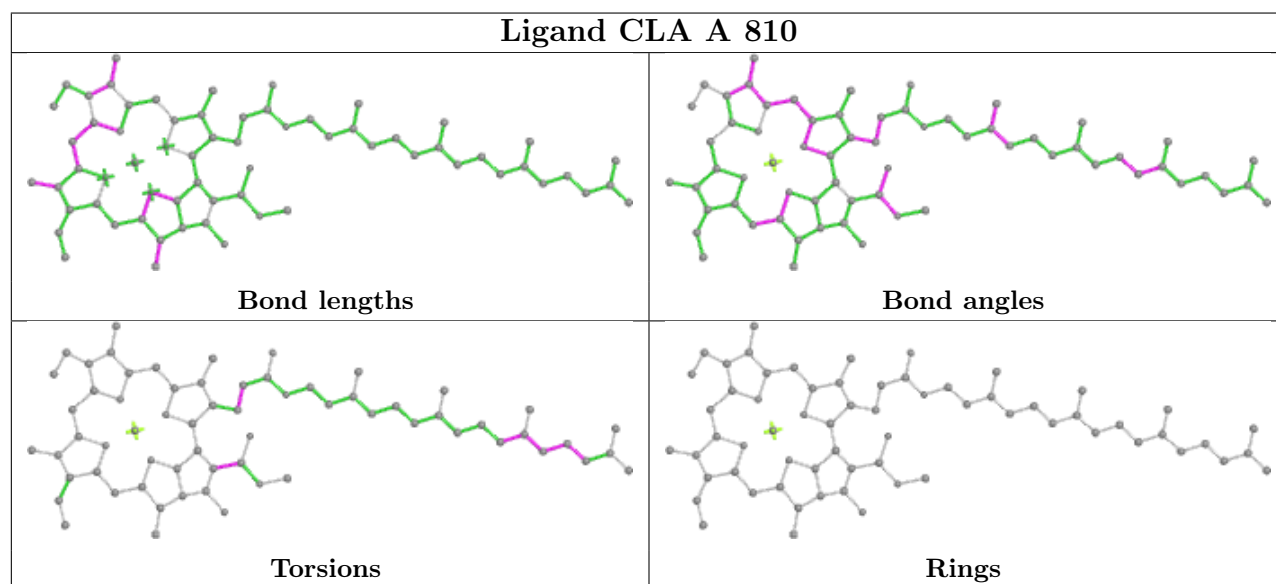
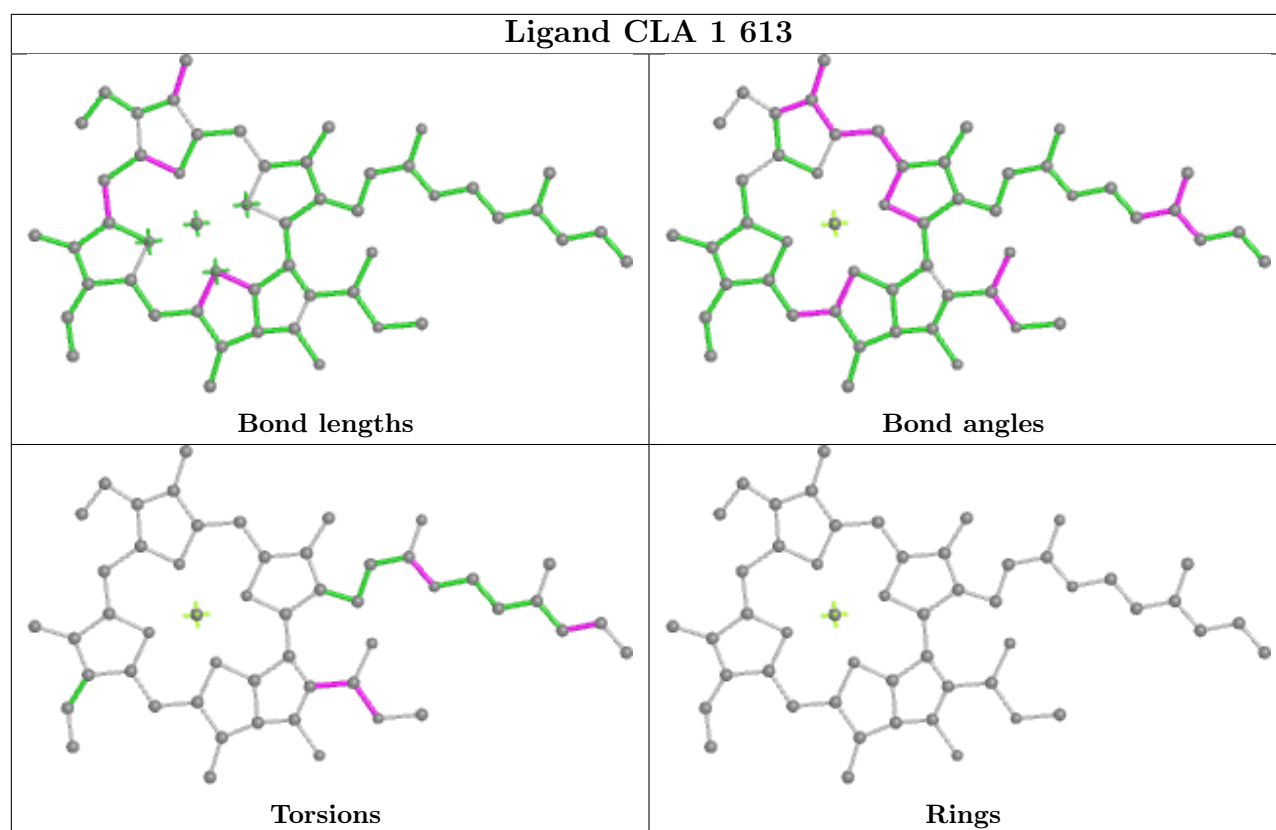
Rings

Ligand CLA A 841

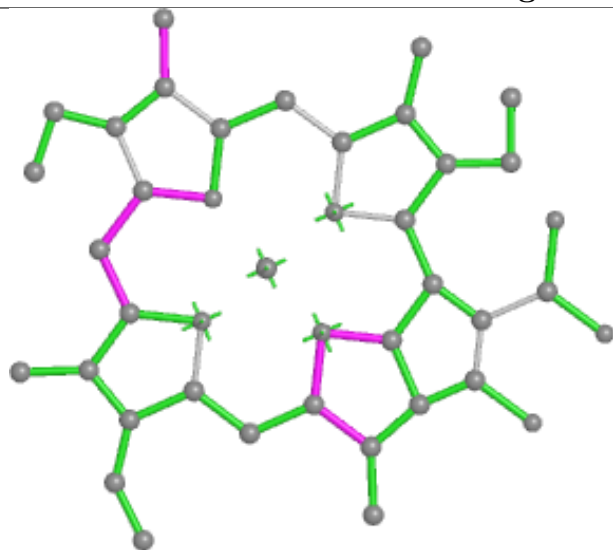


Ligand CLA 1 603

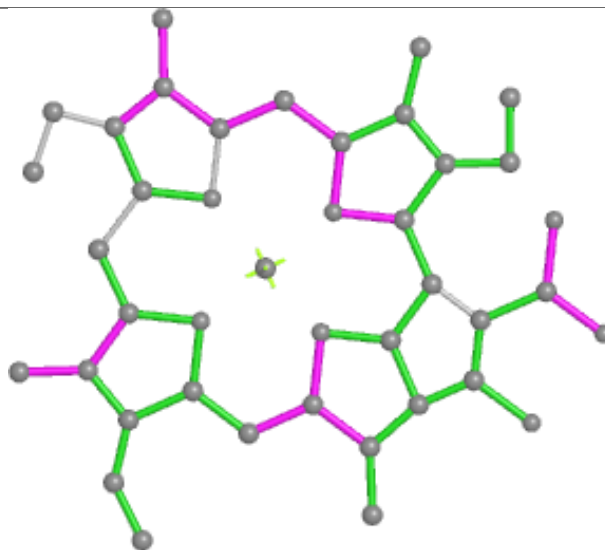




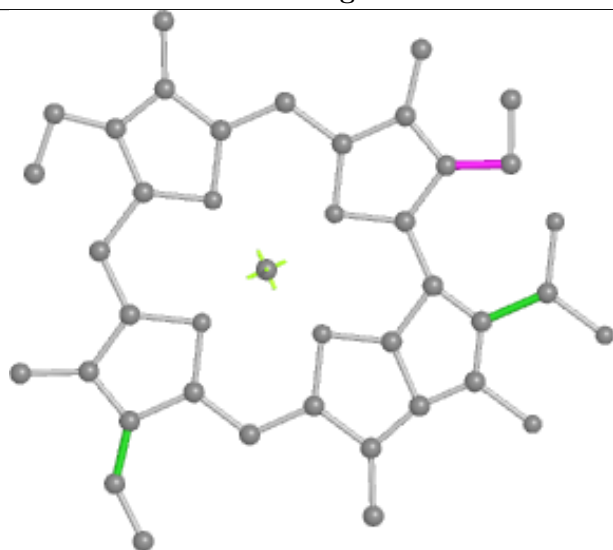
Ligand CLA 3 304



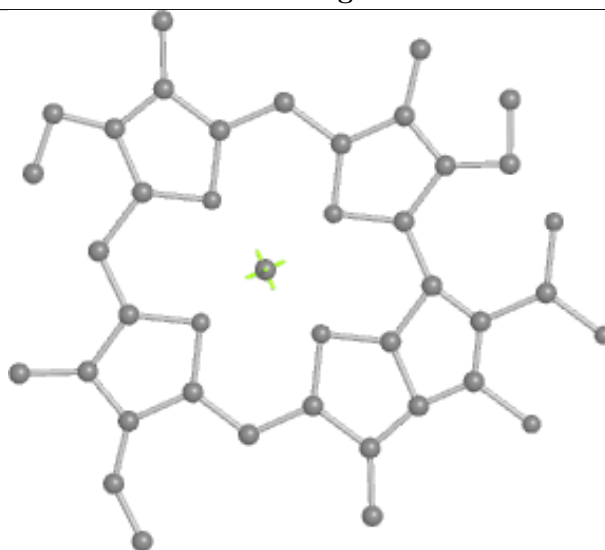
Bond lengths



Bond angles

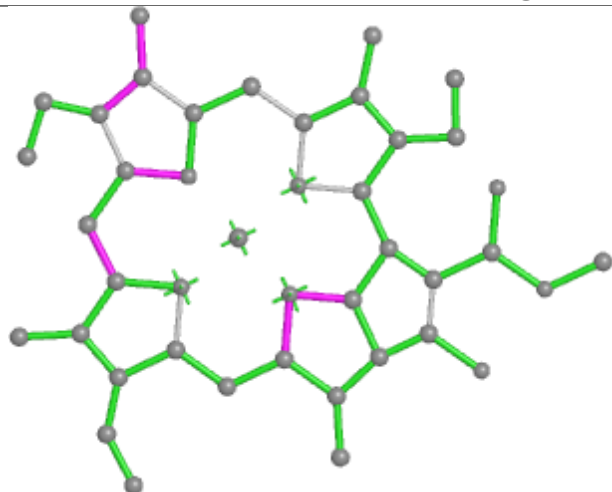


Torsions

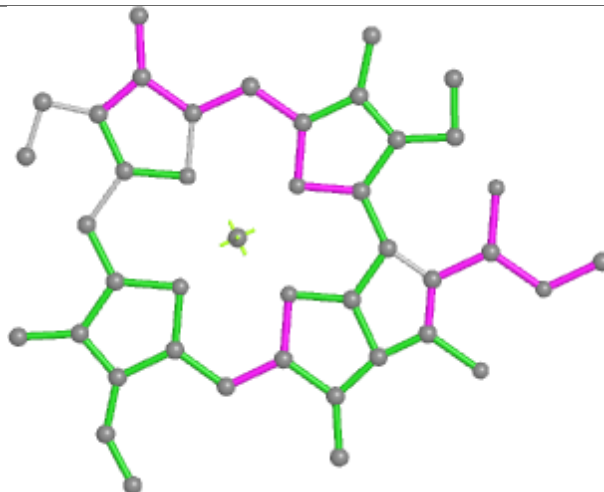


Rings

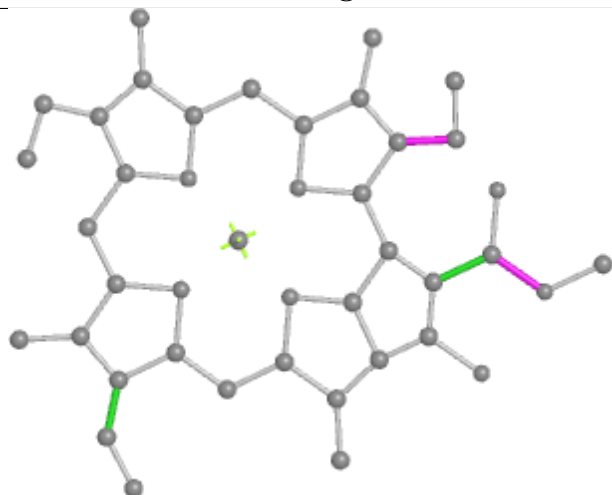
Ligand CLA 4 316



Bond lengths



Bond angles

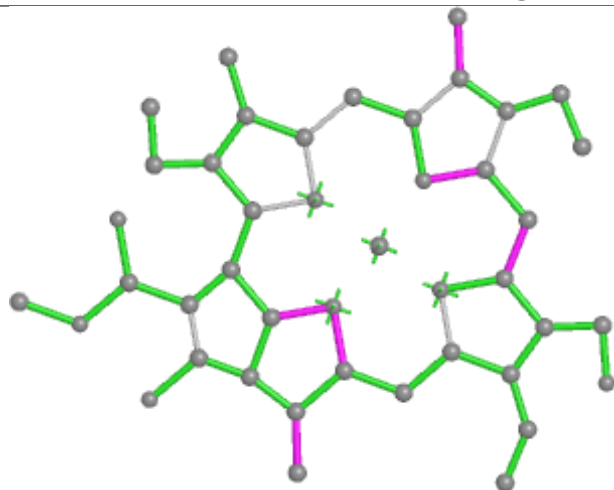


Torsions

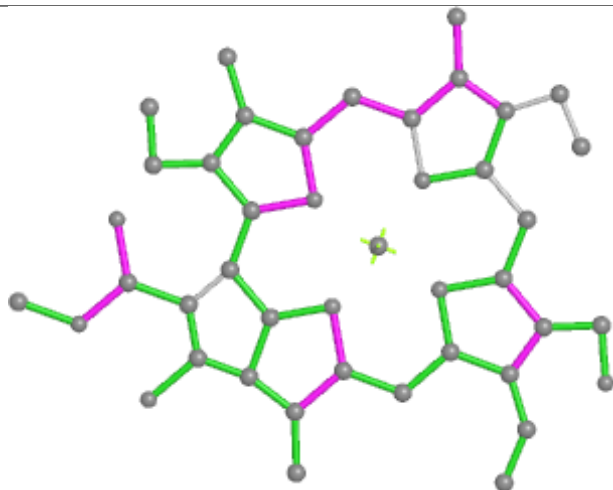


Rings

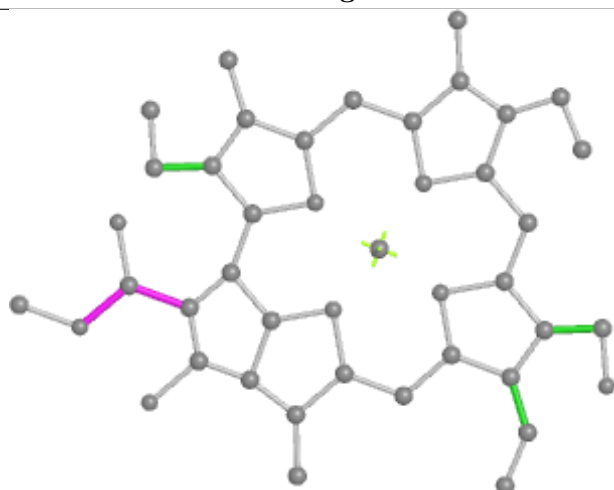
Ligand CHL U 313



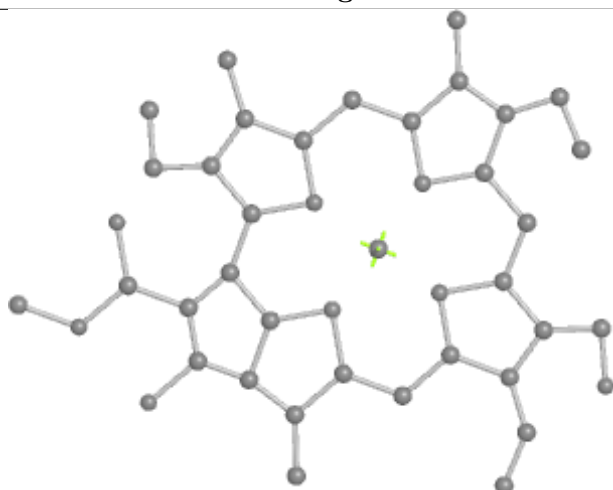
Bond lengths



Bond angles

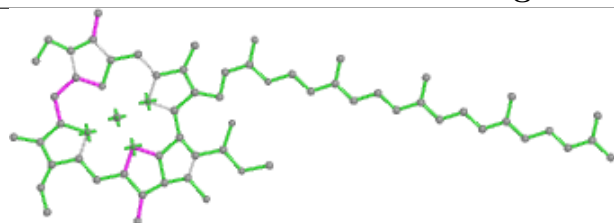


Torsions

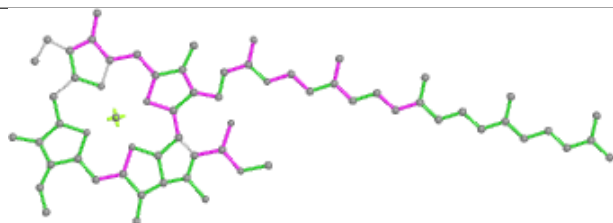


Rings

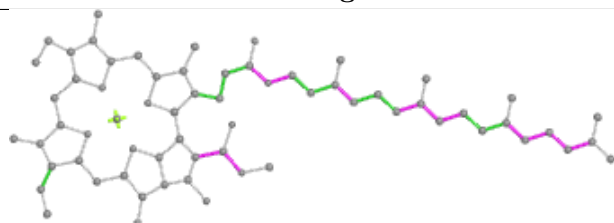
Ligand CLA A 838



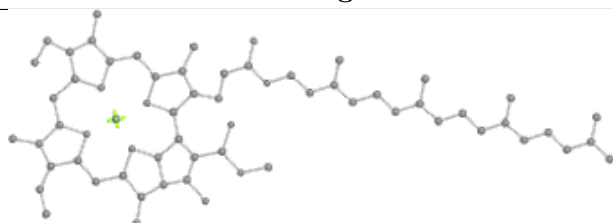
Bond lengths



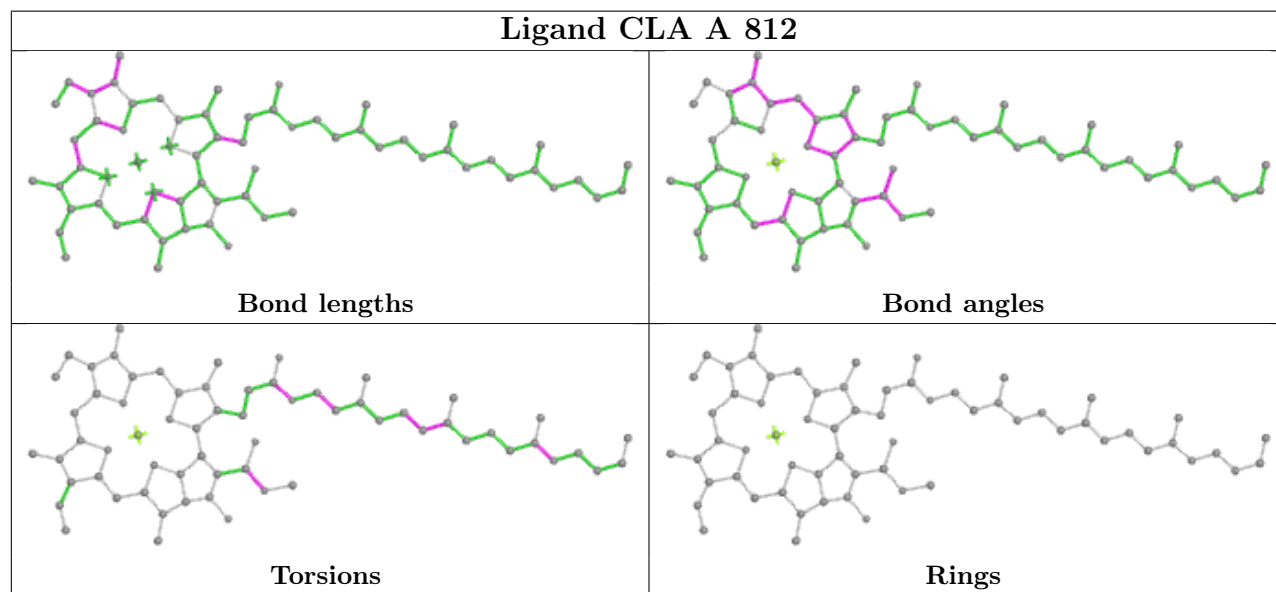
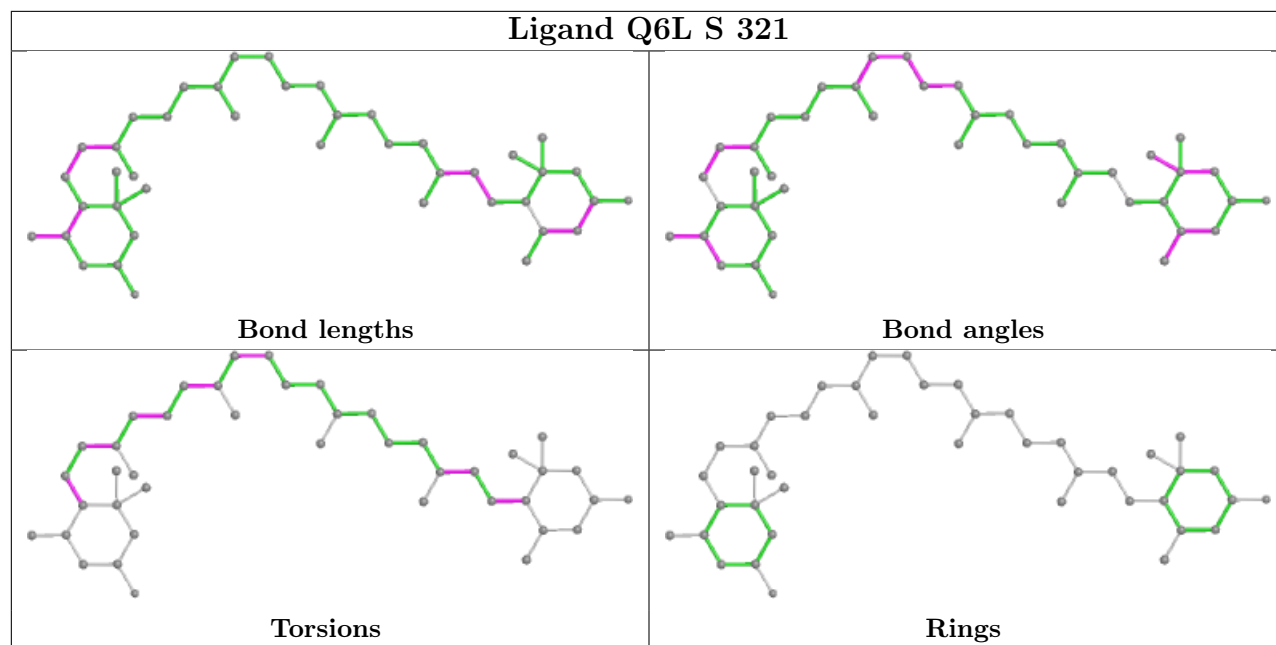
Bond angles



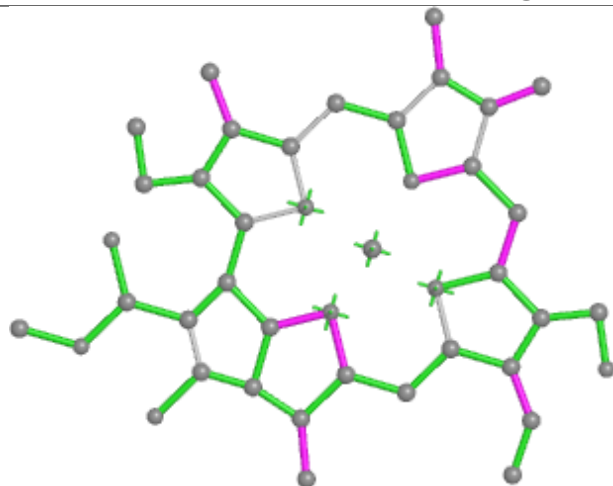
Torsions



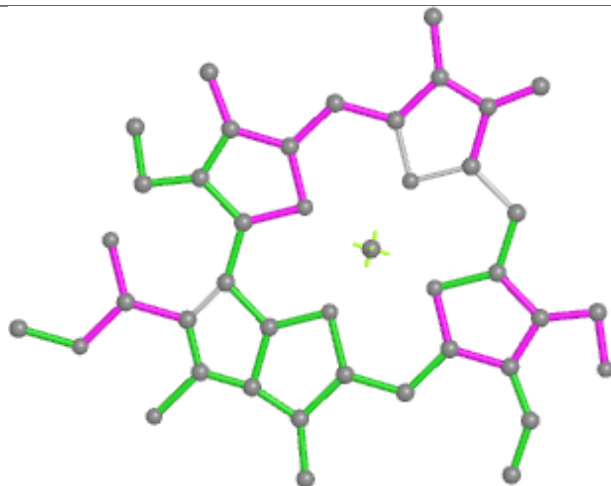
Rings



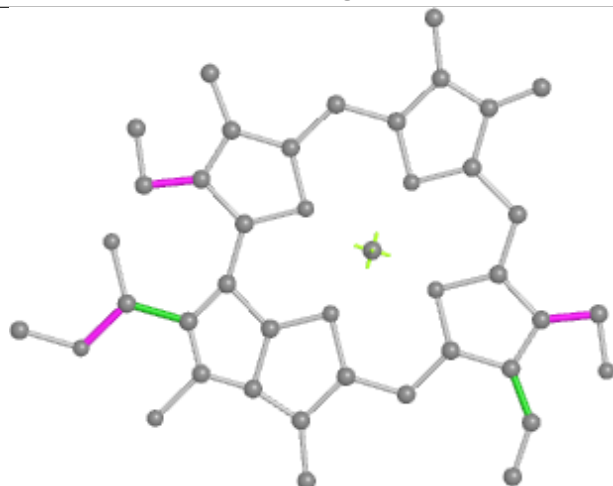
Ligand CHL 4 307



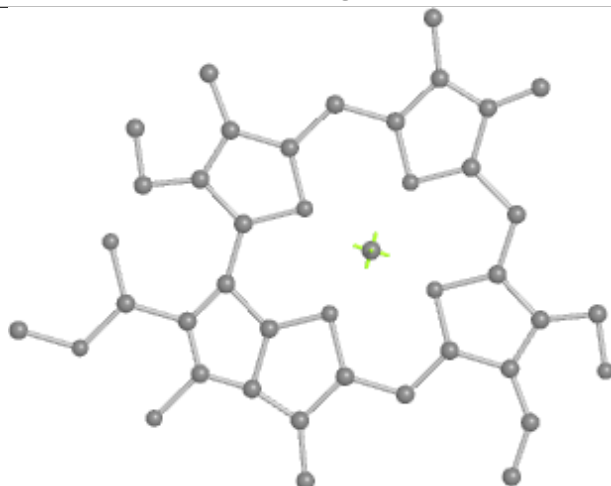
Bond lengths



Bond angles

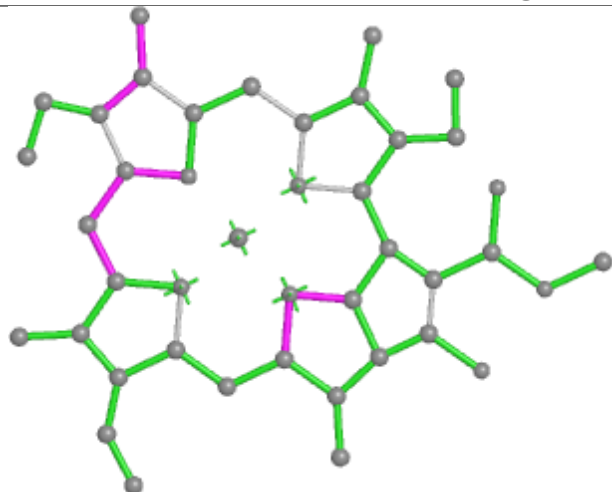


Torsions

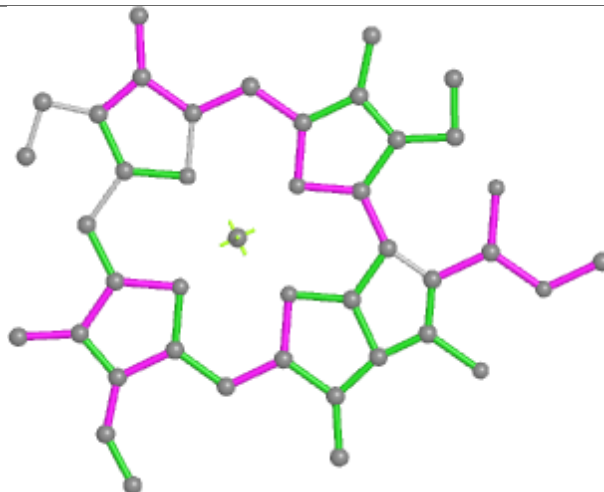


Rings

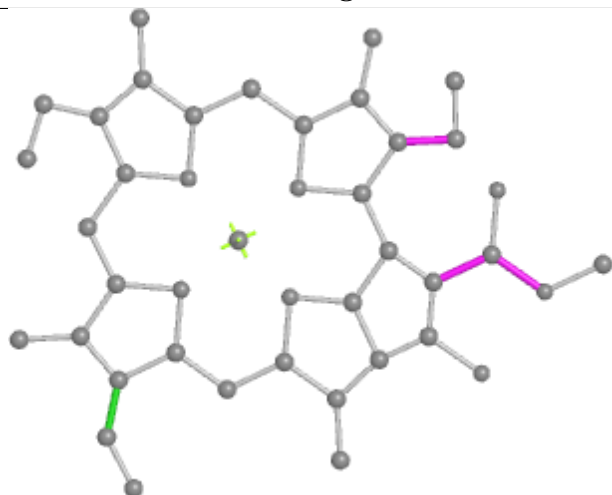
Ligand CLA 4 311



Bond lengths



Bond angles

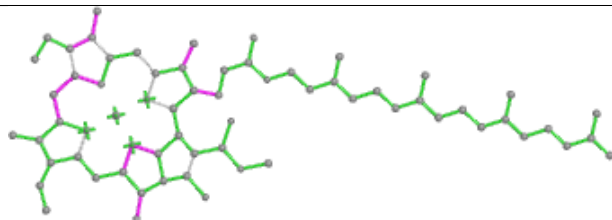


Torsions

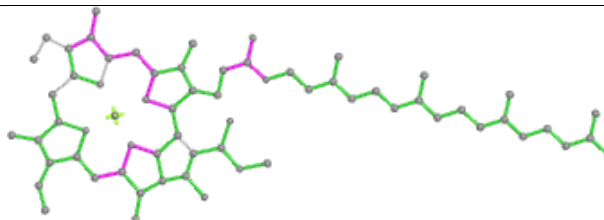


Rings

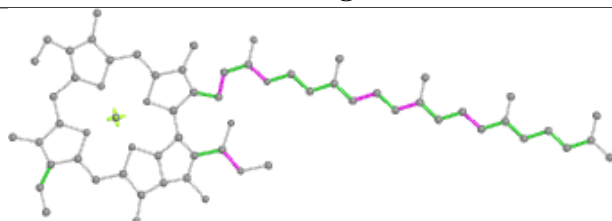
Ligand CLA Q 304



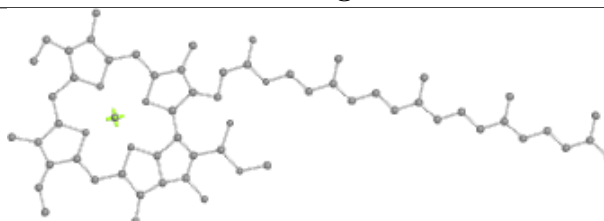
Bond lengths



Bond angles

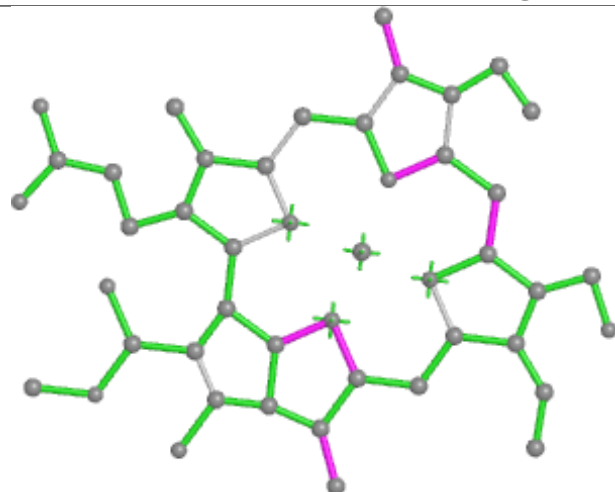


Torsions

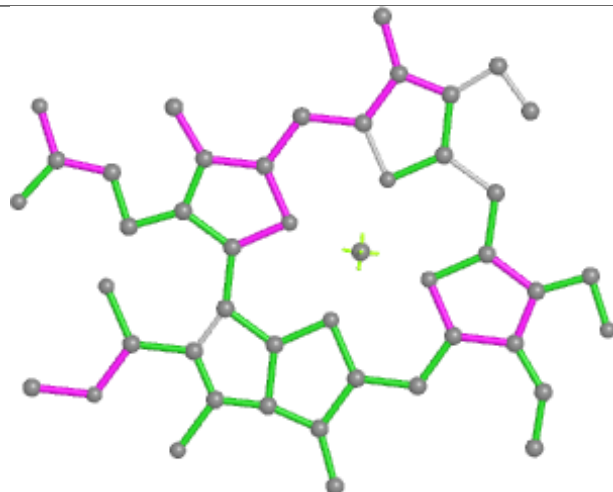


Rings

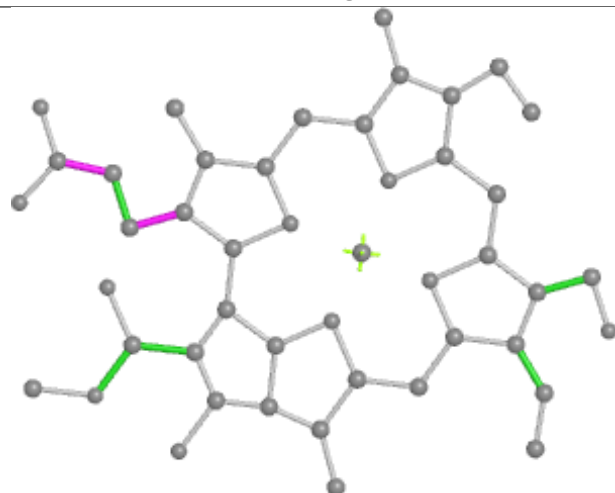
Ligand CHL P 305



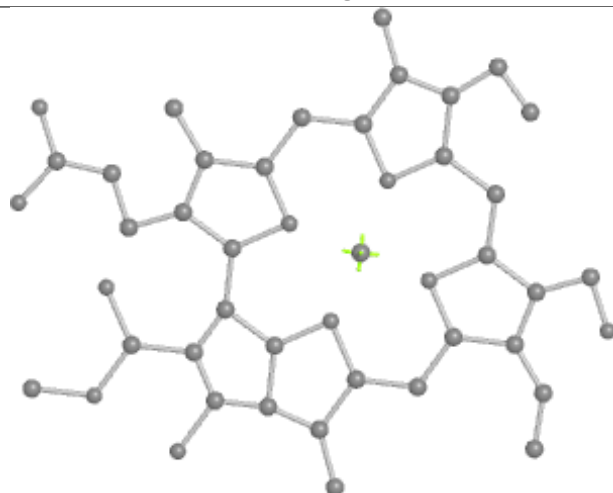
Bond lengths



Bond angles

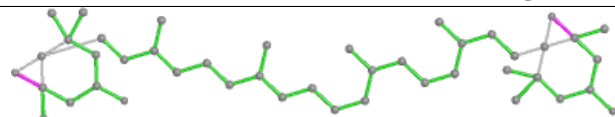


Torsions

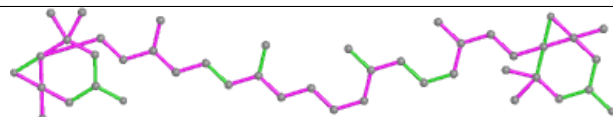


Rings

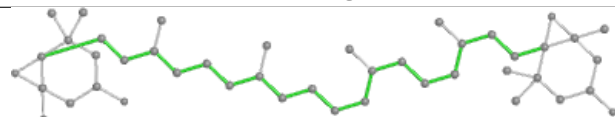
Ligand XAT 5 612



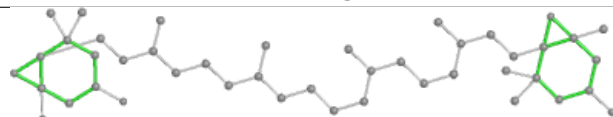
Bond lengths



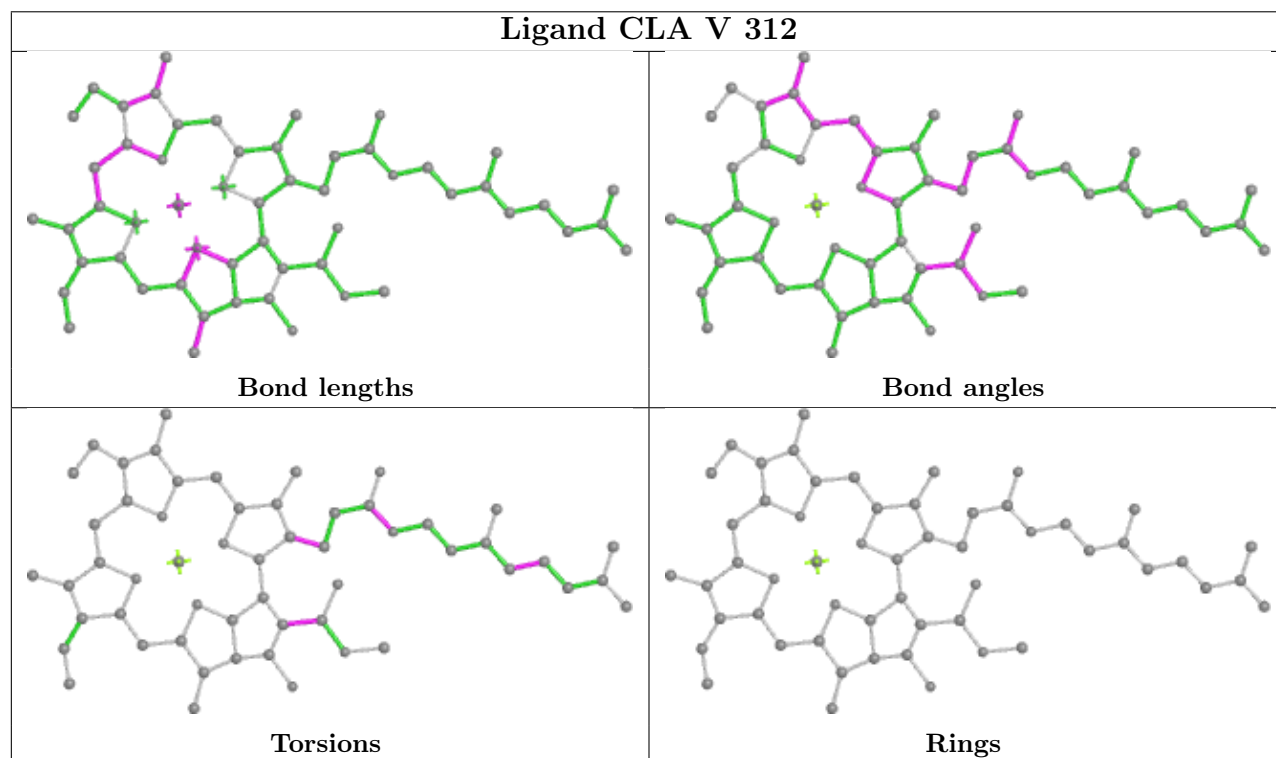
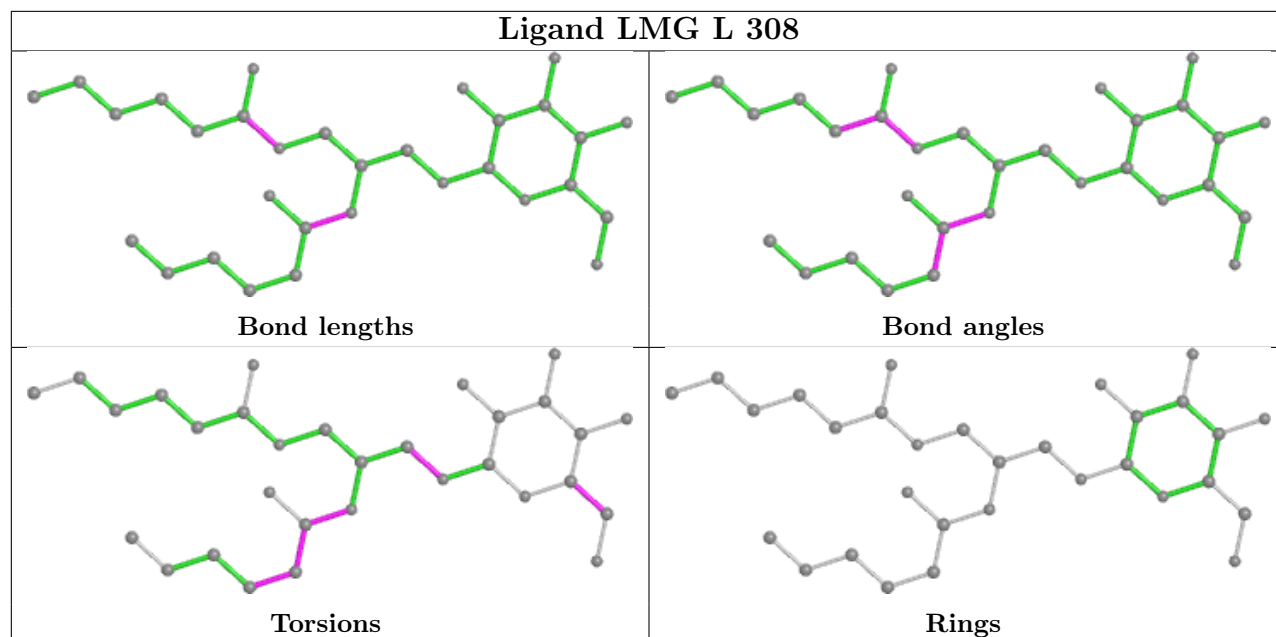
Bond angles

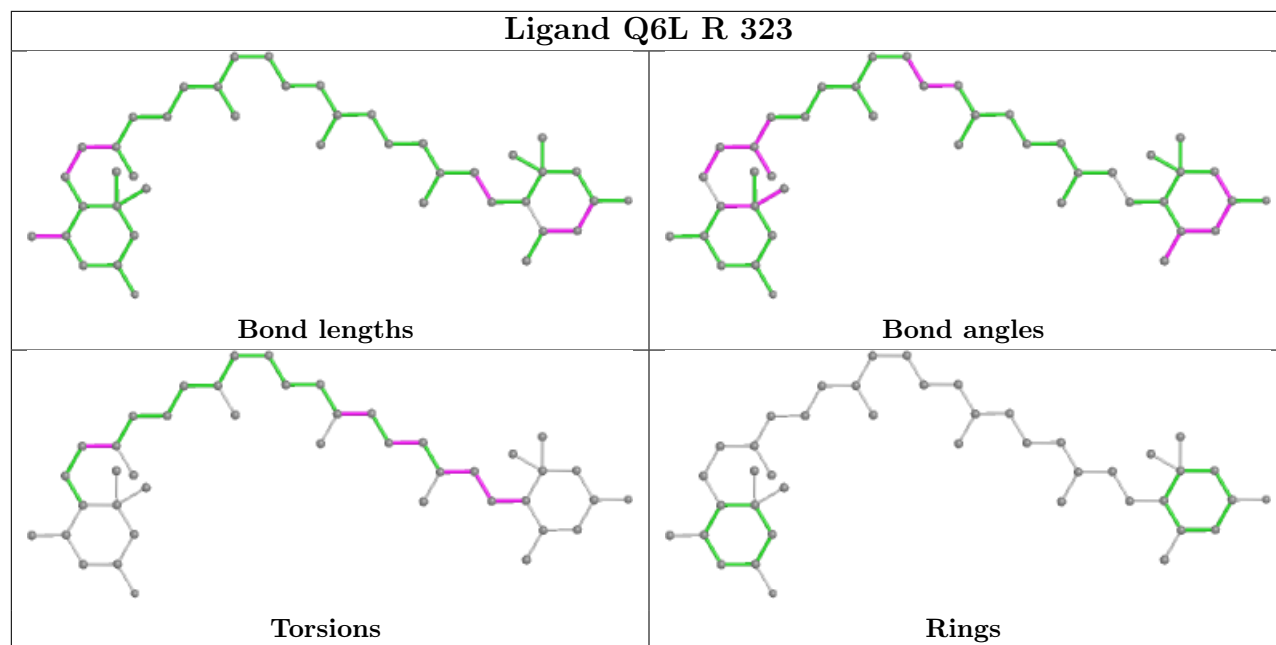
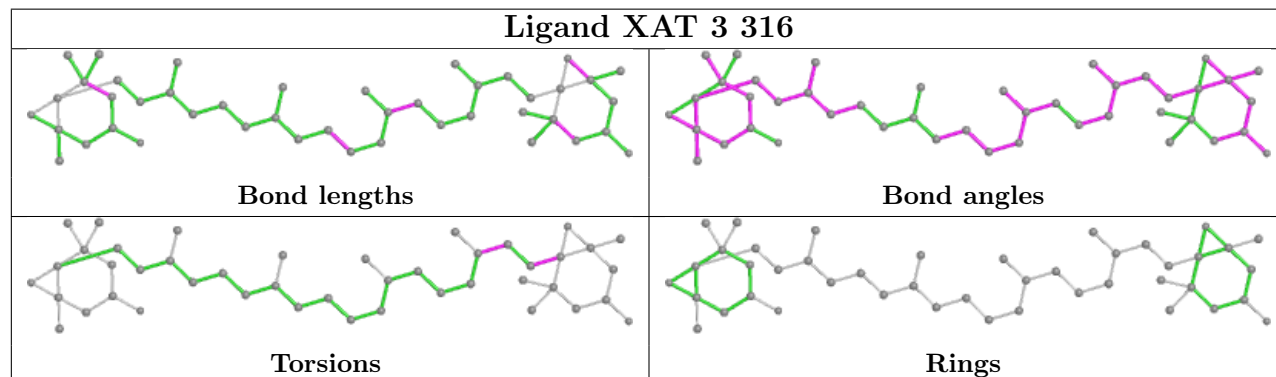


Torsions

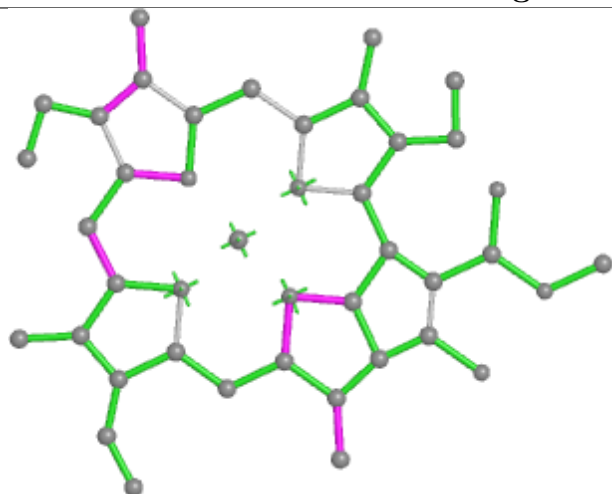


Rings

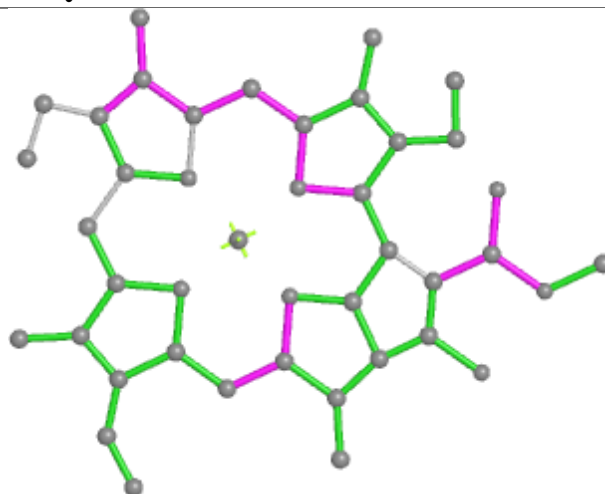


Ligand Q6L R 323**Ligand XAT 3 316**

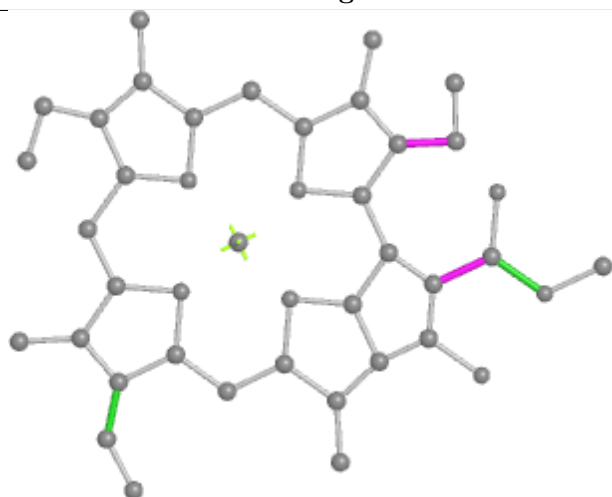
Ligand CLA Q 312



Bond lengths



Bond angles

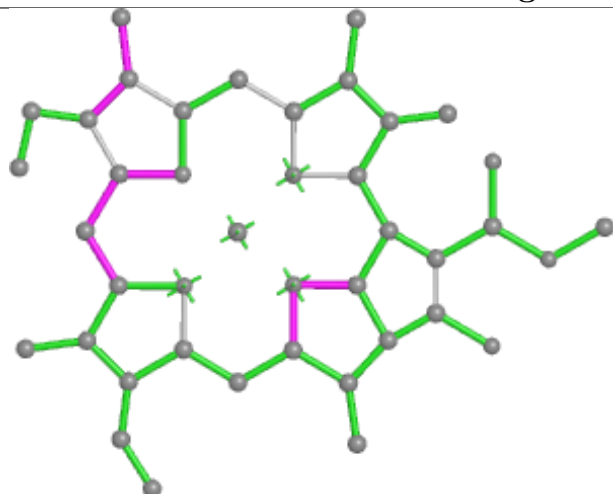


Torsions

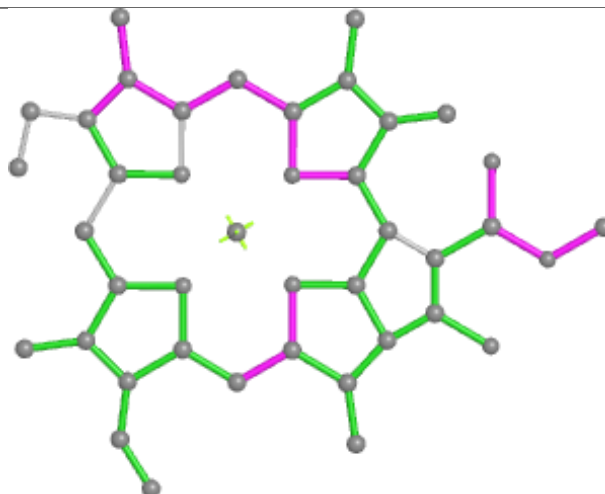


Rings

Ligand CLA 3 313



Bond lengths



Bond angles

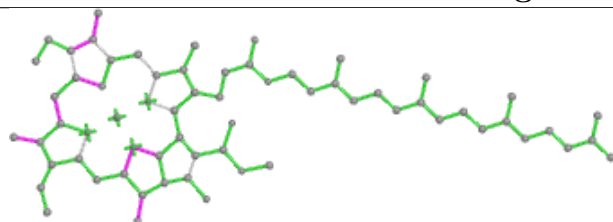


Torsions

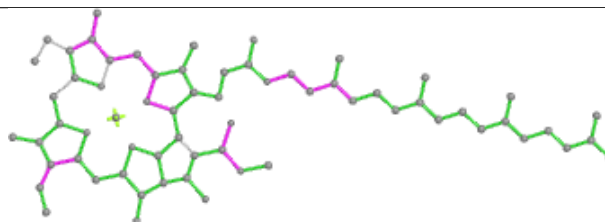


Rings

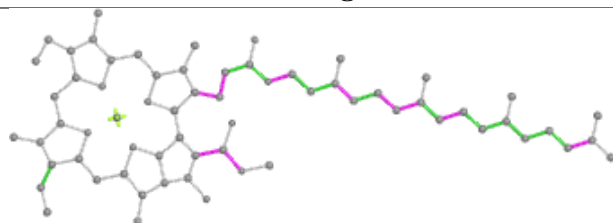
Ligand CLA T 302



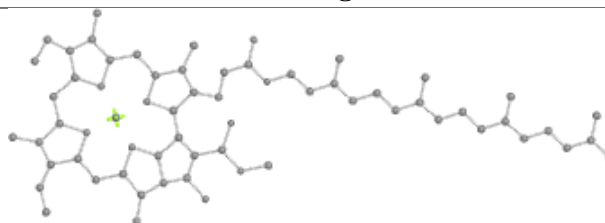
Bond lengths



Bond angles

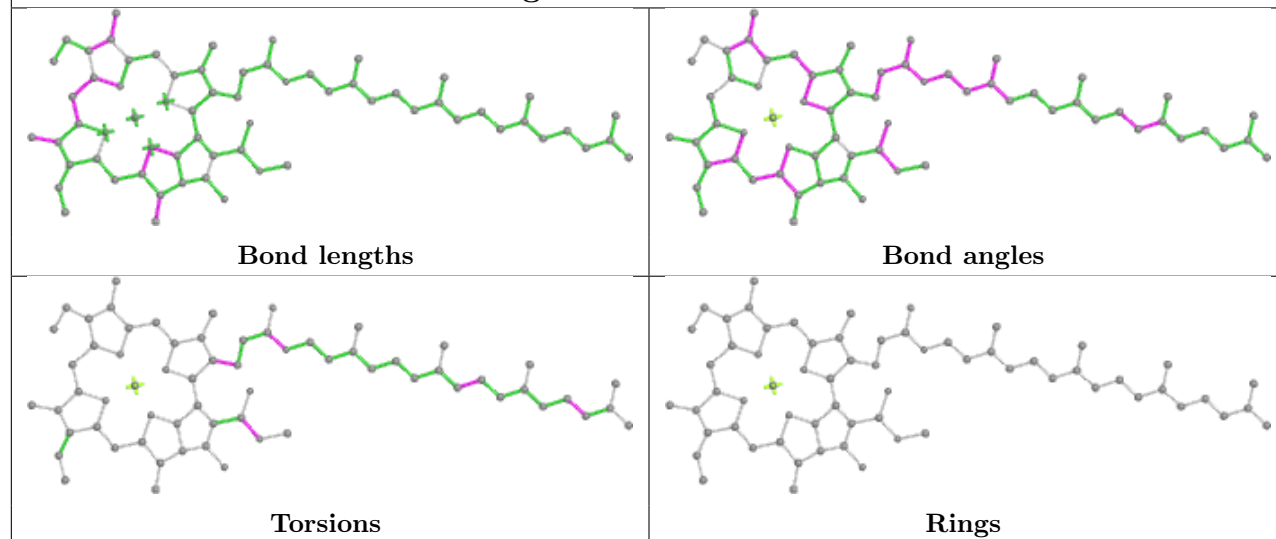


Torsions

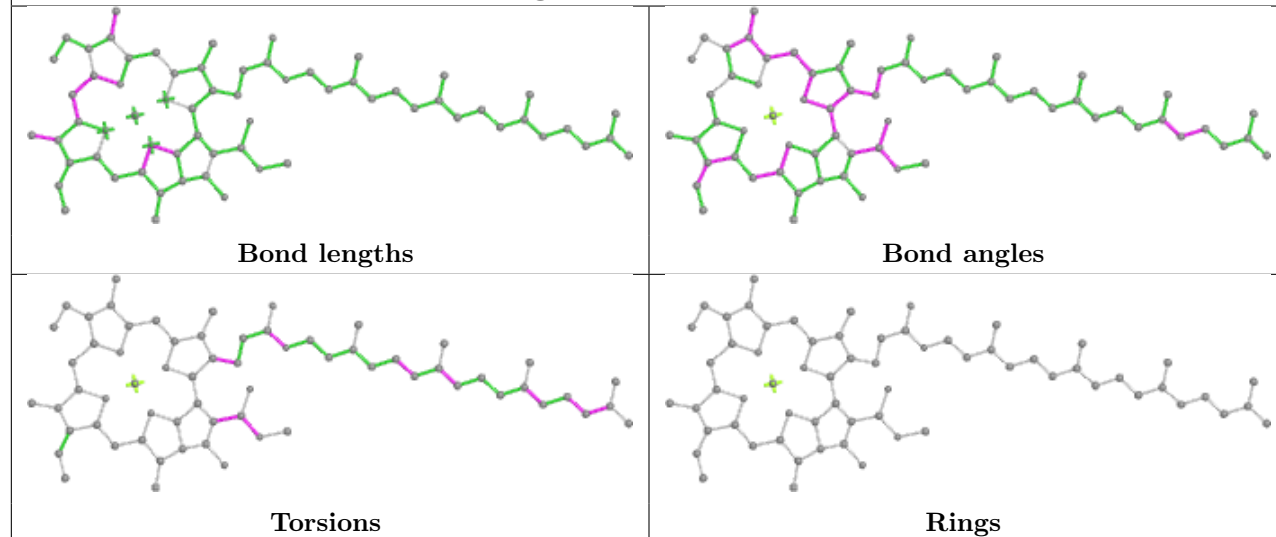


Rings

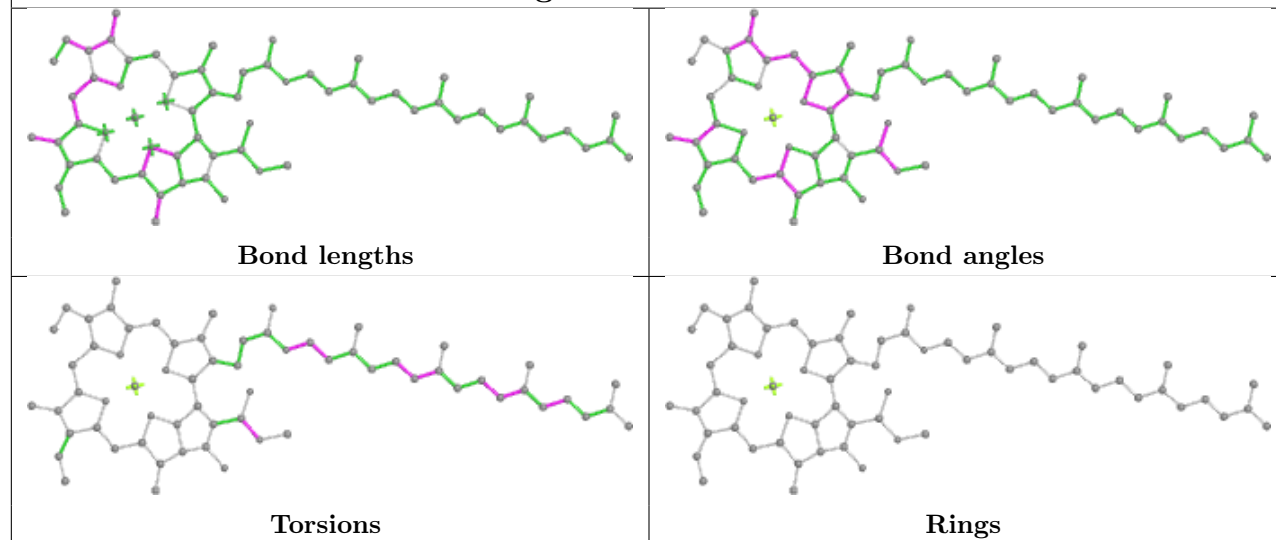
Ligand CLA O 2002

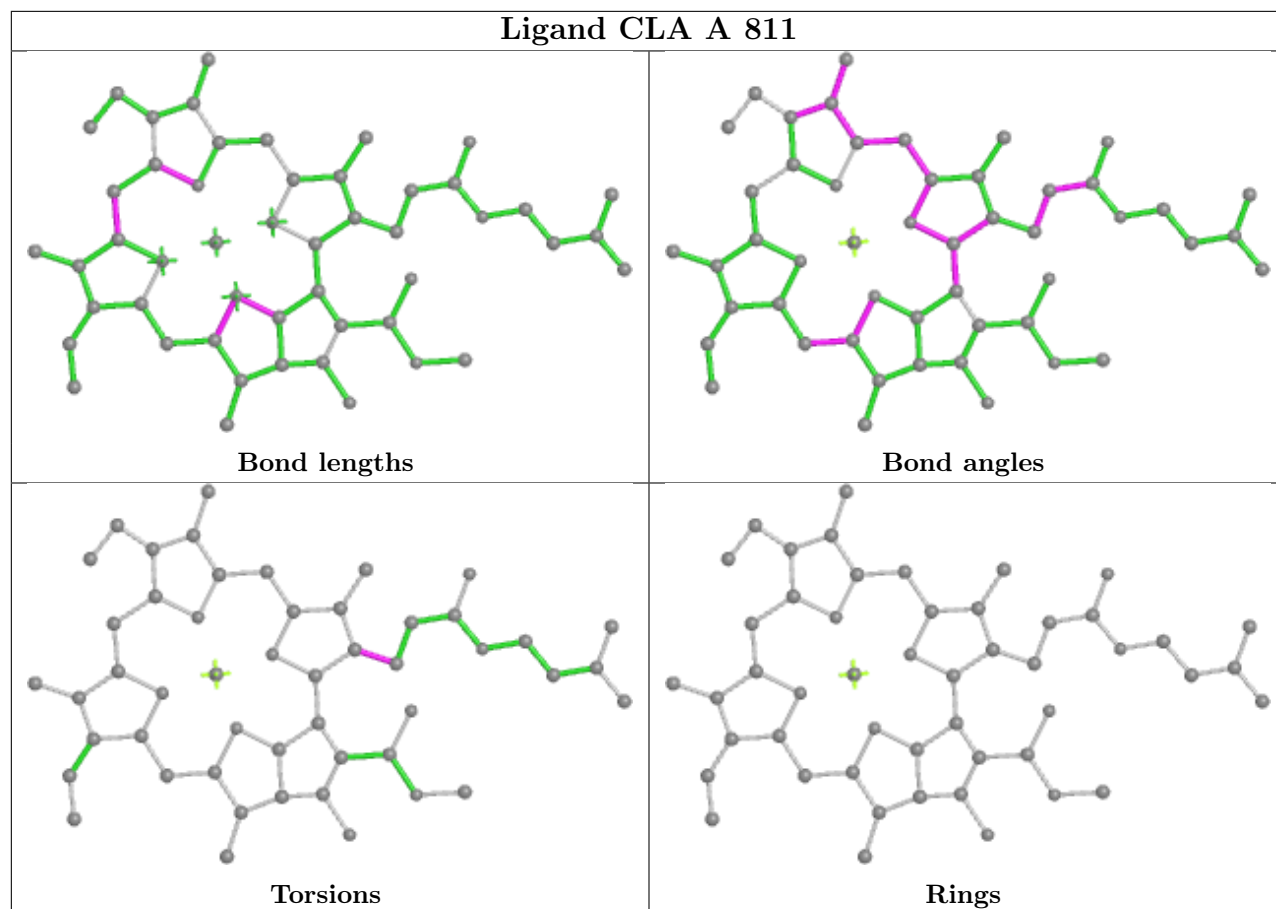


Ligand CLA A 821

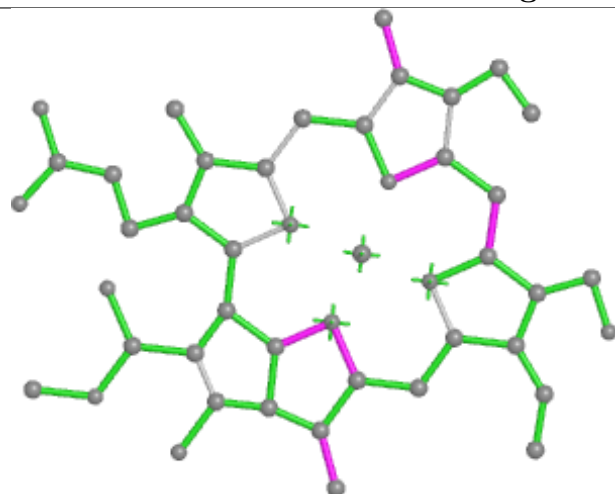


Ligand CLA S 302

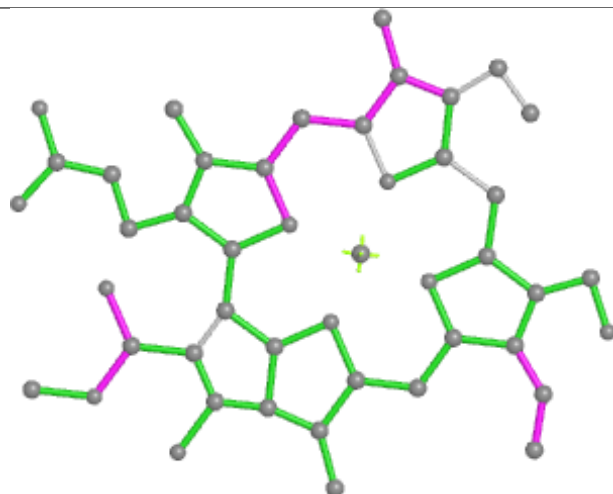




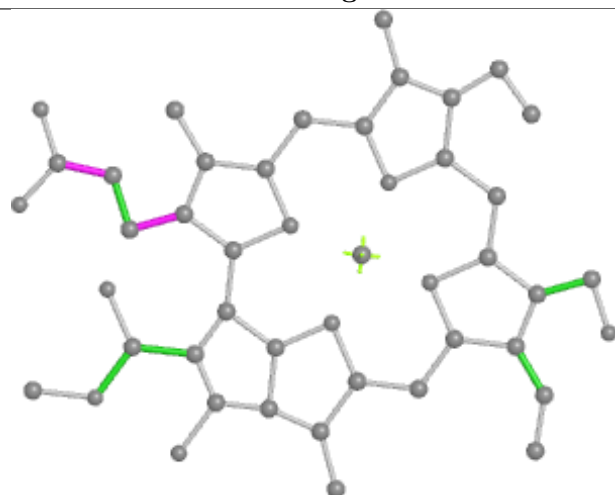
Ligand CHL 4 308



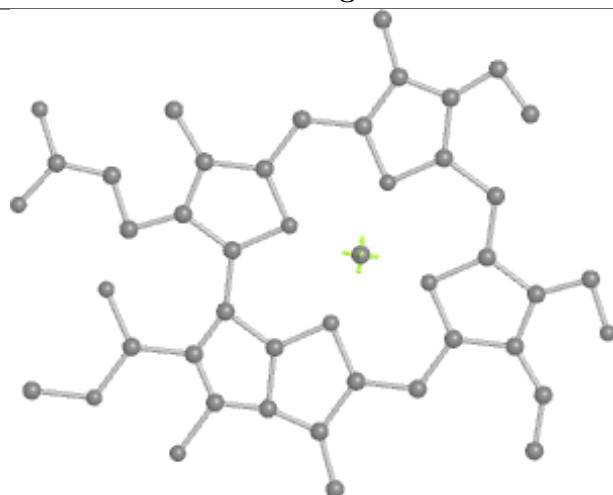
Bond lengths



Bond angles

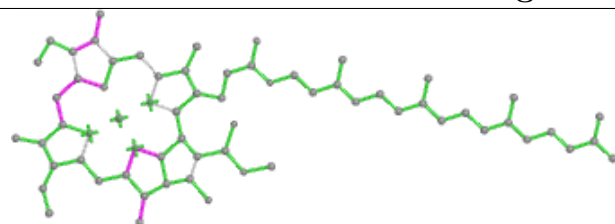


Torsions

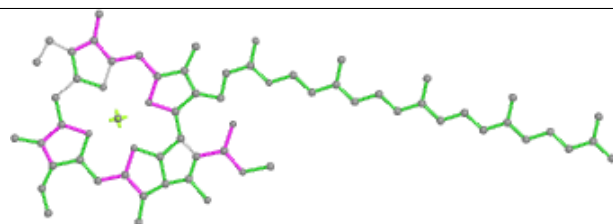


Rings

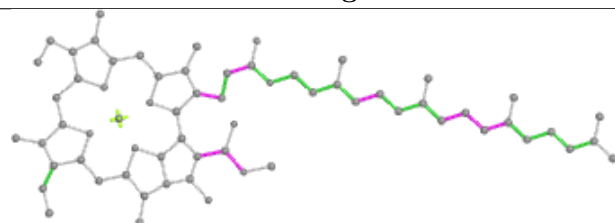
Ligand CLA B 834



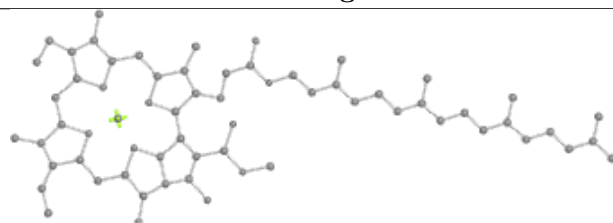
Bond lengths



Bond angles

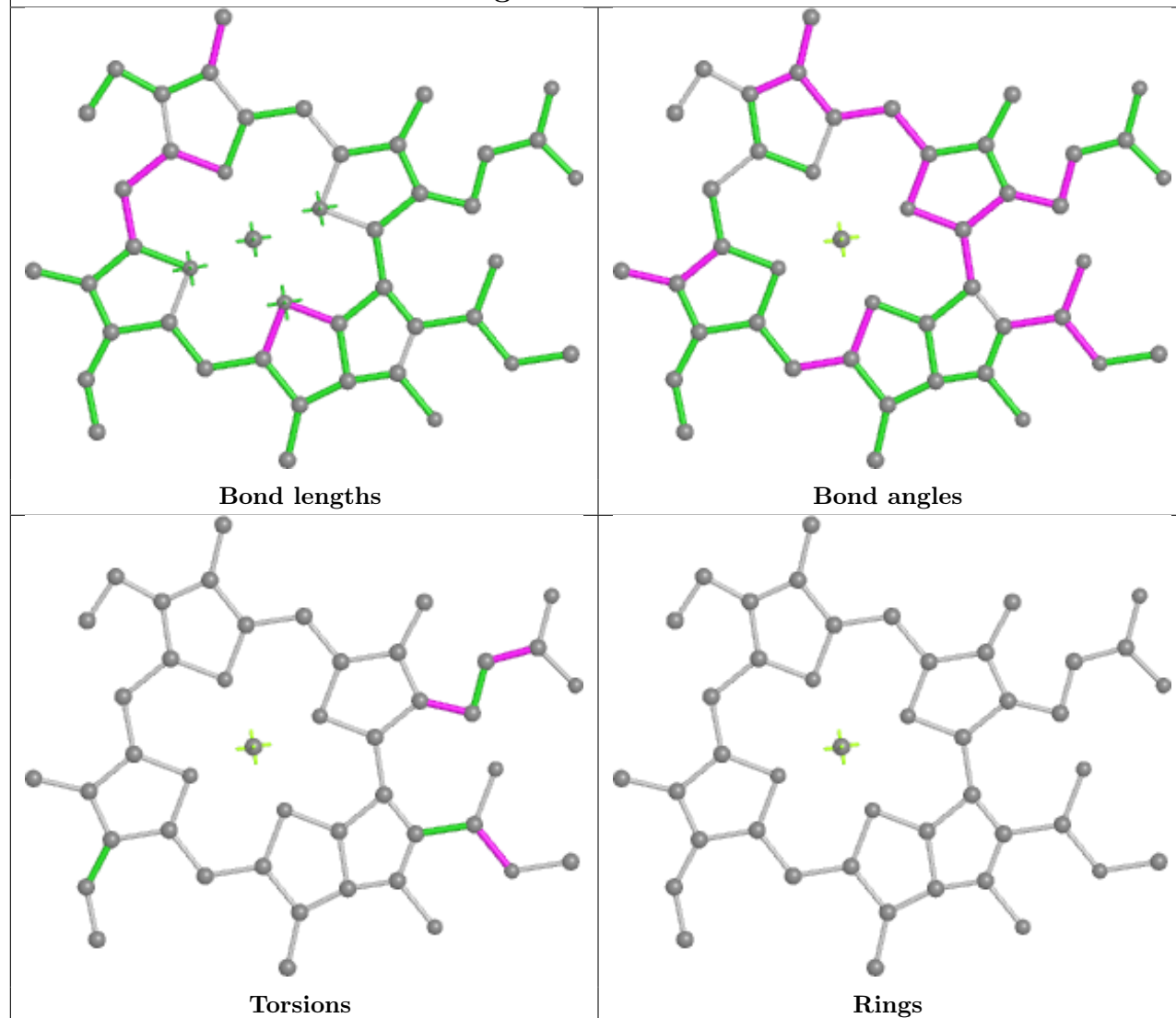


Torsions

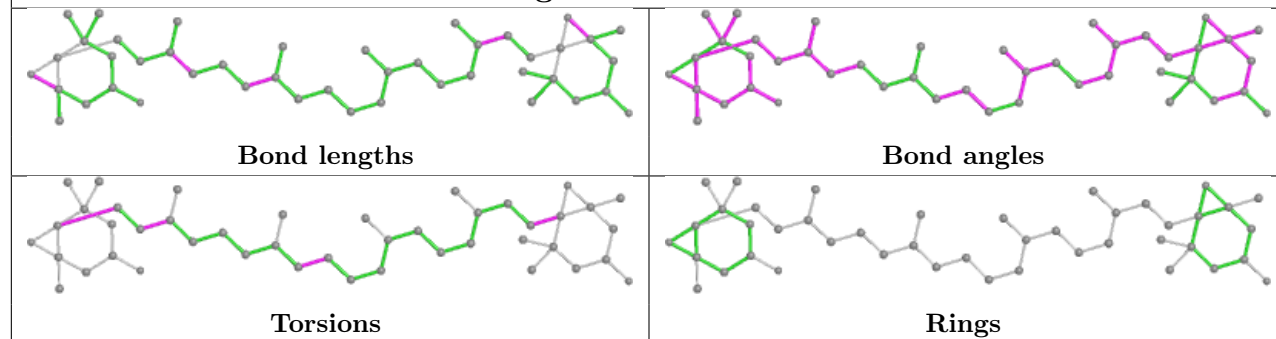


Rings

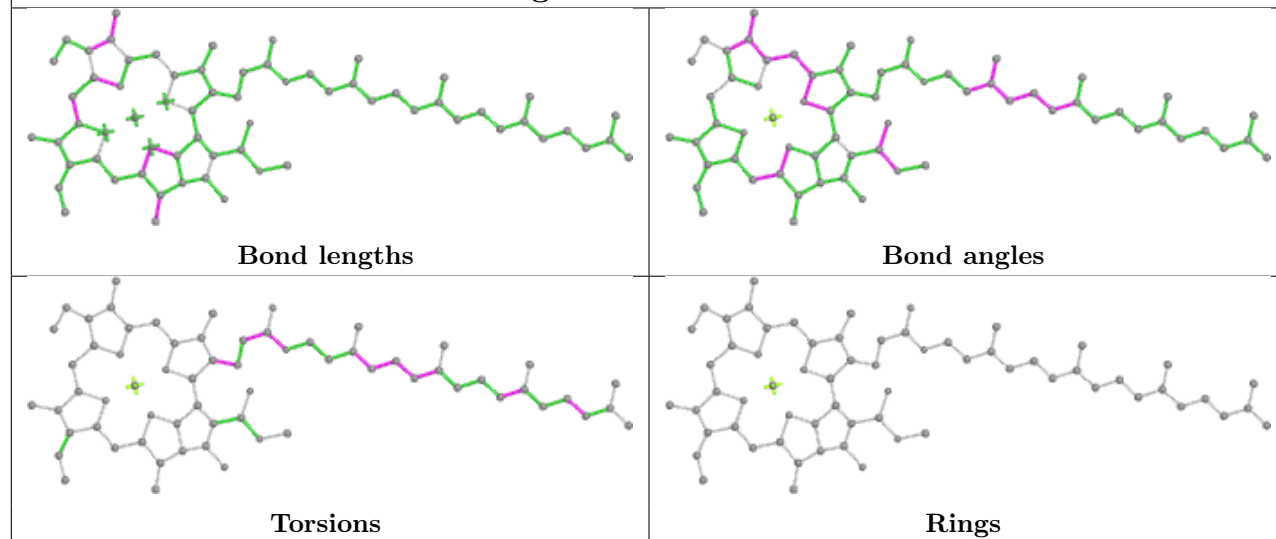
Ligand CLA 2 608



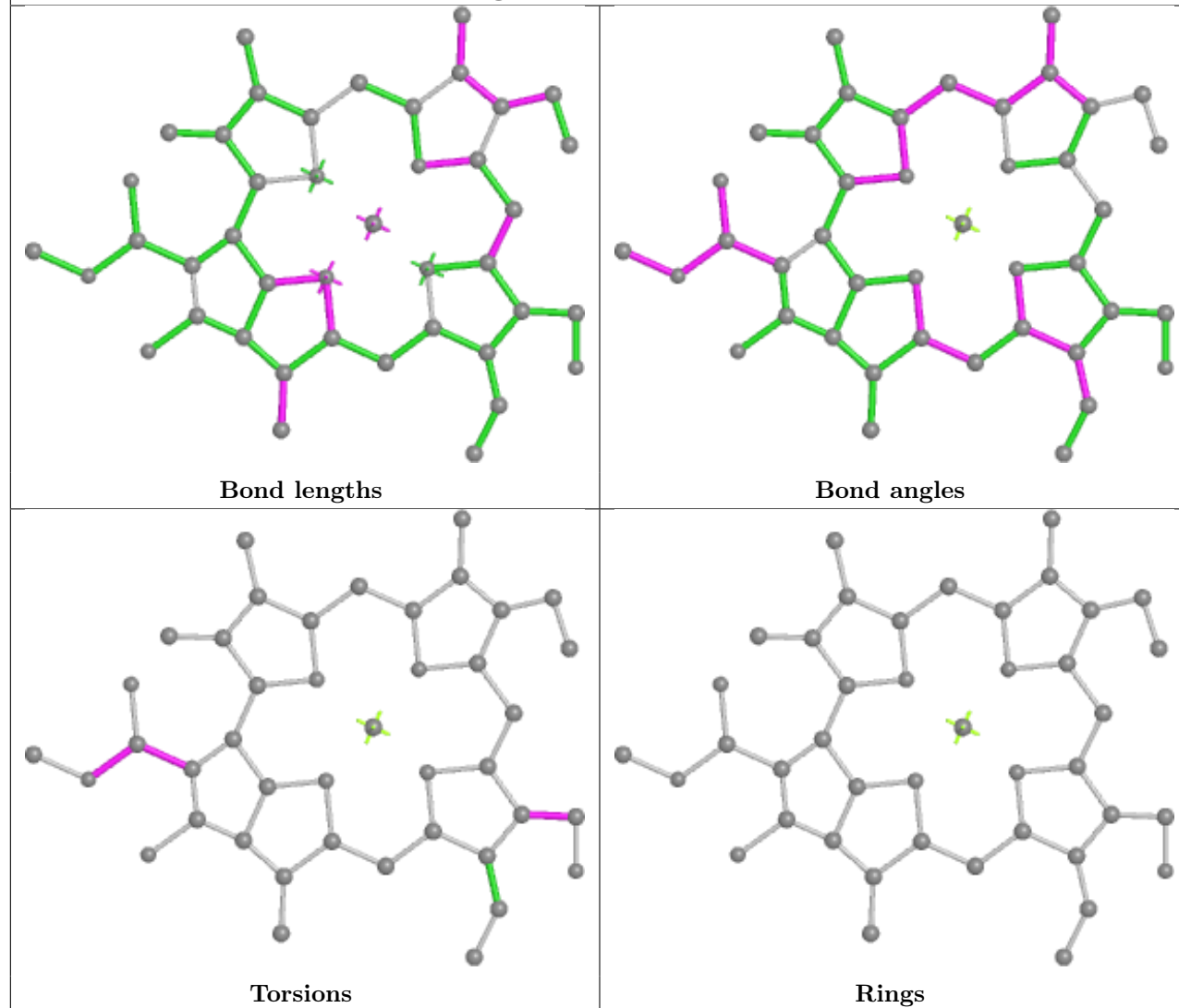
Ligand XAT 4 318



Ligand CLA A 837



Ligand CHL U 304



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.

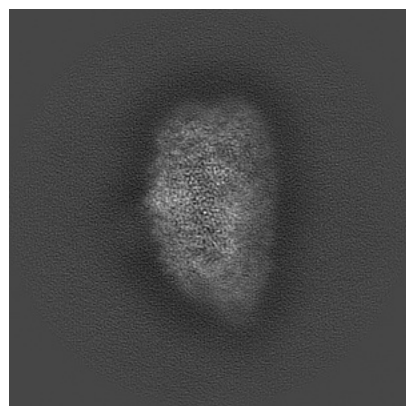
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-33737. These allow visual inspection of the internal detail of the map and identification of artifacts.

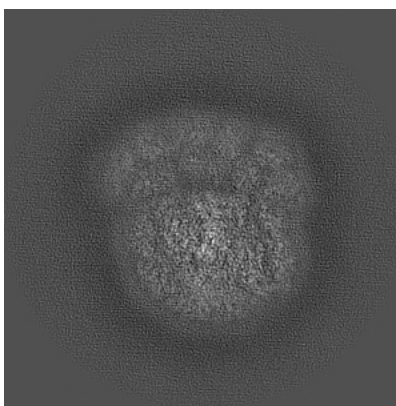
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

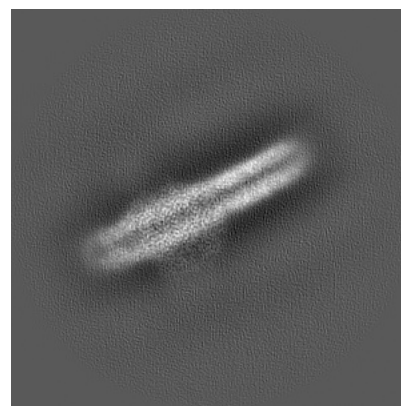
6.1.1 Primary map



X

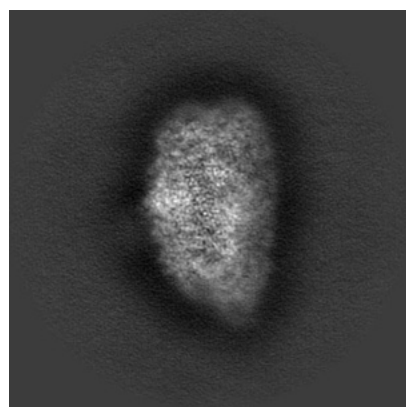


Y

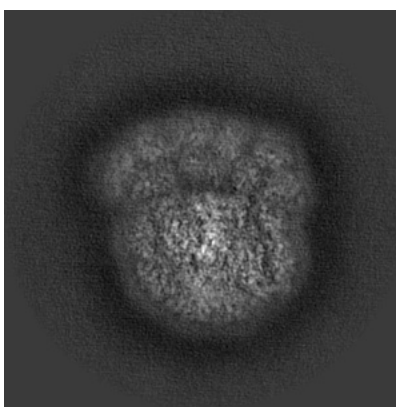


Z

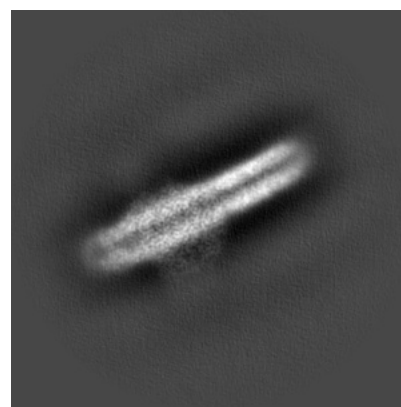
6.1.2 Raw map



X



Y

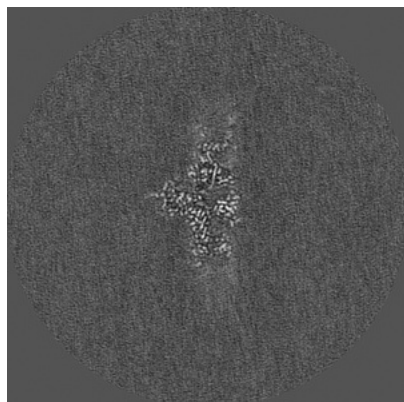


Z

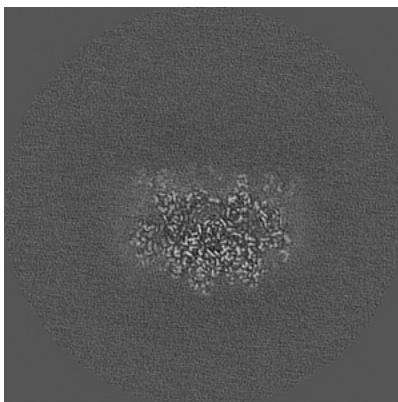
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

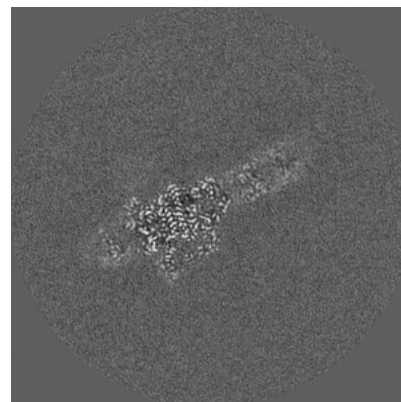
6.2.1 Primary map



X Index: 192

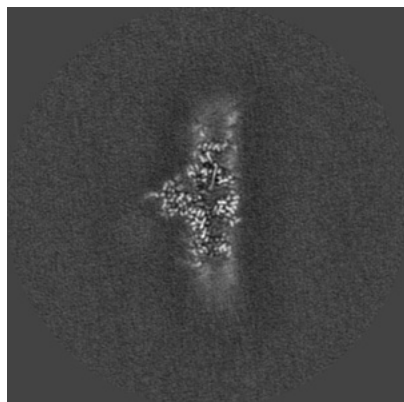


Y Index: 192

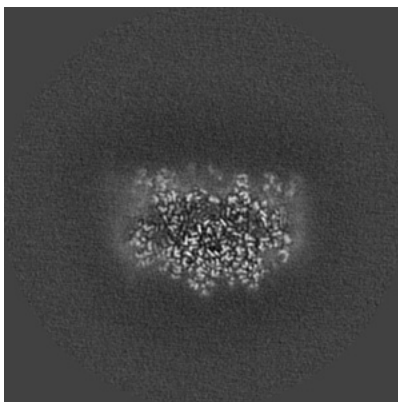


Z Index: 192

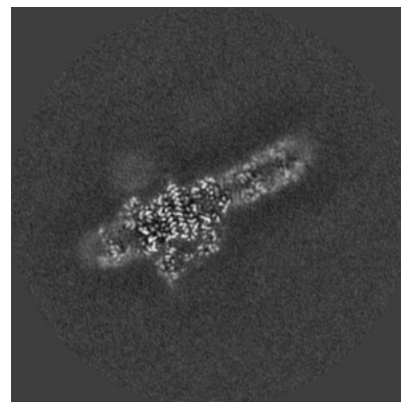
6.2.2 Raw map



X Index: 192



Y Index: 192

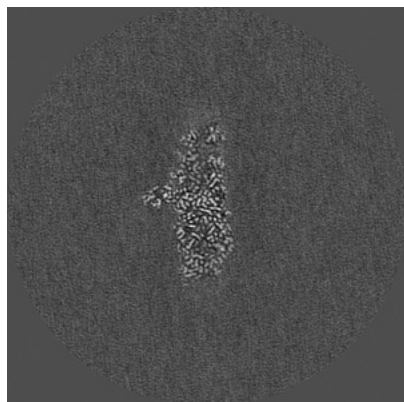


Z Index: 192

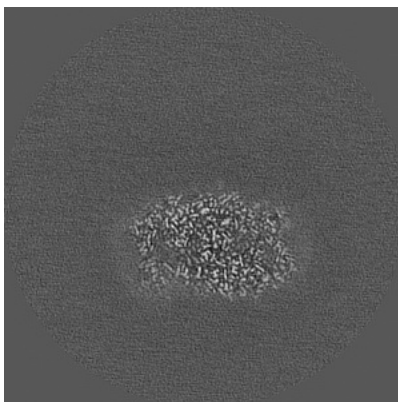
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

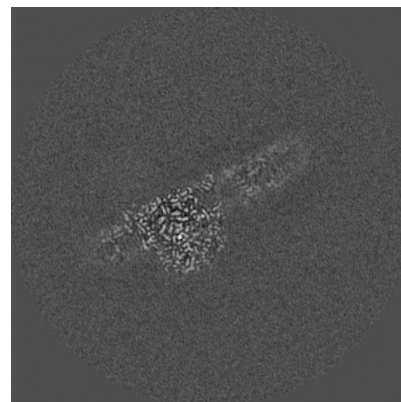
6.3.1 Primary map



X Index: 169

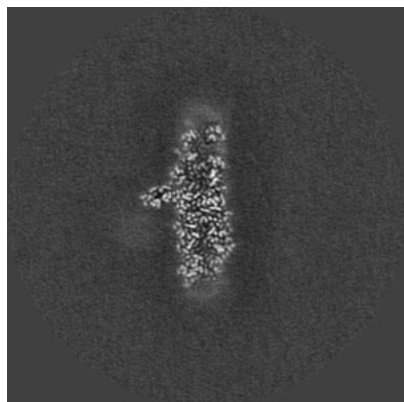


Y Index: 180

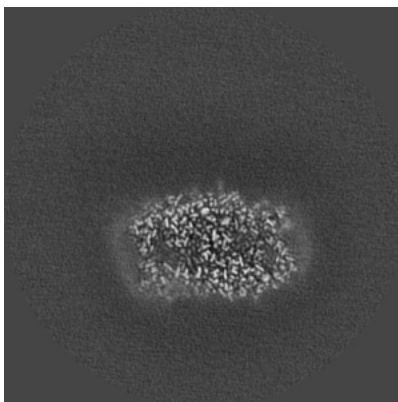


Z Index: 201

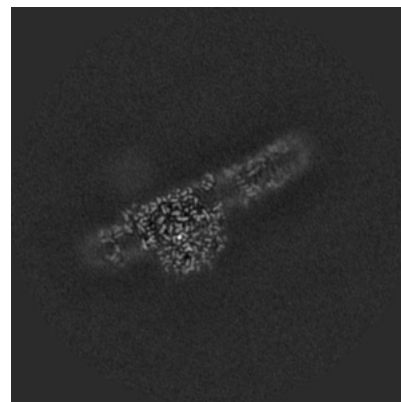
6.3.2 Raw map



X Index: 168



Y Index: 180

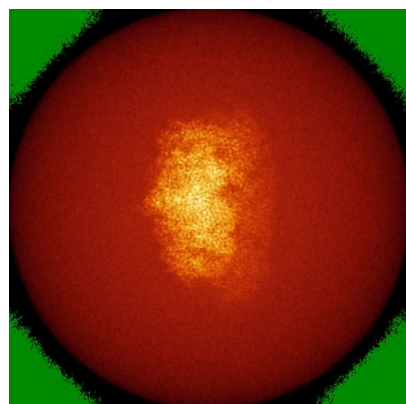


Z Index: 201

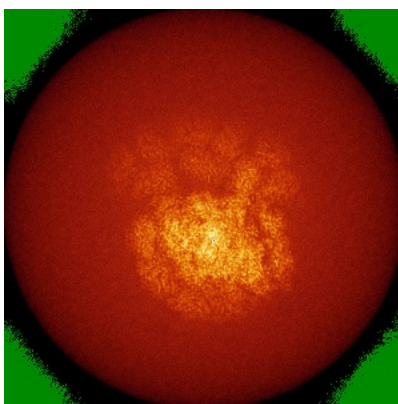
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) ⓘ

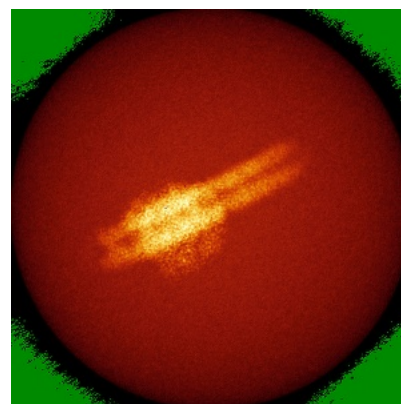
6.4.1 Primary map



X

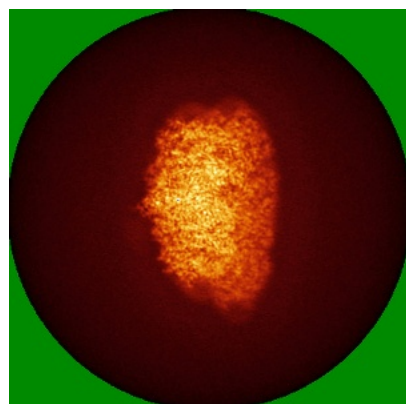


Y

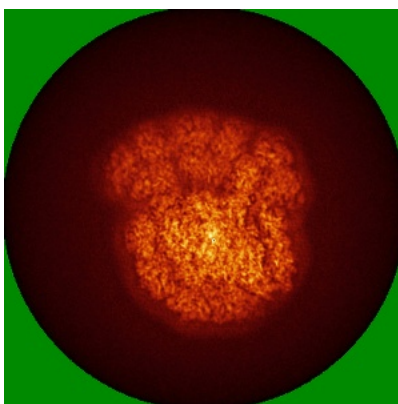


Z

6.4.2 Raw map



X



Y

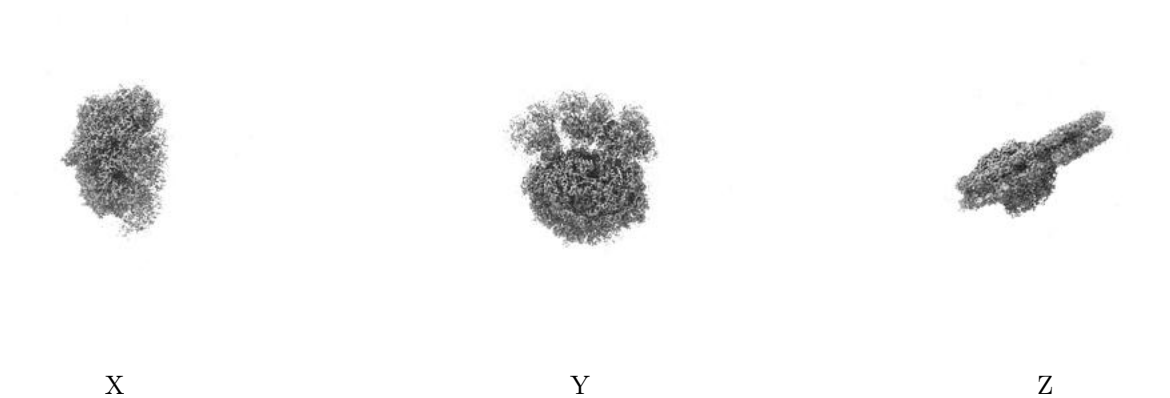


Z

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

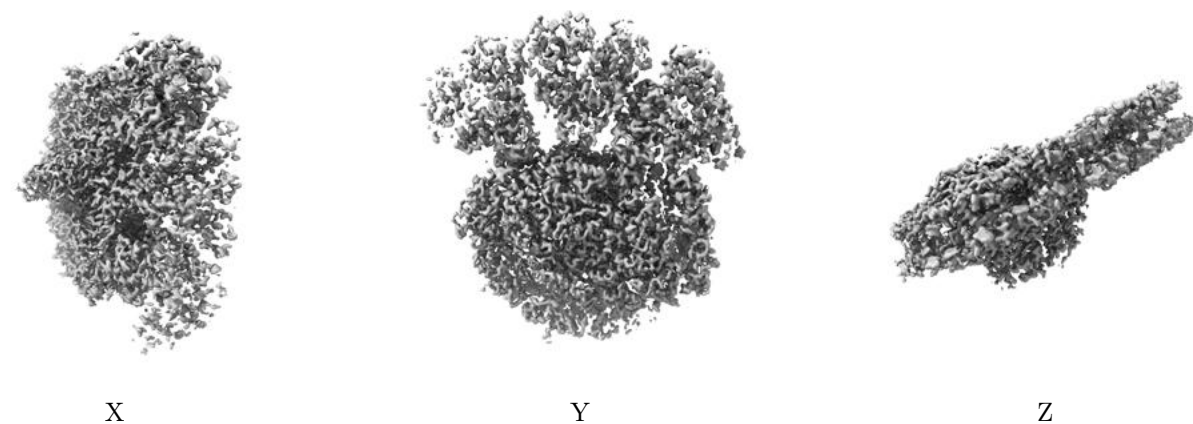
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.025. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

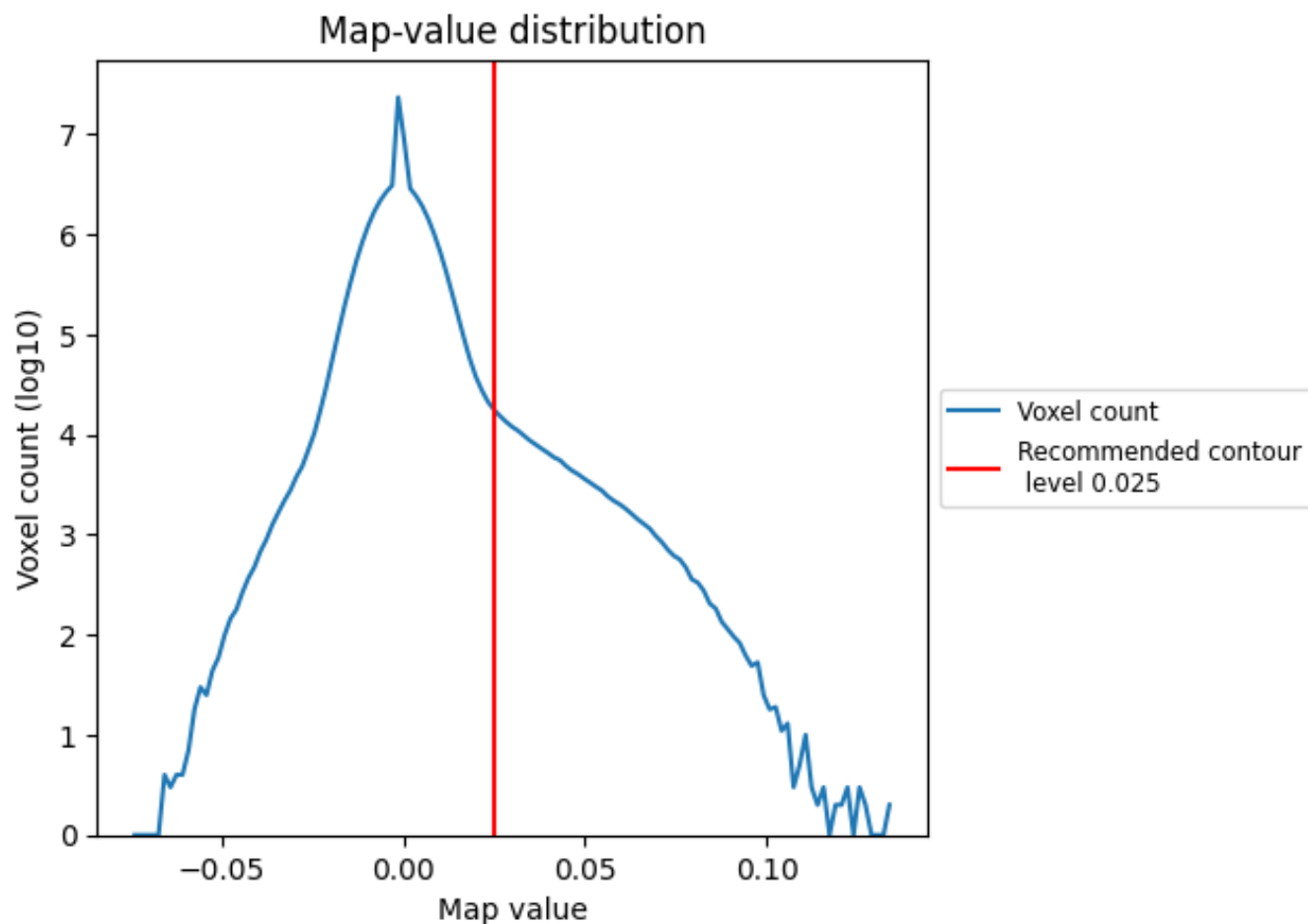
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

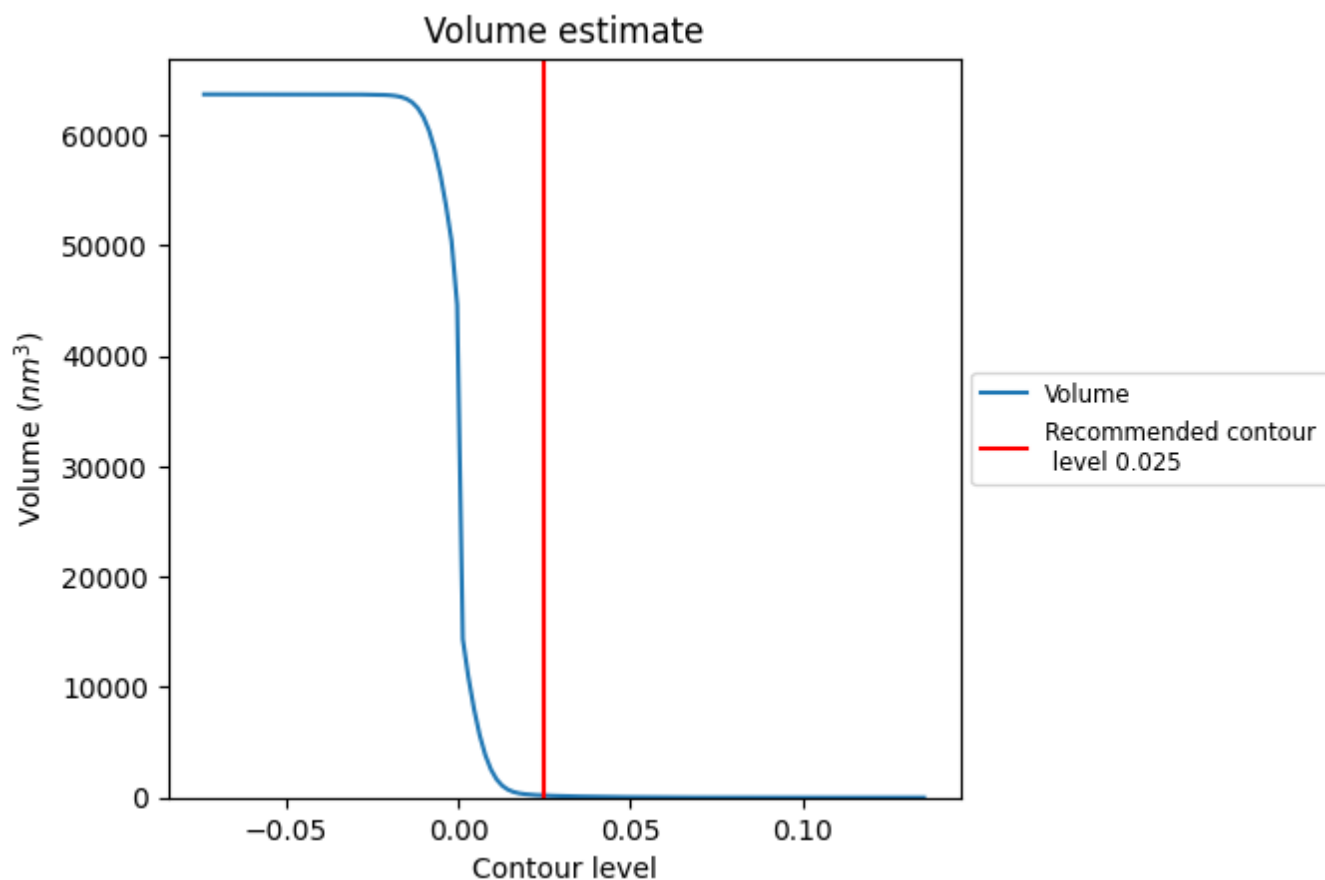
This section contains the results of statistical analysis of the map.

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.

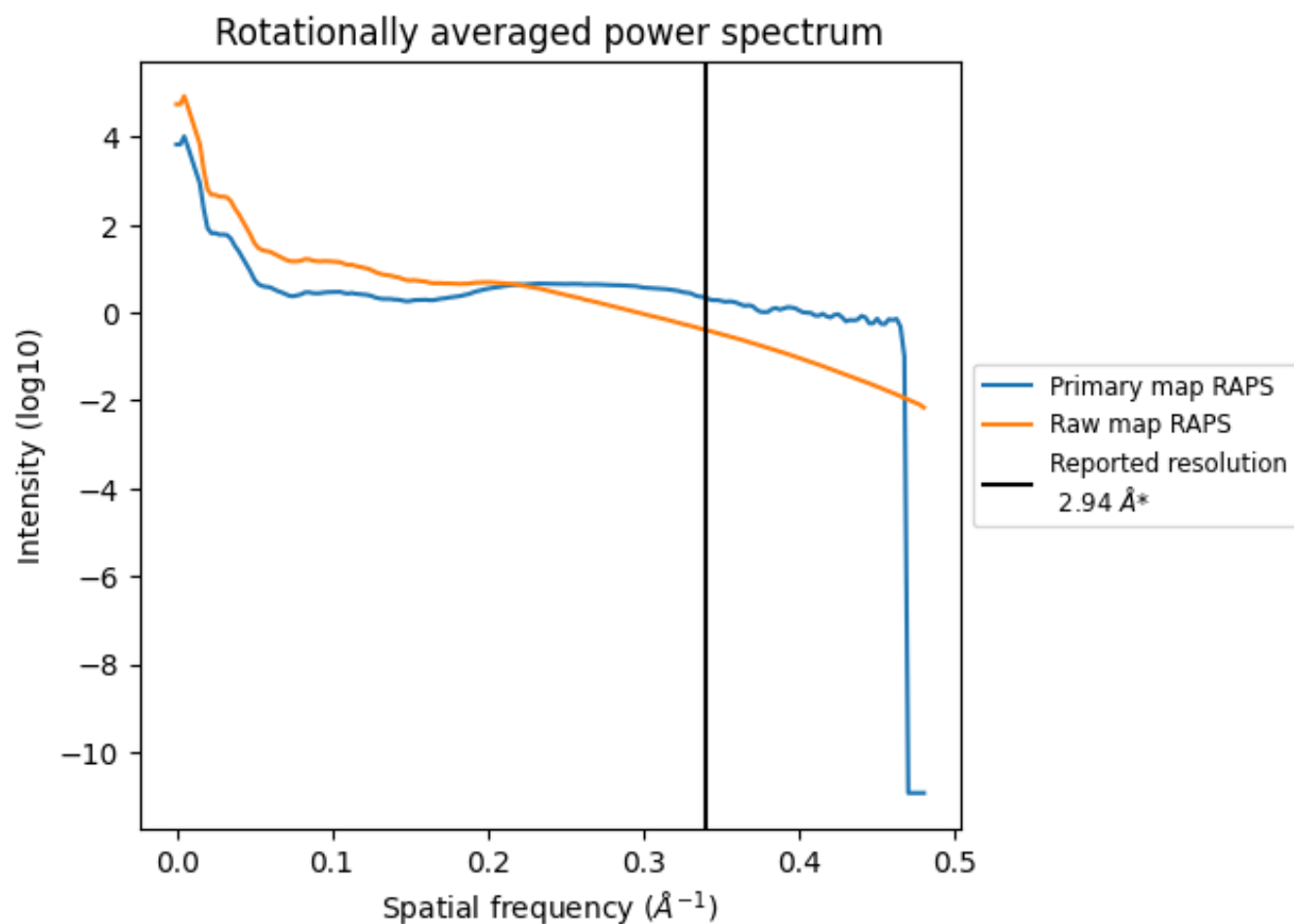
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 188 nm³; this corresponds to an approximate mass of 169 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 ⓘ

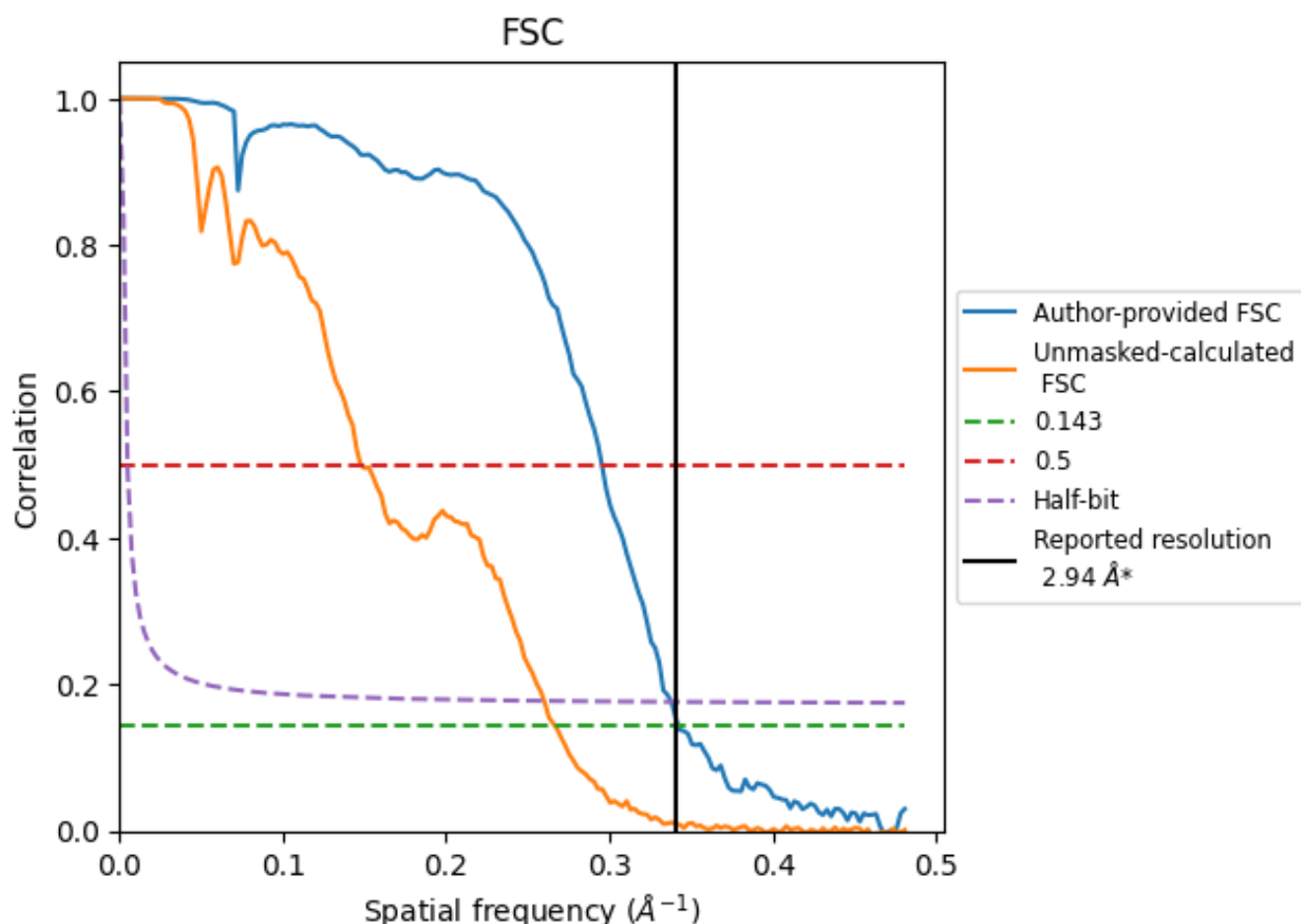


*Reported resolution corresponds to spatial frequency of 0.340 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.340 Å⁻¹

8.2 Resolution estimates [i](#)

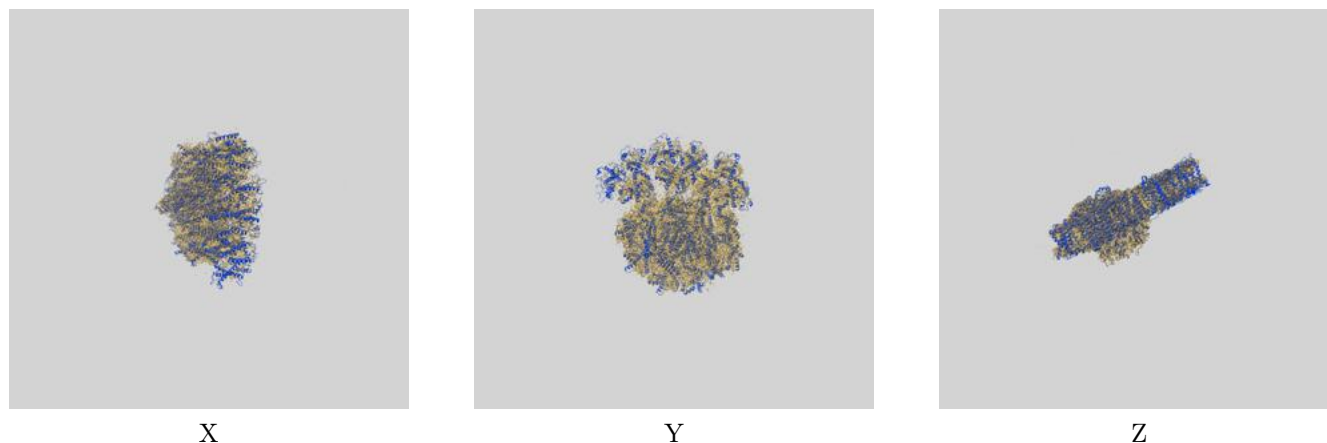
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.94	-	-
Author-provided FSC curve	2.92	3.39	2.96
Unmasked-calculated*	3.75	6.77	3.85

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.75 differs from the reported value 2.94 by more than 10 %

9 Map-model fit [i](#)

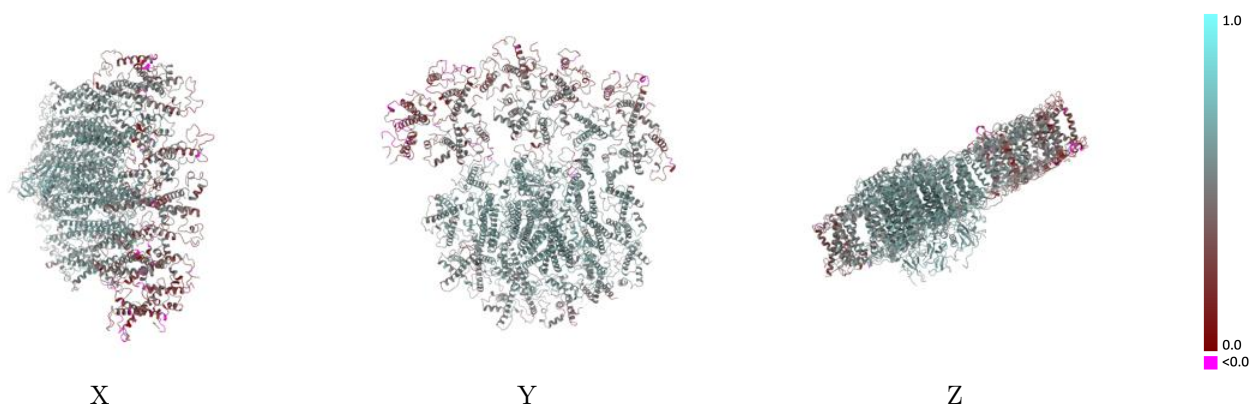
This section contains information regarding the fit between EMDB map EMD-33737 and PDB model 7YCA. Per-residue inclusion information can be found in section [3](#) on page [44](#).

9.1 Map-model overlay [i](#)



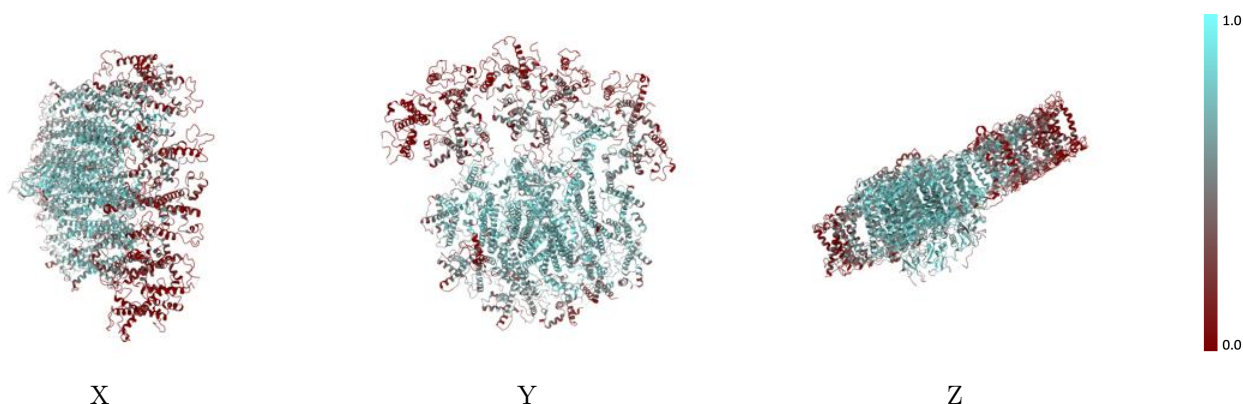
The images above show the 3D surface view of the map at the recommended contour level 0.025 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



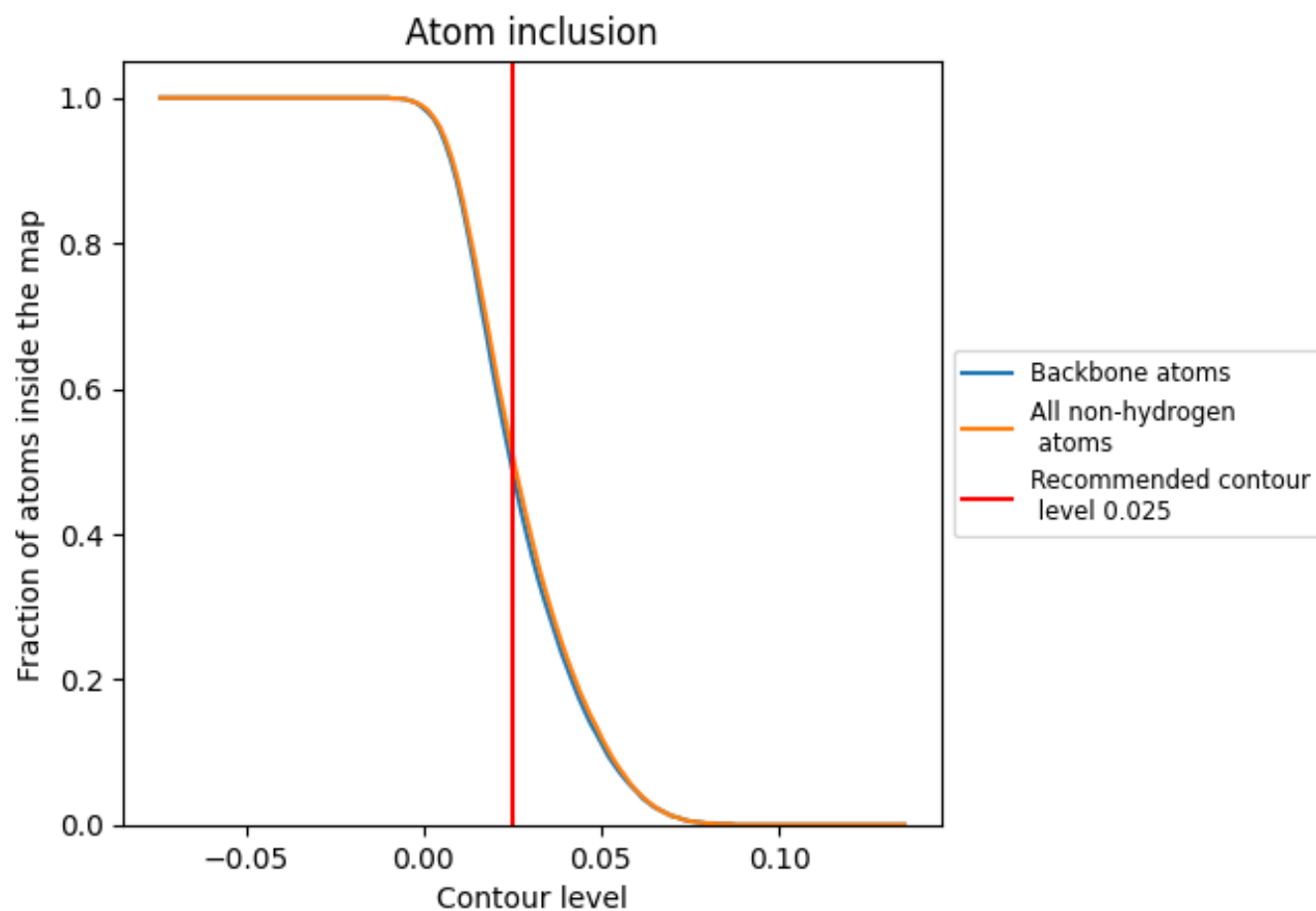
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.025).































































9.4 Atom inclusion [i](#)



At the recommended contour level, 49% of all backbone atoms, 51% 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 (0.025) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5110	 0.5140
1	 0.3170	 0.4450
2	 0.5160	 0.5240
3	 0.5610	 0.5590
4	 0.4200	 0.4810
5	 0.5730	 0.5480
6	 0.6330	 0.5670
A	 0.7720	 0.6190
B	 0.7600	 0.6090
C	 0.7780	 0.6160
D	 0.6260	 0.5840
E	 0.6110	 0.5870
F	 0.5970	 0.5620
G	 0.3990	 0.4970
H	 0.6320	 0.5770
I	 0.6670	 0.5760
J	 0.6620	 0.5760
K	 0.6500	 0.5780
L	 0.7290	 0.6100
M	 0.6490	 0.5930
N	 0.3080	 0.4830
O	 0.6920	 0.5910
P	 0.2520	 0.3960
Q	 0.5640	 0.5220
R	 0.3340	 0.4370
S	 0.2460	 0.4000
T	 0.3560	 0.4660
U	 0.1480	 0.3670
V	 0.1590	 0.3420
W	 0.3080	 0.4200
X	 0.0560	 0.2600

