



Full wwPDB EM Validation Report ⓘ

Mar 20, 2026 – 02:41 AM UTC

PDB ID : 8JZF / pdb_00008jzf
EMDB ID : EMD-36743
Title : PSI-AcpPCI supercomplex from Symbiodinium
Authors : Li, X.Y.; Li, Z.H.; Wang, W.D.
Deposited on : 2023-07-05
Resolution : 2.70 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

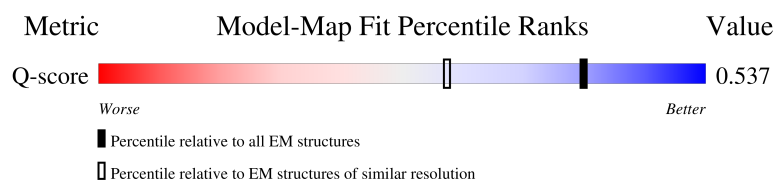
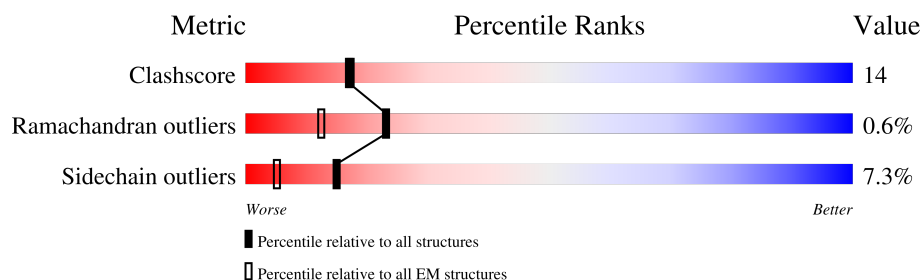
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



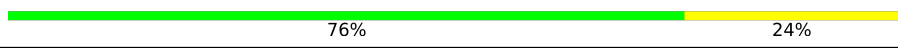
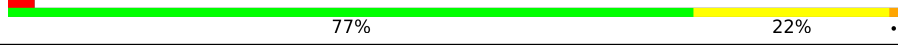
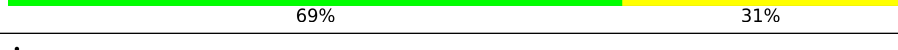
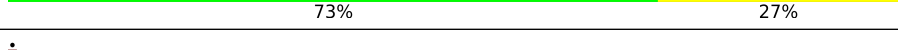
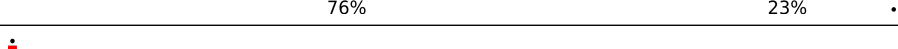
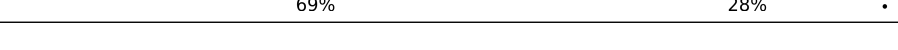
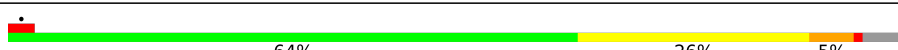
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	10327 (2.20 - 3.20)

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	I	200	
2	K	177	
3	z	78	
4	y	131	

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Mol	Chain	Length	Quality of chain
5	G	224	
6	A	189	
7	c	86	
8	d	218	
9	e	73	
10	f	184	
11	h	131	
12	i	119	
13	j	98	
14	l	250	
15	m	79	
16	a	670	
17	b	663	
18	B	192	
19	D	165	
20	F	176	
21	H	160	
22	J	220	
23	L	185	
24	M	173	
25	N	160	

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
28	CLA	A	307	X	-	-	-
28	CLA	A	308	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
28	CLA	A	309	X	-	-	-
28	CLA	A	310	X	-	-	-
28	CLA	A	311	X	-	-	-
28	CLA	A	312	X	-	-	-
28	CLA	A	313	X	-	-	-
28	CLA	A	315	X	-	-	-
28	CLA	A	316	X	-	-	-
28	CLA	A	317	X	-	-	-
28	CLA	A	319	X	-	-	-
28	CLA	A	320	X	-	-	-
28	CLA	B	301	X	-	-	-
28	CLA	B	307	X	-	-	-
28	CLA	B	308	X	-	-	-
28	CLA	B	309	X	-	-	-
28	CLA	B	310	X	-	-	-
28	CLA	B	311	X	-	-	-
28	CLA	B	312	X	-	-	-
28	CLA	B	313	X	-	-	-
28	CLA	B	315	X	-	-	-
28	CLA	B	316	X	-	-	-
28	CLA	B	317	X	-	-	-
28	CLA	D	308	X	-	-	-
28	CLA	D	309	X	-	-	-
28	CLA	D	311	X	-	-	-
28	CLA	D	312	X	-	-	-
28	CLA	D	313	X	-	-	-
28	CLA	D	314	X	-	-	-
28	CLA	D	316	X	-	-	-
28	CLA	F	307	X	-	-	-
28	CLA	F	308	X	-	-	-
28	CLA	F	310	X	-	-	-
28	CLA	F	311	X	-	-	-
28	CLA	F	312	X	-	-	-
28	CLA	F	313	X	-	-	-
28	CLA	F	315	X	-	-	-
28	CLA	G	509	X	-	-	-
28	CLA	G	510	X	-	-	-
28	CLA	G	511	X	-	-	-
28	CLA	G	512	X	-	-	-
28	CLA	G	513	X	-	-	-
28	CLA	G	514	X	-	-	-
28	CLA	G	516	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
28	CLA	G	517	X	-	-	-
28	CLA	G	518	X	-	-	-
28	CLA	G	519	X	-	-	-
28	CLA	G	520	X	-	-	-
28	CLA	H	304	X	-	-	-
28	CLA	H	305	X	-	-	-
28	CLA	H	307	X	-	-	-
28	CLA	H	308	X	-	-	-
28	CLA	H	309	X	-	-	-
28	CLA	H	312	X	-	-	-
28	CLA	I	306	X	-	-	-
28	CLA	I	307	X	-	-	-
28	CLA	I	308	X	-	-	-
28	CLA	I	309	X	-	-	-
28	CLA	I	310	X	-	-	-
28	CLA	I	311	X	-	-	-
28	CLA	I	312	X	-	-	-
28	CLA	I	313	X	-	-	-
28	CLA	I	315	X	-	-	-
28	CLA	I	316	X	-	-	-
28	CLA	I	319	X	-	-	-
28	CLA	I	321	X	-	-	-
28	CLA	J	301	X	-	-	-
28	CLA	J	306	X	-	-	-
28	CLA	J	307	X	-	-	-
28	CLA	J	308	X	-	-	-
28	CLA	J	309	X	-	-	-
28	CLA	J	310	X	-	-	-
28	CLA	J	311	X	-	-	-
28	CLA	J	312	X	-	-	-
28	CLA	J	314	X	-	-	-
28	CLA	J	315	X	-	-	-
28	CLA	K	306	X	-	-	-
28	CLA	K	307	X	-	-	-
28	CLA	K	308	X	-	-	-
28	CLA	K	309	X	-	-	-
28	CLA	K	310	X	-	-	-
28	CLA	K	311	X	-	-	-
28	CLA	K	312	X	-	-	-
28	CLA	K	313	X	-	-	-
28	CLA	K	315	X	-	-	-
28	CLA	K	316	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
28	CLA	L	308	X	-	-	-
28	CLA	L	309	X	-	-	-
28	CLA	L	310	X	-	-	-
28	CLA	L	311	X	-	-	-
28	CLA	L	312	X	-	-	-
28	CLA	L	313	X	-	-	-
28	CLA	L	314	X	-	-	-
28	CLA	L	316	X	-	-	-
28	CLA	L	317	X	-	-	-
28	CLA	L	318	X	-	-	-
28	CLA	M	308	X	-	-	-
28	CLA	M	309	X	-	-	-
28	CLA	M	310	X	-	-	-
28	CLA	M	311	X	-	-	-
28	CLA	M	312	X	-	-	-
28	CLA	M	313	X	-	-	-
28	CLA	M	315	X	-	-	-
28	CLA	M	316	X	-	-	-
28	CLA	M	317	X	-	-	-
28	CLA	M	318	X	-	-	-
28	CLA	N	304	X	-	-	-
28	CLA	N	305	X	-	-	-
28	CLA	N	307	X	-	-	-
28	CLA	N	309	X	-	-	-
28	CLA	N	310	X	-	-	-
28	CLA	a	701	X	-	-	-
28	CLA	a	702	X	-	-	-
28	CLA	a	703	X	-	-	-
28	CLA	a	704	X	-	-	-
28	CLA	a	705	X	-	-	-
28	CLA	a	706	X	-	-	-
28	CLA	a	707	X	-	-	-
28	CLA	a	708	X	-	-	-
28	CLA	a	709	X	-	-	-
28	CLA	a	710	X	-	-	-
28	CLA	a	711	X	-	-	-
28	CLA	a	712	X	-	-	-
28	CLA	a	713	X	-	-	-
28	CLA	a	714	X	-	-	-
28	CLA	a	715	X	-	-	-
28	CLA	a	716	X	-	-	-
28	CLA	a	717	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
28	CLA	a	718	X	-	-	-
28	CLA	a	719	X	-	-	-
28	CLA	a	720	X	-	-	-
28	CLA	a	721	X	-	-	-
28	CLA	a	722	X	-	-	-
28	CLA	a	723	X	-	-	-
28	CLA	a	724	X	-	-	-
28	CLA	a	725	X	-	-	-
28	CLA	a	726	X	-	-	-
28	CLA	a	727	X	-	-	-
28	CLA	a	728	X	-	-	-
28	CLA	a	729	X	-	-	-
28	CLA	a	730	X	-	-	-
28	CLA	a	731	X	-	-	-
28	CLA	a	735	X	-	-	-
28	CLA	a	738	X	-	-	-
28	CLA	b	701	X	-	-	-
28	CLA	b	703	X	-	-	-
28	CLA	b	704	X	-	-	-
28	CLA	b	705	X	-	-	-
28	CLA	b	706	X	-	-	-
28	CLA	b	707	X	-	-	-
28	CLA	b	708	X	-	-	-
28	CLA	b	709	X	-	-	-
28	CLA	b	710	X	-	-	-
28	CLA	b	711	X	-	-	-
28	CLA	b	712	X	-	-	-
28	CLA	b	713	X	-	-	-
28	CLA	b	714	X	-	-	-
28	CLA	b	715	X	-	-	-
28	CLA	b	716	X	-	-	-
28	CLA	b	717	X	-	-	-
28	CLA	b	718	X	-	-	-
28	CLA	b	719	X	-	-	-
28	CLA	b	720	X	-	-	-
28	CLA	b	721	X	-	-	-
28	CLA	b	722	X	-	-	-
28	CLA	b	723	X	-	-	-
28	CLA	b	724	X	-	-	-
28	CLA	b	725	X	-	-	-
28	CLA	b	726	X	-	-	-
28	CLA	b	727	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
28	CLA	b	728	X	-	-	-
28	CLA	f	301	X	-	-	-
28	CLA	f	302	X	-	-	-
28	CLA	f	303	X	-	-	-
28	CLA	h	202	X	-	-	-
28	CLA	j	104	X	-	-	-
28	CLA	j	106	X	-	-	-
28	CLA	l	303	X	-	-	-
28	CLA	l	304	X	-	-	-
28	CLA	l	305	X	-	-	-
28	CLA	l	308	X	-	-	-
28	CLA	l	309	X	-	-	-
28	CLA	l	311	X	-	-	-
28	CLA	l	312	X	-	-	-
28	CLA	l	313	X	-	-	-
28	CLA	m	202	X	-	-	-

2 Entry composition

There are 37 unique types of molecules in this entry. The entry contains 52237 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Chlorophyll a-chlorophyll c-peridinin-protein-complex I-7, acpPCI-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	I	200	Total	C	N	O	S	0	0
			1480	961	250	259	10		

- Molecule 2 is a protein called Chlorophyll a-chlorophyll c-peridinin-protein-complex I-6, acpPCI-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	K	177	Total	C	N	O	S	0	0
			1349	872	227	238	12		

- Molecule 3 is a protein called Photosystem I unk.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	z	78	Total	C	N	O	0	0
			390	234	78	78		

- Molecule 4 is a protein called Photosystem I unk.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	y	131	Total	C	N	O	0	0
			655	393	131	131		

- Molecule 5 is a protein called Chlorophyll a-chlorophyll c-peridinin-protein-complex I-8, acpPCI-8.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	G	217	Total	C	N	O	S	0	0
			1572	1004	269	289	10		

- Molecule 6 is a protein called Chlorophyll a-chlorophyll c-peridinin-protein-complex I-10, acpPCI-10.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	A	186	Total	C	N	O	S	0	0
			1346	870	225	242	9		

- Molecule 7 is a protein called Photosystem I PsuC.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	c	86	Total	C	N	O	S	0	0
			653	403	109	132	9		

- Molecule 8 is a protein called Photosystem I PsuD.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	d	218	Total	C	N	O	S	0	0
			1731	1096	307	315	13		

- Molecule 9 is a protein called Photosystem I PsuE.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	e	73	Total	C	N	O	0	0
			587	384	99	104		

- Molecule 10 is a protein called Photosystem I PsuF.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	f	184	Total	C	N	O	S	0	0
			1450	930	252	260	8		

- Molecule 11 is a protein called Photosystem I PsuR.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	h	131	Total	C	N	O	S	0	0
			1066	704	165	193	4		

- Molecule 12 is a protein called Photosystem I PsuI.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	i	119	Total	C	N	O	S	0	0
			964	620	167	175	2		

- Molecule 13 is a protein called Photosystem I PsuJ.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	j	98	Total	C	N	O	0	0
			783	505	125	153		

- Molecule 14 is a protein called Photosystem I Psal.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	l	250	Total	C	N	O	S	0	0
			1943	1267	312	354	10		

- Molecule 15 is a protein called Photosystem I Psam.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	m	79	Total	C	N	O	S	0	0
			582	373	100	107	2		

- Molecule 16 is a protein called Photosystem I PsaA.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	a	670	Total	C	N	O	S	0	0
			5194	3393	875	910	16		

- Molecule 17 is a protein called Photosystem I Psab.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	b	663	Total	C	N	O	S	0	0
			5199	3408	851	928	12		

- Molecule 18 is a protein called Chlorophyll a-chlorophyll c-peridinin-protein-complex I-11, acpPCI-11.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	B	192	Total	C	N	O	S	0	0
			1452	934	241	265	12		

- Molecule 19 is a protein called Chlorophyll a-chlorophyll c-peridinin-protein-complex I-9, acpPCI-9.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	D	160	Total	C	N	O	S	0	0
			1158	728	195	228	7		

- Molecule 20 is a protein called Chlorophyll a-chlorophyll c-peridinin-protein-complex I-2,

acpPCI-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	F	169	Total	C	N	O	S	0	0
			1237	777	209	239	12		

- Molecule 21 is a protein called Chlorophyll a-chlorophyll c-peridinin-protein-complex I-12, acpPCI-12.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	H	160	Total	C	N	O	S	0	0
			1202	769	198	228	7		

- Molecule 22 is a protein called Chlorophyll a-chlorophyll c-peridinin-protein-complex I-3, acpPCI-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	J	220	Total	C	N	O	S	0	0
			1496	938	261	290	7		

- Molecule 23 is a protein called Chlorophyll a-chlorophyll c-peridinin-protein-complex I-5, acpPCI-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	L	185	Total	C	N	O	S	0	0
			1427	924	239	258	6		

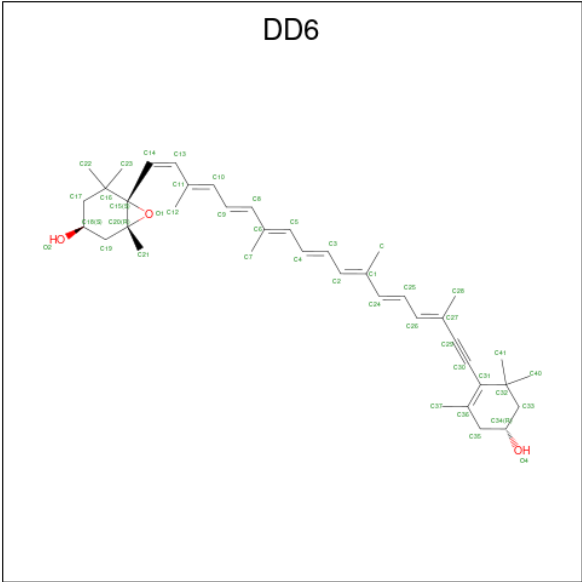
- Molecule 24 is a protein called Chlorophyll a-chlorophyll c-peridinin-protein-complex I-4, acpPCI-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	M	168	Total	C	N	O	S	0	0
			1211	773	208	225	5		

- Molecule 25 is a protein called Chlorophyll a-chlorophyll c-peridinin-protein-complex I-13, acpPCI-13.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	N	153	Total	C	N	O	S	0	0
			993	607	179	202	5		

- Molecule 26 is (3S,3'R,5R,6S,7cis)-7',8'-didehydro-5,6-dihydro-5,6-epoxy-beta,beta-carotene-3,3'-diol (CCD ID: DD6) (formula: C₄₀H₅₄O₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
26	I	1	Total	C	O	0
			43	40	3	
26	I	1	Total	C	O	0
			43	40	3	
26	I	1	Total	C	O	0
			43	40	3	
26	I	1	Total	C	O	0
			43	40	3	
26	K	1	Total	C	O	0
			43	40	3	
26	K	1	Total	C	O	0
			43	40	3	
26	K	1	Total	C	O	0
			43	40	3	
26	K	1	Total	C	O	0
			43	40	3	
26	K	1	Total	C	O	0
			43	40	3	
26	G	1	Total	C	O	0
			43	40	3	
26	G	1	Total	C	O	0
			43	40	3	
26	G	1	Total	C	O	0
			43	40	3	
26	G	1	Total	C	O	0
			43	40	3	
26	A	1	Total	C	O	0
			43	40	3	

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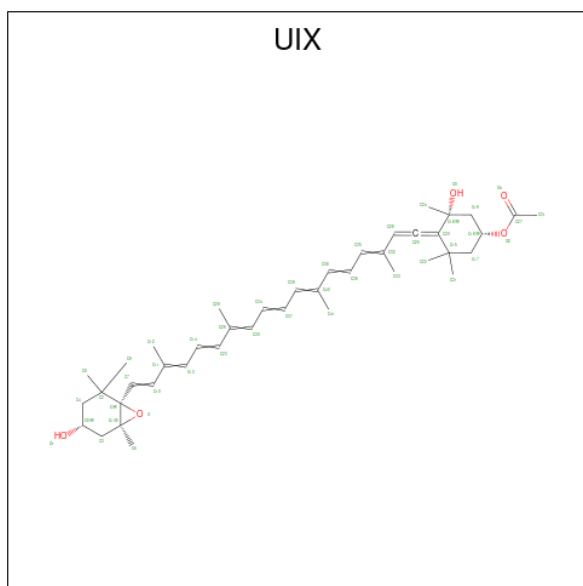
Mol	Chain	Residues	Atoms			AltConf
26	A	1	Total 43	C 40	O 3	0
26	A	1	Total 43	C 40	O 3	0
26	A	1	Total 43	C 40	O 3	0
26	h	1	Total 43	C 40	O 3	0
26	b	1	Total 43	C 40	O 3	0
26	B	1	Total 42	C 39	O 3	0
26	B	1	Total 43	C 40	O 3	0
26	B	1	Total 43	C 40	O 3	0
26	B	1	Total 43	C 40	O 3	0
26	B	1	Total 43	C 40	O 3	0
26	D	1	Total 43	C 40	O 3	0
26	F	1	Total 43	C 40	O 3	0
26	F	1	Total 43	C 40	O 3	0
26	H	1	Total 43	C 40	O 3	0
26	J	1	Total 43	C 40	O 3	0
26	J	1	Total 43	C 40	O 3	0
26	J	1	Total 43	C 40	O 3	0
26	L	1	Total 43	C 40	O 3	0
26	L	1	Total 43	C 40	O 3	0
26	L	1	Total 43	C 40	O 3	0
26	L	1	Total 43	C 40	O 3	0
26	L	1	Total 43	C 40	O 3	0

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Mol	Chain	Residues	Atoms			AltConf
26	M	1	Total	C	O	0
			43	40	3	
26	M	1	Total	C	O	0
			43	40	3	
26	M	1	Total	C	O	0
			43	40	3	
26	M	1	Total	C	O	0
			43	40	3	
26	M	1	Total	C	O	0
			43	40	3	
26	N	1	Total	C	O	0
			43	40	3	

- Molecule 27 is [(1 {S},5 {R})-3,3,5-trimethyl-5-oxidanyl-4-[(3 {E},5 {E},7 {E},9 {E},11 {E},13 {E},15 {E},17 {E})-3,7,12,16-tetramethyl-18-[(1 {S},4 {S},6 {R})-2,2,6-trimethyl-4-oxidanyl-7-oxabicyclo[4.1.0]heptan-1-yl]octadeca-1,3,5,7,9,11,13,15,17-nonaenylidene]cyclohexyl] ethanoate (CCD ID: UIX) (formula: C₄₂H₅₈O₅) (labeled as "Ligand of Interest" by depositor).



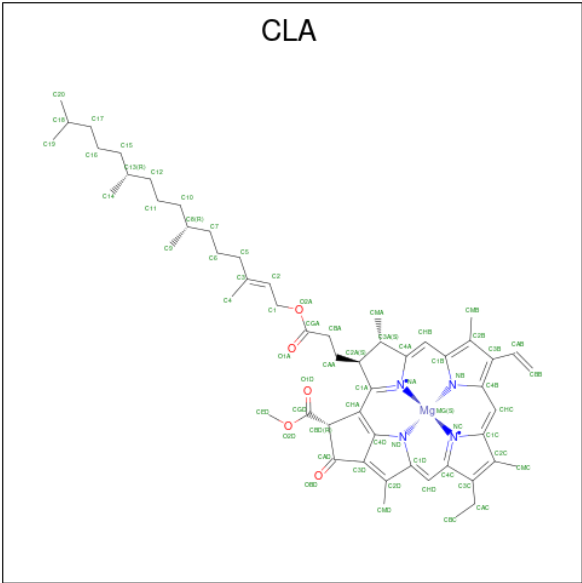
Mol	Chain	Residues	Atoms			AltConf
27	I	1	Total	C	O	0
			47	42	5	
27	K	1	Total	C	O	0
			47	42	5	
27	G	1	Total	C	O	0
			47	42	5	

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Mol	Chain	Residues	Atoms			AltConf
27	A	1	Total	C	O	0
			47	42	5	
27	h	1	Total	C	O	0
			47	42	5	
27	B	1	Total	C	O	0
			47	42	5	
27	J	1	Total	C	O	0
			47	42	5	

- Molecule 28 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
28	I	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
28	I	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
28	I	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
28	I	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
28	I	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
28	I	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
28	I	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
28	I	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
28	I	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
28	I	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
28	I	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
28	I	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
28	K	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
28	K	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
28	K	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
28	K	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
28	K	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
28	K	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
28	K	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
28	K	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
28	K	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
28	K	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
28	G	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
28	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	G	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
28	G	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
28	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	G	1	Total	C	Mg	N	O	0
			53	43	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
28	G	1	Total 41	C 33	Mg 1	N 4	O 3	0
28	G	1	Total 46	C 36	Mg 1	N 4	O 5	0
28	G	1	Total 46	C 36	Mg 1	N 4	O 5	0
28	G	1	Total 61	C 51	Mg 1	N 4	O 5	0
28	G	1	Total 49	C 39	Mg 1	N 4	O 5	0
28	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
28	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
28	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
28	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	A	1	Total 46	C 36	Mg 1	N 4	O 5	0
28	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
28	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
28	A	1	Total 41	C 33	Mg 1	N 4	O 3	0
28	A	1	Total 47	C 37	Mg 1	N 4	O 5	0
28	A	1	Total 41	C 33	Mg 1	N 4	O 3	0
28	A	1	Total 46	C 36	Mg 1	N 4	O 5	0
28	A	1	Total 46	C 36	Mg 1	N 4	O 5	0
28	f	1	Total 55	C 45	Mg 1	N 4	O 5	0
28	f	1	Total 46	C 36	Mg 1	N 4	O 5	0
28	f	1	Total 46	C 36	Mg 1	N 4	O 5	0
28	h	1	Total 55	C 45	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
28	j	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
28	j	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
28	l	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	l	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
28	l	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	l	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
28	l	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
28	l	1	Total	C	N	O		0
			45	36	4	5		
28	l	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	l	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
28	l	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	m	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
28	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
28	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	a	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
28	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	a	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
28	a	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
28	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	a	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
28	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
28	a	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
28	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
28	a	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
28	a	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
28	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
28	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
28	a	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
28	a	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
28	a	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
28	a	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
28	a	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
28	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	a	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
28	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	a	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
28	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	a	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
28	a	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
28	a	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
28	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
28	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	a	1	Total 46	C 36	Mg 1	N 4	O 5	0
28	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	b	1	Total 48	C 38	Mg 1	N 4	O 5	0
28	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	b	1	Total 60	C 50	Mg 1	N 4	O 5	0
28	b	1	Total 52	C 42	Mg 1	N 4	O 5	0
28	b	1	Total 55	C 45	Mg 1	N 4	O 5	0
28	b	1	Total 54	C 44	Mg 1	N 4	O 5	0
28	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	b	1	Total 46	C 36	Mg 1	N 4	O 5	0
28	b	1	Total 60	C 50	Mg 1	N 4	O 5	0
28	b	1	Total 50	C 40	Mg 1	N 4	O 5	0
28	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	b	1	Total 51	C 41	Mg 1	N 4	O 5	0
28	b	1	Total 46	C 36	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
28	b	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
28	b	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
28	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	b	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
28	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	b	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
28	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
28	B	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
28	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
28	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
28	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	B	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
28	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	B	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
28	B	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
28	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
28	D	1	Total	C	Mg	N	O	0
			47	37	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
28	D	1	Total 46	C 36	Mg 1	N 4	O 5	0
28	D	1	Total 46	C 36	Mg 1	N 4	O 5	0
28	D	1	Total 46	C 36	Mg 1	N 4	O 5	0
28	D	1	Total 45	C 35	Mg 1	N 4	O 5	0
28	D	1	Total 46	C 36	Mg 1	N 4	O 5	0
28	D	1	Total 41	C 33	Mg 1	N 4	O 3	0
28	F	1	Total 46	C 36	Mg 1	N 4	O 5	0
28	F	1	Total 46	C 36	Mg 1	N 4	O 5	0
28	F	1	Total 46	C 36	Mg 1	N 4	O 5	0
28	F	1	Total 46	C 36	Mg 1	N 4	O 5	0
28	F	1	Total 46	C 36	Mg 1	N 4	O 5	0
28	F	1	Total 46	C 36	Mg 1	N 4	O 5	0
28	F	1	Total 41	C 33	Mg 1	N 4	O 3	0
28	H	1	Total 47	C 37	Mg 1	N 4	O 5	0
28	H	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	H	1	Total 51	C 41	Mg 1	N 4	O 5	0
28	H	1	Total 46	C 36	Mg 1	N 4	O 5	0
28	H	1	Total 47	C 37	Mg 1	N 4	O 5	0
28	H	1	Total 41	C 33	Mg 1	N 4	O 3	0
28	H	1	Total 46	C 36	Mg 1	N 4	O 5	0
28	J	1	Total 60	C 50	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
28	J	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
28	J	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	J	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
28	J	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
28	J	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
28	J	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
28	J	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
28	J	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
28	J	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
28	J	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
28	L	1	Total	C	Mg	N	O	0
			47	39	1	4	3	
28	L	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
28	L	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
28	L	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
28	L	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
28	L	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
28	L	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
28	L	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
28	L	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
28	L	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
28	M	1	Total	C	Mg	N	O	0
			53	43	1	4	5	

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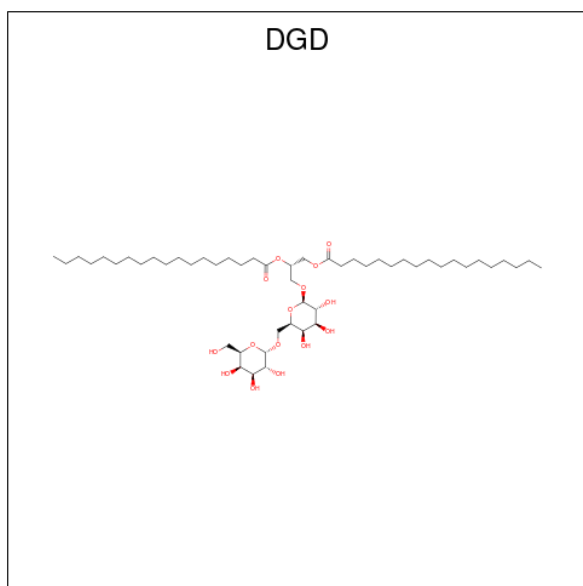
Mol	Chain	Residues	Atoms					AltConf
28	M	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
28	M	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
28	M	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
28	M	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
28	M	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
28	M	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
28	M	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
28	M	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
28	M	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
28	N	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
28	N	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	N	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
28	N	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
28	N	1	Total	C	Mg	N	O	0
			47	37	1	4	5	

- Molecule 29 is Chlorophyll c1 (CCD ID: KC1) (formula: $C_{35}H_{30}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).

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Mol	Chain	Residues	Atoms					AltConf
29	L	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
29	M	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
29	M	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
29	N	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
29	N	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
29	N	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

- Molecule 30 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$) (labeled as "Ligand of Interest" by depositor).



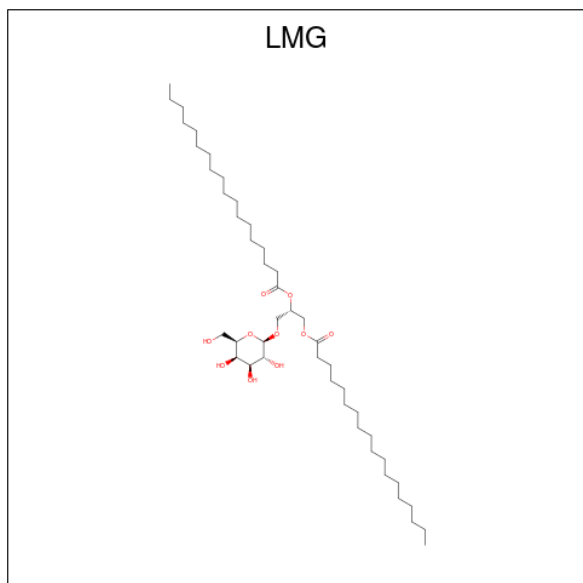
Mol	Chain	Residues	Atoms			AltConf
30	I	1	Total	C	O	0
			39	24	15	
30	y	1	Total	C	O	0
			54	39	15	
30	G	1	Total	C	O	0
			45	30	15	
30	G	1	Total	C	O	0
			44	29	15	
30	j	1	Total	C	O	0
			41	26	15	

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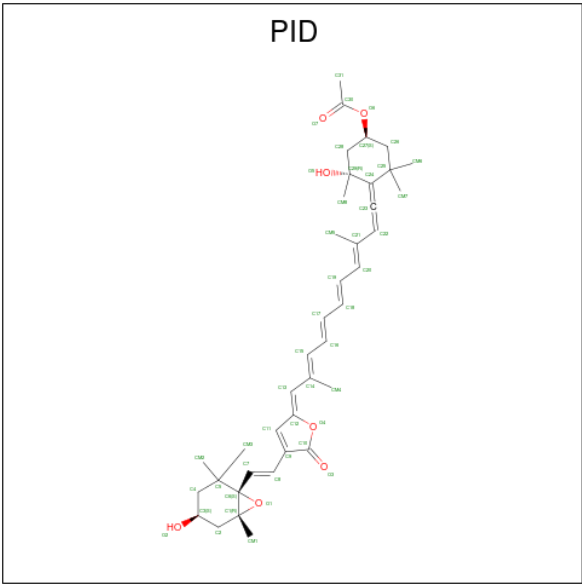
Mol	Chain	Residues	Atoms			AltConf
30	l	1	Total	C	O	0
			50	35	15	
30	L	1	Total	C	O	0
			38	23	15	

- Molecule 31 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
31	I	1	Total	C	O	0
			36	26	10	
31	I	1	Total	C	O	0
			38	28	10	
31	K	1	Total	C	O	0
			27	17	10	
31	K	1	Total	C	O	0
			43	33	10	
31	j	1	Total	C	O	0
			35	25	10	
31	b	1	Total	C	O	0
			44	34	10	
31	b	1	Total	C	O	0
			31	21	10	
31	B	1	Total	C	O	0
			37	27	10	
31	D	1	Total	C	O	0
			49	39	10	

- Molecule 32 is PERIDININ (CCD ID: PID) (formula: C₃₉H₅₀O₇) (labeled as "Ligand of Interest" by depositor).



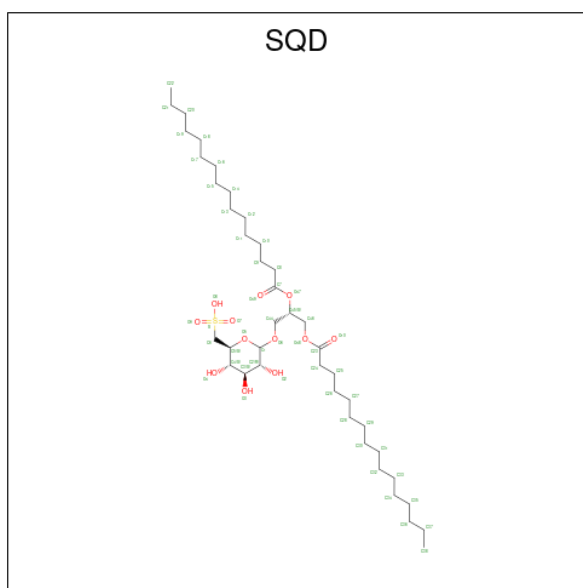
Mol	Chain	Residues	Atoms			AltConf
32	G	1	Total	C	O	0
			46	39	7	
32	G	1	Total	C	O	0
			46	39	7	
32	j	1	Total	C	O	0
			46	39	7	
32	D	1	Total	C	O	0
			46	39	7	
32	D	1	Total	C	O	0
			46	39	7	
32	D	1	Total	C	O	0
			46	39	7	
32	D	1	Total	C	O	0
			46	39	7	
32	D	1	Total	C	O	0
			46	39	7	
32	F	1	Total	C	O	0
			46	39	7	
32	F	1	Total	C	O	0
			46	39	7	
32	F	1	Total	C	O	0
			46	39	7	

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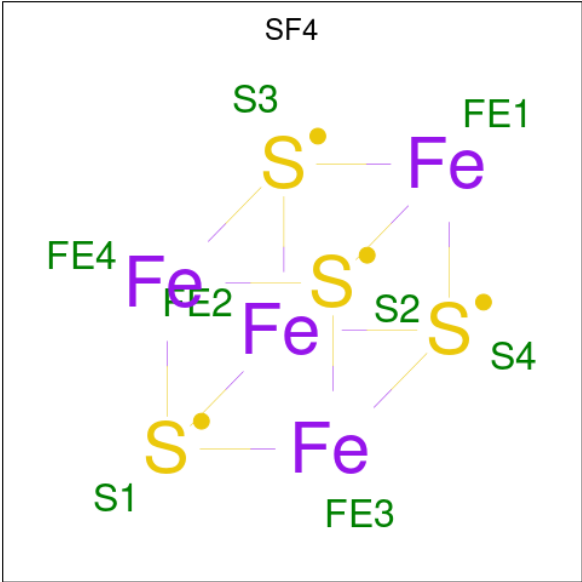
Mol	Chain	Residues	Atoms			AltConf
32	F	1	Total	C	O	0
			46	39	7	
32	H	1	Total	C	O	0
			46	39	7	
32	H	1	Total	C	O	0
			46	39	7	
32	M	1	Total	C	O	0
			46	39	7	
32	N	1	Total	C	O	0
			46	39	7	
32	N	1	Total	C	O	0
			46	39	7	

- Molecule 33 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: $C_{41}H_{78}O_{12}S$) (labeled as "Ligand of Interest" by depositor).



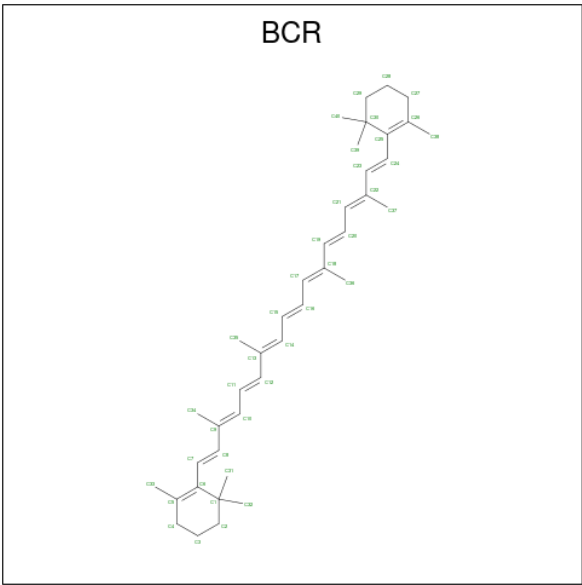
Mol	Chain	Residues	Atoms				AltConf
33	A	1	Total	C	O	S	0
			50	37	12	1	

- Molecule 34 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms			AltConf
34	c	1	Total	Fe	S	0
			8	4	4	
34	c	1	Total	Fe	S	0
			8	4	4	
34	a	1	Total	Fe	S	0
			8	4	4	

- Molecule 35 is BETA-CAROTENE (CCD ID: BCR) (formula: C₄₀H₅₆).



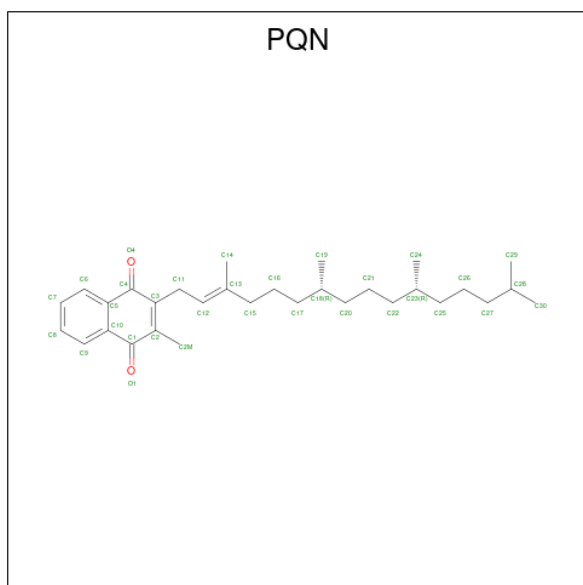
Mol	Chain	Residues	Atoms		AltConf
35	f	1	Total	C	0
			40	40	

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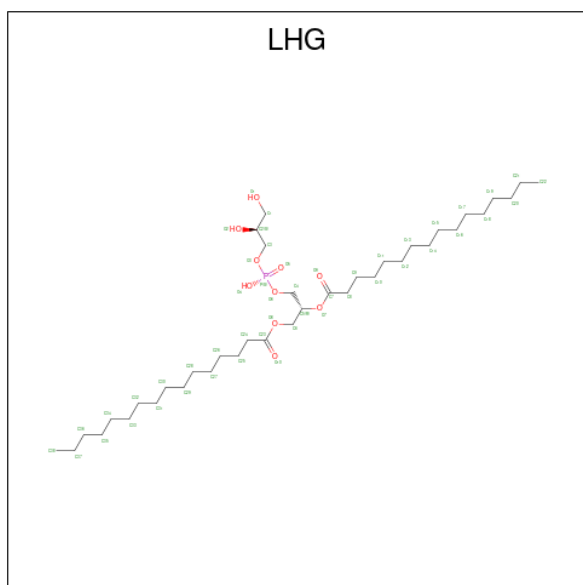
Mol	Chain	Residues	Atoms	AltConf
35	i	1	Total C 40 40	0
35	j	1	Total C 40 40	0
35	l	1	Total C 40 40	0
35	l	1	Total C 40 40	0
35	l	1	Total C 40 40	0
35	m	1	Total C 40 40	0
35	a	1	Total C 40 40	0
35	a	1	Total C 40 40	0
35	b	1	Total C 40 40	0
35	b	1	Total C 40 40	0
35	b	1	Total C 40 40	0

- Molecule 36 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$).



Mol	Chain	Residues	Atoms			AltConf
36	a	1	Total	C	O	0
			33	31	2	
36	b	1	Total	C	O	0
			33	31	2	

- Molecule 37 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$) (labeled as "Ligand of Interest" by depositor).

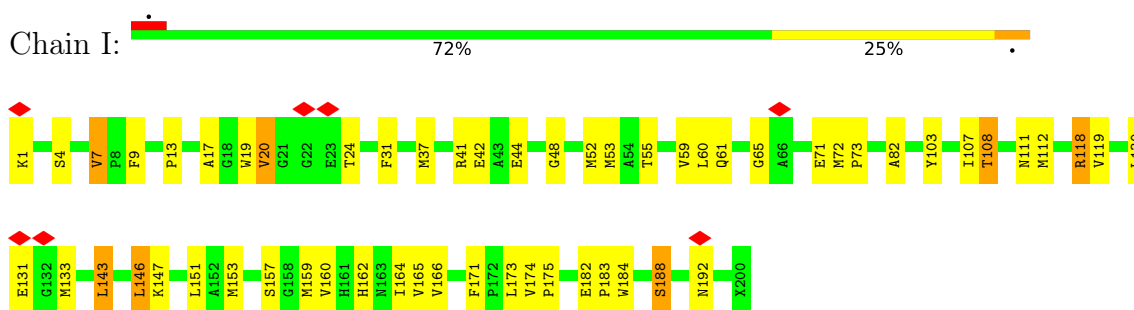


Mol	Chain	Residues	Atoms				AltConf
37	a	1	Total	C	O	P	0
			48	37	10	1	

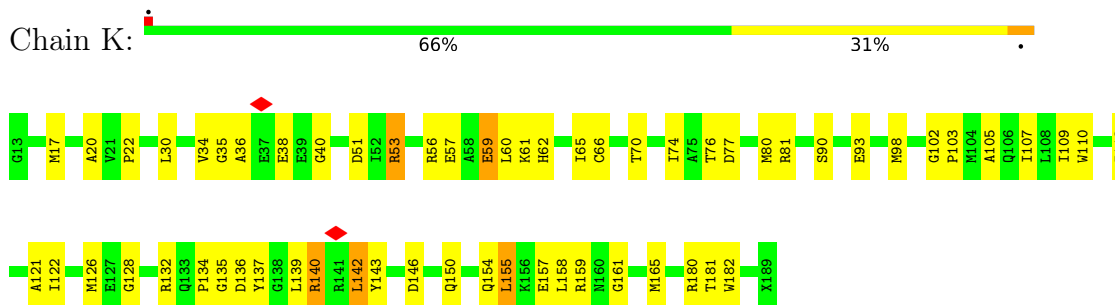
3 Residue-property plots

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.

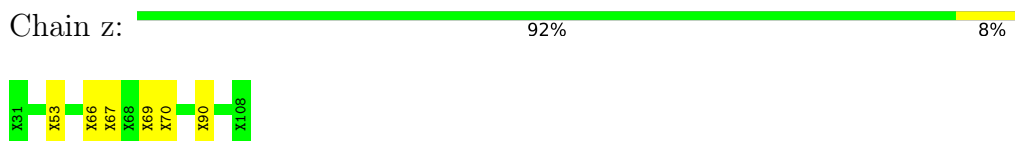
- Molecule 1: Chlorophyll a-chlorophyll c-peridinin-protein-complex I-7, acpPCI-7



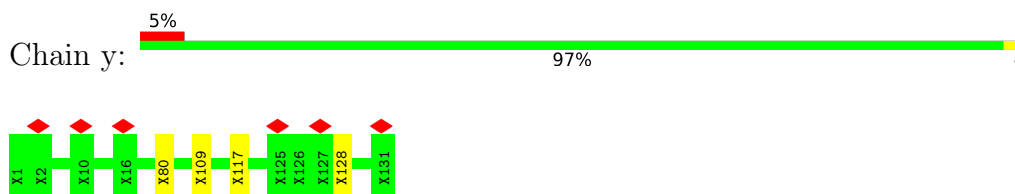
- Molecule 2: Chlorophyll a-chlorophyll c-peridinin-protein-complex I-6, acpPCI-6



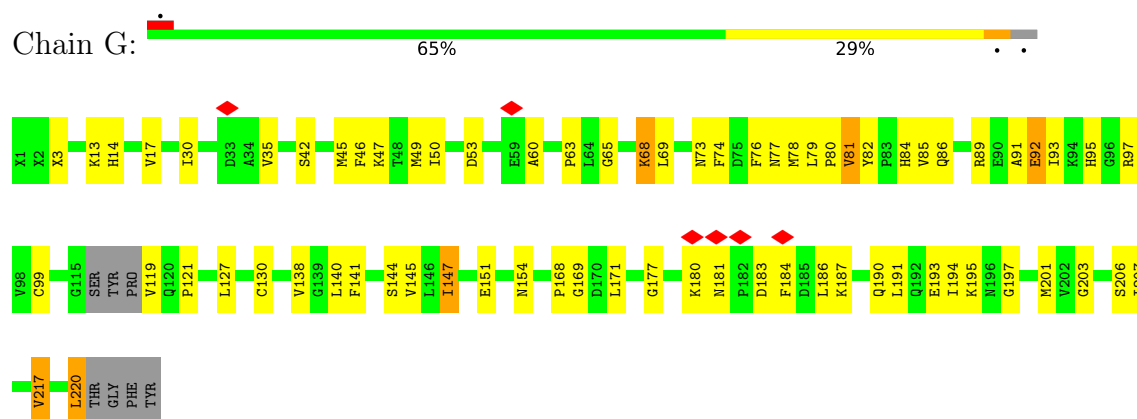
- Molecule 3: Photosystem I unk



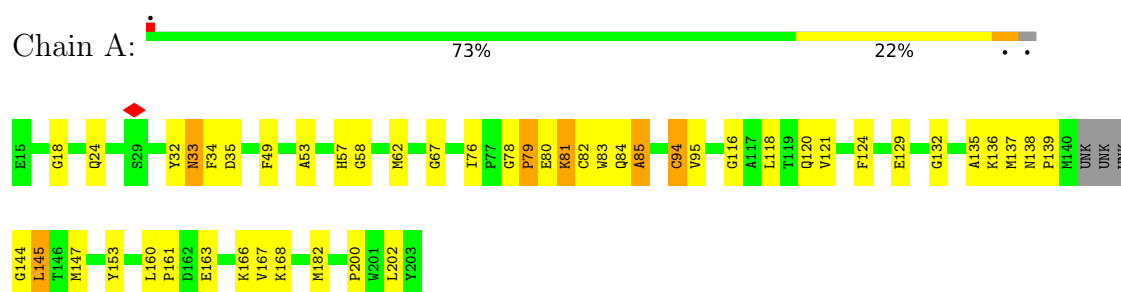
- Molecule 4: Photosystem I unk



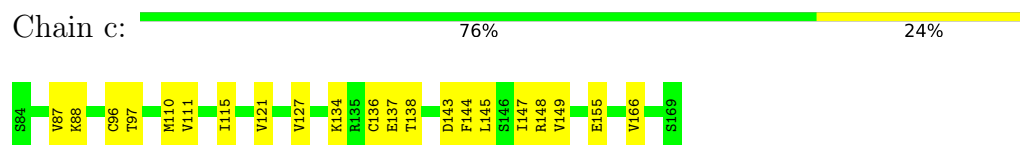
- Molecule 5: Chlorophyll a-chlorophyll c-peridinin-protein-complex I-8, acpPCI-8



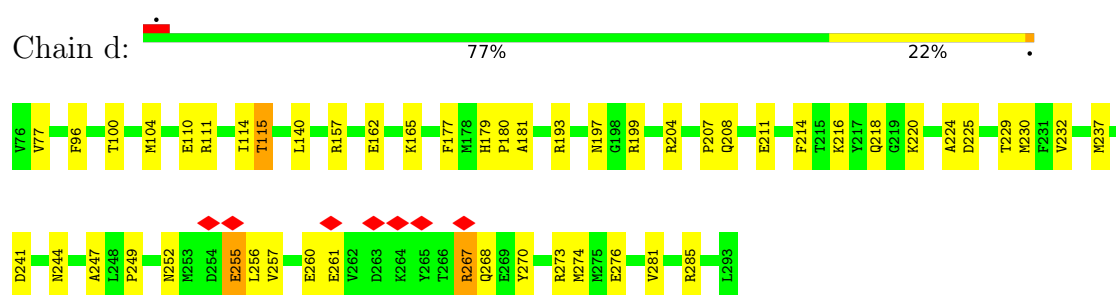
- Molecule 6: Chlorophyll a-chlorophyll c-peridinin-protein-complex I-10, acpPCI-10



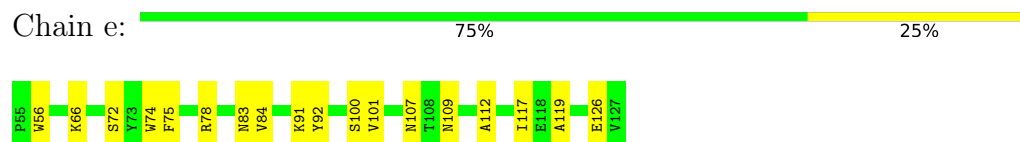
- Molecule 7: Photosystem I Psac



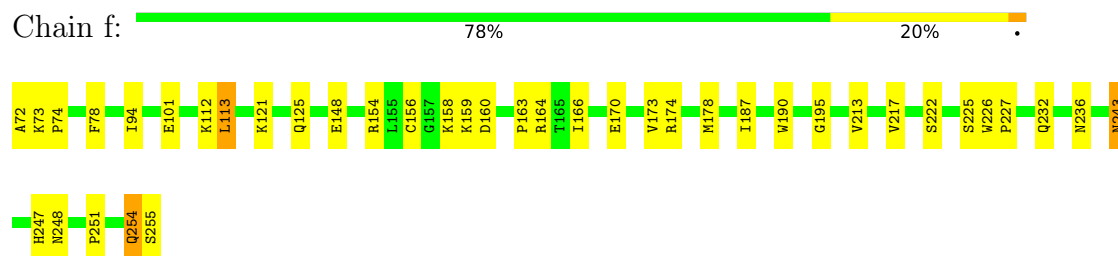
- Molecule 8: Photosystem I Psad



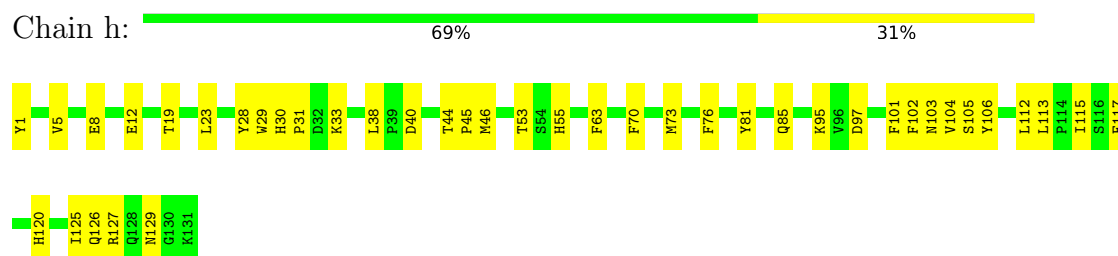
- Molecule 9: Photosystem I Psae



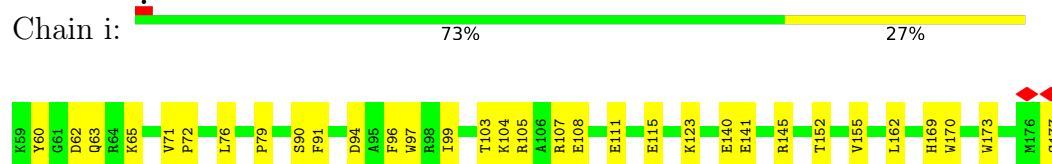
- Molecule 10: Photosystem I Psaf



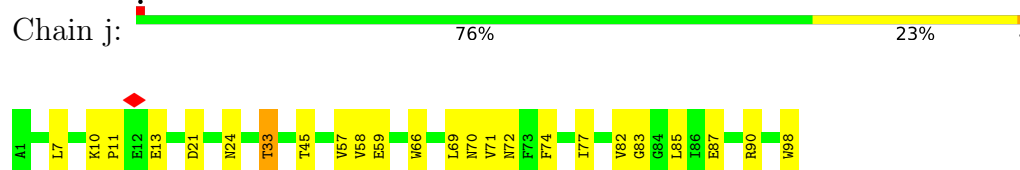
- Molecule 11: Photosystem I Psar



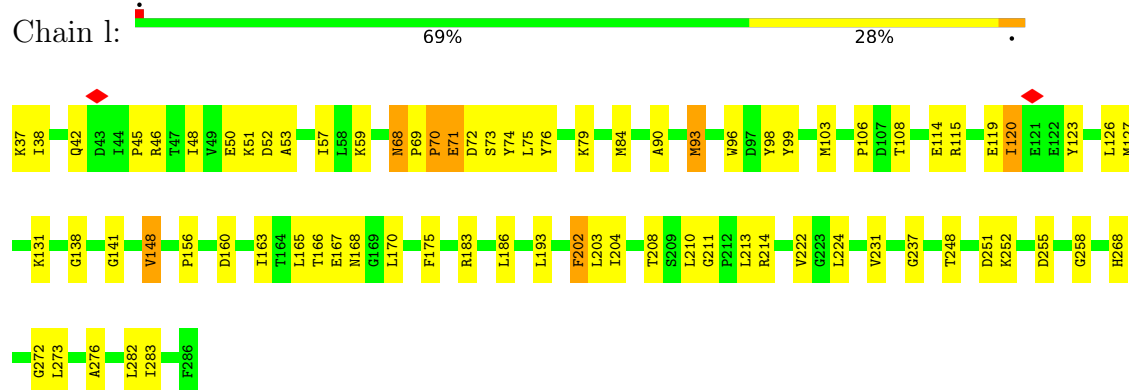
- Molecule 12: Photosystem I Psal



- Molecule 13: Photosystem I Psaj

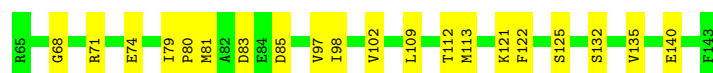


- Molecule 14: Photosystem I Psal



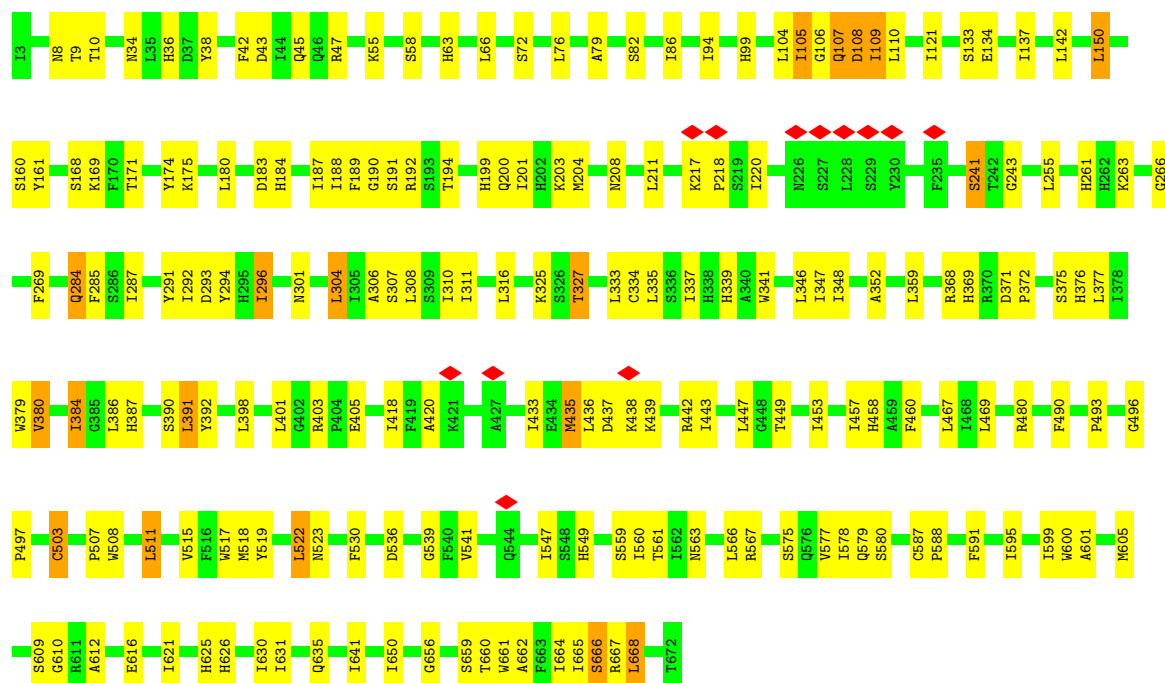
- Molecule 15: Photosystem I Psam

Chain m:  75% 25%



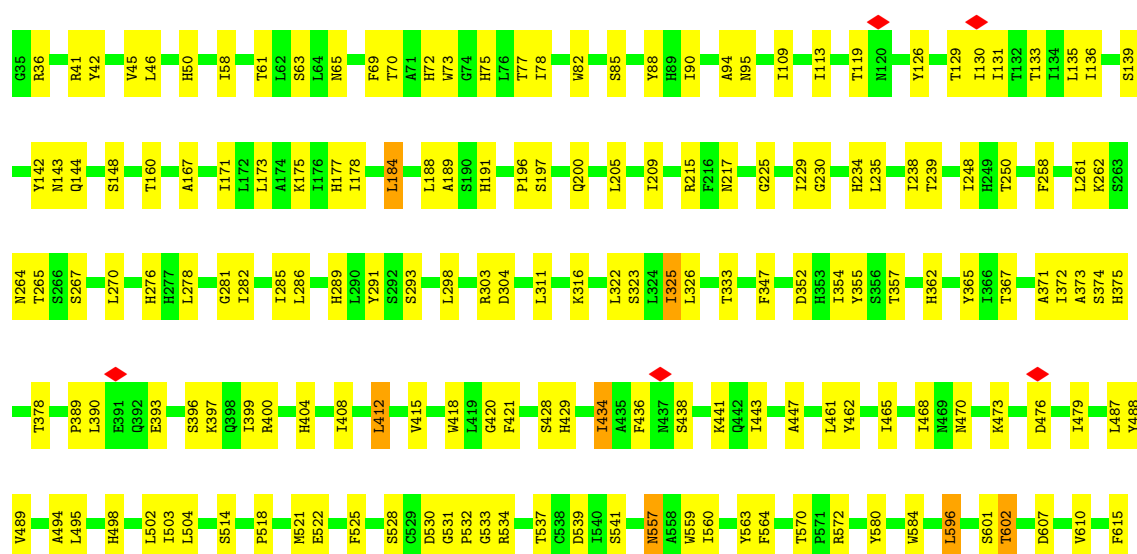
• Molecule 16: Photosystem I PsA

Chain a:  71% 26%

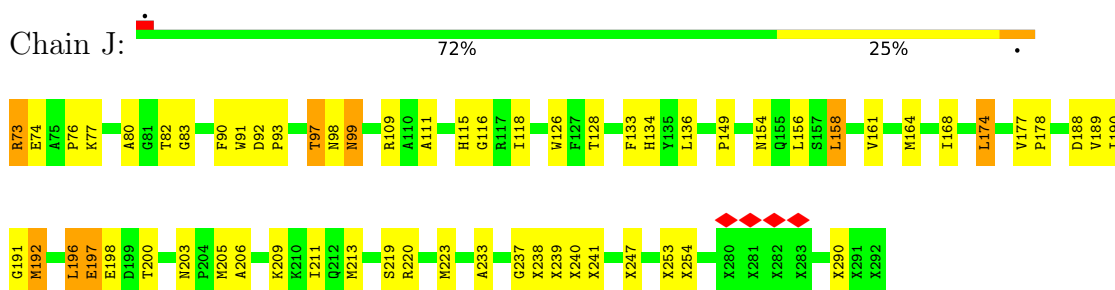


• Molecule 17: Photosystem I PsbB

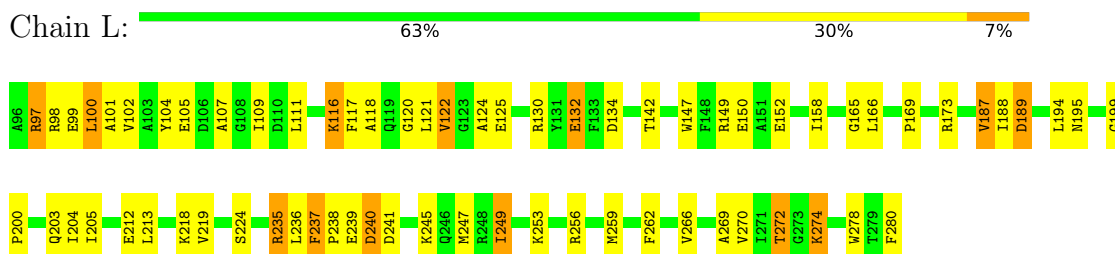
Chain b:  70% 29%



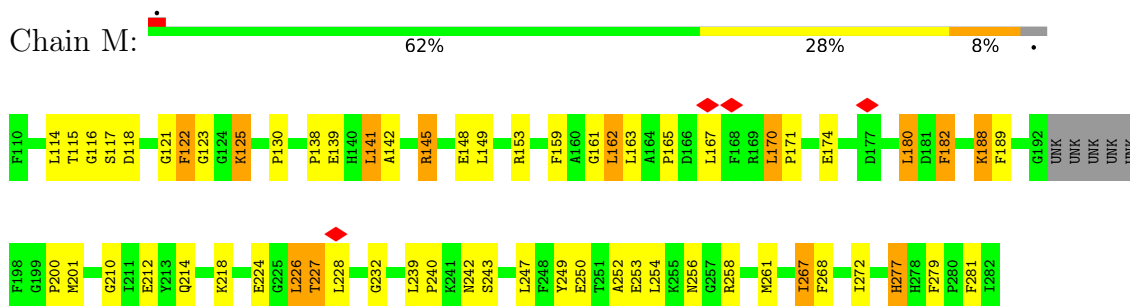
- Molecule 22: Chlorophyll a-chlorophyll c-peridinin-protein-complex I-3, acpPCI-3



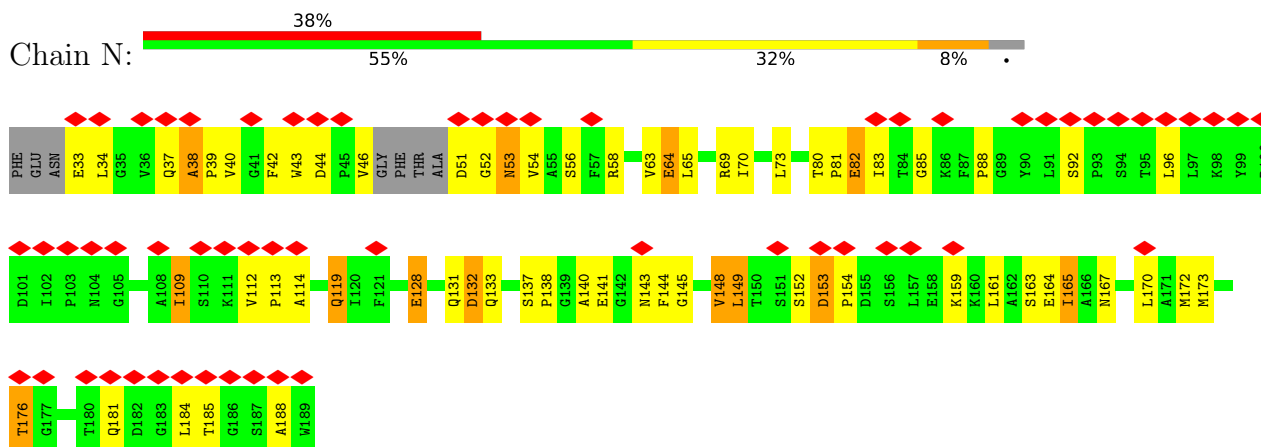
- Molecule 23: Chlorophyll a-chlorophyll c-peridinin-protein-complex I-5, acpPCI-5



- Molecule 24: Chlorophyll a-chlorophyll c-peridinin-protein-complex I-4, acpPCI-4



- Molecule 25: Chlorophyll a-chlorophyll c-peridinin-protein-complex I-13, acpPCI-13



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	216895	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.628	Depositor
Minimum map value	-0.312	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.025	Depositor
Recommended contour level	0.215	Depositor
Map size (Å)	532.48, 532.48, 532.48	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	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: PID, DGD, BCR, DD6, UIX, SF4, CLA, PQN, LHG, SQD, LMG, KC1

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	I	0.13	0/1484	0.33	0/2019
2	K	0.15	0/1357	0.33	1/1838 (0.1%)
5	G	0.35	0/1562	0.52	1/2122 (0.0%)
6	A	0.37	0/1276	0.53	0/1725
7	c	0.12	0/663	0.31	0/902
8	d	0.11	0/1767	0.30	0/2375
9	e	0.24	0/608	0.30	0/833
10	f	0.16	0/1489	0.33	0/2016
11	h	0.12	0/1101	0.27	0/1493
12	i	0.17	0/992	0.33	0/1346
13	j	0.14	0/801	0.31	0/1092
14	l	0.20	0/1998	0.35	0/2706
15	m	0.13	0/590	0.29	0/793
16	a	0.26	0/5344	0.41	2/7280 (0.0%)
17	b	0.20	0/5362	0.33	0/7335
18	B	0.17	0/1382	0.36	1/1862 (0.1%)
19	D	0.25	0/1178	0.47	0/1592
20	F	0.24	0/1263	0.54	4/1708 (0.2%)
21	H	0.19	0/1232	0.42	1/1665 (0.1%)
22	J	0.18	0/1246	0.39	0/1699
23	L	0.24	0/1462	0.43	0/1985
24	M	0.20	0/1241	0.35	0/1681
25	N	0.23	0/1005	0.51	0/1370
All	All	0.22	0/36403	0.39	10/49437 (0.0%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	F	145	LYS	N-CA-C	8.96	123.31	112.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	a	391	LEU	N-CA-C	-6.94	103.77	111.82
21	H	110	MET	N-CA-C	-6.52	104.18	111.28
20	F	146	TYR	N-CA-C	-6.00	104.41	113.89
20	F	148	PHE	CA-C-N	-5.99	113.77	119.76
20	F	148	PHE	C-N-CA	-5.99	113.77	119.76
16	a	82	SER	N-CA-C	5.85	118.07	109.24
2	K	38	GLU	N-CA-C	-5.71	108.11	114.62
18	B	118	PRO	N-CA-C	-5.54	101.07	112.47
5	G	68	LYS	N-CA-C	5.49	119.45	112.87

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	I	1480	0	1381	52	0
2	K	1349	0	1323	55	0
3	z	390	0	87	4	0
4	y	655	0	136	3	0
5	G	1572	0	1440	49	0
6	A	1346	0	1242	40	0
7	c	653	0	629	21	0
8	d	1731	0	1741	40	0
9	e	587	0	575	15	0
10	f	1450	0	1437	31	0
11	h	1066	0	1018	34	0
12	i	964	0	941	27	0
13	j	783	0	774	21	0
14	l	1943	0	1919	66	0
15	m	582	0	603	16	0
16	a	5194	0	5023	158	0
17	b	5199	0	5053	171	0
18	B	1452	0	1368	40	0
19	D	1158	0	1114	51	0
20	F	1237	0	1188	36	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	H	1202	0	1182	46	0
22	J	1496	0	1233	48	0
23	L	1427	0	1392	51	0
24	M	1211	0	1090	42	0
25	N	993	0	844	39	0
26	A	172	0	0	2	0
26	B	171	0	0	1	0
26	D	43	0	0	0	0
26	F	86	0	0	1	0
26	G	172	0	0	5	0
26	H	43	0	0	1	0
26	I	172	0	0	2	0
26	J	129	0	0	5	0
26	K	215	0	0	0	0
26	L	215	0	0	2	0
26	M	215	0	0	2	0
26	N	43	0	0	0	0
26	b	43	0	0	0	0
26	h	43	0	0	0	0
27	A	47	0	0	1	0
27	B	47	0	0	0	0
27	G	47	0	0	0	0
27	I	47	0	0	2	0
27	J	47	0	0	1	0
27	K	47	0	0	1	0
27	h	47	0	0	0	0
28	A	597	0	493	22	0
28	B	587	0	532	20	0
28	D	317	0	229	18	0
28	F	317	0	227	22	0
28	G	592	0	530	22	0
28	H	343	0	278	15	0
28	I	637	0	554	30	0
28	J	552	0	456	29	0
28	K	496	0	398	17	0
28	L	503	0	411	21	0
28	M	481	0	370	18	0
28	N	256	0	216	10	0
28	a	1870	0	1786	112	0
28	b	1563	0	1526	105	0
28	f	147	0	115	10	0
28	h	55	0	49	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	j	113	0	104	8	0
28	l	493	0	471	26	0
28	m	60	0	59	2	0
29	A	90	0	0	0	0
29	B	45	0	0	0	0
29	D	90	0	0	1	0
29	F	90	0	0	2	0
29	G	45	0	0	0	0
29	H	90	0	0	1	0
29	I	45	0	0	0	0
29	J	45	0	0	0	0
29	K	45	0	0	0	0
29	L	90	0	0	0	0
29	M	90	0	0	1	0
29	N	135	0	0	1	0
30	G	89	0	94	2	0
30	I	39	0	36	0	0
30	L	38	0	34	2	0
30	j	41	0	40	4	0
30	l	50	0	58	0	0
30	y	54	0	66	1	0
31	B	37	0	44	1	0
31	D	49	0	64	5	0
31	I	74	0	88	1	0
31	K	70	0	80	0	0
31	b	75	0	90	4	0
31	j	35	0	40	5	0
32	D	276	0	300	12	0
32	F	184	0	200	12	0
32	G	92	0	100	6	0
32	H	92	0	100	8	0
32	M	46	0	50	1	0
32	N	92	0	100	3	0
32	j	46	0	50	5	0
33	A	50	0	64	8	0
34	a	8	0	0	1	0
34	c	16	0	0	1	0
35	a	80	0	112	5	0
35	b	120	0	168	14	0
35	f	40	0	56	3	0
35	i	40	0	56	5	0
35	j	40	0	56	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	l	120	0	168	11	0
35	m	40	0	56	5	0
36	a	33	0	46	5	0
36	b	33	0	46	4	0
37	a	48	0	69	3	0
All	All	52237	0	46068	1357	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 14.

All (1357) 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)
10:f:72:ALA:N	17:b:462:TYR:HH	1.46	1.12
28:K:308:CLA:H2A	28:K:308:CLA:HED3	1.53	0.89
28:b:712:CLA:H12	18:B:124:ILE:HD11	1.56	0.87
17:b:468:ILE:HG22	17:b:470:ASN:H	1.36	0.87
18:B:124:ILE:HG21	28:B:301:CLA:HBB	1.61	0.82
28:a:707:CLA:HBB1	28:a:723:CLA:HAB	1.60	0.81
22:J:116:GLY:HA3	22:J:219:SER:HB2	1.62	0.80
28:a:714:CLA:H3A	35:a:734:BCR:H332	1.64	0.78
6:A:144:GLY:N	33:A:318:SQD:HO2	1.82	0.78
16:a:359:LEU:HD13	16:a:490:PHE:HA	1.65	0.78
6:A:160:LEU:HD13	28:A:313:CLA:HAA2	1.66	0.77
24:M:115:THR:HG21	24:M:250:GLU:HB3	1.64	0.77
28:G:517:CLA:HBB1	11:h:76:PHE:HE2	1.49	0.77
10:f:159:LYS:HD3	17:b:572:ARG:HH12	1.50	0.77
5:G:130:CYS:HB3	5:G:140:LEU:HD21	1.68	0.76
1:I:20:VAL:HG21	1:I:146:LEU:HG	1.69	0.75
28:a:730:CLA:HAB	28:a:730:CLA:H122	1.68	0.74
1:I:159:MET:HG2	27:I:304:UIX:C9	2.18	0.74
28:b:709:CLA:HBB1	28:b:709:CLA:HHC	1.71	0.73
10:f:94:ILE:HG12	10:f:166:ILE:HD12	1.71	0.72
28:G:519:CLA:O1D	11:h:127:ARG:NH2	2.23	0.72
14:l:160:ASP:O	17:b:649:LYS:NZ	2.22	0.72
9:e:91:LYS:HA	11:h:5:VAL:HG21	1.71	0.71
6:A:76:ILE:HB	6:A:83:TRP:CZ3	2.25	0.71
28:b:704:CLA:CGA	28:b:704:CLA:H3A	2.20	0.71
7:c:97:THR:HA	7:c:110:MET:HE3	1.73	0.71
32:G:507:PID:HM83	32:G:507:PID:HM51	1.72	0.71
6:A:79:PRO:O	6:A:83:TRP:HD1	1.74	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:180:ARG:NH1	2:K:181:THR:OG1	2.24	0.70
6:A:144:GLY:N	33:A:318:SQD:HO3	1.88	0.70
25:N:149:LEU:HD13	25:N:149:LEU:H	1.55	0.70
18:B:221:PRO:HB2	18:B:226:LYS:HB3	1.73	0.70
22:J:83:GLY:HA2	22:J:220:ARG:HH12	1.56	0.70
24:M:162:LEU:HD13	24:M:267:ILE:HG21	1.74	0.69
17:b:610:VAL:HG22	28:b:710:CLA:HAC1	1.74	0.69
22:J:98:ASN:O	22:J:99:ASN:ND2	2.24	0.69
8:d:257:VAL:HG13	17:b:191:HIS:HA	1.75	0.69
19:D:55:ASN:HD21	19:D:59:ARG:HE	1.40	0.69
28:a:716:CLA:CGA	28:a:721:CLA:HBB2	2.23	0.69
18:B:129:TRP:HE1	18:B:202:LEU:HD22	1.58	0.69
21:H:100:LYS:HG3	32:H:302:PID:H41	1.72	0.69
21:H:218:LEU:HB3	28:H:311:CLA:HED1	1.73	0.68
2:K:53:ARG:HH21	2:K:126:MET:HA	1.58	0.68
26:G:504:DD6:C24	28:G:510:CLA:HAB	2.23	0.68
16:a:110:LEU:HD22	16:a:588:PRO:HG3	1.75	0.68
17:b:209:ILE:O	17:b:215:ARG:NH2	2.27	0.68
18:B:233:LYS:O	18:B:237:ASN:ND2	2.22	0.68
32:F:305:PID:H17	32:F:305:PID:HM41	1.76	0.68
8:d:214:PHE:H	8:d:218:GLN:HG2	1.57	0.68
19:D:30:GLU:O	19:D:31:ASN:ND2	2.27	0.68
8:d:157:ARG:NH1	8:d:162:GLU:OE1	2.27	0.68
15:m:79:ILE:HD11	17:b:109:ILE:HG12	1.74	0.68
16:a:306:ALA:HB2	16:a:346:LEU:HB2	1.75	0.67
8:d:204:ARG:NH2	17:b:522:GLU:OE2	2.26	0.67
23:L:147:TRP:HH2	28:L:313:CLA:HAA2	1.58	0.67
17:b:530:ASP:OD2	17:b:534:ARG:NH2	2.27	0.67
8:d:211:GLU:HG2	8:d:232:VAL:HB	1.76	0.67
13:j:87:GLU:OE1	13:j:90:ARG:NH2	2.28	0.67
18:B:243:LEU:HD13	26:B:302:DD6:C26	2.24	0.67
28:b:704:CLA:H43	28:b:704:CLA:HMB3	1.77	0.67
16:a:563:ASN:OD1	16:a:567:ARG:NH1	2.27	0.67
26:J:304:DD6:C24	28:J:307:CLA:HAB	2.25	0.67
18:B:124:ILE:HG23	18:B:125:ILE:HG13	1.75	0.67
32:F:304:PID:H7	28:F:315:CLA:HMB2	1.77	0.67
28:b:712:CLA:H42	18:B:124:ILE:HG12	1.76	0.67
8:d:256:LEU:HD21	18:B:78:UNK:HA	1.75	0.66
12:i:141:GLU:OE2	12:i:145:ARG:NH2	2.28	0.66
6:A:82:CYS:SG	6:A:83:TRP:N	2.68	0.66
13:j:24:ASN:ND2	23:L:105:GLU:OE2	2.27	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:a:72:SER:HB2	16:a:150:LEU:HD22	1.77	0.66
28:a:735:CLA:HBB	28:b:703:CLA:H192	1.75	0.66
24:M:252:ALA:O	24:M:256:ASN:ND2	2.22	0.66
25:N:92:SER:H	25:N:96:LEU:HA	1.61	0.66
25:N:163:SER:O	25:N:167:ASN:ND2	2.27	0.66
20:F:88:LEU:HG	20:F:109:LEU:HD11	1.76	0.66
5:G:97:ARG:NH1	5:G:193:GLU:OE2	2.28	0.66
17:b:528:SER:HB3	17:b:669:ILE:HD12	1.78	0.66
21:H:100:LYS:HZ3	32:H:302:PID:H42	1.61	0.66
22:J:97:THR:HG22	28:J:307:CLA:HBA1	1.77	0.66
2:K:76:THR:O	2:K:81:ARG:NH1	2.28	0.66
9:e:101:VAL:HG12	9:e:107:ASN:HB3	1.78	0.66
28:a:704:CLA:H193	28:b:710:CLA:H2	1.77	0.66
23:L:149:ARG:NH1	23:L:152:GLU:OE1	2.28	0.66
11:h:95:LYS:NZ	11:h:101:PHE:O	2.25	0.66
22:J:82:THR:HG21	22:J:109:ARG:HH12	1.61	0.66
22:J:128:THR:HG21	28:J:309:CLA:HAC2	1.78	0.65
5:G:181:ASN:HB2	5:G:184:PHE:HB2	1.79	0.65
5:G:50:ILE:O	5:G:89:ARG:NH2	2.30	0.65
8:d:100:THR:O	16:a:480:ARG:NH2	2.30	0.65
16:a:307:SER:O	16:a:311:ILE:HG12	1.97	0.65
22:J:233:ALA:HA	22:J:237:GLY:O	1.96	0.65
25:N:112:VAL:O	25:N:114:ALA:N	2.26	0.65
5:G:177:GLY:HA2	5:G:180:LYS:HG3	1.77	0.65
33:A:318:SQD:H241	33:A:318:SQD:H91	1.78	0.65
28:l:313:CLA:H51	28:a:720:CLA:HBB2	1.79	0.65
17:b:72:HIS:ND1	28:b:713:CLA:OBD	2.29	0.65
16:a:379:TRP:HB2	28:b:701:CLA:HED2	1.79	0.65
24:M:227:THR:OG1	24:M:228:LEU:N	2.30	0.64
28:A:319:CLA:HAB	17:b:230:GLY:HA2	1.80	0.64
16:a:519:TYR:O	16:a:523:ASN:ND2	2.21	0.64
17:b:286:LEU:HD23	35:b:730:BCR:H14C	1.79	0.64
28:b:703:CLA:H41	28:b:703:CLA:H102	1.79	0.64
16:a:86:ILE:HG13	16:a:94:ILE:HG13	1.79	0.64
28:A:312:CLA:H12	33:A:318:SQD:H322	1.78	0.64
19:D:33:LEU:O	19:D:60:ARG:NH2	2.31	0.64
24:M:161:GLY:O	24:M:165:PRO:HD2	1.97	0.64
2:K:57:GLU:OE1	2:K:132:ARG:NH2	2.31	0.64
6:A:160:LEU:HG	6:A:167:VAL:HG12	1.80	0.64
23:L:256:ARG:HA	23:L:259:MET:HE3	1.79	0.64
16:a:293:ASP:HB3	16:a:296:ILE:HG22	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:M:142:ALA:HB1	24:M:226:LEU:HD22	1.79	0.63
2:K:53:ARG:NH1	30:j:103:DGD:O5E	2.31	0.63
24:M:182:PHE:HE2	24:M:268:PHE:HA	1.63	0.63
10:f:72:ALA:N	17:b:462:TYR:OH	2.26	0.63
17:b:50:HIS:ND1	28:b:707:CLA:O1A	2.32	0.63
13:j:90:ARG:HD3	32:j:105:PID:H41	1.80	0.63
8:d:252:ASN:ND2	8:d:255:GLU:OE1	2.20	0.63
1:I:65:GLY:HA2	28:I:310:CLA:HMD1	1.81	0.63
21:H:135:ASP:O	21:H:145:LYS:NZ	2.31	0.63
16:a:591:PHE:O	16:a:595:ILE:HG12	1.99	0.63
28:b:709:CLA:H43	28:b:720:CLA:H11	1.80	0.63
18:B:118:PRO:C	18:B:120:ARG:H	2.06	0.63
21:H:151:TRP:HB3	28:H:312:CLA:HMC1	1.81	0.63
2:K:70:THR:O	2:K:74:ILE:HG12	1.99	0.62
25:N:132:ASP:OD1	25:N:132:ASP:N	2.28	0.62
16:a:201:ILE:HD13	28:J:301:CLA:HBC2	1.81	0.62
2:K:132:ARG:NH1	2:K:136:ASP:O	2.30	0.62
17:b:270:LEU:HD11	17:b:347:PHE:HZ	1.64	0.62
16:a:334:CYS:HB3	28:a:722:CLA:HMA1	1.81	0.62
16:a:377:LEU:HD22	28:a:729:CLA:HBB1	1.82	0.62
23:L:240:ASP:OD1	23:L:240:ASP:N	2.32	0.62
14:l:126:LEU:HD22	14:l:131:LYS:HB2	1.80	0.62
14:l:204:ILE:HD12	14:l:224:LEU:HA	1.82	0.62
17:b:626:PHE:HB3	28:b:704:CLA:HMC2	1.81	0.62
14:l:53:ALA:HB2	14:l:108:THR:HG22	1.82	0.62
18:B:220:LEU:HD12	18:B:221:PRO:HD2	1.81	0.62
22:J:73:ARG:HG2	22:J:76:PRO:HB2	1.80	0.62
28:l:303:CLA:HAA2	28:F:312:CLA:HBA1	1.81	0.62
18:B:246:SER:HB2	28:B:315:CLA:HMC2	1.81	0.62
24:M:117:SER:HB2	24:M:125:LYS:HG3	1.82	0.62
19:D:66:HIS:NE2	29:D:310:KC1:ND	2.48	0.61
28:b:704:CLA:HBC3	28:b:704:CLA:HHD	1.82	0.61
28:l:311:CLA:H201	22:J:174:LEU:HD12	1.83	0.61
16:a:458:HIS:HB3	28:a:727:CLA:HAB	1.82	0.61
1:I:108:THR:HG23	10:f:222:SER:HB3	1.83	0.61
28:G:511:CLA:HBC1	28:G:513:CLA:HAC1	1.83	0.61
23:L:122:VAL:O	23:L:149:ARG:NH2	2.32	0.61
19:D:167:SER:O	19:D:171:ASN:ND2	2.27	0.61
24:M:159:PHE:HA	24:M:162:LEU:HD12	1.83	0.61
2:K:159:ARG:NH1	28:K:307:CLA:O1D	2.34	0.61
22:J:220:ARG:HA	22:J:223:MET:HE3	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:32:TYR:O	6:A:33:ASN:C	2.44	0.61
15:m:122:PHE:HB2	17:b:189:ALA:HB2	1.82	0.61
18:B:174:MET:HB3	18:B:180:MET:HG2	1.82	0.61
16:a:104:LEU:HG	16:a:105:ILE:HG23	1.82	0.61
16:a:107:GLN:O	16:a:110:LEU:HG	2.01	0.61
17:b:610:VAL:HG11	28:b:709:CLA:HAC1	1.82	0.61
28:a:702:CLA:NA	28:b:703:CLA:HAB	2.16	0.60
20:F:131:GLN:NE2	20:F:132:ASP:O	2.34	0.60
11:h:38:LEU:O	17:b:303:ARG:NH2	2.34	0.60
13:j:59:GLU:HB3	31:j:101:LMG:HC61	1.84	0.60
16:a:243:GLY:O	16:a:442:ARG:NH2	2.32	0.60
5:G:138:VAL:HB	19:D:113:VAL:HG11	1.82	0.60
28:A:309:CLA:HAC1	28:A:316:CLA:HAB	1.82	0.60
15:m:81:MET:HE1	17:b:131:ILE:HG21	1.82	0.60
17:b:333:THR:HB	17:b:367:THR:HB	1.84	0.60
16:a:433:ILE:HB	16:a:443:ILE:HG22	1.84	0.60
20:F:88:LEU:HD23	20:F:99:ILE:HD13	1.83	0.60
25:N:141:GLU:HG3	25:N:143:ASN:H	1.67	0.60
1:I:55:THR:HA	1:I:159:MET:HE1	1.84	0.60
14:l:210:LEU:HD11	28:a:725:CLA:HBB2	1.83	0.60
17:b:412:LEU:HG	17:b:502:LEU:HB2	1.83	0.60
28:I:316:CLA:CHA	28:I:316:CLA:HBA1	2.32	0.60
5:G:127:LEU:HD23	32:G:507:PID:HM23	1.83	0.60
28:l:313:CLA:H193	35:a:736:BCR:H271	1.81	0.60
18:B:253:ASN:HB2	28:B:317:CLA:HMA3	1.84	0.60
15:m:132:SER:HB2	15:m:135:VAL:HG23	1.82	0.60
18:B:239:ARG:HA	18:B:242:MET:HE3	1.83	0.60
15:m:80:PRO:O	17:b:95:ASN:ND2	2.35	0.60
25:N:181:GLN:NE2	25:N:188:ALA:O	2.35	0.60
14:l:103:MET:HE1	28:a:711:CLA:H2A	1.84	0.60
16:a:76:LEU:HD13	28:a:708:CLA:HAC2	1.84	0.60
16:a:316:LEU:O	16:a:325:LYS:NZ	2.34	0.60
6:A:24:GLN:OE1	6:A:168:LYS:NZ	2.34	0.59
8:d:241:ASP:OD2	8:d:244:ASN:ND2	2.35	0.59
21:H:124:TYR:O	21:H:126:SER:N	2.34	0.59
1:I:41:ARG:NH2	28:I:308:CLA:O1D	2.33	0.59
28:G:517:CLA:HBB1	11:h:76:PHE:CE2	2.36	0.59
32:D:305:PID:HM81	28:D:314:CLA:HBC3	1.84	0.59
24:M:121:GLY:HA3	29:M:307:KC1:O1D	2.02	0.59
18:B:183:MET:HG2	28:B:316:CLA:HBC1	1.83	0.59
32:F:305:PID:H22	29:F:309:KC1:CAA	2.33	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:i:140:GLU:HA	12:i:155:VAL:HG21	1.84	0.59
17:b:373:ALA:HB2	28:b:722:CLA:HMC2	1.84	0.59
17:b:173:LEU:O	17:b:177:HIS:ND1	2.30	0.59
17:b:415:VAL:HG23	28:b:725:CLA:HBB1	1.84	0.59
1:l:184:TRP:CE2	28:l:316:CLA:HBA2	2.37	0.59
16:a:621:ILE:HD13	28:a:730:CLA:HMD1	1.85	0.59
17:b:258:PHE:O	17:b:473:LYS:NZ	2.34	0.59
2:K:56:ARG:NH1	2:K:59:GLU:OE2	2.36	0.59
6:A:137:MET:HG2	6:A:145:LEU:HD22	1.85	0.59
28:b:709:CLA:HAB	28:b:710:CLA:H11	1.84	0.59
21:H:67:GLU:HG2	21:H:91:PHE:CZ	2.38	0.59
23:L:147:TRP:CH2	28:L:313:CLA:HAA2	2.37	0.58
20:F:172:SER:O	20:F:176:ASN:ND2	2.30	0.58
23:L:99:GLU:HG3	23:L:101:ALA:H	1.69	0.58
9:e:78:ARG:NH2	9:e:126:GLU:OE2	2.36	0.58
32:G:507:PID:HM31	28:G:517:CLA:HED3	1.86	0.58
11:h:103:ASN:OD1	11:h:105:SER:OG	2.20	0.58
14:l:120:ILE:HG12	16:a:285:PHE:CE2	2.38	0.58
28:l:303:CLA:H101	35:l:307:BCR:H363	1.85	0.58
5:G:97:ARG:NH2	5:G:169:GLY:O	2.37	0.58
20:F:88:LEU:HD21	28:F:310:CLA:HBA2	1.84	0.58
25:N:109:ILE:HA	25:N:114:ALA:HB3	1.85	0.58
8:d:252:ASN:HB3	8:d:256:LEU:HD23	1.85	0.58
11:h:117:PHE:O	11:h:120:HIS:ND1	2.36	0.58
20:F:170:LEU:HG	28:F:313:CLA:HMA1	1.84	0.58
25:N:172:MET:O	25:N:176:THR:OG1	2.21	0.58
15:m:68:GLY:N	17:b:607:ASP:OD1	2.37	0.58
17:b:689:PRO:HG2	28:b:720:CLA:H2	1.86	0.58
14:l:46:ARG:HH22	23:L:142:THR:H	1.51	0.58
19:D:39:THR:HG21	19:D:42:PHE:HD1	1.67	0.58
24:M:189:PHE:HB2	24:M:201:MET:HG2	1.85	0.58
5:G:46:PHE:HB2	5:G:85:VAL:HG21	1.86	0.57
10:f:78:PHE:CG	17:b:479:ILE:HD11	2.39	0.57
20:F:125:GLU:HG2	28:F:312:CLA:C1B	2.34	0.57
25:N:128:GLU:CD	32:N:302:PID:HM32	2.29	0.57
28:l:311:CLA:H62	30:G:501:DGD:HG12	1.86	0.57
6:A:35:ASP:OD1	26:A:303:DD6:O2	2.22	0.57
6:A:84:GLN:O	6:A:85:ALA:HB3	2.04	0.57
28:l:312:CLA:HAB	28:a:729:CLA:HAB	1.87	0.57
16:a:390:SER:HB2	28:a:726:CLA:HHC	1.86	0.57
20:F:145:LYS:HA	28:F:313:CLA:HAA1	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:N:148:VAL:O	25:N:154:PRO:HD2	2.04	0.57
15:m:121:LYS:HE2	15:m:125:SER:HB2	1.87	0.57
16:a:460:PHE:CE1	28:b:704:CLA:HBA2	2.40	0.57
16:a:503:CYS:HB3	34:a:737:SF4:S4	2.44	0.57
28:N:310:CLA:HED2	28:N:310:CLA:HBA1	1.85	0.57
1:I:153:MET:HE1	28:I:308:CLA:HHC	1.86	0.57
11:h:45:PRO:O	11:h:53:THR:OG1	2.20	0.57
2:K:143:TYR:CD1	28:K:313:CLA:HAA2	2.40	0.57
5:G:92:GLU:HG2	28:G:510:CLA:C1B	2.34	0.57
13:j:74:PHE:HA	13:j:77:ILE:HG22	1.87	0.57
25:N:170:LEU:HD23	32:N:301:PID:HM31	1.86	0.57
19:D:173:ARG:HA	19:D:176:MET:HE3	1.85	0.57
32:D:305:PID:H20	28:D:314:CLA:HBB1	1.87	0.57
28:J:301:CLA:HBA2	30:L:301:DGD:HD61	1.85	0.57
1:I:20:VAL:HG11	1:I:146:LEU:HD23	1.85	0.57
7:c:138:THR:HG22	17:b:533:GLY:HA3	1.86	0.57
12:i:99:ILE:HD12	17:b:45:VAL:HG13	1.85	0.57
20:F:186:GLY:O	20:F:190:GLN:HG2	2.05	0.57
25:N:65:LEU:O	25:N:69:ARG:HG2	2.04	0.57
1:I:4:SER:HB3	1:I:13:PRO:HD3	1.86	0.57
2:K:107:ILE:HG22	28:K:316:CLA:HBC1	1.87	0.57
14:l:127:MET:HE3	16:a:368:ARG:HH12	1.68	0.57
28:l:304:CLA:HAC2	35:l:306:BCR:H24C	1.87	0.57
16:a:294:TYR:HB3	28:a:706:CLA:HAC1	1.87	0.57
16:a:304:LEU:HD22	28:a:719:CLA:HAA1	1.87	0.57
16:a:433:ILE:HD13	16:a:547:ILE:HD11	1.85	0.57
18:B:220:LEU:HD13	28:B:313:CLA:HAA2	1.87	0.57
17:b:640:ILE:HD11	35:b:732:BCR:H282	1.86	0.56
14:l:204:ILE:HD11	14:l:276:ALA:HB1	1.88	0.56
28:A:317:CLA:CBB	28:A:320:CLA:HBB1	2.35	0.56
13:j:7:LEU:HD23	13:j:21:ASP:HA	1.86	0.56
16:a:610:GLY:N	17:b:539:ASP:OD2	2.38	0.56
17:b:139:SER:HA	28:b:720:CLA:HMA2	1.88	0.56
17:b:525:PHE:O	17:b:541:SER:OG	2.23	0.56
20:F:46:LEU:HB3	20:F:58:ARG:HH12	1.70	0.56
20:F:74:MET:HB2	28:F:310:CLA:HMC2	1.87	0.56
23:L:189:ASP:OD1	23:L:189:ASP:N	2.34	0.56
2:K:62:HIS:HB3	2:K:165:MET:HE3	1.88	0.56
5:G:13:LYS:HG3	9:e:117:ILE:HG12	1.87	0.56
11:h:125:ILE:O	11:h:129:ASN:ND2	2.37	0.56
16:a:333:LEU:HD21	16:a:664:ILE:HB	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:b:712:CLA:C4D	28:b:712:CLA:H11	2.36	0.56
22:J:177:VAL:HB	22:J:178:PRO:HD3	1.87	0.56
6:A:53:ALA:O	6:A:57:HIS:ND1	2.24	0.56
16:a:335:LEU:O	16:a:339:HIS:ND1	2.36	0.56
28:b:712:CLA:H92	28:B:301:CLA:HMB3	1.87	0.56
28:b:707:CLA:H161	28:b:721:CLA:HBB2	1.87	0.56
23:L:118:ALA:HB3	28:L:309:CLA:HED1	1.88	0.56
37:a:733:LHG:O4	37:a:733:LHG:O2	2.23	0.56
24:M:254:LEU:O	24:M:258:ARG:HD3	2.05	0.56
5:G:183:ASP:O	5:G:186:LEU:N	2.39	0.56
19:D:33:LEU:HD13	19:D:165:LEU:HG	1.88	0.56
23:L:158:ILE:HD12	28:L:313:CLA:HMD3	1.88	0.56
1:I:147:LYS:NZ	26:I:301:DD6:O4	2.39	0.56
14:l:57:ILE:HD11	14:l:106:PRO:HG2	1.87	0.56
17:b:610:VAL:HG22	28:b:710:CLA:HHD	1.88	0.55
28:J:307:CLA:H61	28:J:308:CLA:HBA2	1.88	0.55
23:L:134:ASP:OD1	26:L:304:DD6:O4	2.24	0.55
25:N:159:LYS:O	25:N:163:SER:N	2.34	0.55
28:K:312:CLA:HED2	28:K:312:CLA:H2A	1.88	0.55
17:b:113:ILE:HB	17:b:133:THR:HB	1.88	0.55
15:m:109:LEU:HG	15:m:113:MET:HE2	1.87	0.55
5:G:63:PRO:C	5:G:65:GLY:H	2.15	0.55
35:j:102:BCR:HC31	16:a:66:LEU:HD11	1.88	0.55
16:a:183:ASP:OD1	16:a:184:HIS:N	2.39	0.55
16:a:518:MET:HG2	16:a:522:LEU:HD21	1.87	0.55
28:G:513:CLA:H161	28:G:513:CLA:HMC3	1.89	0.55
14:l:138:GLY:N	14:l:141:GLY:O	2.29	0.55
17:b:94:ALA:HB1	17:b:142:TYR:OH	2.06	0.55
25:N:53:ASN:OD1	25:N:53:ASN:N	2.40	0.55
1:I:173:LEU:HG	1:I:174:VAL:HG23	1.89	0.55
16:a:530:PHE:HE1	16:a:668:LEU:HD23	1.72	0.55
21:H:188:PRO:HD2	21:H:190:SER:HB3	1.89	0.55
22:J:111:ALA:O	22:J:115:HIS:ND1	2.39	0.55
23:L:212:GLU:HG2	28:L:313:CLA:NB	2.20	0.55
5:G:86:GLN:HG3	5:G:168:PRO:HG3	1.88	0.55
28:G:520:CLA:HBC3	35:f:304:BCR:H362	1.89	0.55
28:b:713:CLA:H171	28:b:717:CLA:HBB2	1.87	0.55
33:A:318:SQD:H192	28:b:718:CLA:HBB1	1.89	0.55
11:h:1:TYR:HD2	12:i:152:THR:HG22	1.72	0.55
11:h:28:TYR:HB3	11:h:33:LYS:NZ	2.20	0.55
12:i:94:ASP:CG	12:i:105:ARG:HE	2.14	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:J:303:DD6:C5	28:J:310:CLA:HAC1	2.36	0.55
8:d:274:MET:HE1	17:b:197:SER:HB3	1.88	0.55
16:a:662:ALA:O	16:a:666:SER:OG	2.25	0.55
4:y:80:UNK:N	16:a:433:ILE:O	2.40	0.54
11:h:28:TYR:HB3	11:h:33:LYS:HZ1	1.72	0.54
25:N:70:ILE:HG12	32:N:302:PID:HM22	1.88	0.54
5:G:93:ILE:O	5:G:97:ARG:HG3	2.06	0.54
20:F:87:GLU:HA	20:F:95:LYS:HA	1.88	0.54
21:H:103:ARG:NE	21:H:198:GLU:OE2	2.36	0.54
24:M:212:GLU:HG2	28:M:312:CLA:CHB	2.37	0.54
2:K:126:MET:HB3	31:j:101:LMG:HC72	1.89	0.54
7:c:143:ASP:OD2	9:e:72:SER:OG	2.24	0.54
35:i:201:BCR:H382	35:i:201:BCR:H23C	1.89	0.54
16:a:449:THR:O	16:a:453:ILE:HG13	2.07	0.54
5:G:154:ASN:HB3	5:G:171:LEU:HD22	1.89	0.54
13:j:11:PRO:HB3	14:l:84:MET:SD	2.47	0.54
14:l:93:MET:HE2	23:L:111:LEU:HD11	1.90	0.54
28:l:313:CLA:H201	16:a:296:ILE:HD13	1.90	0.54
16:a:560:ILE:HG13	16:a:561:THR:HG23	1.90	0.54
28:a:707:CLA:H122	28:a:707:CLA:HMA3	1.89	0.54
1:I:1:LYS:NZ	2:K:128:GLY:O	2.31	0.54
35:l:302:BCR:H10C	28:b:728:CLA:H191	1.89	0.54
16:a:188:ILE:O	16:a:192:ARG:HB2	2.08	0.54
17:b:389:PRO:HD2	17:b:399:ILE:HD11	1.88	0.54
20:F:125:GLU:HG2	28:F:312:CLA:CHB	2.37	0.54
20:F:136:ALA:HB3	20:F:139:ASP:HB2	1.90	0.54
1:I:118:ARG:HG3	1:I:119:VAL:H	1.73	0.54
4:y:109:UNK:HA	16:a:217:LYS:HA	1.90	0.54
1:I:108:THR:HG22	1:I:111:ASN:H	1.72	0.54
32:G:506:PID:H21	32:G:507:PID:HM22	1.90	0.54
17:b:217:ASN:ND2	17:b:291:TYR:O	2.40	0.54
19:D:89:TYR:HA	19:D:97:LYS:HA	1.88	0.54
19:D:114:LEU:O	19:D:118:GLN:NE2	2.41	0.54
19:D:121:ALA:HB2	31:D:317:LMG:H182	1.89	0.54
32:F:306:PID:HM51	32:F:306:PID:HM83	1.89	0.54
8:d:207:PRO:HA	10:f:255:SER:HA	1.90	0.54
28:a:703:CLA:O1A	17:b:420:GLY:HA3	2.08	0.54
24:M:163:LEU:HD22	24:M:279:PHE:HB2	1.89	0.54
16:a:517:TRP:HE1	28:b:704:CLA:C1D	2.21	0.54
28:b:701:CLA:H141	28:b:728:CLA:H151	1.89	0.54
19:D:114:LEU:HD23	28:D:312:CLA:HED2	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:D:304:PID:H22	28:D:312:CLA:CHB	2.37	0.54
1:I:143:LEU:O	1:I:147:LYS:HG2	2.07	0.53
1:I:188:SER:OG	28:I:319:CLA:OBD	2.21	0.53
6:A:78:GLY:O	6:A:79:PRO:C	2.50	0.53
28:f:302:CLA:HMB1	13:j:85:LEU:HD11	1.90	0.53
24:M:138:PRO:HA	24:M:141:LEU:HD22	1.90	0.53
25:N:64:GLU:HG3	25:N:165:ILE:HD11	1.89	0.53
17:b:627:MET:HB3	28:b:704:CLA:C1C	2.38	0.53
16:a:327:THR:HG21	16:a:436:LEU:HD23	1.91	0.53
17:b:276:HIS:HB2	28:b:716:CLA:C1B	2.38	0.53
24:M:122:PHE:HD1	24:M:123:GLY:H	1.56	0.53
2:K:136:ASP:OD1	2:K:140:ARG:NH2	2.41	0.53
28:a:703:CLA:HMD3	17:b:503:ILE:HG12	1.90	0.53
23:L:249:ILE:HD12	23:L:253:LYS:HE3	1.89	0.53
15:m:112:THR:OG1	17:b:175:LYS:NZ	2.41	0.53
28:b:715:CLA:C1D	28:b:716:CLA:HBB2	2.38	0.53
18:B:149:ILE:HG12	18:B:260:PHE:HB2	1.90	0.53
16:a:187:ILE:HA	16:a:191:SER:HB2	1.89	0.53
21:H:140:LEU:N	21:H:216:ASP:OD2	2.39	0.53
22:J:200:THR:HG23	22:J:206:ALA:HB2	1.91	0.53
23:L:166:LEU:HA	23:L:187:VAL:HG21	1.91	0.53
17:b:326:LEU:HD13	17:b:373:ALA:HB1	1.90	0.53
25:N:65:LEU:HD12	25:N:140:ALA:HB3	1.90	0.53
9:e:83:ASN:OD1	9:e:84:VAL:N	2.42	0.53
35:f:304:BCR:H333	28:b:724:CLA:H142	1.90	0.53
28:j:104:CLA:H72	36:a:732:PQN:H243	1.90	0.53
19:D:37:ALA:HB2	28:D:308:CLA:HMA2	1.89	0.53
25:N:69:ARG:NE	25:N:164:GLU:OE2	2.41	0.53
2:K:51:ASP:OD1	30:j:103:DGD:O5E	2.24	0.53
7:c:96:CYS:N	34:c:202:SF4:S1	2.81	0.53
17:b:270:LEU:HD11	17:b:347:PHE:CZ	2.43	0.53
21:H:148:ALA:O	21:H:152:ALA:N	2.41	0.53
1:I:103:TYR:HD2	1:I:107:ILE:HG22	1.72	0.52
10:f:154:ARG:HD2	10:f:163:PRO:HB2	1.91	0.52
19:D:133:SER:HB2	19:D:134:PRO:HD3	1.90	0.52
25:N:119:GLN:NE2	29:N:308:KC1:O2D	2.40	0.52
8:d:104:MET:SD	14:l:160:ASP:HB3	2.50	0.52
28:b:717:CLA:H142	28:b:717:CLA:HBC2	1.91	0.52
28:a:702:CLA:C1A	28:b:703:CLA:HAB	2.39	0.52
28:a:725:CLA:HBB1	28:a:726:CLA:H2	1.91	0.52
19:D:141:GLY:O	28:D:314:CLA:HAA2	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:J:82:THR:HA	22:J:213:MET:SD	2.49	0.52
22:J:116:GLY:CA	22:J:219:SER:HB2	2.35	0.52
12:i:62:ASP:O	12:i:65:LYS:NZ	2.32	0.52
13:j:66:TRP:O	13:j:72:ASN:ND2	2.42	0.52
5:G:47:LYS:HZ3	5:G:60:ALA:H	1.56	0.52
12:i:104:LYS:HG3	12:i:108:GLU:OE1	2.09	0.52
28:a:725:CLA:H91	28:b:704:CLA:H171	1.91	0.52
23:L:116:LYS:HB2	23:L:120:GLY:H	1.74	0.52
24:M:117:SER:H	28:M:309:CLA:HED2	1.74	0.52
16:a:36:HIS:HB3	37:a:733:LHG:H121	1.91	0.52
20:F:73:CYS:HB3	32:F:304:PID:HM43	1.91	0.52
15:m:79:ILE:HD12	17:b:136:ILE:HG12	1.92	0.52
28:a:703:CLA:HMB1	28:a:703:CLA:HBB1	1.92	0.52
35:b:702:BCR:HC41	28:b:724:CLA:HBB2	1.91	0.52
19:D:79:THR:HB	19:D:80:PRO:HD3	1.92	0.52
1:I:108:THR:O	1:I:112:MET:N	2.42	0.52
2:K:132:ARG:NH2	2:K:134:PRO:O	2.43	0.52
11:h:44:THR:HG23	11:h:55:HIS:HB3	1.91	0.52
16:a:386:LEU:O	28:a:726:CLA:HBB2	2.09	0.52
16:a:612:ALA:HB2	17:b:537:THR:HA	1.91	0.52
17:b:225:GLY:HA2	17:b:281:GLY:HA2	1.90	0.52
17:b:235:LEU:HA	17:b:239:THR:HB	1.91	0.52
21:H:73:PRO:HB3	28:H:304:CLA:HBB1	1.92	0.52
21:H:124:TYR:HD2	21:H:127:PRO:HA	1.75	0.52
32:H:301:PID:H20	28:H:311:CLA:HBC2	1.92	0.52
23:L:122:VAL:HG12	23:L:249:ILE:HG12	1.90	0.52
1:I:20:VAL:HG12	1:I:143:LEU:HD22	1.92	0.52
6:A:62:MET:SD	28:A:313:CLA:HAB	2.50	0.52
6:A:200:PRO:O	27:A:304:U1X:O1	2.28	0.52
13:j:69:LEU:HB3	13:j:72:ASN:HD22	1.75	0.52
16:a:630:ILE:HD13	28:a:730:CLA:HMB2	1.91	0.52
17:b:647:HIS:CE1	28:b:727:CLA:HAC1	2.45	0.52
21:H:69:GLY:HA3	21:H:203:ARG:HH22	1.75	0.52
24:M:122:PHE:HD1	24:M:123:GLY:N	2.08	0.52
5:G:97:ARG:HD3	28:G:514:CLA:CHD	2.40	0.51
11:h:63:PHE:O	11:h:126:GLN:NE2	2.38	0.51
17:b:354:ILE:HG12	17:b:697:SER:HB3	1.91	0.51
17:b:622:TRP:HB2	17:b:683:GLY:HA3	1.92	0.51
26:M:303:DD6:C35	28:M:309:CLA:H2	2.40	0.51
14:l:115:ARG:O	14:l:119:GLU:HG2	2.10	0.51
16:a:659:SER:HB3	28:a:702:CLA:O1D	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:b:126:TYR:OH	17:b:610:VAL:HG23	2.10	0.51
21:H:216:ASP:OD1	21:H:222:ALA:N	2.42	0.51
23:L:235:ARG:HH21	23:L:236:LEU:HD21	1.75	0.51
10:f:195:GLY:HA2	28:a:730:CLA:H172	1.93	0.51
14:l:167:GLU:HB2	28:l:311:CLA:HBA2	1.92	0.51
21:H:103:ARG:HB3	32:H:302:PID:HM13	1.92	0.51
21:H:135:ASP:OD1	21:H:135:ASP:N	2.42	0.51
25:N:81:PRO:HG3	28:N:307:CLA:C3D	2.41	0.51
2:K:161:GLY:O	2:K:165:MET:HG3	2.11	0.51
28:A:320:CLA:HBB1	28:A:320:CLA:HHC	1.92	0.51
28:a:730:CLA:HED3	28:a:730:CLA:H2A	1.93	0.51
21:H:95:ARG:NH2	28:H:305:CLA:O1D	2.42	0.51
18:B:139:ARG:HA	18:B:142:MET:HE3	1.93	0.51
28:I:306:CLA:HAB	2:K:137:TYR:O	2.10	0.51
2:K:17:MET:CE	23:L:101:ALA:HA	2.40	0.51
6:A:137:MET:HE2	6:A:145:LEU:HD13	1.93	0.51
14:l:193:LEU:HD11	35:l:307:BCR:H381	1.92	0.51
16:a:42:PHE:CD2	28:a:706:CLA:HMC2	2.46	0.51
25:N:148:VAL:O	25:N:152:SER:HB2	2.09	0.51
11:h:106:TYR:HH	31:D:317:LMG:HO4	1.53	0.51
24:M:253:GLU:HG2	28:M:313:CLA:C1B	2.40	0.51
8:d:237:MET:HG2	17:b:390:LEU:HD21	1.92	0.51
14:l:170:LEU:HB3	22:J:191:GLY:HA3	1.93	0.51
28:a:704:CLA:HBB2	28:b:704:CLA:HBA1	1.92	0.51
17:b:396:SER:HB2	17:b:399:ILE:HG12	1.93	0.51
5:G:53:ASP:OD2	5:G:195:LYS:NZ	2.32	0.51
16:a:203:LYS:HB3	16:a:204:MET:HE2	1.93	0.51
19:D:114:LEU:HD12	31:D:317:LMG:H111	1.92	0.51
24:M:149:LEU:O	24:M:153:ARG:HG2	2.11	0.51
24:M:180:LEU:HD11	24:M:188:LYS:HG2	1.93	0.51
5:G:73:ASN:ND2	5:G:80:PRO:HA	2.26	0.51
8:d:274:MET:HE2	8:d:274:MET:HA	1.93	0.51
16:a:180:LEU:HD23	28:a:713:CLA:HBC2	1.92	0.51
16:a:301:ASN:ND2	28:a:706:CLA:OBD	2.42	0.51
17:b:322:LEU:HD11	28:b:722:CLA:HBB1	1.93	0.51
23:L:280:PHE:H	28:L:316:CLA:HED3	1.75	0.51
8:d:220:LYS:HD3	12:i:170:TRP:HE1	1.76	0.50
17:b:626:PHE:CB	28:b:704:CLA:HMC2	2.40	0.50
7:c:143:ASP:HB2	9:e:109:ASN:CG	2.35	0.50
16:a:387:HIS:O	16:a:391:LEU:HG	2.11	0.50
16:a:496:GLY:HA2	17:b:532:PRO:HD3	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:M:242:ASN:CG	24:M:243:SER:H	2.19	0.50
28:a:703:CLA:CGA	28:a:703:CLA:H3A	2.41	0.50
17:b:438:SER:HB3	17:b:441:LYS:HG3	1.93	0.50
20:F:78:VAL:HG21	28:F:310:CLA:HAC2	1.93	0.50
20:F:84:PHE:HB2	20:F:96:PHE:CD2	2.46	0.50
14:l:283:ILE:HG12	28:l:305:CLA:H12	1.91	0.50
17:b:447:ALA:HB2	17:b:487:LEU:HB2	1.93	0.50
23:L:205:ILE:HG12	28:L:317:CLA:HBC2	1.93	0.50
1:I:130:LEU:HG	1:I:131:GLU:H	1.77	0.50
28:G:510:CLA:H42	28:G:510:CLA:C2B	2.42	0.50
28:f:301:CLA:HAB	36:a:732:PQN:H161	1.94	0.50
11:h:40:ASP:OD1	17:b:303:ARG:NH1	2.35	0.50
14:l:268:HIS:CD2	35:l:306:BCR:H291	2.47	0.50
28:a:704:CLA:H71	17:b:617:LEU:HD13	1.93	0.50
35:a:734:BCR:H351	28:L:317:CLA:H42	1.93	0.50
17:b:113:ILE:HD12	17:b:133:THR:HG22	1.93	0.50
24:M:149:LEU:HD13	24:M:232:GLY:HA3	1.94	0.50
19:D:93:SER:OG	19:D:94:GLN:OE1	2.26	0.50
16:a:79:ALA:HB2	16:a:142:LEU:HB3	1.93	0.50
21:H:104:ILE:HD12	28:H:308:CLA:HMD3	1.93	0.50
21:H:117:ILE:HG13	21:H:118:THR:H	1.76	0.50
22:J:77:LYS:HA	22:J:80:ALA:HB2	1.94	0.50
7:c:88:LYS:HD3	8:d:197:ASN:HB3	1.94	0.50
16:a:380:VAL:HG22	28:a:728:CLA:HBB2	1.94	0.50
21:H:78:ASP:OD1	26:H:303:DD6:O2	2.30	0.50
23:L:107:ALA:HA	23:L:224:SER:HB3	1.94	0.50
11:h:19:THR:O	11:h:23:LEU:HG	2.11	0.50
16:a:293:ASP:OD1	16:a:294:TYR:N	2.44	0.50
18:B:186:ILE:HG22	28:B:311:CLA:H121	1.93	0.50
24:M:148:GLU:OE2	24:M:258:ARG:NH1	2.31	0.50
14:l:99:TYR:OH	28:a:711:CLA:O1A	2.30	0.49
17:b:372:ILE:HG13	17:b:504:LEU:HD11	1.92	0.49
1:I:133:MET:SD	1:I:133:MET:N	2.85	0.49
25:N:63:VAL:HG22	28:N:309:CLA:HED1	1.94	0.49
5:G:89:ARG:O	5:G:93:ILE:HG12	2.12	0.49
5:G:147:ILE:O	5:G:151:GLU:HG2	2.12	0.49
28:b:727:CLA:HAB	36:b:729:PQN:H151	1.95	0.49
20:F:35:THR:HG21	20:F:175:ASN:HD21	1.77	0.49
24:M:153:ARG:HD2	28:M:313:CLA:C4C	2.43	0.49
28:K:309:CLA:H2	28:K:309:CLA:HED3	1.95	0.49
14:l:231:VAL:HG11	14:l:272:GLY:HA3	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:a:168:SER:N	16:a:171:THR:OG1	2.33	0.49
16:a:200:GLN:HA	16:a:204:MET:HG2	1.95	0.49
17:b:627:MET:O	17:b:631:SER:OG	2.25	0.49
20:F:36:PRO:N	20:F:37:PRO:HD2	2.27	0.49
20:F:49:ASP:OD1	20:F:49:ASP:N	2.41	0.49
21:H:195:LEU:O	21:H:199:ILE:HG12	2.11	0.49
27:J:305:UIX:C35	28:J:312:CLA:HAB	2.43	0.49
24:M:189:PHE:HB3	24:M:200:PRO:HD2	1.93	0.49
10:f:232:GLN:O	10:f:236:ASN:ND2	2.46	0.49
13:j:13:GLU:N	13:j:13:GLU:OE1	2.45	0.49
17:b:281:GLY:O	17:b:285:ILE:HG12	2.11	0.49
8:d:204:ARG:HG3	10:f:254:GLN:HG3	1.94	0.49
14:l:74:TYR:CD2	14:l:106:PRO:HG3	2.48	0.49
17:b:686:LEU:HD23	28:b:720:CLA:H42	1.93	0.49
19:D:139:ALA:N	28:D:314:CLA:HED3	2.28	0.49
20:F:95:LYS:N	20:F:98:GLU:OE2	2.39	0.49
25:N:137:SER:HB2	25:N:138:PRO:HD3	1.92	0.49
8:d:110:GLU:C	8:d:111:ARG:HD2	2.38	0.49
16:a:261:HIS:HB2	28:a:716:CLA:C1B	2.43	0.49
17:b:461:LEU:O	17:b:465:ILE:HG12	2.12	0.49
22:J:240:UNK:O	22:J:241:UNK:CB	2.61	0.49
16:a:304:LEU:HD13	28:a:719:CLA:HBB	1.95	0.49
16:a:664:ILE:HG13	16:a:665:ILE:N	2.27	0.49
28:a:721:CLA:H11	28:a:721:CLA:H143	1.95	0.49
19:D:144:GLY:HA3	19:D:152:VAL:HG21	1.94	0.49
21:H:166:ASP:HB2	21:H:168:THR:HG23	1.94	0.49
1:I:61:GLN:O	1:I:72:MET:HE1	2.13	0.49
6:A:138:ASN:HB2	6:A:139:PRO:HD3	1.95	0.49
7:c:143:ASP:N	9:e:109:ASN:OD1	2.46	0.49
28:j:106:CLA:HMC1	17:b:428:SER:HB2	1.95	0.49
17:b:421:PHE:HZ	35:b:702:BCR:H372	1.78	0.49
35:b:702:BCR:H323	28:b:724:CLA:HBB1	1.94	0.49
22:J:93:PRO:HD2	26:J:304:DD6:O4	2.13	0.49
2:K:53:ARG:HG3	2:K:134:PRO:HG3	1.95	0.49
28:A:317:CLA:HBB1	28:A:320:CLA:HBB1	1.95	0.49
9:e:101:VAL:O	16:a:635:GLN:NE2	2.45	0.49
16:a:63:HIS:CE1	28:a:706:CLA:HMA2	2.48	0.49
18:B:178:GLY:HA2	18:B:181:GLN:HE22	1.77	0.49
20:F:67:ARG:HA	20:F:70:MET:HE3	1.95	0.49
20:F:170:LEU:HG	28:F:313:CLA:CMA	2.42	0.49
22:J:238:UNK:O	22:J:239:UNK:C	2.61	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:l:183:ARG:NH1	14:l:186:LEU:HD11	2.27	0.48
16:a:380:VAL:O	16:a:384:ILE:HG12	2.12	0.48
1:I:143:LEU:HB3	28:I:307:CLA:HED3	1.95	0.48
5:G:13:LYS:HG2	5:G:14:HIS:H	1.78	0.48
6:A:82:CYS:O	6:A:83:TRP:C	2.55	0.48
14:l:45:PRO:HD2	14:l:48:ILE:HD12	1.95	0.48
16:a:650:ILE:HD13	28:a:724:CLA:H101	1.95	0.48
2:K:57:GLU:HG2	2:K:122:ILE:HD11	1.94	0.48
2:K:60:LEU:HD13	2:K:135:GLY:HA3	1.95	0.48
28:K:308:CLA:H62	28:K:308:CLA:H41	1.56	0.48
5:G:203:GLY:O	5:G:207:ILE:HG13	2.13	0.48
7:c:136:CYS:HB2	7:c:147:ILE:HD13	1.96	0.48
12:i:99:ILE:HD11	28:b:705:CLA:HED1	1.95	0.48
16:a:184:HIS:ND1	28:a:719:CLA:OBD	2.46	0.48
17:b:375:HIS:HB3	17:b:504:LEU:HB3	1.94	0.48
23:L:97:ARG:NH2	23:L:100:LEU:HD13	2.27	0.48
1:I:48:GLY:O	1:I:52:MET:HG3	2.13	0.48
5:G:190:GLN:O	5:G:194:ILE:HG13	2.13	0.48
6:A:163:GLU:OE1	6:A:166:LYS:N	2.44	0.48
7:c:134:LYS:O	7:c:138:THR:HG23	2.14	0.48
28:b:709:CLA:O1A	28:b:720:CLA:HBD	2.14	0.48
19:D:38:PRO:HG2	32:D:301:PID:H22A	1.94	0.48
19:D:124:ALA:HB2	28:D:313:CLA:CAB	2.44	0.48
28:K:311:CLA:HBA1	28:K:311:CLA:H3A	1.52	0.48
3:z:66:UNK:HA	3:z:70:UNK:HA	1.95	0.48
9:e:74:TRP:NE1	9:e:100:SER:O	2.37	0.48
10:f:113:LEU:HD22	10:f:148:GLU:HB2	1.94	0.48
11:h:102:PHE:HB2	28:b:715:CLA:H12	1.94	0.48
16:a:386:LEU:HD23	28:b:704:CLA:H71	1.95	0.48
17:b:262:LYS:HE3	17:b:264:ASN:HD21	1.77	0.48
22:J:253:UNK:O	22:J:254:UNK:C	2.61	0.48
15:m:83:ASP:OD1	15:m:83:ASP:N	2.45	0.48
16:a:420:ALA:HB1	16:a:447:LEU:HD12	1.95	0.48
28:J:301:CLA:HBB1	30:L:301:DGD:HB41	1.95	0.48
1:I:188:SER:O	1:I:192:ASN:N	2.39	0.48
5:G:50:ILE:HG21	5:G:187:LYS:HG3	1.96	0.48
8:d:115:THR:HG22	8:d:140:LEU:HD13	1.96	0.48
17:b:70:THR:HG21	17:b:178:ILE:HD11	1.96	0.48
1:I:42:GLU:OE1	1:I:118:ARG:NH2	2.47	0.48
28:I:311:CLA:OBD	30:G:501:DGD:O2D	2.32	0.48
7:c:111:VAL:HG12	8:d:193:ARG:HB3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:l:204:ILE:O	14:l:208:THR:HG22	2.14	0.48
16:a:304:LEU:HD13	28:a:719:CLA:H3A	1.96	0.48
18:B:118:PRO:C	18:B:120:ARG:N	2.71	0.48
18:B:166:SER:HB3	18:B:169:ASN:HD21	1.78	0.48
32:H:301:PID:HM22	28:H:305:CLA:HAC2	1.95	0.48
25:N:51:ASP:OD1	25:N:52:GLY:N	2.46	0.48
25:N:144:PHE:CB	25:N:149:LEU:HD11	2.43	0.48
2:K:61:LYS:HE2	27:K:302:UIX:O1	2.14	0.48
2:K:61:LYS:O	2:K:65:ILE:HG12	2.14	0.48
6:A:118:LEU:O	6:A:121:VAL:N	2.46	0.48
14:l:46:ARG:NH2	23:L:142:THR:H	2.12	0.48
28:l:313:CLA:HED3	28:a:720:CLA:H72	1.96	0.48
16:a:403:ARG:HG3	17:b:119:THR:HG22	1.95	0.48
16:a:566:LEU:HD22	17:b:616:LEU:HD21	1.95	0.48
28:a:724:CLA:H203	28:a:731:CLA:H121	1.96	0.48
17:b:73:TRP:CE2	28:b:713:CLA:HED1	2.49	0.48
28:M:315:CLA:HBC1	28:M:317:CLA:HAB	1.96	0.48
28:G:520:CLA:HMB2	28:a:730:CLA:HAA2	1.95	0.48
7:c:166:VAL:HG11	17:b:663:THR:OG1	2.14	0.48
8:d:96:PHE:CZ	14:l:156:PRO:HB2	2.49	0.48
12:i:71:VAL:HG22	28:b:708:CLA:HAA1	1.96	0.48
16:a:493:PRO:HB3	16:a:641:ILE:HB	1.95	0.48
18:B:130:LEU:HD13	28:B:309:CLA:H11	1.95	0.48
24:M:114:LEU:HB3	24:M:145:ARG:NH2	2.29	0.48
28:I:311:CLA:HBC1	10:f:225:SER:HA	1.96	0.47
5:G:74:PHE:HA	5:G:78:MET:HA	1.95	0.47
14:l:73:SER:O	14:l:76:TYR:N	2.46	0.47
15:m:98:ILE:O	15:m:102:VAL:HG23	2.14	0.47
17:b:129:THR:OG1	17:b:130:ILE:N	2.47	0.47
28:b:717:CLA:H3A	28:b:717:CLA:HBA2	1.54	0.47
21:H:107:LEU:HD13	28:H:309:CLA:HAC1	1.95	0.47
22:J:92:ASP:CG	22:J:97:THR:HG23	2.39	0.47
28:L:317:CLA:HHC	28:L:317:CLA:HBB1	1.96	0.47
6:A:120:GLN:NE2	28:A:311:CLA:O1D	2.47	0.47
16:a:359:LEU:HD11	16:a:507:PRO:HG2	1.95	0.47
16:a:601:ALA:HB3	28:a:703:CLA:HBB2	1.96	0.47
28:b:705:CLA:H141	28:b:705:CLA:H161	1.66	0.47
25:N:64:GLU:HG2	28:N:305:CLA:C1B	2.44	0.47
1:I:59:VAL:HG13	1:I:171:PHE:CE2	2.49	0.47
28:a:706:CLA:H61	28:a:706:CLA:H41	1.61	0.47
28:a:709:CLA:H8	28:a:709:CLA:H122	1.60	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:84:GLN:O	6:A:85:ALA:CB	2.62	0.47
16:a:199:HIS:HB2	28:a:714:CLA:C1C	2.45	0.47
16:a:519:TYR:OH	16:a:656:GLY:HA3	2.14	0.47
17:b:77:THR:HG23	17:b:167:ALA:HB1	1.95	0.47
23:L:272:THR:HG22	23:L:274:LYS:HG3	1.94	0.47
2:K:36:ALA:O	2:K:40:GLY:N	2.46	0.47
2:K:142:LEU:HB2	28:K:313:CLA:H2	1.96	0.47
6:A:83:TRP:CH2	28:A:310:CLA:O1A	2.67	0.47
11:h:73:MET:HG2	31:D:317:LMG:H221	1.97	0.47
16:a:58:SER:O	16:a:160:SER:OG	2.31	0.47
17:b:36:ARG:NH1	17:b:41:ARG:HH22	2.12	0.47
28:b:701:CLA:HBC1	36:b:729:PQN:H193	1.96	0.47
28:b:703:CLA:H102	28:b:703:CLA:H62	1.67	0.47
25:N:149:LEU:HD13	25:N:149:LEU:N	2.27	0.47
5:G:89:ARG:HD2	5:G:93:ILE:HD11	1.95	0.47
10:f:170:GLU:HG2	10:f:173:VAL:HG13	1.97	0.47
35:m:201:BCR:H11C	35:m:201:BCR:H341	1.73	0.47
28:a:731:CLA:H193	28:a:735:CLA:H191	1.96	0.47
19:D:63:GLU:HB2	28:D:309:CLA:C1B	2.44	0.47
25:N:128:GLU:O	25:N:132:ASP:HB3	2.14	0.47
2:K:66:CYS:SG	2:K:165:MET:HG2	2.55	0.47
28:K:309:CLA:HED1	30:j:103:DGD:HA31	1.97	0.47
28:A:310:CLA:H171	28:A:310:CLA:H111	1.96	0.47
8:d:165:LYS:HB3	8:d:177:PHE:HE1	1.79	0.47
11:h:30:HIS:CG	11:h:31:PRO:HD2	2.49	0.47
13:j:33:THR:HB	16:a:169:LYS:HE3	1.96	0.47
28:a:717:CLA:H91	28:a:721:CLA:HBA2	1.97	0.47
17:b:278:LEU:O	17:b:282:ILE:HG12	2.14	0.47
28:b:723:CLA:HBA2	28:b:723:CLA:H3A	1.43	0.47
28:F:313:CLA:HAA2	28:F:313:CLA:HED2	1.97	0.47
22:J:133:PHE:CD2	28:J:316:CLA:HBA2	2.50	0.47
23:L:121:LEU:HD12	23:L:121:LEU:HA	1.77	0.47
1:I:17:ALA:H	1:I:19:TRP:HZ3	1.63	0.47
6:A:182:MET:HE1	28:A:308:CLA:HHC	1.96	0.47
28:A:313:CLA:H41	28:A:313:CLA:H61	1.67	0.47
11:h:70:PHE:HB2	19:D:128:LEU:HD12	1.97	0.47
16:a:375:SER:HB2	17:b:646:ILE:CG1	2.45	0.47
28:B:309:CLA:C2B	28:B:309:CLA:H42	2.45	0.47
21:H:127:PRO:HD3	32:H:302:PID:HM61	1.97	0.47
26:J:303:DD6:C22	28:J:310:CLA:HAA1	2.44	0.47
24:M:148:GLU:HB2	28:M:309:CLA:C1B	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:M:261:MET:HE1	28:M:309:CLA:HAB	1.97	0.47
1:I:31:PHE:HB2	28:I:308:CLA:O1A	2.15	0.47
28:a:702:CLA:H162	28:a:702:CLA:H122	1.71	0.47
17:b:184:LEU:HD21	17:b:205:LEU:HD22	1.97	0.47
21:H:91:PHE:CD2	21:H:92:LYS:HG2	2.49	0.47
1:I:130:LEU:HB2	28:I:313:CLA:HAA2	1.96	0.47
2:K:17:MET:HE3	23:L:101:ALA:HA	1.96	0.47
7:c:115:ILE:HD11	7:c:121:VAL:HG11	1.97	0.47
10:f:156:CYS:HB3	10:f:163:PRO:HA	1.97	0.47
28:f:301:CLA:H2	28:j:104:CLA:HED2	1.97	0.47
16:a:371:ASP:HB2	16:a:372:PRO:HD3	1.96	0.47
17:b:69:PHE:HE2	17:b:177:HIS:CD2	2.33	0.47
26:F:301:DD6:C40	28:F:307:CLA:HAC2	2.44	0.47
23:L:165:GLY:O	23:L:169:PRO:HD2	2.15	0.47
23:L:247:MET:HE1	28:L:314:CLA:H2	1.96	0.47
17:b:239:THR:HG22	17:b:270:LEU:HD13	1.98	0.46
19:D:68:ARG:HB3	32:D:302:PID:HM32	1.97	0.46
7:c:97:THR:HG22	7:c:110:MET:HG3	1.96	0.46
8:d:230:MET:HE1	12:i:162:LEU:HD13	1.97	0.46
16:a:204:MET:O	16:a:208:ASN:N	2.40	0.46
16:a:371:ASP:O	16:a:375:SER:HB3	2.14	0.46
17:b:82:TRP:O	17:b:85:SER:OG	2.21	0.46
17:b:143:ASN:ND2	17:b:347:PHE:O	2.41	0.46
17:b:316:LYS:HA	17:b:316:LYS:HD3	1.76	0.46
17:b:418:TRP:CZ2	28:b:725:CLA:HMC3	2.50	0.46
32:H:301:PID:HM41	32:H:301:PID:H16	1.61	0.46
24:M:253:GLU:HG2	28:M:313:CLA:NB	2.31	0.46
4:y:117:UNK:N	4:y:128:UNK:O	2.48	0.46
5:G:195:LYS:NZ	28:G:509:CLA:O1D	2.47	0.46
11:h:81:TYR:CZ	11:h:85:GLN:HG3	2.50	0.46
28:j:104:CLA:H51	36:a:732:PQN:H243	1.97	0.46
18:B:118:PRO:O	18:B:120:ARG:N	2.48	0.46
19:D:168:GLU:HB2	28:D:314:CLA:C1B	2.45	0.46
25:N:65:LEU:HD23	25:N:65:LEU:HA	1.79	0.46
1:I:60:LEU:HD22	28:I:310:CLA:HAC2	1.97	0.46
2:K:103:PRO:HB3	28:K:311:CLA:CAD	2.45	0.46
5:G:99:CYS:SG	26:G:504:DD6:C5	3.03	0.46
26:G:505:DD6:C24	28:G:514:CLA:HAB	2.46	0.46
6:A:49:PHE:CD1	33:A:318:SQD:H242	2.51	0.46
10:f:174:ARG:NH2	13:j:98:TRP:O	2.44	0.46
14:l:96:TRP:CE2	28:a:711:CLA:HED2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:m:201:BCR:HC42	28:b:705:CLA:H72	1.97	0.46
16:a:577:VAL:O	16:a:580:SER:OG	2.26	0.46
17:b:615:PHE:CZ	17:b:619:HIS:HE1	2.34	0.46
28:J:307:CLA:C1B	28:J:307:CLA:H42	2.46	0.46
28:M:309:CLA:H71	28:M:310:CLA:HMB1	1.98	0.46
5:G:99:CYS:SG	26:G:504:DD6:C6	3.04	0.46
16:a:348:ILE:HG21	16:a:515:VAL:HG22	1.96	0.46
16:a:605:MET:O	16:a:609:SER:OG	2.26	0.46
17:b:264:ASN:OD1	17:b:265:THR:N	2.48	0.46
1:I:37:MET:HE2	1:I:37:MET:HB2	1.81	0.46
1:I:53:MET:HE3	28:I:313:CLA:HMC3	1.96	0.46
8:d:247:ALA:O	8:d:285:ARG:NH1	2.35	0.46
8:d:261:GLU:OE1	8:d:261:GLU:N	2.47	0.46
14:l:148:VAL:HG22	22:J:205:MET:CB	2.46	0.46
20:F:32:LEU:HD22	20:F:170:LEU:HB3	1.97	0.46
28:L:312:CLA:HBA1	28:L:312:CLA:H3A	1.38	0.46
2:K:136:ASP:CG	2:K:140:ARG:HH22	2.23	0.46
7:c:166:VAL:HG13	17:b:660:ASP:HA	1.97	0.46
10:f:178:MET:HA	10:f:178:MET:HE2	1.97	0.46
28:j:106:CLA:HBA1	28:j:106:CLA:H3A	1.43	0.46
16:a:105:ILE:HD12	28:a:710:CLA:C2B	2.45	0.46
16:a:137:ILE:HD11	16:a:211:LEU:HD11	1.97	0.46
28:a:728:CLA:H41	28:a:728:CLA:H62	1.65	0.46
28:B:308:CLA:H3A	28:B:308:CLA:HBA2	1.61	0.46
22:J:73:ARG:O	22:J:76:PRO:HD2	2.16	0.46
28:N:309:CLA:H2A	28:N:309:CLA:O1D	2.16	0.46
6:A:32:TYR:OH	26:A:305:DD6:O2	2.31	0.46
32:j:105:PID:H11	28:a:710:CLA:HAA2	1.98	0.46
17:b:144:GLN:NE2	17:b:148:SER:OG	2.48	0.46
28:b:709:CLA:H2	28:b:709:CLA:H61	1.75	0.46
18:B:145:THR:HG23	18:B:248:ILE:HD12	1.98	0.46
29:F:309:KC1:CBC	28:F:312:CLA:HAC1	2.45	0.46
21:H:201:ASN:ND2	28:H:304:CLA:OBD	2.48	0.46
22:J:203:ASN:C	22:J:205:MET:H	2.23	0.46
14:l:123:TYR:O	14:l:127:MET:HG2	2.16	0.46
14:l:148:VAL:HG21	22:J:200:THR:HG21	1.98	0.46
16:a:110:LEU:HD21	17:b:436:PHE:CE1	2.51	0.46
16:a:600:TRP:HZ3	28:a:735:CLA:HMD3	1.81	0.46
17:b:262:LYS:N	17:b:267:SER:O	2.49	0.46
35:b:730:BCR:H341	35:b:730:BCR:H11C	1.73	0.46
22:J:164:MET:O	22:J:168:ILE:HG12	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:j:105:PID:HM52	28:a:731:CLA:H142	1.97	0.46
28:l:312:CLA:O2A	28:l:313:CLA:HBB2	2.15	0.46
16:a:661:TRP:O	16:a:665:ILE:HG12	2.16	0.46
17:b:46:LEU:HB3	31:b:733:LMG:H162	1.97	0.46
28:b:707:CLA:H91	31:b:733:LMG:H391	1.98	0.46
6:A:58:GLY:O	6:A:62:MET:HG3	2.16	0.45
28:A:313:CLA:CHB	28:A:313:CLA:H11	2.47	0.45
28:j:106:CLA:H41	28:j:106:CLA:H62	1.65	0.45
14:l:175:PHE:HE2	22:J:174:LEU:HD11	1.81	0.45
16:a:110:LEU:HD21	17:b:436:PHE:HE1	1.80	0.45
16:a:390:SER:OG	28:a:726:CLA:HAB	2.16	0.45
28:a:709:CLA:H3A	28:a:709:CLA:HBA2	1.37	0.45
28:B:313:CLA:H111	28:B:313:CLA:H151	1.74	0.45
28:B:315:CLA:HBC1	28:B:317:CLA:HAB	1.98	0.45
19:D:165:LEU:HD22	28:D:314:CLA:HMA3	1.98	0.45
36:a:732:PQN:H161	36:a:732:PQN:H141	1.64	0.45
28:l:306:CLA:HMB3	2:K:139:LEU:HD23	1.98	0.45
11:h:81:TYR:CE1	19:D:114:LEU:HD11	2.52	0.45
14:l:46:ARG:HH22	23:L:142:THR:N	2.14	0.45
17:b:88:TYR:HB2	17:b:160:THR:HG21	1.98	0.45
17:b:276:HIS:HB2	28:b:716:CLA:CHB	2.47	0.45
20:F:160:ASP:OD1	20:F:160:ASP:N	2.46	0.45
22:J:133:PHE:CE2	28:J:316:CLA:HBA2	2.51	0.45
2:K:30:LEU:HD23	2:K:40:GLY:HA2	1.97	0.45
6:A:81:LYS:HE2	6:A:82:CYS:HB2	1.98	0.45
10:f:251:PRO:HD2	17:b:518:PRO:HB3	1.99	0.45
12:i:63:GLN:NE2	15:m:85:ASP:O	2.31	0.45
12:i:90:SER:HB3	17:b:662:TYR:OH	2.16	0.45
14:l:165:LEU:HD11	22:J:190:ILE:HG22	1.97	0.45
28:a:726:CLA:H203	28:a:726:CLA:H162	1.74	0.45
35:a:736:BCR:H11C	35:a:736:BCR:H341	1.69	0.45
28:b:713:CLA:H112	28:b:717:CLA:H92	1.99	0.45
19:D:60:ARG:NH1	19:D:63:GLU:OE1	2.49	0.45
32:F:304:PID:H16	32:F:304:PID:HM41	1.64	0.45
24:M:116:GLY:H	24:M:145:ARG:HH22	1.64	0.45
9:e:75:PHE:HB3	10:f:247:HIS:CD2	2.51	0.45
11:h:8:GLU:O	11:h:12:GLU:HG2	2.16	0.45
13:j:82:VAL:HG13	35:j:102:BCR:H373	1.98	0.45
14:l:37:LYS:HG2	14:l:38:ILE:H	1.80	0.45
16:a:109:ILE:HD13	16:a:587:CYS:SG	2.55	0.45
16:a:189:PHE:HB3	16:a:269:PHE:CD2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:a:705:CLA:H11	28:a:705:CLA:H51	1.73	0.45
23:L:132:GLU:H	23:L:132:GLU:HG2	1.39	0.45
1:I:4:SER:OG	1:I:7:VAL:O	2.35	0.45
30:y:201:DGD:HA22	30:y:201:DGD:HA51	1.75	0.45
28:f:302:CLA:HBB1	13:j:85:LEU:HD21	1.99	0.45
14:l:273:LEU:HD21	28:l:308:CLA:C3D	2.46	0.45
28:a:731:CLA:HBA1	28:a:731:CLA:H3A	1.58	0.45
18:B:132:GLU:OE2	18:B:208:ARG:NH2	2.39	0.45
20:F:150:MET:O	20:F:158:GLY:N	2.50	0.45
21:H:146:VAL:HB	21:H:151:TRP:NE1	2.32	0.45
22:J:211:ILE:HG12	28:J:312:CLA:HBB	1.98	0.45
28:J:311:CLA:HMB1	28:J:311:CLA:HBB1	1.98	0.45
28:M:308:CLA:H41	28:M:308:CLA:H61	1.63	0.45
28:I:308:CLA:H91	28:I:308:CLA:H111	1.75	0.45
28:A:309:CLA:H2	28:A:309:CLA:H61	1.62	0.45
28:A:312:CLA:H92	28:A:312:CLA:H61	1.79	0.45
17:b:113:ILE:HD11	17:b:135:LEU:HG	1.98	0.45
17:b:323:SER:OG	17:b:374:SER:O	2.34	0.45
18:B:77:UNK:CB	18:B:83:UNK:HA	2.47	0.45
18:B:150:SER:HB2	18:B:155:TRP:HE3	1.82	0.45
19:D:123:GLY:O	19:D:127:GLU:HG2	2.16	0.45
21:H:143:ILE:HG22	21:H:151:TRP:CZ2	2.52	0.45
24:M:170:LEU:HD23	24:M:171:PRO:HD2	1.98	0.45
1:I:61:GLN:HE21	28:I:310:CLA:HED1	1.82	0.45
2:K:157:GLU:HB2	28:K:313:CLA:CHB	2.46	0.45
6:A:95:VAL:O	6:A:116:GLY:HA2	2.17	0.45
11:h:97:ASP:OD2	17:b:468:ILE:HA	2.16	0.45
14:l:50:GLU:OE1	14:l:50:GLU:N	2.49	0.45
16:a:161:TYR:HB2	28:a:712:CLA:HMC2	1.98	0.45
17:b:323:SER:OG	17:b:378:THR:OG1	2.33	0.45
5:G:92:GLU:HG2	28:G:510:CLA:CHB	2.47	0.45
5:G:99:CYS:SG	5:G:201:MET:HG2	2.56	0.45
28:A:308:CLA:HBB1	28:A:308:CLA:HMB3	1.99	0.45
28:a:705:CLA:H92	28:a:705:CLA:H61	1.75	0.45
17:b:674:PHE:HZ	28:b:722:CLA:H61	1.82	0.45
1:I:151:LEU:HD13	28:I:307:CLA:HBC1	1.97	0.45
28:I:312:CLA:H92	28:I:312:CLA:H61	1.72	0.45
6:A:160:LEU:HD12	6:A:161:PRO:HD2	1.98	0.45
8:d:267:ARG:HH21	8:d:268:GLN:HB2	1.81	0.45
28:f:301:CLA:HAC1	16:a:625:HIS:CD2	2.52	0.45
16:a:460:PHE:HE1	28:b:704:CLA:HBA2	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:b:389:PRO:HD2	17:b:399:ILE:CD1	2.47	0.45
28:b:715:CLA:H3A	28:b:715:CLA:HBA2	1.46	0.45
28:b:727:CLA:H3A	36:b:729:PQN:H293	1.98	0.45
19:D:71:MET:HE3	19:D:171:ASN:HB3	1.99	0.45
28:J:309:CLA:HBC1	28:J:316:CLA:C4B	2.47	0.45
28:M:315:CLA:H2A	28:M:315:CLA:CED	2.47	0.45
28:M:318:CLA:HBA2	28:M:318:CLA:H3A	1.34	0.45
1:I:73:PRO:HG3	1:I:82:ALA:HB3	1.99	0.44
2:K:34:VAL:HG11	2:K:154:GLN:HB3	1.99	0.44
2:K:102:GLY:N	2:K:103:PRO:HD2	2.32	0.44
6:A:34:PHE:HB3	28:A:308:CLA:HMD2	1.99	0.44
6:A:135:ALA:O	6:A:139:PRO:HD2	2.17	0.44
6:A:138:ASN:OD1	33:A:318:SQD:H101	2.16	0.44
11:h:30:HIS:CD2	11:h:31:PRO:HD2	2.52	0.44
13:j:45:THR:HG23	14:l:90:ALA:HB1	1.98	0.44
17:b:293:SER:OG	28:b:718:CLA:OBD	2.23	0.44
17:b:420:GLY:N	17:b:495:LEU:HD13	2.32	0.44
28:b:725:CLA:H41	28:b:725:CLA:H61	1.57	0.44
21:H:160:TYR:CD2	28:N:309:CLA:HBA2	2.51	0.44
28:M:308:CLA:HAA2	25:N:145:GLY:O	2.16	0.44
1:I:166:VAL:HG13	1:I:175:PRO:HG3	1.99	0.44
28:I:312:CLA:H142	28:I:312:CLA:H111	1.71	0.44
10:f:164:ARG:HA	10:f:164:ARG:HD3	1.86	0.44
32:j:105:PID:C11	28:a:710:CLA:HMA2	2.48	0.44
16:a:392:TYR:HE2	16:a:457:ILE:HG13	1.81	0.44
36:a:732:PQN:H172	35:b:702:BCR:H382	2.00	0.44
28:b:715:CLA:H61	28:b:715:CLA:H41	1.70	0.44
19:D:176:MET:O	19:D:180:ILE:HG22	2.17	0.44
24:M:139:GLU:H	24:M:139:GLU:CD	2.25	0.44
8:d:208:GLN:HG3	10:f:255:SER:HB3	1.99	0.44
12:i:97:TRP:HA	12:i:103:THR:HG21	1.99	0.44
14:l:120:ILE:HD13	14:l:120:ILE:HA	1.81	0.44
28:a:702:CLA:HBD	28:a:702:CLA:HED2	1.45	0.44
18:B:178:GLY:HA2	18:B:181:GLN:NE2	2.32	0.44
2:K:98:MET:HG3	28:K:310:CLA:HAA2	1.99	0.44
2:K:122:ILE:HD11	28:K:312:CLA:HED3	1.99	0.44
3:z:67:UNK:O	3:z:69:UNK:N	2.49	0.44
8:d:216:LYS:HG3	12:i:123:LYS:O	2.18	0.44
16:a:306:ALA:CB	16:a:347:ILE:HG13	2.48	0.44
28:b:701:CLA:H62	28:b:701:CLA:H41	1.49	0.44
19:D:85:LYS:HE2	28:D:311:CLA:HED3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:F:305:PID:HM41	32:F:305:PID:C17	2.43	0.44
28:J:309:CLA:H41	28:J:316:CLA:HMC3	2.00	0.44
23:L:237:PHE:CD1	23:L:238:PRO:HD2	2.52	0.44
28:L:308:CLA:HBA2	28:L:308:CLA:H3A	1.42	0.44
25:N:53:ASN:CG	25:N:56:SER:HB3	2.42	0.44
1:I:42:GLU:HG2	1:I:112:MET:HE2	1.98	0.44
2:K:146:ASP:O	2:K:150:GLN:HG3	2.17	0.44
16:a:307:SER:O	16:a:310:ILE:HG22	2.17	0.44
16:a:348:ILE:HD13	16:a:469:LEU:HD11	2.00	0.44
28:J:307:CLA:O1D	28:J:307:CLA:H2A	2.18	0.44
24:M:267:ILE:HD12	24:M:281:PHE:CD2	2.52	0.44
1:I:157:SER:HB3	28:I:315:CLA:HBC2	1.98	0.44
28:I:321:CLA:O1D	13:j:90:ARG:NH1	2.45	0.44
8:d:177:PHE:CZ	8:d:180:PRO:HG2	2.53	0.44
35:i:201:BCR:H15C	35:i:201:BCR:H351	1.78	0.44
16:a:375:SER:HB2	17:b:646:ILE:HG12	1.98	0.44
28:a:707:CLA:H143	28:a:707:CLA:H111	1.76	0.44
31:b:734:LMG:H171	31:b:734:LMG:H292	2.00	0.44
20:F:95:LYS:H	20:F:98:GLU:CD	2.25	0.44
32:F:304:PID:HM53	28:F:313:CLA:HAB	2.00	0.44
28:F:311:CLA:H2A	28:F:311:CLA:O1D	2.17	0.44
22:J:90:PHE:CD2	28:J:307:CLA:HED3	2.52	0.44
28:J:307:CLA:H111	28:J:307:CLA:H71	1.55	0.44
28:J:307:CLA:H93	28:J:308:CLA:HMA1	1.98	0.44
23:L:200:PRO:O	23:L:204:ILE:HG13	2.17	0.44
28:I:313:CLA:H62	28:I:313:CLA:H41	1.53	0.44
28:G:518:CLA:H3A	28:G:518:CLA:HBA2	1.33	0.44
13:j:83:GLY:O	13:j:87:GLU:HG2	2.18	0.44
16:a:539:GLY:HA3	16:a:549:HIS:HA	2.00	0.44
28:a:713:CLA:H91	28:a:723:CLA:H71	2.00	0.44
17:b:234:HIS:HB2	28:b:714:CLA:CHC	2.47	0.44
19:D:78:MET:SD	32:D:306:PID:H11	2.57	0.44
21:H:100:LYS:NZ	32:H:302:PID:H42	2.29	0.44
11:h:23:LEU:HD22	11:h:28:TYR:CG	2.52	0.44
11:h:104:VAL:HG13	28:b:715:CLA:H72	2.00	0.44
14:l:52:ASP:OD1	14:l:52:ASP:N	2.50	0.44
16:a:435:MET:SD	16:a:541:VAL:HG11	2.58	0.44
28:a:723:CLA:H162	28:a:723:CLA:H141	1.69	0.44
17:b:494:ALA:O	17:b:498:HIS:ND1	2.38	0.44
28:b:725:CLA:HBB1	28:b:725:CLA:HMB1	2.00	0.44
28:B:309:CLA:CHB	28:B:309:CLA:H12	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:H:98:GLU:OE2	21:H:203:ARG:NE	2.35	0.44
14:l:98:TYR:CG	23:L:109:ILE:HG21	2.53	0.44
16:a:341:TRP:HB3	28:a:722:CLA:HMC2	2.00	0.44
28:a:721:CLA:H143	28:a:721:CLA:H161	1.85	0.44
19:D:89:TYR:C	19:D:91:SER:H	2.26	0.44
20:F:117:MET:H	20:F:117:MET:HG2	1.49	0.44
32:F:302:PID:HM12	28:F:313:CLA:HAC2	1.98	0.44
21:H:149:LEU:O	21:H:153:GLN:N	2.40	0.44
5:G:144:SER:O	5:G:147:ILE:HG22	2.18	0.43
16:a:616:GLU:OE2	17:b:514:SER:OG	2.33	0.43
28:a:713:CLA:H61	28:a:713:CLA:H41	1.56	0.43
28:a:718:CLA:CHA	28:a:718:CLA:HBA1	2.46	0.43
17:b:443:ILE:O	17:b:488:TYR:OH	2.22	0.43
17:b:596:LEU:HD21	17:b:615:PHE:CD2	2.53	0.43
28:b:707:CLA:H111	28:b:707:CLA:H72	1.46	0.43
19:D:143:PHE:HB2	32:D:305:PID:O5	2.18	0.43
22:J:126:TRP:CE2	22:J:149:PRO:HG2	2.52	0.43
22:J:209:LYS:O	22:J:213:MET:HG2	2.18	0.43
7:c:166:VAL:HG21	17:b:663:THR:HG23	2.00	0.43
28:f:301:CLA:HAA2	13:j:74:PHE:CE2	2.53	0.43
35:l:306:BCR:H20C	28:b:701:CLA:HBB2	2.00	0.43
16:a:8:ASN:HB3	16:a:10:THR:HG22	1.99	0.43
16:a:86:ILE:HG23	16:a:94:ILE:HG21	2.00	0.43
28:a:721:CLA:H143	28:a:721:CLA:H111	1.82	0.43
28:a:735:CLA:H41	28:a:735:CLA:H62	1.57	0.43
17:b:36:ARG:HA	17:b:36:ARG:NE	2.32	0.43
28:b:704:CLA:H61	28:b:704:CLA:H41	1.81	0.43
21:H:131:LEU:HD22	21:H:136:ILE:HD11	2.00	0.43
23:L:199:GLY:O	23:L:203:GLN:HG3	2.18	0.43
5:G:45:MET:HG2	5:G:84:HIS:CE1	2.53	0.43
16:a:204:MET:HB3	16:a:255:LEU:HD23	1.99	0.43
16:a:377:LEU:HG	16:a:467:LEU:HB2	2.00	0.43
28:a:722:CLA:O1D	28:a:723:CLA:HBB	2.18	0.43
17:b:248:ILE:O	17:b:250:THR:N	2.48	0.43
18:B:199:LYS:O	18:B:203:LEU:HG	2.18	0.43
22:J:196:LEU:HD22	22:J:197:GLU:H	1.83	0.43
13:j:10:LYS:HD2	13:j:10:LYS:HA	1.86	0.43
14:l:51:LYS:H	14:l:51:LYS:HD2	1.83	0.43
35:l:307:BCR:H351	35:l:307:BCR:H15C	1.77	0.43
16:a:104:LEU:O	16:a:105:ILE:HG12	2.18	0.43
16:a:341:TRP:CE3	16:a:522:LEU:HD12	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:a:497:PRO:HD3	17:b:531:GLY:HA2	2.00	0.43
28:a:722:CLA:HBB1	28:a:722:CLA:HMB3	2.00	0.43
18:B:142:MET:SD	28:B:313:CLA:HAB	2.59	0.43
28:J:307:CLA:H3A	28:J:307:CLA:HBA2	1.34	0.43
23:L:97:ARG:HG3	23:L:237:PHE:HE2	1.83	0.43
1:I:41:ARG:NH1	1:I:44:GLU:OE1	2.51	0.43
2:K:20:ALA:O	2:K:22:PRO:HD3	2.18	0.43
7:c:137:GLU:HB3	7:c:145:LEU:HD13	1.99	0.43
10:f:121:LYS:HG2	10:f:125:GLN:OE1	2.18	0.43
14:l:210:LEU:CD1	28:a:725:CLA:HBB2	2.46	0.43
17:b:285:ILE:HD12	28:b:718:CLA:HAC1	2.01	0.43
18:B:221:PRO:HG2	18:B:227:ALA:HA	1.99	0.43
28:J:311:CLA:HBA1	28:J:311:CLA:H3A	1.63	0.43
1:I:160:VAL:O	1:I:164:ILE:HG13	2.18	0.43
6:A:67:GLY:HA3	28:A:310:CLA:C1C	2.48	0.43
8:d:179:HIS:HB3	8:d:180:PRO:HD3	2.00	0.43
10:f:248:ASN:OD1	10:f:248:ASN:N	2.51	0.43
15:m:81:MET:HE3	15:m:81:MET:HB2	1.77	0.43
16:a:45:GLN:OE1	16:a:55:LYS:NZ	2.40	0.43
16:a:503:CYS:HB2	17:b:632:TRP:HB3	1.99	0.43
19:D:139:ALA:H	28:D:314:CLA:HED3	1.84	0.43
1:I:130:LEU:HA	1:I:133:MET:HE1	2.01	0.43
7:c:145:LEU:H	7:c:145:LEU:HG	1.61	0.43
28:a:717:CLA:H61	28:a:717:CLA:H41	1.82	0.43
17:b:489:VAL:HG11	17:b:563:TYR:HB2	2.01	0.43
19:D:68:ARG:HB3	28:D:314:CLA:HAC2	2.00	0.43
19:D:162:LYS:HE3	19:D:162:LYS:HB2	1.89	0.43
20:F:196:THR:OG1	20:F:197:THR:N	2.51	0.43
25:N:64:GLU:HG2	28:N:305:CLA:NB	2.32	0.43
5:G:206:SER:HB3	5:G:217:VAL:HG21	2.00	0.43
28:l:303:CLA:H72	28:l:303:CLA:H112	1.77	0.43
16:a:106:GLY:C	16:a:108:ASP:N	2.75	0.43
17:b:389:PRO:CB	17:b:393:GLU:HB2	2.49	0.43
28:b:704:CLA:H202	28:b:704:CLA:H161	1.61	0.43
32:M:301:PID:HM41	32:M:301:PID:H16	1.61	0.43
12:i:94:ASP:OD2	12:i:105:ARG:NE	2.50	0.43
14:l:202:PHE:CZ	28:l:304:CLA:HBB1	2.54	0.43
28:l:303:CLA:H2A	28:l:303:CLA:O2D	2.18	0.43
16:a:437:ASP:C	16:a:439:LYS:H	2.27	0.43
28:a:706:CLA:H12	28:a:707:CLA:HAB	2.01	0.43
28:a:717:CLA:H3A	28:a:717:CLA:HBA2	1.36	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:b:229:ILE:HD13	35:b:730:BCR:H373	2.01	0.43
35:b:702:BCR:H20C	35:b:702:BCR:H361	1.86	0.43
18:B:173:LYS:O	18:B:177:MET:HG2	2.19	0.43
23:L:237:PHE:CD1	28:L:314:CLA:HAA2	2.54	0.43
25:N:164:GLU:HB2	28:N:310:CLA:C1B	2.48	0.43
8:d:225:ASP:O	8:d:229:THR:HG23	2.19	0.43
14:l:68:ASN:O	14:l:69:PRO:C	2.61	0.43
28:b:701:CLA:HMD3	35:b:732:BCR:H383	2.01	0.43
28:D:314:CLA:HED2	28:D:314:CLA:HBD	1.78	0.43
20:F:114:TRP:HA	20:F:117:MET:HG3	2.01	0.43
24:M:182:PHE:CE1	24:M:277:HIS:HA	2.54	0.43
33:A:318:SQD:H272	17:b:298:LEU:HD21	1.99	0.42
9:e:66:LYS:HB3	9:e:117:ILE:HG22	2.00	0.42
14:l:213:LEU:HD12	14:l:222:VAL:HG21	2.01	0.42
16:a:418:ILE:HD13	16:a:418:ILE:HA	1.85	0.42
28:a:704:CLA:HBB1	28:a:704:CLA:HMB3	2.00	0.42
28:a:722:CLA:H93	28:a:722:CLA:H62	1.83	0.42
17:b:559:TRP:CD1	28:b:703:CLA:H43	2.54	0.42
35:b:732:BCR:H15C	35:b:732:BCR:H351	1.83	0.42
22:J:196:LEU:HD23	22:J:196:LEU:HA	1.87	0.42
23:L:150:GLU:HG2	23:L:219:VAL:HG13	2.01	0.42
23:L:213:LEU:HG	28:L:313:CLA:HMB2	2.01	0.42
1:I:146:LEU:HD13	1:I:146:LEU:HA	1.81	0.42
1:I:162:HIS:HA	1:I:165:VAL:HG22	2.00	0.42
28:I:321:CLA:HBC2	32:j:105:PID:C12	2.49	0.42
28:I:321:CLA:HBC3	28:I:321:CLA:HHD	2.02	0.42
5:G:197:GLY:O	5:G:201:MET:HG3	2.19	0.42
8:d:177:PHE:HZ	8:d:180:PRO:HG2	1.84	0.42
28:f:302:CLA:HMB1	28:f:302:CLA:HBB1	2.02	0.42
14:l:59:LYS:HZ2	14:l:114:GLU:N	2.17	0.42
16:a:308:LEU:HD11	28:a:723:CLA:H172	2.00	0.42
17:b:75:HIS:CE1	28:b:706:CLA:HMA2	2.54	0.42
17:b:362:HIS:HB2	28:b:720:CLA:C1B	2.49	0.42
19:D:80:PRO:HG3	28:D:311:CLA:C2D	2.49	0.42
19:D:85:LYS:HD3	19:D:85:LYS:HA	1.93	0.42
24:M:261:MET:HE1	28:M:309:CLA:HHC	2.00	0.42
26:I:305:DD6:C4	28:I:309:CLA:HBB2	2.50	0.42
2:K:30:LEU:O	2:K:36:ALA:HB1	2.19	0.42
5:G:89:ARG:HA	5:G:92:GLU:HB2	2.01	0.42
28:G:513:CLA:H102	28:G:517:CLA:HMA2	2.01	0.42
10:f:213:VAL:O	10:f:217:VAL:HG22	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:j:70:ASN:ND2	28:j:104:CLA:OBD	2.41	0.42
16:a:372:PRO:O	16:a:376:HIS:ND1	2.29	0.42
16:a:508:TRP:NE1	28:a:724:CLA:HMD3	2.34	0.42
16:a:595:ILE:HG22	28:a:709:CLA:H191	2.01	0.42
18:B:174:MET:HG2	28:B:311:CLA:HAA2	2.00	0.42
19:D:173:ARG:HB2	32:D:301:PID:HM23	2.01	0.42
27:I:304:UIX:C9	27:I:304:UIX:C3	2.97	0.42
2:K:90:SER:HB3	2:K:93:GLU:OE1	2.20	0.42
3:z:90:UNK:HA	8:d:181:ALA:HB1	2.01	0.42
28:G:520:CLA:H3A	28:G:520:CLA:HBA2	1.63	0.42
9:e:66:LYS:HB2	9:e:119:ALA:HB2	2.01	0.42
35:i:201:BCR:H272	28:a:725:CLA:HMA2	2.01	0.42
35:j:102:BCR:H15C	35:j:102:BCR:H351	1.78	0.42
16:a:190:GLY:HA2	16:a:266:GLY:HA2	2.00	0.42
17:b:371:ALA:O	17:b:374:SER:OG	2.36	0.42
19:D:37:ALA:HB3	19:D:38:PRO:HD3	2.01	0.42
21:H:100:LYS:HD2	28:H:308:CLA:C3D	2.49	0.42
21:H:124:TYR:CZ	21:H:130:LEU:HA	2.54	0.42
28:H:305:CLA:H162	28:H:305:CLA:H141	1.77	0.42
24:M:272:ILE:HD13	28:M:317:CLA:O1D	2.20	0.42
28:I:311:CLA:HBA1	28:I:311:CLA:H3A	1.64	0.42
31:I:320:LMG:H131	31:I:320:LMG:H162	1.76	0.42
32:G:506:PID:H16	32:G:506:PID:HM41	1.71	0.42
28:G:513:CLA:H121	28:G:517:CLA:HED2	2.01	0.42
28:f:301:CLA:CGA	28:j:104:CLA:H43	2.48	0.42
35:i:201:BCR:H383	35:l:302:BCR:H353	2.00	0.42
14:l:203:LEU:HD11	28:b:727:CLA:H192	2.02	0.42
28:l:304:CLA:H111	28:l:304:CLA:H91	1.63	0.42
28:a:731:CLA:H141	28:a:731:CLA:H161	1.83	0.42
17:b:261:LEU:HG	17:b:476:ASP:HB2	2.00	0.42
28:B:310:CLA:H92	28:B:310:CLA:H61	1.68	0.42
23:L:117:PHE:CG	23:L:132:GLU:HB3	2.54	0.42
28:M:310:CLA:HAC1	28:M:316:CLA:CBB	2.48	0.42
25:N:128:GLU:HG2	28:N:309:CLA:HMA3	2.00	0.42
10:f:112:LYS:NZ	10:f:160:ASP:O	2.42	0.42
14:l:214:ARG:NH2	16:a:405:GLU:O	2.51	0.42
16:a:104:LEU:O	16:a:107:GLN:HB2	2.20	0.42
16:a:284:GLN:HE21	16:a:284:GLN:HB2	1.62	0.42
17:b:77:THR:HG21	17:b:171:ILE:HD11	2.02	0.42
17:b:90:ILE:O	17:b:94:ALA:HB3	2.20	0.42
28:L:308:CLA:HBC3	28:L:308:CLA:HHD	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:G:49:MET:HG2	5:G:89:ARG:HH21	1.84	0.42
28:G:511:CLA:H12	28:G:511:CLA:H51	1.81	0.42
14:l:282:LEU:HD13	28:l:305:CLA:H93	2.01	0.42
28:l:303:CLA:HAA1	28:F:312:CLA:H3A	2.01	0.42
16:a:99:HIS:ND1	16:a:121:ILE:HD12	2.34	0.42
16:a:352:ALA:HB2	16:a:511:LEU:HD13	2.01	0.42
28:b:707:CLA:H51	28:b:722:CLA:H52	2.02	0.42
28:b:717:CLA:H203	28:b:721:CLA:CAD	2.50	0.42
21:H:187:ASP:N	21:H:188:PRO:HD3	2.35	0.42
32:G:507:PID:HM41	32:G:507:PID:H16	1.80	0.42
12:i:60:TYR:HB3	17:b:131:ILE:HD11	2.01	0.42
14:l:163:ILE:HG22	14:l:168:ASN:ND2	2.35	0.42
14:l:251:ASP:OD2	14:l:258:GLY:N	2.40	0.42
28:l:305:CLA:H171	28:l:305:CLA:H13	1.88	0.42
16:a:595:ILE:O	16:a:599:ILE:HG12	2.20	0.42
35:a:734:BCR:H351	35:a:734:BCR:H15C	1.73	0.42
17:b:61:THR:O	17:b:65:ASN:ND2	2.29	0.42
19:D:46:GLY:C	19:D:48:SER:H	2.27	0.42
19:D:127:GLU:OE2	32:D:302:PID:H22A	2.20	0.42
20:F:95:LYS:O	20:F:99:ILE:HD12	2.20	0.42
32:F:304:PID:HM52	28:F:313:CLA:HHC	2.01	0.42
28:H:304:CLA:HBD	29:H:310:KC1:OBD	2.20	0.42
24:M:153:ARG:NH2	24:M:232:GLY:O	2.53	0.42
1:I:71:GLU:OE1	1:I:71:GLU:N	2.45	0.42
10:f:190:TRP:CE3	28:f:302:CLA:HBA1	2.55	0.42
35:l:302:BCR:H24C	35:l:302:BCR:H371	1.74	0.42
35:m:201:BCR:H15C	35:m:201:BCR:H351	1.65	0.42
16:a:575:SER:HA	16:a:578:ILE:HG22	2.02	0.42
28:a:704:CLA:H92	28:a:704:CLA:H62	1.88	0.42
17:b:489:VAL:HG11	17:b:563:TYR:CG	2.54	0.42
18:B:182:GLN:O	18:B:186:ILE:HG12	2.20	0.42
21:H:137:PRO:HD2	21:H:145:LYS:HG3	2.02	0.42
21:H:222:ALA:HB1	21:H:223:TRP:HE3	1.85	0.42
22:J:290:UNK:N	28:J:301:CLA:OBD	2.53	0.42
8:d:100:THR:OG1	16:a:371:ASP:OD1	2.37	0.42
12:i:91:PHE:HE2	17:b:661:ILE:HG21	1.85	0.42
16:a:133:SER:HB2	28:a:717:CLA:HED1	2.02	0.42
16:a:134:GLU:O	28:a:714:CLA:HED1	2.20	0.42
16:a:291:TYR:CG	16:a:296:ILE:HG12	2.55	0.42
17:b:616:LEU:HD23	17:b:616:LEU:HA	1.86	0.42
28:b:709:CLA:C1A	28:b:709:CLA:CGA	2.98	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:b:713:CLA:H112	28:b:713:CLA:H71	1.86	0.42
28:b:718:CLA:H43	28:B:301:CLA:C2D	2.50	0.42
18:B:157:PHE:HB2	18:B:162:PHE:CD2	2.55	0.42
21:H:69:GLY:HA3	28:H:305:CLA:O1D	2.20	0.42
21:H:101:HIS:HB3	21:H:206:MET:SD	2.60	0.42
28:L:313:CLA:H11	28:L:313:CLA:H51	1.77	0.42
24:M:239:LEU:N	24:M:240:PRO:HD2	2.35	0.42
28:G:514:CLA:H61	28:G:514:CLA:H41	1.71	0.41
7:c:137:GLU:OE1	7:c:148:ARG:NH1	2.52	0.41
8:d:249:PRO:HG3	8:d:281:VAL:HG11	2.01	0.41
10:f:73:LYS:HB3	10:f:73:LYS:HE2	1.84	0.41
10:f:243:ASN:OD1	10:f:243:ASN:N	2.52	0.41
17:b:352:ASP:HB3	17:b:355:TYR:HB2	2.01	0.41
17:b:357:THR:HA	17:b:564:PHE:HE2	1.84	0.41
17:b:400:ARG:NE	28:b:723:CLA:OBD	2.34	0.41
17:b:646:ILE:HD13	17:b:646:ILE:HA	1.94	0.41
28:L:313:CLA:HBA1	28:L:313:CLA:H3A	1.67	0.41
5:G:91:ALA:O	5:G:95:HIS:ND1	2.42	0.41
5:G:220:LEU:HD22	5:G:220:LEU:HA	1.89	0.41
12:i:96:PHE:CD1	17:b:45:VAL:HG11	2.56	0.41
12:i:123:LYS:HA	12:i:123:LYS:HD3	1.75	0.41
14:l:37:LYS:HD3	14:l:42:GLN:OE1	2.20	0.41
14:l:74:TYR:CG	14:l:106:PRO:HG3	2.55	0.41
16:a:263:LYS:HE3	16:a:263:LYS:HB3	1.81	0.41
17:b:42:TYR:HE2	28:b:727:CLA:HMA1	1.85	0.41
17:b:404:HIS:CE1	17:b:408:ILE:HD11	2.55	0.41
28:b:723:CLA:HAB	28:b:726:CLA:HBB2	2.02	0.41
35:b:730:BCR:H351	35:b:730:BCR:H15C	1.70	0.41
28:B:309:CLA:H41	28:B:309:CLA:H61	1.71	0.41
20:F:165:LYS:HE2	20:F:165:LYS:HB3	1.78	0.41
22:J:92:ASP:HA	26:J:304:DD6:O4	2.20	0.41
22:J:192:MET:HB2	22:J:192:MET:HE3	1.65	0.41
23:L:235:ARG:HB2	26:L:305:DD6:O4	2.19	0.41
23:L:269:ALA:HB2	23:L:278:TRP:CD1	2.55	0.41
28:I:316:CLA:H42	28:I:319:CLA:HMC1	2.02	0.41
2:K:77:ASP:HB3	2:K:182:TRP:H	1.85	0.41
28:f:303:CLA:HBA1	28:f:303:CLA:H3A	1.41	0.41
14:l:73:SER:O	14:l:74:TYR:C	2.63	0.41
16:a:530:PHE:HZ	16:a:667:ARG:HD3	1.85	0.41
32:D:301:PID:H16	32:D:301:PID:HM41	1.82	0.41
32:D:304:PID:H16	32:D:304:PID:HM41	1.76	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:J:76:PRO:HB3	22:J:90:PHE:CZ	2.55	0.41
10:f:74:PRO:HG3	17:b:462:TYR:CE1	2.56	0.41
16:a:174:TYR:CE2	16:a:175:LYS:HG3	2.55	0.41
28:a:707:CLA:H41	37:a:733:LHG:H271	2.02	0.41
28:a:709:CLA:CHC	28:a:710:CLA:HMD2	2.50	0.41
17:b:429:HIS:C	17:b:429:HIS:CD2	2.97	0.41
36:b:729:PQN:H212	36:b:729:PQN:H171	1.66	0.41
19:D:114:LEU:HD22	19:D:114:LEU:H	1.85	0.41
28:J:307:CLA:H52	28:J:308:CLA:HBA2	2.03	0.41
25:N:82:GLU:O	25:N:85:GLY:N	2.50	0.41
1:I:182:GLU:N	1:I:183:PRO:HD3	2.35	0.41
10:f:101:GLU:HB2	10:f:158:LYS:HG2	2.03	0.41
10:f:226:TRP:CD1	10:f:227:PRO:HD3	2.56	0.41
31:j:101:LMG:HC92	31:j:101:LMG:H292	1.78	0.41
16:a:352:ALA:HB2	16:a:511:LEU:CD1	2.50	0.41
17:b:434:ILE:HG21	17:b:580:TYR:CD2	2.56	0.41
28:b:701:CLA:H71	28:b:727:CLA:H102	2.03	0.41
19:D:82:ILE:HG23	19:D:83:THR:OG1	2.21	0.41
22:J:133:PHE:HE1	22:J:247:UNK:CB	2.34	0.41
22:J:158:LEU:HD23	22:J:158:LEU:HA	1.92	0.41
22:J:213:MET:HB2	28:J:306:CLA:HED2	2.02	0.41
2:K:139:LEU:O	28:K:313:CLA:HBD	2.21	0.41
5:G:69:LEU:HB3	5:G:82:TYR:CG	2.55	0.41
28:a:721:CLA:H62	28:a:721:CLA:H102	1.81	0.41
35:b:732:BCR:H11C	35:b:732:BCR:H341	1.97	0.41
18:B:223:GLU:C	18:B:225:ASP:H	2.27	0.41
19:D:118:GLN:HG2	31:D:317:LMG:H332	2.03	0.41
32:D:301:PID:HM22	28:D:309:CLA:HAC2	2.03	0.41
28:J:301:CLA:H62	28:J:301:CLA:H92	1.78	0.41
24:M:258:ARG:HG2	28:M:309:CLA:C4C	2.51	0.41
2:K:35:GLY:H	2:K:155:LEU:HD22	1.84	0.41
2:K:56:ARG:HH11	2:K:59:GLU:HG2	1.86	0.41
6:A:124:PHE:HD1	31:B:318:LMG:H381	1.85	0.41
7:c:87:VAL:HG22	7:c:149:VAL:HG22	2.03	0.41
35:i:201:BCR:H332	28:b:705:CLA:H143	2.02	0.41
35:j:102:BCR:H24C	35:j:102:BCR:H371	1.86	0.41
14:l:237:GLY:HA3	35:l:306:BCR:H19C	2.03	0.41
28:l:313:CLA:H203	28:l:313:CLA:H162	1.73	0.41
28:a:708:CLA:HMB3	28:a:709:CLA:H3A	2.02	0.41
28:a:723:CLA:H142	28:a:723:CLA:H111	1.78	0.41
17:b:678:VAL:HG11	28:b:728:CLA:HED3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:b:702:BCR:H11C	35:b:702:BCR:H341	1.82	0.41
18:B:99:TYR:CE1	28:B:307:CLA:HBB1	2.55	0.41
20:F:109:LEU:HB3	20:F:114:TRP:NE1	2.36	0.41
23:L:97:ARG:NH2	23:L:99:GLU:HA	2.35	0.41
28:L:317:CLA:HHC	28:L:317:CLA:CBB	2.51	0.41
25:N:82:GLU:O	25:N:83:ILE:C	2.63	0.41
1:I:59:VAL:HG13	1:I:171:PHE:HE2	1.82	0.41
2:K:59:GLU:HB2	28:K:308:CLA:C1B	2.51	0.41
3:z:53:UNK:O	14:l:248:THR:OG1	2.39	0.41
7:c:155:GLU:OE2	12:i:173:TRP:HD1	2.04	0.41
9:e:92:TYR:HA	9:e:112:ALA:HA	2.03	0.41
11:h:112:LEU:HD23	11:h:115:ILE:HD12	2.03	0.41
14:l:69:PRO:HD2	14:l:79:LYS:HD3	2.01	0.41
14:l:211:GLY:H	14:l:214:ARG:HB3	1.86	0.41
28:l:310:CLA:H3A	28:l:310:CLA:HBA1	1.85	0.41
16:a:241:SER:HA	28:a:738:CLA:O1D	2.21	0.41
16:a:578:ILE:HG23	16:a:579:GLN:HG3	2.02	0.41
28:a:707:CLA:H141	28:a:723:CLA:HBB2	2.03	0.41
17:b:365:TYR:HA	17:b:557:ASN:OD1	2.21	0.41
17:b:389:PRO:HB3	17:b:393:GLU:HB2	2.03	0.41
17:b:610:VAL:HG21	28:b:710:CLA:HMD3	2.03	0.41
20:F:88:LEU:HD13	20:F:88:LEU:HA	1.81	0.41
23:L:247:MET:CE	28:L:314:CLA:H2	2.51	0.41
1:I:9:PHE:HD2	2:K:121:ALA:HB2	1.86	0.41
1:I:107:ILE:HD11	28:I:311:CLA:CHD	2.50	0.41
2:K:110:TRP:O	2:K:113:ILE:HG22	2.21	0.41
2:K:180:ARG:HH11	2:K:181:THR:H	1.68	0.41
2:K:180:ARG:HH12	2:K:181:THR:HG1	1.67	0.41
5:G:3:UNK:N	9:e:56:TRP:O	2.53	0.41
8:d:273:ARG:HA	8:d:276:GLU:CD	2.45	0.41
35:f:304:BCR:H12C	35:f:304:BCR:H15C	1.85	0.41
11:h:28:TYR:CE2	11:h:30:HIS:HB2	2.56	0.41
12:i:72:PRO:O	12:i:76:LEU:HB2	2.20	0.41
12:i:76:LEU:C	12:i:79:PRO:HD2	2.46	0.41
12:i:107:ARG:NH1	12:i:177:SER:O	2.54	0.41
35:j:102:BCR:H11C	35:j:102:BCR:H341	1.94	0.41
14:l:69:PRO:HG3	14:l:75:LEU:HG	2.03	0.41
28:l:305:CLA:H3A	28:l:305:CLA:HBA1	1.84	0.41
28:l:311:CLA:CHA	28:l:311:CLA:HBA1	2.49	0.41
35:m:201:BCR:HC8	17:b:78:ILE:HG12	2.02	0.41
28:m:202:CLA:H42	28:b:705:CLA:H11	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:a:261:HIS:HB2	28:a:716:CLA:CHB	2.51	0.41
16:a:438:LYS:HB3	16:a:438:LYS:HE2	1.74	0.41
16:a:626:HIS:CE1	16:a:631:ILE:HG22	2.56	0.41
28:a:706:CLA:H61	28:a:706:CLA:H92	1.77	0.41
28:a:731:CLA:H18	28:a:735:CLA:H201	2.01	0.41
17:b:131:ILE:HD12	17:b:131:ILE:HA	1.86	0.41
17:b:397:LYS:HD3	17:b:397:LYS:HA	1.88	0.41
17:b:560:ILE:HD13	31:b:734:LMG:H112	2.03	0.41
28:b:704:CLA:H111	28:b:704:CLA:H142	1.72	0.41
18:B:148:TRP:O	18:B:152:ASP:HB2	2.21	0.41
28:B:313:CLA:H141	28:B:313:CLA:H162	1.89	0.41
20:F:34:VAL:HG23	28:F:308:CLA:HED2	2.02	0.41
32:F:304:PID:HM52	28:F:313:CLA:CHC	2.50	0.41
28:F:310:CLA:H2A	28:F:310:CLA:O2D	2.20	0.41
22:J:91:TRP:CE2	22:J:93:PRO:HG3	2.56	0.41
22:J:192:MET:O	22:J:196:LEU:HB2	2.21	0.41
24:M:130:PRO:HD2	26:M:303:DD6:C33	2.51	0.41
5:G:191:LEU:O	5:G:195:LYS:HG2	2.21	0.41
28:A:312:CLA:H52	28:A:312:CLA:H11	1.78	0.41
8:d:270:TYR:HB3	17:b:196:PRO:HD3	2.03	0.41
16:a:34:ASN:HB3	16:a:38:TYR:CE2	2.55	0.41
16:a:194:THR:HG23	16:a:266:GLY:HA3	2.03	0.41
28:a:726:CLA:H141	28:a:726:CLA:H161	1.75	0.41
28:a:728:CLA:H52	28:a:728:CLA:H11	1.89	0.41
28:b:720:CLA:H11	28:b:720:CLA:H52	1.93	0.41
21:H:71:GLN:OE1	21:H:196:ALA:HB1	2.21	0.41
23:L:204:ILE:HG22	28:L:317:CLA:HBC1	2.03	0.41
23:L:262:PHE:O	23:L:266:VAL:HG22	2.21	0.41
5:G:141:PHE:O	5:G:145:VAL:HG13	2.21	0.40
11:h:29:TRP:HZ3	17:b:200:GLN:HB2	1.86	0.40
28:b:708:CLA:HAA2	28:b:710:CLA:HED1	2.04	0.40
23:L:100:LEU:HG	23:L:104:TYR:CZ	2.56	0.40
23:L:152:GLU:OE2	23:L:256:ARG:NE	2.33	0.40
1:I:162:HIS:CE1	1:I:166:VAL:HG21	2.56	0.40
2:K:66:CYS:SG	2:K:165:MET:HA	2.61	0.40
5:G:46:PHE:CZ	5:G:60:ALA:HB1	2.55	0.40
5:G:99:CYS:SG	5:G:201:MET:HA	2.62	0.40
6:A:202:LEU:HD21	28:A:315:CLA:HMA1	2.04	0.40
14:l:70:PRO:HB2	14:l:71:GLU:H	1.66	0.40
28:l:311:CLA:H161	28:l:311:CLA:H141	1.81	0.40
15:m:71:ARG:HA	15:m:74:GLU:HG2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:a:392:TYR:HE1	16:a:559:SER:O	2.04	0.40
16:a:398:LEU:HD23	16:a:401:LEU:HD12	2.02	0.40
17:b:601:SER:OG	17:b:602:THR:N	2.54	0.40
21:H:95:ARG:O	21:H:99:ILE:HG13	2.21	0.40
28:H:307:CLA:H3A	28:H:307:CLA:HBA2	1.85	0.40
2:K:34:VAL:HG12	2:K:158:LEU:HD12	2.03	0.40
28:K:313:CLA:HBB1	28:K:313:CLA:HMB3	2.03	0.40
26:G:508:DD6:C	28:G:517:CLA:HBB2	2.51	0.40
8:d:199:ARG:NH2	8:d:224:ALA:O	2.42	0.40
8:d:204:ARG:NH2	17:b:521:MET:HE2	2.36	0.40
11:h:46:MET:HE3	17:b:304:ASP:HB3	2.03	0.40
16:a:443:ILE:HD11	16:a:536:ASP:O	2.21	0.40
28:a:712:CLA:H92	28:a:712:CLA:H62	1.90	0.40
17:b:390:LEU:H	17:b:390:LEU:HD22	1.86	0.40
28:b:706:CLA:HBA1	28:b:706:CLA:H3A	1.62	0.40
28:b:713:CLA:H141	28:b:713:CLA:H161	1.80	0.40
20:F:166:ASN:ND2	20:F:169:SER:HB2	2.36	0.40
21:H:163:LEU:HD11	28:J:307:CLA:H101	2.03	0.40
21:H:194:LYS:C	28:H:309:CLA:HMA1	2.46	0.40
22:J:164:MET:HA	28:J:310:CLA:CBC	2.51	0.40
23:L:124:ALA:HB3	23:L:130:ARG:NH2	2.36	0.40
24:M:210:GLY:O	24:M:214:GLN:HG2	2.21	0.40
25:N:69:ARG:HD2	28:N:310:CLA:C4C	2.51	0.40
2:K:126:MET:HG3	31:j:101:LMG:O2	2.22	0.40
5:G:73:ASN:HB3	5:G:79:LEU:O	2.21	0.40
6:A:136:LYS:HD2	6:A:153:TYR:CE1	2.56	0.40
12:i:111:GLU:O	12:i:115:GLU:HG3	2.22	0.40
14:l:70:PRO:O	14:l:76:TYR:CD1	2.75	0.40
35:l:307:BCR:H342	28:l:311:CLA:H143	2.02	0.40
16:a:287:ILE:HG23	16:a:291:TYR:CD2	2.56	0.40
17:b:322:LEU:HA	17:b:325:ILE:HD11	2.03	0.40
17:b:563:TYR:HA	17:b:584:TRP:HH2	1.85	0.40
28:b:717:CLA:H143	28:b:717:CLA:H162	1.81	0.40
19:D:55:ASN:ND2	19:D:59:ARG:HE	2.15	0.40
19:D:140:ALA:HB3	28:D:314:CLA:CAD	2.52	0.40
28:F:310:CLA:CHA	28:F:310:CLA:HBA1	2.51	0.40
28:L:309:CLA:H42	28:L:309:CLA:C2B	2.51	0.40
2:K:105:ALA:O	2:K:109:ILE:HG12	2.21	0.40
5:G:77:ASN:HD21	5:G:81:VAL:HG11	1.85	0.40
6:A:18:GLY:HA3	6:A:147:MET:HE2	2.03	0.40
6:A:94:CYS:SG	28:A:310:CLA:HAA2	2.62	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:c:144:PHE:CZ	17:b:518:PRO:HD2	2.55	0.40
11:h:1:TYR:CD2	12:i:152:THR:HG22	2.55	0.40
12:i:71:VAL:HB	12:i:72:PRO:HD3	2.03	0.40
31:j:101:LMG:H292	30:j:103:DGD:HB32	2.03	0.40
14:l:46:ARG:HG3	14:l:51:LYS:NZ	2.37	0.40
15:m:97:VAL:HG22	35:m:201:BCR:H272	2.04	0.40
28:m:202:CLA:HBA1	28:m:202:CLA:H3A	1.75	0.40
16:a:325:LYS:HB3	16:a:325:LYS:HE3	1.76	0.40
16:a:369:HIS:O	16:a:372:PRO:HD2	2.21	0.40
16:a:380:VAL:HG21	28:a:729:CLA:C2C	2.51	0.40
28:a:704:CLA:H203	28:a:704:CLA:H162	1.87	0.40
28:a:707:CLA:H2	28:a:707:CLA:H61	1.69	0.40
17:b:325:ILE:HD12	28:b:706:CLA:OBD	2.21	0.40
32:F:306:PID:H16	32:F:306:PID:HM41	1.77	0.40
21:H:88:MET:HG3	21:H:92:LYS:NZ	2.37	0.40
22:J:82:THR:C	22:J:213:MET:HE1	2.46	0.40
25:N:38:ALA:HB3	25:N:39:PRO:HD3	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	I	191/200 (96%)	164 (86%)	27 (14%)	0	100	100
2	K	171/177 (97%)	160 (94%)	11 (6%)	0	100	100
5	G	204/224 (91%)	176 (86%)	26 (13%)	2 (1%)	12	32
6	A	162/189 (86%)	144 (89%)	14 (9%)	4 (2%)	4	11
7	c	84/86 (98%)	83 (99%)	1 (1%)	0	100	100
8	d	216/218 (99%)	197 (91%)	19 (9%)	0	100	100
9	e	71/73 (97%)	68 (96%)	3 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	f	182/184 (99%)	177 (97%)	4 (2%)	1 (0%)	24	48
11	h	129/131 (98%)	120 (93%)	9 (7%)	0	100	100
12	i	117/119 (98%)	105 (90%)	12 (10%)	0	100	100
13	j	96/98 (98%)	89 (93%)	7 (7%)	0	100	100
14	l	248/250 (99%)	235 (95%)	12 (5%)	1 (0%)	30	54
15	m	77/79 (98%)	76 (99%)	1 (1%)	0	100	100
16	a	668/670 (100%)	622 (93%)	43 (6%)	3 (0%)	30	54
17	b	661/663 (100%)	613 (93%)	47 (7%)	1 (0%)	43	68
18	B	171/192 (89%)	153 (90%)	15 (9%)	3 (2%)	6	18
19	D	156/165 (94%)	130 (83%)	23 (15%)	3 (2%)	6	17
20	F	165/176 (94%)	153 (93%)	10 (6%)	2 (1%)	10	27
21	H	158/160 (99%)	140 (89%)	16 (10%)	2 (1%)	9	25
22	J	164/220 (74%)	146 (89%)	17 (10%)	1 (1%)	21	44
23	L	183/185 (99%)	161 (88%)	22 (12%)	0	100	100
24	M	164/173 (95%)	151 (92%)	13 (8%)	0	100	100
25	N	149/160 (93%)	119 (80%)	24 (16%)	6 (4%)	2	5
All	All	4587/4792 (96%)	4182 (91%)	376 (8%)	29 (1%)	23	44

All (29) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	G	121	PRO
6	A	85	ALA
14	l	70	PRO
16	a	47	ARG
16	a	218	PRO
19	D	134	PRO
21	H	72	ALA
25	N	88	PRO
25	N	109	ILE
25	N	113	PRO
25	N	153	ASP
5	G	76	PHE
21	H	125	LEU
6	A	79	PRO
10	f	254	GLN

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Mol	Chain	Res	Type
19	D	156	GLU
16	a	220	ILE
18	B	119	LEU
20	F	33	GLY
22	J	74	GLU
18	B	93	MET
20	F	32	LEU
25	N	82	GLU
6	A	33	ASN
17	b	311	LEU
19	D	37	ALA
6	A	132	GLY
18	B	165	VAL
25	N	38	ALA

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	I	139/155 (90%)	131 (94%)	8 (6%)	18	42
2	K	133/138 (96%)	127 (96%)	6 (4%)	24	52
5	G	147/171 (86%)	136 (92%)	11 (8%)	12	31
6	A	122/129 (95%)	117 (96%)	5 (4%)	27	56
7	c	76/76 (100%)	75 (99%)	1 (1%)	61	83
8	d	182/184 (99%)	176 (97%)	6 (3%)	33	63
9	e	63/63 (100%)	63 (100%)	0	100	100
10	f	148/148 (100%)	145 (98%)	3 (2%)	48	76
11	h	112/114 (98%)	111 (99%)	1 (1%)	70	87
12	i	100/101 (99%)	99 (99%)	1 (1%)	68	86
13	j	88/89 (99%)	84 (96%)	4 (4%)	24	52
14	l	199/201 (99%)	189 (95%)	10 (5%)	22	48
15	m	60/63 (95%)	59 (98%)	1 (2%)	53	79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	a	540/592 (91%)	517 (96%)	23 (4%)	26	54
17	b	557/581 (96%)	540 (97%)	17 (3%)	35	65
18	B	142/146 (97%)	123 (87%)	19 (13%)	4	9
19	D	116/123 (94%)	91 (78%)	25 (22%)	1	3
20	F	126/140 (90%)	106 (84%)	20 (16%)	2	7
21	H	123/123 (100%)	111 (90%)	12 (10%)	7	19
22	J	124/136 (91%)	107 (86%)	17 (14%)	3	9
23	L	140/145 (97%)	115 (82%)	25 (18%)	2	5
24	M	106/128 (83%)	86 (81%)	20 (19%)	1	4
25	N	80/124 (64%)	52 (65%)	28 (35%)	0	0
All	All	3623/3870 (94%)	3360 (93%)	263 (7%)	15	32

All (263) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	I	7	VAL
1	I	20	VAL
1	I	24	THR
1	I	108	THR
1	I	118	ARG
1	I	143	LEU
1	I	146	LEU
1	I	188	SER
2	K	53	ARG
2	K	59	GLU
2	K	80	MET
2	K	140	ARG
2	K	142	LEU
2	K	155	LEU
5	G	17	VAL
5	G	30	ILE
5	G	35	VAL
5	G	42	SER
5	G	68	LYS
5	G	81	VAL
5	G	92	GLU
5	G	119	VAL
5	G	147	ILE

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Mol	Chain	Res	Type
5	G	217	VAL
5	G	220	LEU
6	A	80	GLU
6	A	81	LYS
6	A	94	CYS
6	A	129	GLU
6	A	145	LEU
7	c	127	VAL
8	d	77	VAL
8	d	114	ILE
8	d	115	THR
8	d	255	GLU
8	d	260	GLU
8	d	267	ARG
10	f	113	LEU
10	f	187	ILE
10	f	243	ASN
11	h	113	LEU
12	i	169	HIS
13	j	33	THR
13	j	57	VAL
13	j	58	VAL
13	j	71	VAL
14	l	68	ASN
14	l	71	GLU
14	l	72	ASP
14	l	93	MET
14	l	120	ILE
14	l	148	VAL
14	l	166	THR
14	l	202	PHE
14	l	252	LYS
14	l	255	ASP
15	m	140	GLU
16	a	9	THR
16	a	43	ASP
16	a	105	ILE
16	a	107	GLN
16	a	108	ASP
16	a	109	ILE
16	a	150	LEU
16	a	241	SER

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Mol	Chain	Res	Type
16	a	284	GLN
16	a	292	ILE
16	a	296	ILE
16	a	304	LEU
16	a	327	THR
16	a	337	ILE
16	a	380	VAL
16	a	384	ILE
16	a	435	MET
16	a	503	CYS
16	a	511	LEU
16	a	522	LEU
16	a	660	THR
16	a	666	SER
16	a	668	LEU
17	b	58	ILE
17	b	63	SER
17	b	184	LEU
17	b	188	LEU
17	b	238	ILE
17	b	289	HIS
17	b	325	ILE
17	b	412	LEU
17	b	434	ILE
17	b	557	ASN
17	b	570	THR
17	b	596	LEU
17	b	602	THR
17	b	650	THR
17	b	651	PRO
17	b	652	ILE
17	b	667	LEU
18	B	91	VAL
18	B	97	VAL
18	B	105	ARG
18	B	113	GLU
18	B	121	THR
18	B	140	ILE
18	B	152	ASP
18	B	158	GLU
18	B	165	VAL
18	B	169	ASN

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Mol	Chain	Res	Type
18	B	176	GLU
18	B	179	VAL
18	B	215	ILE
18	B	222	LYS
18	B	224	GLU
18	B	226	LYS
18	B	228	LYS
18	B	230	MET
18	B	253	ASN
19	D	30	GLU
19	D	31	ASN
19	D	36	GLN
19	D	39	THR
19	D	64	ILE
19	D	75	MET
19	D	82	ILE
19	D	83	THR
19	D	90	LEU
19	D	113	VAL
19	D	114	LEU
19	D	129	SER
19	D	132	GLN
19	D	142	ASP
19	D	143	PHE
19	D	151	LYS
19	D	153	ILE
19	D	159	GLU
19	D	161	LEU
19	D	162	LYS
19	D	165	LEU
19	D	169	LEU
19	D	177	MET
19	D	180	ILE
19	D	188	LEU
20	F	29	GLU
20	F	32	LEU
20	F	88	LEU
20	F	95	LYS
20	F	99	ILE
20	F	103	MET
20	F	107	LYS
20	F	111	THR

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Mol	Chain	Res	Type
20	F	117	MET
20	F	123	LEU
20	F	125	GLU
20	F	133	GLU
20	F	142	THR
20	F	145	LYS
20	F	164	VAL
20	F	166	ASN
20	F	167	GLN
20	F	170	LEU
20	F	197	THR
20	F	200	GLU
21	H	70	VAL
21	H	85	ASP
21	H	89	LYS
21	H	91	PHE
21	H	92	LYS
21	H	106	MET
21	H	107	LEU
21	H	110	MET
21	H	130	LEU
21	H	143	ILE
21	H	149	LEU
21	H	207	MET
22	J	73	ARG
22	J	97	THR
22	J	99	ASN
22	J	118	ILE
22	J	134	HIS
22	J	136	LEU
22	J	154	ASN
22	J	156	LEU
22	J	158	LEU
22	J	161	VAL
22	J	174	LEU
22	J	188	ASP
22	J	189	VAL
22	J	192	MET
22	J	196	LEU
22	J	197	GLU
22	J	198	GLU
23	L	97	ARG

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Mol	Chain	Res	Type
23	L	98	ARG
23	L	100	LEU
23	L	102	VAL
23	L	116	LYS
23	L	122	VAL
23	L	125	GLU
23	L	132	GLU
23	L	173	ARG
23	L	187	VAL
23	L	188	ILE
23	L	189	ASP
23	L	194	LEU
23	L	195	ASN
23	L	218	LYS
23	L	235	ARG
23	L	237	PHE
23	L	239	GLU
23	L	240	ASP
23	L	241	ASP
23	L	245	LYS
23	L	249	ILE
23	L	270	VAL
23	L	272	THR
23	L	274	LYS
24	M	118	ASP
24	M	122	PHE
24	M	125	LYS
24	M	141	LEU
24	M	145	ARG
24	M	162	LEU
24	M	167	LEU
24	M	170	LEU
24	M	174	GLU
24	M	180	LEU
24	M	182	PHE
24	M	188	LYS
24	M	218	LYS
24	M	224	GLU
24	M	226	LEU
24	M	227	THR
24	M	247	LEU
24	M	249	TYR

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Mol	Chain	Res	Type
24	M	267	ILE
24	M	277	HIS
25	N	33	GLU
25	N	34	LEU
25	N	37	GLN
25	N	40	VAL
25	N	42	PHE
25	N	43	TRP
25	N	44	ASP
25	N	46	VAL
25	N	53	ASN
25	N	54	VAL
25	N	58	ARG
25	N	64	GLU
25	N	73	LEU
25	N	80	THR
25	N	119	GLN
25	N	128	GLU
25	N	131	GLN
25	N	132	ASP
25	N	133	GLN
25	N	148	VAL
25	N	149	LEU
25	N	153	ASP
25	N	161	LEU
25	N	165	ILE
25	N	173	MET
25	N	176	THR
25	N	184	LEU
25	N	185	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	I	61	GLN
1	I	191	ASN
2	K	95	HIS
2	K	124	ASN
2	K	154	GLN
5	G	109	GLN
5	G	210	ASN
8	d	190	ASN

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Mol	Chain	Res	Type
9	e	76	GLN
10	f	247	HIS
13	j	72	ASN
14	l	280	HIS
16	a	46	GLN
16	a	163	HIS
16	a	208	ASN
16	a	284	GLN
16	a	456	HIS
16	a	544	GLN
16	a	546	HIS
16	a	579	GLN
16	a	625	HIS
17	b	44	GLN
17	b	67	GLN
17	b	75	HIS
17	b	219	HIS
18	B	163	GLN
18	B	169	ASN
19	D	55	ASN
20	F	131	GLN
20	F	166	ASN
20	F	191	ASN
22	J	163	GLN
22	J	232	GLN
23	L	268	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

310 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
28	CLA	N	309	25	50,54,73	1.35	7 (14%)	59,90,113	1.41	4 (6%)
26	DD6	L	302	-	40,45,45	1.48	2 (5%)	51,67,67	1.97	16 (31%)
26	DD6	F	303	-	40,45,45	1.55	2 (5%)	51,67,67	2.03	14 (27%)
28	CLA	M	316	-	56,60,73	1.32	8 (14%)	65,97,113	1.36	4 (6%)
28	CLA	L	313	-	59,63,73	1.28	7 (11%)	70,101,113	1.31	5 (7%)
28	CLA	a	723	-	69,73,73	1.17	9 (13%)	82,113,113	1.22	5 (6%)
28	CLA	b	710	-	56,60,73	1.32	8 (14%)	65,97,113	1.36	5 (7%)
28	CLA	F	315	-	45,49,73	1.43	6 (13%)	54,84,113	1.52	6 (11%)
28	CLA	G	512	-	64,68,73	1.23	7 (10%)	76,107,113	1.32	5 (6%)
28	CLA	K	313	-	59,63,73	1.25	6 (10%)	70,101,113	1.32	7 (10%)
32	PID	G	507	-	43,49,49	1.25	3 (6%)	52,76,76	1.34	7 (13%)
32	PID	D	304	-	43,49,49	1.23	3 (6%)	52,76,76	1.72	7 (13%)
28	CLA	G	516	5	45,49,73	1.43	6 (13%)	54,84,113	1.48	5 (9%)
28	CLA	M	309	24	59,63,73	1.27	6 (10%)	70,101,113	1.30	5 (7%)
29	KC1	I	314	1	49,53,53	1.32	6 (12%)	61,89,89	1.75	15 (24%)
31	LMG	I	320	-	38,38,55	0.80	0	46,46,63	1.29	6 (13%)
28	CLA	H	304	-	51,55,73	1.36	6 (11%)	60,91,113	1.38	5 (8%)
26	DD6	L	304	-	40,45,45	1.55	2 (5%)	51,67,67	1.81	12 (23%)
28	CLA	l	312	-	50,54,73	1.36	7 (14%)	59,90,113	1.34	4 (6%)
28	CLA	M	308	29	57,61,73	1.30	8 (14%)	67,98,113	1.38	6 (8%)
28	CLA	H	308	-	50,54,73	1.38	7 (14%)	59,90,113	1.41	4 (6%)
28	CLA	L	316	-	45,49,73	1.42	7 (15%)	54,84,113	1.48	5 (9%)
31	LMG	K	318	-	43,43,55	0.81	1 (2%)	51,51,63	1.32	6 (11%)
31	LMG	I	318	-	36,36,55	0.89	1 (2%)	44,44,63	1.25	3 (6%)
31	LMG	j	101	-	35,35,55	0.87	1 (2%)	43,43,63	1.23	4 (9%)
28	CLA	B	308	-	49,53,73	1.39	5 (10%)	58,89,113	1.44	4 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	CLA	L	312	-	50,54,73	1.37	7 (14%)	59,90,113	1.40	4 (6%)
29	KC1	G	515	5	49,53,53	1.35	6 (12%)	61,89,89	1.71	14 (22%)
28	CLA	I	308	-	64,68,73	1.23	8 (12%)	76,107,113	1.29	7 (9%)
28	CLA	a	728	-	59,63,73	1.27	8 (13%)	70,101,113	1.34	6 (8%)
28	CLA	B	310	-	59,63,73	1.27	7 (11%)	70,101,113	1.32	7 (10%)
28	CLA	a	729	-	60,64,73	1.26	6 (10%)	71,102,113	1.30	6 (8%)
26	DD6	h	203	-	40,45,45	1.55	2 (5%)	51,67,67	1.86	12 (23%)
28	CLA	b	715	-	64,68,73	1.22	5 (7%)	76,107,113	1.31	6 (7%)
26	DD6	L	305	-	40,45,45	1.55	2 (5%)	51,67,67	1.93	14 (27%)
28	CLA	F	307	-	50,54,73	1.37	8 (16%)	59,90,113	1.43	4 (6%)
29	KC1	N	306	-	49,53,53	1.33	5 (10%)	61,89,89	1.72	13 (21%)
26	DD6	M	304	-	40,45,45	1.59	3 (7%)	51,67,67	1.92	14 (27%)
28	CLA	I	312	-	69,73,73	1.18	8 (11%)	82,113,113	1.21	5 (6%)
26	DD6	B	306	-	40,45,45	1.55	2 (5%)	51,67,67	1.95	19 (37%)
28	CLA	a	718	-	50,54,73	1.36	6 (12%)	59,90,113	1.41	4 (6%)
28	CLA	a	715	-	49,53,73	1.39	8 (16%)	58,89,113	1.44	4 (6%)
28	CLA	a	725	-	65,69,73	1.21	7 (10%)	77,108,113	1.30	6 (7%)
28	CLA	A	319	-	50,54,73	1.36	7 (14%)	59,90,113	1.35	4 (6%)
26	DD6	M	303	-	40,45,45	1.76	4 (10%)	51,67,67	2.19	18 (35%)
28	CLA	N	305	-	69,73,73	1.17	8 (11%)	82,113,113	1.27	5 (6%)
27	UIX	I	304	-	43,49,49	1.41	6 (13%)	53,74,74	2.50	16 (30%)
31	LMG	K	317	-	27,27,55	0.99	1 (3%)	35,35,63	1.19	4 (11%)
32	PID	F	305	-	43,49,49	1.25	4 (9%)	52,76,76	1.83	8 (15%)
28	CLA	L	314	-	57,61,73	1.29	8 (14%)	67,98,113	1.36	6 (8%)
28	CLA	H	311	-	45,49,73	1.44	7 (15%)	54,84,113	1.44	5 (9%)
36	PQN	a	732	-	34,34,34	1.60	2 (5%)	43,45,45	1.15	4 (9%)
28	CLA	B	313	18	69,73,73	1.16	7 (10%)	82,113,113	1.27	4 (4%)
28	CLA	K	315	-	45,49,73	1.42	6 (13%)	54,84,113	1.49	7 (12%)
29	KC1	F	309	20	49,53,53	1.35	6 (12%)	61,89,89	1.79	14 (22%)
28	CLA	l	311	-	69,73,73	1.18	6 (8%)	82,113,113	1.26	5 (6%)
26	DD6	L	306	-	40,45,45	1.54	2 (5%)	51,67,67	2.03	15 (29%)
28	CLA	a	708	-	55,59,73	1.32	7 (12%)	64,96,113	1.38	6 (9%)
28	CLA	G	517	-	50,54,73	1.36	6 (12%)	59,90,113	1.39	4 (6%)
28	CLA	K	307	-	50,54,73	1.34	7 (14%)	59,90,113	1.42	5 (8%)
28	CLA	a	713	-	64,68,73	1.21	7 (10%)	76,107,113	1.27	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	CLA	J	311	22	51,55,73	1.36	6 (11%)	60,91,113	1.41	6 (10%)
28	CLA	D	314	-	50,54,73	1.40	8 (16%)	59,90,113	1.46	6 (10%)
28	CLA	a	735	-	69,73,73	1.18	6 (8%)	82,113,113	1.21	5 (6%)
28	CLA	h	202	-	59,63,73	1.28	7 (11%)	70,101,113	1.33	5 (7%)
30	DGD	L	301	-	39,39,67	0.96	2 (5%)	53,53,81	0.99	2 (3%)
28	CLA	G	511	-	59,63,73	1.28	7 (11%)	70,101,113	1.32	5 (7%)
29	KC1	H	310	-	49,53,53	1.35	5 (10%)	61,89,89	1.72	13 (21%)
28	CLA	M	312	-	52,56,73	1.35	8 (15%)	61,92,113	1.40	6 (9%)
28	CLA	D	308	-	51,55,73	1.36	7 (13%)	60,91,113	1.37	4 (6%)
26	DD6	B	304	-	40,45,45	1.54	2 (5%)	51,67,67	1.88	12 (23%)
34	SF4	c	201	7	0,12,12	-	-	-	-	-
28	CLA	l	313	14	69,73,73	1.19	6 (8%)	82,113,113	1.29	5 (6%)
28	CLA	M	318	-	50,54,73	1.38	8 (16%)	59,90,113	1.37	4 (6%)
35	BCR	a	734	-	41,41,41	0.65	0	56,56,56	2.08	20 (35%)
32	PID	D	305	-	43,49,49	1.26	3 (6%)	52,76,76	1.46	9 (17%)
26	DD6	G	505	-	40,45,45	1.84	3 (7%)	51,67,67	2.31	19 (37%)
28	CLA	B	316	-	50,54,73	1.37	7 (14%)	59,90,113	1.35	4 (6%)
28	CLA	b	703	-	69,73,73	1.17	7 (10%)	82,113,113	1.22	6 (7%)
30	DGD	I	317	-	40,40,67	1.10	2 (5%)	54,54,81	1.00	4 (7%)
30	DGD	y	201	-	55,55,67	0.93	2 (3%)	69,69,81	0.97	3 (4%)
28	CLA	a	716	-	51,55,73	1.35	6 (11%)	60,91,113	1.40	5 (8%)
28	CLA	a	705	28	59,63,73	1.27	7 (11%)	70,101,113	1.38	7 (10%)
28	CLA	G	520	-	53,57,73	1.32	7 (13%)	61,93,113	1.35	7 (11%)
28	CLA	M	317	-	50,54,73	1.36	6 (12%)	59,90,113	1.43	5 (8%)
28	CLA	b	708	-	69,73,73	1.17	8 (11%)	82,113,113	1.24	6 (7%)
26	DD6	M	302	-	40,45,45	1.74	3 (7%)	51,67,67	2.23	18 (35%)
28	CLA	K	308	2	58,62,73	1.27	6 (10%)	68,99,113	1.33	6 (8%)
28	CLA	A	308	-	59,63,73	1.26	7 (11%)	70,101,113	1.32	6 (8%)
30	DGD	j	103	-	42,42,67	1.06	2 (4%)	56,56,81	1.01	3 (5%)
28	CLA	D	311	-	50,54,73	1.36	5 (10%)	59,90,113	1.41	4 (6%)
28	CLA	a	724	-	69,73,73	1.19	8 (11%)	82,113,113	1.29	8 (9%)
28	CLA	a	720	-	66,70,73	1.20	7 (10%)	78,109,113	1.29	6 (7%)
33	SQD	A	318	-	48,50,54	0.41	1 (2%)	58,61,65	0.58	0
28	CLA	b	718	-	55,59,73	1.34	6 (10%)	64,96,113	1.41	6 (9%)
26	DD6	K	301	-	40,45,45	1.53	2 (5%)	51,67,67	1.93	15 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	CLA	a	707	-	69,73,73	1.19	6 (8%)	82,113,113	1.21	5 (6%)
28	CLA	f	302	-	50,54,73	1.37	7 (14%)	59,90,113	1.39	5 (8%)
29	KC1	N	311	25	49,53,53	1.33	5 (10%)	61,89,89	1.72	13 (21%)
28	CLA	A	312	-	59,63,73	1.27	7 (11%)	70,101,113	1.30	5 (7%)
28	CLA	L	310	-	59,63,73	1.27	6 (10%)	70,101,113	1.33	6 (8%)
26	DD6	I	301	-	40,45,45	1.57	2 (5%)	51,67,67	2.17	17 (33%)
28	CLA	A	310	-	69,73,73	1.17	8 (11%)	82,113,113	1.30	5 (6%)
28	CLA	a	706	16	62,66,73	1.23	7 (11%)	73,104,113	1.31	4 (5%)
28	CLA	l	303	14	69,73,73	1.18	7 (10%)	82,113,113	1.26	6 (7%)
35	BCR	l	307	-	41,41,41	0.68	0	56,56,56	2.03	19 (33%)
28	CLA	f	301	-	59,63,73	1.27	7 (11%)	70,101,113	1.32	5 (7%)
34	SF4	a	737	17,16	0,12,12	-	-	-	-	-
28	CLA	I	310	-	52,56,73	1.34	6 (11%)	61,92,113	1.42	6 (9%)
28	CLA	a	702	-	69,73,73	1.19	9 (13%)	82,113,113	1.33	5 (6%)
29	KC1	A	314	6	49,53,53	1.33	6 (12%)	61,89,89	1.73	14 (22%)
28	CLA	l	305	-	69,73,73	1.19	8 (11%)	82,113,113	1.26	4 (4%)
27	UIX	J	305	-	43,49,49	1.35	4 (9%)	53,74,74	2.38	18 (33%)
28	CLA	A	307	29	49,53,73	1.41	6 (12%)	58,89,113	1.44	4 (6%)
29	KC1	A	306	26,28	49,53,53	1.34	6 (12%)	61,89,89	1.70	13 (21%)
37	LHG	a	733	-	47,47,48	0.27	0	50,53,54	0.33	0
32	PID	F	306	-	43,49,49	1.23	3 (6%)	52,76,76	1.43	5 (9%)
28	CLA	m	202	-	64,68,73	1.22	7 (10%)	76,107,113	1.33	6 (7%)
28	CLA	D	309	-	50,54,73	1.35	6 (12%)	59,90,113	1.41	4 (6%)
28	CLA	G	519	-	63,67,73	1.23	7 (11%)	74,105,113	1.30	4 (5%)
35	BCR	a	736	-	41,41,41	0.70	0	56,56,56	2.04	18 (32%)
26	DD6	A	303	-	40,45,45	1.49	2 (5%)	51,67,67	1.80	13 (25%)
28	CLA	I	319	28	49,53,73	1.38	7 (14%)	58,89,113	1.46	7 (12%)
32	PID	N	302	-	43,49,49	1.31	3 (6%)	52,76,76	1.64	10 (19%)
28	CLA	K	309	-	54,58,73	1.31	7 (12%)	64,95,113	1.40	6 (9%)
29	KC1	M	307	28	49,53,53	1.36	6 (12%)	61,89,89	1.80	14 (22%)
28	CLA	b	709	-	64,68,73	1.22	8 (12%)	76,107,113	1.32	7 (9%)
28	CLA	K	310	-	59,63,73	1.27	8 (13%)	70,101,113	1.32	5 (7%)
28	CLA	A	315	-	45,49,73	1.42	6 (13%)	54,84,113	1.47	5 (9%)
28	CLA	b	707	-	69,73,73	1.18	6 (8%)	82,113,113	1.29	6 (7%)
28	CLA	I	306	1	53,57,73	1.33	6 (11%)	61,93,113	1.43	6 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	CLA	K	316	-	50,54,73	1.37	8 (16%)	59,90,113	1.42	5 (8%)
26	DD6	J	303	-	40,45,45	1.87	3 (7%)	51,67,67	2.45	16 (31%)
28	CLA	a	703	-	59,63,73	1.25	10 (16%)	70,101,113	1.45	8 (11%)
26	DD6	M	305	-	40,45,45	1.56	3 (7%)	51,67,67	1.88	16 (31%)
27	UIX	h	201	-	43,49,49	1.41	4 (9%)	53,74,74	2.48	20 (37%)
28	CLA	J	312	-	57,61,73	1.28	9 (15%)	67,98,113	1.42	7 (10%)
26	DD6	K	304	-	40,45,45	1.55	2 (5%)	51,67,67	1.99	15 (29%)
28	CLA	H	307	-	55,59,73	1.31	9 (16%)	64,96,113	1.39	6 (9%)
35	BCR	b	730	-	41,41,41	0.70	0	56,56,56	2.27	20 (35%)
28	CLA	a	731	-	69,73,73	1.18	7 (10%)	82,113,113	1.26	6 (7%)
28	CLA	f	303	10	50,54,73	1.36	8 (16%)	59,90,113	1.39	4 (6%)
28	CLA	L	309	-	57,61,73	1.29	5 (8%)	67,98,113	1.37	6 (8%)
28	CLA	N	304	-	51,55,73	1.37	7 (13%)	60,91,113	1.40	5 (8%)
28	CLA	a	726	-	69,73,73	1.17	8 (11%)	82,113,113	1.28	7 (8%)
26	DD6	A	301	-	40,45,45	1.53	2 (5%)	51,67,67	2.05	14 (27%)
28	CLA	I	307	-	50,54,73	1.36	6 (12%)	59,90,113	1.39	4 (6%)
28	CLA	K	311	-	56,60,73	1.31	7 (12%)	65,97,113	1.34	6 (9%)
28	CLA	a	727	-	50,54,73	1.37	7 (14%)	59,90,113	1.36	4 (6%)
28	CLA	K	306	2	53,57,73	1.34	7 (13%)	61,93,113	1.41	6 (9%)
26	DD6	N	303	-	40,45,45	1.53	2 (5%)	51,67,67	2.07	17 (33%)
28	CLA	I	309	-	59,63,73	1.28	7 (11%)	70,101,113	1.33	6 (8%)
32	PID	D	307	-	43,49,49	1.22	4 (9%)	52,76,76	1.36	5 (9%)
26	DD6	M	306	-	40,45,45	1.70	2 (5%)	51,67,67	2.22	20 (39%)
28	CLA	b	706	-	52,56,73	1.36	6 (11%)	61,92,113	1.37	6 (9%)
26	DD6	G	502	-	40,45,45	1.53	2 (5%)	51,67,67	1.87	11 (21%)
26	DD6	D	303	-	40,45,45	1.49	2 (5%)	51,67,67	1.83	14 (27%)
28	CLA	A	313	-	59,63,73	1.26	6 (10%)	70,101,113	1.32	6 (8%)
28	CLA	l	308	-	45,49,73	1.43	7 (15%)	54,84,113	1.45	5 (9%)
28	CLA	b	712	-	58,62,73	1.36	9 (15%)	71,100,113	1.38	6 (8%)
28	CLA	B	307	18	53,57,73	1.35	7 (13%)	61,93,113	1.37	5 (8%)
26	DD6	J	304	-	40,45,45	1.80	4 (10%)	51,67,67	2.14	19 (37%)
28	CLA	G	518	-	50,54,73	1.39	8 (16%)	59,90,113	1.44	5 (8%)
28	CLA	j	106	-	62,66,73	1.24	8 (12%)	73,104,113	1.33	6 (8%)
28	CLA	J	307	-	69,73,73	1.17	7 (10%)	82,113,113	1.31	4 (4%)
28	CLA	l	310	-	39,50,73	2.85	12 (30%)	32,76,113	1.72	6 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	PID	F	304	-	43,49,49	1.24	3 (6%)	52,76,76	1.90	9 (17%)
28	CLA	b	728	-	69,73,73	1.18	7 (10%)	82,113,113	1.29	5 (6%)
26	DD6	J	302	-	40,45,45	1.54	1 (2%)	51,67,67	2.07	14 (27%)
28	CLA	J	301	-	64,68,73	1.22	7 (10%)	76,107,113	1.29	5 (6%)
35	BCR	b	732	-	41,41,41	0.72	0	56,56,56	1.90	18 (32%)
27	UIX	B	305	-	43,49,49	1.36	4 (9%)	53,74,74	2.39	17 (32%)
28	CLA	a	722	-	62,66,73	1.24	7 (11%)	73,104,113	1.30	8 (10%)
26	DD6	L	303	-	40,45,45	1.50	2 (5%)	51,67,67	1.94	14 (27%)
28	CLA	A	316	-	51,55,73	1.35	7 (13%)	60,91,113	1.38	5 (8%)
28	CLA	H	312	-	50,54,73	1.38	7 (14%)	59,90,113	1.39	4 (6%)
28	CLA	a	701	-	49,53,73	1.39	7 (14%)	58,89,113	1.44	4 (6%)
28	CLA	B	311	-	69,73,73	1.17	8 (11%)	82,113,113	1.21	5 (6%)
28	CLA	G	513	5	69,73,73	1.18	8 (11%)	82,113,113	1.27	7 (8%)
28	CLA	D	313	19	49,53,73	1.39	8 (16%)	58,89,113	1.40	4 (6%)
28	CLA	I	311	1	59,63,73	1.28	6 (10%)	70,101,113	1.34	6 (8%)
28	CLA	A	309	-	59,63,73	1.27	6 (10%)	70,101,113	1.32	6 (8%)
27	UIX	A	304	-	43,49,49	1.36	4 (9%)	53,74,74	2.42	21 (39%)
26	DD6	A	305	29	40,45,45	1.52	2 (5%)	51,67,67	1.89	14 (27%)
28	CLA	a	721	-	69,73,73	1.17	8 (11%)	82,113,113	1.24	6 (7%)
30	DGD	G	521	-	45,45,67	1.03	2 (4%)	59,59,81	1.46	8 (13%)
28	CLA	a	704	-	69,73,73	1.18	7 (10%)	82,113,113	1.17	2 (2%)
28	CLA	b	727	-	69,73,73	1.18	7 (10%)	82,113,113	1.26	5 (6%)
29	KC1	H	306	-	49,53,53	1.32	5 (10%)	61,89,89	1.72	13 (21%)
35	BCR	b	702	-	41,41,41	0.66	0	56,56,56	2.19	16 (28%)
28	CLA	L	308	29	49,55,73	1.38	7 (14%)	62,91,113	1.39	7 (11%)
31	LMG	B	318	-	37,37,55	0.85	0	45,45,63	1.34	6 (13%)
28	CLA	I	315	-	56,60,73	1.31	7 (12%)	65,97,113	1.37	7 (10%)
28	CLA	J	314	-	45,49,73	1.43	6 (13%)	54,84,113	1.48	6 (11%)
28	CLA	b	711	-	59,63,73	1.27	5 (8%)	70,101,113	1.31	6 (8%)
27	UIX	G	503	-	43,49,49	1.33	4 (9%)	53,74,74	2.33	19 (35%)
28	CLA	b	713	-	69,73,73	1.18	8 (11%)	82,113,113	1.23	6 (7%)
28	CLA	a	711	-	49,53,73	1.38	7 (14%)	58,89,113	1.46	7 (12%)
28	CLA	a	714	-	49,53,73	1.40	6 (12%)	58,89,113	1.43	4 (6%)
32	PID	H	301	-	43,49,49	1.24	3 (6%)	52,76,76	1.58	7 (13%)
32	PID	G	506	-	43,49,49	1.28	3 (6%)	52,76,76	1.35	7 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
35	BCR	l	306	-	41,41,41	0.68	0	56,56,56	1.93	12 (21%)
28	CLA	a	719	-	51,55,73	1.36	9 (17%)	60,91,113	1.36	5 (8%)
28	CLA	L	318	-	50,54,73	1.36	8 (16%)	59,90,113	1.41	4 (6%)
28	CLA	a	712	28	64,68,73	1.21	8 (12%)	76,107,113	1.29	6 (7%)
28	CLA	G	510	-	69,73,73	1.16	7 (10%)	82,113,113	1.28	7 (8%)
29	KC1	K	314	2	49,53,53	1.33	6 (12%)	61,89,89	1.70	12 (19%)
26	DD6	H	303	-	40,45,45	1.54	3 (7%)	51,67,67	1.92	13 (25%)
28	CLA	J	315	-	50,54,73	1.37	7 (14%)	59,90,113	1.41	4 (6%)
26	DD6	G	508	-	40,45,45	1.55	2 (5%)	51,67,67	2.01	14 (27%)
26	DD6	A	302	-	40,45,45	1.59	3 (7%)	51,67,67	2.10	15 (29%)
29	KC1	N	308	-	49,53,53	1.43	6 (12%)	61,89,89	2.04	15 (24%)
28	CLA	B	317	-	49,53,73	1.40	8 (16%)	58,89,113	1.44	4 (6%)
26	DD6	B	302	-	39,44,45	1.74	2 (5%)	49,65,67	2.08	17 (34%)
35	BCR	i	201	-	41,41,41	0.78	2 (4%)	56,56,56	2.14	21 (37%)
26	DD6	K	303	-	40,45,45	1.65	3 (7%)	51,67,67	1.73	13 (25%)
32	PID	M	301	-	43,49,49	1.22	3 (6%)	52,76,76	1.68	9 (17%)
29	KC1	D	310	-	49,53,53	1.34	6 (12%)	61,89,89	1.74	13 (21%)
28	CLA	I	316	-	59,63,73	1.25	5 (8%)	70,101,113	1.34	7 (10%)
28	CLA	M	311	-	50,54,73	1.37	8 (16%)	59,90,113	1.38	4 (6%)
28	CLA	F	308	-	50,54,73	1.35	8 (16%)	59,90,113	1.39	4 (6%)
31	LMG	D	317	-	48,48,55	0.76	1 (2%)	55,55,63	1.29	5 (9%)
28	CLA	I	313	-	59,63,73	1.26	7 (11%)	70,101,113	1.33	7 (10%)
29	KC1	F	314	20	49,53,53	1.35	5 (10%)	61,89,89	1.73	13 (21%)
26	DD6	B	303	-	40,45,45	1.51	2 (5%)	51,67,67	1.89	13 (25%)
26	DD6	I	303	-	40,45,45	1.83	5 (12%)	51,67,67	2.02	16 (31%)
31	LMG	b	733	-	44,44,55	0.82	1 (2%)	52,52,63	1.31	7 (13%)
28	CLA	G	514	-	57,61,73	1.28	8 (14%)	67,98,113	1.37	6 (8%)
32	PID	D	301	-	43,49,49	1.25	3 (6%)	52,76,76	1.44	7 (13%)
28	CLA	F	310	-	50,54,73	1.36	6 (12%)	59,90,113	1.47	5 (8%)
28	CLA	G	509	5	55,59,73	1.32	6 (10%)	64,96,113	1.38	5 (7%)
28	CLA	l	309	-	45,49,73	1.43	6 (13%)	54,84,113	1.47	5 (9%)
28	CLA	b	721	26	50,54,73	1.37	8 (16%)	59,90,113	1.34	4 (6%)
28	CLA	b	701	-	69,73,73	1.18	8 (11%)	82,113,113	1.28	5 (6%)
28	CLA	N	310	-	51,55,73	1.38	7 (13%)	60,91,113	1.51	6 (10%)
28	CLA	l	304	-	64,68,73	1.21	5 (7%)	76,107,113	1.34	5 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	CLA	F	312	-	50,54,73	1.33	8 (16%)	59,90,113	1.37	4 (6%)
28	CLA	K	312	-	52,56,73	1.35	8 (15%)	61,92,113	1.38	5 (8%)
28	CLA	b	705	-	69,73,73	1.17	7 (10%)	82,113,113	1.26	6 (7%)
35	BCR	j	102	-	41,41,41	0.65	0	56,56,56	2.02	16 (28%)
26	DD6	K	319	-	40,45,45	1.54	2 (5%)	51,67,67	2.05	13 (25%)
28	CLA	b	725	-	69,73,73	1.17	7 (10%)	82,113,113	1.25	6 (7%)
28	CLA	L	311	-	59,63,73	1.27	6 (10%)	70,101,113	1.34	5 (7%)
28	CLA	b	724	-	69,73,73	1.18	8 (11%)	82,113,113	1.23	4 (4%)
28	CLA	b	720	-	57,61,73	1.27	7 (12%)	67,98,113	1.32	5 (7%)
28	CLA	I	321	28	56,60,73	1.31	6 (10%)	65,97,113	1.46	7 (10%)
28	CLA	B	312	-	55,59,73	1.32	7 (12%)	64,96,113	1.37	5 (7%)
32	PID	N	301	-	43,49,49	1.25	3 (6%)	52,76,76	1.44	6 (11%)
29	KC1	M	314	24	49,53,53	1.34	5 (10%)	61,89,89	1.73	14 (22%)
26	DD6	K	305	-	40,45,45	1.51	2 (5%)	51,67,67	1.86	15 (29%)
26	DD6	G	504	-	40,45,45	1.83	6 (15%)	51,67,67	2.12	19 (37%)
28	CLA	H	305	-	69,73,73	1.18	6 (8%)	82,113,113	1.29	6 (7%)
28	CLA	N	307	-	55,59,73	1.32	8 (14%)	64,96,113	1.35	5 (7%)
26	DD6	b	731	28	40,45,45	1.61	2 (5%)	51,67,67	1.98	17 (33%)
28	CLA	J	310	-	50,54,73	1.39	8 (16%)	59,90,113	1.37	4 (6%)
28	CLA	a	717	-	61,65,73	1.26	8 (13%)	72,103,113	1.30	7 (9%)
28	CLA	B	301	-	64,68,73	1.23	6 (9%)	76,107,113	1.26	5 (6%)
28	CLA	b	723	-	54,58,73	1.32	8 (14%)	64,95,113	1.38	7 (10%)
32	PID	D	302	-	43,49,49	1.26	3 (6%)	52,76,76	1.40	9 (17%)
26	DD6	I	305	-	40,45,45	1.80	4 (10%)	51,67,67	2.24	17 (33%)
28	CLA	H	309	-	51,55,73	1.35	6 (11%)	60,91,113	1.40	5 (8%)
26	DD6	I	302	-	40,45,45	1.60	2 (5%)	51,67,67	2.16	18 (35%)
28	CLA	M	315	-	45,49,73	1.42	6 (13%)	54,84,113	1.56	8 (14%)
28	CLA	J	308	-	50,54,73	1.38	8 (16%)	59,90,113	1.41	6 (10%)
30	DGD	l	301	-	51,51,67	0.96	2 (3%)	65,65,81	0.89	2 (3%)
36	PQN	b	729	-	34,34,34	1.58	2 (5%)	43,45,45	1.28	5 (11%)
32	PID	j	105	-	43,49,49	1.28	4 (9%)	52,76,76	1.54	11 (21%)
28	CLA	a	730	-	69,73,73	1.17	8 (11%)	82,113,113	1.30	6 (7%)
32	PID	H	302	-	43,49,49	1.29	3 (6%)	52,76,76	1.39	9 (17%)
28	CLA	a	738	22	50,54,73	1.37	5 (10%)	59,90,113	1.45	5 (8%)
30	DGD	G	501	-	46,46,67	1.02	2 (4%)	60,60,81	1.01	4 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
35	BCR	m	201	-	41,41,41	0.68	0	56,56,56	2.35	17 (30%)
35	BCR	l	302	-	41,41,41	0.68	0	56,56,56	2.20	22 (39%)
26	DD6	F	301	-	40,45,45	1.53	2 (5%)	51,67,67	2.31	16 (31%)
28	CLA	D	312	19	50,54,73	1.37	8 (16%)	59,90,113	1.37	4 (6%)
28	CLA	F	313	-	50,54,73	1.38	7 (14%)	59,90,113	1.48	6 (10%)
29	KC1	D	315	19	49,53,53	1.32	6 (12%)	61,89,89	1.73	15 (24%)
28	CLA	a	710	16	59,63,73	1.28	8 (13%)	70,101,113	1.35	7 (10%)
28	CLA	J	309	-	60,64,73	1.25	8 (13%)	71,102,113	1.39	6 (8%)
28	CLA	A	320	-	50,54,73	1.38	8 (16%)	59,90,113	1.41	4 (6%)
28	CLA	J	306	-	50,54,73	1.37	7 (14%)	59,90,113	1.42	4 (6%)
28	CLA	F	311	-	50,54,73	1.37	8 (16%)	59,90,113	1.44	5 (8%)
29	KC1	B	314	18	49,53,53	1.33	5 (10%)	61,89,89	1.71	13 (21%)
28	CLA	j	104	-	59,63,73	1.29	7 (11%)	70,101,113	1.30	6 (8%)
28	CLA	b	704	-	69,73,73	1.16	8 (11%)	82,113,113	1.34	6 (7%)
28	CLA	b	716	-	54,58,73	1.32	7 (12%)	64,95,113	1.39	5 (7%)
28	CLA	b	717	-	69,73,73	1.19	8 (11%)	82,113,113	1.22	5 (6%)
28	CLA	D	316	-	45,49,73	1.43	7 (15%)	54,84,113	1.47	5 (9%)
28	CLA	M	310	-	52,56,73	1.35	6 (11%)	61,92,113	1.39	5 (8%)
32	PID	F	302	-	43,49,49	1.24	3 (6%)	52,76,76	1.59	7 (13%)
28	CLA	b	714	-	50,54,73	1.37	7 (14%)	59,90,113	1.42	5 (8%)
35	BCR	f	304	-	41,41,41	0.67	0	56,56,56	2.08	17 (30%)
27	UIX	K	302	-	43,49,49	1.40	4 (9%)	53,74,74	2.71	22 (41%)
28	CLA	b	726	-	51,55,73	1.36	7 (13%)	60,91,113	1.36	5 (8%)
28	CLA	a	709	-	69,73,73	1.18	8 (11%)	82,113,113	1.24	6 (7%)
28	CLA	B	315	-	45,49,73	1.41	7 (15%)	54,84,113	1.52	5 (9%)
28	CLA	M	313	-	50,54,73	1.37	7 (14%)	59,90,113	1.37	4 (6%)
31	LMG	b	734	-	31,31,55	0.99	1 (3%)	39,39,63	1.18	4 (10%)
29	KC1	J	313	-	49,53,53	1.34	6 (12%)	61,89,89	1.71	13 (21%)
34	SF4	c	202	7	0,12,12	-	-	-	-	-
32	PID	D	306	-	43,49,49	1.25	3 (6%)	52,76,76	1.37	5 (9%)
28	CLA	b	719	-	50,54,73	1.37	8 (16%)	59,90,113	1.44	4 (6%)
29	KC1	L	307	28	49,53,53	1.33	5 (10%)	61,89,89	1.74	15 (24%)
28	CLA	J	316	-	50,54,73	1.38	7 (14%)	59,90,113	1.38	4 (6%)
28	CLA	A	311	6	50,54,73	1.37	7 (14%)	59,90,113	1.38	4 (6%)
28	CLA	L	317	-	56,60,73	1.32	7 (12%)	65,97,113	1.37	6 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	CLA	B	309	18	69,73,73	1.17	6 (8%)	82,113,113	1.26	6 (7%)
28	CLA	A	317	-	45,49,73	1.42	7 (15%)	54,84,113	1.49	6 (11%)
29	KC1	L	315	-	49,53,53	1.35	6 (12%)	61,89,89	1.75	14 (22%)
28	CLA	b	722	-	69,73,73	1.19	8 (11%)	82,113,113	1.31	7 (8%)

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
28	CLA	N	309	25	1/1/11/20	4/17/93/115	-
26	DD6	L	302	-	-	4/26/80/80	0/3/3/3
28	CLA	M	316	-	1/1/12/20	10/24/100/115	-
26	DD6	F	303	-	-	2/26/80/80	0/3/3/3
28	CLA	L	313	-	1/1/13/20	11/27/103/115	-
28	CLA	a	723	-	1/1/15/20	13/39/115/115	-
28	CLA	b	710	-	1/1/12/20	4/24/100/115	-
28	CLA	F	315	-	1/1/10/20	4/10/86/115	-
28	CLA	G	512	-	1/1/14/20	11/33/109/115	-
28	CLA	K	313	-	1/1/13/20	7/27/103/115	-
32	PID	G	507	-	-	0/24/93/93	1/4/4/4
32	PID	D	304	-	-	3/24/93/93	0/4/4/4
28	CLA	G	516	5	1/1/10/20	6/10/86/115	-
28	CLA	M	309	24	1/1/13/20	5/27/103/115	-
29	KC1	I	314	1	-	9/15/71/71	-
31	LMG	I	320	-	-	14/33/53/70	0/1/1/1
28	CLA	H	304	-	1/1/11/20	6/18/94/115	-
28	CLA	l	312	-	1/1/11/20	6/17/93/115	-
26	DD6	L	304	-	-	0/26/80/80	0/3/3/3
28	CLA	M	308	29	1/1/12/20	10/25/101/115	-
28	CLA	H	308	-	1/1/11/20	4/17/93/115	-
28	CLA	L	316	-	1/1/10/20	4/10/86/115	-
31	LMG	K	318	-	-	19/38/58/70	0/1/1/1
31	LMG	I	318	-	-	21/31/51/70	0/1/1/1
31	LMG	j	101	-	-	14/30/50/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	CLA	B	308	-	1/1/11/20	5/15/91/115	-
28	CLA	L	312	-	1/1/11/20	7/17/93/115	-
29	KC1	G	515	5	-	6/15/71/71	-
28	CLA	I	308	-	1/1/14/20	12/33/109/115	-
28	CLA	a	728	-	1/1/13/20	8/27/103/115	-
28	CLA	B	310	-	1/1/13/20	8/27/103/115	-
28	CLA	a	729	-	1/1/13/20	7/29/105/115	-
26	DD6	h	203	-	-	1/26/80/80	0/3/3/3
28	CLA	b	715	-	1/1/14/20	12/33/109/115	-
26	DD6	L	305	-	-	3/26/80/80	0/3/3/3
28	CLA	F	307	-	1/1/11/20	3/17/93/115	-
29	KC1	N	306	-	-	6/15/71/71	-
26	DD6	M	304	-	-	0/26/80/80	0/3/3/3
28	CLA	I	312	-	1/1/15/20	15/39/115/115	-
26	DD6	B	306	-	-	2/26/80/80	0/3/3/3
28	CLA	a	718	-	1/1/11/20	9/17/93/115	-
28	CLA	a	715	-	1/1/11/20	7/15/91/115	-
28	CLA	a	725	-	1/1/14/20	13/35/111/115	-
28	CLA	A	319	-	1/1/11/20	9/17/93/115	-
28	CLA	N	305	-	1/1/15/20	9/39/115/115	-
26	DD6	M	303	-	-	2/26/80/80	0/3/3/3
27	UIX	I	304	-	-	4/31/87/87	0/3/3/3
31	LMG	K	317	-	-	9/22/42/70	0/1/1/1
32	PID	F	305	-	-	8/24/93/93	0/4/4/4
28	CLA	L	314	-	1/1/12/20	6/25/101/115	-
28	CLA	H	311	-	-	6/10/86/115	-
36	PQN	a	732	-	-	8/23/43/43	0/2/2/2
28	CLA	B	313	18	1/1/15/20	9/39/115/115	-
28	CLA	K	315	-	1/1/10/20	2/10/86/115	-
29	KC1	F	309	20	-	9/15/71/71	-
28	CLA	l	311	-	1/1/15/20	14/39/115/115	-
26	DD6	L	306	-	-	3/26/80/80	0/3/3/3
28	CLA	a	708	-	1/1/12/20	5/23/99/115	-
28	CLA	G	517	-	1/1/11/20	4/17/93/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	CLA	K	307	-	1/1/11/20	2/17/93/115	-
28	CLA	a	713	-	1/1/14/20	11/33/109/115	-
28	CLA	J	311	22	1/1/11/20	7/18/94/115	-
28	CLA	D	314	-	1/1/11/20	8/17/93/115	-
28	CLA	a	735	-	1/1/15/20	18/39/115/115	-
28	CLA	h	202	-	1/1/13/20	9/27/103/115	-
30	DGD	L	301	-	-	1/26/66/95	0/2/2/2
28	CLA	G	511	-	1/1/13/20	4/27/103/115	-
29	KC1	H	310	-	-	6/15/71/71	-
28	CLA	M	312	-	1/1/11/20	5/19/95/115	-
28	CLA	D	308	-	1/1/11/20	4/18/94/115	-
26	DD6	B	304	-	-	0/26/80/80	0/3/3/3
34	SF4	c	201	7	-	-	0/6/5/5
28	CLA	l	313	14	1/1/15/20	20/39/115/115	-
26	DD6	G	505	-	-	4/26/80/80	0/3/3/3
35	BCR	a	734	-	-	2/29/63/63	0/2/2/2
32	PID	D	305	-	-	2/24/93/93	0/4/4/4
28	CLA	M	318	-	1/1/11/20	9/17/93/115	-
28	CLA	B	316	-	1/1/11/20	9/17/93/115	-
28	CLA	b	703	-	1/1/15/20	12/39/115/115	-
30	DGD	I	317	-	-	3/28/68/95	0/2/2/2
30	DGD	y	201	-	-	7/43/83/95	0/2/2/2
28	CLA	a	716	-	1/1/11/20	6/18/94/115	-
28	CLA	a	705	28	1/1/13/20	8/27/103/115	-
28	CLA	G	520	-	1/1/11/20	5/20/96/115	-
28	CLA	M	317	-	1/1/11/20	8/17/93/115	-
28	CLA	b	708	-	1/1/15/20	10/39/115/115	-
26	DD6	M	302	-	-	3/26/80/80	0/3/3/3
28	CLA	K	308	2	1/1/12/20	10/26/102/115	-
28	CLA	A	308	-	1/1/13/20	4/27/103/115	-
30	DGD	j	103	-	-	8/30/70/95	0/2/2/2
28	CLA	D	311	-	1/1/11/20	3/17/93/115	-
28	CLA	a	724	-	1/1/15/20	13/39/115/115	-
28	CLA	a	720	-	1/1/14/20	7/36/112/115	-
33	SQD	A	318	-	-	5/45/65/69	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	CLA	b	718	-	1/1/12/20	3/23/99/115	-
28	CLA	a	707	-	1/1/15/20	17/39/115/115	-
26	DD6	K	301	-	-	5/26/80/80	0/3/3/3
28	CLA	f	302	-	1/1/11/20	6/17/93/115	-
29	KC1	N	311	25	-	7/15/71/71	-
28	CLA	A	312	-	1/1/13/20	6/27/103/115	-
28	CLA	L	310	-	1/1/13/20	0/27/103/115	-
26	DD6	I	301	-	-	3/26/80/80	0/3/3/3
28	CLA	A	310	-	1/1/15/20	15/39/115/115	-
28	CLA	a	706	16	1/1/13/20	15/31/107/115	-
28	CLA	l	303	14	1/1/15/20	14/39/115/115	-
35	BCR	l	307	-	-	0/29/63/63	0/2/2/2
28	CLA	f	301	-	1/1/13/20	11/27/103/115	-
34	SF4	a	737	17,16	-	-	0/6/5/5
28	CLA	I	310	-	1/1/11/20	8/19/95/115	-
28	CLA	a	702	-	1/1/15/20	11/39/115/115	-
29	KC1	A	314	6	-	5/15/71/71	-
28	CLA	l	305	-	1/1/15/20	12/39/115/115	-
28	CLA	A	307	29	1/1/11/20	1/15/91/115	-
27	UIX	J	305	-	-	11/31/87/87	0/3/3/3
29	KC1	A	306	26,28	-	7/15/71/71	-
37	LHG	a	733	-	-	16/52/52/53	-
32	PID	F	306	-	-	0/24/93/93	0/4/4/4
28	CLA	m	202	-	1/1/14/20	10/33/109/115	-
28	CLA	D	309	-	1/1/11/20	7/17/93/115	-
28	CLA	G	519	-	1/1/13/20	13/32/108/115	-
35	BCR	a	736	-	-	2/29/63/63	0/2/2/2
26	DD6	A	303	-	-	1/26/80/80	0/3/3/3
28	CLA	I	319	28	1/1/11/20	7/15/91/115	-
32	PID	N	302	-	-	2/24/93/93	0/4/4/4
28	CLA	K	309	-	1/1/12/20	2/21/97/115	-
29	KC1	M	307	28	-	6/15/71/71	-
28	CLA	b	709	-	1/1/14/20	8/33/109/115	-
28	CLA	K	310	-	1/1/13/20	5/27/103/115	-
28	CLA	A	315	-	1/1/10/20	4/10/86/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	CLA	b	707	-	1/1/15/20	18/39/115/115	-
28	CLA	I	306	1	1/1/11/20	9/20/96/115	-
28	CLA	K	316	-	1/1/11/20	3/17/93/115	-
26	DD6	J	303	-	-	2/26/80/80	0/3/3/3
28	CLA	a	703	-	1/1/13/20	6/27/103/115	-
26	DD6	M	305	-	-	1/26/80/80	0/3/3/3
28	CLA	J	312	-	1/1/12/20	6/25/101/115	-
27	UIX	h	201	-	-	2/31/87/87	0/3/3/3
26	DD6	K	304	-	-	1/26/80/80	0/3/3/3
28	CLA	H	307	-	1/1/12/20	5/23/99/115	-
35	BCR	b	730	-	-	6/29/63/63	0/2/2/2
28	CLA	a	731	-	1/1/15/20	13/39/115/115	-
28	CLA	f	303	10	1/1/11/20	8/17/93/115	-
28	CLA	L	309	-	1/1/12/20	7/25/101/115	-
28	CLA	N	304	-	1/1/11/20	4/18/94/115	-
28	CLA	a	726	-	1/1/15/20	13/39/115/115	-
26	DD6	A	301	-	-	3/26/80/80	0/3/3/3
28	CLA	K	311	-	1/1/12/20	11/24/100/115	-
28	CLA	I	307	-	1/1/11/20	7/17/93/115	-
28	CLA	a	727	-	1/1/11/20	9/17/93/115	-
28	CLA	K	306	2	1/1/11/20	4/20/96/115	-
26	DD6	N	303	-	-	0/26/80/80	0/3/3/3
28	CLA	I	309	-	1/1/13/20	6/27/103/115	-
32	PID	D	307	-	-	4/24/93/93	0/4/4/4
26	DD6	M	306	-	-	4/26/80/80	0/3/3/3
28	CLA	b	706	-	1/1/11/20	4/19/95/115	-
26	DD6	G	502	-	-	6/26/80/80	0/3/3/3
26	DD6	D	303	-	-	6/26/80/80	0/3/3/3
28	CLA	A	313	-	1/1/13/20	10/27/103/115	-
28	CLA	l	308	-	1/1/10/20	3/10/86/115	-
28	CLA	b	712	-	1/1/13/20	9/25/101/115	-
28	CLA	B	307	18	1/1/11/20	3/20/96/115	-
26	DD6	J	304	-	-	2/26/80/80	0/3/3/3
28	CLA	G	518	-	1/1/11/20	7/17/93/115	-
28	CLA	j	106	-	1/1/13/20	10/31/107/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	CLA	J	307	-	1/1/15/20	19/39/115/115	-
28	CLA	l	310	-	-	10/15/65/115	0/5/5/9
32	PID	F	304	-	-	3/24/93/93	0/4/4/4
28	CLA	b	728	-	1/1/15/20	9/39/115/115	-
26	DD6	J	302	-	-	3/26/80/80	0/3/3/3
28	CLA	J	301	-	1/1/14/20	12/33/109/115	-
35	BCR	b	732	-	-	0/29/63/63	0/2/2/2
27	UIX	B	305	-	-	2/31/87/87	0/3/3/3
28	CLA	a	722	-	1/1/13/20	8/31/107/115	-
26	DD6	L	303	-	-	0/26/80/80	0/3/3/3
28	CLA	A	316	-	1/1/11/20	4/18/94/115	-
28	CLA	H	312	-	1/1/11/20	9/17/93/115	-
28	CLA	a	701	-	1/1/11/20	2/15/91/115	-
28	CLA	B	311	-	1/1/15/20	21/39/115/115	-
28	CLA	G	513	5	1/1/15/20	7/39/115/115	-
28	CLA	D	313	19	1/1/11/20	2/15/91/115	-
28	CLA	I	311	1	1/1/13/20	10/27/103/115	-
28	CLA	A	309	-	1/1/13/20	5/27/103/115	-
27	UIX	A	304	-	-	0/31/87/87	0/3/3/3
26	DD6	A	305	29	-	1/26/80/80	0/3/3/3
28	CLA	a	721	-	1/1/15/20	18/39/115/115	-
30	DGD	G	521	-	-	18/33/73/95	0/2/2/2
28	CLA	a	704	-	1/1/15/20	6/39/115/115	-
28	CLA	b	727	-	1/1/15/20	7/39/115/115	-
29	KC1	H	306	-	-	4/15/71/71	-
35	BCR	b	702	-	-	2/29/63/63	0/2/2/2
28	CLA	L	308	29	1/1/11/20	9/15/91/115	-
31	LMG	B	318	-	-	15/32/52/70	0/1/1/1
28	CLA	I	315	-	1/1/12/20	8/24/100/115	-
28	CLA	J	314	-	1/1/10/20	2/10/86/115	-
28	CLA	b	711	-	1/1/13/20	11/27/103/115	-
28	CLA	b	713	-	1/1/15/20	8/39/115/115	-
27	UIX	G	503	-	-	5/31/87/87	0/3/3/3
28	CLA	a	711	-	1/1/11/20	6/15/91/115	-
28	CLA	a	714	-	1/1/11/20	4/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	PID	H	301	-	-	4/24/93/93	0/4/4/4
32	PID	G	506	-	-	3/24/93/93	0/4/4/4
35	BCR	l	306	-	-	7/29/63/63	0/2/2/2
28	CLA	a	719	-	1/1/11/20	7/18/94/115	-
28	CLA	L	318	-	1/1/11/20	8/17/93/115	-
28	CLA	a	712	28	1/1/14/20	8/33/109/115	-
28	CLA	G	510	-	1/1/15/20	10/39/115/115	-
29	KC1	K	314	2	-	9/15/71/71	-
26	DD6	H	303	-	-	1/26/80/80	0/3/3/3
28	CLA	J	315	-	1/1/11/20	3/17/93/115	-
26	DD6	G	508	-	-	1/26/80/80	0/3/3/3
26	DD6	A	302	-	-	3/26/80/80	0/3/3/3
29	KC1	N	308	-	-	8/15/71/71	-
28	CLA	B	317	-	1/1/11/20	7/15/91/115	-
26	DD6	B	302	-	-	3/24/78/80	0/3/3/3
35	BCR	i	201	-	-	8/29/63/63	0/2/2/2
26	DD6	K	303	-	-	0/26/80/80	0/3/3/3
32	PID	M	301	-	-	1/24/93/93	0/4/4/4
29	KC1	D	310	-	-	10/15/71/71	-
28	CLA	I	316	-	1/1/13/20	13/27/103/115	-
28	CLA	M	311	-	1/1/11/20	4/17/93/115	-
28	CLA	F	308	-	1/1/11/20	3/17/93/115	-
31	LMG	D	317	-	-	17/41/61/70	0/1/1/1
28	CLA	I	313	-	1/1/13/20	11/27/103/115	-
29	KC1	F	314	20	-	5/15/71/71	-
26	DD6	B	303	-	-	2/26/80/80	0/3/3/3
26	DD6	I	303	-	-	2/26/80/80	0/3/3/3
31	LMG	b	733	-	-	19/39/59/70	0/1/1/1
28	CLA	G	514	-	1/1/12/20	11/25/101/115	-
32	PID	D	301	-	-	2/24/93/93	0/4/4/4
28	CLA	F	310	-	1/1/11/20	8/17/93/115	-
28	CLA	G	509	5	1/1/12/20	4/23/99/115	-
28	CLA	l	309	-	1/1/10/20	3/10/86/115	-
28	CLA	b	721	26	1/1/11/20	1/17/93/115	-
28	CLA	b	701	-	1/1/15/20	13/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	CLA	N	310	-	1/1/11/20	10/18/94/115	-
28	CLA	l	304	-	1/1/14/20	9/33/109/115	-
28	CLA	F	312	-	1/1/11/20	3/17/93/115	-
28	CLA	K	312	-	1/1/11/20	5/19/95/115	-
28	CLA	b	705	-	1/1/15/20	11/39/115/115	-
35	BCR	j	102	-	-	5/29/63/63	0/2/2/2
26	DD6	K	319	-	-	4/26/80/80	0/3/3/3
28	CLA	b	725	-	1/1/15/20	9/39/115/115	-
28	CLA	L	311	-	1/1/13/20	5/27/103/115	-
28	CLA	b	724	-	1/1/15/20	15/39/115/115	-
28	CLA	b	720	-	1/1/12/20	9/25/101/115	-
28	CLA	I	321	28	1/1/12/20	8/24/100/115	-
28	CLA	B	312	-	1/1/12/20	4/23/99/115	-
32	PID	N	301	-	-	6/24/93/93	0/4/4/4
29	KC1	M	314	24	-	9/15/71/71	-
26	DD6	K	305	-	-	4/26/80/80	0/3/3/3
26	DD6	G	504	-	-	5/26/80/80	0/3/3/3
28	CLA	H	305	-	1/1/15/20	8/39/115/115	-
28	CLA	N	307	-	1/1/12/20	3/23/99/115	-
26	DD6	b	731	28	-	3/26/80/80	0/3/3/3
28	CLA	J	310	-	1/1/11/20	8/17/93/115	-
28	CLA	a	717	-	1/1/13/20	13/30/106/115	-
28	CLA	B	301	-	1/1/14/20	10/33/109/115	-
28	CLA	b	723	-	1/1/12/20	9/21/97/115	-
32	PID	D	302	-	-	3/24/93/93	0/4/4/4
26	DD6	I	305	-	-	5/26/80/80	0/3/3/3
28	CLA	H	309	-	1/1/11/20	8/18/94/115	-
28	CLA	M	315	-	1/1/10/20	5/10/86/115	-
26	DD6	I	302	-	-	5/26/80/80	0/3/3/3
28	CLA	J	308	-	1/1/11/20	9/17/93/115	-
30	DGD	l	301	-	-	8/39/79/95	0/2/2/2
36	PQN	b	729	-	-	4/23/43/43	0/2/2/2
32	PID	j	105	-	-	4/24/93/93	0/4/4/4
28	CLA	a	730	-	1/1/15/20	4/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	PID	H	302	-	-	2/24/93/93	0/4/4/4
28	CLA	a	738	22	1/1/11/20	4/17/93/115	-
30	DGD	G	501	-	-	10/34/74/95	0/2/2/2
35	BCR	m	201	-	-	5/29/63/63	0/2/2/2
35	BCR	l	302	-	-	3/29/63/63	0/2/2/2
28	CLA	D	312	19	1/1/11/20	7/17/93/115	-
26	DD6	F	301	-	-	2/26/80/80	0/3/3/3
28	CLA	F	313	-	1/1/11/20	5/17/93/115	-
29	KC1	D	315	19	-	4/15/71/71	-
28	CLA	a	710	16	1/1/13/20	6/27/103/115	-
28	CLA	J	309	-	1/1/13/20	9/29/105/115	-
28	CLA	A	320	-	1/1/11/20	6/17/93/115	-
28	CLA	J	306	-	1/1/11/20	6/17/93/115	-
28	CLA	F	311	-	1/1/11/20	7/17/93/115	-
29	KC1	B	314	18	-	7/15/71/71	-
28	CLA	j	104	-	1/1/13/20	6/27/103/115	-
28	CLA	b	704	-	1/1/15/20	19/39/115/115	-
28	CLA	b	716	-	1/1/12/20	4/21/97/115	-
28	CLA	b	717	-	1/1/15/20	18/39/115/115	-
28	CLA	D	316	-	1/1/10/20	0/10/86/115	-
28	CLA	M	310	-	1/1/11/20	8/19/95/115	-
32	PID	F	302	-	-	2/24/93/93	0/4/4/4
28	CLA	b	714	-	1/1/11/20	3/17/93/115	-
35	BCR	f	304	-	-	2/29/63/63	0/2/2/2
27	UIX	K	302	-	-	5/31/87/87	0/3/3/3
28	CLA	b	726	-	1/1/11/20	2/18/94/115	-
28	CLA	a	709	-	1/1/15/20	16/39/115/115	-
28	CLA	B	315	-	1/1/10/20	4/10/86/115	-
28	CLA	M	313	-	1/1/11/20	2/17/93/115	-
31	LMG	b	734	-	-	12/26/46/70	0/1/1/1
29	KC1	J	313	-	-	7/15/71/71	-
34	SF4	c	202	7	-	-	0/6/5/5
32	PID	D	306	-	-	8/24/93/93	0/4/4/4
28	CLA	b	719	-	1/1/11/20	9/17/93/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	KC1	L	307	28	-	6/15/71/71	-
28	CLA	J	316	-	-	3/17/93/115	-
28	CLA	A	311	6	1/1/11/20	5/17/93/115	-
28	CLA	L	317	-	1/1/12/20	11/24/100/115	-
28	CLA	B	309	18	1/1/15/20	19/39/115/115	-
28	CLA	A	317	-	1/1/10/20	0/10/86/115	-
29	KC1	L	315	-	-	8/15/71/71	-
28	CLA	b	722	-	1/1/15/20	7/39/115/115	-

All (1669) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	I	310	CLA	C1B-C2B	9.21	1.49	1.39
26	I	305	DD6	C30-C31	-9.00	1.25	1.42
26	J	303	DD6	C30-C31	-8.99	1.25	1.42
26	M	306	DD6	C30-C31	-8.99	1.25	1.42
26	G	505	DD6	C30-C31	-8.96	1.25	1.42
26	M	303	DD6	C30-C31	-8.92	1.25	1.42
26	b	731	DD6	C30-C31	-8.80	1.25	1.42
26	G	504	DD6	C30-C31	-8.77	1.25	1.42
26	I	303	DD6	C30-C31	-8.75	1.25	1.42
26	B	302	DD6	C30-C31	-8.73	1.25	1.42
26	J	304	DD6	C30-C31	-8.72	1.25	1.42
26	M	302	DD6	C30-C31	-8.68	1.25	1.42
26	h	203	DD6	C30-C31	-8.55	1.25	1.42
26	N	303	DD6	C30-C31	-8.52	1.25	1.42
26	I	301	DD6	C30-C31	-8.52	1.25	1.42
26	M	304	DD6	C30-C31	-8.50	1.26	1.42
26	B	306	DD6	C30-C31	-8.50	1.26	1.42
26	G	508	DD6	C30-C31	-8.47	1.26	1.42
26	A	302	DD6	C30-C31	-8.45	1.26	1.42
26	G	502	DD6	C30-C31	-8.43	1.26	1.42
26	K	304	DD6	C30-C31	-8.43	1.26	1.42
26	K	303	DD6	C30-C31	-8.42	1.26	1.42
26	A	301	DD6	C30-C31	-8.42	1.26	1.42
26	I	302	DD6	C30-C31	-8.41	1.26	1.42
26	B	303	DD6	C30-C31	-8.41	1.26	1.42
26	M	305	DD6	C30-C31	-8.41	1.26	1.42
26	F	303	DD6	C30-C31	-8.39	1.26	1.42
26	L	305	DD6	C30-C31	-8.38	1.26	1.42
26	F	301	DD6	C30-C31	-8.38	1.26	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	K	319	DD6	C30-C31	-8.38	1.26	1.42
26	L	306	DD6	C30-C31	-8.35	1.26	1.42
26	A	305	DD6	C30-C31	-8.34	1.26	1.42
26	B	304	DD6	C30-C31	-8.31	1.26	1.42
26	K	305	DD6	C30-C31	-8.30	1.26	1.42
26	D	303	DD6	C30-C31	-8.26	1.26	1.42
26	L	303	DD6	C30-C31	-8.24	1.26	1.42
26	L	304	DD6	C30-C31	-8.22	1.26	1.42
28	l	310	CLA	C1D-C2D	8.21	1.48	1.39
26	H	303	DD6	C30-C31	-8.21	1.26	1.42
26	J	302	DD6	C30-C31	-8.21	1.26	1.42
26	K	301	DD6	C30-C31	-8.19	1.26	1.42
26	A	303	DD6	C30-C31	-8.18	1.26	1.42
26	L	302	DD6	C30-C31	-8.12	1.26	1.42
28	l	310	CLA	C3B-C4B	8.10	1.49	1.41
36	a	732	PQN	C3-C2	7.65	1.48	1.35
36	b	729	PQN	C3-C2	7.48	1.48	1.35
32	N	302	PID	C13-C14	-6.22	1.34	1.45
32	H	302	PID	C13-C14	-6.00	1.34	1.45
32	G	506	PID	C13-C14	-5.96	1.34	1.45
32	D	302	PID	C13-C14	-5.79	1.34	1.45
32	D	305	PID	C13-C14	-5.79	1.34	1.45
32	D	301	PID	C13-C14	-5.72	1.34	1.45
32	j	105	PID	C13-C14	-5.71	1.35	1.45
32	G	507	PID	C13-C14	-5.71	1.35	1.45
32	D	306	PID	C13-C14	-5.70	1.35	1.45
32	N	301	PID	C13-C14	-5.66	1.35	1.45
32	F	306	PID	C13-C14	-5.57	1.35	1.45
32	H	301	PID	C13-C14	-5.54	1.35	1.45
32	F	304	PID	C13-C14	-5.46	1.35	1.45
32	F	302	PID	C13-C14	-5.46	1.35	1.45
32	F	305	PID	C13-C14	-5.44	1.35	1.45
32	D	307	PID	C13-C14	-5.40	1.35	1.45
32	D	304	PID	C13-C14	-5.32	1.35	1.45
32	M	301	PID	C13-C14	-5.27	1.35	1.45
29	N	308	KC1	MG-ND	-5.11	1.95	2.05
29	L	315	KC1	MG-ND	-5.07	1.95	2.05
29	F	309	KC1	MG-ND	-5.06	1.95	2.05
28	l	310	CLA	C3D-C4D	5.04	1.48	1.41
29	H	310	KC1	MG-ND	-5.03	1.95	2.05
29	M	307	KC1	MG-ND	-5.01	1.95	2.05
29	F	314	KC1	MG-ND	-5.00	1.95	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	B	305	UIX	O2-C27	4.99	1.46	1.35
29	G	515	KC1	MG-ND	-4.98	1.95	2.05
29	N	311	KC1	MG-ND	-4.97	1.95	2.05
29	J	313	KC1	MG-ND	-4.96	1.95	2.05
29	M	314	KC1	MG-ND	-4.95	1.96	2.05
29	A	306	KC1	MG-ND	-4.95	1.96	2.05
29	N	306	KC1	MG-ND	-4.92	1.96	2.05
36	b	729	PQN	C10-C5	4.92	1.48	1.40
27	J	305	UIX	O2-C27	4.92	1.46	1.35
27	h	201	UIX	O2-C27	4.91	1.46	1.35
29	B	314	KC1	MG-ND	-4.89	1.96	2.05
27	G	503	UIX	O2-C27	4.87	1.46	1.35
29	D	315	KC1	MG-ND	-4.87	1.96	2.05
29	I	314	KC1	MG-ND	-4.86	1.96	2.05
29	L	307	KC1	MG-ND	-4.86	1.96	2.05
36	a	732	PQN	C10-C5	4.86	1.48	1.40
29	H	306	KC1	MG-ND	-4.86	1.96	2.05
29	D	310	KC1	MG-ND	-4.83	1.96	2.05
27	K	302	UIX	O2-C27	4.83	1.45	1.35
29	A	314	KC1	MG-ND	-4.82	1.96	2.05
29	K	314	KC1	MG-ND	-4.81	1.96	2.05
27	A	304	UIX	O2-C27	4.79	1.45	1.35
29	M	307	KC1	MG-NB	-4.75	1.96	2.05
29	H	310	KC1	MG-NB	-4.69	1.96	2.05
29	F	314	KC1	MG-NB	-4.68	1.96	2.05
29	N	311	KC1	MG-NB	-4.65	1.96	2.05
29	F	309	KC1	MG-NB	-4.64	1.96	2.05
29	D	310	KC1	MG-NB	-4.63	1.96	2.05
29	M	314	KC1	MG-NB	-4.63	1.96	2.05
29	N	306	KC1	MG-NB	-4.61	1.96	2.05
29	H	306	KC1	MG-NB	-4.61	1.96	2.05
29	N	308	KC1	MG-NB	-4.60	1.96	2.05
29	I	314	KC1	MG-NB	-4.59	1.96	2.05
29	A	314	KC1	MG-NB	-4.58	1.96	2.05
29	J	313	KC1	MG-NB	-4.57	1.96	2.05
29	L	315	KC1	MG-NB	-4.57	1.96	2.05
29	K	314	KC1	MG-NB	-4.56	1.96	2.05
29	L	307	KC1	MG-NB	-4.54	1.96	2.05
29	B	314	KC1	MG-NB	-4.53	1.96	2.05
29	A	306	KC1	MG-NB	-4.53	1.96	2.05
29	G	515	KC1	MG-NB	-4.50	1.96	2.05
29	D	315	KC1	MG-NB	-4.46	1.97	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	I	304	UIX	O2-C27	4.33	1.44	1.35
30	I	317	DGD	O1G-C1A	4.26	1.45	1.33
30	G	501	DGD	O1G-C1A	4.24	1.45	1.33
27	h	201	UIX	C25-C20	-4.24	1.25	1.30
30	j	103	DGD	O1G-C1A	4.24	1.45	1.33
30	l	301	DGD	O1G-C1A	4.24	1.45	1.33
30	y	201	DGD	O1G-C1A	4.21	1.45	1.33
26	J	303	DD6	C19-C20	4.19	1.58	1.52
27	K	302	UIX	C25-C20	-4.19	1.25	1.30
30	G	521	DGD	O2G-C1B	4.17	1.46	1.34
30	G	501	DGD	O2G-C1B	4.15	1.46	1.34
30	l	301	DGD	O2G-C1B	4.12	1.45	1.34
30	j	103	DGD	O2G-C1B	4.12	1.45	1.34
27	A	304	UIX	C25-C20	-4.07	1.25	1.30
30	y	201	DGD	O2G-C1B	4.04	1.45	1.34
30	L	301	DGD	O2G-C1B	4.03	1.45	1.34
30	I	317	DGD	O2G-C1B	4.01	1.45	1.34
30	G	521	DGD	O1G-C1A	4.00	1.45	1.33
27	I	304	UIX	C25-C20	-3.94	1.26	1.30
27	B	305	UIX	C25-C20	-3.94	1.26	1.30
27	h	201	UIX	C25-C28	-3.87	1.25	1.31
27	I	304	UIX	C25-C28	-3.83	1.25	1.31
26	G	505	DD6	C19-C20	3.83	1.57	1.52
27	K	302	UIX	C25-C28	-3.78	1.25	1.31
28	b	718	CLA	C1D-ND	3.75	1.42	1.37
28	M	318	CLA	C1D-ND	3.73	1.42	1.37
28	J	316	CLA	C1D-ND	3.73	1.42	1.37
27	A	304	UIX	C25-C28	-3.72	1.25	1.31
28	H	304	CLA	C1D-ND	3.71	1.42	1.37
28	H	311	CLA	C1D-ND	3.71	1.42	1.37
28	L	317	CLA	C1D-ND	3.71	1.42	1.37
28	K	306	CLA	C1D-ND	3.69	1.42	1.37
28	A	307	CLA	C1D-ND	3.69	1.42	1.37
28	N	307	CLA	C1D-ND	3.69	1.42	1.37
28	N	310	CLA	C1D-ND	3.69	1.42	1.37
28	G	518	CLA	C1D-ND	3.67	1.42	1.37
28	a	738	CLA	C1D-ND	3.66	1.42	1.37
28	F	313	CLA	C1D-ND	3.66	1.42	1.37
28	H	312	CLA	C1D-ND	3.66	1.42	1.37
28	H	308	CLA	C1D-ND	3.66	1.42	1.37
28	L	313	CLA	C1D-ND	3.66	1.42	1.37
28	G	509	CLA	C1D-ND	3.65	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	J	311	CLA	C1D-ND	3.65	1.42	1.37
28	M	308	CLA	C1D-ND	3.65	1.42	1.37
28	G	512	CLA	C1D-ND	3.64	1.42	1.37
28	B	307	CLA	C1D-ND	3.64	1.42	1.37
28	j	104	CLA	C1D-ND	3.64	1.42	1.37
28	F	315	CLA	C1D-ND	3.64	1.42	1.37
28	b	705	CLA	C1D-ND	3.63	1.42	1.37
28	K	312	CLA	C1D-ND	3.63	1.42	1.37
28	J	308	CLA	C1D-ND	3.63	1.42	1.37
28	J	314	CLA	C1D-ND	3.63	1.42	1.37
28	b	726	CLA	C1D-ND	3.62	1.42	1.37
28	l	309	CLA	C1D-ND	3.62	1.42	1.37
28	b	708	CLA	C1D-ND	3.62	1.42	1.37
27	B	305	UIX	C25-C28	-3.62	1.26	1.31
28	h	202	CLA	C1D-ND	3.62	1.42	1.37
28	b	717	CLA	C1D-ND	3.62	1.42	1.37
28	G	516	CLA	C1D-ND	3.62	1.42	1.37
28	K	307	CLA	C1D-ND	3.61	1.42	1.37
28	a	726	CLA	C1D-ND	3.61	1.42	1.37
28	K	316	CLA	C1D-ND	3.61	1.42	1.37
27	G	503	UIX	C25-C20	-3.61	1.26	1.30
28	A	315	CLA	C1D-ND	3.61	1.42	1.37
28	a	714	CLA	C1D-ND	3.61	1.42	1.37
26	G	504	DD6	C19-C20	3.61	1.57	1.52
28	B	316	CLA	C1D-ND	3.61	1.42	1.37
28	L	318	CLA	C1D-ND	3.61	1.42	1.37
28	a	717	CLA	C1D-ND	3.60	1.42	1.37
28	D	314	CLA	C1D-ND	3.60	1.42	1.37
28	a	728	CLA	C1D-ND	3.60	1.42	1.37
28	N	305	CLA	C1D-ND	3.60	1.42	1.37
28	l	303	CLA	C1D-ND	3.60	1.42	1.37
28	I	311	CLA	C1D-ND	3.60	1.42	1.37
28	l	305	CLA	C1D-ND	3.60	1.42	1.37
28	A	312	CLA	C1D-ND	3.60	1.42	1.37
28	b	707	CLA	C1D-ND	3.60	1.42	1.37
28	b	711	CLA	C1D-ND	3.59	1.42	1.37
28	a	707	CLA	C1D-ND	3.59	1.42	1.37
28	A	311	CLA	C1D-ND	3.59	1.42	1.37
28	M	315	CLA	C1D-ND	3.59	1.42	1.37
28	K	311	CLA	C1D-ND	3.59	1.42	1.37
28	b	719	CLA	C1D-ND	3.59	1.42	1.37
28	D	316	CLA	C1D-ND	3.59	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	M	309	CLA	C1D-ND	3.59	1.42	1.37
28	B	301	CLA	C1D-ND	3.59	1.42	1.37
28	G	511	CLA	C1D-ND	3.59	1.42	1.37
28	A	316	CLA	C1D-ND	3.58	1.42	1.37
28	b	714	CLA	C1D-ND	3.58	1.42	1.37
28	J	310	CLA	C1D-ND	3.58	1.42	1.37
26	K	303	DD6	C28-C27	-3.58	1.48	1.50
28	N	304	CLA	C1D-ND	3.58	1.42	1.37
28	b	715	CLA	C1D-ND	3.57	1.42	1.37
28	H	305	CLA	C1D-ND	3.57	1.42	1.37
28	a	708	CLA	C1D-ND	3.57	1.42	1.37
28	K	310	CLA	C1D-ND	3.57	1.42	1.37
28	m	202	CLA	C1D-ND	3.57	1.42	1.37
28	a	705	CLA	C1D-ND	3.57	1.42	1.37
28	D	313	CLA	C1D-ND	3.57	1.42	1.37
28	I	315	CLA	C1D-ND	3.57	1.42	1.37
28	F	311	CLA	C1D-ND	3.57	1.42	1.37
28	D	311	CLA	C1D-ND	3.56	1.42	1.37
28	a	722	CLA	C1D-ND	3.56	1.42	1.37
28	F	310	CLA	C1D-ND	3.56	1.42	1.37
28	I	306	CLA	C1D-ND	3.56	1.42	1.37
28	G	517	CLA	C1D-ND	3.56	1.42	1.37
28	a	723	CLA	C1D-ND	3.56	1.42	1.37
28	A	309	CLA	C1D-ND	3.56	1.42	1.37
28	I	308	CLA	C1D-ND	3.56	1.42	1.37
28	l	311	CLA	C1D-ND	3.56	1.42	1.37
28	B	312	CLA	C1D-ND	3.56	1.42	1.37
28	J	301	CLA	C1D-ND	3.56	1.42	1.37
28	I	307	CLA	C1D-ND	3.55	1.42	1.37
28	F	307	CLA	C1D-ND	3.55	1.42	1.37
28	G	513	CLA	C1D-ND	3.55	1.42	1.37
28	a	721	CLA	C1D-ND	3.55	1.42	1.37
28	f	302	CLA	C1D-ND	3.55	1.42	1.37
28	f	301	CLA	C1D-ND	3.55	1.42	1.37
28	D	309	CLA	C1D-ND	3.55	1.42	1.37
28	M	312	CLA	C1D-ND	3.54	1.42	1.37
28	a	718	CLA	C1D-ND	3.54	1.42	1.37
28	L	316	CLA	C1D-ND	3.54	1.42	1.37
28	l	308	CLA	C1D-ND	3.54	1.42	1.37
28	B	308	CLA	C1D-ND	3.54	1.42	1.37
28	A	313	CLA	C1D-ND	3.54	1.42	1.37
28	K	315	CLA	C1D-ND	3.54	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	a	715	CLA	C1D-ND	3.54	1.42	1.37
28	L	308	CLA	C1D-ND	3.54	1.42	1.37
28	M	317	CLA	C1D-ND	3.54	1.42	1.37
28	a	720	CLA	C1D-ND	3.53	1.42	1.37
28	b	724	CLA	C1D-ND	3.53	1.42	1.37
28	B	317	CLA	C1D-ND	3.53	1.42	1.37
28	a	731	CLA	C1D-ND	3.53	1.42	1.37
28	a	704	CLA	C1D-ND	3.53	1.42	1.37
28	J	315	CLA	C1D-ND	3.53	1.42	1.37
28	j	106	CLA	C1D-ND	3.53	1.42	1.37
28	a	709	CLA	C1D-ND	3.53	1.42	1.37
28	a	706	CLA	C1D-ND	3.53	1.42	1.37
28	b	716	CLA	C1D-ND	3.53	1.42	1.37
28	D	312	CLA	C1D-ND	3.53	1.42	1.37
28	M	310	CLA	C1D-ND	3.52	1.42	1.37
28	L	312	CLA	C1D-ND	3.52	1.42	1.37
28	a	729	CLA	C1D-ND	3.52	1.42	1.37
28	H	307	CLA	C1D-ND	3.52	1.42	1.37
28	M	311	CLA	C1D-ND	3.52	1.42	1.37
28	f	303	CLA	C1D-ND	3.51	1.42	1.37
28	I	312	CLA	C1D-ND	3.51	1.42	1.37
28	A	319	CLA	C1D-ND	3.51	1.42	1.37
28	l	313	CLA	C1D-ND	3.51	1.42	1.37
28	I	310	CLA	C1D-ND	3.51	1.42	1.37
28	L	314	CLA	C1D-ND	3.51	1.42	1.37
28	G	510	CLA	C1D-ND	3.51	1.42	1.37
28	B	310	CLA	C1D-ND	3.51	1.42	1.37
28	B	313	CLA	C1D-ND	3.51	1.42	1.37
28	D	308	CLA	C1D-ND	3.51	1.42	1.37
28	L	311	CLA	C1D-ND	3.51	1.42	1.37
28	M	313	CLA	C1D-ND	3.51	1.42	1.37
28	a	716	CLA	C1D-ND	3.51	1.42	1.37
28	A	317	CLA	C1D-ND	3.51	1.42	1.37
28	a	725	CLA	C1D-ND	3.51	1.42	1.37
28	J	306	CLA	C1D-ND	3.51	1.42	1.37
28	b	706	CLA	C1D-ND	3.50	1.42	1.37
28	B	309	CLA	C1D-ND	3.50	1.42	1.37
28	L	310	CLA	C1D-ND	3.50	1.42	1.37
28	b	701	CLA	C1D-ND	3.50	1.42	1.37
28	L	309	CLA	C1D-ND	3.50	1.42	1.37
28	a	711	CLA	C1D-ND	3.49	1.42	1.37
28	N	309	CLA	C1D-ND	3.49	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	J	309	CLA	C1D-ND	3.49	1.42	1.37
28	b	720	CLA	C1D-ND	3.49	1.42	1.37
28	b	722	CLA	C1D-ND	3.48	1.42	1.37
28	K	308	CLA	C1D-ND	3.48	1.42	1.37
28	H	309	CLA	C1D-ND	3.48	1.42	1.37
28	I	316	CLA	C1D-ND	3.48	1.42	1.37
28	b	727	CLA	C1D-ND	3.48	1.42	1.37
28	b	725	CLA	C1D-ND	3.48	1.42	1.37
28	b	710	CLA	C1D-ND	3.47	1.42	1.37
28	F	308	CLA	C1D-ND	3.47	1.42	1.37
27	J	305	UIX	C25-C20	-3.47	1.26	1.30
28	a	701	CLA	C1D-ND	3.47	1.42	1.37
28	b	728	CLA	C1D-ND	3.46	1.42	1.37
28	A	310	CLA	C1D-ND	3.45	1.42	1.37
28	I	309	CLA	C1D-ND	3.45	1.42	1.37
28	J	312	CLA	C1D-ND	3.44	1.42	1.37
28	G	519	CLA	C1D-ND	3.44	1.42	1.37
28	A	308	CLA	C1D-ND	3.44	1.42	1.37
28	M	316	CLA	C1D-ND	3.43	1.42	1.37
28	a	727	CLA	C1D-ND	3.43	1.42	1.37
28	a	730	CLA	C1D-ND	3.43	1.42	1.37
28	a	735	CLA	C1D-ND	3.43	1.42	1.37
28	I	319	CLA	C1D-ND	3.43	1.42	1.37
28	b	713	CLA	C1D-ND	3.43	1.42	1.37
28	J	307	CLA	C1D-ND	3.43	1.42	1.37
28	G	520	CLA	C1D-ND	3.43	1.42	1.37
28	b	723	CLA	C1D-ND	3.43	1.42	1.37
28	I	313	CLA	C1D-ND	3.42	1.42	1.37
28	b	712	CLA	C1D-ND	3.42	1.42	1.37
28	K	309	CLA	C1D-ND	3.42	1.42	1.37
28	l	312	CLA	C1D-ND	3.41	1.42	1.37
28	G	514	CLA	C1D-ND	3.41	1.42	1.37
28	l	304	CLA	C1D-ND	3.41	1.42	1.37
28	a	719	CLA	C1D-ND	3.41	1.42	1.37
28	b	703	CLA	C1D-ND	3.41	1.42	1.37
28	a	710	CLA	C1D-ND	3.40	1.42	1.37
28	b	709	CLA	C1D-ND	3.40	1.42	1.37
28	K	313	CLA	C1D-ND	3.40	1.42	1.37
28	B	315	CLA	C1D-ND	3.39	1.42	1.37
27	G	503	UIX	C25-C28	-3.39	1.26	1.31
28	A	320	CLA	C1D-ND	3.39	1.42	1.37
28	I	321	CLA	C1D-ND	3.38	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	J	305	UIX	C25-C28	-3.38	1.26	1.31
28	a	712	CLA	C1D-ND	3.37	1.42	1.37
26	J	303	DD6	O1-C20	-3.36	1.41	1.46
28	I	311	CLA	C4B-NB	3.34	1.42	1.37
28	A	320	CLA	C4B-NB	3.34	1.42	1.37
28	a	713	CLA	C1D-ND	3.34	1.42	1.37
28	B	311	CLA	C1D-ND	3.32	1.42	1.37
28	a	724	CLA	C1D-ND	3.32	1.42	1.37
28	b	721	CLA	C1D-ND	3.31	1.42	1.37
28	B	307	CLA	C4B-NB	3.30	1.42	1.37
28	b	718	CLA	C4B-NB	3.29	1.42	1.37
26	J	304	DD6	O1-C20	-3.29	1.42	1.46
28	b	709	CLA	C4B-NB	3.28	1.42	1.37
28	N	307	CLA	C4B-NB	3.25	1.42	1.37
28	G	518	CLA	C4B-NB	3.25	1.42	1.37
28	J	310	CLA	C4B-NB	3.24	1.42	1.37
28	b	719	CLA	C4B-NB	3.22	1.42	1.37
28	l	303	CLA	C4B-NB	3.22	1.42	1.37
28	A	307	CLA	C4B-NB	3.21	1.42	1.37
28	a	707	CLA	C4B-NB	3.21	1.42	1.37
28	j	104	CLA	C4B-NB	3.21	1.42	1.37
28	a	727	CLA	C4B-NB	3.20	1.42	1.37
28	a	735	CLA	C4B-NB	3.20	1.42	1.37
28	M	313	CLA	C4B-NB	3.19	1.42	1.37
28	a	731	CLA	C4B-NB	3.19	1.42	1.37
28	D	308	CLA	C4B-NB	3.19	1.42	1.37
28	a	724	CLA	C4B-NB	3.18	1.42	1.37
28	M	316	CLA	C4B-NB	3.17	1.42	1.37
28	b	728	CLA	C4B-NB	3.17	1.42	1.37
28	b	706	CLA	C4B-NB	3.17	1.42	1.37
28	b	723	CLA	C4B-NB	3.16	1.42	1.37
28	H	308	CLA	C4B-NB	3.16	1.42	1.37
28	G	516	CLA	C4B-NB	3.16	1.42	1.37
28	b	721	CLA	C4B-NB	3.16	1.42	1.37
28	N	304	CLA	C4B-NB	3.16	1.42	1.37
28	L	317	CLA	C4B-NB	3.15	1.42	1.37
28	K	316	CLA	C4B-NB	3.15	1.42	1.37
28	H	311	CLA	C4B-NB	3.15	1.42	1.37
28	M	311	CLA	C4B-NB	3.14	1.42	1.37
28	I	321	CLA	C4B-NB	3.14	1.42	1.37
28	J	306	CLA	C4B-NB	3.14	1.42	1.37
28	L	309	CLA	C4B-NB	3.14	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	b	712	CLA	C4B-NB	3.14	1.42	1.37
28	l	309	CLA	C4B-NB	3.14	1.42	1.37
26	M	302	DD6	C19-C20	3.14	1.56	1.52
28	I	307	CLA	C4B-NB	3.14	1.42	1.37
28	A	316	CLA	C4B-NB	3.13	1.42	1.37
28	a	738	CLA	C4B-NB	3.13	1.42	1.37
28	B	317	CLA	C4B-NB	3.13	1.42	1.37
28	I	309	CLA	C4B-NB	3.13	1.42	1.37
28	l	308	CLA	C4B-NB	3.13	1.42	1.37
28	b	712	CLA	CAB-C3B	-3.13	1.44	1.50
28	b	701	CLA	C4B-NB	3.13	1.42	1.37
28	a	710	CLA	C4B-NB	3.13	1.42	1.37
28	a	714	CLA	C4B-NB	3.13	1.42	1.37
28	F	311	CLA	C4B-NB	3.12	1.42	1.37
28	K	306	CLA	C4B-NB	3.12	1.42	1.37
28	M	318	CLA	C4B-NB	3.12	1.42	1.37
28	H	304	CLA	C4B-NB	3.12	1.42	1.37
28	H	312	CLA	C4B-NB	3.12	1.42	1.37
28	I	308	CLA	C4B-NB	3.12	1.42	1.37
28	a	716	CLA	C4B-NB	3.12	1.42	1.37
28	B	308	CLA	C4B-NB	3.12	1.42	1.37
28	l	310	CLA	C4D-ND	-3.11	1.33	1.38
28	J	316	CLA	C4B-NB	3.11	1.42	1.37
28	G	511	CLA	C4B-NB	3.11	1.41	1.37
28	B	301	CLA	C4B-NB	3.11	1.41	1.37
28	I	313	CLA	C4B-NB	3.11	1.41	1.37
28	L	311	CLA	C4B-NB	3.11	1.41	1.37
28	A	317	CLA	C4B-NB	3.11	1.41	1.37
28	A	319	CLA	C4B-NB	3.11	1.41	1.37
28	a	718	CLA	C4B-NB	3.11	1.41	1.37
28	G	519	CLA	C4B-NB	3.11	1.41	1.37
28	b	722	CLA	C4B-NB	3.11	1.41	1.37
26	I	303	DD6	O1-C20	-3.10	1.42	1.46
28	b	711	CLA	C4B-NB	3.10	1.41	1.37
28	a	719	CLA	C4B-NB	3.10	1.41	1.37
28	L	316	CLA	C4B-NB	3.10	1.41	1.37
32	N	302	PID	C8-C9	-3.10	1.39	1.46
28	L	308	CLA	C4B-NB	3.10	1.41	1.37
28	l	311	CLA	C4B-NB	3.10	1.41	1.37
28	l	304	CLA	C4B-NB	3.10	1.41	1.37
28	b	726	CLA	C4B-NB	3.10	1.41	1.37
28	b	707	CLA	C4B-NB	3.10	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	b	727	CLA	C4B-NB	3.10	1.41	1.37
28	a	704	CLA	C4B-NB	3.10	1.41	1.37
28	F	310	CLA	C4B-NB	3.10	1.41	1.37
28	b	710	CLA	C4B-NB	3.10	1.41	1.37
28	J	314	CLA	C4B-NB	3.10	1.41	1.37
28	B	315	CLA	C4B-NB	3.09	1.41	1.37
28	F	307	CLA	C4B-NB	3.09	1.41	1.37
28	M	310	CLA	C4B-NB	3.09	1.41	1.37
28	m	202	CLA	C4B-NB	3.09	1.41	1.37
28	a	722	CLA	C4B-NB	3.09	1.41	1.37
28	b	716	CLA	C4B-NB	3.09	1.41	1.37
28	D	311	CLA	C4B-NB	3.09	1.41	1.37
28	D	312	CLA	C4B-NB	3.09	1.41	1.37
28	A	311	CLA	C4B-NB	3.09	1.41	1.37
28	D	316	CLA	C4B-NB	3.09	1.41	1.37
28	K	315	CLA	C4B-NB	3.09	1.41	1.37
28	a	709	CLA	C4B-NB	3.08	1.41	1.37
28	I	306	CLA	C4B-NB	3.08	1.41	1.37
28	M	308	CLA	C4B-NB	3.08	1.41	1.37
28	I	315	CLA	C4B-NB	3.08	1.41	1.37
28	l	305	CLA	C4B-NB	3.08	1.41	1.37
28	l	313	CLA	C4B-NB	3.08	1.41	1.37
28	J	315	CLA	C4B-NB	3.08	1.41	1.37
28	J	312	CLA	C4B-NB	3.08	1.41	1.37
28	L	310	CLA	C4B-NB	3.08	1.41	1.37
28	K	311	CLA	C4B-NB	3.08	1.41	1.37
28	A	308	CLA	C4B-NB	3.08	1.41	1.37
28	b	714	CLA	C4B-NB	3.07	1.41	1.37
28	L	312	CLA	C4B-NB	3.07	1.41	1.37
28	H	305	CLA	C4B-NB	3.07	1.41	1.37
28	l	312	CLA	C4B-NB	3.07	1.41	1.37
28	J	308	CLA	C4B-NB	3.07	1.41	1.37
28	a	708	CLA	C4B-NB	3.06	1.41	1.37
28	a	717	CLA	C4B-NB	3.06	1.41	1.37
28	a	713	CLA	C4B-NB	3.06	1.41	1.37
28	M	315	CLA	C4B-NB	3.06	1.41	1.37
28	B	316	CLA	C4B-NB	3.06	1.41	1.37
28	j	106	CLA	C4B-NB	3.06	1.41	1.37
28	N	310	CLA	C4B-NB	3.06	1.41	1.37
28	D	314	CLA	C4B-NB	3.06	1.41	1.37
32	G	506	PID	C8-C9	-3.06	1.39	1.46
28	a	712	CLA	C4B-NB	3.05	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	I	316	CLA	C4B-NB	3.05	1.41	1.37
28	f	301	CLA	C4B-NB	3.05	1.41	1.37
28	H	307	CLA	C4B-NB	3.05	1.41	1.37
28	b	703	CLA	C4B-NB	3.05	1.41	1.37
28	B	311	CLA	C4B-NB	3.05	1.41	1.37
28	b	715	CLA	C4B-NB	3.04	1.41	1.37
28	I	319	CLA	C4B-NB	3.04	1.41	1.37
28	F	315	CLA	C4B-NB	3.04	1.41	1.37
28	K	310	CLA	C4B-NB	3.04	1.41	1.37
28	K	308	CLA	C4B-NB	3.04	1.41	1.37
28	A	315	CLA	C4B-NB	3.04	1.41	1.37
28	A	312	CLA	C4B-NB	3.03	1.41	1.37
28	b	713	CLA	C4B-NB	3.03	1.41	1.37
28	H	309	CLA	C4B-NB	3.03	1.41	1.37
28	B	310	CLA	C4B-NB	3.03	1.41	1.37
28	a	706	CLA	C4B-NB	3.03	1.41	1.37
28	J	307	CLA	C4B-NB	3.03	1.41	1.37
28	a	701	CLA	C4B-NB	3.03	1.41	1.37
28	h	202	CLA	C4B-NB	3.03	1.41	1.37
28	f	302	CLA	C4B-NB	3.02	1.41	1.37
28	b	717	CLA	C4B-NB	3.02	1.41	1.37
28	a	705	CLA	C4B-NB	3.02	1.41	1.37
28	G	517	CLA	C4B-NB	3.02	1.41	1.37
28	K	313	CLA	C4B-NB	3.02	1.41	1.37
28	b	724	CLA	C4B-NB	3.02	1.41	1.37
28	B	309	CLA	C4B-NB	3.02	1.41	1.37
28	D	309	CLA	C4B-NB	3.02	1.41	1.37
26	G	505	DD6	O1-C20	-3.01	1.42	1.46
28	G	512	CLA	C4B-NB	3.01	1.41	1.37
28	G	520	CLA	C4B-NB	3.01	1.41	1.37
28	I	310	CLA	C4B-NB	3.01	1.41	1.37
28	M	317	CLA	C4B-NB	3.00	1.41	1.37
28	a	725	CLA	C4B-NB	3.00	1.41	1.37
28	A	309	CLA	C4B-NB	2.99	1.41	1.37
28	M	309	CLA	C4B-NB	2.99	1.41	1.37
28	G	509	CLA	C4B-NB	2.99	1.41	1.37
28	J	311	CLA	C4B-NB	2.99	1.41	1.37
28	a	711	CLA	C4B-NB	2.99	1.41	1.37
26	I	305	DD6	O1-C20	-2.99	1.42	1.46
28	b	720	CLA	C4B-NB	2.98	1.41	1.37
28	B	312	CLA	C4B-NB	2.98	1.41	1.37
28	a	729	CLA	C4B-NB	2.98	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	A	310	CLA	C4B-NB	2.98	1.41	1.37
28	f	303	CLA	C4B-NB	2.98	1.41	1.37
28	J	301	CLA	C4B-NB	2.98	1.41	1.37
28	a	723	CLA	C4B-NB	2.97	1.41	1.37
28	L	314	CLA	C4B-NB	2.97	1.41	1.37
28	I	312	CLA	C4B-NB	2.97	1.41	1.37
28	a	715	CLA	C4B-NB	2.97	1.41	1.37
28	F	308	CLA	C4B-NB	2.96	1.41	1.37
28	L	313	CLA	C4B-NB	2.96	1.41	1.37
28	L	318	CLA	C4B-NB	2.96	1.41	1.37
28	K	312	CLA	C4B-NB	2.96	1.41	1.37
28	M	312	CLA	C4B-NB	2.96	1.41	1.37
28	a	720	CLA	C4B-NB	2.96	1.41	1.37
28	b	725	CLA	C4B-NB	2.95	1.41	1.37
27	K	302	UIX	O-C1	-2.95	1.42	1.46
28	J	309	CLA	C4B-NB	2.95	1.41	1.37
28	F	313	CLA	C4B-NB	2.95	1.41	1.37
28	G	510	CLA	C4B-NB	2.95	1.41	1.37
28	B	313	CLA	C4B-NB	2.95	1.41	1.37
28	G	514	CLA	C4B-NB	2.95	1.41	1.37
28	b	708	CLA	C4B-NB	2.95	1.41	1.37
28	a	726	CLA	C4B-NB	2.94	1.41	1.37
28	N	305	CLA	C4B-NB	2.94	1.41	1.37
28	a	730	CLA	C4B-NB	2.93	1.41	1.37
28	a	728	CLA	C4B-NB	2.93	1.41	1.37
28	K	309	CLA	C4B-NB	2.93	1.41	1.37
28	B	301	CLA	C1B-C2B	2.91	1.50	1.43
28	a	721	CLA	C4B-NB	2.91	1.41	1.37
28	b	705	CLA	C4B-NB	2.91	1.41	1.37
26	J	304	DD6	C19-C20	2.90	1.56	1.52
28	b	703	CLA	C1B-C2B	2.88	1.49	1.43
28	A	313	CLA	C4B-NB	2.87	1.41	1.37
28	D	313	CLA	C4B-NB	2.87	1.41	1.37
28	N	309	CLA	C4B-NB	2.86	1.41	1.37
28	G	513	CLA	C4B-NB	2.85	1.41	1.37
28	K	312	CLA	C1B-C2B	2.85	1.49	1.43
28	B	309	CLA	C1B-C2B	2.84	1.49	1.43
28	F	315	CLA	C1B-C2B	2.83	1.49	1.43
28	b	707	CLA	C1B-C2B	2.83	1.49	1.43
32	H	302	PID	C8-C9	-2.83	1.39	1.46
28	G	512	CLA	C1B-C2B	2.83	1.49	1.43
28	B	313	CLA	C1B-C2B	2.82	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	N	308	KC1	C4A-C3A	-2.81	1.38	1.44
28	L	308	CLA	C1B-C2B	2.81	1.49	1.43
28	J	314	CLA	C1B-C2B	2.81	1.49	1.43
26	M	303	DD6	O1-C20	-2.81	1.42	1.46
28	l	305	CLA	C1B-C2B	2.81	1.49	1.43
28	L	311	CLA	C1B-C2B	2.81	1.49	1.43
28	M	315	CLA	C1B-C2B	2.81	1.49	1.43
28	h	202	CLA	C1B-C2B	2.80	1.49	1.43
28	b	714	CLA	C1B-C2B	2.80	1.49	1.43
28	K	311	CLA	C1B-C2B	2.80	1.49	1.43
28	a	729	CLA	C1B-C2B	2.80	1.49	1.43
28	b	711	CLA	C1B-C2B	2.80	1.49	1.43
28	M	308	CLA	C1B-C2B	2.80	1.49	1.43
28	J	309	CLA	C1B-C2B	2.80	1.49	1.43
28	l	304	CLA	C1B-C2B	2.80	1.49	1.43
28	F	308	CLA	C1B-C2B	2.80	1.49	1.43
28	a	715	CLA	C1B-C2B	2.80	1.49	1.43
28	a	720	CLA	C1B-C2B	2.80	1.49	1.43
28	b	728	CLA	C1B-C2B	2.80	1.49	1.43
28	D	308	CLA	C1B-C2B	2.79	1.49	1.43
28	M	309	CLA	C1B-C2B	2.79	1.49	1.43
28	F	307	CLA	C1B-C2B	2.79	1.49	1.43
28	H	308	CLA	C1B-C2B	2.79	1.49	1.43
28	G	511	CLA	C1B-C2B	2.79	1.49	1.43
28	G	517	CLA	C1B-C2B	2.79	1.49	1.43
28	b	706	CLA	C1B-C2B	2.79	1.49	1.43
28	N	304	CLA	C1B-C2B	2.79	1.49	1.43
28	K	315	CLA	C1B-C2B	2.79	1.49	1.43
28	M	310	CLA	C1B-C2B	2.79	1.49	1.43
28	J	306	CLA	C1B-C2B	2.79	1.49	1.43
28	G	519	CLA	C1B-C2B	2.79	1.49	1.43
28	a	714	CLA	C1B-C2B	2.79	1.49	1.43
32	D	302	PID	C8-C9	-2.78	1.39	1.46
28	a	706	CLA	C1B-C2B	2.78	1.49	1.43
28	a	730	CLA	C1B-C2B	2.78	1.49	1.43
26	I	305	DD6	C36-C31	-2.78	1.31	1.35
28	f	303	CLA	C1B-C2B	2.78	1.49	1.43
28	A	308	CLA	C1B-C2B	2.78	1.49	1.43
28	H	305	CLA	C1B-C2B	2.78	1.49	1.43
28	L	309	CLA	C1B-C2B	2.78	1.49	1.43
28	I	319	CLA	C1B-C2B	2.78	1.49	1.43
28	D	311	CLA	C1B-C2B	2.78	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	a	707	CLA	C1B-C2B	2.78	1.49	1.43
32	D	304	PID	C13-C12	2.78	1.44	1.36
28	l	308	CLA	C1B-C2B	2.77	1.49	1.43
28	B	308	CLA	C1B-C2B	2.77	1.49	1.43
32	F	304	PID	C13-C12	2.77	1.44	1.36
28	A	309	CLA	C1B-C2B	2.77	1.49	1.43
28	H	309	CLA	C1B-C2B	2.77	1.49	1.43
28	L	314	CLA	C1B-C2B	2.77	1.49	1.43
28	G	509	CLA	C1B-C2B	2.77	1.49	1.43
28	D	316	CLA	C1B-C2B	2.77	1.49	1.43
28	M	317	CLA	C1B-C2B	2.77	1.49	1.43
28	D	313	CLA	C1B-C2B	2.77	1.49	1.43
32	F	306	PID	C8-C9	-2.77	1.39	1.46
28	B	312	CLA	C1B-C2B	2.76	1.49	1.43
28	I	310	CLA	C1B-C2B	2.76	1.49	1.43
28	A	315	CLA	C1B-C2B	2.76	1.49	1.43
28	l	309	CLA	C1B-C2B	2.76	1.49	1.43
28	J	315	CLA	C1B-C2B	2.76	1.49	1.43
28	b	725	CLA	C1B-C2B	2.76	1.49	1.43
28	K	307	CLA	C1B-C2B	2.76	1.49	1.43
28	F	311	CLA	C1B-C2B	2.76	1.49	1.43
28	J	301	CLA	C1B-C2B	2.76	1.49	1.43
28	H	304	CLA	C1B-C2B	2.76	1.49	1.43
28	b	716	CLA	C1B-C2B	2.76	1.49	1.43
28	F	310	CLA	C1B-C2B	2.76	1.49	1.43
28	f	301	CLA	C1B-C2B	2.75	1.49	1.43
28	A	312	CLA	C1B-C2B	2.75	1.49	1.43
28	b	727	CLA	C1B-C2B	2.75	1.49	1.43
28	b	726	CLA	C1B-C2B	2.75	1.49	1.43
28	b	720	CLA	C1B-C2B	2.75	1.49	1.43
28	H	311	CLA	C1B-C2B	2.75	1.49	1.43
28	N	310	CLA	C1B-C2B	2.75	1.49	1.43
28	a	722	CLA	C1B-C2B	2.75	1.49	1.43
28	b	723	CLA	C1B-C2B	2.74	1.49	1.43
28	I	307	CLA	C1B-C2B	2.74	1.49	1.43
28	G	516	CLA	C1B-C2B	2.74	1.49	1.43
28	a	710	CLA	C1B-C2B	2.74	1.49	1.43
28	I	306	CLA	C1B-C2B	2.74	1.49	1.43
28	A	316	CLA	C1B-C2B	2.74	1.49	1.43
28	D	309	CLA	C1B-C2B	2.74	1.49	1.43
28	G	514	CLA	C1B-C2B	2.74	1.49	1.43
28	a	728	CLA	C1B-C2B	2.74	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	A	313	CLA	C1B-C2B	2.74	1.49	1.43
32	D	306	PID	C8-C9	-2.74	1.39	1.46
32	M	301	PID	C13-C12	2.73	1.44	1.36
28	a	725	CLA	C1B-C2B	2.73	1.49	1.43
28	b	705	CLA	C1B-C2B	2.73	1.49	1.43
26	G	504	DD6	O1-C20	-2.73	1.42	1.46
32	F	302	PID	C8-C9	-2.73	1.39	1.46
28	D	312	CLA	C1B-C2B	2.73	1.49	1.43
28	H	307	CLA	C1B-C2B	2.73	1.49	1.43
28	F	312	CLA	C1D-ND	2.73	1.41	1.37
29	N	308	KC1	C4B-NB	-2.73	1.34	1.37
28	H	312	CLA	C1B-C2B	2.73	1.49	1.43
27	h	201	UIX	O-C1	-2.73	1.42	1.46
28	l	310	CLA	C4D-CHA	2.73	1.43	1.39
28	G	513	CLA	C1B-C2B	2.73	1.49	1.43
28	a	718	CLA	C1B-C2B	2.73	1.49	1.43
28	b	715	CLA	C1B-C2B	2.73	1.49	1.43
28	a	731	CLA	C1B-C2B	2.73	1.49	1.43
28	b	701	CLA	C1B-C2B	2.73	1.49	1.43
28	a	703	CLA	MG-NB	-2.73	2.00	2.05
27	G	503	UIX	O-C1	-2.73	1.42	1.46
28	K	307	CLA	C4B-NB	2.73	1.41	1.37
32	D	305	PID	C8-C9	-2.73	1.39	1.46
32	G	507	PID	C8-C9	-2.72	1.39	1.46
28	G	520	CLA	C1B-C2B	2.72	1.49	1.43
28	b	721	CLA	C1B-C2B	2.72	1.49	1.43
28	a	738	CLA	C1B-C2B	2.72	1.49	1.43
28	j	106	CLA	C1B-C2B	2.72	1.49	1.43
28	B	317	CLA	C1B-C2B	2.72	1.49	1.43
28	L	318	CLA	C1B-C2B	2.72	1.49	1.43
28	K	310	CLA	C1B-C2B	2.72	1.49	1.43
28	l	311	CLA	C1B-C2B	2.72	1.49	1.43
28	M	318	CLA	C1B-C2B	2.72	1.49	1.43
28	L	317	CLA	C1B-C2B	2.72	1.49	1.43
29	J	313	KC1	C4B-NB	-2.72	1.34	1.37
28	N	309	CLA	C1B-C2B	2.72	1.49	1.43
32	F	305	PID	C8-C9	-2.72	1.39	1.46
28	B	316	CLA	C1B-C2B	2.72	1.49	1.43
28	A	319	CLA	C1B-C2B	2.72	1.49	1.43
28	B	315	CLA	C1B-C2B	2.71	1.49	1.43
28	L	316	CLA	C1B-C2B	2.71	1.49	1.43
28	l	313	CLA	C1B-C2B	2.71	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	A	307	CLA	C1B-C2B	2.71	1.49	1.43
28	A	311	CLA	C1B-C2B	2.71	1.49	1.43
28	A	310	CLA	C1B-C2B	2.71	1.49	1.43
32	F	302	PID	C13-C12	2.71	1.44	1.36
28	L	312	CLA	C1B-C2B	2.71	1.49	1.43
28	a	711	CLA	C1B-C2B	2.71	1.49	1.43
28	a	702	CLA	C1D-ND	2.71	1.41	1.37
28	J	311	CLA	C1B-C2B	2.71	1.49	1.43
28	B	311	CLA	C1B-C2B	2.71	1.49	1.43
28	j	104	CLA	C1B-C2B	2.71	1.49	1.43
28	B	310	CLA	C1B-C2B	2.70	1.49	1.43
28	a	719	CLA	C1B-C2B	2.70	1.49	1.43
28	f	302	CLA	C1B-C2B	2.70	1.49	1.43
28	a	701	CLA	C1B-C2B	2.70	1.49	1.43
28	a	702	CLA	MG-NB	-2.70	2.00	2.05
28	b	713	CLA	C1B-C2B	2.70	1.49	1.43
28	K	306	CLA	C1B-C2B	2.69	1.49	1.43
28	b	724	CLA	C1B-C2B	2.69	1.49	1.43
28	K	308	CLA	C1B-C2B	2.69	1.49	1.43
28	I	311	CLA	C1B-C2B	2.69	1.49	1.43
28	J	316	CLA	C1B-C2B	2.69	1.49	1.43
28	G	510	CLA	C1B-C2B	2.69	1.49	1.43
28	a	727	CLA	C1B-C2B	2.69	1.49	1.43
28	b	718	CLA	C1B-C2B	2.69	1.49	1.43
28	I	313	CLA	C1B-C2B	2.68	1.49	1.43
32	H	301	PID	C8-C9	-2.68	1.40	1.46
28	J	307	CLA	C1B-C2B	2.68	1.49	1.43
28	N	305	CLA	C1B-C2B	2.68	1.49	1.43
28	F	313	CLA	C1B-C2B	2.68	1.49	1.43
32	D	307	PID	C13-C12	2.68	1.43	1.36
28	a	717	CLA	C1B-C2B	2.68	1.49	1.43
26	M	302	DD6	O1-C20	-2.68	1.42	1.46
28	a	704	CLA	C1B-C2B	2.68	1.49	1.43
28	b	709	CLA	C3B-C4B	2.68	1.50	1.42
28	K	316	CLA	C1B-C2B	2.67	1.49	1.43
28	K	309	CLA	C1B-C2B	2.67	1.49	1.43
28	M	311	CLA	C1B-C2B	2.67	1.49	1.43
28	L	310	CLA	C1B-C2B	2.67	1.49	1.43
28	b	708	CLA	C1B-C2B	2.67	1.49	1.43
28	b	719	CLA	C1B-C2B	2.67	1.49	1.43
32	F	305	PID	C13-C12	2.67	1.43	1.36
26	K	301	DD6	O1-C20	-2.67	1.42	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	I	315	CLA	C1B-C2B	2.67	1.49	1.43
28	b	712	CLA	C4B-C3B	2.67	1.49	1.43
28	I	309	CLA	C1B-C2B	2.67	1.49	1.43
28	b	717	CLA	C1B-C2B	2.66	1.49	1.43
28	a	712	CLA	C1B-C2B	2.66	1.49	1.43
28	a	708	CLA	C1B-C2B	2.66	1.49	1.43
28	M	316	CLA	C1B-C2B	2.66	1.49	1.43
28	l	303	CLA	C1B-C2B	2.66	1.49	1.43
28	a	705	CLA	C1B-C2B	2.66	1.49	1.43
28	a	716	CLA	C1B-C2B	2.66	1.49	1.43
28	J	312	CLA	C1B-C2B	2.66	1.49	1.43
28	a	735	CLA	C1B-C2B	2.65	1.49	1.43
29	M	314	KC1	C4B-NB	-2.65	1.34	1.37
26	I	302	DD6	O1-C20	-2.65	1.42	1.46
28	I	308	CLA	C1B-C2B	2.65	1.49	1.43
28	I	312	CLA	C1B-C2B	2.65	1.49	1.43
28	a	709	CLA	C1B-C2B	2.65	1.49	1.43
32	j	105	PID	C8-C9	-2.65	1.40	1.46
28	l	310	CLA	CMD-C2D	-2.64	1.46	1.51
29	B	314	KC1	C4B-NB	-2.64	1.34	1.37
28	K	313	CLA	C1B-C2B	2.64	1.49	1.43
28	I	321	CLA	C1B-C2B	2.64	1.49	1.43
29	F	314	KC1	C4B-NB	-2.64	1.34	1.37
28	a	723	CLA	C1B-C2B	2.64	1.49	1.43
32	N	301	PID	C13-C12	2.63	1.43	1.36
29	K	314	KC1	C4B-NB	-2.63	1.34	1.37
29	A	306	KC1	CBA-CGA	-2.63	1.41	1.48
26	L	304	DD6	O1-C20	-2.63	1.42	1.46
28	b	704	CLA	MG-NB	-2.63	2.00	2.05
28	b	710	CLA	C1B-C2B	2.63	1.49	1.43
32	M	301	PID	C8-C9	-2.63	1.40	1.46
29	M	307	KC1	C4B-NB	-2.63	1.34	1.37
28	L	313	CLA	C1B-C2B	2.63	1.49	1.43
28	A	320	CLA	C1B-C2B	2.63	1.49	1.43
32	H	301	PID	C13-C12	2.63	1.43	1.36
29	K	314	KC1	CBA-CGA	-2.62	1.41	1.48
28	A	317	CLA	C1B-C2B	2.62	1.49	1.43
32	F	306	PID	C13-C12	2.62	1.43	1.36
28	a	721	CLA	C1B-C2B	2.62	1.49	1.43
32	j	105	PID	C13-C12	2.62	1.43	1.36
28	I	316	CLA	C1B-C2B	2.62	1.49	1.43
32	D	301	PID	C8-C9	-2.62	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	B	302	DD6	O1-C20	-2.62	1.42	1.46
28	I	312	CLA	C1B-C2B	2.62	1.49	1.43
29	D	310	KC1	C4B-NB	-2.61	1.34	1.37
28	N	307	CLA	C1B-C2B	2.61	1.49	1.43
29	H	306	KC1	C4B-NB	-2.60	1.34	1.37
29	L	315	KC1	C4B-NB	-2.60	1.34	1.37
29	M	307	KC1	CBA-CGA	-2.60	1.41	1.48
28	B	307	CLA	C1B-C2B	2.60	1.49	1.43
28	b	722	CLA	CMB-C2B	-2.60	1.45	1.50
28	a	703	CLA	CMD-C2D	-2.60	1.45	1.50
28	F	312	CLA	MG-NB	-2.60	2.00	2.05
26	I	305	DD6	C19-C20	2.59	1.55	1.52
28	M	313	CLA	C3B-C4B	2.59	1.50	1.42
29	L	307	KC1	CBA-CGA	-2.59	1.41	1.48
28	D	314	CLA	C3B-C4B	2.59	1.50	1.42
29	G	515	KC1	C4B-NB	-2.59	1.34	1.37
28	A	320	CLA	C3B-C4B	2.58	1.50	1.42
28	b	708	CLA	C3B-C4B	2.58	1.50	1.42
28	b	704	CLA	C1D-ND	2.58	1.41	1.37
28	m	202	CLA	C1B-C2B	2.58	1.49	1.43
32	D	304	PID	C8-C9	-2.58	1.40	1.46
28	M	313	CLA	C1B-C2B	2.57	1.49	1.43
29	N	308	KC1	C1B-NB	-2.57	1.34	1.37
28	a	723	CLA	C3B-C4B	2.57	1.50	1.42
29	L	307	KC1	C4B-NB	-2.57	1.34	1.37
30	L	301	DGD	O1G-C1A	2.56	1.45	1.33
32	N	301	PID	C8-C9	-2.56	1.40	1.46
28	a	726	CLA	CHC-C1C	2.56	1.43	1.38
29	J	313	KC1	CBA-CGA	-2.56	1.42	1.48
26	G	504	DD6	C36-C31	-2.56	1.32	1.35
29	L	315	KC1	CBA-CGA	-2.55	1.42	1.48
27	A	304	UIX	O-C1	-2.55	1.42	1.46
32	G	507	PID	C13-C12	2.55	1.43	1.36
28	M	316	CLA	C3B-C4B	2.55	1.50	1.42
29	H	310	KC1	C4B-NB	-2.55	1.34	1.37
28	J	316	CLA	C3B-C4B	2.55	1.50	1.42
28	j	104	CLA	C3B-C4B	2.55	1.50	1.42
29	N	306	KC1	C4B-NB	-2.54	1.34	1.37
27	J	305	UIX	O-C1	-2.54	1.42	1.46
29	B	314	KC1	CBA-CGA	-2.54	1.42	1.48
29	A	314	KC1	C4B-NB	-2.54	1.34	1.37
28	G	518	CLA	C1B-C2B	2.54	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	a	735	CLA	CHC-C1C	2.54	1.43	1.38
28	B	307	CLA	C3B-C4B	2.54	1.50	1.42
28	I	311	CLA	C3B-C4B	2.53	1.50	1.42
29	A	314	KC1	CBA-CGA	-2.53	1.42	1.48
28	J	308	CLA	C1B-C2B	2.53	1.49	1.43
29	A	306	KC1	C4B-NB	-2.53	1.34	1.37
28	b	712	CLA	C1B-C2B	2.53	1.49	1.43
29	H	310	KC1	CBA-CGA	-2.53	1.42	1.48
27	B	305	UIX	O-C1	-2.52	1.43	1.46
29	N	311	KC1	C4B-NB	-2.52	1.34	1.37
28	K	308	CLA	C3B-C4B	2.52	1.50	1.42
28	a	735	CLA	C3B-C4B	2.52	1.50	1.42
32	D	306	PID	C13-C12	2.52	1.43	1.36
28	l	311	CLA	C3B-C4B	2.52	1.50	1.42
32	D	301	PID	C13-C12	2.52	1.43	1.36
28	a	724	CLA	C1B-C2B	2.52	1.49	1.43
28	a	713	CLA	C1B-C2B	2.52	1.49	1.43
28	a	731	CLA	C3B-C4B	2.51	1.50	1.42
28	M	313	CLA	CHC-C1C	2.51	1.43	1.38
29	D	310	KC1	CBA-CGA	-2.51	1.42	1.48
29	F	309	KC1	C4B-NB	-2.51	1.34	1.37
28	l	310	CLA	CMB-C2B	-2.50	1.46	1.51
29	H	306	KC1	CBA-CGA	-2.50	1.42	1.48
29	N	311	KC1	CBA-CGA	-2.50	1.42	1.48
29	I	314	KC1	C4B-NB	-2.50	1.34	1.37
28	l	310	CLA	CMC-C2C	-2.50	1.46	1.50
28	a	702	CLA	CMD-C2D	-2.50	1.45	1.50
29	F	309	KC1	CBA-CGA	-2.50	1.42	1.48
29	G	515	KC1	CBA-CGA	-2.50	1.42	1.48
29	F	314	KC1	CBA-CGA	-2.49	1.42	1.48
29	M	314	KC1	CBA-CGA	-2.49	1.42	1.48
26	K	304	DD6	O1-C20	-2.49	1.43	1.46
28	L	316	CLA	C3B-C4B	2.49	1.50	1.42
28	a	726	CLA	C3B-C4B	2.49	1.50	1.42
28	a	727	CLA	C3B-C4B	2.49	1.50	1.42
28	F	312	CLA	CMD-C2D	-2.49	1.45	1.50
28	I	309	CLA	C3B-C4B	2.49	1.50	1.42
28	F	312	CLA	CMB-C2B	-2.48	1.45	1.50
26	B	304	DD6	O1-C20	-2.48	1.43	1.46
26	G	508	DD6	O1-C20	-2.48	1.43	1.46
28	a	702	CLA	CMB-C2B	-2.48	1.45	1.50
32	H	302	PID	C13-C12	2.48	1.43	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	A	313	CLA	C3B-C4B	2.48	1.50	1.42
28	a	705	CLA	C3B-C4B	2.48	1.50	1.42
28	a	711	CLA	C3B-C4B	2.48	1.49	1.42
29	N	306	KC1	CBA-CGA	-2.48	1.42	1.48
28	I	308	CLA	CHC-C1C	2.48	1.43	1.38
28	D	314	CLA	C1B-C2B	2.48	1.48	1.43
28	I	309	CLA	CHC-C1C	2.47	1.43	1.38
29	I	314	KC1	CBA-CGA	-2.47	1.42	1.48
28	A	317	CLA	C3B-C4B	2.47	1.49	1.42
26	b	731	DD6	O1-C20	-2.47	1.43	1.46
28	b	722	CLA	C1B-C2B	2.47	1.48	1.43
32	D	305	PID	C13-C12	2.47	1.43	1.36
32	D	307	PID	C8-C9	-2.46	1.40	1.46
28	I	315	CLA	C3B-C4B	2.46	1.49	1.42
28	I	316	CLA	C3B-C4B	2.46	1.49	1.42
28	L	317	CLA	C3B-C4B	2.46	1.49	1.42
28	I	316	CLA	CHC-C1C	2.46	1.43	1.38
28	a	705	CLA	CHC-C1C	2.46	1.43	1.38
28	a	704	CLA	C3B-C4B	2.46	1.49	1.42
28	a	716	CLA	C3B-C4B	2.46	1.49	1.42
27	I	304	UIX	O-C1	-2.46	1.43	1.46
28	K	313	CLA	C3B-C4B	2.46	1.49	1.42
28	I	308	CLA	C3B-C4B	2.46	1.49	1.42
32	F	304	PID	C8-C9	-2.45	1.40	1.46
28	J	301	CLA	C3B-C4B	2.45	1.49	1.42
28	K	309	CLA	CHC-C1C	2.45	1.43	1.38
28	b	725	CLA	C3B-C4B	2.45	1.49	1.42
26	F	303	DD6	O1-C20	-2.45	1.43	1.46
28	a	707	CLA	C3B-C4B	2.45	1.49	1.42
26	M	304	DD6	O1-C20	-2.45	1.43	1.46
28	a	724	CLA	CMB-C2B	-2.45	1.45	1.50
28	l	303	CLA	C3B-C4B	2.44	1.49	1.42
28	F	310	CLA	C3B-C4B	2.44	1.49	1.42
28	b	704	CLA	CMD-C2D	-2.44	1.45	1.50
28	J	310	CLA	CMB-C2B	-2.44	1.45	1.50
28	G	510	CLA	C3B-C4B	2.44	1.49	1.42
32	D	302	PID	C13-C12	2.44	1.43	1.36
28	J	312	CLA	C3B-C4B	2.44	1.49	1.42
28	A	307	CLA	C3B-C4B	2.44	1.49	1.42
28	J	314	CLA	C3B-C4B	2.44	1.49	1.42
28	K	306	CLA	C3B-C4B	2.44	1.49	1.42
28	a	717	CLA	C3B-C4B	2.43	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	B	309	CLA	C3B-C4B	2.43	1.49	1.42
28	M	318	CLA	C3B-C4B	2.43	1.49	1.42
29	D	315	KC1	CBA-CGA	-2.43	1.42	1.48
28	M	312	CLA	C1B-C2B	2.43	1.48	1.43
28	A	319	CLA	CHC-C1C	2.43	1.43	1.38
28	b	709	CLA	C1B-C2B	2.43	1.48	1.43
28	a	724	CLA	CMD-C2D	-2.43	1.45	1.50
28	b	714	CLA	C3B-C4B	2.43	1.49	1.42
28	J	310	CLA	C1B-C2B	2.43	1.48	1.43
28	b	715	CLA	C3B-C4B	2.42	1.49	1.42
28	A	308	CLA	C3B-C4B	2.42	1.49	1.42
28	b	724	CLA	C3B-C4B	2.42	1.49	1.42
26	K	303	DD6	O1-C20	-2.42	1.43	1.46
28	G	513	CLA	C3B-C4B	2.42	1.49	1.42
28	B	315	CLA	C3B-C4B	2.42	1.49	1.42
28	A	311	CLA	CHC-C1C	2.42	1.43	1.38
28	a	718	CLA	C3B-C4B	2.42	1.49	1.42
26	B	306	DD6	O1-C20	-2.42	1.43	1.46
28	b	725	CLA	CHC-C1C	2.42	1.43	1.38
28	b	715	CLA	CHC-C1C	2.42	1.43	1.38
28	G	516	CLA	C3B-C4B	2.41	1.49	1.42
28	H	307	CLA	C3B-C4B	2.41	1.49	1.42
28	D	312	CLA	C3B-C4B	2.41	1.49	1.42
28	J	311	CLA	C3B-C4B	2.41	1.49	1.42
28	K	309	CLA	C3B-C4B	2.41	1.49	1.42
28	L	310	CLA	C3B-C4B	2.41	1.49	1.42
28	L	310	CLA	CHC-C1C	2.41	1.43	1.38
28	a	711	CLA	CHC-C1C	2.41	1.43	1.38
28	a	709	CLA	C3B-C4B	2.41	1.49	1.42
28	a	703	CLA	C1D-ND	2.41	1.41	1.37
28	I	321	CLA	C3B-C4B	2.41	1.49	1.42
28	D	316	CLA	CHC-C1C	2.41	1.43	1.38
28	a	709	CLA	CHC-C1C	2.41	1.43	1.38
28	I	312	CLA	C3B-C4B	2.41	1.49	1.42
28	b	728	CLA	C3B-C4B	2.41	1.49	1.42
28	F	310	CLA	CHC-C1C	2.41	1.43	1.38
28	I	319	CLA	C3B-C4B	2.41	1.49	1.42
28	a	701	CLA	CHC-C1C	2.41	1.43	1.38
28	L	313	CLA	CHC-C1C	2.41	1.43	1.38
28	L	314	CLA	C3B-C4B	2.41	1.49	1.42
28	K	308	CLA	CHC-C1C	2.41	1.43	1.38
28	G	519	CLA	C3B-C4B	2.40	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	a	706	CLA	C3B-C4B	2.40	1.49	1.42
28	b	724	CLA	CHC-C1C	2.40	1.43	1.38
28	H	309	CLA	C3B-C4B	2.40	1.49	1.42
28	b	704	CLA	CMB-C2B	-2.40	1.45	1.50
28	L	316	CLA	CHC-C1C	2.40	1.43	1.38
28	N	309	CLA	C3B-C4B	2.40	1.49	1.42
28	B	312	CLA	C3B-C4B	2.40	1.49	1.42
28	L	313	CLA	C3B-C4B	2.40	1.49	1.42
28	A	313	CLA	CHC-C1C	2.40	1.43	1.38
28	j	106	CLA	C3B-C4B	2.40	1.49	1.42
31	K	318	LMG	O7-C8	-2.40	1.41	1.46
28	G	518	CLA	C3B-C4B	2.40	1.49	1.42
28	L	309	CLA	C3B-C4B	2.40	1.49	1.42
28	A	311	CLA	C3B-C4B	2.40	1.49	1.42
28	M	315	CLA	C3B-C4B	2.40	1.49	1.42
28	I	307	CLA	C3B-C4B	2.40	1.49	1.42
28	A	309	CLA	C3B-C4B	2.40	1.49	1.42
28	L	312	CLA	C3B-C4B	2.40	1.49	1.42
28	D	314	CLA	CHC-C1C	2.40	1.43	1.38
26	H	303	DD6	O1-C20	-2.39	1.43	1.46
28	J	315	CLA	C3B-C4B	2.39	1.49	1.42
28	H	304	CLA	C3B-C4B	2.39	1.49	1.42
28	D	311	CLA	C3B-C4B	2.39	1.49	1.42
28	J	307	CLA	C3B-C4B	2.39	1.49	1.42
28	a	701	CLA	C3B-C4B	2.39	1.49	1.42
28	a	738	CLA	C3B-C4B	2.39	1.49	1.42
28	J	312	CLA	CHC-C1C	2.39	1.43	1.38
28	b	714	CLA	CHC-C1C	2.39	1.43	1.38
26	M	305	DD6	O1-C20	-2.39	1.43	1.46
28	K	316	CLA	C3B-C4B	2.39	1.49	1.42
28	b	726	CLA	C3B-C4B	2.39	1.49	1.42
28	G	511	CLA	C3B-C4B	2.39	1.49	1.42
28	M	311	CLA	C3B-C4B	2.39	1.49	1.42
28	j	104	CLA	CHC-C1C	2.39	1.43	1.38
28	A	309	CLA	CHC-C1C	2.39	1.43	1.38
28	I	313	CLA	C3B-C4B	2.39	1.49	1.42
28	f	303	CLA	C3B-C4B	2.39	1.49	1.42
28	D	316	CLA	C3B-C4B	2.39	1.49	1.42
28	J	301	CLA	CHC-C1C	2.39	1.43	1.38
28	a	714	CLA	C3B-C4B	2.38	1.49	1.42
28	a	721	CLA	C3B-C4B	2.38	1.49	1.42
28	a	722	CLA	C3B-C4B	2.38	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	K	315	CLA	C3B-C4B	2.38	1.49	1.42
28	J	308	CLA	C3B-C4B	2.38	1.49	1.42
28	D	308	CLA	C3B-C4B	2.38	1.49	1.42
28	H	312	CLA	C3B-C4B	2.38	1.49	1.42
26	I	303	DD6	C28-C27	-2.38	1.49	1.50
28	b	711	CLA	C3B-C4B	2.38	1.49	1.42
28	b	706	CLA	C3B-C4B	2.38	1.49	1.42
28	A	312	CLA	C3B-C4B	2.38	1.49	1.42
28	b	710	CLA	CMB-C2B	-2.38	1.45	1.50
28	J	311	CLA	CHC-C1C	2.38	1.43	1.38
26	M	306	DD6	O1-C20	-2.38	1.43	1.46
28	N	309	CLA	CHC-C1C	2.38	1.43	1.38
28	l	305	CLA	C3B-C4B	2.38	1.49	1.42
28	B	310	CLA	C3B-C4B	2.38	1.49	1.42
28	b	706	CLA	CHC-C1C	2.38	1.43	1.38
28	l	312	CLA	CHC-C1C	2.38	1.43	1.38
28	b	727	CLA	C3B-C4B	2.38	1.49	1.42
28	L	311	CLA	C3B-C4B	2.38	1.49	1.42
26	A	302	DD6	C26-C27	-2.38	1.32	1.37
28	F	315	CLA	C3B-C4B	2.38	1.49	1.42
28	K	310	CLA	CHC-C1C	2.38	1.43	1.38
28	b	703	CLA	CHC-C1C	2.37	1.43	1.38
28	K	311	CLA	C3B-C4B	2.37	1.49	1.42
28	l	309	CLA	C3B-C4B	2.37	1.49	1.42
28	l	309	CLA	CHC-C1C	2.37	1.43	1.38
28	L	314	CLA	CHC-C1C	2.37	1.43	1.38
28	I	313	CLA	CHC-C1C	2.37	1.43	1.38
28	b	719	CLA	C3B-C4B	2.37	1.49	1.42
28	f	303	CLA	CHC-C1C	2.37	1.43	1.38
28	b	707	CLA	CHC-C1C	2.37	1.43	1.38
28	l	312	CLA	C3B-C4B	2.37	1.49	1.42
28	a	708	CLA	C3B-C4B	2.37	1.49	1.42
28	H	305	CLA	CHC-C1C	2.37	1.43	1.38
28	M	310	CLA	CHC-C1C	2.37	1.43	1.38
28	B	316	CLA	C3B-C4B	2.37	1.49	1.42
28	G	509	CLA	C3B-C4B	2.37	1.49	1.42
28	b	707	CLA	C3B-C4B	2.37	1.49	1.42
28	G	520	CLA	C3B-C4B	2.37	1.49	1.42
28	l	308	CLA	C3B-C4B	2.37	1.49	1.42
28	a	730	CLA	C3B-C4B	2.37	1.49	1.42
28	a	719	CLA	C3B-C4B	2.37	1.49	1.42
28	H	305	CLA	C3B-C4B	2.36	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	N	305	CLA	C3B-C4B	2.36	1.49	1.42
28	N	304	CLA	C3B-C4B	2.36	1.49	1.42
28	F	311	CLA	C3B-C4B	2.36	1.49	1.42
28	M	317	CLA	C3B-C4B	2.36	1.49	1.42
28	b	718	CLA	C3B-C4B	2.36	1.49	1.42
28	I	321	CLA	CHC-C1C	2.36	1.43	1.38
28	b	723	CLA	C3B-C4B	2.36	1.49	1.42
28	b	727	CLA	CHC-C1C	2.36	1.43	1.38
28	a	710	CLA	CMD-C2D	-2.36	1.45	1.50
28	K	312	CLA	C3B-C4B	2.36	1.49	1.42
28	B	311	CLA	CMD-C2D	-2.36	1.45	1.50
28	K	313	CLA	CHC-C1C	2.36	1.43	1.38
28	I	308	CLA	CHC-C1C	2.36	1.43	1.38
28	D	311	CLA	CHC-C1C	2.36	1.43	1.38
29	D	315	KC1	C4B-NB	-2.36	1.34	1.37
28	b	705	CLA	C3B-C4B	2.36	1.49	1.42
28	G	514	CLA	C3B-C4B	2.36	1.49	1.42
28	a	724	CLA	C3B-C4B	2.36	1.49	1.42
28	M	309	CLA	C3B-C4B	2.36	1.49	1.42
28	B	317	CLA	CHC-C1C	2.36	1.43	1.38
28	a	717	CLA	CHC-C1C	2.36	1.43	1.38
28	M	318	CLA	CHC-C1C	2.36	1.43	1.38
32	G	506	PID	C13-C12	2.36	1.43	1.36
28	F	312	CLA	C4B-NB	2.36	1.41	1.37
28	a	704	CLA	CHC-C1C	2.36	1.43	1.38
28	b	704	CLA	C1B-C2B	2.36	1.48	1.43
28	B	313	CLA	C3B-C4B	2.35	1.49	1.42
28	B	317	CLA	C3B-C4B	2.35	1.49	1.42
28	L	308	CLA	CHC-C1C	2.35	1.43	1.38
28	M	309	CLA	CHC-C1C	2.35	1.43	1.38
28	a	713	CLA	C3B-C4B	2.35	1.49	1.42
28	N	307	CLA	C3B-C4B	2.35	1.49	1.42
28	M	311	CLA	CHC-C1C	2.35	1.43	1.38
29	N	308	KC1	CBA-CGA	-2.35	1.42	1.48
28	b	716	CLA	C3B-C4B	2.35	1.49	1.42
28	B	312	CLA	CHC-C1C	2.35	1.43	1.38
28	b	712	CLA	CMB-C2B	-2.35	1.46	1.50
28	J	314	CLA	CHC-C1C	2.35	1.43	1.38
28	m	202	CLA	C3B-C4B	2.35	1.49	1.42
28	M	310	CLA	C3B-C4B	2.35	1.49	1.42
28	b	713	CLA	C3B-C4B	2.35	1.49	1.42
28	b	716	CLA	CHC-C1C	2.34	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	M	308	CLA	C3B-C4B	2.34	1.49	1.42
28	G	510	CLA	CHC-C1C	2.34	1.43	1.38
28	A	312	CLA	CHC-C1C	2.34	1.43	1.38
28	f	301	CLA	C3B-C4B	2.34	1.49	1.42
28	I	319	CLA	CHC-C1C	2.34	1.43	1.38
28	I	306	CLA	C3B-C4B	2.34	1.49	1.42
28	l	304	CLA	C3B-C4B	2.34	1.49	1.42
28	A	310	CLA	C3B-C4B	2.34	1.49	1.42
28	l	313	CLA	CHC-C1C	2.34	1.43	1.38
28	a	714	CLA	CHC-C1C	2.34	1.43	1.38
28	L	311	CLA	CHC-C1C	2.34	1.43	1.38
28	h	202	CLA	C3B-C4B	2.34	1.49	1.42
28	A	315	CLA	C3B-C4B	2.34	1.49	1.42
26	h	203	DD6	O1-C20	-2.34	1.43	1.46
28	M	312	CLA	CMB-C2B	-2.34	1.46	1.50
28	G	513	CLA	CHC-C1C	2.34	1.43	1.38
28	b	704	CLA	CMC-C2C	-2.34	1.46	1.50
28	B	308	CLA	C3B-C4B	2.34	1.49	1.42
28	K	310	CLA	C3B-C4B	2.34	1.49	1.42
31	I	318	LMG	C4-C5	2.34	1.58	1.53
28	a	707	CLA	CHC-C1C	2.34	1.43	1.38
28	L	309	CLA	CHC-C1C	2.34	1.43	1.38
28	A	319	CLA	C3B-C4B	2.34	1.49	1.42
28	b	726	CLA	CHC-C1C	2.34	1.43	1.38
28	a	728	CLA	C3B-C4B	2.33	1.49	1.42
28	L	308	CLA	C3B-C4B	2.33	1.49	1.42
28	a	703	CLA	CMB-C2B	-2.33	1.46	1.50
26	L	305	DD6	O1-C20	-2.33	1.43	1.46
28	G	520	CLA	CHC-C1C	2.33	1.43	1.38
28	j	106	CLA	CHC-C1C	2.33	1.43	1.38
28	H	308	CLA	CHC-C1C	2.33	1.43	1.38
28	a	708	CLA	CHC-C1C	2.33	1.43	1.38
28	f	302	CLA	C3B-C4B	2.33	1.49	1.42
28	J	315	CLA	CHC-C1C	2.33	1.43	1.38
28	b	720	CLA	C3B-C4B	2.33	1.49	1.42
28	L	318	CLA	C3B-C4B	2.33	1.49	1.42
28	A	315	CLA	CHC-C1C	2.33	1.43	1.38
28	F	315	CLA	CHC-C1C	2.33	1.43	1.38
28	l	313	CLA	C3B-C4B	2.33	1.49	1.42
28	a	725	CLA	CHC-C1C	2.33	1.43	1.38
28	a	702	CLA	CMC-C2C	-2.33	1.46	1.50
28	a	729	CLA	CHC-C1C	2.33	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	H	308	CLA	C3B-C4B	2.33	1.49	1.42
28	f	301	CLA	CHC-C1C	2.33	1.43	1.38
28	H	307	CLA	CHC-C1C	2.33	1.43	1.38
28	A	316	CLA	C3B-C4B	2.33	1.49	1.42
28	I	312	CLA	CHC-C1C	2.33	1.43	1.38
28	a	722	CLA	CHC-C1C	2.33	1.43	1.38
28	a	727	CLA	CHC-C1C	2.33	1.43	1.38
28	L	312	CLA	CHC-C1C	2.33	1.43	1.38
28	B	309	CLA	CHC-C1C	2.33	1.43	1.38
28	G	519	CLA	CHC-C1C	2.33	1.43	1.38
28	G	517	CLA	C3B-C4B	2.33	1.49	1.42
28	a	726	CLA	C1B-C2B	2.33	1.48	1.43
28	a	720	CLA	C3B-C4B	2.33	1.49	1.42
28	K	315	CLA	CHC-C1C	2.33	1.43	1.38
28	a	719	CLA	CHC-C1C	2.33	1.43	1.38
28	a	706	CLA	CHC-C1C	2.32	1.43	1.38
28	D	309	CLA	CHC-C1C	2.32	1.43	1.38
28	N	310	CLA	C3B-C4B	2.32	1.49	1.42
28	A	317	CLA	CHC-C1C	2.32	1.43	1.38
28	b	701	CLA	C3B-C4B	2.32	1.49	1.42
28	J	306	CLA	C3B-C4B	2.32	1.49	1.42
28	b	705	CLA	CHC-C1C	2.32	1.43	1.38
28	a	729	CLA	C3B-C4B	2.32	1.49	1.42
28	l	305	CLA	CHC-C1C	2.32	1.43	1.38
28	M	316	CLA	CHC-C1C	2.32	1.43	1.38
28	a	710	CLA	CHC-C1C	2.32	1.43	1.38
28	b	721	CLA	CMD-C2D	-2.32	1.46	1.50
29	F	309	KC1	C1B-NB	-2.32	1.34	1.37
29	D	315	KC1	C1B-NB	-2.32	1.34	1.37
28	f	302	CLA	CHC-C1C	2.32	1.43	1.38
28	D	309	CLA	C3B-C4B	2.32	1.49	1.42
28	G	512	CLA	C3B-C4B	2.32	1.49	1.42
28	a	710	CLA	C3B-C4B	2.32	1.49	1.42
28	a	702	CLA	C1B-C2B	2.32	1.48	1.43
28	l	311	CLA	CHC-C1C	2.32	1.43	1.38
28	D	312	CLA	CHC-C1C	2.31	1.43	1.38
28	a	716	CLA	CHC-C1C	2.31	1.43	1.38
26	K	305	DD6	O1-C20	-2.31	1.43	1.46
28	K	312	CLA	CHC-C1C	2.31	1.43	1.38
28	a	723	CLA	CHC-C1C	2.31	1.43	1.38
28	H	312	CLA	CHC-C1C	2.31	1.43	1.38
35	i	201	BCR	C1-C6	-2.31	1.50	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	M	315	CLA	CHC-C1C	2.31	1.43	1.38
26	L	306	DD6	O1-C20	-2.31	1.43	1.46
28	B	308	CLA	CHC-C1C	2.31	1.43	1.38
28	b	709	CLA	CHC-C1C	2.31	1.43	1.38
28	l	304	CLA	CHC-C1C	2.31	1.43	1.38
28	I	310	CLA	C3B-C4B	2.31	1.49	1.42
28	b	721	CLA	C3B-C4B	2.31	1.49	1.42
28	F	313	CLA	C3B-C4B	2.30	1.49	1.42
28	A	308	CLA	CHC-C1C	2.30	1.43	1.38
28	b	723	CLA	CHC-C1C	2.30	1.43	1.38
28	a	718	CLA	CHC-C1C	2.30	1.43	1.38
28	b	713	CLA	CHC-C1C	2.30	1.43	1.38
28	a	712	CLA	CHC-C1C	2.30	1.43	1.38
26	K	319	DD6	O1-C20	-2.30	1.43	1.46
28	L	318	CLA	CHC-C1C	2.30	1.43	1.38
28	b	720	CLA	CHC-C1C	2.30	1.43	1.38
28	M	317	CLA	CHC-C1C	2.30	1.43	1.38
27	I	304	UIX	C15-C20	-2.30	1.50	1.54
28	B	315	CLA	CHC-C1C	2.30	1.43	1.38
28	a	712	CLA	C3B-C4B	2.30	1.49	1.42
28	H	311	CLA	CHC-C1C	2.30	1.43	1.38
28	H	311	CLA	C3B-C4B	2.30	1.49	1.42
28	G	514	CLA	CHC-C1C	2.30	1.43	1.38
28	D	308	CLA	CHC-C1C	2.29	1.43	1.38
28	F	308	CLA	C3B-C4B	2.29	1.49	1.42
28	l	310	CLA	CAC-C3C	-2.29	1.47	1.51
28	b	717	CLA	C3B-C4B	2.29	1.49	1.42
31	b	733	LMG	O7-C8	-2.29	1.41	1.46
28	J	308	CLA	CHC-C1C	2.29	1.43	1.38
28	h	202	CLA	CHC-C1C	2.29	1.43	1.38
28	b	701	CLA	CHC-C1C	2.29	1.43	1.38
26	I	303	DD6	C21-C20	-2.29	1.48	1.51
28	A	310	CLA	CHC-C1C	2.28	1.43	1.38
28	B	311	CLA	CHC-C1C	2.28	1.43	1.38
28	B	310	CLA	CHC-C1C	2.28	1.43	1.38
28	a	730	CLA	CHC-C1C	2.28	1.43	1.38
28	B	301	CLA	C3B-C4B	2.28	1.49	1.42
28	N	307	CLA	CHC-C1C	2.28	1.43	1.38
28	G	516	CLA	CHC-C1C	2.28	1.43	1.38
28	m	202	CLA	CHC-C1C	2.28	1.43	1.38
28	F	311	CLA	CHC-C1C	2.28	1.43	1.38
28	a	721	CLA	CHC-C1C	2.28	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	G	517	CLA	CHC-C1C	2.28	1.43	1.38
28	G	511	CLA	CHC-C1C	2.28	1.43	1.38
28	b	722	CLA	C3B-C4B	2.28	1.49	1.42
28	l	303	CLA	CHC-C1C	2.28	1.43	1.38
28	a	715	CLA	C3B-C4B	2.28	1.49	1.42
28	b	712	CLA	CHC-C1C	2.28	1.43	1.38
29	D	310	KC1	C1B-NB	-2.27	1.34	1.37
28	I	315	CLA	CHC-C1C	2.27	1.43	1.38
28	K	311	CLA	CHC-C1C	2.27	1.43	1.38
28	a	713	CLA	CHC-C1C	2.27	1.43	1.38
28	a	720	CLA	CHC-C1C	2.27	1.43	1.38
28	B	307	CLA	CHC-C1C	2.27	1.43	1.38
28	G	518	CLA	CHC-C1C	2.27	1.43	1.38
26	M	304	DD6	C28-C27	-2.27	1.49	1.50
28	a	725	CLA	C3B-C4B	2.27	1.49	1.42
29	L	307	KC1	C1B-NB	-2.27	1.34	1.37
28	b	728	CLA	CHC-C1C	2.26	1.43	1.38
28	D	313	CLA	C3B-C4B	2.26	1.49	1.42
28	a	703	CLA	CMC-C2C	-2.26	1.46	1.50
28	b	722	CLA	CMD-C2D	-2.26	1.46	1.50
26	H	303	DD6	C28-C27	-2.26	1.49	1.50
28	I	310	CLA	CHC-C1C	2.26	1.43	1.38
28	M	308	CLA	CHC-C1C	2.26	1.43	1.38
28	b	711	CLA	CHC-C1C	2.26	1.43	1.38
28	a	738	CLA	CHC-C1C	2.26	1.43	1.38
28	N	304	CLA	CHC-C1C	2.26	1.43	1.38
28	b	703	CLA	C3B-C4B	2.26	1.49	1.42
26	N	303	DD6	O1-C20	-2.26	1.43	1.46
28	A	320	CLA	CHC-C1C	2.26	1.43	1.38
28	a	715	CLA	CHC-C1C	2.26	1.43	1.38
28	H	309	CLA	CHC-C1C	2.26	1.43	1.38
28	F	307	CLA	C3B-C4B	2.26	1.49	1.42
28	B	311	CLA	C3B-C4B	2.26	1.49	1.42
28	G	509	CLA	CHC-C1C	2.26	1.43	1.38
28	a	731	CLA	CHC-C1C	2.25	1.43	1.38
26	A	301	DD6	O1-C20	-2.25	1.43	1.46
28	J	316	CLA	CHC-C1C	2.25	1.43	1.38
28	J	310	CLA	C3B-C4B	2.25	1.49	1.42
28	b	710	CLA	CHC-C1C	2.25	1.43	1.38
28	B	313	CLA	CHC-C1C	2.25	1.43	1.38
28	a	728	CLA	CHC-C1C	2.25	1.43	1.38
28	H	304	CLA	CHC-C1C	2.25	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	A	306	KC1	C1B-NB	-2.24	1.34	1.37
28	F	312	CLA	CMC-C2C	-2.24	1.46	1.50
28	I	307	CLA	CHC-C1C	2.24	1.43	1.38
28	K	306	CLA	CHC-C1C	2.24	1.43	1.38
28	b	719	CLA	CHC-C1C	2.24	1.43	1.38
28	b	721	CLA	CMB-C2B	-2.24	1.46	1.50
28	B	301	CLA	CHC-C1C	2.24	1.43	1.38
32	j	105	PID	C20-C21	2.24	1.41	1.35
28	b	710	CLA	C3B-C4B	2.24	1.49	1.42
28	J	307	CLA	CHC-C1C	2.24	1.43	1.38
28	b	721	CLA	CHC-C1C	2.24	1.43	1.38
28	B	316	CLA	CHC-C1C	2.24	1.43	1.38
28	l	313	CLA	CMB-C2B	-2.24	1.46	1.50
31	D	317	LMG	O7-C8	-2.24	1.41	1.46
28	l	310	CLA	C1D-ND	2.24	1.42	1.38
29	G	515	KC1	C1B-NB	-2.23	1.34	1.37
26	I	303	DD6	C19-C20	2.23	1.55	1.52
28	M	312	CLA	C3B-C4B	2.23	1.49	1.42
28	I	311	CLA	CHC-C1C	2.23	1.43	1.38
35	i	201	BCR	C30-C25	-2.23	1.50	1.53
28	J	309	CLA	C3B-C4B	2.23	1.49	1.42
28	N	305	CLA	CHC-C1C	2.23	1.42	1.38
28	A	307	CLA	CHC-C1C	2.23	1.42	1.38
26	L	302	DD6	O1-C20	-2.22	1.43	1.46
28	b	718	CLA	CMB-C2B	-2.22	1.46	1.50
28	J	306	CLA	CHC-C1C	2.22	1.42	1.38
28	J	308	CLA	CMD-C2D	-2.22	1.46	1.50
26	A	302	DD6	C28-C27	2.22	1.52	1.50
32	N	302	PID	C13-C12	2.22	1.42	1.36
28	A	320	CLA	CMD-C2D	-2.22	1.46	1.50
28	M	312	CLA	CHC-C1C	2.22	1.42	1.38
28	b	713	CLA	CMB-C2B	-2.21	1.46	1.50
28	N	309	CLA	CMD-C2D	-2.20	1.46	1.50
28	N	309	CLA	CMC-C2C	-2.20	1.46	1.50
28	b	708	CLA	CHC-C1C	2.20	1.42	1.38
26	M	303	DD6	C36-C31	-2.20	1.32	1.35
29	I	314	KC1	C1B-NB	-2.20	1.35	1.37
28	I	306	CLA	CHC-C1C	2.20	1.42	1.38
28	b	717	CLA	CMB-C2B	-2.19	1.46	1.50
28	a	702	CLA	MG-ND	-2.19	2.01	2.05
28	b	717	CLA	CHC-C1C	2.19	1.42	1.38
28	a	712	CLA	CMB-C2B	-2.19	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	F	312	CLA	C1B-C2B	2.19	1.48	1.43
28	b	719	CLA	CMB-C2B	-2.19	1.46	1.50
28	l	305	CLA	CMD-C2D	-2.19	1.46	1.50
26	J	304	DD6	C36-C31	-2.18	1.32	1.35
29	J	313	KC1	C1B-NB	-2.18	1.35	1.37
28	a	703	CLA	C1B-C2B	2.18	1.48	1.43
28	b	710	CLA	CMD-C2D	-2.18	1.46	1.50
28	J	308	CLA	MG-NB	-2.18	2.01	2.05
32	F	305	PID	C20-C21	2.18	1.40	1.35
28	D	313	CLA	CMD-C2D	-2.18	1.46	1.50
29	A	314	KC1	C1B-NB	-2.18	1.35	1.37
28	a	703	CLA	MG-ND	-2.18	2.01	2.05
28	M	316	CLA	CMD-C2D	-2.18	1.46	1.50
29	H	310	KC1	C1B-NB	-2.18	1.35	1.37
28	b	709	CLA	CMB-C2B	-2.17	1.46	1.50
28	M	312	CLA	MG-NB	-2.17	2.01	2.05
28	a	711	CLA	CMD-C2D	-2.17	1.46	1.50
29	F	314	KC1	C1B-NB	-2.17	1.35	1.37
28	K	307	CLA	C3B-C4B	2.17	1.49	1.42
28	b	704	CLA	MG-ND	-2.17	2.01	2.05
26	I	301	DD6	O1-C20	-2.17	1.43	1.46
28	J	309	CLA	CHC-C1C	2.17	1.42	1.38
28	B	311	CLA	MG-NB	-2.17	2.01	2.05
28	F	308	CLA	CHC-C1C	2.17	1.42	1.38
28	a	724	CLA	MG-NB	-2.17	2.01	2.05
28	I	312	CLA	CMB-C2B	-2.17	1.46	1.50
28	a	712	CLA	MG-NB	-2.17	2.01	2.05
28	G	512	CLA	CMC-C2C	-2.17	1.46	1.50
26	F	301	DD6	O1-C20	-2.17	1.43	1.46
28	a	719	CLA	CMD-C2D	-2.17	1.46	1.50
28	G	512	CLA	CHC-C1C	2.16	1.42	1.38
28	K	311	CLA	CMD-C2D	-2.16	1.46	1.50
26	G	502	DD6	O1-C20	-2.16	1.43	1.46
28	b	701	CLA	CMB-C2B	-2.16	1.46	1.50
29	K	314	KC1	C1B-NB	-2.16	1.35	1.37
28	D	313	CLA	CHC-C1C	2.16	1.42	1.38
28	G	518	CLA	CMB-C2B	-2.16	1.46	1.50
28	a	719	CLA	CMC-C2C	-2.16	1.46	1.50
28	K	307	CLA	MG-NB	-2.16	2.01	2.05
28	a	724	CLA	CHC-C1C	2.16	1.42	1.38
28	b	709	CLA	CMD-C2D	-2.16	1.46	1.50
28	b	704	CLA	C4B-NB	2.16	1.40	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	b	713	CLA	MG-NB	-2.16	2.01	2.05
28	a	709	CLA	CMB-C2B	-2.15	1.46	1.50
28	a	719	CLA	CMB-C2B	-2.15	1.46	1.50
28	b	703	CLA	CMD-C2D	-2.15	1.46	1.50
28	a	703	CLA	C4B-NB	2.15	1.40	1.37
29	M	314	KC1	C1B-NB	-2.15	1.35	1.37
28	a	723	CLA	CMD-C2D	-2.15	1.46	1.50
29	G	515	KC1	C4A-C3A	-2.15	1.40	1.44
26	L	303	DD6	O1-C20	-2.15	1.43	1.46
28	b	722	CLA	MG-NB	-2.15	2.01	2.05
33	A	318	SQD	O8-S	2.15	1.55	1.47
28	K	315	CLA	CMD-C2D	-2.15	1.46	1.50
28	K	316	CLA	CHC-C1C	2.15	1.42	1.38
28	F	307	CLA	CHC-C1C	2.14	1.42	1.38
28	a	713	CLA	MG-NB	-2.14	2.01	2.05
28	j	106	CLA	CMD-C2D	-2.14	1.46	1.50
28	b	717	CLA	CMC-C2C	-2.14	1.46	1.50
26	A	303	DD6	O1-C20	-2.14	1.43	1.46
28	a	727	CLA	CMD-C2D	-2.14	1.46	1.50
28	b	701	CLA	CMD-C2D	-2.14	1.46	1.50
28	K	316	CLA	CMB-C2B	-2.14	1.46	1.50
28	J	306	CLA	CMD-C2D	-2.14	1.46	1.50
28	J	308	CLA	CMB-C2B	-2.14	1.46	1.50
26	A	305	DD6	O1-C20	-2.14	1.43	1.46
28	a	706	CLA	CMC-C2C	-2.13	1.46	1.50
28	F	313	CLA	CHC-C1C	2.13	1.42	1.38
28	L	317	CLA	CHC-C1C	2.13	1.42	1.38
28	b	721	CLA	MG-NB	-2.13	2.01	2.05
29	A	314	KC1	C4A-C3A	-2.13	1.40	1.44
28	I	311	CLA	CMB-C2B	-2.13	1.46	1.50
26	M	303	DD6	C21-C20	2.13	1.55	1.51
28	a	701	CLA	CMD-C2D	-2.13	1.46	1.50
29	N	306	KC1	C1B-NB	-2.13	1.35	1.37
28	G	511	CLA	CMD-C2D	-2.13	1.46	1.50
28	l	312	CLA	CMB-C2B	-2.13	1.46	1.50
29	L	315	KC1	C1B-NB	-2.13	1.35	1.37
28	A	316	CLA	CHC-C1C	2.12	1.42	1.38
28	b	718	CLA	CHC-C1C	2.12	1.42	1.38
29	A	306	KC1	C4A-C3A	-2.12	1.40	1.44
29	M	307	KC1	C1B-NB	-2.12	1.35	1.37
28	A	310	CLA	CMB-C2B	-2.12	1.46	1.50
28	a	715	CLA	CMD-C2D	-2.12	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	K	311	CLA	CMB-C2B	-2.12	1.46	1.50
28	b	712	CLA	MG-NB	-2.12	2.01	2.05
29	F	309	KC1	C4A-C3A	-2.12	1.40	1.44
29	B	314	KC1	C1B-NB	-2.12	1.35	1.37
28	N	307	CLA	CMD-C2D	-2.11	1.46	1.50
28	l	303	CLA	CMB-C2B	-2.11	1.46	1.50
29	N	311	KC1	C1B-NB	-2.11	1.35	1.37
28	F	313	CLA	CMD-C2D	-2.11	1.46	1.50
26	M	305	DD6	C28-C27	-2.11	1.49	1.50
28	A	315	CLA	CMD-C2D	-2.11	1.46	1.50
26	G	504	DD6	C28-C27	-2.11	1.49	1.50
28	N	310	CLA	CHC-C1C	2.11	1.42	1.38
29	D	310	KC1	C4A-C3A	-2.11	1.40	1.44
28	B	301	CLA	CMB-C2B	-2.11	1.46	1.50
28	b	706	CLA	CMB-C2B	-2.10	1.46	1.50
28	a	702	CLA	C4B-NB	2.10	1.40	1.37
28	D	314	CLA	CMB-C2B	-2.10	1.46	1.50
28	H	308	CLA	CMD-C2D	-2.10	1.46	1.50
28	b	723	CLA	CMB-C2B	-2.10	1.46	1.50
29	J	313	KC1	C4A-C3A	-2.10	1.40	1.44
28	A	319	CLA	CMD-C2D	-2.10	1.46	1.50
28	A	310	CLA	CMD-C2D	-2.10	1.46	1.50
29	H	306	KC1	C1B-NB	-2.10	1.35	1.37
28	B	316	CLA	CMB-C2B	-2.09	1.46	1.50
28	a	729	CLA	CMD-C2D	-2.09	1.46	1.50
28	a	717	CLA	CMB-C2B	-2.09	1.46	1.50
28	b	713	CLA	CMD-C2D	-2.09	1.46	1.50
28	N	305	CLA	CMB-C2B	-2.09	1.46	1.50
28	F	312	CLA	MG-ND	-2.09	2.01	2.05
28	G	512	CLA	CMB-C2B	-2.09	1.46	1.50
28	J	310	CLA	CMD-C2D	-2.09	1.46	1.50
28	M	311	CLA	CMB-C2B	-2.09	1.46	1.50
28	b	701	CLA	MG-NB	-2.09	2.01	2.05
28	K	310	CLA	MG-NB	-2.09	2.01	2.05
28	M	311	CLA	MG-NB	-2.09	2.01	2.05
28	F	308	CLA	CMC-C2C	-2.09	1.46	1.50
28	H	311	CLA	CMD-C2D	-2.09	1.46	1.50
32	D	307	PID	C20-C21	2.09	1.40	1.35
28	b	710	CLA	MG-NB	-2.09	2.01	2.05
28	D	316	CLA	CMC-C2C	-2.09	1.46	1.50
28	I	308	CLA	CMB-C2B	-2.08	1.46	1.50
28	J	310	CLA	CHC-C1C	2.08	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	A	320	CLA	CMB-C2B	-2.08	1.46	1.50
28	a	704	CLA	CMD-C2D	-2.08	1.46	1.50
28	a	728	CLA	MG-NB	-2.08	2.01	2.05
28	J	310	CLA	MG-NB	-2.08	2.01	2.05
28	K	312	CLA	CMD-C2D	-2.08	1.46	1.50
28	D	314	CLA	MG-NB	-2.08	2.01	2.05
28	f	302	CLA	MG-NB	-2.08	2.01	2.05
28	K	313	CLA	CMC-C2C	-2.08	1.46	1.50
28	L	312	CLA	CMB-C2B	-2.08	1.46	1.50
28	B	317	CLA	CMB-C2B	-2.08	1.46	1.50
28	a	707	CLA	CMD-C2D	-2.08	1.46	1.50
28	H	312	CLA	CMD-C2D	-2.08	1.46	1.50
28	B	317	CLA	CMD-C2D	-2.08	1.46	1.50
28	b	726	CLA	CMB-C2B	-2.08	1.46	1.50
28	M	317	CLA	CMD-C2D	-2.08	1.46	1.50
28	b	712	CLA	CMD-C2D	-2.07	1.46	1.50
28	I	313	CLA	CMD-C2D	-2.07	1.46	1.50
28	K	310	CLA	CMB-C2B	-2.07	1.46	1.50
28	K	312	CLA	CMC-C2C	-2.07	1.46	1.50
31	b	734	LMG	O7-C8	-2.07	1.41	1.46
28	a	715	CLA	CMB-C2B	-2.07	1.46	1.50
28	F	307	CLA	CMD-C2D	-2.07	1.46	1.50
28	a	730	CLA	CMC-C2C	-2.07	1.46	1.50
28	L	318	CLA	CMB-C2B	-2.07	1.46	1.50
28	L	317	CLA	CMD-C2D	-2.07	1.46	1.50
28	G	513	CLA	CMD-C2D	-2.07	1.46	1.50
28	A	316	CLA	CMC-C2C	-2.07	1.46	1.50
28	H	309	CLA	CMB-C2B	-2.07	1.46	1.50
28	J	316	CLA	CMB-C2B	-2.07	1.46	1.50
28	M	310	CLA	CMD-C2D	-2.07	1.46	1.50
28	a	731	CLA	CMD-C2D	-2.07	1.46	1.50
28	L	316	CLA	CMB-C2B	-2.07	1.46	1.50
28	a	717	CLA	CMC-C2C	-2.07	1.46	1.50
28	K	316	CLA	CMD-C2D	-2.06	1.46	1.50
28	b	727	CLA	CMC-C2C	-2.06	1.46	1.50
28	N	305	CLA	MG-NB	-2.06	2.01	2.05
28	b	724	CLA	CMD-C2D	-2.06	1.46	1.50
27	I	304	UIX	O2-C18	-2.06	1.41	1.46
28	b	705	CLA	CMD-C2D	-2.06	1.46	1.50
28	a	714	CLA	CMD-C2D	-2.06	1.46	1.50
28	B	312	CLA	CMB-C2B	-2.06	1.46	1.50
28	I	312	CLA	CMD-C2D	-2.06	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	J	316	CLA	CMD-C2D	-2.06	1.46	1.50
28	G	514	CLA	CMC-C2C	-2.06	1.46	1.50
28	b	719	CLA	CMD-C2D	-2.06	1.46	1.50
28	b	725	CLA	CMC-C2C	-2.06	1.46	1.50
28	b	717	CLA	MG-NB	-2.06	2.01	2.05
28	G	519	CLA	CMB-C2B	-2.06	1.46	1.50
28	A	317	CLA	CMB-C2B	-2.06	1.46	1.50
28	l	311	CLA	CMD-C2D	-2.06	1.46	1.50
28	b	728	CLA	CMB-C2B	-2.06	1.46	1.50
28	L	308	CLA	CMB-C2B	-2.06	1.46	1.50
28	N	310	CLA	CMB-C2B	-2.06	1.46	1.50
28	L	318	CLA	CMC-C2C	-2.06	1.46	1.50
28	M	316	CLA	CMB-C2B	-2.06	1.46	1.50
28	A	312	CLA	CMD-C2D	-2.06	1.46	1.50
28	N	304	CLA	CMB-C2B	-2.06	1.46	1.50
28	I	319	CLA	CMD-C2D	-2.06	1.46	1.50
28	G	518	CLA	MG-NB	-2.06	2.01	2.05
28	L	318	CLA	CMD-C2D	-2.05	1.46	1.50
28	M	313	CLA	CMD-C2D	-2.05	1.46	1.50
28	a	712	CLA	CMD-C2D	-2.05	1.46	1.50
28	M	318	CLA	CMD-C2D	-2.05	1.46	1.50
28	a	702	CLA	C1B-NB	-2.05	1.35	1.37
29	D	315	KC1	C4A-C3A	-2.05	1.40	1.44
28	f	301	CLA	CMB-C2B	-2.05	1.46	1.50
28	L	311	CLA	CMD-C2D	-2.05	1.46	1.50
28	I	321	CLA	CMC-C2C	-2.05	1.46	1.50
28	a	725	CLA	CMD-C2D	-2.05	1.46	1.50
28	b	727	CLA	CMD-C2D	-2.05	1.46	1.50
28	a	725	CLA	CMB-C2B	-2.05	1.46	1.50
28	b	708	CLA	CMD-C2D	-2.05	1.46	1.50
28	F	310	CLA	CMD-C2D	-2.05	1.46	1.50
28	a	701	CLA	CMB-C2B	-2.05	1.46	1.50
28	K	306	CLA	CMB-C2B	-2.05	1.46	1.50
28	M	311	CLA	CMD-C2D	-2.05	1.46	1.50
28	h	202	CLA	CMD-C2D	-2.05	1.46	1.50
28	a	713	CLA	CMD-C2D	-2.05	1.46	1.50
28	a	721	CLA	CMD-C2D	-2.05	1.46	1.50
28	J	307	CLA	CMD-C2D	-2.05	1.46	1.50
28	L	314	CLA	CMD-C2D	-2.05	1.46	1.50
28	b	724	CLA	MG-NB	-2.05	2.01	2.05
28	J	309	CLA	MG-NB	-2.05	2.01	2.05
26	D	303	DD6	O1-C20	-2.05	1.43	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	N	310	CLA	CMD-C2D	-2.05	1.46	1.50
28	a	710	CLA	MG-NB	-2.05	2.01	2.05
28	L	310	CLA	MG-NB	-2.05	2.01	2.05
28	G	514	CLA	CMB-C2B	-2.05	1.46	1.50
28	A	316	CLA	CMB-C2B	-2.05	1.46	1.50
28	A	319	CLA	CMC-C2C	-2.05	1.46	1.50
28	M	318	CLA	CMB-C2B	-2.05	1.46	1.50
28	I	310	CLA	CMD-C2D	-2.05	1.46	1.50
26	G	504	DD6	C17-C16	-2.05	1.51	1.54
28	I	306	CLA	CMB-C2B	-2.05	1.46	1.50
28	I	319	CLA	MG-NB	-2.05	2.01	2.05
28	j	106	CLA	CMC-C2C	-2.05	1.46	1.50
28	l	303	CLA	CMD-C2D	-2.05	1.46	1.50
28	L	313	CLA	CMD-C2D	-2.05	1.46	1.50
28	I	315	CLA	CMD-C2D	-2.04	1.46	1.50
28	A	308	CLA	CMD-C2D	-2.04	1.46	1.50
29	M	307	KC1	C4A-C3A	-2.04	1.40	1.44
28	a	726	CLA	CMD-C2D	-2.04	1.46	1.50
28	a	722	CLA	CMC-C2C	-2.04	1.46	1.50
28	B	307	CLA	CMB-C2B	-2.04	1.46	1.50
28	F	307	CLA	CMB-C2B	-2.04	1.46	1.50
28	a	726	CLA	MG-NB	-2.04	2.01	2.05
28	B	309	CLA	CMD-C2D	-2.04	1.46	1.50
28	D	314	CLA	CMD-C2D	-2.04	1.46	1.50
28	F	308	CLA	CMB-C2B	-2.04	1.46	1.50
28	G	518	CLA	CMD-C2D	-2.04	1.46	1.50
28	J	314	CLA	CMD-C2D	-2.04	1.46	1.50
28	f	301	CLA	CMD-C2D	-2.04	1.46	1.50
28	a	708	CLA	CMB-C2B	-2.04	1.46	1.50
28	M	318	CLA	MG-NB	-2.04	2.01	2.05
28	K	310	CLA	CMD-C2D	-2.04	1.46	1.50
28	G	519	CLA	CMD-C2D	-2.04	1.46	1.50
28	l	312	CLA	CMD-C2D	-2.04	1.46	1.50
28	J	315	CLA	CMD-C2D	-2.04	1.46	1.50
28	F	311	CLA	MG-NB	-2.04	2.01	2.05
28	I	315	CLA	CMB-C2B	-2.04	1.46	1.50
28	F	311	CLA	CMD-C2D	-2.04	1.46	1.50
28	L	317	CLA	CMB-C2B	-2.04	1.46	1.50
28	a	723	CLA	CMC-C2C	-2.04	1.46	1.50
28	a	730	CLA	CMD-C2D	-2.04	1.46	1.50
29	L	315	KC1	C4A-C3A	-2.04	1.40	1.44
28	D	312	CLA	MG-NB	-2.04	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	I	313	CLA	CMC-C2C	-2.04	1.46	1.50
28	H	308	CLA	MG-NB	-2.04	2.01	2.05
28	a	716	CLA	CMB-C2B	-2.04	1.46	1.50
28	D	313	CLA	MG-NB	-2.04	2.01	2.05
28	l	308	CLA	CMB-C2B	-2.04	1.46	1.50
28	H	312	CLA	MG-NB	-2.04	2.01	2.05
28	D	309	CLA	MG-NB	-2.03	2.01	2.05
28	I	309	CLA	CMD-C2D	-2.03	1.46	1.50
28	J	312	CLA	CMD-C2D	-2.03	1.46	1.50
28	N	307	CLA	CMC-C2C	-2.03	1.46	1.50
28	K	306	CLA	CMD-C2D	-2.03	1.46	1.50
28	m	202	CLA	CMD-C2D	-2.03	1.46	1.50
28	b	705	CLA	CMB-C2B	-2.03	1.46	1.50
28	b	720	CLA	CMD-C2D	-2.03	1.46	1.50
28	b	728	CLA	CMC-C2C	-2.03	1.46	1.50
28	H	311	CLA	CMB-C2B	-2.03	1.46	1.50
28	F	311	CLA	CMB-C2B	-2.03	1.46	1.50
28	A	311	CLA	CMB-C2B	-2.03	1.46	1.50
28	b	726	CLA	CMD-C2D	-2.03	1.46	1.50
28	J	301	CLA	MG-NB	-2.03	2.01	2.05
28	a	709	CLA	CMD-C2D	-2.03	1.46	1.50
28	b	714	CLA	CMD-C2D	-2.03	1.46	1.50
28	B	317	CLA	MG-NB	-2.03	2.01	2.05
28	G	510	CLA	CMC-C2C	-2.03	1.46	1.50
28	a	705	CLA	CMD-C2D	-2.03	1.46	1.50
28	b	724	CLA	CMB-C2B	-2.03	1.46	1.50
28	b	722	CLA	CHC-C1C	2.03	1.42	1.38
28	A	307	CLA	CMD-C2D	-2.03	1.46	1.50
28	a	706	CLA	CMD-C2D	-2.03	1.46	1.50
29	K	314	KC1	C4A-C3A	-2.03	1.40	1.44
28	a	726	CLA	CMB-C2B	-2.03	1.46	1.50
28	K	309	CLA	MG-NB	-2.03	2.01	2.05
28	G	520	CLA	CMD-C2D	-2.03	1.46	1.50
28	I	312	CLA	MG-NB	-2.03	2.01	2.05
28	G	511	CLA	CMB-C2B	-2.03	1.46	1.50
28	B	310	CLA	MG-NB	-2.03	2.01	2.05
28	J	315	CLA	MG-NB	-2.03	2.01	2.05
28	m	202	CLA	MG-NB	-2.03	2.01	2.05
28	G	513	CLA	CMC-C2C	-2.03	1.46	1.50
28	J	312	CLA	CMB-C2B	-2.03	1.46	1.50
28	I	308	CLA	MG-NB	-2.03	2.01	2.05
28	G	513	CLA	MG-NB	-2.03	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	B	303	DD6	O1-C20	-2.03	1.43	1.46
28	f	303	CLA	CMC-C2C	-2.03	1.46	1.50
28	B	307	CLA	CMD-C2D	-2.03	1.46	1.50
28	f	303	CLA	MG-NB	-2.03	2.01	2.05
28	K	307	CLA	CMB-C2B	-2.03	1.46	1.50
28	J	301	CLA	CMD-C2D	-2.03	1.46	1.50
28	a	728	CLA	CMB-C2B	-2.03	1.46	1.50
28	l	310	CLA	C4B-NB	2.03	1.42	1.38
28	b	703	CLA	CMC-C2C	-2.02	1.46	1.50
28	a	727	CLA	CMB-C2B	-2.02	1.46	1.50
28	H	307	CLA	CMD-C2D	-2.02	1.46	1.50
28	b	716	CLA	CMC-C2C	-2.02	1.46	1.50
28	F	315	CLA	CMD-C2D	-2.02	1.46	1.50
28	h	202	CLA	CMB-C2B	-2.02	1.46	1.50
28	a	720	CLA	CMD-C2D	-2.02	1.46	1.50
28	H	307	CLA	CMB-C2B	-2.02	1.46	1.50
28	K	312	CLA	CMB-C2B	-2.02	1.46	1.50
28	B	315	CLA	CMC-C2C	-2.02	1.46	1.50
28	F	307	CLA	MG-NB	-2.02	2.01	2.05
28	b	723	CLA	CMD-C2D	-2.02	1.46	1.50
28	A	310	CLA	MG-NB	-2.02	2.01	2.05
28	I	308	CLA	CMD-C2D	-2.02	1.46	1.50
28	a	728	CLA	CMD-C2D	-2.02	1.46	1.50
28	M	308	CLA	MG-NB	-2.02	2.01	2.05
28	B	315	CLA	CMD-C2D	-2.02	1.46	1.50
28	F	308	CLA	CMD-C2D	-2.02	1.46	1.50
28	A	309	CLA	MG-NB	-2.02	2.01	2.05
28	a	709	CLA	MG-NB	-2.02	2.01	2.05
28	a	723	CLA	CMB-C2B	-2.02	1.46	1.50
28	a	719	CLA	MG-NB	-2.02	2.01	2.05
28	a	703	CLA	CAA-C2A	-2.02	1.50	1.54
28	A	311	CLA	CMD-C2D	-2.02	1.46	1.50
28	b	707	CLA	CMD-C2D	-2.02	1.46	1.50
28	L	314	CLA	MG-NB	-2.02	2.01	2.05
31	K	317	LMG	O7-C8	-2.02	1.41	1.46
28	G	514	CLA	CMD-C2D	-2.02	1.46	1.50
28	b	720	CLA	CMC-C2C	-2.02	1.46	1.50
28	M	308	CLA	CMB-C2B	-2.02	1.46	1.50
28	N	305	CLA	CMD-C2D	-2.02	1.46	1.50
28	D	312	CLA	CMB-C2B	-2.02	1.46	1.50
28	F	313	CLA	CMC-C2C	-2.02	1.46	1.50
28	l	305	CLA	MG-NB	-2.02	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	K	308	CLA	CMD-C2D	-2.02	1.46	1.50
28	K	309	CLA	CMC-C2C	-2.02	1.46	1.50
28	a	722	CLA	CMD-C2D	-2.02	1.46	1.50
28	L	313	CLA	CMB-C2B	-2.02	1.46	1.50
28	a	710	CLA	CMC-C2C	-2.02	1.46	1.50
28	L	308	CLA	CMD-C2D	-2.02	1.46	1.50
28	L	312	CLA	CMD-C2D	-2.02	1.46	1.50
28	D	312	CLA	CMD-C2D	-2.02	1.46	1.50
28	M	309	CLA	CMD-C2D	-2.02	1.46	1.50
28	M	312	CLA	CMD-C2D	-2.02	1.46	1.50
28	N	304	CLA	CMD-C2D	-2.02	1.46	1.50
28	a	721	CLA	MG-NB	-2.02	2.01	2.05
28	a	720	CLA	CMB-C2B	-2.02	1.46	1.50
28	b	714	CLA	CMC-C2C	-2.02	1.46	1.50
28	G	517	CLA	MG-NB	-2.02	2.01	2.05
28	J	312	CLA	MG-NB	-2.02	2.01	2.05
28	G	510	CLA	CMB-C2B	-2.01	1.46	1.50
31	j	101	LMG	O7-C8	-2.01	1.41	1.46
28	a	704	CLA	CMB-C2B	-2.01	1.46	1.50
28	B	313	CLA	CMD-C2D	-2.01	1.46	1.50
28	D	313	CLA	CMC-C2C	-2.01	1.46	1.50
28	A	317	CLA	CMC-C2C	-2.01	1.46	1.50
28	a	735	CLA	CMD-C2D	-2.01	1.46	1.50
28	a	715	CLA	MG-NB	-2.01	2.01	2.05
28	j	104	CLA	CMB-C2B	-2.01	1.46	1.50
28	B	311	CLA	CMB-C2B	-2.01	1.46	1.50
28	b	708	CLA	CMB-C2B	-2.01	1.46	1.50
28	L	316	CLA	CMD-C2D	-2.01	1.46	1.50
28	M	315	CLA	CMD-C2D	-2.01	1.46	1.50
28	l	308	CLA	CMD-C2D	-2.01	1.46	1.50
28	A	320	CLA	MG-NB	-2.01	2.01	2.05
28	J	309	CLA	CMB-C2B	-2.01	1.46	1.50
28	M	313	CLA	CMC-C2C	-2.01	1.46	1.50
28	A	312	CLA	CMC-C2C	-2.01	1.46	1.50
28	D	316	CLA	CMD-C2D	-2.01	1.46	1.50
28	A	313	CLA	CMD-C2D	-2.01	1.46	1.50
28	l	309	CLA	MG-NB	-2.01	2.01	2.05
28	M	316	CLA	MG-NB	-2.01	2.01	2.05
28	D	308	CLA	CMB-C2B	-2.01	1.46	1.50
28	J	309	CLA	CMC-C2C	-2.01	1.46	1.50
28	M	308	CLA	CMD-C2D	-2.01	1.46	1.50
28	J	307	CLA	MG-NB	-2.01	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	a	721	CLA	CMB-C2B	-2.01	1.46	1.50
28	b	716	CLA	CMD-C2D	-2.01	1.46	1.50
28	H	305	CLA	CMD-C2D	-2.01	1.46	1.50
28	I	309	CLA	MG-NB	-2.01	2.01	2.05
28	a	723	CLA	MG-NB	-2.01	2.01	2.05
28	a	730	CLA	MG-NB	-2.01	2.01	2.05
28	J	311	CLA	CMB-C2B	-2.01	1.46	1.50
28	B	312	CLA	CMD-C2D	-2.01	1.46	1.50
28	J	312	CLA	CMC-C2C	-2.01	1.46	1.50
28	G	509	CLA	CMB-C2B	-2.01	1.46	1.50
28	K	316	CLA	MG-NB	-2.01	2.01	2.05
28	B	313	CLA	CMB-C2B	-2.01	1.46	1.50
28	G	520	CLA	MG-NB	-2.01	2.01	2.05
28	I	307	CLA	CMD-C2D	-2.01	1.46	1.50
28	a	708	CLA	CMD-C2D	-2.01	1.46	1.50
28	b	709	CLA	CMC-C2C	-2.01	1.46	1.50
28	f	302	CLA	CMB-C2B	-2.00	1.46	1.50
28	b	725	CLA	CMD-C2D	-2.00	1.46	1.50
28	b	723	CLA	MG-NB	-2.00	2.01	2.05
28	N	307	CLA	MG-NB	-2.00	2.01	2.05
28	G	516	CLA	CMD-C2D	-2.00	1.46	1.50
28	j	104	CLA	CMD-C2D	-2.00	1.46	1.50
28	l	305	CLA	CMB-C2B	-2.00	1.46	1.50
28	a	705	CLA	CMC-C2C	-2.00	1.46	1.50
28	B	310	CLA	CMB-C2B	-2.00	1.46	1.50
28	B	316	CLA	CMD-C2D	-2.00	1.46	1.50
28	a	717	CLA	MG-NB	-2.00	2.01	2.05
28	a	711	CLA	CMB-C2B	-2.00	1.46	1.50
28	a	731	CLA	CMB-C2B	-2.00	1.46	1.50
28	H	307	CLA	CMC-C2C	-2.00	1.46	1.50
28	j	106	CLA	MG-NB	-2.00	2.01	2.05
28	H	304	CLA	MG-NB	-2.00	2.01	2.05
28	L	314	CLA	CMC-C2C	-2.00	1.46	1.50
28	a	703	CLA	C1B-NB	-2.00	1.35	1.37
28	b	719	CLA	MG-NB	-2.00	2.01	2.05
28	J	306	CLA	MG-NB	-2.00	2.01	2.05
28	K	307	CLA	CMD-C2D	-2.00	1.46	1.50
28	A	308	CLA	MG-NB	-2.00	2.01	2.05
29	I	314	KC1	C4A-C3A	-2.00	1.40	1.44
28	f	303	CLA	CMB-C2B	-2.00	1.46	1.50
28	D	308	CLA	CMD-C2D	-2.00	1.46	1.50
28	a	718	CLA	CMD-C2D	-2.00	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	b	708	CLA	MG-NB	-2.00	2.01	2.05
28	H	307	CLA	MG-NB	-2.00	2.01	2.05

All (2478) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	I	304	UIX	C6-C1-C	-9.09	107.34	122.30
35	m	201	BCR	C7-C8-C9	-8.29	113.98	126.23
28	l	304	CLA	C4A-NA-C1A	7.47	110.09	106.68
27	G	503	UIX	C6-C1-C	-7.23	110.40	122.30
27	I	304	UIX	O-C1-C3	7.23	120.27	113.49
26	J	303	DD6	C3-C2-C1	-7.20	117.18	127.28
28	J	307	CLA	C4A-NA-C1A	7.14	109.94	106.68
27	h	201	UIX	C6-C1-C	-7.09	110.63	122.30
28	N	310	CLA	C4A-NA-C1A	7.05	109.89	106.68
27	J	305	UIX	O-C1-C3	7.04	120.09	113.49
28	B	308	CLA	C4A-NA-C1A	7.02	109.88	106.68
28	a	702	CLA	C4A-NA-C1A	7.01	109.88	106.68
27	J	305	UIX	C6-C1-C	-7.00	110.78	122.30
28	G	512	CLA	C4A-NA-C1A	6.99	109.87	106.68
28	J	309	CLA	C4A-NA-C1A	6.98	109.86	106.68
28	L	309	CLA	C4A-NA-C1A	6.98	109.86	106.68
28	a	738	CLA	C4A-NA-C1A	6.97	109.86	106.68
28	b	714	CLA	C4A-NA-C1A	6.97	109.86	106.68
28	A	310	CLA	C4A-NA-C1A	6.97	109.86	106.68
28	M	317	CLA	C4A-NA-C1A	6.96	109.85	106.68
28	b	704	CLA	C4A-NA-C1A	6.95	109.85	106.68
28	L	311	CLA	C4A-NA-C1A	6.94	109.84	106.68
27	B	305	UIX	C6-C1-C	-6.93	110.89	122.30
28	a	730	CLA	C4A-NA-C1A	6.93	109.84	106.68
28	a	715	CLA	C4A-NA-C1A	6.92	109.84	106.68
28	b	719	CLA	C4A-NA-C1A	6.91	109.83	106.68
28	J	312	CLA	C4A-NA-C1A	6.90	109.83	106.68
28	M	315	CLA	C4A-NA-C1A	6.90	109.83	106.68
28	b	728	CLA	C4A-NA-C1A	6.90	109.83	106.68
28	B	317	CLA	C4A-NA-C1A	6.88	109.82	106.68
28	b	718	CLA	C4A-NA-C1A	6.87	109.81	106.68
28	L	318	CLA	C4A-NA-C1A	6.87	109.81	106.68
28	D	311	CLA	C4A-NA-C1A	6.86	109.81	106.68
28	J	306	CLA	C4A-NA-C1A	6.83	109.80	106.68
28	K	312	CLA	C4A-NA-C1A	6.82	109.79	106.68
28	a	703	CLA	C4A-NA-C1A	6.81	109.79	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	l	303	CLA	C4A-NA-C1A	6.81	109.79	106.68
28	B	313	CLA	C4A-NA-C1A	6.81	109.79	106.68
28	N	309	CLA	C4A-NA-C1A	6.81	109.79	106.68
28	h	202	CLA	C4A-NA-C1A	6.80	109.78	106.68
28	B	315	CLA	C4A-NA-C1A	6.80	109.78	106.68
35	b	702	BCR	C24-C23-C22	-6.79	116.19	126.23
28	M	310	CLA	C4A-NA-C1A	6.78	109.77	106.68
28	F	310	CLA	C4A-NA-C1A	6.78	109.77	106.68
35	b	730	BCR	C7-C8-C9	-6.77	116.22	126.23
28	a	714	CLA	C4A-NA-C1A	6.76	109.76	106.68
28	I	306	CLA	C4A-NA-C1A	6.76	109.76	106.68
28	A	308	CLA	C4A-NA-C1A	6.76	109.76	106.68
28	J	315	CLA	C4A-NA-C1A	6.76	109.76	106.68
28	A	307	CLA	C4A-NA-C1A	6.75	109.76	106.68
28	G	514	CLA	C4A-NA-C1A	6.75	109.76	106.68
28	b	720	CLA	C4A-NA-C1A	6.75	109.76	106.68
28	a	720	CLA	C4A-NA-C1A	6.74	109.76	106.68
28	I	307	CLA	C4A-NA-C1A	6.74	109.75	106.68
28	a	705	CLA	C4A-NA-C1A	6.73	109.75	106.68
28	F	313	CLA	C4A-NA-C1A	6.73	109.75	106.68
28	A	316	CLA	C4A-NA-C1A	6.72	109.75	106.68
28	A	320	CLA	C4A-NA-C1A	6.72	109.74	106.68
26	M	303	DD6	C9-C10-C11	-6.71	117.87	127.28
28	b	705	CLA	C4A-NA-C1A	6.71	109.74	106.68
28	b	707	CLA	C4A-NA-C1A	6.70	109.74	106.68
28	a	701	CLA	C4A-NA-C1A	6.70	109.73	106.68
28	b	701	CLA	C4A-NA-C1A	6.70	109.73	106.68
28	a	731	CLA	C4A-NA-C1A	6.68	109.73	106.68
28	b	709	CLA	C4A-NA-C1A	6.68	109.73	106.68
28	I	319	CLA	C4A-NA-C1A	6.68	109.72	106.68
28	F	308	CLA	C4A-NA-C1A	6.68	109.72	106.68
28	F	315	CLA	C4A-NA-C1A	6.67	109.72	106.68
28	K	316	CLA	C4A-NA-C1A	6.66	109.72	106.68
28	b	727	CLA	C4A-NA-C1A	6.65	109.72	106.68
28	G	517	CLA	C4A-NA-C1A	6.64	109.71	106.68
28	a	718	CLA	C4A-NA-C1A	6.64	109.71	106.68
28	I	311	CLA	C4A-NA-C1A	6.64	109.71	106.68
28	G	519	CLA	C4A-NA-C1A	6.63	109.71	106.68
28	N	304	CLA	C4A-NA-C1A	6.63	109.70	106.68
28	b	716	CLA	C4A-NA-C1A	6.63	109.70	106.68
28	B	312	CLA	C4A-NA-C1A	6.63	109.70	106.68
28	B	309	CLA	C4A-NA-C1A	6.62	109.70	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	a	716	CLA	C4A-NA-C1A	6.62	109.70	106.68
28	M	308	CLA	C4A-NA-C1A	6.62	109.70	106.68
28	K	307	CLA	C4A-NA-C1A	6.61	109.70	106.68
28	G	518	CLA	C4A-NA-C1A	6.61	109.70	106.68
27	A	304	UIX	C6-C1-C	-6.61	111.43	122.30
28	a	711	CLA	C4A-NA-C1A	6.61	109.69	106.68
28	H	308	CLA	C4A-NA-C1A	6.60	109.69	106.68
28	a	722	CLA	C4A-NA-C1A	6.60	109.69	106.68
28	D	313	CLA	C4A-NA-C1A	6.60	109.69	106.68
28	L	312	CLA	C4A-NA-C1A	6.60	109.69	106.68
28	F	307	CLA	C4A-NA-C1A	6.60	109.69	106.68
28	N	305	CLA	C4A-NA-C1A	6.59	109.69	106.68
28	K	306	CLA	C4A-NA-C1A	6.59	109.68	106.68
28	D	312	CLA	C4A-NA-C1A	6.58	109.68	106.68
28	a	725	CLA	C4A-NA-C1A	6.58	109.68	106.68
28	L	316	CLA	C4A-NA-C1A	6.58	109.68	106.68
28	A	311	CLA	C4A-NA-C1A	6.58	109.68	106.68
28	f	303	CLA	C4A-NA-C1A	6.56	109.67	106.68
27	B	305	UIX	O-C1-C3	6.55	119.63	113.49
28	l	313	CLA	C4A-NA-C1A	6.55	109.67	106.68
28	D	309	CLA	C4A-NA-C1A	6.55	109.67	106.68
28	D	316	CLA	C4A-NA-C1A	6.55	109.67	106.68
32	F	305	PID	C17-C16-C15	6.54	136.91	123.52
28	H	312	CLA	C4A-NA-C1A	6.54	109.66	106.68
28	H	305	CLA	C4A-NA-C1A	6.54	109.66	106.68
28	a	710	CLA	C4A-NA-C1A	6.54	109.66	106.68
28	a	728	CLA	C4A-NA-C1A	6.54	109.66	106.68
28	l	311	CLA	C4A-NA-C1A	6.53	109.66	106.68
28	K	308	CLA	C4A-NA-C1A	6.53	109.66	106.68
28	b	724	CLA	C4A-NA-C1A	6.52	109.66	106.68
28	I	310	CLA	C4A-NA-C1A	6.50	109.65	106.68
28	K	311	CLA	C4A-NA-C1A	6.50	109.65	106.68
28	A	317	CLA	C4A-NA-C1A	6.50	109.65	106.68
28	G	510	CLA	C4A-NA-C1A	6.49	109.64	106.68
28	G	516	CLA	C4A-NA-C1A	6.49	109.64	106.68
35	l	302	BCR	C24-C23-C22	-6.49	116.64	126.23
28	J	311	CLA	C4A-NA-C1A	6.49	109.64	106.68
26	F	301	DD6	C9-C10-C11	-6.48	118.19	127.28
28	D	308	CLA	C4A-NA-C1A	6.48	109.64	106.68
28	L	314	CLA	C4A-NA-C1A	6.48	109.64	106.68
28	G	509	CLA	C4A-NA-C1A	6.47	109.63	106.68
28	A	312	CLA	C4A-NA-C1A	6.47	109.63	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	b	726	CLA	C4A-NA-C1A	6.47	109.63	106.68
28	I	315	CLA	C4A-NA-C1A	6.46	109.63	106.68
28	j	106	CLA	C4A-NA-C1A	6.46	109.62	106.68
28	b	712	CLA	C4A-NA-C1A	6.46	109.62	106.68
28	a	708	CLA	C4A-NA-C1A	6.46	109.62	106.68
28	F	311	CLA	C4A-NA-C1A	6.46	109.62	106.68
28	H	307	CLA	C4A-NA-C1A	6.45	109.62	106.68
28	a	707	CLA	C4A-NA-C1A	6.44	109.62	106.68
28	J	316	CLA	C4A-NA-C1A	6.44	109.62	106.68
26	K	319	DD6	C9-C10-C11	-6.44	118.25	127.28
28	f	301	CLA	C4A-NA-C1A	6.44	109.62	106.68
28	I	321	CLA	C4A-NA-C1A	6.44	109.61	106.68
28	a	723	CLA	C4A-NA-C1A	6.44	109.61	106.68
28	M	316	CLA	C4A-NA-C1A	6.44	109.61	106.68
28	l	308	CLA	C4A-NA-C1A	6.43	109.61	106.68
28	I	313	CLA	C4A-NA-C1A	6.43	109.61	106.68
28	b	710	CLA	C4A-NA-C1A	6.43	109.61	106.68
28	b	715	CLA	C4A-NA-C1A	6.43	109.61	106.68
28	a	706	CLA	C4A-NA-C1A	6.41	109.60	106.68
28	K	315	CLA	C4A-NA-C1A	6.41	109.60	106.68
28	l	309	CLA	C4A-NA-C1A	6.40	109.60	106.68
28	G	511	CLA	C4A-NA-C1A	6.40	109.60	106.68
28	A	313	CLA	C4A-NA-C1A	6.39	109.59	106.68
28	b	723	CLA	C4A-NA-C1A	6.39	109.59	106.68
28	A	319	CLA	C4A-NA-C1A	6.38	109.59	106.68
28	G	513	CLA	C4A-NA-C1A	6.38	109.59	106.68
28	a	727	CLA	C4A-NA-C1A	6.38	109.59	106.68
28	J	301	CLA	C4A-NA-C1A	6.37	109.58	106.68
26	M	302	DD6	C3-C2-C1	-6.37	118.35	127.28
28	A	315	CLA	C4A-NA-C1A	6.37	109.58	106.68
28	B	301	CLA	C4A-NA-C1A	6.37	109.58	106.68
28	K	310	CLA	C4A-NA-C1A	6.36	109.58	106.68
28	b	708	CLA	C4A-NA-C1A	6.36	109.58	106.68
26	A	302	DD6	C9-C10-C11	-6.36	118.36	127.28
28	a	729	CLA	C4A-NA-C1A	6.35	109.58	106.68
28	b	722	CLA	C4A-NA-C1A	6.35	109.58	106.68
28	f	302	CLA	C4A-NA-C1A	6.34	109.57	106.68
28	H	309	CLA	C4A-NA-C1A	6.34	109.57	106.68
28	b	717	CLA	C4A-NA-C1A	6.33	109.57	106.68
28	b	703	CLA	C4A-NA-C1A	6.32	109.56	106.68
28	A	309	CLA	C4A-NA-C1A	6.32	109.56	106.68
28	I	316	CLA	C4A-NA-C1A	6.31	109.56	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	b	725	CLA	C4A-NA-C1A	6.31	109.56	106.68
32	F	305	PID	C18-C19-C20	6.31	136.43	123.52
26	F	301	DD6	C4-C5-C6	-6.31	118.43	127.28
28	L	310	CLA	C4A-NA-C1A	6.31	109.56	106.68
28	J	314	CLA	C4A-NA-C1A	6.30	109.55	106.68
28	m	202	CLA	C4A-NA-C1A	6.29	109.55	106.68
28	M	311	CLA	C4A-NA-C1A	6.28	109.55	106.68
28	a	712	CLA	C4A-NA-C1A	6.28	109.54	106.68
28	K	309	CLA	C4A-NA-C1A	6.28	109.54	106.68
28	b	713	CLA	C4A-NA-C1A	6.28	109.54	106.68
28	M	318	CLA	C4A-NA-C1A	6.28	109.54	106.68
28	B	316	CLA	C4A-NA-C1A	6.27	109.54	106.68
28	b	721	CLA	C4A-NA-C1A	6.26	109.53	106.68
28	a	721	CLA	C4A-NA-C1A	6.26	109.53	106.68
28	H	304	CLA	C4A-NA-C1A	6.26	109.53	106.68
28	l	305	CLA	C4A-NA-C1A	6.24	109.53	106.68
28	K	313	CLA	C4A-NA-C1A	6.24	109.52	106.68
28	b	706	CLA	C4A-NA-C1A	6.23	109.52	106.68
28	b	711	CLA	C4A-NA-C1A	6.23	109.52	106.68
27	K	302	UIX	C6-C1-C	-6.21	112.07	122.30
28	L	317	CLA	C4A-NA-C1A	6.20	109.51	106.68
28	B	307	CLA	C4A-NA-C1A	6.20	109.51	106.68
28	M	309	CLA	C4A-NA-C1A	6.18	109.50	106.68
28	I	312	CLA	C4A-NA-C1A	6.18	109.50	106.68
28	J	308	CLA	C4A-NA-C1A	6.17	109.49	106.68
28	a	724	CLA	C4A-NA-C1A	6.17	109.49	106.68
28	H	311	CLA	C4A-NA-C1A	6.16	109.49	106.68
28	D	314	CLA	C4A-NA-C1A	6.16	109.49	106.68
28	I	308	CLA	C4A-NA-C1A	6.15	109.48	106.68
28	j	104	CLA	C4A-NA-C1A	6.15	109.48	106.68
28	G	520	CLA	C4A-NA-C1A	6.14	109.48	106.68
28	N	307	CLA	C4A-NA-C1A	6.12	109.47	106.68
28	L	308	CLA	C4A-NA-C1A	6.11	109.47	106.68
28	B	311	CLA	C4A-NA-C1A	6.10	109.46	106.68
32	H	301	PID	C17-C16-C15	6.09	135.98	123.52
28	M	313	CLA	C4A-NA-C1A	6.09	109.46	106.68
28	a	709	CLA	C4A-NA-C1A	6.08	109.45	106.68
28	l	312	CLA	C4A-NA-C1A	6.06	109.44	106.68
27	K	302	UIX	C14-C13-C11	-6.04	118.80	127.28
28	F	312	CLA	C4A-NA-C1A	6.03	109.43	106.68
28	M	312	CLA	C4A-NA-C1A	6.01	109.42	106.68
35	m	201	BCR	C15-C14-C13	-6.01	118.85	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	a	717	CLA	C4A-NA-C1A	6.00	109.42	106.68
28	L	313	CLA	C4A-NA-C1A	6.00	109.42	106.68
28	a	719	CLA	C4A-NA-C1A	6.00	109.42	106.68
26	J	304	DD6	C9-C10-C11	-5.99	118.87	127.28
28	I	309	CLA	C4A-NA-C1A	5.99	109.41	106.68
35	a	736	BCR	C7-C8-C9	-5.98	117.38	126.23
27	G	503	UIX	O-C1-C3	5.98	119.09	113.49
29	N	308	KC1	C1D-ND-C4D	5.94	110.48	106.31
26	A	302	DD6	C14-C13-C11	-5.92	116.34	125.53
29	N	308	KC1	O2D-CGD-CBD	5.90	121.54	111.23
27	J	305	UIX	C34-C30-C26	-5.84	119.08	127.28
26	A	301	DD6	C21-C20-C19	5.83	120.79	114.24
35	j	102	BCR	C16-C17-C18	-5.83	119.10	127.28
26	M	306	DD6	C3-C2-C1	-5.83	119.11	127.28
26	J	302	DD6	C3-C2-C1	-5.80	119.14	127.28
28	a	704	CLA	C4A-NA-C1A	5.80	109.32	106.68
26	I	305	DD6	C4-C5-C6	-5.79	119.16	127.28
32	M	301	PID	C17-C16-C15	5.78	135.35	123.52
35	b	702	BCR	C16-C17-C18	-5.78	119.18	127.28
26	G	504	DD6	C4-C5-C6	-5.77	119.18	127.28
26	G	505	DD6	O1-C20-C21	5.76	121.48	115.05
32	F	304	PID	C17-C16-C15	5.76	135.30	123.52
28	a	735	CLA	C4A-NA-C1A	5.75	109.30	106.68
27	h	201	UIX	O-C1-C3	5.73	118.86	113.49
26	I	305	DD6	C3-C2-C1	-5.72	119.25	127.28
27	K	302	UIX	C34-C30-C26	-5.71	119.28	127.28
28	a	726	CLA	C4A-NA-C1A	5.68	109.27	106.68
28	J	310	CLA	C4A-NA-C1A	5.68	109.27	106.68
26	J	304	DD6	C3-C2-C1	-5.67	119.33	127.28
32	F	302	PID	C18-C19-C20	5.64	135.06	123.52
26	G	505	DD6	C3-C2-C1	-5.64	119.37	127.28
32	D	304	PID	C17-C16-C15	5.62	135.01	123.52
35	i	201	BCR	C24-C23-C22	-5.58	117.98	126.23
26	J	303	DD6	C4-C5-C6	-5.56	119.48	127.28
26	A	303	DD6	C21-C20-C19	5.56	120.48	114.24
32	F	304	PID	C7-C8-C9	5.54	133.04	126.06
28	B	310	CLA	C4A-NA-C1A	5.54	109.20	106.68
28	a	713	CLA	C4A-NA-C1A	5.52	109.20	106.68
26	F	301	DD6	C21-C20-C19	5.52	120.44	114.24
35	a	736	BCR	C11-C10-C9	-5.52	119.54	127.28
32	N	302	PID	C18-C19-C20	5.52	134.81	123.52
26	M	305	DD6	C3-C2-C1	-5.51	119.55	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	b	702	BCR	C20-C21-C22	-5.51	119.55	127.28
26	A	301	DD6	C9-C10-C11	-5.50	119.57	127.28
26	L	306	DD6	C9-C10-C11	-5.49	119.58	127.28
26	I	301	DD6	C21-C20-C19	5.48	120.40	114.24
26	G	502	DD6	C21-C20-C19	5.45	120.37	114.24
26	B	303	DD6	C21-C20-C19	5.45	120.36	114.24
26	A	305	DD6	C21-C20-C19	5.44	120.35	114.24
26	F	303	DD6	C4-C5-C6	-5.44	119.66	127.28
26	I	302	DD6	C9-C10-C11	-5.42	119.68	127.28
26	I	301	DD6	C9-C10-C11	-5.42	119.68	127.28
26	J	303	DD6	C9-C10-C11	-5.40	119.70	127.28
35	b	730	BCR	C15-C14-C13	-5.38	119.73	127.28
27	K	302	UIX	O-C1-C3	5.32	118.48	113.49
26	I	301	DD6	C4-C5-C6	-5.31	119.83	127.28
26	J	302	DD6	C9-C10-C11	-5.30	119.84	127.28
29	M	307	KC1	C1D-ND-C4D	5.29	110.03	106.31
35	b	730	BCR	C3-C4-C5	-5.29	104.62	114.06
26	K	304	DD6	C21-C20-C19	5.28	120.17	114.24
27	I	304	UIX	O-C1-C6	5.27	120.94	115.05
35	f	304	BCR	C15-C14-C13	-5.27	119.89	127.28
26	A	302	DD6	C3-C2-C1	-5.24	119.94	127.28
26	J	302	DD6	C14-C13-C11	-5.23	117.41	125.53
27	B	305	UIX	O2-C27-C31	5.22	120.40	111.09
26	G	508	DD6	C21-C20-C19	5.21	120.10	114.24
27	h	201	UIX	C37-C39-C40	-5.21	119.97	127.28
26	L	302	DD6	C14-C13-C11	-5.21	117.45	125.53
32	D	304	PID	C18-C19-C20	5.21	134.17	123.52
26	B	302	DD6	C3-C2-C1	-5.20	119.98	127.28
29	L	307	KC1	O2D-CGD-CBD	5.20	120.32	111.23
35	l	307	BCR	C3-C4-C5	-5.19	104.80	114.06
27	K	302	UIX	O-C1-C6	5.18	120.83	115.05
26	N	303	DD6	C4-C5-C6	-5.14	120.06	127.28
35	b	730	BCR	C11-C10-C9	-5.14	120.07	127.28
26	K	305	DD6	C3-C2-C1	-5.13	120.09	127.28
26	B	306	DD6	C3-C2-C1	-5.12	120.09	127.28
35	a	734	BCR	C15-C14-C13	-5.12	120.10	127.28
29	F	309	KC1	O2D-CGD-CBD	5.11	120.17	111.23
26	F	301	DD6	C3-C2-C1	-5.11	120.11	127.28
27	A	304	UIX	O-C1-C3	5.11	118.28	113.49
29	M	314	KC1	O2D-CGD-CBD	5.10	120.14	111.23
27	A	304	UIX	O-C1-C6	5.10	120.75	115.05
29	A	306	KC1	O2D-CGD-CBD	5.09	120.13	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	M	304	DD6	C21-C20-C19	5.09	119.96	114.24
26	H	303	DD6	C21-C20-C19	5.08	119.95	114.24
26	G	502	DD6	C4-C5-C6	-5.07	120.17	127.28
26	G	508	DD6	C3-C2-C1	-5.06	120.17	127.28
26	B	304	DD6	C21-C20-C19	5.04	119.90	114.24
29	H	310	KC1	C1D-ND-C4D	5.04	109.85	106.31
29	F	314	KC1	C1D-ND-C4D	5.03	109.84	106.31
26	G	508	DD6	C4-C5-C6	-5.03	120.23	127.28
29	J	313	KC1	O2D-CGD-CBD	5.02	120.01	111.23
26	G	504	DD6	C3-C2-C1	-5.02	120.23	127.28
35	f	304	BCR	C11-C10-C9	-5.02	120.24	127.28
35	m	201	BCR	C11-C10-C9	-5.01	120.25	127.28
26	K	304	DD6	C3-C2-C1	-5.01	120.25	127.28
26	K	301	DD6	C21-C20-C19	5.01	119.87	114.24
26	L	306	DD6	C4-C5-C6	-5.00	120.27	127.28
26	M	306	DD6	C4-C5-C6	-4.98	120.29	127.28
27	h	201	UIX	O2-C27-C31	4.98	119.97	111.09
29	A	306	KC1	C1D-ND-C4D	4.98	109.81	106.31
26	B	306	DD6	C21-C20-C19	4.98	119.84	114.24
26	N	303	DD6	C21-C20-C19	4.97	119.83	114.24
26	K	305	DD6	C21-C20-C19	4.97	119.83	114.24
28	l	310	CLA	C4D-CHA-CBD	-4.97	106.07	108.45
29	L	315	KC1	O2D-CGD-CBD	4.97	119.92	111.23
29	D	315	KC1	O2D-CGD-CBD	4.97	119.91	111.23
29	H	310	KC1	O2D-CGD-CBD	4.96	119.91	111.23
29	D	310	KC1	C1D-ND-C4D	4.96	109.79	106.31
26	L	303	DD6	C21-C20-C19	4.96	119.81	114.24
29	N	311	KC1	O2D-CGD-CBD	4.96	119.89	111.23
29	J	313	KC1	C1D-ND-C4D	4.94	109.78	106.31
26	I	305	DD6	C15-C14-C13	-4.94	115.56	125.99
29	F	309	KC1	C1D-ND-C4D	4.93	109.77	106.31
26	L	303	DD6	C3-C2-C1	-4.92	120.37	127.28
29	N	306	KC1	C1D-ND-C4D	4.92	109.77	106.31
26	h	203	DD6	C21-C20-C19	4.91	119.76	114.24
26	L	305	DD6	C21-C20-C19	4.91	119.75	114.24
26	K	303	DD6	C21-C20-C19	4.90	119.75	114.24
29	G	515	KC1	C1D-ND-C4D	4.89	109.74	106.31
27	K	302	UIX	C16-C20-C15	4.88	124.54	119.70
29	M	314	KC1	C1D-ND-C4D	4.88	109.73	106.31
26	L	306	DD6	C21-C20-C19	4.86	119.70	114.24
26	G	505	DD6	C9-C10-C11	-4.86	120.47	127.28
35	l	306	BCR	C7-C8-C9	-4.85	119.07	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	N	311	KC1	C1D-ND-C4D	4.84	109.71	106.31
26	L	302	DD6	C21-C20-C19	4.84	119.68	114.24
35	a	736	BCR	C16-C17-C18	-4.84	120.49	127.28
29	F	314	KC1	O2D-CGD-CBD	4.83	119.68	111.23
26	F	303	DD6	C21-C20-C19	4.83	119.66	114.24
27	A	304	UIX	O2-C27-C31	4.83	119.69	111.09
32	N	301	PID	C17-C16-C15	4.82	133.38	123.52
26	G	505	DD6	C4-C5-C6	-4.81	120.53	127.28
35	l	306	BCR	C33-C5-C6	-4.81	119.24	124.48
29	H	306	KC1	O2D-CGD-CBD	4.81	119.64	111.23
26	I	301	DD6	C3-C2-C1	-4.81	120.54	127.28
29	A	314	KC1	O2D-CGD-CBD	4.80	119.62	111.23
27	K	302	UIX	C17-C15-C20	4.79	113.87	109.21
26	K	319	DD6	C4-C5-C6	-4.78	120.57	127.28
35	i	201	BCR	C20-C21-C22	-4.78	120.57	127.28
26	M	302	DD6	C15-C14-C13	-4.78	115.89	125.99
26	M	305	DD6	C21-C20-C19	4.77	119.60	114.24
26	K	319	DD6	C3-C2-C1	-4.77	120.59	127.28
26	M	304	DD6	C3-C2-C1	-4.77	120.59	127.28
29	I	314	KC1	C1D-ND-C4D	4.76	109.66	106.31
29	I	314	KC1	O2D-CGD-CBD	4.76	119.56	111.23
26	M	306	DD6	C9-C10-C11	-4.76	120.60	127.28
26	I	302	DD6	C21-C20-C19	4.75	119.57	114.24
29	L	315	KC1	C1D-ND-C4D	4.74	109.64	106.31
29	D	315	KC1	C1D-ND-C4D	4.74	109.64	106.31
35	l	306	BCR	C16-C17-C18	-4.74	120.64	127.28
26	K	301	DD6	C4-C5-C6	-4.73	120.64	127.28
29	M	307	KC1	O2D-CGD-CBD	4.73	119.50	111.23
29	N	308	KC1	O2D-CGD-O1D	-4.72	114.67	123.85
35	j	102	BCR	C15-C14-C13	-4.72	120.66	127.28
29	B	314	KC1	C1D-ND-C4D	4.69	109.61	106.31
26	D	303	DD6	C21-C20-C19	4.68	119.50	114.24
35	f	304	BCR	C16-C17-C18	-4.68	120.71	127.28
26	L	305	DD6	C3-C2-C1	-4.68	120.72	127.28
29	L	307	KC1	C1D-ND-C4D	4.66	109.58	106.31
29	G	515	KC1	O2D-CGD-CBD	4.66	119.37	111.23
26	M	303	DD6	C4-C5-C6	-4.65	120.75	127.28
29	B	314	KC1	O2D-CGD-CBD	4.65	119.37	111.23
35	i	201	BCR	C15-C14-C13	-4.65	120.76	127.28
26	I	303	DD6	C9-C10-C11	-4.65	120.76	127.28
29	K	314	KC1	C1D-ND-C4D	4.64	109.57	106.31
26	J	303	DD6	O1-C15-C14	-4.64	103.58	116.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	l	302	BCR	C28-C27-C26	-4.64	105.79	114.06
26	A	301	DD6	C3-C2-C1	-4.64	120.78	127.28
29	K	314	KC1	O2D-CGD-CBD	4.63	119.32	111.23
26	b	731	DD6	C21-C20-C19	4.62	119.44	114.24
26	I	303	DD6	C21-C20-C19	4.62	119.43	114.24
26	B	302	DD6	C9-C10-C11	-4.62	120.80	127.28
26	J	303	DD6	O1-C20-C21	4.62	120.21	115.05
26	D	303	DD6	C10-C9-C8	-4.62	109.82	123.20
27	K	302	UIX	O2-C27-C31	4.62	119.32	111.09
29	A	314	KC1	C1D-ND-C4D	4.61	109.55	106.31
26	N	303	DD6	C9-C10-C11	-4.61	120.81	127.28
29	H	306	KC1	C1D-ND-C4D	4.61	109.55	106.31
29	N	308	KC1	O1D-CGD-CBD	-4.61	115.43	124.52
27	G	503	UIX	O2-C27-C31	4.59	119.28	111.09
35	a	736	BCR	C15-C14-C13	-4.58	120.86	127.28
26	G	505	DD6	O1-C15-C14	-4.56	103.80	116.88
26	I	302	DD6	C3-C2-C1	-4.54	120.91	127.28
35	a	734	BCR	C16-C17-C18	-4.54	120.91	127.28
27	J	305	UIX	O2-C27-C31	4.54	119.18	111.09
26	L	304	DD6	C21-C20-C19	4.54	119.34	114.24
35	l	302	BCR	C16-C17-C18	-4.53	120.92	127.28
26	M	303	DD6	C3-C2-C1	-4.53	120.92	127.28
26	b	731	DD6	C4-C5-C6	-4.53	120.93	127.28
27	I	304	UIX	O2-C27-C31	4.52	119.16	111.09
35	b	732	BCR	C33-C5-C6	-4.52	119.55	124.48
32	F	304	PID	C6-C7-C8	4.52	135.54	125.99
29	N	306	KC1	O2D-CGD-CBD	4.51	119.12	111.23
26	J	302	DD6	C4-C5-C6	-4.51	120.95	127.28
26	I	305	DD6	O1-C15-C14	-4.51	103.95	116.88
32	M	301	PID	CM4-C14-C15	-4.51	115.51	122.82
27	B	305	UIX	O-C1-C6	4.51	120.09	115.05
26	G	504	DD6	O1-C20-C19	4.49	117.70	113.49
35	l	307	BCR	C15-C14-C13	-4.49	120.98	127.28
26	G	502	DD6	C9-C10-C11	-4.48	120.99	127.28
26	N	303	DD6	C3-C2-C1	-4.48	121.00	127.28
27	G	503	UIX	O-C1-C6	4.47	120.05	115.05
27	K	302	UIX	O-C-C7	-4.46	104.09	116.88
35	j	102	BCR	C20-C21-C22	-4.46	121.03	127.28
32	D	301	PID	C17-C16-C15	4.46	132.64	123.52
35	l	306	BCR	C38-C26-C25	-4.45	119.63	124.48
26	J	303	DD6	O1-C20-C19	4.45	117.66	113.49
26	B	304	DD6	C3-C2-C1	-4.45	121.04	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	D	304	PID	C12-O4-C10	4.45	109.84	107.68
32	M	301	PID	C12-O4-C10	4.44	109.83	107.68
26	M	303	DD6	O1-C15-C14	-4.44	104.16	116.88
27	h	201	UIX	O-C1-C6	4.43	120.00	115.05
26	M	302	DD6	O1-C20-C21	4.43	119.99	115.05
26	L	305	DD6	C9-C10-C11	-4.42	121.07	127.28
26	J	303	DD6	C15-C14-C13	-4.42	116.64	125.99
32	D	304	PID	CM4-C14-C15	-4.42	115.65	122.82
29	D	310	KC1	O2D-CGD-CBD	4.42	118.96	111.23
27	h	201	UIX	C-C7-C10	-4.42	116.65	125.99
27	A	304	UIX	C6-C1-C3	4.41	119.20	114.24
26	I	305	DD6	C21-C20-C19	4.41	119.19	114.24
27	K	302	UIX	C21-C15-C20	-4.40	106.53	110.47
26	h	203	DD6	C3-C2-C1	-4.39	121.12	127.28
26	F	303	DD6	C9-C10-C11	-4.38	121.13	127.28
32	D	305	PID	C18-C19-C20	4.35	132.42	123.52
26	L	306	DD6	C3-C2-C1	-4.35	121.18	127.28
36	b	729	PQN	C11-C12-C13	-4.34	119.36	126.83
26	b	731	DD6	C15-C14-C13	-4.33	116.83	125.99
26	H	303	DD6	C4-C5-C6	-4.33	121.21	127.28
26	A	301	DD6	O1-C20-C19	-4.33	109.44	113.49
32	F	302	PID	C12-O4-C10	4.33	109.78	107.68
32	H	301	PID	CM4-C14-C15	-4.32	115.82	122.82
26	M	303	DD6	O1-C20-C21	4.31	119.87	115.05
35	b	732	BCR	C16-C17-C18	-4.30	121.24	127.28
35	i	201	BCR	C16-C17-C18	-4.30	121.25	127.28
26	M	306	DD6	C25-C24-C1	-4.30	114.57	126.36
26	L	304	DD6	C3-C2-C1	-4.29	121.25	127.28
26	K	301	DD6	C15-C14-C13	-4.28	116.95	125.99
26	K	319	DD6	O1-C20-C21	-4.27	110.27	115.05
27	I	304	UIX	C7-C10-C11	-4.24	118.95	125.53
32	F	304	PID	CM4-C14-C15	-4.24	115.95	122.82
26	I	302	DD6	C7-C6-C8	4.24	124.56	118.09
35	m	201	BCR	C38-C26-C25	-4.23	119.86	124.48
26	B	303	DD6	C4-C5-C6	-4.23	121.35	127.28
26	H	303	DD6	C3-C2-C1	-4.22	121.36	127.28
32	H	301	PID	C12-O4-C10	4.21	109.72	107.68
26	A	305	DD6	C4-C5-C6	-4.20	121.38	127.28
32	D	306	PID	C18-C19-C20	4.19	132.09	123.52
32	F	304	PID	C12-O4-C10	4.18	109.71	107.68
32	F	302	PID	CM4-C14-C15	-4.17	116.05	122.82
26	L	303	DD6	C9-C10-C11	-4.16	121.44	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	G	521	DGD	O2G-C1B-C2B	4.16	120.48	111.48
26	K	304	DD6	C15-C14-C13	-4.16	117.20	125.99
26	L	305	DD6	C4-C5-C6	-4.16	121.44	127.28
26	L	302	DD6	C3-C2-C1	-4.16	121.45	127.28
26	F	301	DD6	O1-C20-C19	-4.15	109.60	113.49
26	B	302	DD6	C14-C13-C11	-4.14	119.10	125.53
32	N	301	PID	C12-O4-C10	4.14	109.69	107.68
27	A	304	UIX	C16-C20-C15	4.14	123.80	119.70
35	a	734	BCR	C11-C10-C9	-4.12	121.50	127.28
32	D	306	PID	C17-C16-C15	4.11	131.94	123.52
30	j	103	DGD	O2G-C1B-C2B	4.11	120.37	111.48
35	a	734	BCR	C33-C5-C6	-4.10	120.01	124.48
26	I	302	DD6	C12-C11-C13	4.09	124.33	118.09
30	L	301	DGD	O2G-C1B-C2B	4.07	120.29	111.48
26	K	319	DD6	C14-C13-C11	-4.07	119.22	125.53
26	A	301	DD6	C4-C5-C6	-4.07	121.58	127.28
35	b	732	BCR	C15-C14-C13	-4.07	121.58	127.28
32	D	307	PID	C12-O4-C10	4.06	109.65	107.68
27	J	305	UIX	C34-C37-C39	-4.05	115.22	123.52
27	h	201	UIX	O-C-C7	-4.05	105.29	116.88
32	D	301	PID	C18-C19-C20	4.04	131.79	123.52
26	L	302	DD6	C9-C10-C11	-4.04	121.61	127.28
26	J	304	DD6	O1-C15-C14	-4.04	105.31	116.88
32	N	301	PID	CM4-C14-C15	-4.04	116.28	122.82
29	D	315	KC1	CHB-C1B-NB	4.02	130.47	124.80
35	l	306	BCR	C20-C21-C22	-4.02	121.64	127.28
30	y	201	DGD	O2G-C1B-C2B	4.02	120.17	111.48
26	I	303	DD6	O1-C15-C14	-4.01	105.39	116.88
32	F	306	PID	C12-O4-C10	4.01	109.62	107.68
26	L	302	DD6	C4-C5-C6	-4.00	121.67	127.28
35	i	201	BCR	C7-C8-C9	-4.00	120.32	126.23
26	B	303	DD6	O1-C20-C19	-4.00	109.75	113.49
26	M	302	DD6	O1-C20-C19	3.99	117.23	113.49
26	M	306	DD6	O1-C15-C14	-3.99	105.43	116.88
35	b	730	BCR	C4-C5-C6	-3.99	117.31	122.70
27	B	305	UIX	C37-C39-C40	-3.99	121.68	127.28
29	D	310	KC1	CHC-C4B-NB	3.98	130.41	124.80
35	a	734	BCR	C28-C27-C26	-3.98	106.95	114.06
26	H	303	DD6	C15-C14-C13	-3.98	117.58	125.99
27	h	201	UIX	C6-C1-C3	3.98	118.71	114.24
27	h	201	UIX	C16-C20-C15	3.97	123.64	119.70
29	H	310	KC1	CHB-C1B-NB	3.97	130.39	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	B	304	DD6	C4-C5-C6	-3.96	121.72	127.28
32	D	301	PID	C12-O4-C10	3.96	109.60	107.68
27	G	503	UIX	O-C-C7	-3.95	105.56	116.88
32	D	301	PID	CM4-C14-C15	-3.95	116.42	122.82
26	I	303	DD6	C4-C5-C6	-3.94	121.75	127.28
27	A	304	UIX	C34-C30-C26	-3.94	121.75	127.28
29	F	309	KC1	CHC-C4B-NB	3.94	130.35	124.80
35	m	201	BCR	C3-C4-C5	-3.94	107.03	114.06
26	M	302	DD6	C21-C20-C15	-3.94	115.82	122.30
35	f	304	BCR	C33-C5-C6	-3.93	120.19	124.48
35	j	102	BCR	C24-C23-C22	-3.92	120.43	126.23
29	F	314	KC1	CHB-C1B-NB	3.92	130.33	124.80
26	B	304	DD6	C15-C14-C13	-3.92	117.70	125.99
29	H	306	KC1	CHB-C1B-NB	3.92	130.32	124.80
27	J	305	UIX	O-C1-C6	3.92	119.43	115.05
35	m	201	BCR	C15-C16-C17	-3.92	115.50	123.52
29	M	314	KC1	CHB-C1B-NB	3.92	130.31	124.80
32	F	306	PID	C17-C16-C15	3.92	131.53	123.52
26	L	304	DD6	C4-C5-C6	-3.91	121.79	127.28
29	D	310	KC1	CHB-C1B-NB	3.91	130.31	124.80
26	b	731	DD6	C9-C10-C11	-3.91	121.80	127.28
26	G	508	DD6	C9-C10-C11	-3.90	121.81	127.28
35	b	730	BCR	C16-C17-C18	-3.89	121.82	127.28
35	l	302	BCR	C33-C5-C6	-3.89	120.24	124.48
26	F	303	DD6	C3-C2-C1	-3.87	121.84	127.28
29	A	314	KC1	CHB-C1B-NB	3.87	130.25	124.80
26	K	303	DD6	C15-C14-C13	-3.87	117.81	125.99
30	G	501	DGD	O2G-C1B-C2B	3.87	119.85	111.48
30	I	317	DGD	O2G-C1B-C2B	3.87	119.85	111.48
29	L	315	KC1	CHB-C1B-NB	3.86	130.24	124.80
32	F	305	PID	C12-O4-C10	3.86	109.56	107.68
32	G	506	PID	CM4-C14-C15	-3.86	116.56	122.82
26	M	304	DD6	C15-C14-C13	-3.86	117.83	125.99
35	f	304	BCR	C20-C21-C22	-3.86	121.87	127.28
27	J	305	UIX	C14-C13-C11	-3.85	121.87	127.28
29	B	314	KC1	CHB-C1B-NB	3.85	130.23	124.80
32	F	306	PID	CM4-C14-C15	-3.85	116.58	122.82
26	I	303	DD6	C3-C2-C1	-3.85	121.88	127.28
26	F	303	DD6	C15-C14-C13	-3.85	117.86	125.99
26	M	302	DD6	C4-C5-C6	-3.85	121.88	127.28
27	G	503	UIX	C6-C1-C3	3.85	118.56	114.24
27	G	503	UIX	C-C7-C10	-3.84	117.87	125.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	I	314	KC1	CHB-C1B-NB	3.83	130.20	124.80
29	N	311	KC1	CHC-C4B-NB	3.83	130.19	124.80
30	l	301	DGD	O2G-C1B-C2B	3.83	119.76	111.48
29	H	306	KC1	CHC-C4B-NB	3.82	130.18	124.80
35	b	702	BCR	C16-C15-C14	-3.82	115.71	123.52
29	N	306	KC1	CHB-C1B-NB	3.82	130.17	124.80
27	I	304	UIX	C37-C39-C40	-3.81	121.93	127.28
35	f	304	BCR	C7-C8-C9	-3.81	120.59	126.23
26	K	301	DD6	O1-C20-C21	-3.81	110.79	115.05
29	L	307	KC1	CHC-C4B-NB	3.81	130.17	124.80
29	K	314	KC1	CHC-C4B-NB	3.80	130.16	124.80
27	I	304	UIX	C14-C13-C11	-3.80	121.95	127.28
32	G	506	PID	C17-C16-C15	3.80	131.29	123.52
32	F	302	PID	C17-C16-C15	3.80	131.29	123.52
35	f	304	BCR	C28-C27-C26	-3.78	107.31	114.06
26	A	302	DD6	C4-C5-C6	-3.78	121.98	127.28
29	F	314	KC1	CHC-C4B-NB	3.78	130.12	124.80
29	N	311	KC1	CHB-C1B-NB	3.78	130.12	124.80
29	F	309	KC1	CHD-C1D-ND	3.77	129.71	124.05
26	B	302	DD6	O1-C20-C21	3.77	119.26	115.05
32	D	306	PID	C12-O4-C10	3.77	109.51	107.68
26	A	302	DD6	C21-C20-C19	3.77	118.47	114.24
29	K	314	KC1	CHB-C1B-NB	3.77	130.10	124.80
29	F	309	KC1	CHB-C1B-NB	3.77	130.10	124.80
29	N	308	KC1	CHD-C1D-ND	3.76	129.69	124.05
26	I	302	DD6	C14-C13-C11	3.76	131.36	125.53
29	J	313	KC1	CHB-C1B-NB	3.76	130.09	124.80
26	M	306	DD6	C21-C20-C19	3.75	118.45	114.24
29	L	307	KC1	CHB-C1B-NB	3.75	130.08	124.80
32	G	507	PID	C12-O4-C10	3.74	109.50	107.68
29	N	306	KC1	CHC-C4B-NB	3.74	130.07	124.80
26	G	502	DD6	C3-C2-C1	-3.74	122.03	127.28
29	I	314	KC1	CHC-C4B-NB	3.74	130.07	124.80
26	J	304	DD6	C4-C5-C6	-3.73	122.04	127.28
29	N	308	KC1	CHB-C1B-NB	3.73	130.06	124.80
26	M	302	DD6	O1-C15-C14	-3.73	106.20	116.88
26	F	303	DD6	O1-C20-C19	-3.73	110.00	113.49
26	B	302	DD6	C21-C20-C19	3.72	118.42	114.24
32	D	307	PID	CM4-C14-C15	-3.72	116.79	122.82
27	J	305	UIX	C14-C23-C26	-3.72	116.17	126.36
28	a	726	CLA	C3B-C4B-NB	-3.71	107.22	110.53
32	D	305	PID	C12-O4-C10	3.71	109.48	107.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	I	301	DD6	O1-C20-C19	-3.71	110.01	113.49
32	D	302	PID	C18-C19-C20	3.70	131.10	123.52
29	M	314	KC1	CHC-C4B-NB	3.70	130.02	124.80
29	A	314	KC1	CHC-C4B-NB	3.70	130.01	124.80
32	G	506	PID	C12-O4-C10	3.69	109.47	107.68
27	B	305	UIX	C34-C30-C26	-3.69	122.10	127.28
35	l	306	BCR	C11-C10-C9	-3.69	122.11	127.28
29	G	515	KC1	CHB-C1B-NB	3.68	129.99	124.80
29	B	314	KC1	CHC-C4B-NB	3.68	129.99	124.80
29	L	315	KC1	CHC-C4B-NB	3.68	129.99	124.80
29	A	306	KC1	CHB-C1B-NB	3.68	129.98	124.80
32	D	306	PID	CM4-C14-C15	-3.68	116.86	122.82
27	G	503	UIX	C34-C30-C26	-3.68	122.12	127.28
26	I	301	DD6	C15-C14-C13	-3.67	118.22	125.99
32	N	302	PID	CM4-C14-C15	-3.67	116.87	122.82
26	J	304	DD6	C24-C1-C2	3.67	124.78	119.01
29	H	310	KC1	CHC-C4B-NB	3.66	129.96	124.80
29	M	307	KC1	CHC-C4B-NB	3.66	129.95	124.80
26	A	305	DD6	C3-C2-C1	-3.65	122.16	127.28
29	D	315	KC1	CHD-C1D-ND	3.65	129.52	124.05
29	A	306	KC1	CHC-C4B-NB	3.65	129.94	124.80
26	G	508	DD6	C15-C14-C13	-3.64	118.29	125.99
27	A	304	UIX	C18-O2-C27	-3.64	111.42	117.85
26	L	303	DD6	C4-C5-C6	-3.62	122.20	127.28
32	G	507	PID	CM4-C14-C15	-3.62	116.95	122.82
26	I	303	DD6	C14-C13-C11	-3.62	119.92	125.53
32	F	305	PID	C16-C15-C14	3.61	132.35	127.28
29	M	307	KC1	CHB-C1B-NB	3.61	129.89	124.80
29	M	307	KC1	O1D-CGD-CBD	-3.61	117.40	124.52
32	H	302	PID	C18-C19-C20	3.60	130.90	123.52
28	F	311	CLA	O2D-CGD-O1D	-3.60	116.83	123.85
26	K	319	DD6	C21-C20-C19	3.60	118.29	114.24
29	J	313	KC1	CHC-C4B-NB	3.60	129.86	124.80
27	I	304	UIX	C6-C1-C3	3.59	118.28	114.24
32	j	105	PID	C12-O4-C10	3.58	109.42	107.68
29	M	307	KC1	O2D-CGD-O1D	-3.58	116.88	123.85
26	J	304	DD6	C21-C20-C19	3.58	118.26	114.24
35	f	304	BCR	C24-C23-C22	-3.58	120.94	126.23
26	L	306	DD6	C14-C13-C11	-3.57	119.99	125.53
35	a	734	BCR	C7-C8-C9	-3.57	120.96	126.23
26	h	203	DD6	C4-C5-C6	-3.56	122.28	127.28
26	K	304	DD6	C9-C10-C11	-3.55	122.30	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	b	702	BCR	C11-C10-C9	-3.55	122.30	127.28
26	h	203	DD6	C15-C14-C13	-3.55	118.49	125.99
26	J	302	DD6	C21-C20-C19	3.54	118.21	114.24
26	B	303	DD6	C3-C2-C1	-3.53	122.32	127.28
26	F	303	DD6	O1-C15-C14	-3.53	106.76	116.88
35	l	307	BCR	C4-C5-C6	-3.53	117.93	122.70
27	K	302	UIX	C18-O2-C27	-3.53	111.61	117.85
26	N	303	DD6	O1-C20-C19	-3.53	110.18	113.49
32	G	507	PID	C18-C19-C20	3.53	130.74	123.52
26	L	304	DD6	C15-C14-C13	-3.52	118.54	125.99
35	l	302	BCR	C15-C14-C13	-3.52	122.34	127.28
30	G	521	DGD	C4D-C3D-C2D	3.52	117.01	110.83
35	b	732	BCR	C21-C20-C19	-3.52	113.01	123.20
35	m	201	BCR	C4-C5-C6	-3.52	117.95	122.70
26	N	303	DD6	C15-C14-C13	-3.51	118.57	125.99
26	K	304	DD6	O1-C15-C14	-3.51	106.82	116.88
29	D	310	KC1	CHD-C1D-ND	3.51	129.31	124.05
26	A	303	DD6	C3-C2-C1	-3.50	122.37	127.28
26	I	302	DD6	O1-C15-C14	-3.49	106.87	116.88
26	B	306	DD6	C4-C5-C6	-3.49	122.38	127.28
26	G	505	DD6	C14-C13-C11	-3.49	120.11	125.53
29	L	307	KC1	CHD-C1D-ND	3.49	129.29	124.05
32	j	105	PID	C17-C16-C15	3.48	130.65	123.52
27	B	305	UIX	C14-C13-C11	-3.48	122.39	127.28
35	l	307	BCR	C7-C8-C9	-3.48	121.08	126.23
32	D	307	PID	C17-C16-C15	3.47	130.63	123.52
29	M	314	KC1	CHD-C1D-ND	3.47	129.26	124.05
32	H	302	PID	C12-O4-C10	3.47	109.36	107.68
27	A	304	UIX	C17-C15-C20	3.46	112.58	109.21
26	I	305	DD6	C9-C8-C6	-3.46	116.88	126.36
35	b	702	BCR	C33-C5-C6	-3.46	120.71	124.48
35	l	307	BCR	C11-C10-C9	-3.45	122.44	127.28
29	F	314	KC1	CHD-C1D-ND	3.45	129.22	124.05
29	I	314	KC1	CHD-C1D-ND	3.44	129.22	124.05
26	M	304	DD6	C4-C5-C6	-3.44	122.45	127.28
35	l	302	BCR	C20-C21-C22	-3.44	122.45	127.28
29	N	311	KC1	CHD-C1D-ND	3.44	129.21	124.05
26	G	504	DD6	C21-C20-C19	3.43	118.10	114.24
32	D	302	PID	C12-O4-C10	3.43	109.35	107.68
26	J	303	DD6	C21-C20-C15	-3.42	116.67	122.30
28	l	310	CLA	O2D-CGD-CBD	3.42	114.70	110.95
35	m	201	BCR	C11-C12-C13	-3.42	116.99	126.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	N	308	KC1	CHC-C4B-NB	3.41	129.61	124.80
35	I	307	BCR	C38-C26-C25	-3.41	120.76	124.48
29	N	306	KC1	CHD-C1D-ND	3.40	129.15	124.05
26	I	301	DD6	C37-C36-C35	3.40	120.66	114.42
29	K	314	KC1	CHD-C1D-ND	3.39	129.14	124.05
26	B	306	DD6	C15-C14-C13	-3.39	118.83	125.99
29	L	315	KC1	CHD-C1D-ND	3.39	129.13	124.05
35	j	102	BCR	C33-C5-C6	-3.39	120.79	124.48
32	F	306	PID	C18-C19-C20	3.38	130.44	123.52
29	B	314	KC1	CHD-C1D-ND	3.38	129.12	124.05
29	G	515	KC1	CHC-C4B-NB	3.38	129.56	124.80
29	G	515	KC1	CHD-C1D-ND	3.37	129.11	124.05
26	b	731	DD6	C3-C2-C1	-3.37	122.55	127.28
29	H	306	KC1	CHD-C1D-ND	3.37	129.11	124.05
35	a	734	BCR	C20-C21-C22	-3.37	122.56	127.28
32	N	301	PID	C18-C19-C20	3.36	130.40	123.52
28	J	312	CLA	O2D-CGD-O1D	-3.36	117.31	123.85
29	A	314	KC1	CHD-C1D-ND	3.36	129.09	124.05
28	F	310	CLA	O2D-CGD-O1D	-3.35	117.33	123.85
26	D	303	DD6	O1-C20-C19	3.34	116.62	113.49
28	D	314	CLA	C3B-C4B-NB	-3.34	107.55	110.53
32	N	302	PID	C26-C25-C24	3.33	112.45	109.21
35	m	201	BCR	C20-C21-C22	-3.33	122.61	127.28
26	G	505	DD6	C24-C1-C2	3.33	124.24	119.01
26	F	301	DD6	C14-C13-C11	-3.33	120.37	125.53
29	H	310	KC1	CHD-C1D-ND	3.32	129.03	124.05
28	M	315	CLA	O2D-CGD-O1D	-3.32	117.39	123.85
26	I	305	DD6	C3-C4-C5	-3.31	116.74	123.52
35	i	201	BCR	C27-C26-C25	-3.31	118.23	122.70
26	M	306	DD6	C25-C26-C27	-3.31	117.36	126.61
32	D	307	PID	C18-C19-C20	3.31	130.29	123.52
27	J	305	UIX	C6-C1-C3	3.30	117.95	114.24
36	a	732	PQN	C14-C13-C15	3.30	120.95	115.23
26	A	303	DD6	C15-C14-C13	-3.29	119.03	125.99
26	B	302	DD6	C21-C20-C15	-3.29	116.89	122.30
26	I	303	DD6	O1-C20-C19	-3.29	110.41	113.49
27	B	305	UIX	C6-C1-C3	3.28	117.93	114.24
28	I	310	CLA	C3D-C4D-ND	3.28	111.91	107.71
29	A	306	KC1	CHD-C1D-ND	3.28	128.97	124.05
26	I	305	DD6	O1-C20-C21	3.28	118.71	115.05
27	K	302	UIX	C34-C37-C39	-3.28	116.81	123.52
26	H	303	DD6	C9-C10-C11	-3.28	122.68	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	j	102	BCR	C3-C4-C5	-3.27	108.22	114.06
32	D	302	PID	CM4-C14-C15	-3.27	117.51	122.82
29	M	307	KC1	CHD-C1D-ND	3.27	128.96	124.05
26	K	304	DD6	C4-C5-C6	-3.27	122.69	127.28
26	I	305	DD6	C37-C36-C35	3.26	120.42	114.42
26	G	504	DD6	O1-C20-C21	3.26	118.69	115.05
26	F	301	DD6	C25-C26-C27	-3.26	117.50	126.61
26	L	303	DD6	C21-C20-C15	-3.25	116.95	122.30
28	I	319	CLA	O2D-CGD-O1D	-3.25	117.52	123.85
29	J	313	KC1	CHD-C1D-ND	3.25	128.92	124.05
32	j	105	PID	CM4-C14-C15	-3.25	117.56	122.82
32	N	302	PID	C12-O4-C10	3.25	109.25	107.68
28	F	312	CLA	C3B-C4B-NB	-3.25	107.63	110.53
26	b	731	DD6	C4-C3-C2	-3.24	116.89	123.52
26	I	303	DD6	C24-C1-C2	3.24	124.10	119.01
35	i	201	BCR	C15-C16-C17	-3.24	116.89	123.52
26	G	508	DD6	O1-C20-C21	-3.24	111.43	115.05
26	L	305	DD6	C15-C14-C13	-3.24	119.15	125.99
28	N	309	CLA	O2D-CGD-O1D	-3.23	117.55	123.85
26	L	304	DD6	O1-C20-C21	-3.23	111.44	115.05
35	l	307	BCR	C16-C17-C18	-3.23	122.75	127.28
26	B	304	DD6	O1-C20-C21	-3.23	111.44	115.05
35	i	201	BCR	C11-C10-C9	-3.23	122.75	127.28
28	a	726	CLA	O2D-CGD-O1D	-3.23	117.57	123.85
26	G	502	DD6	C14-C13-C11	-3.22	120.53	125.53
32	G	507	PID	C17-C16-C15	3.22	130.10	123.52
26	M	302	DD6	C21-C20-C19	3.21	117.85	114.24
35	l	302	BCR	C38-C26-C25	-3.21	120.98	124.48
30	G	521	DGD	C1D-C2D-C3D	3.21	116.76	110.01
26	J	302	DD6	O1-C20-C21	-3.21	111.47	115.05
26	K	305	DD6	C15-C14-C13	-3.20	119.23	125.99
26	A	305	DD6	O1-C20-C19	-3.20	110.49	113.49
26	h	203	DD6	C9-C10-C11	-3.19	122.80	127.28
26	D	303	DD6	C14-C13-C11	3.18	130.47	125.53
26	F	301	DD6	C9-C8-C6	-3.18	117.64	126.36
26	J	304	DD6	C25-C24-C1	-3.17	117.66	126.36
28	A	307	CLA	O2D-CGD-O1D	-3.17	117.67	123.85
27	A	304	UIX	O-C-C7	-3.17	107.79	116.88
28	b	723	CLA	O2D-CGD-O1D	-3.17	117.67	123.85
28	a	702	CLA	C3B-C4B-NB	-3.17	107.70	110.53
28	b	724	CLA	C3B-C4B-NB	-3.17	107.70	110.53
28	D	314	CLA	O2D-CGD-O1D	-3.17	117.68	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	m	201	BCR	C23-C24-C25	-3.17	118.53	127.00
26	D	303	DD6	C21-C20-C15	-3.17	117.09	122.30
28	G	516	CLA	O2D-CGD-O1D	-3.17	117.69	123.85
26	M	305	DD6	C9-C10-C11	-3.16	122.84	127.28
27	A	304	UIX	C35-C36-C38	-3.16	114.04	123.20
28	K	315	CLA	CAA-C2A-C3A	-3.16	108.98	116.23
26	M	305	DD6	C4-C5-C6	-3.16	122.85	127.28
28	l	310	CLA	O2D-CGD-O1D	-3.16	117.71	123.85
27	J	305	UIX	C7-C10-C11	-3.15	120.64	125.53
28	b	704	CLA	C3B-C4B-NB	-3.14	107.72	110.53
28	I	311	CLA	O2D-CGD-O1D	-3.14	117.73	123.85
35	i	201	BCR	C30-C25-C26	-3.14	118.35	122.64
28	L	309	CLA	O2D-CGD-O1D	-3.14	117.74	123.85
35	b	702	BCR	C28-C27-C26	-3.14	108.46	114.06
29	D	315	KC1	CHC-C4B-NB	3.13	129.22	124.80
27	K	302	UIX	C35-C36-C38	-3.13	114.14	123.20
28	b	709	CLA	O2D-CGD-O1D	-3.13	117.76	123.85
28	L	308	CLA	CBD-CHA-C1A	3.13	132.10	127.38
26	M	306	DD6	C37-C36-C35	3.13	120.17	114.42
26	I	302	DD6	C12-C11-C10	-3.12	117.76	122.82
28	H	307	CLA	O2D-CGD-O1D	-3.12	117.77	123.85
26	I	305	DD6	C25-C24-C1	-3.12	117.80	126.36
28	I	306	CLA	O2D-CGD-O1D	-3.12	117.77	123.85
26	G	504	DD6	C21-C20-C15	-3.12	117.16	122.30
26	J	303	DD6	C32-C33-C34	-3.12	106.75	113.59
26	M	306	DD6	C14-C13-C11	-3.12	120.69	125.53
27	B	305	UIX	O-C-C7	-3.12	107.94	116.88
28	F	315	CLA	O2D-CGD-O1D	-3.12	117.78	123.85
26	K	303	DD6	C3-C2-C1	-3.12	122.91	127.28
26	K	305	DD6	C4-C5-C6	-3.12	122.91	127.28
26	A	305	DD6	C37-C36-C35	3.12	120.15	114.42
26	K	304	DD6	O1-C20-C19	-3.11	110.58	113.49
28	l	303	CLA	O2D-CGD-O1D	-3.11	117.79	123.85
35	l	307	BCR	C20-C21-C22	-3.11	122.92	127.28
32	M	301	PID	C26-C25-C24	3.11	112.23	109.21
35	b	732	BCR	C8-C7-C6	-3.11	118.70	127.00
28	B	310	CLA	O2D-CGD-O1D	-3.11	117.80	123.85
26	A	305	DD6	C37-C36-C31	-3.10	118.36	124.16
26	M	302	DD6	C-C1-C2	-3.10	117.79	122.82
28	a	738	CLA	O2D-CGD-O1D	-3.10	117.81	123.85
26	K	301	DD6	C9-C10-C11	-3.10	122.93	127.28
35	b	732	BCR	C10-C11-C12	-3.10	114.23	123.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	H	308	CLA	O2D-CGD-O1D	-3.09	117.83	123.85
27	A	304	UIX	C37-C39-C40	-3.09	122.94	127.28
32	D	305	PID	CM4-C14-C15	-3.09	117.81	122.82
26	K	301	DD6	O1-C15-C14	-3.09	108.03	116.88
27	K	302	UIX	C6-C1-C3	3.09	117.71	114.24
26	L	303	DD6	C15-C14-C13	-3.09	119.47	125.99
26	A	303	DD6	C4-C5-C6	-3.09	122.95	127.28
26	A	302	DD6	C21-C20-C15	-3.09	117.22	122.30
26	I	302	DD6	O1-C20-C21	-3.08	111.60	115.05
28	K	316	CLA	O2D-CGD-O1D	-3.08	117.85	123.85
32	M	301	PID	C17-C18-C19	3.08	131.85	124.72
35	l	302	BCR	C29-C30-C25	3.08	114.91	110.44
35	f	304	BCR	C38-C26-C25	-3.07	121.13	124.48
28	I	309	CLA	C3B-C4B-NB	-3.07	107.79	110.53
28	M	316	CLA	C3B-C4B-NB	-3.07	107.79	110.53
28	M	318	CLA	C3B-C4B-NB	-3.07	107.79	110.53
28	b	722	CLA	O2D-CGD-O1D	-3.07	117.87	123.85
28	L	317	CLA	O2D-CGD-O1D	-3.07	117.87	123.85
35	l	307	BCR	C24-C23-C22	-3.07	121.69	126.23
32	H	301	PID	C17-C18-C19	3.07	131.81	124.72
27	h	201	UIX	C37-C34-C30	-3.06	117.25	123.52
30	G	501	DGD	O1G-C1A-C2A	3.06	121.18	111.83
26	G	504	DD6	C37-C36-C35	3.06	120.05	114.42
28	a	729	CLA	O2D-CGD-O1D	-3.06	117.89	123.85
28	a	703	CLA	O2D-CGD-O1D	-3.06	117.89	123.85
28	J	308	CLA	O2D-CGD-O1D	-3.05	117.90	123.85
28	a	724	CLA	O2D-CGD-O1D	-3.05	117.91	123.85
28	b	719	CLA	O2D-CGD-O1D	-3.05	117.91	123.85
35	b	730	BCR	C21-C20-C19	-3.05	114.37	123.20
26	b	731	DD6	C32-C33-C34	-3.05	106.91	113.59
26	b	731	DD6	C37-C36-C35	3.05	120.02	114.42
26	A	303	DD6	O1-C20-C19	-3.05	110.64	113.49
29	D	310	KC1	CHC-C4B-C3B	-3.05	120.07	125.21
35	a	736	BCR	C20-C21-C22	-3.04	123.02	127.28
27	B	305	UIX	C-C7-C10	-3.04	119.57	125.99
26	K	303	DD6	O1-C15-C14	-3.04	108.18	116.88
28	F	313	CLA	CHB-C4A-NA	3.03	128.78	124.40
28	A	317	CLA	C3B-C4B-NB	-3.03	107.82	110.53
35	b	702	BCR	C8-C7-C6	-3.03	118.90	127.00
28	I	310	CLA	O2D-CGD-O1D	-3.03	117.95	123.85
26	B	302	DD6	O1-C15-C14	-3.03	108.20	116.88
32	H	302	PID	CM4-C14-C15	-3.03	117.92	122.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	a	734	BCR	C3-C4-C5	-3.02	108.66	114.06
28	J	314	CLA	O2D-CGD-O1D	-3.02	117.97	123.85
35	b	730	BCR	C28-C27-C26	-3.02	108.67	114.06
28	J	301	CLA	O2D-CGD-O1D	-3.02	117.97	123.85
27	I	304	UIX	C35-C36-C38	-3.02	114.46	123.20
28	G	518	CLA	O2D-CGD-O1D	-3.02	117.98	123.85
32	F	304	PID	C17-C18-C19	3.02	131.69	124.72
28	I	315	CLA	O2D-CGD-O1D	-3.02	117.98	123.85
26	H	303	DD6	O1-C15-C14	-3.01	108.25	116.88
28	L	312	CLA	O2D-CGD-O1D	-3.01	117.98	123.85
26	M	304	DD6	O1-C15-C14	-3.01	108.25	116.88
26	A	301	DD6	C14-C13-C11	-3.01	120.86	125.53
28	a	716	CLA	C3B-C4B-NB	-3.01	107.84	110.53
27	B	305	UIX	C18-O2-C27	-3.01	112.53	117.85
26	M	306	DD6	O1-C20-C21	3.01	118.41	115.05
28	l	311	CLA	C3B-C4B-NB	-3.01	107.84	110.53
28	B	311	CLA	O2D-CGD-O1D	-3.00	118.00	123.85
28	J	308	CLA	C3B-C4B-NB	-3.00	107.85	110.53
32	D	304	PID	C17-C18-C19	3.00	131.66	124.72
28	L	316	CLA	CAA-C2A-C3A	-3.00	109.35	116.23
30	G	521	DGD	O6E-C5E-C4E	-3.00	104.30	109.70
26	M	305	DD6	C15-C14-C13	-3.00	119.65	125.99
29	F	309	KC1	CHC-C4B-C3B	-3.00	120.16	125.21
32	F	305	PID	C29-C24-C25	2.99	122.67	119.70
28	a	714	CLA	O2D-CGD-O1D	-2.99	118.02	123.85
29	M	307	KC1	C2D-C1D-ND	-2.99	107.22	110.33
27	G	503	UIX	C36-C35-C32	-2.99	123.09	127.28
32	j	105	PID	C6-C7-C8	-2.99	119.67	125.99
28	J	310	CLA	O2D-CGD-O1D	-2.99	118.03	123.85
29	N	308	KC1	CHB-C1B-C2B	-2.99	119.28	125.49
28	J	307	CLA	O2D-CGD-O1D	-2.99	118.04	123.85
26	A	305	DD6	C9-C10-C11	-2.98	123.09	127.28
28	a	712	CLA	O2D-CGD-O1D	-2.98	118.04	123.85
32	F	302	PID	CM5-C21-C20	-2.98	117.98	122.82
28	K	306	CLA	O2D-CGD-O1D	-2.98	118.04	123.85
28	H	309	CLA	O2D-CGD-O1D	-2.98	118.05	123.85
28	a	721	CLA	C3B-C4B-NB	-2.98	107.87	110.53
27	G	503	UIX	C18-O2-C27	-2.98	112.58	117.85
26	J	304	DD6	C14-C13-C11	-2.98	120.91	125.53
28	a	723	CLA	O2D-CGD-O1D	-2.98	118.06	123.85
28	B	315	CLA	O2D-CGD-O1D	-2.98	118.06	123.85
28	J	301	CLA	C3B-C4B-NB	-2.97	107.88	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	M	306	DD6	C24-C1-C2	2.97	123.69	119.01
35	b	702	BCR	C3-C4-C5	-2.97	108.75	114.06
35	l	307	BCR	C33-C5-C4	2.97	119.93	113.60
32	N	302	PID	CM5-C21-C20	-2.97	118.01	122.82
28	a	725	CLA	O2D-CGD-O1D	-2.97	118.07	123.85
26	L	304	DD6	O1-C15-C14	-2.97	108.38	116.88
28	a	727	CLA	C3B-C4B-NB	-2.97	107.88	110.53
26	K	303	DD6	C10-C9-C8	-2.97	114.60	123.20
26	G	508	DD6	C4-C3-C2	-2.97	117.45	123.52
26	B	306	DD6	C25-C26-C27	-2.96	118.32	126.61
27	B	305	UIX	C7-C10-C11	-2.96	120.93	125.53
26	N	303	DD6	O1-C15-C14	-2.96	108.39	116.88
28	G	510	CLA	O2D-CGD-O1D	-2.96	118.08	123.85
28	L	316	CLA	C3B-C4B-NB	-2.96	107.89	110.53
28	D	312	CLA	C3B-C4B-NB	-2.96	107.89	110.53
28	L	313	CLA	C3B-C4B-NB	-2.96	107.89	110.53
28	a	702	CLA	C1-C2-C3	-2.95	121.36	126.20
26	B	303	DD6	C37-C36-C31	-2.95	118.64	124.16
28	H	304	CLA	C3B-C4B-NB	-2.95	107.90	110.53
27	h	201	UIX	C13-C14-C23	-2.95	114.65	123.20
28	D	309	CLA	O2D-CGD-O1D	-2.95	118.11	123.85
32	H	302	PID	C17-C16-C15	2.95	129.55	123.52
26	L	303	DD6	C37-C36-C31	-2.95	118.65	124.16
32	F	305	PID	C19-C20-C21	2.95	131.41	127.28
28	f	301	CLA	C3B-C4B-NB	-2.94	107.90	110.53
28	I	308	CLA	O2D-CGD-O1D	-2.94	118.12	123.85
28	F	313	CLA	O2D-CGD-O1D	-2.94	118.12	123.85
28	a	717	CLA	O2D-CGD-O1D	-2.94	118.12	123.85
35	b	732	BCR	C24-C23-C22	-2.94	121.89	126.23
35	i	201	BCR	C10-C11-C12	-2.94	114.69	123.20
28	M	313	CLA	C3B-C4B-NB	-2.93	107.91	110.53
28	H	311	CLA	O2D-CGD-O1D	-2.93	118.14	123.85
35	b	702	BCR	C10-C11-C12	-2.93	114.70	123.20
28	J	315	CLA	O2D-CGD-O1D	-2.93	118.14	123.85
29	N	308	KC1	C2D-C1D-ND	-2.93	107.28	110.33
26	B	304	DD6	C37-C36-C31	-2.93	118.68	124.16
35	a	734	BCR	C8-C7-C6	-2.93	119.17	127.00
28	K	309	CLA	O2D-CGD-O1D	-2.93	118.15	123.85
29	D	310	KC1	C2D-C1D-ND	-2.93	107.29	110.33
31	K	317	LMG	O6-C1-O1	-2.93	103.13	110.04
28	B	310	CLA	C1-C2-C3	-2.92	121.41	126.20
29	L	307	KC1	CHC-C4B-C3B	-2.92	120.28	125.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	I	309	CLA	O2D-CGD-O1D	-2.92	118.16	123.85
26	B	304	DD6	O1-C15-C14	-2.92	108.50	116.88
28	A	315	CLA	O2D-CGD-O1D	-2.92	118.16	123.85
28	a	703	CLA	C3B-C4B-NB	-2.92	107.92	110.53
28	b	707	CLA	O2D-CGD-O1D	-2.92	118.16	123.85
28	B	307	CLA	O2D-CGD-O1D	-2.92	118.16	123.85
28	M	313	CLA	O2D-CGD-O1D	-2.92	118.16	123.85
28	A	320	CLA	O2D-CGD-O1D	-2.92	118.16	123.85
28	b	715	CLA	O2D-CGD-O1D	-2.92	118.16	123.85
26	I	303	DD6	C37-C36-C31	-2.92	118.70	124.16
26	J	302	DD6	C25-C24-C1	-2.92	118.36	126.36
26	G	505	DD6	O1-C20-C15	-2.92	56.62	58.93
28	a	708	CLA	C3B-C4B-NB	-2.92	107.92	110.53
28	l	309	CLA	O2D-CGD-O1D	-2.92	118.17	123.85
28	B	309	CLA	O2D-CGD-O1D	-2.91	118.17	123.85
29	N	306	KC1	C2D-C1D-ND	-2.91	107.31	110.33
28	B	315	CLA	CAA-C2A-C3A	-2.91	109.55	116.23
26	K	304	DD6	C3-C4-C5	-2.91	117.56	123.52
26	G	504	DD6	C9-C10-C11	-2.91	123.20	127.28
26	M	303	DD6	C14-C13-C11	-2.91	121.02	125.53
29	H	310	KC1	C2D-C1D-ND	-2.91	107.31	110.33
35	l	302	BCR	C3-C4-C5	-2.91	108.87	114.06
28	b	705	CLA	C3B-C4B-NB	-2.91	107.94	110.53
35	l	302	BCR	C38-C26-C27	2.91	119.79	113.60
28	L	316	CLA	O2D-CGD-O1D	-2.90	118.19	123.85
28	b	718	CLA	O2D-CGD-O1D	-2.90	118.19	123.85
28	a	718	CLA	C3B-C4B-NB	-2.90	107.94	110.53
26	B	306	DD6	C9-C10-C11	-2.90	123.21	127.28
28	F	307	CLA	O2D-CGD-O1D	-2.90	118.20	123.85
28	b	716	CLA	O2D-CGD-O1D	-2.90	118.20	123.85
28	J	316	CLA	O2D-CGD-O1D	-2.90	118.20	123.85
32	F	304	PID	C8-C9-C10	2.90	129.28	123.60
28	a	709	CLA	C3B-C4B-NB	-2.90	107.94	110.53
26	K	301	DD6	C3-C2-C1	-2.90	123.21	127.28
28	a	715	CLA	O2D-CGD-O1D	-2.89	118.21	123.85
35	l	302	BCR	C16-C15-C14	-2.89	117.60	123.52
27	K	302	UIX	C7-C10-C11	-2.89	121.04	125.53
28	b	724	CLA	O2D-CGD-O1D	-2.89	118.22	123.85
28	H	304	CLA	O2D-CGD-O1D	-2.89	118.22	123.85
29	A	306	KC1	C2D-C1D-ND	-2.89	107.33	110.33
26	L	302	DD6	C28-C27-C26	-2.89	118.57	124.18
28	B	301	CLA	O2D-CGD-O1D	-2.89	118.23	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	b	709	CLA	C3B-C4B-NB	-2.89	107.95	110.53
28	B	307	CLA	C3B-C4B-NB	-2.89	107.95	110.53
28	b	723	CLA	C3B-C4B-NB	-2.89	107.95	110.53
28	b	710	CLA	O2D-CGD-O1D	-2.89	118.23	123.85
28	a	705	CLA	O2D-CGD-O1D	-2.88	118.23	123.85
28	A	317	CLA	O2D-CGD-O1D	-2.88	118.23	123.85
27	h	201	UIX	C34-C30-C26	-2.88	123.23	127.28
35	l	307	BCR	C15-C16-C17	-2.88	117.62	123.52
29	N	308	KC1	C4B-CHC-C1C	-2.88	119.89	126.02
28	N	304	CLA	O2D-CGD-O1D	-2.88	118.24	123.85
26	B	306	DD6	O1-C15-C14	-2.88	108.62	116.88
28	A	308	CLA	O2D-CGD-O1D	-2.88	118.24	123.85
30	I	317	DGD	O1G-C1A-C2A	2.88	119.89	111.15
28	j	104	CLA	C3B-C4B-NB	-2.88	107.96	110.53
28	L	312	CLA	C3B-C4B-NB	-2.88	107.96	110.53
35	b	702	BCR	C34-C9-C8	2.88	122.48	118.09
26	G	505	DD6	C21-C20-C19	2.88	117.47	114.24
26	I	301	DD6	C25-C26-C27	-2.88	118.57	126.61
26	G	508	DD6	O1-C15-C14	-2.88	108.64	116.88
26	M	303	DD6	C21-C20-C15	-2.87	117.57	122.30
28	K	308	CLA	O2D-CGD-O1D	-2.87	118.26	123.85
28	H	307	CLA	C3B-C4B-NB	-2.87	107.97	110.53
29	J	313	KC1	C2D-C1D-ND	-2.87	107.35	110.33
28	I	307	CLA	O2D-CGD-O1D	-2.87	118.27	123.85
28	b	725	CLA	O2D-CGD-O1D	-2.87	118.27	123.85
26	G	504	DD6	C24-C1-C2	2.87	123.52	119.01
28	H	305	CLA	O2D-CGD-O1D	-2.87	118.27	123.85
28	L	310	CLA	O2D-CGD-O1D	-2.86	118.28	123.85
28	a	728	CLA	O2D-CGD-O1D	-2.86	118.28	123.85
28	l	308	CLA	O2D-CGD-O1D	-2.86	118.28	123.85
26	J	303	DD6	C37-C36-C31	-2.86	118.81	124.16
28	a	718	CLA	O2D-CGD-O1D	-2.86	118.28	123.85
28	N	305	CLA	O2D-CGD-O1D	-2.86	118.28	123.85
28	b	717	CLA	O2D-CGD-O1D	-2.86	118.28	123.85
26	K	303	DD6	C4-C5-C6	-2.86	123.27	127.28
29	M	314	KC1	C2D-C1D-ND	-2.86	107.36	110.33
28	M	317	CLA	O2D-CGD-O1D	-2.86	118.29	123.85
32	N	302	PID	C29-C24-C25	2.86	122.53	119.70
26	M	305	DD6	C21-C20-C15	-2.86	117.60	122.30
29	I	314	KC1	C2D-C1D-ND	-2.85	107.37	110.33
27	G	503	UIX	C14-C13-C11	-2.85	123.28	127.28
28	l	304	CLA	O2D-CGD-O1D	-2.85	118.30	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	L	314	CLA	O2D-CGD-O1D	-2.85	118.30	123.85
31	b	734	LMG	O6-C1-O1	-2.85	103.30	110.04
28	l	313	CLA	O2D-CGD-O1D	-2.85	118.30	123.85
28	I	321	CLA	O2D-CGD-O1D	-2.85	118.30	123.85
29	K	314	KC1	CHC-C4B-C3B	-2.85	120.40	125.21
28	B	312	CLA	C3B-C4B-NB	-2.85	107.98	110.53
28	B	313	CLA	O2D-CGD-O1D	-2.85	118.30	123.85
28	m	202	CLA	O2D-CGD-O1D	-2.85	118.30	123.85
28	A	315	CLA	CAA-C2A-C3A	-2.85	109.69	116.23
28	K	310	CLA	O2D-CGD-O1D	-2.85	118.30	123.85
28	A	320	CLA	C3B-C4B-NB	-2.85	107.99	110.53
28	N	307	CLA	O2D-CGD-O1D	-2.85	118.31	123.85
26	H	303	DD6	O1-C20-C21	-2.85	111.87	115.05
35	b	730	BCR	C27-C26-C25	-2.85	118.86	122.70
26	b	731	DD6	C26-C25-C24	-2.85	114.96	123.20
28	f	303	CLA	O2D-CGD-O1D	-2.85	118.31	123.85
28	b	706	CLA	O2D-CGD-O1D	-2.84	118.31	123.85
28	b	711	CLA	O2D-CGD-O1D	-2.84	118.31	123.85
28	F	308	CLA	O2D-CGD-O1D	-2.84	118.31	123.85
28	a	722	CLA	O2D-CGD-O1D	-2.84	118.31	123.85
29	N	311	KC1	CHC-C4B-C3B	-2.84	120.41	125.21
29	F	314	KC1	C2D-C1D-ND	-2.84	107.38	110.33
29	A	314	KC1	CHB-C1B-C2B	-2.84	119.58	125.49
28	a	716	CLA	O2D-CGD-O1D	-2.84	118.32	123.85
28	j	104	CLA	O2D-CGD-O1D	-2.84	118.32	123.85
28	M	308	CLA	O2D-CGD-O1D	-2.84	118.32	123.85
28	N	304	CLA	C3B-C4B-NB	-2.84	108.00	110.53
26	F	301	DD6	C37-C36-C35	2.84	119.64	114.42
28	M	312	CLA	C3B-C4B-NB	-2.84	108.00	110.53
28	a	719	CLA	C3B-C4B-NB	-2.84	108.00	110.53
26	J	302	DD6	C37-C36-C35	2.84	119.64	114.42
28	b	712	CLA	O2D-CGD-O1D	-2.84	118.33	123.85
35	l	302	BCR	C10-C11-C12	-2.84	114.98	123.20
28	A	319	CLA	O2D-CGD-O1D	-2.84	118.33	123.85
26	D	303	DD6	C9-C10-C11	-2.84	123.30	127.28
35	l	306	BCR	C28-C27-C26	-2.84	109.00	114.06
28	M	309	CLA	O2D-CGD-O1D	-2.83	118.33	123.85
28	B	317	CLA	C3B-C4B-NB	-2.83	108.00	110.53
28	G	509	CLA	O2D-CGD-O1D	-2.83	118.33	123.85
27	G	503	UIX	C34-C37-C39	-2.83	117.72	123.52
26	J	302	DD6	C37-C36-C31	-2.83	118.86	124.16
32	D	305	PID	CM5-C21-C20	-2.83	118.23	122.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	N	306	KC1	O1D-CGD-CBD	-2.83	118.94	124.52
28	M	318	CLA	O2D-CGD-O1D	-2.83	118.34	123.85
29	H	306	KC1	CHC-C4B-C3B	-2.83	120.44	125.21
26	M	303	DD6	C25-C24-C1	-2.83	118.61	126.36
28	K	315	CLA	O2D-CGD-O1D	-2.83	118.34	123.85
28	M	316	CLA	O2D-CGD-O1D	-2.83	118.34	123.85
26	I	301	DD6	O1-C15-C14	-2.83	108.78	116.88
26	I	305	DD6	C24-C1-C2	2.83	123.45	119.01
26	D	303	DD6	C12-C11-C13	2.83	122.41	118.09
28	K	311	CLA	O2D-CGD-O1D	-2.83	118.35	123.85
29	N	311	KC1	C2D-C1D-ND	-2.83	107.40	110.33
29	G	515	KC1	C2D-C1D-ND	-2.82	107.40	110.33
28	K	313	CLA	O2D-CGD-O1D	-2.82	118.35	123.85
28	a	701	CLA	O2D-CGD-O1D	-2.82	118.35	123.85
28	H	305	CLA	C1-C2-C3	-2.82	121.57	126.20
28	J	309	CLA	C1-C2-C3	-2.82	121.57	126.20
28	B	311	CLA	C3B-C4B-NB	-2.82	108.01	110.53
28	D	308	CLA	C3B-C4B-NB	-2.82	108.01	110.53
28	A	313	CLA	O2D-CGD-O1D	-2.82	118.36	123.85
32	F	305	PID	CM4-C14-C15	-2.82	118.25	122.82
28	a	738	CLA	C3B-C4B-NB	-2.82	108.01	110.53
28	M	312	CLA	O2D-CGD-O1D	-2.82	118.36	123.85
26	b	731	DD6	O1-C15-C14	-2.82	108.81	116.88
28	M	317	CLA	C3B-C4B-NB	-2.82	108.02	110.53
36	b	729	PQN	C11-C3-C2	-2.82	120.06	124.89
28	K	307	CLA	O2D-CGD-O1D	-2.82	118.37	123.85
28	M	311	CLA	O2D-CGD-O1D	-2.81	118.37	123.85
29	I	314	KC1	CHC-C4B-C3B	-2.81	120.46	125.21
28	l	305	CLA	O2D-CGD-O1D	-2.81	118.37	123.85
28	H	309	CLA	C3B-C4B-NB	-2.81	108.02	110.53
28	A	312	CLA	O2D-CGD-O1D	-2.81	118.37	123.85
28	a	735	CLA	O2D-CGD-O1D	-2.81	118.37	123.85
29	L	315	KC1	C2D-C1D-ND	-2.81	107.41	110.33
35	b	730	BCR	C15-C16-C17	-2.81	117.77	123.52
28	F	315	CLA	CAA-C2A-C3A	-2.81	109.78	116.23
28	a	708	CLA	O2D-CGD-O1D	-2.81	118.38	123.85
28	I	307	CLA	C3B-C4B-NB	-2.81	108.02	110.53
35	j	102	BCR	C11-C10-C9	-2.81	123.34	127.28
35	j	102	BCR	C7-C8-C9	-2.81	122.08	126.23
26	G	508	DD6	C14-C13-C11	-2.81	121.17	125.53
26	F	301	DD6	C28-C27-C26	-2.81	118.73	124.18
28	I	312	CLA	O2D-CGD-O1D	-2.81	118.39	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	B	317	CLA	O2D-CGD-O1D	-2.81	118.39	123.85
26	K	305	DD6	O1-C15-C14	-2.81	108.84	116.88
29	D	315	KC1	CHB-C1B-C2B	-2.81	119.65	125.49
35	j	102	BCR	C28-C27-C26	-2.81	109.05	114.06
28	b	720	CLA	O2D-CGD-O1D	-2.81	118.39	123.85
28	G	512	CLA	O2D-CGD-O1D	-2.80	118.39	123.85
28	L	318	CLA	O2D-CGD-O1D	-2.80	118.39	123.85
29	F	309	KC1	C2D-C1D-ND	-2.80	107.42	110.33
26	J	304	DD6	O1-C20-C21	2.80	118.18	115.05
28	B	308	CLA	O2D-CGD-O1D	-2.80	118.40	123.85
28	A	316	CLA	O2D-CGD-O1D	-2.80	118.40	123.85
28	b	705	CLA	O2D-CGD-O1D	-2.80	118.40	123.85
28	D	313	CLA	O2D-CGD-O1D	-2.80	118.40	123.85
27	I	304	UIX	C18-O2-C27	-2.80	112.90	117.85
28	b	703	CLA	O2D-CGD-O1D	-2.80	118.40	123.85
28	a	731	CLA	C3B-C4B-NB	-2.80	108.03	110.53
31	D	317	LMG	O6-C1-O1	-2.80	103.43	110.04
35	m	201	BCR	C16-C17-C18	-2.80	123.35	127.28
28	J	311	CLA	O2D-CGD-O1D	-2.80	118.40	123.85
28	N	310	CLA	CHB-C4A-NA	2.80	128.44	124.40
26	G	505	DD6	C25-C24-C1	-2.80	118.69	126.36
35	j	102	BCR	C8-C7-C6	-2.80	119.53	127.00
28	a	709	CLA	O2D-CGD-O1D	-2.80	118.41	123.85
27	A	304	UIX	C21-C15-C20	-2.80	107.97	110.47
29	N	306	KC1	CHC-C4B-C3B	-2.79	120.50	125.21
28	G	516	CLA	C3B-C4B-NB	-2.79	108.04	110.53
26	L	306	DD6	C37-C36-C35	2.79	119.56	114.42
27	K	302	UIX	C14-C23-C26	-2.79	118.70	126.36
27	I	304	UIX	C37-C34-C30	-2.79	117.80	123.52
32	j	105	PID	C18-C19-C20	2.79	129.24	123.52
26	K	304	DD6	C37-C36-C35	2.79	119.56	114.42
28	K	306	CLA	C3B-C4B-NB	-2.79	108.04	110.53
29	H	306	KC1	C2D-C1D-ND	-2.79	107.43	110.33
35	b	702	BCR	C15-C14-C13	-2.79	123.36	127.28
26	M	304	DD6	C3-C4-C5	-2.79	117.81	123.52
28	A	313	CLA	C3B-C4B-NB	-2.79	108.04	110.53
28	D	314	CLA	CHB-C4A-NA	2.79	128.43	124.40
28	B	316	CLA	C3B-C4B-NB	-2.79	108.04	110.53
35	j	102	BCR	C16-C15-C14	-2.79	117.81	123.52
28	f	301	CLA	O2D-CGD-O1D	-2.79	118.42	123.85
35	a	736	BCR	C38-C26-C25	-2.79	121.44	124.48
35	a	734	BCR	C24-C23-C22	-2.79	122.11	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	I	320	LMG	O6-C1-O1	-2.79	103.46	110.04
29	A	314	KC1	C2D-C1D-ND	-2.78	107.44	110.33
26	A	303	DD6	C9-C10-C11	-2.78	123.37	127.28
28	b	727	CLA	O2D-CGD-O1D	-2.78	118.43	123.85
28	a	706	CLA	O2D-CGD-O1D	-2.78	118.43	123.85
28	I	313	CLA	O2D-CGD-O1D	-2.78	118.43	123.85
28	a	730	CLA	O2D-CGD-O1D	-2.78	118.43	123.85
29	B	314	KC1	CHC-C4B-C3B	-2.78	120.52	125.21
35	b	702	BCR	C20-C19-C18	-2.78	118.73	126.36
35	m	201	BCR	C28-C27-C26	-2.78	109.09	114.06
28	b	726	CLA	O2D-CGD-O1D	-2.78	118.43	123.85
29	M	314	KC1	CHB-C1B-C2B	-2.78	119.70	125.49
32	j	105	PID	C7-C8-C9	2.78	129.56	126.06
28	J	312	CLA	C3B-C4B-NB	-2.78	108.05	110.53
26	K	305	DD6	C21-C20-C15	-2.78	117.73	122.30
26	B	302	DD6	C25-C24-C1	-2.78	118.75	126.36
28	J	306	CLA	O2D-CGD-O1D	-2.78	118.44	123.85
35	i	201	BCR	C1-C6-C5	-2.78	118.84	122.64
32	M	301	PID	C29-C24-C25	2.78	122.45	119.70
28	a	705	CLA	C3B-C4B-NB	-2.77	108.05	110.53
28	a	727	CLA	O2D-CGD-O1D	-2.77	118.45	123.85
26	G	505	DD6	C37-C36-C31	-2.77	118.97	124.16
28	l	313	CLA	CHB-C4A-NA	2.77	128.40	124.40
26	B	303	DD6	C15-C14-C13	-2.77	120.13	125.99
28	a	725	CLA	C3B-C4B-NB	-2.77	108.06	110.53
28	B	310	CLA	C3B-C4B-NB	-2.77	108.06	110.53
28	D	311	CLA	C3B-C4B-NB	-2.77	108.06	110.53
28	l	311	CLA	O2D-CGD-O1D	-2.77	118.46	123.85
26	G	505	DD6	C-C1-C2	-2.77	118.33	122.82
28	G	520	CLA	O2D-CGD-O1D	-2.77	118.46	123.85
28	I	311	CLA	C3B-C4B-NB	-2.77	108.06	110.53
28	D	316	CLA	C3B-C4B-NB	-2.77	108.06	110.53
29	A	314	KC1	CHC-C4B-C3B	-2.77	120.54	125.21
28	a	701	CLA	C3B-C4B-NB	-2.77	108.06	110.53
26	K	301	DD6	C37-C36-C31	-2.77	118.99	124.16
31	b	733	LMG	O6-C1-O1	-2.77	103.51	110.04
27	B	305	UIX	C16-C20-C15	2.76	122.44	119.70
29	I	314	KC1	CHB-C1B-C2B	-2.76	119.74	125.49
28	D	312	CLA	O2D-CGD-O1D	-2.76	118.47	123.85
28	b	728	CLA	O2D-CGD-O1D	-2.76	118.47	123.85
35	a	736	BCR	C33-C5-C6	-2.76	121.47	124.48
28	I	321	CLA	CHB-C4A-NA	2.76	128.38	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	b	731	DD6	C14-C13-C11	-2.76	121.25	125.53
28	a	712	CLA	C3B-C4B-NB	-2.76	108.07	110.53
28	l	312	CLA	O2D-CGD-O1D	-2.76	118.48	123.85
29	B	314	KC1	O1D-CGD-CBD	-2.76	119.08	124.52
26	F	301	DD6	C25-C24-C1	-2.75	118.81	126.36
28	A	319	CLA	C3B-C4B-NB	-2.75	108.07	110.53
28	h	202	CLA	C3B-C4B-NB	-2.75	108.07	110.53
28	a	707	CLA	C3B-C4B-NB	-2.75	108.08	110.53
28	D	311	CLA	O2D-CGD-O1D	-2.75	118.50	123.85
26	G	504	DD6	C15-C14-C13	-2.75	120.18	125.99
28	l	309	CLA	C3B-C4B-NB	-2.75	108.08	110.53
30	G	521	DGD	C3E-C4E-C5E	2.75	115.22	110.23
28	j	106	CLA	O2D-CGD-O1D	-2.75	118.50	123.85
28	L	311	CLA	O2D-CGD-O1D	-2.75	118.50	123.85
35	a	736	BCR	C3-C4-C5	-2.75	109.16	114.06
28	b	721	CLA	O2D-CGD-O1D	-2.74	118.51	123.85
26	K	305	DD6	C14-C13-C11	-2.74	121.27	125.53
28	B	312	CLA	O2D-CGD-O1D	-2.74	118.51	123.85
28	J	309	CLA	O2D-CGD-O1D	-2.74	118.51	123.85
28	a	724	CLA	CMB-C2B-C1B	-2.74	121.24	125.42
26	L	303	DD6	C37-C36-C35	2.74	119.46	114.42
28	A	311	CLA	O2D-CGD-O1D	-2.74	118.51	123.85
32	G	506	PID	C18-C19-C20	2.74	129.13	123.52
32	D	302	PID	CM2-C5-C4	-2.74	104.15	108.97
28	h	202	CLA	O2D-CGD-O1D	-2.74	118.51	123.85
29	B	314	KC1	CHB-C1B-C2B	-2.74	119.79	125.49
28	b	728	CLA	C3B-C4B-NB	-2.74	108.08	110.53
26	L	304	DD6	C37-C36-C31	-2.74	119.04	124.16
28	K	309	CLA	C3B-C4B-NB	-2.74	108.08	110.53
35	b	732	BCR	C11-C10-C9	-2.74	123.44	127.28
28	b	711	CLA	C3B-C4B-NB	-2.74	108.09	110.53
28	b	727	CLA	C3B-C4B-NB	-2.74	108.09	110.53
29	K	314	KC1	C2D-C1D-ND	-2.74	107.49	110.33
35	l	306	BCR	C23-C24-C25	-2.74	119.69	127.00
28	D	316	CLA	O2D-CGD-O1D	-2.74	118.52	123.85
28	J	314	CLA	C3B-C4B-NB	-2.74	108.09	110.53
27	K	302	UIX	C37-C39-C40	-2.74	123.44	127.28
28	a	711	CLA	O2D-CGD-O1D	-2.74	118.52	123.85
28	J	315	CLA	C3B-C4B-NB	-2.73	108.09	110.53
29	D	310	KC1	CHB-C1B-C2B	-2.73	119.80	125.49
29	B	314	KC1	C2D-C1D-ND	-2.73	107.49	110.33
28	A	316	CLA	C3B-C4B-NB	-2.73	108.09	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	a	704	CLA	O2D-CGD-O1D	-2.73	118.53	123.85
29	L	315	KC1	CHB-C1B-C2B	-2.73	119.81	125.49
28	K	310	CLA	C3B-C4B-NB	-2.73	108.09	110.53
28	a	730	CLA	C3B-C4B-NB	-2.73	108.09	110.53
28	I	321	CLA	CAC-C3C-C4C	2.73	128.34	124.79
28	D	308	CLA	O2D-CGD-O1D	-2.73	118.54	123.85
28	b	708	CLA	C3B-C4B-NB	-2.73	108.10	110.53
28	A	309	CLA	O2D-CGD-O1D	-2.73	118.54	123.85
28	M	311	CLA	C3B-C4B-NB	-2.73	108.10	110.53
31	I	318	LMG	C1-C2-C3	-2.72	104.28	110.01
28	B	315	CLA	C3B-C4B-NB	-2.72	108.10	110.53
28	B	316	CLA	O2D-CGD-O1D	-2.72	118.55	123.85
35	b	732	BCR	C7-C8-C9	-2.72	122.21	126.23
31	K	318	LMG	O6-C1-O1	-2.72	103.61	110.04
26	L	304	DD6	C10-C9-C8	-2.72	115.32	123.20
28	f	302	CLA	O2D-CGD-O1D	-2.72	118.55	123.85
29	M	314	KC1	CHC-C4B-C3B	-2.72	120.62	125.21
26	F	301	DD6	O1-C20-C21	-2.72	112.01	115.05
26	M	304	DD6	C32-C33-C34	-2.72	107.63	113.59
32	D	301	PID	CM5-C21-C20	-2.72	118.41	122.82
27	B	305	UIX	C35-C36-C38	-2.72	115.33	123.20
28	b	709	CLA	O2A-CGA-O1A	-2.71	116.84	123.63
28	b	708	CLA	O2D-CGD-O1D	-2.71	118.56	123.85
28	l	309	CLA	CAA-C2A-C3A	-2.71	110.01	116.23
26	B	302	DD6	C32-C33-C34	-2.71	107.64	113.59
28	I	306	CLA	C3B-C4B-NB	-2.71	108.11	110.53
26	F	303	DD6	C9-C8-C6	-2.71	118.92	126.36
28	F	310	CLA	C3B-C4B-NB	-2.71	108.11	110.53
31	B	318	LMG	O6-C1-O1	-2.71	103.64	110.04
32	F	305	PID	C26-C25-C24	2.71	111.84	109.21
29	F	314	KC1	CHB-C1B-C2B	-2.71	119.85	125.49
28	K	312	CLA	C3B-C4B-NB	-2.71	108.11	110.53
35	a	734	BCR	C38-C26-C25	-2.71	121.53	124.48
26	B	302	DD6	C24-C1-C2	2.71	123.27	119.01
35	l	302	BCR	C8-C7-C6	-2.71	119.77	127.00
35	j	102	BCR	C38-C26-C25	-2.71	121.53	124.48
35	b	732	BCR	C16-C15-C14	-2.71	117.98	123.52
28	A	317	CLA	CAA-C2A-C3A	-2.71	110.03	116.23
28	a	710	CLA	O2D-CGD-O1D	-2.70	118.58	123.85
35	l	307	BCR	C2-C1-C6	2.70	114.37	110.44
28	a	731	CLA	O2D-CGD-O1D	-2.70	118.58	123.85
28	a	710	CLA	C3B-C4B-NB	-2.70	108.12	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	K	302	UIX	C3-C5-C4	-2.70	105.73	110.79
28	B	317	CLA	CHB-C4A-NA	2.70	128.30	124.40
28	F	310	CLA	CHB-C4A-NA	2.70	128.30	124.40
35	l	302	BCR	C7-C8-C9	-2.70	122.24	126.23
26	D	303	DD6	C37-C36-C31	-2.70	119.11	124.16
28	A	310	CLA	O2D-CGD-O1D	-2.70	118.59	123.85
26	I	303	DD6	C25-C24-C1	-2.70	118.95	126.36
28	J	312	CLA	O2D-CGD-CBD	2.70	115.95	111.23
26	L	302	DD6	C21-C20-C15	-2.70	117.86	122.30
28	A	315	CLA	C3B-C4B-NB	-2.70	108.12	110.53
28	F	311	CLA	C3B-C4B-NB	-2.70	108.12	110.53
28	L	310	CLA	C3B-C4B-NB	-2.70	108.12	110.53
26	G	504	DD6	C14-C13-C11	-2.70	121.34	125.53
28	a	721	CLA	O2D-CGD-O1D	-2.70	118.60	123.85
29	I	314	KC1	O1D-CGD-CBD	-2.70	119.20	124.52
28	l	311	CLA	CHB-C4A-NA	2.70	128.29	124.40
35	j	102	BCR	C20-C19-C18	-2.69	118.97	126.36
32	F	306	PID	CM5-C21-C20	-2.69	118.45	122.82
28	L	318	CLA	CHB-C4A-NA	2.69	128.29	124.40
28	G	511	CLA	O2D-CGD-O1D	-2.69	118.60	123.85
36	b	729	PQN	C2M-C2-C3	-2.69	120.03	124.45
26	M	305	DD6	C14-C13-C11	-2.69	121.35	125.53
32	D	301	PID	CM2-C5-C4	-2.69	104.24	108.97
28	N	310	CLA	O2D-CGD-O1D	-2.69	118.61	123.85
28	M	310	CLA	O2D-CGD-O1D	-2.69	118.61	123.85
28	b	715	CLA	C3B-C4B-NB	-2.69	108.13	110.53
26	A	303	DD6	C21-C20-C15	-2.69	117.88	122.30
28	b	704	CLA	O2D-CGD-O1D	-2.69	118.61	123.85
28	I	319	CLA	C3B-C4B-NB	-2.69	108.13	110.53
28	I	315	CLA	C3B-C4B-NB	-2.69	108.13	110.53
28	G	517	CLA	O2D-CGD-O1D	-2.69	118.62	123.85
28	G	518	CLA	C3B-C4B-NB	-2.69	108.13	110.53
28	L	308	CLA	C3B-C4B-NB	-2.69	108.13	110.53
28	J	312	CLA	CHB-C4A-NA	2.69	128.28	124.40
29	F	314	KC1	CHC-C4B-C3B	-2.68	120.68	125.21
28	N	309	CLA	C3B-C4B-NB	-2.68	108.13	110.53
26	J	303	DD6	C25-C24-C1	-2.68	119.00	126.36
26	M	302	DD6	C3-C4-C5	-2.68	118.03	123.52
28	L	317	CLA	C3B-C4B-NB	-2.68	108.14	110.53
28	M	315	CLA	CAA-C2A-C3A	-2.68	110.08	116.23
35	m	201	BCR	C21-C20-C19	-2.68	115.43	123.20
29	F	309	KC1	CHB-C1B-C2B	-2.68	119.91	125.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	D	303	DD6	C4-C5-C6	-2.68	123.52	127.28
35	b	732	BCR	C23-C24-C25	-2.68	119.84	127.00
28	l	304	CLA	CHB-C4A-NA	2.68	128.27	124.40
28	J	307	CLA	CHB-C4A-NA	2.68	128.27	124.40
29	L	315	KC1	CHC-C4B-C3B	-2.68	120.69	125.21
27	h	201	UIX	C18-O2-C27	-2.68	113.12	117.85
28	H	312	CLA	C3B-C4B-NB	-2.68	108.14	110.53
28	a	719	CLA	O2D-CGD-O1D	-2.67	118.64	123.85
29	F	309	KC1	C2A-C3A-C4A	2.67	108.42	106.41
29	K	314	KC1	CHB-C1B-C2B	-2.67	119.93	125.49
28	M	317	CLA	CHB-C4A-NA	2.67	128.26	124.40
29	H	310	KC1	CHB-C1B-C2B	-2.67	119.93	125.49
28	b	713	CLA	C3B-C4B-NB	-2.67	108.14	110.53
26	L	305	DD6	O1-C15-C14	-2.67	109.22	116.88
28	G	519	CLA	O2D-CGD-O1D	-2.67	118.65	123.85
29	H	306	KC1	CHB-C1B-C2B	-2.67	119.93	125.49
29	N	306	KC1	CHB-C1B-C2B	-2.67	119.93	125.49
29	N	308	KC1	CHB-C4A-C3A	-2.67	120.81	125.03
35	b	702	BCR	C27-C26-C25	-2.67	119.10	122.70
28	b	703	CLA	C1-C2-C3	-2.67	121.82	126.20
29	L	307	KC1	CHB-C1B-C2B	-2.67	119.94	125.49
35	b	732	BCR	C20-C21-C22	-2.67	123.54	127.28
26	h	203	DD6	C37-C36-C35	2.67	119.33	114.42
28	b	713	CLA	O2D-CGD-O1D	-2.67	118.66	123.85
29	A	306	KC1	CHC-C4B-C3B	-2.67	120.71	125.21
26	h	203	DD6	C21-C20-C15	-2.67	117.91	122.30
28	b	716	CLA	C3B-C4B-NB	-2.67	108.15	110.53
26	I	302	DD6	O1-C20-C19	-2.67	110.99	113.49
26	L	305	DD6	C21-C20-C15	-2.66	117.92	122.30
28	a	703	CLA	C1-C2-C3	-2.66	121.83	126.20
35	i	201	BCR	C4-C5-C6	-2.66	119.11	122.70
29	L	315	KC1	O1D-CGD-CBD	-2.66	119.27	124.52
28	J	314	CLA	CAA-C2A-C3A	-2.66	110.13	116.23
29	D	315	KC1	C2D-C1D-ND	-2.66	107.57	110.33
28	A	311	CLA	C3B-C4B-NB	-2.66	108.16	110.53
28	G	514	CLA	O2D-CGD-O1D	-2.66	118.67	123.85
28	a	715	CLA	C3B-C4B-NB	-2.66	108.16	110.53
26	B	304	DD6	C10-C9-C8	-2.66	115.50	123.20
28	H	308	CLA	C3B-C4B-NB	-2.66	108.16	110.53
28	a	707	CLA	O2D-CGD-O1D	-2.66	118.68	123.85
28	L	314	CLA	C3B-C4B-NB	-2.66	108.16	110.53
29	G	515	KC1	CHB-C1B-C2B	-2.65	119.97	125.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	M	302	DD6	C37-C36-C31	-2.65	119.20	124.16
28	b	705	CLA	C1-C2-C3	-2.65	121.85	126.20
28	M	308	CLA	C3B-C4B-NB	-2.65	108.16	110.53
28	a	720	CLA	O2D-CGD-O1D	-2.65	118.68	123.85
28	K	316	CLA	C3B-C4B-NB	-2.65	108.16	110.53
26	G	505	DD6	C21-C20-C15	-2.65	117.94	122.30
29	H	310	KC1	CHC-C4B-C3B	-2.65	120.74	125.21
28	b	725	CLA	C3B-C4B-NB	-2.65	108.16	110.53
28	b	707	CLA	CHB-C4A-NA	2.65	128.22	124.40
26	L	306	DD6	C15-C14-C13	-2.65	120.39	125.99
30	j	103	DGD	C2G-O2G-C1B	-2.65	111.46	117.80
27	J	305	UIX	O-C-C7	-2.65	109.30	116.88
28	K	312	CLA	O2D-CGD-O1D	-2.65	118.70	123.85
28	a	713	CLA	O2D-CGD-O1D	-2.65	118.70	123.85
29	D	315	KC1	C2A-C3A-C4A	2.64	108.40	106.41
28	b	707	CLA	C1-C2-C3	-2.64	121.86	126.20
31	j	101	LMG	O6-C1-O1	-2.64	103.80	110.04
26	A	302	DD6	C28-C27-C26	-2.64	119.05	124.18
27	h	201	UIX	C22-C15-C20	-2.64	108.11	110.47
28	I	308	CLA	C3B-C4B-NB	-2.64	108.17	110.53
28	b	723	CLA	CHB-C4A-NA	2.64	128.21	124.40
27	B	305	UIX	C37-C34-C30	-2.64	118.12	123.52
35	b	730	BCR	C33-C5-C4	2.64	119.22	113.60
26	M	303	DD6	C9-C8-C6	-2.64	119.13	126.36
28	J	316	CLA	C3B-C4B-NB	-2.64	108.17	110.53
26	I	305	DD6	C21-C20-C15	-2.64	117.96	122.30
27	J	305	UIX	C35-C36-C38	-2.64	115.56	123.20
28	G	516	CLA	CAA-C2A-C3A	-2.64	110.19	116.23
28	G	514	CLA	CHB-C4A-NA	2.63	128.20	124.40
28	L	313	CLA	O2D-CGD-O1D	-2.63	118.72	123.85
26	K	301	DD6	C26-C25-C24	-2.63	115.57	123.20
30	G	521	DGD	O1G-C1A-C2A	2.63	119.86	111.83
30	L	301	DGD	C2G-O2G-C1B	-2.63	111.50	117.80
29	H	306	KC1	O1D-CGD-CBD	-2.63	119.33	124.52
28	J	309	CLA	C3B-C4B-NB	-2.63	108.18	110.53
28	l	313	CLA	C3B-C4B-NB	-2.63	108.18	110.53
28	b	701	CLA	C3B-C4B-NB	-2.63	108.18	110.53
28	H	305	CLA	C3B-C4B-NB	-2.63	108.18	110.53
29	M	307	KC1	C1D-CHD-C4C	-2.63	120.06	126.25
28	I	321	CLA	C3B-C4B-NB	-2.63	108.18	110.53
28	a	716	CLA	CHB-C4A-NA	2.63	128.19	124.40
28	I	312	CLA	C3B-C4B-NB	-2.63	108.19	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	J	304	DD6	C37-C36-C35	2.62	119.25	114.42
28	D	316	CLA	CAA-C2A-C3A	-2.62	110.21	116.23
28	b	701	CLA	O2D-CGD-O1D	-2.62	118.74	123.85
28	H	312	CLA	O2D-CGD-O1D	-2.62	118.74	123.85
28	N	310	CLA	C3B-C4B-NB	-2.62	108.19	110.53
29	A	314	KC1	C1D-CHD-C4C	-2.62	120.08	126.25
36	a	732	PQN	C11-C3-C2	-2.62	120.40	124.89
35	i	201	BCR	C3-C4-C5	-2.62	109.38	114.06
28	m	202	CLA	CMB-C2B-C1B	-2.62	121.43	125.42
27	K	302	UIX	C22-C15-C20	-2.62	108.13	110.47
28	L	311	CLA	C3B-C4B-NB	-2.62	108.19	110.53
28	b	726	CLA	C3B-C4B-NB	-2.62	108.19	110.53
28	A	313	CLA	C1-C2-C3	-2.62	121.91	126.20
26	J	302	DD6	C32-C33-C34	-2.62	107.85	113.59
29	F	309	KC1	C4B-CHC-C1C	-2.62	120.46	126.02
28	N	305	CLA	CHB-C4A-NA	2.62	128.18	124.40
26	K	305	DD6	C25-C26-C27	-2.62	119.29	126.61
28	A	307	CLA	C3B-C4B-NB	-2.62	108.19	110.53
26	M	304	DD6	C21-C20-C15	-2.62	118.00	122.30
28	B	308	CLA	C3B-C4B-NB	-2.61	108.20	110.53
28	a	701	CLA	CHB-C4A-NA	2.61	128.17	124.40
28	B	312	CLA	CHB-C4A-NA	2.61	128.17	124.40
28	M	315	CLA	CHB-C4A-NA	2.61	128.17	124.40
28	M	309	CLA	C3B-C4B-NB	-2.61	108.20	110.53
32	G	506	PID	CM5-C21-C20	-2.61	118.58	122.82
29	A	314	KC1	O1D-CGD-CBD	-2.61	119.37	124.52
29	M	307	KC1	CHC-C4B-C3B	-2.61	120.81	125.21
28	A	310	CLA	O2A-CGA-O1A	-2.61	117.10	123.63
28	a	728	CLA	C3B-C4B-NB	-2.61	108.20	110.53
29	F	309	KC1	C1D-CHD-C4C	-2.61	120.11	126.25
29	J	313	KC1	C4B-CHC-C1C	-2.61	120.47	126.02
28	a	718	CLA	CHB-C4A-NA	2.61	128.17	124.40
28	b	715	CLA	O2A-CGA-O1A	-2.61	117.10	123.63
29	N	308	KC1	CHC-C4B-C3B	-2.61	120.81	125.21
26	L	303	DD6	C14-C13-C11	-2.61	121.48	125.53
28	N	305	CLA	C3B-C4B-NB	-2.61	108.20	110.53
29	D	315	KC1	C1D-CHD-C4C	-2.61	120.12	126.25
28	G	513	CLA	CHB-C4A-NA	2.61	128.16	124.40
28	I	316	CLA	O2D-CGD-O1D	-2.61	118.78	123.85
28	G	517	CLA	C3B-C4B-NB	-2.61	108.20	110.53
29	D	310	KC1	C4B-CHC-C1C	-2.61	120.48	126.02
28	l	308	CLA	C3B-C4B-NB	-2.60	108.20	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	a	726	CLA	CHB-C4A-NA	2.60	128.16	124.40
29	H	306	KC1	C1D-CHD-C4C	-2.60	120.12	126.25
29	A	306	KC1	CHB-C1B-C2B	-2.60	120.07	125.49
29	L	307	KC1	C2D-C1D-ND	-2.60	107.63	110.33
28	b	703	CLA	C3B-C4B-NB	-2.60	108.21	110.53
28	G	519	CLA	CHB-C4A-NA	2.60	128.15	124.40
26	M	305	DD6	C3-C4-C5	-2.60	118.20	123.52
35	l	302	BCR	C27-C26-C25	-2.60	119.19	122.70
28	a	729	CLA	C3B-C4B-NB	-2.60	108.21	110.53
35	m	201	BCR	C33-C5-C4	2.60	119.14	113.60
26	B	306	DD6	C21-C20-C15	-2.60	118.03	122.30
29	B	314	KC1	O2D-CGD-O1D	-2.60	118.79	123.85
28	a	705	CLA	CHB-C4A-NA	2.60	128.15	124.40
29	J	313	KC1	CHC-C4B-C3B	-2.59	120.83	125.21
26	L	303	DD6	C3-C4-C5	-2.59	118.21	123.52
29	H	310	KC1	C1D-CHD-C4C	-2.59	120.15	126.25
29	J	313	KC1	CHB-C1B-C2B	-2.59	120.09	125.49
35	a	734	BCR	C23-C24-C25	-2.59	120.07	127.00
28	G	510	CLA	CHB-C4A-NA	2.59	128.14	124.40
28	L	311	CLA	CHB-C4A-NA	2.59	128.13	124.40
26	L	306	DD6	C37-C36-C31	-2.59	119.32	124.16
28	I	316	CLA	CHB-C4A-NA	2.59	128.13	124.40
29	L	307	KC1	C1D-CHD-C4C	-2.59	120.16	126.25
29	N	311	KC1	CHB-C1B-C2B	-2.59	120.11	125.49
35	b	732	BCR	C15-C16-C17	-2.59	118.23	123.52
28	b	714	CLA	O2D-CGD-O1D	-2.59	118.82	123.85
28	a	721	CLA	CHB-C4A-NA	2.58	128.13	124.40
28	a	730	CLA	CHB-C4A-NA	2.58	128.13	124.40
28	G	510	CLA	C3B-C4B-NB	-2.58	108.22	110.53
28	F	313	CLA	C3B-C4B-NB	-2.58	108.22	110.53
29	G	515	KC1	CHC-C4B-C3B	-2.58	120.85	125.21
27	G	503	UIX	C37-C39-C40	-2.58	123.65	127.28
28	b	701	CLA	CHB-C4A-NA	2.58	128.13	124.40
28	J	306	CLA	CHB-C4A-NA	2.58	128.13	124.40
28	L	308	CLA	C1-C2-C3	-2.58	122.58	126.76
28	L	318	CLA	C3B-C4B-NB	-2.58	108.22	110.53
28	a	713	CLA	C3B-C4B-NB	-2.58	108.23	110.53
26	M	303	DD6	C24-C1-C2	2.58	123.07	119.01
28	F	315	CLA	C3B-C4B-NB	-2.58	108.23	110.53
35	a	734	BCR	C33-C5-C4	2.58	119.10	113.60
26	J	304	DD6	C25-C26-C27	-2.58	119.40	126.61
28	K	312	CLA	CHB-C4A-NA	2.58	128.12	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	a	711	CLA	C3B-C4B-NB	-2.58	108.23	110.53
28	A	311	CLA	CHB-C4A-NA	2.58	128.12	124.40
29	I	314	KC1	C1D-CHD-C4C	-2.58	120.19	126.25
28	f	303	CLA	C3B-C4B-NB	-2.58	108.23	110.53
28	b	714	CLA	C3B-C4B-NB	-2.58	108.23	110.53
28	a	721	CLA	C1-C2-C3	-2.58	121.97	126.20
26	M	305	DD6	C25-C26-C27	-2.58	119.41	126.61
29	M	314	KC1	C1D-CHD-C4C	-2.58	120.19	126.25
28	A	310	CLA	CHB-C4A-NA	2.58	128.12	124.40
28	b	718	CLA	C3B-C4B-NB	-2.58	108.23	110.53
28	J	307	CLA	C3B-C4B-NB	-2.58	108.23	110.53
26	A	302	DD6	C3-C4-C5	-2.58	118.25	123.52
32	D	306	PID	CM5-C21-C20	-2.57	118.64	122.82
26	G	502	DD6	O1-C20-C21	-2.57	112.17	115.05
27	I	304	UIX	O2-C27-O4	-2.57	118.02	122.99
28	M	310	CLA	C3B-C4B-NB	-2.57	108.23	110.53
26	K	305	DD6	C9-C10-C11	-2.57	123.67	127.28
28	G	517	CLA	CHB-C4A-NA	2.57	128.11	124.40
28	B	308	CLA	CHB-C4A-NA	2.57	128.11	124.40
26	A	305	DD6	C25-C26-C27	-2.57	119.42	126.61
28	L	312	CLA	CHB-C4A-NA	2.57	128.11	124.40
26	L	303	DD6	O1-C15-C14	-2.57	109.51	116.88
28	A	309	CLA	C3B-C4B-NB	-2.57	108.24	110.53
31	I	318	LMG	O7-C10-O9	-2.57	117.70	123.70
29	L	307	KC1	O2A-CGA-O1A	-2.57	117.47	122.70
35	b	730	BCR	C2-C1-C6	2.57	114.17	110.44
29	D	310	KC1	C1D-CHD-C4C	-2.57	120.21	126.25
26	M	306	DD6	C19-C18-C17	-2.57	105.99	110.79
32	G	507	PID	CM5-C21-C20	-2.56	118.66	122.82
29	F	314	KC1	C1D-CHD-C4C	-2.56	120.22	126.25
28	M	310	CLA	CHB-C4A-NA	2.56	128.10	124.40
26	B	302	DD6	C8-C6-C5	-2.56	118.79	124.72
26	K	303	DD6	C21-C20-C15	-2.56	118.08	122.30
29	N	308	KC1	C1D-CHD-C4C	-2.56	120.22	126.25
26	N	303	DD6	C14-C13-C11	-2.56	121.55	125.53
29	H	306	KC1	C2A-C3A-C4A	2.56	108.33	106.41
28	b	709	CLA	C1-C2-C3	-2.56	122.00	126.20
28	J	309	CLA	CHB-C4A-NA	2.56	128.09	124.40
27	B	305	UIX	O2-C27-O4	-2.56	118.05	122.99
30	G	521	DGD	C6E-C5E-C4E	2.56	119.30	113.02
29	G	515	KC1	O1D-CGD-CBD	-2.56	119.47	124.52
26	M	304	DD6	C37-C36-C31	-2.56	119.38	124.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	B	314	KC1	C1D-CHD-C4C	-2.56	120.24	126.25
30	I	317	DGD	C2G-O2G-C1B	-2.56	111.68	117.80
28	a	731	CLA	C1-C2-C3	-2.55	122.01	126.20
32	N	301	PID	CM5-C21-C20	-2.55	118.68	122.82
28	A	310	CLA	C3B-C4B-NB	-2.55	108.25	110.53
36	b	729	PQN	C14-C13-C15	2.55	119.66	115.23
29	N	306	KC1	C1D-CHD-C4C	-2.55	120.24	126.25
28	J	301	CLA	CHB-C4A-NA	2.55	128.09	124.40
26	D	303	DD6	C4-C3-C2	-2.55	118.30	123.52
28	D	311	CLA	CHB-C4A-NA	2.55	128.08	124.40
28	l	310	CLA	CMB-C2B-C3B	2.55	129.78	124.68
28	j	104	CLA	C1-C2-C3	-2.55	122.02	126.20
29	G	515	KC1	C2A-C3A-C4A	2.55	108.33	106.41
28	F	311	CLA	CHB-C4A-NA	2.55	128.08	124.40
28	I	308	CLA	C1-C2-C3	-2.55	122.02	126.20
30	y	201	DGD	C2G-O2G-C1B	-2.55	111.70	117.80
28	I	306	CLA	CHB-C4A-NA	2.55	128.07	124.40
26	M	306	DD6	C21-C20-C15	-2.55	118.11	122.30
28	G	514	CLA	C3B-C4B-NB	-2.54	108.26	110.53
26	L	306	DD6	C25-C26-C27	-2.54	119.50	126.61
32	j	105	PID	C8-C9-C10	2.54	128.58	123.60
29	K	314	KC1	C1D-CHD-C4C	-2.54	120.27	126.25
26	F	303	DD6	C4-C3-C2	-2.54	118.32	123.52
28	a	706	CLA	CHB-C4A-NA	2.54	128.07	124.40
29	N	311	KC1	C1D-CHD-C4C	-2.54	120.27	126.25
28	b	719	CLA	C3B-C4B-NB	-2.54	108.26	110.53
28	b	714	CLA	CHB-C4A-NA	2.54	128.06	124.40
26	H	303	DD6	O1-C20-C19	-2.54	111.11	113.49
29	M	307	KC1	CHB-C1B-C2B	-2.54	120.21	125.49
26	h	203	DD6	O1-C15-C14	-2.54	109.61	116.88
26	B	306	DD6	C10-C9-C8	-2.53	115.86	123.20
27	A	304	UIX	C13-C14-C23	-2.53	115.86	123.20
26	K	304	DD6	O1-C20-C21	-2.53	112.22	115.05
28	G	518	CLA	CHB-C4A-NA	2.53	128.05	124.40
28	I	319	CLA	CHB-C4A-NA	2.53	128.05	124.40
28	M	315	CLA	C3B-C4B-NB	-2.53	108.27	110.53
28	a	710	CLA	C1-C2-C3	-2.53	122.05	126.20
28	a	711	CLA	CHB-C4A-NA	2.53	128.05	124.40
28	l	308	CLA	CAA-C2A-C3A	-2.53	110.43	116.23
26	L	305	DD6	C37-C36-C31	-2.53	119.43	124.16
28	K	308	CLA	C3B-C4B-NB	-2.53	108.27	110.53
27	A	304	UIX	C22-C15-C20	-2.52	108.21	110.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	M	307	KC1	C4B-CHC-C1C	-2.52	120.66	126.02
28	L	317	CLA	CHB-C4A-NA	2.52	128.04	124.40
28	l	312	CLA	C3B-C4B-NB	-2.52	108.28	110.53
26	G	504	DD6	O1-C20-C15	-2.52	56.93	58.93
28	b	704	CLA	CAC-C3C-C4C	2.52	128.07	124.79
27	A	304	UIX	O2-C27-O4	-2.52	118.12	122.99
28	I	310	CLA	CHB-C4A-NA	2.52	128.04	124.40
26	I	302	DD6	C37-C36-C31	-2.52	119.45	124.16
35	l	307	BCR	C21-C20-C19	-2.52	115.90	123.20
28	a	715	CLA	CHB-C4A-NA	2.52	128.03	124.40
28	b	727	CLA	CHB-C4A-NA	2.52	128.03	124.40
28	B	309	CLA	CHB-C4A-NA	2.52	128.03	124.40
28	B	313	CLA	CHB-C4A-NA	2.52	128.03	124.40
28	H	307	CLA	CHB-C4A-NA	2.52	128.03	124.40
26	B	303	DD6	C9-C10-C11	-2.52	123.75	127.28
28	l	305	CLA	C3B-C4B-NB	-2.52	108.28	110.53
32	M	301	PID	C19-C20-C21	2.52	130.81	127.28
28	A	313	CLA	CHB-C4A-NA	2.52	128.03	124.40
26	M	304	DD6	C10-C9-C8	-2.51	115.91	123.20
28	F	311	CLA	O2D-CGD-CBD	2.51	115.62	111.23
28	b	716	CLA	CHB-C4A-NA	2.51	128.03	124.40
26	G	505	DD6	C32-C33-C34	-2.51	108.08	113.59
28	K	313	CLA	CHB-C4A-NA	2.51	128.03	124.40
28	b	709	CLA	CHB-C4A-NA	2.51	128.03	124.40
29	D	315	KC1	O1D-CGD-CBD	-2.51	119.56	124.52
28	K	306	CLA	CHB-C4A-NA	2.51	128.03	124.40
28	h	202	CLA	CHB-C4A-NA	2.51	128.03	124.40
28	I	316	CLA	C1-C2-C3	-2.51	122.08	126.20
28	K	309	CLA	C1-C2-C3	-2.51	122.70	126.76
29	J	313	KC1	C1D-CHD-C4C	-2.51	120.35	126.25
28	J	306	CLA	C3B-C4B-NB	-2.51	108.29	110.53
26	L	306	DD6	O1-C20-C21	-2.51	112.25	115.05
35	f	304	BCR	C29-C30-C25	2.51	114.08	110.44
28	b	712	CLA	CMB-C2B-C3B	2.51	130.19	123.53
28	l	309	CLA	CHB-C4A-NA	2.51	128.02	124.40
32	D	304	PID	CM5-C21-C20	-2.51	118.75	122.82
28	A	317	CLA	CHB-C4A-NA	2.50	128.01	124.40
26	M	302	DD6	C9-C10-C11	-2.50	123.77	127.28
28	K	311	CLA	C3B-C4B-NB	-2.50	108.29	110.53
29	H	310	KC1	C4B-CHC-C1C	-2.50	120.70	126.02
29	F	314	KC1	C4B-CHC-C1C	-2.50	120.70	126.02
28	M	313	CLA	CHB-C4A-NA	2.50	128.01	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	a	714	CLA	C3B-C4B-NB	-2.50	108.30	110.53
35	a	734	BCR	C29-C30-C25	2.50	114.07	110.44
26	N	303	DD6	C4-C3-C2	-2.50	118.40	123.52
28	B	313	CLA	C3B-C4B-NB	-2.50	108.30	110.53
28	J	316	CLA	CHB-C4A-NA	2.50	128.01	124.40
29	L	315	KC1	O2D-CGD-O1D	-2.50	118.98	123.85
28	D	314	CLA	CAA-C2A-C3A	-2.50	106.24	113.00
28	b	704	CLA	CHB-C4A-NA	2.50	128.01	124.40
26	A	302	DD6	C37-C36-C31	-2.50	119.49	124.16
28	a	724	CLA	C3B-C4B-NB	-2.50	108.30	110.53
29	F	309	KC1	O1D-CGD-CBD	-2.50	119.59	124.52
28	a	738	CLA	CHB-C4A-NA	2.50	128.00	124.40
29	M	307	KC1	O2A-CGA-O1A	-2.50	117.62	122.70
28	B	315	CLA	CHB-C4A-NA	2.50	128.00	124.40
30	j	103	DGD	O1G-C1A-C2A	2.50	119.45	111.83
35	m	201	BCR	C38-C26-C27	2.50	118.92	113.60
28	b	705	CLA	CHB-C4A-NA	2.49	128.00	124.40
28	N	304	CLA	CHB-C4A-NA	2.49	128.00	124.40
28	G	513	CLA	O2D-CGD-O1D	-2.49	118.99	123.85
31	b	733	LMG	C1-C2-C3	-2.49	104.76	110.01
26	N	303	DD6	C21-C20-C15	-2.49	118.20	122.30
26	M	305	DD6	C37-C36-C31	-2.49	119.50	124.16
32	D	302	PID	CM5-C21-C20	-2.49	118.78	122.82
28	J	315	CLA	CHB-C4A-NA	2.49	128.00	124.40
35	a	736	BCR	C24-C23-C22	-2.49	122.55	126.23
28	b	728	CLA	CHB-C4A-NA	2.49	127.99	124.40
28	F	315	CLA	CHB-C4A-NA	2.49	127.99	124.40
28	a	720	CLA	CHB-C4A-NA	2.49	127.99	124.40
28	a	731	CLA	CHB-C4A-NA	2.49	127.99	124.40
35	j	102	BCR	C10-C11-C12	-2.49	115.99	123.20
28	A	315	CLA	CHB-C4A-NA	2.49	127.99	124.40
35	l	306	BCR	C35-C13-C12	2.49	121.89	118.09
28	I	309	CLA	CHB-C4A-NA	2.49	127.99	124.40
26	M	303	DD6	C37-C36-C35	2.49	118.99	114.42
26	J	304	DD6	C28-C27-C26	-2.49	119.36	124.18
28	b	718	CLA	CHB-C4A-NA	2.48	127.99	124.40
28	I	313	CLA	CHB-C4A-NA	2.48	127.98	124.40
28	J	314	CLA	CHB-C4A-NA	2.48	127.98	124.40
26	K	301	DD6	C10-C9-C8	-2.48	116.00	123.20
28	G	511	CLA	CHB-C4A-NA	2.48	127.98	124.40
35	f	304	BCR	C11-C12-C13	-2.48	119.56	126.36
29	K	314	KC1	C4B-CHC-C1C	-2.48	120.75	126.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	G	520	CLA	C3B-C4B-NB	-2.48	108.31	110.53
35	a	734	BCR	C15-C16-C17	-2.48	118.44	123.52
28	b	712	CLA	CHB-C4A-NA	2.48	127.98	124.40
28	L	316	CLA	CHB-C4A-NA	2.48	127.98	124.40
28	G	511	CLA	C3B-C4B-NB	-2.48	108.32	110.53
26	L	302	DD6	O1-C20-C19	-2.48	111.17	113.49
26	G	502	DD6	C37-C36-C31	-2.48	119.52	124.16
28	G	519	CLA	C3B-C4B-NB	-2.48	108.32	110.53
28	D	309	CLA	C3B-C4B-NB	-2.48	108.32	110.53
28	G	516	CLA	CHB-C4A-NA	2.48	127.97	124.40
28	D	312	CLA	CHB-C4A-NA	2.48	127.97	124.40
35	l	307	BCR	C28-C27-C26	-2.48	109.64	114.06
28	f	303	CLA	CHB-C4A-NA	2.48	127.97	124.40
28	I	321	CLA	O2A-CGA-O1A	-2.47	117.44	123.63
28	a	714	CLA	CHB-C4A-NA	2.47	127.97	124.40
28	F	308	CLA	CHB-C4A-NA	2.47	127.97	124.40
28	H	309	CLA	CHB-C4A-NA	2.47	127.97	124.40
26	I	302	DD6	C3-C4-C5	-2.47	118.46	123.52
28	F	307	CLA	CHB-C4A-NA	2.47	127.97	124.40
32	N	302	PID	CM4-C14-C13	2.47	124.51	119.05
27	G	503	UIX	C13-C14-C23	-2.47	116.03	123.20
29	A	306	KC1	C1D-CHD-C4C	-2.47	120.43	126.25
29	L	315	KC1	C2A-C3A-C4A	2.47	108.27	106.41
29	L	307	KC1	O2D-CGD-O1D	-2.47	119.04	123.85
28	L	313	CLA	O2A-CGA-O1A	-2.47	117.45	123.63
28	b	719	CLA	CHB-C4A-NA	2.47	127.97	124.40
26	M	302	DD6	C10-C9-C8	-2.47	116.05	123.20
27	A	304	UIX	C34-C37-C39	-2.47	118.47	123.52
28	A	309	CLA	CHB-C4A-NA	2.47	127.96	124.40
28	A	316	CLA	CHB-C4A-NA	2.47	127.96	124.40
26	M	304	DD6	O1-C20-C21	-2.47	112.29	115.05
28	A	308	CLA	CHB-C4A-NA	2.47	127.96	124.40
28	K	315	CLA	C3B-C4B-NB	-2.47	108.33	110.53
28	F	308	CLA	C3B-C4B-NB	-2.47	108.33	110.53
26	M	304	DD6	C9-C10-C11	-2.46	123.82	127.28
26	b	731	DD6	C10-C9-C8	-2.46	116.06	123.20
28	M	308	CLA	CHB-C4A-NA	2.46	127.96	124.40
28	I	313	CLA	C3B-C4B-NB	-2.46	108.33	110.53
27	h	201	UIX	O2-C27-O4	-2.46	118.23	122.99
29	F	314	KC1	O1D-CGD-CBD	-2.46	119.66	124.52
35	a	736	BCR	C33-C5-C4	2.46	118.85	113.60
28	f	301	CLA	CHB-C4A-NA	2.46	127.95	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	F	307	CLA	C3B-C4B-NB	-2.46	108.33	110.53
28	G	509	CLA	CHB-C4A-NA	2.46	127.95	124.40
26	A	301	DD6	O1-C20-C21	-2.46	112.30	115.05
28	a	709	CLA	CHB-C4A-NA	2.46	127.95	124.40
28	b	721	CLA	C3B-C4B-NB	-2.46	108.33	110.53
28	K	309	CLA	CHB-C4A-NA	2.46	127.95	124.40
28	J	311	CLA	CHB-C4A-NA	2.46	127.95	124.40
28	H	308	CLA	CHB-C4A-NA	2.46	127.95	124.40
26	I	303	DD6	C12-C11-C10	-2.46	118.84	122.82
28	b	710	CLA	C3B-C4B-NB	-2.46	108.34	110.53
26	K	319	DD6	C37-C36-C31	-2.46	119.57	124.16
28	A	307	CLA	CHB-C4A-NA	2.46	127.94	124.40
28	J	311	CLA	C3B-C4B-NB	-2.46	108.34	110.53
29	I	314	KC1	C4B-CHC-C1C	-2.45	120.80	126.02
29	A	306	KC1	C4B-CHC-C1C	-2.45	120.80	126.02
28	M	316	CLA	CHB-C4A-NA	2.45	127.94	124.40
29	N	311	KC1	C4B-CHC-C1C	-2.45	120.81	126.02
26	N	303	DD6	C37-C36-C35	2.45	118.93	114.42
29	N	311	KC1	O1D-CGD-CBD	-2.45	119.68	124.52
28	L	314	CLA	CHB-C4A-NA	2.45	127.94	124.40
27	h	201	UIX	C12-C11-C10	2.45	121.83	118.09
28	b	709	CLA	O2D-CGD-CBD	2.45	115.51	111.23
28	D	316	CLA	CHB-C4A-NA	2.45	127.94	124.40
28	J	308	CLA	CHB-C4A-NA	2.45	127.94	124.40
28	a	706	CLA	C3B-C4B-NB	-2.45	108.34	110.53
26	L	306	DD6	C21-C20-C15	-2.45	118.27	122.30
35	i	201	BCR	C28-C27-C26	-2.45	109.69	114.06
35	l	306	BCR	C10-C11-C12	-2.45	116.10	123.20
28	D	309	CLA	CHB-C4A-NA	2.45	127.93	124.40
28	L	309	CLA	CHB-C4A-NA	2.45	127.93	124.40
28	f	302	CLA	C3B-C4B-NB	-2.45	108.34	110.53
29	G	515	KC1	C4B-CHC-C1C	-2.45	120.82	126.02
26	G	504	DD6	C28-C27-C26	-2.45	119.43	124.18
28	H	312	CLA	CHB-C4A-NA	2.45	127.93	124.40
26	h	203	DD6	C3-C4-C5	-2.45	118.52	123.52
26	G	505	DD6	O1-C20-C19	2.45	115.78	113.49
28	K	313	CLA	C3B-C4B-NB	-2.45	108.35	110.53
28	G	509	CLA	C3B-C4B-NB	-2.45	108.35	110.53
26	I	301	DD6	C28-C27-C26	-2.45	119.43	124.18
26	A	303	DD6	C37-C36-C31	-2.45	119.59	124.16
28	b	724	CLA	CHB-C4A-NA	2.44	127.93	124.40
35	a	734	BCR	C21-C20-C19	-2.44	116.12	123.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	a	728	CLA	CHB-C4A-NA	2.44	127.93	124.40
28	b	715	CLA	CHB-C4A-NA	2.44	127.93	124.40
28	B	307	CLA	CHB-C4A-NA	2.44	127.93	124.40
26	I	303	DD6	C19-C18-C17	-2.44	106.22	110.79
29	N	308	KC1	CGD-CBD-CAD	-2.44	102.94	110.85
28	j	104	CLA	CHB-C4A-NA	2.44	127.92	124.40
26	H	303	DD6	C37-C36-C31	-2.44	119.60	124.16
27	I	304	UIX	C41-C40-C38	2.44	121.81	118.09
26	G	502	DD6	C37-C36-C35	2.44	118.91	114.42
28	K	308	CLA	CHB-C4A-NA	2.44	127.92	124.40
28	M	311	CLA	CHB-C4A-NA	2.44	127.92	124.40
26	K	304	DD6	C32-C33-C34	-2.44	108.25	113.59
28	a	708	CLA	CHB-C4A-NA	2.44	127.92	124.40
26	I	305	DD6	C37-C36-C31	-2.44	119.61	124.16
26	I	305	DD6	C-C1-C2	-2.44	118.87	122.82
28	b	728	CLA	C1-C2-C3	-2.44	122.21	126.20
29	L	307	KC1	C4B-CHC-C1C	-2.43	120.84	126.02
26	L	305	DD6	C37-C36-C35	2.43	118.90	114.42
30	G	521	DGD	C1D-O6D-C5D	-2.43	108.97	113.72
26	G	504	DD6	C25-C24-C1	-2.43	119.69	126.36
28	a	723	CLA	C3B-C4B-NB	-2.43	108.36	110.53
26	G	504	DD6	O1-C15-C14	-2.43	109.91	116.88
28	b	708	CLA	CHB-C4A-NA	2.43	127.91	124.40
26	L	306	DD6	C28-C27-C26	-2.43	119.46	124.18
27	h	201	UIX	C35-C36-C38	-2.43	116.16	123.20
28	a	735	CLA	C1-C2-C3	-2.43	122.22	126.20
35	b	732	BCR	C38-C26-C25	-2.43	121.83	124.48
35	m	201	BCR	C36-C18-C19	2.43	121.80	118.09
29	N	306	KC1	C4B-CHC-C1C	-2.43	120.86	126.02
28	b	722	CLA	CMB-C2B-C1B	-2.43	121.73	125.42
26	A	305	DD6	C21-C20-C15	-2.42	118.31	122.30
28	H	305	CLA	CHB-C4A-NA	2.42	127.90	124.40
26	G	508	DD6	C37-C36-C35	2.42	118.88	114.42
28	l	303	CLA	CHB-C4A-NA	2.42	127.90	124.40
28	a	707	CLA	CHB-C4A-NA	2.42	127.90	124.40
29	A	314	KC1	C4B-CHC-C1C	-2.42	120.87	126.02
28	b	713	CLA	CHB-C4A-NA	2.42	127.89	124.40
28	K	311	CLA	CHB-C4A-NA	2.42	127.89	124.40
35	l	302	BCR	C37-C22-C21	-2.42	118.89	122.82
26	A	301	DD6	C37-C36-C31	-2.42	119.64	124.16
26	N	303	DD6	C25-C26-C27	-2.42	119.84	126.61
26	J	304	DD6	C-C1-C2	-2.42	118.90	122.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	I	316	CLA	C3B-C4B-NB	-2.42	108.37	110.53
28	b	711	CLA	CHB-C4A-NA	2.42	127.89	124.40
28	I	308	CLA	CHB-C4A-NA	2.42	127.89	124.40
32	H	302	PID	CM5-C21-C20	-2.42	118.90	122.82
28	l	303	CLA	C3B-C4B-NB	-2.42	108.37	110.53
28	a	725	CLA	CHB-C4A-NA	2.41	127.88	124.40
26	M	303	DD6	C12-C11-C10	-2.41	118.91	122.82
28	I	307	CLA	CHB-C4A-NA	2.41	127.88	124.40
28	J	312	CLA	O2A-CGA-O1A	-2.41	117.59	123.63
26	A	302	DD6	C25-C26-C27	-2.41	119.86	126.61
29	L	315	KC1	C4B-CHC-C1C	-2.41	120.89	126.02
32	j	105	PID	CM5-C21-C20	-2.41	118.91	122.82
28	a	703	CLA	CHB-C4A-NA	2.41	127.88	124.40
28	a	720	CLA	C3B-C4B-NB	-2.41	108.38	110.53
28	a	712	CLA	CHB-C4A-NA	2.41	127.88	124.40
28	L	310	CLA	CHB-C4A-NA	2.41	127.88	124.40
26	B	303	DD6	C10-C9-C8	-2.41	116.22	123.20
26	A	302	DD6	O1-C20-C21	-2.41	112.36	115.05
28	K	310	CLA	CHB-C4A-NA	2.41	127.88	124.40
35	b	730	BCR	C36-C18-C19	2.41	121.77	118.09
28	H	311	CLA	CAA-C2A-C3A	-2.41	110.71	116.23
28	N	309	CLA	CHB-C4A-NA	2.41	127.87	124.40
29	G	515	KC1	CAC-C3C-C4C	2.41	127.92	124.79
29	L	315	KC1	C1D-CHD-C4C	-2.41	120.59	126.25
26	L	302	DD6	C37-C36-C31	-2.41	119.66	124.16
28	G	512	CLA	CHB-C4A-NA	2.41	127.87	124.40
28	B	301	CLA	C3B-C4B-NB	-2.41	108.38	110.53
35	a	736	BCR	C21-C20-C19	-2.40	116.23	123.20
28	b	707	CLA	C3B-C4B-NB	-2.40	108.38	110.53
28	K	316	CLA	CHB-C4A-NA	2.40	127.87	124.40
28	L	309	CLA	O2D-CGD-CBD	2.40	115.43	111.23
26	G	505	DD6	C25-C26-C27	-2.40	119.89	126.61
26	B	306	DD6	C25-C24-C1	-2.40	119.78	126.36
32	D	305	PID	CM4-C14-C13	2.40	124.34	119.05
31	B	318	LMG	O7-C10-O9	-2.40	118.10	123.70
28	l	308	CLA	CHB-C4A-NA	2.40	127.86	124.40
29	F	314	KC1	O2D-CGD-O1D	-2.40	119.18	123.85
26	K	301	DD6	C4-C3-C2	-2.40	118.61	123.52
26	h	203	DD6	C10-C9-C8	-2.40	116.25	123.20
28	D	313	CLA	CHB-C4A-NA	2.40	127.86	124.40
26	F	303	DD6	C21-C20-C15	-2.40	118.36	122.30
28	K	307	CLA	CHB-C4A-NA	2.40	127.86	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	D	310	KC1	O1D-CGD-CBD	-2.39	119.80	124.52
28	A	320	CLA	CHB-C4A-NA	2.39	127.85	124.40
28	B	309	CLA	C3B-C4B-NB	-2.39	108.39	110.53
26	B	306	DD6	C37-C36-C35	2.39	118.82	114.42
28	b	712	CLA	CAB-C3B-C2B	2.39	129.88	123.53
29	I	314	KC1	O2D-CGD-O1D	-2.39	119.20	123.85
28	b	720	CLA	CHB-C4A-NA	2.39	127.85	124.40
28	M	312	CLA	CHB-C4A-NA	2.39	127.85	124.40
32	D	305	PID	C18-C17-C16	2.39	130.24	124.72
29	N	306	KC1	O2D-CGD-O1D	-2.39	119.20	123.85
28	a	725	CLA	C1-C2-C3	-2.39	122.29	126.20
29	M	307	KC1	C2A-C3A-C4A	2.39	108.20	106.41
28	a	727	CLA	CHB-C4A-NA	2.39	127.84	124.40
28	a	728	CLA	C1-C2-C3	-2.39	122.29	126.20
28	a	722	CLA	CHB-C4A-NA	2.39	127.84	124.40
26	B	303	DD6	C3-C4-C5	-2.38	118.64	123.52
28	a	717	CLA	C3B-C4B-NB	-2.38	108.40	110.53
32	H	302	PID	C8-C9-C10	2.38	128.27	123.60
28	b	726	CLA	CHB-C4A-NA	2.38	127.84	124.40
26	B	306	DD6	O1-C20-C21	-2.38	112.39	115.05
26	K	305	DD6	C37-C36-C31	-2.38	119.71	124.16
28	b	706	CLA	CHB-C4A-NA	2.38	127.84	124.40
28	M	315	CLA	O2D-CGD-CBD	2.38	115.39	111.23
26	G	505	DD6	C19-C18-C17	-2.38	106.34	110.79
28	m	202	CLA	CHB-C4A-NA	2.38	127.83	124.40
28	I	321	CLA	C1-C2-C3	-2.38	122.30	126.20
26	J	304	DD6	C12-C11-C10	-2.38	118.96	122.82
28	a	710	CLA	CHB-C4A-NA	2.38	127.83	124.40
28	M	318	CLA	CHB-C4A-NA	2.38	127.83	124.40
28	l	305	CLA	CHB-C4A-NA	2.38	127.83	124.40
28	J	309	CLA	O2A-CGA-O1A	-2.38	117.68	123.63
28	a	723	CLA	CHB-C4A-NA	2.38	127.83	124.40
32	D	302	PID	CM4-C14-C13	2.37	124.29	119.05
28	a	713	CLA	C1-C2-C3	-2.37	122.31	126.20
29	B	314	KC1	C4B-CHC-C1C	-2.37	120.98	126.02
26	L	303	DD6	O1-C20-C19	-2.37	111.27	113.49
26	M	305	DD6	C37-C36-C35	2.37	118.78	114.42
26	I	302	DD6	C7-C6-C5	-2.37	118.98	122.82
28	K	315	CLA	CHB-C4A-NA	2.37	127.82	124.40
26	J	302	DD6	C25-C26-C27	-2.37	119.98	126.61
28	H	304	CLA	CHB-C4A-NA	2.37	127.82	124.40
26	b	731	DD6	C37-C36-C31	-2.37	119.74	124.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	H	306	KC1	C4B-CHC-C1C	-2.36	120.99	126.02
26	B	306	DD6	C28-C27-C26	-2.36	119.59	124.18
26	G	508	DD6	C37-C36-C31	-2.36	119.74	124.16
29	M	314	KC1	C4B-CHC-C1C	-2.36	121.00	126.02
26	B	302	DD6	C8-C9-C10	-2.36	118.69	123.52
32	D	305	PID	O1-C6-C7	-2.36	110.11	116.88
26	I	302	DD6	C4-C5-C6	-2.36	123.97	127.28
26	h	203	DD6	C14-C13-C11	-2.36	121.87	125.53
29	K	314	KC1	C2A-C3A-C4A	2.36	108.18	106.41
28	A	312	CLA	CHB-C4A-NA	2.36	127.81	124.40
28	G	514	CLA	C1-C2-C3	-2.36	122.33	126.20
28	I	316	CLA	O2A-CGA-O1A	-2.36	117.72	123.63
26	B	303	DD6	C21-C20-C15	-2.36	118.42	122.30
35	l	306	BCR	C21-C20-C19	-2.36	116.36	123.20
26	G	504	DD6	C-C1-C2	-2.36	119.00	122.82
35	a	736	BCR	C23-C24-C25	-2.36	120.70	127.00
28	J	311	CLA	O2A-CGA-O1A	-2.36	117.73	123.63
28	f	302	CLA	CHB-C4A-NA	2.36	127.80	124.40
26	M	305	DD6	C10-C9-C8	-2.36	116.37	123.20
28	I	311	CLA	CHB-C4A-NA	2.36	127.80	124.40
28	a	702	CLA	O2A-CGA-O1A	-2.36	117.74	123.63
28	j	106	CLA	CHB-C4A-NA	2.35	127.80	124.40
28	b	723	CLA	O2A-CGA-O1A	-2.35	117.74	123.63
28	H	311	CLA	C3B-C4B-NB	-2.35	108.43	110.53
28	a	717	CLA	CHB-C4A-NA	2.35	127.79	124.40
28	G	513	CLA	C3B-C4B-NB	-2.35	108.43	110.53
28	a	717	CLA	C1-C2-C3	-2.35	122.34	126.20
35	b	730	BCR	C30-C25-C26	-2.35	119.42	122.64
26	M	303	DD6	C13-C11-C10	2.35	122.71	119.01
35	b	702	BCR	C35-C13-C12	2.35	121.68	118.09
26	A	301	DD6	C3-C4-C5	-2.35	118.71	123.52
31	b	733	LMG	C38-C37-C36	-2.35	102.50	114.37
26	I	301	DD6	C14-C13-C11	-2.35	121.89	125.53
28	I	315	CLA	CHB-C4A-NA	2.35	127.79	124.40
28	b	703	CLA	O2A-CGA-O1A	-2.35	117.76	123.63
28	A	308	CLA	C3B-C4B-NB	-2.35	108.44	110.53
28	N	307	CLA	C3B-C4B-NB	-2.35	108.44	110.53
26	M	303	DD6	C37-C36-C31	-2.35	119.77	124.16
28	l	312	CLA	CHB-C4A-NA	2.35	127.78	124.40
28	N	305	CLA	O2A-CGA-O1A	-2.34	117.77	123.63
26	J	303	DD6	C37-C36-C35	2.34	118.73	114.42
29	M	314	KC1	C2A-C3A-C4A	2.34	108.17	106.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	b	708	CLA	C1-C2-C3	-2.34	122.36	126.20
26	G	504	DD6	C25-C26-C27	-2.34	120.06	126.61
28	K	307	CLA	C3B-C4B-NB	-2.34	108.44	110.53
28	b	725	CLA	CHB-C4A-NA	2.34	127.78	124.40
28	G	520	CLA	CHB-C4A-NA	2.34	127.78	124.40
26	M	303	DD6	C21-C20-C19	2.34	116.87	114.24
26	M	305	DD6	O1-C15-C14	-2.34	110.18	116.88
28	b	707	CLA	O2A-CGA-O1A	-2.34	117.78	123.63
28	G	510	CLA	O2A-CGA-O1A	-2.34	117.79	123.63
31	I	320	LMG	O1-C7-C8	-2.33	105.14	110.82
28	j	106	CLA	C1-C2-C3	-2.33	122.37	126.20
26	F	303	DD6	C41-C32-C31	-2.33	106.34	110.52
29	A	306	KC1	O1D-CGD-CBD	-2.33	119.92	124.52
28	L	313	CLA	CHB-C4A-NA	2.33	127.76	124.40
26	K	305	DD6	C28-C27-C26	-2.33	119.66	124.18
28	j	106	CLA	C3B-C4B-NB	-2.33	108.45	110.53
26	A	302	DD6	C9-C8-C6	-2.33	119.98	126.36
29	J	313	KC1	O1D-CGD-CBD	-2.33	119.93	124.52
26	K	301	DD6	C37-C36-C35	2.33	118.70	114.42
35	b	732	BCR	C34-C9-C8	2.33	121.64	118.09
28	K	313	CLA	O2A-CGA-O1A	-2.33	117.81	123.63
29	M	314	KC1	O1D-CGD-CBD	-2.33	119.93	124.52
28	L	309	CLA	O2A-CGA-O1A	-2.33	117.81	123.63
28	A	319	CLA	CHB-C4A-NA	2.33	127.76	124.40
26	M	302	DD6	C37-C36-C35	2.32	118.70	114.42
28	I	315	CLA	O2D-CGD-CBD	2.32	115.29	111.23
28	b	706	CLA	O2A-CGA-O1A	-2.32	117.81	123.63
26	h	203	DD6	C37-C36-C31	-2.32	119.81	124.16
32	H	301	PID	CM5-C21-C20	-2.32	119.05	122.82
26	B	302	DD6	O1-C20-C19	2.32	115.67	113.49
26	L	306	DD6	C9-C8-C6	-2.32	120.00	126.36
28	M	309	CLA	CHB-C4A-NA	2.32	127.75	124.40
26	F	301	DD6	O1-C15-C14	-2.32	110.23	116.88
28	m	202	CLA	CMB-C2B-C3B	2.32	132.00	126.55
28	I	311	CLA	O2D-CGD-CBD	2.32	115.28	111.23
31	I	320	LMG	O7-C10-O9	-2.32	118.29	123.70
29	G	515	KC1	C1D-CHD-C4C	-2.32	120.80	126.25
28	D	308	CLA	CHB-C4A-NA	2.32	127.74	124.40
29	H	306	KC1	O2D-CGD-O1D	-2.31	119.34	123.85
28	a	724	CLA	CHB-C4A-NA	2.31	127.74	124.40
28	B	316	CLA	CHB-C4A-NA	2.31	127.74	124.40
28	a	717	CLA	O2A-CGA-O1A	-2.31	117.84	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	a	730	CLA	O2A-CGA-O1A	-2.31	117.84	123.63
27	A	304	UIX	C-C7-C10	-2.31	121.10	125.99
26	N	303	DD6	C37-C36-C31	-2.31	119.84	124.16
28	l	304	CLA	C3B-C4B-NB	-2.31	108.47	110.53
27	K	302	UIX	O2-C27-O4	-2.31	118.53	122.99
28	I	312	CLA	CHB-C4A-NA	2.31	127.73	124.40
36	a	732	PQN	C2M-C2-C3	-2.31	120.65	124.45
26	A	301	DD6	C37-C36-C35	2.31	118.67	114.42
27	I	304	UIX	C34-C30-C26	-2.31	124.04	127.28
26	K	304	DD6	C37-C36-C31	-2.31	119.84	124.16
28	F	310	CLA	O2D-CGD-CBD	2.31	115.27	111.23
31	B	318	LMG	C38-C37-C36	-2.31	102.70	114.37
35	b	730	BCR	C24-C23-C22	-2.31	122.82	126.23
27	G	503	UIX	O2-C27-O4	-2.31	118.54	122.99
28	a	705	CLA	CAA-CBA-CGA	-2.30	106.66	113.21
28	B	310	CLA	O2D-CGD-CBD	2.30	115.26	111.23
28	L	308	CLA	CHB-C4A-NA	2.30	127.72	124.40
35	b	732	BCR	C37-C22-C23	2.30	121.61	118.09
32	N	301	PID	C15-C14-C13	2.30	122.72	116.80
28	I	313	CLA	O2A-CGA-O1A	-2.30	117.87	123.63
35	b	730	BCR	C38-C26-C27	2.30	118.50	113.60
26	A	301	DD6	O1-C15-C14	-2.30	110.29	116.88
26	K	303	DD6	C37-C36-C31	-2.30	119.86	124.16
26	G	505	DD6	C28-C27-C26	-2.30	119.72	124.18
26	I	303	DD6	C28-C27-C26	-2.30	119.72	124.18
26	B	304	DD6	C37-C36-C35	2.30	118.64	114.42
26	F	301	DD6	C4-C3-C2	-2.30	118.82	123.52
26	N	303	DD6	C9-C8-C6	-2.30	120.06	126.36
32	N	302	PID	C8-C9-C10	2.30	128.10	123.60
28	H	311	CLA	CHB-C4A-NA	2.30	127.71	124.40
26	A	303	DD6	C26-C25-C24	-2.30	116.55	123.20
35	b	732	BCR	C35-C13-C12	2.30	121.59	118.09
28	a	711	CLA	CMB-C2B-C1B	-2.30	121.92	125.42
26	B	304	DD6	C3-C4-C5	-2.30	118.82	123.52
32	M	301	PID	C7-C8-C9	-2.29	123.16	126.06
27	J	305	UIX	C18-O2-C27	-2.29	113.79	117.85
28	a	719	CLA	CHB-C4A-NA	2.29	127.71	124.40
28	a	729	CLA	CHB-C4A-NA	2.29	127.71	124.40
28	L	314	CLA	C1-C2-C3	-2.29	122.44	126.20
35	l	307	BCR	C8-C7-C6	-2.29	120.87	127.00
28	b	727	CLA	O2A-CGA-O1A	-2.29	117.89	123.63
28	F	312	CLA	O2D-CGD-O1D	-2.29	119.39	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	B	310	CLA	O2A-CGA-O1A	-2.29	117.90	123.63
32	D	302	PID	C17-C16-C15	2.29	128.21	123.52
26	B	303	DD6	C26-C25-C24	-2.29	116.56	123.20
26	b	731	DD6	C21-C20-C15	-2.29	118.53	122.30
35	b	730	BCR	C37-C22-C23	2.29	121.58	118.09
28	b	716	CLA	C1-C2-C3	-2.29	123.06	126.76
26	K	319	DD6	C3-C4-C5	-2.28	118.84	123.52
26	B	302	DD6	C4-C3-C2	-2.28	118.84	123.52
26	A	303	DD6	C4-C3-C2	-2.28	118.85	123.52
28	L	309	CLA	C3B-C4B-NB	-2.28	108.49	110.53
26	K	319	DD6	C9-C8-C6	-2.28	120.11	126.36
31	D	317	LMG	O1-C7-C8	-2.28	105.27	110.82
26	B	306	DD6	O1-C20-C19	-2.28	111.35	113.49
36	a	732	PQN	C12-C11-C3	-2.28	106.47	112.08
35	i	201	BCR	C33-C5-C4	2.28	118.45	113.60
30	y	201	DGD	O1G-C1A-C2A	2.28	118.78	111.83
31	K	318	LMG	O1-C1-C2	-2.28	104.82	108.27
26	J	303	DD6	C-C1-C2	-2.28	119.13	122.82
26	K	319	DD6	C37-C36-C35	2.28	118.61	114.42
28	G	512	CLA	C3B-C4B-NB	-2.28	108.50	110.53
28	a	729	CLA	C1-C2-C3	-2.27	122.47	126.20
28	b	717	CLA	CHB-C4A-NA	2.27	127.68	124.40
32	j	105	PID	O1-C6-C7	-2.27	110.36	116.88
28	L	308	CLA	CAC-C3C-C4C	2.27	127.75	124.79
28	a	735	CLA	C3B-C4B-NB	-2.27	108.50	110.53
35	a	736	BCR	C4-C5-C6	-2.27	119.64	122.70
26	M	302	DD6	C28-C27-C26	-2.27	119.78	124.18
35	l	302	BCR	C11-C10-C9	-2.27	124.10	127.28
27	A	304	UIX	C7-C10-C11	-2.27	122.02	125.53
32	D	307	PID	CM5-C21-C20	-2.26	119.15	122.82
26	J	303	DD6	C9-C8-C6	-2.26	120.16	126.36
26	G	502	DD6	C25-C24-C1	-2.26	120.16	126.36
35	f	304	BCR	C8-C7-C6	-2.26	120.96	127.00
31	K	317	LMG	O7-C10-O9	-2.26	118.42	123.70
26	K	304	DD6	C21-C20-C15	-2.26	118.58	122.30
26	I	303	DD6	C37-C36-C35	2.26	118.58	114.42
27	G	503	UIX	C12-C11-C10	2.26	121.54	118.09
26	I	305	DD6	C9-C10-C11	-2.26	124.11	127.28
28	G	518	CLA	O2D-CGD-CBD	2.26	115.18	111.23
28	b	706	CLA	C3B-C4B-NB	-2.26	108.51	110.53
28	b	701	CLA	O2A-CGA-O1A	-2.26	117.98	123.63
27	J	305	UIX	C29-C26-C30	-2.26	119.16	122.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	K	305	DD6	C37-C36-C35	2.26	118.57	114.42
28	M	308	CLA	O2A-CGA-O1A	-2.26	117.98	123.63
28	B	301	CLA	O2A-CGA-O1A	-2.26	117.99	123.63
29	D	315	KC1	CAB-C3B-C4B	2.26	130.21	124.82
28	J	311	CLA	CMB-C2B-C1B	-2.25	121.99	125.42
32	N	302	PID	C6-C7-C8	-2.25	121.23	125.99
26	A	302	DD6	C25-C24-C1	-2.25	120.18	126.36
29	J	313	KC1	C2A-C3A-C4A	2.25	108.10	106.41
28	A	317	CLA	CMA-C3A-C2A	-2.25	111.06	116.23
26	L	305	DD6	C28-C27-C26	-2.25	119.81	124.18
28	B	311	CLA	CHB-C4A-NA	2.25	127.65	124.40
28	F	312	CLA	CHB-C4A-NA	2.25	127.65	124.40
26	K	301	DD6	C-C1-C24	2.25	121.52	118.09
28	I	310	CLA	O2A-CGA-O1A	-2.24	118.02	123.63
26	L	302	DD6	C32-C33-C34	-2.24	108.67	113.59
35	l	302	BCR	C34-C9-C8	2.24	121.52	118.09
32	D	305	PID	C8-C9-C10	2.24	127.99	123.60
28	a	728	CLA	O2A-CGA-O1A	-2.24	118.02	123.63
31	b	733	LMG	O1-C7-C8	-2.24	105.36	110.82
35	l	307	BCR	C10-C11-C12	-2.24	116.70	123.20
26	F	303	DD6	C25-C26-C27	-2.24	120.34	126.61
26	M	306	DD6	O1-C20-C15	-2.24	57.15	58.93
35	b	730	BCR	C20-C21-C22	-2.24	124.14	127.28
29	D	310	KC1	C2A-C3A-C4A	2.24	108.09	106.41
28	L	310	CLA	CMB-C2B-C1B	-2.24	122.01	125.42
27	h	201	UIX	C21-C15-C20	-2.24	108.47	110.47
28	a	730	CLA	C1-C2-C3	-2.24	122.53	126.20
28	B	310	CLA	CHB-C4A-NA	2.23	127.62	124.40
28	a	738	CLA	O2D-CGD-CBD	2.23	115.14	111.23
35	l	302	BCR	C33-C5-C4	2.23	118.36	113.60
26	J	302	DD6	C21-C20-C15	-2.23	118.63	122.30
28	G	520	CLA	CMB-C2B-C1B	-2.23	122.02	125.42
28	H	309	CLA	O2A-CGA-O1A	-2.23	118.05	123.63
26	M	303	DD6	C19-C18-C17	-2.23	106.62	110.79
26	A	305	DD6	C28-C27-C26	-2.23	119.86	124.18
28	a	726	CLA	O2A-CGA-O1A	-2.23	118.06	123.63
32	H	302	PID	O1-C6-C7	-2.23	110.50	116.88
29	N	306	KC1	C2A-C3A-C4A	2.23	108.08	106.41
28	a	722	CLA	O2A-CGA-O1A	-2.23	118.06	123.63
26	N	303	DD6	O1-C20-C21	-2.23	112.56	115.05
26	I	301	DD6	C21-C20-C15	-2.23	118.64	122.30
28	D	314	CLA	O2D-CGD-CBD	2.23	115.12	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	b	710	CLA	CHB-C4A-NA	2.23	127.61	124.40
29	A	314	KC1	O2A-CGA-O1A	-2.22	118.17	122.70
29	D	315	KC1	CHC-C4B-C3B	-2.22	121.46	125.21
32	G	506	PID	CM4-C14-C13	2.22	123.96	119.05
31	j	101	LMG	O7-C10-O9	-2.22	118.51	123.70
29	N	311	KC1	O2D-CGD-O1D	-2.22	119.53	123.85
26	A	305	DD6	C10-C9-C8	-2.22	116.77	123.20
35	i	201	BCR	C38-C26-C27	2.22	118.33	113.60
28	a	713	CLA	O2A-CGA-O1A	-2.22	118.08	123.63
35	b	730	BCR	C23-C24-C25	-2.22	121.07	127.00
26	B	306	DD6	C37-C36-C31	-2.22	120.01	124.16
28	a	705	CLA	O2A-CGA-O1A	-2.22	118.08	123.63
26	B	303	DD6	C37-C36-C35	2.22	118.50	114.42
28	L	314	CLA	O2A-CGA-O1A	-2.22	118.08	123.63
26	D	303	DD6	C-C1-C24	2.21	121.47	118.09
28	f	302	CLA	CMB-C2B-C1B	-2.21	122.05	125.42
27	A	304	UIX	C19-C18-C17	-2.21	105.91	109.89
26	K	304	DD6	C25-C24-C1	-2.21	120.29	126.36
28	f	301	CLA	O2A-CGA-O1A	-2.21	118.09	123.63
28	l	310	CLA	C4D-ND-C1D	-2.21	106.22	108.87
26	L	305	DD6	C25-C26-C27	-2.21	120.43	126.61
26	N	303	DD6	C25-C24-C1	-2.21	120.30	126.36
35	b	732	BCR	C36-C18-C19	2.21	121.47	118.09
28	G	514	CLA	O2A-CGA-O1A	-2.21	118.10	123.63
26	K	304	DD6	C14-C13-C11	-2.21	122.10	125.53
26	A	305	DD6	C15-C14-C13	-2.21	121.32	125.99
35	a	736	BCR	C16-C15-C14	-2.21	119.00	123.52
26	B	302	DD6	C37-C36-C35	2.21	118.48	114.42
28	a	710	CLA	CAA-CBA-CGA	-2.21	106.94	113.21
29	L	315	KC1	CAC-C3C-C4C	2.21	127.66	124.79
31	j	101	LMG	O3-C3-C2	-2.21	105.18	110.38
29	N	311	KC1	C2A-C3A-C4A	2.20	108.07	106.41
28	l	313	CLA	O2A-CGA-O1A	-2.20	118.11	123.63
32	G	507	PID	CM4-C14-C13	2.20	123.91	119.05
29	L	307	KC1	C2A-C3A-C4A	2.20	108.06	106.41
28	K	313	CLA	CMB-C2B-C1B	-2.20	122.07	125.42
26	I	301	DD6	C25-C24-C1	-2.20	120.33	126.36
26	I	301	DD6	C9-C8-C6	-2.20	120.33	126.36
28	B	309	CLA	O2A-CGA-O1A	-2.20	118.12	123.63
29	H	310	KC1	O1D-CGD-CBD	-2.20	120.18	124.52
28	a	724	CLA	O2A-CGA-O1A	-2.20	118.13	123.63
28	a	726	CLA	O2D-CGD-CBD	2.20	115.07	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	H	301	PID	C16-C15-C14	-2.20	124.20	127.28
29	K	314	KC1	O1D-CGD-CBD	-2.20	120.18	124.52
26	J	303	DD6	C21-C20-C19	2.20	116.71	114.24
29	D	310	KC1	O2D-CGD-O1D	-2.20	119.57	123.85
29	F	309	KC1	O2D-CGD-O1D	-2.20	119.57	123.85
28	A	309	CLA	CMB-C2B-C1B	-2.20	122.08	125.42
28	I	308	CLA	O2A-CGA-O1A	-2.20	118.14	123.63
31	j	101	LMG	O2-C2-C1	-2.19	104.85	110.08
28	K	316	CLA	O2D-CGD-CBD	2.19	115.07	111.23
26	L	304	DD6	C28-C27-C26	-2.19	119.92	124.18
29	H	310	KC1	O2D-CGD-O1D	-2.19	119.58	123.85
28	J	301	CLA	O2A-CGA-O1A	-2.19	118.14	123.63
26	L	305	DD6	O1-C20-C21	-2.19	112.60	115.05
26	L	306	DD6	C4-C3-C2	-2.19	119.04	123.52
32	j	105	PID	O4-C12-C13	2.19	127.56	122.89
31	K	318	LMG	O1-C7-C8	-2.19	105.49	110.82
26	G	504	DD6	C4-C3-C2	-2.19	119.04	123.52
28	I	306	CLA	O2D-CGD-CBD	2.19	115.05	111.23
28	D	313	CLA	C3B-C4B-NB	-2.19	108.58	110.53
28	M	308	CLA	C1-C2-C3	-2.19	122.61	126.20
26	K	303	DD6	C3-C4-C5	-2.19	119.05	123.52
26	M	303	DD6	C32-C33-C34	-2.19	108.80	113.59
28	a	713	CLA	CHB-C4A-NA	2.18	127.55	124.40
29	I	314	KC1	O2A-CGA-O1A	-2.18	118.25	122.70
31	K	318	LMG	O2-C2-C1	-2.18	104.88	110.08
32	F	304	PID	C19-C20-C21	2.18	130.34	127.28
32	D	304	PID	O1-C6-C7	-2.18	110.63	116.88
26	G	508	DD6	C21-C20-C15	-2.18	118.71	122.30
26	L	302	DD6	O1-C15-C14	-2.18	110.64	116.88
28	b	718	CLA	O2A-CGA-O1A	-2.18	118.18	123.63
31	b	734	LMG	O3-C3-C2	-2.18	105.24	110.38
35	b	730	BCR	C11-C12-C13	-2.18	120.39	126.36
28	b	725	CLA	O2A-CGA-O1A	-2.18	118.18	123.63
35	l	307	BCR	C33-C5-C6	-2.18	122.11	124.48
28	b	720	CLA	C3B-C4B-NB	-2.18	108.59	110.53
31	B	318	LMG	O2-C2-C1	-2.18	104.89	110.08
35	l	302	BCR	C23-C22-C21	2.17	122.43	119.01
31	D	317	LMG	O2-C2-C1	-2.17	104.89	110.08
26	G	502	DD6	C4-C3-C2	-2.17	119.07	123.52
28	I	310	CLA	C3B-C4B-NB	-2.17	108.59	110.53
28	a	722	CLA	C3B-C4B-NB	-2.17	108.59	110.53
32	F	304	PID	CM5-C21-C20	-2.17	119.30	122.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	B	306	DD6	C3-C4-C5	-2.17	119.08	123.52
28	b	710	CLA	O2A-CGA-O1A	-2.17	118.20	123.63
28	b	722	CLA	CHB-C4A-NA	2.17	127.53	124.40
28	a	712	CLA	O2A-CGA-O1A	-2.17	118.20	123.63
26	L	302	DD6	C37-C36-C35	2.17	118.41	114.42
28	H	307	CLA	C1-C2-C3	-2.17	122.64	126.20
28	G	513	CLA	CMB-C2B-C1B	-2.17	122.12	125.42
28	H	304	CLA	O2A-CGA-O1A	-2.17	118.21	123.63
31	I	320	LMG	O2-C2-C1	-2.17	104.91	110.08
26	M	303	DD6	C25-C26-C27	-2.16	120.56	126.61
28	l	303	CLA	O2A-CGA-O1A	-2.16	118.22	123.63
29	L	307	KC1	O1D-CGD-CBD	-2.16	120.25	124.52
28	b	705	CLA	O2A-CGA-O1A	-2.16	118.22	123.63
32	D	301	PID	C15-C14-C13	2.16	122.36	116.80
31	I	320	LMG	O3-C3-C2	-2.16	105.28	110.38
26	L	302	DD6	C25-C26-C27	-2.16	120.58	126.61
26	I	303	DD6	C25-C26-C27	-2.16	120.58	126.61
28	I	309	CLA	C1-C2-C3	-2.16	122.66	126.20
26	M	306	DD6	C12-C11-C10	-2.16	119.32	122.82
35	f	304	BCR	C23-C24-C25	-2.16	121.24	127.00
28	a	703	CLA	CAA-CBA-CGA	-2.16	107.09	113.21
28	K	311	CLA	C1-C2-C3	-2.16	122.67	126.20
28	a	716	CLA	O2A-CGA-O1A	-2.15	118.24	123.63
32	j	105	PID	CM4-C14-C13	2.15	123.80	119.05
28	G	512	CLA	O2A-CGA-O1A	-2.15	118.25	123.63
28	M	312	CLA	CMB-C2B-C1B	-2.15	122.14	125.42
28	I	313	CLA	C1-C2-C3	-2.15	122.67	126.20
28	a	705	CLA	C1-C2-C3	-2.15	122.67	126.20
35	l	302	BCR	C35-C13-C12	2.15	121.37	118.09
28	F	313	CLA	C2A-C1A-CHA	2.15	127.60	123.87
28	a	702	CLA	CHB-C4A-NA	2.15	127.50	124.40
29	B	314	KC1	C2A-C3A-C4A	2.15	108.03	106.41
32	H	301	PID	C15-C14-C13	2.15	122.33	116.80
26	I	303	DD6	O1-C20-C15	-2.15	57.23	58.93
28	G	513	CLA	O2A-CGA-O1A	-2.15	118.25	123.63
26	I	302	DD6	C9-C8-C6	2.15	132.26	126.36
31	b	733	LMG	O7-C10-O9	-2.15	118.68	123.70
28	I	310	CLA	CMB-C2B-C1B	-2.15	122.15	125.42
28	A	312	CLA	C3B-C4B-NB	-2.15	108.61	110.53
31	I	320	LMG	O1-C1-C2	-2.15	105.01	108.27
26	M	306	DD6	C7-C6-C5	-2.15	119.34	122.82
31	D	317	LMG	O1-C1-C2	-2.15	105.01	108.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	G	511	CLA	C1-C2-C3	-2.15	122.68	126.20
28	a	720	CLA	C1-C2-C3	-2.15	122.68	126.20
28	A	312	CLA	CMB-C2B-C1B	-2.14	122.15	125.42
26	M	302	DD6	C26-C25-C24	-2.14	116.98	123.20
35	i	201	BCR	C20-C19-C18	-2.14	120.48	126.36
28	a	726	CLA	C1-C2-C3	-2.14	122.69	126.20
26	M	305	DD6	C25-C24-C1	-2.14	120.49	126.36
26	I	301	DD6	C3-C4-C5	-2.14	119.13	123.52
26	K	303	DD6	C28-C27-C26	-2.14	120.02	124.18
27	K	302	UIX	C41-C40-C38	2.14	121.36	118.09
26	b	731	DD6	C-C1-C24	2.14	121.36	118.09
28	b	703	CLA	CHB-C4A-NA	2.14	127.49	124.40
28	K	315	CLA	CMA-C3A-C2A	-2.14	111.32	116.23
31	b	734	LMG	O2-C2-C1	-2.14	104.98	110.08
26	L	303	DD6	C25-C24-C1	-2.14	120.50	126.36
28	H	305	CLA	O2A-CGA-O1A	-2.14	118.28	123.63
27	J	305	UIX	C3-C5-C4	-2.14	106.79	110.79
26	A	305	DD6	C25-C24-C1	-2.14	120.51	126.36
28	K	306	CLA	O2A-CGA-O1A	-2.13	118.29	123.63
26	G	505	DD6	C37-C36-C35	2.13	118.34	114.42
28	K	309	CLA	CMB-C2B-C1B	-2.13	122.17	125.42
29	G	515	KC1	O2D-CGD-O1D	-2.13	119.70	123.85
29	I	314	KC1	C2A-C3A-C4A	2.13	108.01	106.41
26	K	305	DD6	C3-C4-C5	-2.13	119.16	123.52
28	b	720	CLA	O2A-CGA-O1A	-2.13	118.30	123.63
26	B	306	DD6	C14-C13-C11	-2.13	122.22	125.53
27	J	305	UIX	O2-C27-O4	-2.13	118.88	122.99
35	b	702	BCR	C33-C5-C4	2.13	118.14	113.60
26	M	306	DD6	C28-C27-C26	-2.13	120.05	124.18
28	I	312	CLA	O2A-CGA-O1A	-2.13	118.30	123.63
26	H	303	DD6	C28-C27-C26	-2.13	120.05	124.18
26	J	304	DD6	C15-C14-C13	-2.13	121.49	125.99
26	G	504	DD6	C10-C9-C8	-2.13	117.03	123.20
26	A	302	DD6	C12-C11-C10	-2.13	119.37	122.82
29	A	314	KC1	O2D-CGD-O1D	-2.13	119.71	123.85
35	i	201	BCR	C35-C13-C12	2.13	121.34	118.09
26	K	305	DD6	C25-C24-C1	-2.13	120.53	126.36
26	A	301	DD6	C9-C8-C6	-2.13	120.53	126.36
30	l	301	DGD	O1G-C1A-C2A	2.13	118.32	111.83
26	D	303	DD6	C7-C6-C8	2.12	121.33	118.09
28	I	311	CLA	O2A-CGA-O1A	-2.12	118.31	123.63
26	F	303	DD6	O1-C20-C21	-2.12	112.67	115.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	L	317	CLA	O2D-CGD-CBD	2.12	114.94	111.23
31	I	318	LMG	O3-C3-C2	-2.12	105.37	110.38
28	b	723	CLA	C1-C2-C3	-2.12	123.33	126.76
35	i	201	BCR	C21-C20-C19	-2.12	117.05	123.20
28	M	309	CLA	O2A-CGA-O1A	-2.12	118.33	123.63
26	K	303	DD6	C25-C26-C27	-2.12	120.69	126.61
27	B	305	UIX	C22-C15-C20	-2.12	108.58	110.47
26	L	304	DD6	C25-C26-C27	-2.12	120.69	126.61
28	B	311	CLA	O2A-CGA-O1A	-2.12	118.34	123.63
28	N	304	CLA	O2A-CGA-O1A	-2.11	118.34	123.63
31	D	317	LMG	O3-C3-C2	-2.11	105.39	110.38
26	L	302	DD6	O1-C20-C21	-2.11	112.69	115.05
26	L	304	DD6	C12-C11-C13	2.11	121.32	118.09
28	a	724	CLA	O2D-CGD-CBD	2.11	114.92	111.23
28	N	307	CLA	CHB-C4A-NA	2.11	127.45	124.40
28	m	202	CLA	O2A-CGA-O1A	-2.11	118.34	123.63
35	a	734	BCR	C16-C15-C14	-2.11	119.20	123.52
26	K	305	DD6	C10-C9-C8	-2.11	117.08	123.20
28	A	313	CLA	O2A-CGA-O1A	-2.11	118.35	123.63
28	a	731	CLA	O2A-CGA-O1A	-2.11	118.35	123.63
31	K	318	LMG	O3-C3-C2	-2.11	105.40	110.38
35	f	304	BCR	C3-C4-C5	-2.11	110.29	114.06
30	G	501	DGD	C2G-O2G-C1B	-2.11	112.75	117.80
35	a	736	BCR	C37-C22-C23	2.11	121.31	118.09
28	b	723	CLA	O2D-CGD-CBD	2.11	114.92	111.23
28	J	310	CLA	CMB-C2B-C1B	-2.11	122.21	125.42
28	a	708	CLA	C1-C2-C3	-2.11	122.74	126.20
35	j	102	BCR	C33-C5-C4	2.11	118.09	113.60
26	b	731	DD6	C12-C11-C13	2.11	121.31	118.09
26	F	301	DD6	C34-C35-C36	-2.11	106.93	112.18
26	M	305	DD6	O1-C20-C21	-2.11	112.69	115.05
35	a	736	BCR	C15-C16-C17	-2.11	119.21	123.52
30	I	317	DGD	O6D-C5D-C6D	2.11	110.87	106.69
28	h	202	CLA	O2A-CGA-O1A	-2.11	118.36	123.63
35	f	304	BCR	C38-C26-C27	2.11	118.08	113.60
26	H	303	DD6	C21-C20-C15	-2.11	118.84	122.30
26	B	306	DD6	C7-C6-C8	2.10	121.30	118.09
35	l	307	BCR	C23-C24-C25	-2.10	121.38	127.00
28	a	722	CLA	C1-C2-C3	-2.10	122.75	126.20
28	J	308	CLA	O2D-CGD-CBD	2.10	114.91	111.23
28	K	312	CLA	O2A-CGA-O1A	-2.10	118.36	123.63
26	J	302	DD6	C28-C27-C26	-2.10	120.10	124.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	M	317	CLA	O2D-CGD-CBD	2.10	114.91	111.23
28	I	319	CLA	CMB-C2B-C1B	-2.10	122.22	125.42
35	a	736	BCR	C11-C12-C13	-2.10	120.60	126.36
26	J	304	DD6	C37-C36-C31	-2.10	120.23	124.16
35	l	307	BCR	C36-C18-C19	2.10	121.30	118.09
28	N	310	CLA	C2A-C1A-CHA	2.10	127.50	123.87
35	l	306	BCR	C15-C16-C17	-2.10	119.23	123.52
28	j	106	CLA	O2A-CGA-O1A	-2.09	118.39	123.63
31	B	318	LMG	O1-C7-C8	-2.09	105.72	110.82
35	i	201	BCR	C34-C9-C8	2.09	121.29	118.09
28	b	726	CLA	O2A-CGA-O1A	-2.09	118.39	123.63
28	b	708	CLA	O2A-CGA-O1A	-2.09	118.39	123.63
31	K	317	LMG	O3-C3-C2	-2.09	105.44	110.38
28	b	725	CLA	C1-C2-C3	-2.09	122.77	126.20
26	K	319	DD6	O1-C15-C14	-2.09	110.88	116.88
32	G	506	PID	C7-C8-C9	-2.09	123.42	126.06
28	G	510	CLA	CMB-C2B-C1B	-2.09	122.23	125.42
28	G	513	CLA	C1-C2-C3	-2.09	122.77	126.20
28	K	310	CLA	O2A-CGA-O1A	-2.09	118.40	123.63
26	M	302	DD6	C24-C1-C2	2.09	122.30	119.01
28	a	708	CLA	O2A-CGA-O1A	-2.09	118.40	123.63
28	I	308	CLA	O2D-CGD-CBD	2.09	114.88	111.23
26	M	305	DD6	C28-C27-C26	-2.09	120.13	124.18
35	a	734	BCR	C37-C22-C23	2.09	121.28	118.09
27	G	503	UIX	C3-C5-C4	-2.09	106.89	110.79
29	A	306	KC1	O2D-CGD-O1D	-2.09	119.78	123.85
26	B	302	DD6	C37-C36-C31	-2.09	120.26	124.16
32	H	302	PID	C6-C7-C8	-2.09	121.58	125.99
28	a	712	CLA	C1-C2-C3	-2.09	122.78	126.20
28	B	301	CLA	CHB-C4A-NA	2.09	127.41	124.40
28	J	312	CLA	C1-C2-C3	-2.09	122.78	126.20
28	M	312	CLA	O2A-CGA-O1A	-2.09	118.41	123.63
28	I	313	CLA	CMB-C2B-C1B	-2.09	122.24	125.42
29	A	314	KC1	C2A-C3A-C4A	2.09	107.98	106.41
28	G	520	CLA	O2A-CGA-O1A	-2.09	118.41	123.63
32	F	302	PID	C17-C18-C19	2.08	129.53	124.72
26	L	306	DD6	O1-C15-C14	-2.08	110.91	116.88
28	I	315	CLA	O2A-CGA-O1A	-2.08	118.42	123.63
28	a	720	CLA	O2A-CGA-O1A	-2.08	118.42	123.63
26	A	303	DD6	O1-C15-C14	-2.08	110.91	116.88
31	B	318	LMG	O3-C3-C2	-2.08	105.47	110.38
26	B	304	DD6	C21-C20-C15	-2.08	118.88	122.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	I	304	UIX	C13-C14-C23	-2.08	117.18	123.20
26	N	303	DD6	C28-C27-C26	-2.08	120.15	124.18
28	b	717	CLA	O2A-CGA-O1A	-2.08	118.43	123.63
29	F	314	KC1	C2A-C3A-C4A	2.08	107.97	106.41
29	D	315	KC1	O2D-CGD-O1D	-2.08	119.80	123.85
28	L	311	CLA	O2A-CGA-O1A	-2.08	118.43	123.63
26	K	319	DD6	C12-C11-C10	-2.08	119.45	122.82
28	I	315	CLA	C1-C2-C3	-2.08	122.80	126.20
28	b	711	CLA	C1-C2-C3	-2.08	122.80	126.20
27	h	201	UIX	C3-C5-C4	-2.08	106.91	110.79
27	I	304	UIX	O-C-C7	-2.08	110.93	116.88
28	b	722	CLA	C3B-C4B-NB	-2.07	108.68	110.53
26	J	304	DD6	C19-C18-C17	-2.07	106.91	110.79
28	a	710	CLA	O2A-CGA-O1A	-2.07	118.44	123.63
28	M	315	CLA	CMB-C2B-C1B	-2.07	122.26	125.42
35	m	201	BCR	C24-C23-C22	-2.07	123.17	126.23
32	G	507	PID	C28-C27-C26	2.07	113.61	109.89
26	B	306	DD6	C4-C3-C2	-2.07	119.28	123.52
27	h	201	UIX	C36-C35-C32	-2.07	124.37	127.28
28	B	307	CLA	O2A-CGA-O1A	-2.07	118.44	123.63
28	F	315	CLA	O2D-CGD-CBD	2.07	114.85	111.23
35	a	734	BCR	C38-C26-C27	2.07	118.01	113.60
28	b	704	CLA	O1D-CGD-CBD	2.07	128.60	124.52
32	D	302	PID	C8-C9-C10	2.07	127.65	123.60
26	I	301	DD6	C37-C36-C31	-2.07	120.29	124.16
26	B	303	DD6	C12-C11-C13	2.07	121.25	118.09
31	K	318	LMG	C1-C2-C3	-2.07	105.66	110.01
29	A	306	KC1	C2A-C3A-C4A	2.07	107.96	106.41
26	D	303	DD6	C28-C27-C26	-2.07	120.17	124.18
28	L	308	CLA	O2A-CGA-O1A	-2.07	118.46	123.63
26	I	301	DD6	C4-C3-C2	-2.07	119.29	123.52
28	A	309	CLA	O2A-CGA-O1A	-2.07	118.46	123.63
28	l	304	CLA	CMB-C2B-C1B	-2.07	122.27	125.42
35	i	201	BCR	C16-C15-C14	-2.07	119.29	123.52
26	A	303	DD6	C37-C36-C35	2.06	118.22	114.42
36	b	729	PQN	C16-C15-C13	-2.06	108.44	113.47
29	M	314	KC1	O2A-CGA-O1A	-2.06	118.50	122.70
28	j	104	CLA	O2A-CGA-O1A	-2.06	118.46	123.63
28	b	722	CLA	O2A-CGA-O1A	-2.06	118.46	123.63
28	a	703	CLA	CMB-C2B-C1B	-2.06	122.28	125.42
28	b	714	CLA	CMB-C2B-C1B	-2.06	122.28	125.42
27	J	305	UIX	C37-C39-C40	-2.06	124.38	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	I	303	CLA	O2D-CGD-CBD	2.06	114.84	111.23
29	D	315	KC1	C4B-CHC-C1C	-2.06	121.64	126.02
28	K	307	CLA	CMB-C2B-C1B	-2.06	122.28	125.42
28	J	308	CLA	CMB-C2B-C1B	-2.06	122.28	125.42
26	I	302	DD6	C37-C36-C35	2.06	118.21	114.42
28	B	312	CLA	O2A-CGA-O1A	-2.06	118.47	123.63
26	J	303	DD6	C3-C4-C5	-2.06	119.30	123.52
26	G	502	DD6	C9-C8-C6	-2.06	120.71	126.36
26	J	304	DD6	O1-C20-C19	-2.06	111.56	113.49
29	F	309	KC1	O2A-CGA-O1A	-2.06	118.51	122.70
28	K	306	CLA	O2D-CGD-CBD	2.06	114.83	111.23
29	N	308	KC1	O2A-CGA-O1A	-2.06	118.51	122.70
28	b	721	CLA	CHB-C4A-NA	2.06	127.37	124.40
26	K	303	DD6	O1-C20-C21	-2.06	112.75	115.05
28	G	509	CLA	O2A-CGA-O1A	-2.06	118.48	123.63
27	G	503	UIX	C41-C40-C38	2.06	121.23	118.09
28	a	725	CLA	O2A-CGA-O1A	-2.06	118.49	123.63
28	a	707	CLA	O2A-CGA-O1A	-2.06	118.49	123.63
28	H	307	CLA	O2A-CGA-O1A	-2.06	118.49	123.63
28	b	717	CLA	CMB-C2B-C1B	-2.05	122.29	125.42
28	A	316	CLA	O2A-CGA-O1A	-2.05	118.49	123.63
26	L	303	DD6	C25-C26-C27	-2.05	120.87	126.61
28	J	314	CLA	CMA-C3A-C2A	-2.05	111.52	116.23
28	M	310	CLA	O2A-CGA-O1A	-2.05	118.49	123.63
27	K	302	UIX	C19-C18-C17	-2.05	106.20	109.89
28	I	309	CLA	O2A-CGA-O1A	-2.05	118.49	123.63
28	b	712	CLA	O2A-CGA-O1A	-2.05	118.50	123.63
26	M	306	DD6	C37-C36-C31	-2.05	120.32	124.16
26	K	301	DD6	C28-C27-C26	-2.05	120.20	124.18
26	D	303	DD6	C32-C33-C34	-2.05	109.10	113.59
29	H	310	KC1	C2A-C3A-C4A	2.05	107.95	106.41
28	a	723	CLA	O2A-CGA-O1A	-2.05	118.51	123.63
32	F	302	PID	CM1-C1-C6	-2.05	118.94	122.30
28	A	308	CLA	O2A-CGA-O1A	-2.05	118.51	123.63
31	b	733	LMG	O3-C3-C2	-2.05	105.55	110.38
27	A	304	UIX	C37-C34-C30	-2.04	119.34	123.52
28	a	719	CLA	O2A-CGA-O1A	-2.04	118.52	123.63
28	a	721	CLA	O2A-CGA-O1A	-2.04	118.52	123.63
28	L	317	CLA	O2A-CGA-O1A	-2.04	118.52	123.63
26	M	306	DD6	C3-C4-C5	-2.04	119.34	123.52
28	I	311	CLA	O2A-CGA-O1A	-2.04	118.52	123.63
26	M	302	DD6	O1-C20-C15	-2.04	57.31	58.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	A	302	DD6	C37-C36-C35	2.04	118.17	114.42
28	b	713	CLA	C1-C2-C3	-2.04	122.85	126.20
26	H	303	DD6	C3-C4-C5	-2.04	119.34	123.52
28	A	308	CLA	CMB-C2B-C1B	-2.04	122.31	125.42
31	K	317	LMG	C6-C5-C4	-2.04	108.02	113.02
28	K	315	CLA	CMB-C2B-C1B	-2.04	122.32	125.42
28	a	722	CLA	CMB-C2B-C1B	-2.04	122.32	125.42
26	I	302	DD6	C15-C14-C13	2.04	130.30	125.99
28	b	713	CLA	O2A-CGA-O1A	-2.04	118.53	123.63
35	j	102	BCR	C34-C9-C8	2.04	121.20	118.09
26	L	305	DD6	O1-C20-C19	-2.04	111.58	113.49
28	b	711	CLA	O2A-CGA-O1A	-2.03	118.54	123.63
28	M	315	CLA	CMA-C3A-C2A	-2.03	111.56	116.23
26	A	303	DD6	C10-C9-C8	-2.03	117.31	123.20
28	K	308	CLA	O2A-CGA-O1A	-2.03	118.54	123.63
29	I	314	KC1	C1A-C2A-C3A	-2.03	105.41	107.28
26	M	306	DD6	C7-C6-C8	2.03	121.19	118.09
28	I	319	CLA	O2D-CGD-CBD	2.03	114.78	111.23
35	f	304	BCR	C21-C20-C19	-2.03	117.31	123.20
28	I	306	CLA	O2A-CGA-O1A	-2.03	118.55	123.63
26	H	303	DD6	C25-C26-C27	-2.03	120.94	126.61
28	a	703	CLA	O2A-CGA-O1A	-2.03	118.55	123.63
26	A	301	DD6	C26-C25-C24	-2.03	117.33	123.20
28	b	718	CLA	C1-C2-C3	-2.03	122.88	126.20
32	H	302	PID	CM4-C14-C13	2.03	123.52	119.05
26	b	731	DD6	C3-C4-C5	-2.03	119.37	123.52
27	G	503	UIX	C35-C36-C38	-2.03	117.33	123.20
28	b	722	CLA	CHB-C1B-NB	2.02	127.08	124.05
26	A	301	DD6	C25-C26-C27	-2.02	120.95	126.61
28	K	308	CLA	C1-C2-C3	-2.02	122.88	126.20
26	M	304	DD6	C37-C36-C35	2.02	118.14	114.42
32	N	302	PID	O4-C12-C13	2.02	127.20	122.89
31	b	733	LMG	O2-C2-C1	-2.02	105.26	110.08
29	L	307	KC1	CAA-CBA-CGA	-2.02	116.78	127.05
28	a	735	CLA	CAA-CBA-CGA	-2.02	107.48	113.21
32	D	302	PID	O1-C6-C7	-2.02	111.10	116.88
26	L	304	DD6	C3-C4-C5	-2.02	119.39	123.52
28	F	313	CLA	CHA-C1A-NA	-2.02	121.82	126.39
26	G	508	DD6	C10-C9-C8	-2.02	117.36	123.20
29	M	314	KC1	O2D-CGD-O1D	-2.02	119.92	123.85
28	a	709	CLA	O2A-CGA-O1A	-2.02	118.59	123.63
26	L	302	DD6	C3-C4-C5	-2.02	119.40	123.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	b	706	CLA	CMB-C2B-C1B	-2.01	122.35	125.42
28	a	711	CLA	CMB-C2B-C3B	2.01	131.29	126.55
26	K	303	DD6	C7-C6-C8	2.01	121.17	118.09
28	a	709	CLA	C1-C2-C3	-2.01	122.90	126.20
27	J	305	UIX	C-C7-C10	-2.01	121.74	125.99
26	L	302	DD6	C4-C3-C2	-2.01	119.40	123.52
28	a	711	CLA	O2A-CGA-O1A	-2.01	118.16	123.33
30	G	501	DGD	O1G-C1A-O1A	-2.01	118.59	123.63
26	I	305	DD6	C19-C18-C17	-2.01	107.03	110.79
28	G	510	CLA	O2D-CGD-CBD	2.01	114.75	111.23
28	I	316	CLA	CAA-C2A-C3A	-2.01	107.56	113.00
28	a	724	CLA	C1-C2-C3	-2.01	122.90	126.20
28	L	310	CLA	O2A-CGA-O1A	-2.01	118.60	123.63
28	N	307	CLA	O2A-CGA-O1A	-2.01	118.60	123.63
28	I	319	CLA	O2A-CGA-O1A	-2.01	118.16	123.33
26	B	302	DD6	C-C1-C2	-2.01	119.56	122.82
26	F	301	DD6	C7-C6-C5	-2.01	119.56	122.82
28	B	309	CLA	CMB-C2B-C1B	-2.01	122.36	125.42
35	l	302	BCR	C40-C30-C25	-2.01	107.09	110.24
26	A	305	DD6	C4-C3-C2	-2.01	119.41	123.52
26	B	304	DD6	C25-C26-C27	-2.01	120.99	126.61
26	J	304	DD6	C9-C8-C6	-2.01	120.86	126.36
26	G	508	DD6	C25-C24-C1	-2.01	120.86	126.36
32	M	301	PID	CM5-C21-C20	-2.01	119.56	122.82
32	D	305	PID	C17-C16-C15	2.01	127.63	123.52
28	G	520	CLA	CMB-C2B-C3B	2.01	131.27	126.55
26	I	305	DD6	O1-C20-C15	-2.01	57.34	58.93
28	N	310	CLA	C3A-C2A-C1A	2.01	104.34	101.34
28	b	715	CLA	C1-C2-C3	-2.01	122.91	126.20
31	b	734	LMG	O7-C10-O9	-2.01	119.02	123.70
28	K	313	CLA	CMB-C2B-C3B	2.01	131.27	126.55
35	a	734	BCR	C10-C11-C12	-2.00	117.39	123.20
29	D	315	KC1	O2A-CGA-O1A	-2.00	118.62	122.70
29	J	313	KC1	O2A-CGA-O1A	-2.00	118.62	122.70
28	a	717	CLA	O2D-CGD-CBD	2.00	114.73	111.23
26	I	302	DD6	C21-C20-C15	-2.00	119.00	122.30
26	F	303	DD6	C28-C27-C26	-2.00	120.29	124.18
26	K	319	DD6	C26-C25-C24	-2.00	117.40	123.20
28	K	311	CLA	O2A-CGA-O1A	-2.00	118.62	123.63
26	L	305	DD6	C25-C24-C1	-2.00	120.87	126.36
26	K	301	DD6	C21-C20-C15	-2.00	119.01	122.30
28	a	722	CLA	CMB-C2B-C3B	2.00	131.26	126.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	J	302	DD6	C12-C11-C10	-2.00	119.57	122.82
28	a	729	CLA	O2D-CGD-CBD	2.00	114.73	111.23
35	a	736	BCR	C1-C6-C5	-2.00	119.90	122.64
26	M	304	DD6	C7-C6-C8	2.00	121.14	118.09
35	f	304	BCR	C15-C16-C17	-2.00	119.43	123.52
28	J	310	CLA	O2D-CGD-CBD	2.00	114.73	111.23

All (186) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
28	I	306	CLA	ND
28	I	307	CLA	ND
28	I	308	CLA	ND
28	I	309	CLA	ND
28	I	310	CLA	ND
28	I	311	CLA	ND
28	I	312	CLA	ND
28	I	313	CLA	ND
28	I	315	CLA	ND
28	I	316	CLA	ND
28	I	319	CLA	ND
28	I	321	CLA	ND
28	K	306	CLA	ND
28	K	307	CLA	ND
28	K	308	CLA	ND
28	K	309	CLA	ND
28	K	310	CLA	ND
28	K	311	CLA	ND
28	K	312	CLA	ND
28	K	313	CLA	ND
28	K	315	CLA	ND
28	K	316	CLA	ND
28	G	509	CLA	ND
28	G	510	CLA	ND
28	G	511	CLA	ND
28	G	512	CLA	ND
28	G	513	CLA	ND
28	G	514	CLA	ND
28	G	516	CLA	ND
28	G	517	CLA	ND
28	G	518	CLA	ND
28	G	519	CLA	ND

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Mol	Chain	Res	Type	Atom
28	G	520	CLA	ND
28	A	307	CLA	ND
28	A	308	CLA	ND
28	A	309	CLA	ND
28	A	310	CLA	ND
28	A	311	CLA	ND
28	A	312	CLA	ND
28	A	313	CLA	ND
28	A	315	CLA	ND
28	A	316	CLA	ND
28	A	317	CLA	ND
28	A	319	CLA	ND
28	A	320	CLA	ND
28	f	301	CLA	ND
28	f	302	CLA	ND
28	f	303	CLA	ND
28	h	202	CLA	ND
28	j	104	CLA	ND
28	j	106	CLA	ND
28	l	303	CLA	ND
28	l	304	CLA	ND
28	l	305	CLA	ND
28	l	308	CLA	ND
28	l	309	CLA	ND
28	l	311	CLA	ND
28	l	312	CLA	ND
28	l	313	CLA	ND
28	m	202	CLA	ND
28	a	701	CLA	ND
28	a	702	CLA	ND
28	a	703	CLA	ND
28	a	704	CLA	ND
28	a	705	CLA	ND
28	a	706	CLA	ND
28	a	707	CLA	ND
28	a	708	CLA	ND
28	a	709	CLA	ND
28	a	710	CLA	ND
28	a	711	CLA	ND
28	a	712	CLA	ND
28	a	713	CLA	ND
28	a	714	CLA	ND

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Mol	Chain	Res	Type	Atom
28	a	715	CLA	ND
28	a	716	CLA	ND
28	a	717	CLA	ND
28	a	718	CLA	ND
28	a	719	CLA	ND
28	a	720	CLA	ND
28	a	721	CLA	ND
28	a	722	CLA	ND
28	a	723	CLA	ND
28	a	724	CLA	ND
28	a	725	CLA	ND
28	a	726	CLA	ND
28	a	727	CLA	ND
28	a	728	CLA	ND
28	a	729	CLA	ND
28	a	730	CLA	ND
28	a	731	CLA	ND
28	a	735	CLA	ND
28	a	738	CLA	ND
28	b	701	CLA	ND
28	b	703	CLA	ND
28	b	704	CLA	ND
28	b	705	CLA	ND
28	b	706	CLA	ND
28	b	707	CLA	ND
28	b	708	CLA	ND
28	b	709	CLA	ND
28	b	710	CLA	ND
28	b	711	CLA	ND
28	b	712	CLA	ND
28	b	713	CLA	ND
28	b	714	CLA	ND
28	b	715	CLA	ND
28	b	716	CLA	ND
28	b	717	CLA	ND
28	b	718	CLA	ND
28	b	719	CLA	ND
28	b	720	CLA	ND
28	b	721	CLA	ND
28	b	722	CLA	ND
28	b	723	CLA	ND
28	b	724	CLA	ND

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Mol	Chain	Res	Type	Atom
28	b	725	CLA	ND
28	b	726	CLA	ND
28	b	727	CLA	ND
28	b	728	CLA	ND
28	B	301	CLA	ND
28	B	307	CLA	ND
28	B	308	CLA	ND
28	B	309	CLA	ND
28	B	310	CLA	ND
28	B	311	CLA	ND
28	B	312	CLA	ND
28	B	313	CLA	ND
28	B	315	CLA	ND
28	B	316	CLA	ND
28	B	317	CLA	ND
28	D	308	CLA	ND
28	D	309	CLA	ND
28	D	311	CLA	ND
28	D	312	CLA	ND
28	D	313	CLA	ND
28	D	314	CLA	ND
28	D	316	CLA	ND
28	F	307	CLA	ND
28	F	308	CLA	ND
28	F	310	CLA	ND
28	F	311	CLA	ND
28	F	312	CLA	ND
28	F	313	CLA	ND
28	F	315	CLA	ND
28	H	304	CLA	ND
28	H	305	CLA	ND
28	H	307	CLA	ND
28	H	308	CLA	ND
28	H	309	CLA	ND
28	H	312	CLA	ND
28	J	301	CLA	ND
28	J	306	CLA	ND
28	J	307	CLA	ND
28	J	308	CLA	ND
28	J	309	CLA	ND
28	J	310	CLA	ND
28	J	311	CLA	ND

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Mol	Chain	Res	Type	Atom
28	J	312	CLA	ND
28	J	314	CLA	ND
28	J	315	CLA	ND
28	L	308	CLA	ND
28	L	309	CLA	ND
28	L	310	CLA	ND
28	L	311	CLA	ND
28	L	312	CLA	ND
28	L	313	CLA	ND
28	L	314	CLA	ND
28	L	316	CLA	ND
28	L	317	CLA	ND
28	L	318	CLA	ND
28	M	308	CLA	ND
28	M	309	CLA	ND
28	M	310	CLA	ND
28	M	311	CLA	ND
28	M	312	CLA	ND
28	M	313	CLA	ND
28	M	315	CLA	ND
28	M	316	CLA	ND
28	M	317	CLA	ND
28	M	318	CLA	ND
28	N	304	CLA	ND
28	N	305	CLA	ND
28	N	307	CLA	ND
28	N	309	CLA	ND
28	N	310	CLA	ND

All (2075) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
26	K	301	DD6	C12-C11-C13-C14
26	G	502	DD6	C-C1-C24-C25
26	G	502	DD6	C2-C1-C24-C25
26	G	504	DD6	C10-C11-C13-C14
26	G	504	DD6	C12-C11-C13-C14
26	G	505	DD6	C5-C6-C8-C9
26	A	301	DD6	C13-C14-C15-C16
26	A	305	DD6	C13-C14-C15-O1
26	B	303	DD6	C13-C14-C15-O1
26	B	306	DD6	C13-C14-C15-O1

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Mol	Chain	Res	Type	Atoms
26	D	303	DD6	C13-C14-C15-O1
26	F	301	DD6	C10-C11-C13-C14
26	F	301	DD6	C12-C11-C13-C14
26	J	302	DD6	C10-C11-C13-C14
26	J	302	DD6	C12-C11-C13-C14
26	J	303	DD6	C10-C11-C13-C14
26	J	303	DD6	C12-C11-C13-C14
26	J	304	DD6	C10-C11-C13-C14
26	L	302	DD6	C13-C14-C15-O1
26	L	305	DD6	C13-C14-C15-O1
26	M	305	DD6	C13-C14-C15-O1
26	M	306	DD6	C10-C11-C13-C14
26	M	306	DD6	C12-C11-C13-C14
27	I	304	UIX	C2-C-C7-C10
27	K	302	UIX	O4-C27-O2-C18
27	K	302	UIX	C31-C27-O2-C18
27	G	503	UIX	C31-C27-O2-C18
27	h	201	UIX	O4-C27-O2-C18
27	J	305	UIX	O-C-C7-C10
27	J	305	UIX	C14-C23-C26-C29
27	J	305	UIX	C14-C23-C26-C30
28	I	306	CLA	CHA-CBD-CGD-O1D
28	I	306	CLA	CHA-CBD-CGD-O2D
28	I	307	CLA	CBA-CGA-O2A-C1
28	I	307	CLA	O1A-CGA-O2A-C1
28	I	310	CLA	CAD-CBD-CGD-O1D
28	I	310	CLA	CAD-CBD-CGD-O2D
28	I	311	CLA	C1A-C2A-CAA-CBA
28	I	311	CLA	C3A-C2A-CAA-CBA
28	I	311	CLA	CHA-CBD-CGD-O1D
28	I	311	CLA	CHA-CBD-CGD-O2D
28	I	312	CLA	C2-C3-C5-C6
28	I	312	CLA	C4-C3-C5-C6
28	I	313	CLA	CBD-CGD-O2D-CED
28	I	316	CLA	C1A-C2A-CAA-CBA
28	I	316	CLA	C3A-C2A-CAA-CBA
28	I	319	CLA	CHA-CBD-CGD-O1D
28	I	319	CLA	CHA-CBD-CGD-O2D
28	K	308	CLA	CBD-CGD-O2D-CED
28	K	311	CLA	C1A-C2A-CAA-CBA
28	K	311	CLA	C3A-C2A-CAA-CBA
28	K	311	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
28	K	315	CLA	CBD-CGD-O2D-CED
28	G	509	CLA	C2-C3-C5-C6
28	G	509	CLA	C4-C3-C5-C6
28	G	514	CLA	C4-C3-C5-C6
28	G	516	CLA	CAD-CBD-CGD-O1D
28	G	516	CLA	CAD-CBD-CGD-O2D
28	G	516	CLA	CBD-CGD-O2D-CED
28	G	517	CLA	CBA-CGA-O2A-C1
28	G	518	CLA	C1A-C2A-CAA-CBA
28	G	518	CLA	C3A-C2A-CAA-CBA
28	G	519	CLA	C1A-C2A-CAA-CBA
28	G	519	CLA	C3A-C2A-CAA-CBA
28	G	520	CLA	C1A-C2A-CAA-CBA
28	G	520	CLA	C3A-C2A-CAA-CBA
28	A	311	CLA	CBA-CGA-O2A-C1
28	A	315	CLA	CAD-CBD-CGD-O1D
28	A	315	CLA	CAD-CBD-CGD-O2D
28	A	319	CLA	C2B-C3B-CAB-CBB
28	A	319	CLA	C4B-C3B-CAB-CBB
28	A	319	CLA	CAD-CBD-CGD-O1D
28	A	319	CLA	CAD-CBD-CGD-O2D
28	A	320	CLA	CBA-CGA-O2A-C1
28	A	320	CLA	CHA-CBD-CGD-O1D
28	A	320	CLA	CHA-CBD-CGD-O2D
28	f	301	CLA	C1A-C2A-CAA-CBA
28	f	301	CLA	C3A-C2A-CAA-CBA
28	f	301	CLA	CBD-CGD-O2D-CED
28	f	302	CLA	CBA-CGA-O2A-C1
28	f	303	CLA	C1A-C2A-CAA-CBA
28	f	303	CLA	C3A-C2A-CAA-CBA
28	j	106	CLA	C1A-C2A-CAA-CBA
28	j	106	CLA	C3A-C2A-CAA-CBA
28	l	304	CLA	CHA-CBD-CGD-O1D
28	l	304	CLA	CHA-CBD-CGD-O2D
28	l	309	CLA	CAD-CBD-CGD-O1D
28	l	309	CLA	CAD-CBD-CGD-O2D
28	l	310	CLA	CBD-CGD-O2D-CED
28	l	311	CLA	C1A-C2A-CAA-CBA
28	l	312	CLA	C3A-C2A-CAA-CBA
28	l	312	CLA	CBD-CGD-O2D-CED
28	l	313	CLA	CHA-CBD-CGD-O1D
28	l	313	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
28	a	702	CLA	CBD-CGD-O2D-CED
28	a	705	CLA	C1A-C2A-CAA-CBA
28	a	705	CLA	C3A-C2A-CAA-CBA
28	a	706	CLA	CAD-CBD-CGD-O1D
28	a	706	CLA	CAD-CBD-CGD-O2D
28	a	707	CLA	C3A-C2A-CAA-CBA
28	a	707	CLA	CBD-CGD-O2D-CED
28	a	709	CLA	C1A-C2A-CAA-CBA
28	a	709	CLA	C3A-C2A-CAA-CBA
28	a	709	CLA	CHA-CBD-CGD-O1D
28	a	709	CLA	CHA-CBD-CGD-O2D
28	a	710	CLA	C2B-C3B-CAB-CBB
28	a	710	CLA	C4B-C3B-CAB-CBB
28	a	713	CLA	CBD-CGD-O2D-CED
28	a	714	CLA	CHA-CBD-CGD-O1D
28	a	714	CLA	CHA-CBD-CGD-O2D
28	a	715	CLA	CBD-CGD-O2D-CED
28	a	716	CLA	C1A-C2A-CAA-CBA
28	a	716	CLA	C3A-C2A-CAA-CBA
28	a	717	CLA	C3A-C2A-CAA-CBA
28	a	717	CLA	C6-C7-C8-C9
28	a	718	CLA	C1A-C2A-CAA-CBA
28	a	718	CLA	CAD-CBD-CGD-O2D
28	a	719	CLA	C2B-C3B-CAB-CBB
28	a	719	CLA	C4B-C3B-CAB-CBB
28	a	720	CLA	C3A-C2A-CAA-CBA
28	a	721	CLA	CAD-CBD-CGD-O2D
28	a	721	CLA	CBD-CGD-O2D-CED
28	a	722	CLA	CBD-CGD-O2D-CED
28	a	724	CLA	CHA-CBD-CGD-O1D
28	a	724	CLA	CHA-CBD-CGD-O2D
28	a	726	CLA	CHA-CBD-CGD-O1D
28	a	726	CLA	CHA-CBD-CGD-O2D
28	a	727	CLA	CBA-CGA-O2A-C1
28	a	727	CLA	O1A-CGA-O2A-C1
28	a	727	CLA	CHA-CBD-CGD-O1D
28	a	727	CLA	CHA-CBD-CGD-O2D
28	a	728	CLA	C4-C3-C5-C6
28	a	731	CLA	C1A-C2A-CAA-CBA
28	a	731	CLA	C3A-C2A-CAA-CBA
28	a	731	CLA	CBD-CGD-O2D-CED
28	a	735	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
28	a	735	CLA	CAD-CBD-CGD-O2D
28	a	738	CLA	CHA-CBD-CGD-O1D
28	a	738	CLA	CHA-CBD-CGD-O2D
28	b	701	CLA	CBD-CGD-O2D-CED
28	b	703	CLA	C2B-C3B-CAB-CBB
28	b	703	CLA	C4B-C3B-CAB-CBB
28	b	703	CLA	CBD-CGD-O2D-CED
28	b	704	CLA	C1A-C2A-CAA-CBA
28	b	704	CLA	C3A-C2A-CAA-CBA
28	b	704	CLA	CBD-CGD-O2D-CED
28	b	704	CLA	C14-C13-C15-C16
28	b	707	CLA	CHA-CBD-CGD-O2D
28	b	709	CLA	CHA-CBD-CGD-O1D
28	b	709	CLA	CHA-CBD-CGD-O2D
28	b	710	CLA	C1A-C2A-CAA-CBA
28	b	710	CLA	C3A-C2A-CAA-CBA
28	b	711	CLA	CAD-CBD-CGD-O1D
28	b	711	CLA	CAD-CBD-CGD-O2D
28	b	711	CLA	CBD-CGD-O2D-CED
28	b	715	CLA	C1A-C2A-CAA-CBA
28	b	715	CLA	C3A-C2A-CAA-CBA
28	b	717	CLA	C1A-C2A-CAA-CBA
28	b	717	CLA	C3A-C2A-CAA-CBA
28	b	717	CLA	C14-C13-C15-C16
28	b	719	CLA	CAD-CBD-CGD-O1D
28	b	719	CLA	CAD-CBD-CGD-O2D
28	b	720	CLA	CBD-CGD-O2D-CED
28	b	723	CLA	C3A-C2A-CAA-CBA
28	b	723	CLA	CHA-CBD-CGD-O1D
28	b	723	CLA	CHA-CBD-CGD-O2D
28	b	724	CLA	C1A-C2A-CAA-CBA
28	b	725	CLA	C2-C3-C5-C6
28	b	725	CLA	C4-C3-C5-C6
28	B	308	CLA	C1A-C2A-CAA-CBA
28	B	311	CLA	CBD-CGD-O2D-CED
28	B	311	CLA	C14-C13-C15-C16
28	B	315	CLA	CAD-CBD-CGD-O1D
28	B	315	CLA	CAD-CBD-CGD-O2D
28	B	315	CLA	CBD-CGD-O2D-CED
28	B	317	CLA	C1A-C2A-CAA-CBA
28	D	312	CLA	CBA-CGA-O2A-C1
28	D	314	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
28	D	314	CLA	CBD-CGD-O2D-CED
28	F	310	CLA	C1A-C2A-CAA-CBA
28	F	310	CLA	CHA-CBD-CGD-O1D
28	F	310	CLA	CHA-CBD-CGD-O2D
28	F	311	CLA	C4B-C3B-CAB-CBB
28	F	313	CLA	CBD-CGD-O2D-CED
28	F	315	CLA	CHA-CBD-CGD-O1D
28	F	315	CLA	CHA-CBD-CGD-O2D
28	H	307	CLA	CBD-CGD-O2D-CED
28	H	308	CLA	CBA-CGA-O2A-C1
28	H	309	CLA	C3A-C2A-CAA-CBA
28	H	309	CLA	CBD-CGD-O2D-CED
28	H	311	CLA	CAD-CBD-CGD-O1D
28	H	311	CLA	CAD-CBD-CGD-O2D
28	H	311	CLA	CBD-CGD-O2D-CED
28	H	312	CLA	C1A-C2A-CAA-CBA
28	H	312	CLA	C3A-C2A-CAA-CBA
28	H	312	CLA	CBD-CGD-O2D-CED
28	J	301	CLA	C4B-C3B-CAB-CBB
28	J	307	CLA	C1A-C2A-CAA-CBA
28	J	307	CLA	C3A-C2A-CAA-CBA
28	J	307	CLA	CAD-CBD-CGD-O2D
28	J	309	CLA	CHA-CBD-CGD-O1D
28	J	309	CLA	CHA-CBD-CGD-O2D
28	J	311	CLA	C1A-C2A-CAA-CBA
28	J	311	CLA	C3A-C2A-CAA-CBA
28	L	308	CLA	C1A-C2A-CAA-CBA
28	L	308	CLA	C3A-C2A-CAA-CBA
28	L	308	CLA	C2B-C3B-CAB-CBB
28	L	308	CLA	C4B-C3B-CAB-CBB
28	L	312	CLA	C3A-C2A-CAA-CBA
28	L	312	CLA	CBD-CGD-O2D-CED
28	L	313	CLA	C3A-C2A-CAA-CBA
28	L	317	CLA	C3-C5-C6-C7
28	L	318	CLA	C4B-C3B-CAB-CBB
28	L	318	CLA	CBD-CGD-O2D-CED
28	M	315	CLA	CHA-CBD-CGD-O1D
28	M	315	CLA	CHA-CBD-CGD-O2D
28	M	317	CLA	CBD-CGD-O2D-CED
28	M	317	CLA	O1D-CGD-O2D-CED
28	M	318	CLA	C1A-C2A-CAA-CBA
28	M	318	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
28	M	318	CLA	CAD-CBD-CGD-O1D
28	M	318	CLA	CAD-CBD-CGD-O2D
28	N	309	CLA	C1A-C2A-CAA-CBA
28	N	310	CLA	C1A-C2A-CAA-CBA
28	N	310	CLA	CBD-CGD-O2D-CED
29	I	314	KC1	C2B-C3B-CAB-CBB
29	I	314	KC1	C4B-C3B-CAB-CBB
29	I	314	KC1	C2A-CAA-CBA-CGA
29	I	314	KC1	CHA-CBD-CGD-O1D
29	I	314	KC1	CHA-CBD-CGD-O2D
29	K	314	KC1	C2B-C3B-CAB-CBB
29	K	314	KC1	CHA-CBD-CGD-O1D
29	K	314	KC1	CHA-CBD-CGD-O2D
29	G	515	KC1	CHA-CBD-CGD-O1D
29	A	306	KC1	C2B-C3B-CAB-CBB
29	A	306	KC1	CHA-CBD-CGD-O1D
29	A	306	KC1	CHA-CBD-CGD-O2D
29	A	314	KC1	C2B-C3B-CAB-CBB
29	A	314	KC1	C4B-C3B-CAB-CBB
29	A	314	KC1	C2A-CAA-CBA-CGA
29	B	314	KC1	C2B-C3B-CAB-CBB
29	B	314	KC1	CBD-CGD-O2D-CED
29	D	310	KC1	C3A-C2A-CAA-CBA
29	D	310	KC1	C2B-C3B-CAB-CBB
29	D	310	KC1	C2A-CAA-CBA-CGA
29	D	310	KC1	CHA-CBD-CGD-O1D
29	D	310	KC1	CHA-CBD-CGD-O2D
29	D	315	KC1	C1A-C2A-CAA-CBA
29	F	309	KC1	C1A-C2A-CAA-CBA
29	F	309	KC1	C2B-C3B-CAB-CBB
29	F	309	KC1	CHA-CBD-CGD-O1D
29	F	309	KC1	CHA-CBD-CGD-O2D
29	F	314	KC1	C2B-C3B-CAB-CBB
29	H	306	KC1	C3A-C2A-CAA-CBA
29	H	306	KC1	C2B-C3B-CAB-CBB
29	H	310	KC1	C1A-C2A-CAA-CBA
29	H	310	KC1	C3A-C2A-CAA-CBA
29	H	310	KC1	C2B-C3B-CAB-CBB
29	H	310	KC1	CBD-CGD-O2D-CED
29	J	313	KC1	C2B-C3B-CAB-CBB
29	L	307	KC1	CHA-CBD-CGD-O1D
29	L	307	KC1	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
29	L	315	KC1	C1A-C2A-CAA-CBA
29	L	315	KC1	C3A-C2A-CAA-CBA
29	L	315	KC1	C2B-C3B-CAB-CBB
29	L	315	KC1	C2A-CAA-CBA-CGA
29	L	315	KC1	CBD-CGD-O2D-CED
29	M	307	KC1	C2B-C3B-CAB-CBB
29	M	307	KC1	CHA-CBD-CGD-O2D
29	M	314	KC1	C3A-C2A-CAA-CBA
29	M	314	KC1	C2B-C3B-CAB-CBB
29	M	314	KC1	CBD-CGD-O2D-CED
29	N	306	KC1	C3A-C2A-CAA-CBA
29	N	306	KC1	C2B-C3B-CAB-CBB
29	N	308	KC1	C2B-C3B-CAB-CBB
29	N	308	KC1	C2A-CAA-CBA-CGA
29	N	308	KC1	CHA-CBD-CGD-O1D
29	N	311	KC1	C3A-C2A-CAA-CBA
29	N	311	KC1	C2B-C3B-CAB-CBB
29	N	311	KC1	CBD-CGD-O2D-CED
30	G	521	DGD	O6E-C1E-O5D-C6D
30	j	103	DGD	C2B-C1B-O2G-C2G
31	I	318	LMG	O6-C1-O1-C7
31	K	317	LMG	C2-C1-O1-C7
31	K	317	LMG	O6-C1-O1-C7
31	K	317	LMG	C11-C10-O7-C8
31	K	318	LMG	O7-C8-C9-O8
31	K	318	LMG	C11-C10-O7-C8
31	j	101	LMG	O9-C10-O7-C8
31	j	101	LMG	C11-C10-O7-C8
31	b	734	LMG	C2-C1-O1-C7
31	b	734	LMG	O6-C1-O1-C7
31	b	734	LMG	O1-C7-C8-O7
31	b	734	LMG	C11-C10-O7-C8
31	B	318	LMG	O10-C28-O8-C9
32	G	506	PID	O1-C6-C7-C8
32	j	105	PID	C20-C21-C22-C23
32	j	105	PID	CM5-C21-C22-C23
32	j	105	PID	O7-C30-O6-C27
32	D	301	PID	O1-C6-C7-C8
32	D	301	PID	O4-C12-C13-C14
32	D	306	PID	O1-C6-C7-C8
32	D	307	PID	O1-C6-C7-C8
32	F	304	PID	O7-C30-O6-C27

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Mol	Chain	Res	Type	Atoms
32	F	305	PID	O7-C30-O6-C27
32	H	301	PID	O1-C6-C7-C8
32	N	301	PID	O4-C12-C13-C14
32	N	301	PID	C12-C13-C14-CM4
32	N	301	PID	O7-C30-O6-C27
32	N	302	PID	O7-C30-O6-C27
33	A	318	SQD	C46-C45-O47-C7
33	A	318	SQD	C8-C7-O47-C45
35	i	201	BCR	C5-C6-C7-C8
35	i	201	BCR	C7-C8-C9-C10
35	i	201	BCR	C21-C22-C23-C24
35	i	201	BCR	C37-C22-C23-C24
35	i	201	BCR	C23-C24-C25-C26
35	i	201	BCR	C23-C24-C25-C30
35	j	102	BCR	C7-C8-C9-C10
35	m	201	BCR	C7-C8-C9-C10
35	m	201	BCR	C7-C8-C9-C34
35	a	734	BCR	C7-C8-C9-C10
35	a	736	BCR	C7-C8-C9-C10
35	b	730	BCR	C21-C22-C23-C24
35	b	730	BCR	C37-C22-C23-C24
28	a	722	CLA	O1D-CGD-O2D-CED
28	a	731	CLA	O1D-CGD-O2D-CED
28	H	309	CLA	O1D-CGD-O2D-CED
28	H	311	CLA	O1D-CGD-O2D-CED
29	I	314	KC1	O1D-CGD-O2D-CED
29	H	310	KC1	O1D-CGD-O2D-CED
29	L	315	KC1	O1D-CGD-O2D-CED
29	M	314	KC1	O1D-CGD-O2D-CED
29	N	311	KC1	O1D-CGD-O2D-CED
27	I	304	UIX	C31-C27-O2-C18
27	h	201	UIX	C31-C27-O2-C18
32	F	304	PID	C31-C30-O6-C27
32	F	305	PID	C31-C30-O6-C27
32	N	301	PID	C31-C30-O6-C27
32	N	302	PID	C31-C30-O6-C27
28	K	312	CLA	O1D-CGD-O2D-CED
28	a	712	CLA	O1D-CGD-O2D-CED
28	a	715	CLA	O1D-CGD-O2D-CED
28	B	311	CLA	O1D-CGD-O2D-CED
28	F	312	CLA	O1D-CGD-O2D-CED
28	L	312	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
28	N	310	CLA	O1D-CGD-O2D-CED
29	B	314	KC1	O1D-CGD-O2D-CED
27	G	503	UIX	O4-C27-O2-C18
32	H	302	PID	C31-C30-O6-C27
32	H	302	PID	O7-C30-O6-C27
28	I	309	CLA	CBD-CGD-O2D-CED
28	I	316	CLA	CBD-CGD-O2D-CED
28	K	312	CLA	CBD-CGD-O2D-CED
28	A	313	CLA	CBD-CGD-O2D-CED
28	A	319	CLA	CBD-CGD-O2D-CED
28	j	106	CLA	CBD-CGD-O2D-CED
28	a	704	CLA	CBD-CGD-O2D-CED
28	a	712	CLA	CBD-CGD-O2D-CED
28	a	714	CLA	CBD-CGD-O2D-CED
28	a	730	CLA	CBD-CGD-O2D-CED
28	B	317	CLA	CBD-CGD-O2D-CED
28	D	313	CLA	CBD-CGD-O2D-CED
28	F	310	CLA	CBD-CGD-O2D-CED
28	F	312	CLA	CBD-CGD-O2D-CED
28	L	316	CLA	CBD-CGD-O2D-CED
28	M	315	CLA	CBD-CGD-O2D-CED
28	M	316	CLA	CBD-CGD-O2D-CED
28	M	318	CLA	CBD-CGD-O2D-CED
28	N	307	CLA	CBD-CGD-O2D-CED
29	I	314	KC1	CBD-CGD-O2D-CED
28	b	701	CLA	O1A-CGA-O2A-C1
28	H	304	CLA	O1A-CGA-O2A-C1
28	J	307	CLA	O1A-CGA-O2A-C1
28	J	311	CLA	O1A-CGA-O2A-C1
28	N	310	CLA	O1A-CGA-O2A-C1
28	A	311	CLA	O1A-CGA-O2A-C1
28	A	320	CLA	O1A-CGA-O2A-C1
28	D	312	CLA	O1A-CGA-O2A-C1
28	D	314	CLA	O1A-CGA-O2A-C1
28	H	308	CLA	O1A-CGA-O2A-C1
28	D	314	CLA	O1D-CGD-O2D-CED
27	J	305	UIX	C31-C27-O2-C18
32	j	105	PID	C31-C30-O6-C27
27	J	305	UIX	C19-C18-O2-C27
32	D	302	PID	C26-C27-O6-C30
28	l	310	CLA	CBA-CGA-O2A-C1
28	D	309	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
28	F	311	CLA	CBA-CGA-O2A-C1
28	I	309	CLA	O1D-CGD-O2D-CED
28	a	702	CLA	O1D-CGD-O2D-CED
28	D	313	CLA	O1D-CGD-O2D-CED
28	F	313	CLA	O1D-CGD-O2D-CED
28	M	318	CLA	O1D-CGD-O2D-CED
28	N	307	CLA	O1D-CGD-O2D-CED
28	b	701	CLA	CBA-CGA-O2A-C1
28	H	304	CLA	CBA-CGA-O2A-C1
28	J	307	CLA	CBA-CGA-O2A-C1
28	J	311	CLA	CBA-CGA-O2A-C1
30	G	521	DGD	C2A-C1A-O1G-C1G
31	K	318	LMG	C29-C28-O8-C9
31	j	101	LMG	C29-C28-O8-C9
28	I	308	CLA	O1A-CGA-O2A-C1
28	I	315	CLA	O1A-CGA-O2A-C1
28	K	308	CLA	O1A-CGA-O2A-C1
28	G	513	CLA	O1A-CGA-O2A-C1
28	a	706	CLA	O1A-CGA-O2A-C1
28	a	721	CLA	O1A-CGA-O2A-C1
28	b	707	CLA	O1A-CGA-O2A-C1
28	b	717	CLA	O1A-CGA-O2A-C1
28	B	311	CLA	O1A-CGA-O2A-C1
28	H	309	CLA	O1A-CGA-O2A-C1
28	L	313	CLA	O1A-CGA-O2A-C1
30	G	521	DGD	O1A-C1A-O1G-C1G
31	I	318	LMG	O10-C28-O8-C9
31	K	318	LMG	O10-C28-O8-C9
31	j	101	LMG	O10-C28-O8-C9
31	b	733	LMG	O10-C28-O8-C9
28	G	517	CLA	O1A-CGA-O2A-C1
28	f	302	CLA	O1A-CGA-O2A-C1
28	F	311	CLA	O1A-CGA-O2A-C1
28	I	316	CLA	O1D-CGD-O2D-CED
28	K	308	CLA	O1D-CGD-O2D-CED
28	H	312	CLA	O1D-CGD-O2D-CED
29	K	314	KC1	CAA-CBA-CGA-O1A
29	B	314	KC1	CAA-CBA-CGA-O1A
29	D	310	KC1	CAA-CBA-CGA-O2A
28	I	313	CLA	O1D-CGD-O2D-CED
28	f	301	CLA	O1D-CGD-O2D-CED
28	l	312	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
28	a	707	CLA	O1D-CGD-O2D-CED
28	b	701	CLA	O1D-CGD-O2D-CED
28	b	703	CLA	O1D-CGD-O2D-CED
28	b	711	CLA	O1D-CGD-O2D-CED
28	B	315	CLA	O1D-CGD-O2D-CED
28	H	307	CLA	O1D-CGD-O2D-CED
30	j	103	DGD	O1B-C1B-O2G-C2G
31	I	318	LMG	O9-C10-O7-C8
31	I	320	LMG	O9-C10-O7-C8
31	K	318	LMG	O9-C10-O7-C8
31	b	734	LMG	O9-C10-O7-C8
31	B	318	LMG	O9-C10-O7-C8
33	A	318	SQD	O49-C7-O47-C45
27	I	304	UIX	O4-C27-O2-C18
32	G	506	PID	C31-C30-O6-C27
28	G	518	CLA	CBA-CGA-O2A-C1
28	J	310	CLA	CBA-CGA-O2A-C1
28	a	718	CLA	O1A-CGA-O2A-C1
28	F	310	CLA	O1A-CGA-O2A-C1
28	I	311	CLA	C3-C5-C6-C7
28	I	312	CLA	C3-C5-C6-C7
28	I	316	CLA	C3-C5-C6-C7
28	K	313	CLA	C3-C5-C6-C7
28	G	514	CLA	C3-C5-C6-C7
28	G	519	CLA	C3-C5-C6-C7
28	j	104	CLA	C3-C5-C6-C7
28	l	305	CLA	C3-C5-C6-C7
28	a	702	CLA	C3-C5-C6-C7
28	a	705	CLA	C3-C5-C6-C7
28	a	706	CLA	C3-C5-C6-C7
28	b	701	CLA	C3-C5-C6-C7
28	b	707	CLA	C3-C5-C6-C7
28	b	717	CLA	C3-C5-C6-C7
28	B	310	CLA	C3-C5-C6-C7
28	J	307	CLA	C3-C5-C6-C7
28	L	309	CLA	C3-C5-C6-C7
28	K	315	CLA	O1D-CGD-O2D-CED
28	I	315	CLA	CBA-CGA-O2A-C1
28	K	308	CLA	CBA-CGA-O2A-C1
28	G	513	CLA	CBA-CGA-O2A-C1
28	a	706	CLA	CBA-CGA-O2A-C1
28	a	728	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
28	b	720	CLA	CBA-CGA-O2A-C1
28	B	310	CLA	CBA-CGA-O2A-C1
28	H	309	CLA	CBA-CGA-O2A-C1
28	L	314	CLA	CBA-CGA-O2A-C1
28	L	317	CLA	CBA-CGA-O2A-C1
28	N	310	CLA	CBA-CGA-O2A-C1
31	b	733	LMG	C29-C28-O8-C9
32	G	506	PID	O7-C30-O6-C27
28	I	319	CLA	CBD-CGD-O2D-CED
28	I	321	CLA	CBD-CGD-O2D-CED
28	A	315	CLA	CBD-CGD-O2D-CED
28	l	308	CLA	CBD-CGD-O2D-CED
28	m	202	CLA	CBD-CGD-O2D-CED
28	a	711	CLA	CBD-CGD-O2D-CED
28	a	725	CLA	CBD-CGD-O2D-CED
28	a	726	CLA	CBD-CGD-O2D-CED
28	b	707	CLA	CBD-CGD-O2D-CED
28	b	713	CLA	CBD-CGD-O2D-CED
28	H	304	CLA	CBD-CGD-O2D-CED
28	H	308	CLA	CBD-CGD-O2D-CED
28	J	306	CLA	CBD-CGD-O2D-CED
28	J	307	CLA	CBD-CGD-O2D-CED
28	J	308	CLA	CBD-CGD-O2D-CED
28	J	315	CLA	CBD-CGD-O2D-CED
28	L	313	CLA	CBD-CGD-O2D-CED
28	M	308	CLA	CBD-CGD-O2D-CED
28	M	309	CLA	CBD-CGD-O2D-CED
28	M	310	CLA	CBD-CGD-O2D-CED
31	I	318	LMG	C11-C10-O7-C8
31	I	320	LMG	C11-C10-O7-C8
31	B	318	LMG	C11-C10-O7-C8
28	l	310	CLA	O1D-CGD-O2D-CED
28	a	721	CLA	O1D-CGD-O2D-CED
28	b	704	CLA	O1D-CGD-O2D-CED
28	b	720	CLA	O1D-CGD-O2D-CED
28	F	310	CLA	O1D-CGD-O2D-CED
28	L	318	CLA	O1D-CGD-O2D-CED
28	M	315	CLA	O1D-CGD-O2D-CED
32	D	305	PID	O7-C30-O6-C27
28	N	304	CLA	O1A-CGA-O2A-C1
28	D	309	CLA	O1A-CGA-O2A-C1
28	F	313	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
28	G	516	CLA	O1D-CGD-O2D-CED
28	a	713	CLA	O1D-CGD-O2D-CED
32	D	305	PID	C31-C30-O6-C27
29	F	309	KC1	CAA-CBA-CGA-O2A
28	I	308	CLA	C4-C3-C5-C6
28	I	313	CLA	C4-C3-C5-C6
28	K	308	CLA	C4-C3-C5-C6
28	K	313	CLA	C4-C3-C5-C6
28	A	313	CLA	C4-C3-C5-C6
28	j	106	CLA	C4-C3-C5-C6
28	a	706	CLA	C4-C3-C5-C6
28	a	713	CLA	C4-C3-C5-C6
28	a	724	CLA	C4-C3-C5-C6
28	a	731	CLA	C4-C3-C5-C6
28	a	735	CLA	C4-C3-C5-C6
28	b	701	CLA	C4-C3-C5-C6
28	b	715	CLA	C4-C3-C5-C6
28	J	307	CLA	C4-C3-C5-C6
28	M	308	CLA	C4-C3-C5-C6
36	a	732	PQN	C14-C13-C15-C16
28	I	313	CLA	C2-C3-C5-C6
28	K	308	CLA	C2-C3-C5-C6
28	K	313	CLA	C2-C3-C5-C6
28	G	514	CLA	C2-C3-C5-C6
28	j	106	CLA	C2-C3-C5-C6
28	a	706	CLA	C2-C3-C5-C6
28	a	728	CLA	C2-C3-C5-C6
28	a	731	CLA	C2-C3-C5-C6
28	b	701	CLA	C2-C3-C5-C6
28	b	715	CLA	C2-C3-C5-C6
28	J	307	CLA	C2-C3-C5-C6
28	M	308	CLA	C2-C3-C5-C6
36	a	732	PQN	C12-C13-C15-C16
28	a	718	CLA	CBA-CGA-O2A-C1
28	F	310	CLA	CBA-CGA-O2A-C1
28	F	313	CLA	CBA-CGA-O2A-C1
28	a	711	CLA	C2A-CAA-CBA-CGA
28	b	714	CLA	C2A-CAA-CBA-CGA
28	J	308	CLA	C2A-CAA-CBA-CGA
28	M	316	CLA	C3-C5-C6-C7
28	M	318	CLA	C2A-CAA-CBA-CGA
28	A	308	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
28	A	312	CLA	C3-C5-C6-C7
28	h	202	CLA	C3-C5-C6-C7
28	I	308	CLA	CBA-CGA-O2A-C1
28	G	514	CLA	CBA-CGA-O2A-C1
28	a	721	CLA	CBA-CGA-O2A-C1
28	b	707	CLA	CBA-CGA-O2A-C1
28	b	717	CLA	CBA-CGA-O2A-C1
28	B	311	CLA	CBA-CGA-O2A-C1
28	L	313	CLA	CBA-CGA-O2A-C1
28	N	304	CLA	CBA-CGA-O2A-C1
31	I	318	LMG	C29-C28-O8-C9
31	B	318	LMG	C29-C28-O8-C9
28	G	518	CLA	O1A-CGA-O2A-C1
28	J	310	CLA	O1A-CGA-O2A-C1
26	I	301	DD6	C24-C25-C26-C27
26	G	502	DD6	C24-C25-C26-C27
26	M	302	DD6	C1-C2-C3-C4
32	F	305	PID	C14-C15-C16-C17
32	F	305	PID	C18-C19-C20-C21
28	G	514	CLA	O1A-CGA-O2A-C1
28	l	313	CLA	O1A-CGA-O2A-C1
28	a	728	CLA	O1A-CGA-O2A-C1
28	b	720	CLA	O1A-CGA-O2A-C1
28	L	317	CLA	O1A-CGA-O2A-C1
27	J	305	UIX	O4-C27-O2-C18
28	F	307	CLA	CBA-CGA-O2A-C1
28	l	310	CLA	O1A-CGA-O2A-C1
28	F	307	CLA	O1A-CGA-O2A-C1
28	j	106	CLA	O1D-CGD-O2D-CED
28	B	317	CLA	O1D-CGD-O2D-CED
28	G	511	CLA	C3-C5-C6-C7
28	A	309	CLA	C3-C5-C6-C7
28	A	312	CLA	CBD-CGD-O2D-CED
28	b	715	CLA	CBD-CGD-O2D-CED
28	J	311	CLA	CBD-CGD-O2D-CED
28	M	311	CLA	CBD-CGD-O2D-CED
28	A	319	CLA	O1D-CGD-O2D-CED
28	a	714	CLA	O1D-CGD-O2D-CED
28	a	730	CLA	O1D-CGD-O2D-CED
28	J	301	CLA	CBA-CGA-O2A-C1
28	B	310	CLA	O1A-CGA-O2A-C1
28	L	314	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
31	B	318	LMG	C4-C5-C6-O5
28	A	313	CLA	O1D-CGD-O2D-CED
28	M	316	CLA	O1D-CGD-O2D-CED
27	B	305	UIX	O4-C27-O2-C18
27	B	305	UIX	C31-C27-O2-C18
32	F	302	PID	C31-C30-O6-C27
32	F	302	PID	O7-C30-O6-C27
32	H	301	PID	C31-C30-O6-C27
32	H	301	PID	O7-C30-O6-C27
28	G	512	CLA	CBD-CGD-O2D-CED
28	L	314	CLA	CBD-CGD-O2D-CED
29	M	307	KC1	CBD-CGD-O2D-CED
28	K	316	CLA	CBA-CGA-O2A-C1
28	H	312	CLA	CBA-CGA-O2A-C1
31	K	318	LMG	O6-C5-C6-O5
28	b	703	CLA	C3-C5-C6-C7
28	a	723	CLA	CBD-CGD-O2D-CED
28	B	312	CLA	CBD-CGD-O2D-CED
28	a	704	CLA	O1D-CGD-O2D-CED
28	L	316	CLA	O1D-CGD-O2D-CED
28	l	313	CLA	CBA-CGA-O2A-C1
29	D	315	KC1	CAA-CBA-CGA-O2A
29	J	313	KC1	CAA-CBA-CGA-O2A
28	G	510	CLA	C4-C3-C5-C6
28	l	305	CLA	C4-C3-C5-C6
28	l	311	CLA	C4-C3-C5-C6
28	L	309	CLA	C4-C3-C5-C6
28	L	317	CLA	C4-C3-C5-C6
28	M	316	CLA	C4-C3-C5-C6
28	G	510	CLA	C2-C3-C5-C6
28	a	713	CLA	C2-C3-C5-C6
28	a	724	CLA	C2-C3-C5-C6
28	a	735	CLA	C2-C3-C5-C6
28	J	301	CLA	O1A-CGA-O2A-C1
31	K	317	LMG	O6-C5-C6-O5
28	b	704	CLA	C2C-C3C-CAC-CBC
28	a	721	CLA	C2A-CAA-CBA-CGA
30	G	501	DGD	O6E-C1E-O5D-C6D
31	D	317	LMG	O6-C1-O1-C7
28	a	708	CLA	CBA-CGA-O2A-C1
28	a	709	CLA	CBA-CGA-O2A-C1
28	b	723	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
28	B	309	CLA	CBA-CGA-O2A-C1
28	M	308	CLA	CBA-CGA-O2A-C1
28	I	306	CLA	CBD-CGD-O2D-CED
28	I	311	CLA	CBD-CGD-O2D-CED
28	A	308	CLA	CBD-CGD-O2D-CED
28	A	320	CLA	CBD-CGD-O2D-CED
28	f	303	CLA	CBD-CGD-O2D-CED
28	l	313	CLA	CBD-CGD-O2D-CED
28	a	705	CLA	CBD-CGD-O2D-CED
28	a	709	CLA	CBD-CGD-O2D-CED
28	b	712	CLA	CBD-CGD-O2D-CED
28	b	727	CLA	CBD-CGD-O2D-CED
28	J	301	CLA	CBD-CGD-O2D-CED
28	J	314	CLA	CBD-CGD-O2D-CED
28	L	317	CLA	CBD-CGD-O2D-CED
29	D	310	KC1	CBD-CGD-O2D-CED
29	B	314	KC1	CAA-CBA-CGA-O2A
29	F	309	KC1	CAA-CBA-CGA-O1A
31	B	318	LMG	O6-C5-C6-O5
28	G	519	CLA	CBD-CGD-O2D-CED
28	a	710	CLA	CBD-CGD-O2D-CED
28	B	316	CLA	CBD-CGD-O2D-CED
28	J	309	CLA	CBD-CGD-O2D-CED
29	N	306	KC1	CBD-CGD-O2D-CED
28	a	708	CLA	O1A-CGA-O2A-C1
28	b	723	CLA	O1A-CGA-O2A-C1
28	M	308	CLA	O1A-CGA-O2A-C1
28	I	321	CLA	CBA-CGA-O2A-C1
28	G	519	CLA	CBA-CGA-O2A-C1
28	A	313	CLA	CBA-CGA-O2A-C1
28	l	311	CLA	CBA-CGA-O2A-C1
28	a	707	CLA	CBA-CGA-O2A-C1
28	a	712	CLA	CBA-CGA-O2A-C1
28	M	312	CLA	CBA-CGA-O2A-C1
29	A	314	KC1	CAA-CBA-CGA-O2A
29	N	308	KC1	CAA-CBA-CGA-O2A
28	b	703	CLA	C4-C3-C5-C6
28	I	308	CLA	C2-C3-C5-C6
28	A	313	CLA	C2-C3-C5-C6
28	b	703	CLA	C2-C3-C5-C6
28	L	309	CLA	C2-C3-C5-C6
28	M	316	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
28	b	728	CLA	C3-C5-C6-C7
28	M	308	CLA	C3-C5-C6-C7
28	I	312	CLA	C14-C13-C15-C16
28	l	303	CLA	C11-C12-C13-C14
28	l	304	CLA	C11-C10-C8-C9
28	l	305	CLA	C11-C12-C13-C14
28	a	707	CLA	C11-C10-C8-C9
28	a	720	CLA	C11-C12-C13-C14
28	a	721	CLA	C14-C13-C15-C16
28	a	722	CLA	C6-C7-C8-C9
28	a	724	CLA	C6-C7-C8-C9
28	a	731	CLA	C11-C12-C13-C14
28	b	704	CLA	C6-C7-C8-C9
28	b	708	CLA	C6-C7-C8-C9
28	B	311	CLA	C6-C7-C8-C9
28	b	707	CLA	O1D-CGD-O2D-CED
28	H	308	CLA	O1D-CGD-O2D-CED
28	M	309	CLA	O1D-CGD-O2D-CED
30	G	521	DGD	C2E-C1E-O5D-C6D
28	K	316	CLA	O1A-CGA-O2A-C1
28	H	312	CLA	O1A-CGA-O2A-C1
28	b	719	CLA	CBA-CGA-O2A-C1
28	M	317	CLA	CBA-CGA-O2A-C1
28	J	308	CLA	O1D-CGD-O2D-CED
28	a	707	CLA	O1A-CGA-O2A-C1
28	a	735	CLA	CBD-CGD-O2D-CED
28	I	319	CLA	O1D-CGD-O2D-CED
28	b	713	CLA	O1D-CGD-O2D-CED
28	J	307	CLA	O1D-CGD-O2D-CED
26	G	504	DD6	C7-C6-C8-C9
26	G	505	DD6	C7-C6-C8-C9
26	D	303	DD6	C12-C11-C13-C14
26	L	302	DD6	C12-C11-C13-C14
35	i	201	BCR	C7-C8-C9-C34
35	j	102	BCR	C7-C8-C9-C34
35	l	306	BCR	C37-C22-C23-C24
35	a	734	BCR	C7-C8-C9-C34
35	a	736	BCR	C7-C8-C9-C34
35	b	702	BCR	C37-C22-C23-C24
35	b	730	BCR	C7-C8-C9-C34
26	K	301	DD6	C10-C11-C13-C14
26	B	302	DD6	C10-C11-C13-C14

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Mol	Chain	Res	Type	Atoms
26	D	303	DD6	C10-C11-C13-C14
26	L	302	DD6	C10-C11-C13-C14
35	l	306	BCR	C21-C22-C23-C24
35	b	702	BCR	C21-C22-C23-C24
35	b	730	BCR	C7-C8-C9-C10
28	G	520	CLA	C2A-CAA-CBA-CGA
30	y	201	DGD	C1B-C2B-C3B-C4B
28	G	519	CLA	O1A-CGA-O2A-C1
28	A	313	CLA	O1A-CGA-O2A-C1
28	M	312	CLA	O1A-CGA-O2A-C1
28	G	514	CLA	CBD-CGD-O2D-CED
29	K	314	KC1	CAA-CBA-CGA-O2A
29	L	307	KC1	CAA-CBA-CGA-O2A
29	M	307	KC1	CAA-CBA-CGA-O2A
30	y	201	DGD	O2G-C2G-C3G-O3G
31	K	317	LMG	C4-C5-C6-O5
28	b	717	CLA	C5-C6-C7-C8
28	A	315	CLA	O1D-CGD-O2D-CED
28	J	306	CLA	O1D-CGD-O2D-CED
28	J	315	CLA	O1D-CGD-O2D-CED
28	L	313	CLA	O1D-CGD-O2D-CED
28	a	721	CLA	C10-C11-C12-C13
28	a	730	CLA	C5-C6-C7-C8
28	a	725	CLA	O1D-CGD-O2D-CED
28	H	304	CLA	O1D-CGD-O2D-CED
28	M	308	CLA	O1D-CGD-O2D-CED
28	l	311	CLA	O1A-CGA-O2A-C1
28	b	713	CLA	C10-C11-C12-C13
28	F	315	CLA	CBD-CGD-O2D-CED
28	b	717	CLA	C6-C7-C8-C10
28	l	308	CLA	O1D-CGD-O2D-CED
29	D	310	KC1	CAA-CBA-CGA-O1A
29	N	308	KC1	CAA-CBA-CGA-O1A
28	a	706	CLA	C5-C6-C7-C8
28	B	313	CLA	C10-C11-C12-C13
26	I	305	DD6	C11-C10-C9-C8
26	M	302	DD6	C24-C25-C26-C27
26	M	306	DD6	C24-C25-C26-C27
28	I	321	CLA	C2C-C3C-CAC-CBC
28	a	711	CLA	O1D-CGD-O2D-CED
28	a	726	CLA	O1D-CGD-O2D-CED
28	I	313	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
31	I	318	LMG	C10-C11-C12-C13
28	B	313	CLA	CBD-CGD-O2D-CED
28	J	310	CLA	CBD-CGD-O2D-CED
28	I	312	CLA	C13-C15-C16-C17
28	j	106	CLA	C5-C6-C7-C8
28	l	303	CLA	C8-C10-C11-C12
28	b	722	CLA	C15-C16-C17-C18
28	B	313	CLA	C8-C10-C11-C12
28	J	307	CLA	C8-C10-C11-C12
28	K	308	CLA	C2A-CAA-CBA-CGA
28	G	513	CLA	C2A-CAA-CBA-CGA
28	A	319	CLA	C2A-CAA-CBA-CGA
28	a	709	CLA	C2A-CAA-CBA-CGA
28	a	719	CLA	C2A-CAA-CBA-CGA
28	b	719	CLA	C2A-CAA-CBA-CGA
28	b	724	CLA	C2A-CAA-CBA-CGA
28	H	312	CLA	C2A-CAA-CBA-CGA
28	M	310	CLA	C2A-CAA-CBA-CGA
28	N	305	CLA	C2A-CAA-CBA-CGA
28	I	309	CLA	C5-C6-C7-C8
28	I	312	CLA	C15-C16-C17-C18
28	m	202	CLA	C5-C6-C7-C8
28	a	713	CLA	C10-C11-C12-C13
28	a	724	CLA	C15-C16-C17-C18
28	b	713	CLA	C8-C10-C11-C12
28	J	307	CLA	C13-C15-C16-C17
28	J	309	CLA	C5-C6-C7-C8
31	I	318	LMG	C28-C29-C30-C31
31	j	101	LMG	C28-C29-C30-C31
28	I	321	CLA	O1D-CGD-O2D-CED
28	m	202	CLA	O1D-CGD-O2D-CED
28	I	321	CLA	O1A-CGA-O2A-C1
28	a	712	CLA	O1A-CGA-O2A-C1
31	j	101	LMG	O6-C1-O1-C7
28	a	707	CLA	C5-C6-C7-C8
28	a	723	CLA	C13-C15-C16-C17
28	a	726	CLA	C15-C16-C17-C18
28	b	707	CLA	C10-C11-C12-C13
28	B	310	CLA	C5-C6-C7-C8
28	K	313	CLA	CBA-CGA-O2A-C1
29	F	314	KC1	CBD-CGD-O2D-CED
28	a	709	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
28	B	309	CLA	O1A-CGA-O2A-C1
28	H	305	CLA	C15-C16-C17-C18
28	b	715	CLA	O1D-CGD-O2D-CED
28	J	311	CLA	O1D-CGD-O2D-CED
28	M	310	CLA	O1D-CGD-O2D-CED
28	G	510	CLA	C5-C6-C7-C8
28	l	313	CLA	C5-C6-C7-C8
28	a	709	CLA	C5-C6-C7-C8
28	a	735	CLA	C13-C15-C16-C17
28	b	705	CLA	C13-C15-C16-C17
28	B	309	CLA	C13-C15-C16-C17
28	L	317	CLA	C2-C3-C5-C6
28	M	311	CLA	O1D-CGD-O2D-CED
30	G	521	DGD	C4A-C5A-C6A-C7A
28	I	312	CLA	C10-C11-C12-C13
28	l	305	CLA	C5-C6-C7-C8
28	b	722	CLA	C5-C6-C7-C8
28	A	309	CLA	CBD-CGD-O2D-CED
28	a	706	CLA	CBD-CGD-O2D-CED
29	K	314	KC1	C2A-CAA-CBA-CGA
29	B	314	KC1	C2A-CAA-CBA-CGA
29	F	314	KC1	C2A-CAA-CBA-CGA
29	J	313	KC1	C2A-CAA-CBA-CGA
28	A	312	CLA	O1D-CGD-O2D-CED
28	b	705	CLA	C10-C11-C12-C13
28	A	313	CLA	C3-C5-C6-C7
30	G	501	DGD	O6D-C5D-C6D-O5D
27	J	305	UIX	C11-C13-C14-C23
30	G	521	DGD	O1B-C1B-O2G-C2G
28	a	722	CLA	C2A-CAA-CBA-CGA
28	b	727	CLA	C2A-CAA-CBA-CGA
28	L	312	CLA	C2A-CAA-CBA-CGA
28	I	306	CLA	CBA-CGA-O2A-C1
28	b	716	CLA	CBA-CGA-O2A-C1
28	B	313	CLA	CBA-CGA-O2A-C1
28	L	309	CLA	CBA-CGA-O2A-C1
28	I	311	CLA	C5-C6-C7-C8
28	h	202	CLA	C5-C6-C7-C8
28	l	311	CLA	C8-C10-C11-C12
28	a	705	CLA	C5-C6-C7-C8
28	a	723	CLA	C5-C6-C7-C8
28	B	311	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
28	I	313	CLA	C3-C5-C6-C7
28	I	308	CLA	C8-C10-C11-C12
28	l	311	CLA	C5-C6-C7-C8
28	b	707	CLA	C15-C16-C17-C18
28	B	311	CLA	C10-C11-C12-C13
28	L	314	CLA	O1D-CGD-O2D-CED
31	j	101	LMG	O6-C5-C6-O5
28	I	312	CLA	C5-C6-C7-C8
28	I	316	CLA	C5-C6-C7-C8
28	a	723	CLA	C15-C16-C17-C18
29	I	314	KC1	CAA-CBA-CGA-O2A
28	l	305	CLA	C2-C3-C5-C6
28	l	311	CLA	C2-C3-C5-C6
28	G	512	CLA	O1D-CGD-O2D-CED
36	b	729	PQN	C20-C21-C22-C23
28	b	709	CLA	C3-C5-C6-C7
28	b	720	CLA	C3-C5-C6-C7
28	L	313	CLA	C3-C5-C6-C7
28	L	314	CLA	C3-C5-C6-C7
30	G	521	DGD	C2B-C1B-O2G-C2G
31	K	317	LMG	O9-C10-O7-C8
28	K	312	CLA	O2A-C1-C2-C3
30	G	521	DGD	C2D-C1D-O3G-C3G
31	I	318	LMG	C2-C1-O1-C7
31	j	101	LMG	C2-C1-O1-C7
33	A	318	SQD	C2-C1-O6-C44
30	G	521	DGD	C1A-C2A-C3A-C4A
28	a	723	CLA	O1D-CGD-O2D-CED
28	m	202	CLA	C11-C12-C13-C15
28	B	309	CLA	C15-C16-C17-C18
32	D	307	PID	C19-C20-C21-CM5
32	F	305	PID	C19-C20-C21-CM5
29	M	307	KC1	CAA-CBA-CGA-O1A
28	a	716	CLA	CBD-CGD-O2D-CED
26	I	305	DD6	C7-C6-C8-C9
26	K	305	DD6	C12-C11-C13-C14
26	K	319	DD6	C12-C11-C13-C14
26	A	301	DD6	C12-C11-C13-C14
26	b	731	DD6	C12-C11-C13-C14
26	B	302	DD6	C12-C11-C13-C14
26	J	304	DD6	C12-C11-C13-C14
26	M	303	DD6	C12-C11-C13-C14

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Mol	Chain	Res	Type	Atoms
27	J	305	UIX	C7-C10-C11-C12
26	K	319	DD6	C10-C11-C13-C14
26	A	301	DD6	C10-C11-C13-C14
26	M	303	DD6	C10-C11-C13-C14
27	J	305	UIX	C7-C10-C11-C13
28	f	303	CLA	C2A-CAA-CBA-CGA
28	j	106	CLA	C2A-CAA-CBA-CGA
28	a	717	CLA	C2A-CAA-CBA-CGA
28	B	309	CLA	C2A-CAA-CBA-CGA
28	B	317	CLA	C2A-CAA-CBA-CGA
28	F	311	CLA	C2A-CAA-CBA-CGA
28	J	315	CLA	C2A-CAA-CBA-CGA
28	N	310	CLA	C2A-CAA-CBA-CGA
32	F	305	PID	C16-C17-C18-C19
28	a	707	CLA	C8-C10-C11-C12
31	B	318	LMG	C7-C8-O7-C10
28	G	512	CLA	C11-C12-C13-C14
28	h	202	CLA	C6-C7-C8-C9
28	b	715	CLA	C11-C12-C13-C15
28	B	311	CLA	C16-C17-C18-C20
28	J	307	CLA	C16-C17-C18-C19
28	B	312	CLA	O1D-CGD-O2D-CED
28	I	309	CLA	C3-C5-C6-C7
36	a	732	PQN	C13-C15-C16-C17
28	G	513	CLA	C5-C6-C7-C8
32	D	306	PID	C19-C20-C21-C22
32	D	307	PID	C19-C20-C21-C22
32	F	305	PID	C19-C20-C21-C22
30	y	201	DGD	O6D-C1D-O3G-C3G
30	G	521	DGD	O6D-C1D-O3G-C3G
33	A	318	SQD	O5-C1-O6-C44
29	N	308	KC1	CBD-CGD-O2D-CED
28	I	316	CLA	C6-C7-C8-C9
28	G	512	CLA	C11-C12-C13-C15
28	j	104	CLA	C6-C7-C8-C10
28	b	708	CLA	C16-C17-C18-C20
28	b	717	CLA	C16-C17-C18-C20
28	B	311	CLA	C16-C17-C18-C19
36	a	732	PQN	C26-C27-C28-C29
28	L	309	CLA	O1A-CGA-O2A-C1
28	D	309	CLA	CBD-CGD-O2D-CED
32	D	307	PID	C17-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
28	I	311	CLA	O1D-CGD-O2D-CED
29	A	314	KC1	CAA-CBA-CGA-O1A
31	D	317	LMG	C15-C16-C17-C18
28	K	313	CLA	O1A-CGA-O2A-C1
28	B	301	CLA	CBA-CGA-O2A-C1
31	I	318	LMG	C29-C30-C31-C32
30	G	501	DGD	C4D-C5D-C6D-O5D
28	f	301	CLA	C4B-C3B-CAB-CBB
28	l	313	CLA	C4B-C3B-CAB-CBB
28	a	708	CLA	C4B-C3B-CAB-CBB
28	B	317	CLA	C4B-C3B-CAB-CBB
28	F	308	CLA	C4B-C3B-CAB-CBB
28	J	310	CLA	C4B-C3B-CAB-CBB
28	N	309	CLA	C4B-C3B-CAB-CBB
30	l	301	DGD	C2B-C3B-C4B-C5B
31	D	317	LMG	C32-C33-C34-C35
28	h	202	CLA	C6-C7-C8-C10
28	j	104	CLA	C6-C7-C8-C9
28	l	311	CLA	C16-C17-C18-C20
28	b	717	CLA	C16-C17-C18-C19
28	B	301	CLA	C11-C12-C13-C14
28	J	307	CLA	C16-C17-C18-C20
28	L	313	CLA	C6-C7-C8-C10
36	a	732	PQN	C26-C27-C28-C30
28	b	716	CLA	O1A-CGA-O2A-C1
28	I	319	CLA	C2A-CAA-CBA-CGA
28	D	312	CLA	C2A-CAA-CBA-CGA
28	L	308	CLA	C2A-CAA-CBA-CGA
28	A	312	CLA	C5-C6-C7-C8
28	a	735	CLA	C15-C16-C17-C18
28	L	308	CLA	C2C-C3C-CAC-CBC
31	K	318	LMG	C4-C5-C6-O5
28	b	707	CLA	C11-C10-C8-C7
31	K	318	LMG	C32-C33-C34-C35
28	j	104	CLA	C5-C6-C7-C8
28	a	702	CLA	C8-C10-C11-C12
31	K	318	LMG	C34-C35-C36-C37
29	D	315	KC1	CAA-CBA-CGA-O1A
29	J	313	KC1	CAA-CBA-CGA-O1A
29	L	307	KC1	CAA-CBA-CGA-O1A
29	N	306	KC1	CAA-CBA-CGA-O2A
28	f	302	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
28	a	718	CLA	C3A-C2A-CAA-CBA
28	a	719	CLA	C3A-C2A-CAA-CBA
28	a	725	CLA	C3A-C2A-CAA-CBA
28	a	727	CLA	C3A-C2A-CAA-CBA
28	a	735	CLA	C3A-C2A-CAA-CBA
28	B	308	CLA	C3A-C2A-CAA-CBA
28	D	314	CLA	C3A-C2A-CAA-CBA
28	F	310	CLA	C3A-C2A-CAA-CBA
28	J	308	CLA	C3A-C2A-CAA-CBA
28	L	317	CLA	C3A-C2A-CAA-CBA
28	N	310	CLA	C3A-C2A-CAA-CBA
28	a	709	CLA	O1D-CGD-O2D-CED
28	J	301	CLA	O1D-CGD-O2D-CED
28	L	317	CLA	O1D-CGD-O2D-CED
36	a	732	PQN	C18-C20-C21-C22
28	a	705	CLA	O1D-CGD-O2D-CED
28	J	314	CLA	O1D-CGD-O2D-CED
30	I	317	DGD	C1B-C2B-C3B-C4B
28	l	311	CLA	C16-C17-C18-C19
28	b	715	CLA	C11-C12-C13-C14
28	B	301	CLA	C11-C12-C13-C15
28	L	313	CLA	C6-C7-C8-C9
30	G	521	DGD	O6D-C5D-C6D-O5D
28	I	306	CLA	O1A-CGA-O2A-C1
28	B	313	CLA	O1A-CGA-O2A-C1
28	b	717	CLA	CBD-CGD-O2D-CED
31	b	733	LMG	C36-C37-C38-C39
28	I	313	CLA	CBA-CGA-O2A-C1
28	b	703	CLA	CBA-CGA-O2A-C1
28	b	724	CLA	C3-C5-C6-C7
28	b	727	CLA	O1D-CGD-O2D-CED
31	b	733	LMG	C33-C34-C35-C36
28	M	317	CLA	O1A-CGA-O2A-C1
31	B	318	LMG	C31-C32-C33-C34
28	b	704	CLA	C4C-C3C-CAC-CBC
31	K	318	LMG	C31-C32-C33-C34
30	G	521	DGD	C4D-C5D-C6D-O5D
28	G	519	CLA	O1D-CGD-O2D-CED
28	A	308	CLA	O1D-CGD-O2D-CED
28	b	712	CLA	O1D-CGD-O2D-CED
31	D	317	LMG	C33-C34-C35-C36
28	I	316	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
28	a	728	CLA	C6-C7-C8-C9
28	b	708	CLA	C16-C17-C18-C19
28	f	301	CLA	C2B-C3B-CAB-CBB
28	a	708	CLA	C2B-C3B-CAB-CBB
28	B	317	CLA	C2B-C3B-CAB-CBB
28	F	311	CLA	C2B-C3B-CAB-CBB
28	J	301	CLA	C2B-C3B-CAB-CBB
28	J	310	CLA	C2B-C3B-CAB-CBB
28	L	318	CLA	C2B-C3B-CAB-CBB
35	i	201	BCR	C1-C6-C7-C8
35	b	730	BCR	C1-C6-C7-C8
35	b	730	BCR	C5-C6-C7-C8
31	b	733	LMG	C37-C38-C39-C40
28	B	301	CLA	CBD-CGD-O2D-CED
28	G	510	CLA	CBA-CGA-O2A-C1
28	h	202	CLA	CBA-CGA-O2A-C1
28	a	705	CLA	CBA-CGA-O2A-C1
28	a	704	CLA	C15-C16-C17-C18
28	K	308	CLA	C3-C5-C6-C7
28	J	312	CLA	C3-C5-C6-C7
28	I	306	CLA	O1D-CGD-O2D-CED
28	A	320	CLA	O1D-CGD-O2D-CED
28	f	303	CLA	O1D-CGD-O2D-CED
28	I	308	CLA	C2A-CAA-CBA-CGA
28	f	302	CLA	C2A-CAA-CBA-CGA
28	b	701	CLA	C2A-CAA-CBA-CGA
28	B	308	CLA	C2A-CAA-CBA-CGA
28	J	316	CLA	C2A-CAA-CBA-CGA
28	M	311	CLA	C2A-CAA-CBA-CGA
28	l	303	CLA	C10-C11-C12-C13
28	I	313	CLA	O1A-CGA-O2A-C1
28	B	301	CLA	O1A-CGA-O2A-C1
31	b	733	LMG	C32-C33-C34-C35
28	b	722	CLA	C4-C3-C5-C6
28	l	313	CLA	O1D-CGD-O2D-CED
31	j	101	LMG	C33-C34-C35-C36
31	K	318	LMG	C28-C29-C30-C31
31	D	317	LMG	C10-C11-C12-C13
28	K	311	CLA	CBA-CGA-O2A-C1
28	a	735	CLA	CBA-CGA-O2A-C1
30	l	301	DGD	C2A-C1A-O1G-C1G
28	b	725	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
28	a	723	CLA	C11-C12-C13-C14
28	b	717	CLA	C11-C12-C13-C14
28	b	719	CLA	O1A-CGA-O2A-C1
31	I	320	LMG	O6-C1-O1-C7
31	D	317	LMG	O6-C5-C6-O5
28	J	309	CLA	O1D-CGD-O2D-CED
31	D	317	LMG	C30-C31-C32-C33
28	f	301	CLA	CBA-CGA-O2A-C1
30	G	501	DGD	C2B-C1B-O2G-C2G
37	a	733	LHG	C8-C7-O7-C5
28	l	311	CLA	C10-C11-C12-C13
28	b	712	CLA	C5-C6-C7-C8
37	a	733	LHG	C26-C27-C28-C29
28	a	712	CLA	C10-C11-C12-C13
26	I	301	DD6	C12-C11-C13-C14
26	G	502	DD6	C12-C11-C13-C14
28	a	729	CLA	C3-C5-C6-C7
26	I	301	DD6	C10-C11-C13-C14
26	I	305	DD6	C5-C6-C8-C9
28	B	311	CLA	C5-C6-C7-C8
28	A	311	CLA	C2A-CAA-CBA-CGA
28	M	316	CLA	C2A-CAA-CBA-CGA
28	I	313	CLA	C6-C7-C8-C9
28	I	313	CLA	C6-C7-C8-C10
28	m	202	CLA	C11-C12-C13-C14
28	a	728	CLA	C6-C7-C8-C10
28	a	735	CLA	C16-C17-C18-C20
29	G	515	KC1	C2B-C3B-CAB-CBB
29	L	307	KC1	C2B-C3B-CAB-CBB
31	B	318	LMG	C32-C33-C34-C35
29	G	515	KC1	C2C-C3C-CAC-CBC
28	b	722	CLA	CBD-CGD-O2D-CED
28	a	705	CLA	O1A-CGA-O2A-C1
28	b	701	CLA	C10-C11-C12-C13
30	L	301	DGD	O6E-C5E-C6E-O5E
28	b	704	CLA	C13-C15-C16-C17
36	a	732	PQN	C15-C16-C17-C18
29	K	314	KC1	C4B-C3B-CAB-CBB
29	A	306	KC1	C4B-C3B-CAB-CBB
29	F	309	KC1	C4B-C3B-CAB-CBB
29	L	307	KC1	C4B-C3B-CAB-CBB
29	L	315	KC1	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
29	M	307	KC1	C4B-C3B-CAB-CBB
29	N	308	KC1	C4B-C3B-CAB-CBB
28	A	310	CLA	C16-C17-C18-C20
29	M	314	KC1	CAA-CBA-CGA-O2A
28	b	703	CLA	O1A-CGA-O2A-C1
28	a	731	CLA	C8-C10-C11-C12
28	a	710	CLA	O1D-CGD-O2D-CED
28	B	316	CLA	O1D-CGD-O2D-CED
31	I	318	LMG	C14-C15-C16-C17
31	I	318	LMG	C30-C31-C32-C33
31	K	318	LMG	C30-C31-C32-C33
31	B	318	LMG	C33-C34-C35-C36
28	b	712	CLA	C6-C7-C8-C10
28	l	304	CLA	C8-C10-C11-C12
28	I	316	CLA	C2A-CAA-CBA-CGA
28	G	510	CLA	C2A-CAA-CBA-CGA
28	G	514	CLA	C2A-CAA-CBA-CGA
28	m	202	CLA	C2A-CAA-CBA-CGA
28	b	708	CLA	C2A-CAA-CBA-CGA
28	b	718	CLA	C2A-CAA-CBA-CGA
28	b	723	CLA	C2A-CAA-CBA-CGA
28	D	309	CLA	C2A-CAA-CBA-CGA
28	J	312	CLA	C2A-CAA-CBA-CGA
31	I	320	LMG	C16-C17-C18-C19
31	K	318	LMG	C12-C13-C14-C15
27	J	305	UIX	C17-C18-O2-C27
28	b	711	CLA	C5-C6-C7-C8
36	b	729	PQN	C23-C25-C26-C27
28	b	712	CLA	C6-C7-C8-C9
30	I	317	DGD	O6E-C5E-C6E-O5E
28	G	510	CLA	O1A-CGA-O2A-C1
28	h	202	CLA	O1A-CGA-O2A-C1
28	I	315	CLA	C1A-C2A-CAA-CBA
28	A	319	CLA	C1A-C2A-CAA-CBA
28	f	302	CLA	C1A-C2A-CAA-CBA
28	l	312	CLA	C1A-C2A-CAA-CBA
28	a	707	CLA	C1A-C2A-CAA-CBA
28	a	711	CLA	C1A-C2A-CAA-CBA
28	a	712	CLA	C1A-C2A-CAA-CBA
28	a	715	CLA	C1A-C2A-CAA-CBA
28	a	717	CLA	C1A-C2A-CAA-CBA
28	a	719	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
28	a	720	CLA	C1A-C2A-CAA-CBA
28	a	725	CLA	C1A-C2A-CAA-CBA
28	a	727	CLA	C1A-C2A-CAA-CBA
28	a	735	CLA	C1A-C2A-CAA-CBA
28	b	706	CLA	C1A-C2A-CAA-CBA
28	b	720	CLA	C1A-C2A-CAA-CBA
28	b	721	CLA	C1A-C2A-CAA-CBA
28	b	723	CLA	C1A-C2A-CAA-CBA
28	D	314	CLA	C1A-C2A-CAA-CBA
28	F	308	CLA	C1A-C2A-CAA-CBA
28	H	309	CLA	C1A-C2A-CAA-CBA
28	J	301	CLA	C1A-C2A-CAA-CBA
28	J	308	CLA	C1A-C2A-CAA-CBA
28	L	312	CLA	C1A-C2A-CAA-CBA
28	L	313	CLA	C1A-C2A-CAA-CBA
28	L	317	CLA	C1A-C2A-CAA-CBA
28	M	313	CLA	C1A-C2A-CAA-CBA
28	N	305	CLA	C1A-C2A-CAA-CBA
30	l	301	DGD	O1A-C1A-O1G-C1G
31	D	317	LMG	C13-C14-C15-C16
28	I	310	CLA	CBD-CGD-O2D-CED
30	G	501	DGD	O1B-C1B-O2G-C2G
28	l	304	CLA	C3-C5-C6-C7
28	I	312	CLA	C12-C13-C15-C16
28	G	510	CLA	C11-C12-C13-C15
28	G	519	CLA	C6-C7-C8-C10
28	G	519	CLA	C11-C10-C8-C7
28	l	313	CLA	C6-C7-C8-C10
28	a	702	CLA	C12-C13-C15-C16
28	a	709	CLA	C12-C13-C15-C16
28	a	717	CLA	C11-C10-C8-C7
28	b	703	CLA	C11-C10-C8-C7
28	b	709	CLA	C11-C10-C8-C7
28	B	301	CLA	C11-C10-C8-C7
28	B	309	CLA	C6-C7-C8-C10
28	B	309	CLA	C11-C12-C13-C15
28	B	311	CLA	C11-C12-C13-C15
28	B	311	CLA	C12-C13-C15-C16
28	B	313	CLA	C11-C10-C8-C7
28	J	307	CLA	C11-C10-C8-C7
28	N	305	CLA	C11-C12-C13-C15
28	l	303	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
28	A	310	CLA	C8-C10-C11-C12
28	K	311	CLA	O1A-CGA-O2A-C1
28	f	301	CLA	O1A-CGA-O2A-C1
28	a	735	CLA	O1A-CGA-O2A-C1
29	A	306	KC1	CAA-CBA-CGA-O2A
28	G	512	CLA	C5-C6-C7-C8
28	a	731	CLA	C15-C16-C17-C18
28	b	701	CLA	C5-C6-C7-C8
28	b	707	CLA	C5-C6-C7-C8
28	b	709	CLA	C2-C3-C5-C6
28	a	721	CLA	C8-C10-C11-C12
28	b	704	CLA	C10-C11-C12-C13
28	b	717	CLA	C13-C15-C16-C17
28	a	735	CLA	C3-C5-C6-C7
28	I	307	CLA	C2A-CAA-CBA-CGA
28	I	313	CLA	C2A-CAA-CBA-CGA
28	I	315	CLA	C2A-CAA-CBA-CGA
28	A	310	CLA	C2A-CAA-CBA-CGA
28	H	307	CLA	C2A-CAA-CBA-CGA
28	J	301	CLA	C2A-CAA-CBA-CGA
28	G	510	CLA	C11-C12-C13-C14
28	G	512	CLA	C11-C10-C8-C9
28	A	310	CLA	C14-C13-C15-C16
28	a	709	CLA	C14-C13-C15-C16
28	B	309	CLA	C11-C12-C13-C14
28	N	305	CLA	C11-C12-C13-C14
31	b	734	LMG	O6-C5-C6-O5
35	l	306	BCR	C13-C14-C15-C16
28	D	311	CLA	CBA-CGA-O2A-C1
28	L	308	CLA	CBA-CGA-O2A-C1
28	I	310	CLA	O2A-C1-C2-C3
30	G	501	DGD	C1G-C2G-C3G-O3G
31	K	318	LMG	C7-C8-C9-O8
31	b	734	LMG	O1-C7-C8-C9
28	G	514	CLA	O1D-CGD-O2D-CED
31	D	317	LMG	C14-C15-C16-C17
28	a	735	CLA	O1D-CGD-O2D-CED
28	A	312	CLA	CBA-CGA-O2A-C1
28	b	704	CLA	CBA-CGA-O2A-C1
28	b	705	CLA	CBA-CGA-O2A-C1
31	b	734	LMG	C29-C28-O8-C9
28	a	721	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
28	b	711	CLA	C6-C7-C8-C9
31	b	733	LMG	C15-C16-C17-C18
28	l	310	CLA	CHA-CBD-CGD-O1D
28	l	310	CLA	CHA-CBD-CGD-O2D
32	D	306	PID	C19-C20-C21-CM5
28	a	729	CLA	C5-C6-C7-C8
31	D	317	LMG	C18-C19-C20-C21
26	G	505	DD6	C12-C11-C13-C14
26	L	305	DD6	C12-C11-C13-C14
28	A	310	CLA	C16-C17-C18-C19
26	I	303	DD6	C10-C11-C13-C14
26	G	505	DD6	C10-C11-C13-C14
28	a	723	CLA	C2A-CAA-CBA-CGA
28	f	303	CLA	CBA-CGA-O2A-C1
31	b	733	LMG	C14-C15-C16-C17
28	b	704	CLA	C15-C16-C17-C18
30	G	521	DGD	C1B-C2B-C3B-C4B
28	I	312	CLA	CBA-CGA-O2A-C1
28	l	311	CLA	C13-C15-C16-C17
28	l	313	CLA	C15-C16-C17-C18
28	a	731	CLA	C5-C6-C7-C8
31	K	318	LMG	C29-C30-C31-C32
28	l	303	CLA	C16-C17-C18-C19
28	a	721	CLA	C16-C17-C18-C20
28	J	306	CLA	CBA-CGA-O2A-C1
28	a	713	CLA	C8-C10-C11-C12
30	l	301	DGD	C3B-C4B-C5B-C6B
28	L	308	CLA	O1A-CGA-O2A-C1
28	B	309	CLA	C4-C3-C5-C6
31	I	320	LMG	C32-C33-C34-C35
30	G	521	DGD	O2G-C2G-C3G-O3G
28	K	308	CLA	C6-C7-C8-C9
31	I	318	LMG	C15-C16-C17-C18
28	F	315	CLA	O1D-CGD-O2D-CED
28	M	310	CLA	O2A-C1-C2-C3
28	l	303	CLA	CBD-CGD-O2D-CED
28	B	313	CLA	O1D-CGD-O2D-CED
28	K	306	CLA	CBA-CGA-O2A-C1
28	a	724	CLA	CBA-CGA-O2A-C1
28	a	726	CLA	CBA-CGA-O2A-C1
28	b	712	CLA	CBA-CGA-O2A-C1
28	K	310	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
28	A	309	CLA	O1D-CGD-O2D-CED
28	J	310	CLA	O1D-CGD-O2D-CED
28	I	311	CLA	C6-C7-C8-C10
28	f	301	CLA	C6-C7-C8-C10
28	H	305	CLA	C4-C3-C5-C6
28	a	707	CLA	C2-C3-C5-C6
28	b	728	CLA	CBA-CGA-O2A-C1
28	a	723	CLA	C10-C11-C12-C13
26	K	301	DD6	C27-C29-C30-C31
26	K	305	DD6	C27-C29-C30-C31
26	K	319	DD6	C27-C29-C30-C31
26	G	502	DD6	C27-C29-C30-C31
26	G	508	DD6	C27-C29-C30-C31
26	A	303	DD6	C27-C29-C30-C31
26	B	303	DD6	C27-C29-C30-C31
26	D	303	DD6	C27-C29-C30-C31
26	J	302	DD6	C27-C29-C30-C31
28	A	311	CLA	CBD-CGD-O2D-CED
28	I	312	CLA	C11-C12-C13-C14
28	G	519	CLA	C6-C7-C8-C9
28	l	313	CLA	C6-C7-C8-C9
28	m	202	CLA	C6-C7-C8-C9
28	a	707	CLA	C11-C12-C13-C14
28	a	717	CLA	C11-C10-C8-C9
28	b	703	CLA	C11-C10-C8-C9
28	b	705	CLA	C14-C13-C15-C16
28	b	709	CLA	C11-C10-C8-C9
28	B	309	CLA	C6-C7-C8-C9
36	a	732	PQN	C21-C22-C23-C24
37	a	733	LHG	C2-C3-O3-P
28	K	307	CLA	C4B-C3B-CAB-CBB
28	G	516	CLA	C4B-C3B-CAB-CBB
28	h	202	CLA	C4B-C3B-CAB-CBB
28	a	718	CLA	C4B-C3B-CAB-CBB
28	a	725	CLA	C4B-C3B-CAB-CBB
28	a	726	CLA	C4B-C3B-CAB-CBB
28	b	726	CLA	C4B-C3B-CAB-CBB
28	B	311	CLA	C4B-C3B-CAB-CBB
28	B	312	CLA	C4B-C3B-CAB-CBB
28	H	311	CLA	C4B-C3B-CAB-CBB
28	J	308	CLA	C4B-C3B-CAB-CBB
28	L	316	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
28	M	317	CLA	C4B-C3B-CAB-CBB
28	L	318	CLA	CAA-CBA-CGA-O2A
28	a	724	CLA	C5-C6-C7-C8
31	I	320	LMG	C17-C18-C19-C20
28	I	310	CLA	C2A-CAA-CBA-CGA
28	b	711	CLA	C3-C5-C6-C7
28	G	512	CLA	C11-C10-C8-C7
28	A	310	CLA	C12-C13-C15-C16
28	m	202	CLA	C6-C7-C8-C10
28	a	709	CLA	C11-C10-C8-C7
28	a	713	CLA	C11-C10-C8-C7
28	a	717	CLA	C6-C7-C8-C10
28	a	725	CLA	C11-C10-C8-C7
28	b	704	CLA	C12-C13-C15-C16
28	J	309	CLA	C6-C7-C8-C10
28	a	720	CLA	C10-C11-C12-C13
28	b	704	CLA	O1A-CGA-O2A-C1
31	b	733	LMG	C38-C39-C40-C41
28	A	312	CLA	O1A-CGA-O2A-C1
28	b	705	CLA	O1A-CGA-O2A-C1
28	I	310	CLA	C3A-C2A-CAA-CBA
28	b	706	CLA	C3A-C2A-CAA-CBA
28	b	709	CLA	C4-C3-C5-C6
28	b	724	CLA	C3A-C2A-CAA-CBA
28	B	317	CLA	C3A-C2A-CAA-CBA
28	b	714	CLA	CAA-CBA-CGA-O2A
26	I	305	DD6	C1-C2-C3-C4
26	I	305	DD6	C3-C4-C5-C6
26	I	303	DD6	C12-C11-C13-C14
35	j	102	BCR	C36-C18-C19-C20
28	I	312	CLA	O1A-CGA-O2A-C1
26	G	504	DD6	C5-C6-C8-C9
26	L	305	DD6	C10-C11-C13-C14
28	b	706	CLA	O2A-C1-C2-C3
30	y	201	DGD	C1G-C2G-C3G-O3G
31	I	318	LMG	C7-C8-C9-O8
31	B	318	LMG	C7-C8-C9-O8
31	D	317	LMG	C7-C8-C9-O8
28	a	726	CLA	C3-C5-C6-C7
28	I	311	CLA	C6-C7-C8-C9
28	a	735	CLA	C16-C17-C18-C19
31	I	318	LMG	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
28	a	707	CLA	C4-C3-C5-C6
28	B	311	CLA	C2-C3-C5-C6
28	a	716	CLA	O1D-CGD-O2D-CED
28	D	309	CLA	O1D-CGD-O2D-CED
31	j	101	LMG	C31-C32-C33-C34
28	a	718	CLA	C2B-C3B-CAB-CBB
28	b	726	CLA	C2B-C3B-CAB-CBB
28	B	316	CLA	CBA-CGA-O2A-C1
28	a	721	CLA	C5-C6-C7-C8
31	I	320	LMG	C31-C32-C33-C34
28	f	301	CLA	C6-C7-C8-C9
30	G	521	DGD	O1G-C1G-C2G-O2G
30	j	103	DGD	O1G-C1G-C2G-O2G
30	l	301	DGD	O2G-C2G-C3G-O3G
31	I	318	LMG	O1-C7-C8-O7
31	I	318	LMG	O7-C8-C9-O8
31	j	101	LMG	O7-C8-C9-O8
31	b	734	LMG	O7-C8-C9-O8
29	G	515	KC1	CAA-CBA-CGA-O2A
31	b	733	LMG	C28-C29-C30-C31
28	B	311	CLA	C4-C3-C5-C6
28	b	722	CLA	C2-C3-C5-C6
31	I	318	LMG	C32-C33-C34-C35
28	a	706	CLA	O1D-CGD-O2D-CED
28	a	709	CLA	C11-C10-C8-C9
28	a	713	CLA	C11-C10-C8-C9
28	a	725	CLA	C11-C10-C8-C9
28	b	704	CLA	C11-C12-C13-C14
28	b	728	CLA	C6-C7-C8-C9
28	B	313	CLA	C11-C10-C8-C9
28	J	301	CLA	C11-C10-C8-C9
28	b	708	CLA	C5-C6-C7-C8
28	l	313	CLA	C2C-C3C-CAC-CBC
32	D	306	PID	C15-C16-C17-C18
28	B	310	CLA	C6-C7-C8-C9
31	b	734	LMG	C11-C12-C13-C14
28	a	704	CLA	C5-C6-C7-C8
28	b	717	CLA	O1D-CGD-O2D-CED
28	a	713	CLA	C3-C5-C6-C7
28	a	724	CLA	C13-C15-C16-C17
32	D	306	PID	CM4-C14-C15-C16
28	B	301	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
28	b	711	CLA	C6-C7-C8-C10
26	L	306	DD6	C12-C11-C13-C14
27	K	302	UIX	C7-C10-C11-C12
28	A	310	CLA	C11-C10-C8-C7
28	l	305	CLA	C11-C12-C13-C15
28	l	313	CLA	C11-C12-C13-C15
28	b	704	CLA	C6-C7-C8-C10
28	b	705	CLA	C11-C12-C13-C15
28	b	707	CLA	C6-C7-C8-C10
28	b	728	CLA	C6-C7-C8-C10
28	B	309	CLA	C12-C13-C15-C16
28	H	305	CLA	C11-C12-C13-C15
28	J	301	CLA	C11-C10-C8-C7
29	L	315	KC1	C2C-C3C-CAC-CBC
31	I	318	LMG	C31-C32-C33-C34
26	K	305	DD6	C10-C11-C13-C14
26	b	731	DD6	C10-C11-C13-C14
26	L	306	DD6	C10-C11-C13-C14
27	K	302	UIX	C7-C10-C11-C13
35	j	102	BCR	C17-C18-C19-C20
35	m	201	BCR	C11-C12-C13-C14
28	a	717	CLA	CBA-CGA-O2A-C1
28	a	720	CLA	CBA-CGA-O2A-C1
28	b	712	CLA	O1A-CGA-O2A-C1
28	b	728	CLA	O1A-CGA-O2A-C1
28	l	310	CLA	C2A-CAA-CBA-CGA
28	b	712	CLA	C2A-CAA-CBA-CGA
28	B	310	CLA	C6-C7-C8-C10
28	I	307	CLA	CBD-CGD-O2D-CED
28	b	719	CLA	CBD-CGD-O2D-CED
28	b	722	CLA	O1D-CGD-O2D-CED
30	G	521	DGD	C1G-C2G-O2G-C1B
31	K	317	LMG	C28-C29-C30-C31
28	K	306	CLA	O1A-CGA-O2A-C1
28	a	724	CLA	O1A-CGA-O2A-C1
28	a	726	CLA	O1A-CGA-O2A-C1
28	G	519	CLA	C10-C11-C12-C13
28	a	702	CLA	C15-C16-C17-C18
32	D	306	PID	C13-C14-C15-C16
30	G	521	DGD	O1G-C1G-C2G-C3G
30	l	301	DGD	C1G-C2G-C3G-O3G
31	I	318	LMG	O1-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
31	b	734	LMG	C7-C8-C9-O8
29	G	515	KC1	C4B-C3B-CAB-CBB
29	B	314	KC1	C4B-C3B-CAB-CBB
29	D	310	KC1	C4B-C3B-CAB-CBB
29	F	314	KC1	C4B-C3B-CAB-CBB
29	H	306	KC1	C4B-C3B-CAB-CBB
29	H	310	KC1	C4B-C3B-CAB-CBB
29	J	313	KC1	C4B-C3B-CAB-CBB
29	M	314	KC1	C4B-C3B-CAB-CBB
29	N	306	KC1	C4B-C3B-CAB-CBB
29	N	311	KC1	C4B-C3B-CAB-CBB
28	a	722	CLA	C5-C6-C7-C8
36	b	729	PQN	C14-C13-C15-C16
28	K	310	CLA	C2A-CAA-CBA-CGA
28	L	309	CLA	C2A-CAA-CBA-CGA
28	a	703	CLA	C3-C5-C6-C7
30	G	501	DGD	O2G-C2G-C3G-O3G
31	B	318	LMG	O7-C8-C9-O8
28	G	510	CLA	C14-C13-C15-C16
28	A	310	CLA	C11-C10-C8-C9
28	b	727	CLA	C11-C12-C13-C14
28	H	305	CLA	C11-C12-C13-C14
28	J	308	CLA	CAA-CBA-CGA-O2A
31	I	320	LMG	C14-C15-C16-C17
31	I	318	LMG	C11-C12-C13-C14
32	N	301	PID	C12-C13-C14-C15
26	D	303	DD6	C11-C10-C9-C8
28	K	311	CLA	C2-C1-O2A-CGA
28	M	312	CLA	O2A-C1-C2-C3
28	a	709	CLA	C8-C10-C11-C12
37	a	733	LHG	C24-C25-C26-C27
28	K	311	CLA	C4-C3-C5-C6
28	N	305	CLA	C3-C5-C6-C7
28	I	321	CLA	C4C-C3C-CAC-CBC
28	a	704	CLA	C2A-CAA-CBA-CGA
28	b	705	CLA	C2A-CAA-CBA-CGA
28	A	313	CLA	C6-C7-C8-C9
28	N	305	CLA	C16-C17-C18-C20
31	b	733	LMG	C35-C36-C37-C38
28	b	720	CLA	C5-C6-C7-C8
26	I	302	DD6	C27-C29-C30-C31
26	K	304	DD6	C27-C29-C30-C31

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Mol	Chain	Res	Type	Atoms
26	H	303	DD6	C27-C29-C30-C31
26	L	306	DD6	C27-C29-C30-C31
28	J	301	CLA	C8-C10-C11-C12
26	A	302	DD6	C7-C6-C8-C9
28	I	306	CLA	C4B-C3B-CAB-CBB
28	I	307	CLA	C4B-C3B-CAB-CBB
28	I	312	CLA	C4B-C3B-CAB-CBB
28	K	306	CLA	C4B-C3B-CAB-CBB
28	K	311	CLA	C4B-C3B-CAB-CBB
28	G	518	CLA	C4B-C3B-CAB-CBB
28	l	303	CLA	C4B-C3B-CAB-CBB
28	a	707	CLA	C4B-C3B-CAB-CBB
28	a	713	CLA	C4B-C3B-CAB-CBB
28	a	716	CLA	C4B-C3B-CAB-CBB
28	a	724	CLA	C1A-C2A-CAA-CBA
28	a	738	CLA	C4B-C3B-CAB-CBB
28	b	718	CLA	C4B-C3B-CAB-CBB
28	b	719	CLA	C4B-C3B-CAB-CBB
28	b	724	CLA	C4B-C3B-CAB-CBB
28	b	728	CLA	C4B-C3B-CAB-CBB
28	B	316	CLA	C4B-C3B-CAB-CBB
28	D	308	CLA	C4B-C3B-CAB-CBB
28	D	312	CLA	C4B-C3B-CAB-CBB
28	D	314	CLA	C4B-C3B-CAB-CBB
28	H	304	CLA	C4B-C3B-CAB-CBB
28	H	305	CLA	C1A-C2A-CAA-CBA
28	H	309	CLA	C4B-C3B-CAB-CBB
28	L	312	CLA	C4B-C3B-CAB-CBB
28	M	318	CLA	C4B-C3B-CAB-CBB
28	N	304	CLA	C4B-C3B-CAB-CBB
28	N	310	CLA	C4B-C3B-CAB-CBB
37	a	733	LHG	C24-C23-O8-C6
28	b	707	CLA	C4-C3-C5-C6
26	G	502	DD6	C10-C11-C13-C14
28	a	717	CLA	O1A-CGA-O2A-C1
28	a	720	CLA	O1A-CGA-O2A-C1
28	a	721	CLA	C13-C15-C16-C17
28	a	725	CLA	C5-C6-C7-C8
37	a	733	LHG	O9-C7-O7-C5
28	l	312	CLA	CBA-CGA-O2A-C1
28	a	708	CLA	C2-C3-C5-C6
28	I	310	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
28	A	310	CLA	C6-C7-C8-C10
28	A	310	CLA	C11-C12-C13-C15
28	l	303	CLA	C11-C12-C13-C15
28	a	722	CLA	C11-C10-C8-C7
28	a	724	CLA	C6-C7-C8-C10
28	b	708	CLA	C11-C10-C8-C7
28	B	301	CLA	C6-C7-C8-C10
28	B	311	CLA	C6-C7-C8-C10
28	N	305	CLA	C12-C13-C15-C16
28	b	709	CLA	C11-C12-C13-C14
28	b	725	CLA	CBA-CGA-O2A-C1
28	a	706	CLA	C3A-C2A-CAA-CBA
28	F	312	CLA	C2C-C3C-CAC-CBC
29	M	314	KC1	C2C-C3C-CAC-CBC
32	D	306	PID	C17-C18-C19-C20
28	A	311	CLA	O1D-CGD-O2D-CED
31	K	317	LMG	C10-C11-C12-C13
28	l	303	CLA	O1D-CGD-O2D-CED
28	A	310	CLA	C11-C12-C13-C14
28	l	304	CLA	C6-C7-C8-C9
28	l	311	CLA	C14-C13-C15-C16
28	l	313	CLA	C11-C12-C13-C14
28	b	705	CLA	C11-C12-C13-C14
28	b	707	CLA	C6-C7-C8-C9
28	b	715	CLA	C6-C7-C8-C9
28	B	309	CLA	C14-C13-C15-C16
28	J	309	CLA	C6-C7-C8-C9
28	K	313	CLA	C6-C7-C8-C10
28	B	309	CLA	C10-C11-C12-C13
31	b	733	LMG	C31-C32-C33-C34
28	G	520	CLA	C1-C2-C3-C4
29	K	314	KC1	C1A-C2A-CAA-CBA
29	A	306	KC1	C1A-C2A-CAA-CBA
29	N	306	KC1	C1A-C2A-CAA-CBA
29	N	308	KC1	C1A-C2A-CAA-CBA
28	b	712	CLA	C3-C5-C6-C7
31	D	317	LMG	O7-C8-C9-O8
28	A	313	CLA	C6-C7-C8-C10
30	G	521	DGD	C1G-C2G-C3G-O3G
30	j	103	DGD	O1G-C1G-C2G-C3G
28	l	313	CLA	C13-C15-C16-C17
28	A	319	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
28	b	703	CLA	CAA-CBA-CGA-O2A
28	K	311	CLA	C2-C3-C5-C6
28	K	310	CLA	CAD-CBD-CGD-O2D
28	G	512	CLA	CAD-CBD-CGD-O2D
28	a	729	CLA	CAD-CBD-CGD-O2D
28	F	311	CLA	CAD-CBD-CGD-O2D
28	H	312	CLA	CAD-CBD-CGD-O2D
32	D	306	PID	O4-C12-C13-C14
32	H	301	PID	O4-C12-C13-C14
31	D	317	LMG	C28-C29-C30-C31
28	b	704	CLA	C16-C17-C18-C20
28	K	310	CLA	CAD-CBD-CGD-O1D
28	G	512	CLA	CAD-CBD-CGD-O1D
28	j	104	CLA	CHA-CBD-CGD-O1D
28	j	104	CLA	CHA-CBD-CGD-O2D
28	a	707	CLA	CHA-CBD-CGD-O1D
28	a	707	CLA	CHA-CBD-CGD-O2D
28	a	718	CLA	CAD-CBD-CGD-O1D
28	a	719	CLA	CHA-CBD-CGD-O1D
28	a	719	CLA	CHA-CBD-CGD-O2D
28	a	720	CLA	CHA-CBD-CGD-O1D
28	a	721	CLA	CAD-CBD-CGD-O1D
28	a	729	CLA	CAD-CBD-CGD-O1D
28	b	707	CLA	CHA-CBD-CGD-O1D
28	b	717	CLA	CHA-CBD-CGD-O1D
28	B	307	CLA	CHA-CBD-CGD-O2D
28	F	311	CLA	CAD-CBD-CGD-O1D
28	H	312	CLA	CAD-CBD-CGD-O1D
28	J	307	CLA	CAD-CBD-CGD-O1D
28	L	311	CLA	CHA-CBD-CGD-O1D
28	L	311	CLA	CHA-CBD-CGD-O2D
28	M	310	CLA	CHA-CBD-CGD-O1D
28	M	310	CLA	CHA-CBD-CGD-O2D
37	a	733	LHG	C3-O3-P-O5
37	a	733	LHG	C4-O6-P-O5
28	b	725	CLA	O1A-CGA-O2A-C1
28	a	726	CLA	C13-C15-C16-C17
28	K	307	CLA	C2B-C3B-CAB-CBB
28	K	311	CLA	C2B-C3B-CAB-CBB
28	G	516	CLA	C2B-C3B-CAB-CBB
28	l	313	CLA	C2B-C3B-CAB-CBB
28	B	312	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
28	D	312	CLA	C2B-C3B-CAB-CBB
28	D	314	CLA	C2B-C3B-CAB-CBB
28	F	308	CLA	C2B-C3B-CAB-CBB
28	J	308	CLA	C2B-C3B-CAB-CBB
28	L	312	CLA	C2B-C3B-CAB-CBB
28	L	316	CLA	C2B-C3B-CAB-CBB
28	N	304	CLA	C2B-C3B-CAB-CBB
28	N	309	CLA	C2B-C3B-CAB-CBB
36	b	729	PQN	C12-C13-C15-C16
29	F	309	KC1	C2A-CAA-CBA-CGA
35	m	201	BCR	C11-C12-C13-C35
28	a	703	CLA	C6-C7-C8-C9
28	N	305	CLA	C16-C17-C18-C19
31	I	318	LMG	C9-C8-O7-C10
31	b	733	LMG	C34-C35-C36-C37
26	I	302	DD6	C6-C8-C9-C10
28	l	303	CLA	C15-C16-C17-C18
28	b	724	CLA	C5-C6-C7-C8
28	l	304	CLA	C11-C12-C13-C14
28	D	311	CLA	O1A-CGA-O2A-C1
28	M	310	CLA	CBA-CGA-O2A-C1
28	M	310	CLA	O1A-CGA-O2A-C1
28	G	513	CLA	C14-C13-C15-C16
28	l	313	CLA	C14-C13-C15-C16
28	a	723	CLA	C14-C13-C15-C16
28	a	726	CLA	C14-C13-C15-C16
28	b	719	CLA	O1D-CGD-O2D-CED
28	G	513	CLA	C12-C13-C15-C16
28	l	304	CLA	C11-C10-C8-C7
28	l	313	CLA	C12-C13-C15-C16
28	B	309	CLA	C11-C10-C8-C7
28	f	303	CLA	O1A-CGA-O2A-C1
32	D	304	PID	C19-C20-C21-C22
37	a	733	LHG	C23-C24-C25-C26
28	b	710	CLA	CBA-CGA-O2A-C1
28	M	316	CLA	CBA-CGA-O2A-C1
31	D	317	LMG	C29-C28-O8-C9
28	A	316	CLA	CAA-CBA-CGA-O2A
28	a	702	CLA	CAA-CBA-CGA-O2A
28	M	317	CLA	CAA-CBA-CGA-O2A
28	b	710	CLA	O1A-CGA-O2A-C1
28	M	316	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
28	B	309	CLA	C2-C3-C5-C6
26	F	303	DD6	C11-C10-C9-C8
31	b	733	LMG	C11-C10-O7-C8
29	M	314	KC1	C4C-C3C-CAC-CBC
31	B	318	LMG	C36-C37-C38-C39
28	b	707	CLA	C2-C1-O2A-CGA
28	a	717	CLA	C4-C3-C5-C6
28	f	303	CLA	CAA-CBA-CGA-O2A
31	B	318	LMG	C34-C35-C36-C37
28	G	513	CLA	C8-C10-C11-C12
31	b	733	LMG	C29-C30-C31-C32
28	K	313	CLA	C6-C7-C8-C9
30	y	201	DGD	C9B-CAB-CBB-CCB
28	G	512	CLA	C2A-CAA-CBA-CGA
28	L	318	CLA	C2A-CAA-CBA-CGA
28	J	307	CLA	C10-C11-C12-C13
26	B	306	DD6	C27-C29-C30-C31
26	F	303	DD6	C27-C29-C30-C31
28	b	707	CLA	C16-C17-C18-C20
28	J	306	CLA	O1A-CGA-O2A-C1
28	a	722	CLA	C11-C10-C8-C9
28	B	301	CLA	C6-C7-C8-C9
28	b	728	CLA	C5-C6-C7-C8
28	I	315	CLA	C4B-C3B-CAB-CBB
28	a	721	CLA	C4B-C3B-CAB-CBB
28	J	306	CLA	C4B-C3B-CAB-CBB
37	a	733	LHG	C32-C33-C34-C35
26	G	504	DD6	C24-C25-C26-C27
26	M	302	DD6	C3-C4-C5-C6
28	b	708	CLA	C6-C7-C8-C10
28	b	713	CLA	C11-C10-C8-C7
28	l	305	CLA	C10-C11-C12-C13
31	b	733	LMG	C30-C31-C32-C33
28	I	307	CLA	O1D-CGD-O2D-CED
28	l	304	CLA	C11-C12-C13-C15
28	b	716	CLA	C3A-C2A-CAA-CBA
28	b	719	CLA	C3A-C2A-CAA-CBA
28	B	307	CLA	C3A-C2A-CAA-CBA
28	F	313	CLA	C3A-C2A-CAA-CBA
28	H	305	CLA	C16-C17-C18-C20
26	I	302	DD6	C9-C10-C11-C12
32	D	304	PID	C19-C20-C21-CM5

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Mol	Chain	Res	Type	Atoms
35	f	304	BCR	C35-C13-C14-C15
35	l	302	BCR	C20-C21-C22-C37
28	L	308	CLA	C4C-C3C-CAC-CBC
31	b	734	LMG	C14-C15-C16-C17
28	B	316	CLA	O1A-CGA-O2A-C1
28	a	721	CLA	C11-C12-C13-C14
28	b	704	CLA	C11-C10-C8-C9
28	b	724	CLA	C11-C10-C8-C9
28	b	724	CLA	C11-C12-C13-C14
28	b	727	CLA	C6-C7-C8-C9
28	N	305	CLA	C14-C13-C15-C16
37	a	733	LHG	C29-C30-C31-C32
31	I	320	LMG	C7-C8-O7-C10
37	a	733	LHG	C4-C5-O7-C7
37	a	733	LHG	C6-C5-O7-C7
30	G	501	DGD	C3A-C4A-C5A-C6A
31	I	320	LMG	C2-C1-O1-C7
28	G	518	CLA	C2A-CAA-CBA-CGA
28	L	311	CLA	C2A-CAA-CBA-CGA
26	I	302	DD6	C9-C10-C11-C13
28	I	308	CLA	C1A-C2A-CAA-CBA
28	I	310	CLA	C1A-C2A-CAA-CBA
28	a	706	CLA	C1A-C2A-CAA-CBA
28	b	716	CLA	C1A-C2A-CAA-CBA
28	B	313	CLA	C1A-C2A-CAA-CBA
35	f	304	BCR	C12-C13-C14-C15
35	l	302	BCR	C20-C21-C22-C23
28	D	308	CLA	CBA-CGA-O2A-C1
28	D	308	CLA	O1A-CGA-O2A-C1
28	I	308	CLA	C10-C11-C12-C13
28	I	306	CLA	C2B-C3B-CAB-CBB
28	I	307	CLA	C2B-C3B-CAB-CBB
28	I	312	CLA	C2B-C3B-CAB-CBB
28	I	315	CLA	C2B-C3B-CAB-CBB
28	K	306	CLA	C2B-C3B-CAB-CBB
28	K	312	CLA	C2B-C3B-CAB-CBB
28	G	518	CLA	C2B-C3B-CAB-CBB
28	h	202	CLA	C2B-C3B-CAB-CBB
28	l	303	CLA	C2B-C3B-CAB-CBB
28	a	707	CLA	C2B-C3B-CAB-CBB
28	a	712	CLA	C2B-C3B-CAB-CBB
28	a	713	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
28	a	716	CLA	C2B-C3B-CAB-CBB
28	a	725	CLA	C2B-C3B-CAB-CBB
28	a	726	CLA	C2B-C3B-CAB-CBB
28	a	738	CLA	C2B-C3B-CAB-CBB
28	b	718	CLA	C2B-C3B-CAB-CBB
28	b	723	CLA	C2B-C3B-CAB-CBB
28	b	724	CLA	C2B-C3B-CAB-CBB
28	b	728	CLA	C2B-C3B-CAB-CBB
28	B	311	CLA	C2B-C3B-CAB-CBB
28	B	316	CLA	C2B-C3B-CAB-CBB
28	D	308	CLA	C2B-C3B-CAB-CBB
28	H	304	CLA	C2B-C3B-CAB-CBB
28	H	309	CLA	C2B-C3B-CAB-CBB
28	J	306	CLA	C2B-C3B-CAB-CBB
28	M	312	CLA	C2B-C3B-CAB-CBB
28	M	317	CLA	C2B-C3B-CAB-CBB
28	M	318	CLA	C2B-C3B-CAB-CBB
28	N	310	CLA	C2B-C3B-CAB-CBB
35	j	102	BCR	C23-C24-C25-C30
35	l	306	BCR	C1-C6-C7-C8
35	l	306	BCR	C23-C24-C25-C30
28	a	723	CLA	C3-C5-C6-C7
28	L	318	CLA	CAA-CBA-CGA-O1A
28	a	704	CLA	C11-C10-C8-C7
28	a	709	CLA	C6-C7-C8-C10
28	a	731	CLA	C11-C12-C13-C15
28	a	735	CLA	C12-C13-C15-C16
28	b	704	CLA	C11-C10-C8-C7
28	b	717	CLA	C12-C13-C15-C16
28	b	724	CLA	C11-C12-C13-C15
28	b	727	CLA	C16-C17-C18-C20
28	I	315	CLA	C4C-C3C-CAC-CBC
28	a	728	CLA	C2A-CAA-CBA-CGA
28	D	311	CLA	C2A-CAA-CBA-CGA
30	j	103	DGD	C2A-C3A-C4A-C5A
28	b	707	CLA	C16-C17-C18-C19
28	a	729	CLA	C11-C10-C8-C7
27	G	503	UIX	C36-C38-C40-C41
28	L	311	CLA	C4-C3-C5-C6
28	H	305	CLA	C2-C3-C5-C6
37	a	733	LHG	O2-C2-C3-O3
28	b	715	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
29	N	311	KC1	C2A-CAA-CBA-CGA
28	l	303	CLA	C14-C13-C15-C16
28	b	701	CLA	C11-C12-C13-C14
28	b	724	CLA	C14-C13-C15-C16
28	B	311	CLA	C11-C10-C8-C9
26	K	301	DD6	C24-C25-C26-C27
27	J	305	UIX	C26-C30-C34-C37
28	A	310	CLA	C13-C15-C16-C17
28	B	316	CLA	C2C-C3C-CAC-CBC
28	B	307	CLA	O2A-C1-C2-C3
30	G	501	DGD	O1G-C1G-C2G-C3G
28	A	308	CLA	C2A-CAA-CBA-CGA
28	b	725	CLA	C2A-CAA-CBA-CGA
28	L	314	CLA	C2A-CAA-CBA-CGA
28	I	316	CLA	O1A-CGA-O2A-C1
28	l	312	CLA	O1A-CGA-O2A-C1
26	h	203	DD6	C27-C29-C30-C31
26	b	731	DD6	C27-C29-C30-C31
26	B	302	DD6	C27-C29-C30-C31
26	L	302	DD6	C27-C29-C30-C31
28	b	720	CLA	C4-C3-C5-C6
28	L	313	CLA	C4-C3-C5-C6
31	j	101	LMG	C4-C5-C6-O5
28	l	308	CLA	C4B-C3B-CAB-CBB
28	l	309	CLA	C4B-C3B-CAB-CBB
28	a	702	CLA	C4B-C3B-CAB-CBB
28	a	712	CLA	C4B-C3B-CAB-CBB
28	b	723	CLA	C4B-C3B-CAB-CBB
28	F	307	CLA	C4B-C3B-CAB-CBB
28	M	312	CLA	C4B-C3B-CAB-CBB
28	b	715	CLA	O1A-CGA-O2A-C1
37	a	733	LHG	O10-C23-O8-C6
28	B	308	CLA	CAA-CBA-CGA-O2A
28	l	305	CLA	CAA-CBA-CGA-O2A
28	a	729	CLA	CAA-CBA-CGA-O2A
28	A	316	CLA	O1A-CGA-O2A-C1
28	a	703	CLA	C6-C7-C8-C10
28	b	714	CLA	CAA-CBA-CGA-O1A
32	D	304	PID	CM4-C14-C15-C16
28	a	710	CLA	C6-C7-C8-C10
28	a	728	CLA	C5-C6-C7-C8
28	B	309	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
31	b	733	LMG	C17-C18-C19-C20
28	l	303	CLA	C13-C15-C16-C17
28	a	725	CLA	CBA-CGA-O2A-C1
28	I	312	CLA	C6-C7-C8-C9
28	A	310	CLA	C6-C7-C8-C9
28	a	702	CLA	C11-C12-C13-C14
28	b	717	CLA	C6-C7-C8-C9
28	G	509	CLA	O1A-CGA-O2A-C1
28	a	725	CLA	O1A-CGA-O2A-C1
30	j	103	DGD	C2G-C3G-O3G-C1D
31	b	733	LMG	C8-C7-O1-C1
28	b	720	CLA	C2A-CAA-CBA-CGA
28	J	309	CLA	C2A-CAA-CBA-CGA
28	a	703	CLA	C2-C1-O2A-CGA
28	b	725	CLA	C2-C1-O2A-CGA
28	M	309	CLA	C2-C1-O2A-CGA
28	H	305	CLA	C16-C17-C18-C19
28	l	311	CLA	C3A-C2A-CAA-CBA
28	H	307	CLA	C3A-C2A-CAA-CBA
28	L	318	CLA	C3A-C2A-CAA-CBA
28	M	311	CLA	C3A-C2A-CAA-CBA
28	b	707	CLA	C2-C3-C5-C6
28	a	715	CLA	CAA-CBA-CGA-O2A
28	a	727	CLA	O1D-CGD-O2D-CED
31	I	320	LMG	C9-C8-O7-C10
28	a	711	CLA	CAA-CBA-CGA-O2A
28	A	316	CLA	CBA-CGA-O2A-C1
26	K	301	DD6	C13-C14-C15-O1
26	K	305	DD6	C13-C14-C15-O1
26	K	319	DD6	C13-C14-C15-O1
26	A	302	DD6	C13-C14-C15-O1
26	M	306	DD6	C13-C14-C15-O1
27	I	304	UIX	O-C-C7-C10
32	F	305	PID	O1-C6-C7-C8
32	M	301	PID	O1-C6-C7-C8
32	N	301	PID	O1-C6-C7-C8
28	a	711	CLA	CAA-CBA-CGA-O1A
31	D	317	LMG	C16-C17-C18-C19
28	G	520	CLA	O2A-C1-C2-C3
28	G	509	CLA	CBA-CGA-O2A-C1
28	I	315	CLA	C2C-C3C-CAC-CBC
31	K	318	LMG	C18-C19-C20-C21

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Mol	Chain	Res	Type	Atoms
31	j	101	LMG	O1-C7-C8-C9
29	G	515	KC1	C4C-C3C-CAC-CBC
28	B	308	CLA	CAA-CBA-CGA-O1A
28	a	710	CLA	C2A-CAA-CBA-CGA
31	D	317	LMG	C20-C21-C22-C23
28	l	305	CLA	C15-C16-C17-C18
28	a	715	CLA	CAA-CBA-CGA-O1A
28	l	313	CLA	C3-C5-C6-C7
28	a	730	CLA	C3-C5-C6-C7
28	a	729	CLA	C6-C7-C8-C9
28	b	708	CLA	C11-C10-C8-C9
28	b	727	CLA	C14-C13-C15-C16
28	B	311	CLA	C11-C12-C13-C14
28	b	725	CLA	C16-C17-C18-C20
26	A	302	DD6	C5-C6-C8-C9
28	m	202	CLA	CAA-CBA-CGA-O2A
28	B	310	CLA	CAA-CBA-CGA-O2A
28	I	308	CLA	C11-C12-C13-C15
28	a	731	CLA	C16-C17-C18-C19
28	G	517	CLA	C2A-CAA-CBA-CGA
28	a	702	CLA	C11-C12-C13-C15
28	a	707	CLA	C11-C10-C8-C7
28	a	721	CLA	C12-C13-C15-C16
28	b	701	CLA	C11-C12-C13-C15
28	b	724	CLA	C12-C13-C15-C16
28	B	311	CLA	C11-C10-C8-C7
30	j	103	DGD	O6D-C5D-C6D-O5D
28	a	701	CLA	C2B-C3B-CAB-CBB
28	a	702	CLA	C2B-C3B-CAB-CBB
28	a	715	CLA	C2B-C3B-CAB-CBB
28	a	721	CLA	C2B-C3B-CAB-CBB
28	H	311	CLA	C2B-C3B-CAB-CBB
28	M	308	CLA	C2B-C3B-CAB-CBB
35	l	306	BCR	C5-C6-C7-C8
35	l	306	BCR	C23-C24-C25-C26
28	b	713	CLA	CAA-CBA-CGA-O2A
28	f	301	CLA	C2-C1-O2A-CGA
26	I	302	DD6	C11-C13-C14-C15
26	D	303	DD6	C11-C13-C14-C15
32	F	304	PID	C6-C7-C8-C9
30	l	301	DGD	C3A-C4A-C5A-C6A
28	b	724	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
28	J	312	CLA	CBD-CGD-O2D-CED
28	L	317	CLA	CAA-CBA-CGA-O2A
28	l	305	CLA	O1A-CGA-O2A-C1
28	b	722	CLA	C2A-CAA-CBA-CGA
31	K	318	LMG	C19-C20-C21-C22
28	I	319	CLA	CAA-CBA-CGA-O2A
28	I	309	CLA	O1A-CGA-O2A-C1
28	I	308	CLA	CAA-CBA-CGA-O2A
28	G	511	CLA	CAA-CBA-CGA-O2A
28	a	717	CLA	CAA-CBA-CGA-O2A
28	a	723	CLA	CAA-CBA-CGA-O2A
31	I	320	LMG	O8-C28-C29-C30
28	A	310	CLA	CAA-CBA-CGA-O2A
28	l	310	CLA	CAA-CBA-CGA-O2A
28	a	706	CLA	CAA-CBA-CGA-O2A
31	D	317	LMG	C36-C37-C38-C39
28	l	313	CLA	C4-C3-C5-C6
31	j	101	LMG	C10-C11-C12-C13
28	I	316	CLA	CAA-CBA-CGA-O2A
28	L	309	CLA	C5-C6-C7-C8
28	a	717	CLA	C2-C3-C5-C6
28	D	309	CLA	CAA-CBA-CGA-O2A
28	l	305	CLA	CBA-CGA-O2A-C1
28	I	306	CLA	O2A-C1-C2-C3
32	D	302	PID	C28-C27-O6-C30
28	a	723	CLA	C11-C10-C8-C9
28	a	735	CLA	C14-C13-C15-C16
28	B	309	CLA	C11-C10-C8-C9
28	J	307	CLA	C11-C10-C8-C9
35	m	201	BCR	C37-C22-C23-C24
28	J	310	CLA	CAA-CBA-CGA-O2A
28	K	312	CLA	C4B-C3B-CAB-CBB
28	K	316	CLA	C4B-C3B-CAB-CBB
28	A	307	CLA	C4B-C3B-CAB-CBB
28	A	316	CLA	C4B-C3B-CAB-CBB
28	a	701	CLA	C4B-C3B-CAB-CBB
28	a	715	CLA	C4B-C3B-CAB-CBB
28	a	727	CLA	C4B-C3B-CAB-CBB
28	b	705	CLA	C4B-C3B-CAB-CBB
28	b	711	CLA	C4B-C3B-CAB-CBB
28	b	728	CLA	C1A-C2A-CAA-CBA
28	B	309	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
28	J	309	CLA	C4B-C3B-CAB-CBB
28	J	316	CLA	C4B-C3B-CAB-CBB
28	M	308	CLA	C4B-C3B-CAB-CBB
28	a	706	CLA	C10-C11-C12-C13
28	M	316	CLA	CAA-CBA-CGA-O2A
27	G	503	UIX	C36-C38-C40-C39
28	I	309	CLA	CBA-CGA-O2A-C1
28	K	309	CLA	CAA-CBA-CGA-O2A
28	G	514	CLA	CAA-CBA-CGA-O2A
28	b	708	CLA	CAA-CBA-CGA-O2A
28	b	711	CLA	CAA-CBA-CGA-O2A
28	A	313	CLA	C2A-CAA-CBA-CGA
28	a	735	CLA	C2A-CAA-CBA-CGA
28	G	511	CLA	C6-C7-C8-C10
28	b	713	CLA	C13-C15-C16-C17
30	G	501	DGD	C2A-C3A-C4A-C5A
28	N	307	CLA	C2-C3-C5-C6
30	y	201	DGD	C2A-C3A-C4A-C5A
28	I	308	CLA	C2-C1-O2A-CGA
28	I	321	CLA	C2-C1-O2A-CGA
28	G	514	CLA	C2-C1-O2A-CGA
28	A	309	CLA	C2-C1-O2A-CGA
28	L	313	CLA	C2-C1-O2A-CGA
28	a	722	CLA	C6-C7-C8-C10
28	a	725	CLA	C6-C7-C8-C10
28	b	717	CLA	C11-C12-C13-C15
28	b	701	CLA	C8-C10-C11-C12
28	a	726	CLA	C5-C6-C7-C8
28	I	316	CLA	CBA-CGA-O2A-C1
28	B	316	CLA	C4C-C3C-CAC-CBC
28	I	321	CLA	C2A-CAA-CBA-CGA
28	l	305	CLA	C2A-CAA-CBA-CGA
28	J	307	CLA	C2A-CAA-CBA-CGA
28	M	313	CLA	C2A-CAA-CBA-CGA
28	b	705	CLA	C5-C6-C7-C8
28	J	312	CLA	O1D-CGD-O2D-CED
28	b	724	CLA	C16-C17-C18-C20
28	B	309	CLA	C16-C17-C18-C19
30	I	317	DGD	O6D-C5D-C6D-O5D
28	A	310	CLA	CAA-CBA-CGA-O1A
28	G	519	CLA	C4-C3-C5-C6
28	J	301	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
28	N	309	CLA	C3A-C2A-CAA-CBA
28	J	312	CLA	CAA-CBA-CGA-O2A
28	a	727	CLA	CBD-CGD-O2D-CED
28	m	202	CLA	CAA-CBA-CGA-O1A
28	a	717	CLA	CAA-CBA-CGA-O1A
28	j	106	CLA	O1A-CGA-O2A-C1
37	a	733	LHG	C31-C32-C33-C34
30	j	103	DGD	C1A-C2A-C3A-C4A
28	I	319	CLA	CAA-CBA-CGA-O1A
28	I	308	CLA	CAA-CBA-CGA-O1A
28	a	706	CLA	CAA-CBA-CGA-O1A
28	B	310	CLA	CAA-CBA-CGA-O1A
28	J	311	CLA	C2-C1-O2A-CGA
28	G	510	CLA	C6-C7-C8-C9
28	a	724	CLA	C14-C13-C15-C16
28	a	725	CLA	C6-C7-C8-C9
28	B	301	CLA	C11-C10-C8-C9
28	K	308	CLA	CAA-CBA-CGA-O2A
28	b	724	CLA	CAA-CBA-CGA-O1A
28	J	308	CLA	CAA-CBA-CGA-O1A
30	y	201	DGD	C2B-C3B-C4B-C5B
28	b	713	CLA	CAA-CBA-CGA-O1A
28	J	310	CLA	CAA-CBA-CGA-O1A
28	M	316	CLA	CAA-CBA-CGA-O1A
28	b	706	CLA	CAA-CBA-CGA-O2A
28	G	519	CLA	C11-C12-C13-C14
29	I	314	KC1	C1A-C2A-CAA-CBA
29	K	314	KC1	C3A-C2A-CAA-CBA
29	A	306	KC1	C3A-C2A-CAA-CBA
29	D	310	KC1	C1A-C2A-CAA-CBA
29	D	315	KC1	C3A-C2A-CAA-CBA
29	F	309	KC1	C3A-C2A-CAA-CBA
29	H	306	KC1	C1A-C2A-CAA-CBA
29	J	313	KC1	C1A-C2A-CAA-CBA
29	J	313	KC1	C3A-C2A-CAA-CBA
29	M	314	KC1	C1A-C2A-CAA-CBA
29	N	311	KC1	C1A-C2A-CAA-CBA
28	I	316	CLA	CAA-CBA-CGA-O1A
28	D	312	CLA	CBD-CGD-O2D-CED
35	l	302	BCR	C17-C18-C19-C20
28	a	723	CLA	CAA-CBA-CGA-O1A
31	K	317	LMG	C8-C7-O1-C1

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Mol	Chain	Res	Type	Atoms
31	K	318	LMG	C8-C7-O1-C1
28	G	511	CLA	CAA-CBA-CGA-O1A
28	D	309	CLA	CAA-CBA-CGA-O1A
31	B	318	LMG	O9-C10-C11-C12
28	l	303	CLA	C2A-CAA-CBA-CGA
28	l	311	CLA	C2A-CAA-CBA-CGA
28	a	703	CLA	C2A-CAA-CBA-CGA
28	M	309	CLA	C2A-CAA-CBA-CGA
29	F	314	KC1	CAA-CBA-CGA-O2A
28	b	715	CLA	C8-C10-C11-C12
28	a	731	CLA	CAA-CBA-CGA-O2A
28	N	310	CLA	C2-C1-O2A-CGA
31	K	318	LMG	C16-C17-C18-C19
28	l	310	CLA	CAA-CBA-CGA-O1A
31	I	320	LMG	O9-C10-C11-C12
28	K	311	CLA	CAD-CBD-CGD-O2D
28	G	517	CLA	CAD-CBD-CGD-O2D
28	f	302	CLA	CAD-CBD-CGD-O2D
28	l	310	CLA	CAD-CBD-CGD-O2D
28	B	316	CLA	CAD-CBD-CGD-O2D
28	H	307	CLA	CAD-CBD-CGD-O2D
28	J	316	CLA	CAD-CBD-CGD-O2D
32	D	302	PID	O4-C12-C13-C14
28	A	309	CLA	CAA-CBA-CGA-O2A
28	G	514	CLA	CAA-CBA-CGA-O1A
28	b	708	CLA	CAA-CBA-CGA-O1A
28	J	312	CLA	CAA-CBA-CGA-O1A
28	L	317	CLA	CAA-CBA-CGA-O1A
30	l	301	DGD	O6D-C5D-C6D-O5D
28	j	106	CLA	C2-C1-O2A-CGA
28	M	308	CLA	C2-C1-O2A-CGA
31	I	320	LMG	O10-C28-C29-C30
28	G	512	CLA	CAA-CBA-CGA-O2A
28	M	317	CLA	C2A-CAA-CBA-CGA
28	K	309	CLA	CAA-CBA-CGA-O1A
28	b	711	CLA	CAA-CBA-CGA-O1A
28	h	202	CLA	CAA-CBA-CGA-O2A
28	a	718	CLA	CAA-CBA-CGA-O2A
28	L	311	CLA	CAA-CBA-CGA-O2A
28	M	309	CLA	CAA-CBA-CGA-O2A
28	b	725	CLA	C16-C17-C18-C19
28	M	315	CLA	C2C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
28	K	310	CLA	CAA-CBA-CGA-O2A
28	a	703	CLA	CAA-CBA-CGA-O2A
28	b	705	CLA	CAA-CBA-CGA-O2A
28	D	312	CLA	O1D-CGD-O2D-CED
31	b	733	LMG	C10-C11-C12-C13
27	K	302	UIX	C19-C18-O2-C27
27	G	503	UIX	C17-C18-O2-C27

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
32	G	507	PID	C24-C25-C26-C27-C28-C29

238 monomers are involved in 601 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
28	N	309	CLA	4	0
28	M	316	CLA	1	0
28	L	313	CLA	7	0
28	a	723	CLA	7	0
28	b	710	CLA	6	0
28	F	315	CLA	1	0
28	K	313	CLA	5	0
32	G	507	PID	5	0
32	D	304	PID	2	0
28	M	309	CLA	7	0
31	I	320	LMG	1	0
28	H	304	CLA	3	0
26	L	304	DD6	1	0
28	l	312	CLA	2	0
28	M	308	CLA	2	0
28	H	308	CLA	2	0
28	L	316	CLA	1	0
31	j	101	LMG	5	0
28	B	308	CLA	1	0
28	L	312	CLA	1	0
28	I	308	CLA	4	0
28	a	728	CLA	3	0
28	B	310	CLA	1	0
28	a	729	CLA	3	0
28	b	715	CLA	5	0
26	L	305	DD6	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
28	F	307	CLA	1	0
28	I	312	CLA	2	0
28	a	718	CLA	1	0
28	a	725	CLA	5	0
28	A	319	CLA	1	0
26	M	303	DD6	2	0
28	N	305	CLA	2	0
27	I	304	UIX	2	0
32	F	305	PID	3	0
28	L	314	CLA	3	0
28	H	311	CLA	2	0
36	a	732	PQN	5	0
28	B	313	CLA	4	0
29	F	309	KC1	2	0
28	l	311	CLA	5	0
28	a	708	CLA	2	0
28	G	517	CLA	6	0
28	K	307	CLA	1	0
28	a	713	CLA	3	0
28	J	311	CLA	2	0
28	D	314	CLA	10	0
28	a	735	CLA	5	0
30	L	301	DGD	2	0
28	G	511	CLA	2	0
29	H	310	KC1	1	0
28	M	312	CLA	1	0
28	D	308	CLA	1	0
28	l	313	CLA	6	0
28	M	318	CLA	1	0
35	a	734	BCR	3	0
32	D	305	PID	3	0
26	G	505	DD6	1	0
28	B	316	CLA	1	0
28	b	703	CLA	6	0
30	y	201	DGD	1	0
28	a	716	CLA	3	0
28	a	705	CLA	2	0
28	G	520	CLA	3	0
28	M	317	CLA	2	0
28	b	708	CLA	2	0
28	K	308	CLA	3	0
28	A	308	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	j	103	DGD	4	0
28	D	311	CLA	2	0
28	a	724	CLA	3	0
28	a	720	CLA	2	0
33	A	318	SQD	8	0
28	b	718	CLA	4	0
28	a	707	CLA	7	0
28	f	302	CLA	4	0
28	A	312	CLA	3	0
26	I	301	DD6	1	0
28	A	310	CLA	4	0
28	a	706	CLA	7	0
28	l	303	CLA	5	0
35	l	307	BCR	4	0
28	f	301	CLA	5	0
34	a	737	SF4	1	0
28	I	310	CLA	3	0
28	a	702	CLA	5	0
28	l	305	CLA	4	0
27	J	305	UIX	1	0
37	a	733	LHG	3	0
32	F	306	PID	2	0
28	m	202	CLA	2	0
28	D	309	CLA	2	0
28	G	519	CLA	1	0
35	a	736	BCR	2	0
26	A	303	DD6	1	0
28	I	319	CLA	2	0
32	N	302	PID	2	0
28	K	309	CLA	2	0
29	M	307	KC1	1	0
28	b	709	CLA	7	0
28	K	310	CLA	1	0
28	A	315	CLA	1	0
28	b	707	CLA	5	0
28	I	306	CLA	2	0
28	K	316	CLA	1	0
26	J	303	DD6	2	0
28	a	703	CLA	5	0
28	J	312	CLA	2	0
28	H	307	CLA	1	0
35	b	730	BCR	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
28	a	731	CLA	6	0
28	f	303	CLA	1	0
28	L	309	CLA	2	0
28	a	726	CLA	6	0
28	I	307	CLA	2	0
28	K	311	CLA	2	0
28	a	727	CLA	1	0
28	I	309	CLA	1	0
28	b	706	CLA	3	0
28	A	313	CLA	4	0
28	l	308	CLA	1	0
28	b	712	CLA	4	0
28	B	307	CLA	1	0
26	J	304	DD6	3	0
28	G	518	CLA	1	0
28	j	106	CLA	3	0
28	J	307	CLA	11	0
28	l	310	CLA	1	0
32	F	304	PID	6	0
28	b	728	CLA	3	0
28	J	301	CLA	5	0
35	b	732	BCR	4	0
28	a	722	CLA	5	0
28	A	316	CLA	1	0
28	H	312	CLA	1	0
28	B	311	CLA	2	0
28	G	513	CLA	4	0
28	D	313	CLA	1	0
28	I	311	CLA	5	0
28	A	309	CLA	2	0
27	A	304	UIX	1	0
26	A	305	DD6	1	0
28	a	721	CLA	6	0
28	a	704	CLA	6	0
28	b	727	CLA	6	0
35	b	702	BCR	6	0
28	L	308	CLA	2	0
31	B	318	LMG	1	0
28	I	315	CLA	1	0
28	b	713	CLA	6	0
28	a	711	CLA	3	0
28	a	714	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	H	301	PID	3	0
32	G	506	PID	2	0
35	l	306	BCR	4	0
28	a	719	CLA	4	0
28	a	712	CLA	2	0
28	G	510	CLA	4	0
26	H	303	DD6	1	0
26	G	508	DD6	1	0
29	N	308	KC1	1	0
28	B	317	CLA	2	0
26	B	302	DD6	1	0
35	i	201	BCR	5	0
32	M	301	PID	1	0
29	D	310	KC1	1	0
28	I	316	CLA	3	0
28	F	308	CLA	1	0
31	D	317	LMG	5	0
28	I	313	CLA	3	0
31	b	733	LMG	2	0
28	G	514	CLA	3	0
32	D	301	PID	4	0
28	F	310	CLA	5	0
28	G	509	CLA	1	0
28	b	721	CLA	2	0
28	b	701	CLA	7	0
28	N	310	CLA	3	0
28	l	304	CLA	3	0
28	F	312	CLA	5	0
28	K	312	CLA	2	0
28	b	705	CLA	5	0
35	j	102	BCR	5	0
28	b	725	CLA	4	0
28	b	724	CLA	3	0
28	b	720	CLA	7	0
28	I	321	CLA	3	0
32	N	301	PID	1	0
26	G	504	DD6	3	0
28	H	305	CLA	4	0
28	N	307	CLA	1	0
28	J	310	CLA	3	0
28	a	717	CLA	4	0
28	B	301	CLA	3	0

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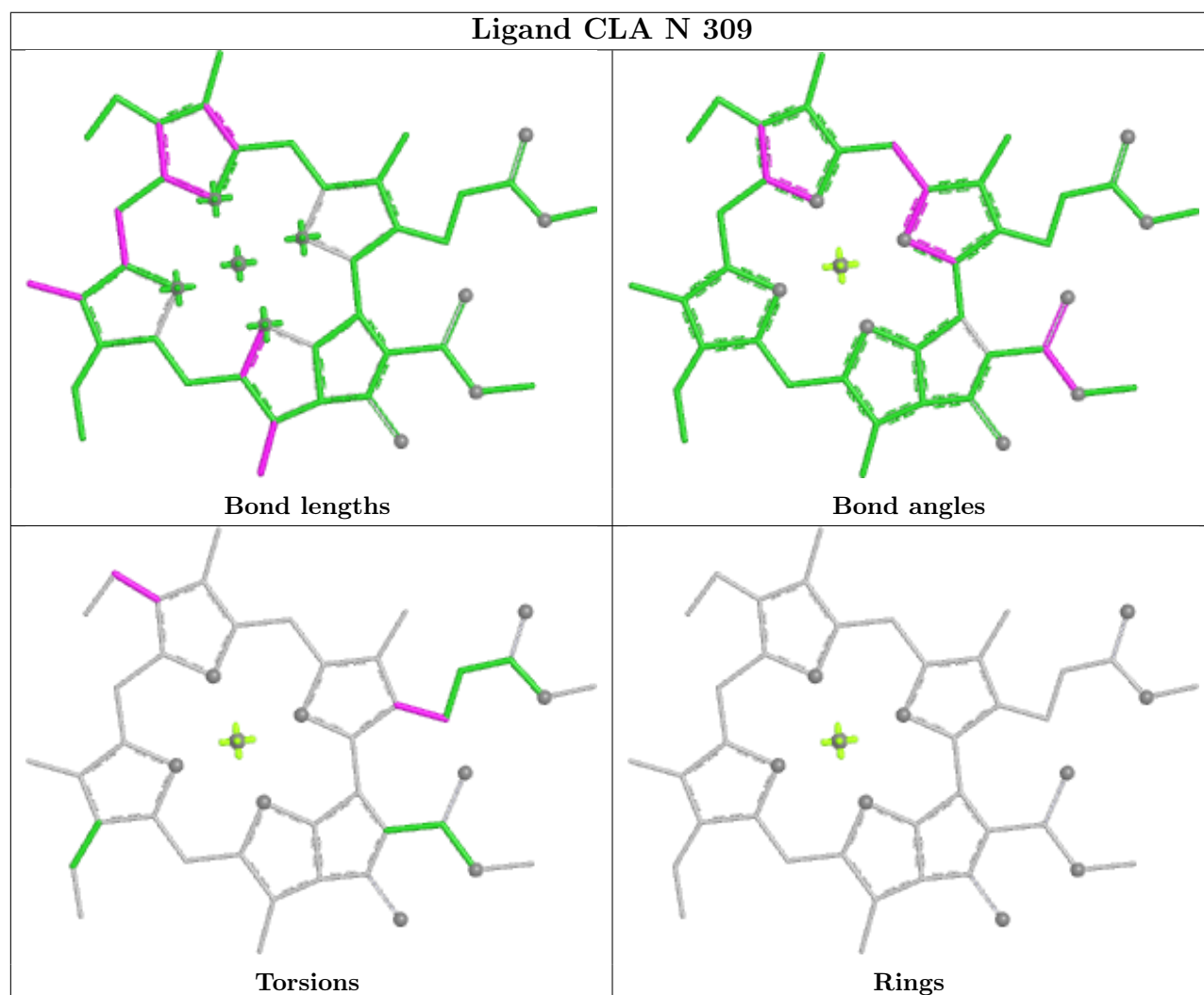
Mol	Chain	Res	Type	Clashes	Symm-Clashes
28	b	723	CLA	3	0
32	D	302	PID	2	0
26	I	305	DD6	1	0
28	H	309	CLA	2	0
28	M	315	CLA	2	0
28	J	308	CLA	3	0
36	b	729	PQN	4	0
32	j	105	PID	5	0
28	a	730	CLA	6	0
32	H	302	PID	5	0
28	a	738	CLA	1	0
30	G	501	DGD	2	0
35	m	201	BCR	5	0
35	l	302	BCR	3	0
26	F	301	DD6	1	0
28	D	312	CLA	2	0
28	F	313	CLA	8	0
28	a	710	CLA	4	0
28	J	309	CLA	3	0
28	A	320	CLA	3	0
28	J	306	CLA	1	0
28	F	311	CLA	1	0
28	j	104	CLA	5	0
28	b	704	CLA	15	0
28	b	716	CLA	3	0
28	b	717	CLA	6	0
28	M	310	CLA	2	0
32	F	302	PID	1	0
28	b	714	CLA	1	0
35	f	304	BCR	3	0
27	K	302	UIX	1	0
28	b	726	CLA	1	0
28	a	709	CLA	5	0
28	B	315	CLA	2	0
28	M	313	CLA	3	0
31	b	734	LMG	2	0
34	c	202	SF4	1	0
32	D	306	PID	1	0
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28	A	311	CLA	1	0
28	L	317	CLA	5	0
28	B	309	CLA	4	0

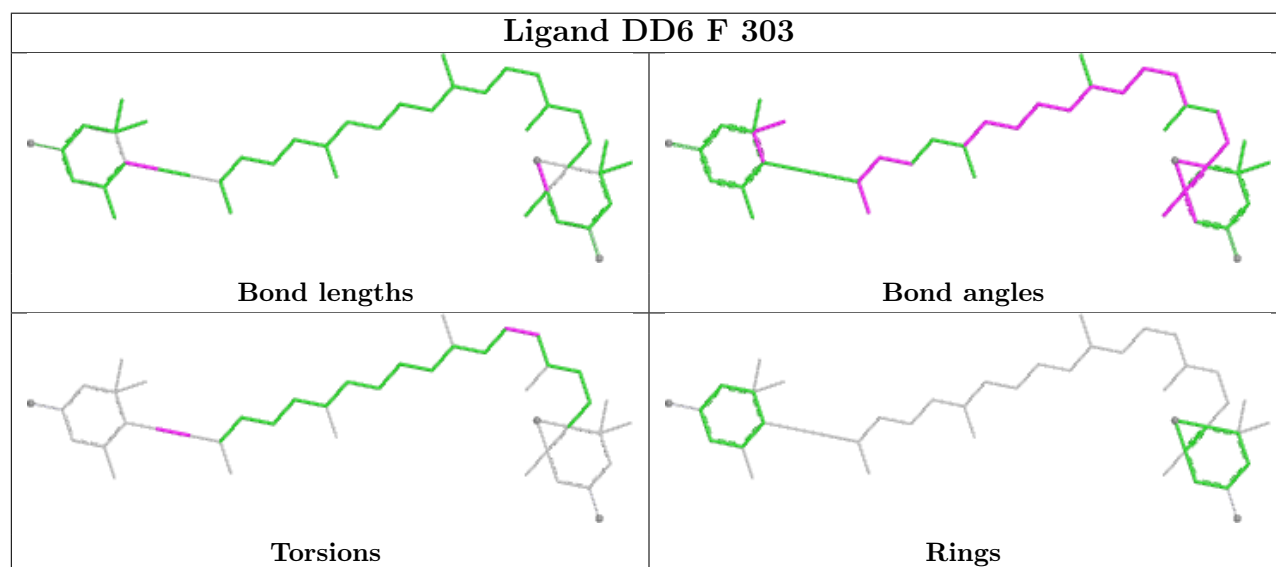
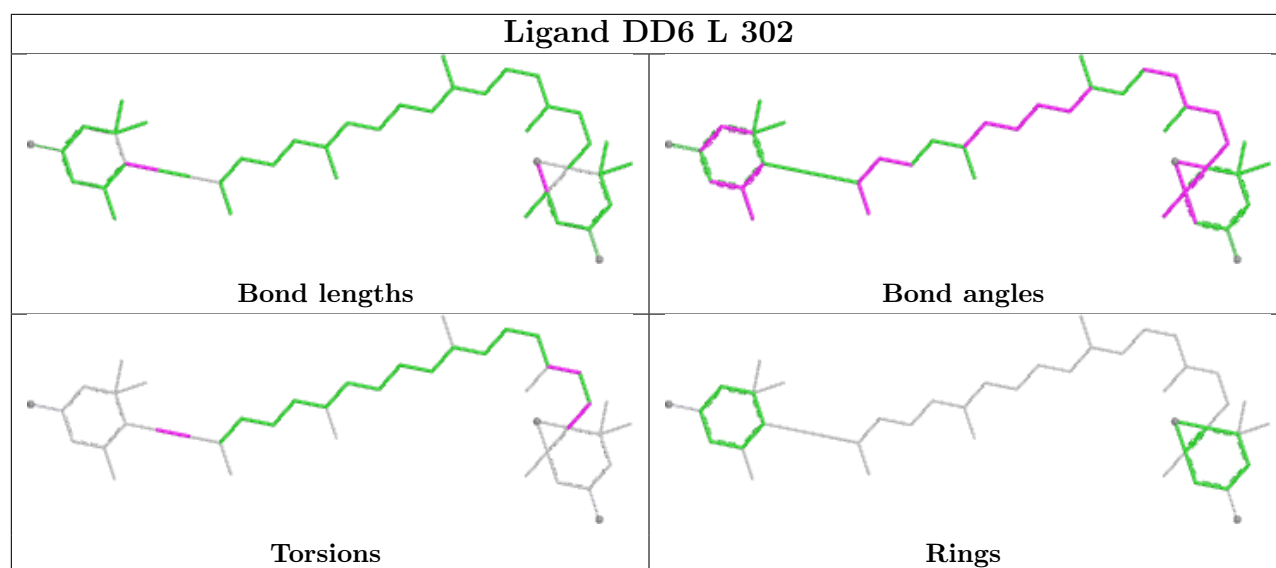
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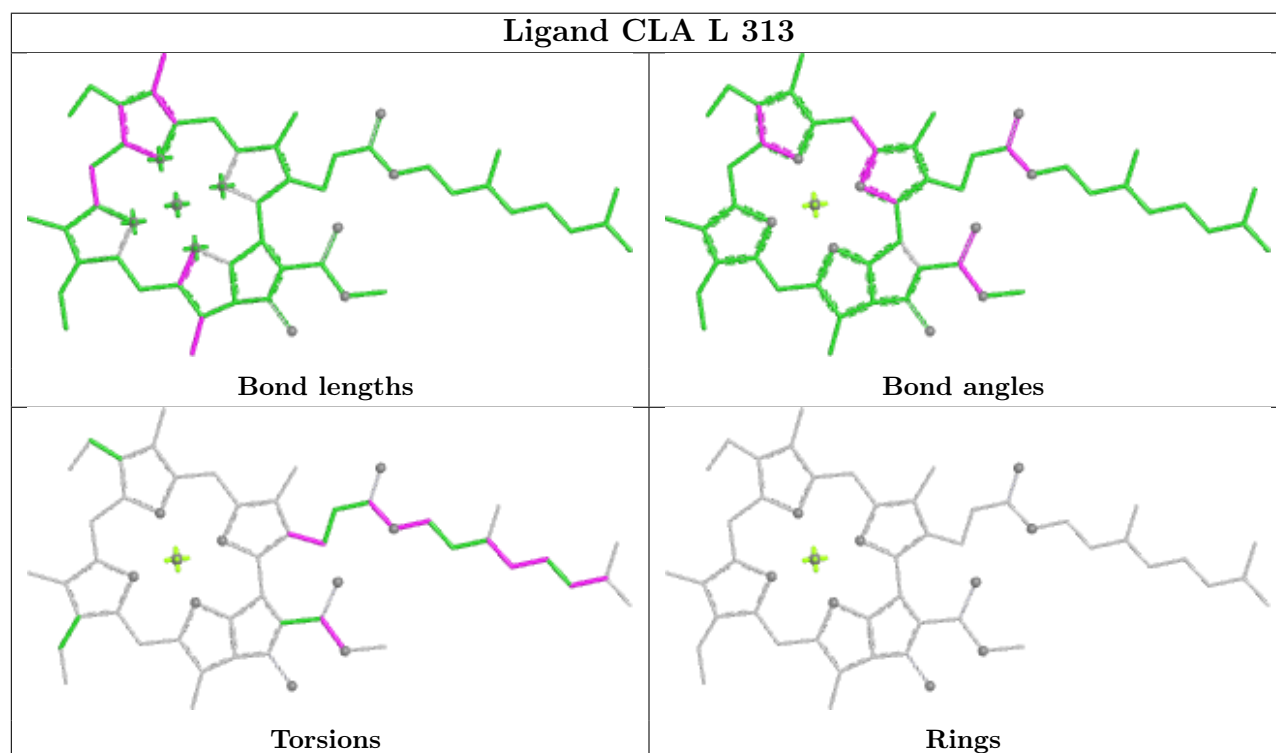
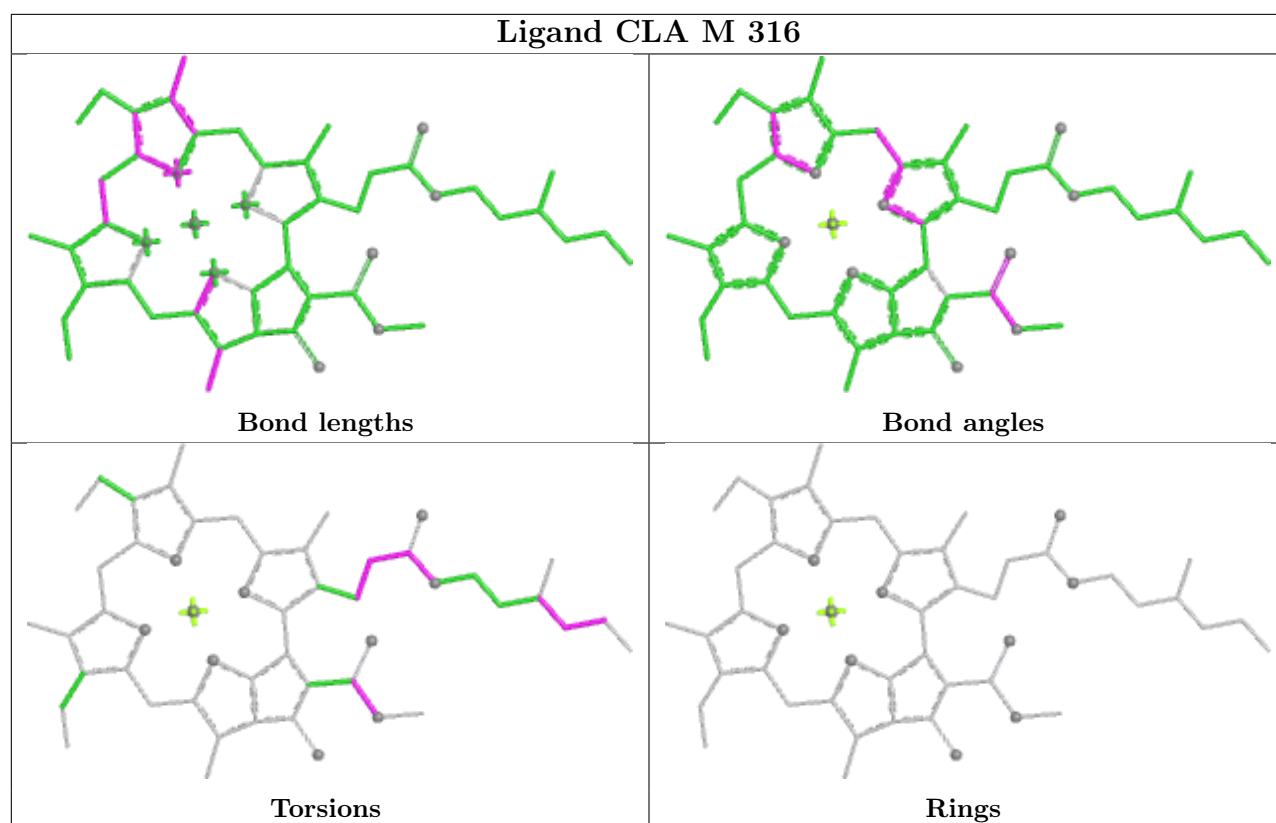
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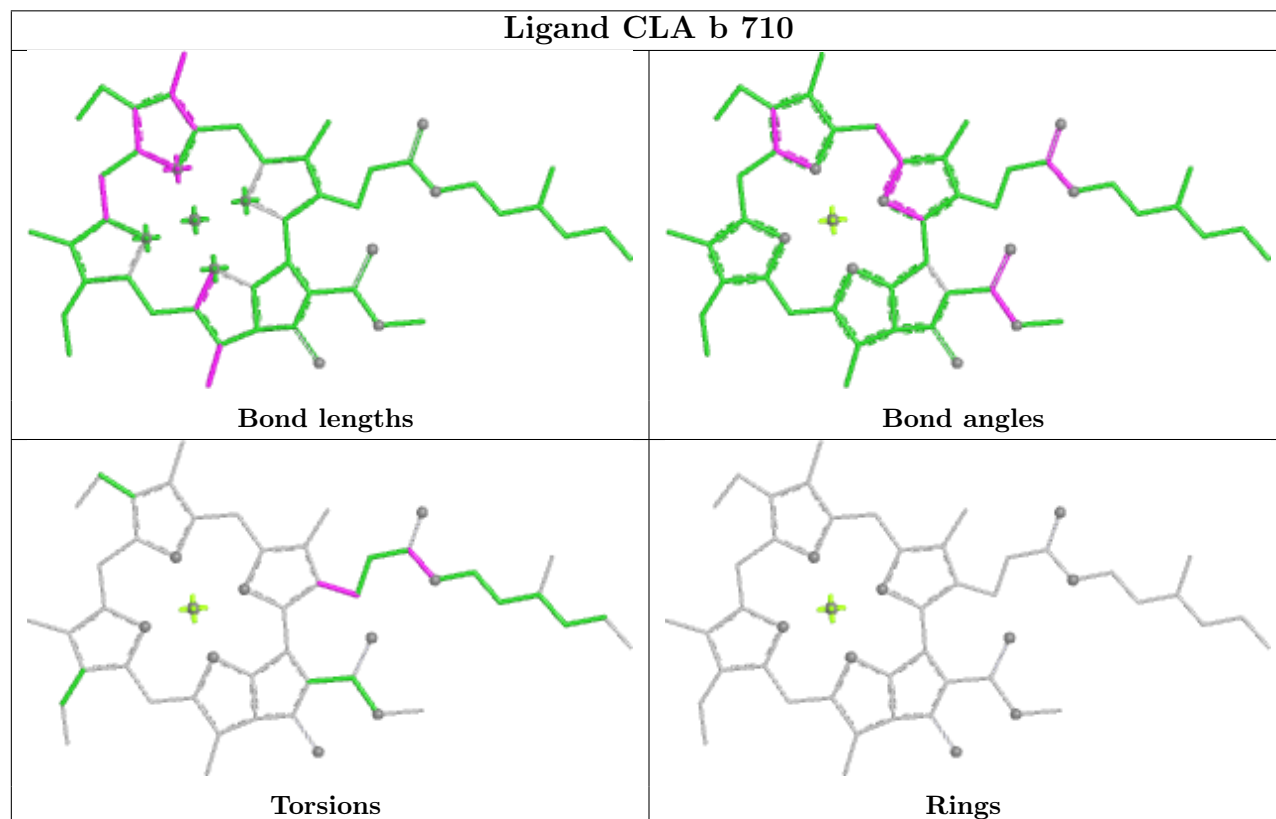
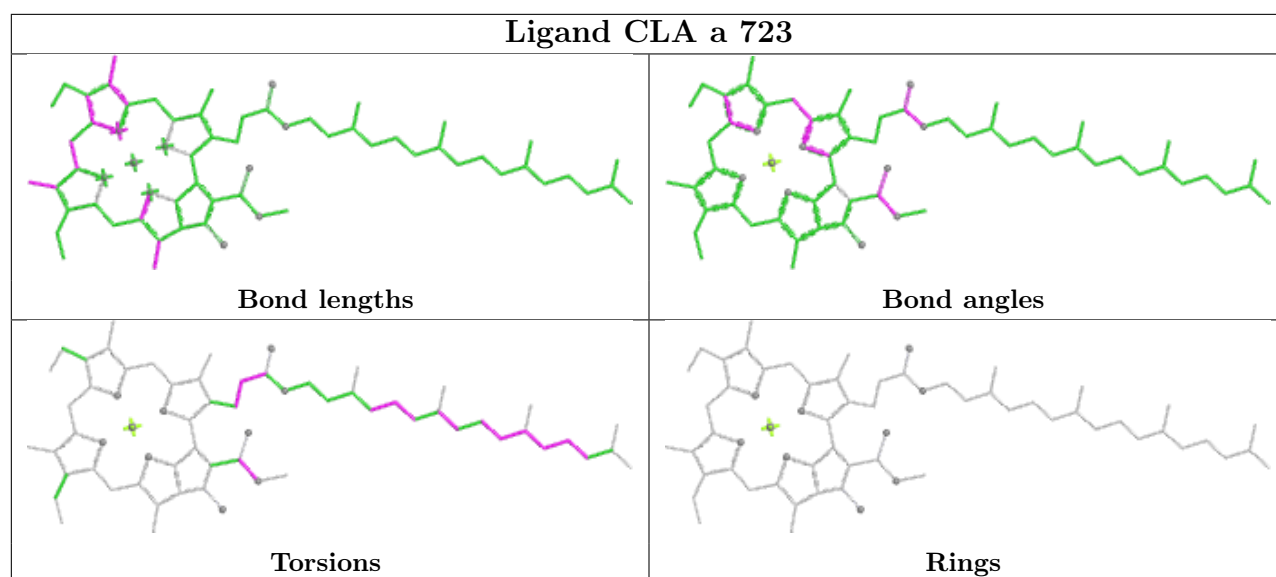
Mol	Chain	Res	Type	Clashes	Symm-Clashes
28	A	317	CLA	2	0
28	b	722	CLA	4	0

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

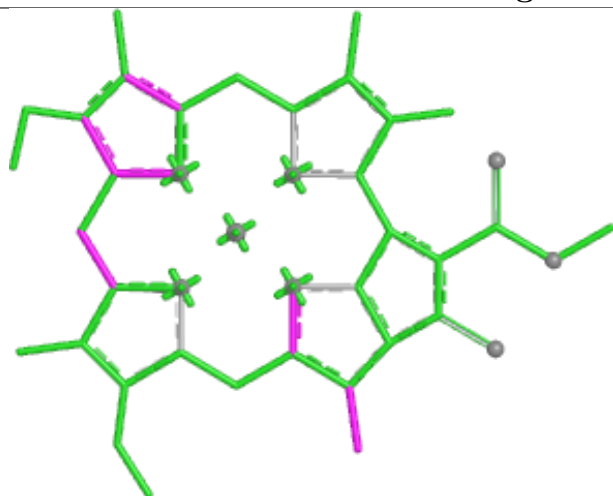




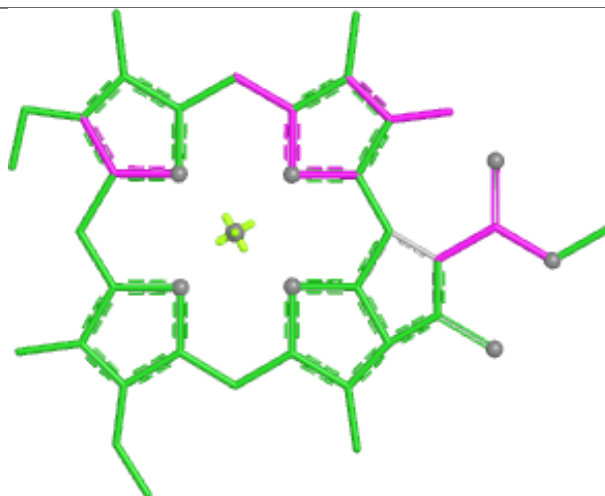




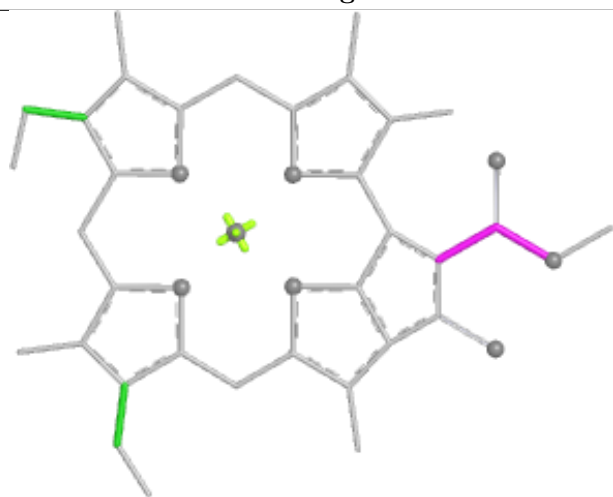
Ligand CLA F 315



Bond lengths



Bond angles

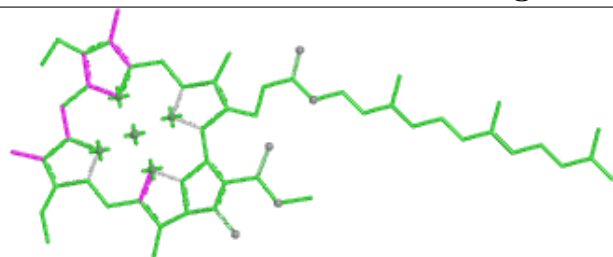


Torsions

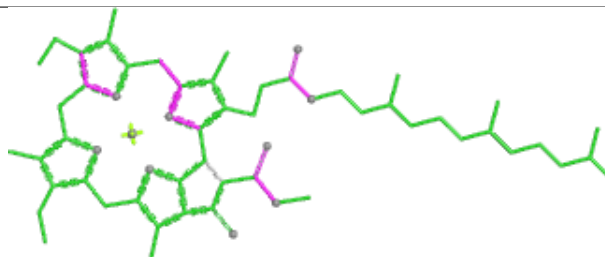


Rings

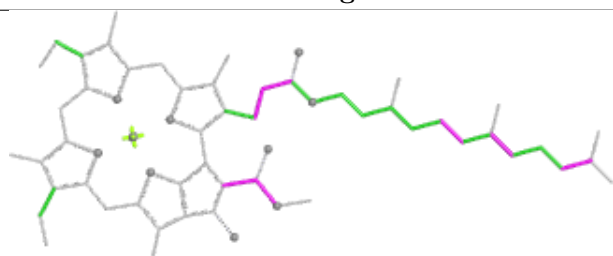
Ligand CLA G 512



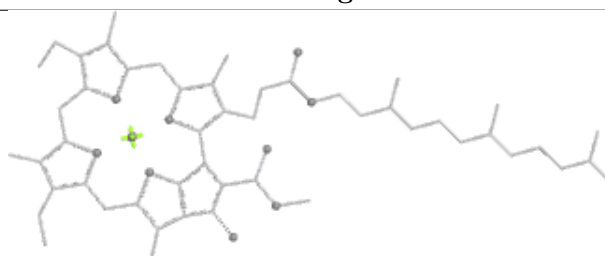
Bond lengths



Bond angles

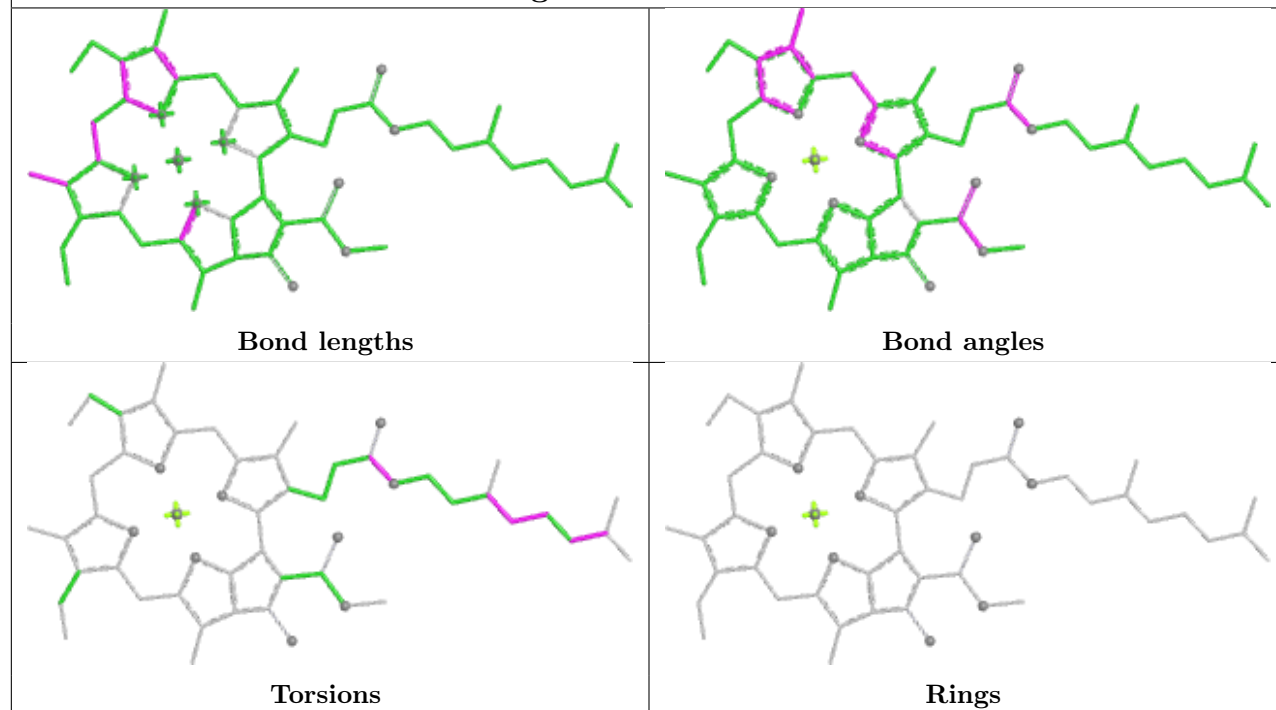


Torsions

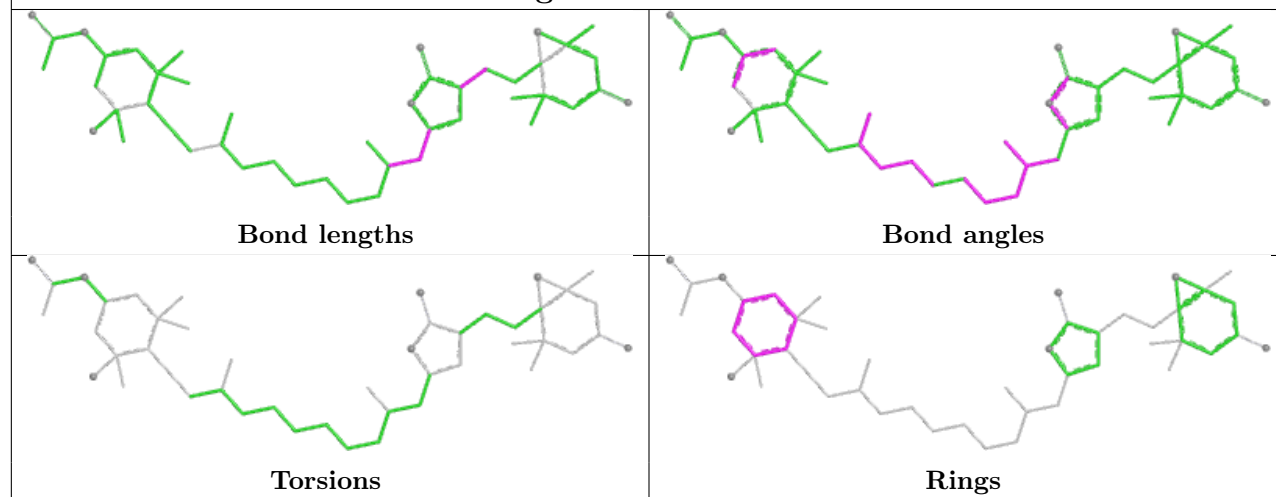


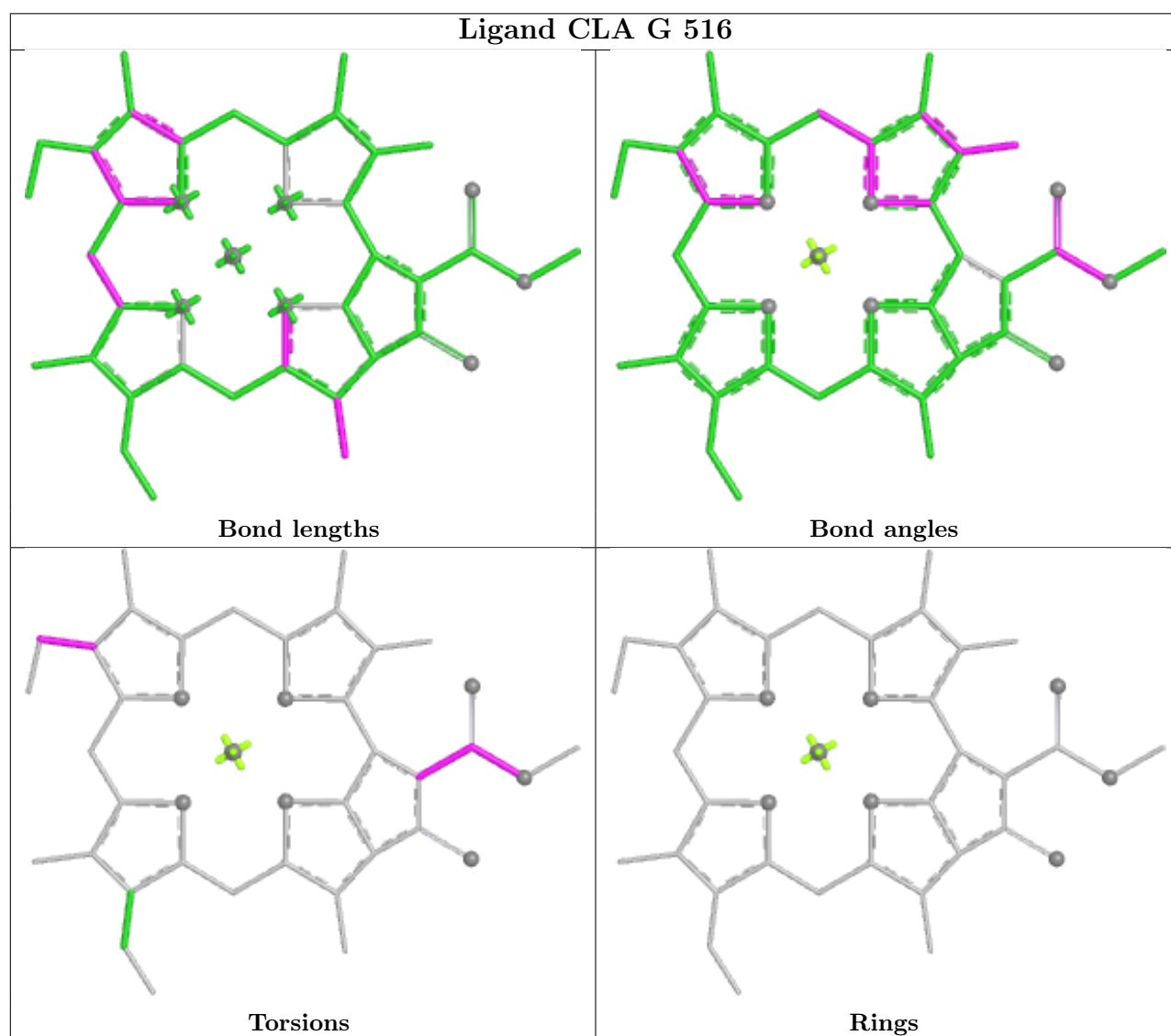
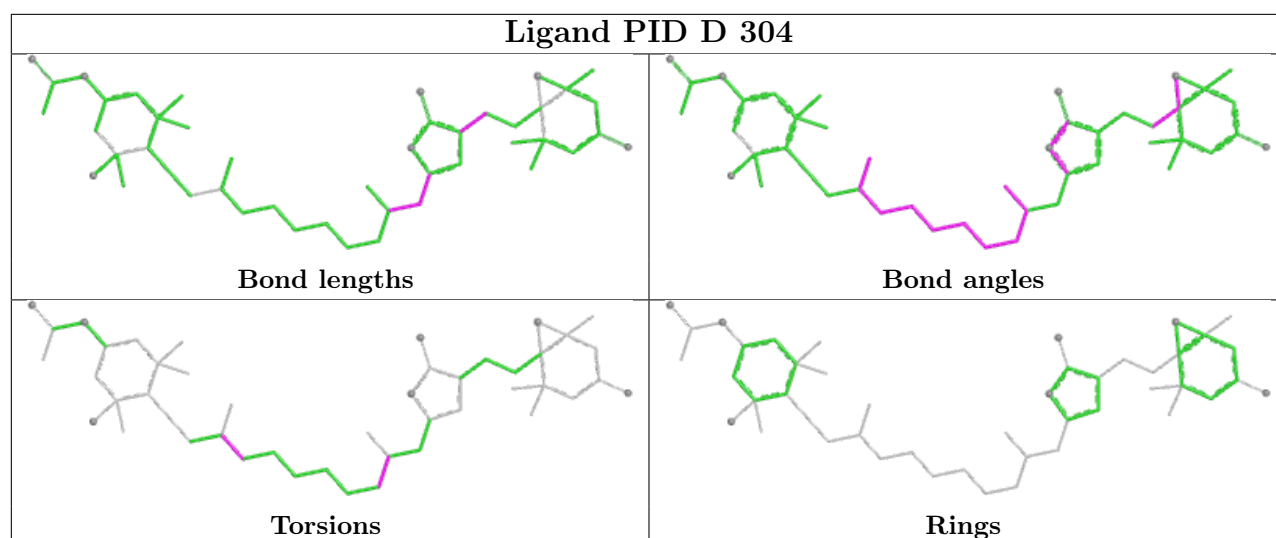
Rings

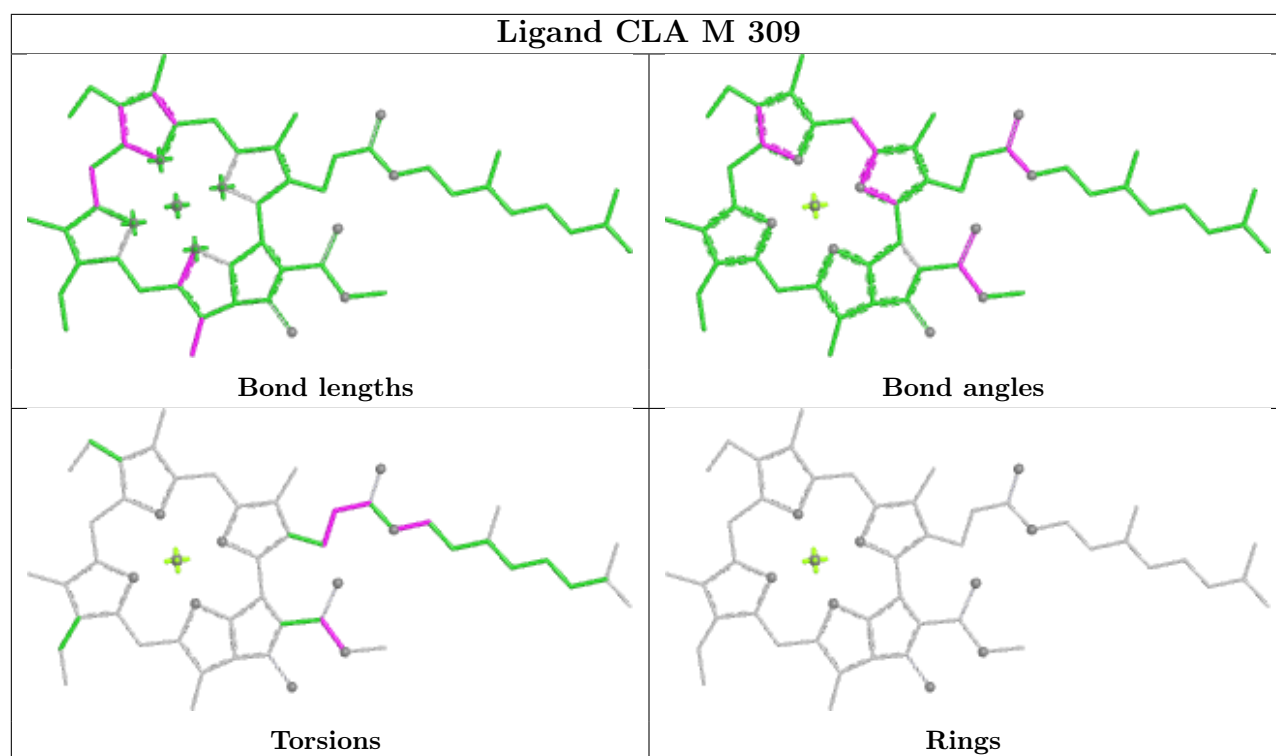
Ligand CLA K 313



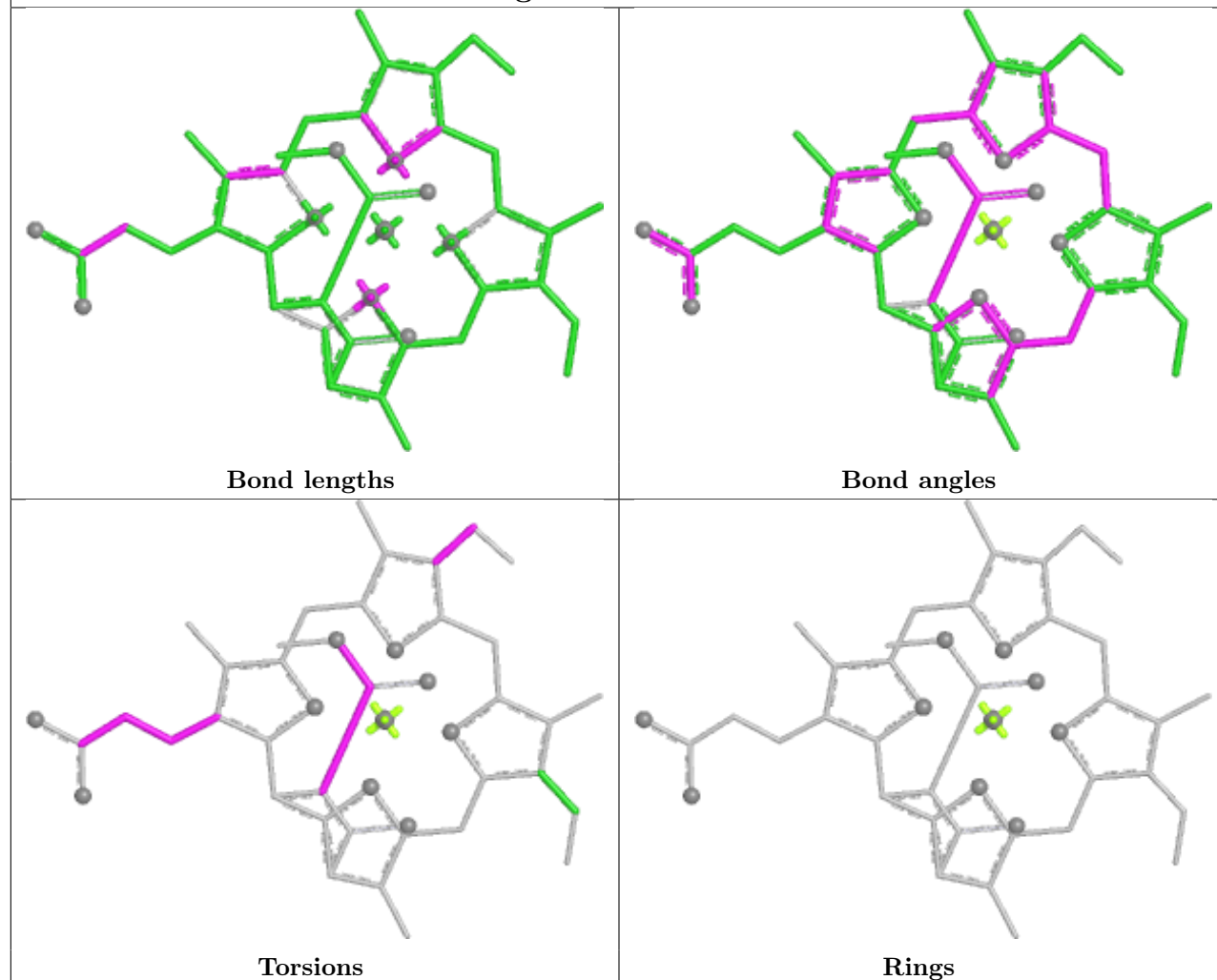
Ligand PID G 507



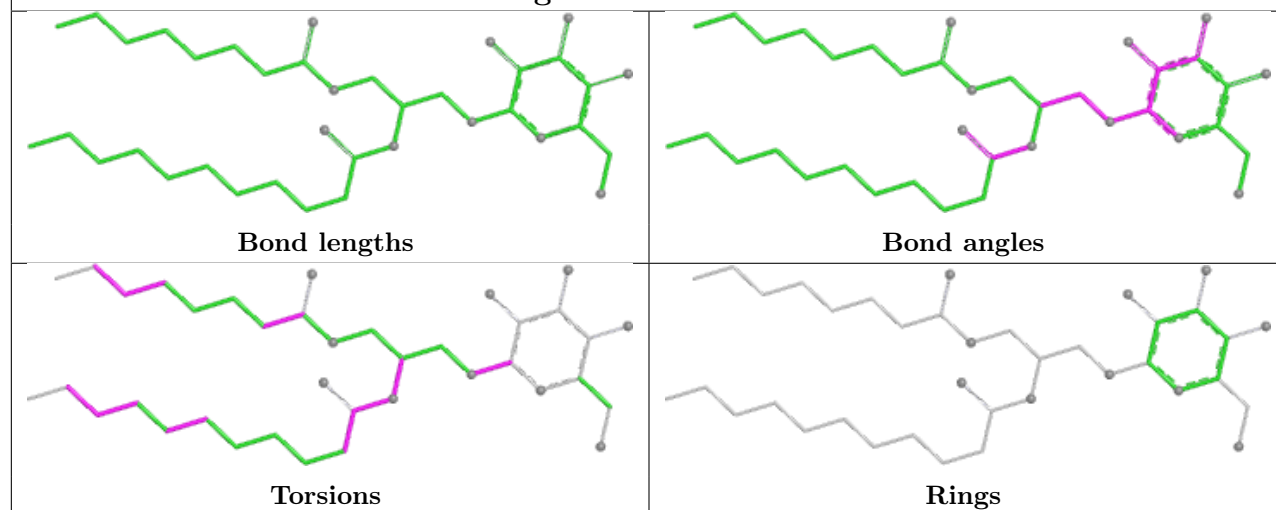




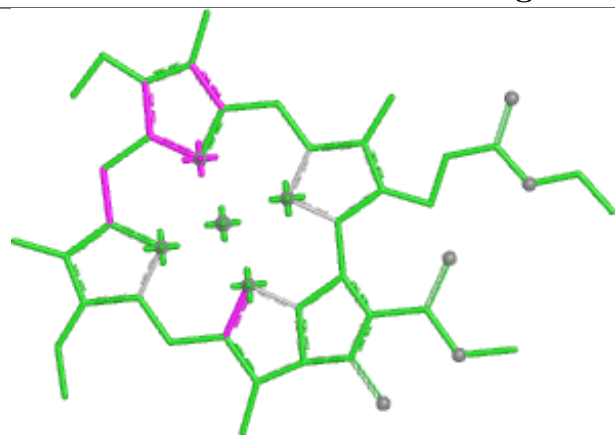
Ligand KC1 I 314



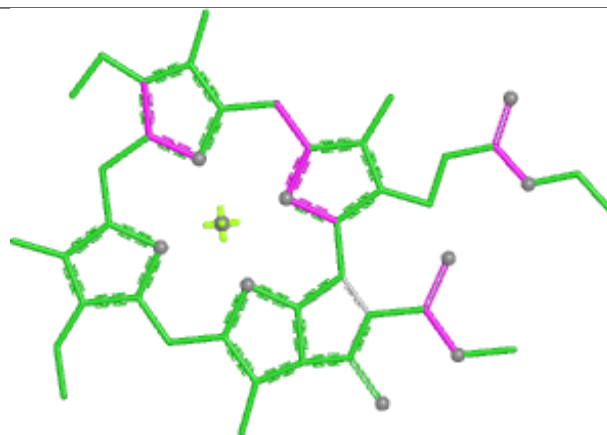
Ligand LMG I 320



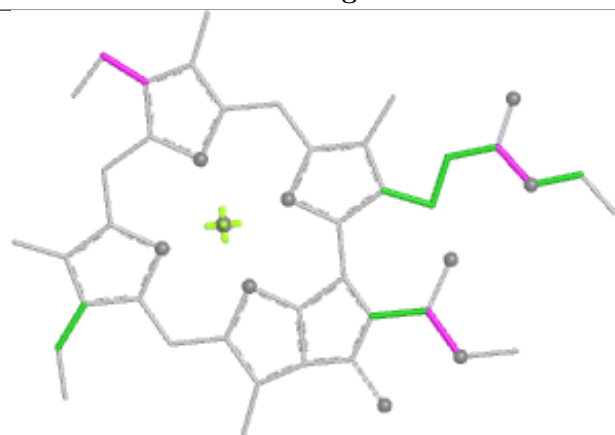
Ligand CLA H 304



Bond lengths



Bond angles

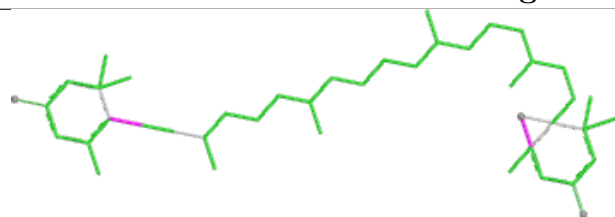


Torsions

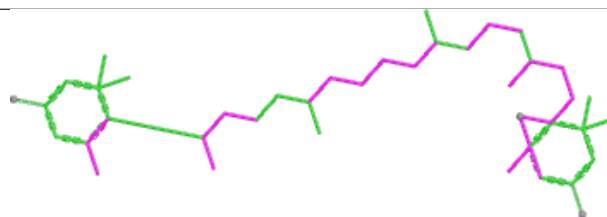


Rings

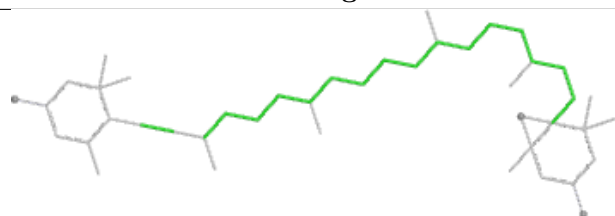
Ligand DD6 L 304



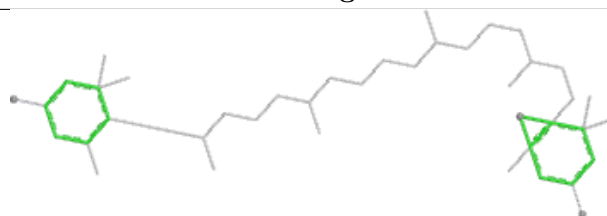
Bond lengths



Bond angles

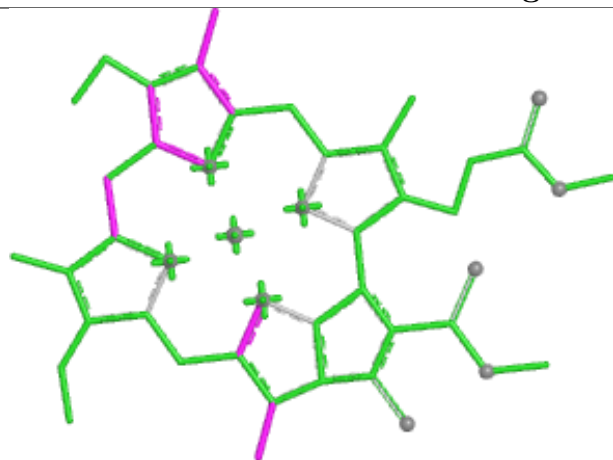


Torsions

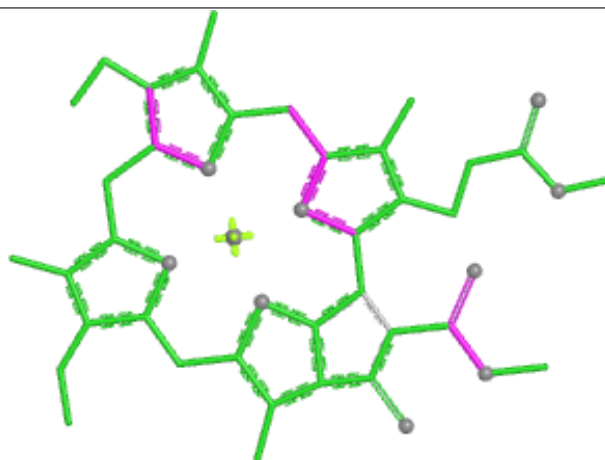


Rings

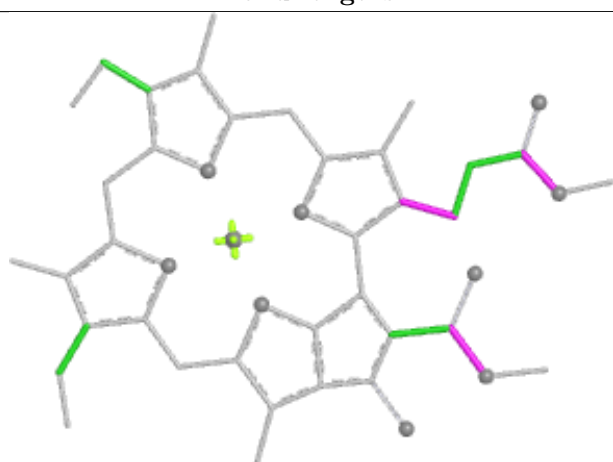
Ligand CLA 1 312



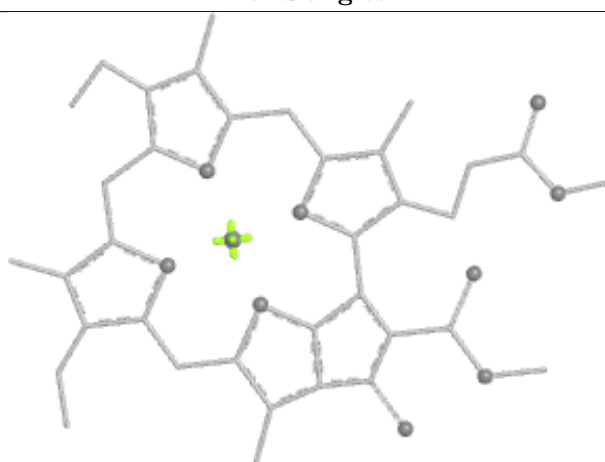
Bond lengths



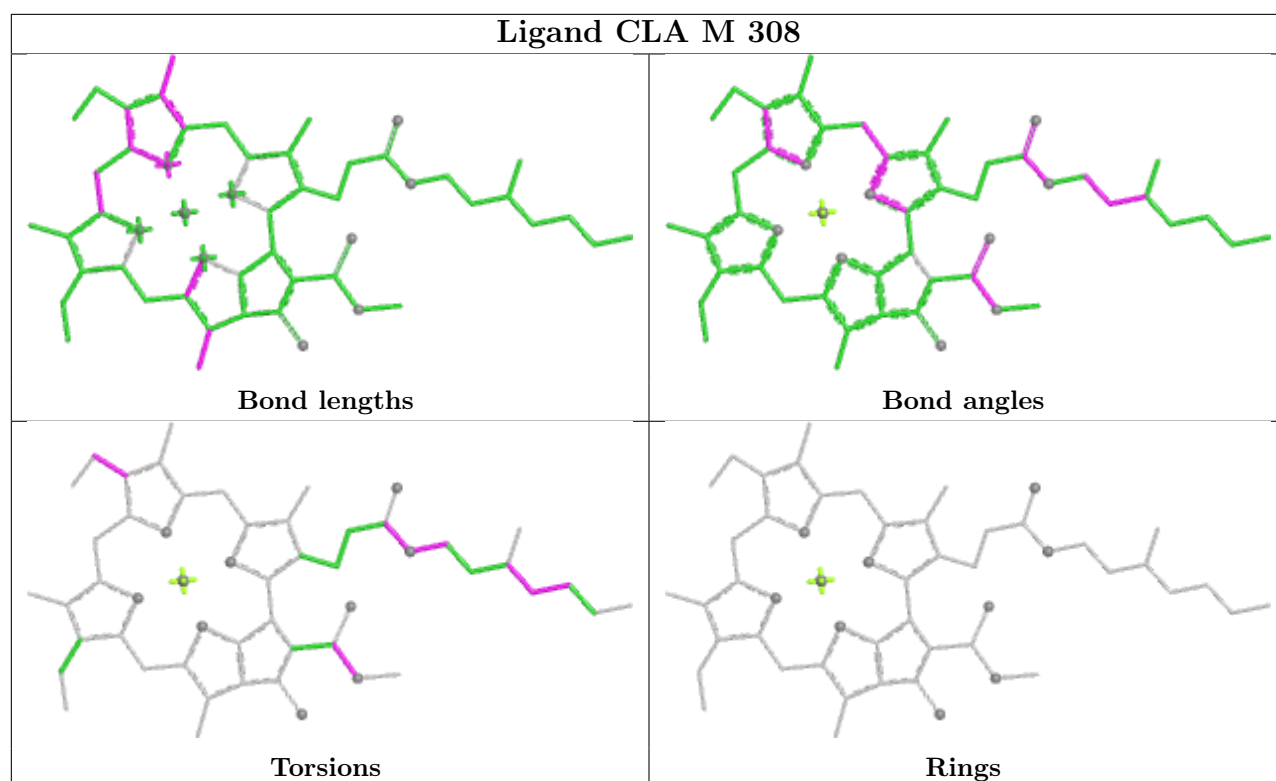
Bond angles

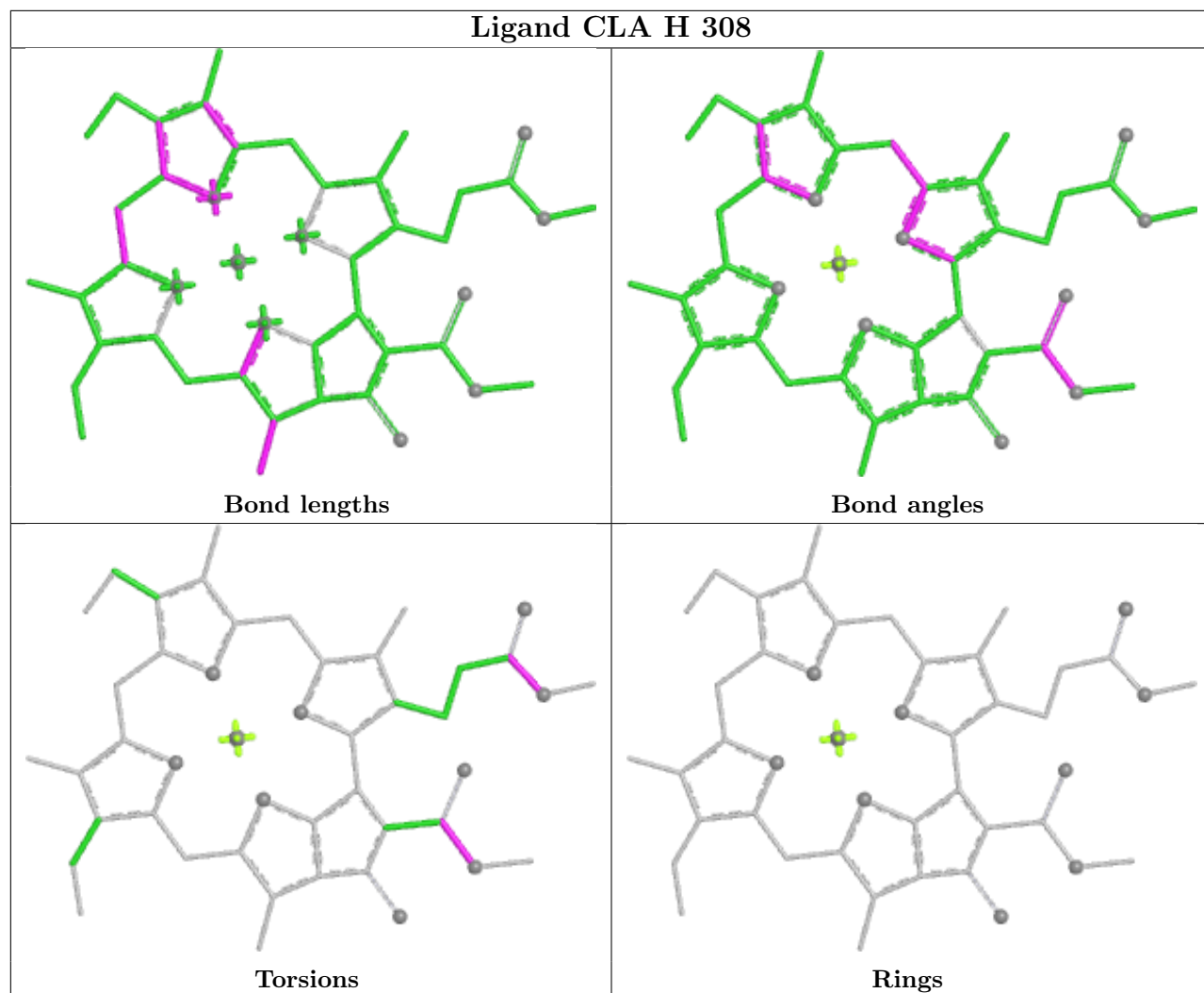


Torsions

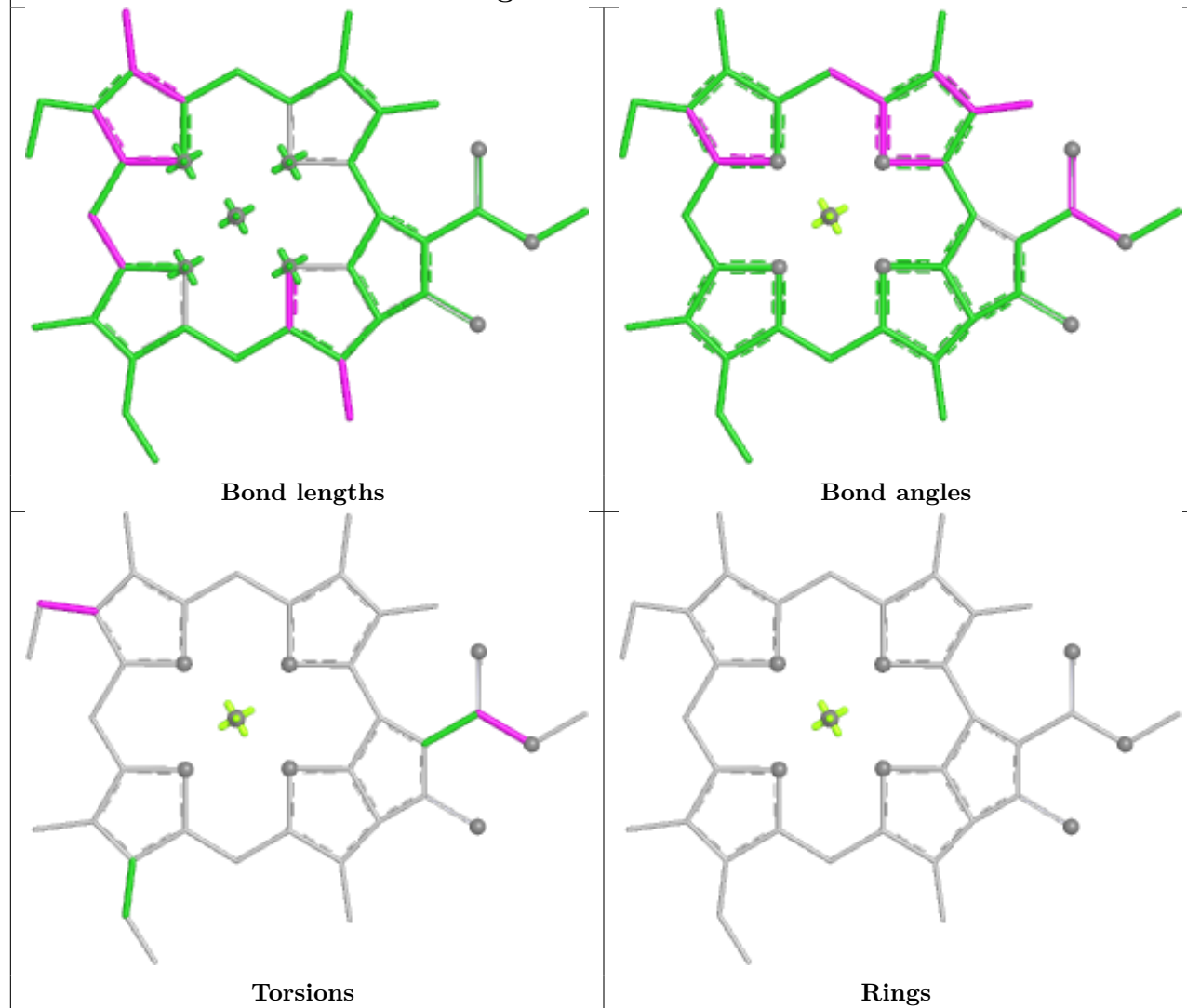


Rings

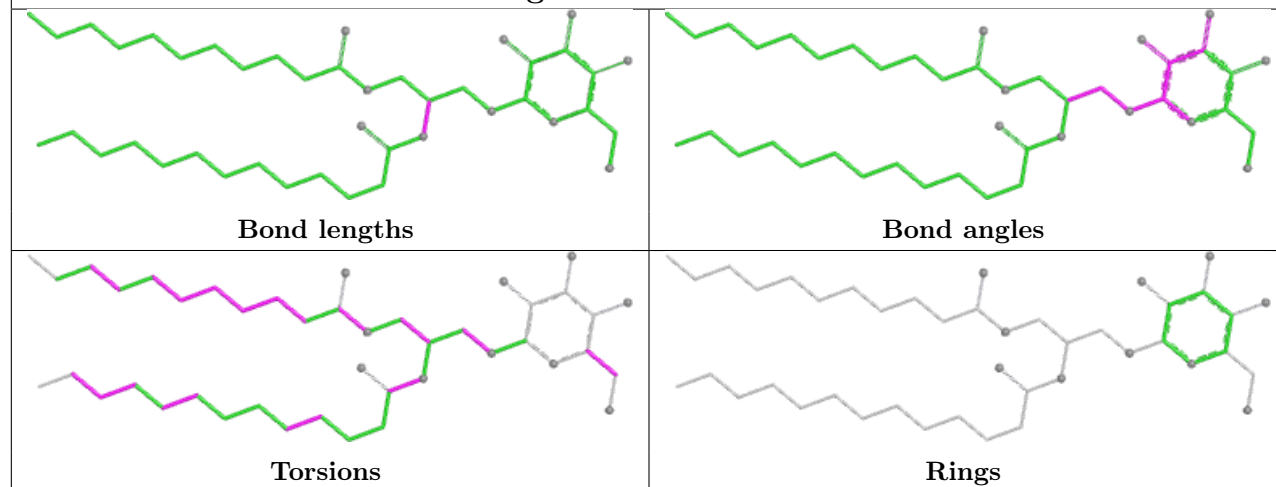


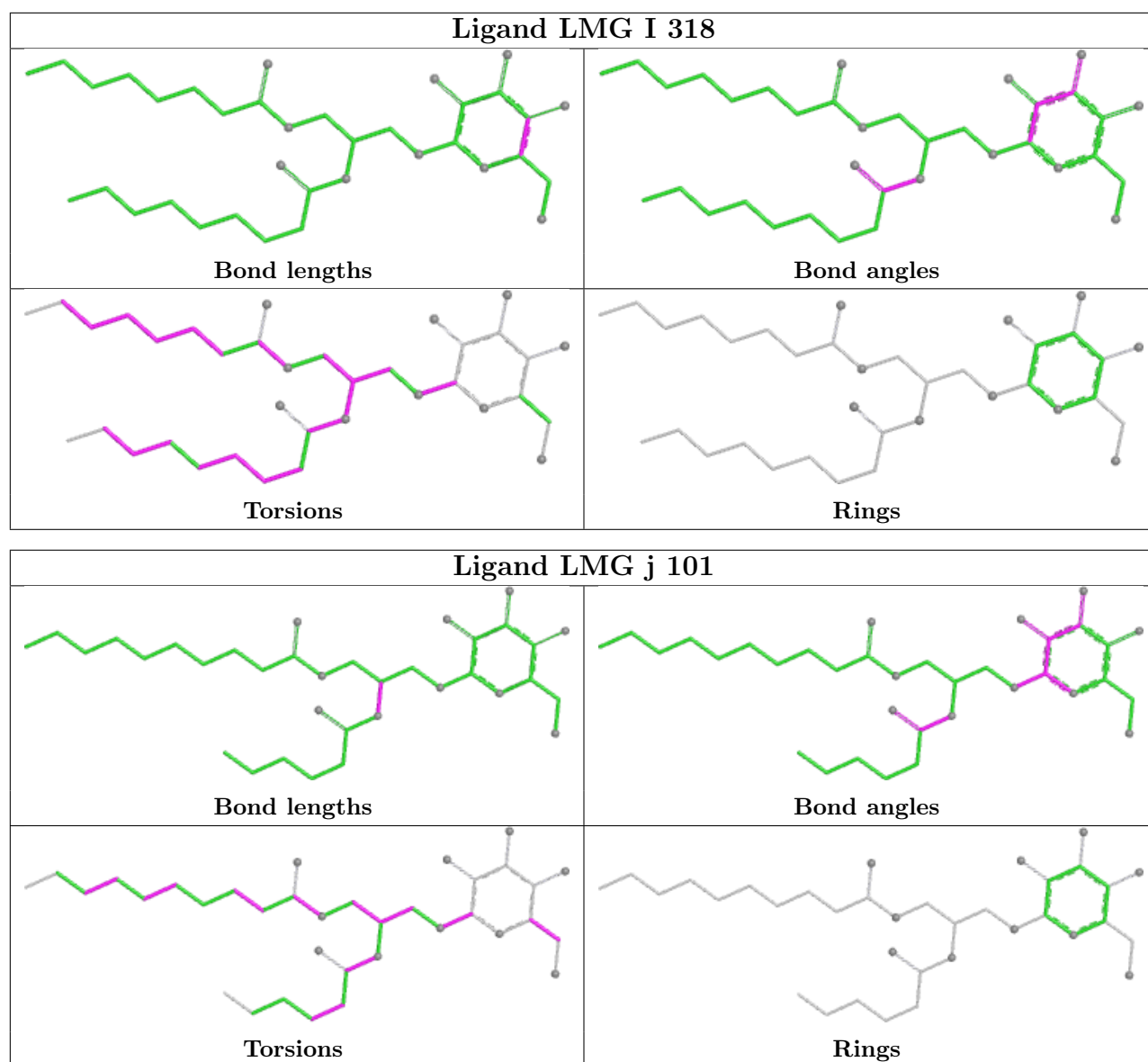


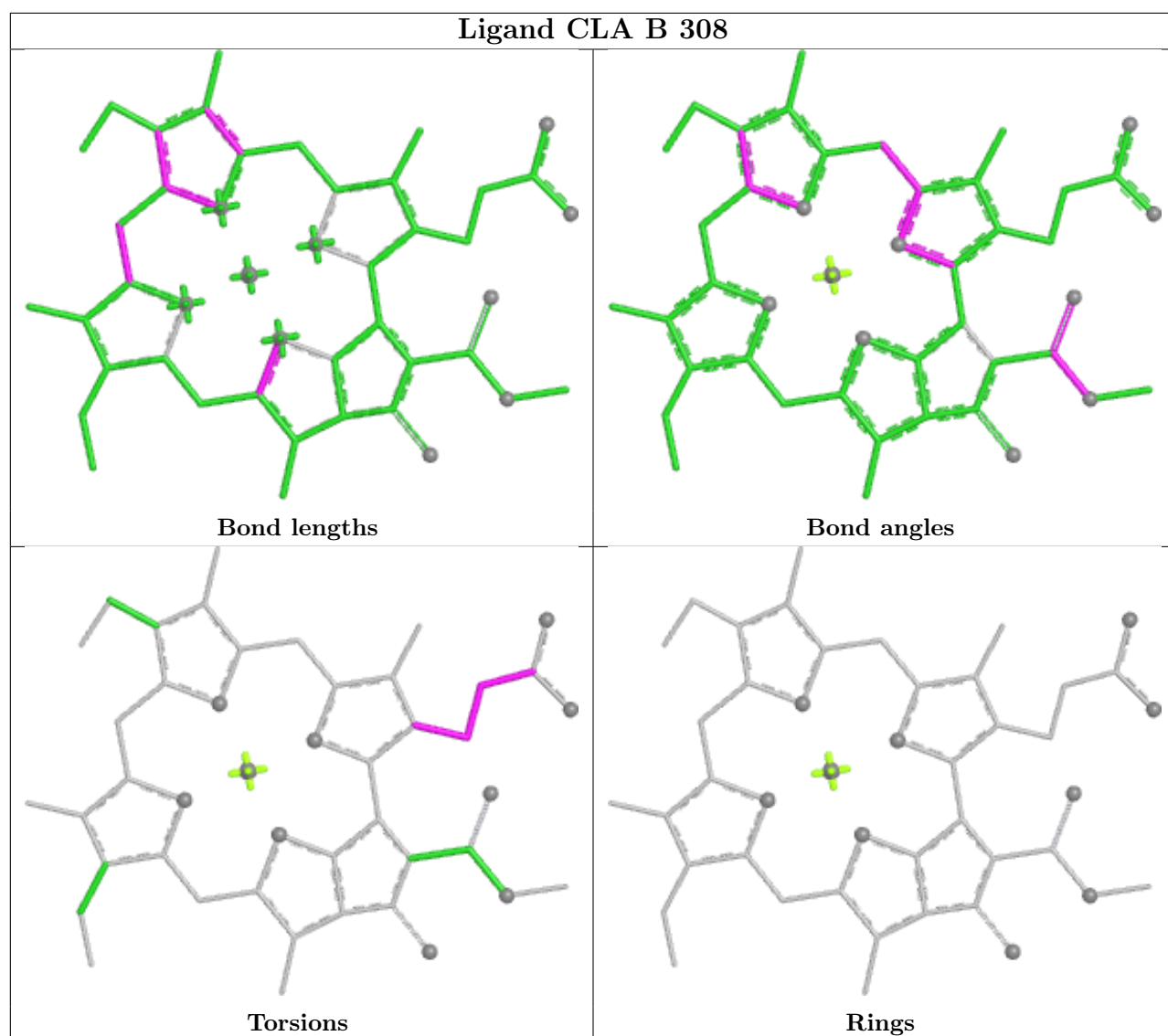
Ligand CLA L 316



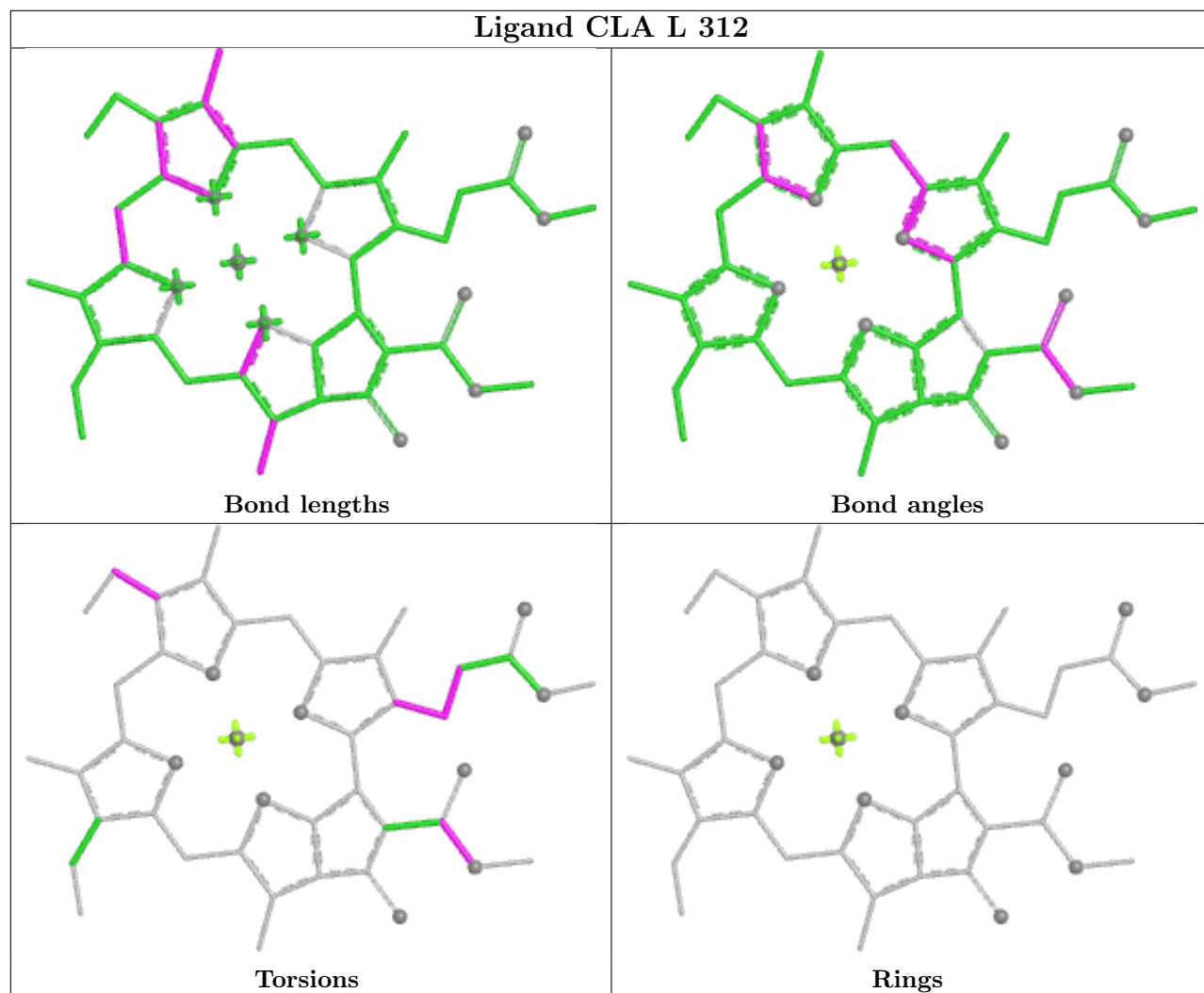
Ligand LMG K 318



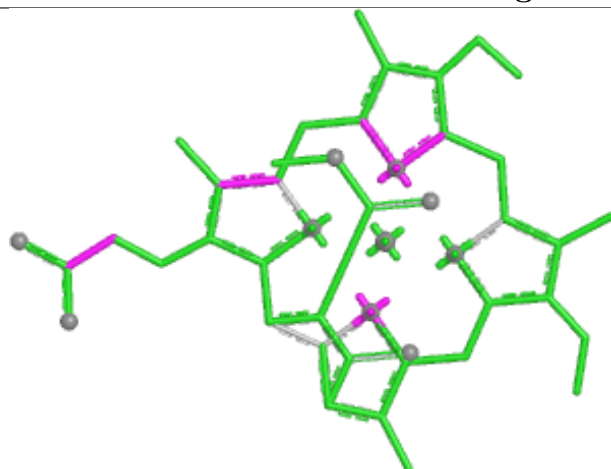




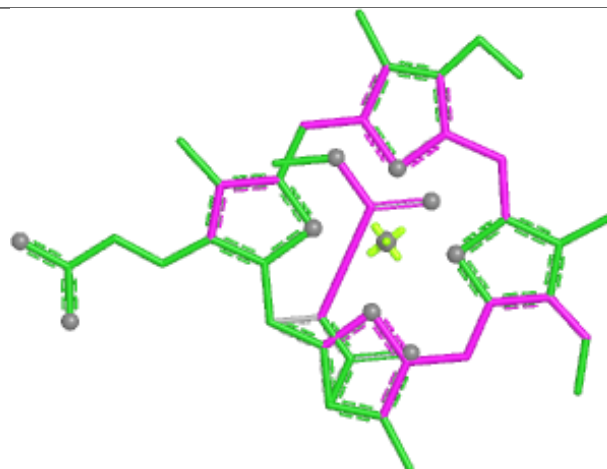
Ligand CLA L 312



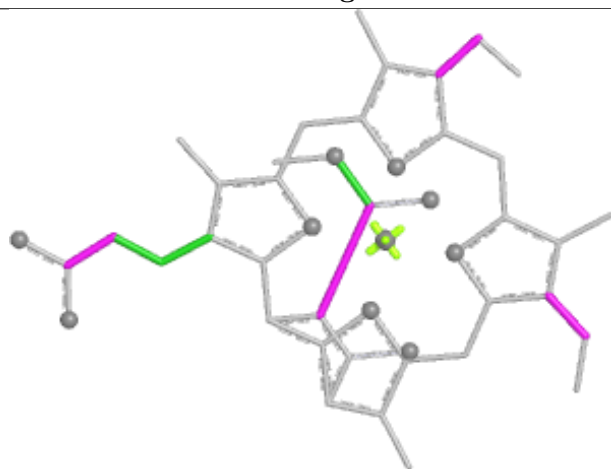
Ligand KC1 G 515



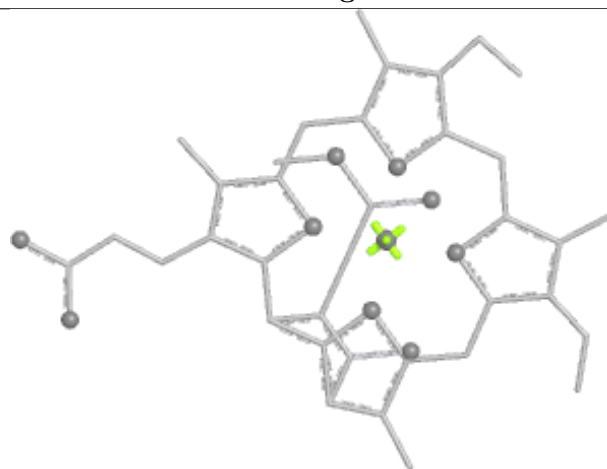
Bond lengths



Bond angles

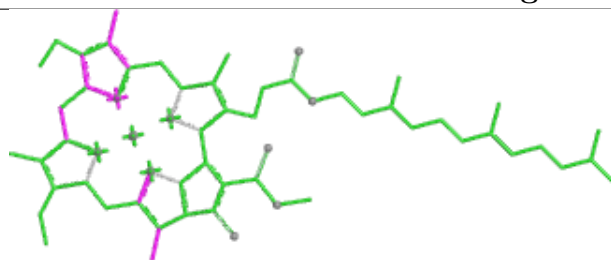


Torsions

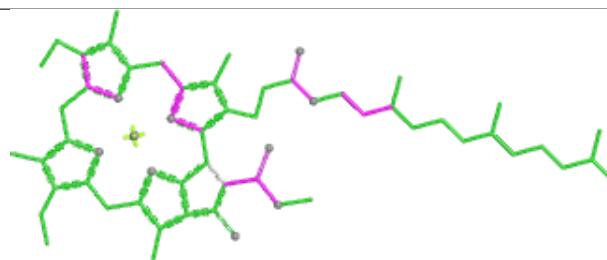


Rings

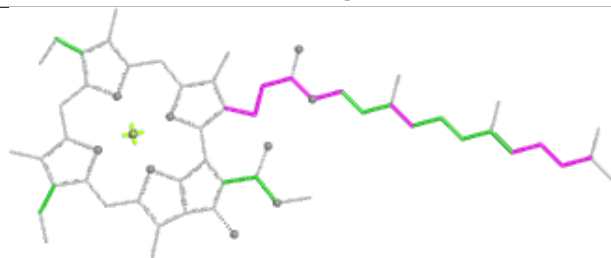
Ligand CLA I 308



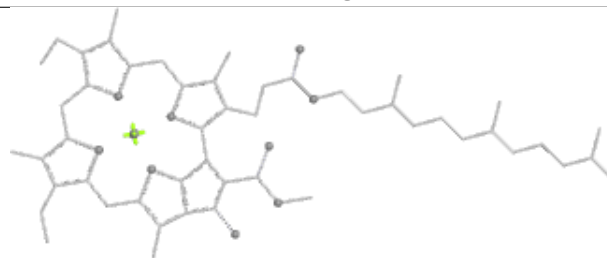
Bond lengths



Bond angles

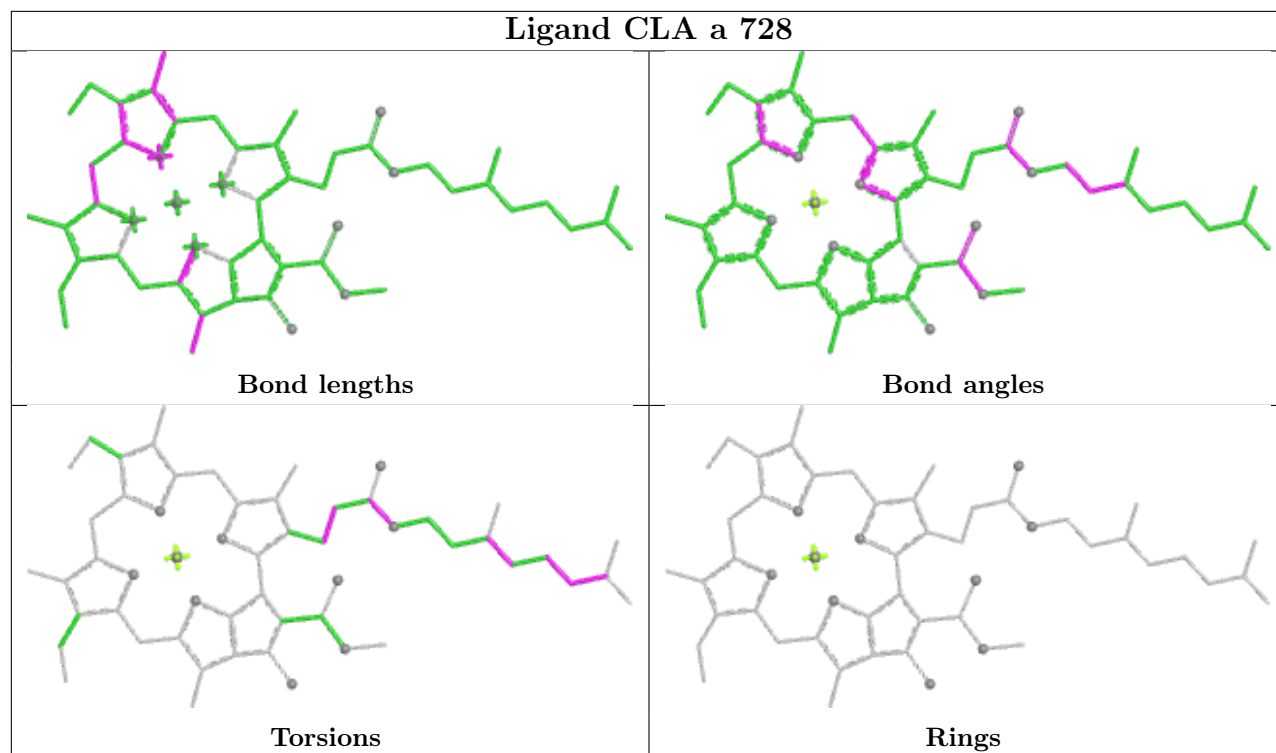


Torsions

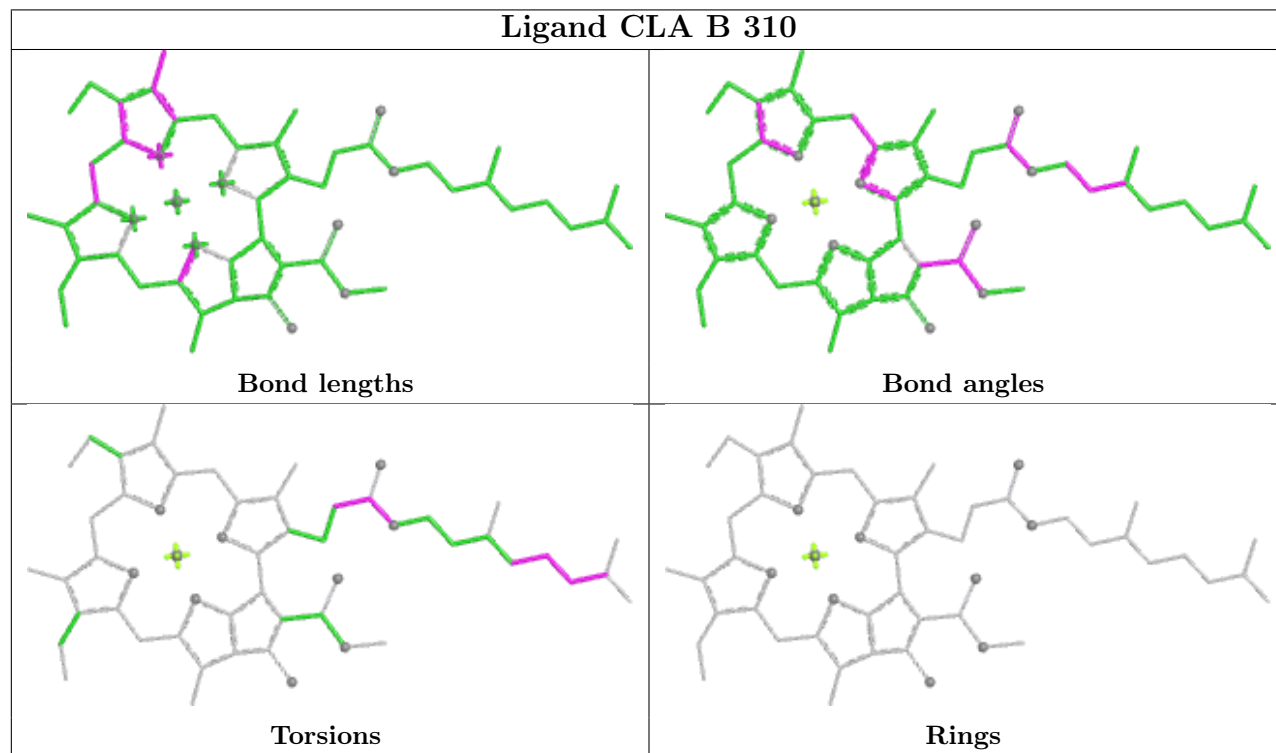


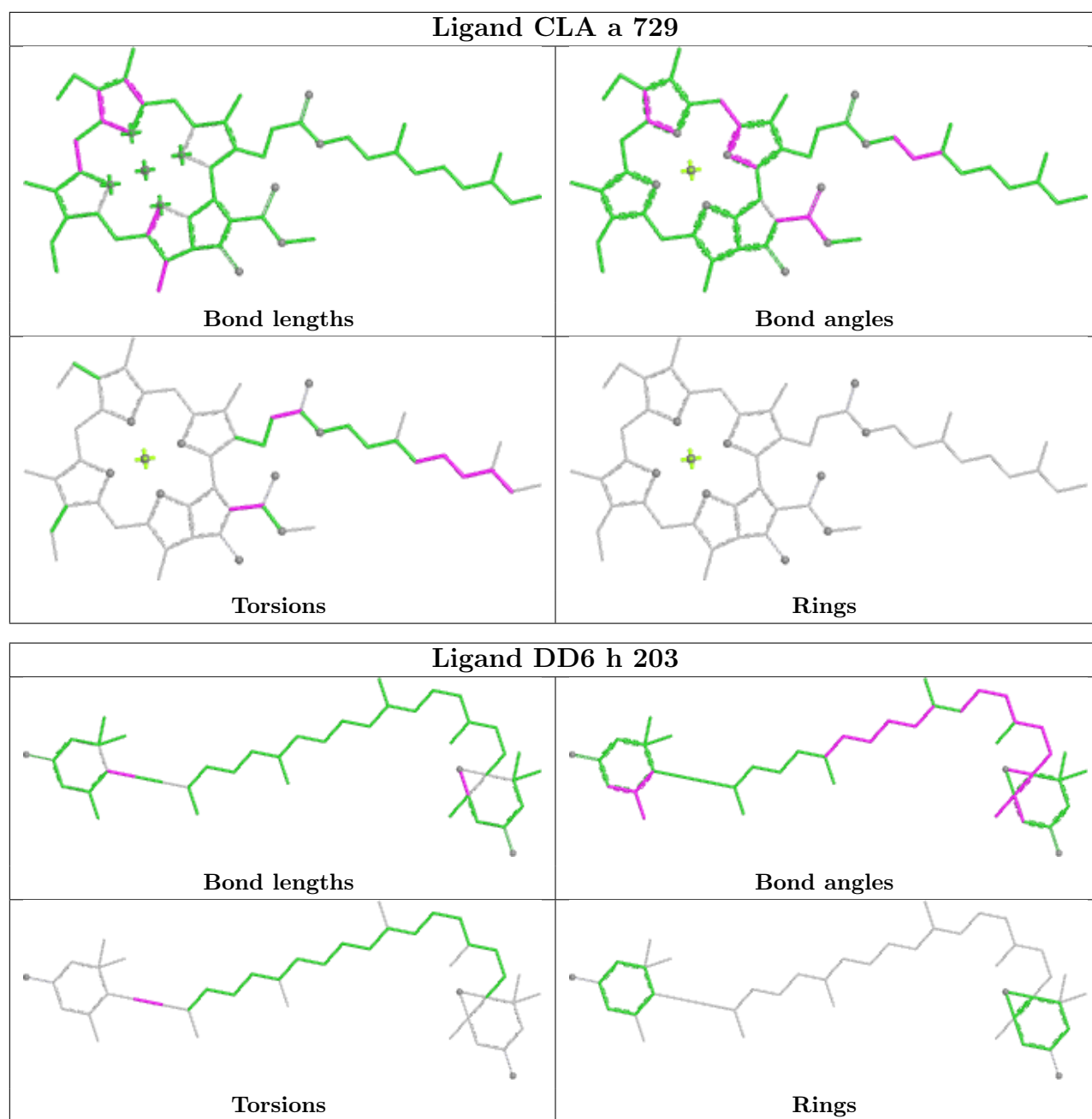
Rings

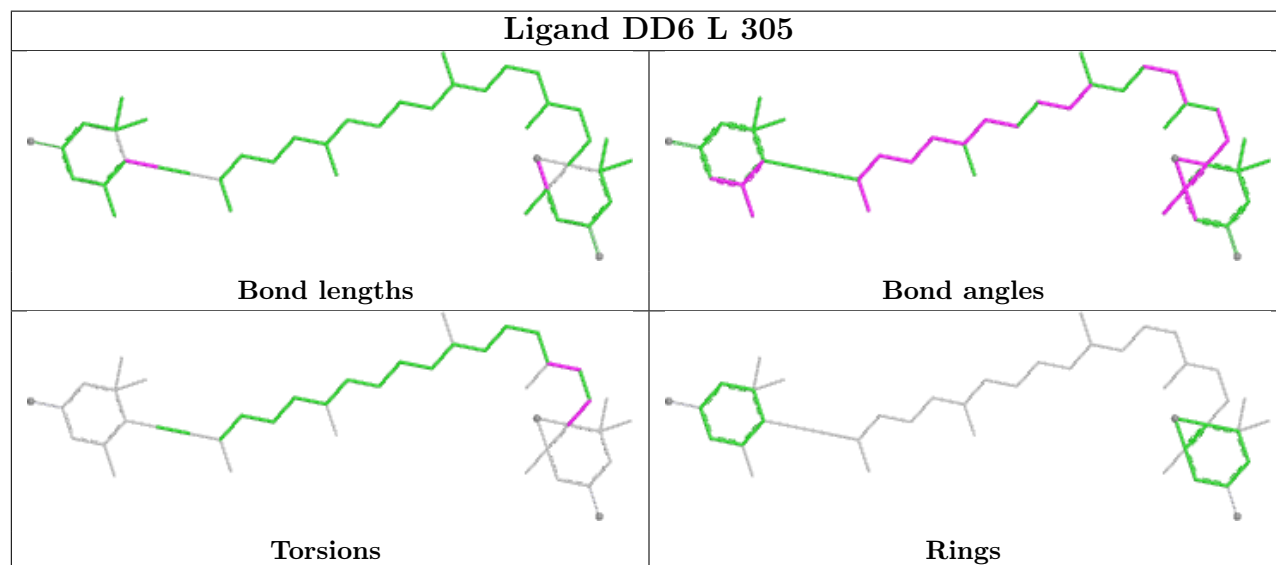
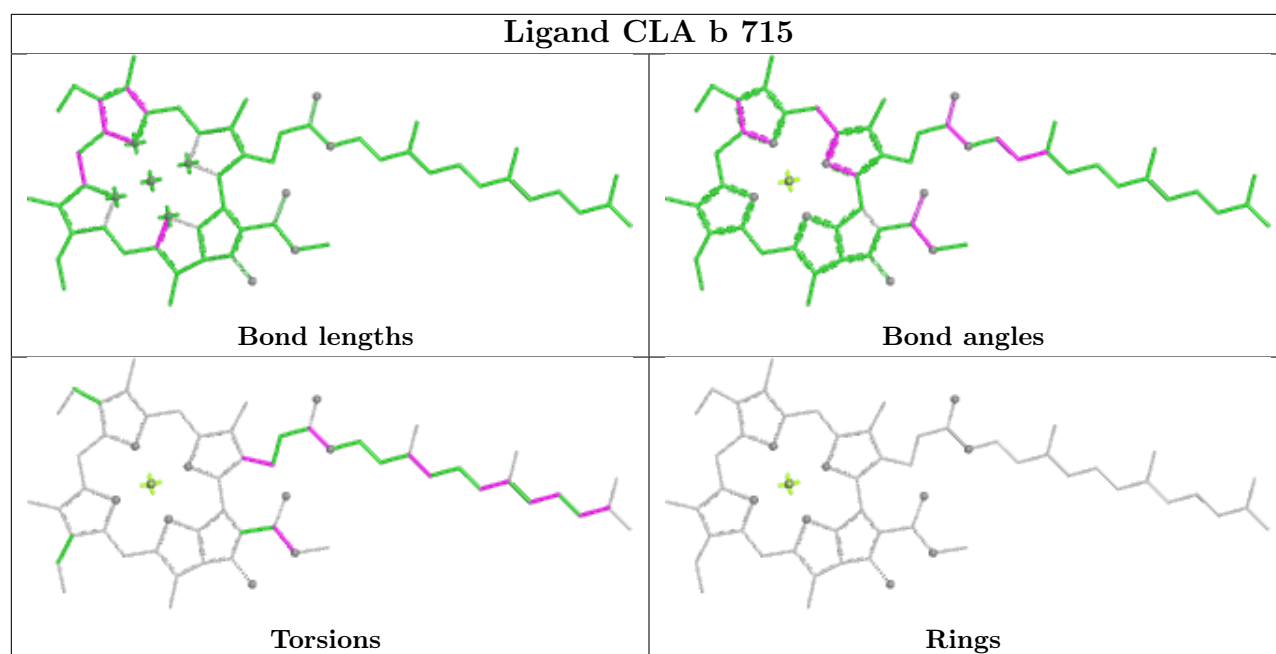
Ligand CLA a 728



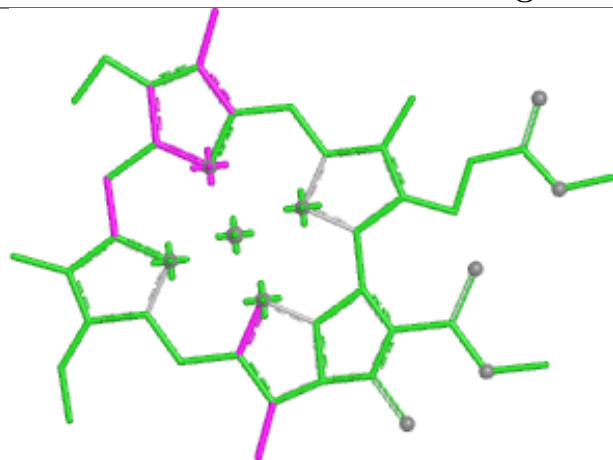
Ligand CLA B 310



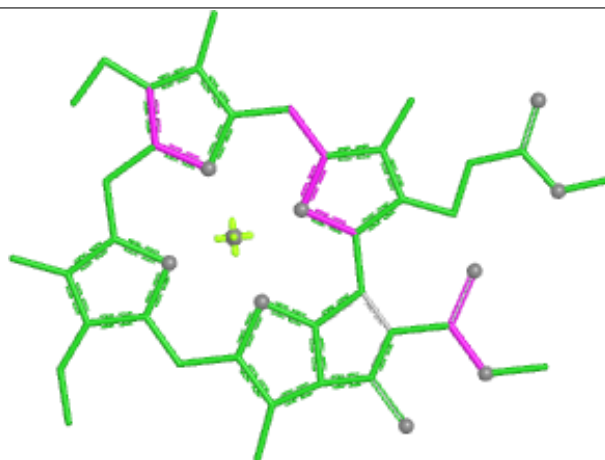




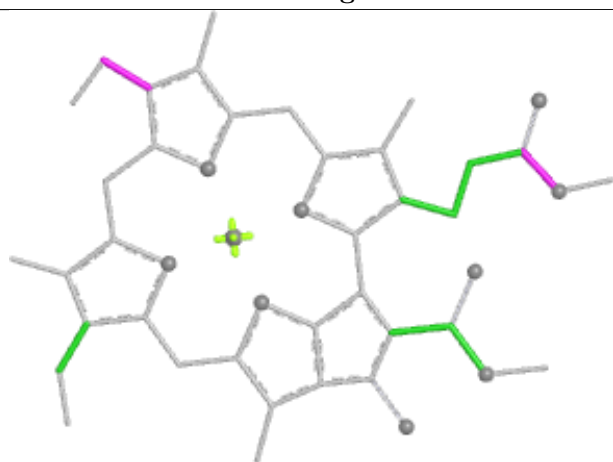
Ligand CLA F 307



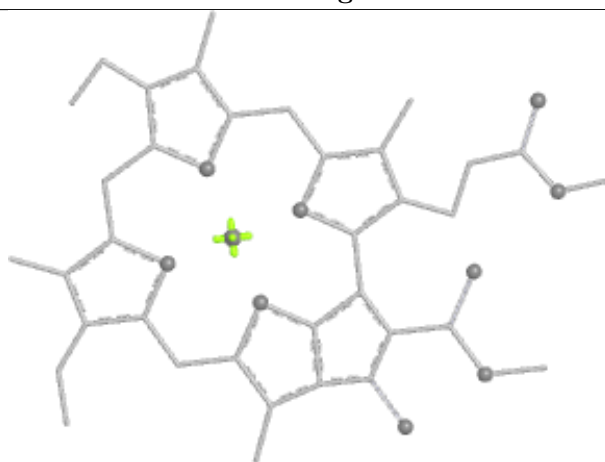
Bond lengths



Bond angles

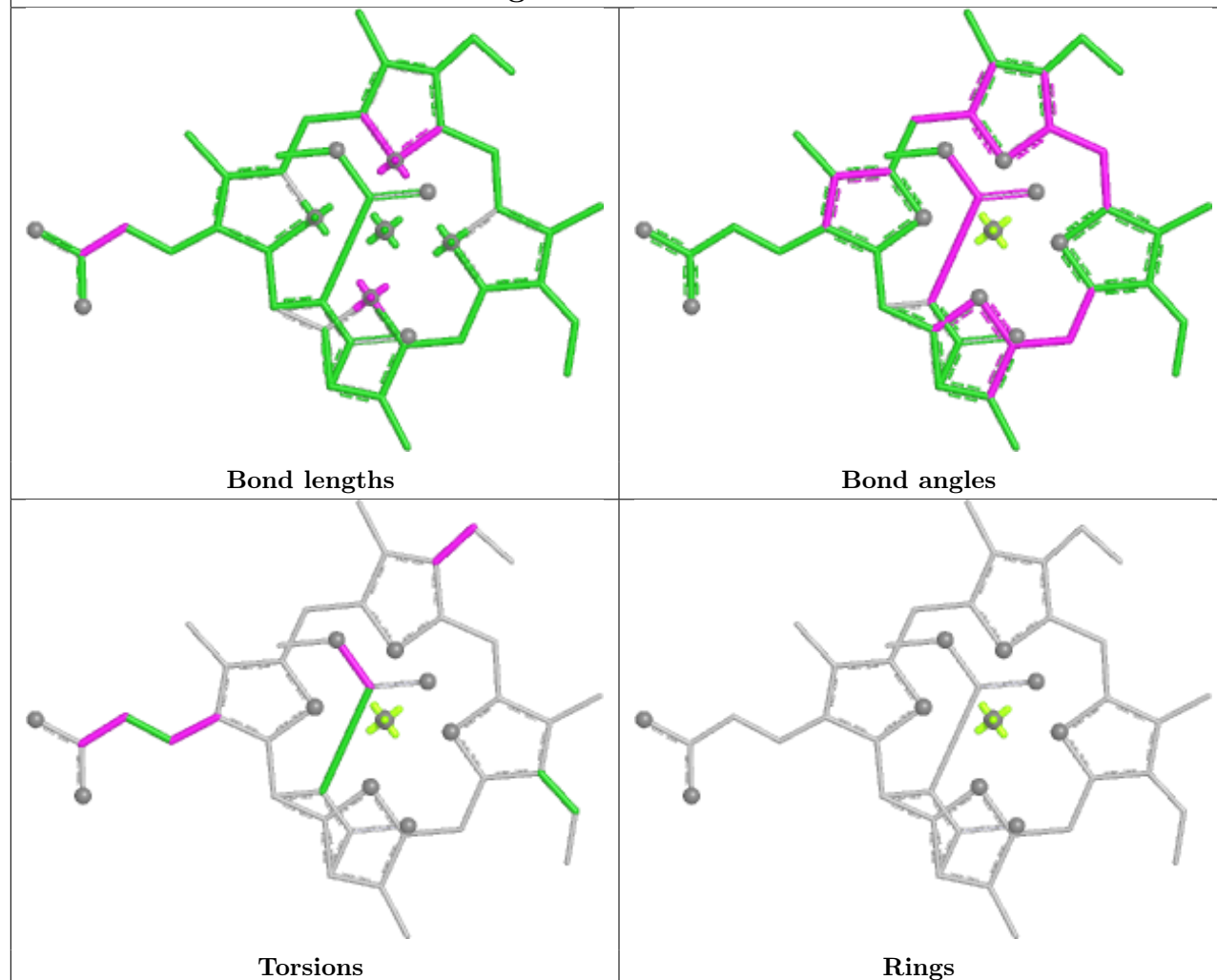


Torsions

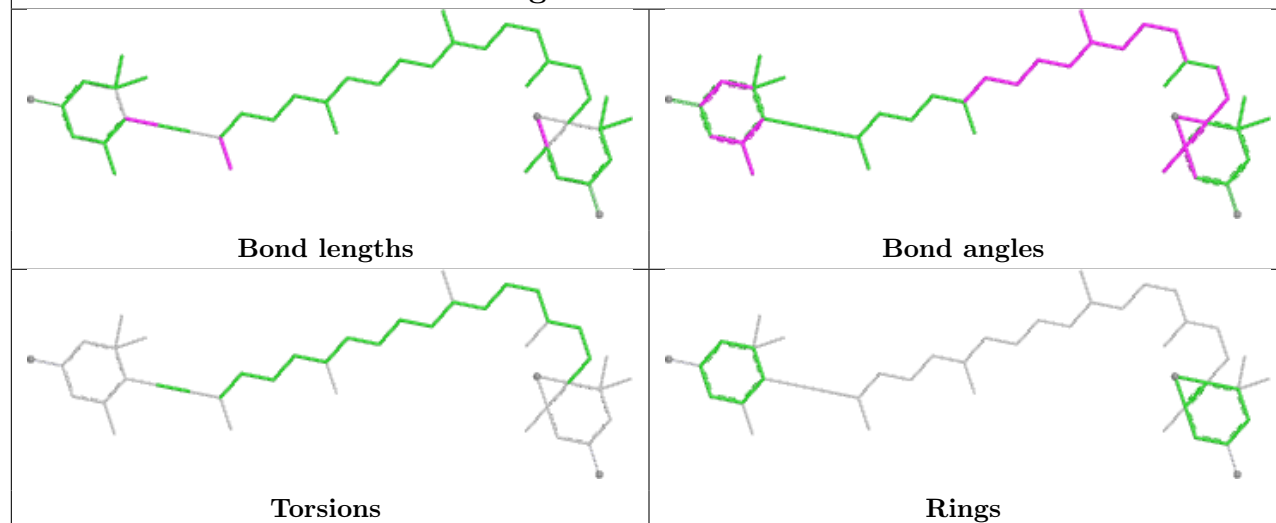


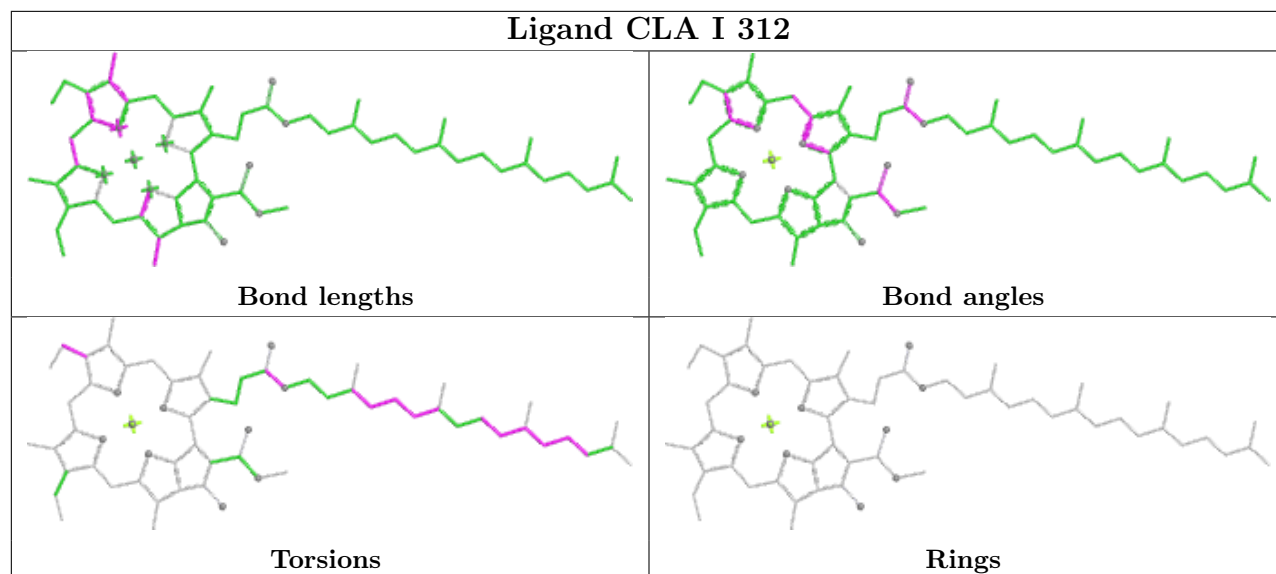
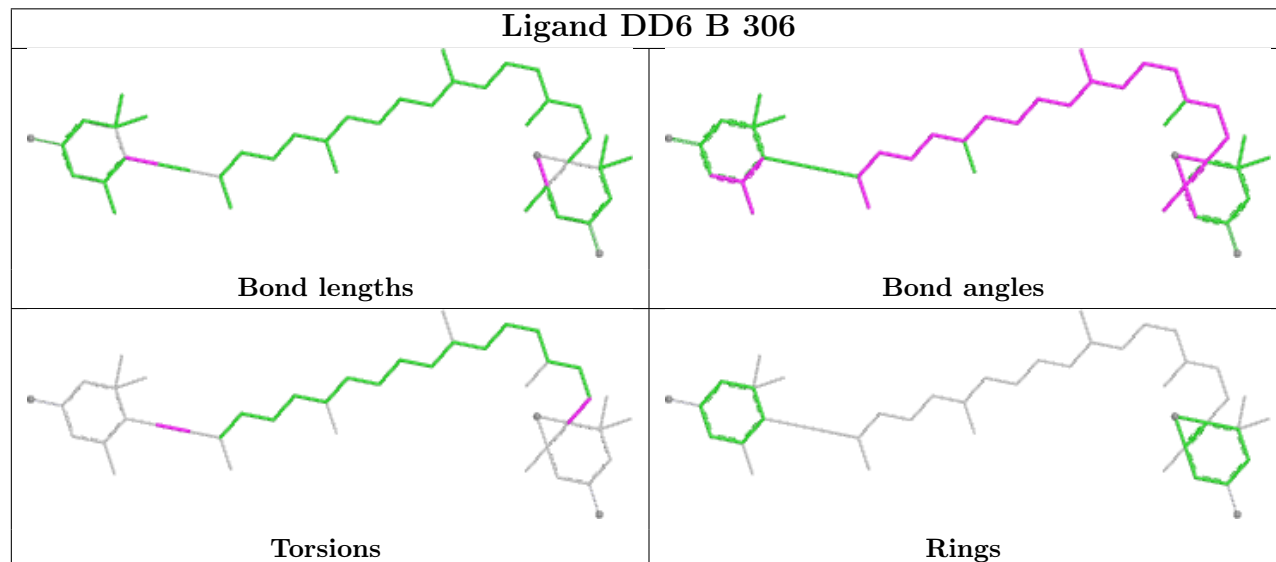
Rings

Ligand KC1 N 306

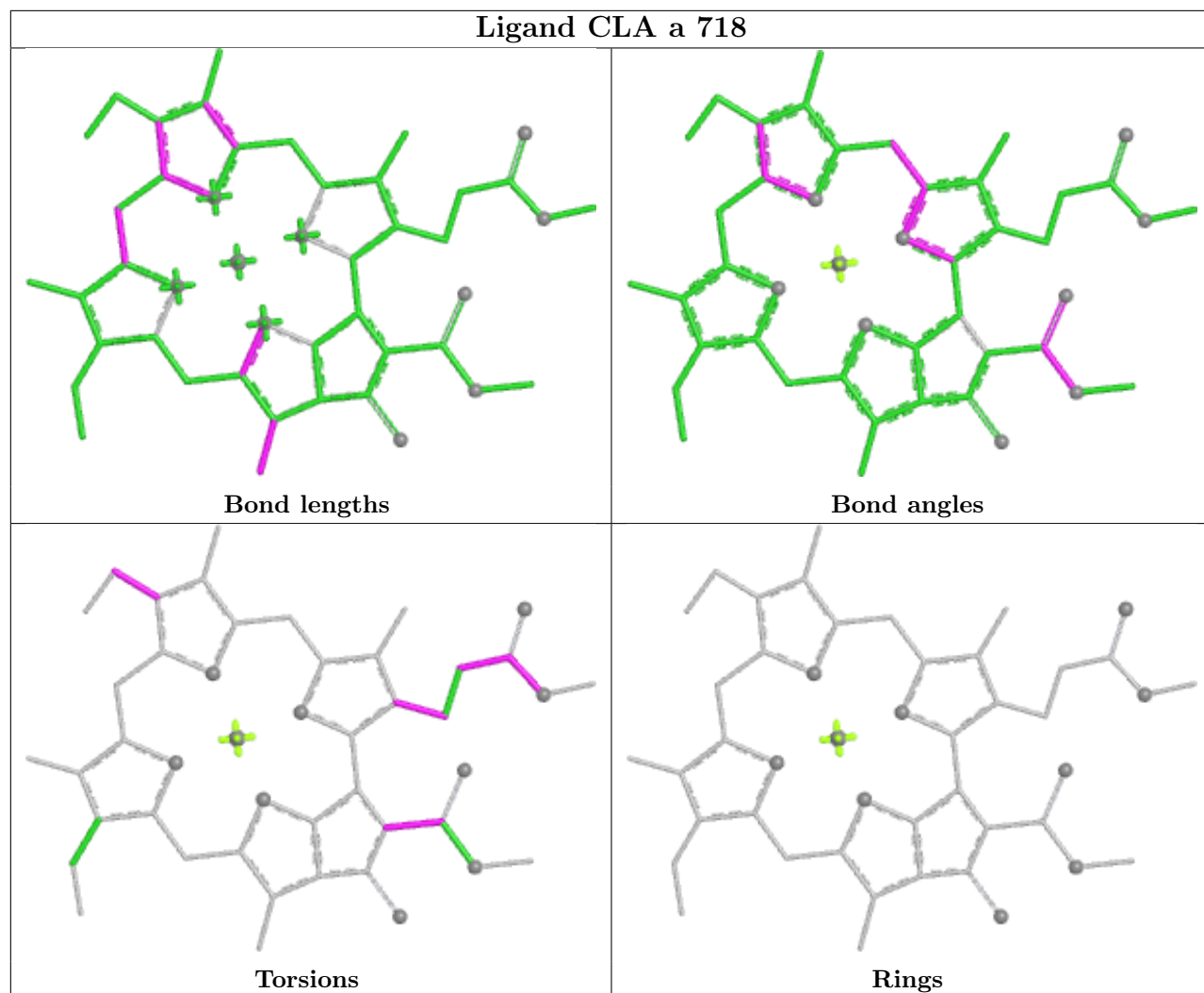


Ligand DD6 M 304

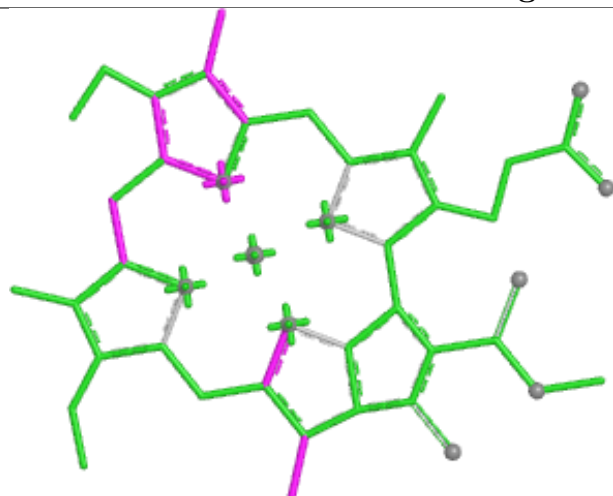


Ligand CLA I 312**Ligand DD6 B 306**

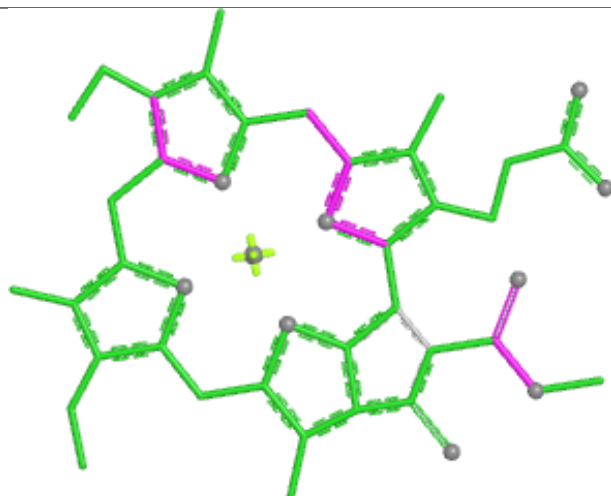
Ligand CLA a 718



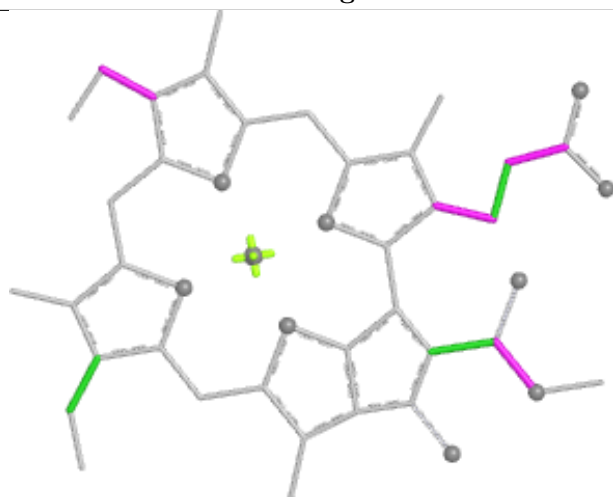
Ligand CLA a 715



Bond lengths



Bond angles

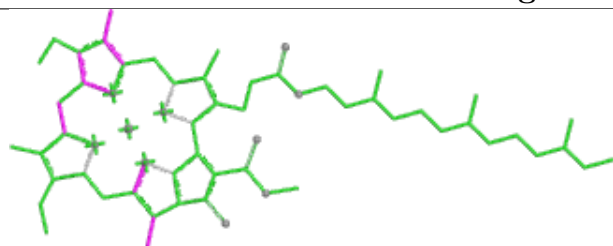


Torsions

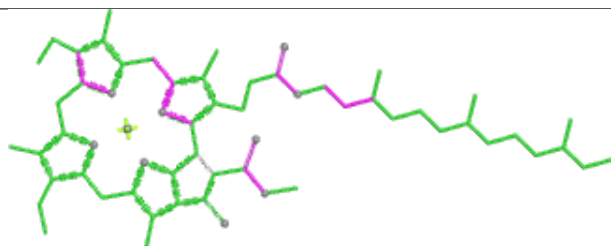


Rings

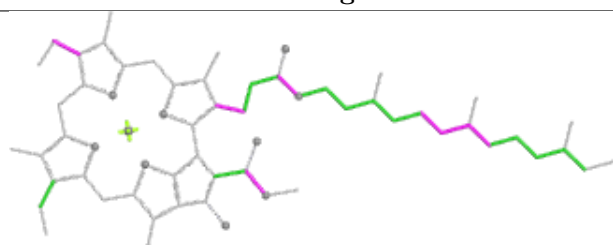
Ligand CLA a 725



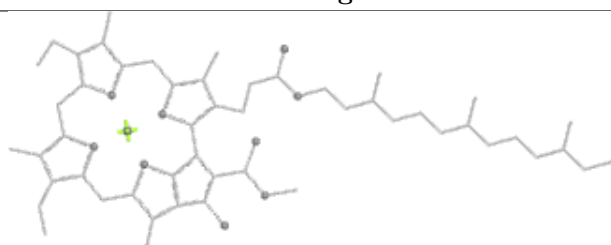
Bond lengths



Bond angles

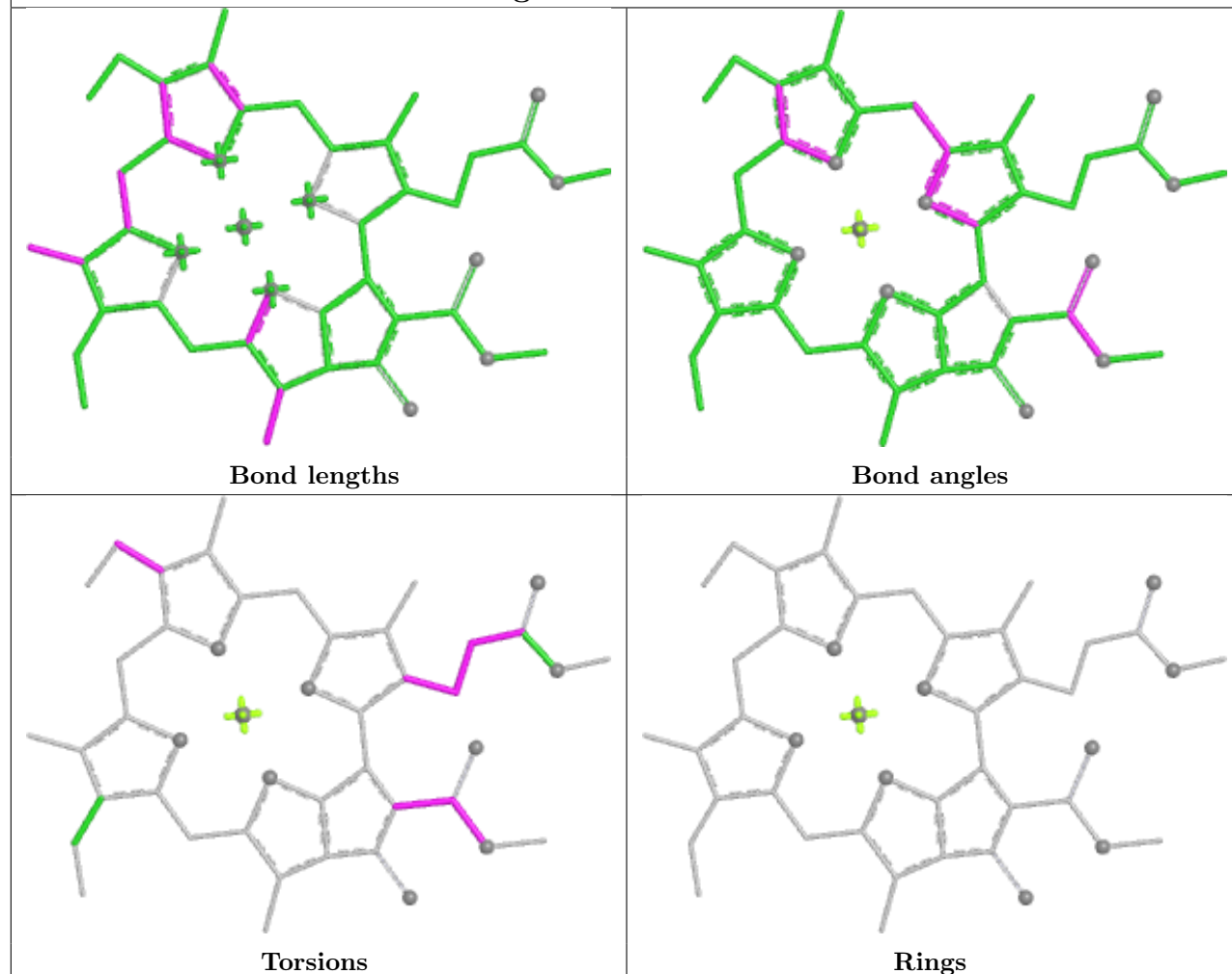


Torsions

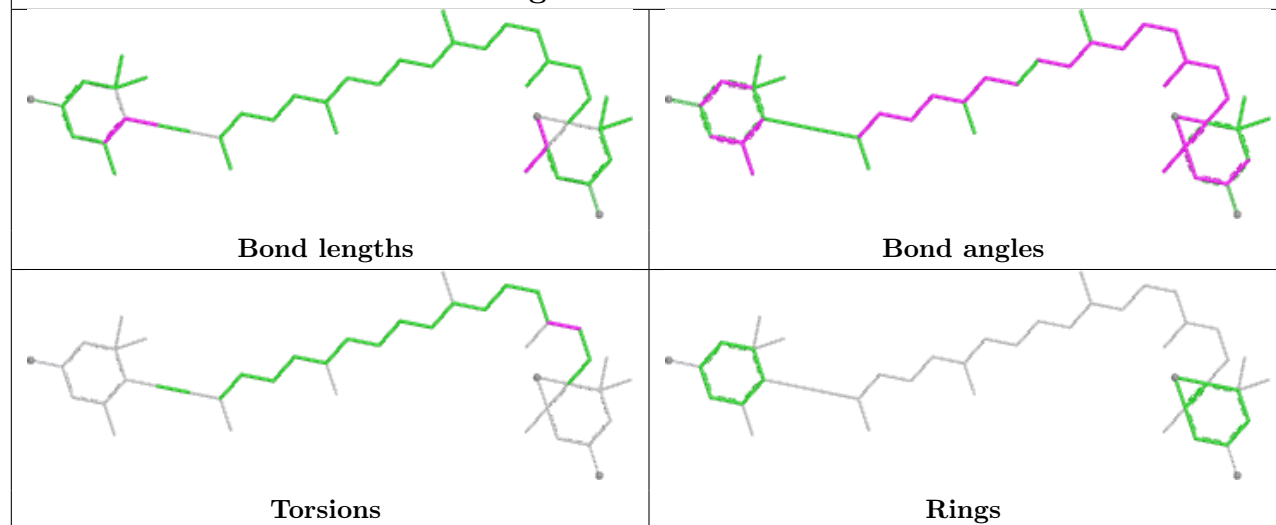


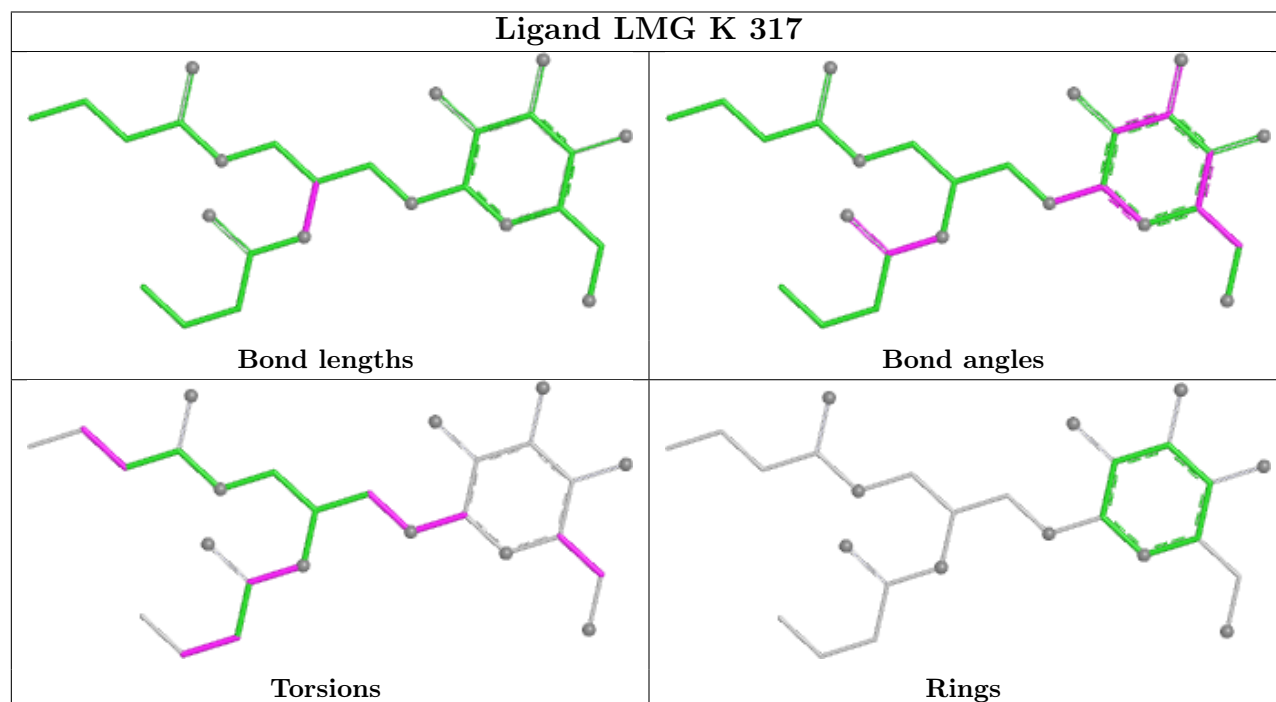
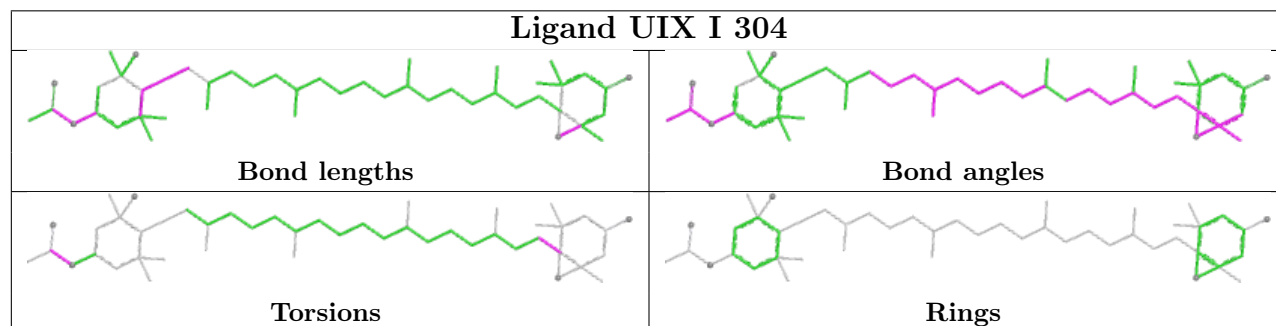
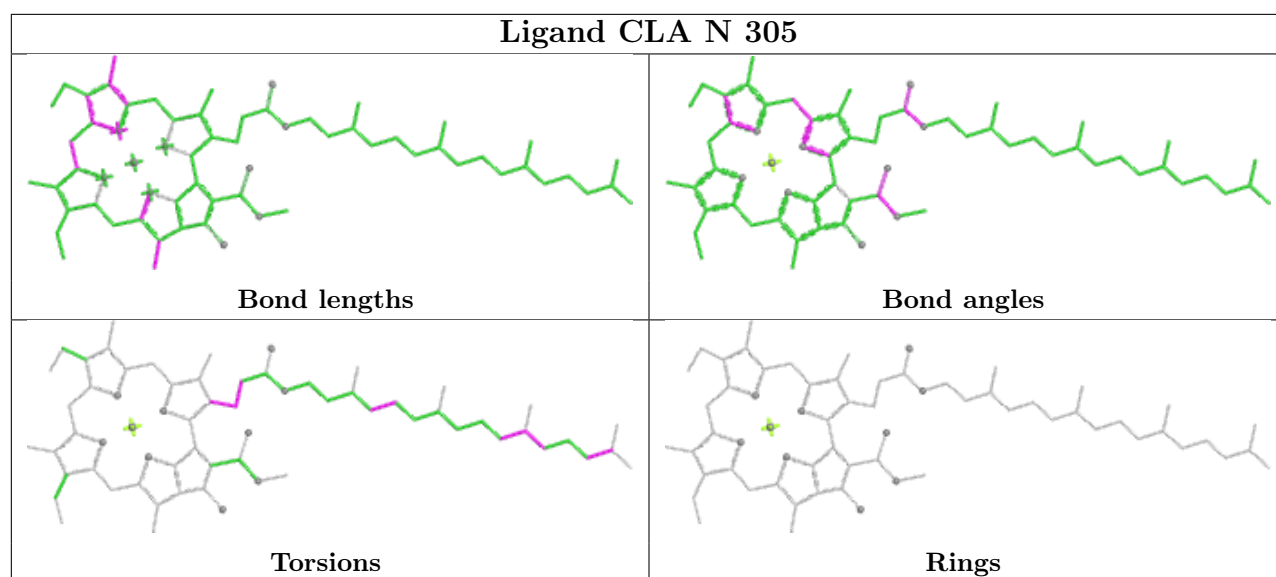
Rings

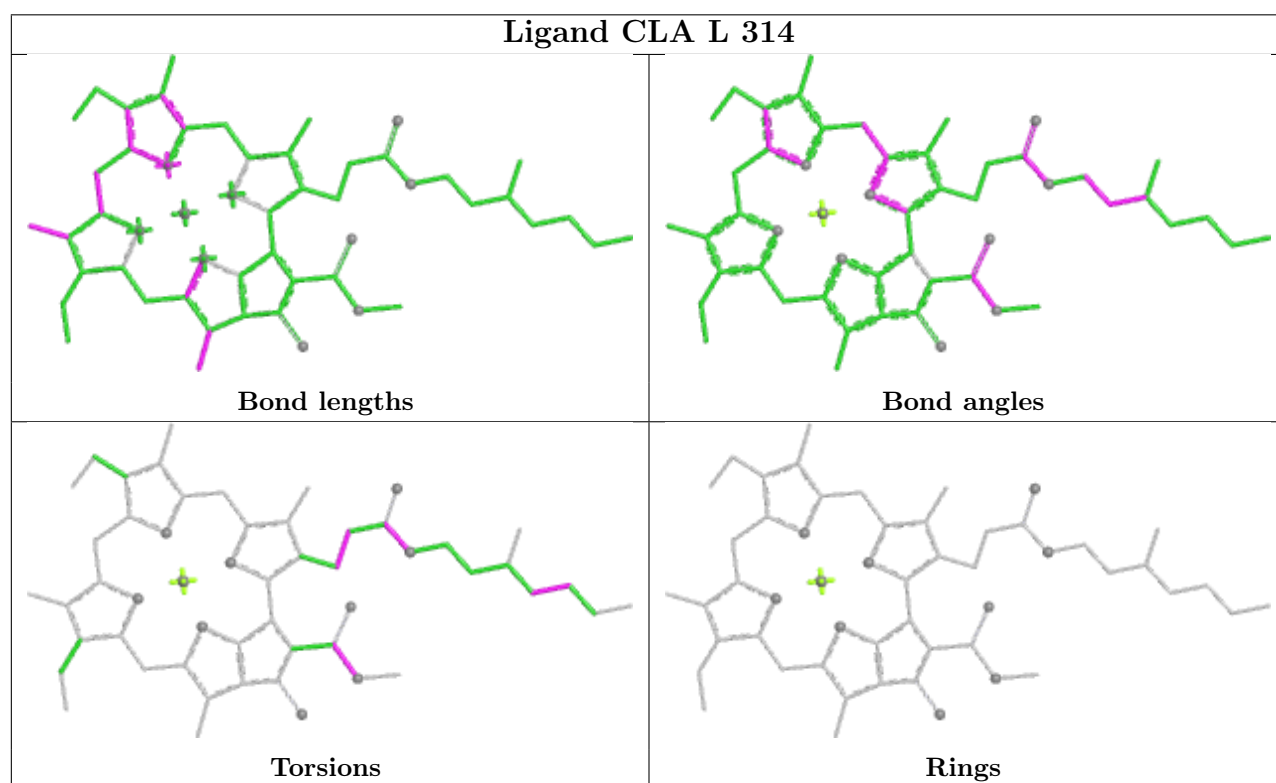
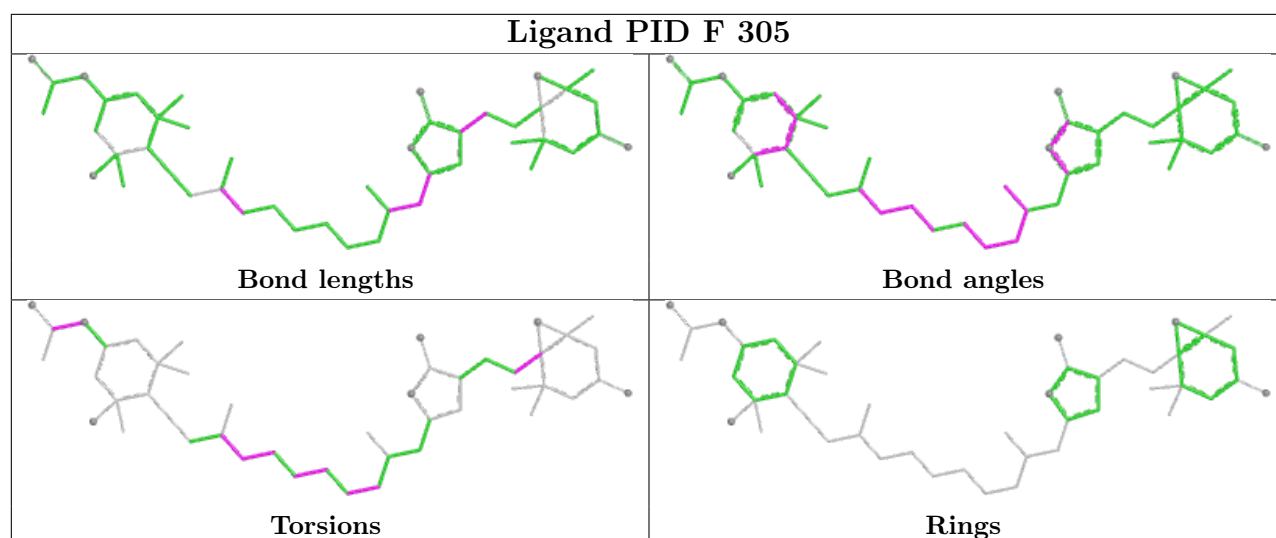
Ligand CLA A 319



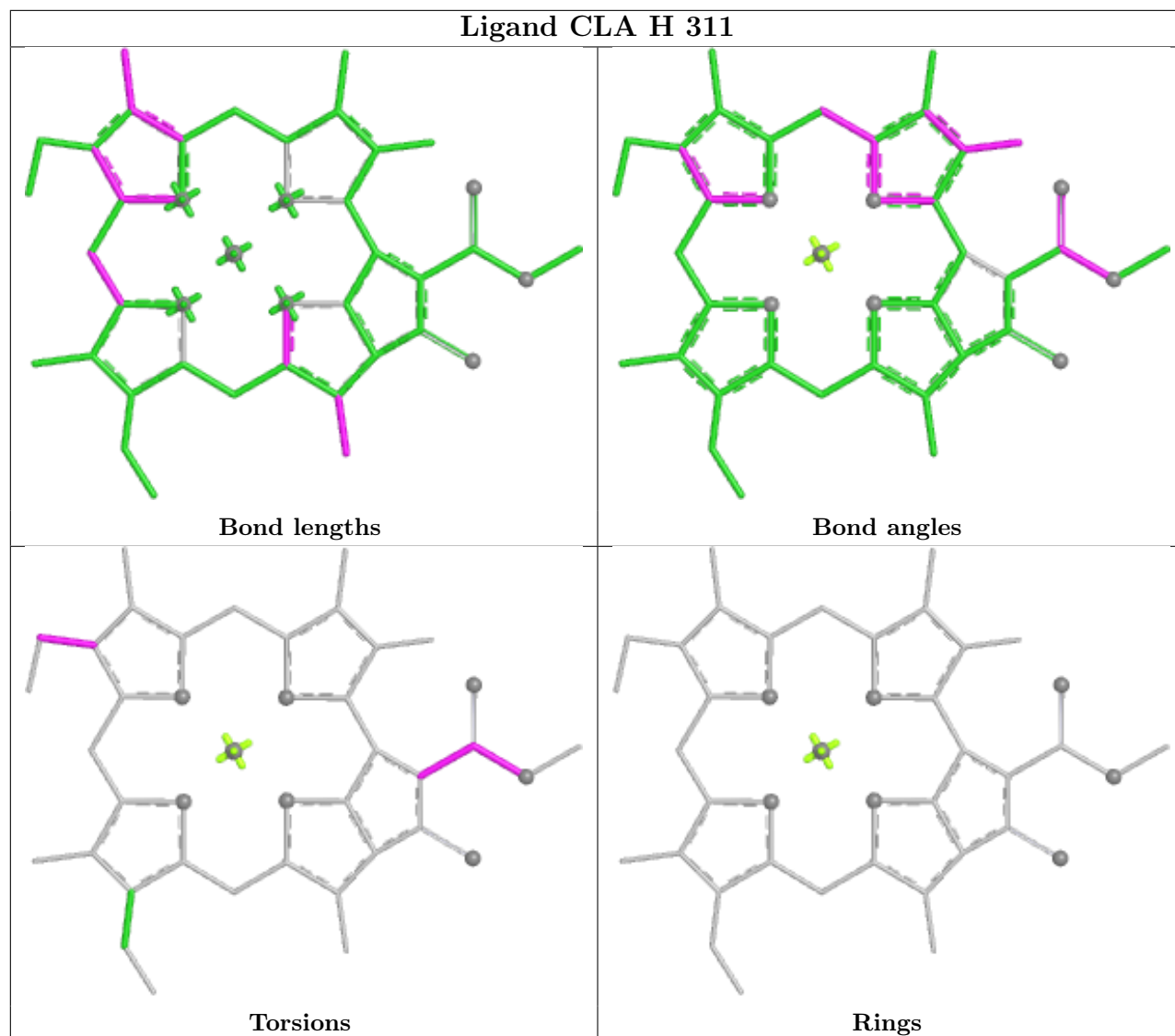
Ligand DD6 M 303



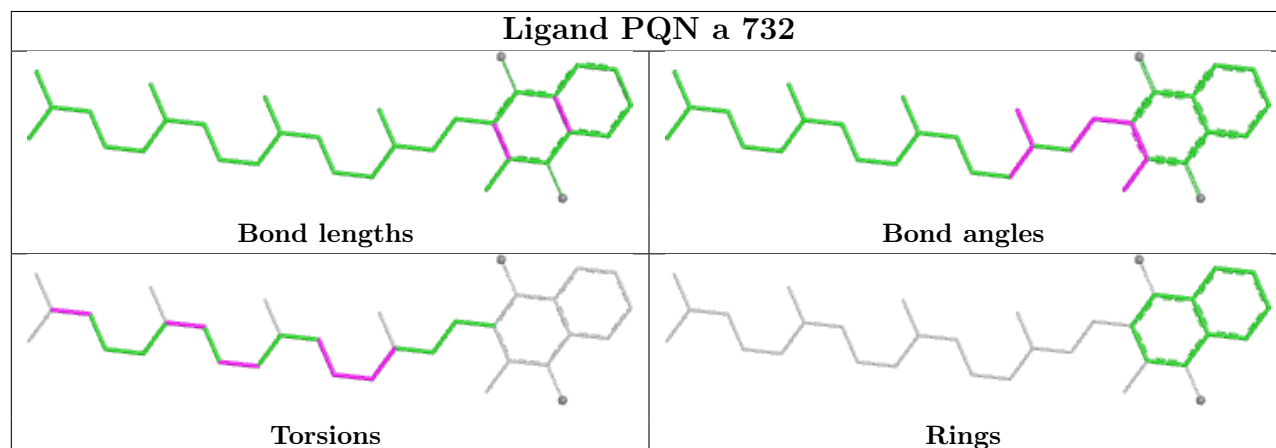




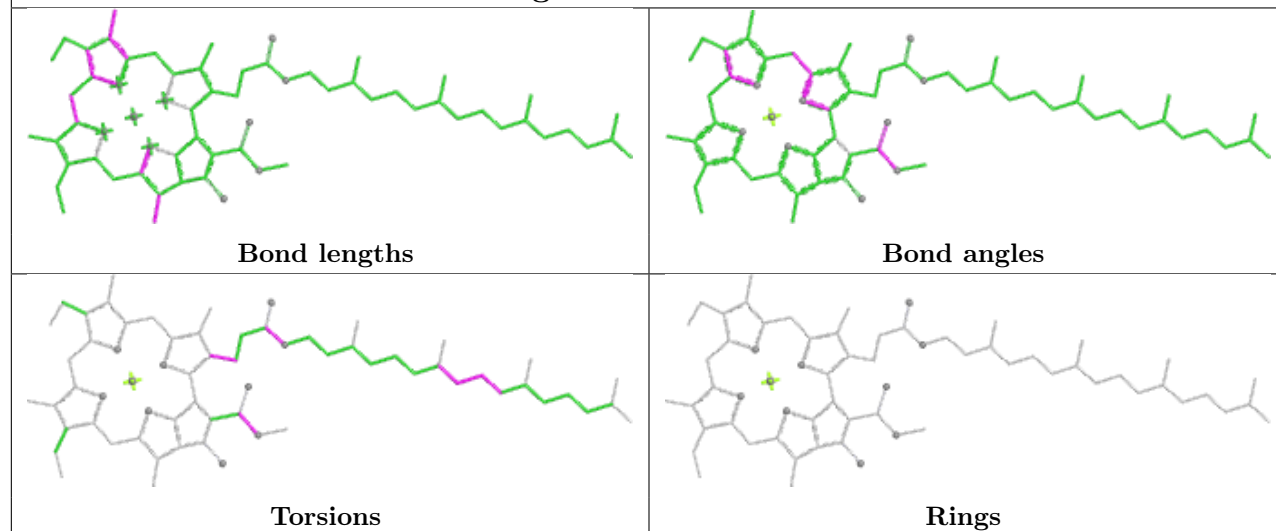
Ligand CLA H 311



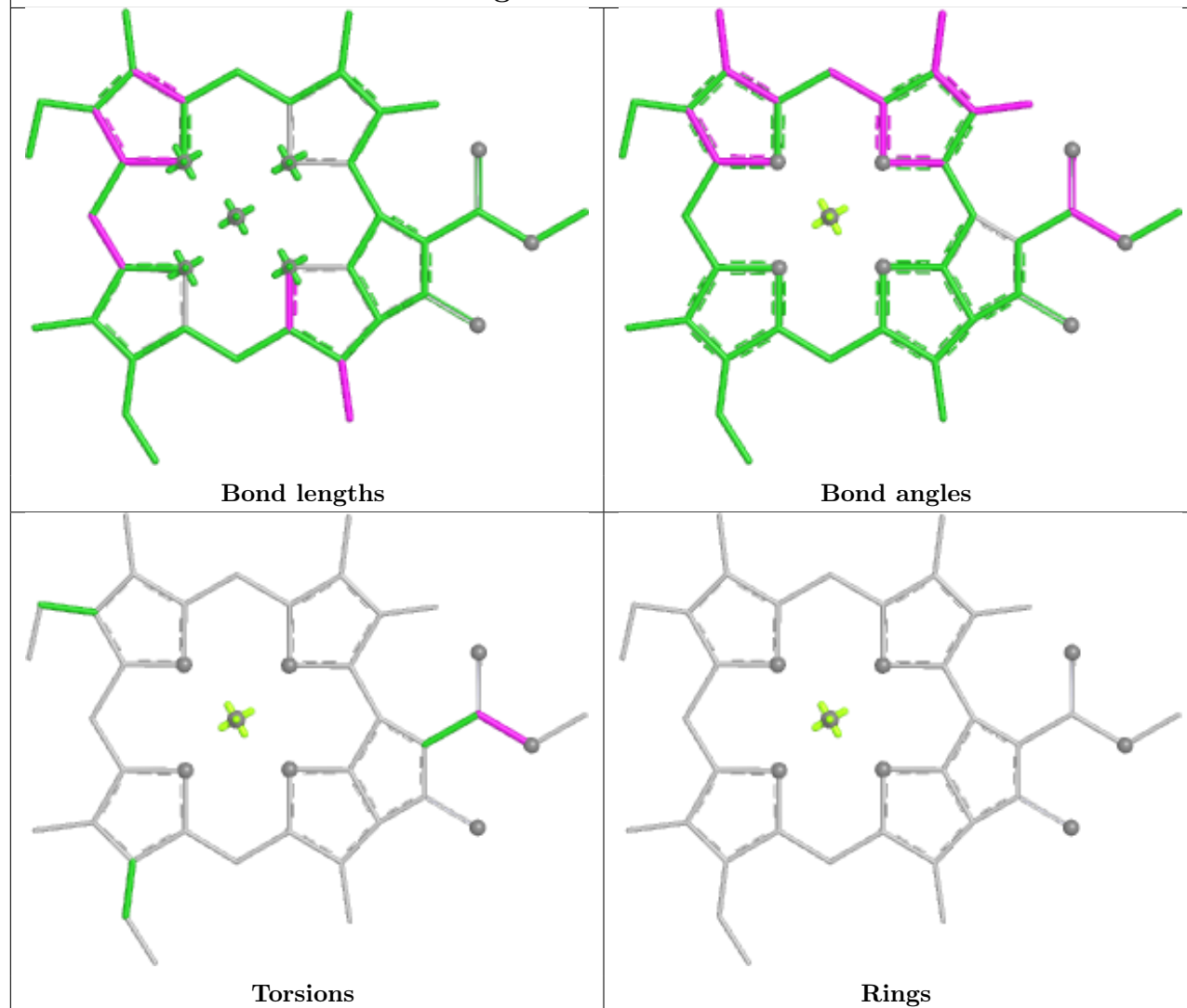
Ligand PQN a 732



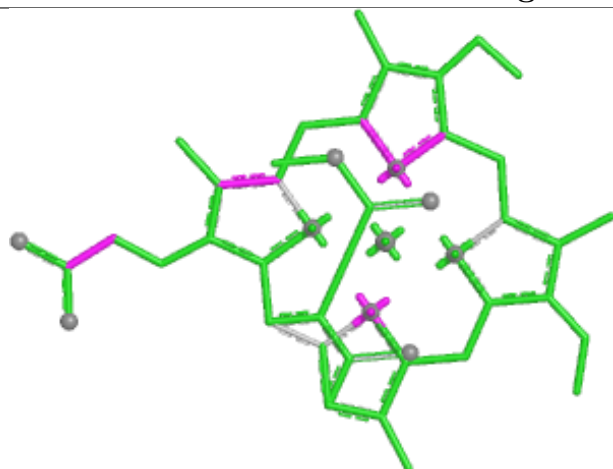
Ligand CLA B 313



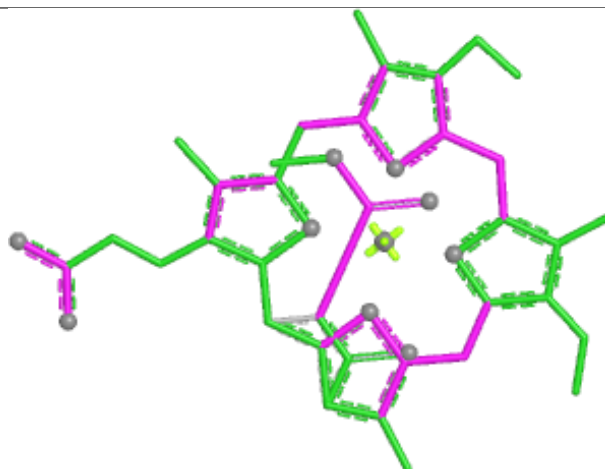
Ligand CLA K 315



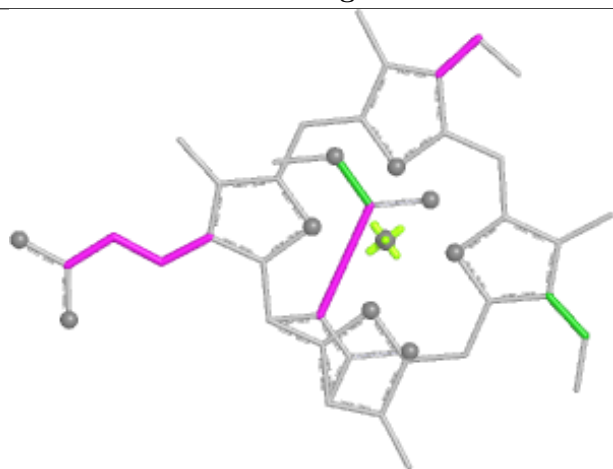
Ligand KC1 F 309



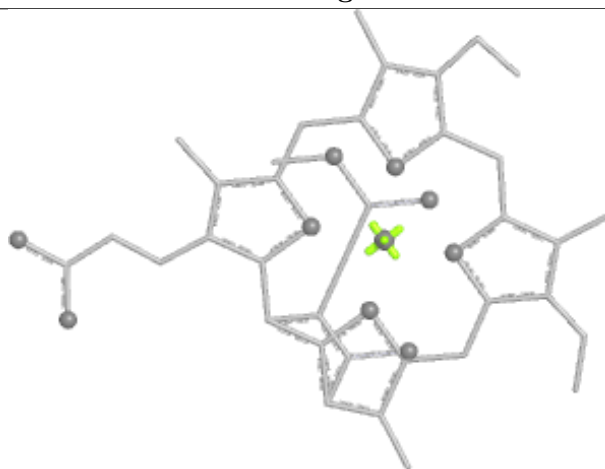
Bond lengths



Bond angles

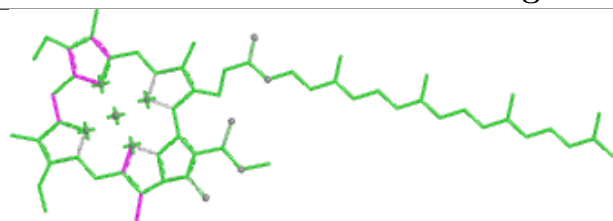


Torsions

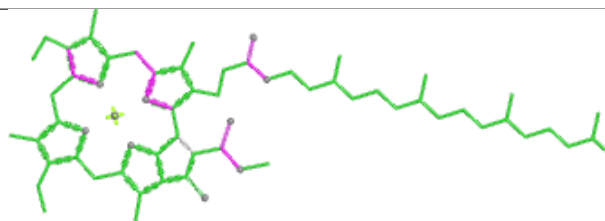


Rings

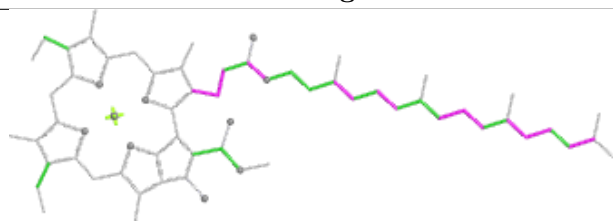
Ligand CLA I 311



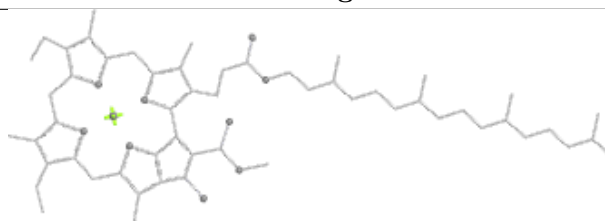
Bond lengths



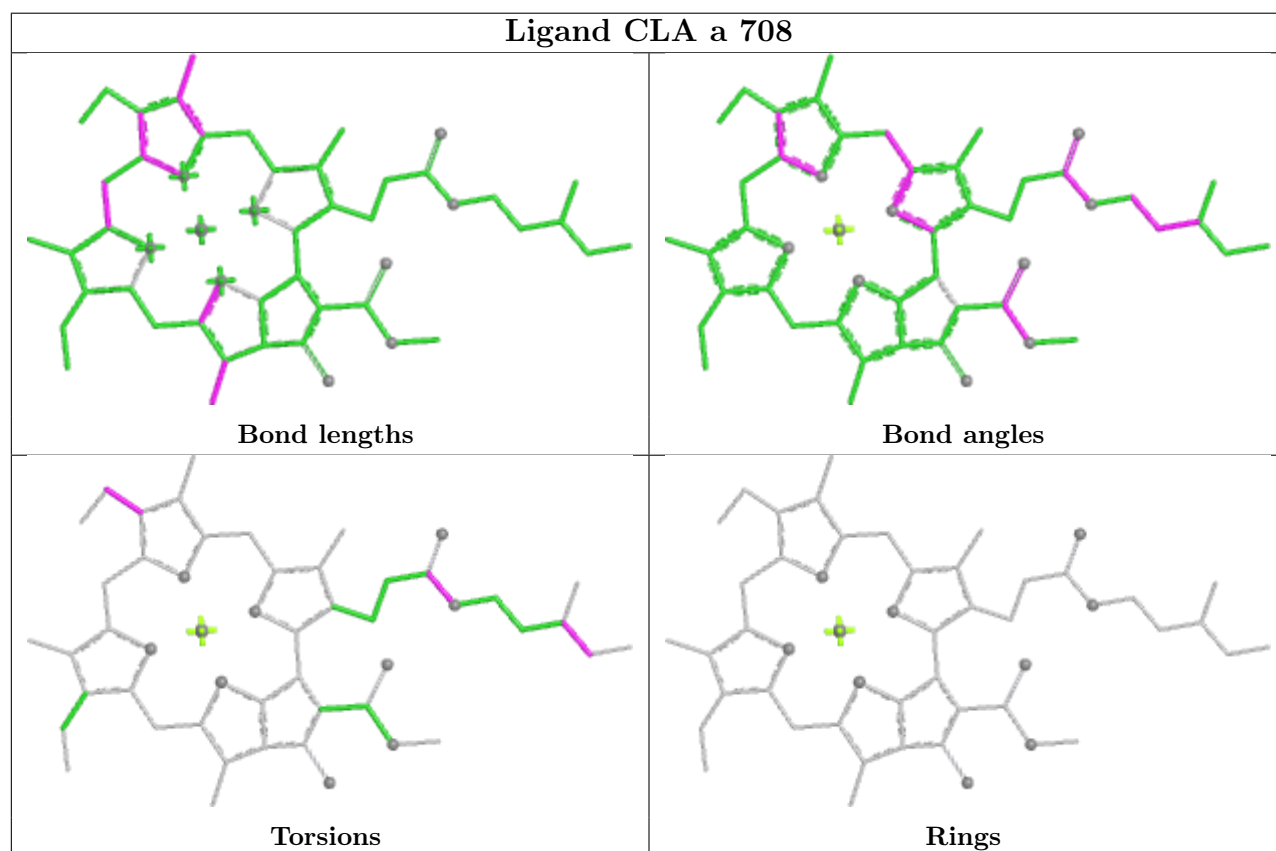
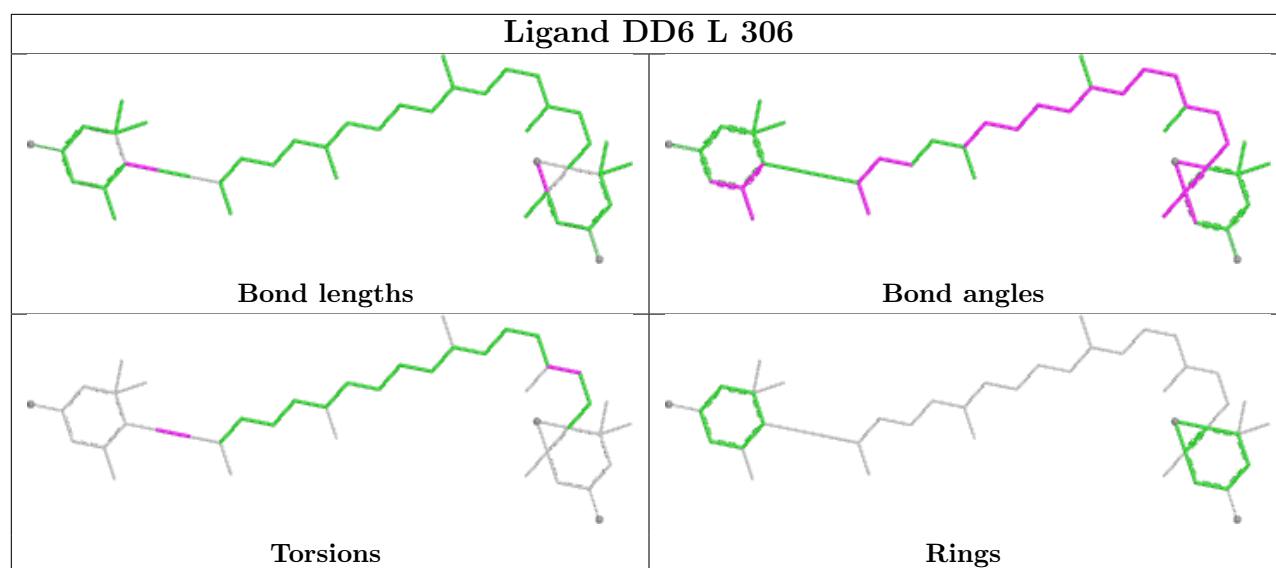
Bond angles

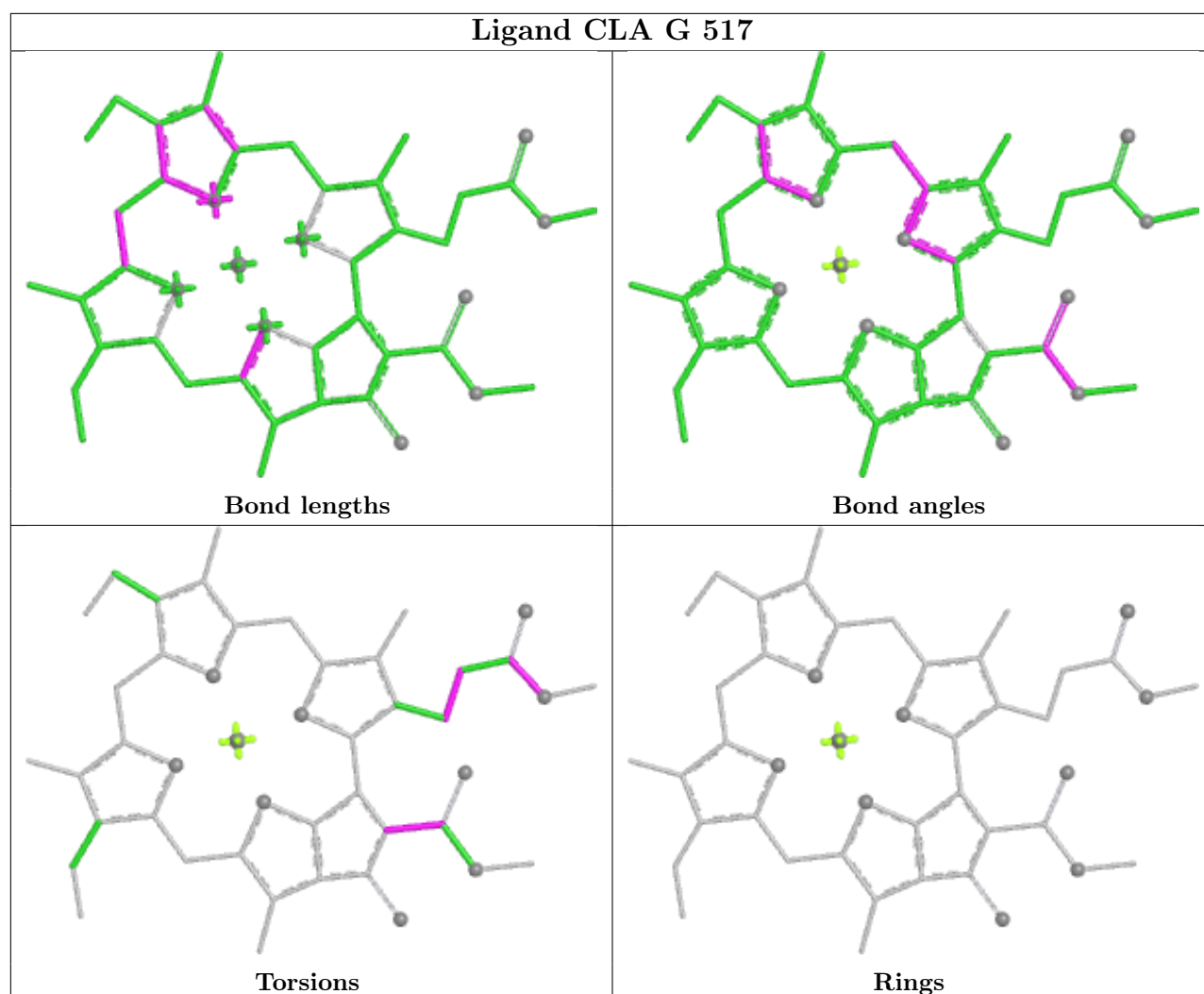


Torsions

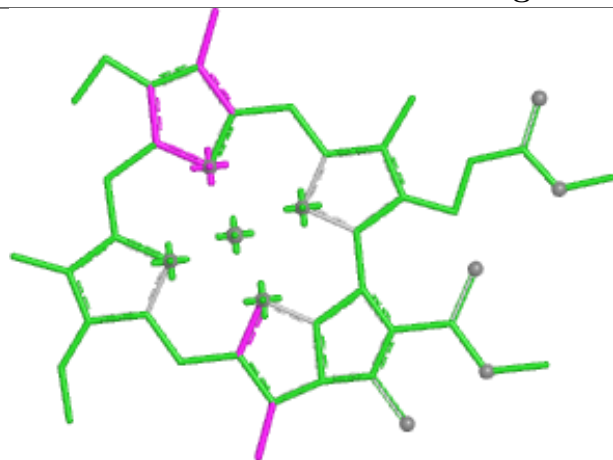


Rings

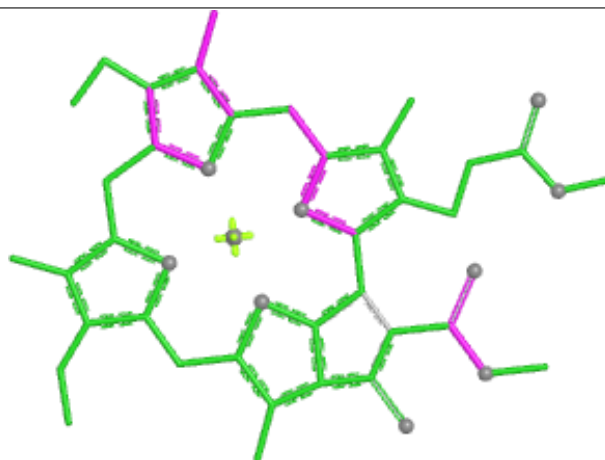




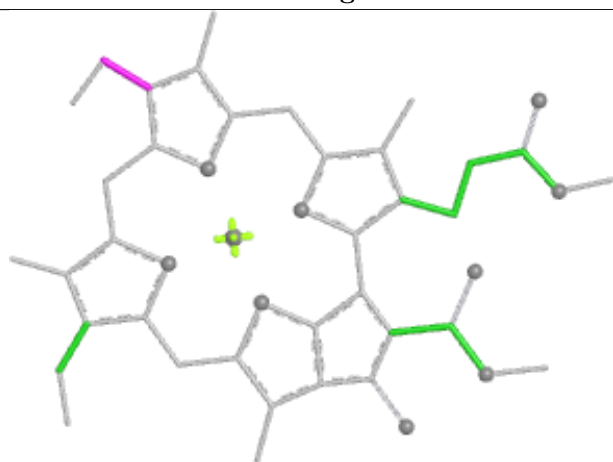
Ligand CLA K 307



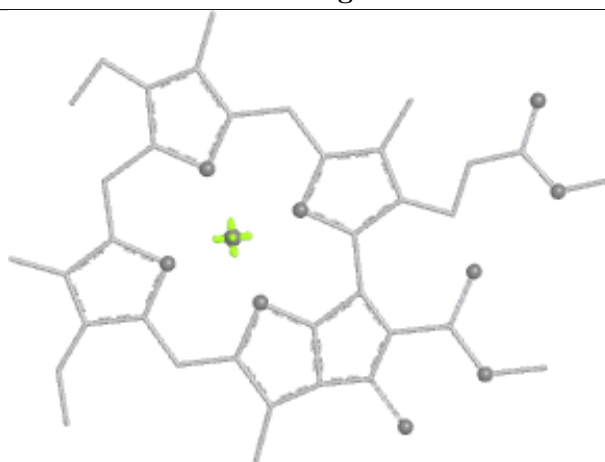
Bond lengths



Bond angles

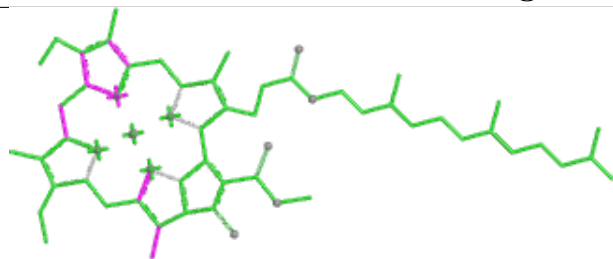


Torsions

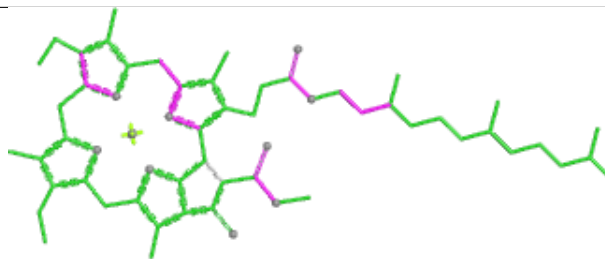


Rings

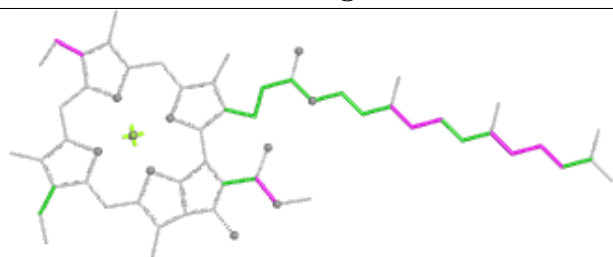
Ligand CLA a 713



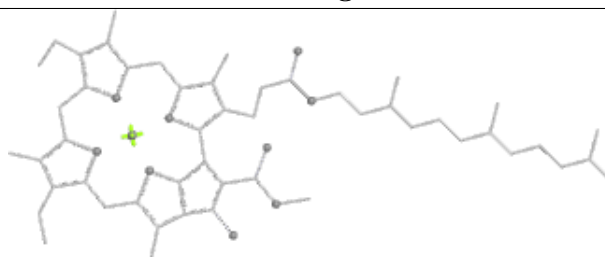
Bond lengths



Bond angles

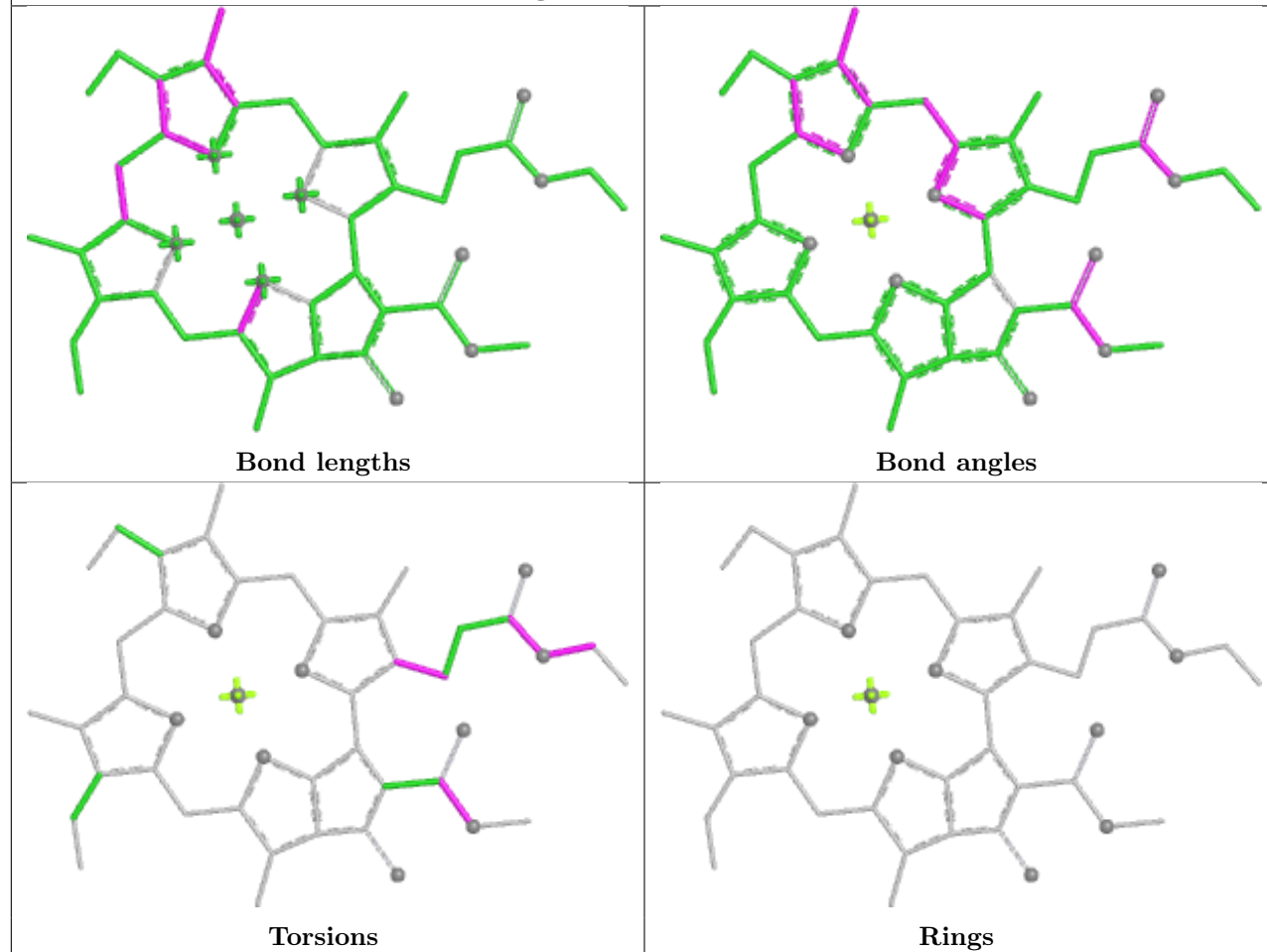


Torsions

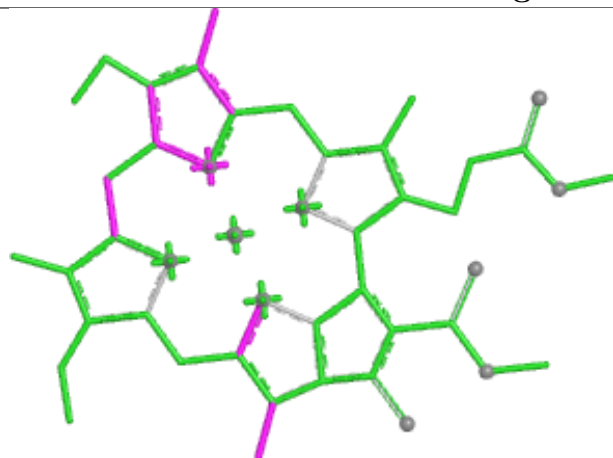


Rings

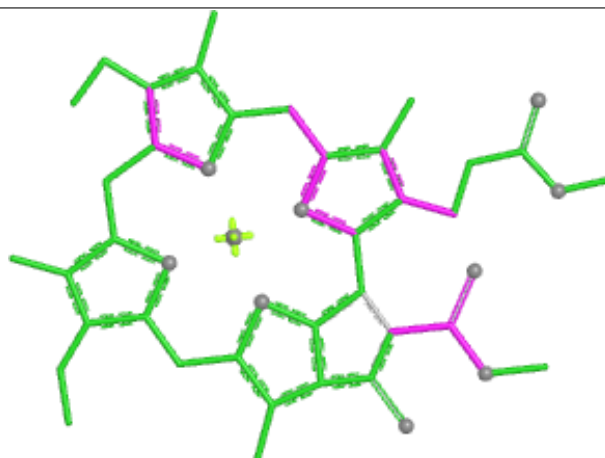
Ligand CLA J 311



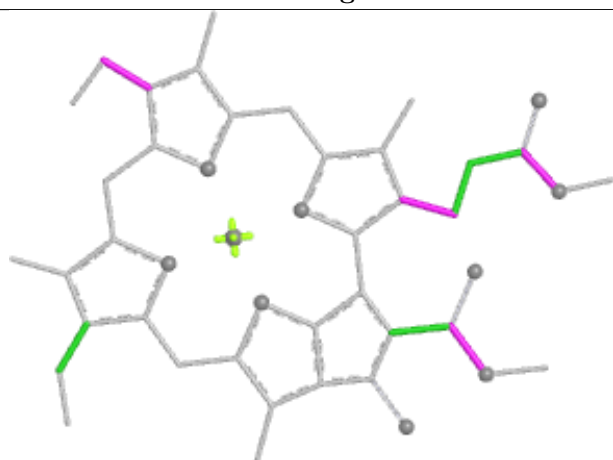
Ligand CLA D 314



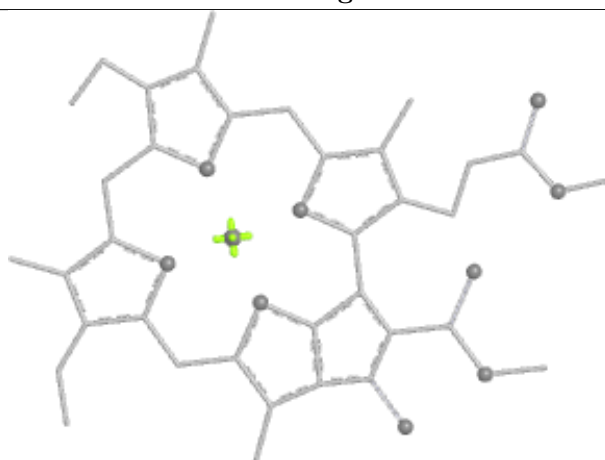
Bond lengths



Bond angles

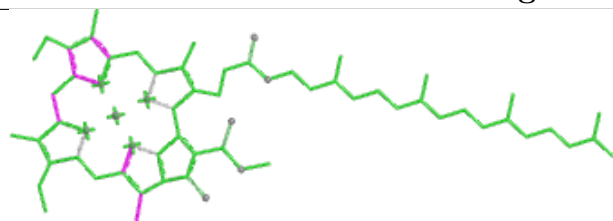


Torsions

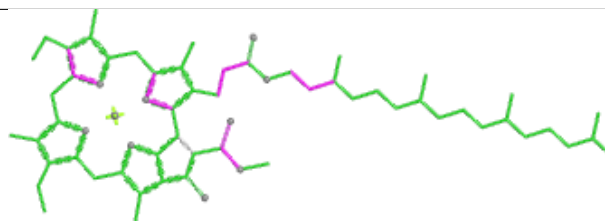


Rings

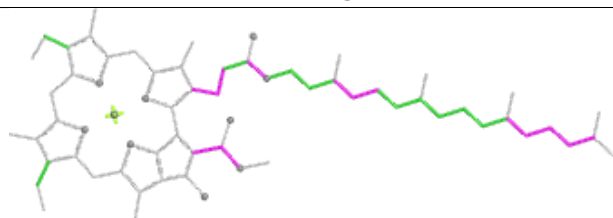
Ligand CLA a 735



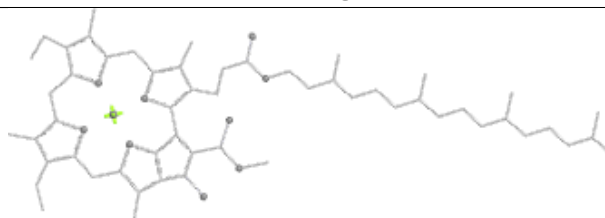
Bond lengths



Bond angles

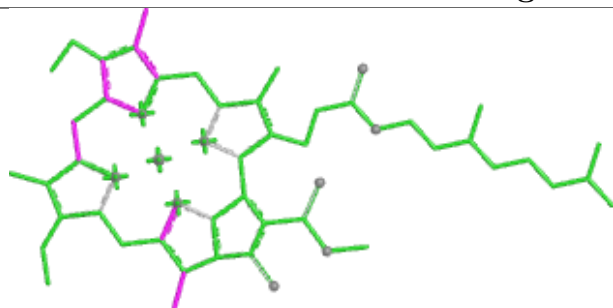


Torsions

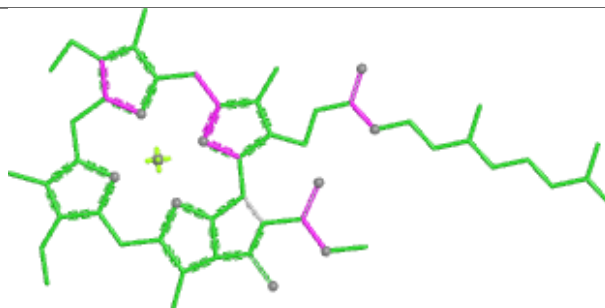


Rings

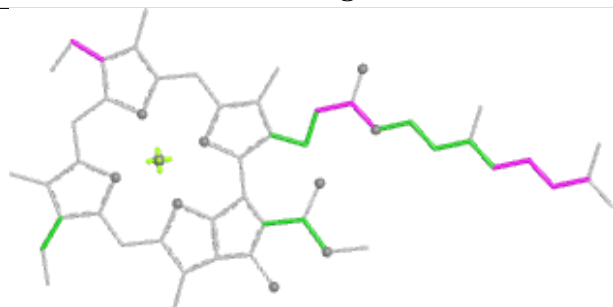
Ligand CLA h 202



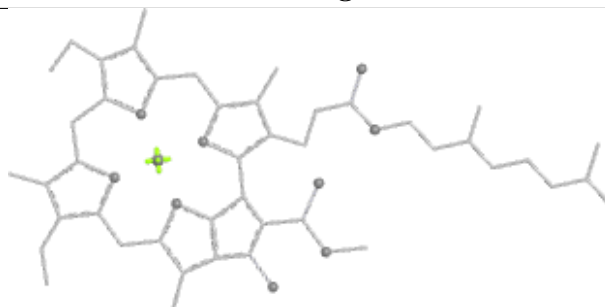
Bond lengths



Bond angles

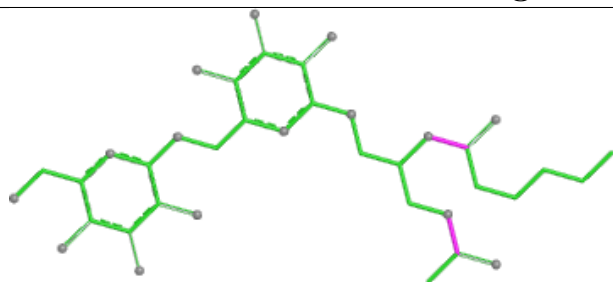


Torsions

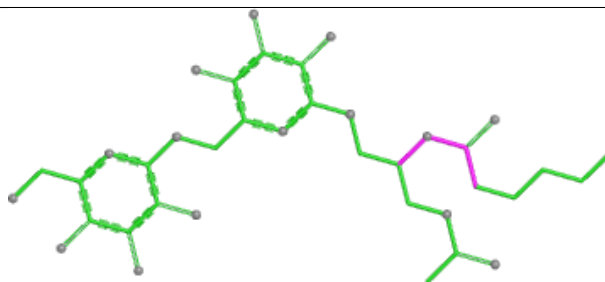


Rings

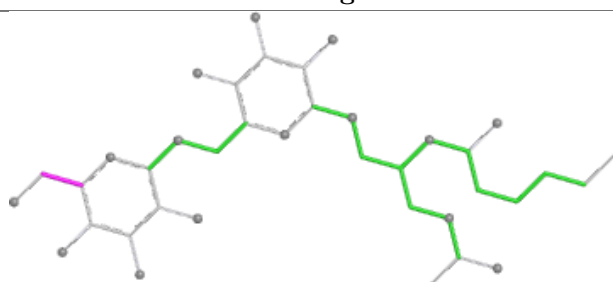
Ligand DGD L 301



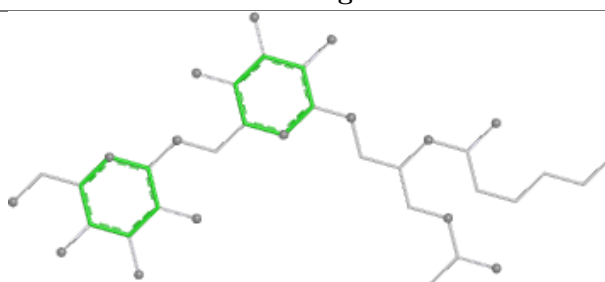
Bond lengths



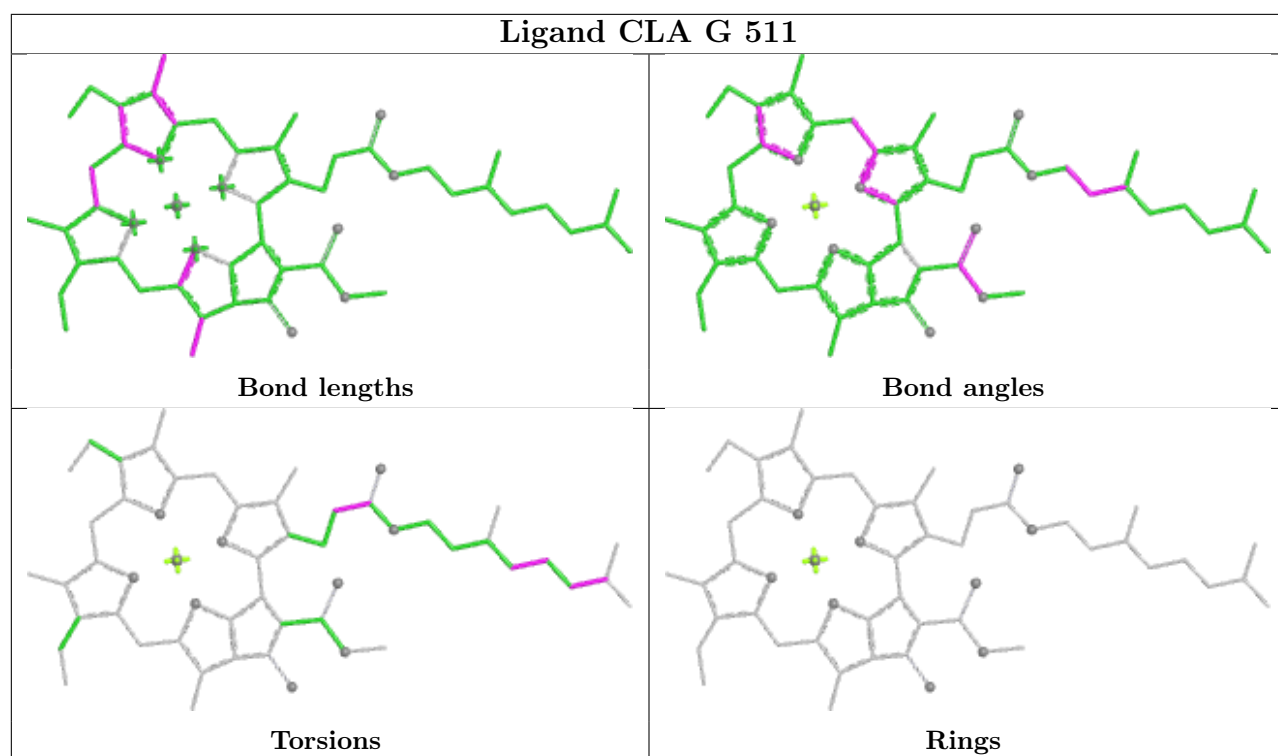
Bond angles



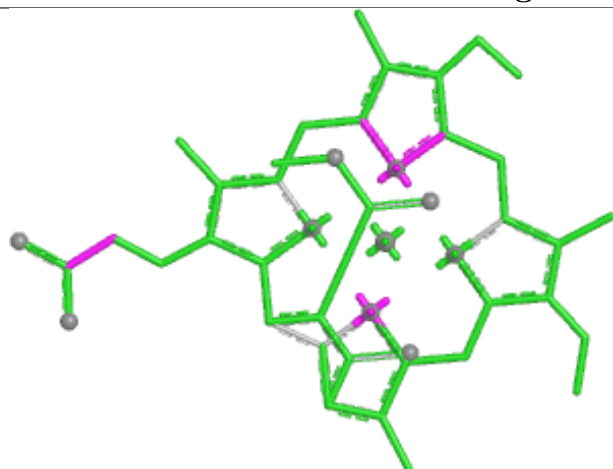
Torsions



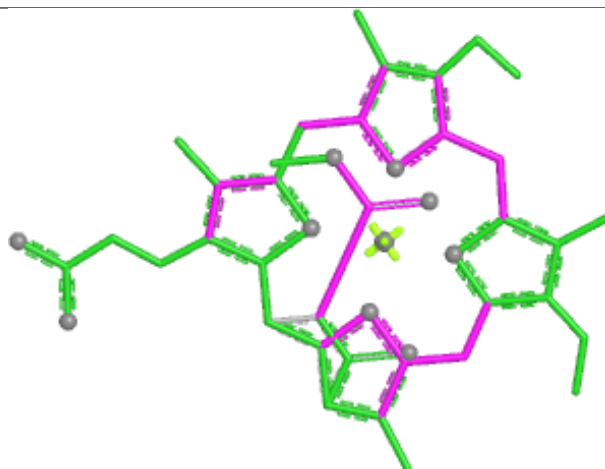
Rings



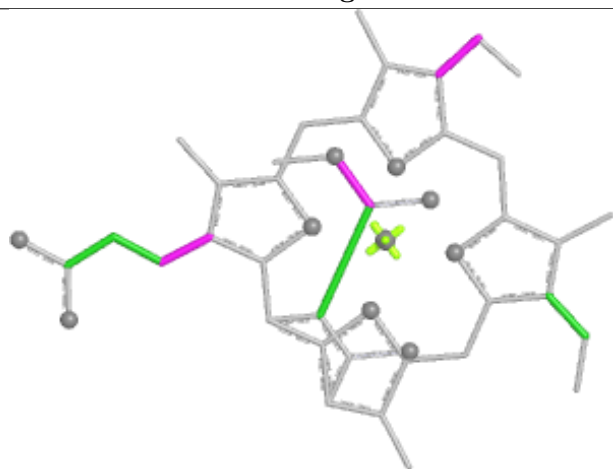
Ligand KC1 H 310



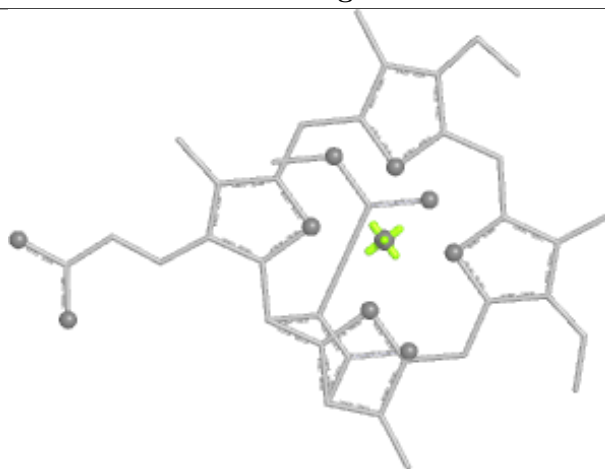
Bond lengths



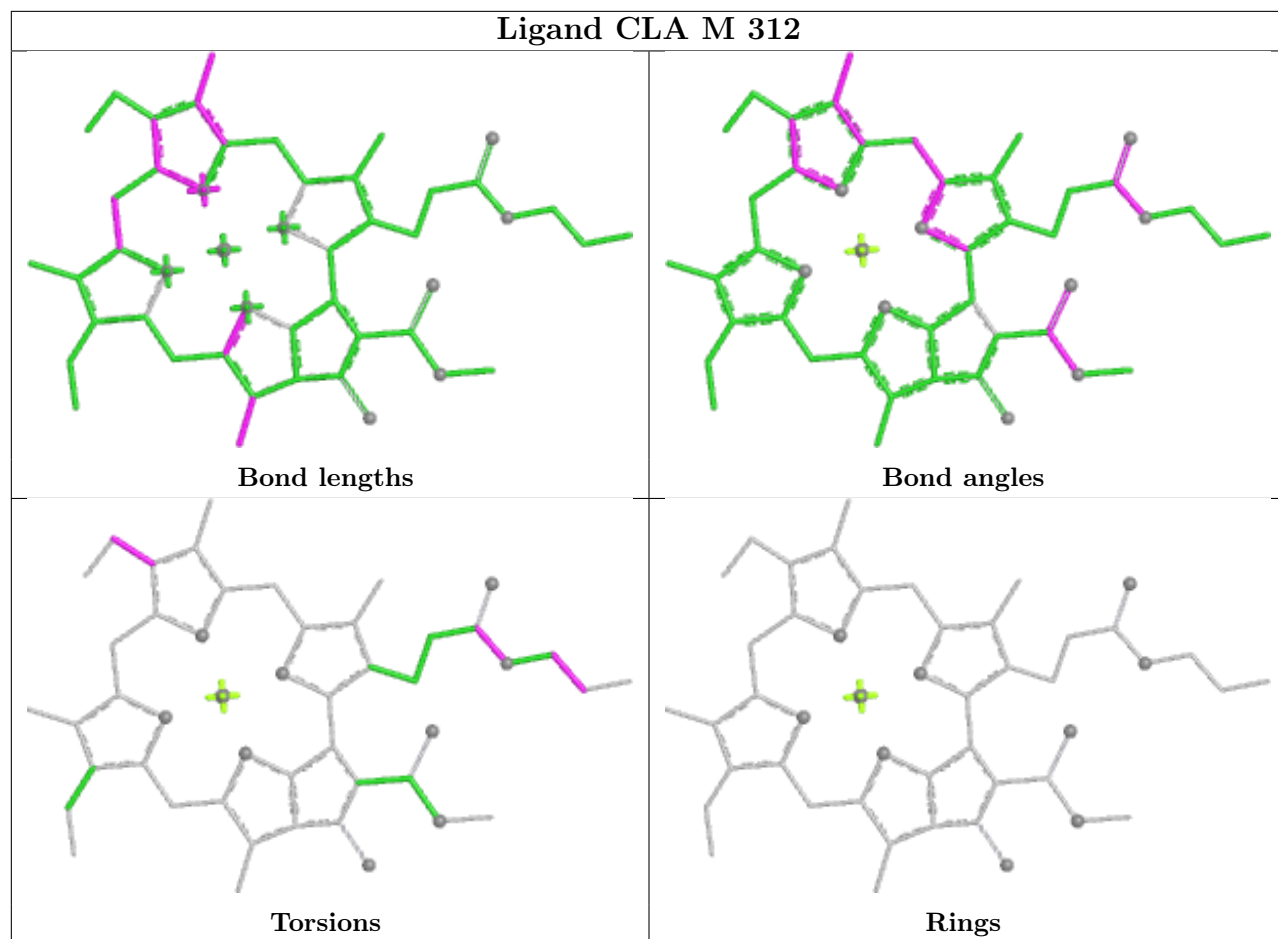
Bond angles



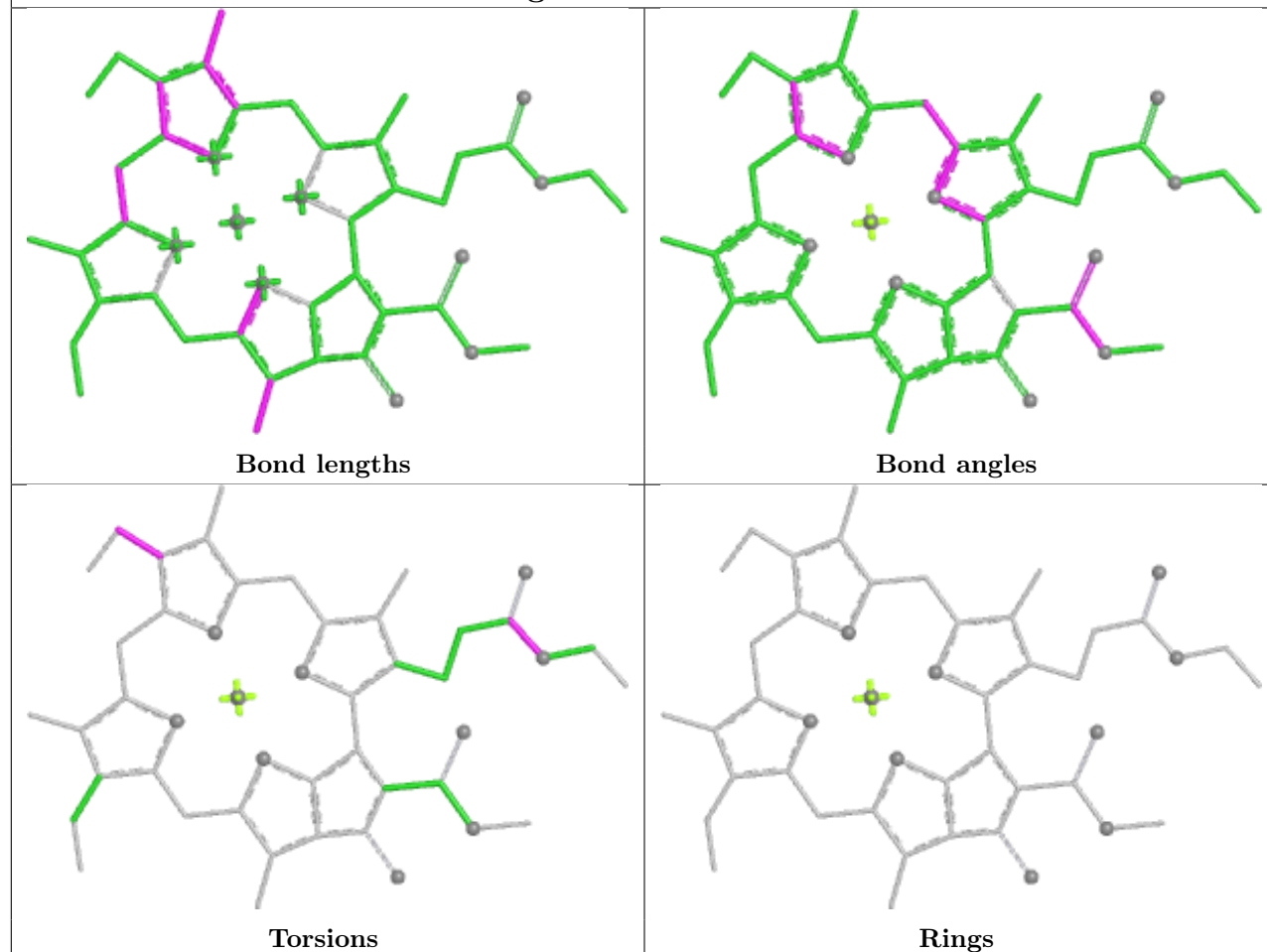
Torsions



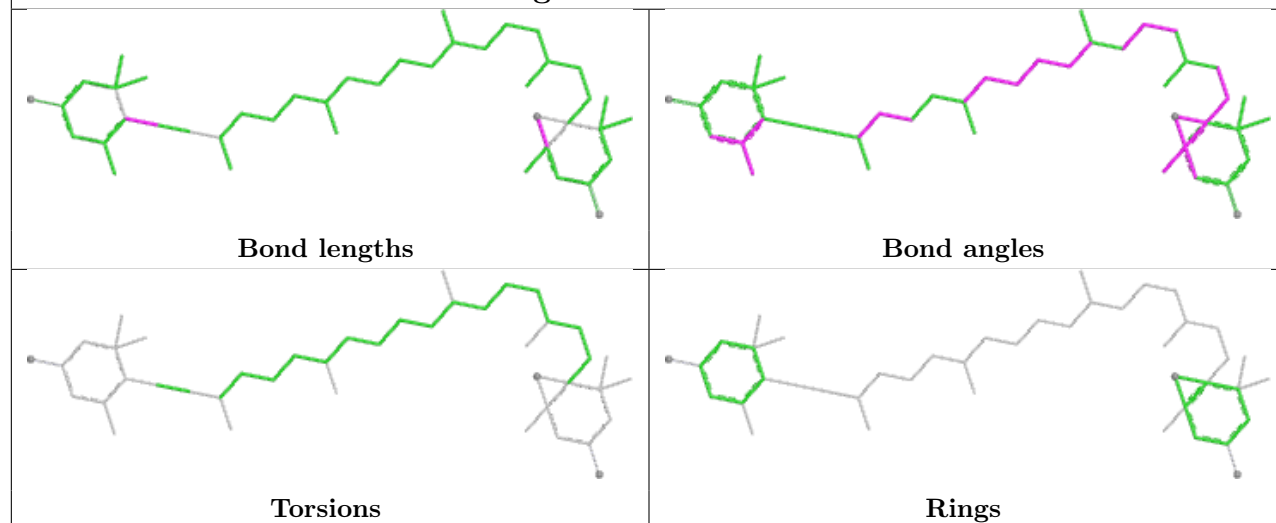
Rings



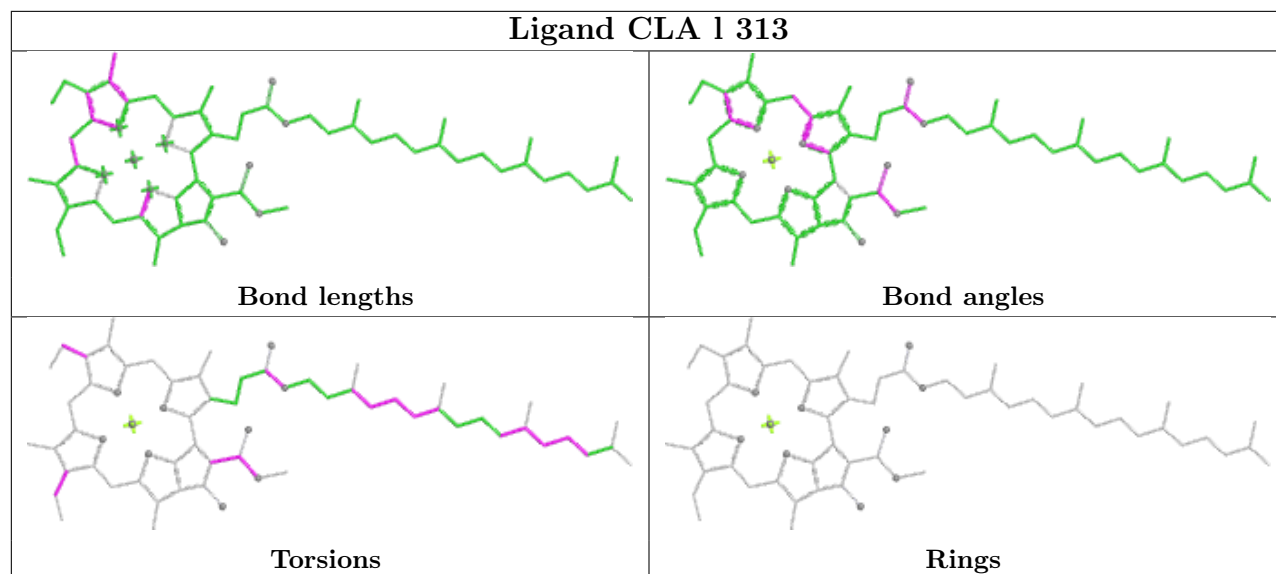
Ligand CLA D 308



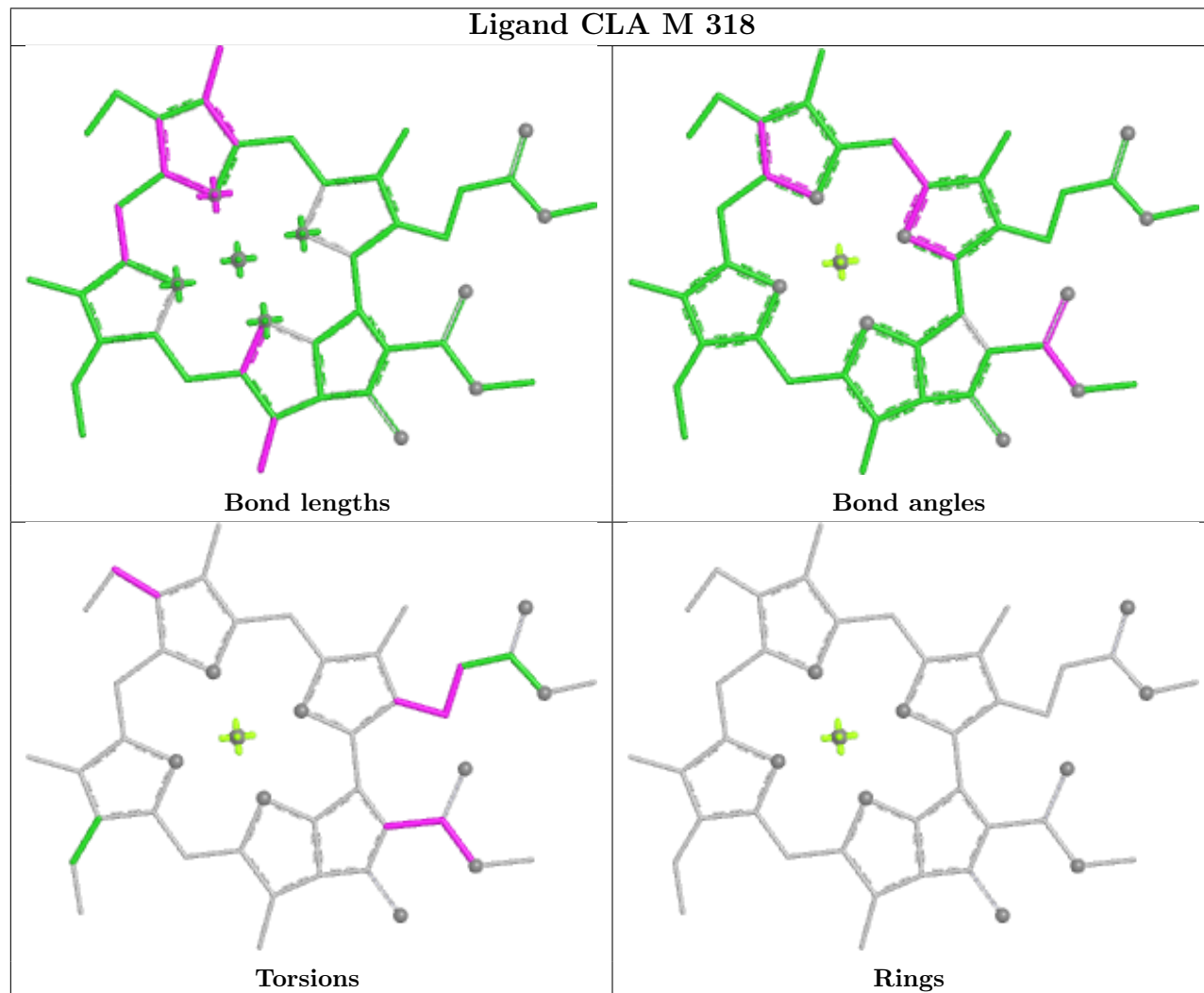
Ligand DD6 B 304

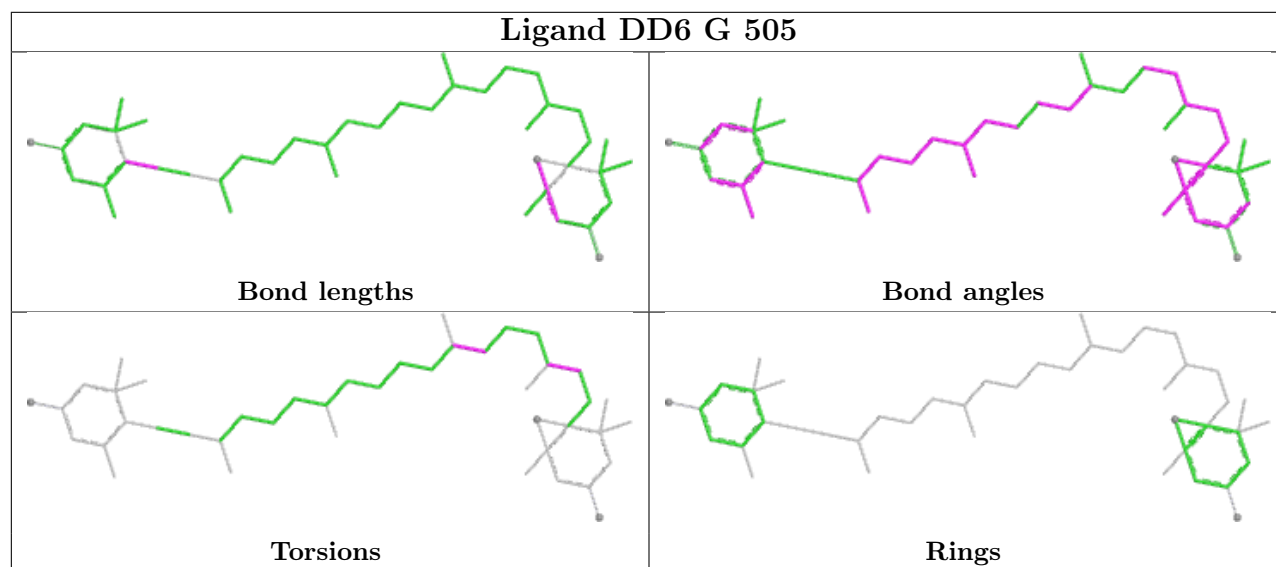
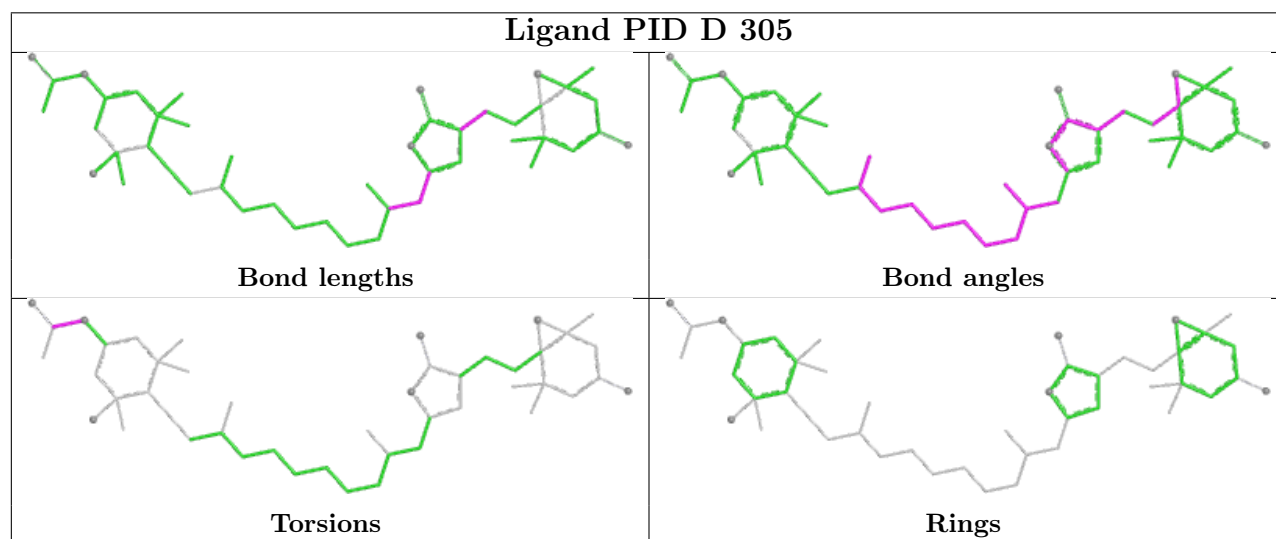
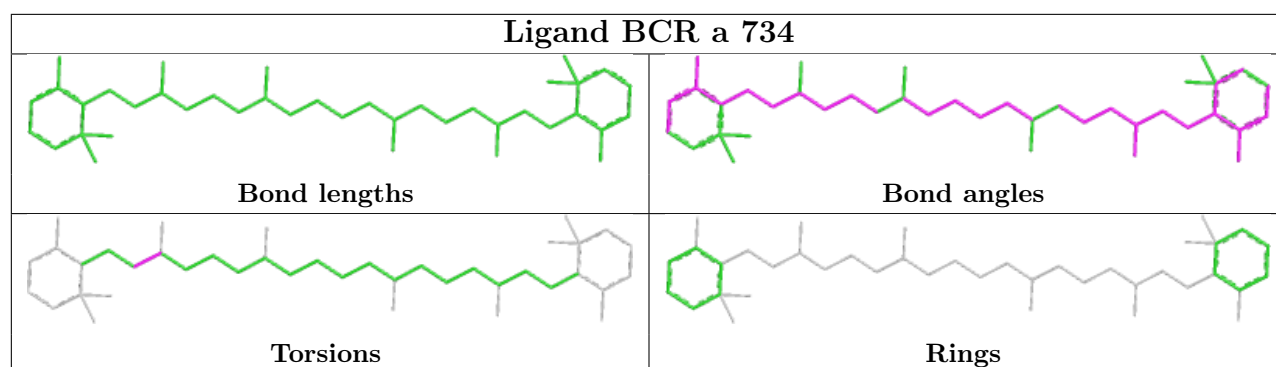


Ligand CLA I 313

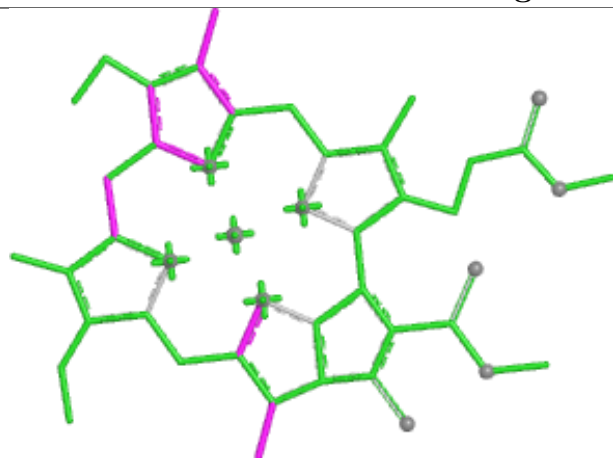


Ligand CLA M 318

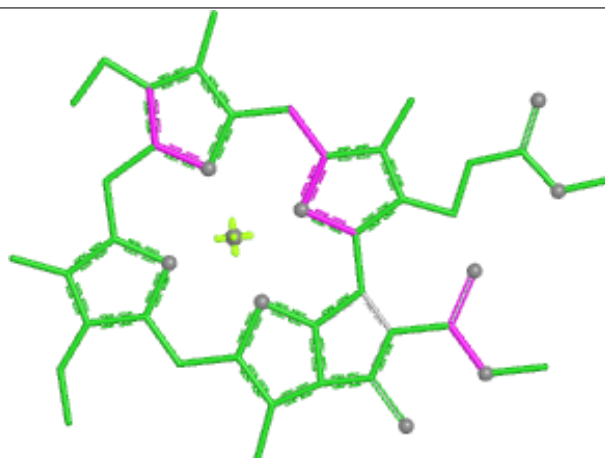




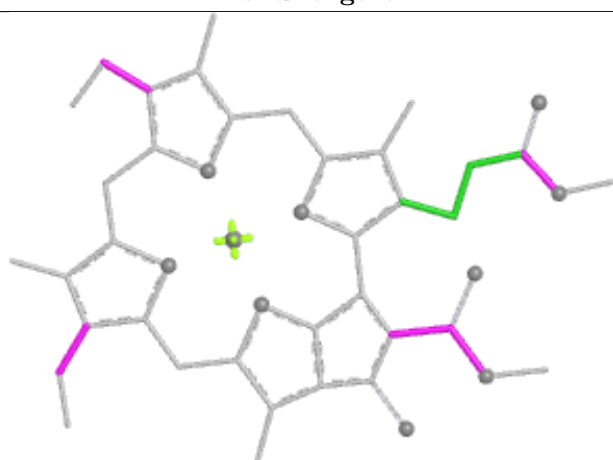
Ligand CLA B 316



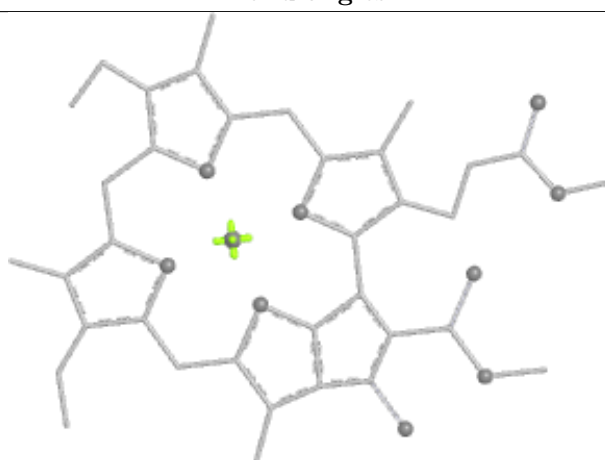
Bond lengths



Bond angles

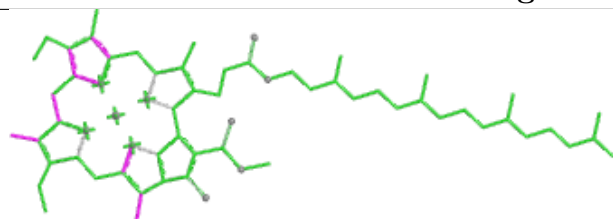


Torsions

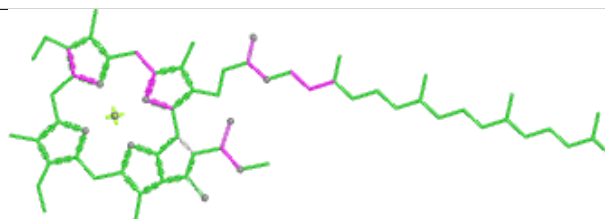


Rings

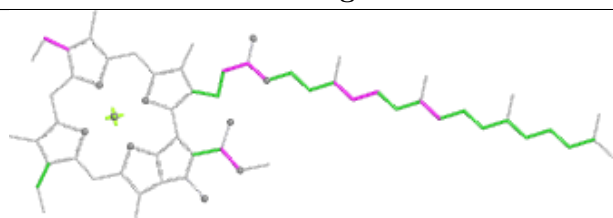
Ligand CLA b 703



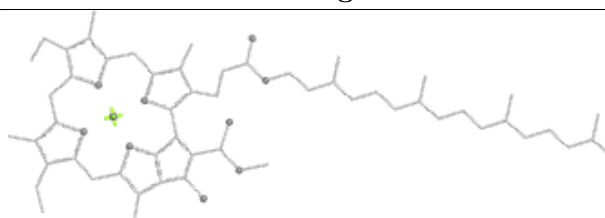
Bond lengths



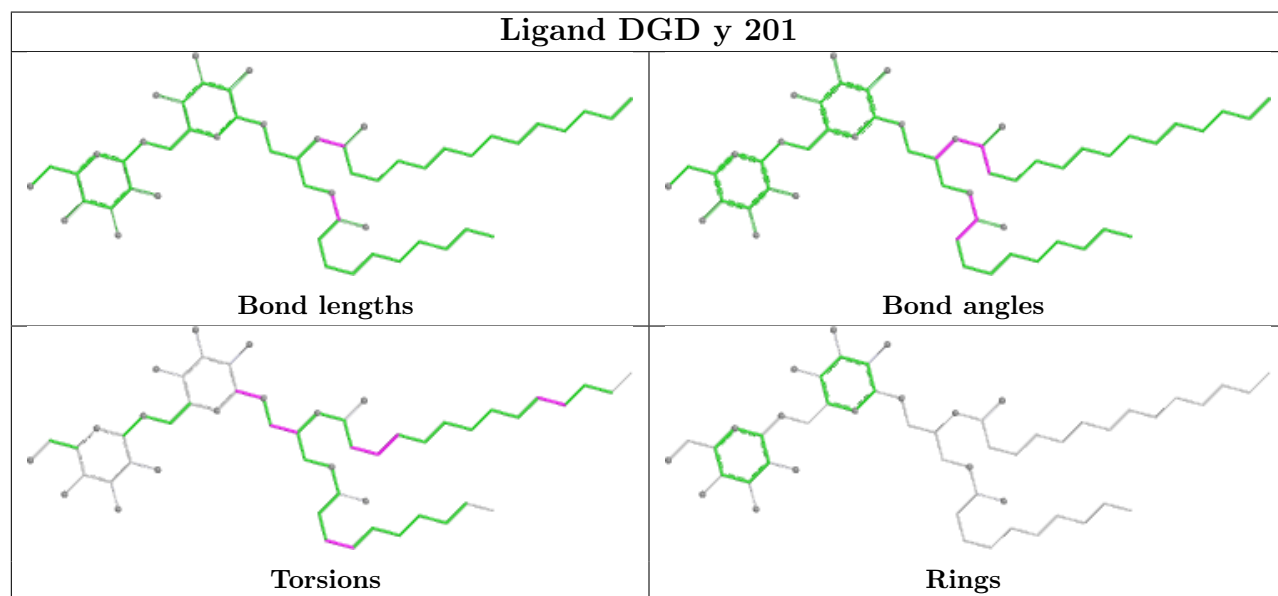
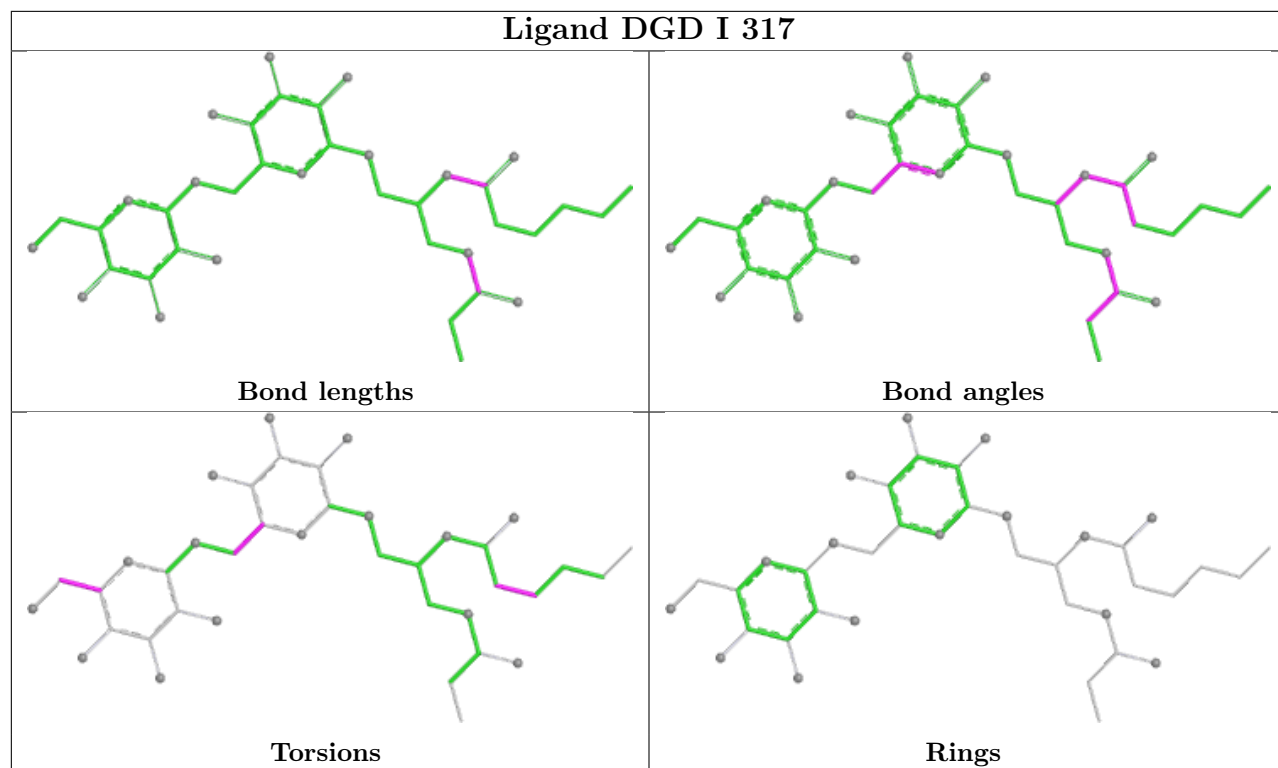
Bond angles



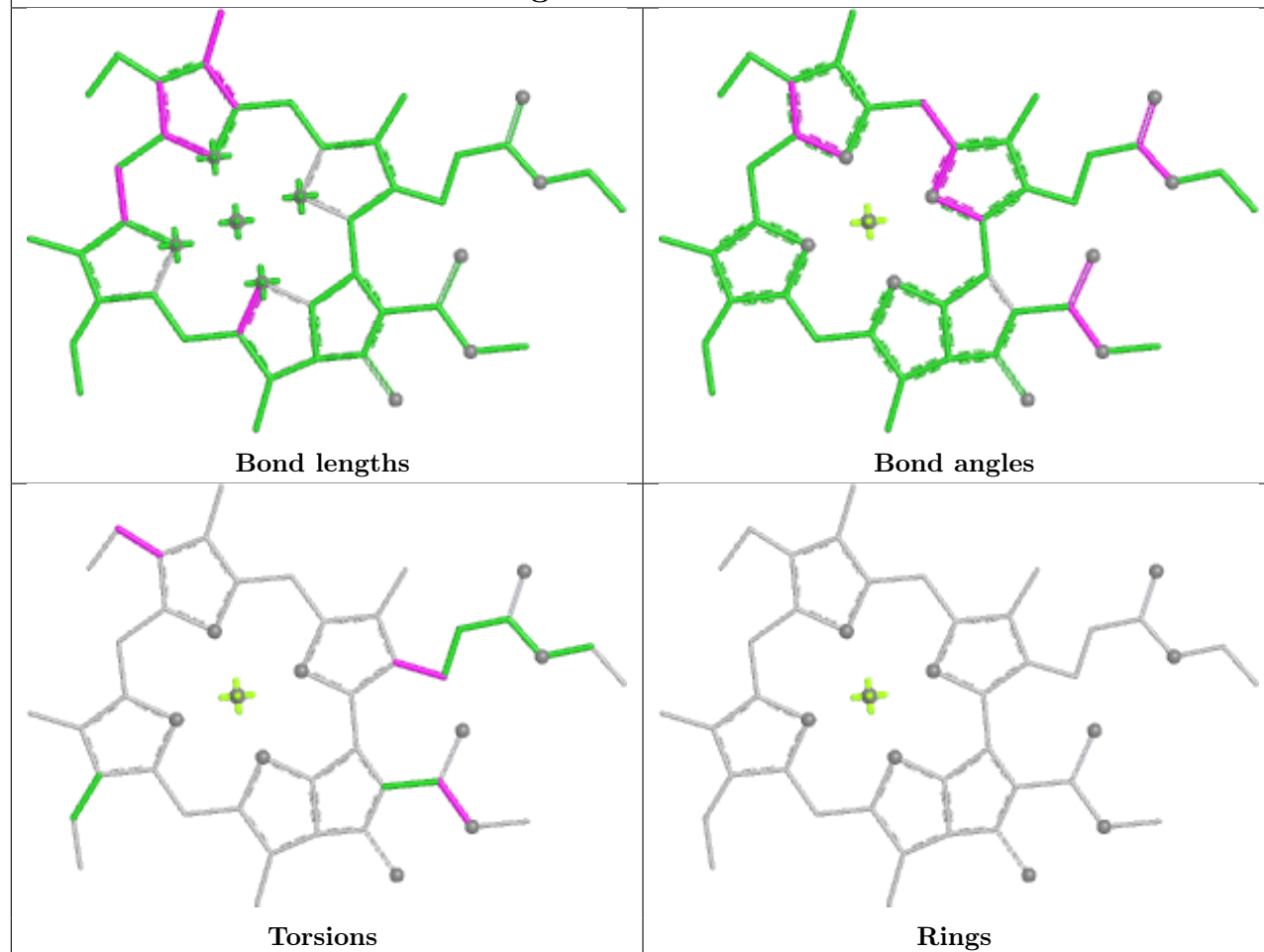
Torsions



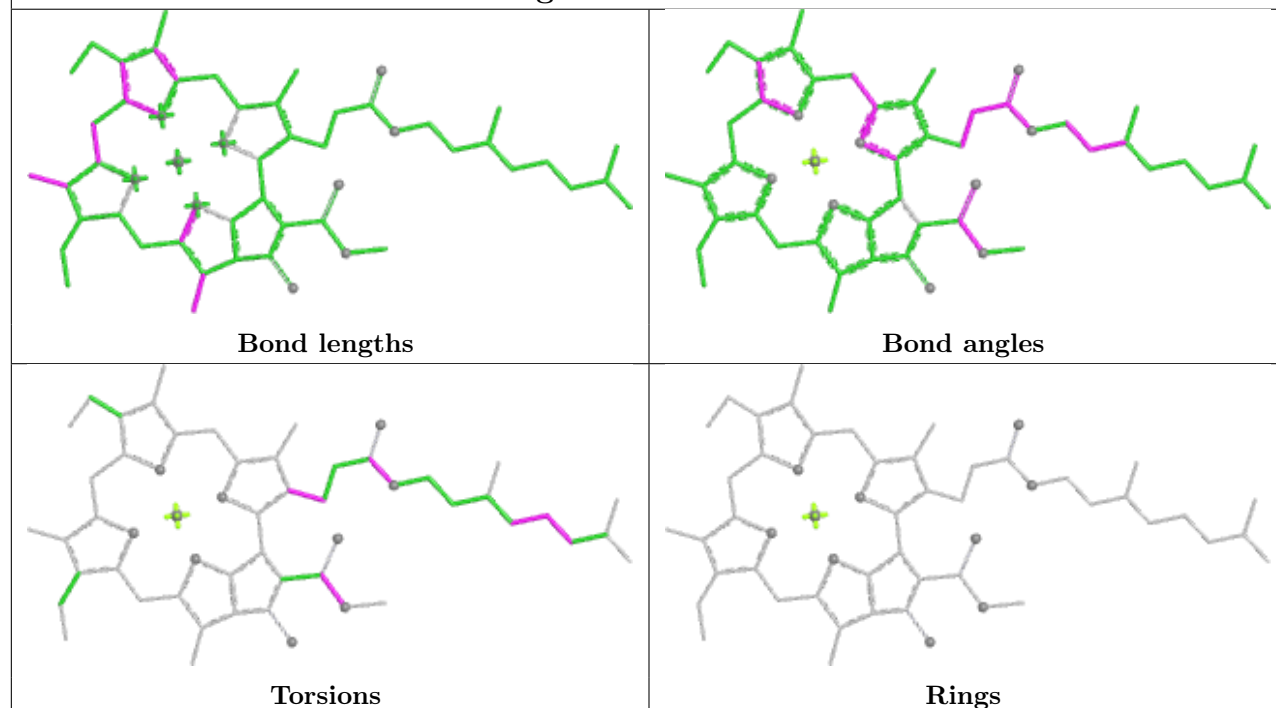
Rings

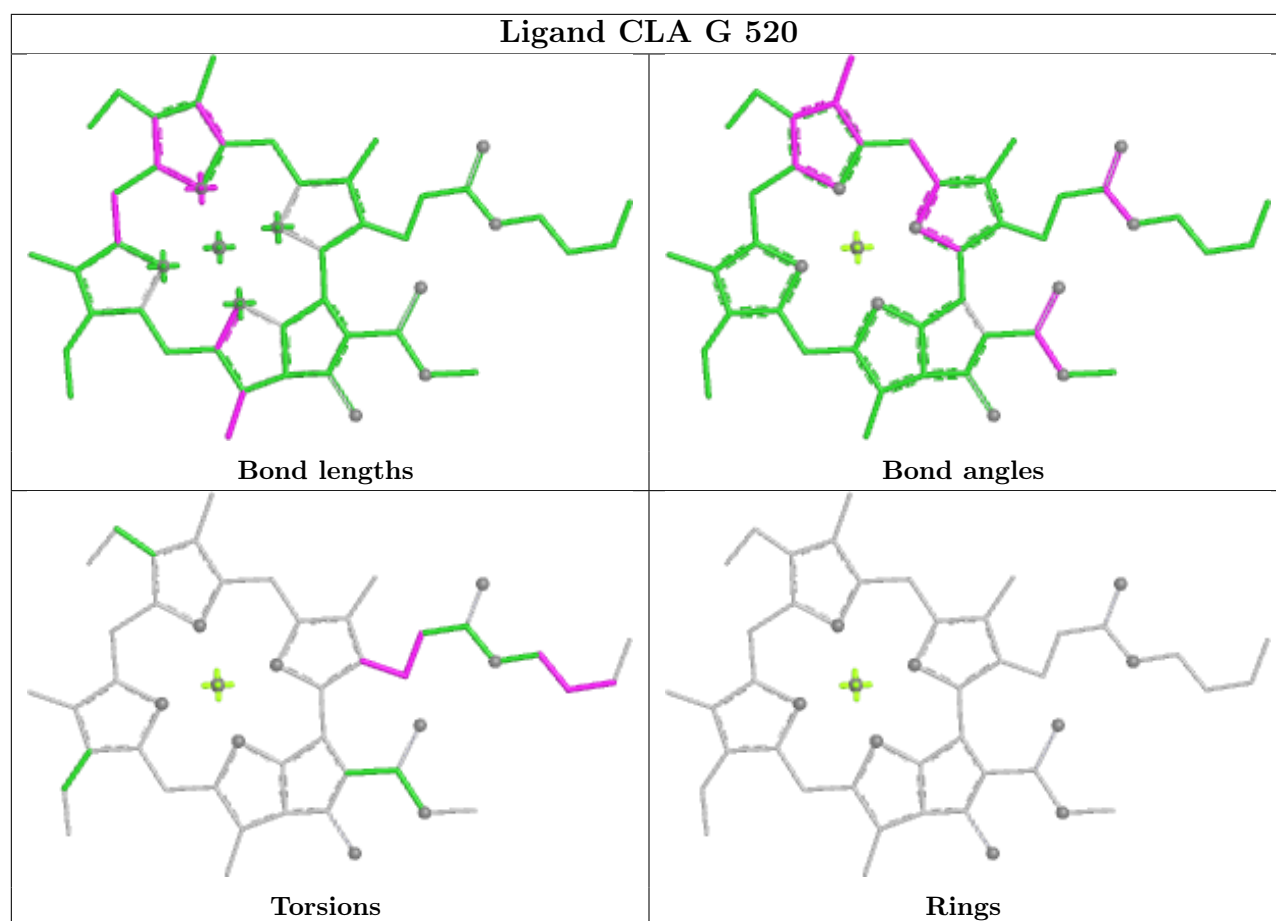


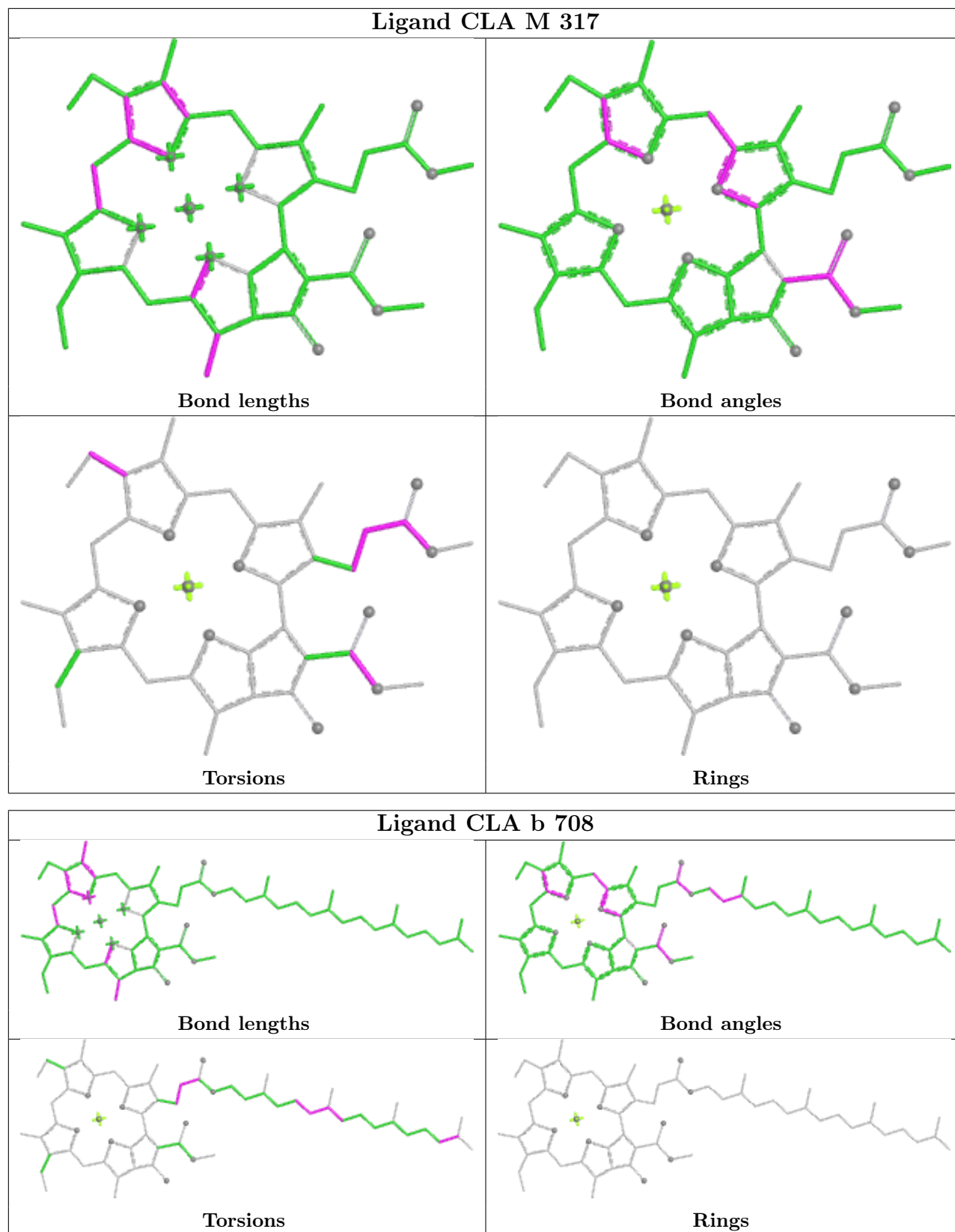
Ligand CLA a 716

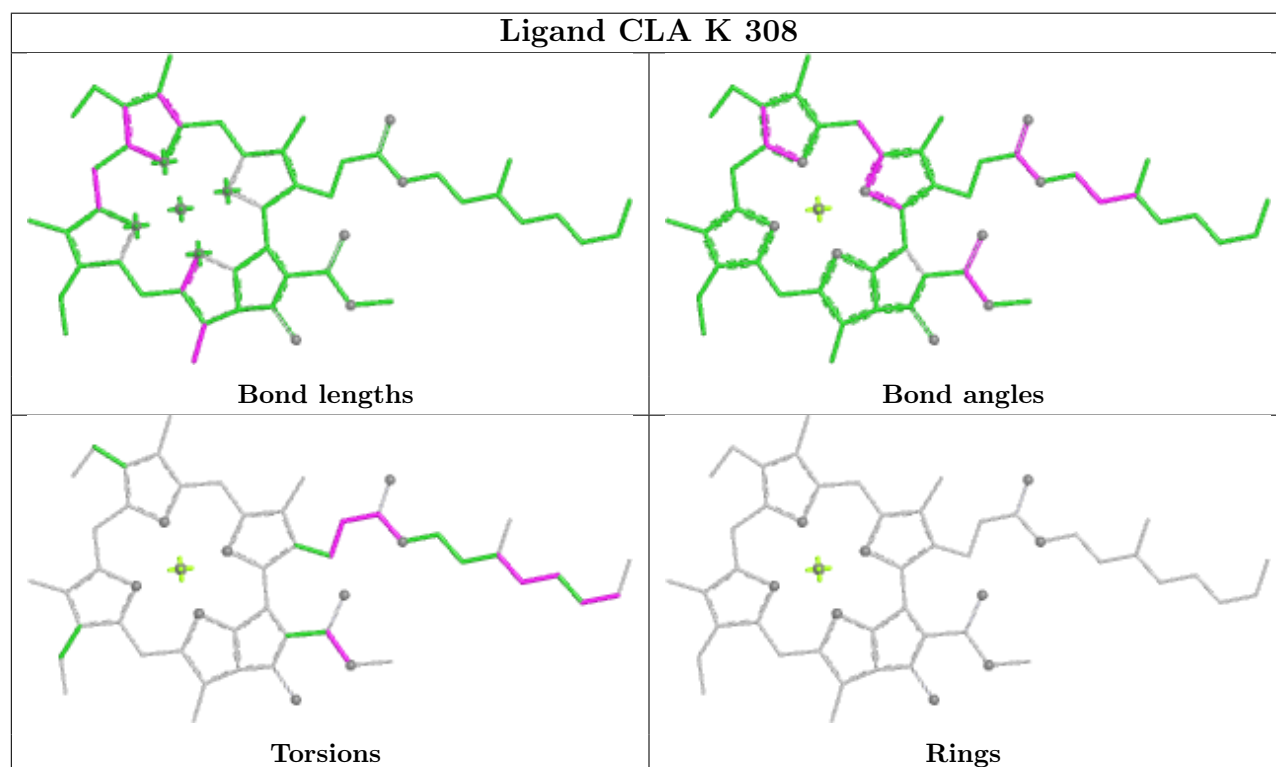
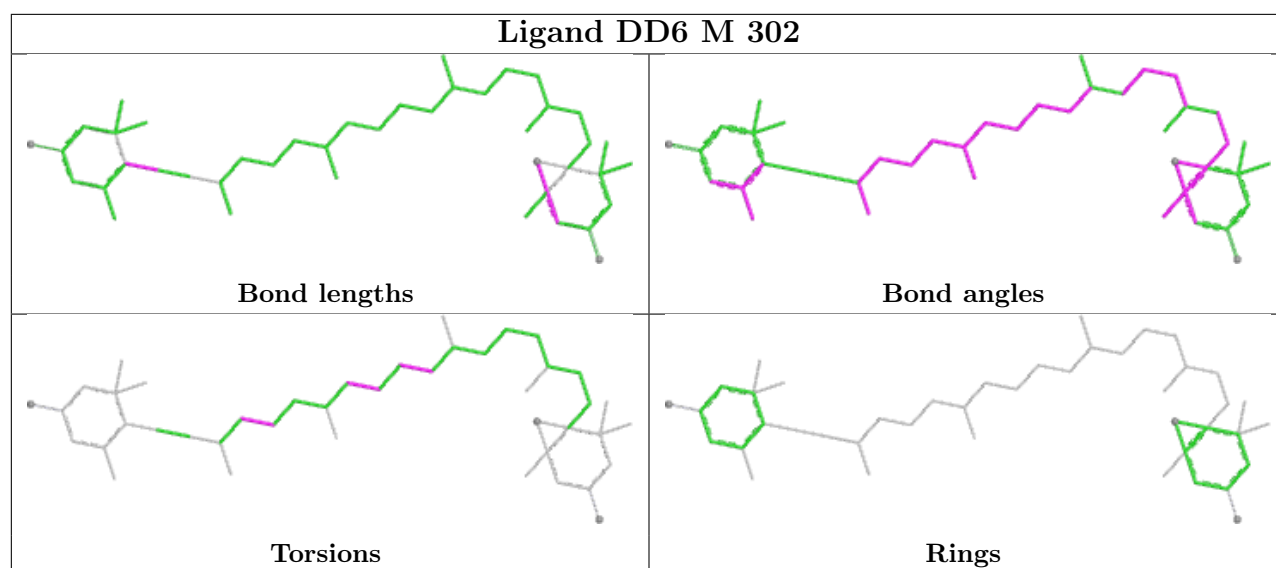


Ligand CLA a 705

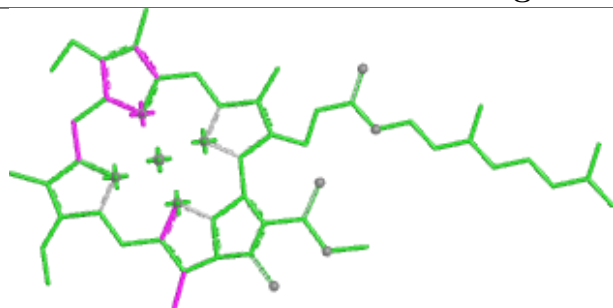




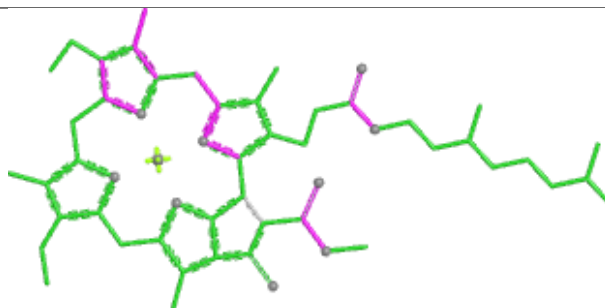




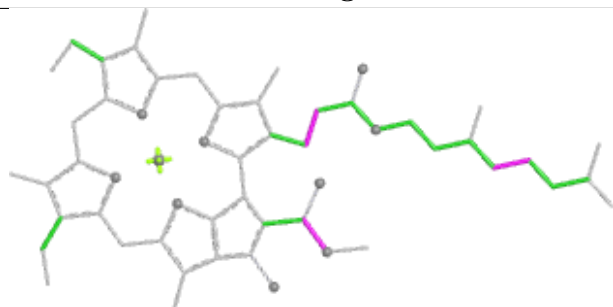
Ligand CLA A 308



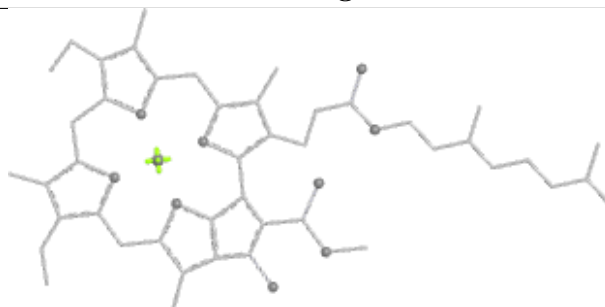
Bond lengths



Bond angles

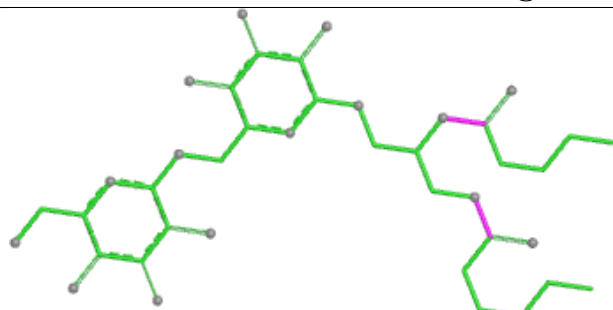


Torsions

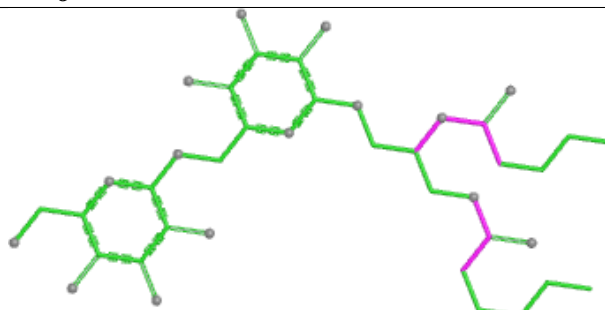


Rings

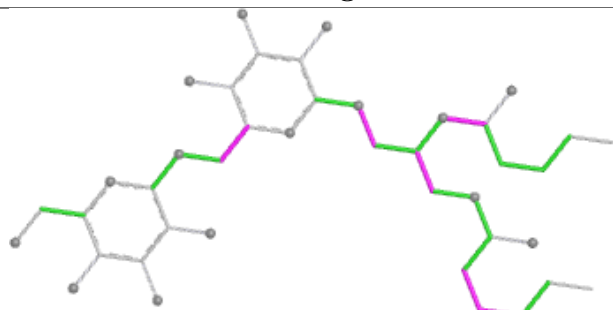
Ligand DGD j 103



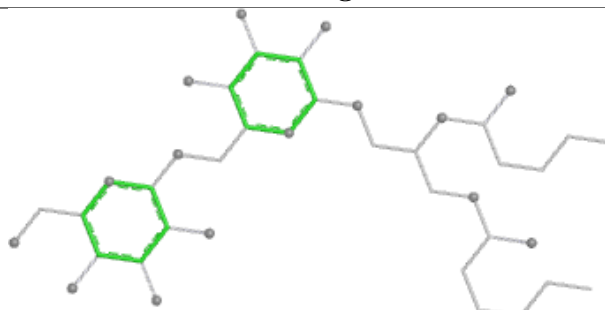
Bond lengths



Bond angles

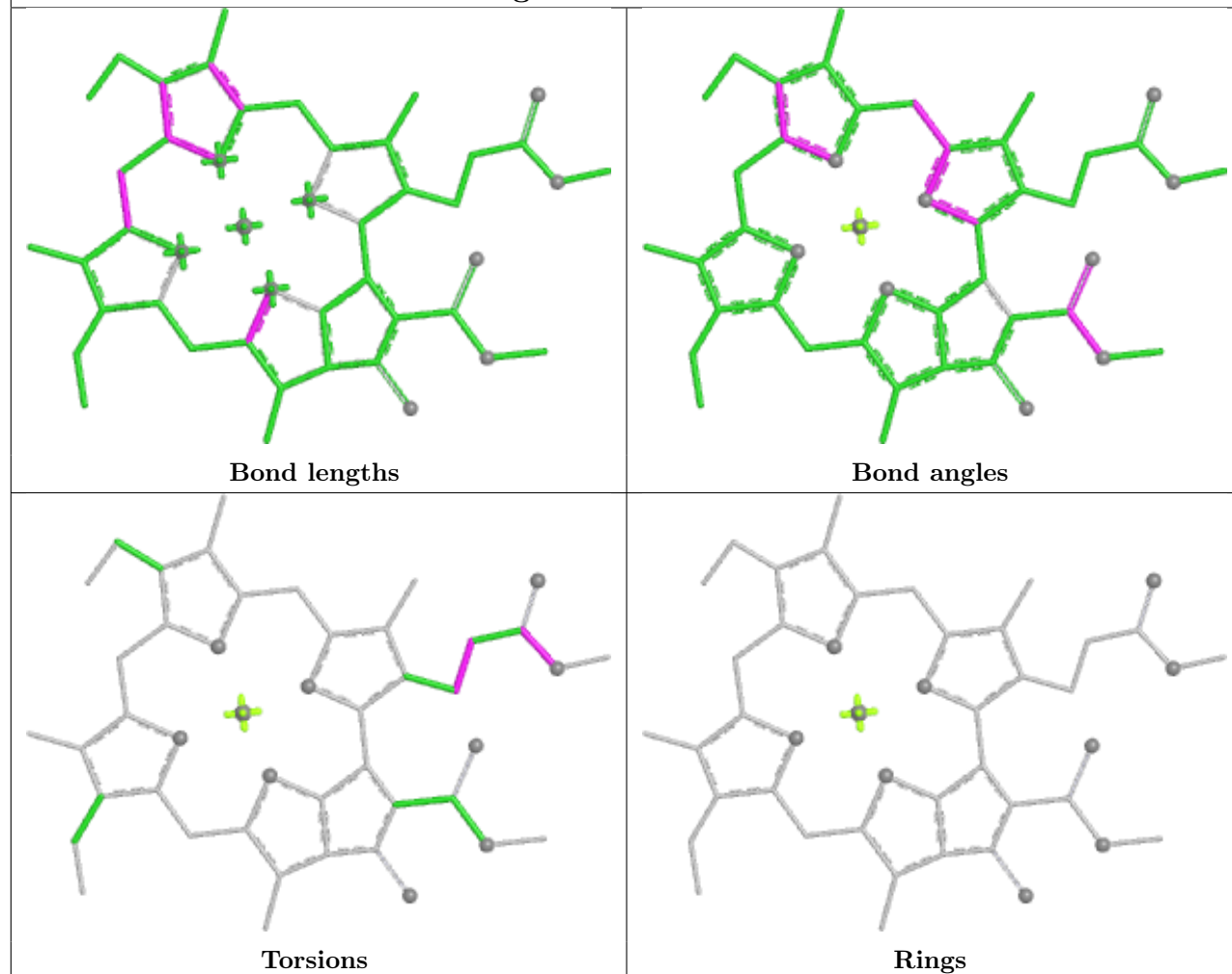


Torsions

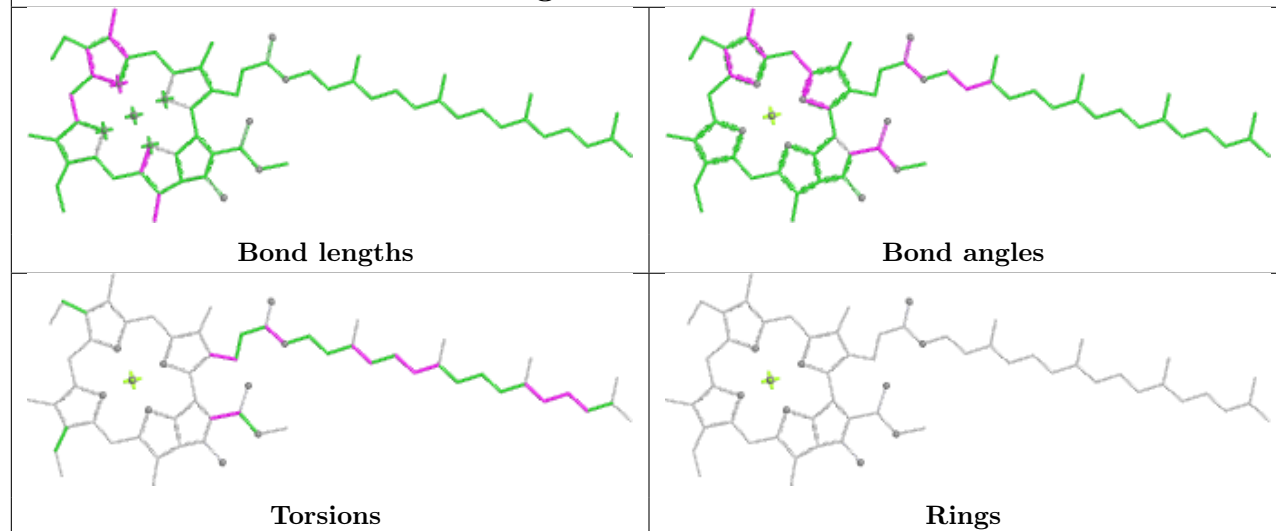


Rings

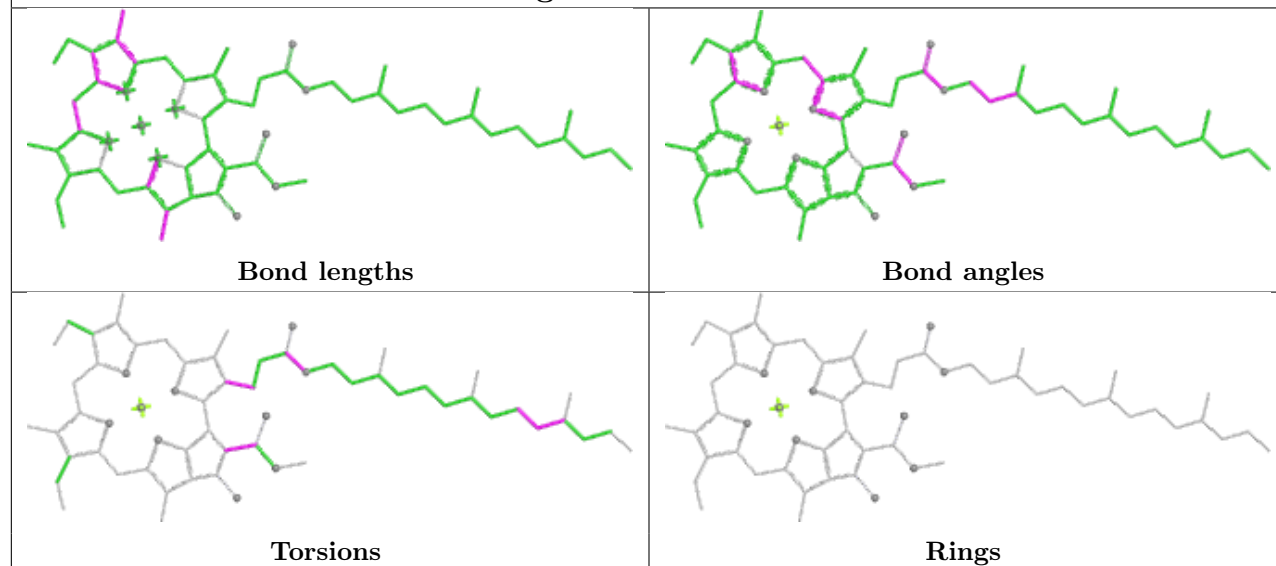
Ligand CLA D 311



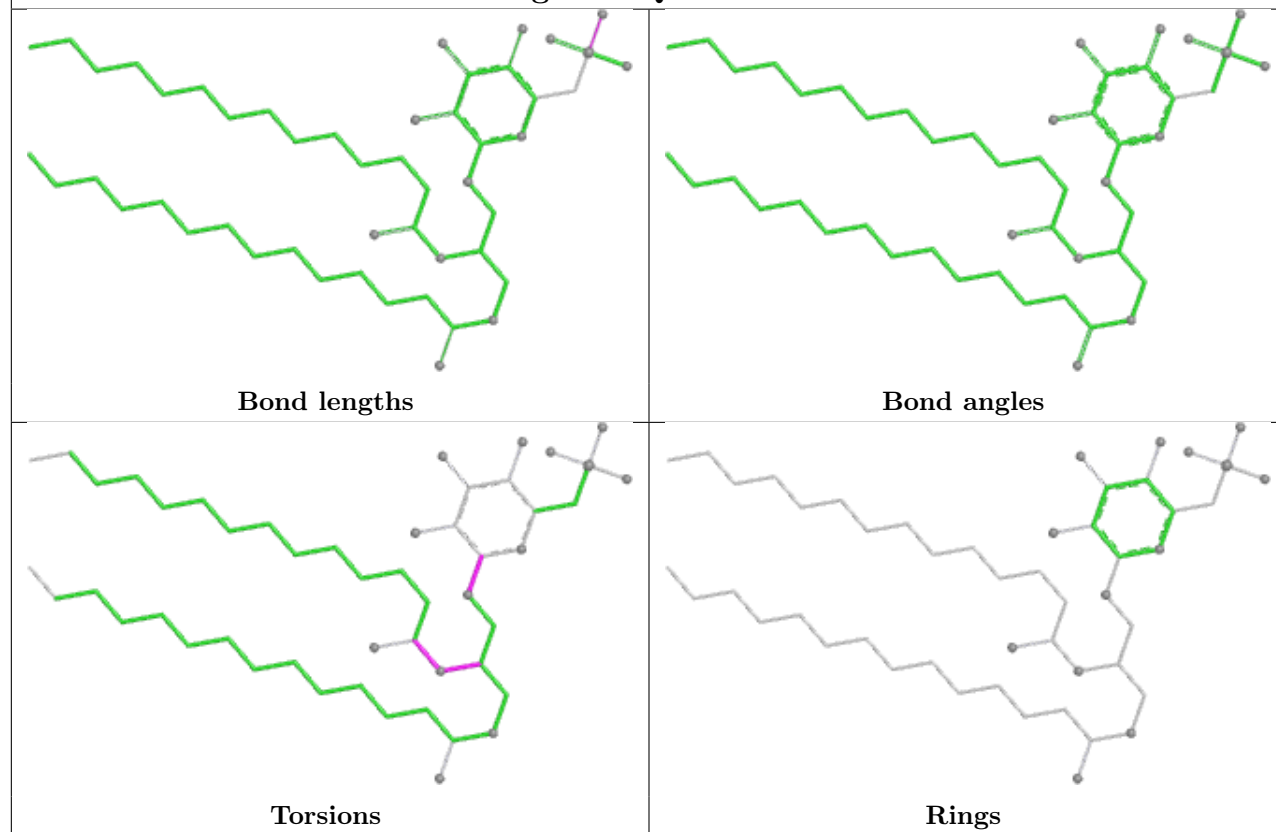
Ligand CLA a 724



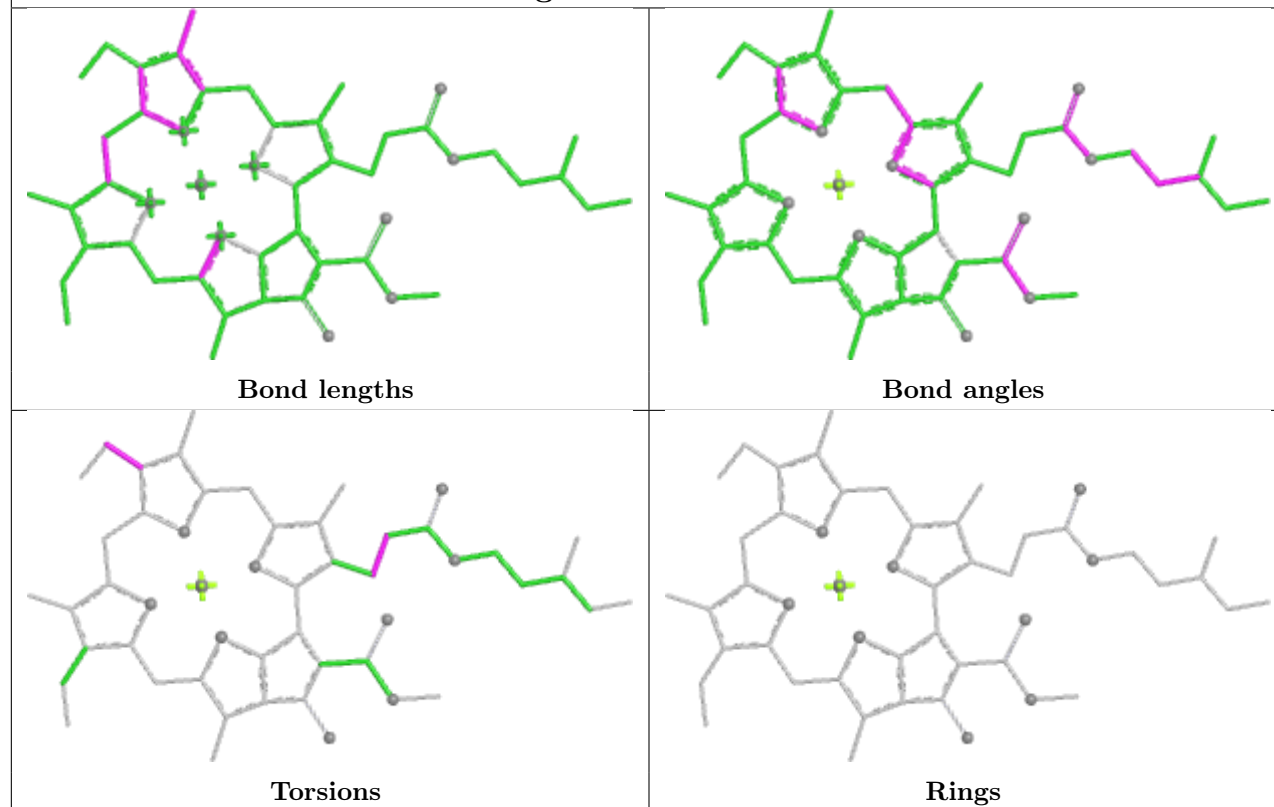
Ligand CLA a 720



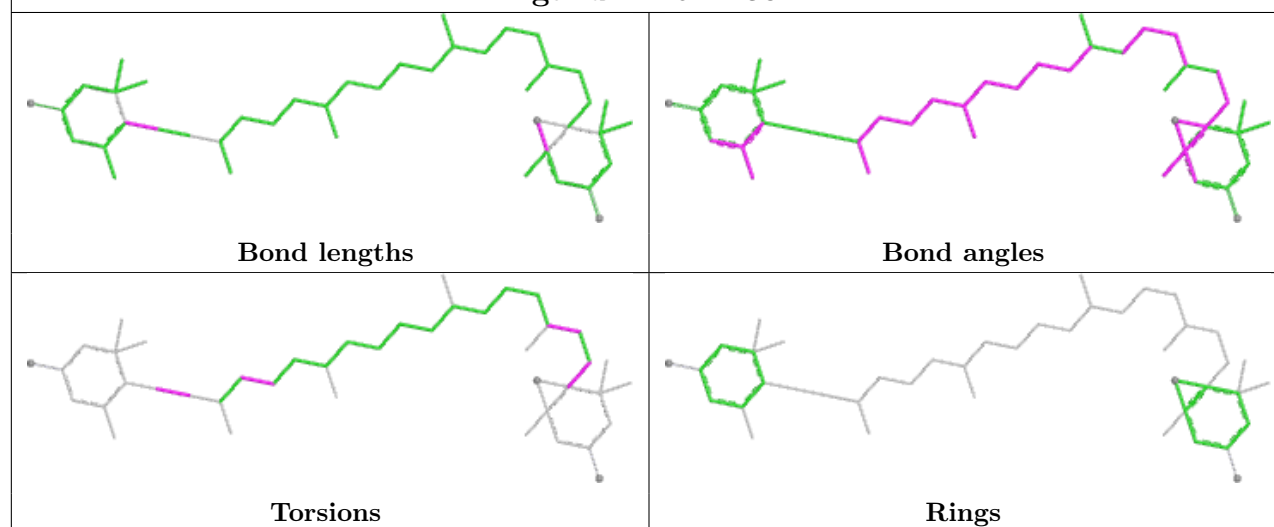
Ligand SQD A 318



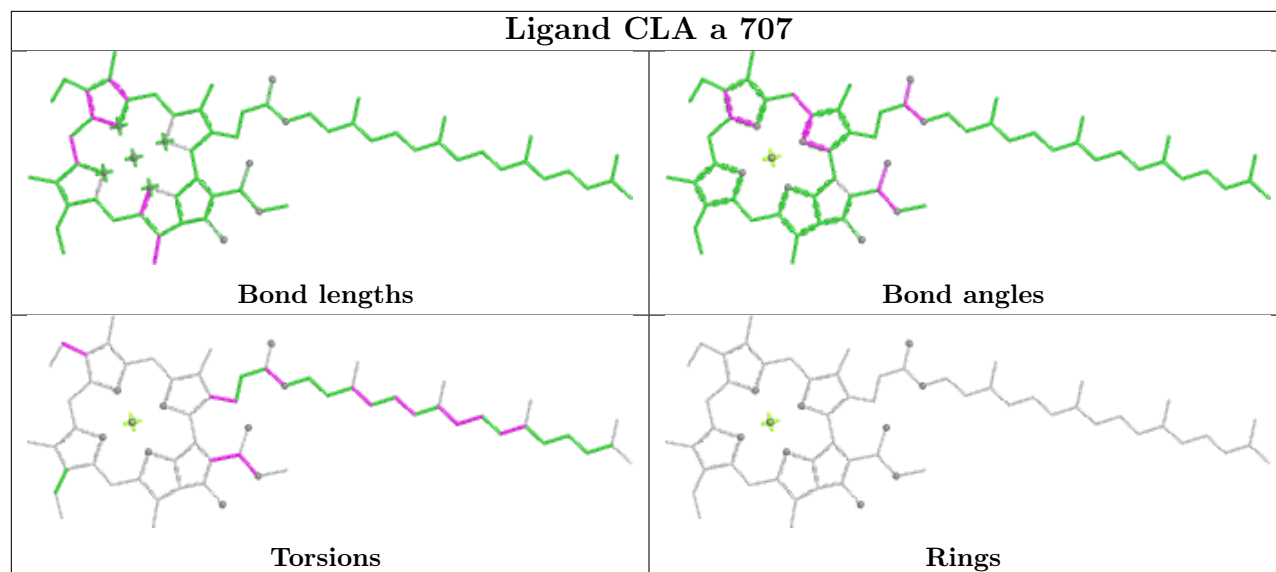
Ligand CLA b 718



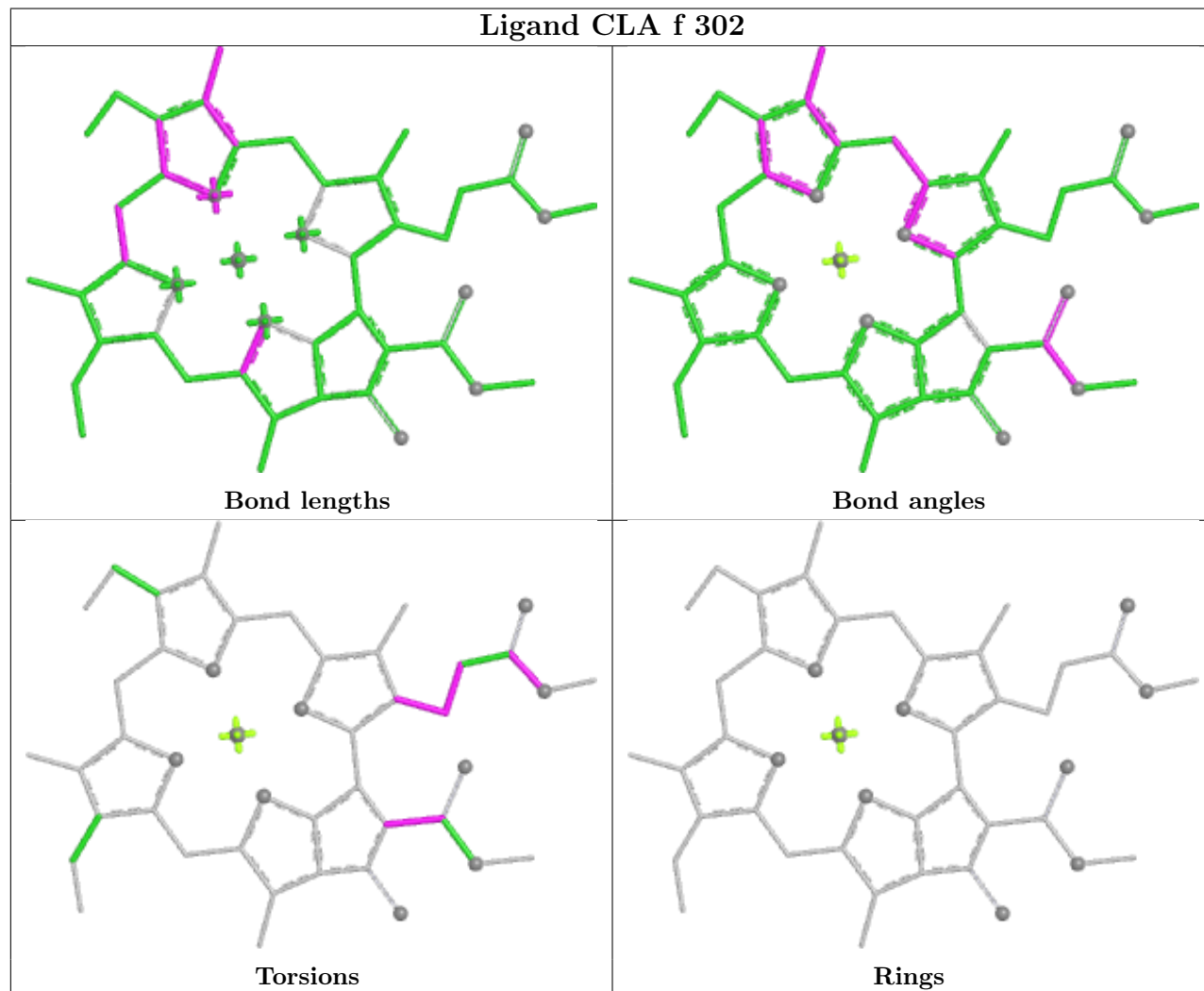
Ligand DD6 K 301



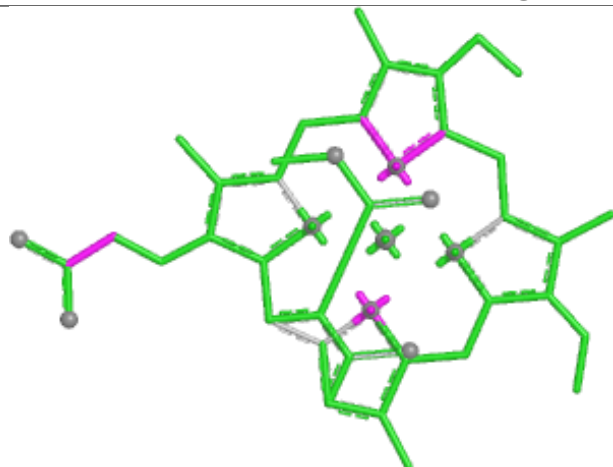
Ligand CLA a 707



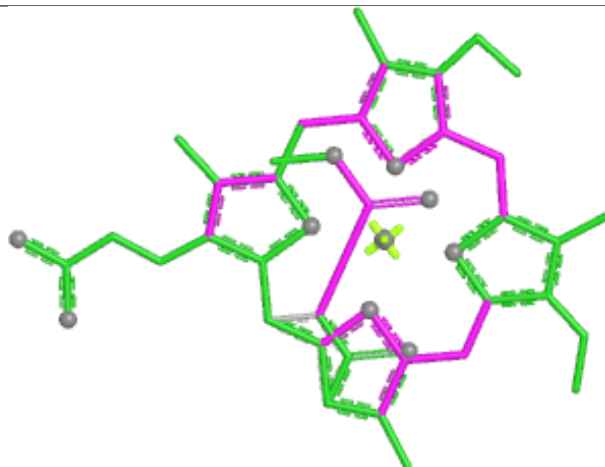
Ligand CLA f 302



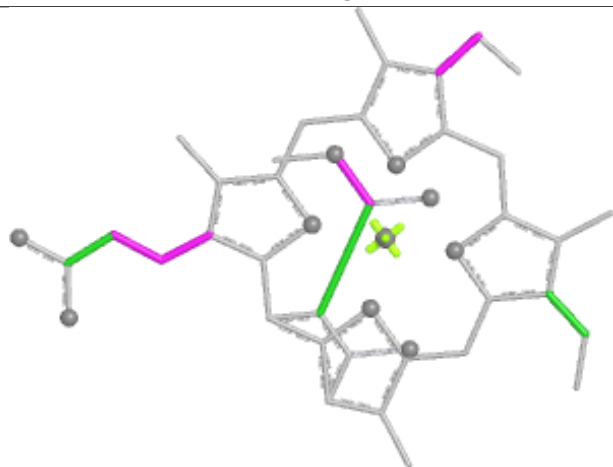
Ligand KC1 N 311



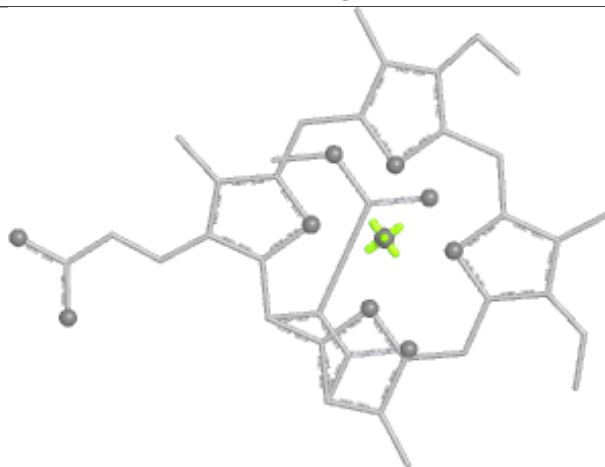
Bond lengths



Bond angles

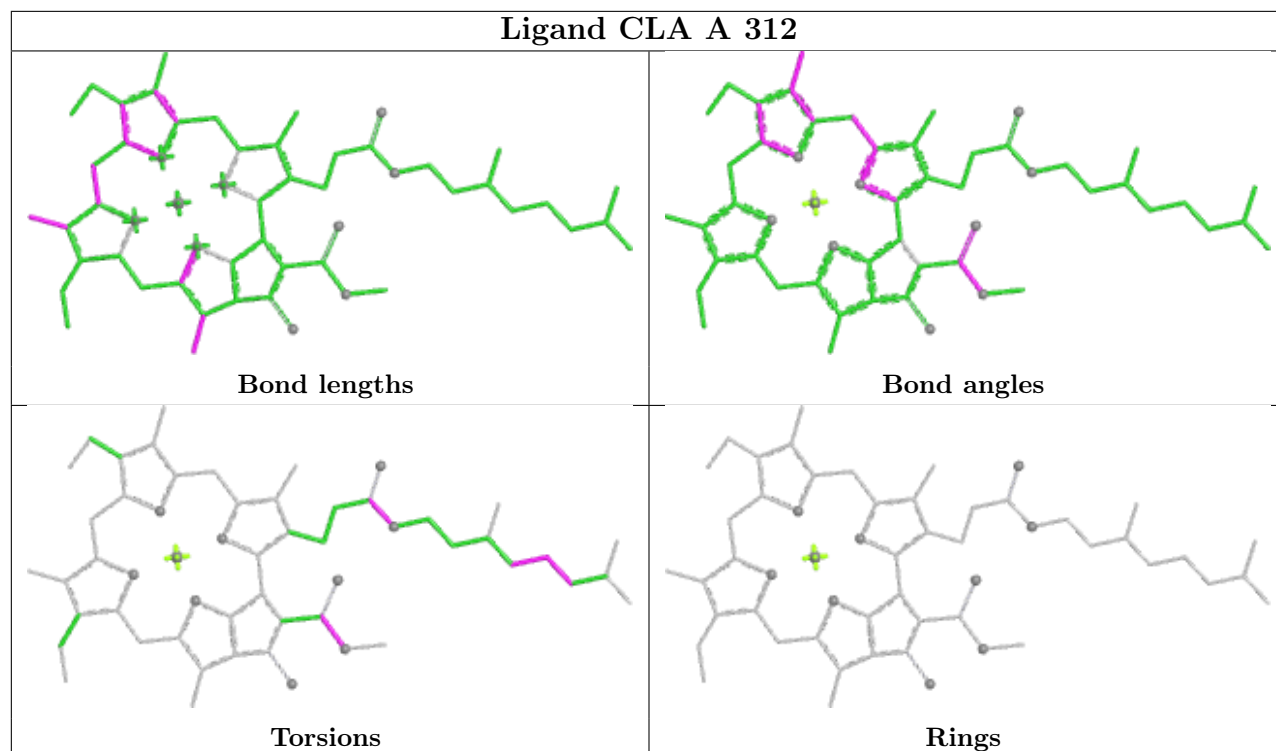


Torsions

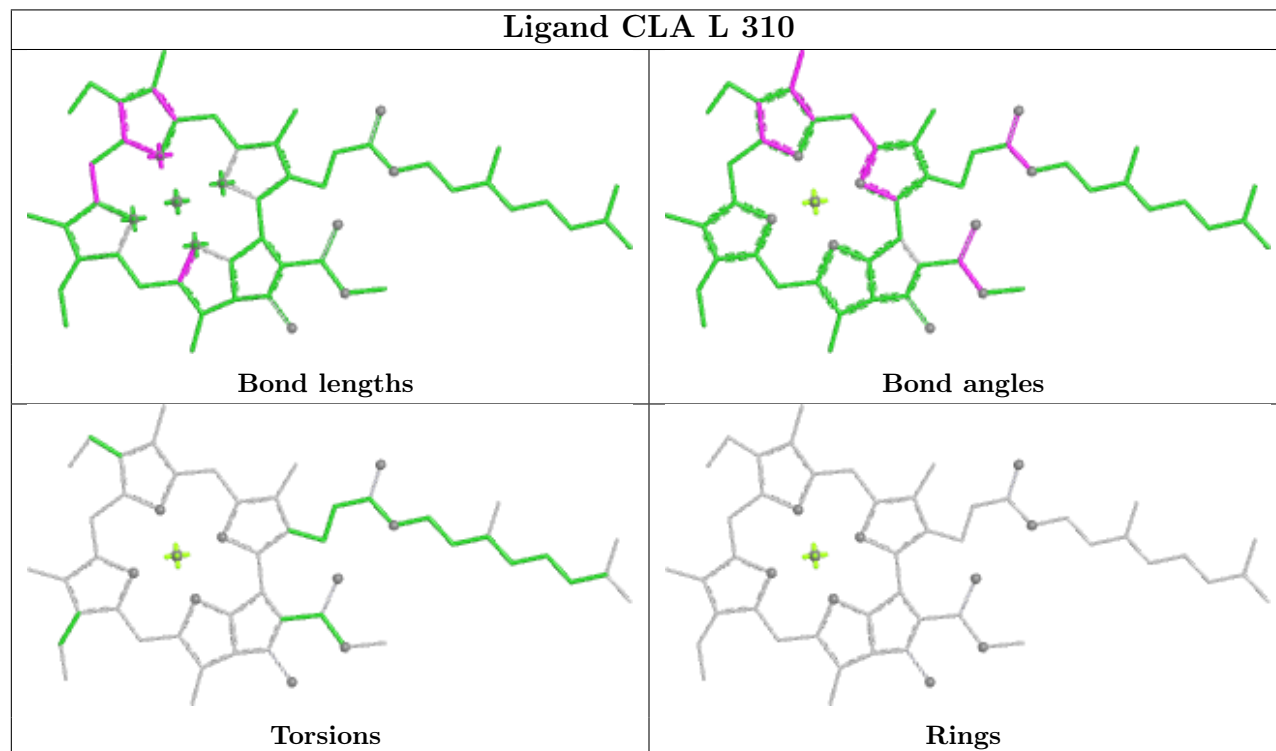


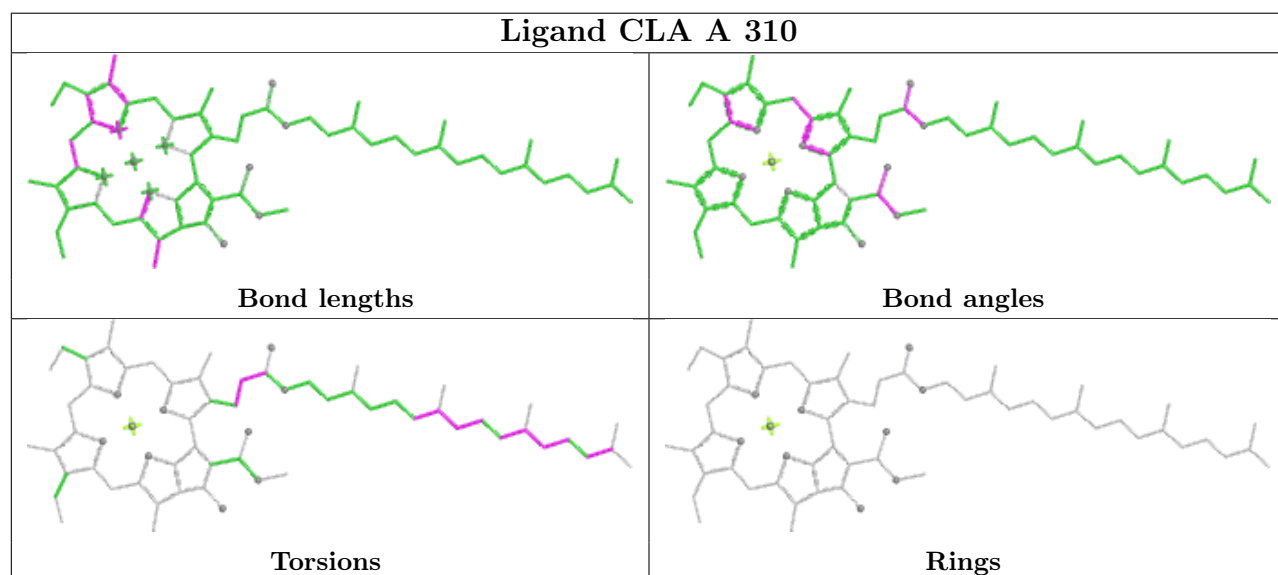
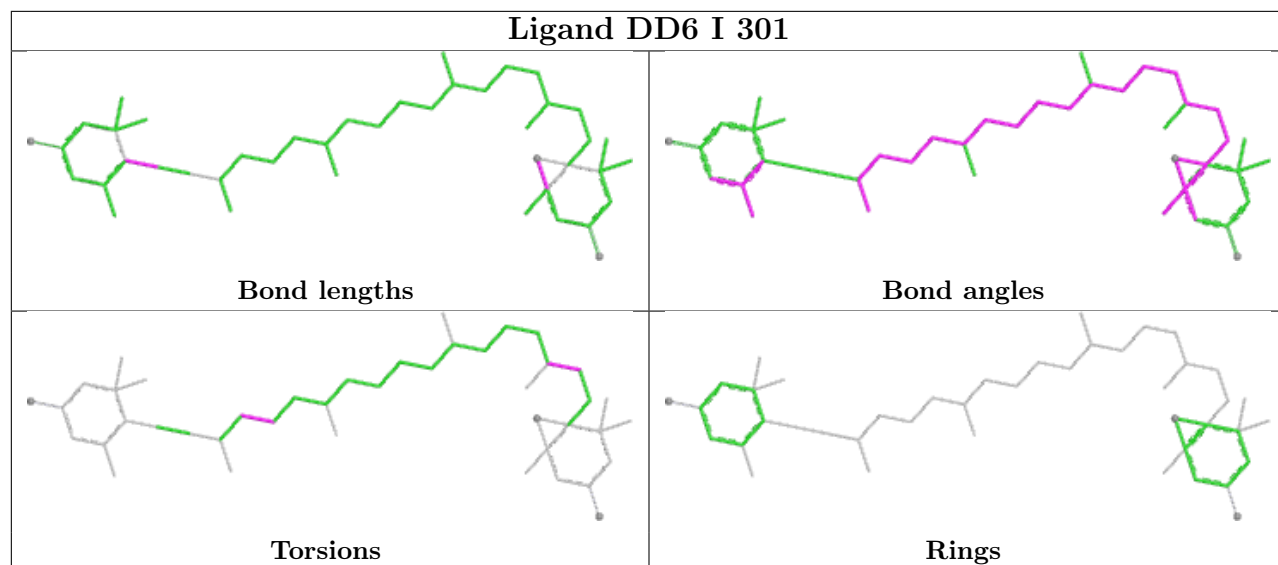
Rings

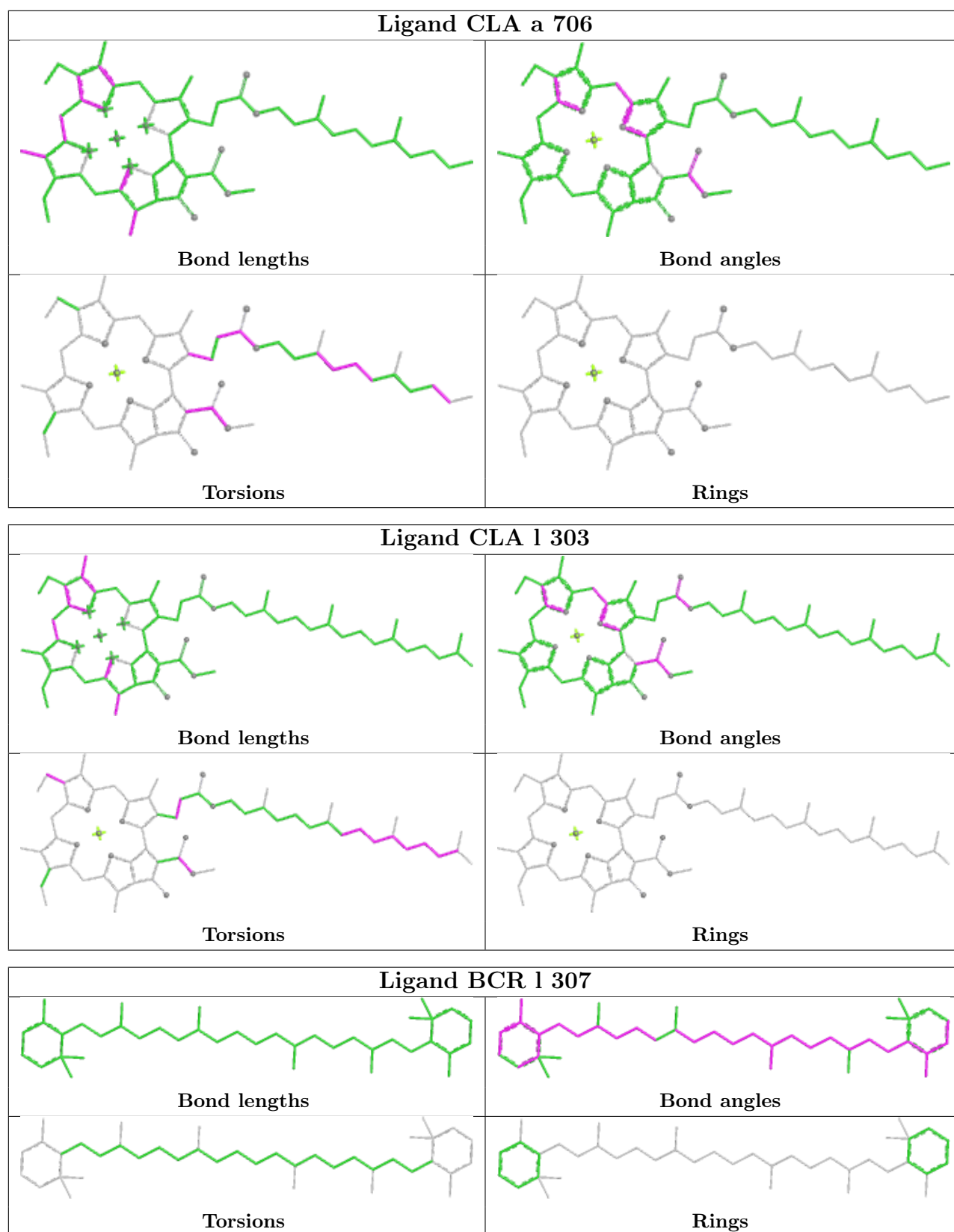
Ligand CLA A 312



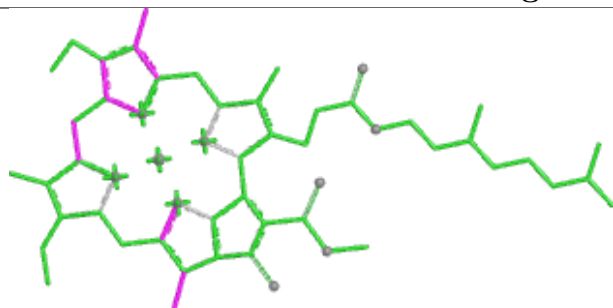
Ligand CLA L 310



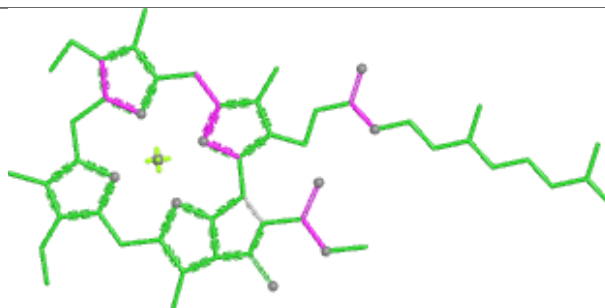




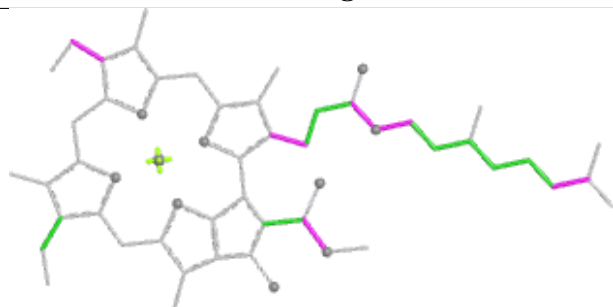
Ligand CLA f 301



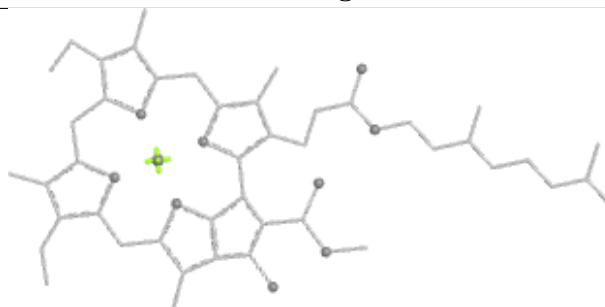
Bond lengths



Bond angles

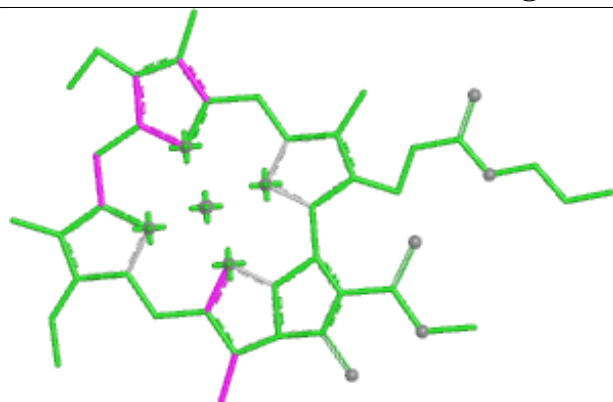


Torsions

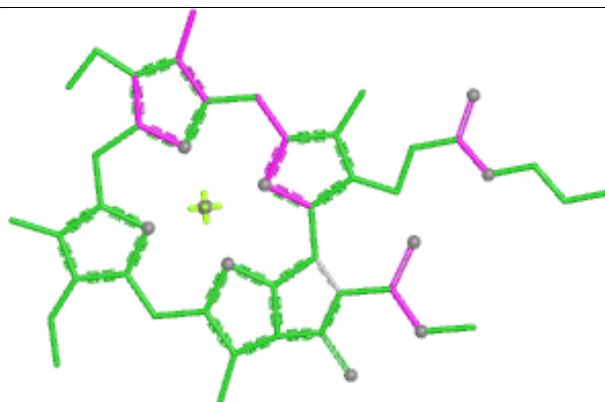


Rings

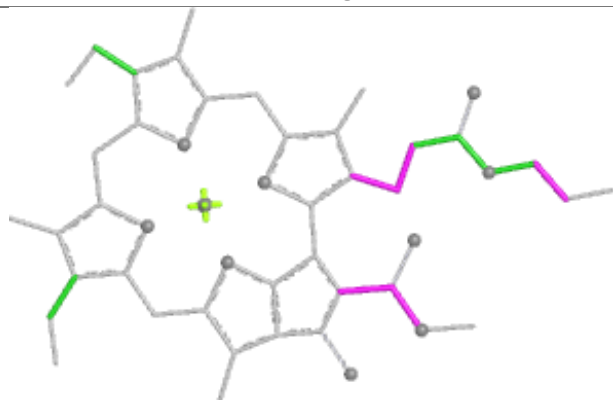
Ligand CLA I 310



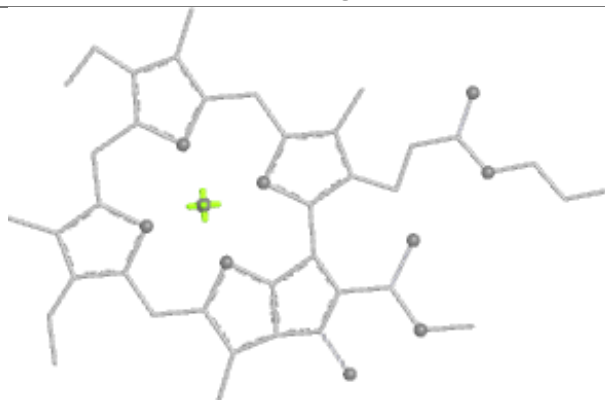
Bond lengths



Bond angles

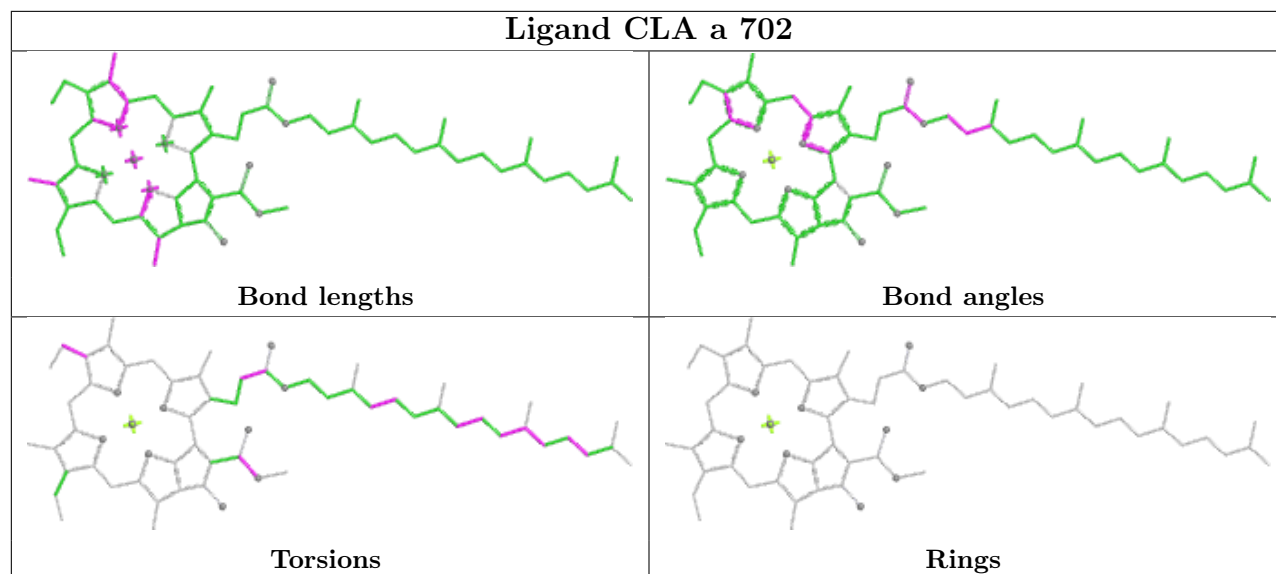


Torsions

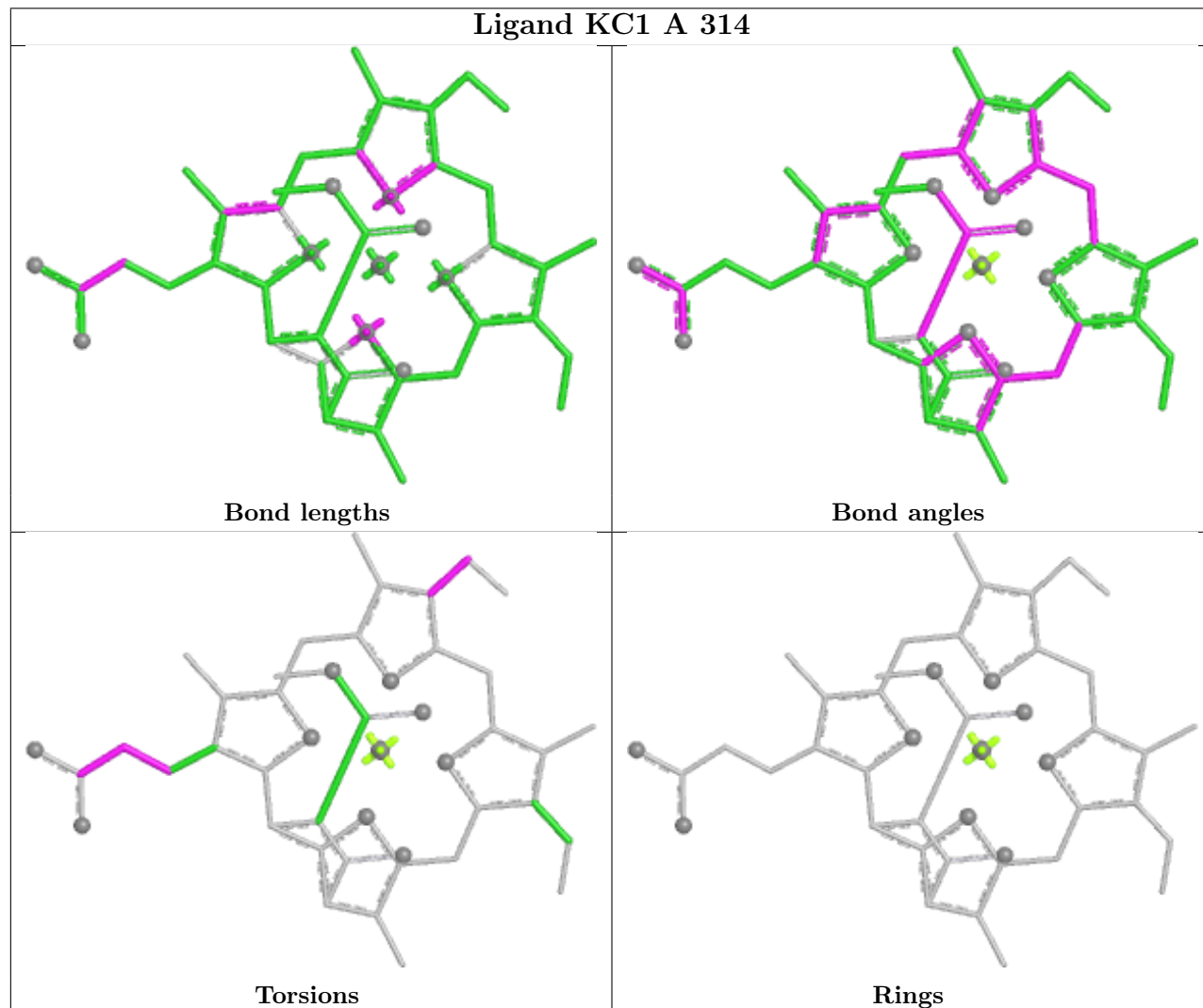


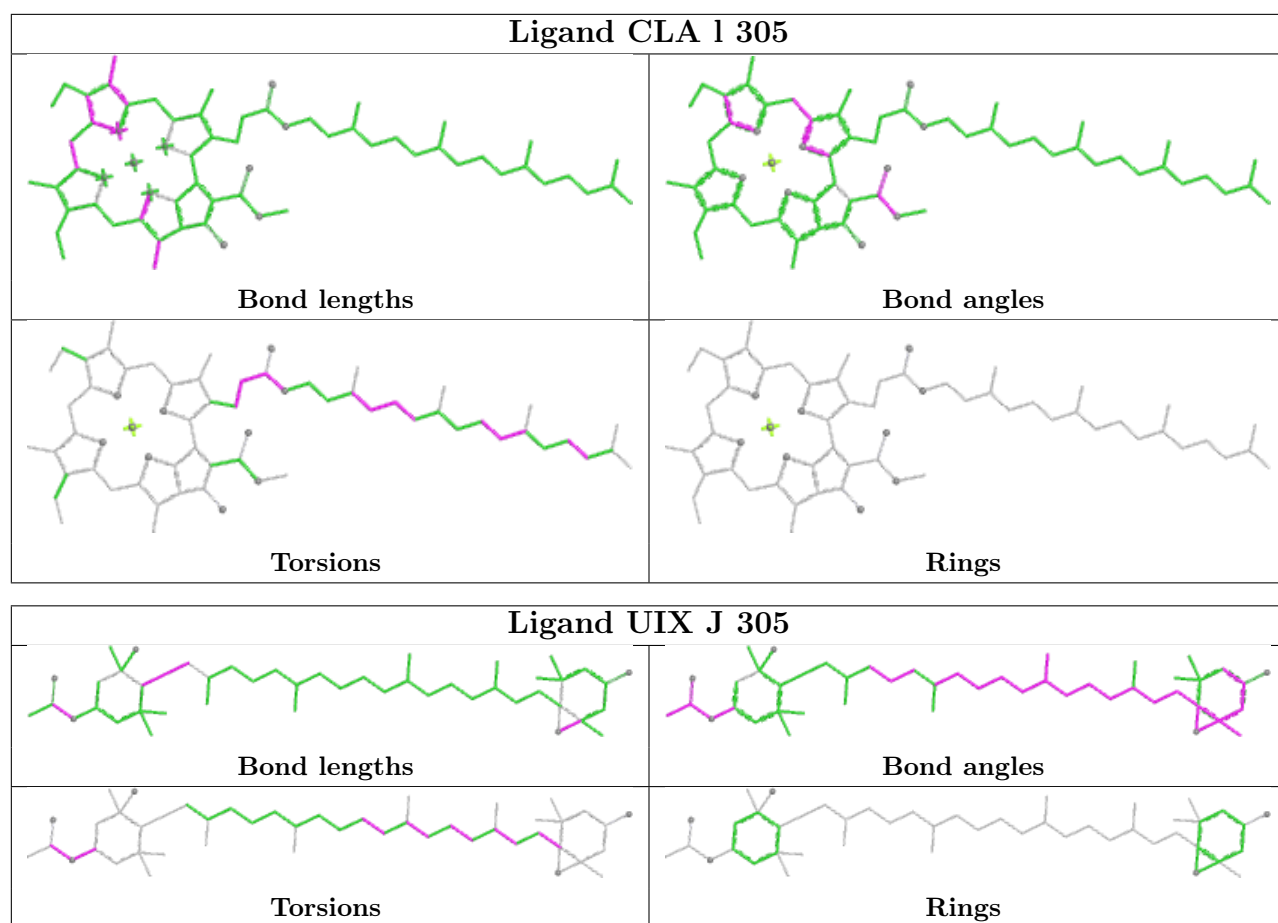
Rings

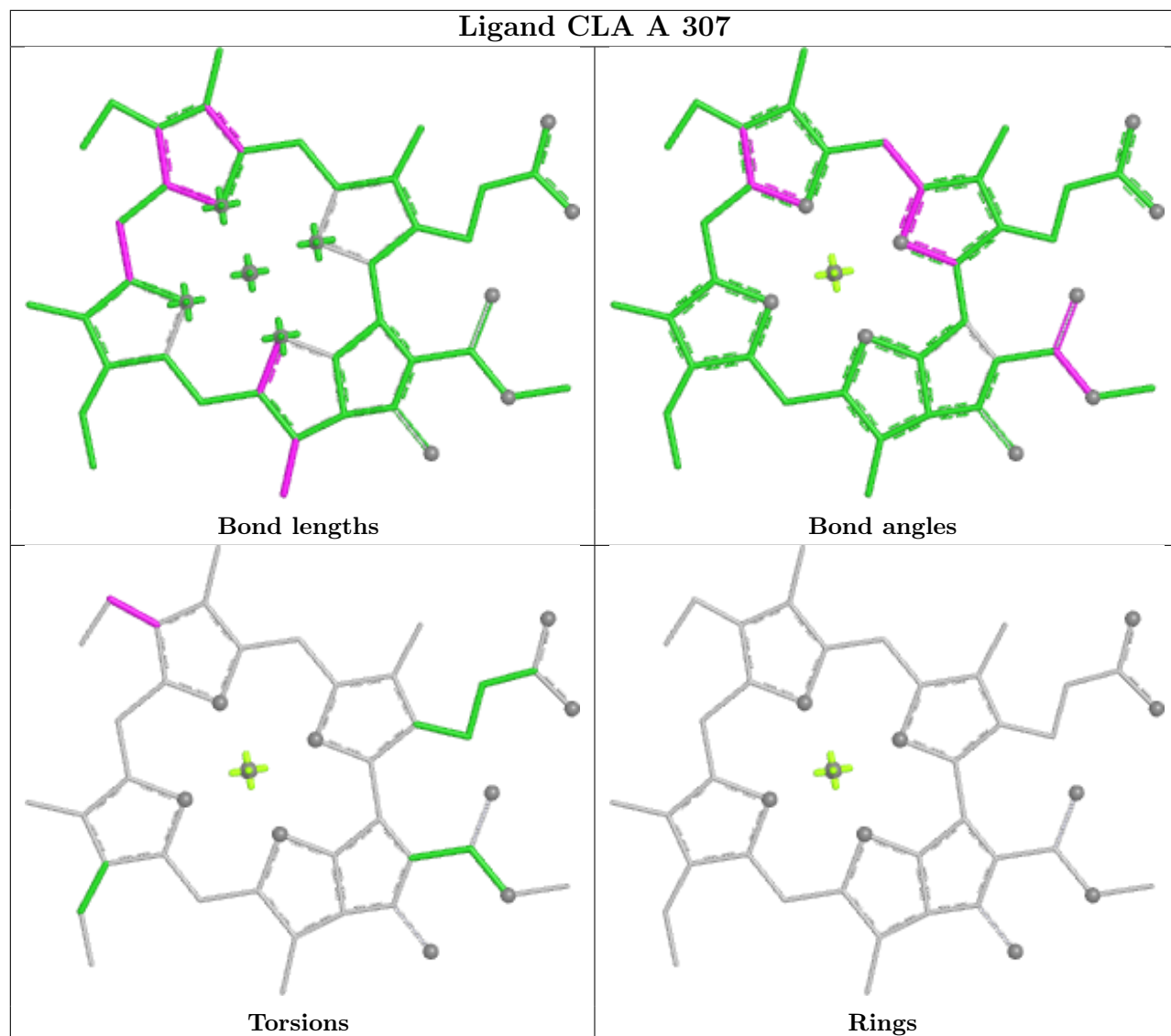
Ligand CLA a 702



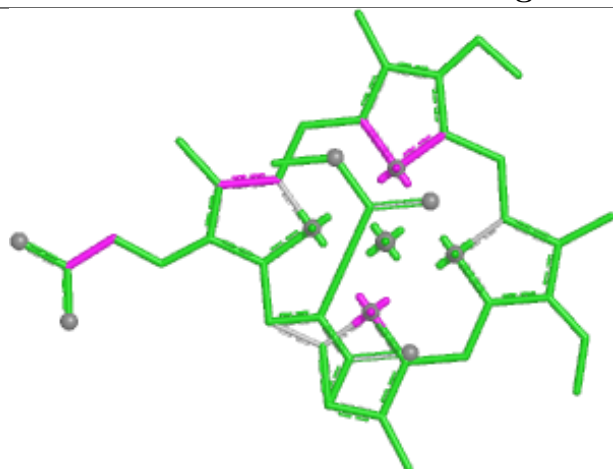
Ligand KC1 A 314



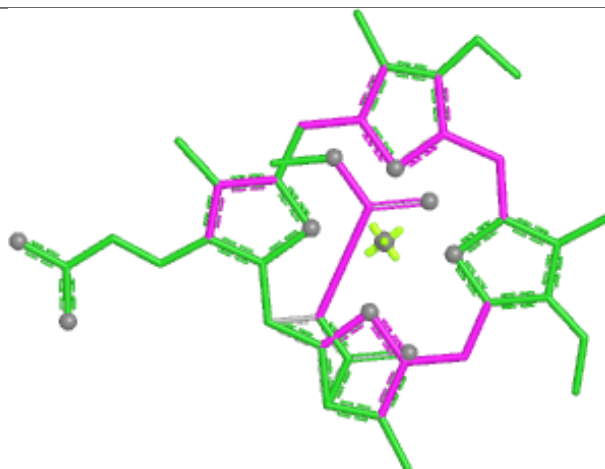




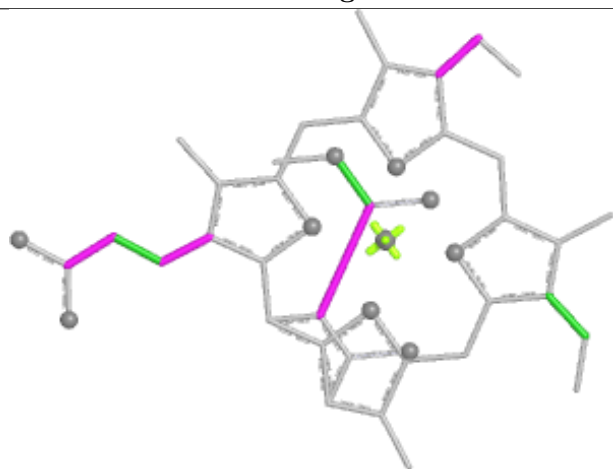
Ligand KC1 A 306



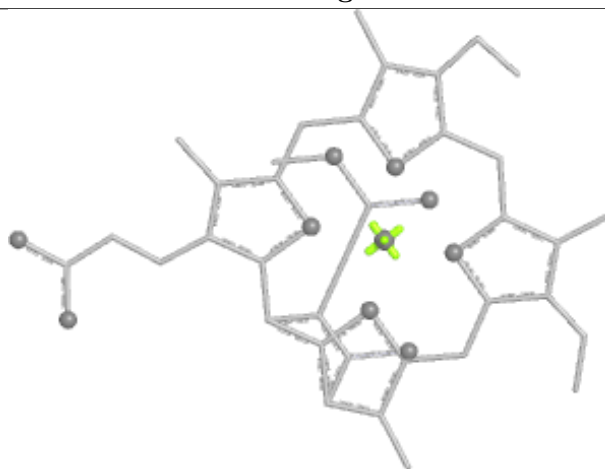
Bond lengths



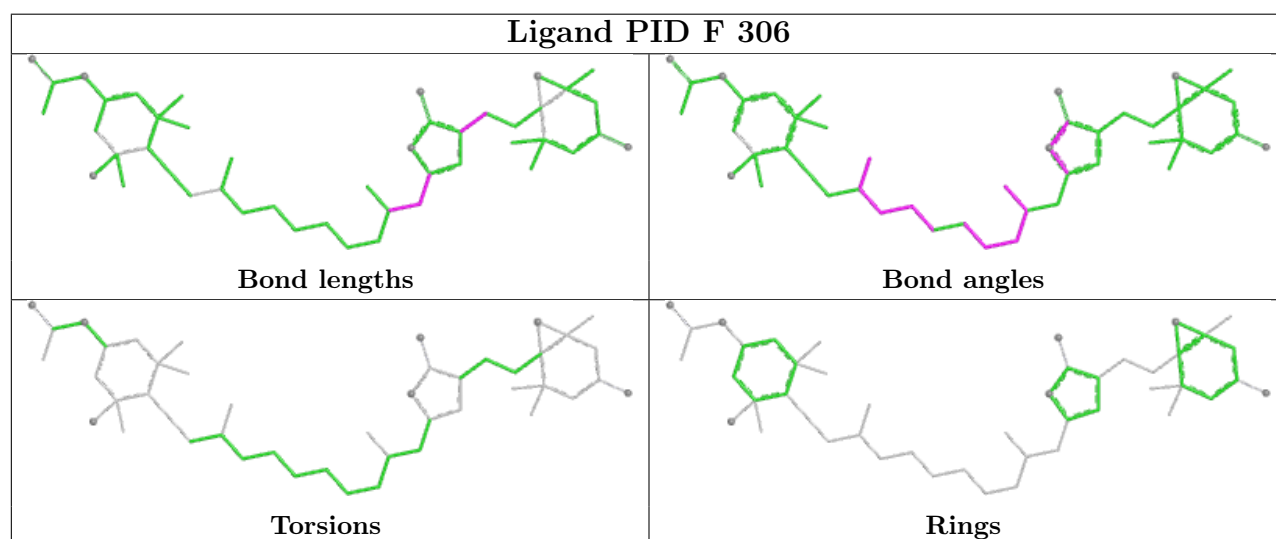
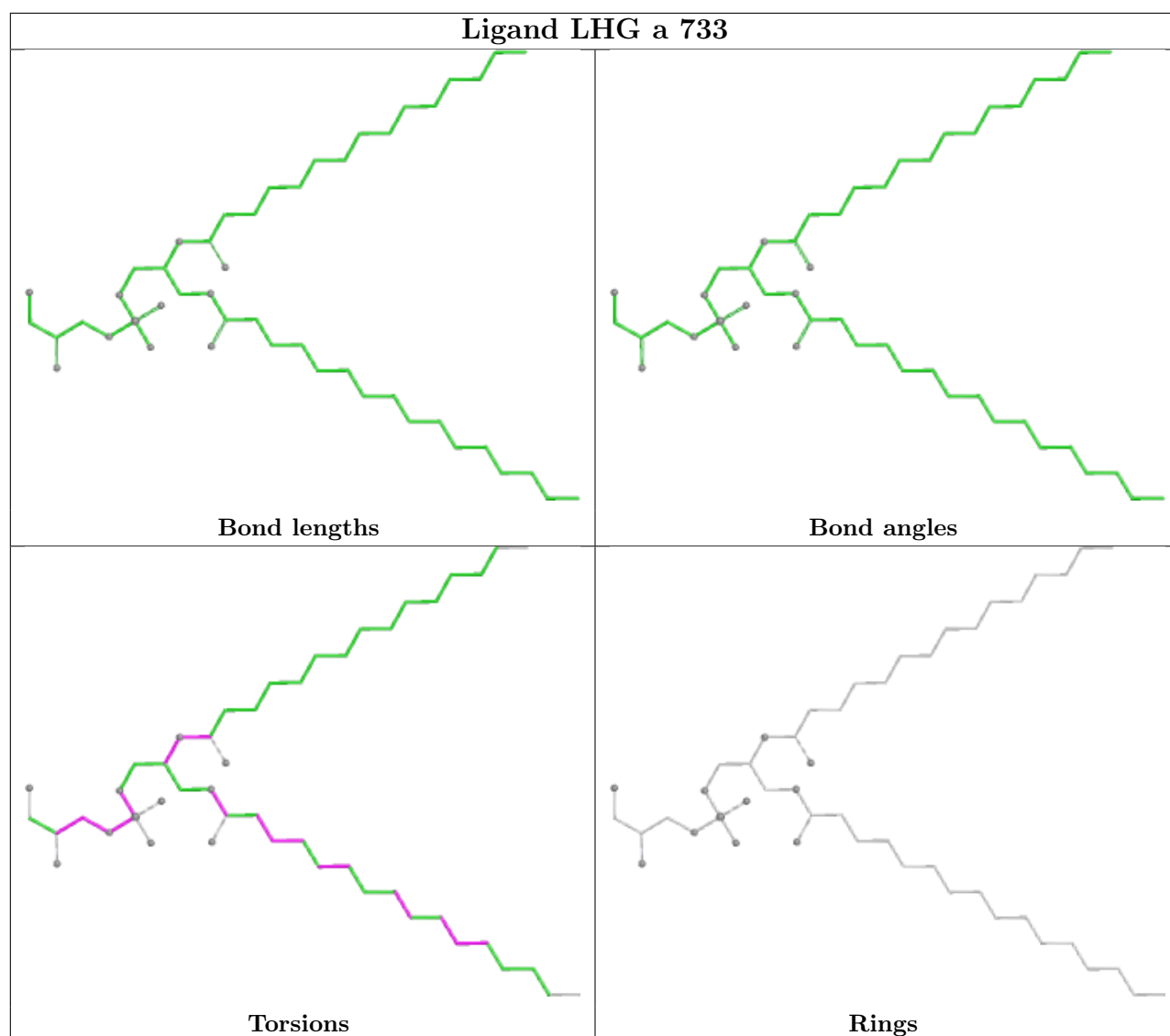
Bond angles

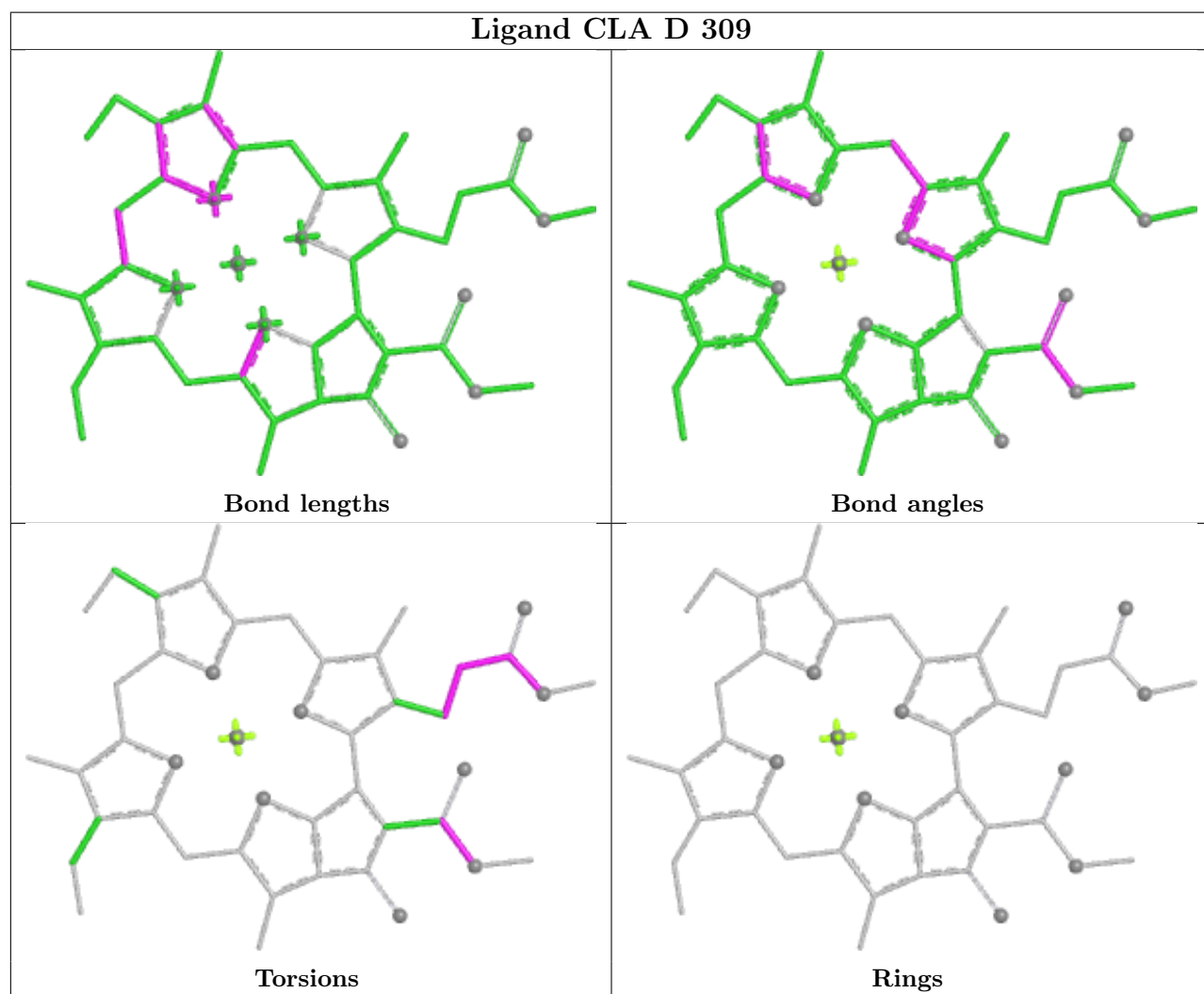
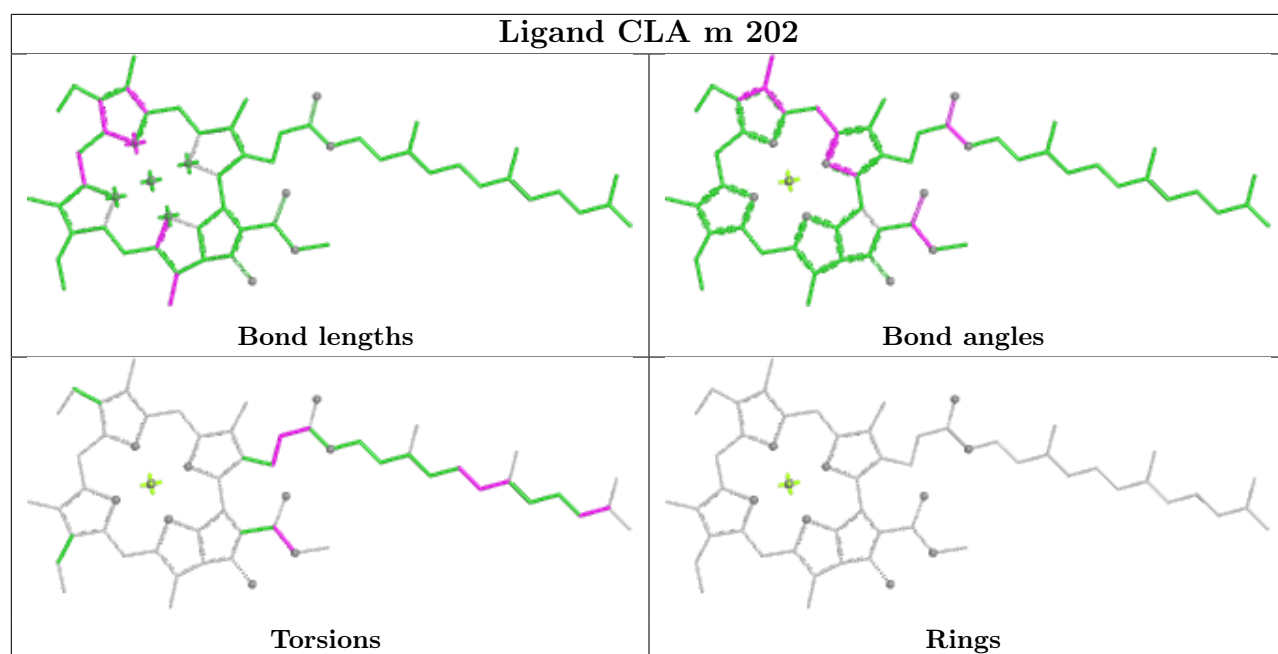


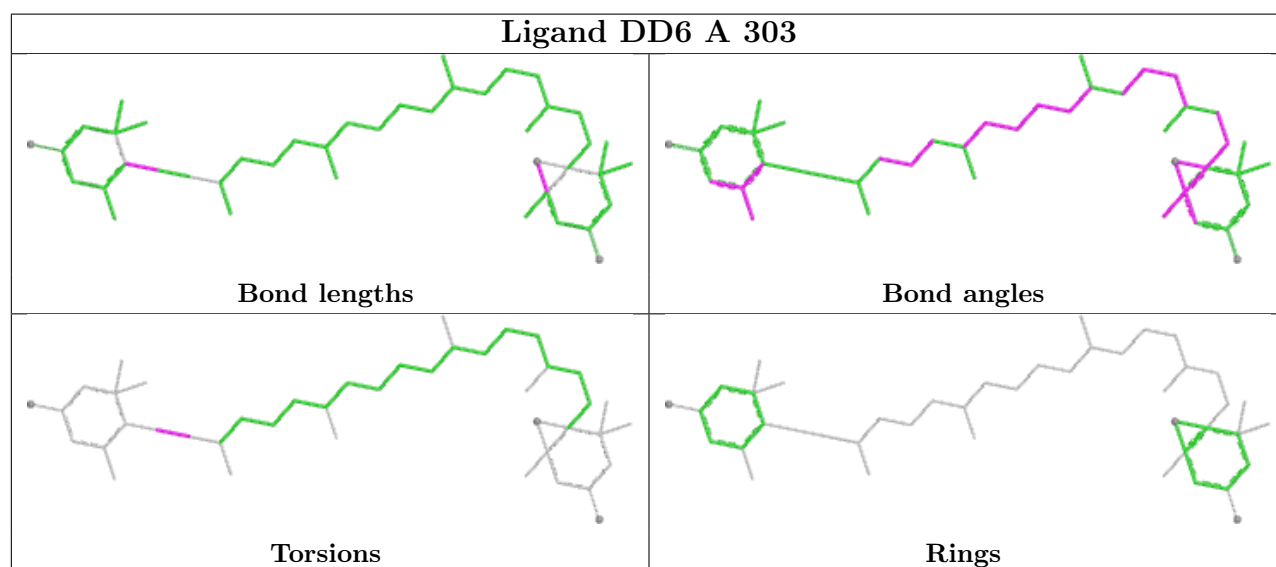
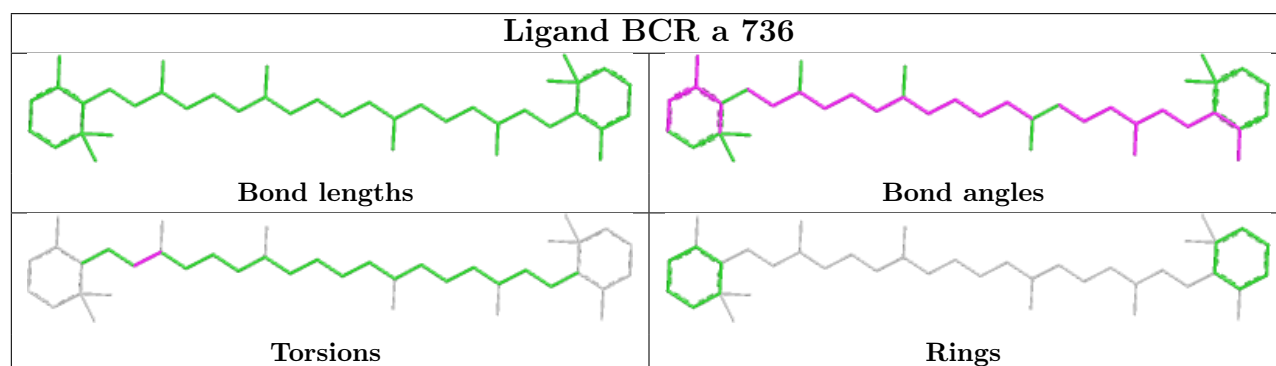
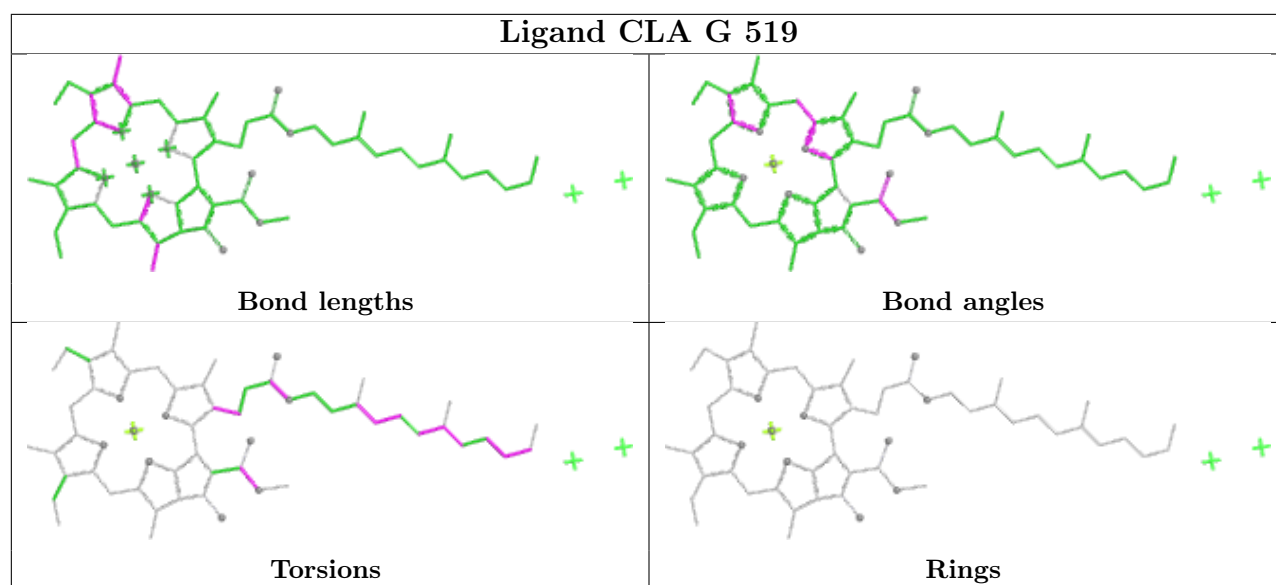
Torsions



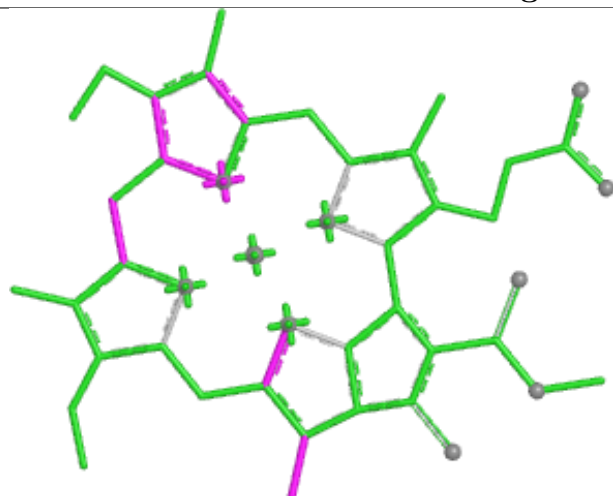
Rings



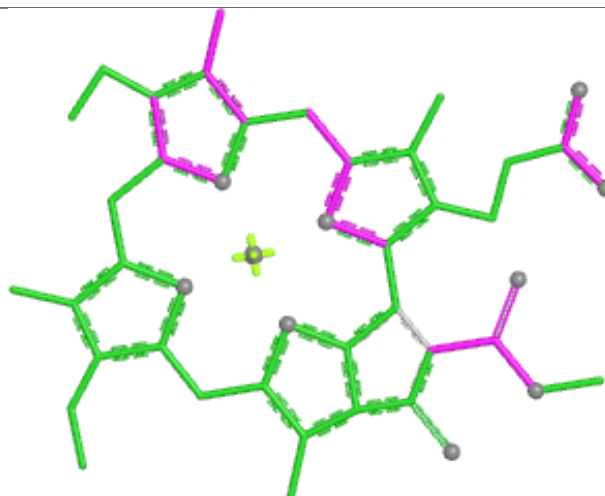




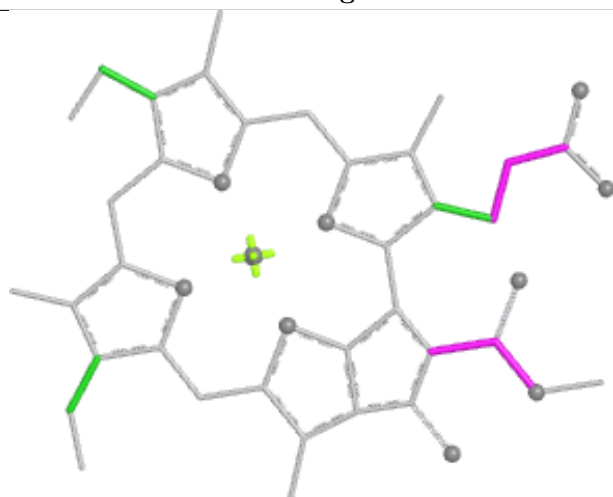
Ligand CLA I 319



Bond lengths



Bond angles

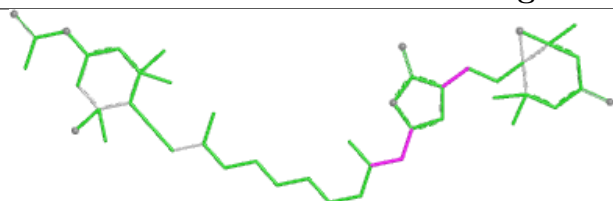


Torsions

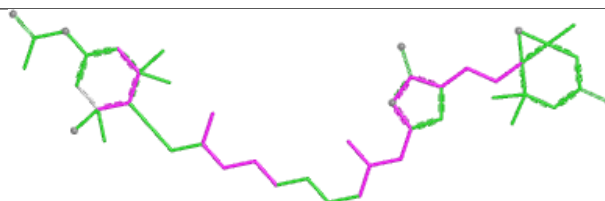


Rings

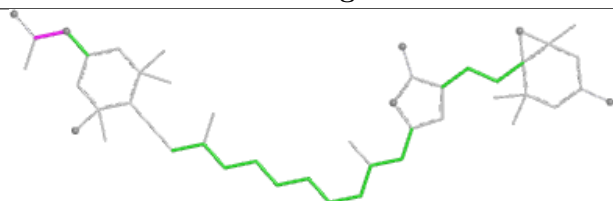
Ligand PID N 302



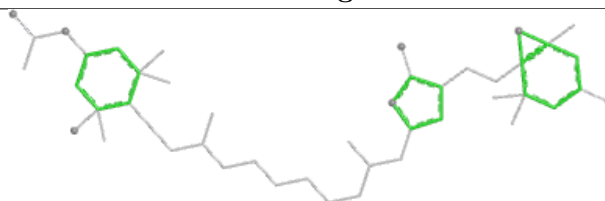
Bond lengths



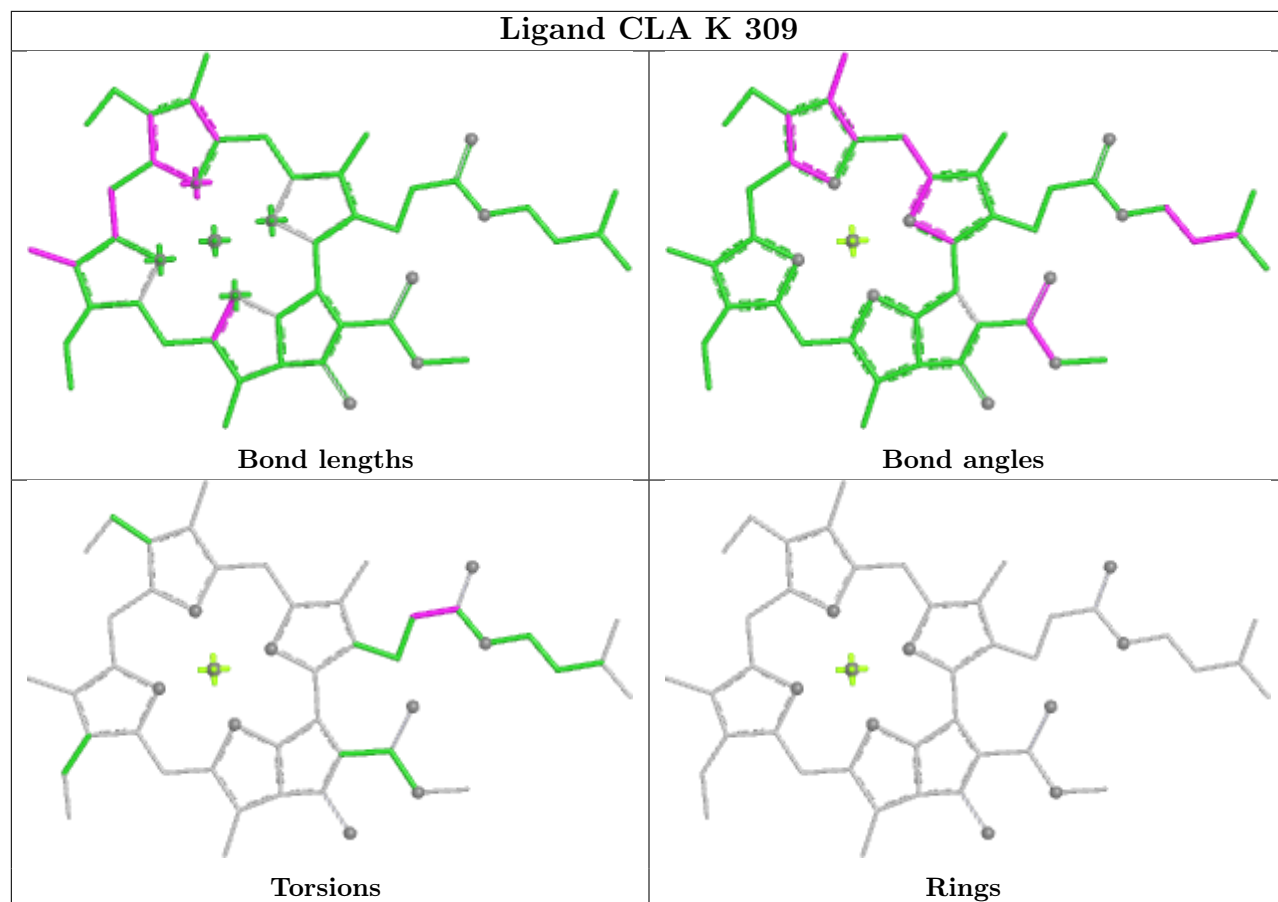
Bond angles

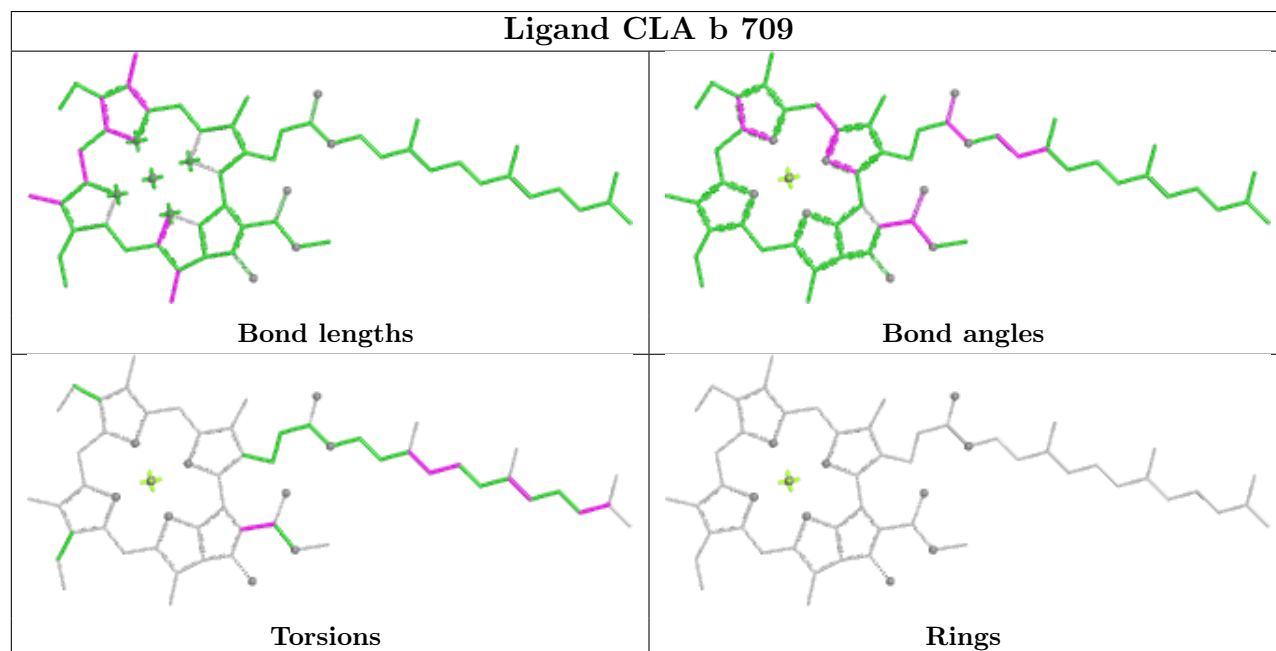
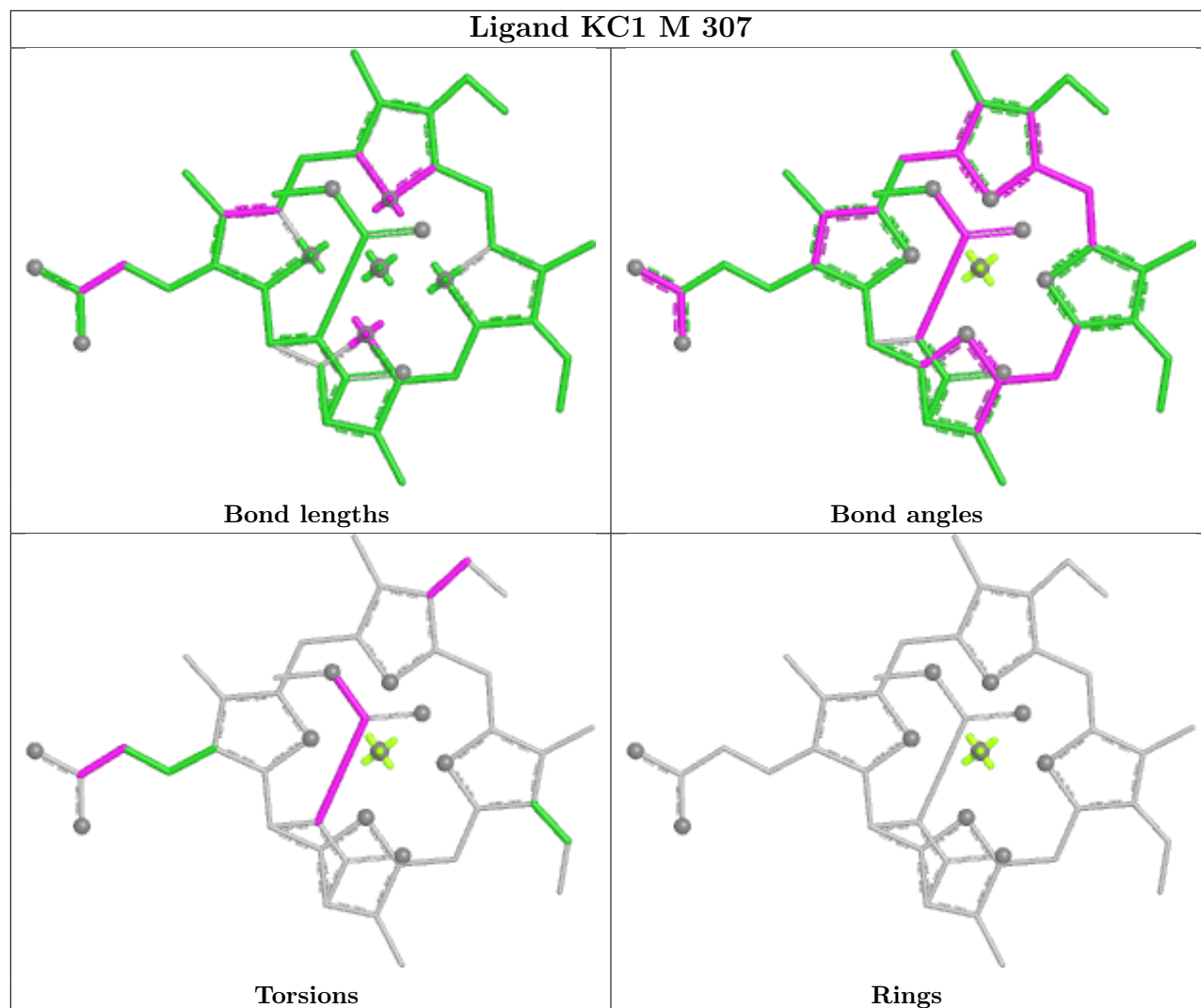


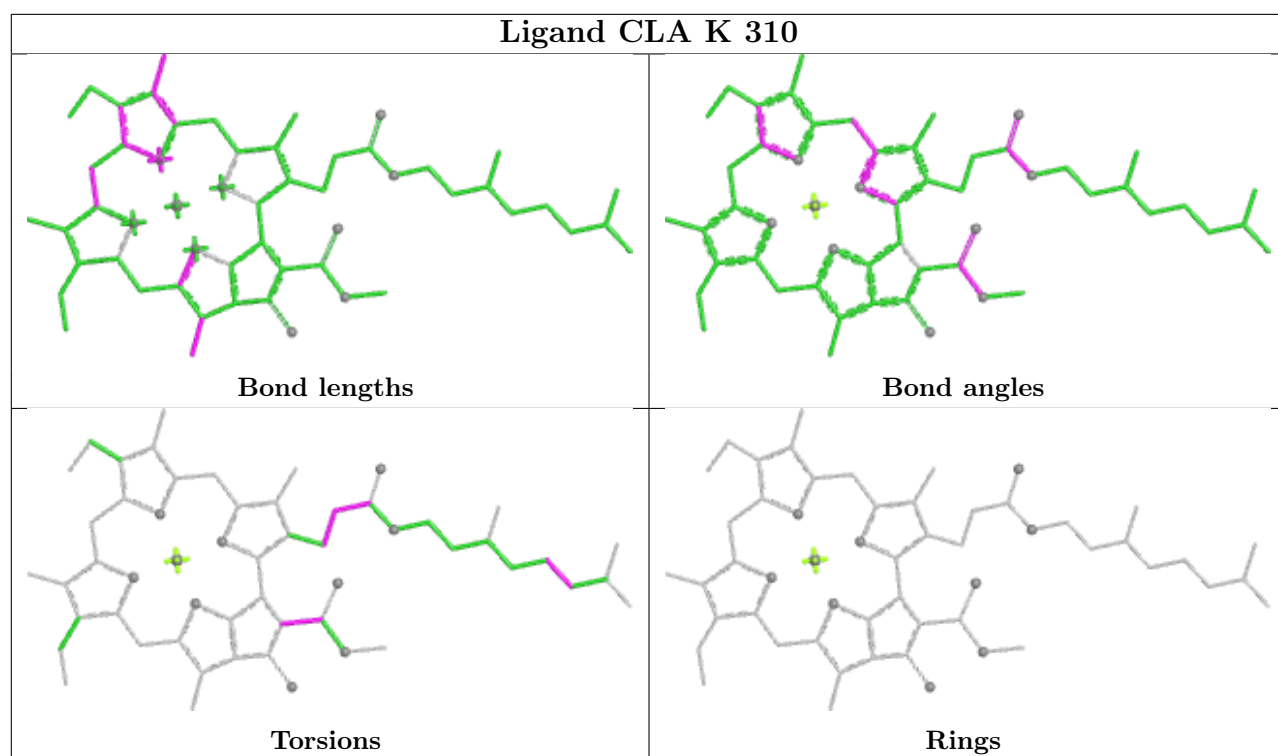
Torsions



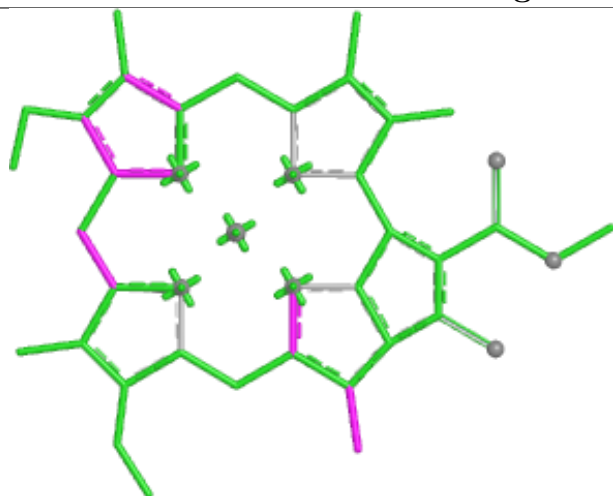
Rings



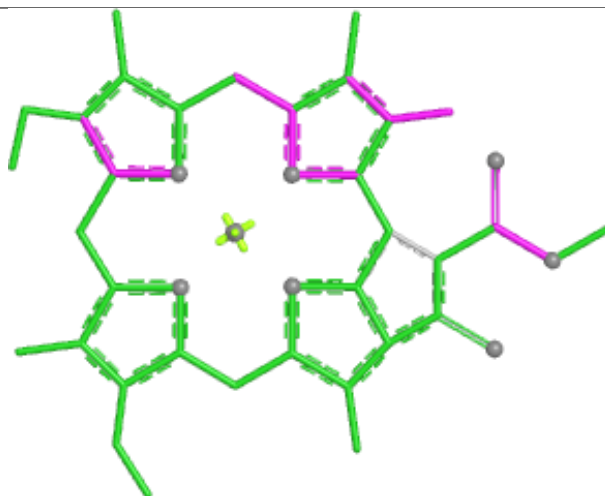




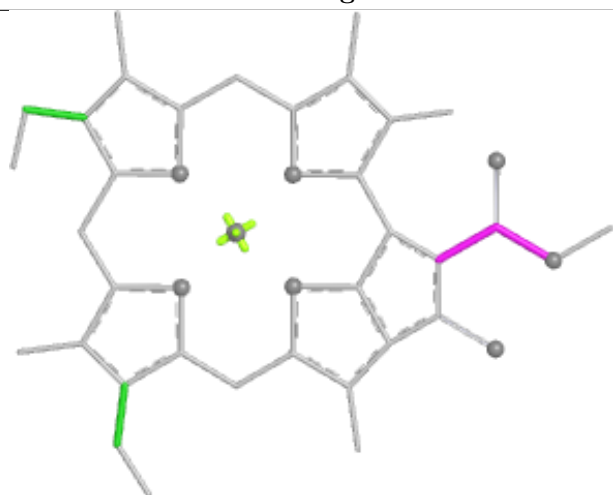
Ligand CLA A 315



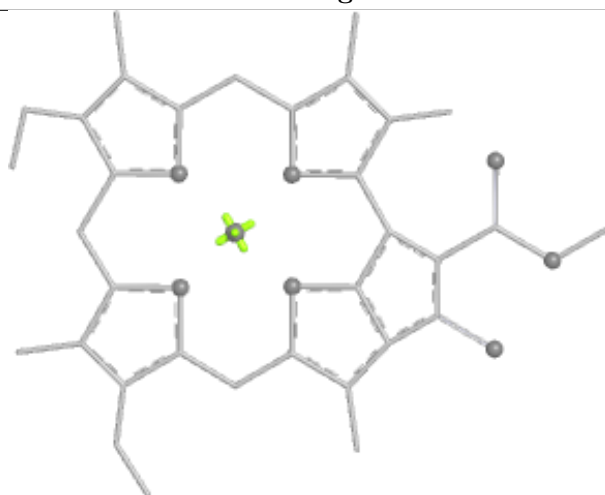
Bond lengths



Bond angles

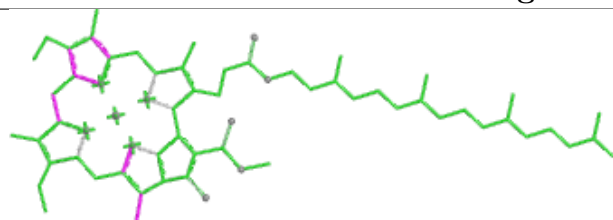


Torsions

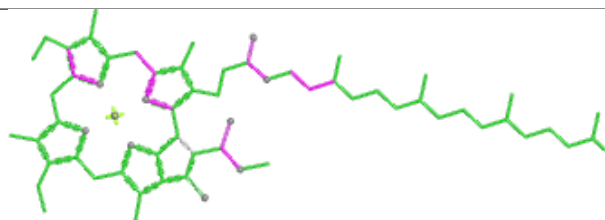


Rings

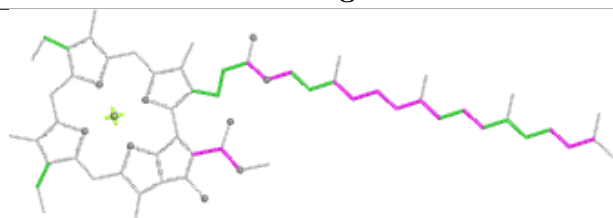
Ligand CLA b 707



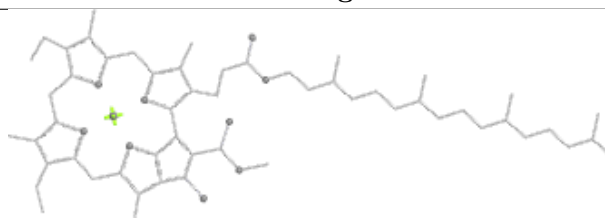
Bond lengths



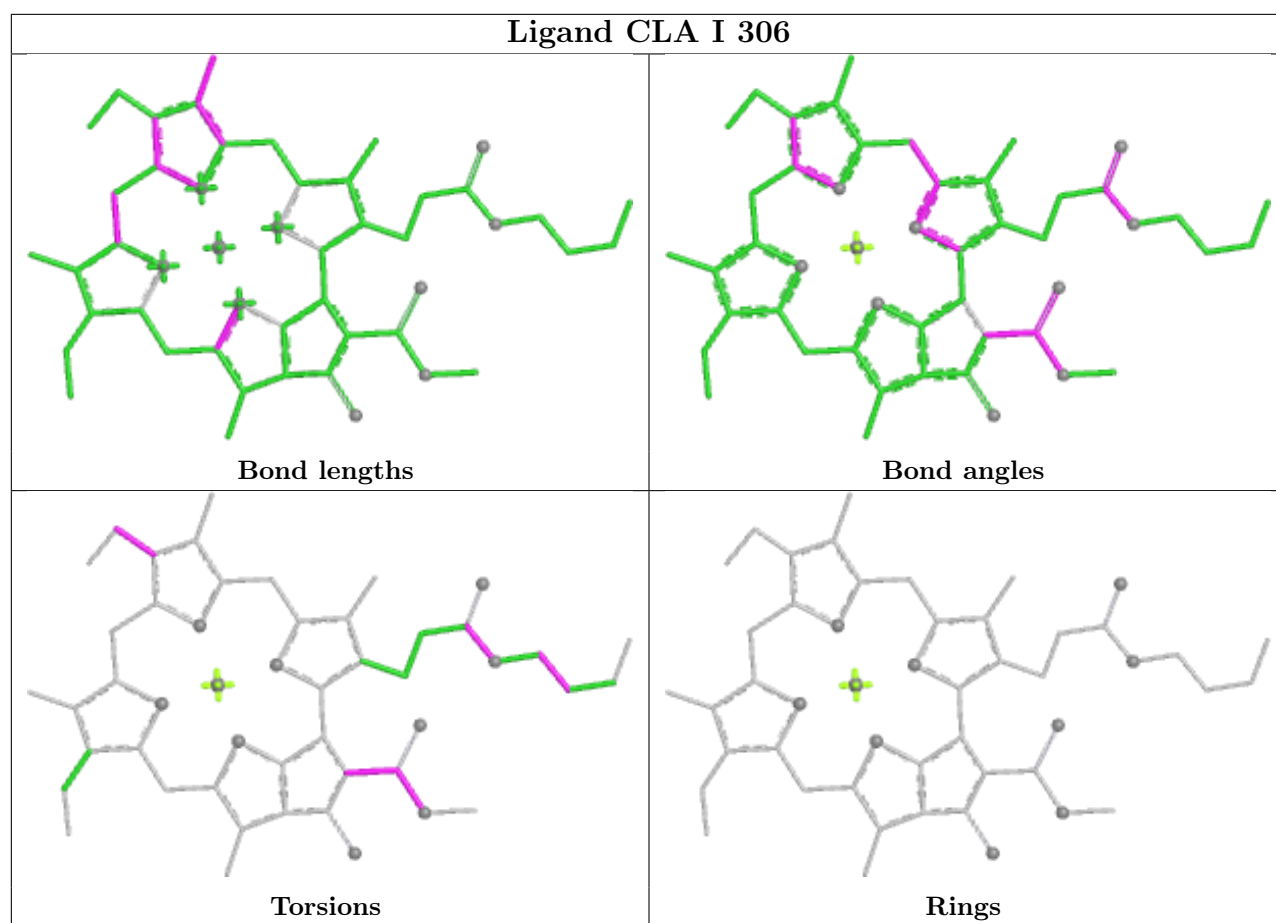
Bond angles



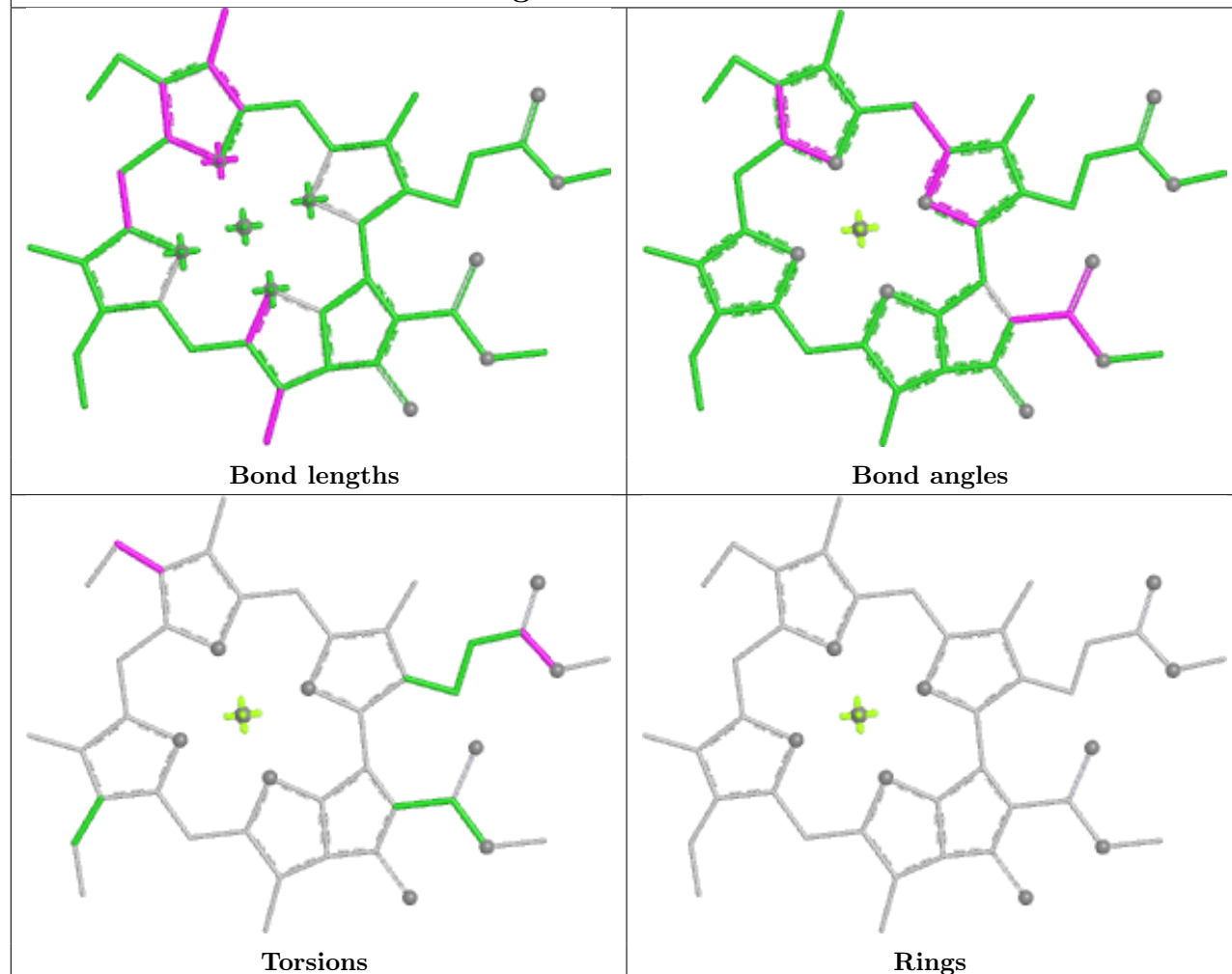
Torsions



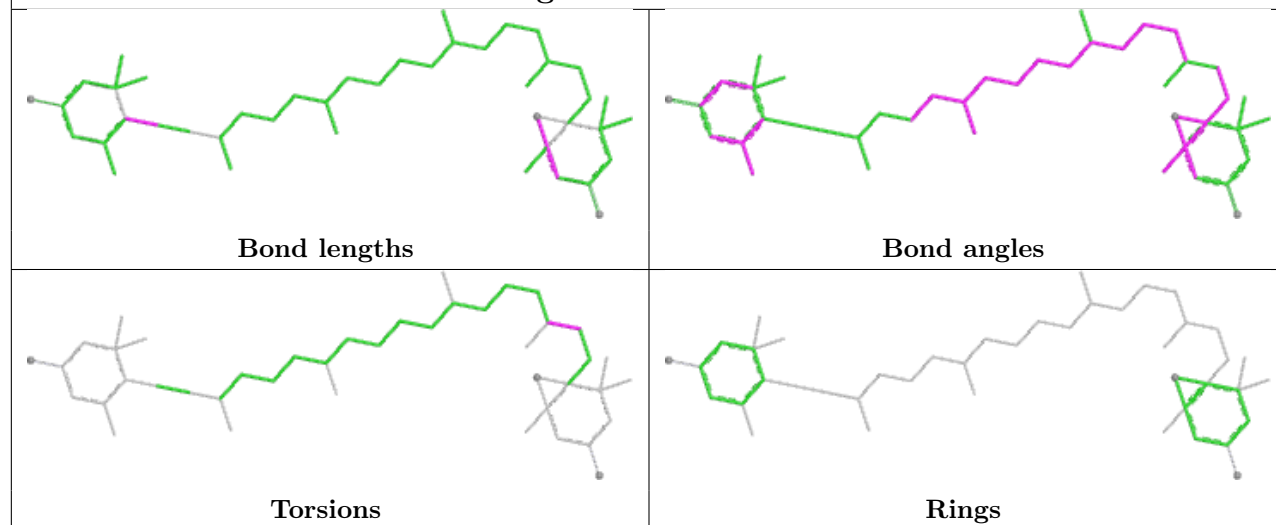
Rings



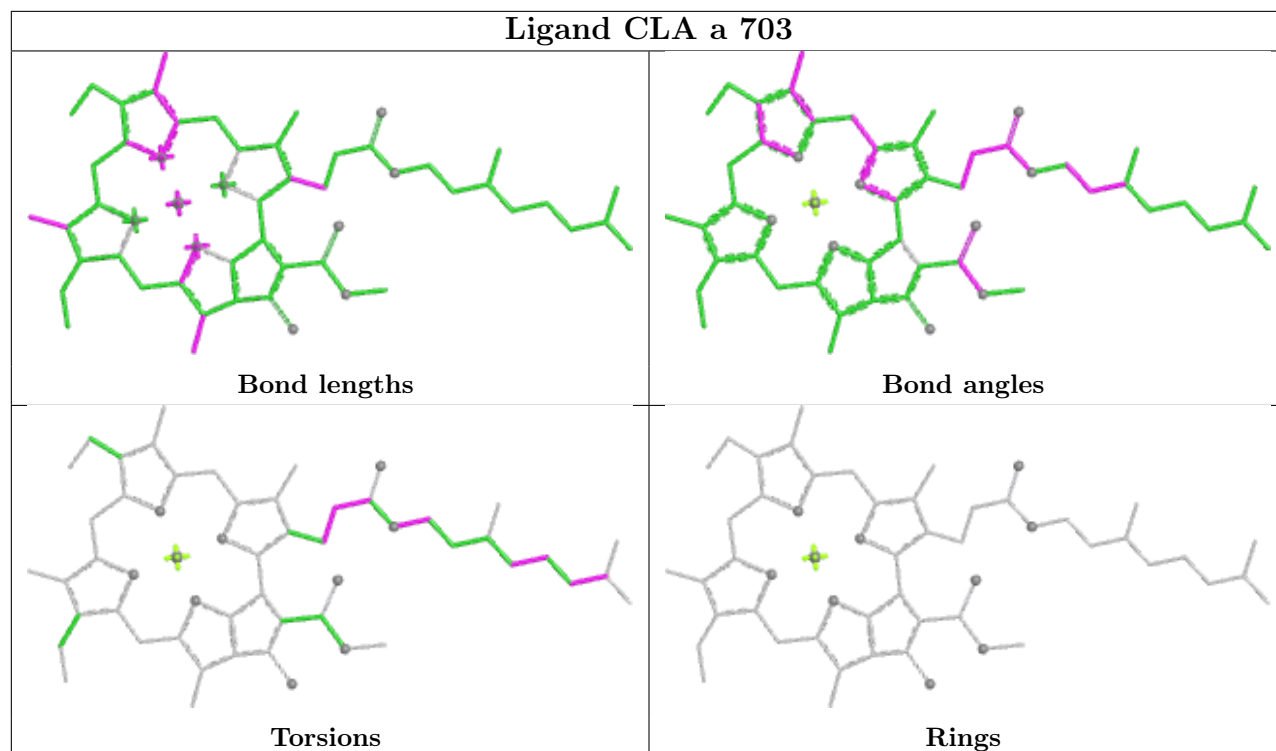
Ligand CLA K 316



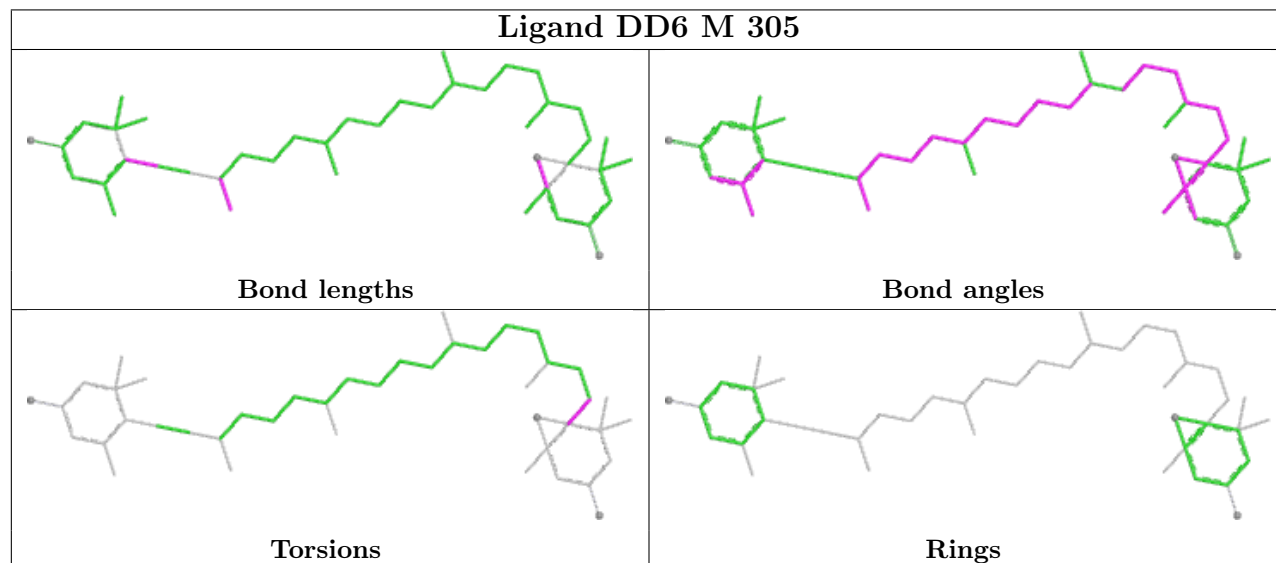
Ligand DD6 J 303



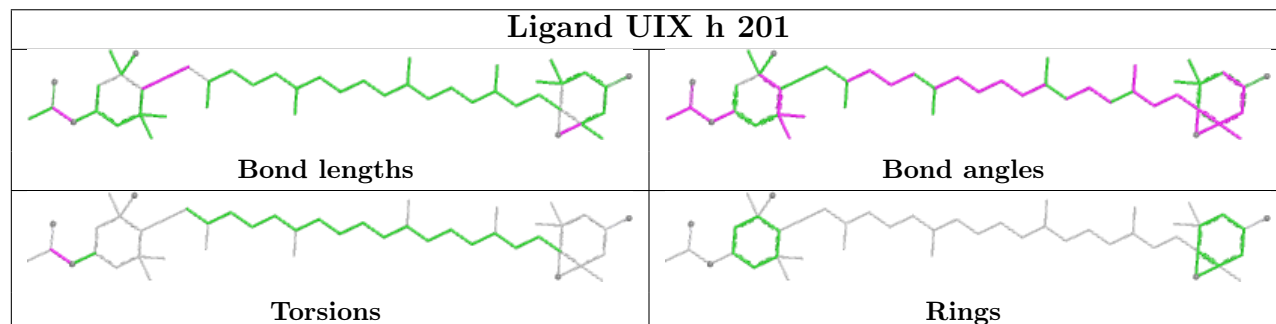
Ligand CLA a 703

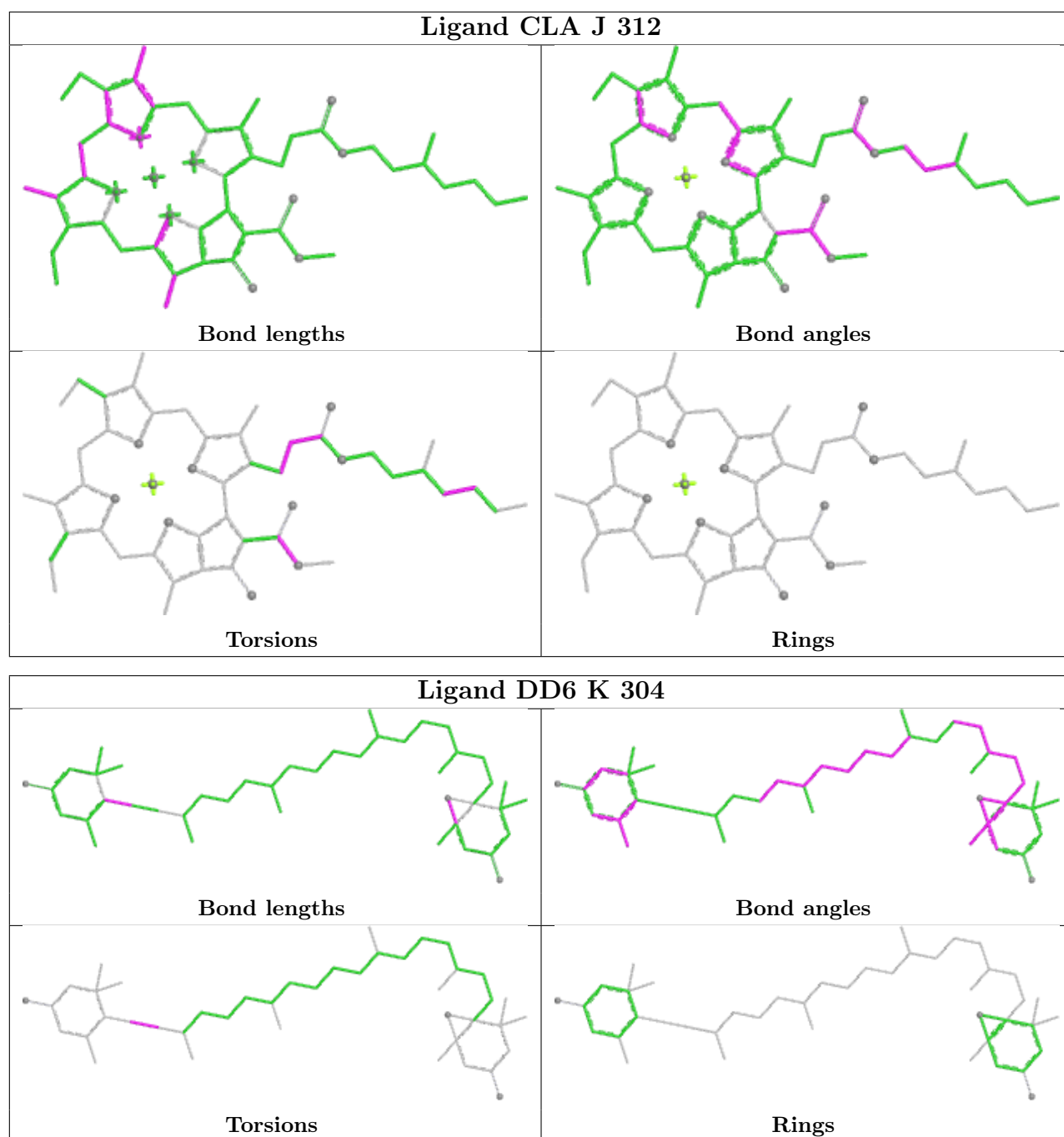


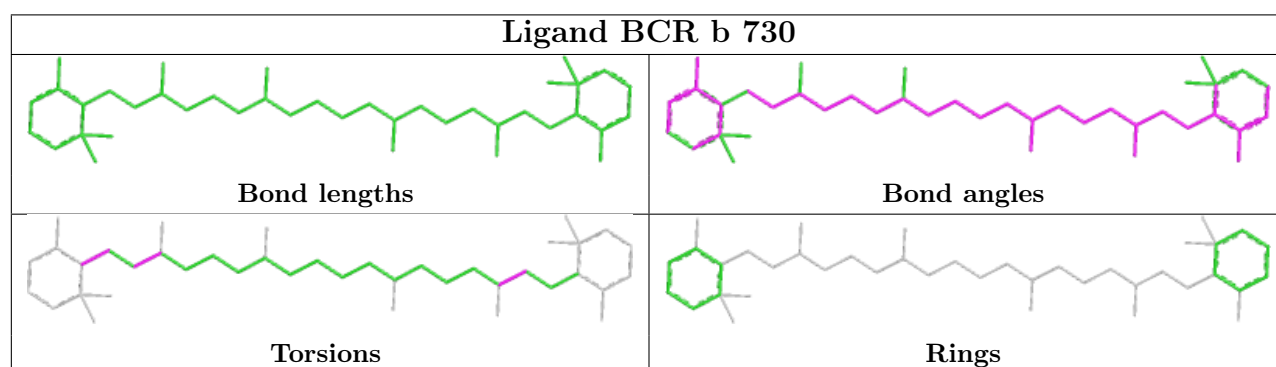
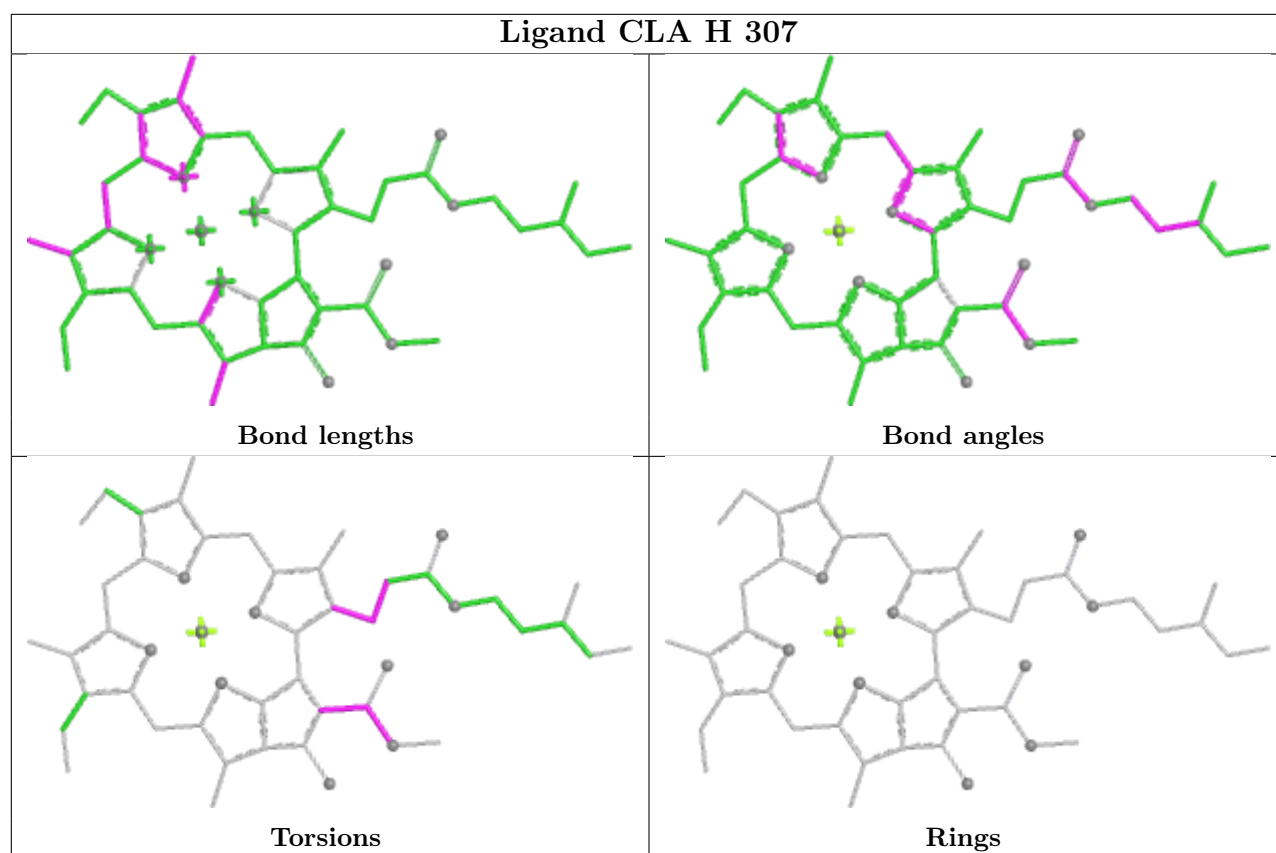
Ligand DD6 M 305



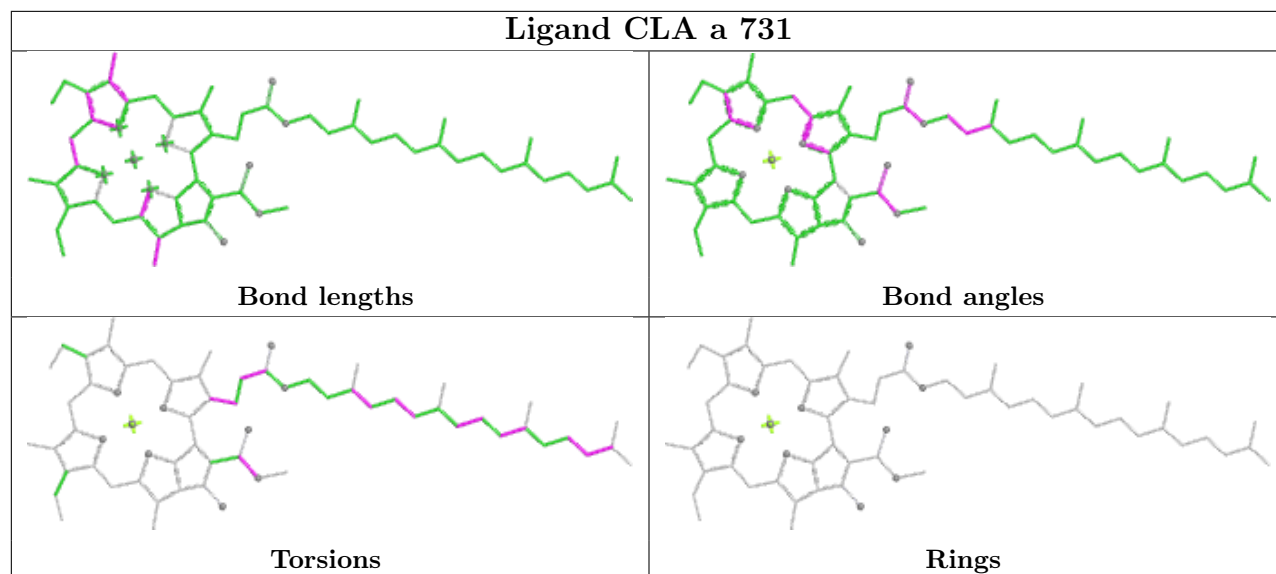
Ligand UIX h 201



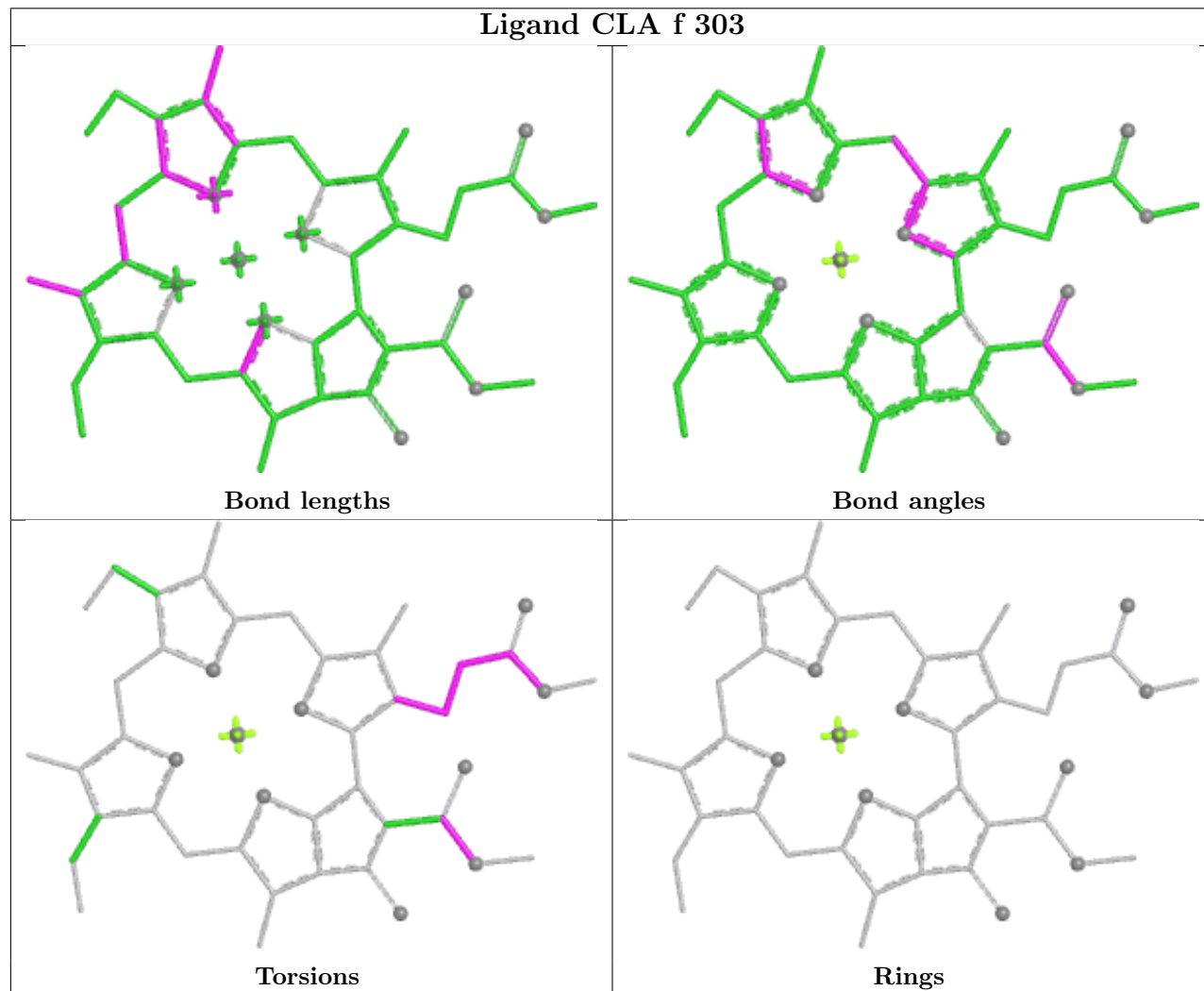




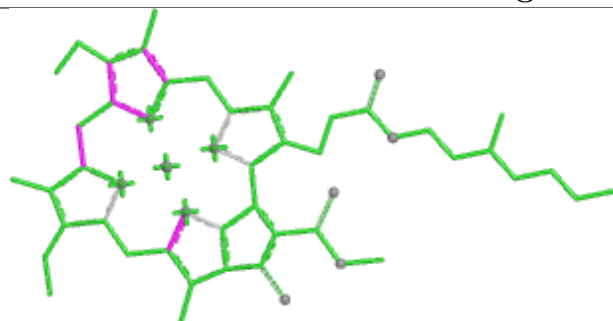
Ligand CLA a 731



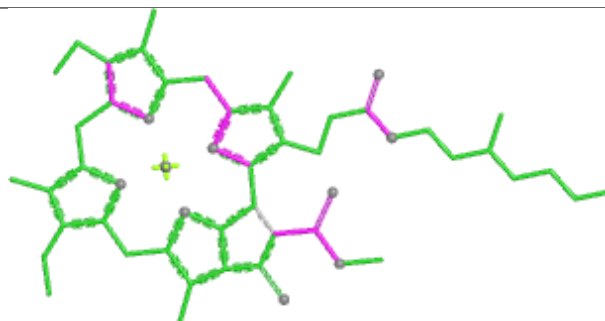
Ligand CLA f 303



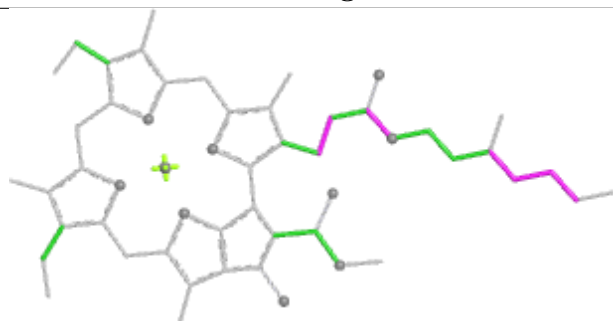
Ligand CLA L 309



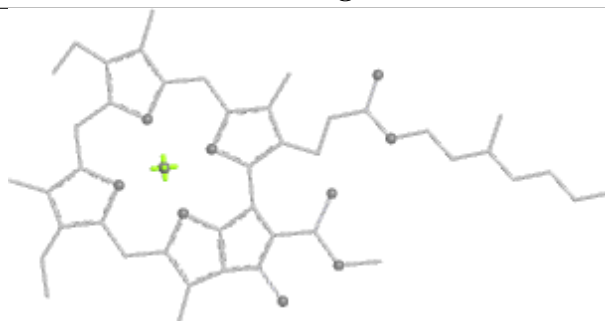
Bond lengths



Bond angles

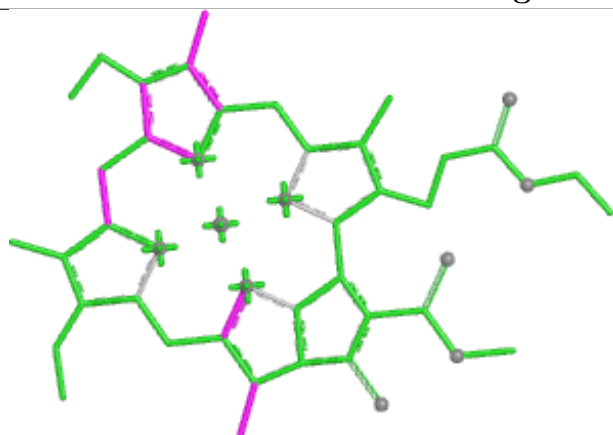


Torsions

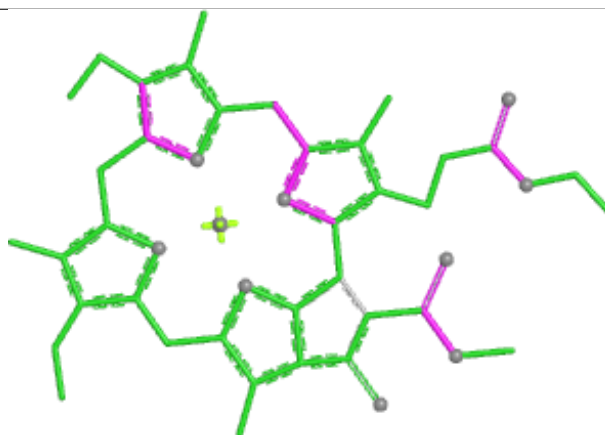


Rings

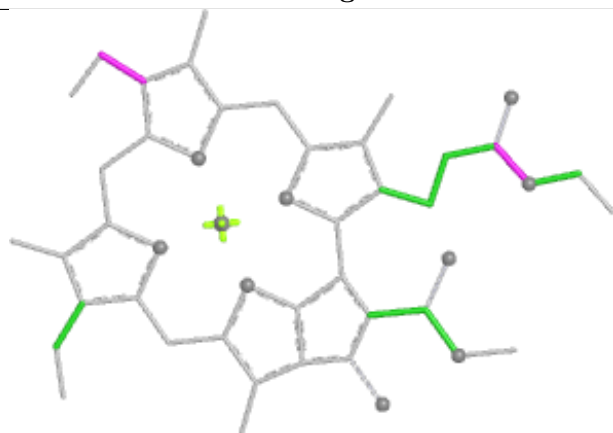
Ligand CLA N 304



Bond lengths



Bond angles

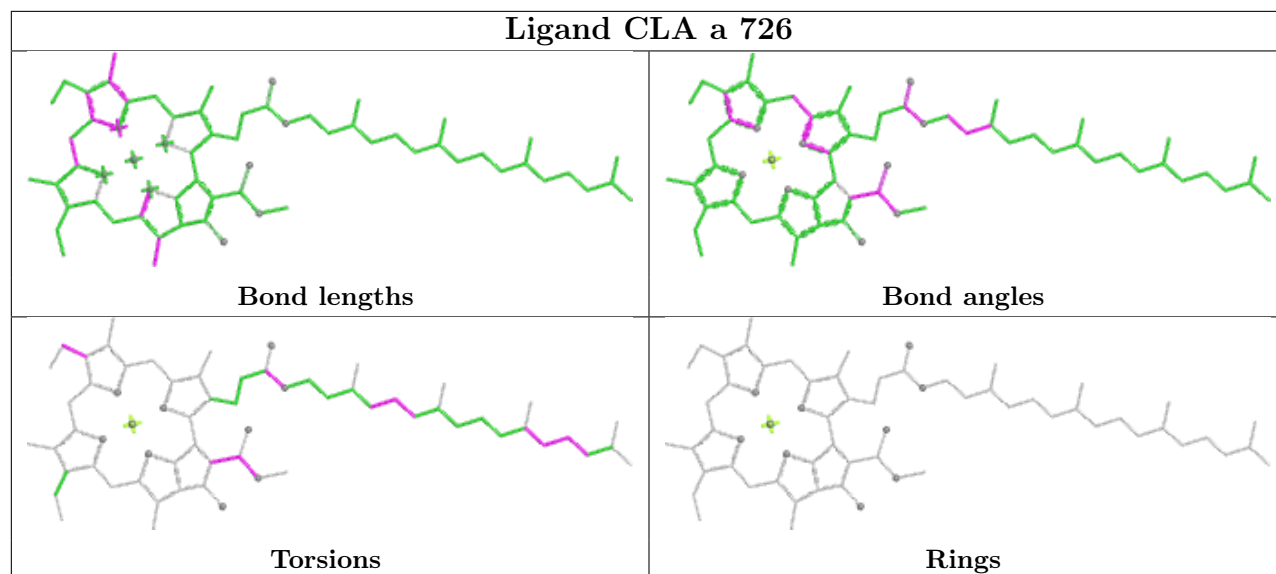


Torsions

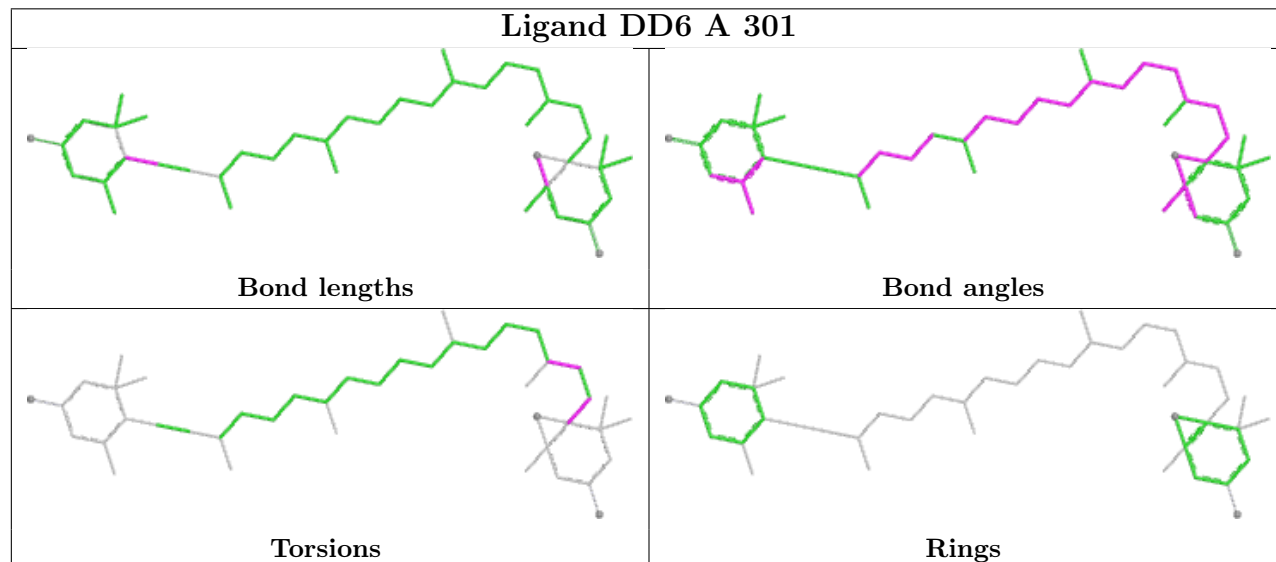


Rings

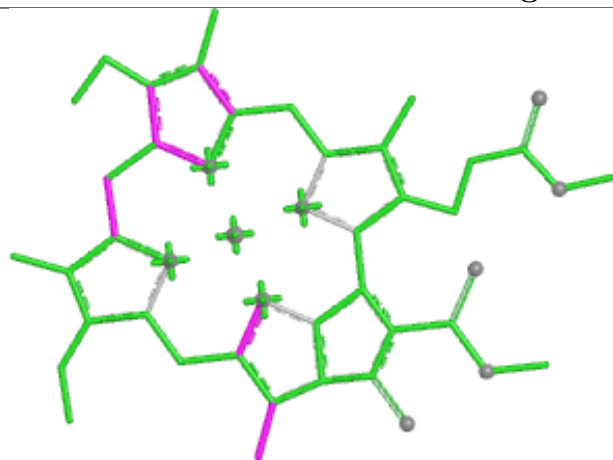
Ligand CLA a 726



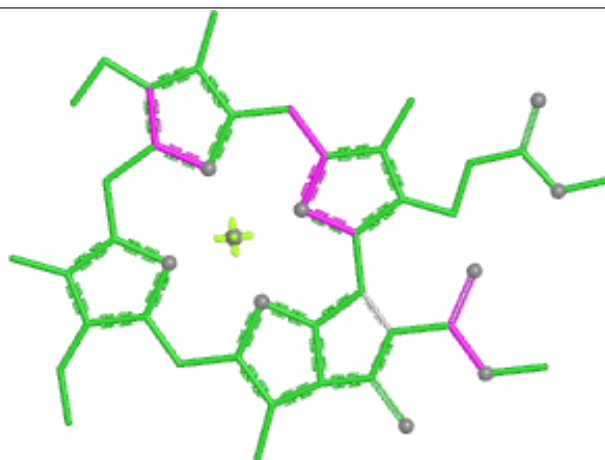
Ligand DD6 A 301



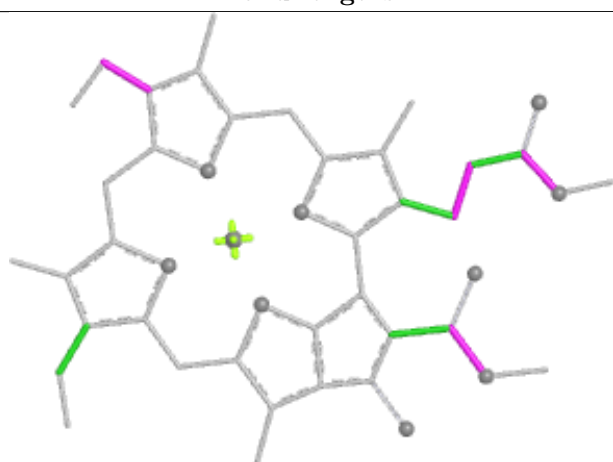
Ligand CLA I 307



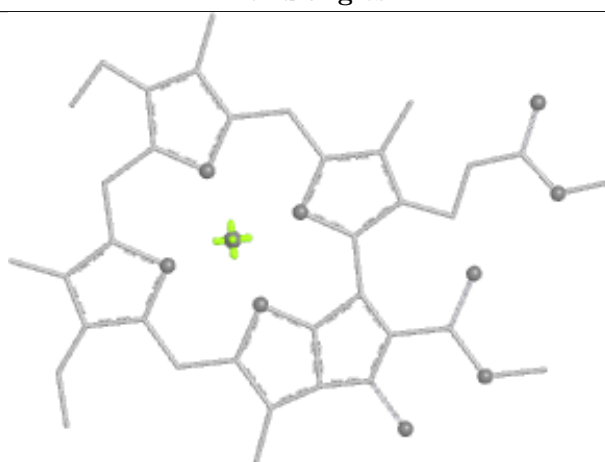
Bond lengths



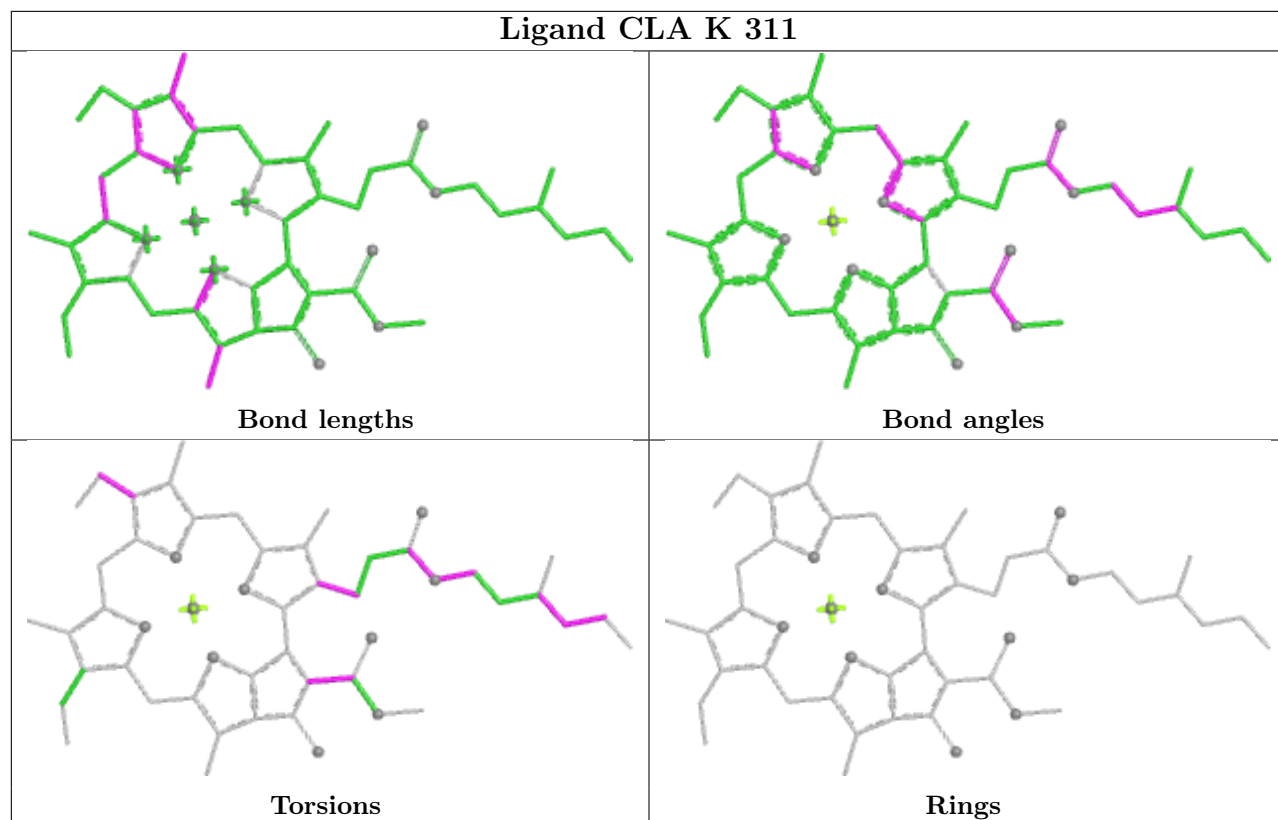
Bond angles



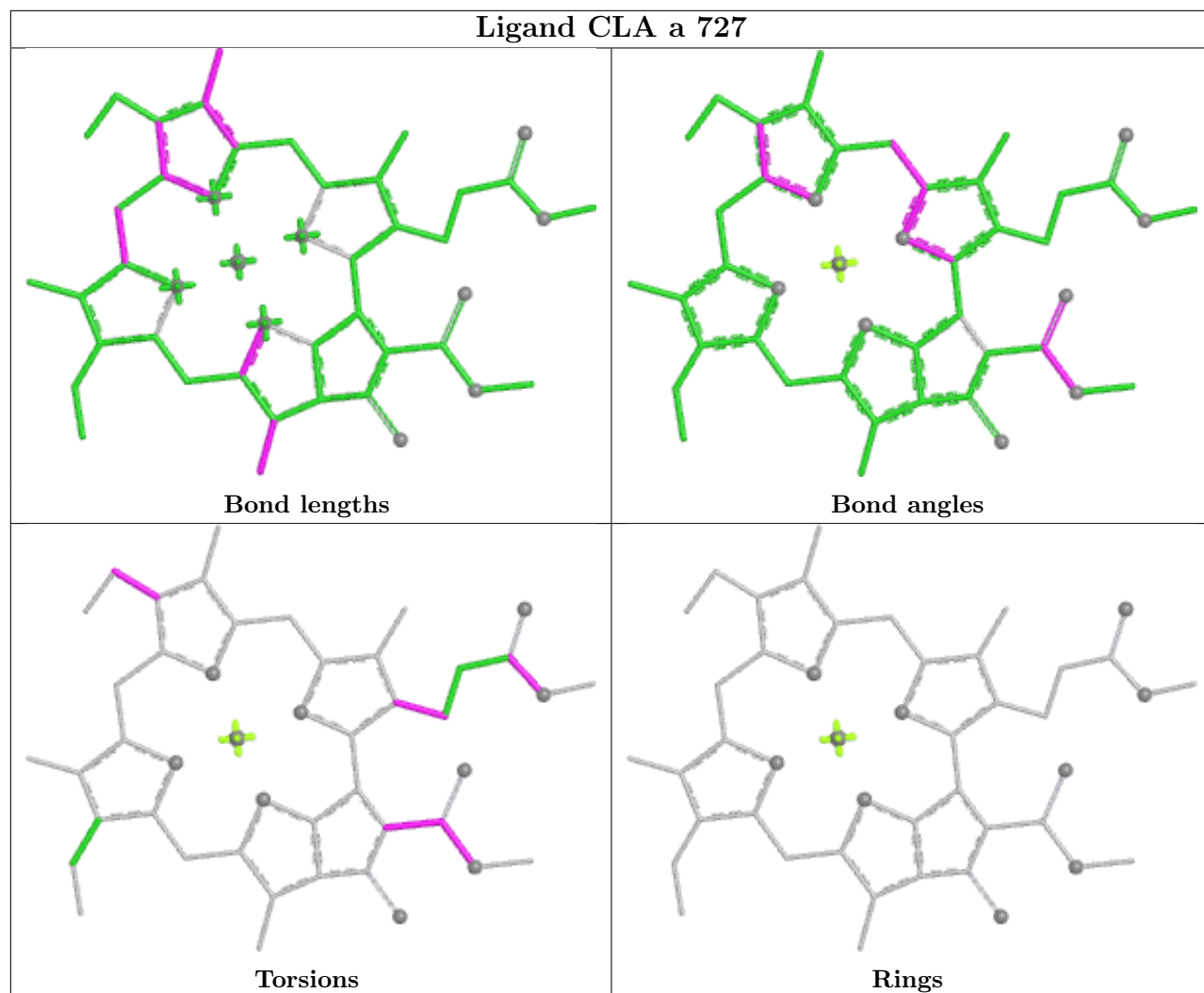
Torsions



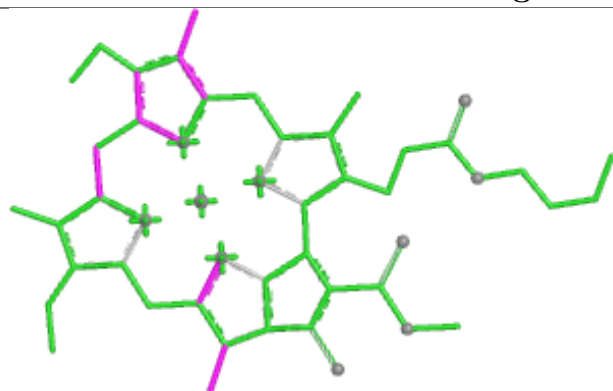
Rings



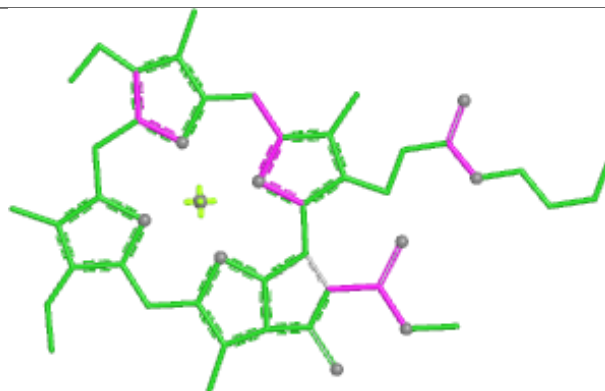
Ligand CLA a 727



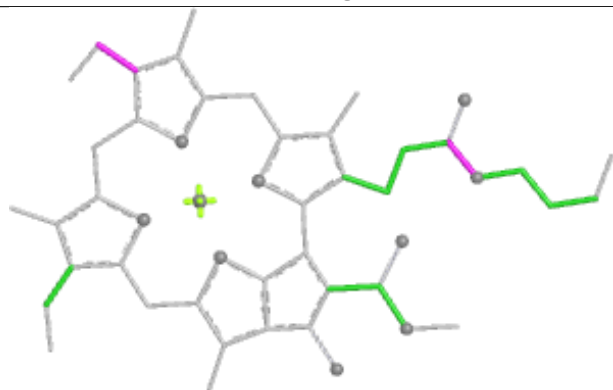
Ligand CLA K 306



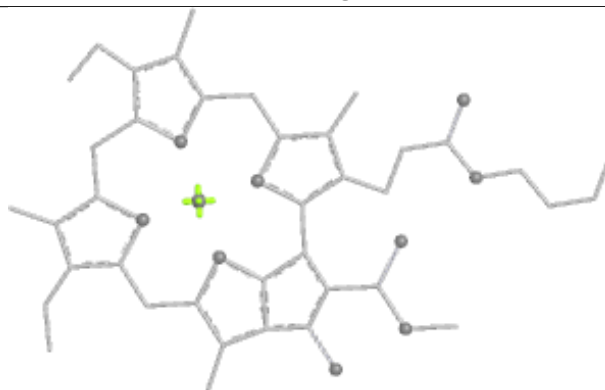
Bond lengths



Bond angles



Torsions

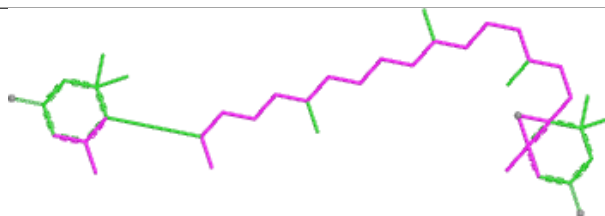


Rings

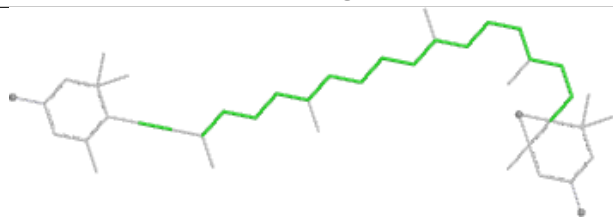
Ligand DD6 N 303



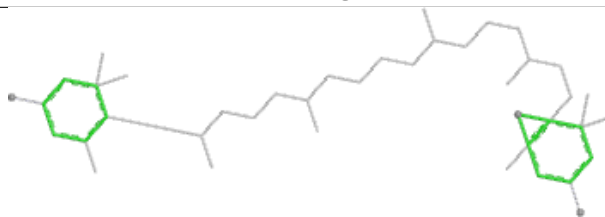
Bond lengths



Bond angles

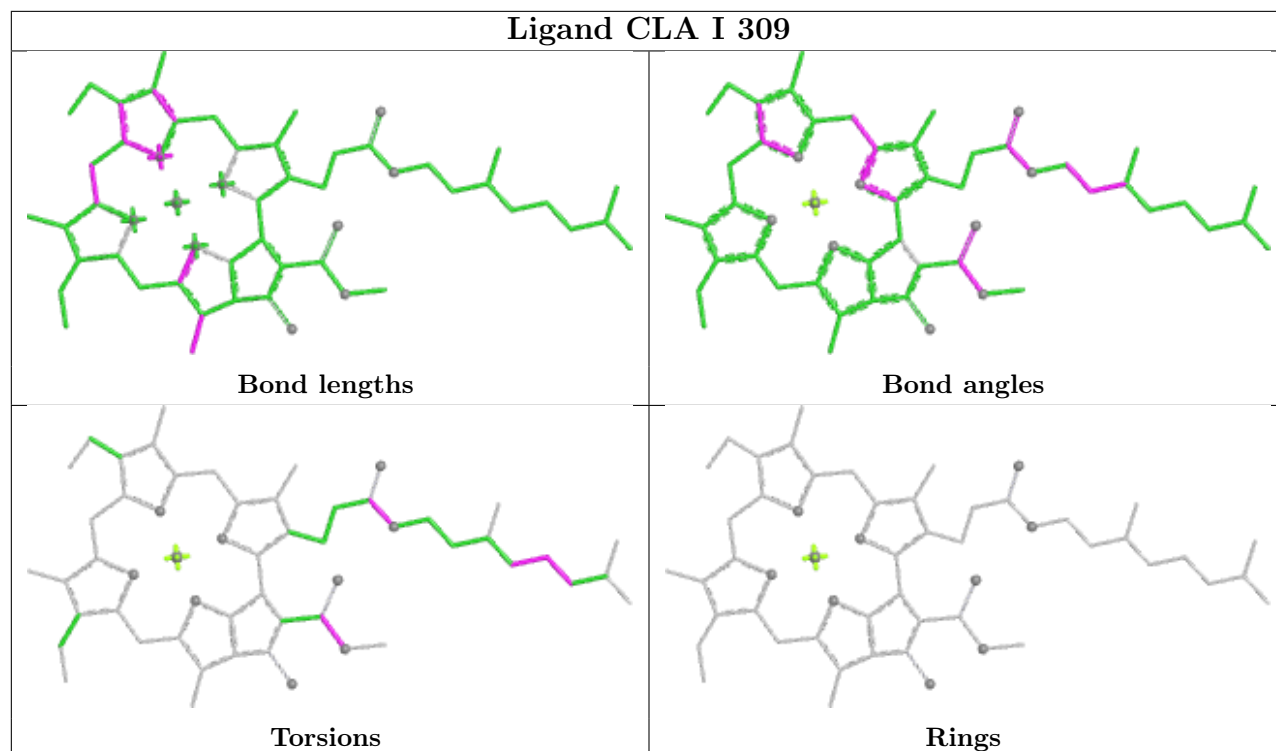


Torsions

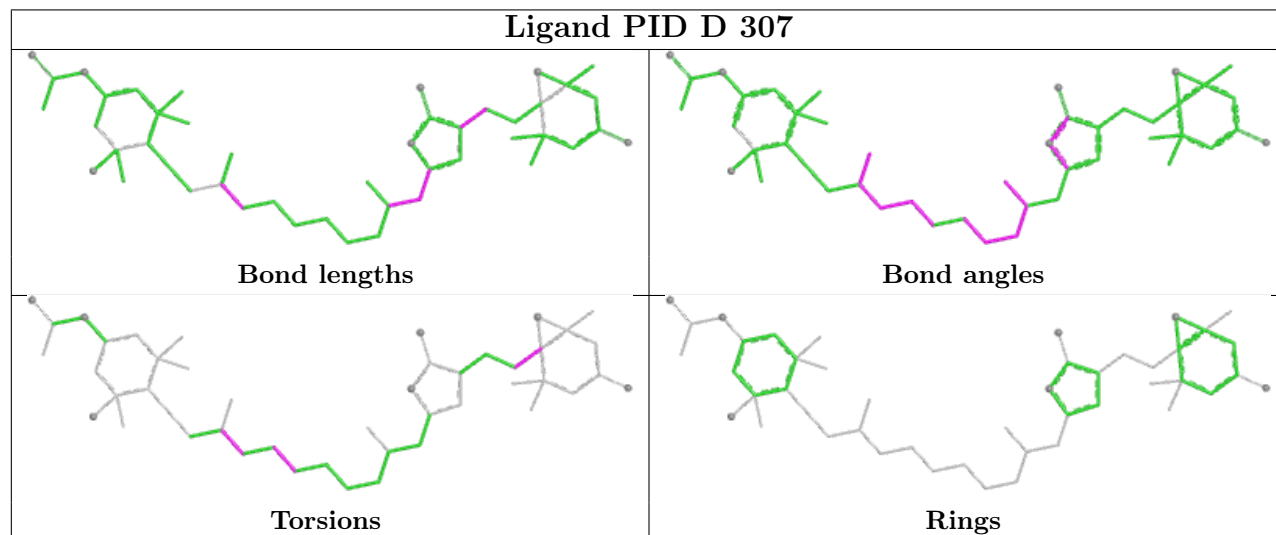


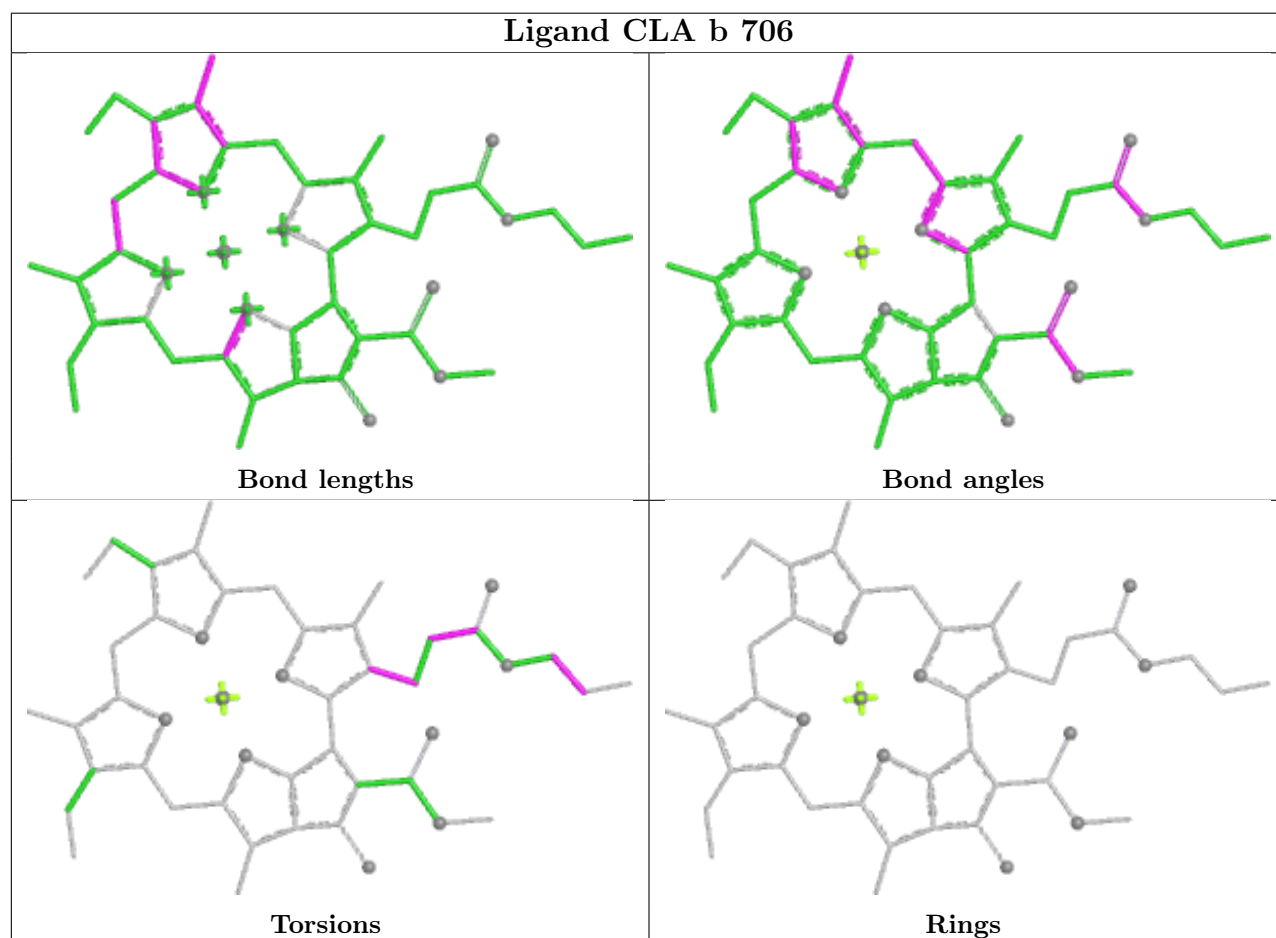
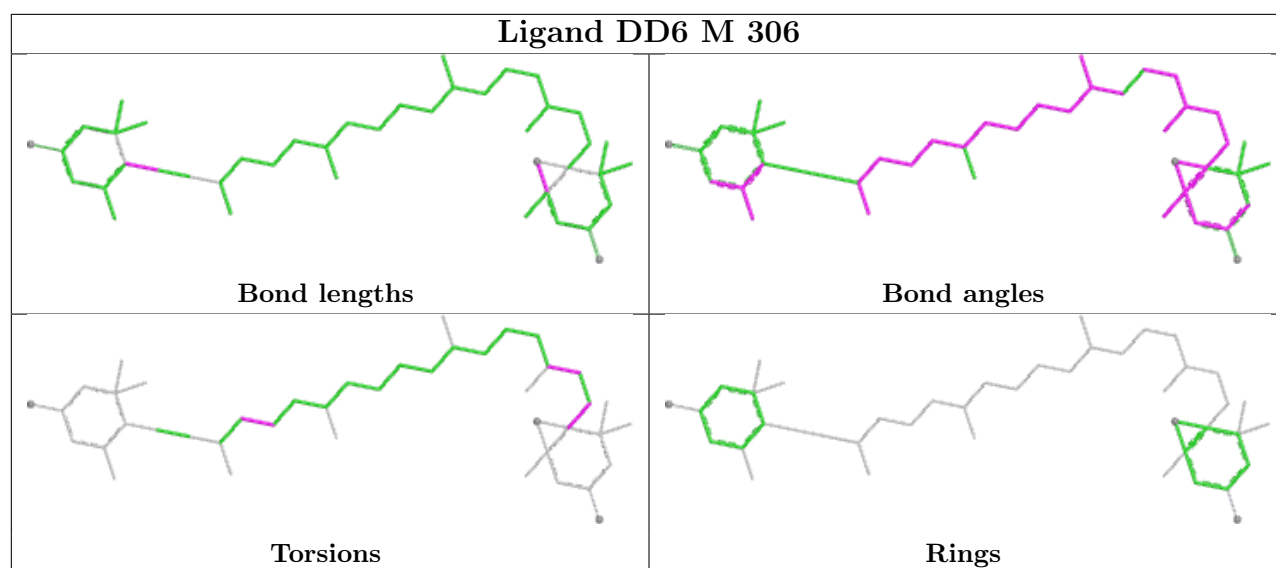
Rings

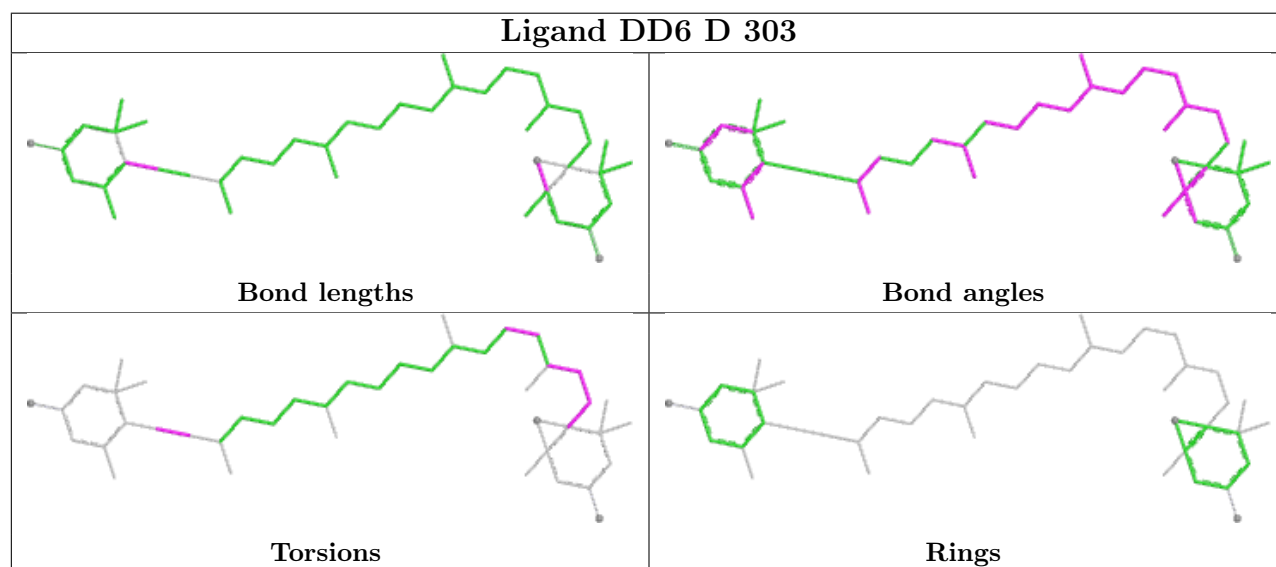
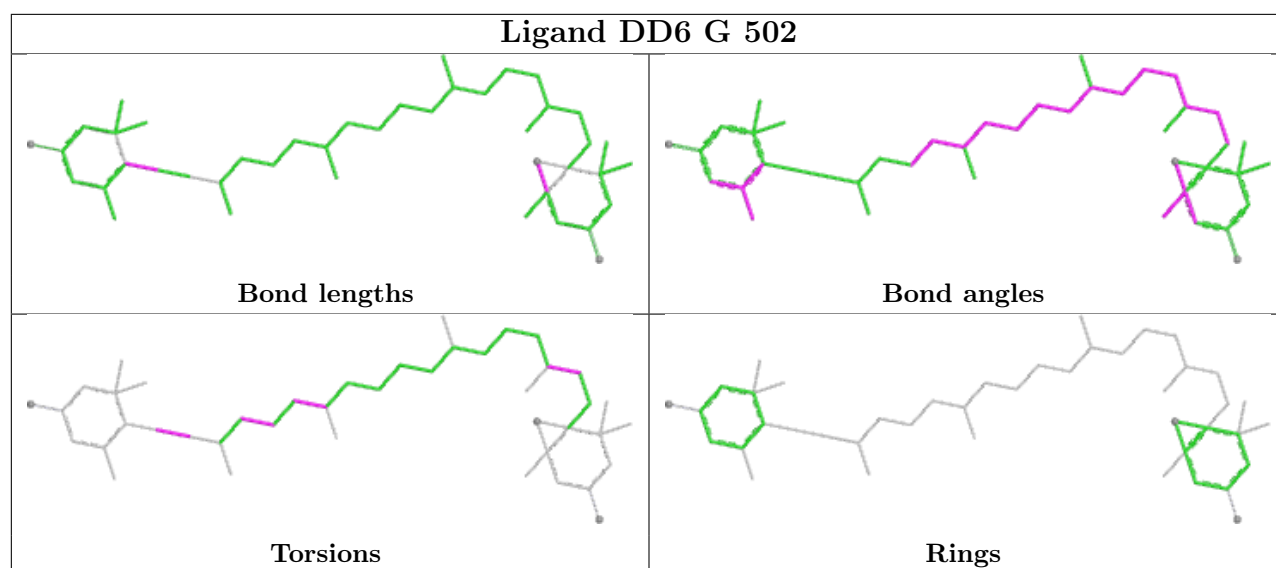
Ligand CLA I 309

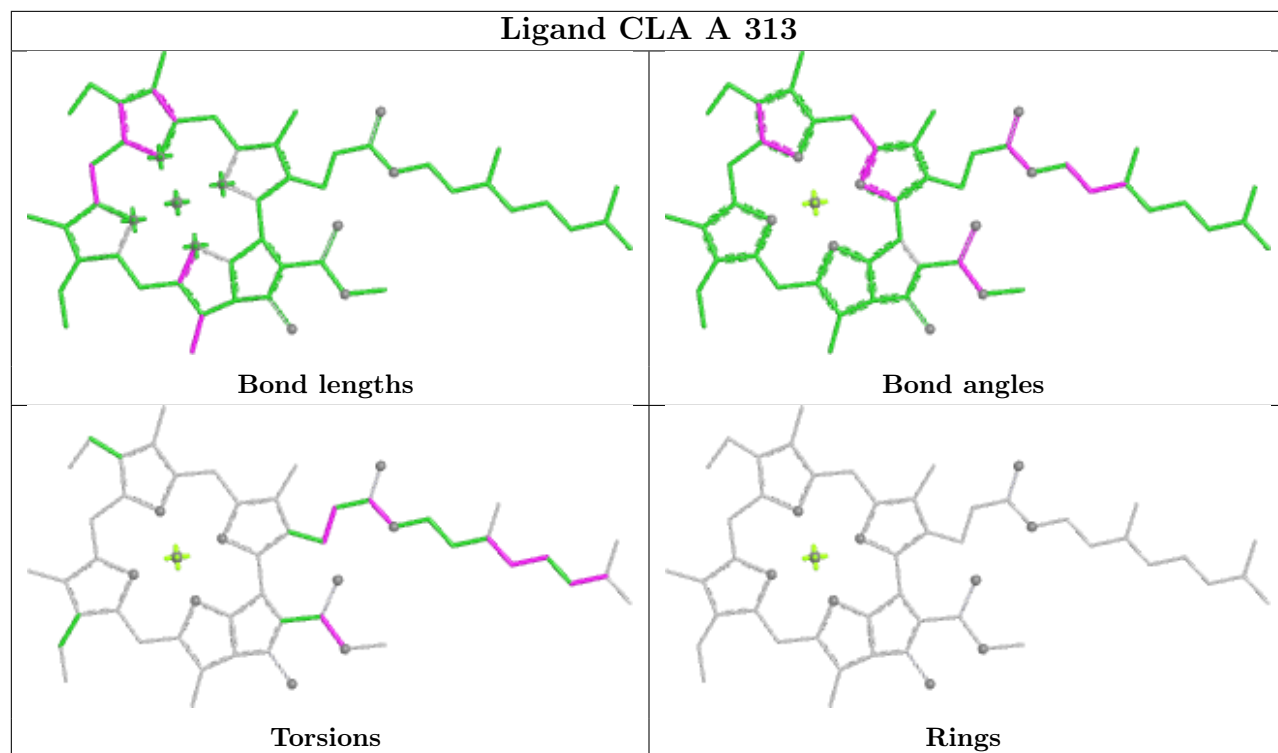


Ligand PID D 307

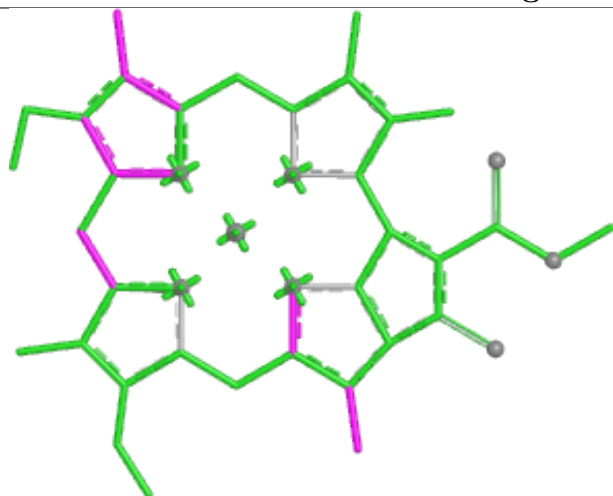




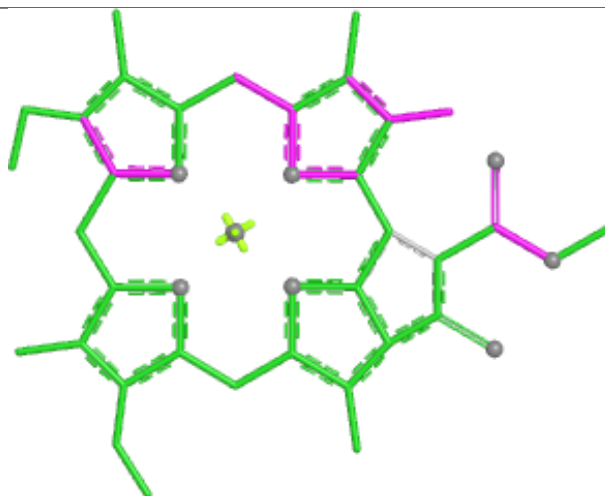




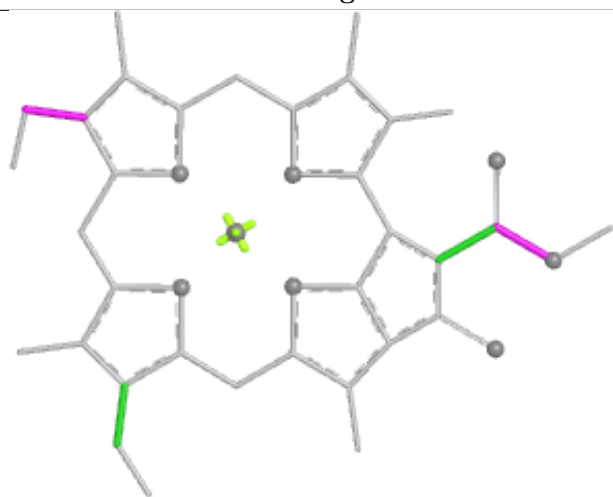
Ligand CLA 1 308



Bond lengths



Bond angles

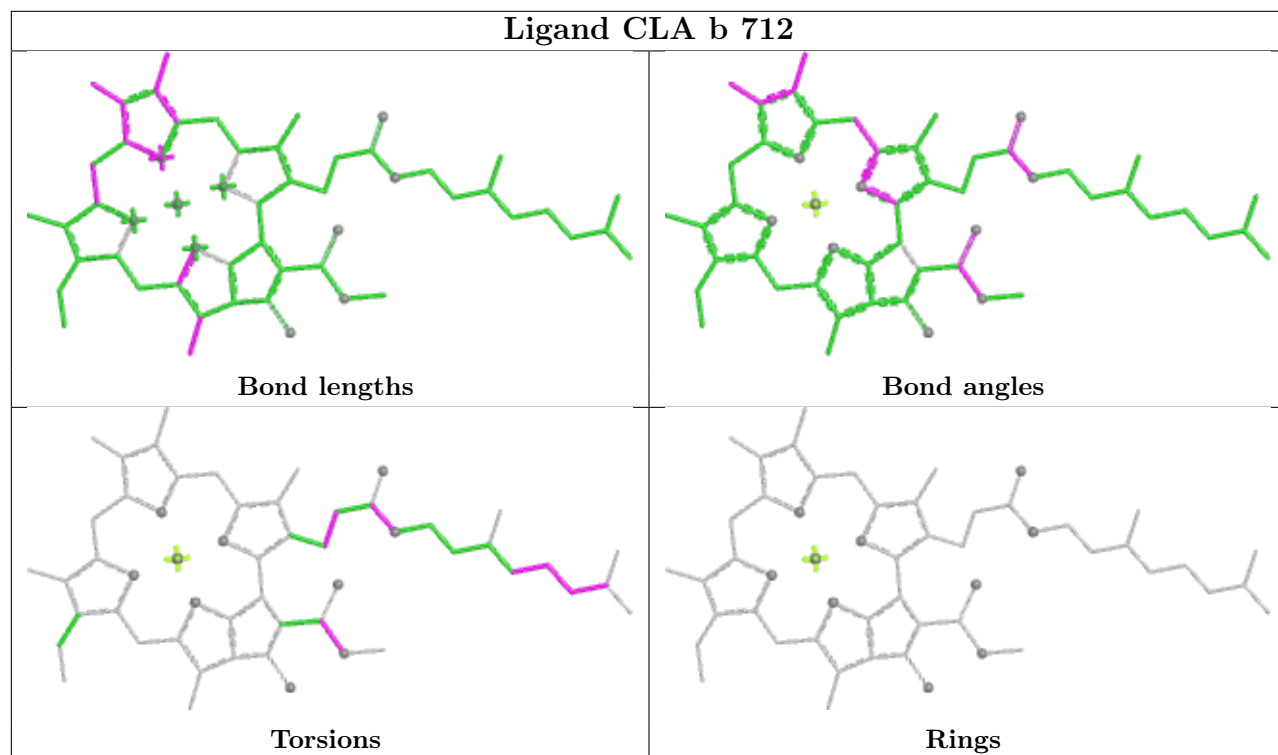


Torsions

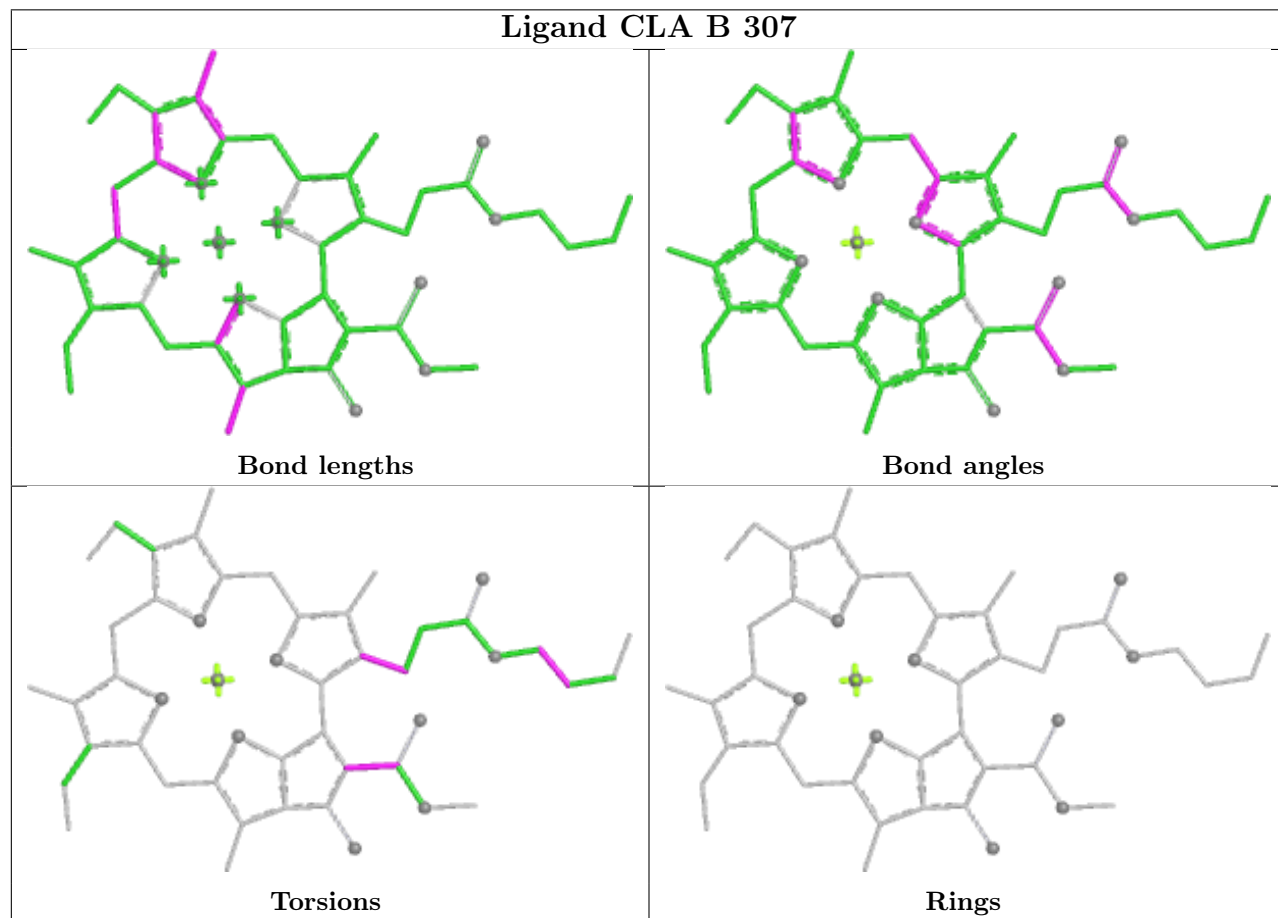


Rings

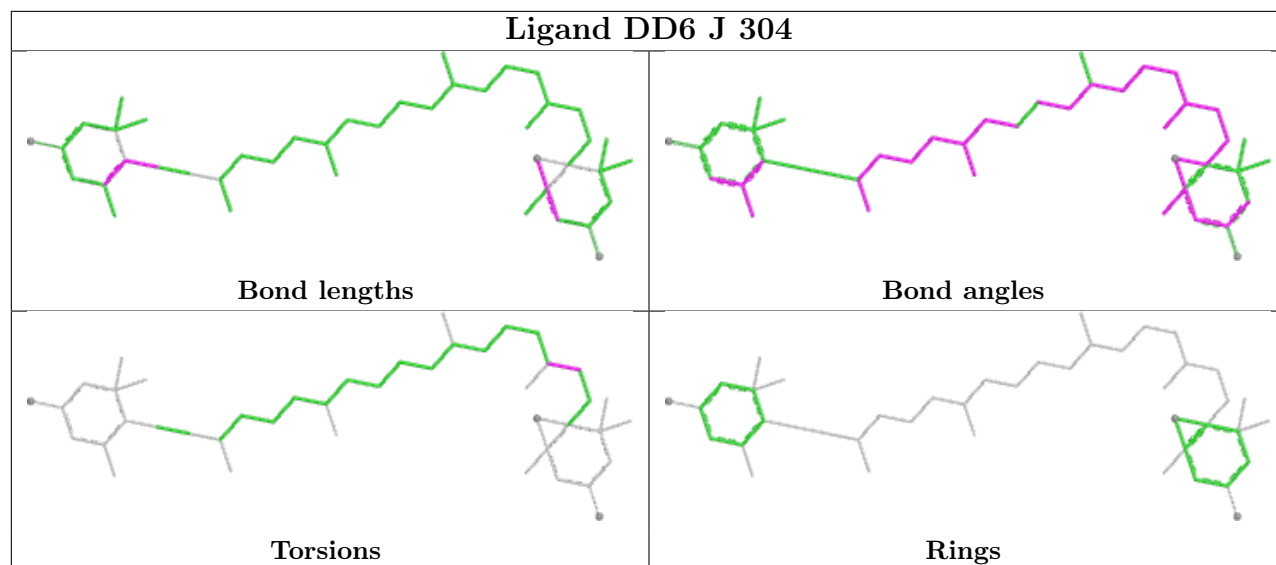
Ligand CLA b 712



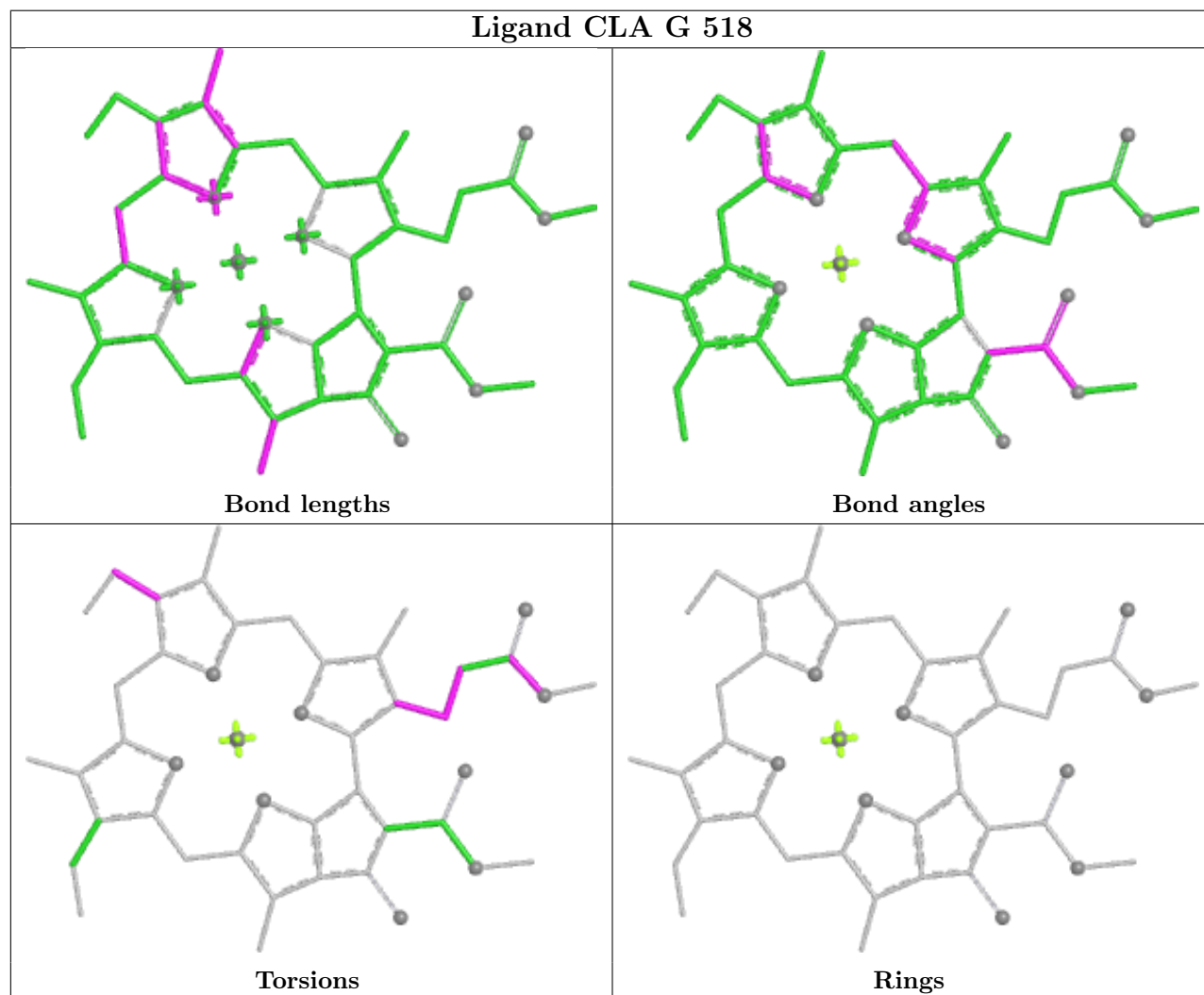
Ligand CLA B 307



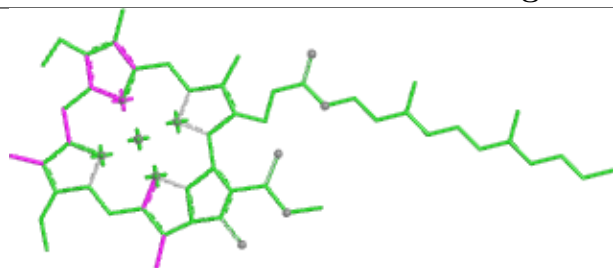
Ligand DD6 J 304



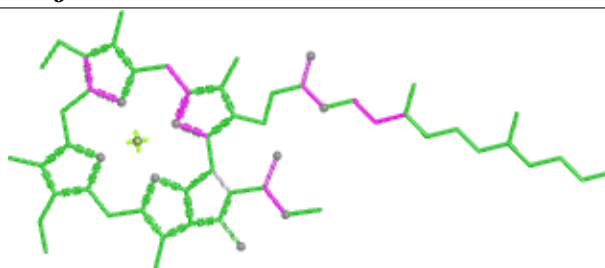
Ligand CLA G 518



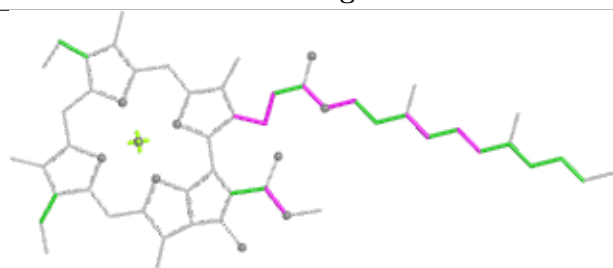
Ligand CLA j 106



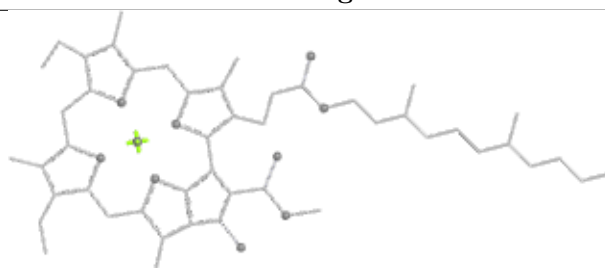
Bond lengths



Bond angles

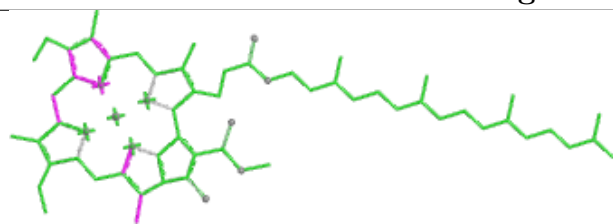


Torsions

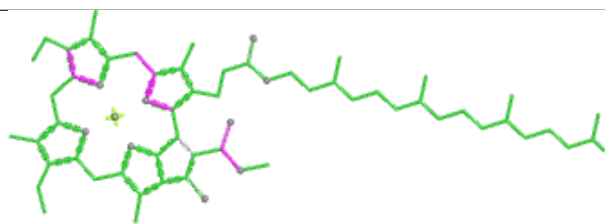


Rings

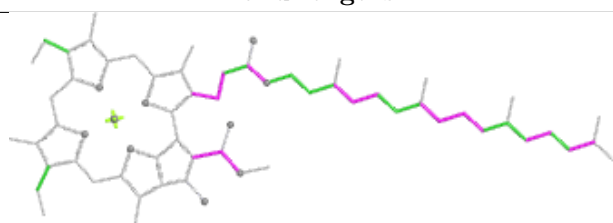
Ligand CLA J 307



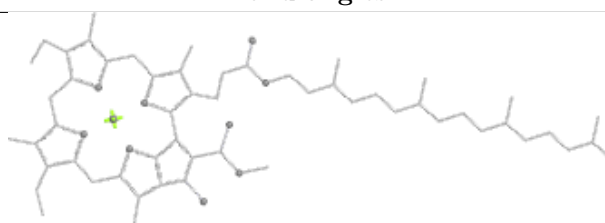
Bond lengths



Bond angles

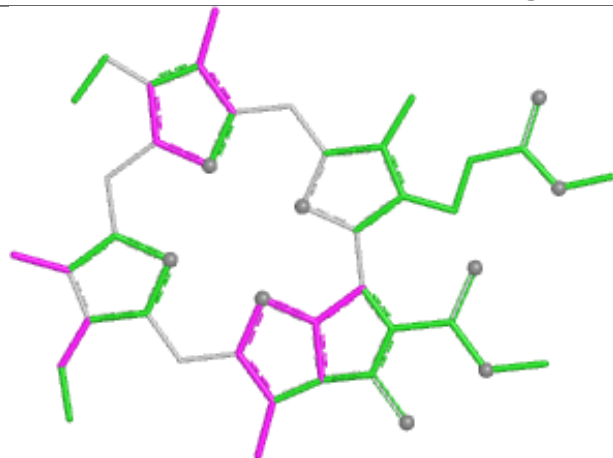


Torsions

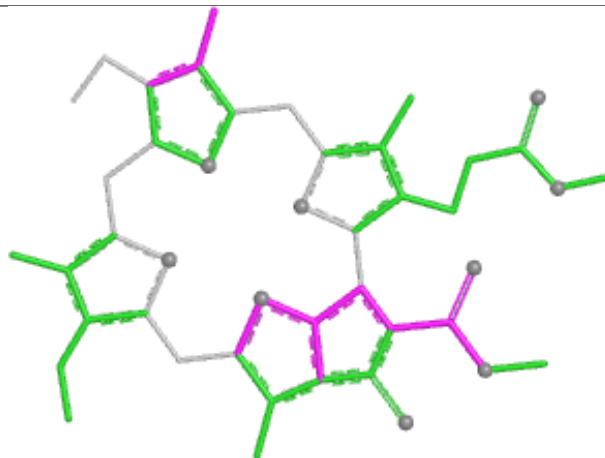


Rings

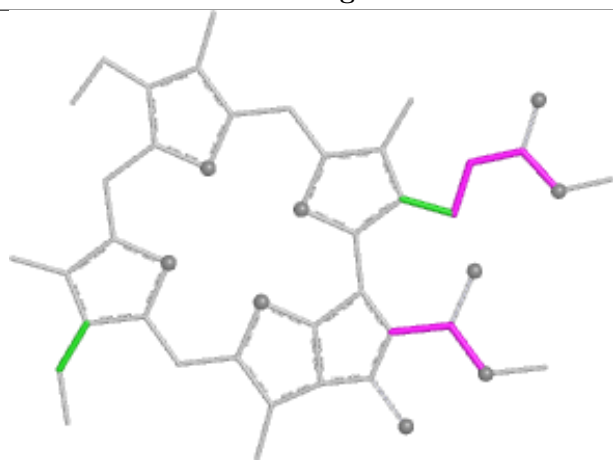
Ligand CLA I 310



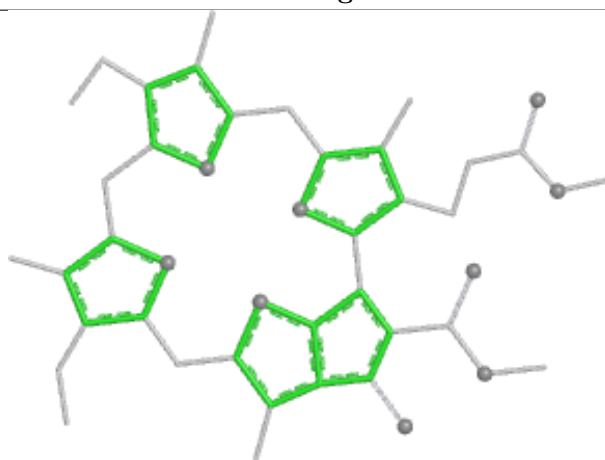
Bond lengths



Bond angles

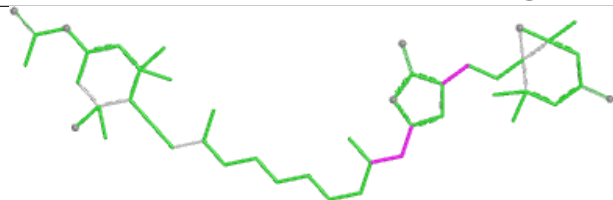


Torsions

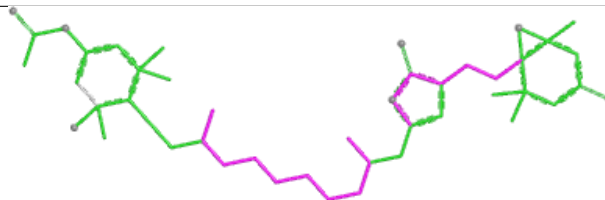


Rings

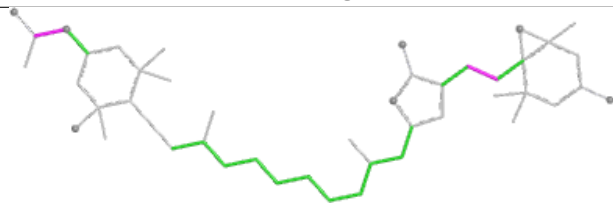
Ligand PID F 304



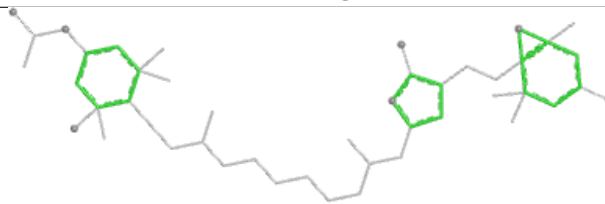
Bond lengths



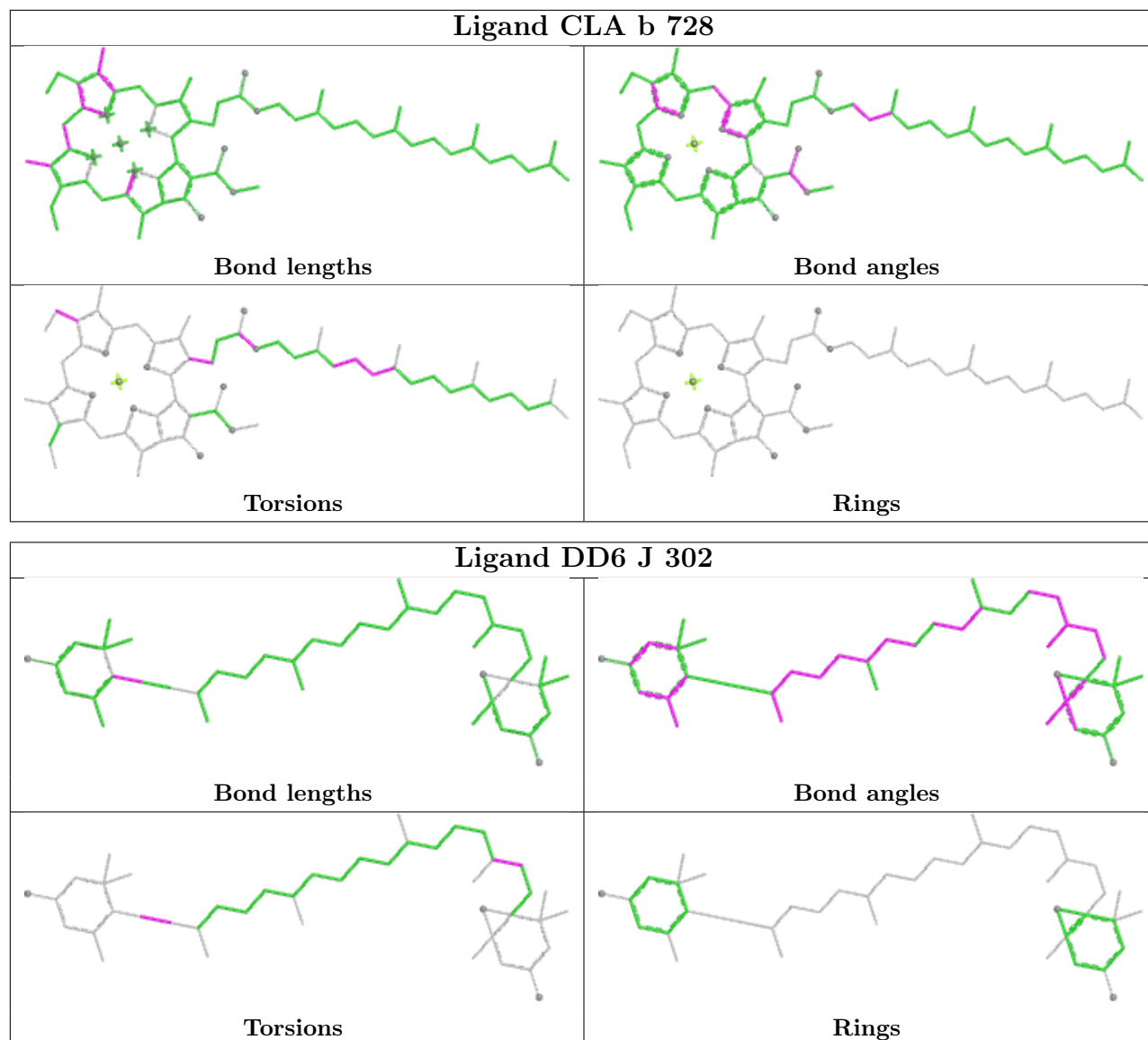
Bond angles

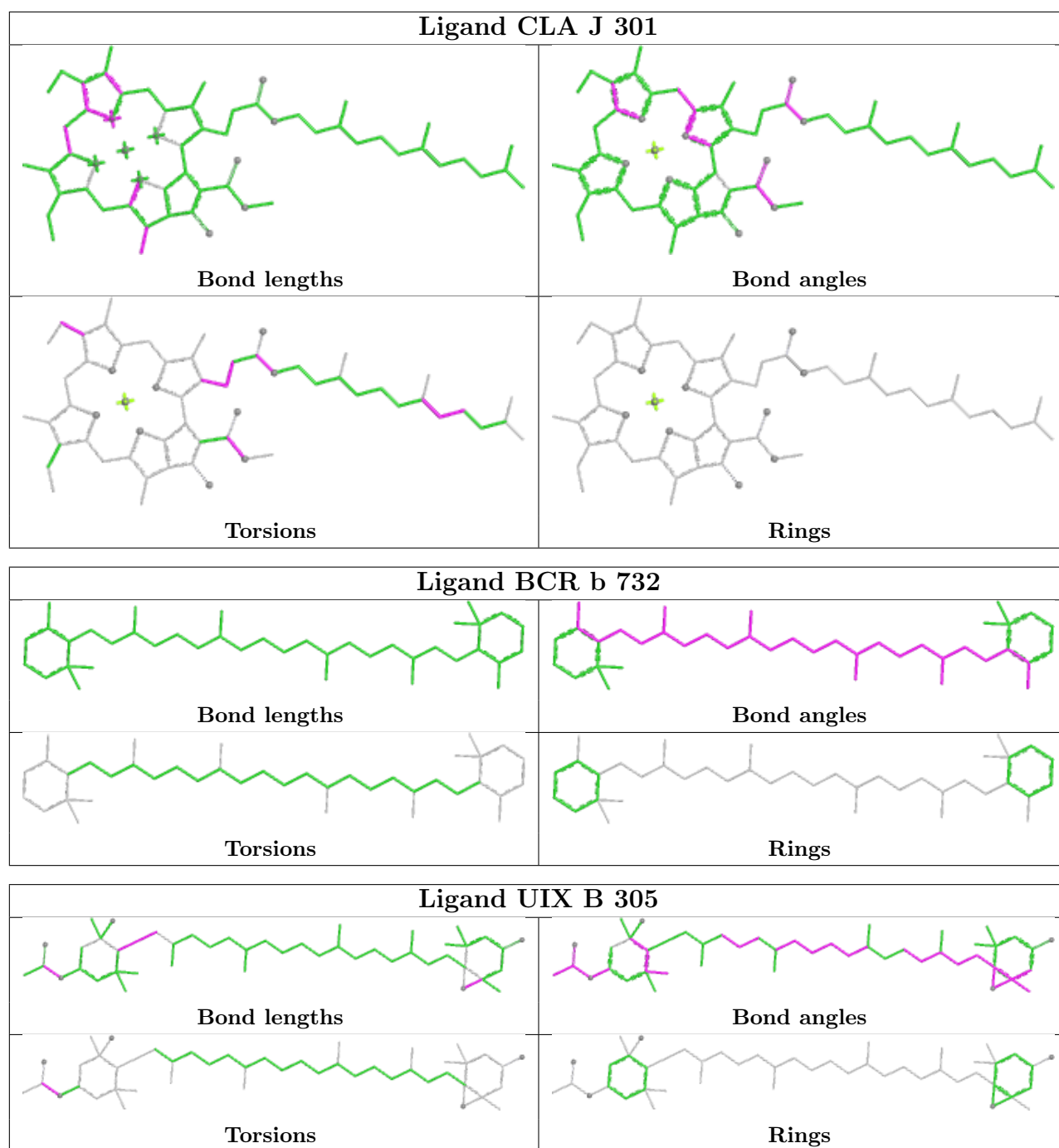


Torsions

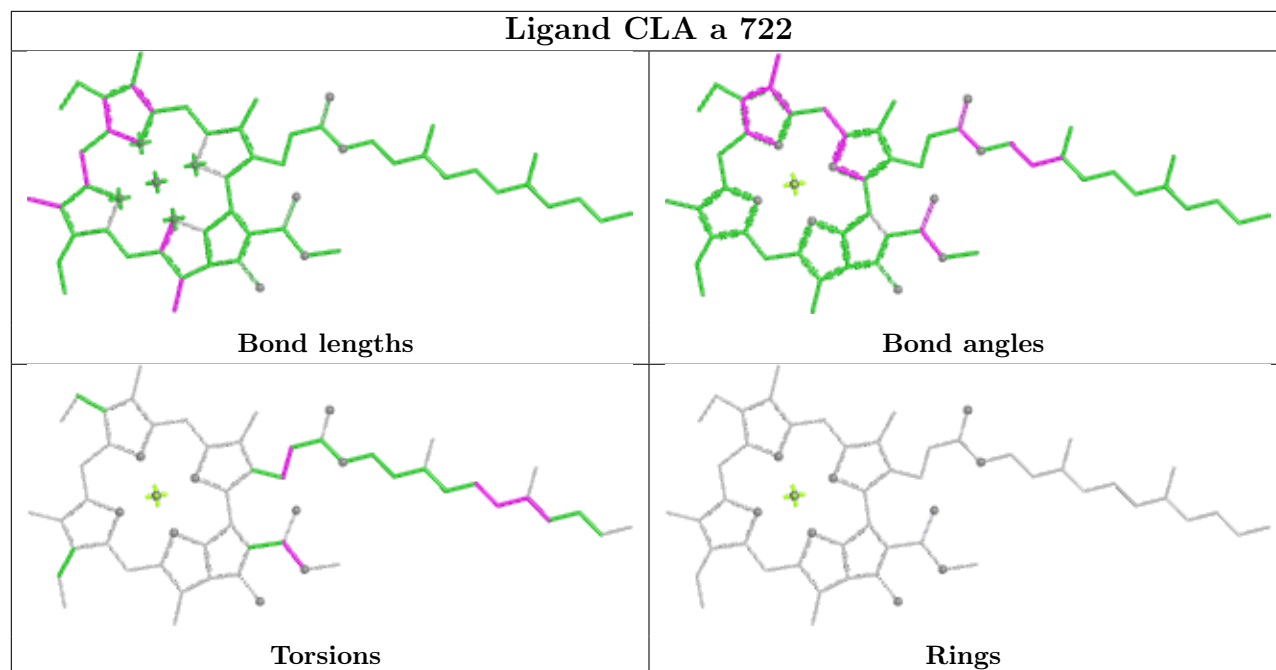


Rings

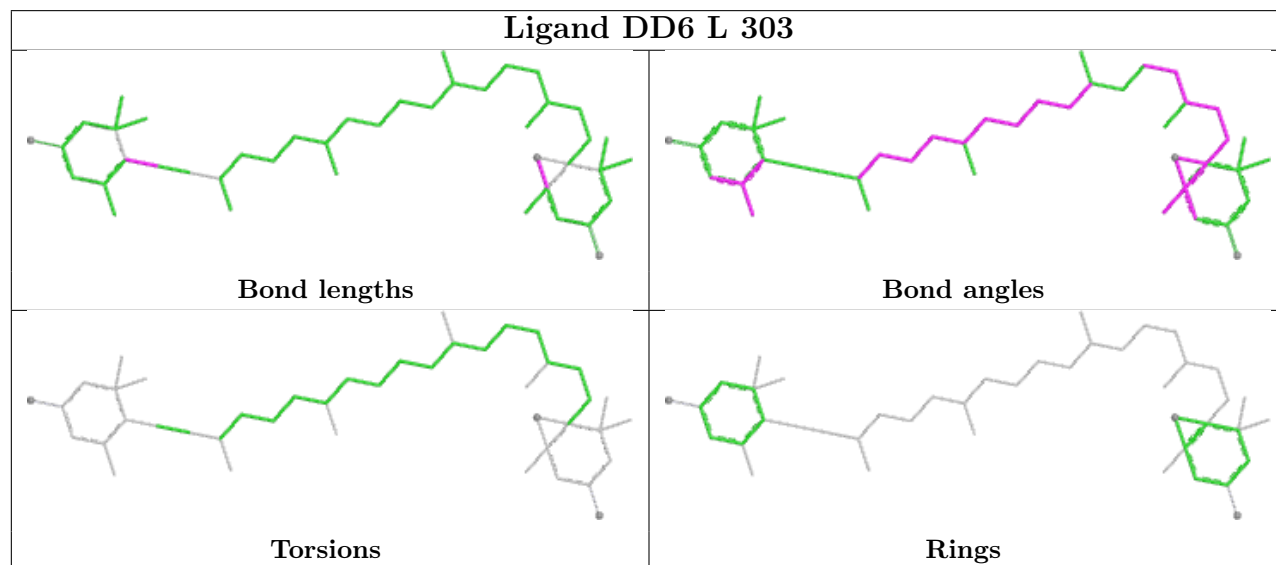




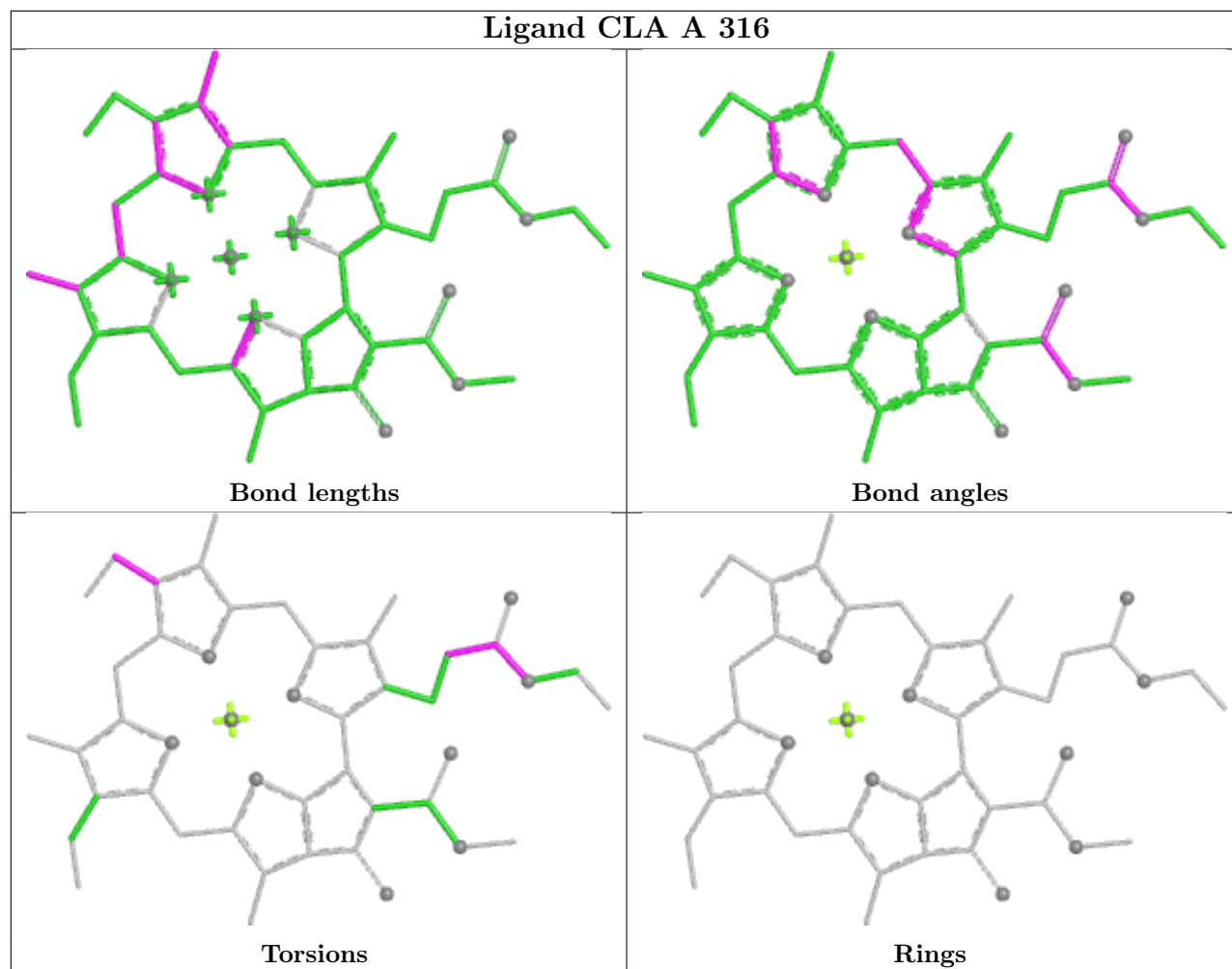
Ligand CLA a 722

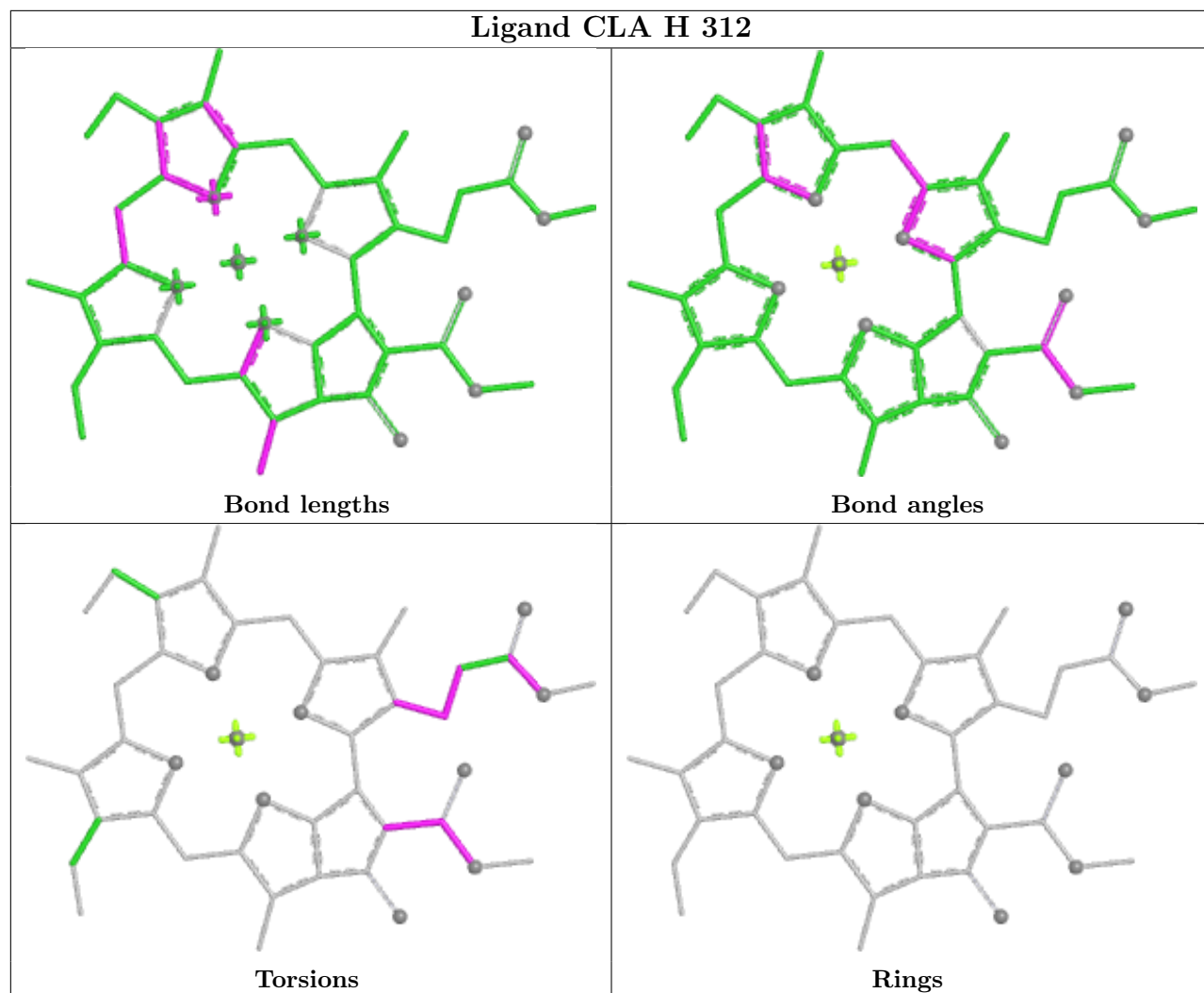


Ligand DD6 L 303

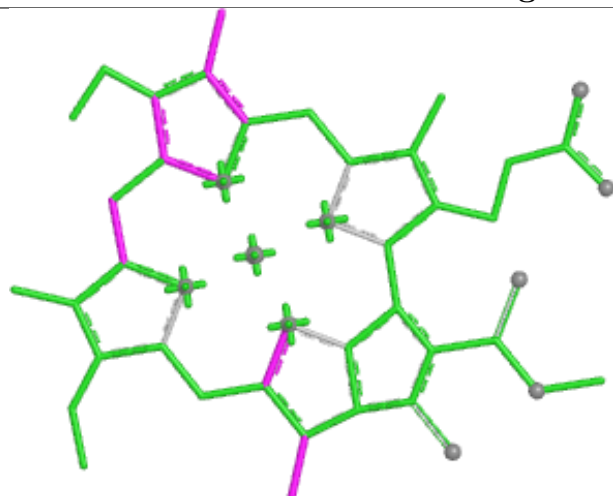


Ligand CLA A 316

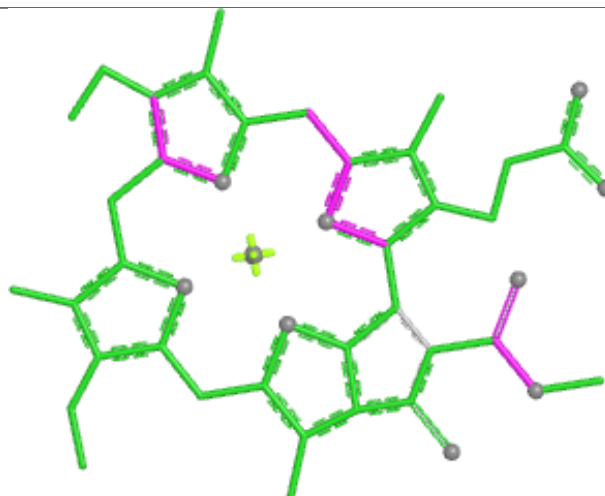




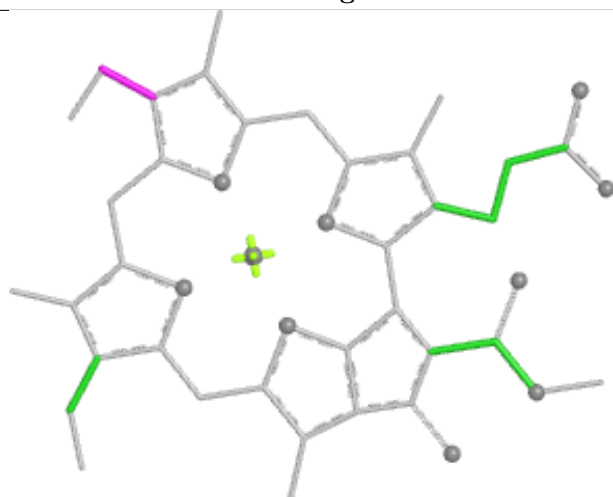
Ligand CLA a 701



Bond lengths



Bond angles

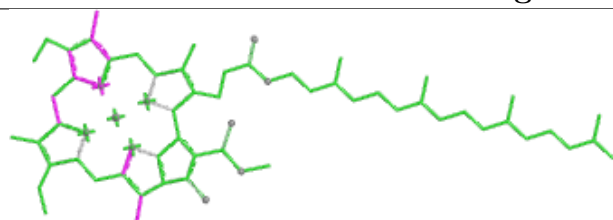


Torsions

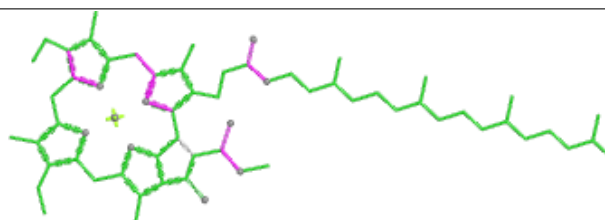


Rings

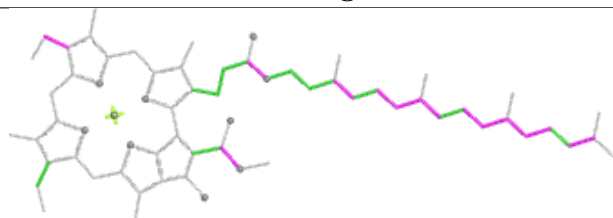
Ligand CLA B 311



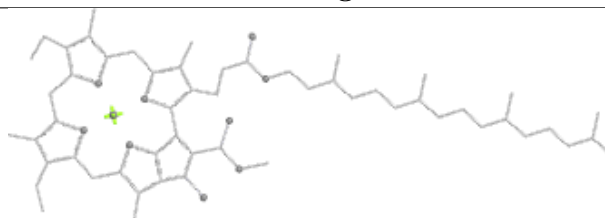
Bond lengths



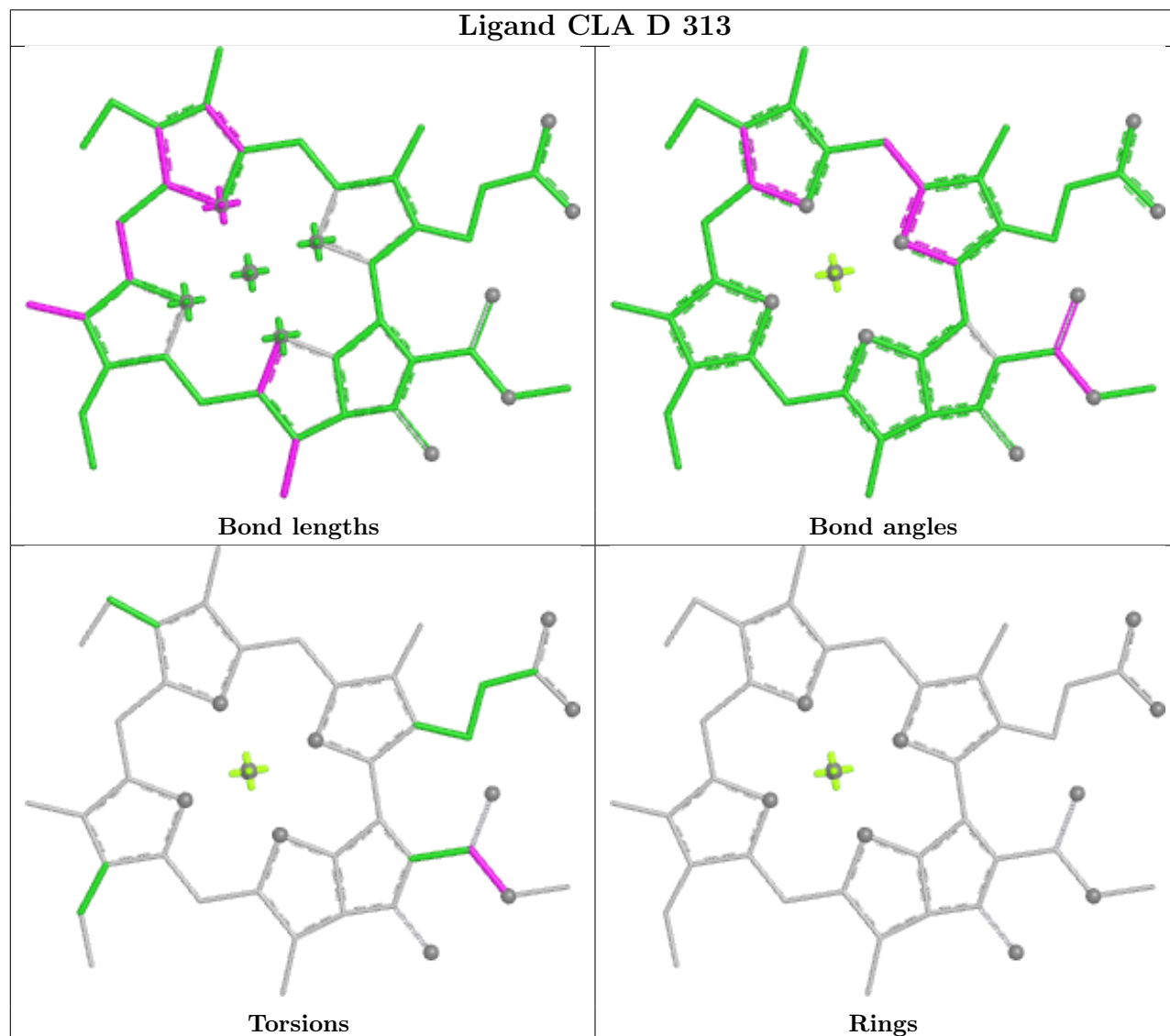
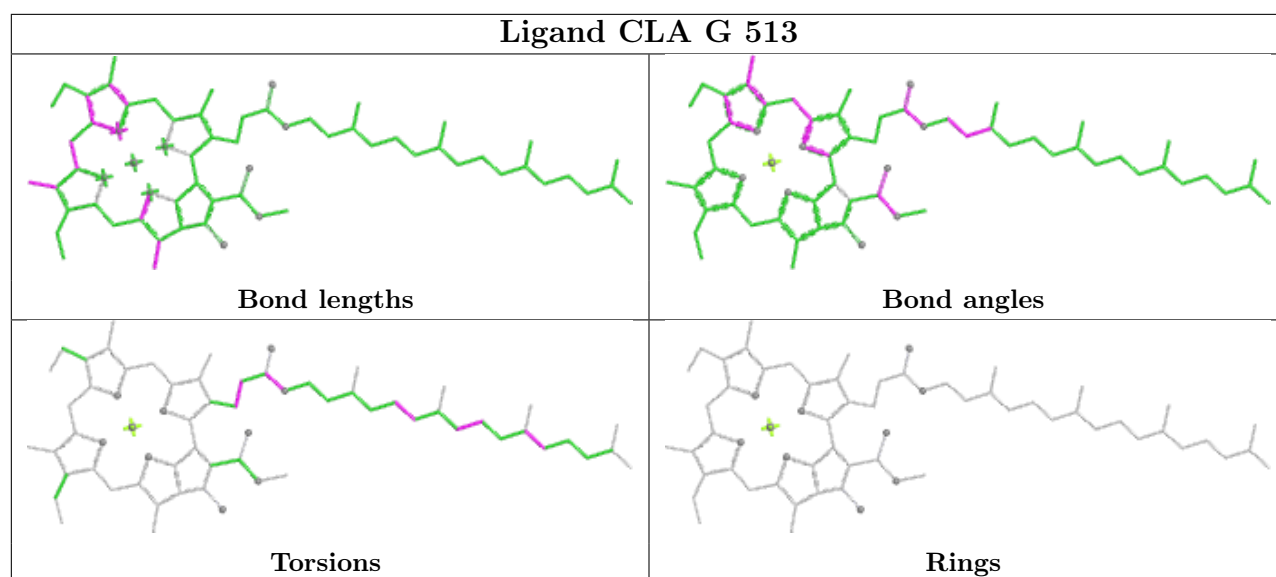
Bond angles



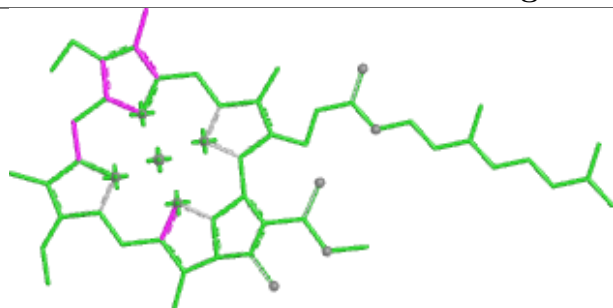
Torsions



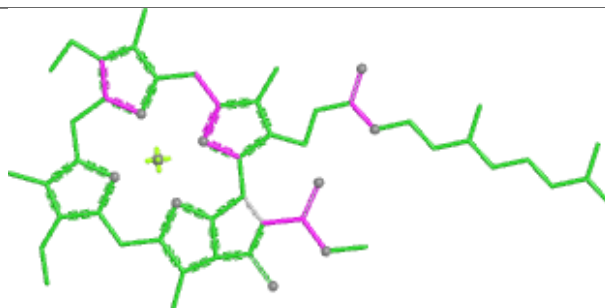
Rings



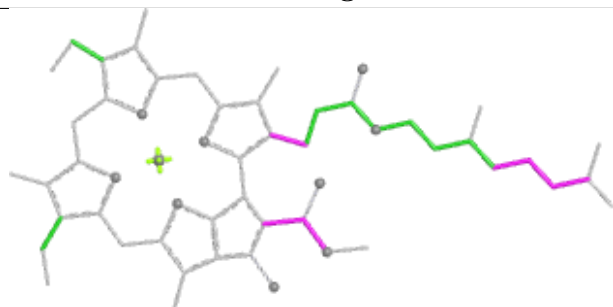
Ligand CLA I 311



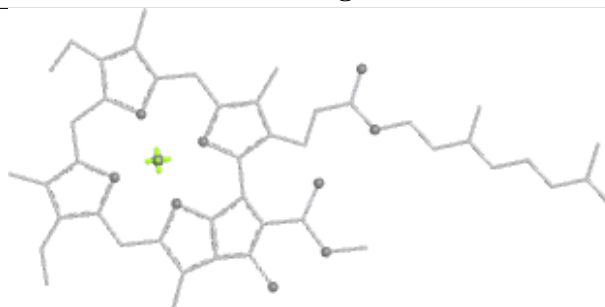
Bond lengths



Bond angles

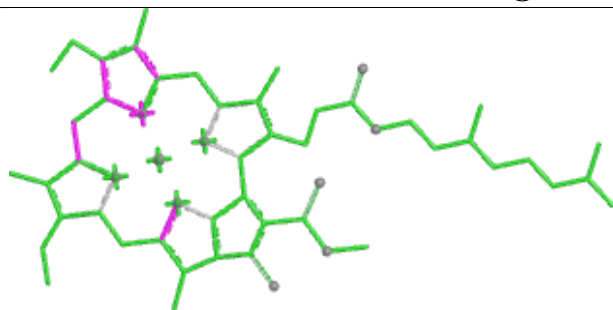


Torsions

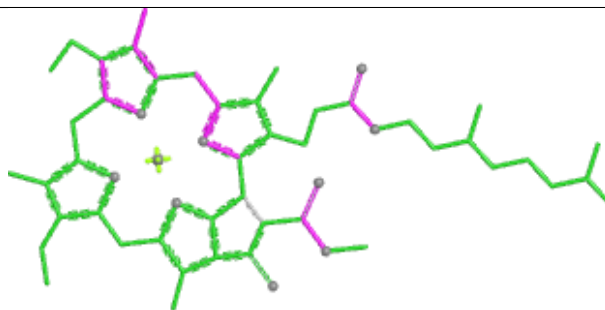


Rings

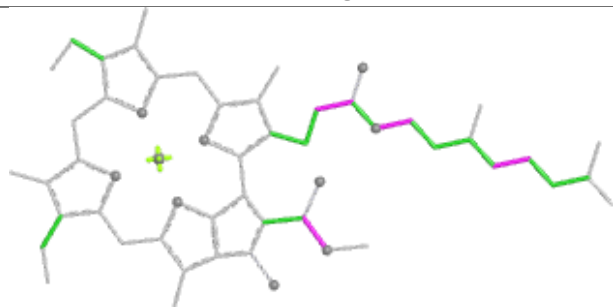
Ligand CLA A 309



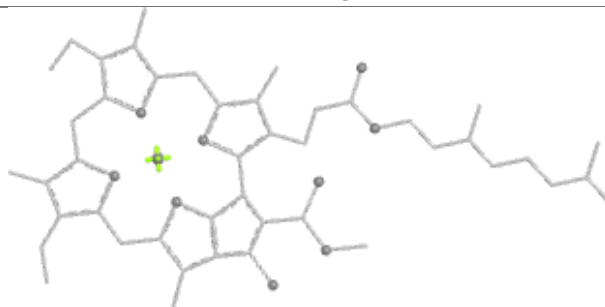
Bond lengths



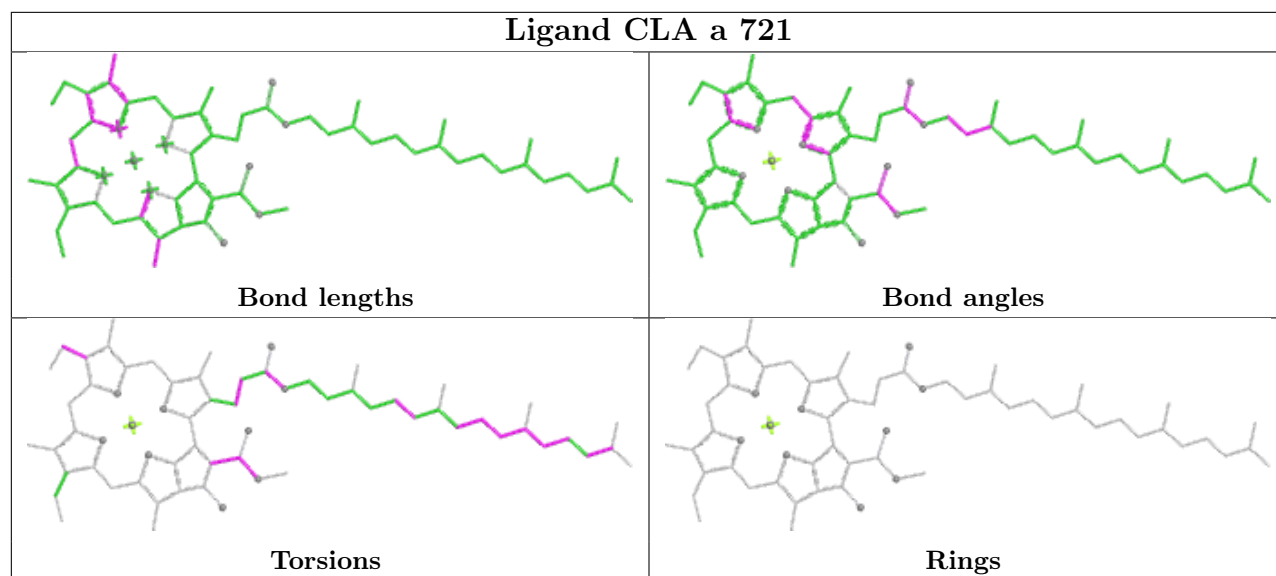
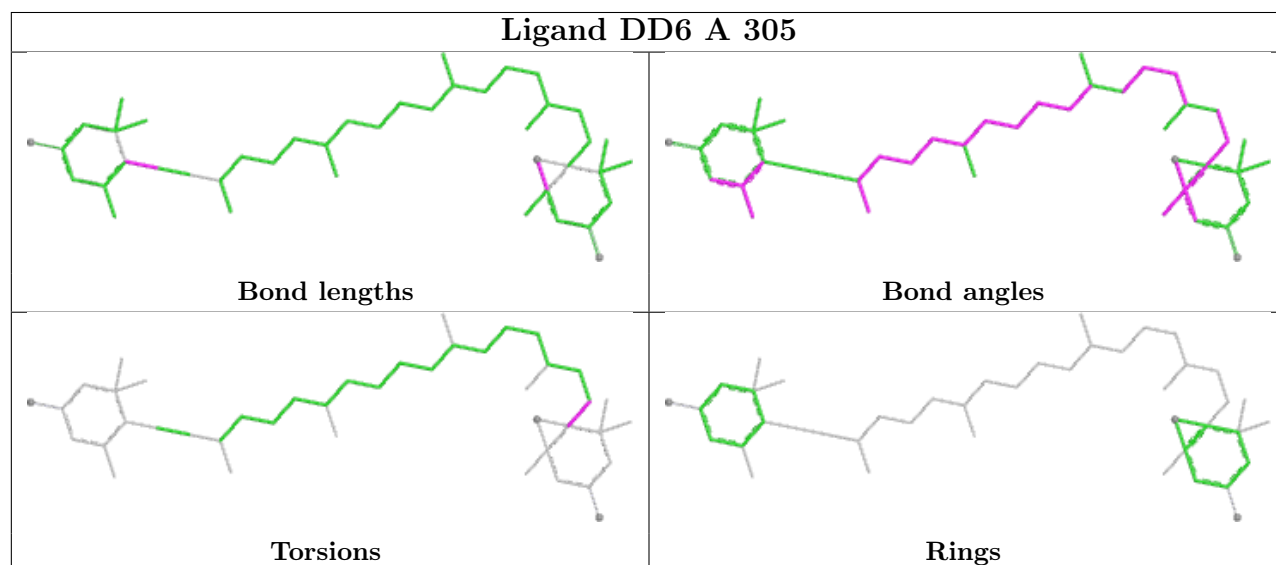
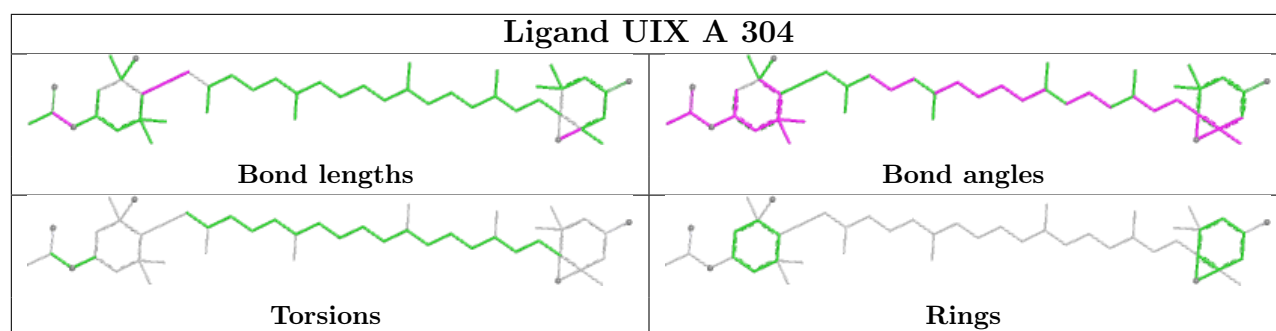
Bond angles

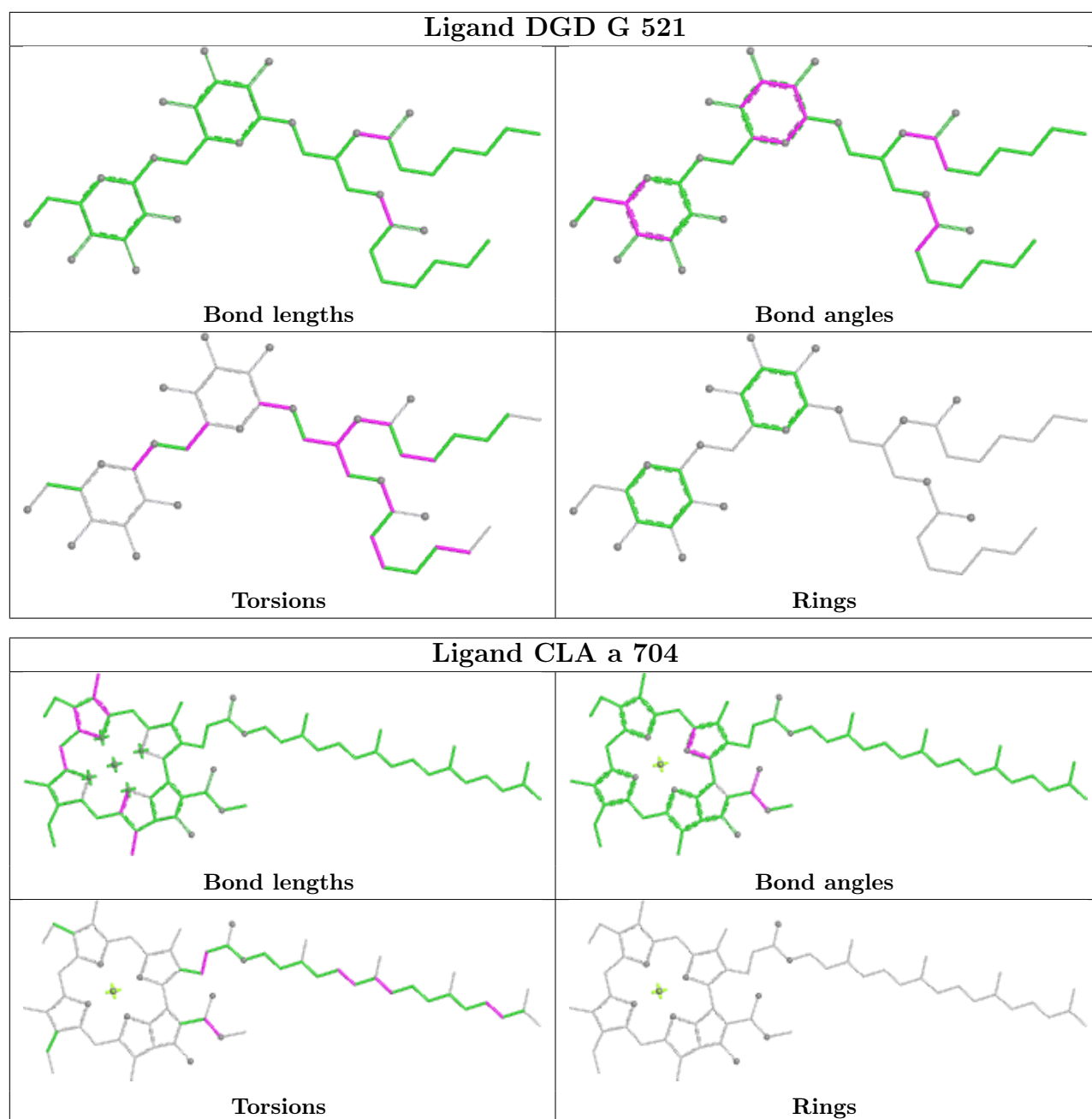


Torsions

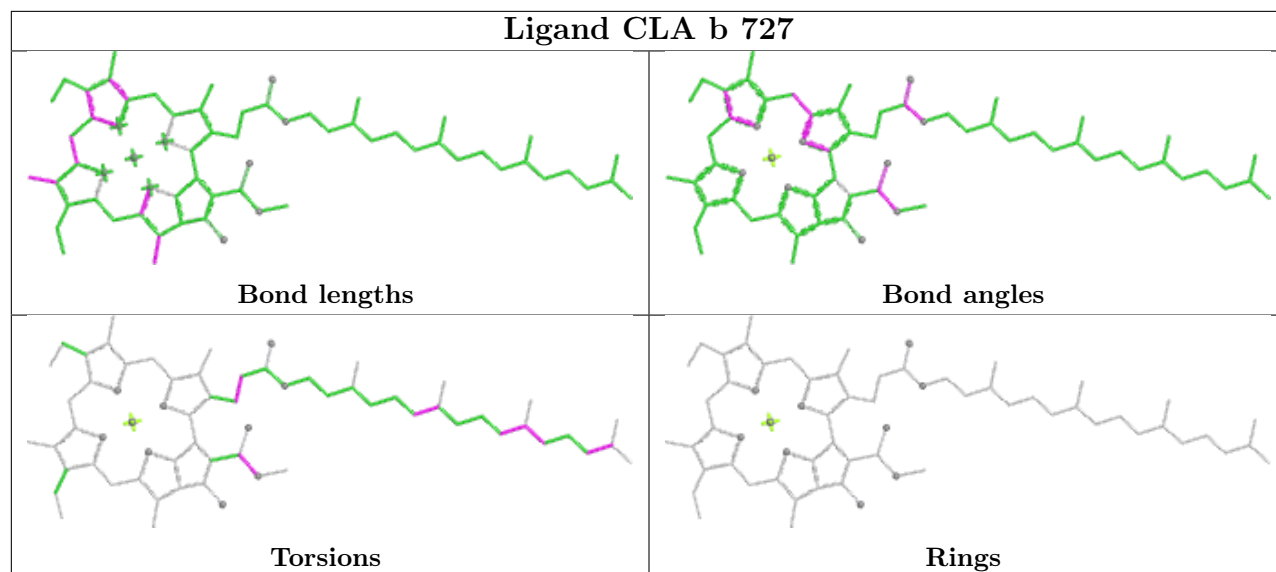


Rings

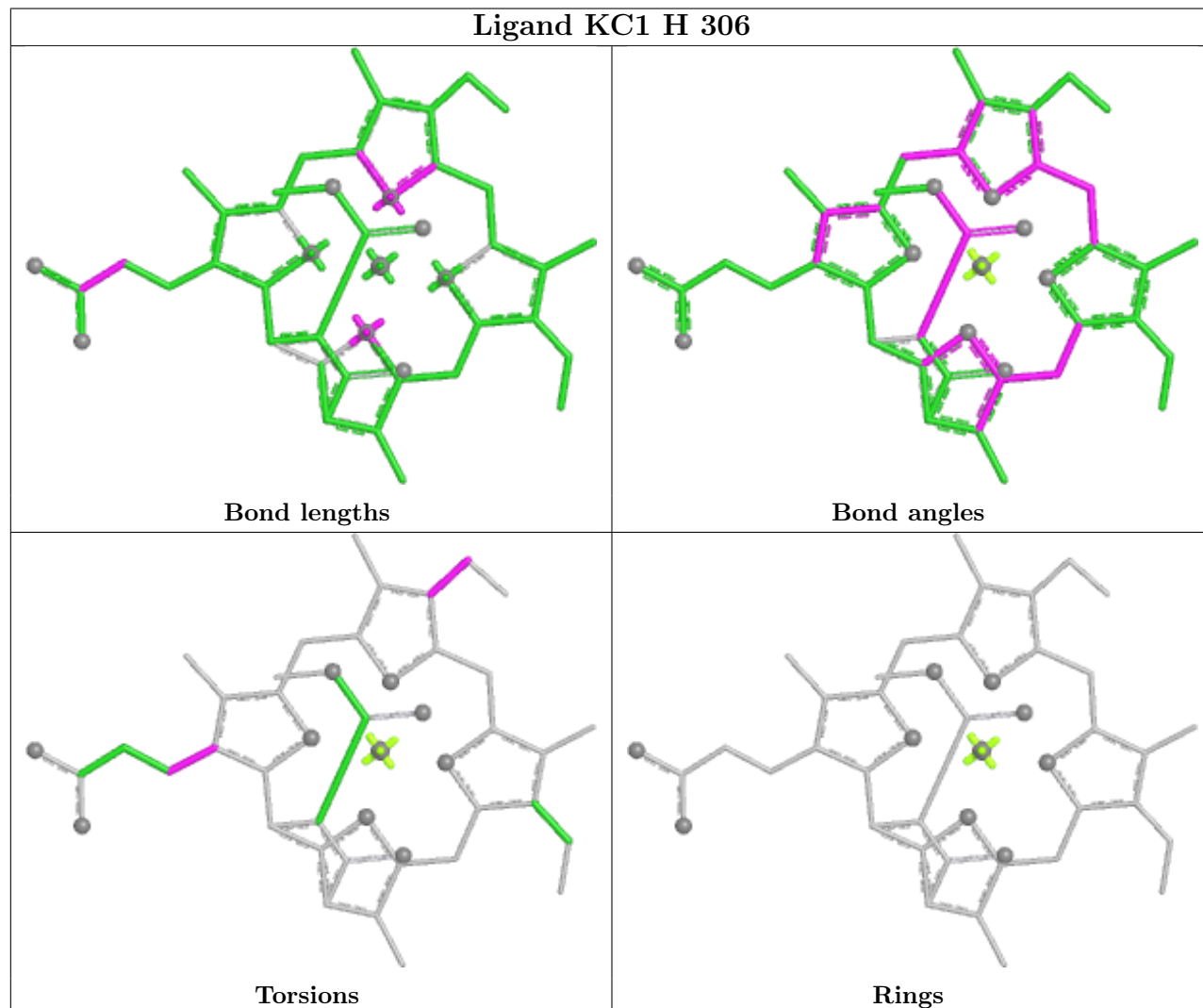


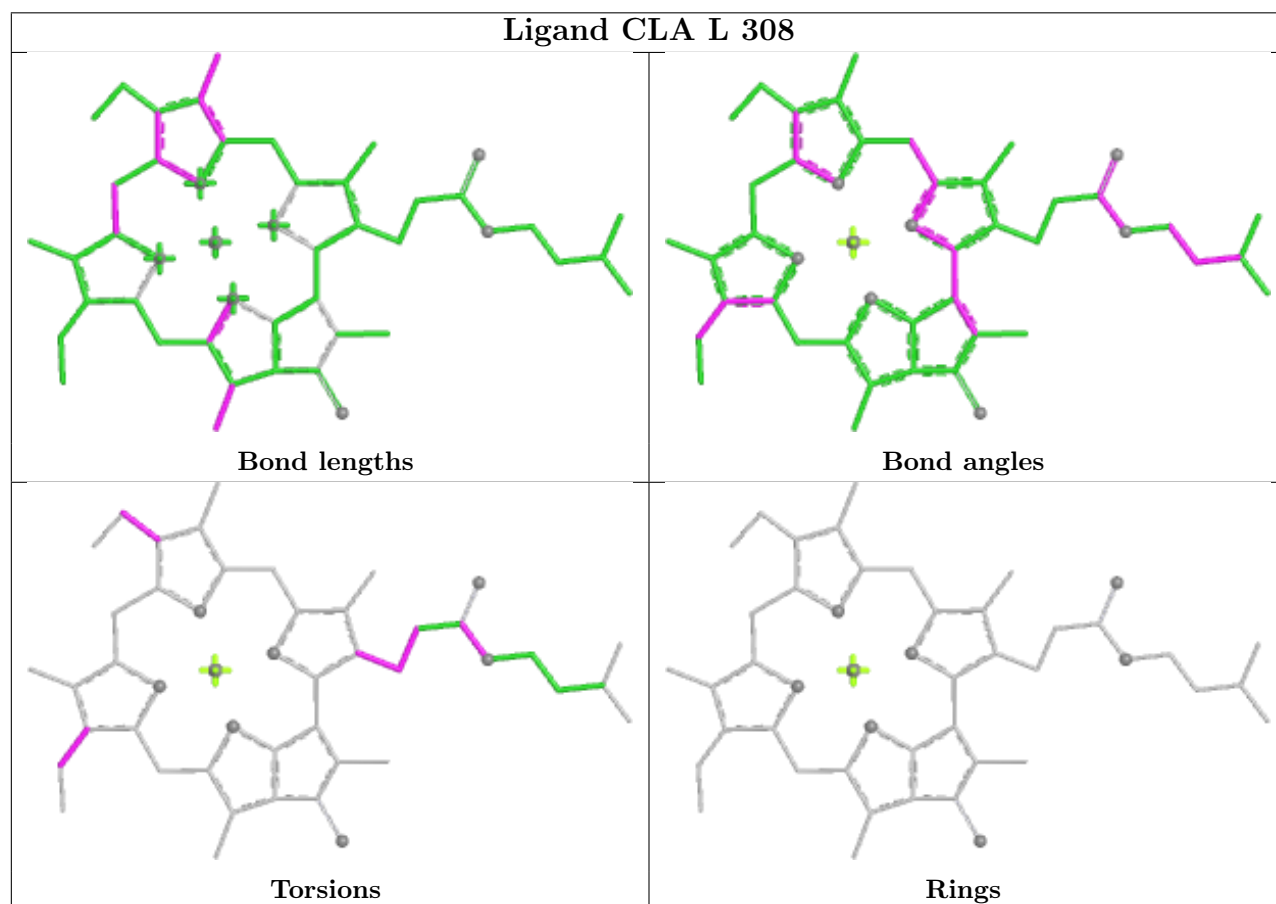
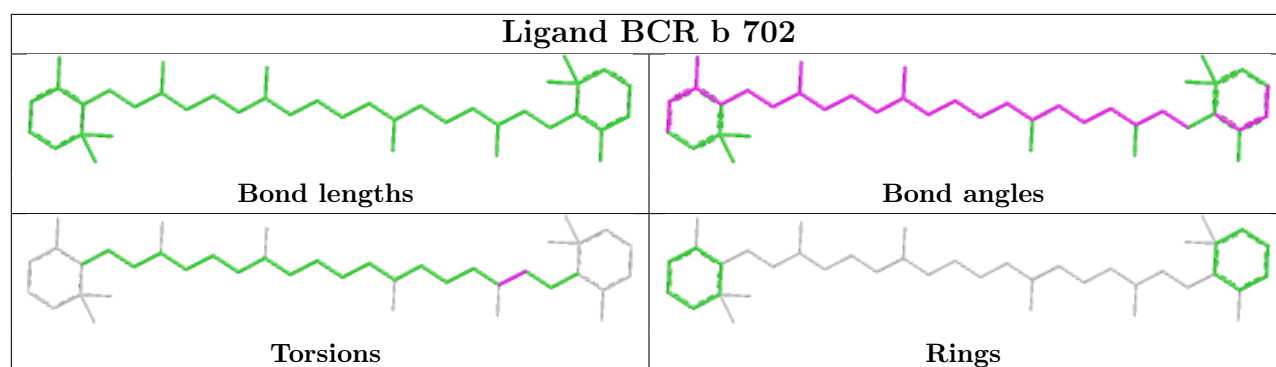


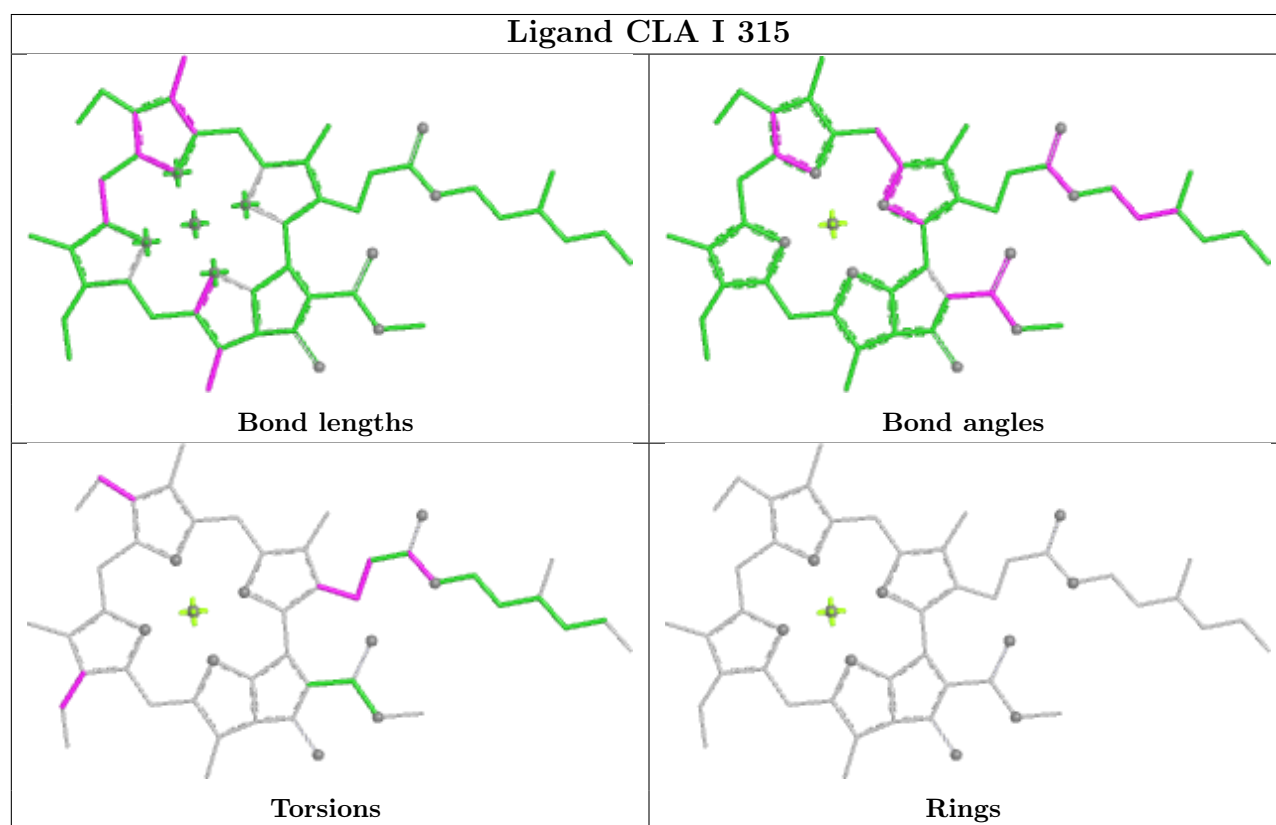
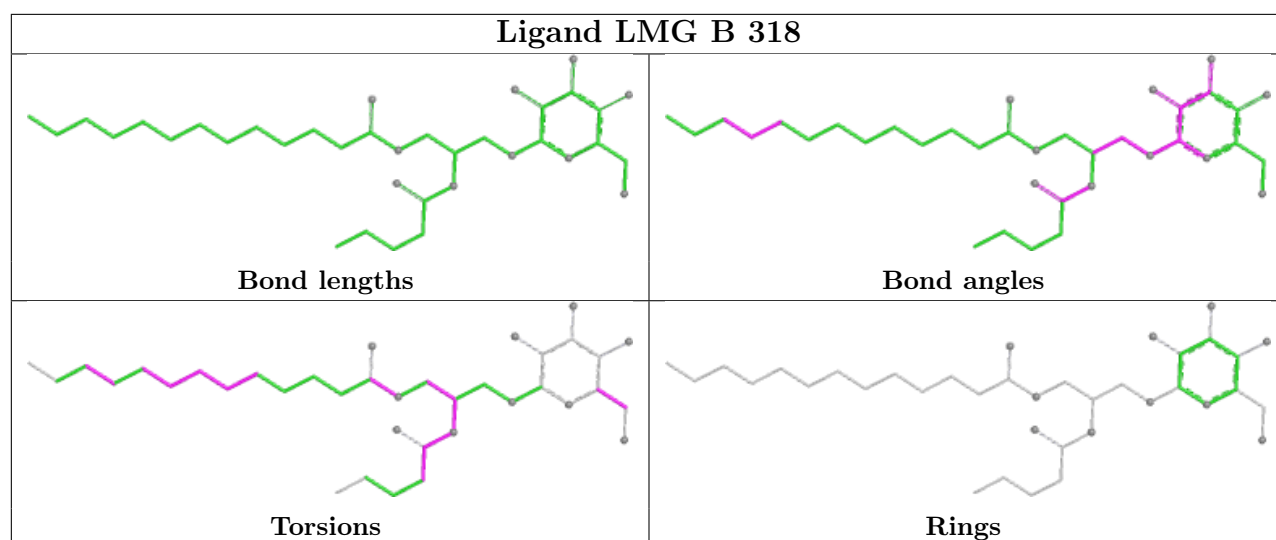
Ligand CLA b 727



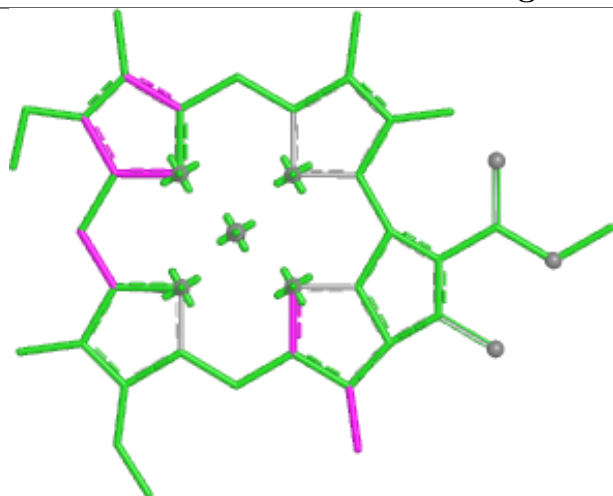
Ligand KC1 H 306



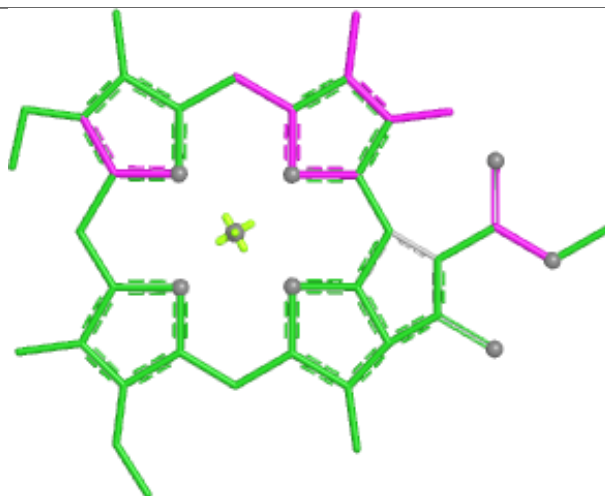




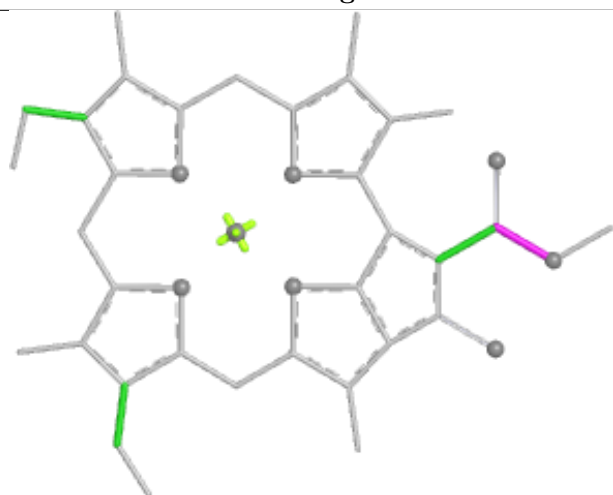
Ligand CLA J 314



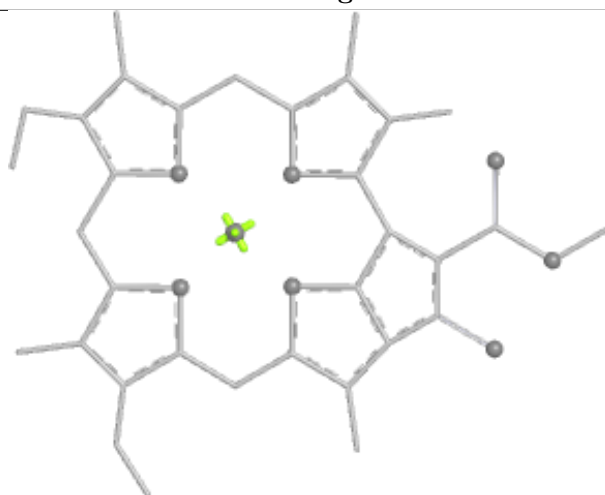
Bond lengths



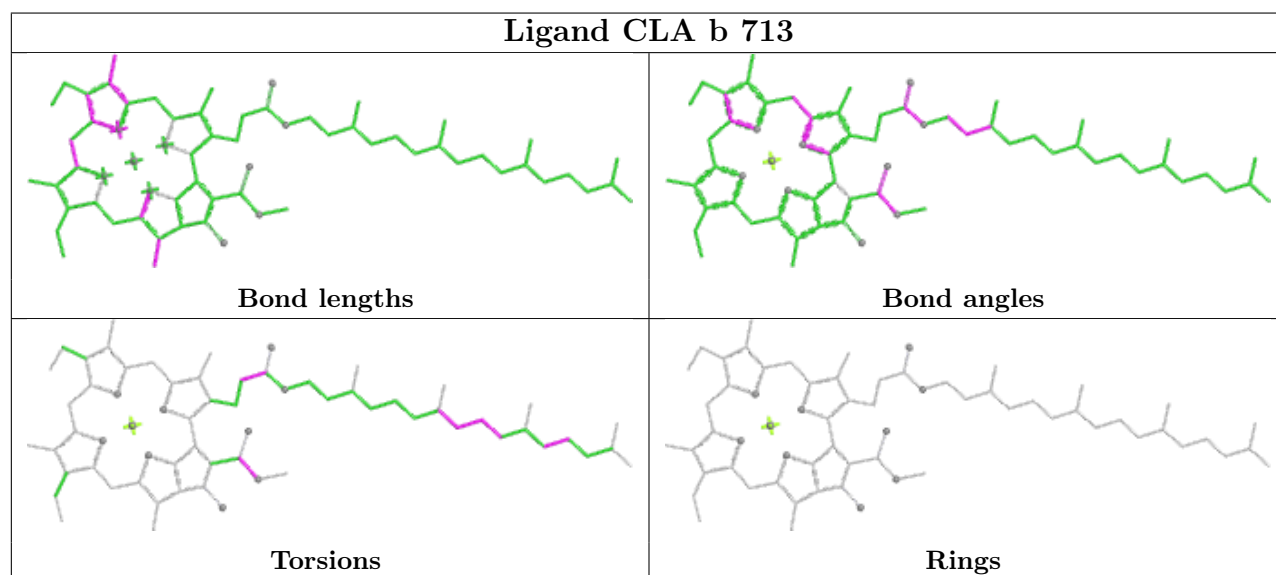
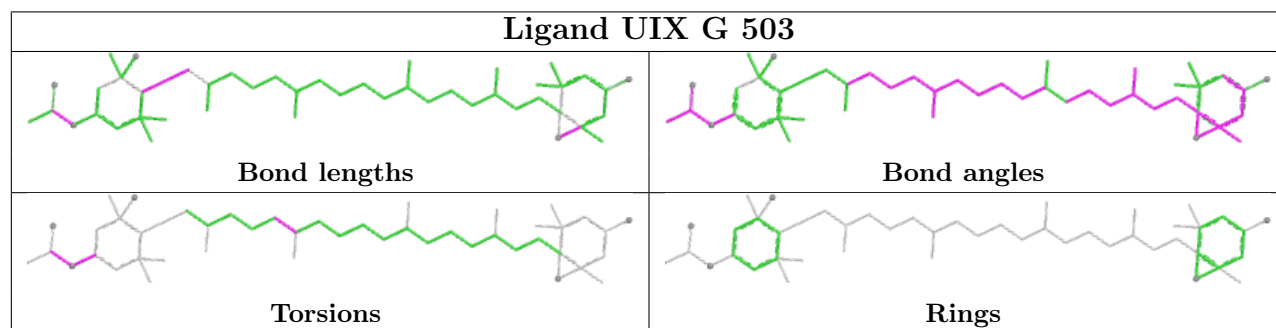
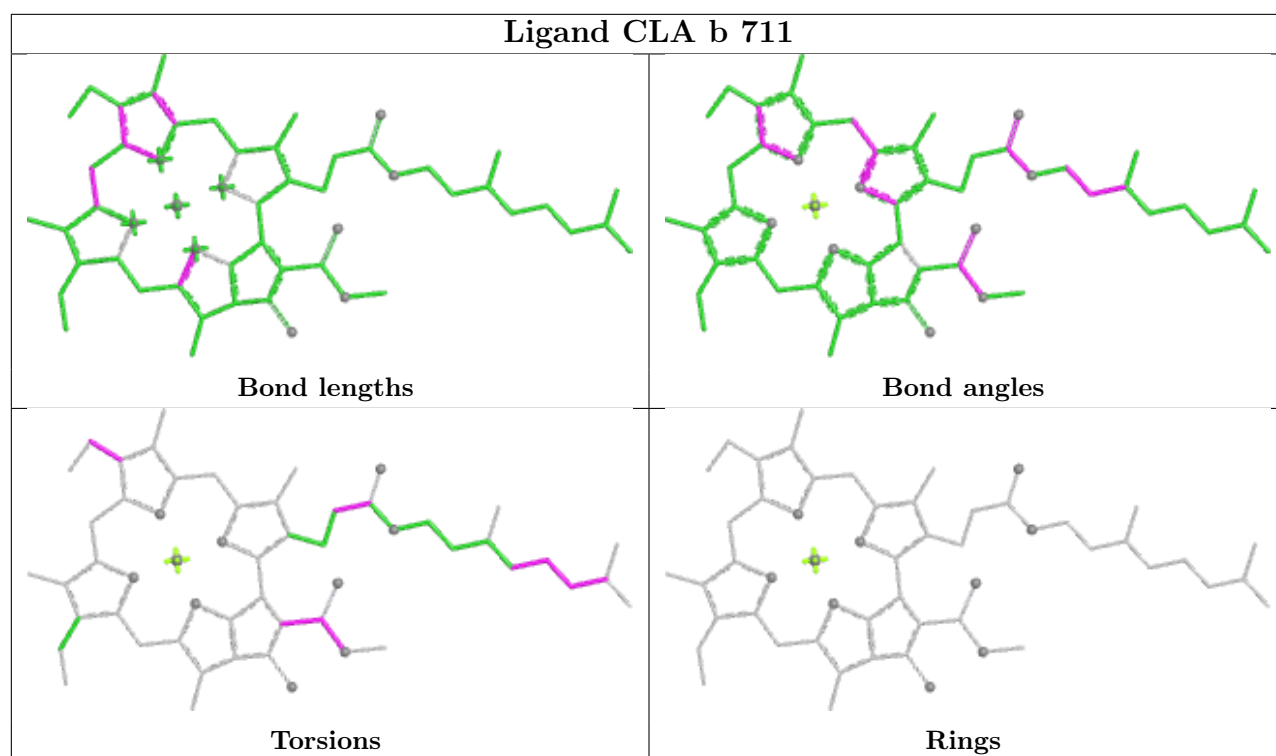
Bond angles



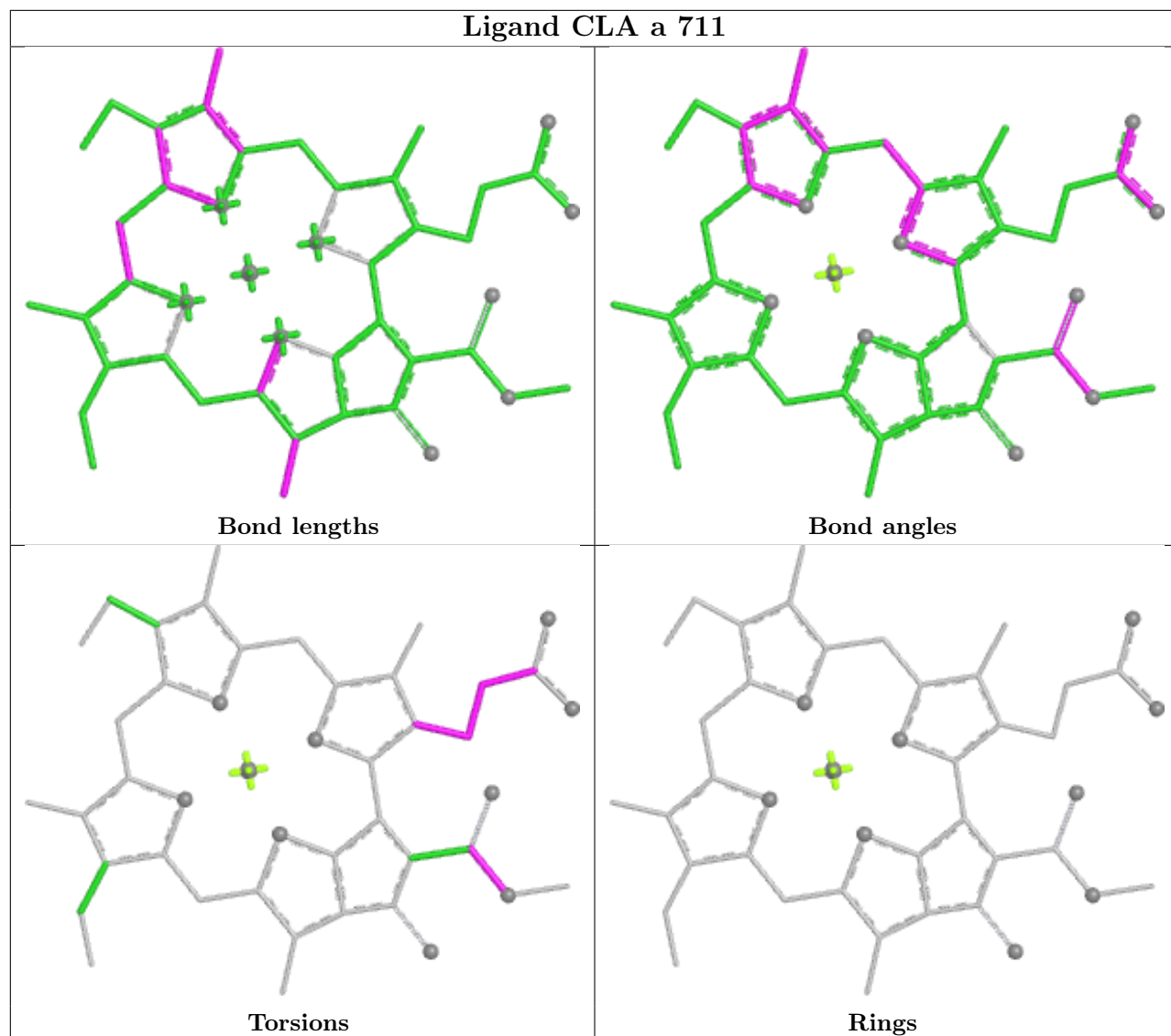
Torsions



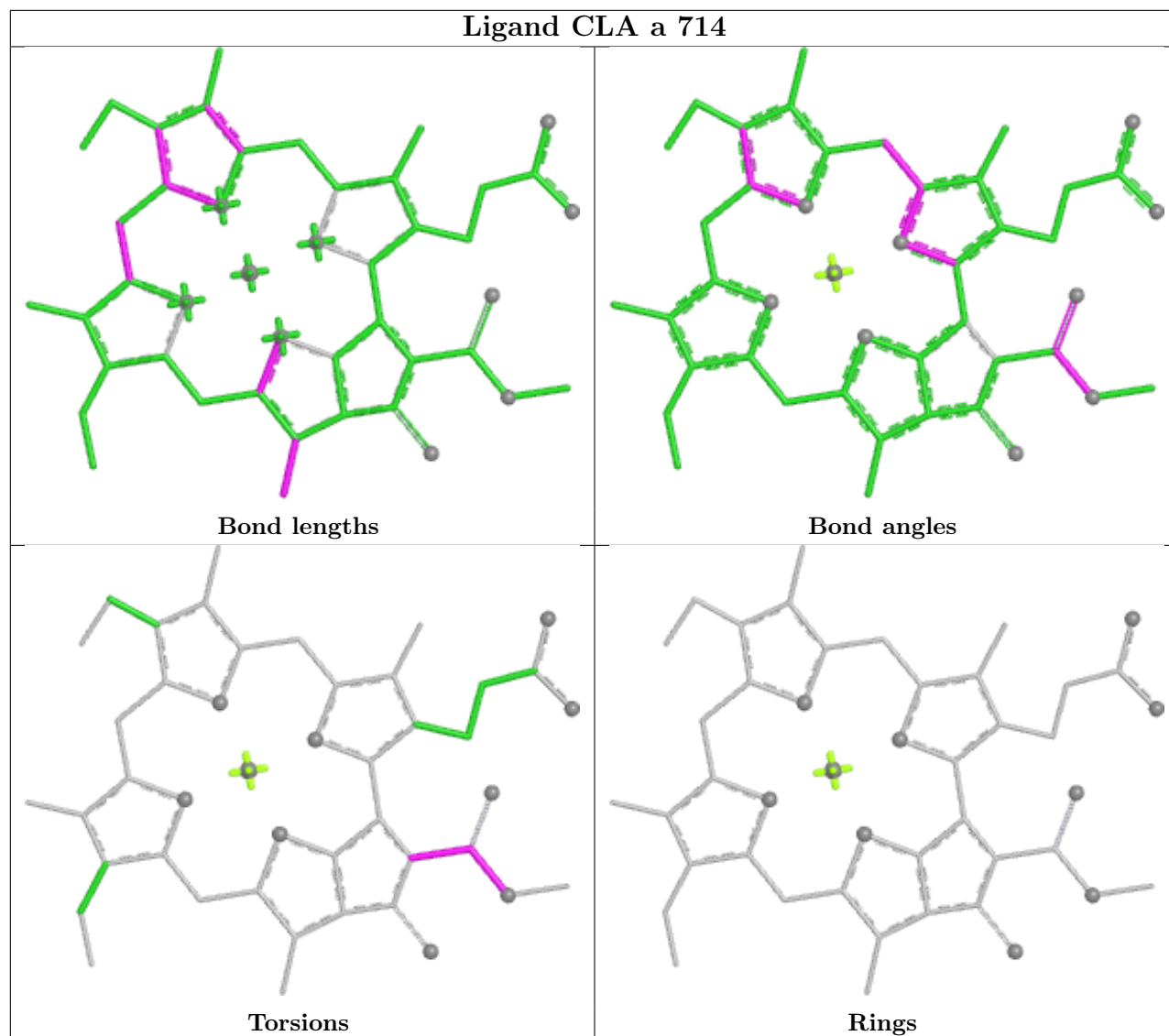
Rings



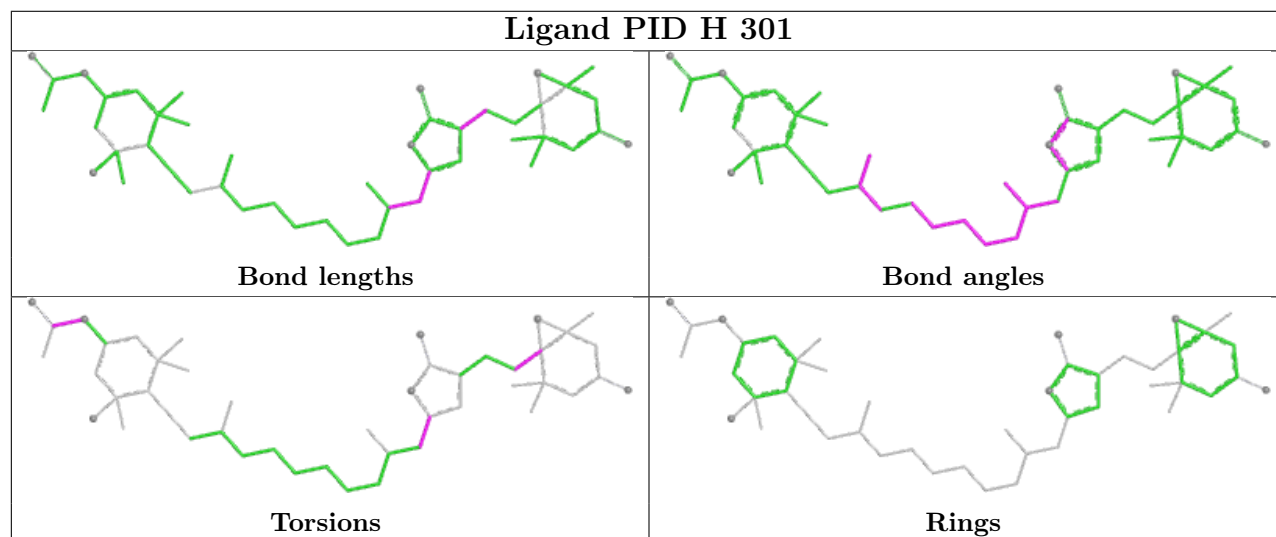
Ligand CLA a 711

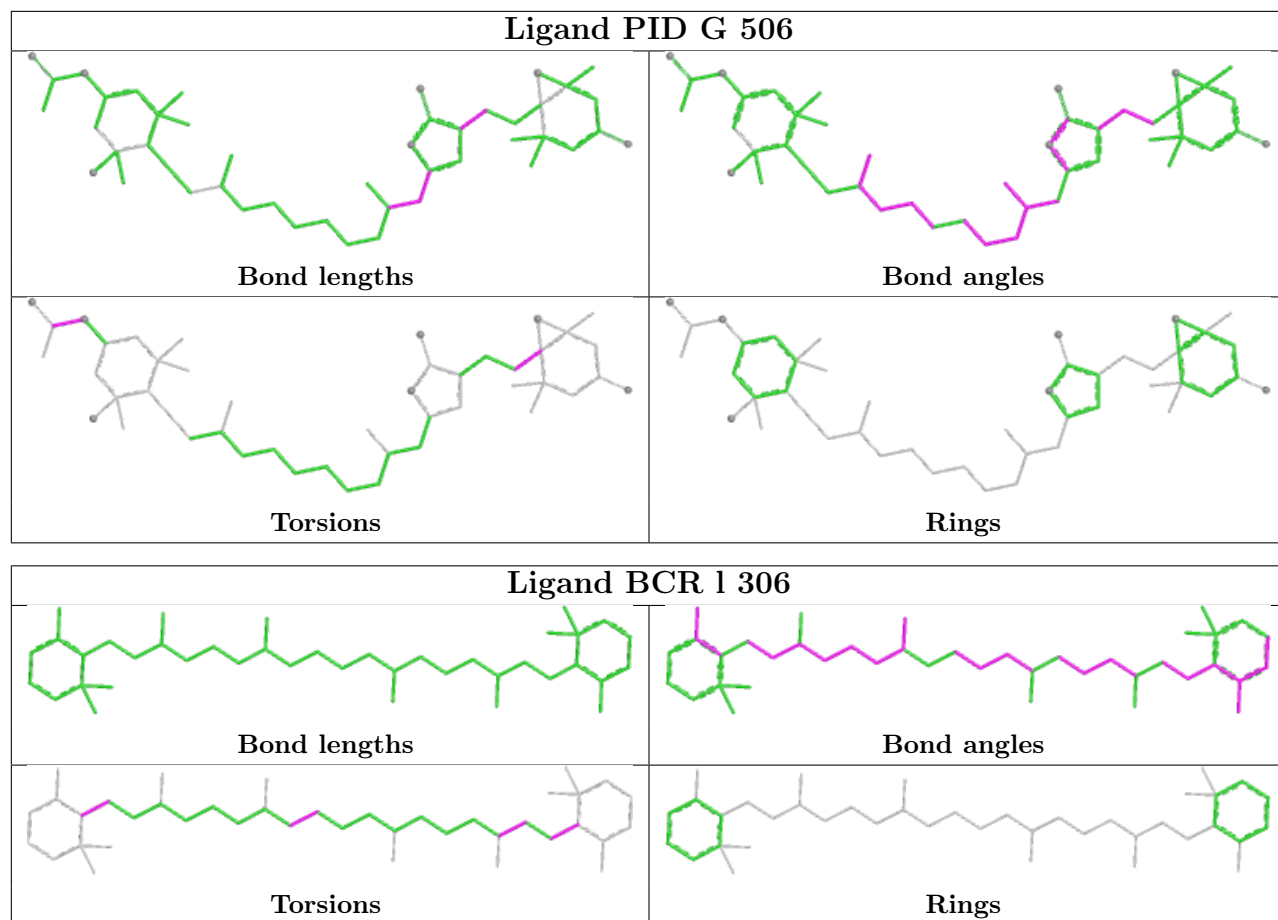


Ligand CLA a 714

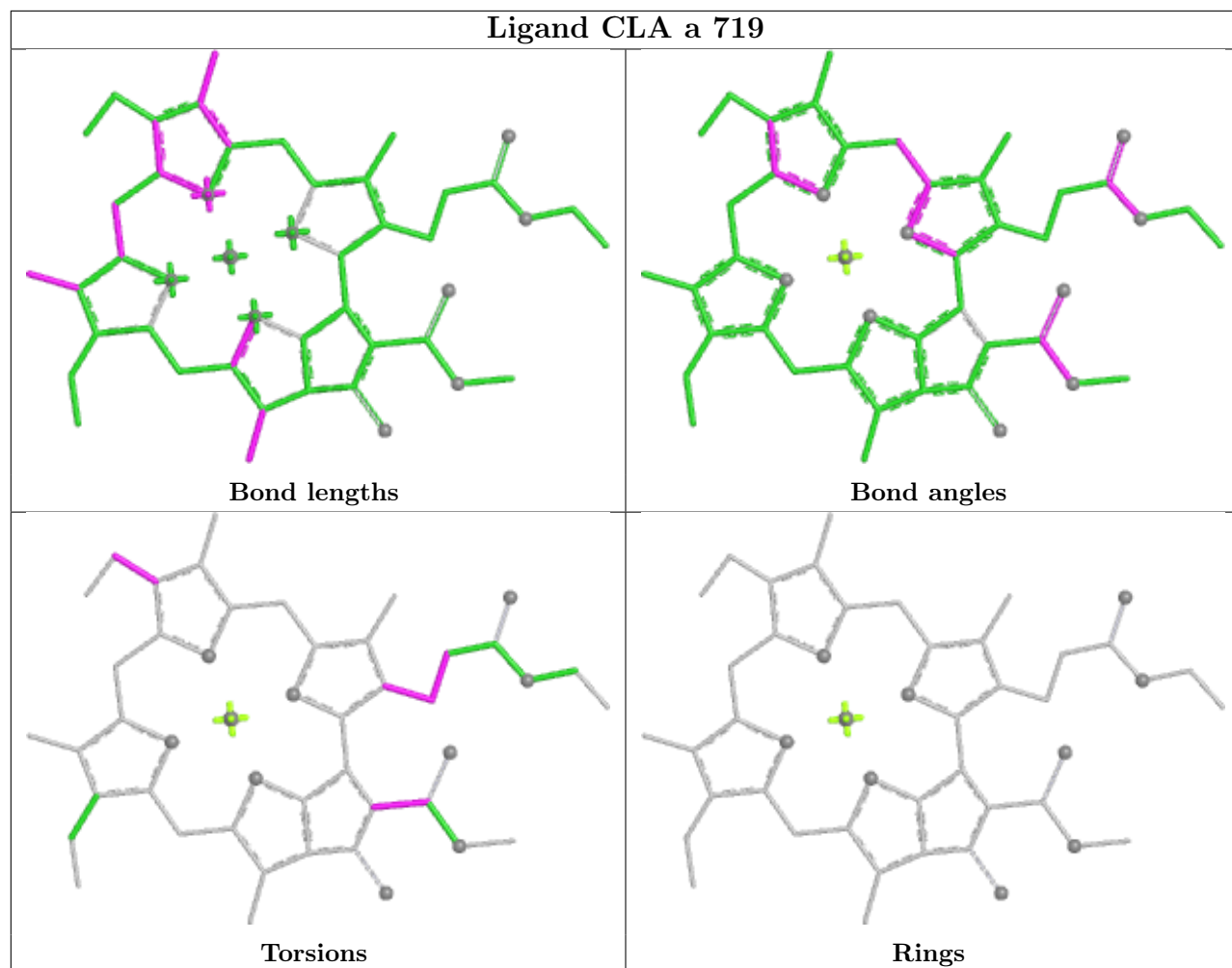


Ligand PID H 301

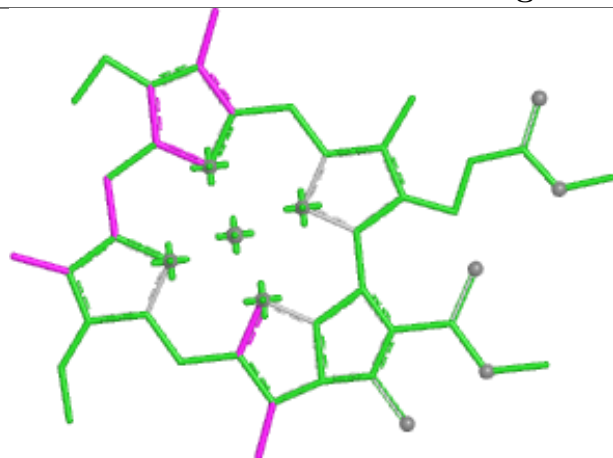




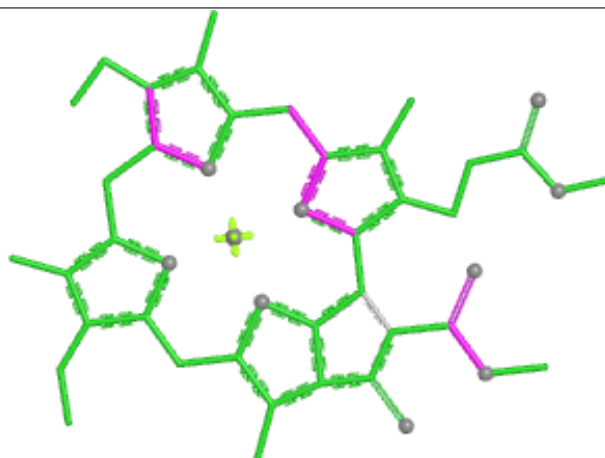
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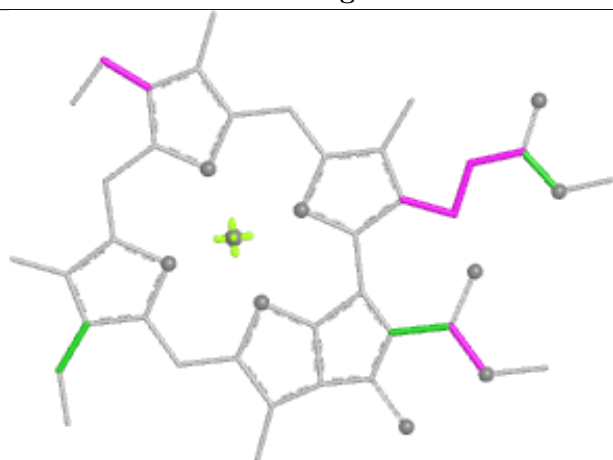
Ligand CLA L 318



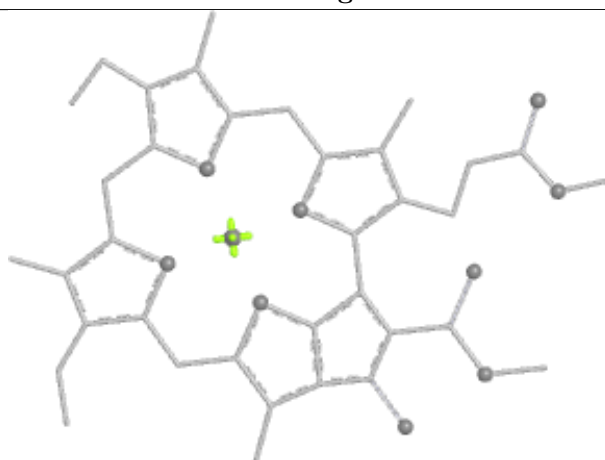
Bond lengths



Bond angles

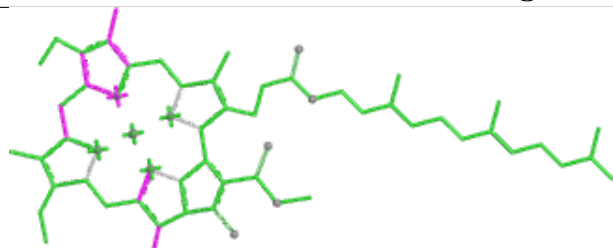


Torsions

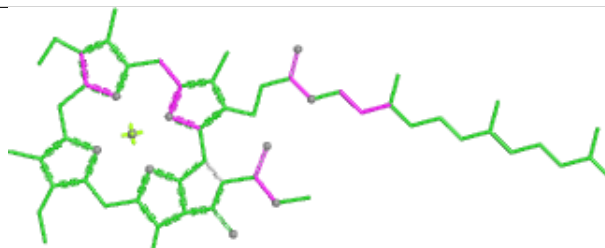


Rings

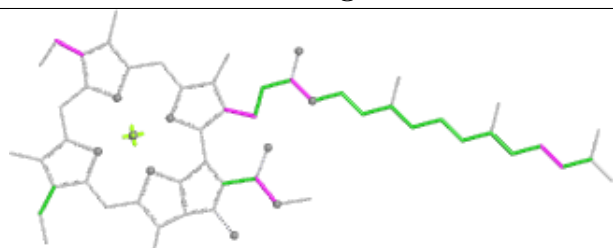
Ligand CLA a 712



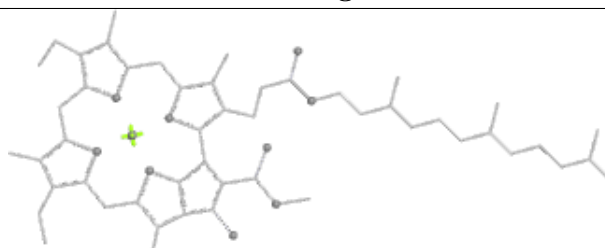
Bond lengths



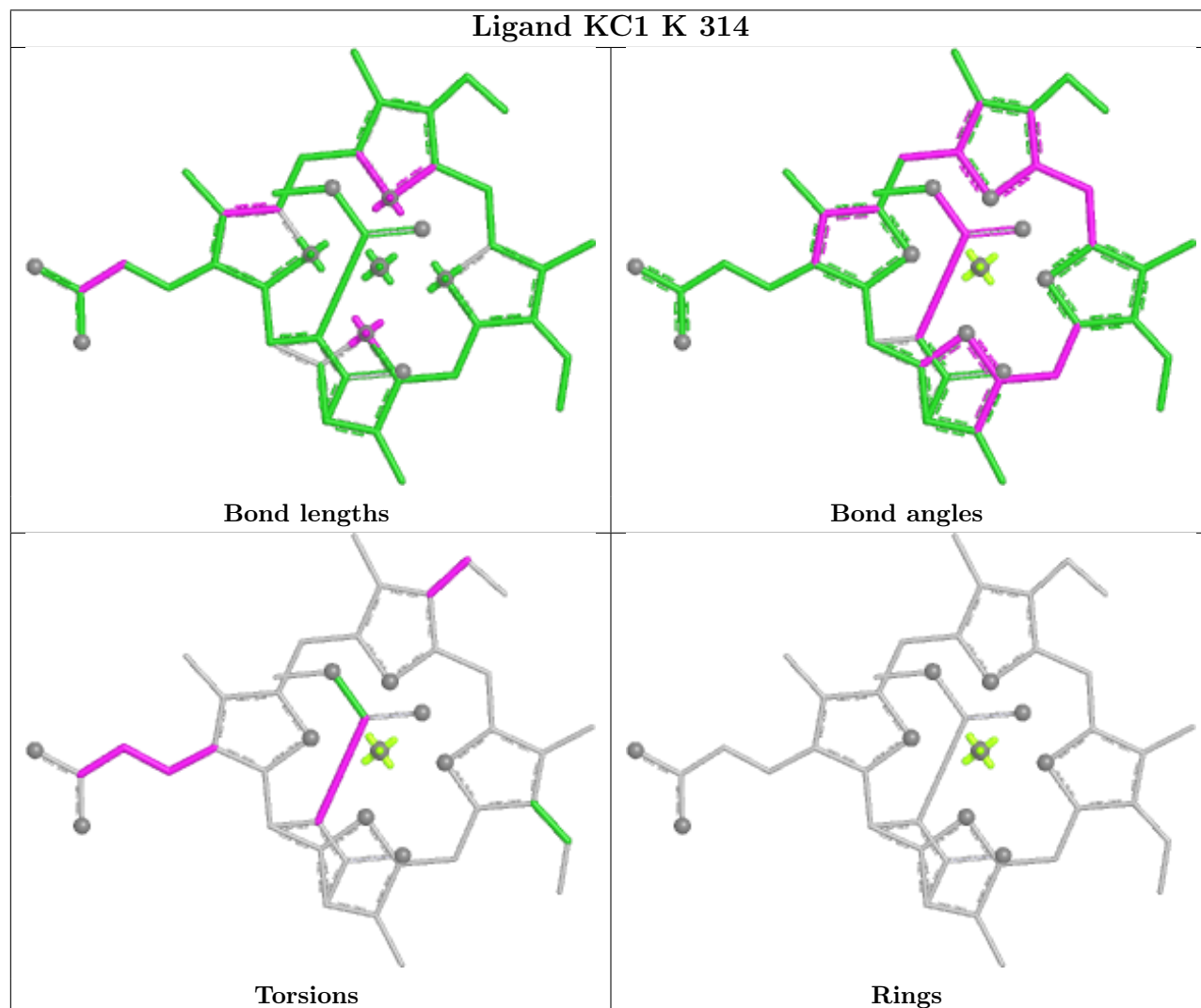
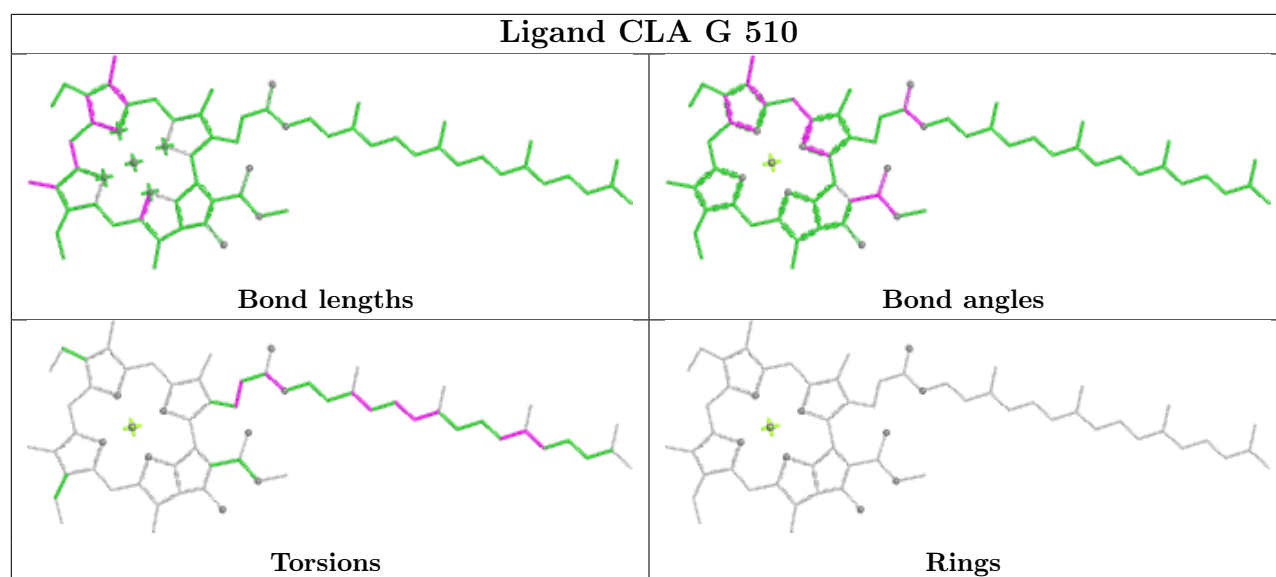
Bond angles



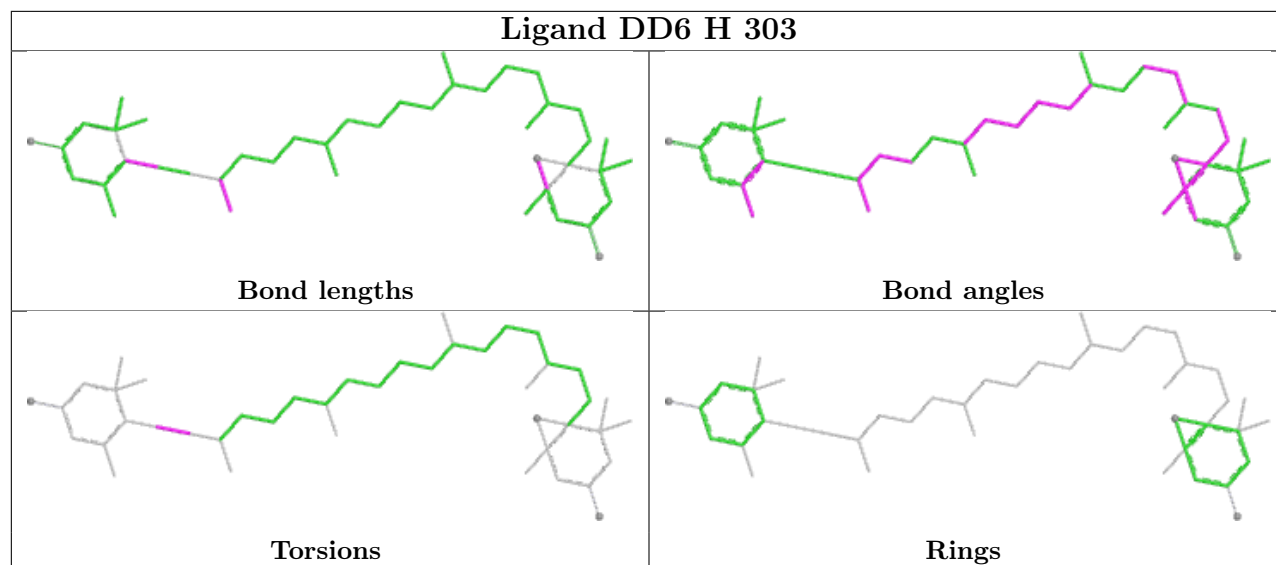
Torsions



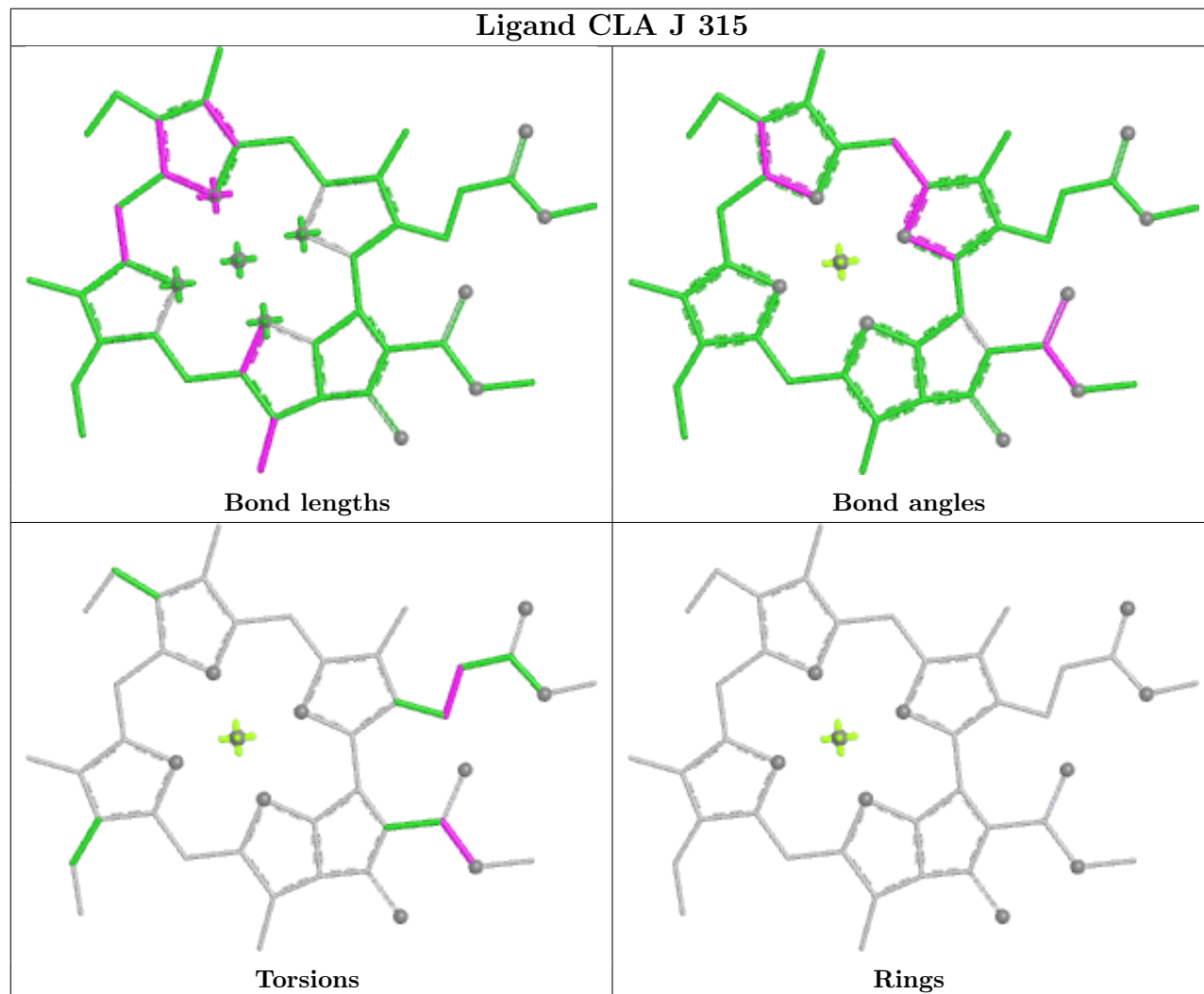
Rings

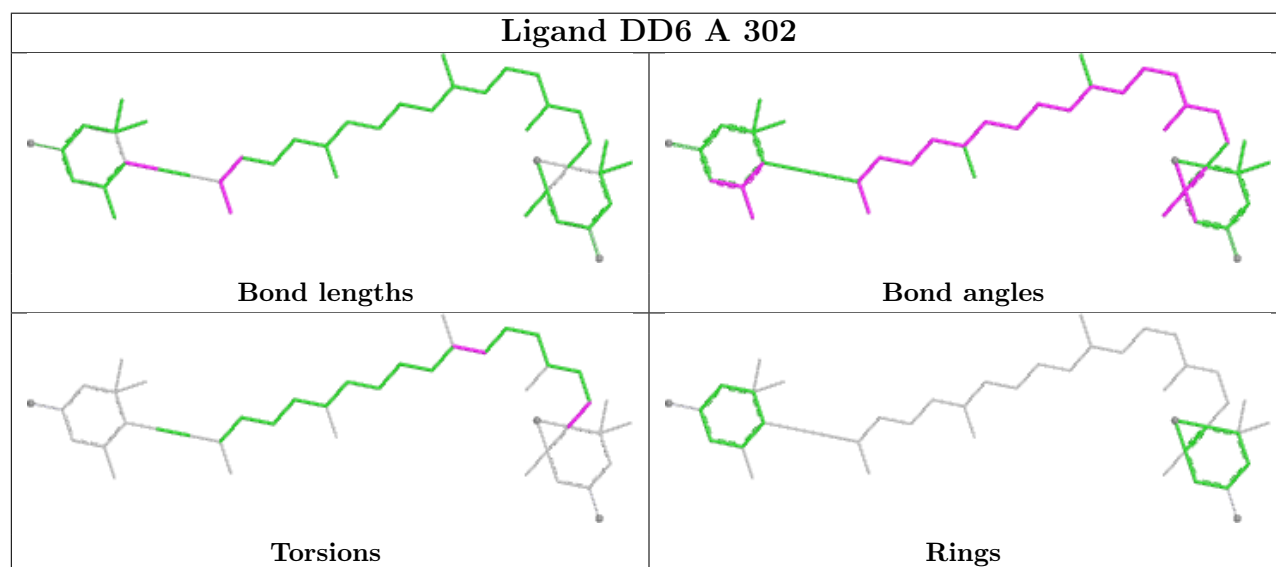
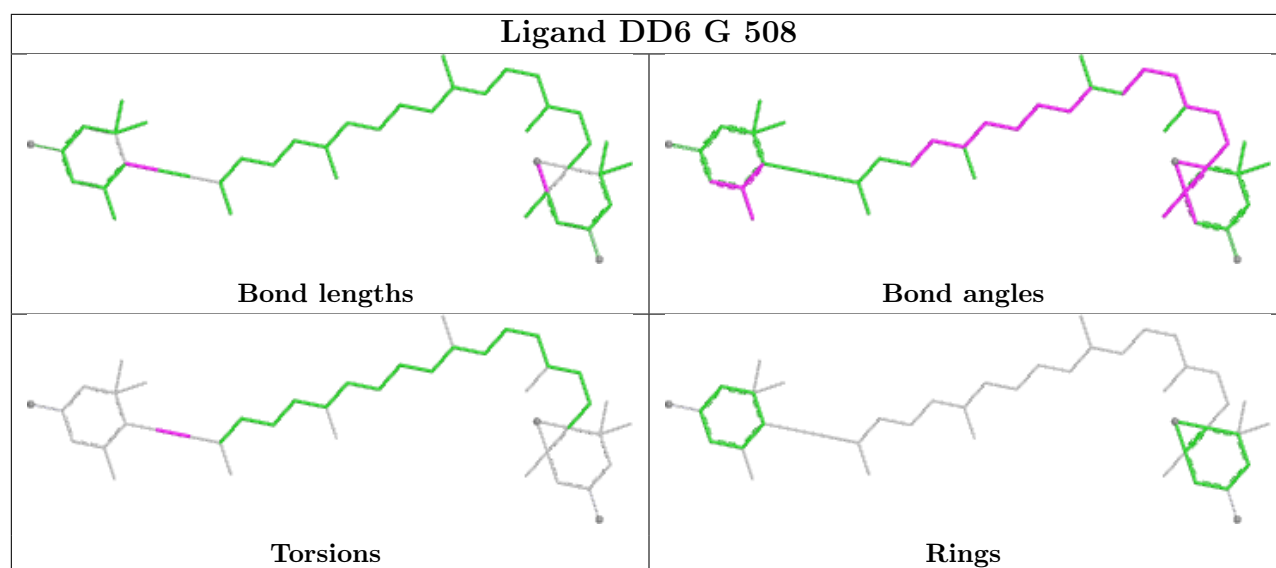


Ligand DD6 H 303

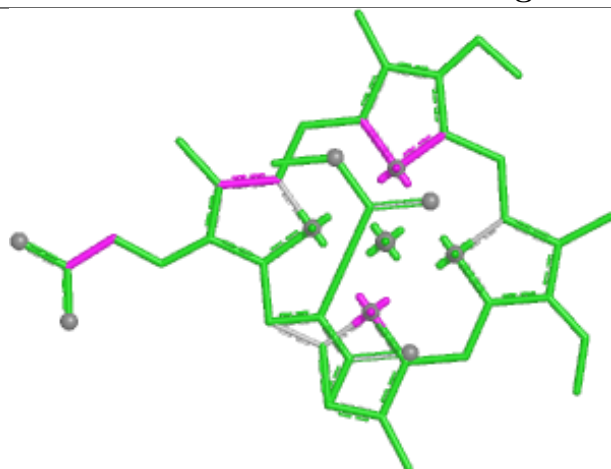


Ligand CLA J 315

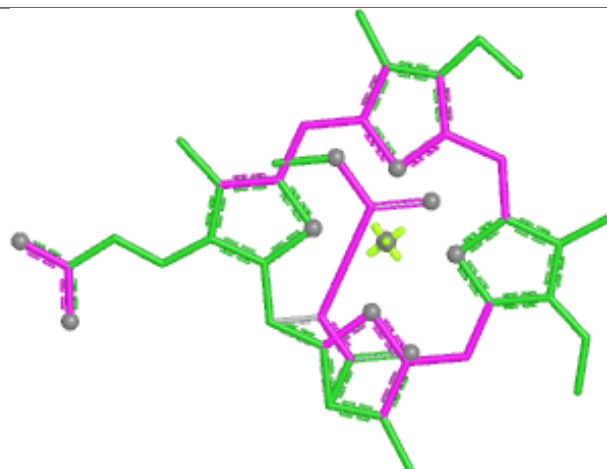




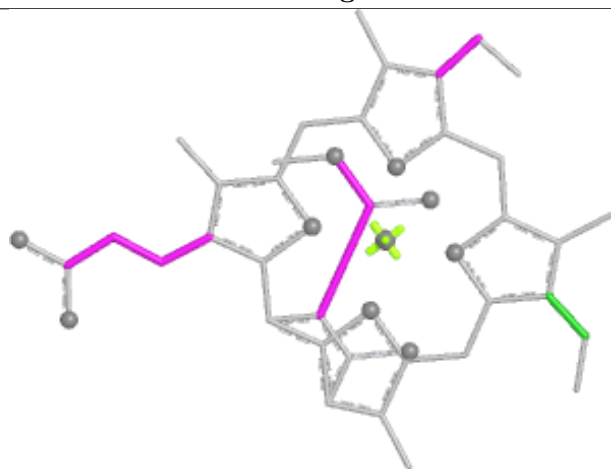
Ligand KC1 N 308



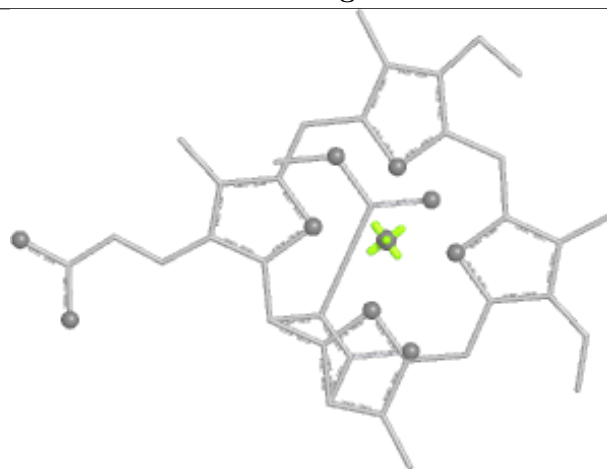
Bond lengths



Bond angles

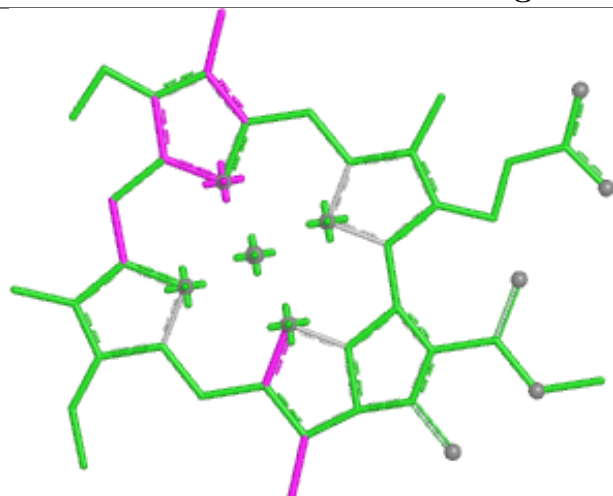


Torsions

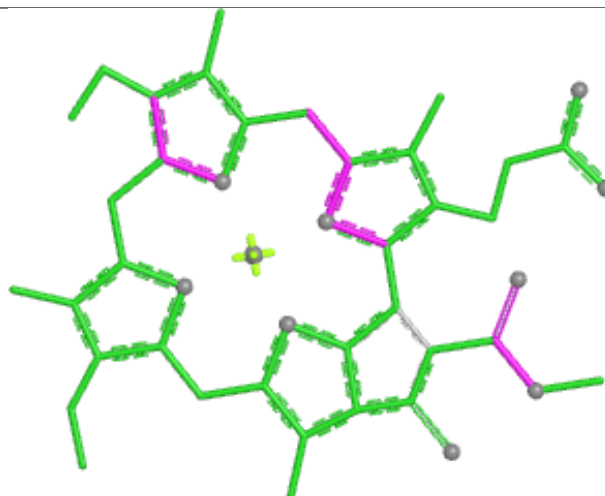


Rings

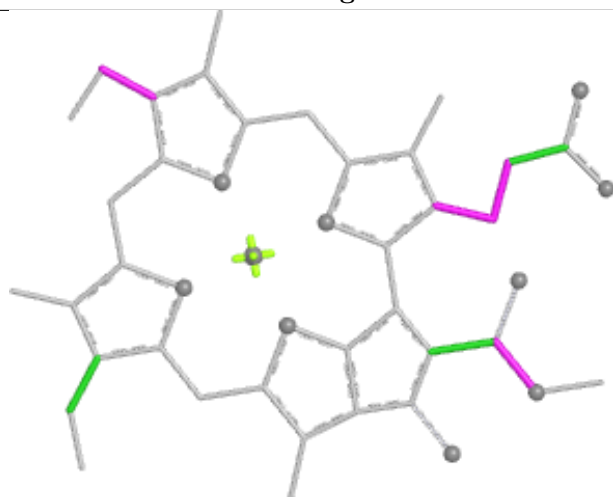
Ligand CLA B 317



Bond lengths



Bond angles

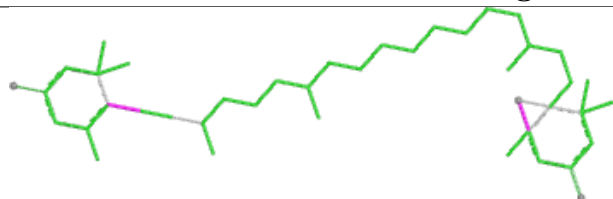


Torsions

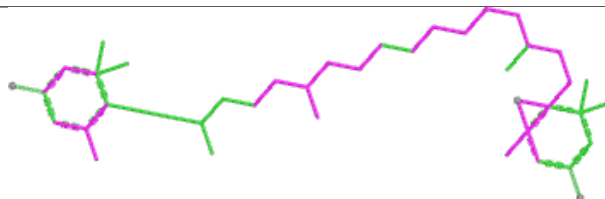


Rings

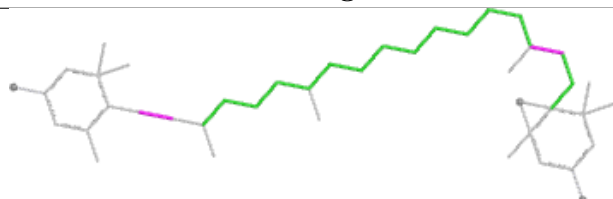
Ligand DD6 B 302



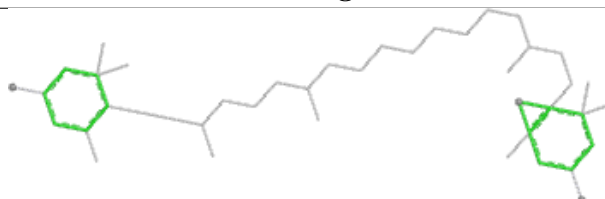
Bond lengths



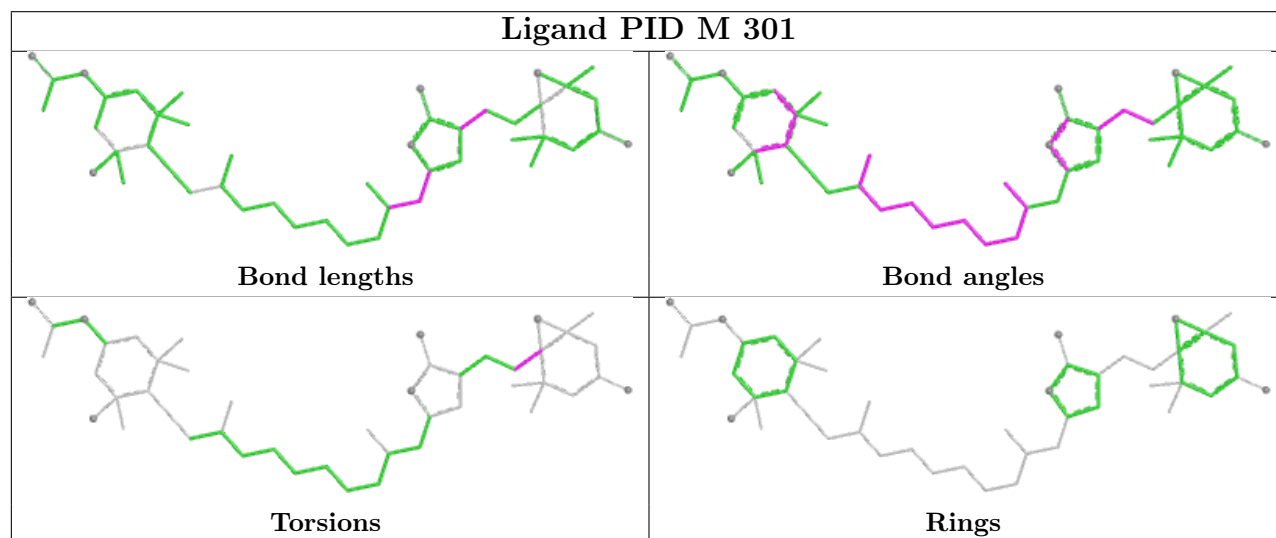
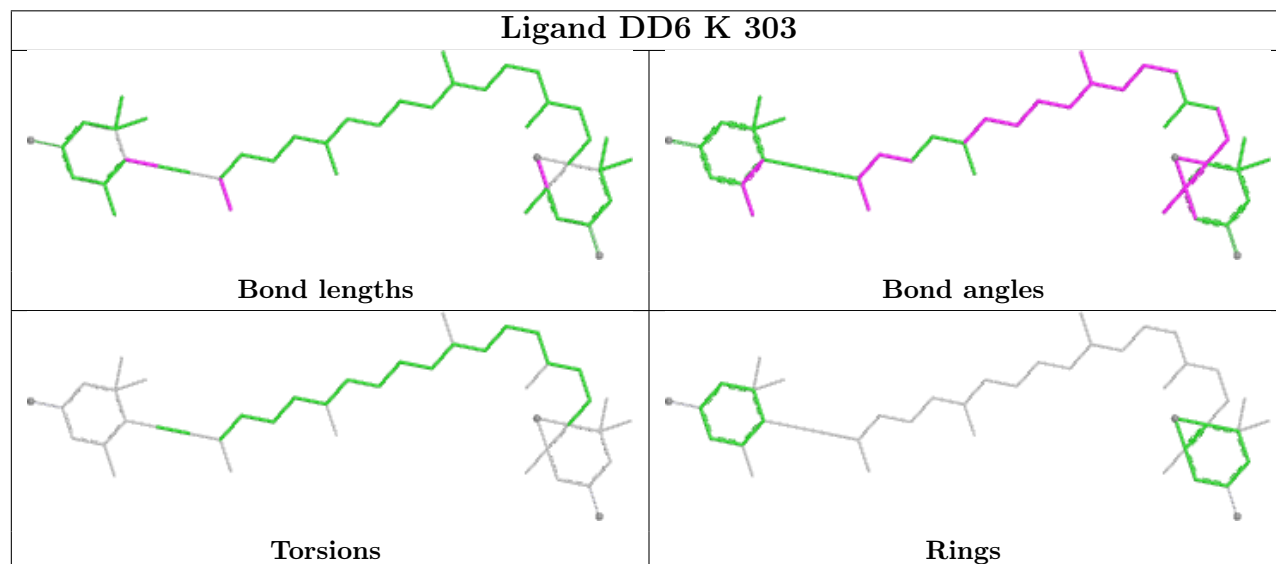
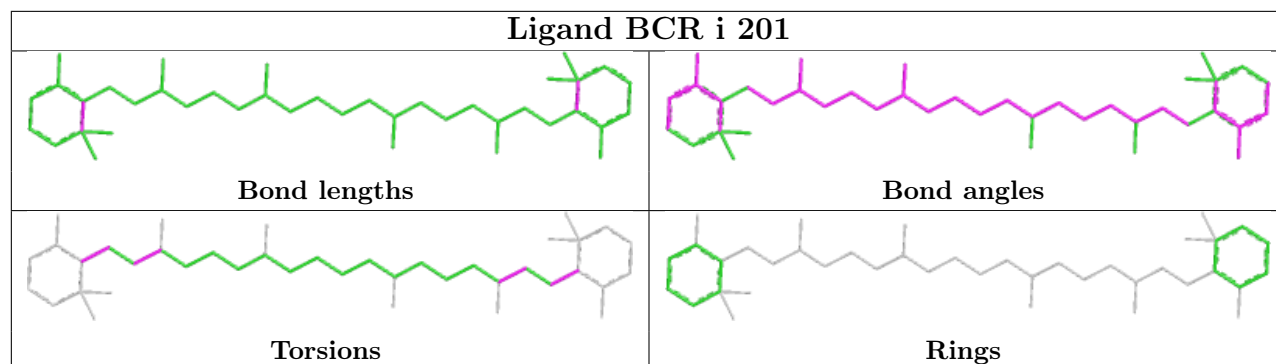
Bond angles



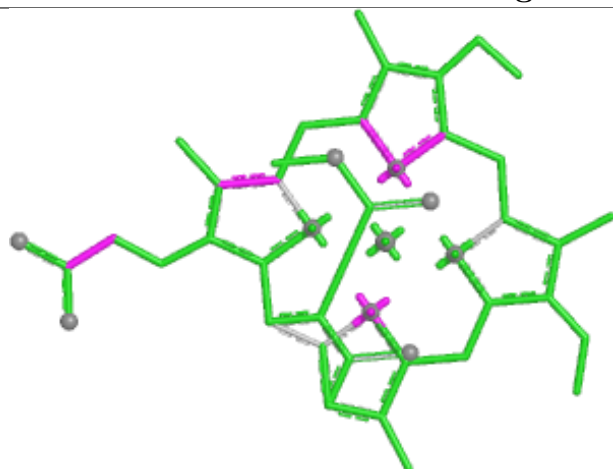
Torsions



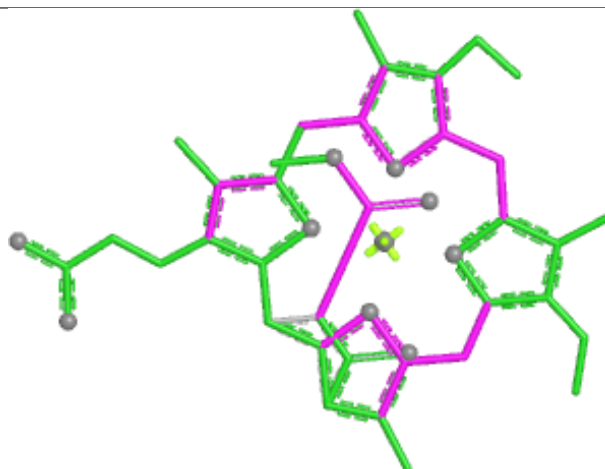
Rings



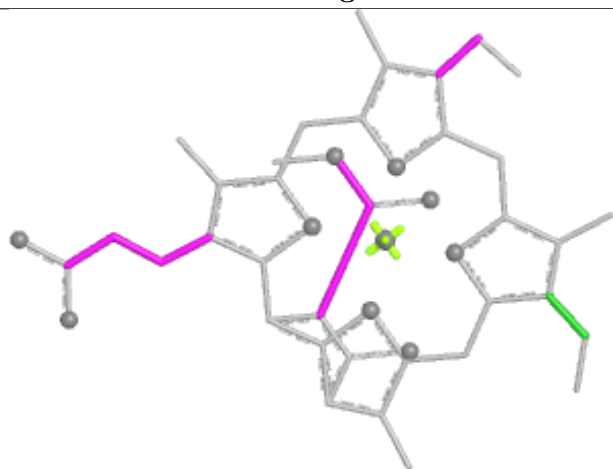
Ligand KC1 D 310



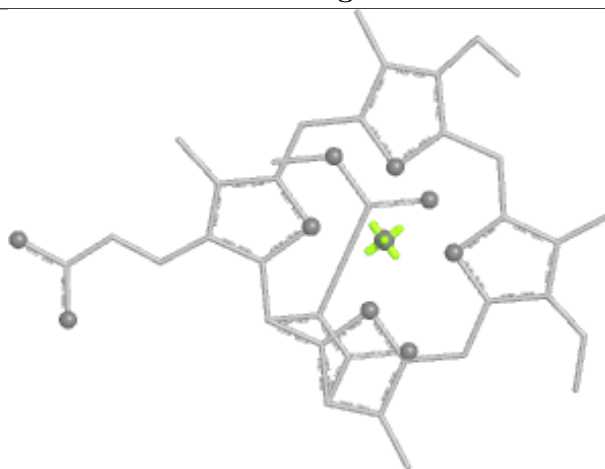
Bond lengths



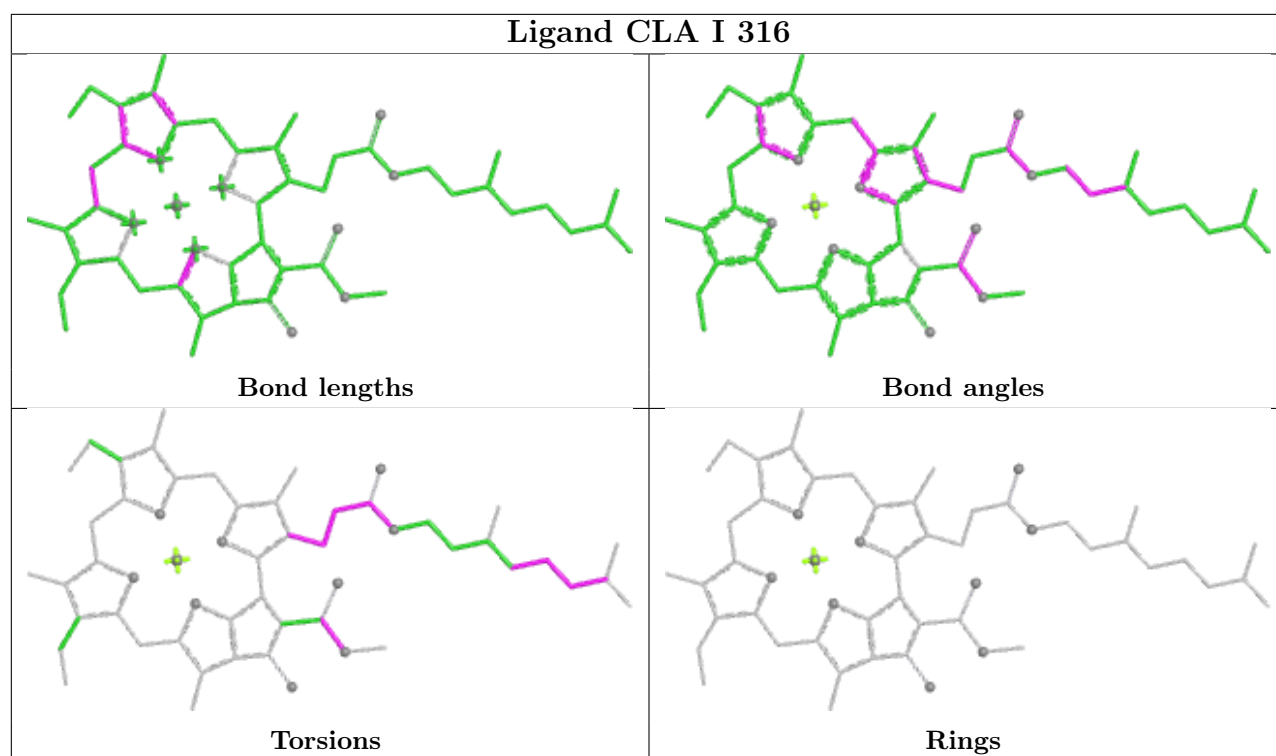
Bond angles

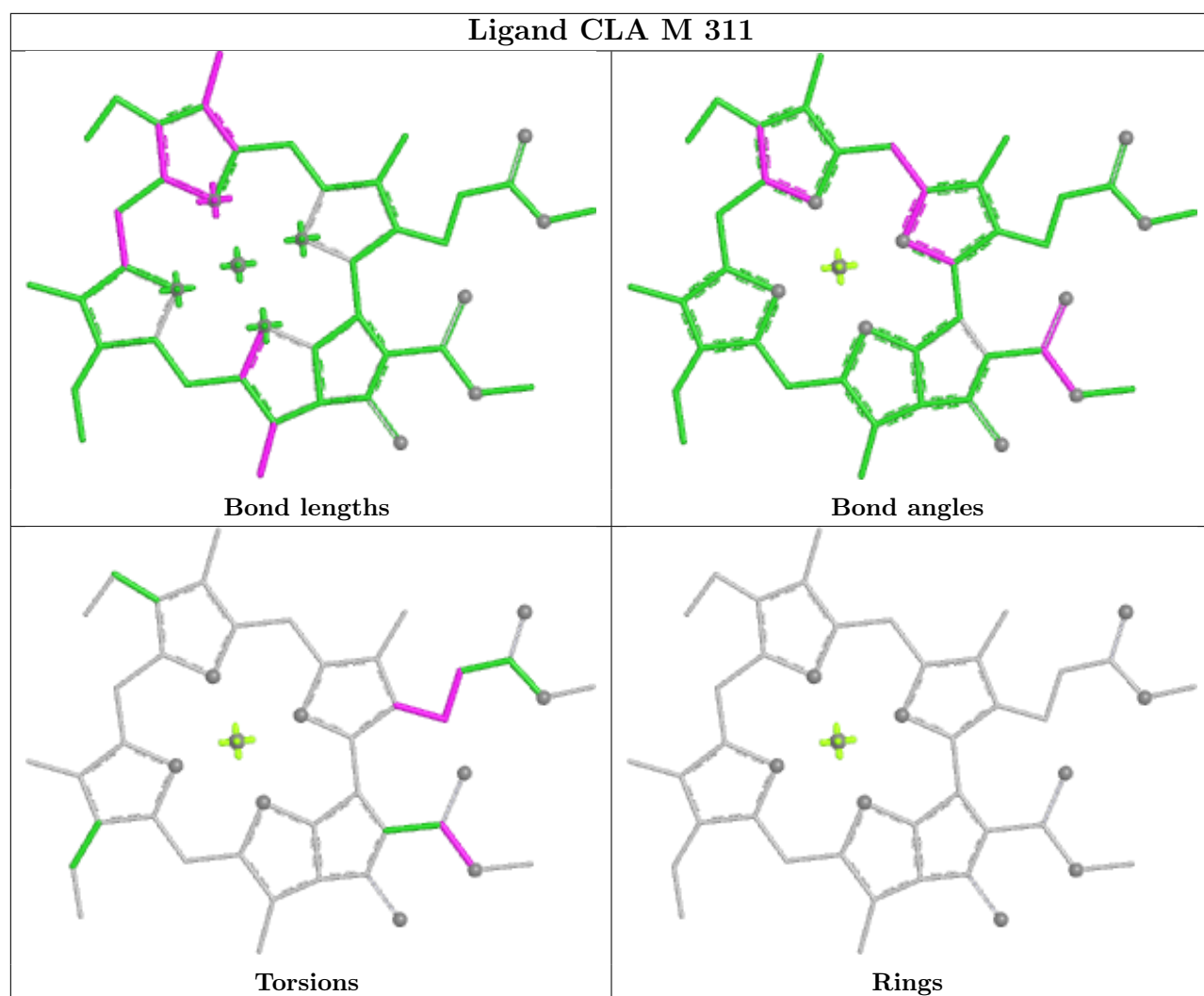


Torsions

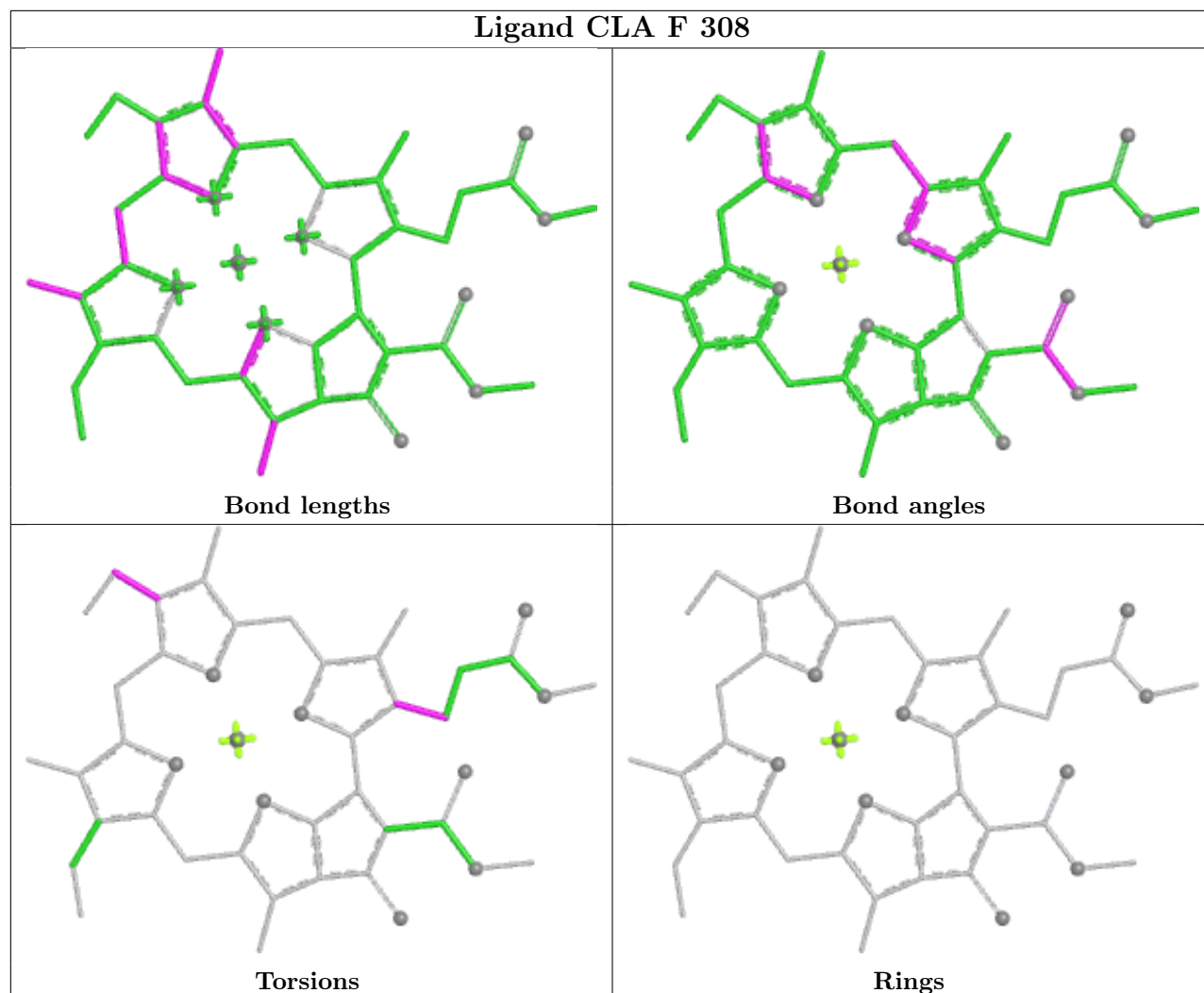


Rings

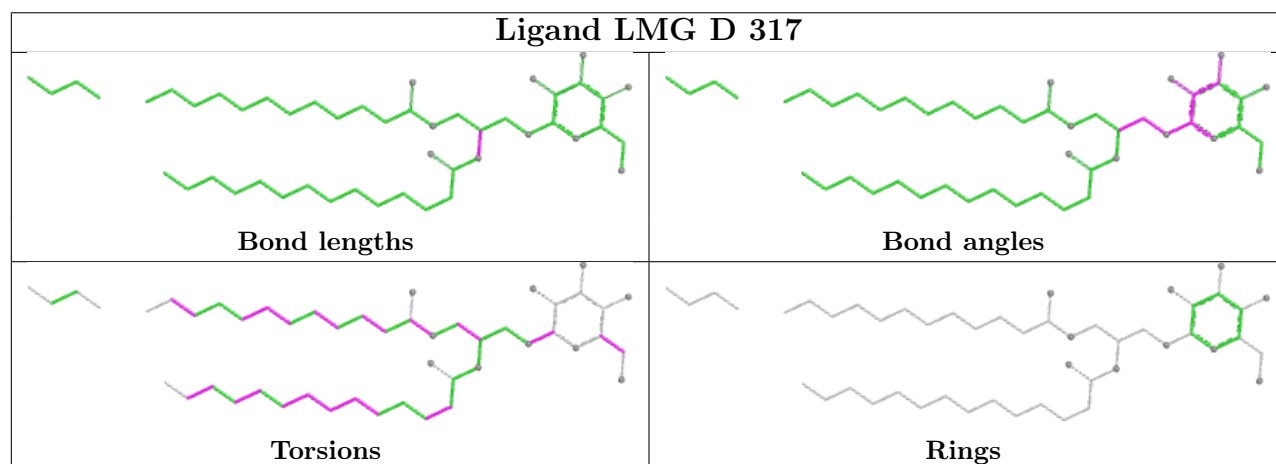


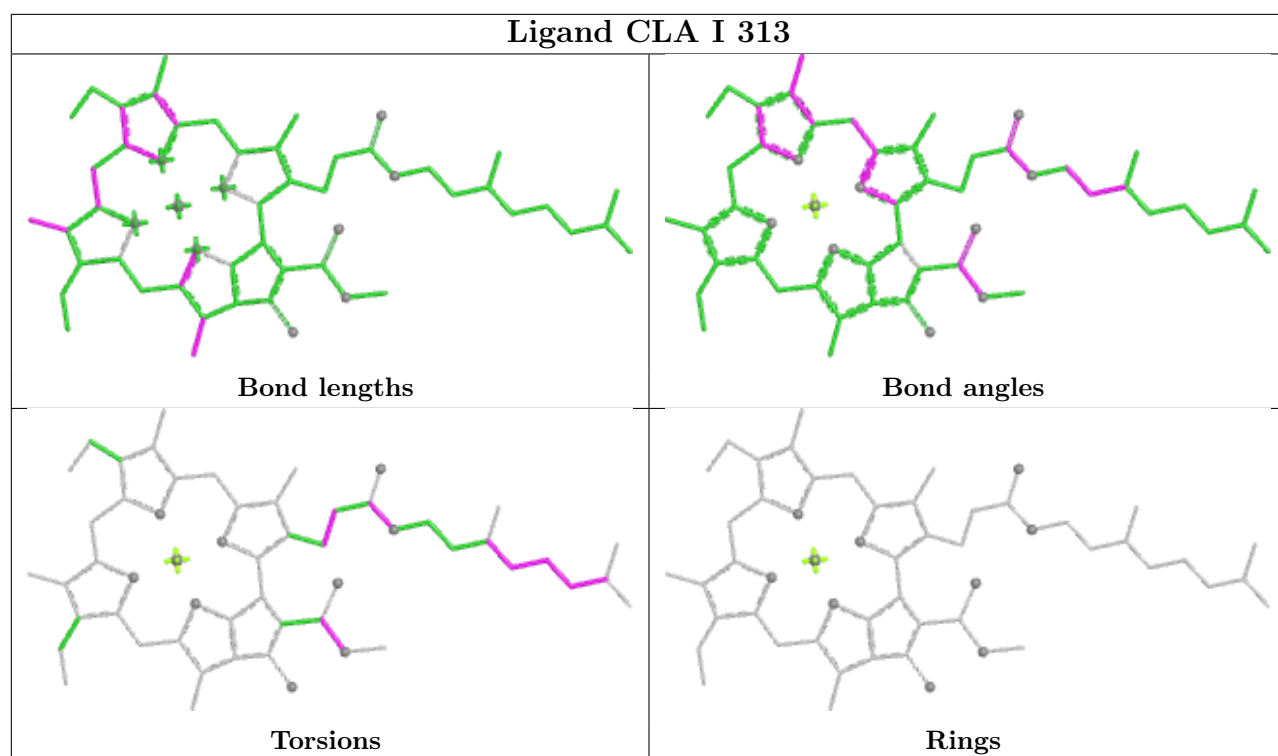


Ligand CLA F 308

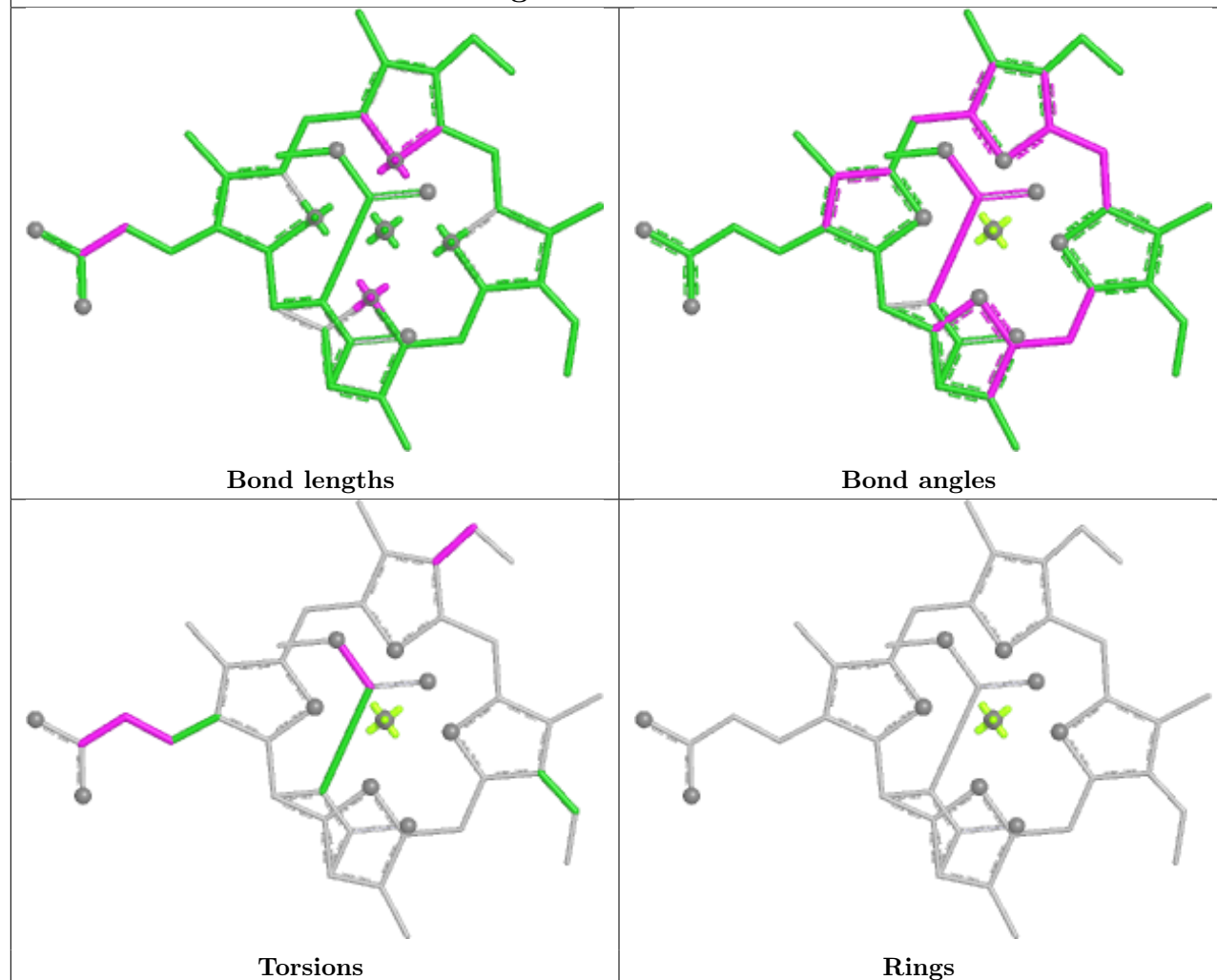


Ligand LMG D 317

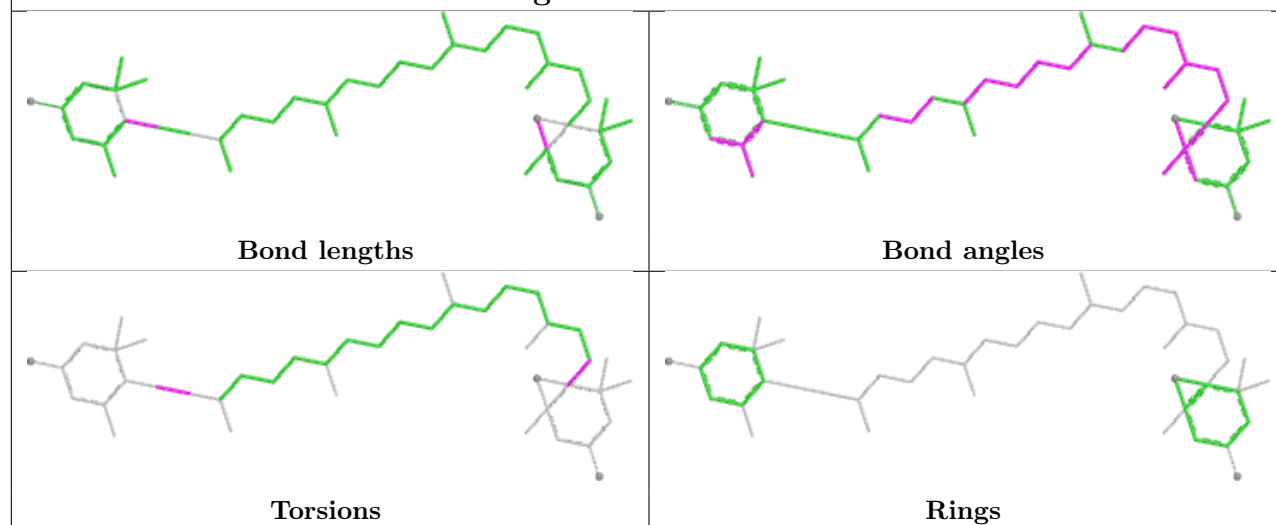


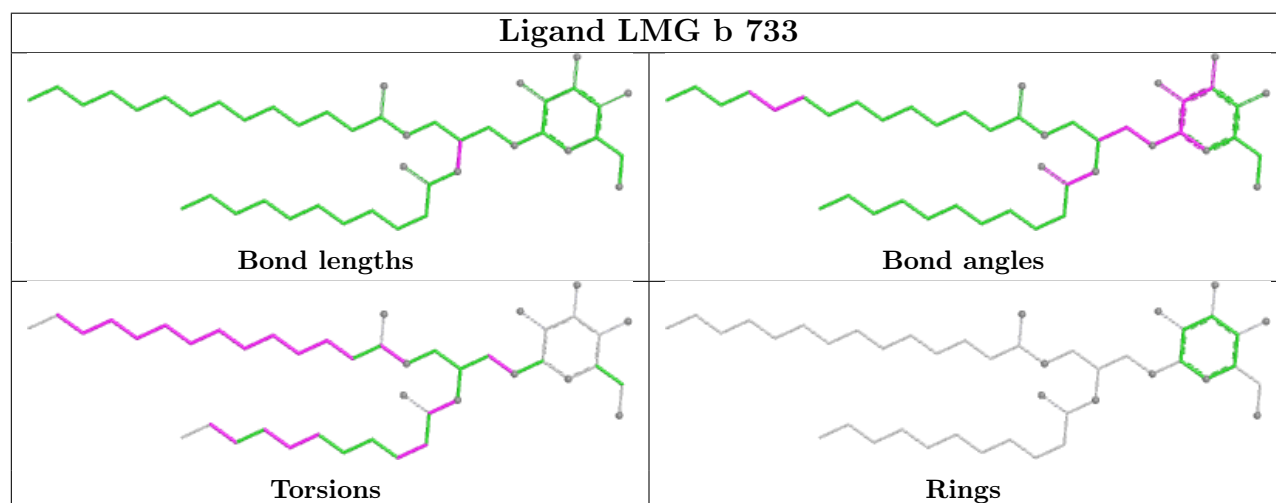
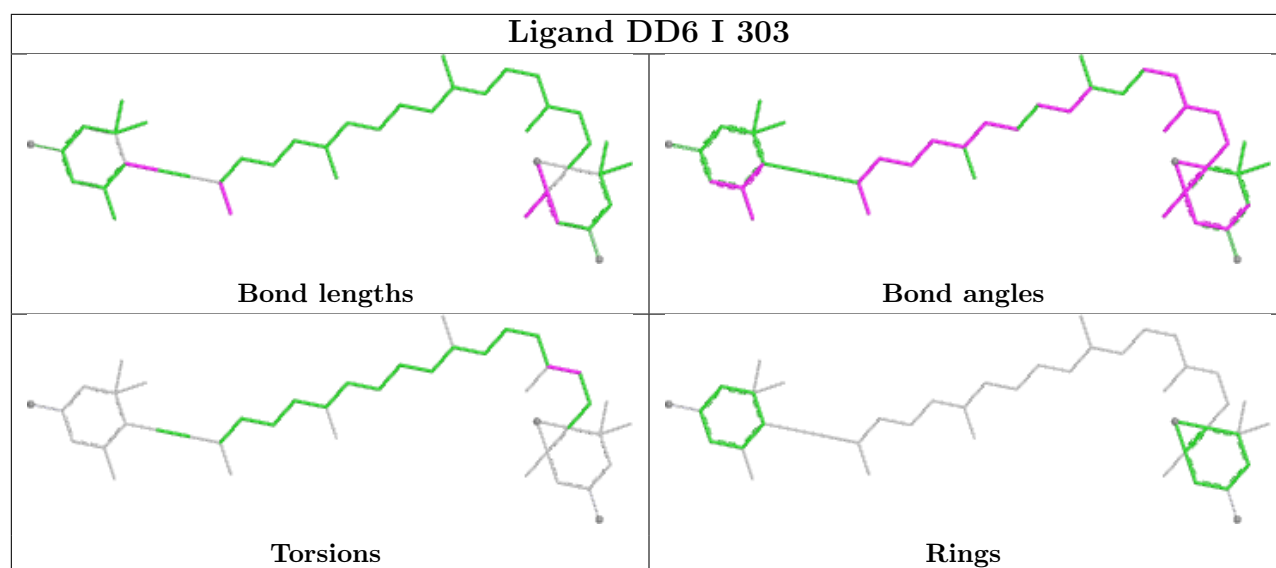


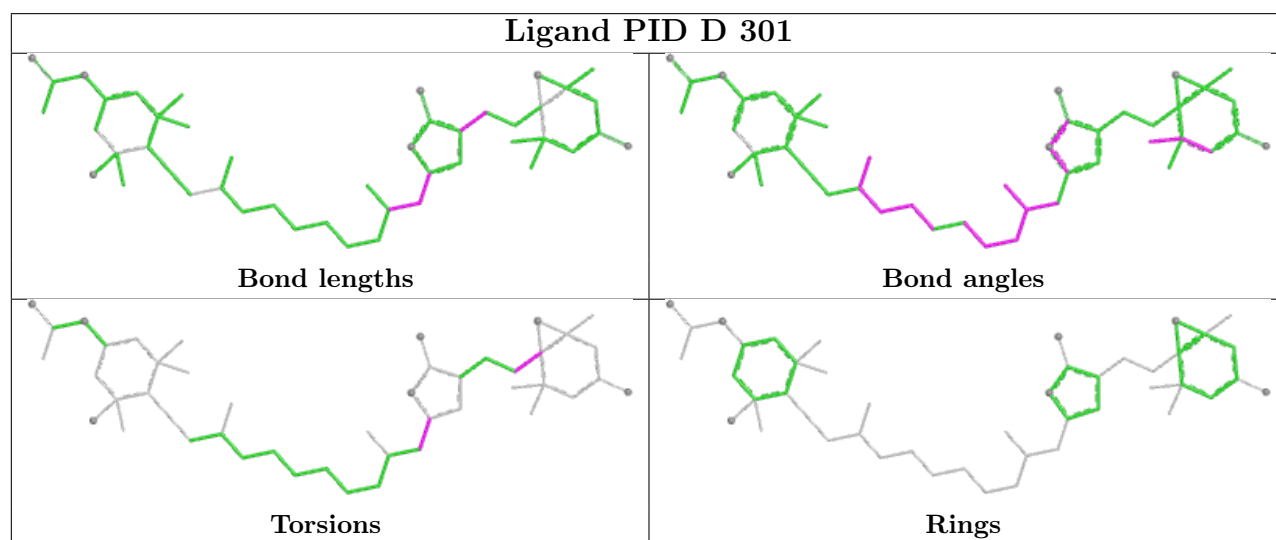
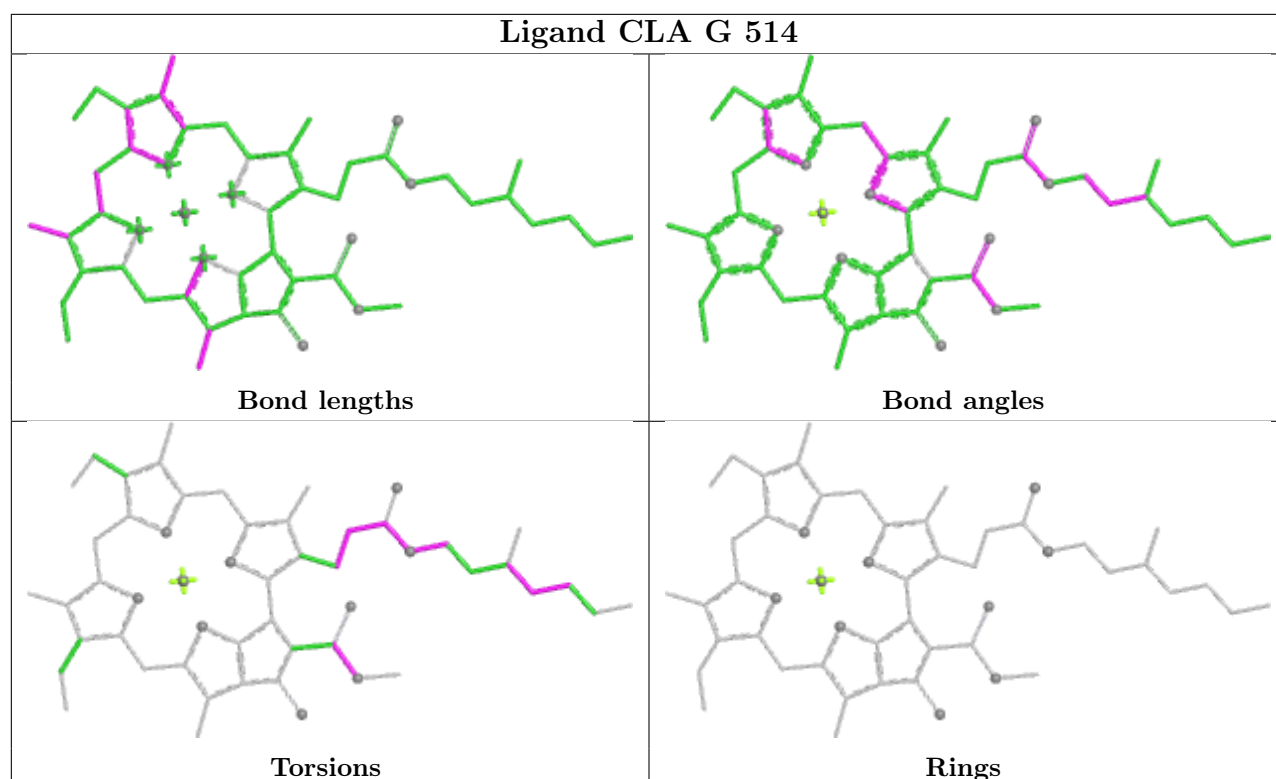
Ligand KC1 F 314



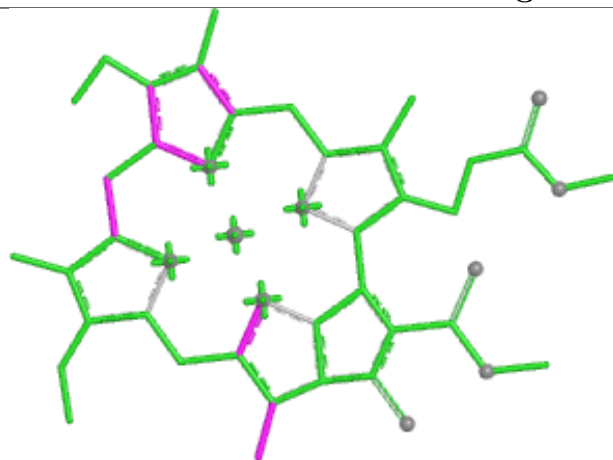
Ligand DD6 B 303



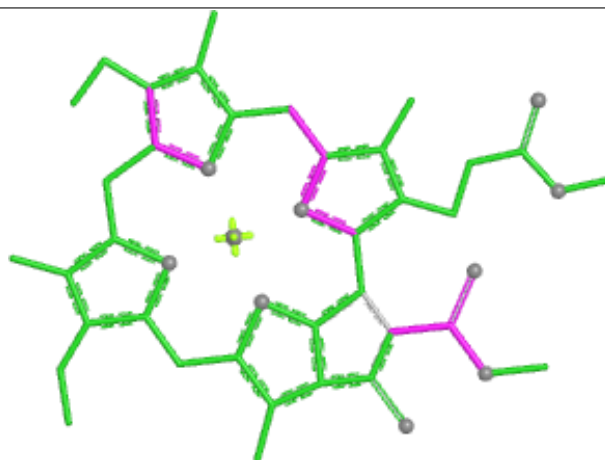




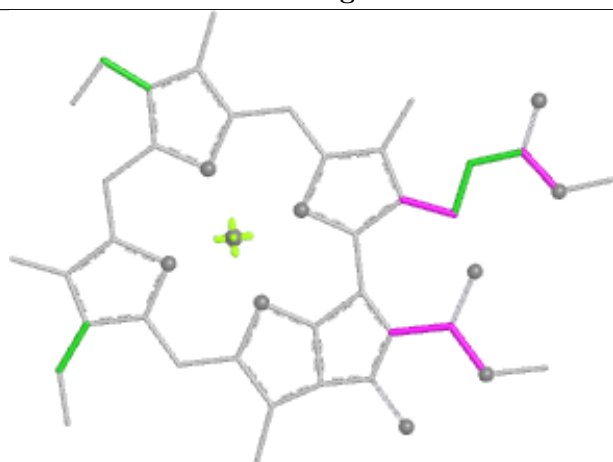
Ligand CLA F 310



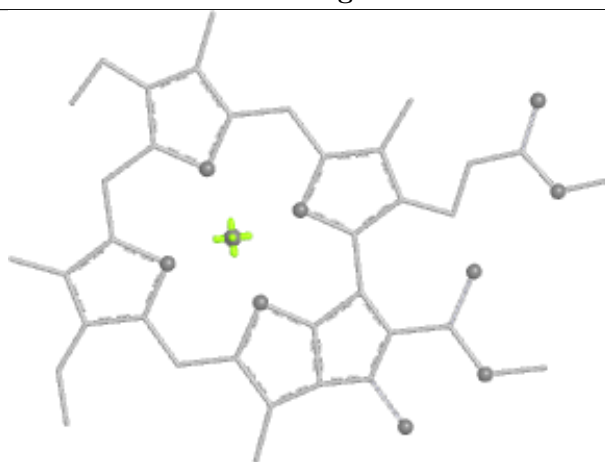
Bond lengths



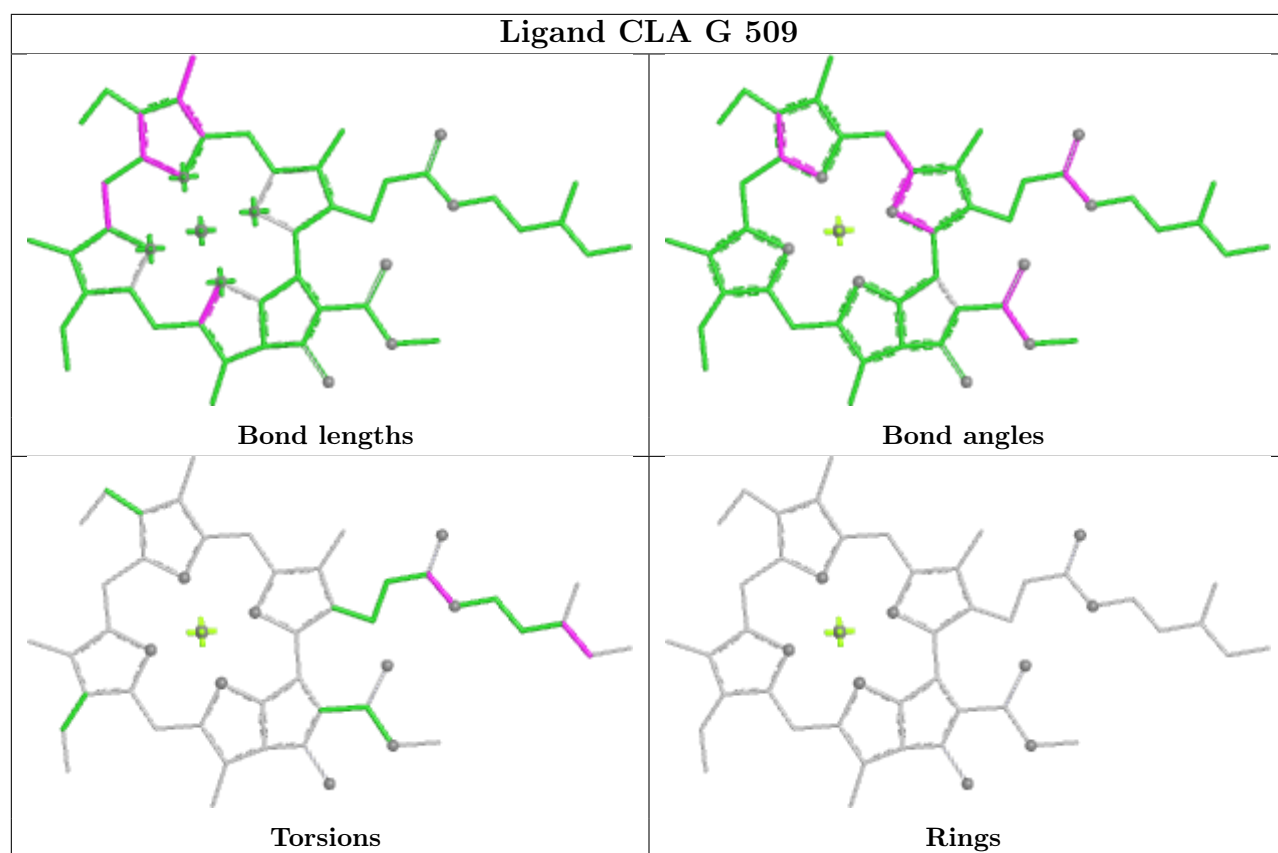
Bond angles



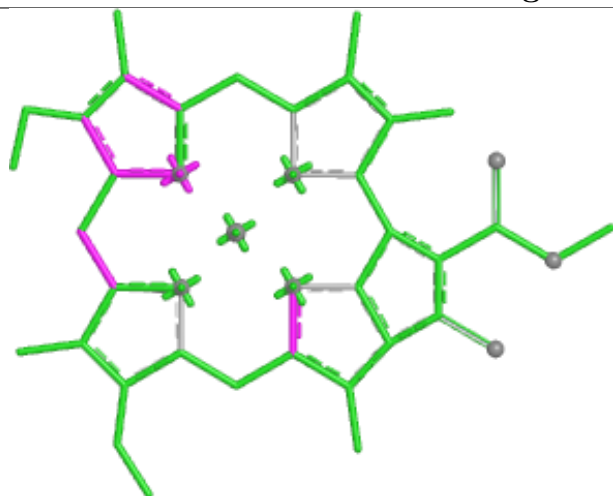
Torsions



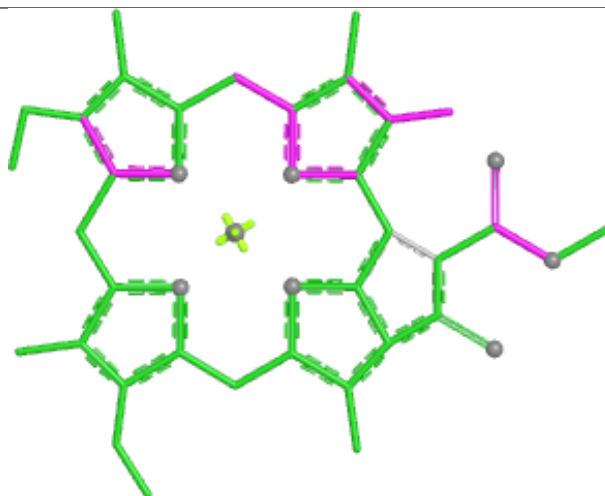
Rings



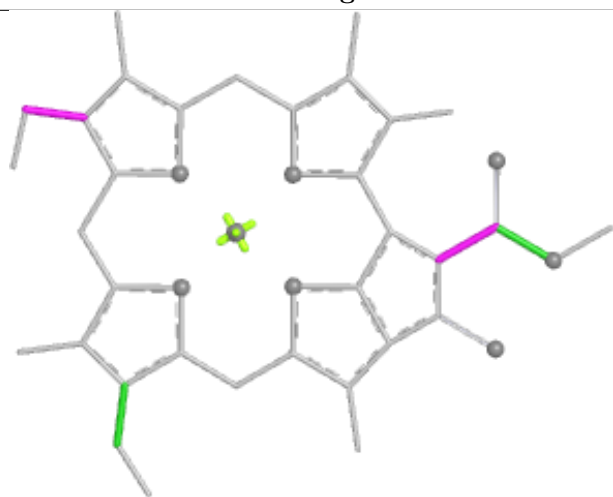
Ligand CLA 1 309



Bond lengths



Bond angles

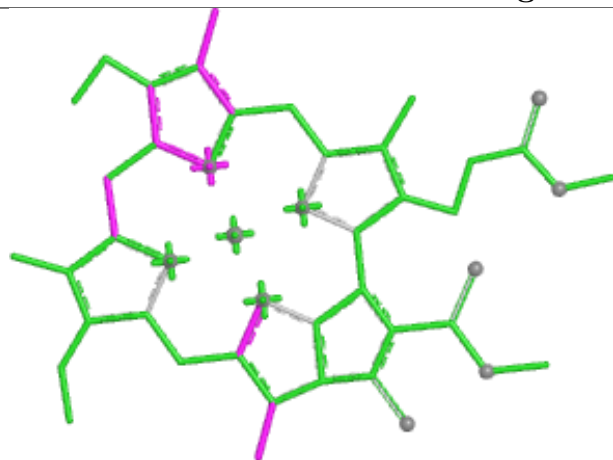


Torsions

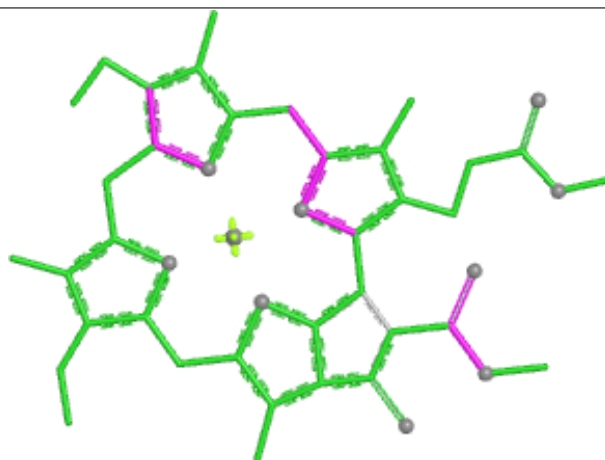


Rings

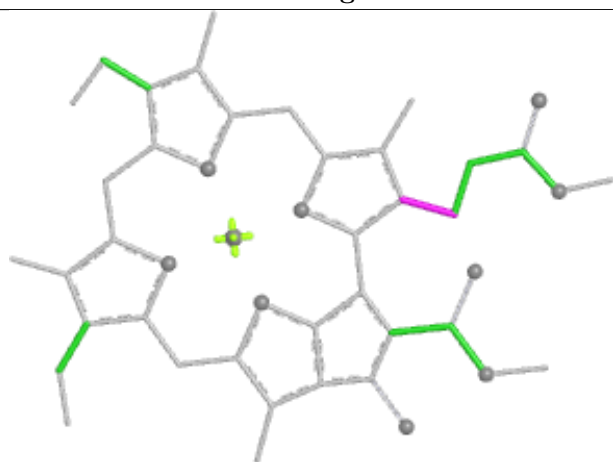
Ligand CLA b 721



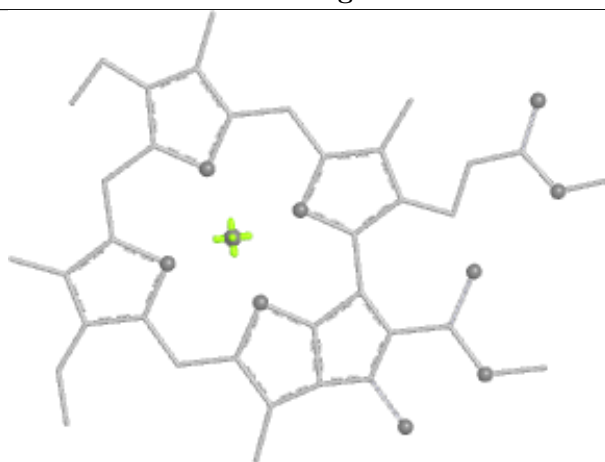
Bond lengths



Bond angles

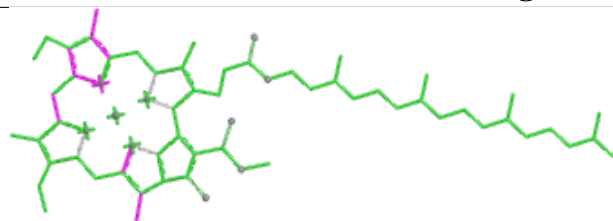


Torsions

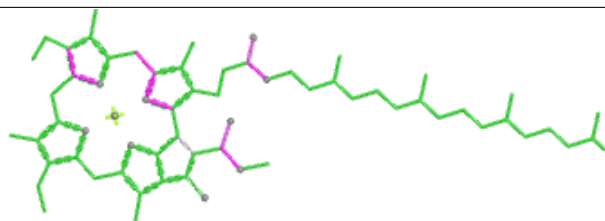


Rings

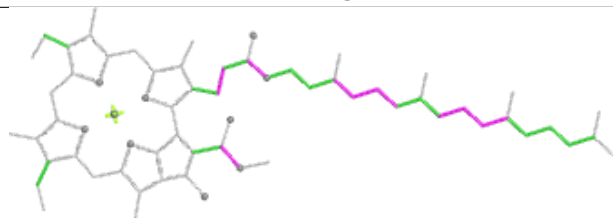
Ligand CLA b 701



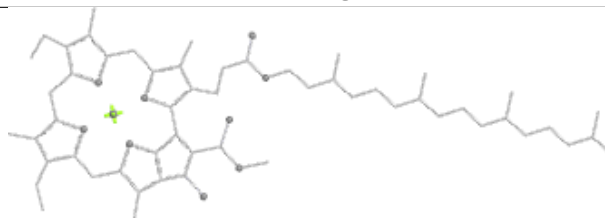
Bond lengths



Bond angles

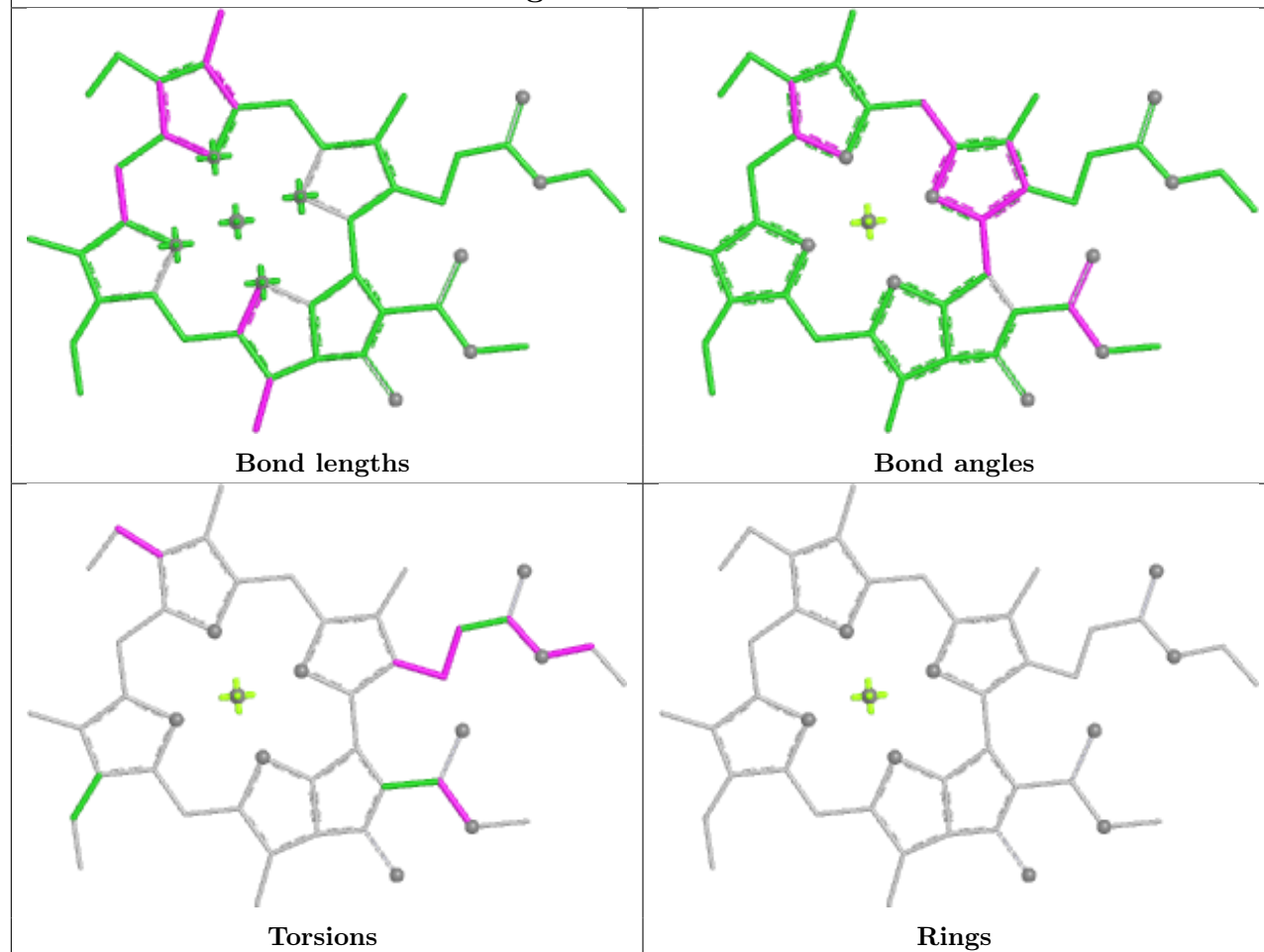


Torsions

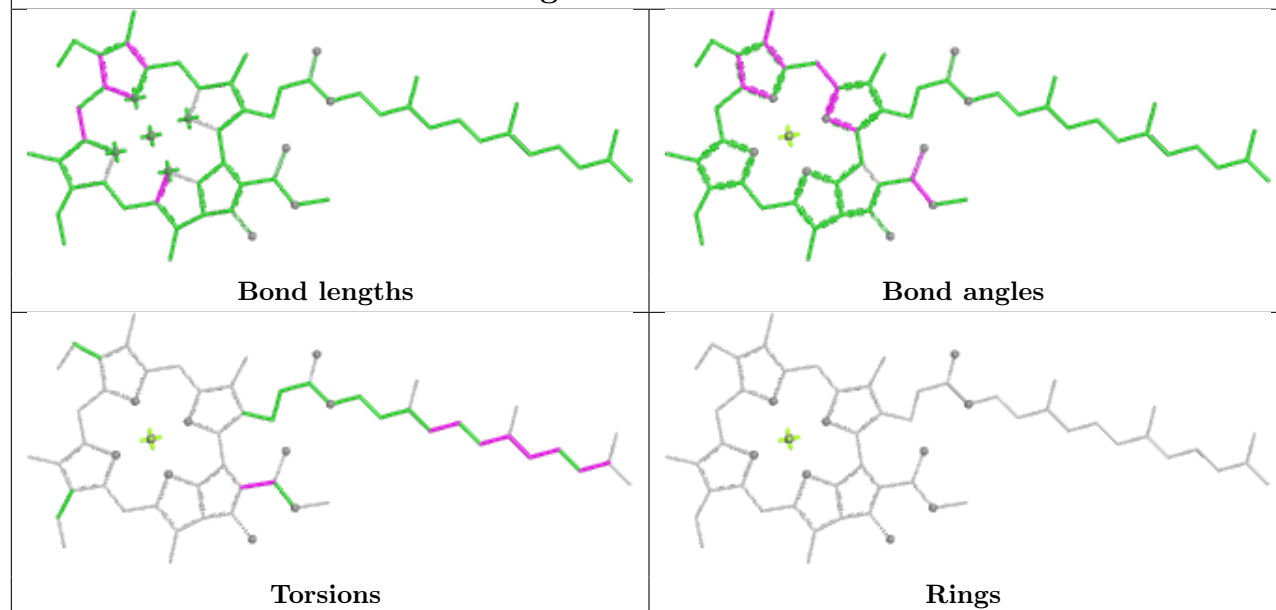


Rings

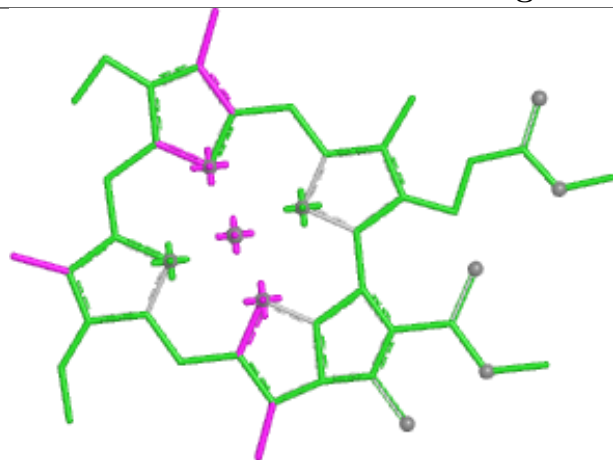
Ligand CLA N 310



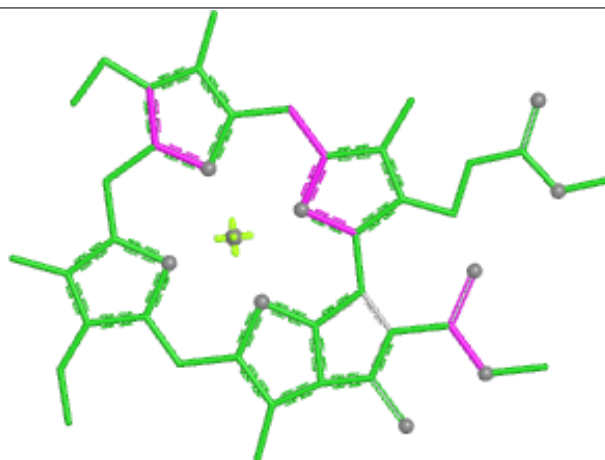
Ligand CLA I 304



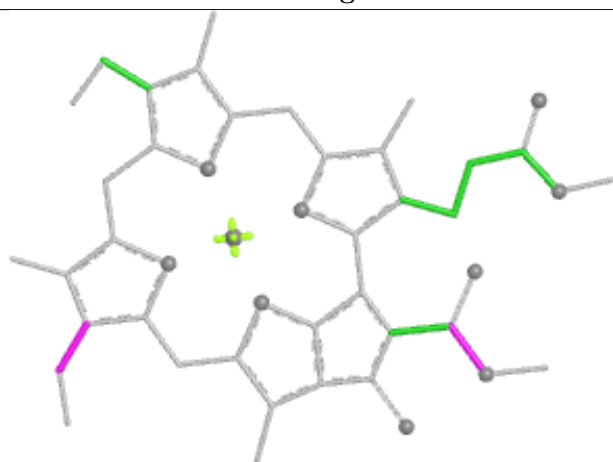
Ligand CLA F 312



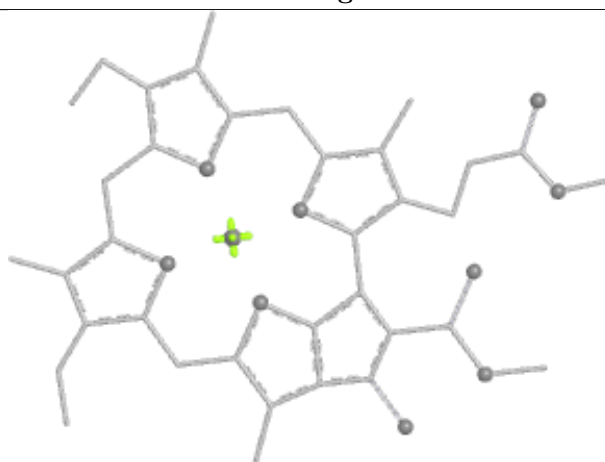
Bond lengths



Bond angles

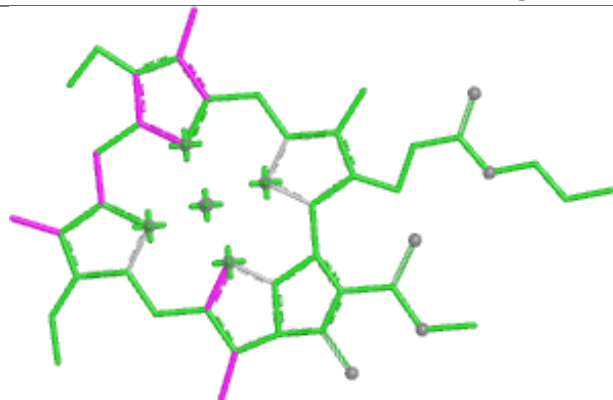


Torsions

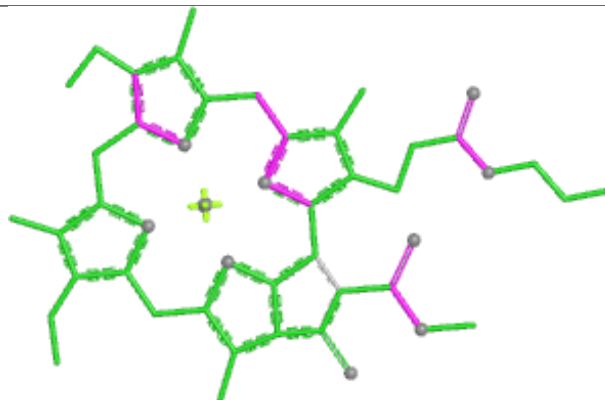


Rings

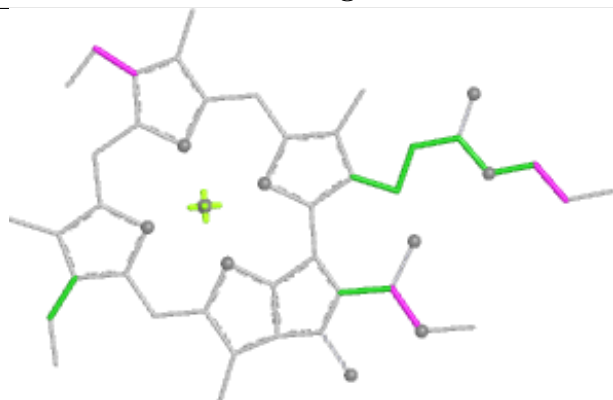
Ligand CLA K 312



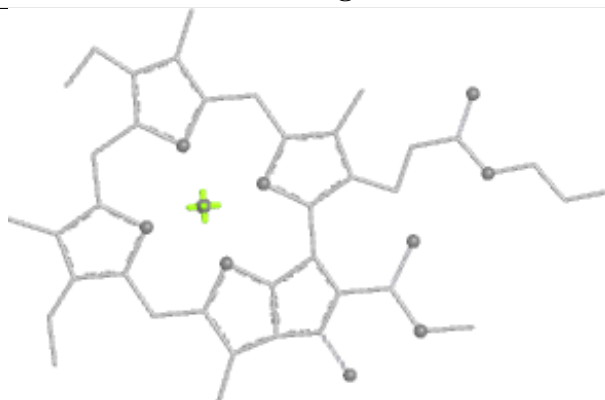
Bond lengths



Bond angles

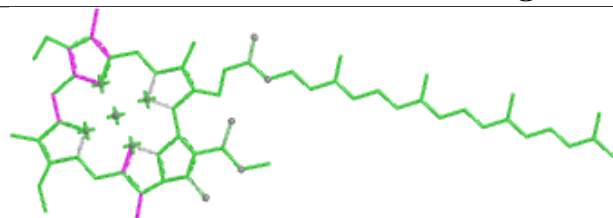


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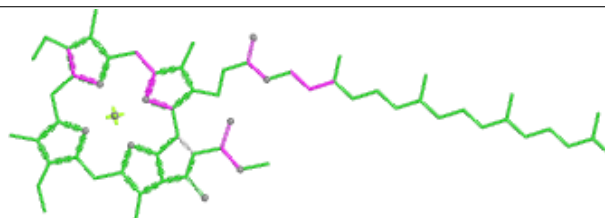


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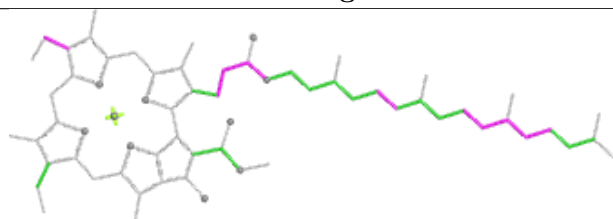
Ligand CLA b 705



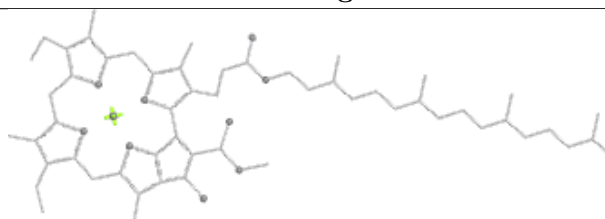
Bond lengths



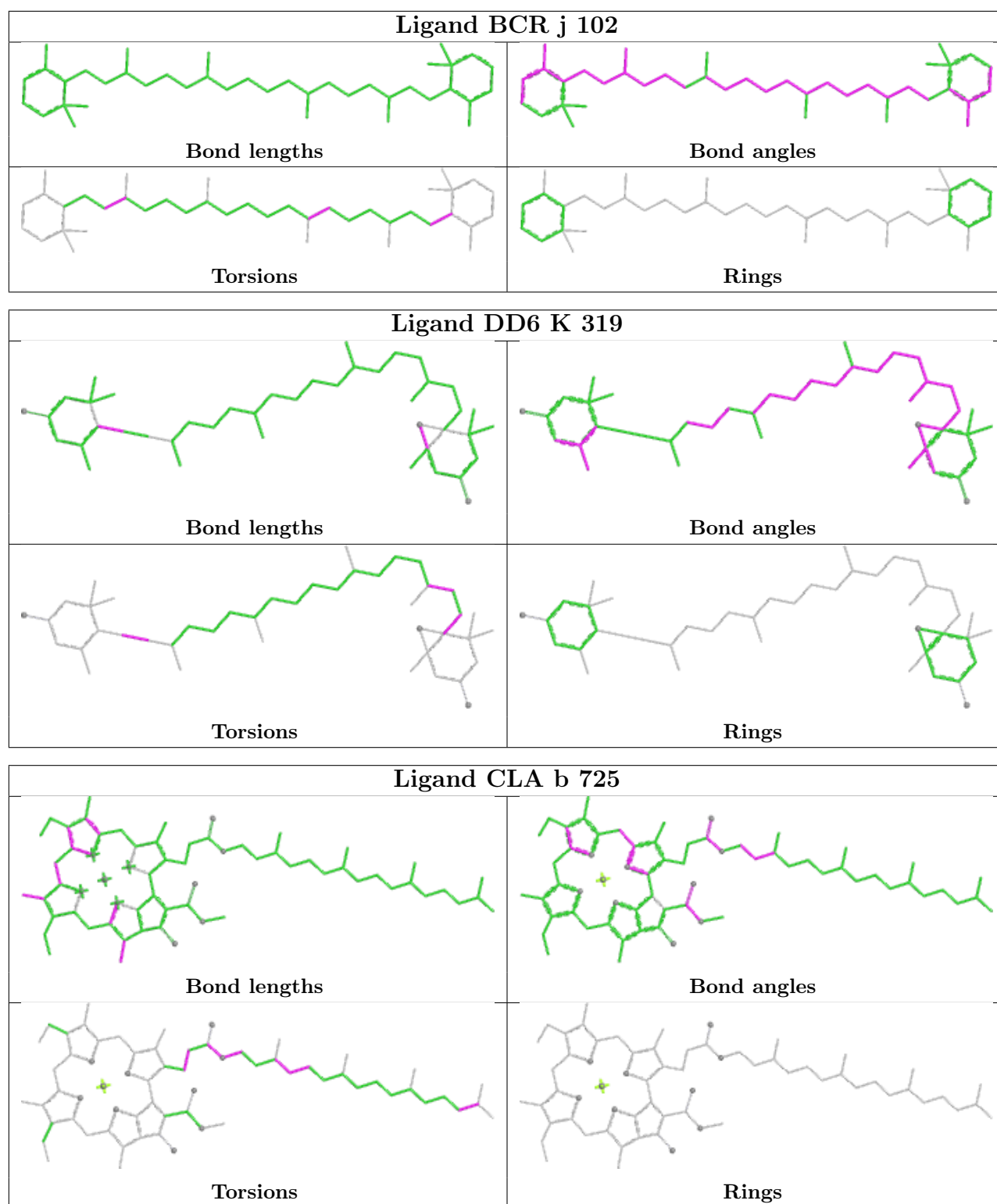
Bond angles



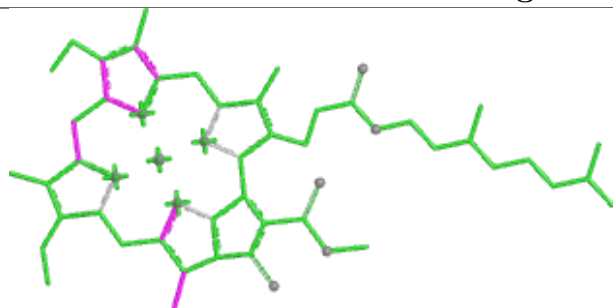
Torsions



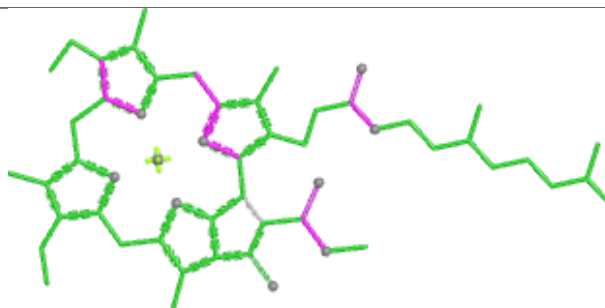
Rings



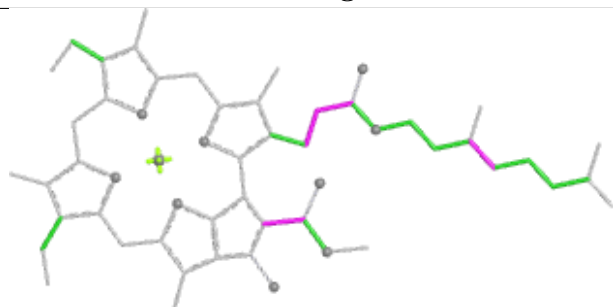
Ligand CLA L 311



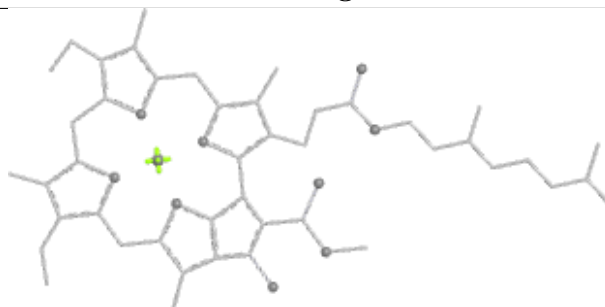
Bond lengths



Bond angles

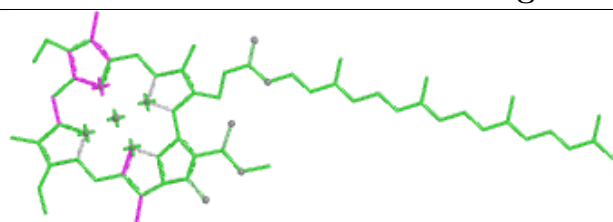


Torsions

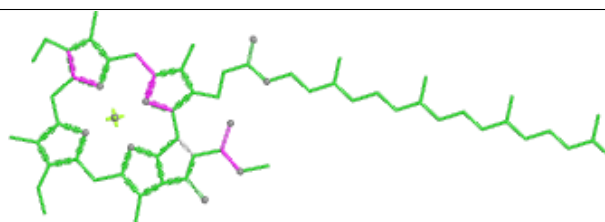


Rings

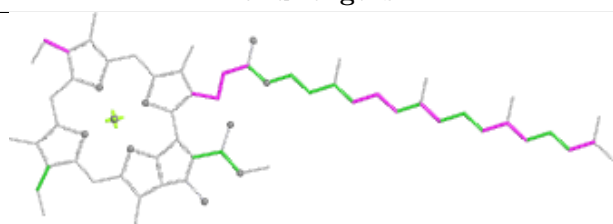
Ligand CLA b 724



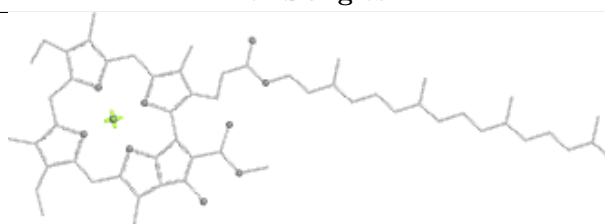
Bond lengths



Bond angles

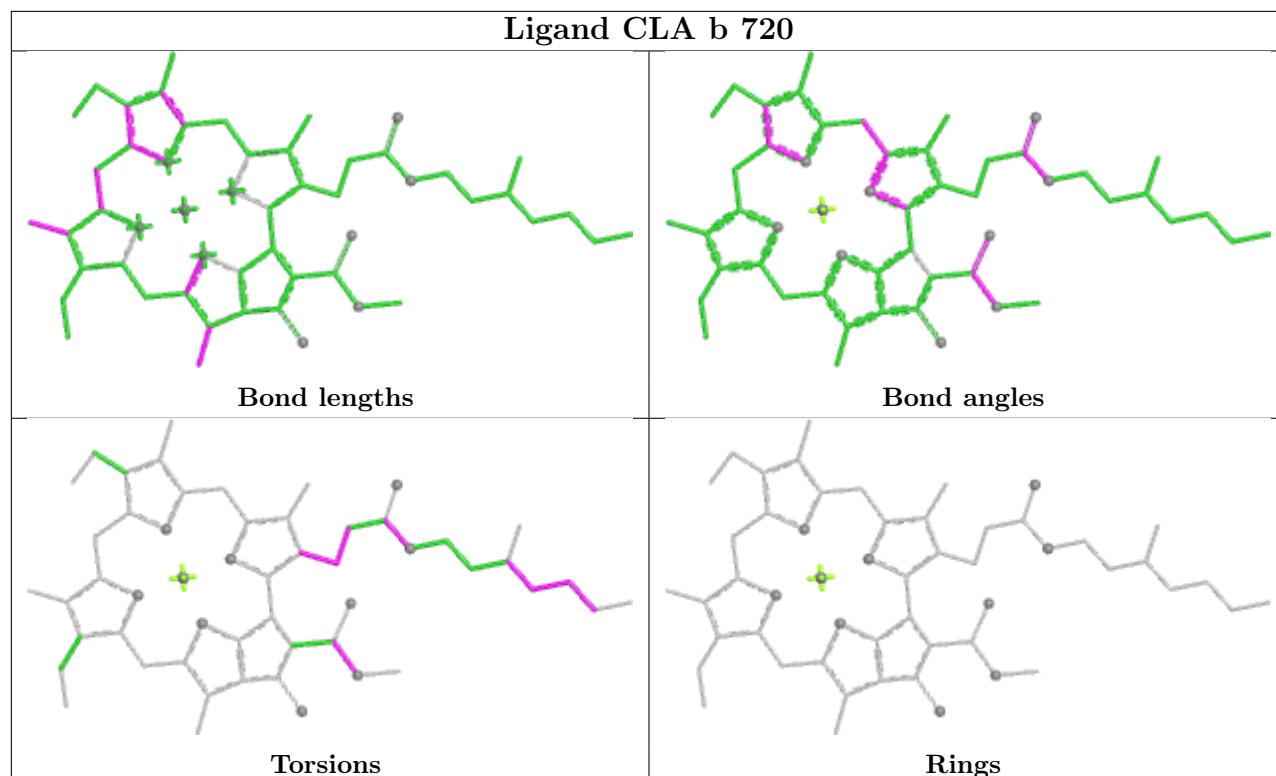


Torsions

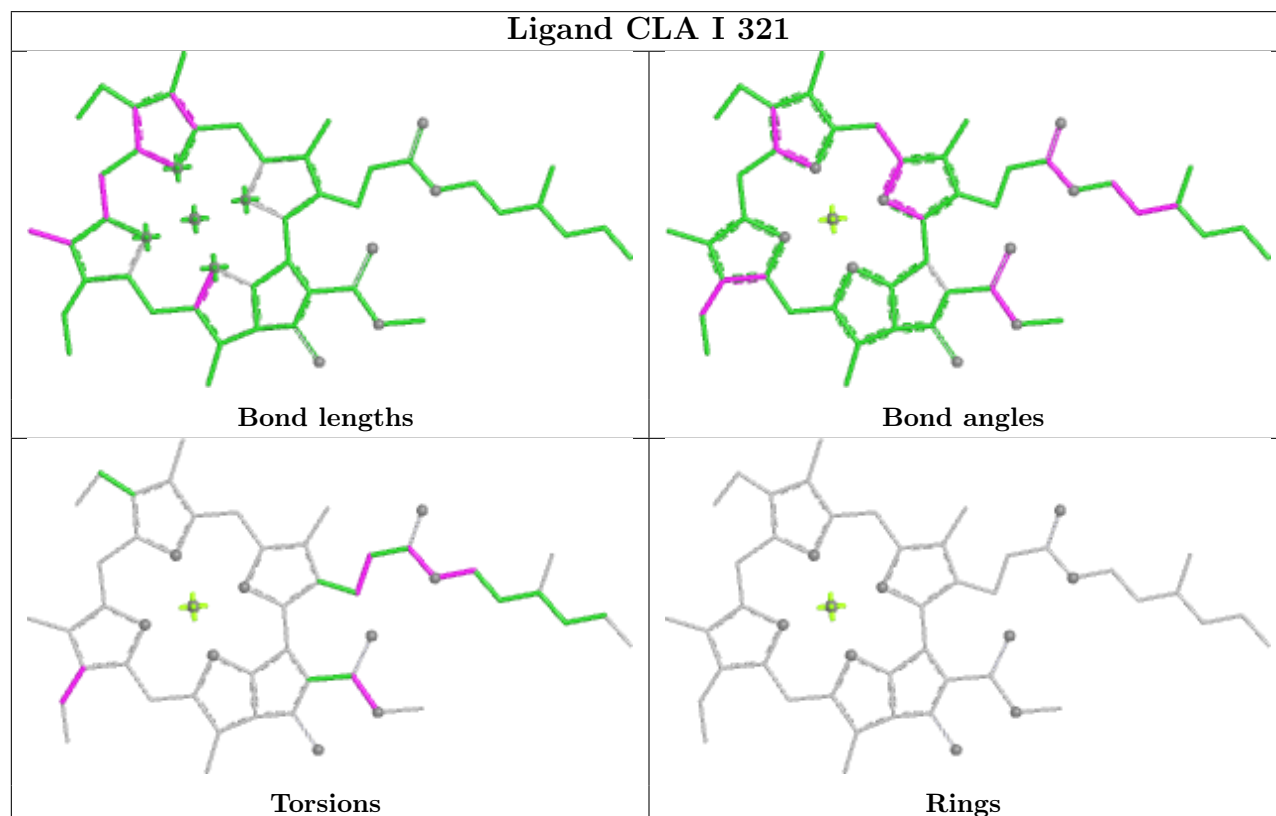


Rings

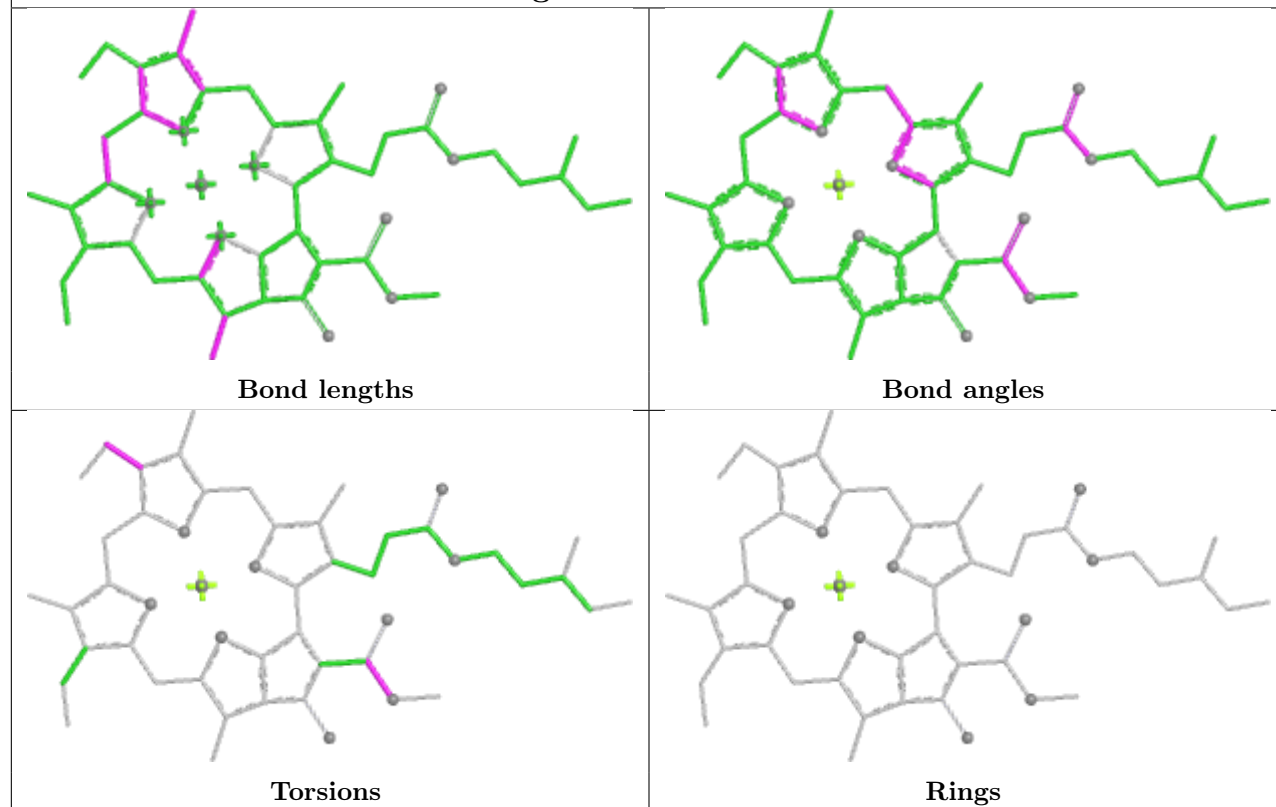
Ligand CLA b 720



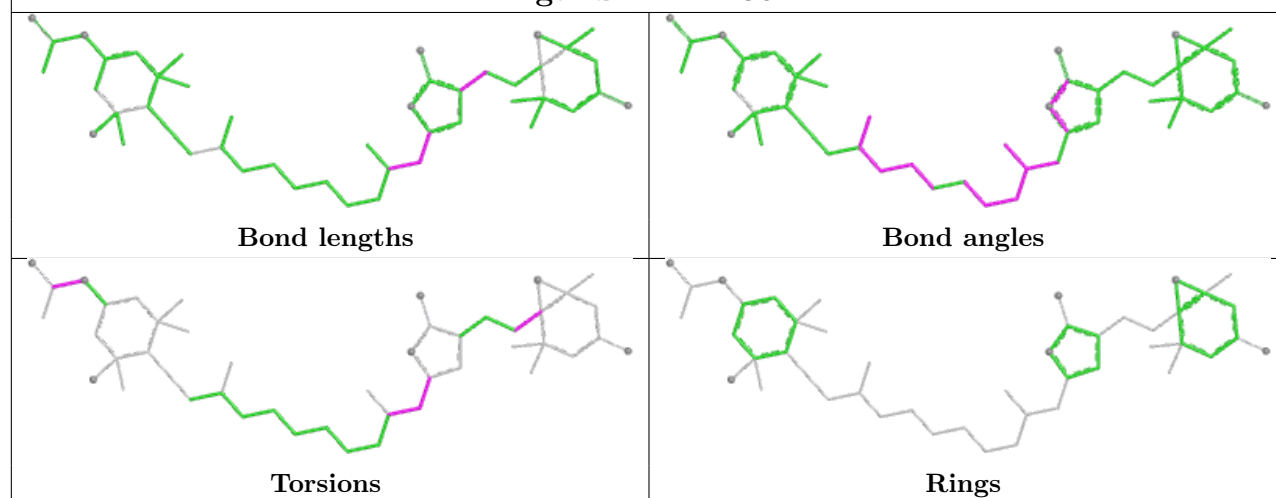
Ligand CLA I 321

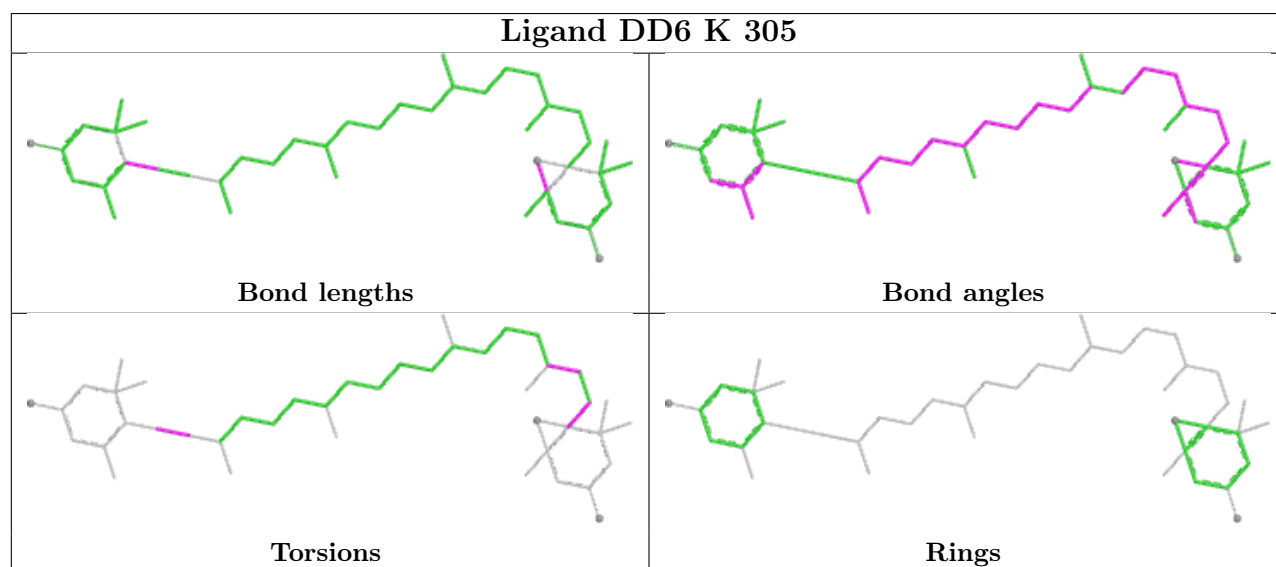
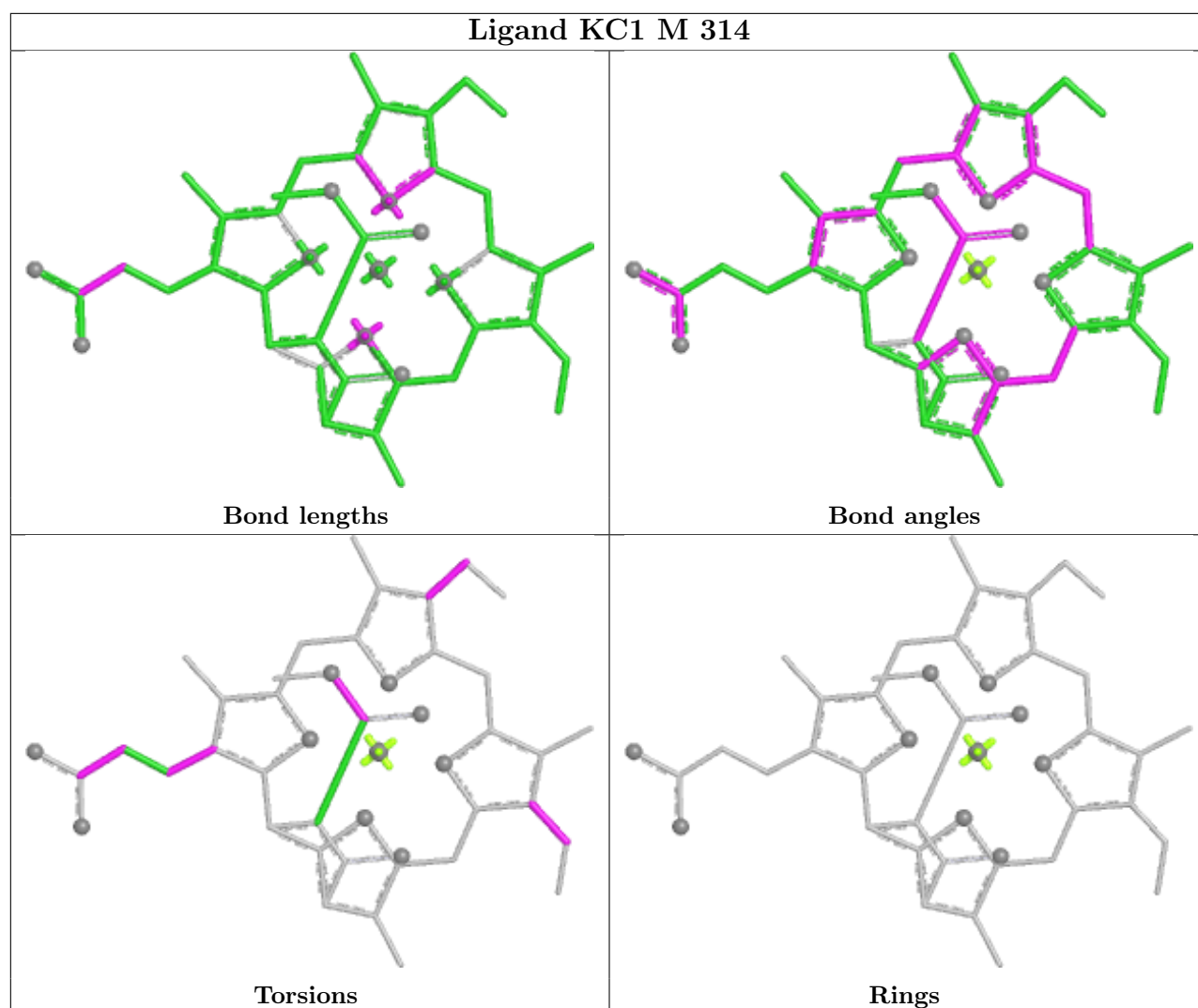


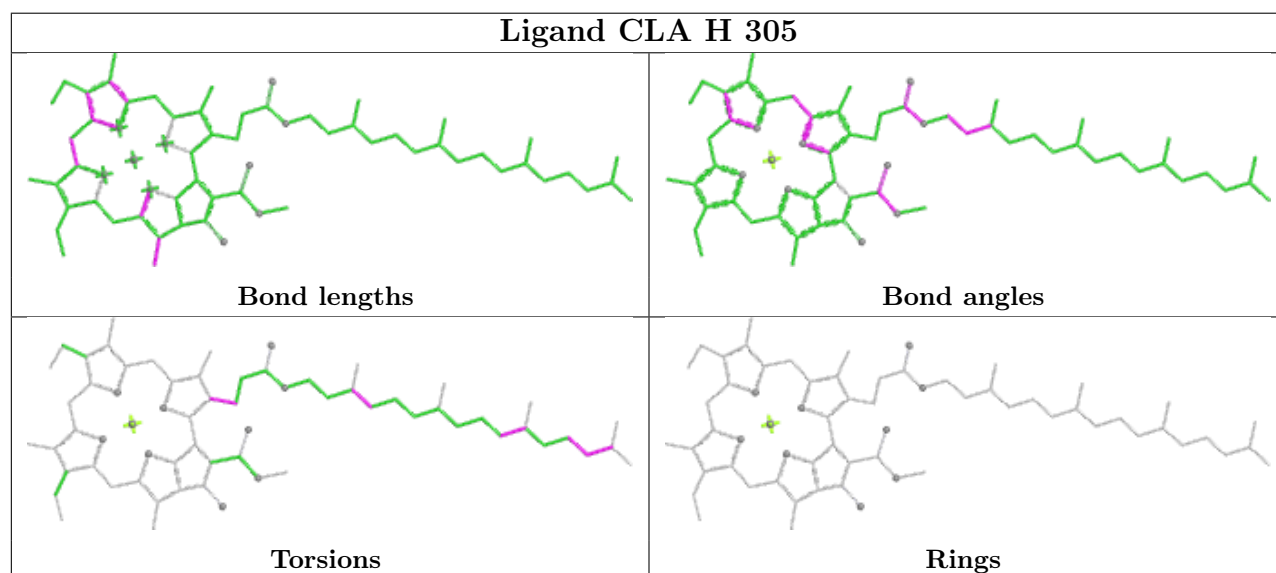
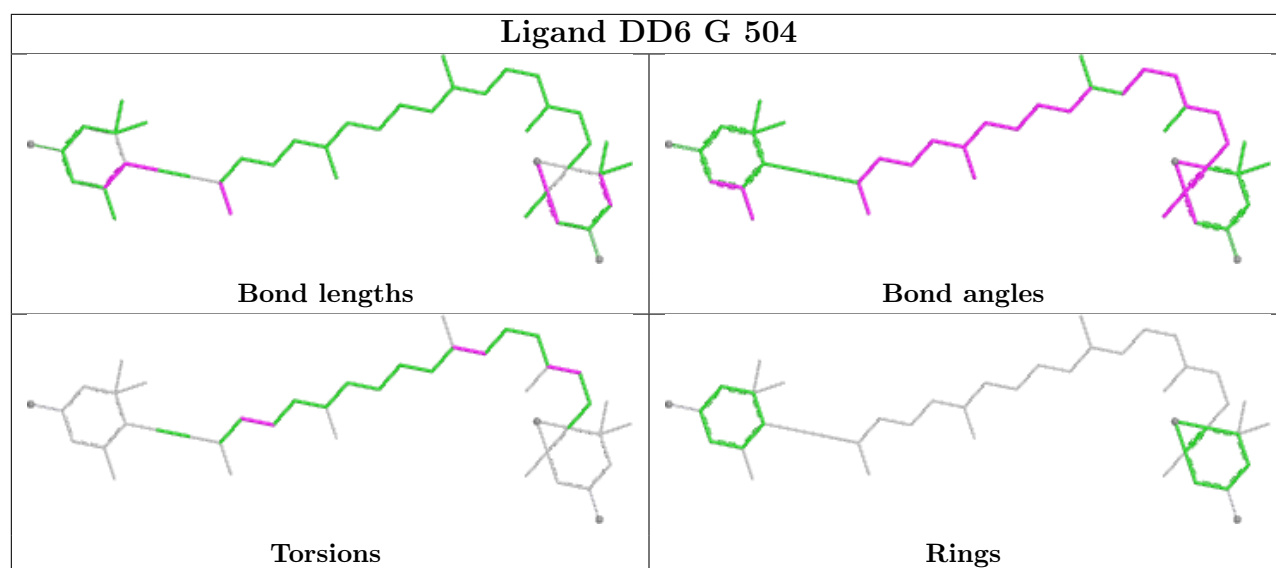
Ligand CLA B 312

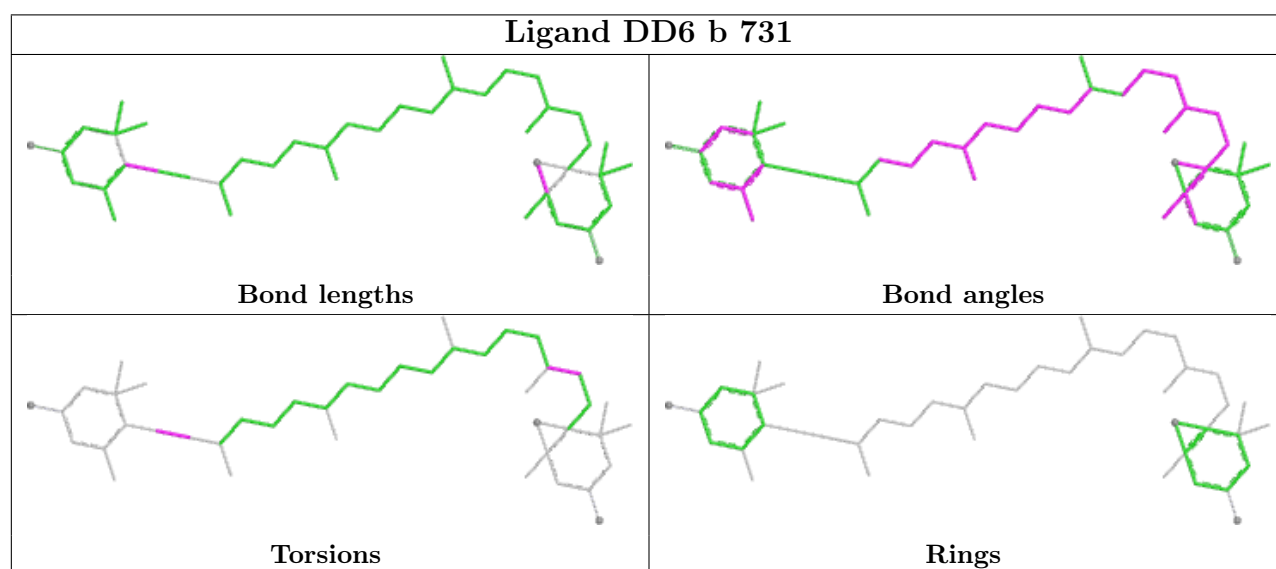
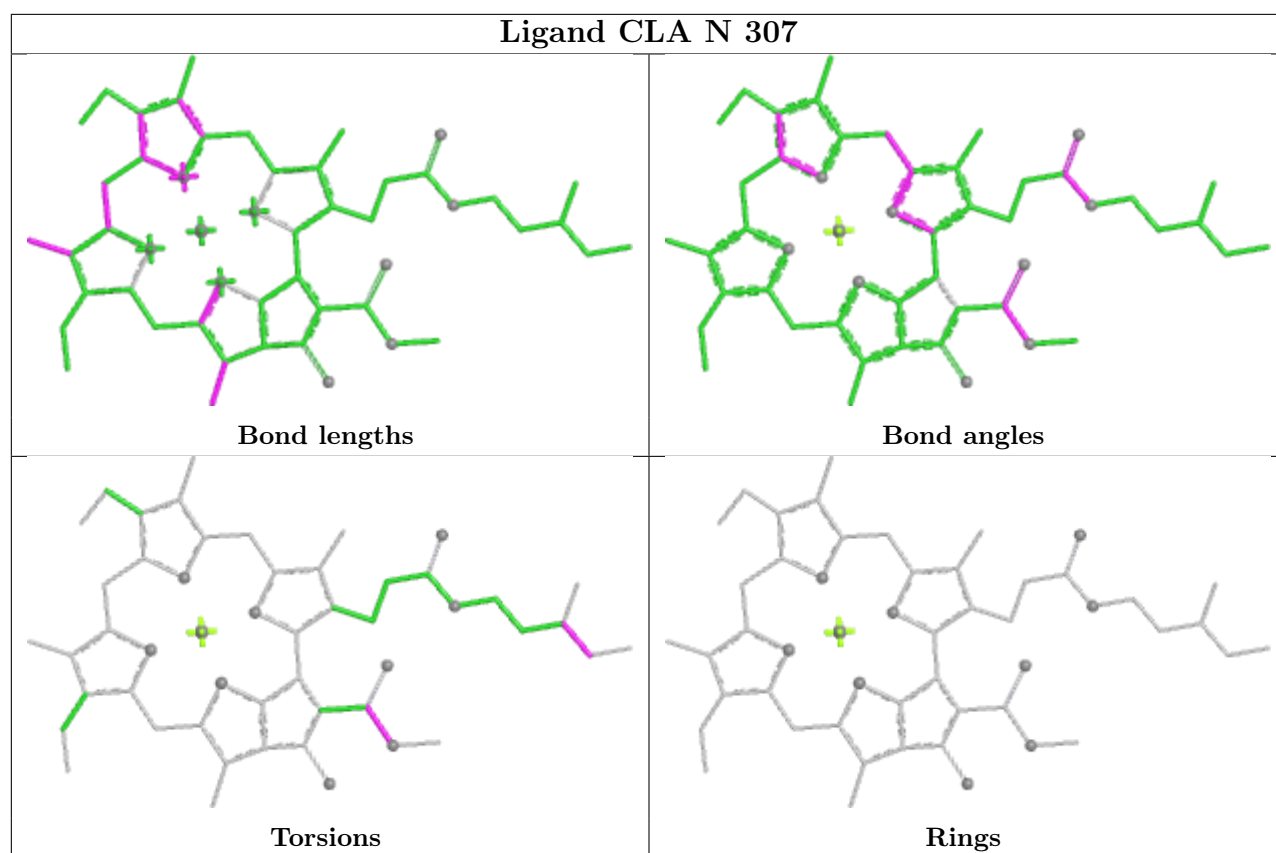


Ligand PID N 301

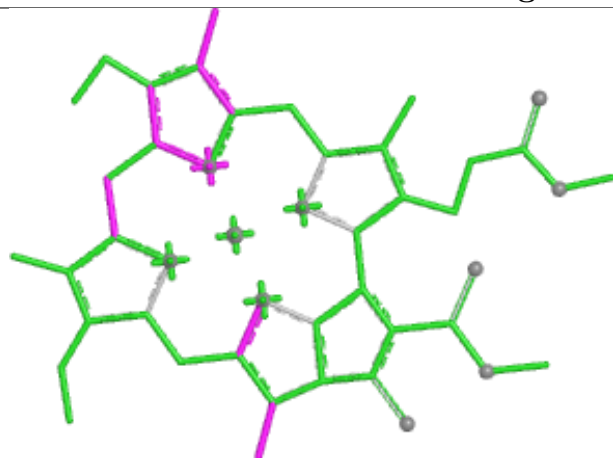




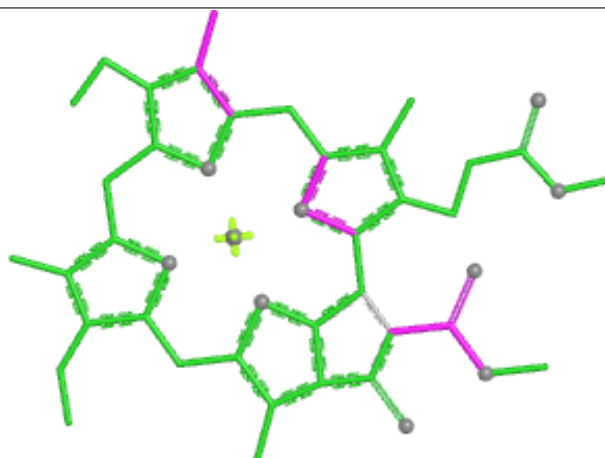




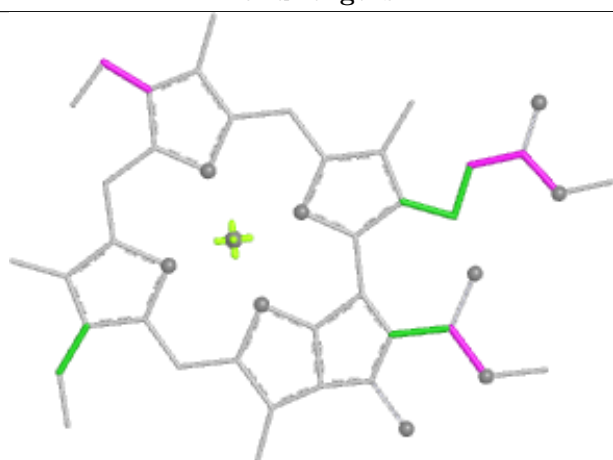
Ligand CLA J 310



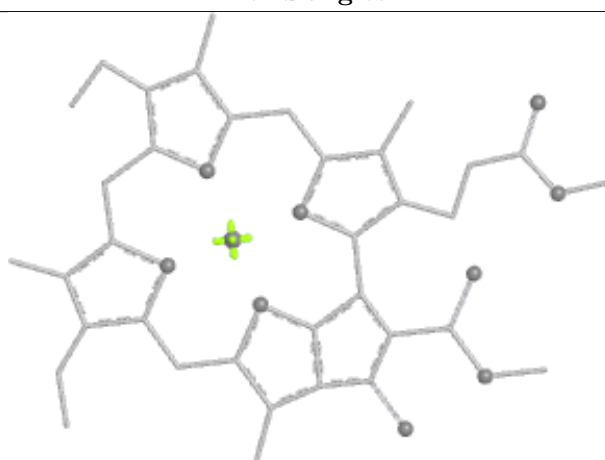
Bond lengths



Bond angles

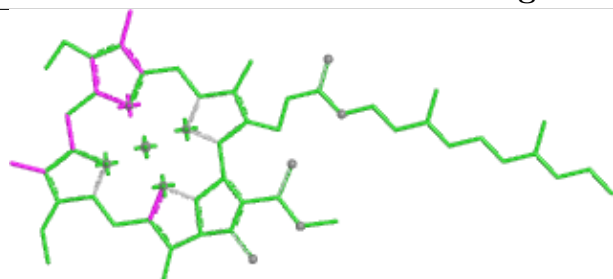


Torsions

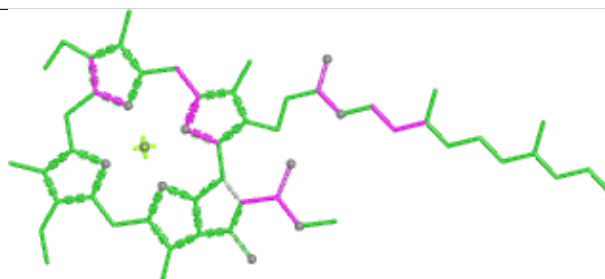


Rings

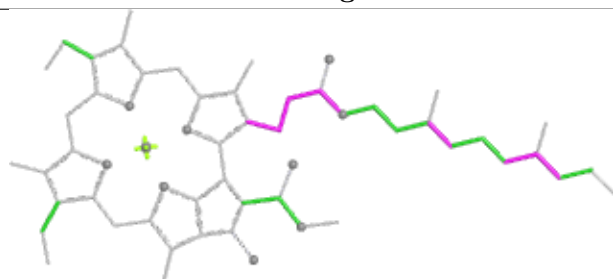
Ligand CLA a 717



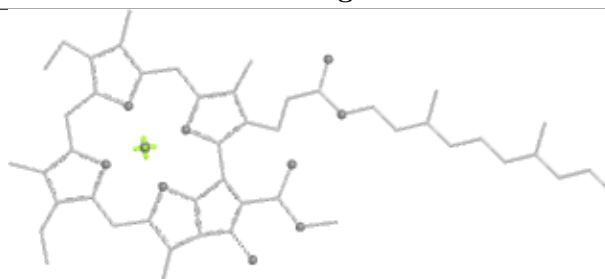
Bond lengths



Bond angles

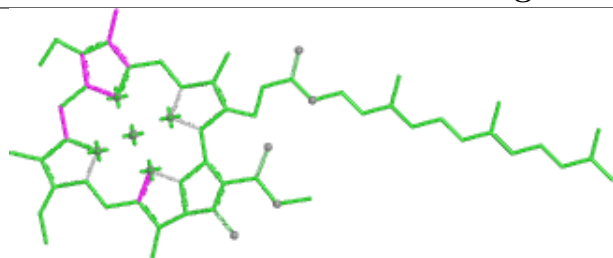


Torsions

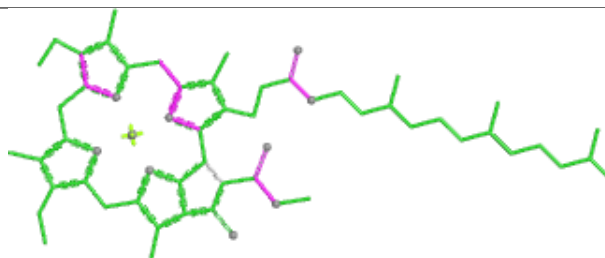


Rings

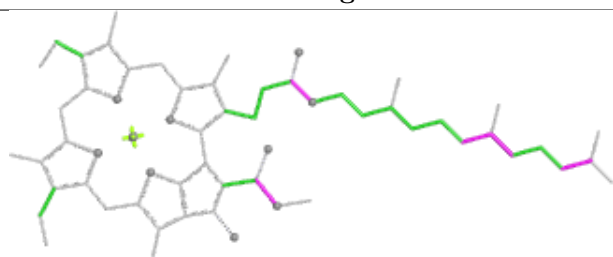
Ligand CLA B 301



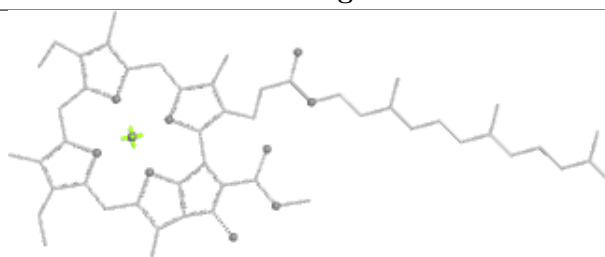
Bond lengths



Bond angles

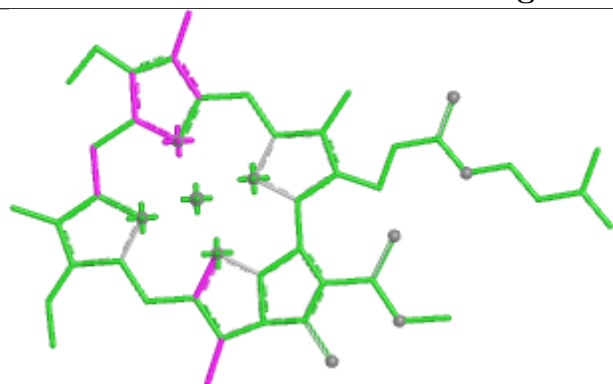


Torsions

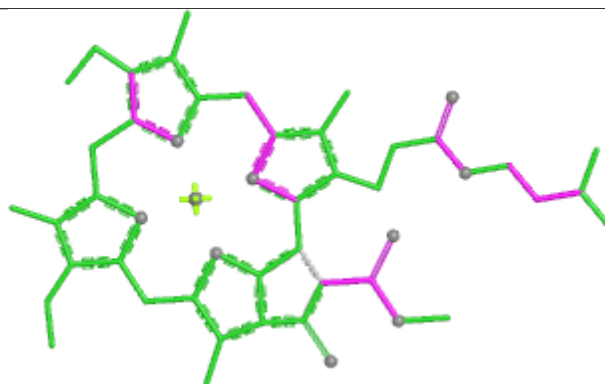


Rings

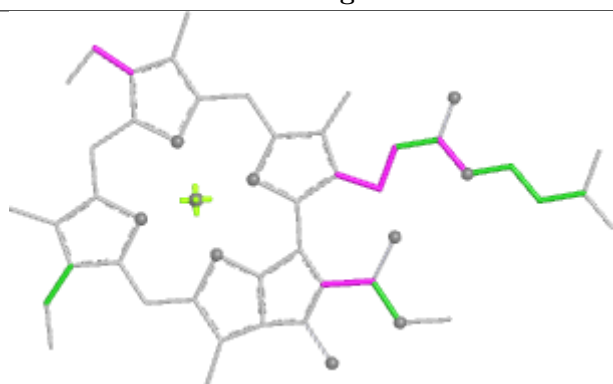
Ligand CLA b 723



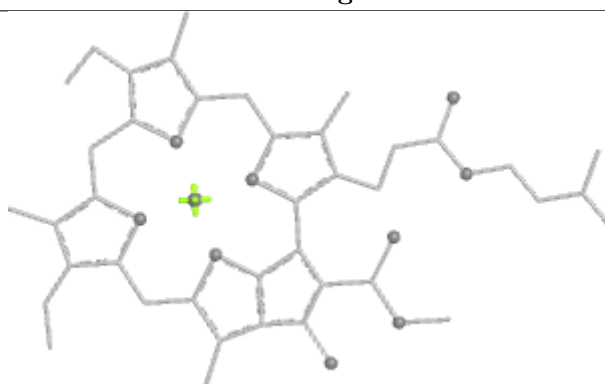
Bond lengths



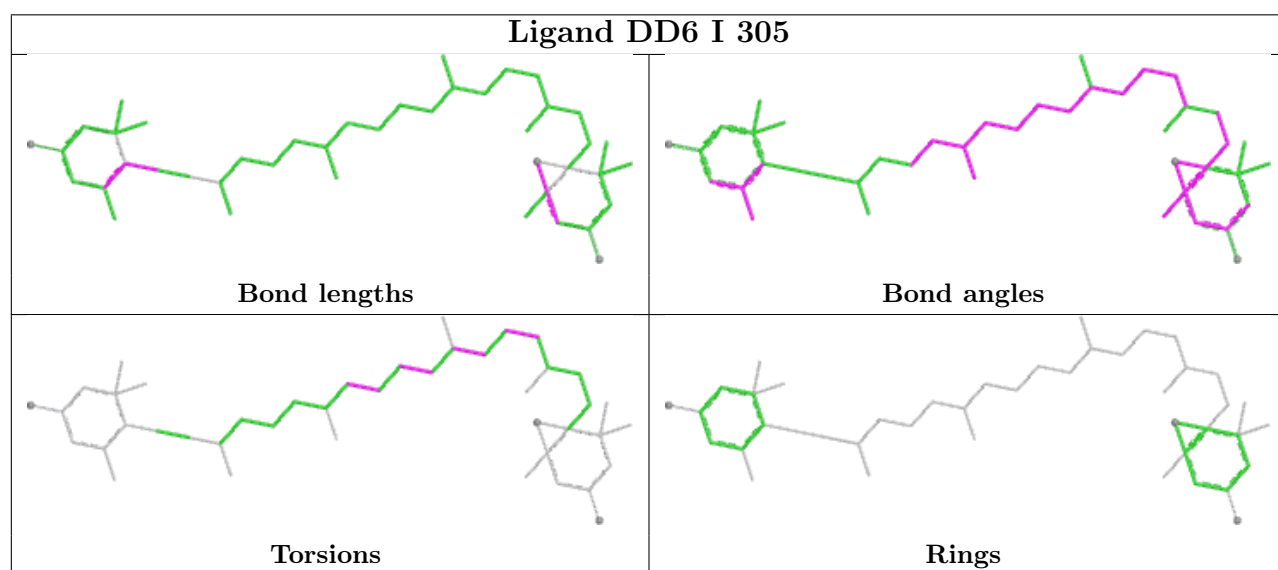
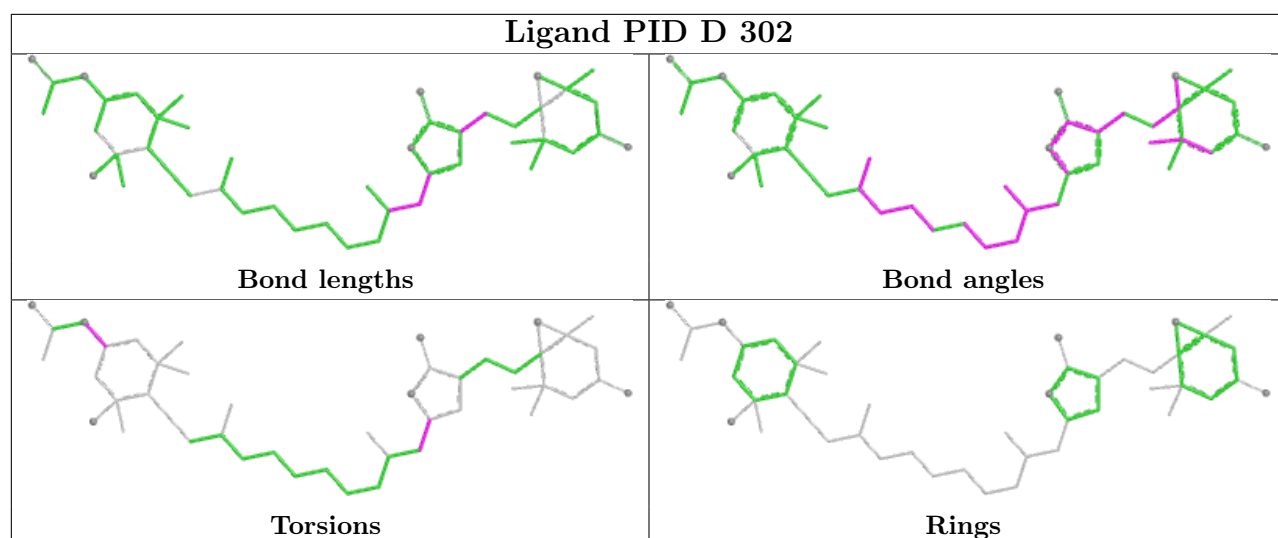
Bond angles



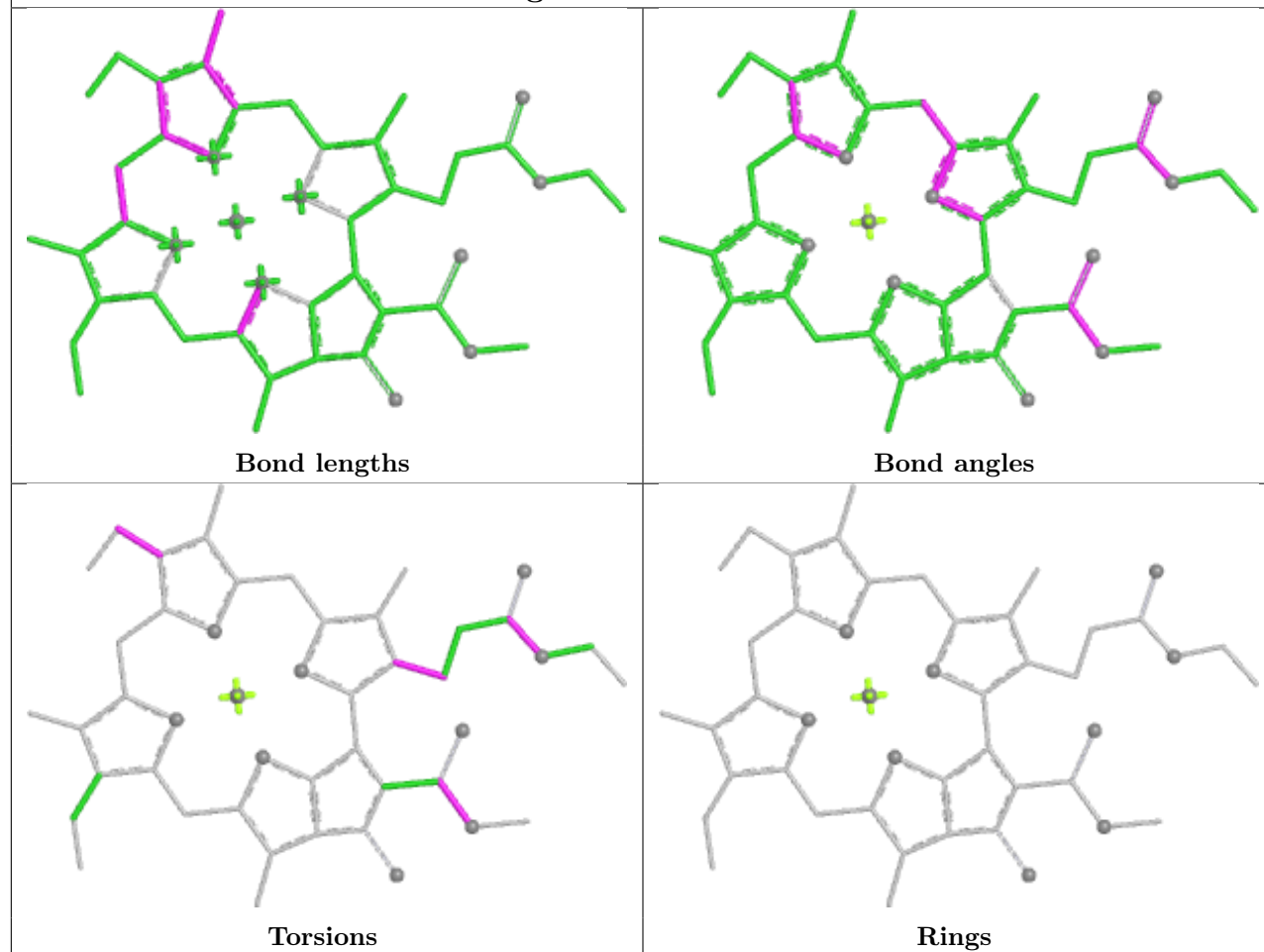
Torsions



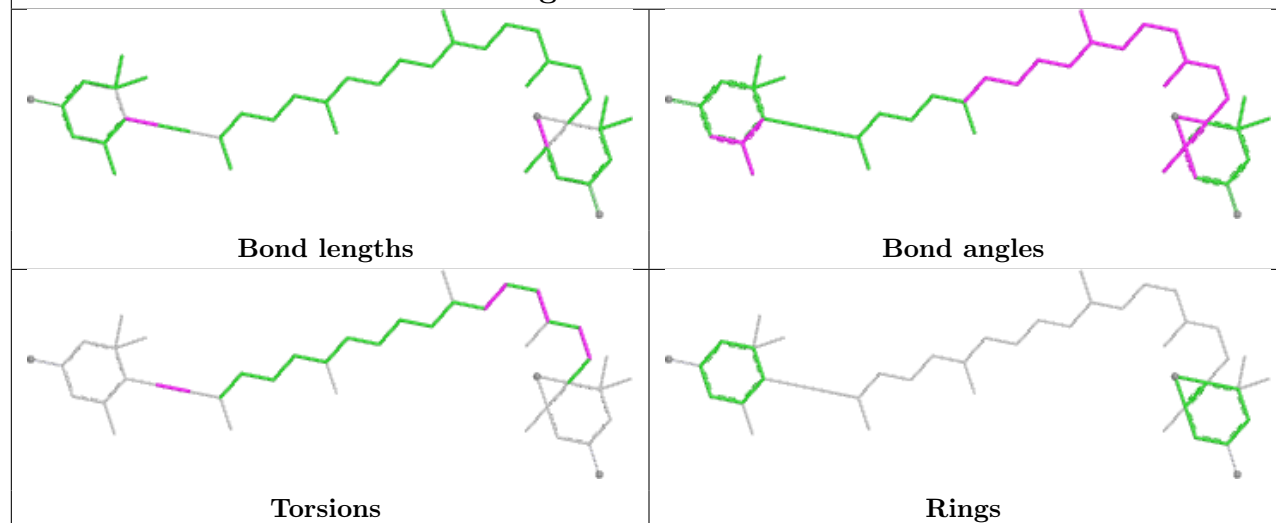
Rings

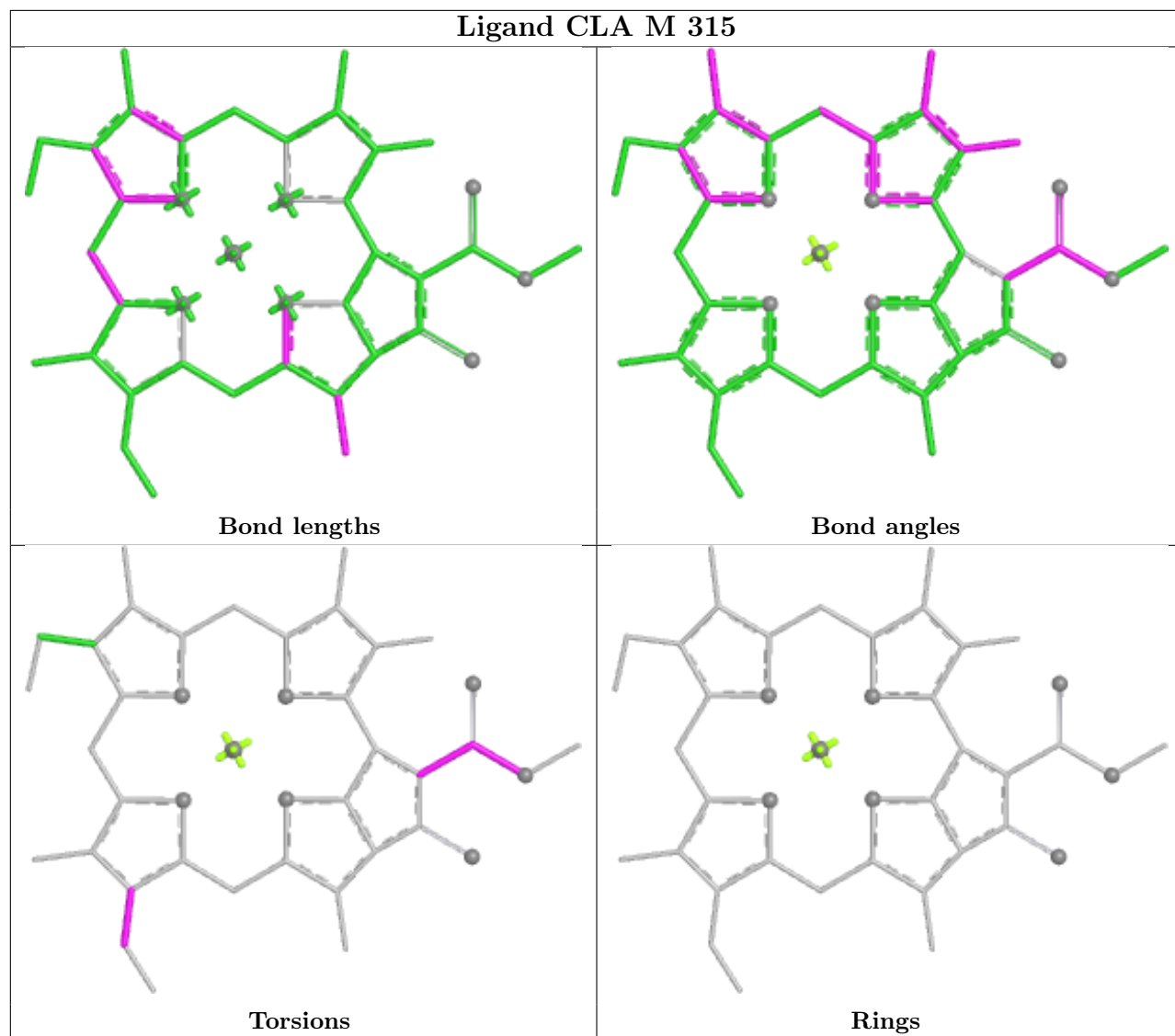


Ligand CLA H 309

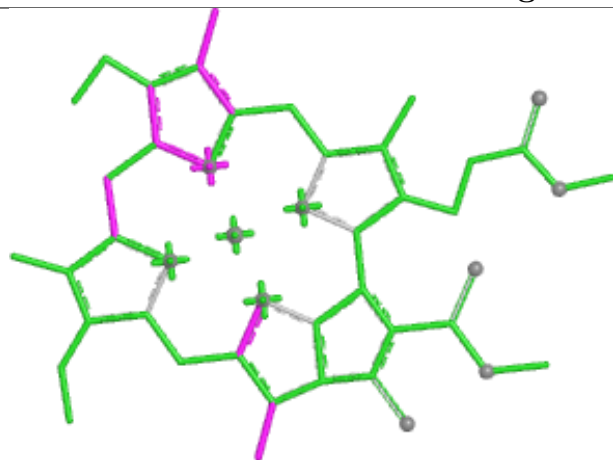


Ligand DD6 I 302

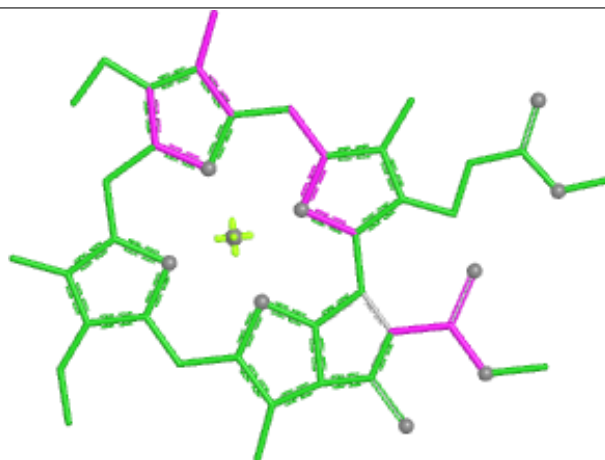




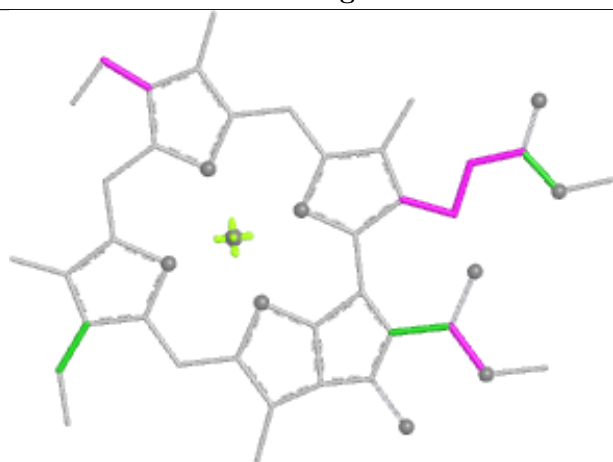
Ligand CLA J 308



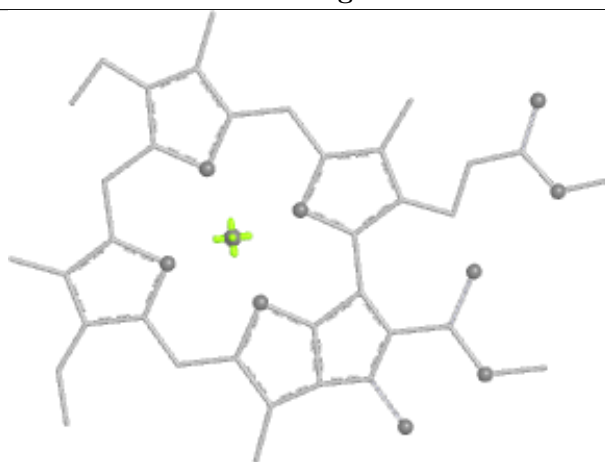
Bond lengths



Bond angles

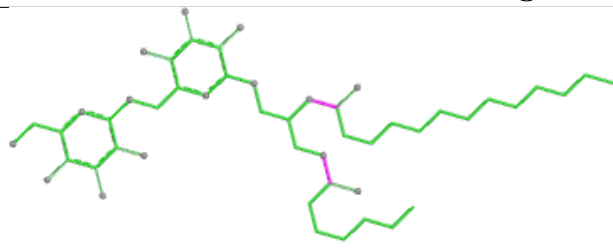


Torsions

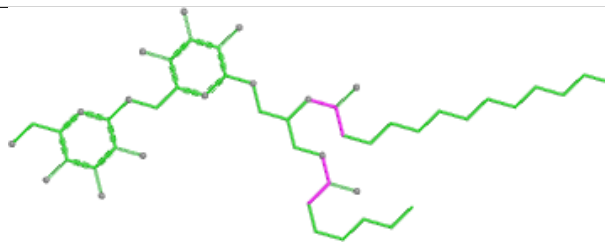


Rings

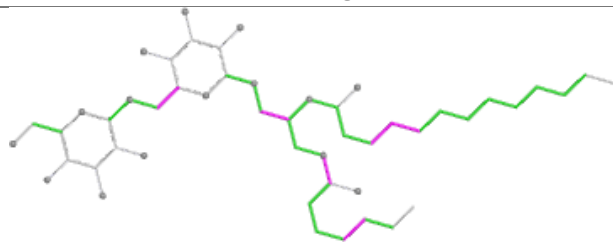
Ligand DGD 1 301



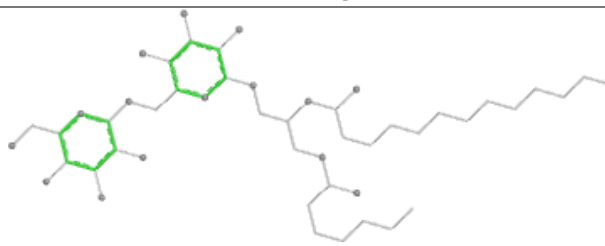
Bond lengths



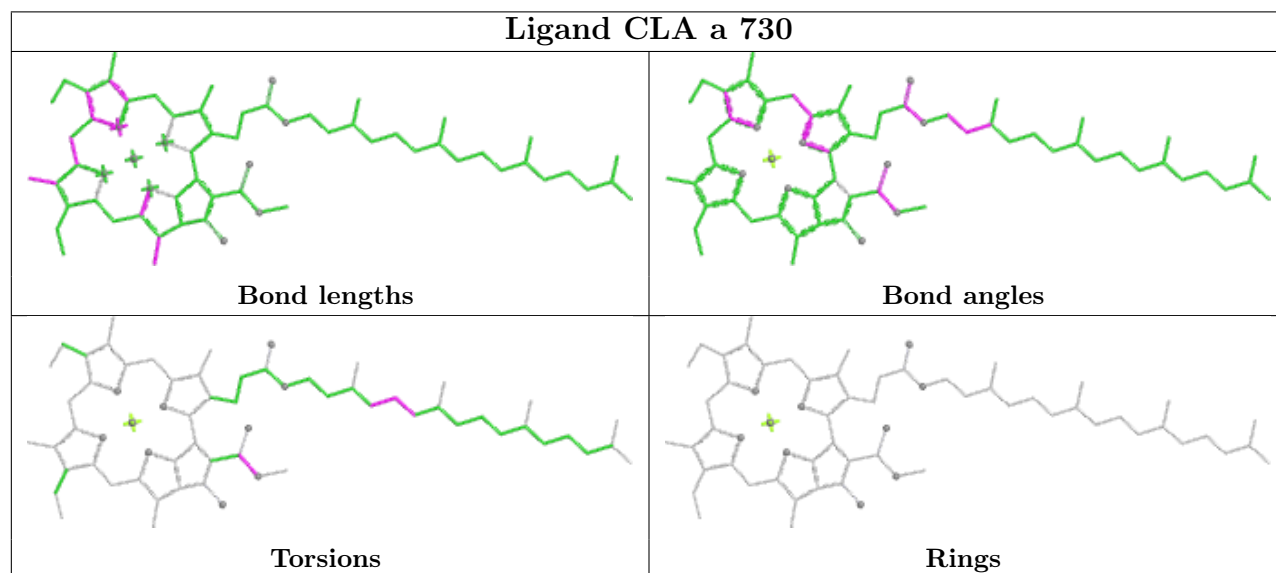
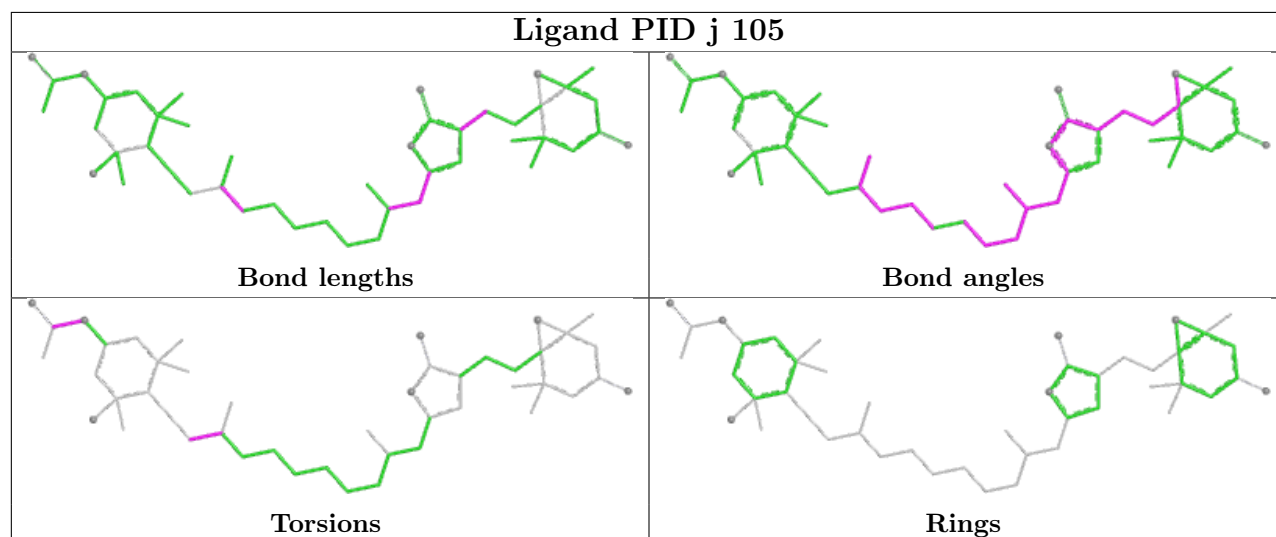
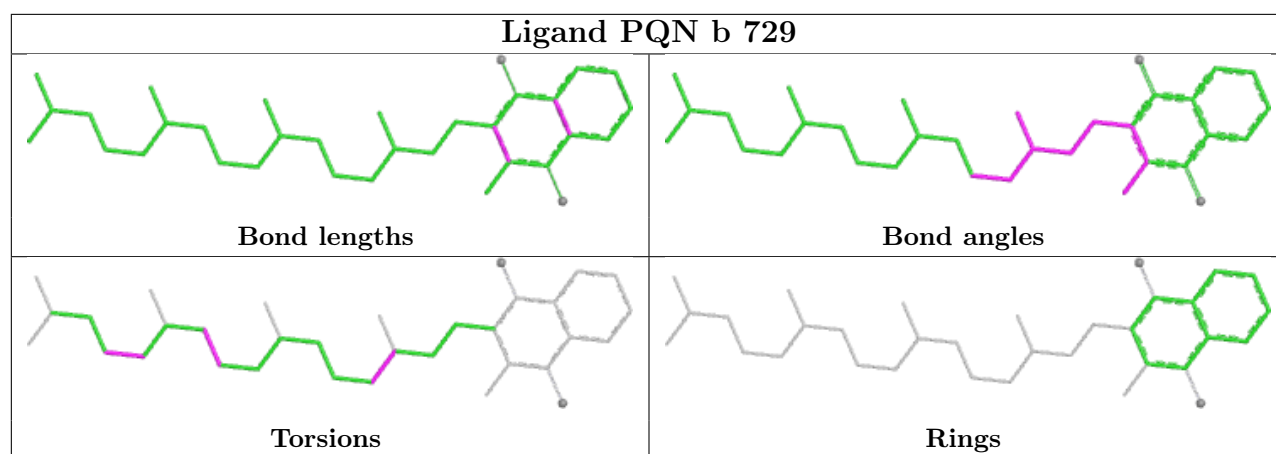
Bond angles

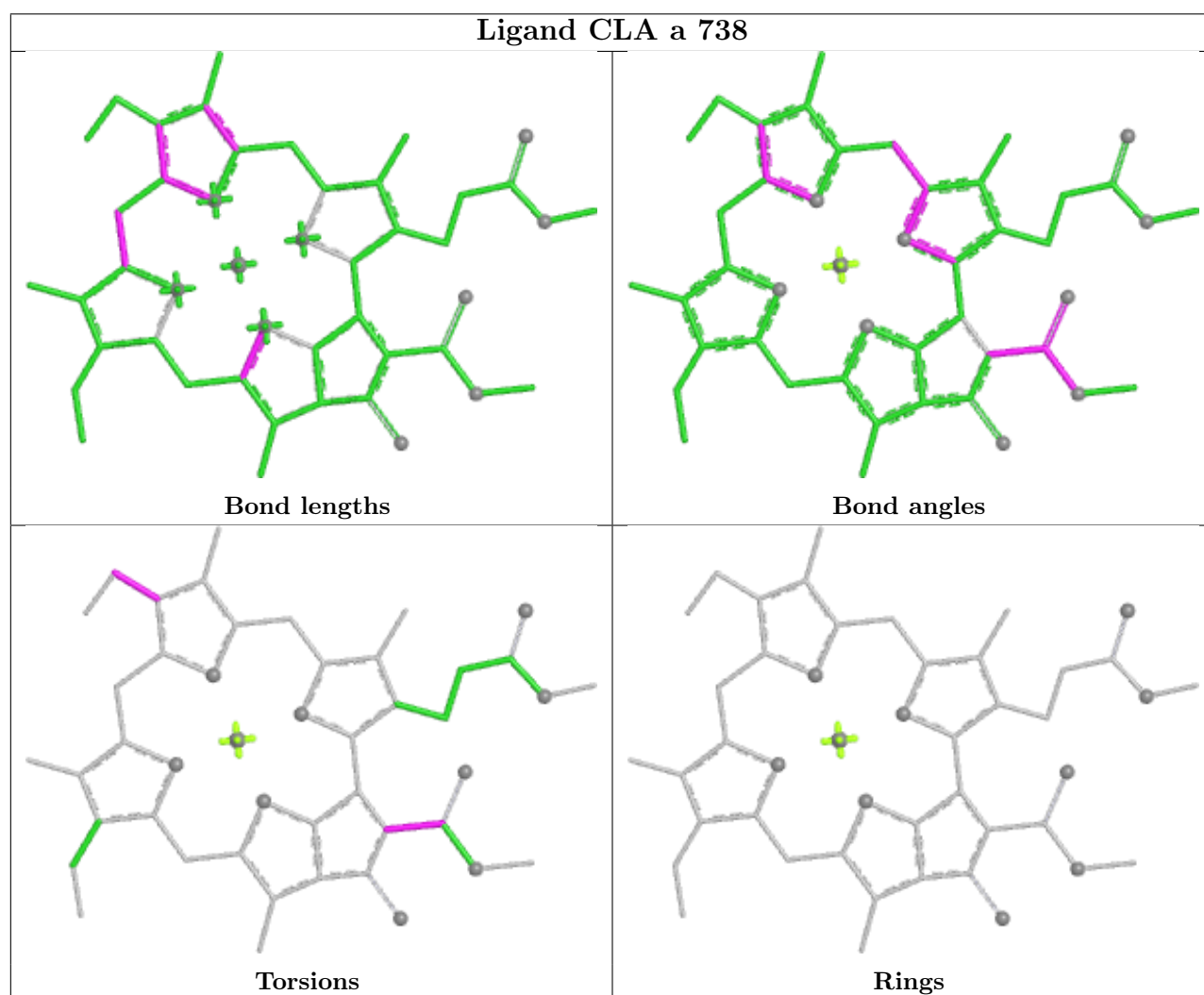
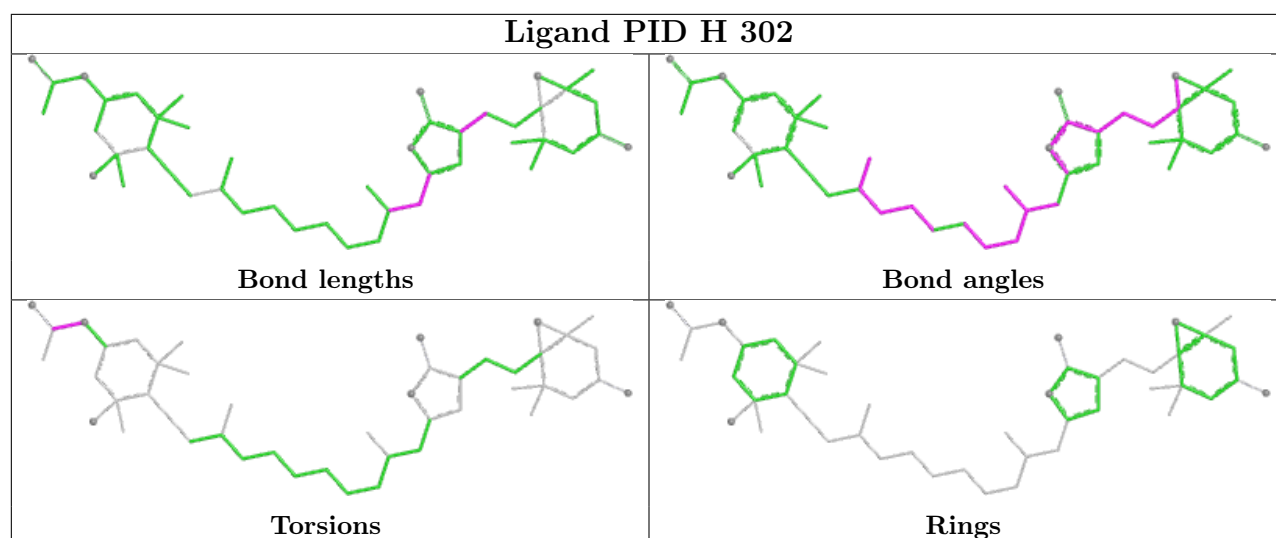


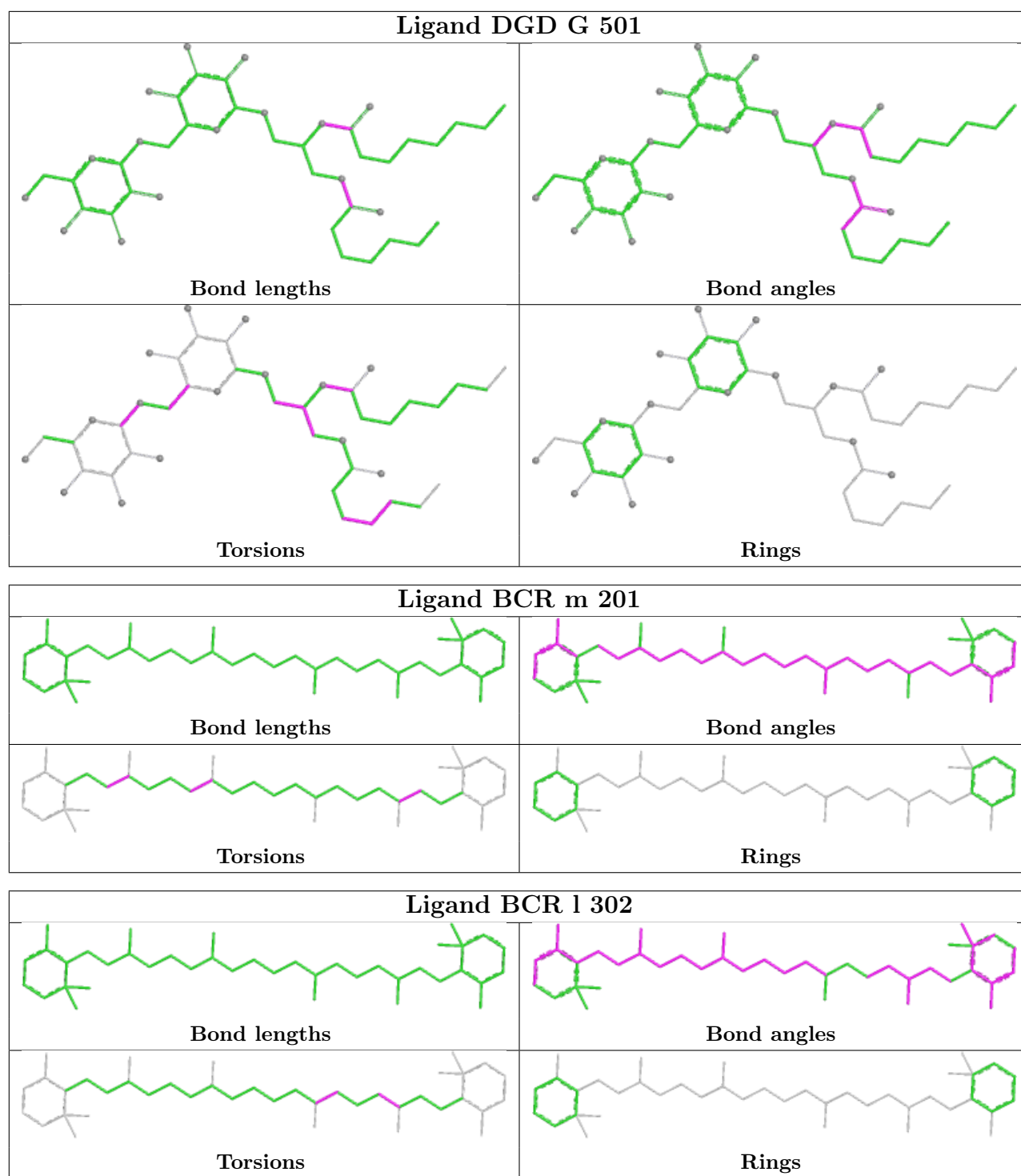
Torsions

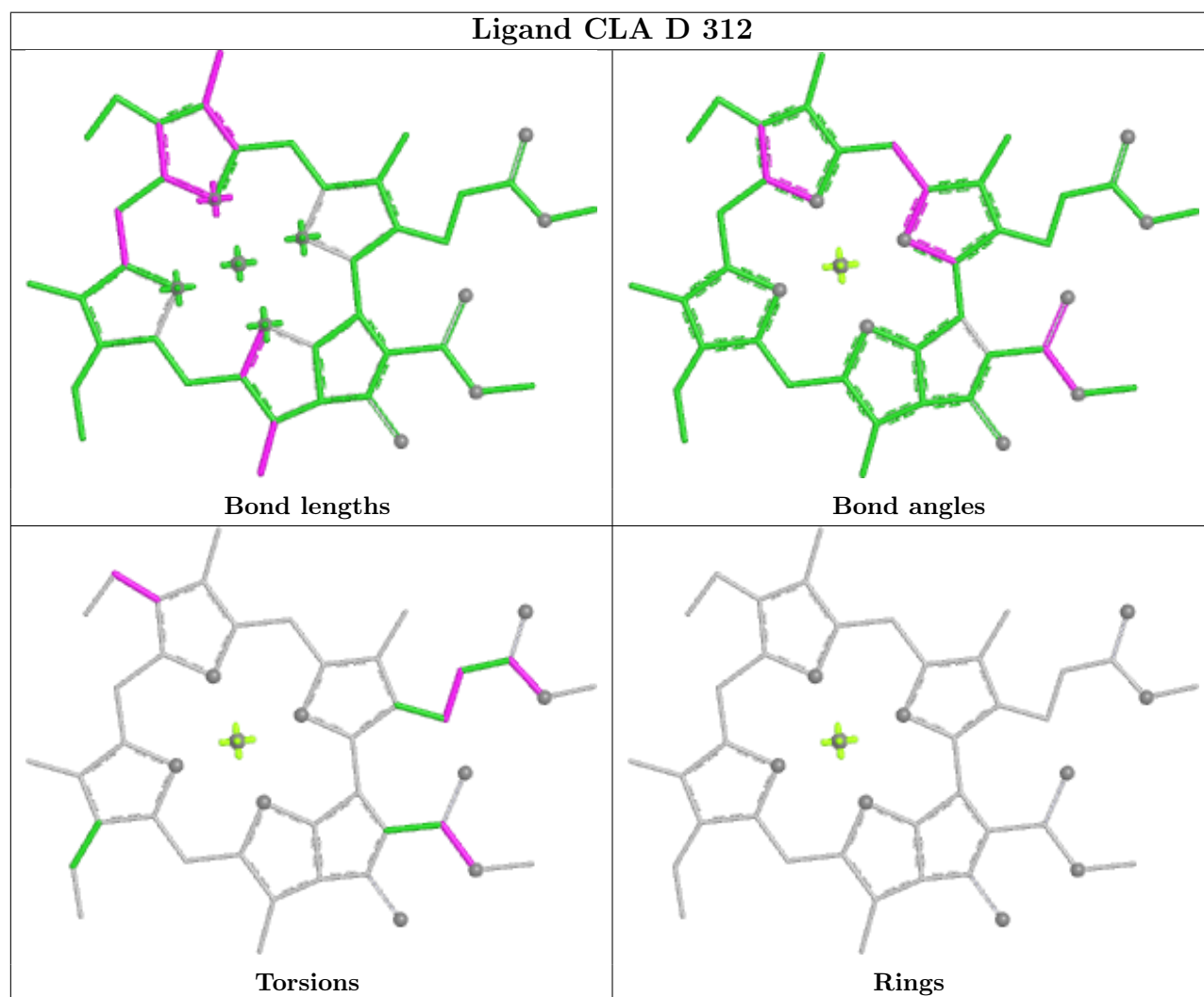
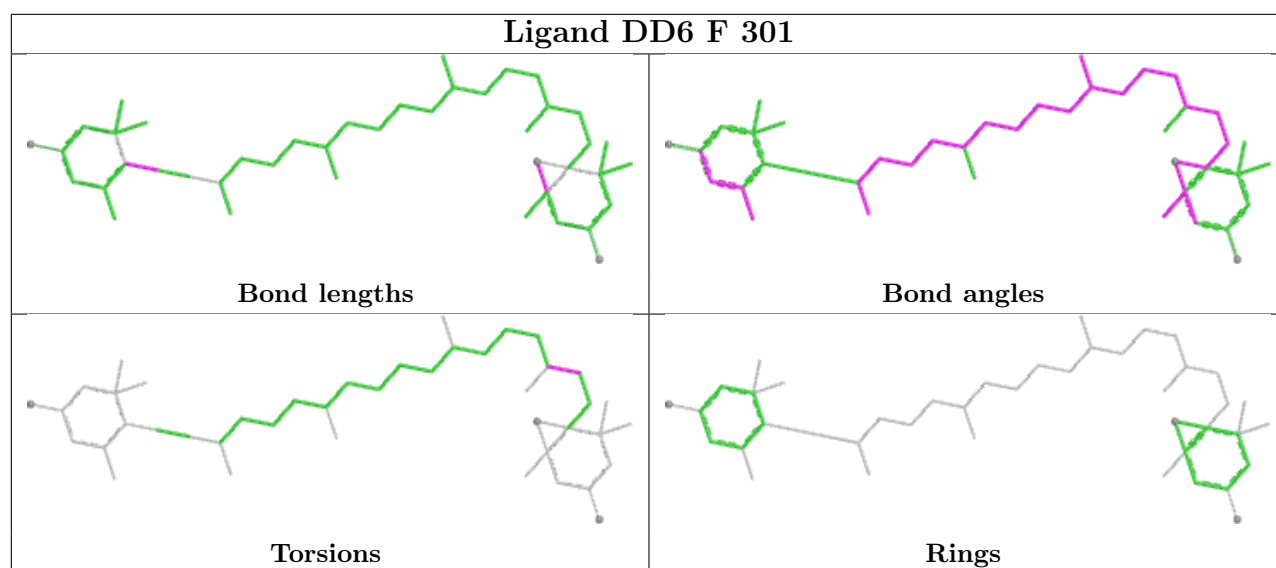


Rings

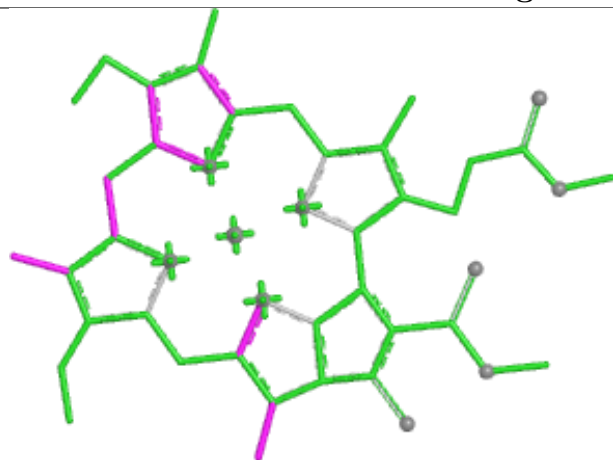




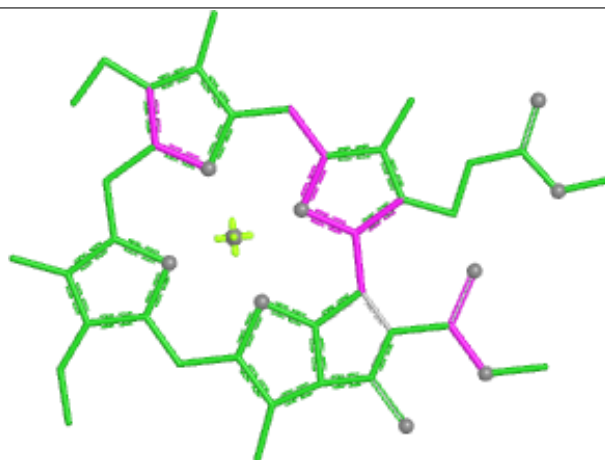




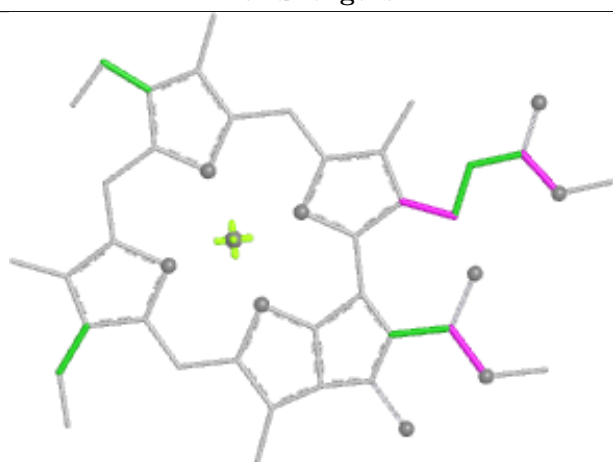
Ligand CLA F 313



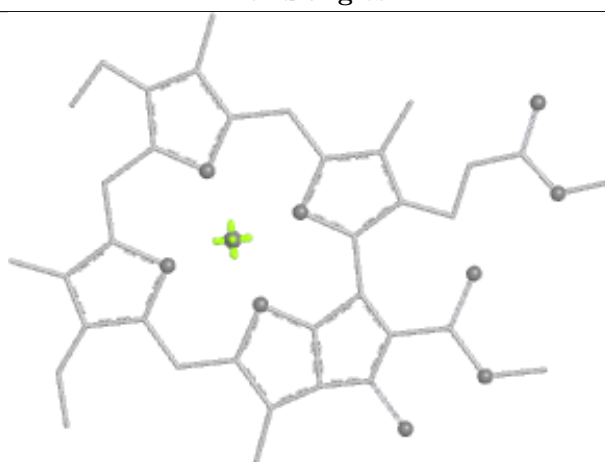
Bond lengths



Bond angles

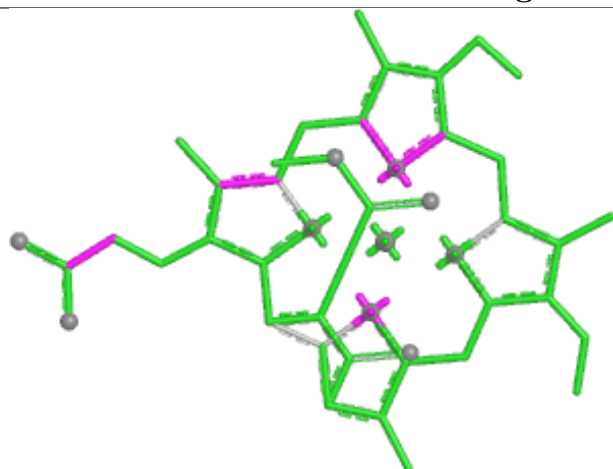


Torsions

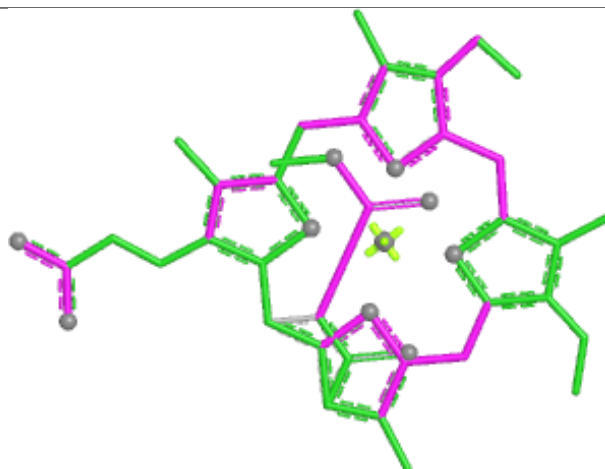


Rings

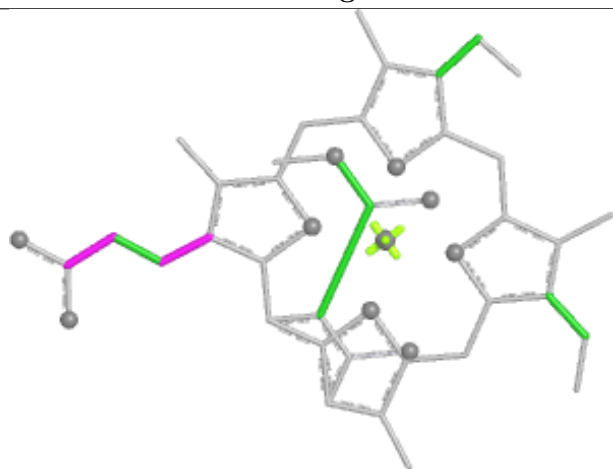
Ligand KC1 D 315



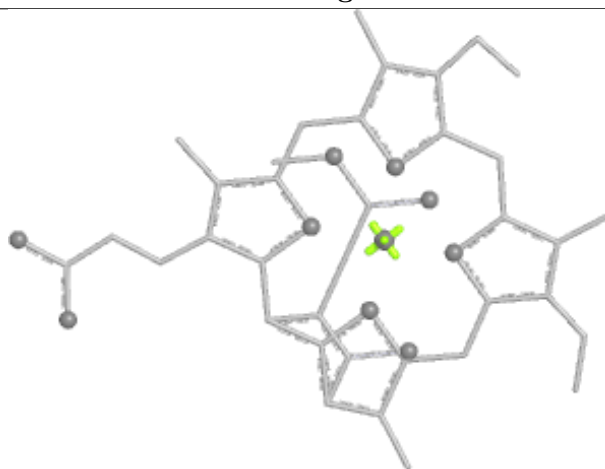
Bond lengths



Bond angles

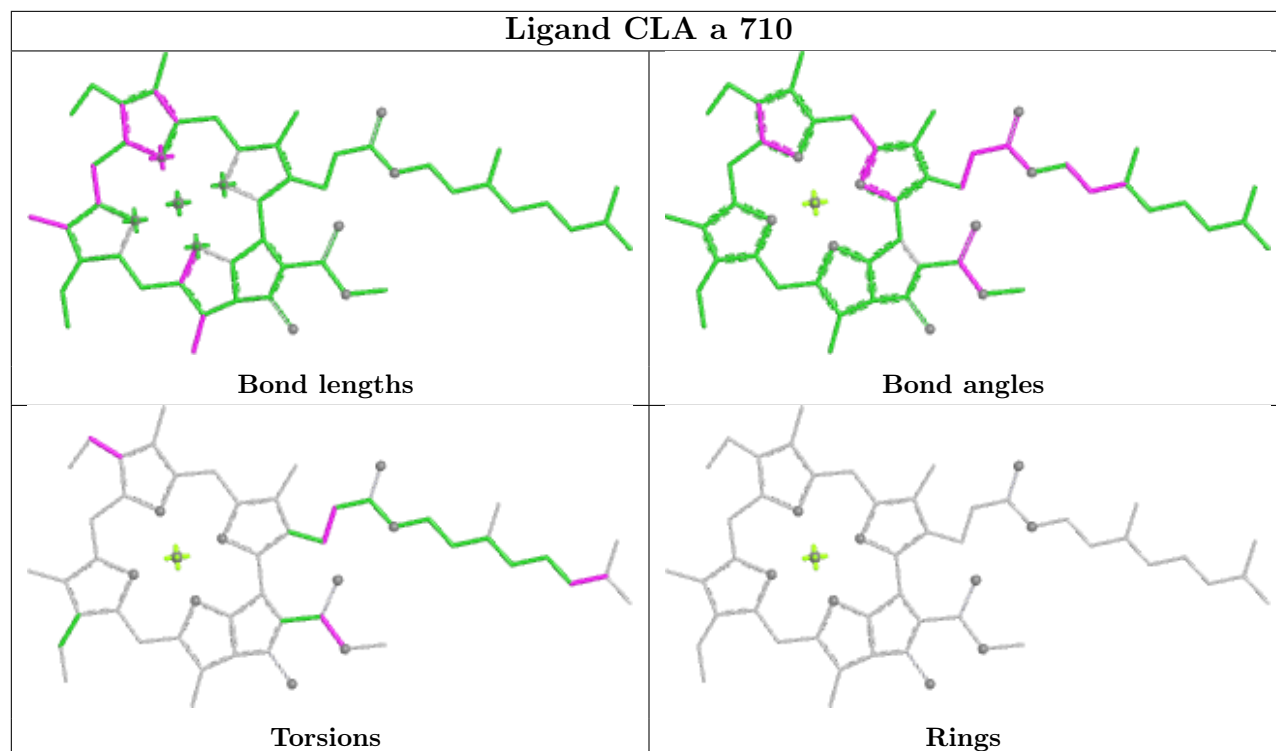


Torsions

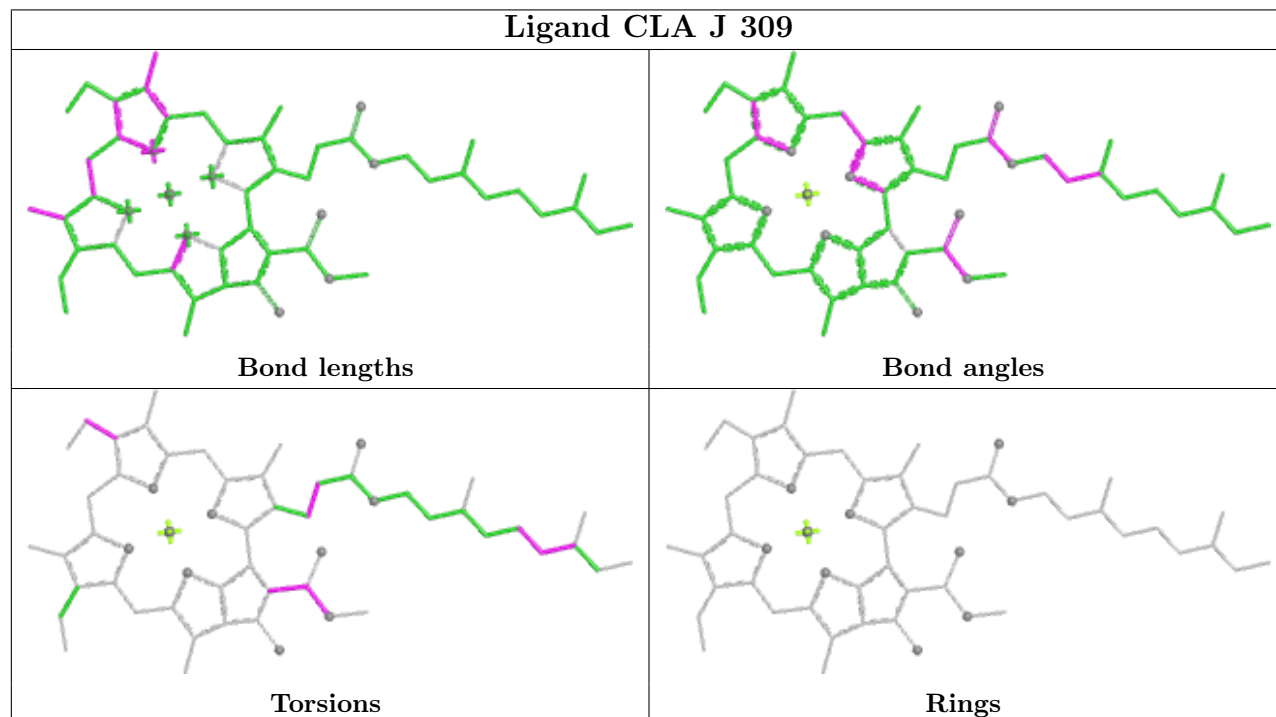


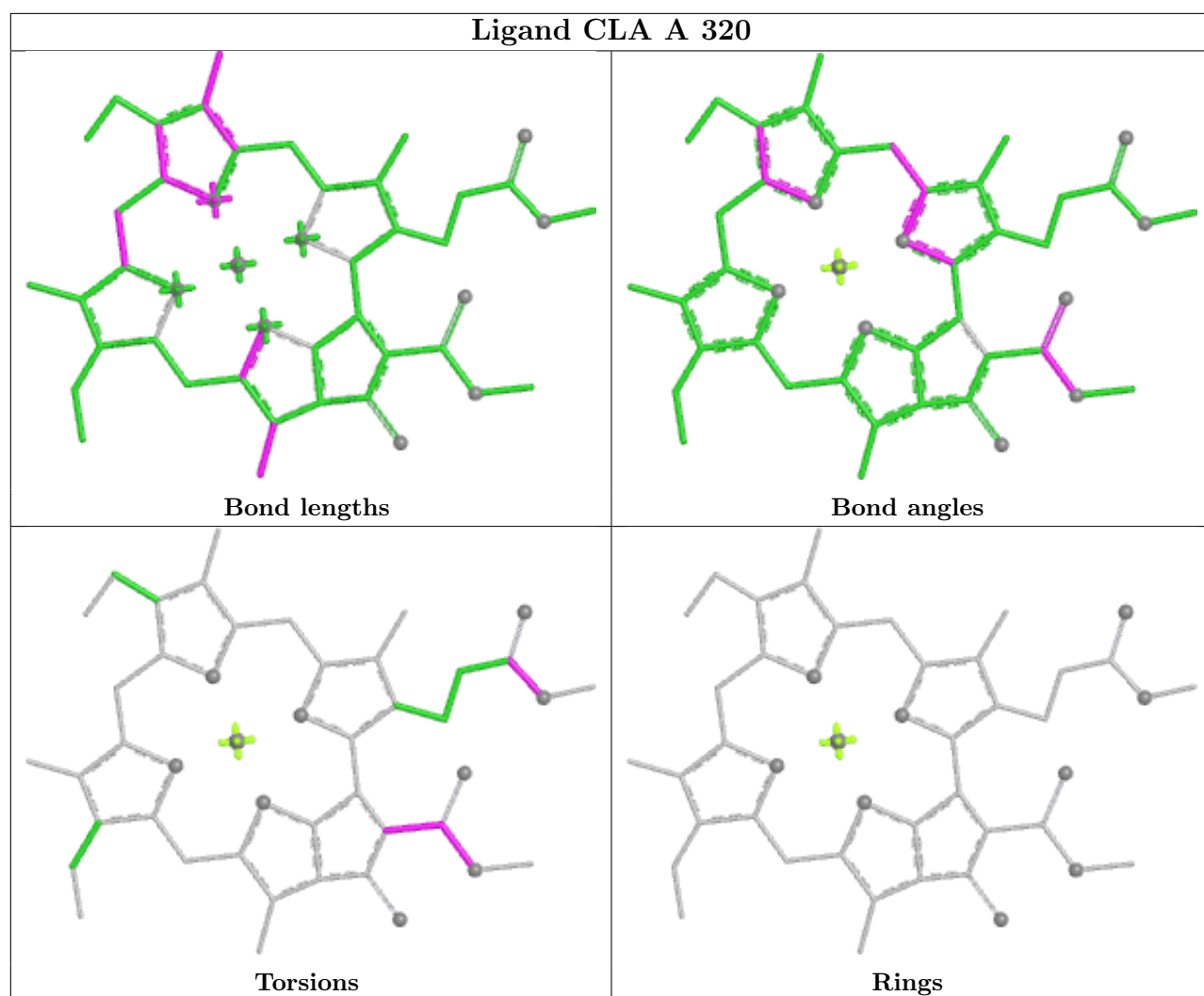
Rings

Ligand CLA a 710

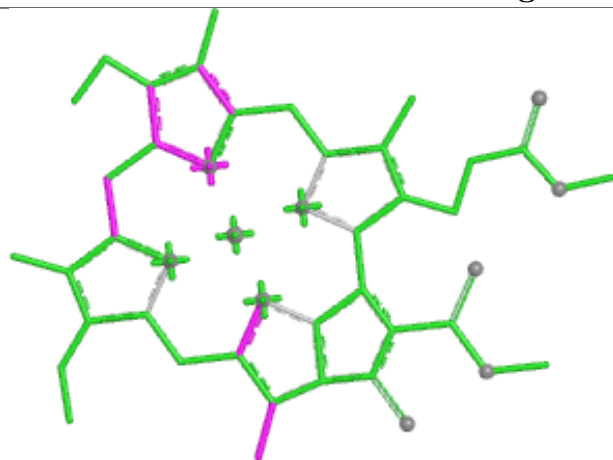


Ligand CLA J 309

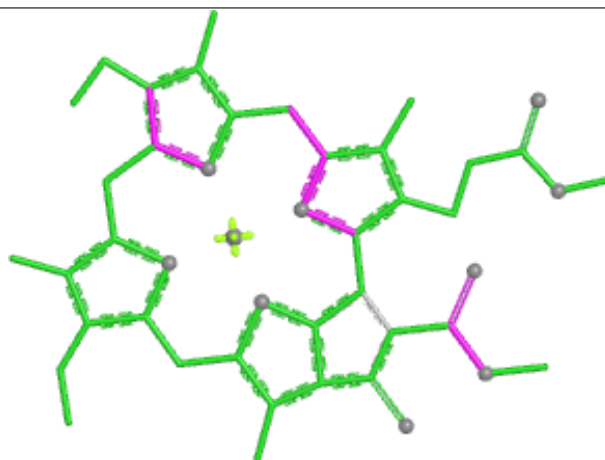




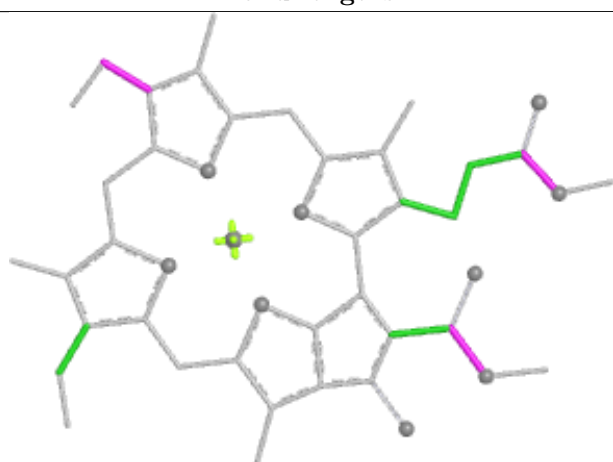
Ligand CLA J 306



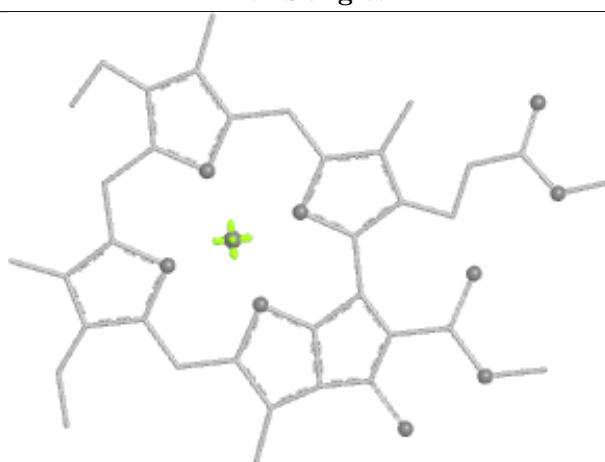
Bond lengths



Bond angles

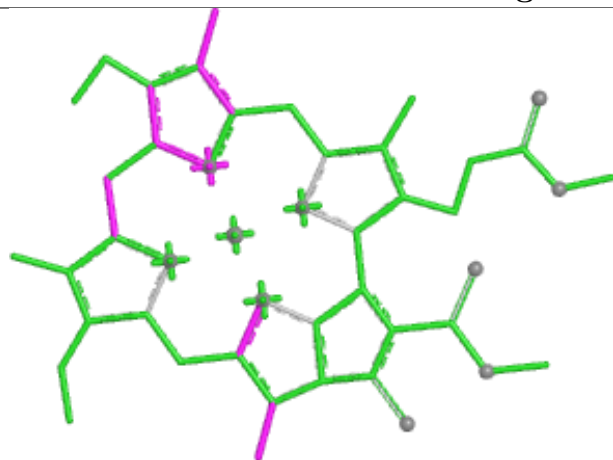


Torsions

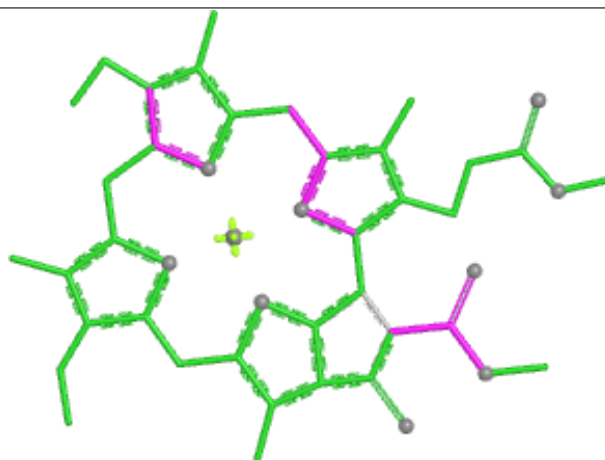


Rings

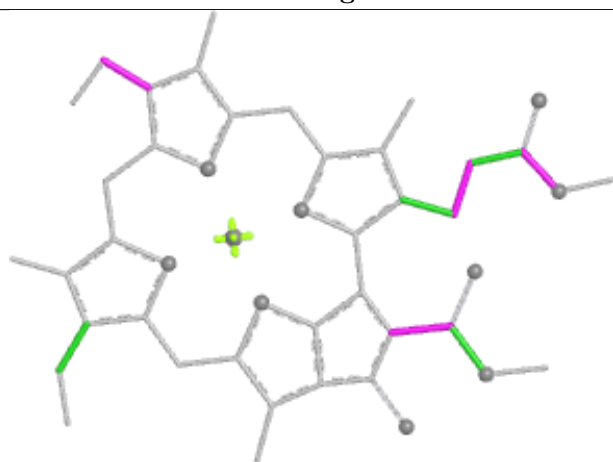
Ligand CLA F 311



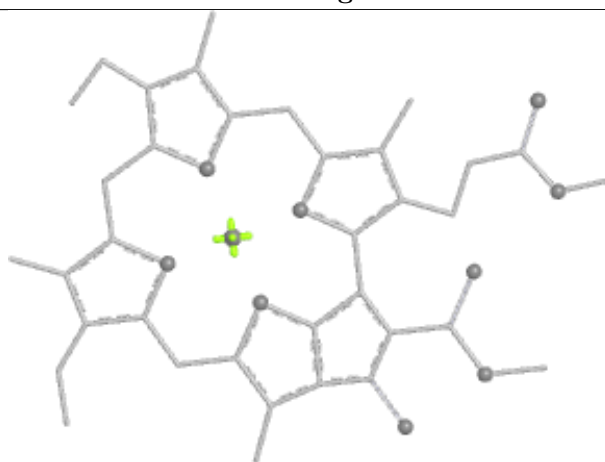
Bond lengths



Bond angles

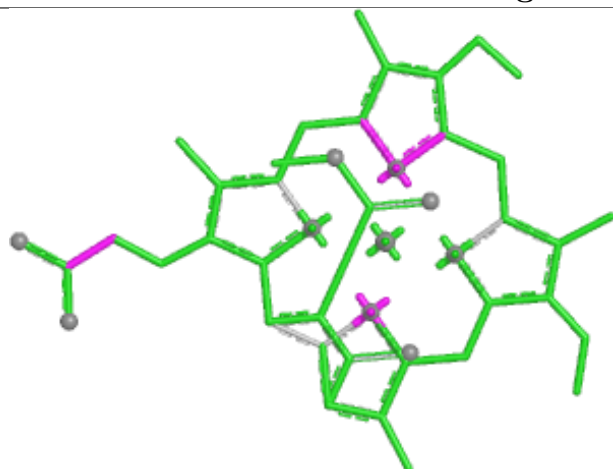


Torsions

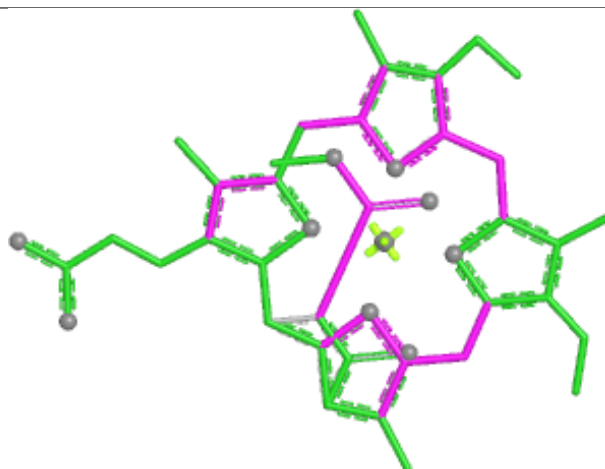


Rings

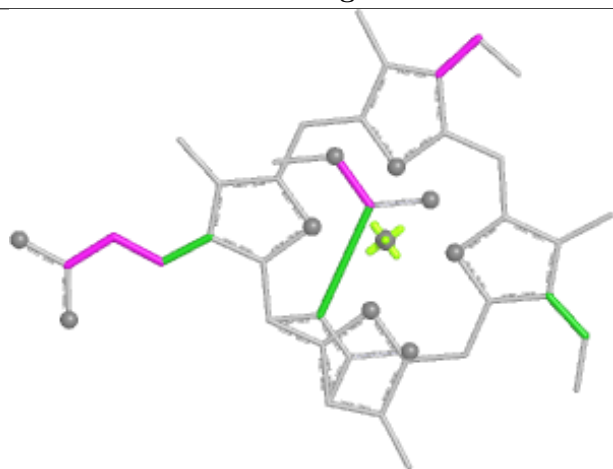
Ligand KC1 B 314



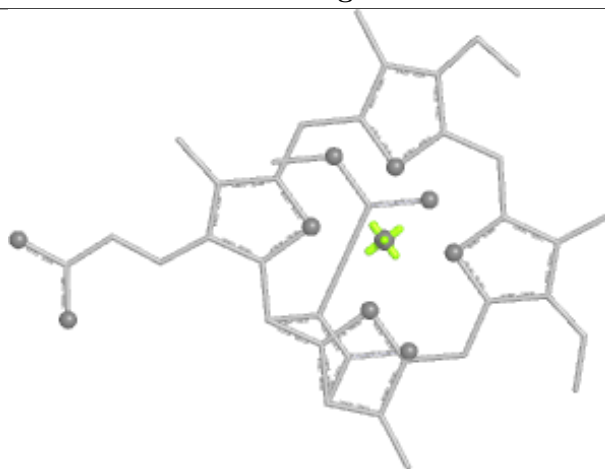
Bond lengths



Bond angles

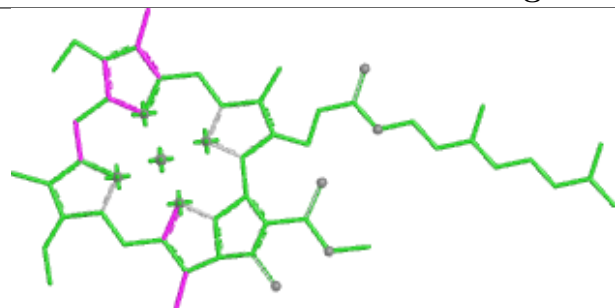


Torsions

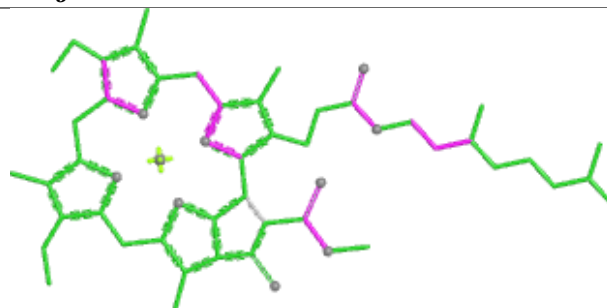


Rings

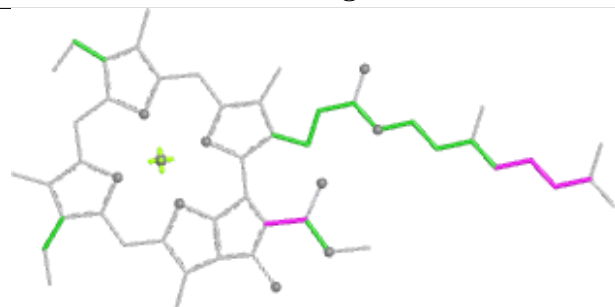
Ligand CLA j 104



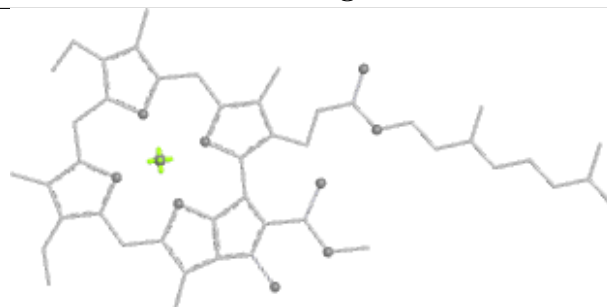
Bond lengths



Bond angles

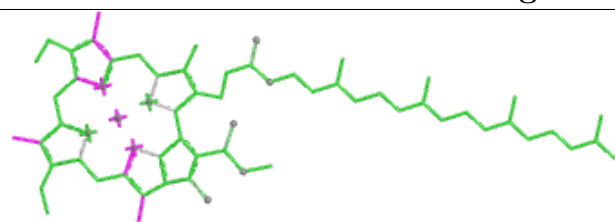


Torsions

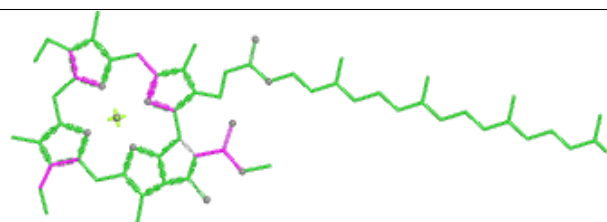


Rings

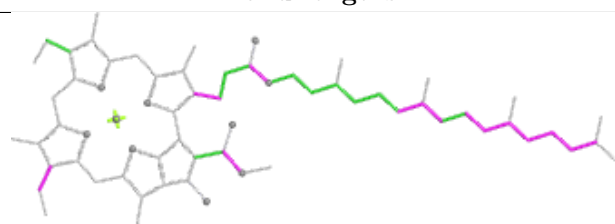
Ligand CLA b 704



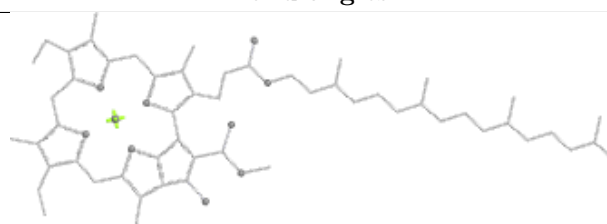
Bond lengths



Bond angles

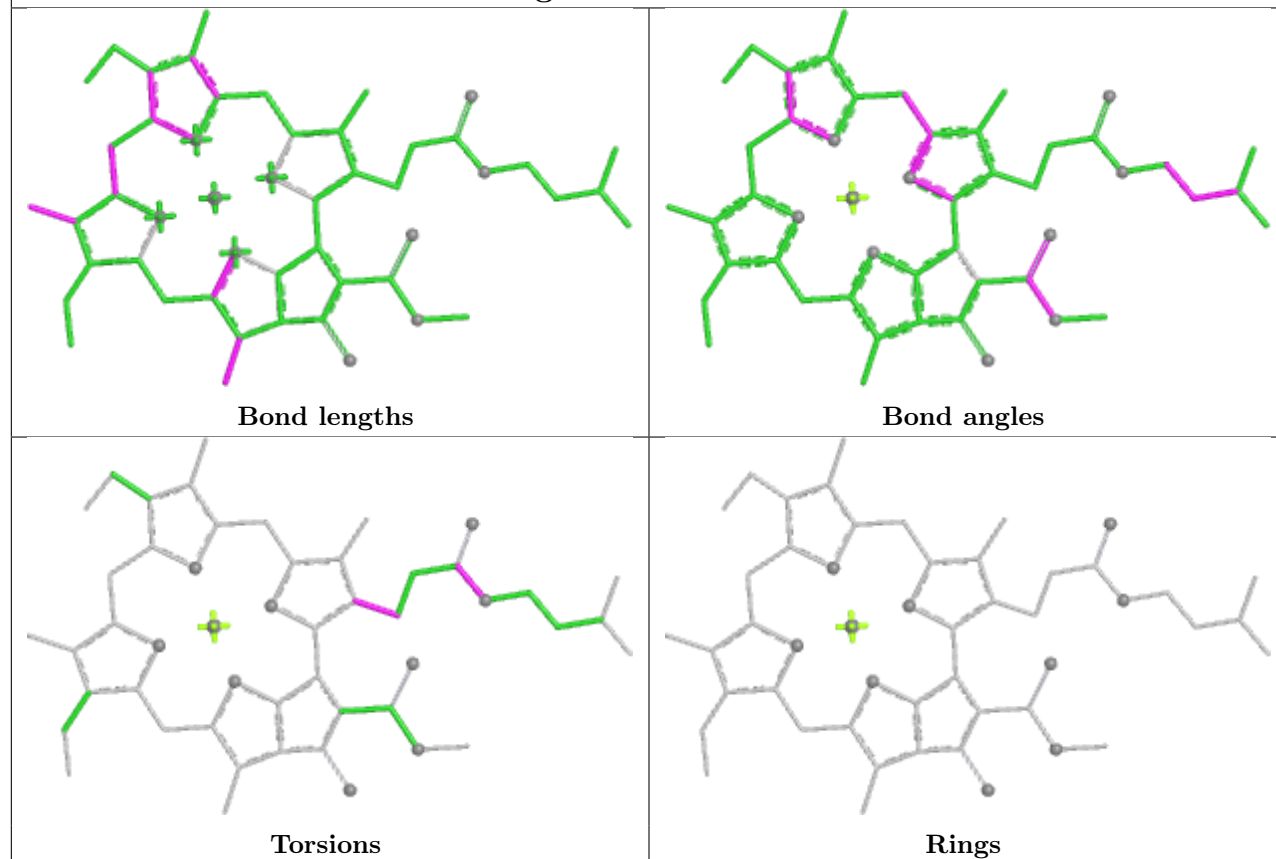


Torsions

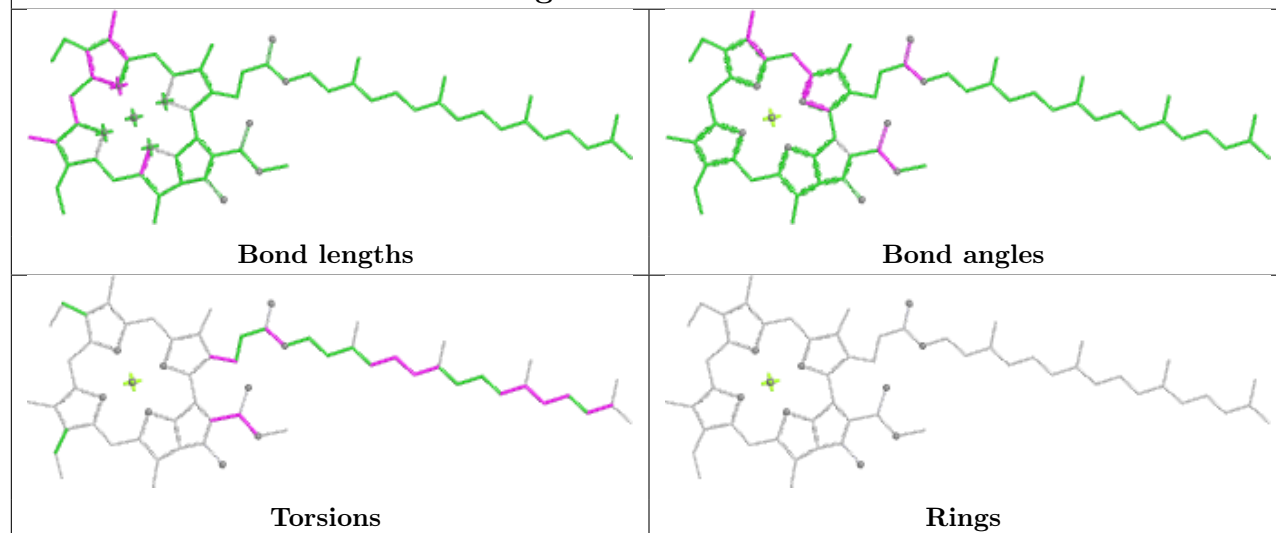


Rings

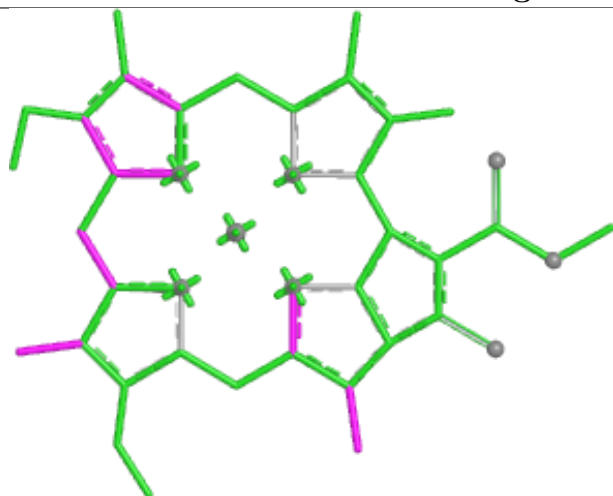
Ligand CLA b 716



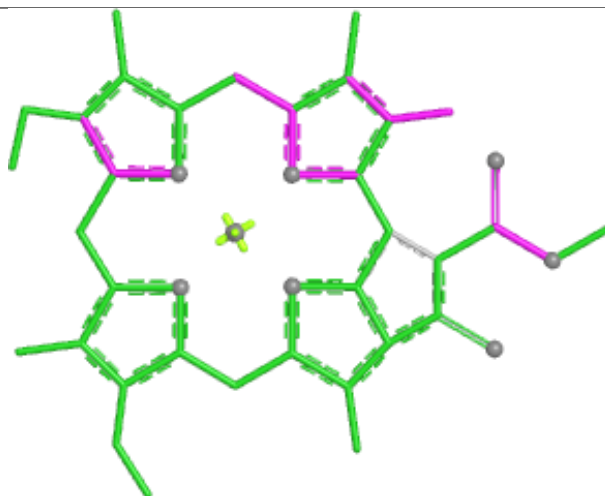
Ligand CLA b 717



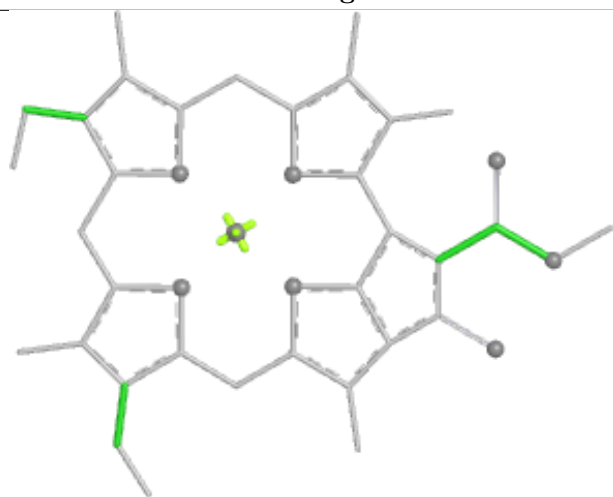
Ligand CLA D 316



Bond lengths



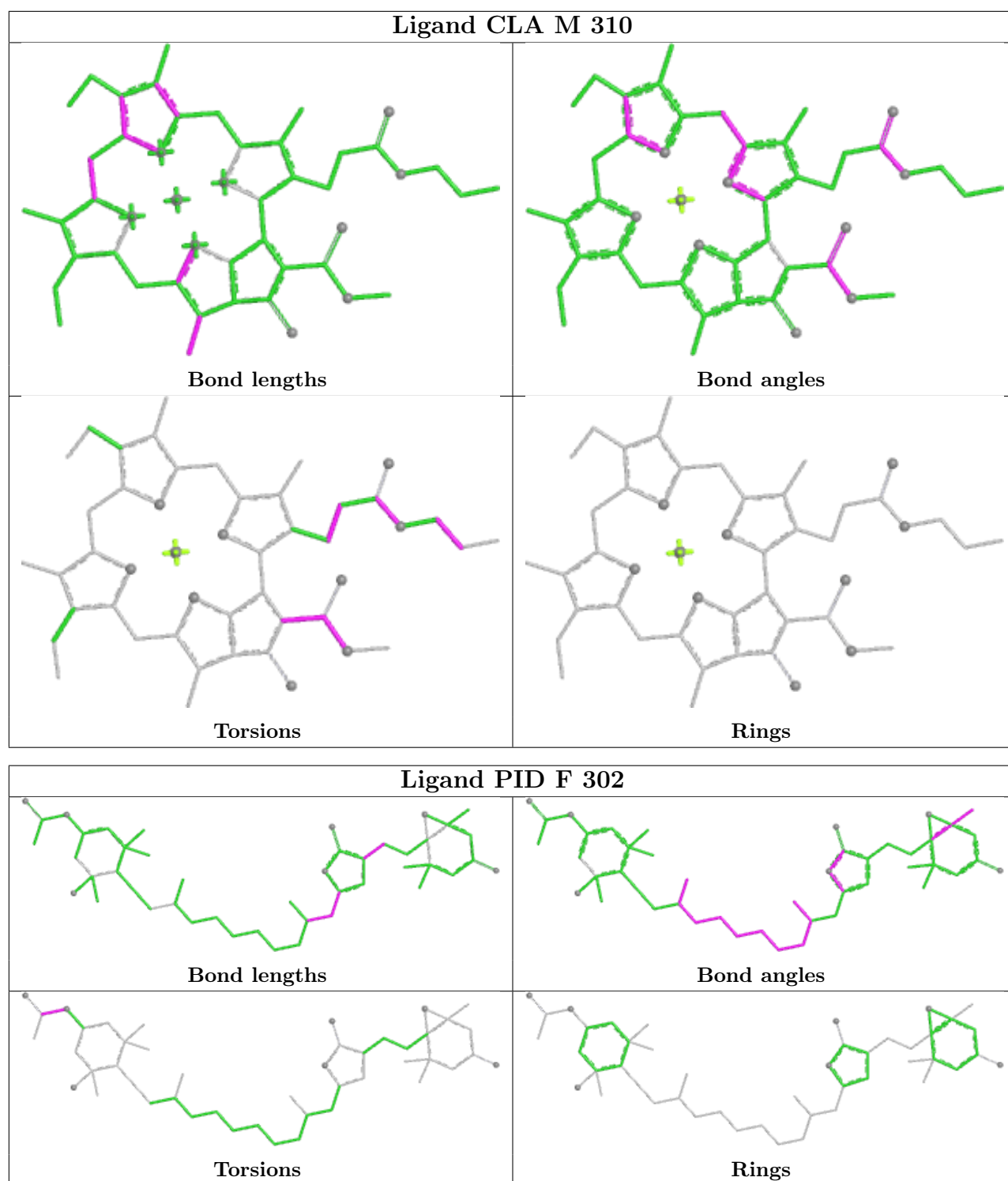
Bond angles

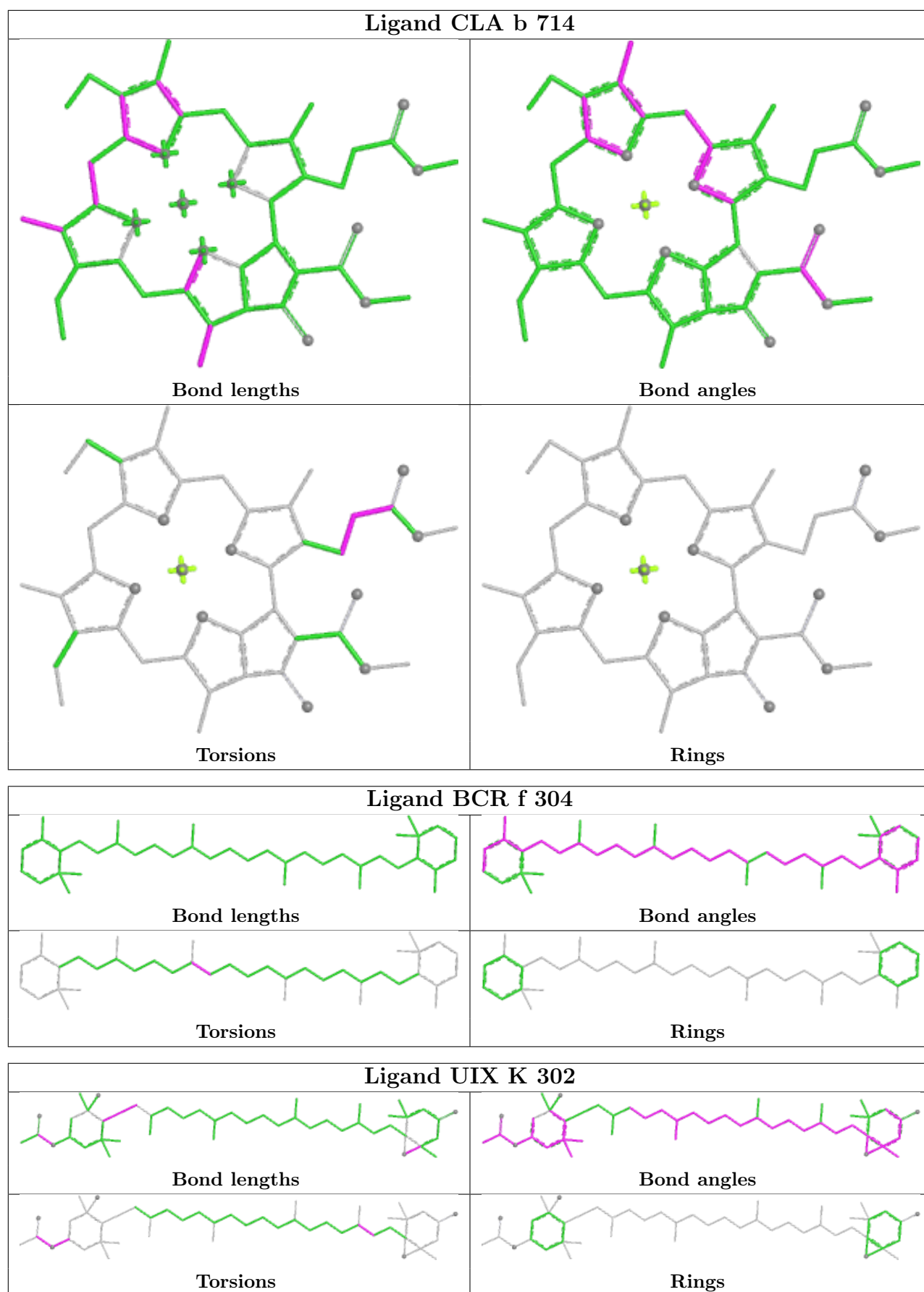


Torsions

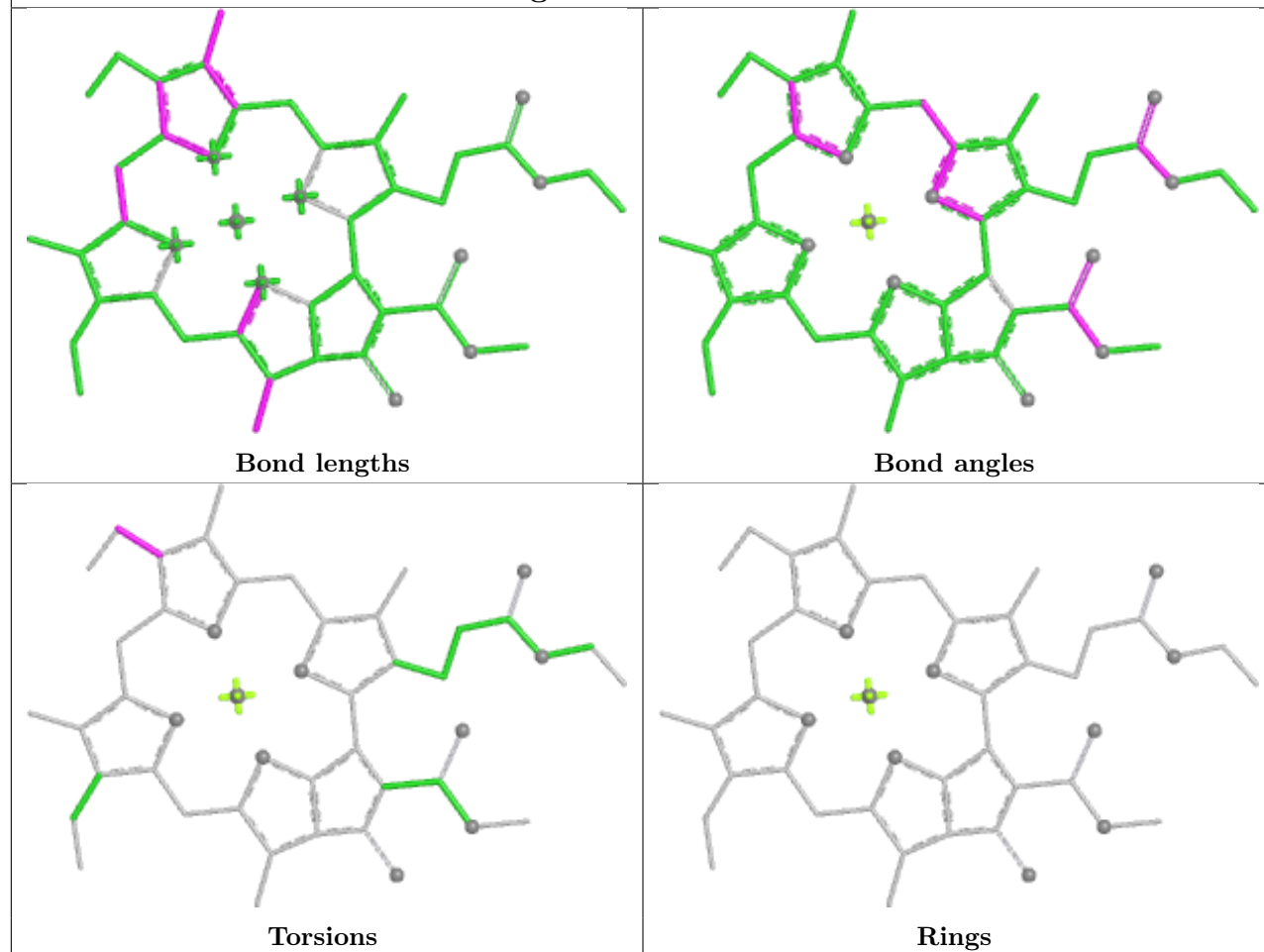


Rings

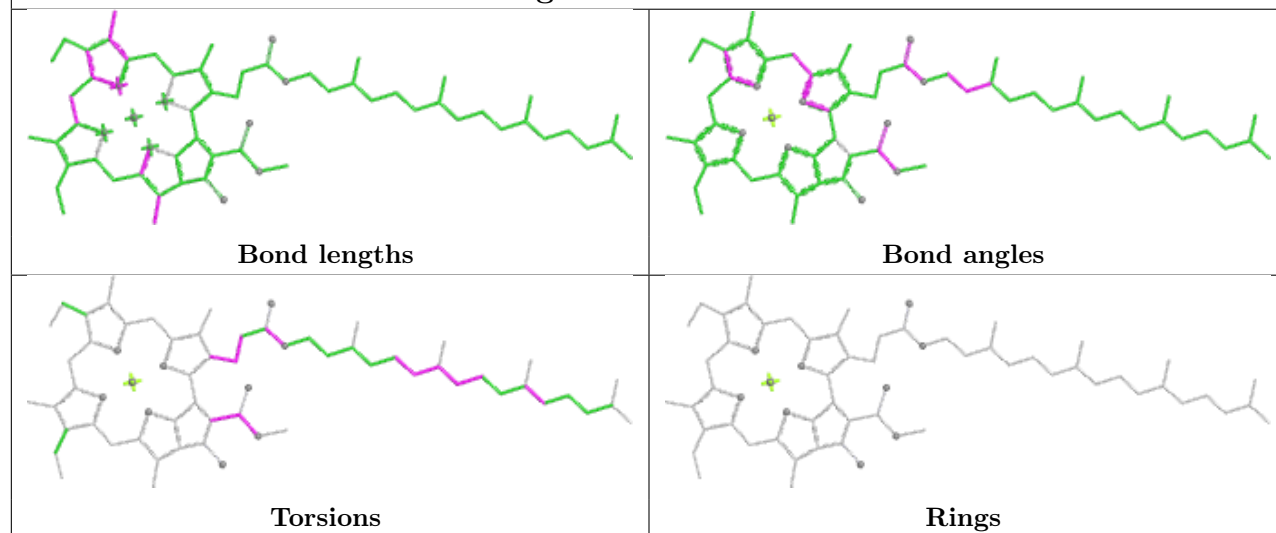


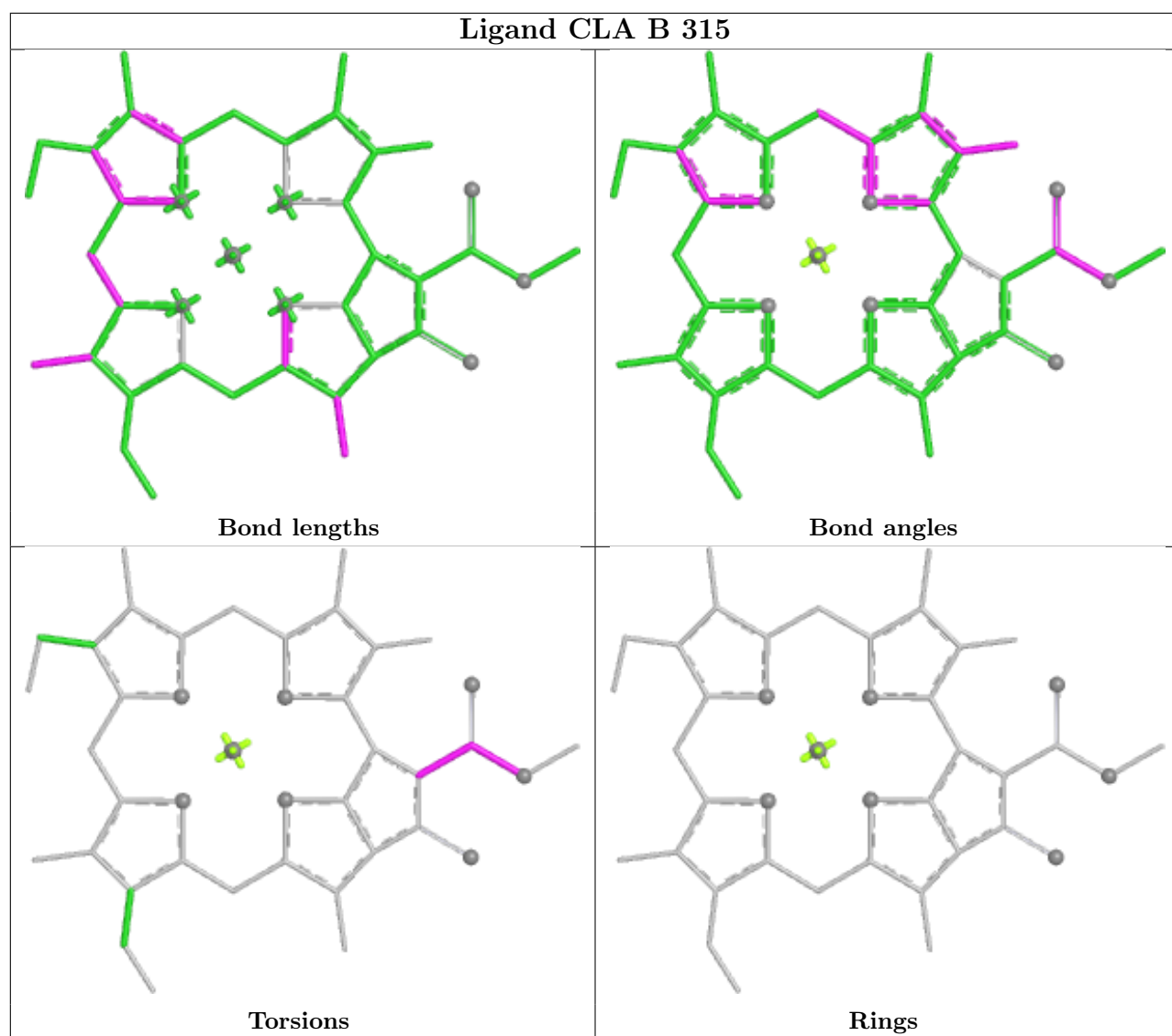


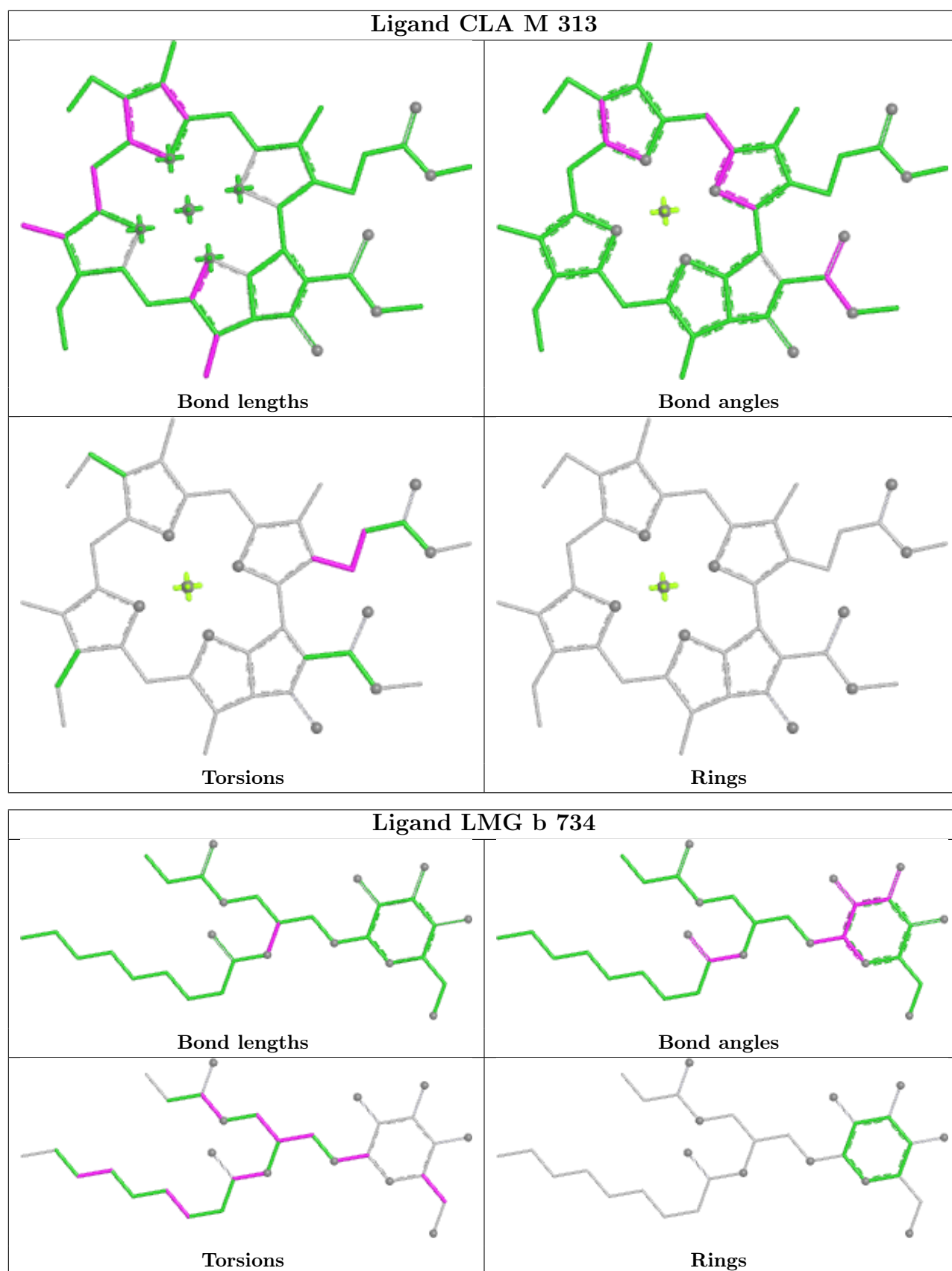
Ligand CLA b 726



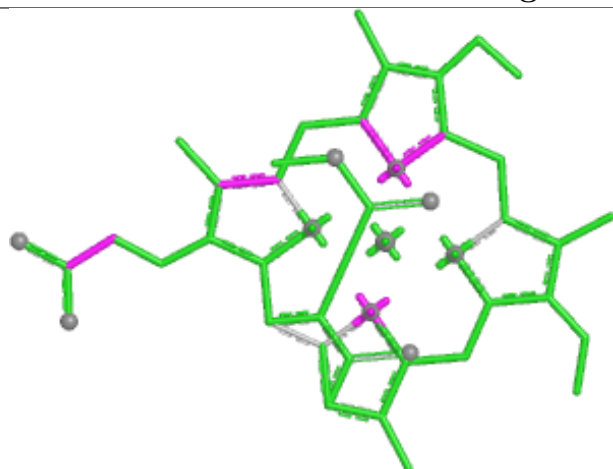
Ligand CLA a 709



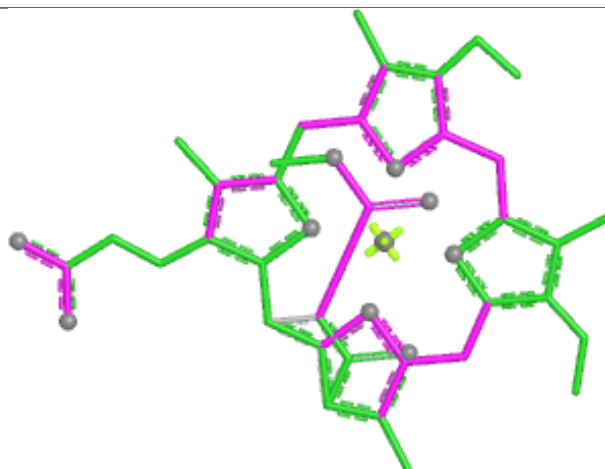




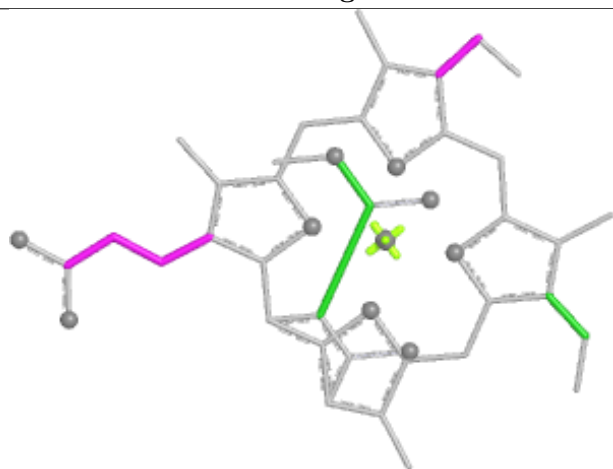
Ligand KC1 J 313



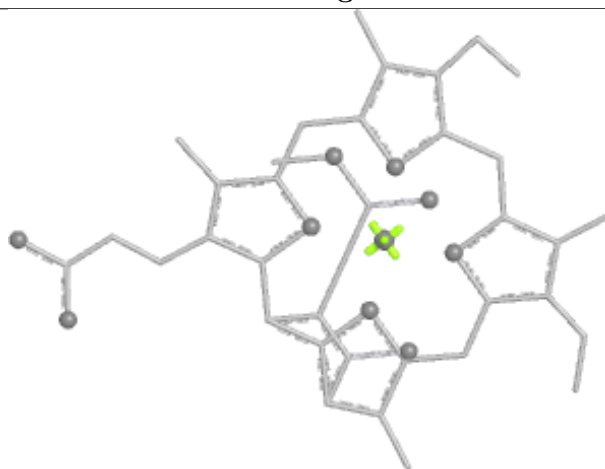
Bond lengths



Bond angles

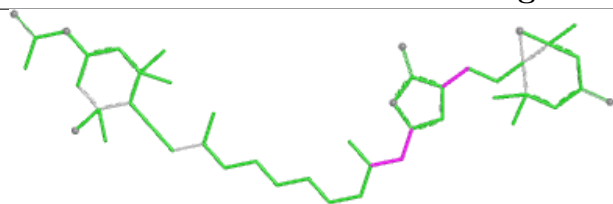


Torsions

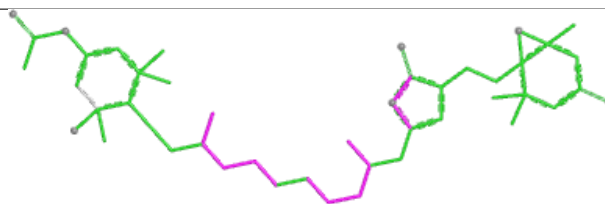


Rings

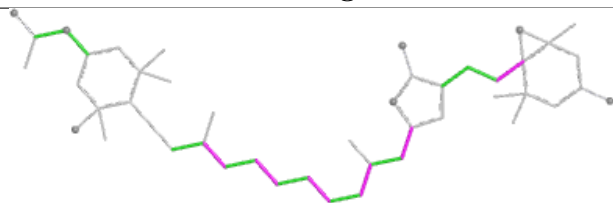
Ligand PID D 306



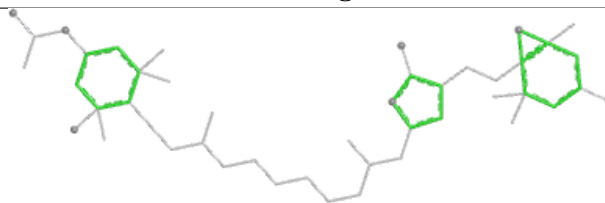
Bond lengths



Bond angles

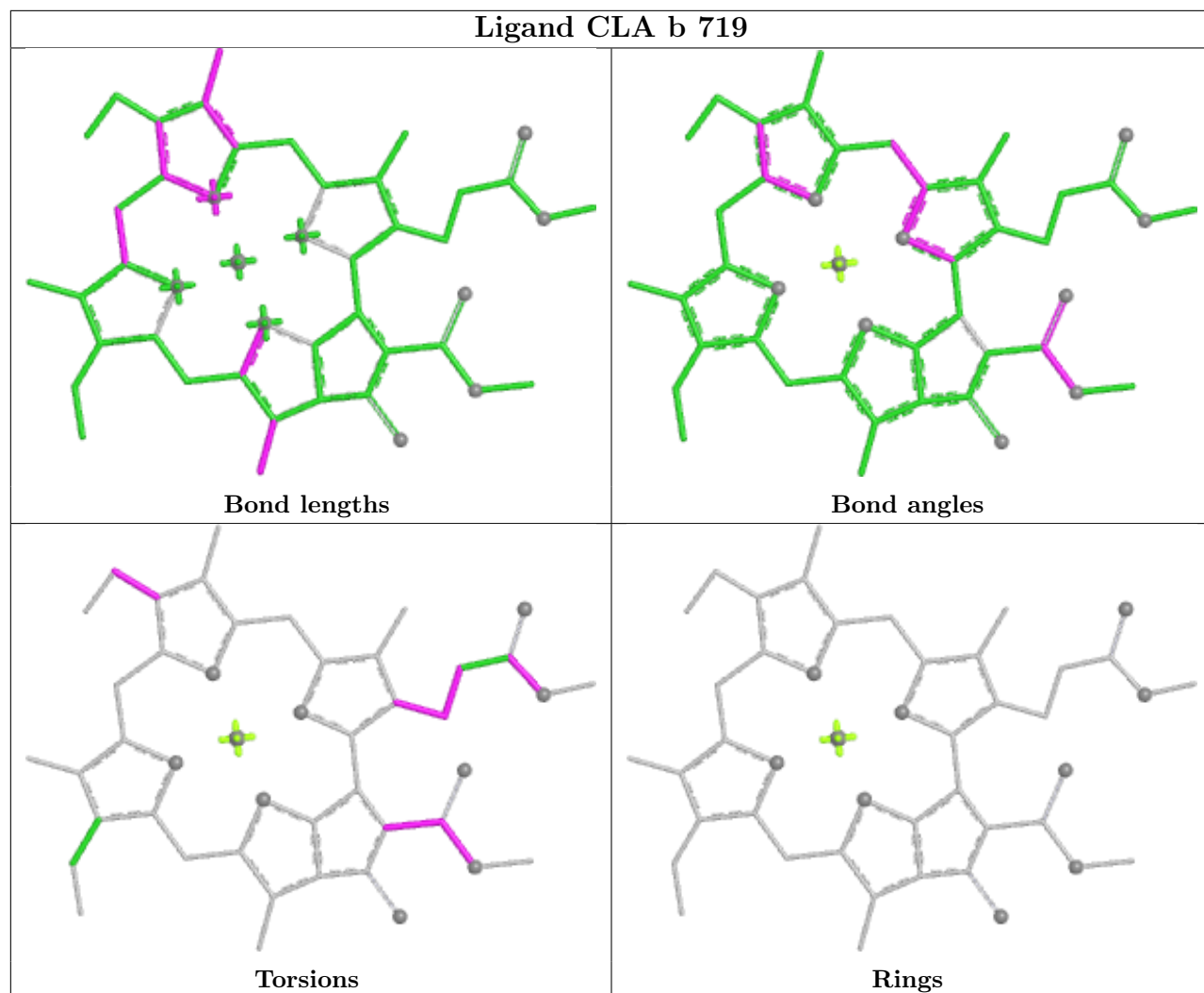


Torsions

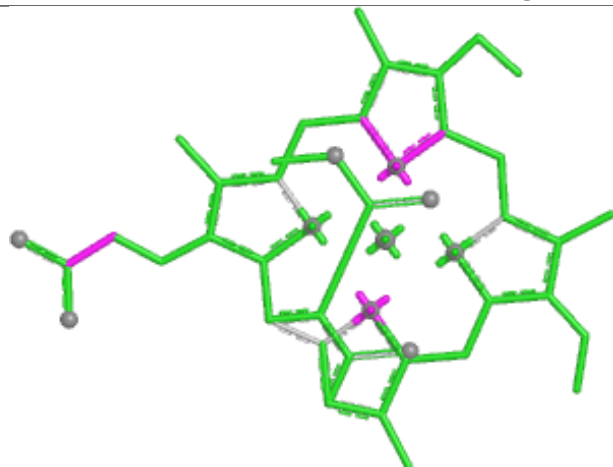


Rings

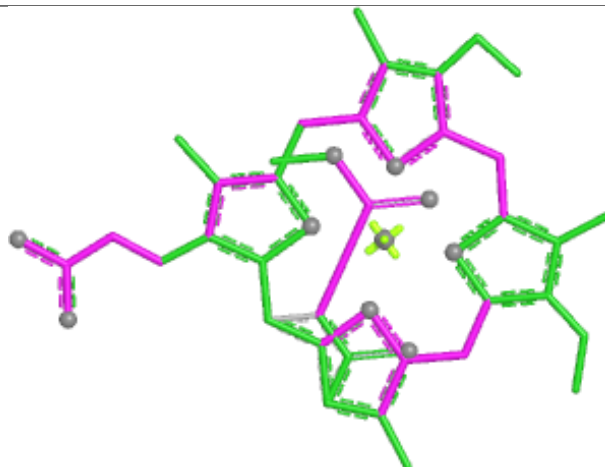
Ligand CLA b 719



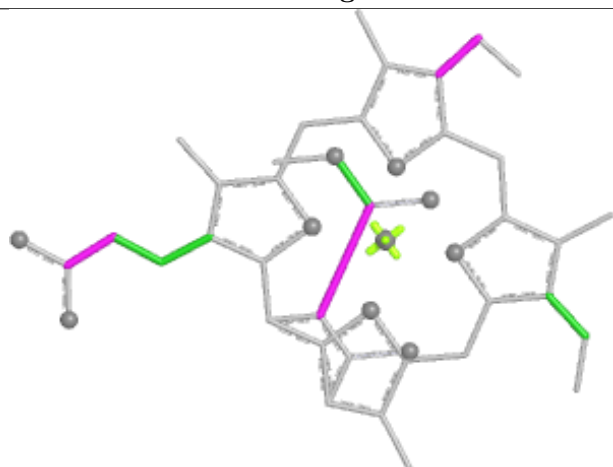
Ligand KC1 L 307



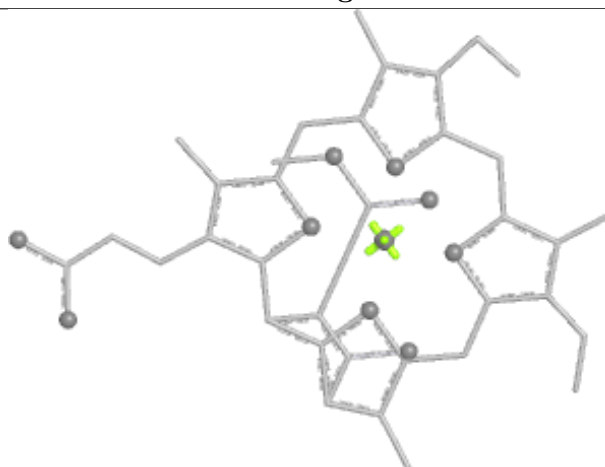
Bond lengths



Bond angles

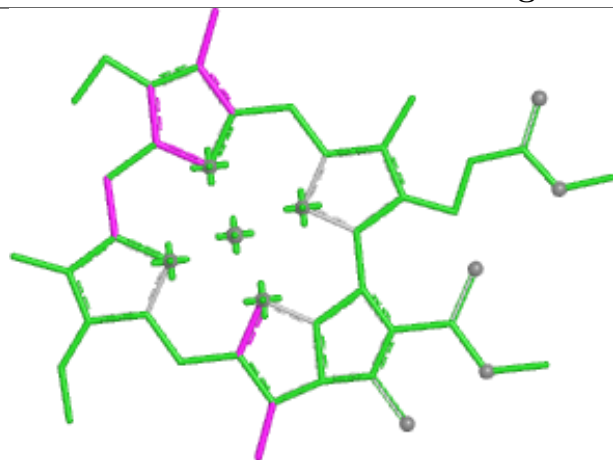


Torsions

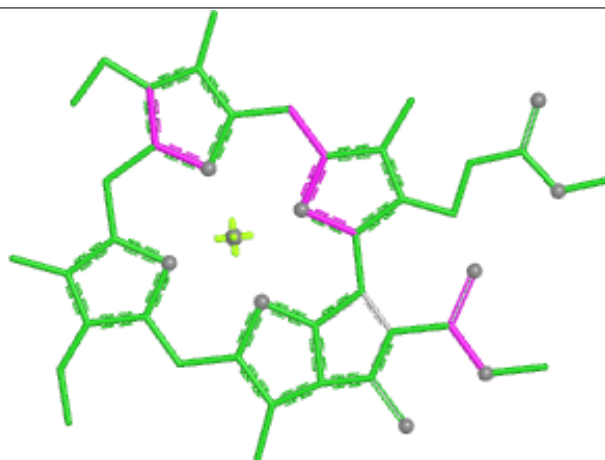


Rings

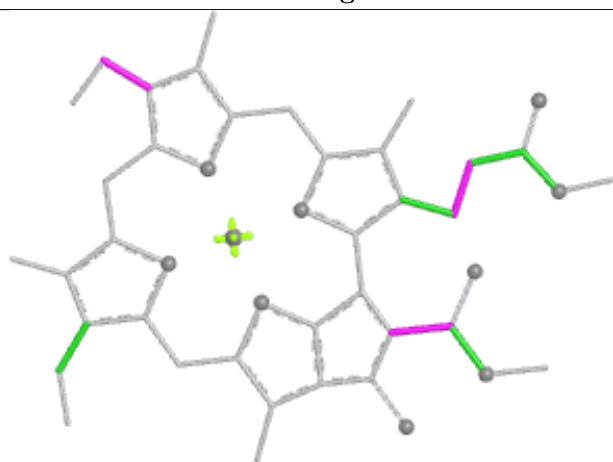
Ligand CLA J 316



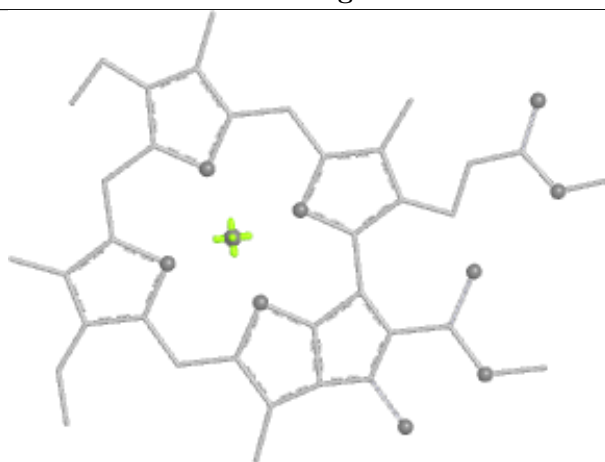
Bond lengths



Bond angles

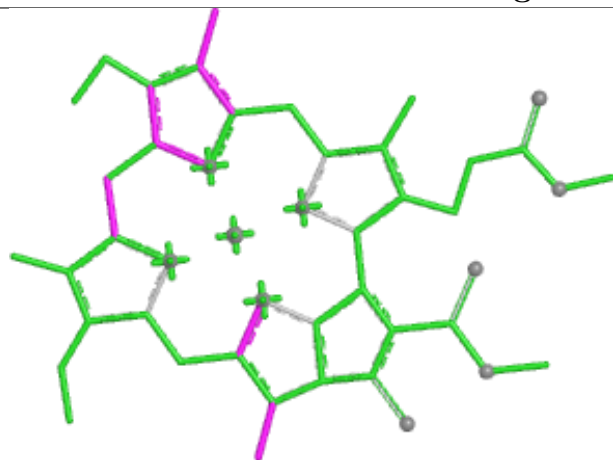


Torsions

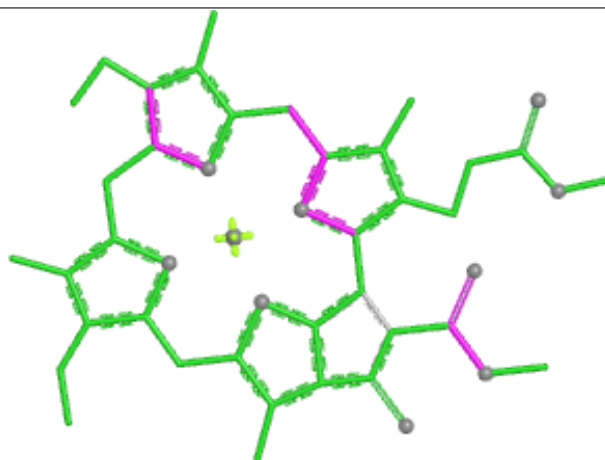


Rings

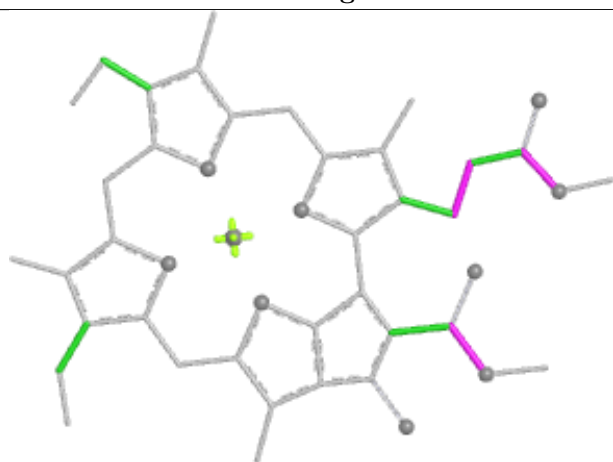
Ligand CLA A 311



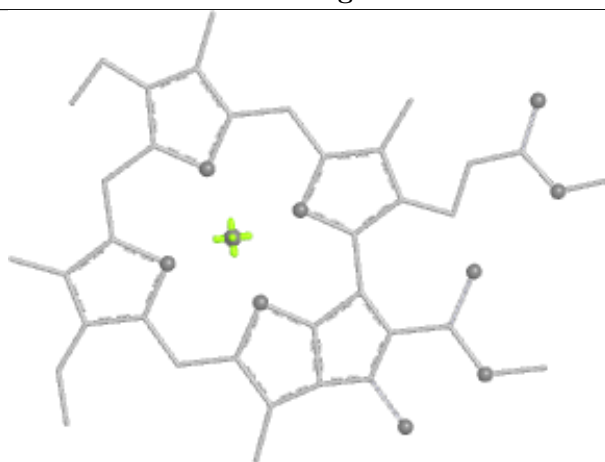
Bond lengths



Bond angles

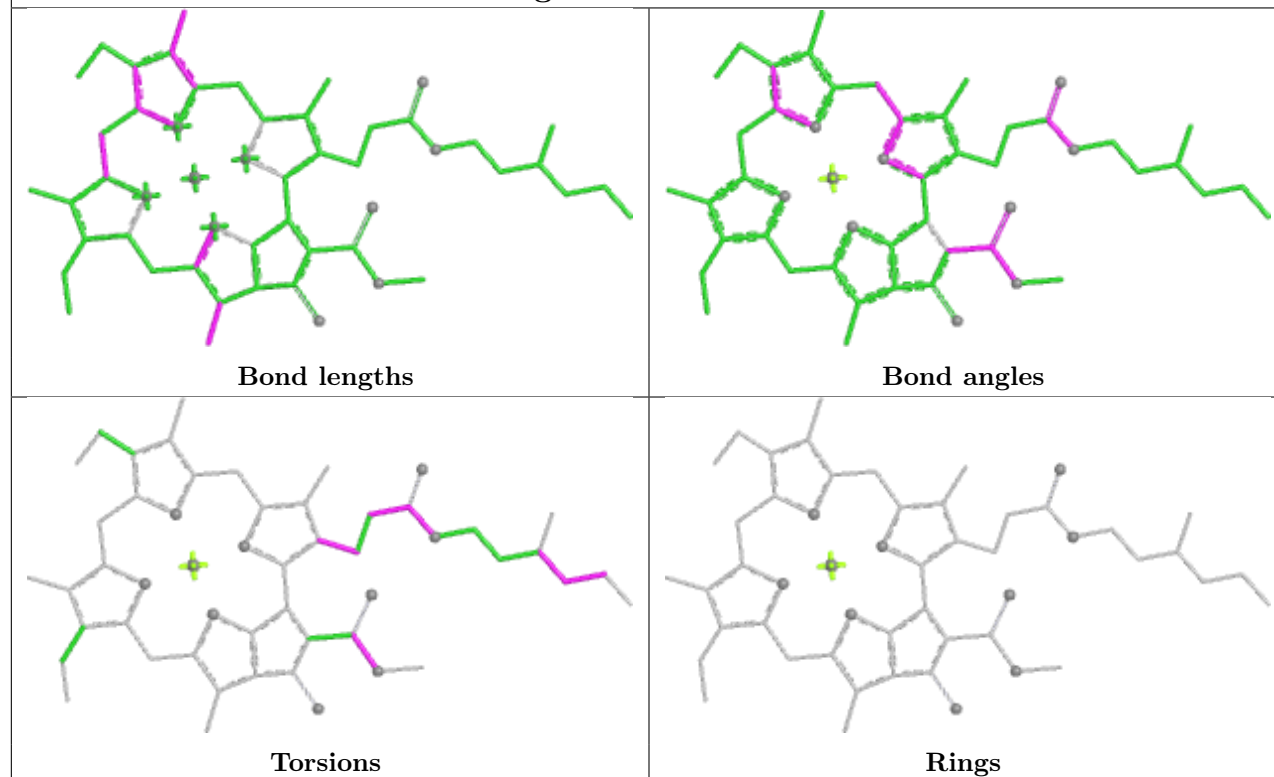


Torsions

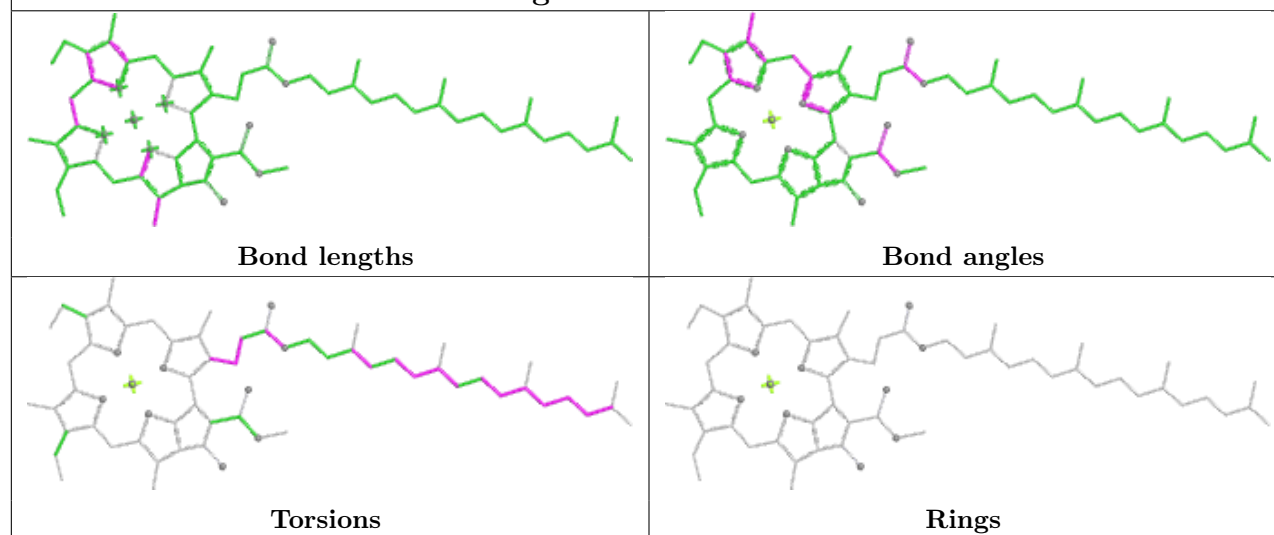


Rings

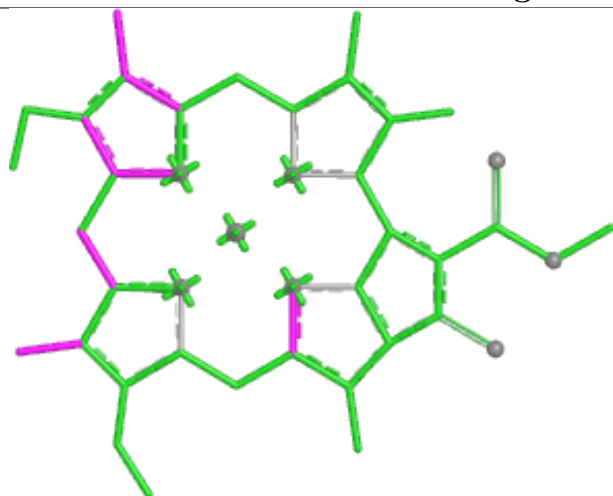
Ligand CLA L 317



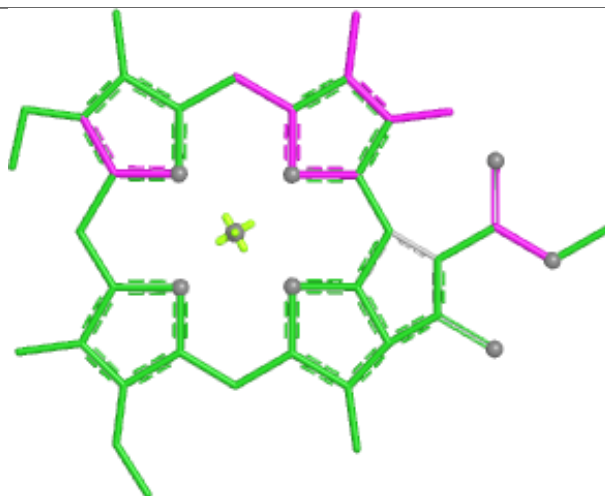
Ligand CLA B 309



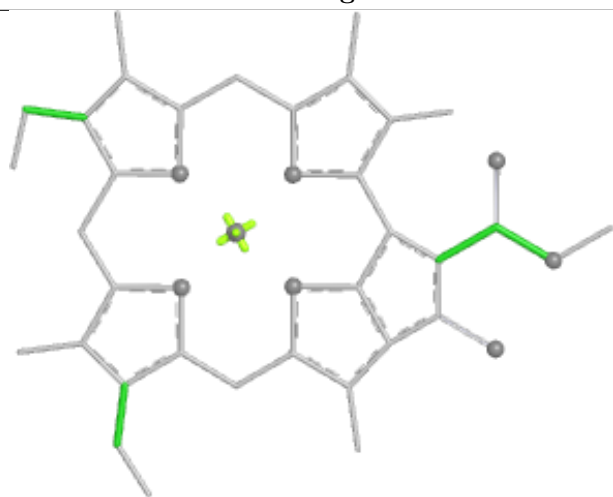
Ligand CLA A 317



Bond lengths



Bond angles

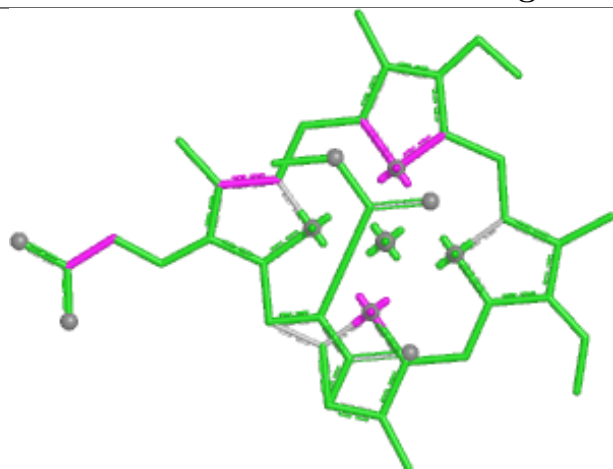


Torsions

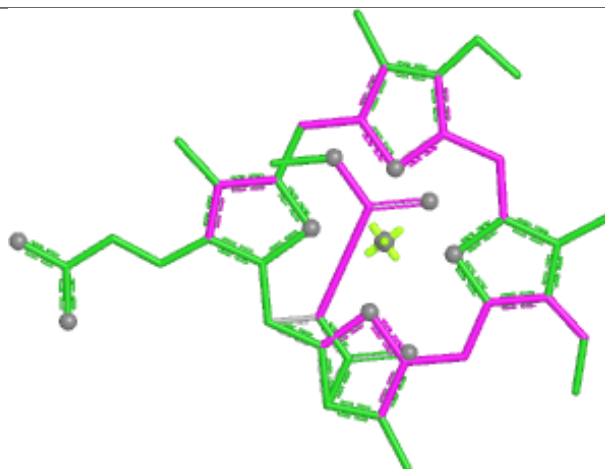


Rings

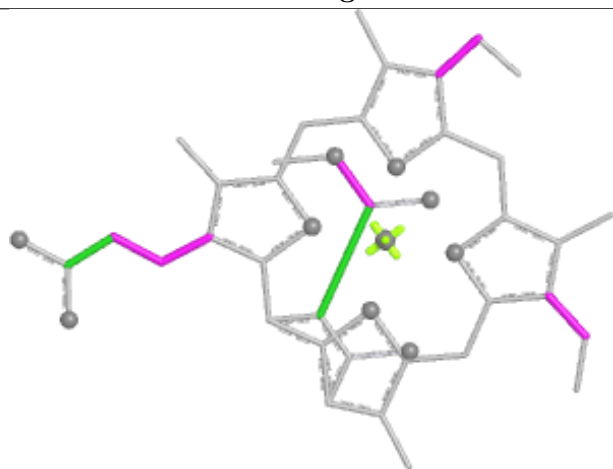
Ligand KC1 L 315



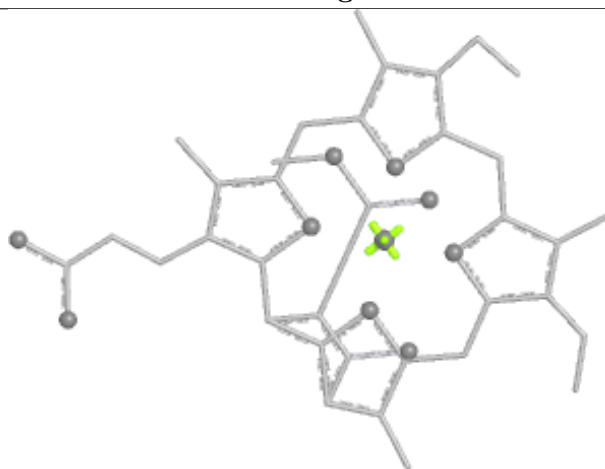
Bond lengths



Bond angles

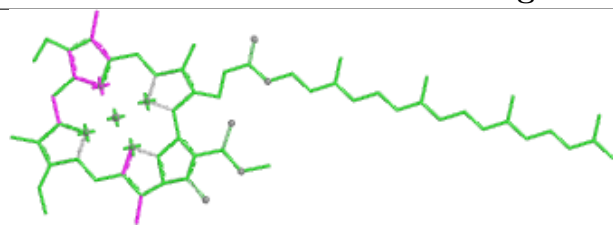


Torsions

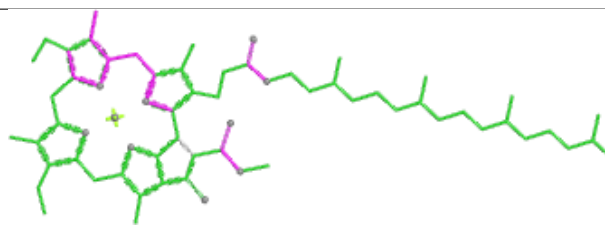


Rings

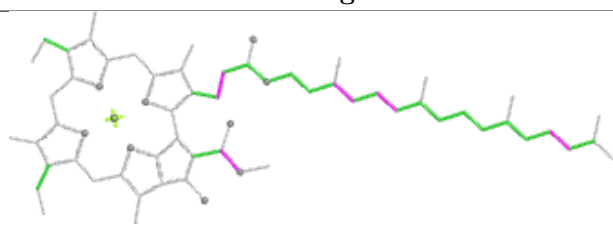
Ligand CLA b 722



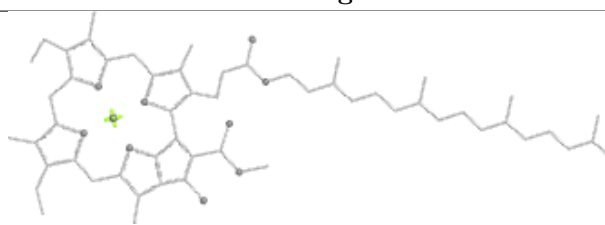
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

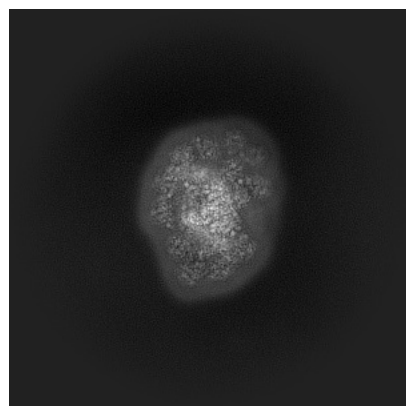
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-36743. These allow visual inspection of the internal detail of the map and identification of artifacts.

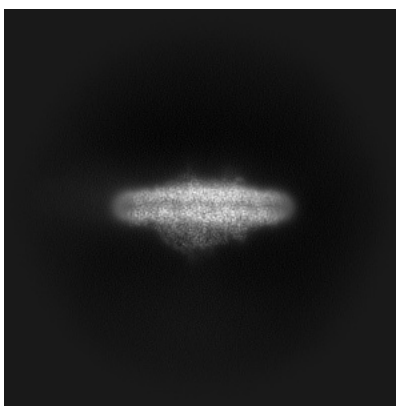
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

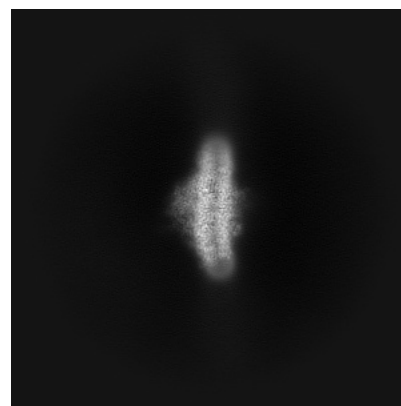
6.1.1 Primary map



X

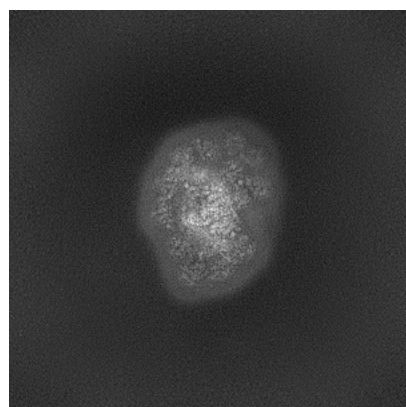


Y

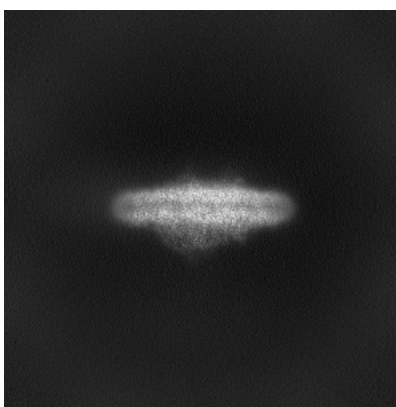


Z

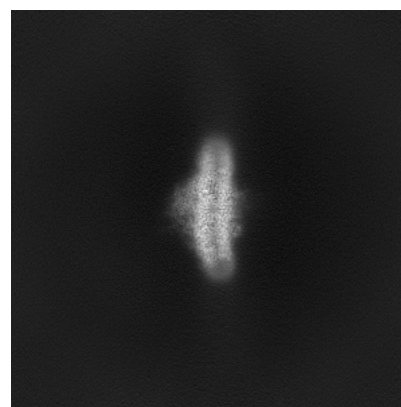
6.1.2 Raw map



X



Y

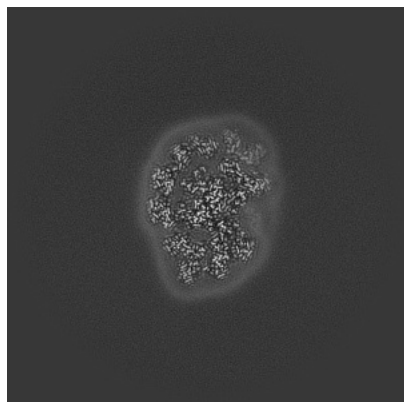


Z

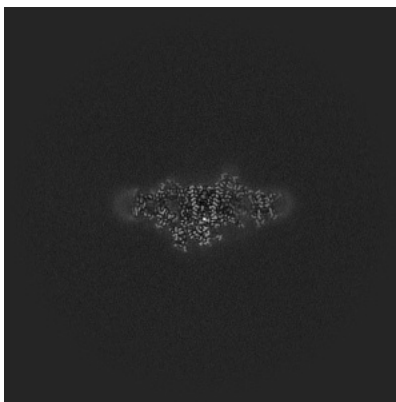
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

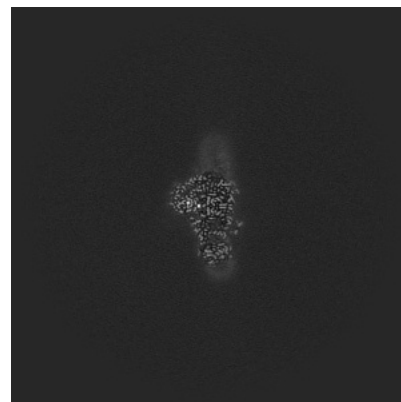
6.2.1 Primary map



X Index: 256

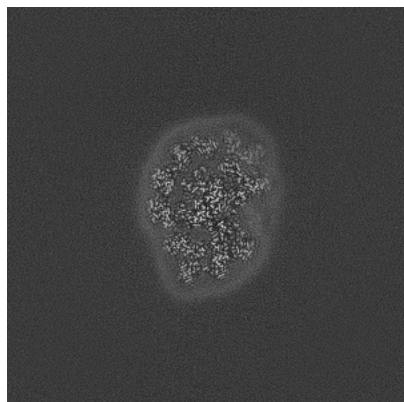


Y Index: 256

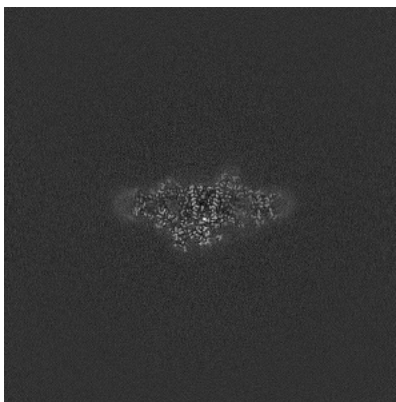


Z Index: 256

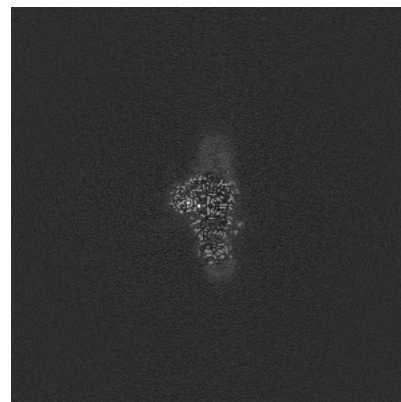
6.2.2 Raw map



X Index: 256



Y Index: 256

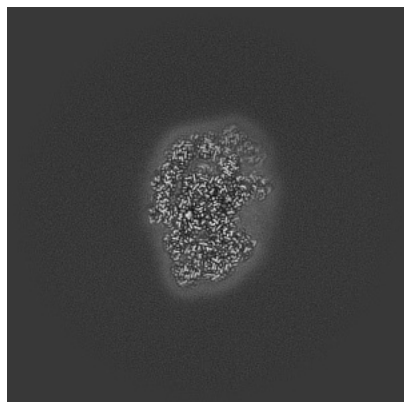


Z Index: 256

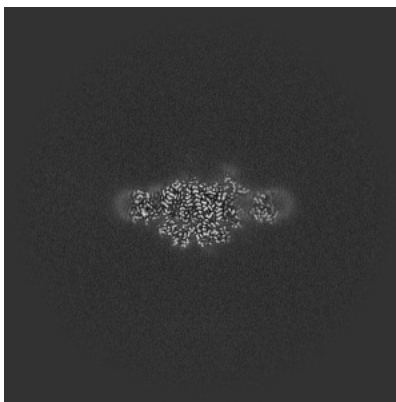
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

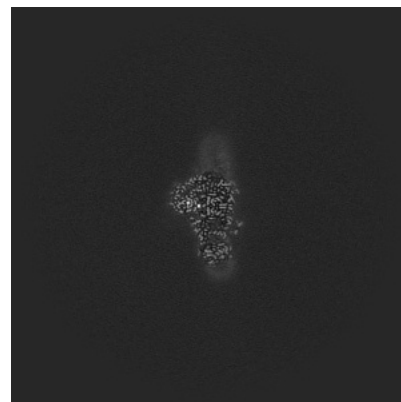
6.3.1 Primary map



X Index: 248

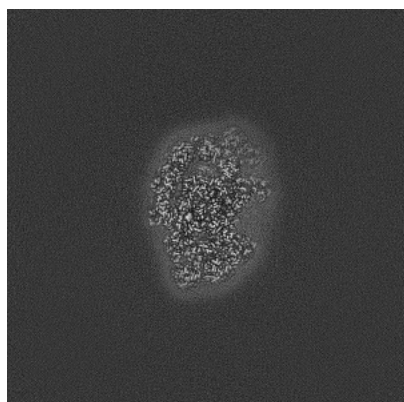


Y Index: 263

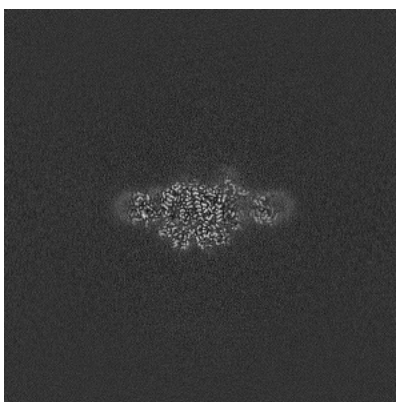


Z Index: 256

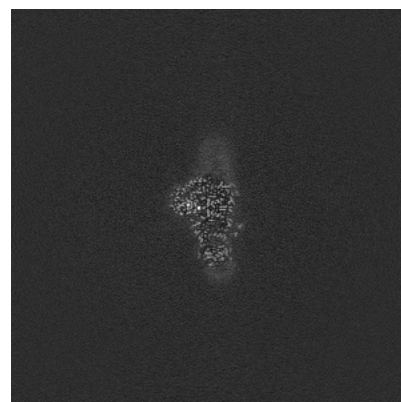
6.3.2 Raw map



X Index: 248



Y Index: 263

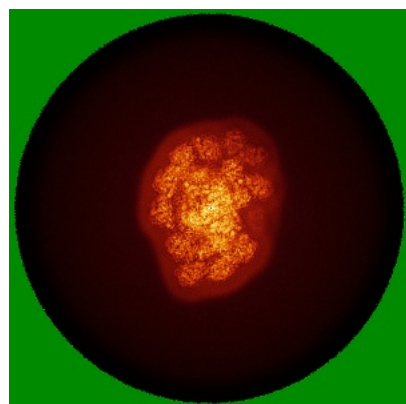


Z Index: 256

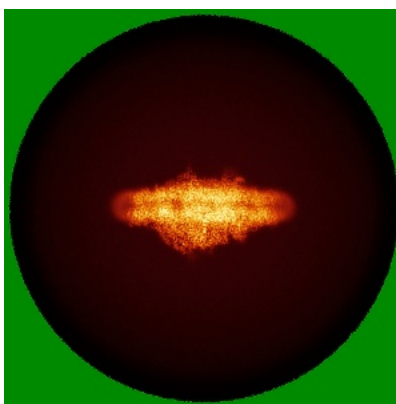
The images above show the largest variance slices of the map in three orthogonal directions.

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

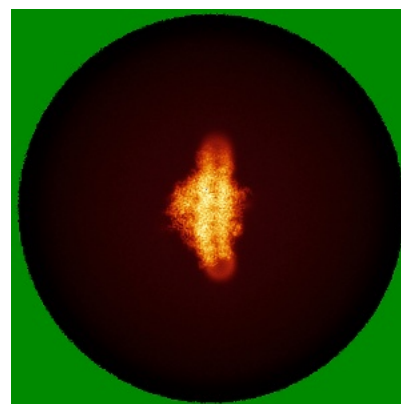
6.4.1 Primary map



X

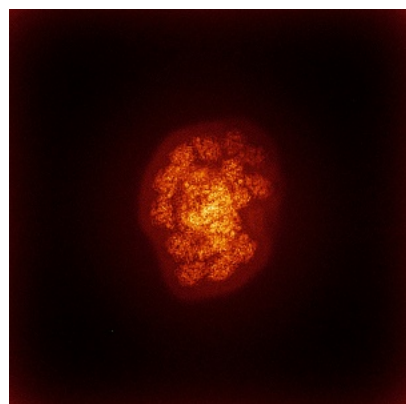


Y

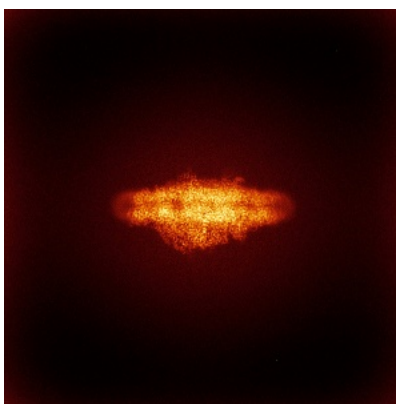


Z

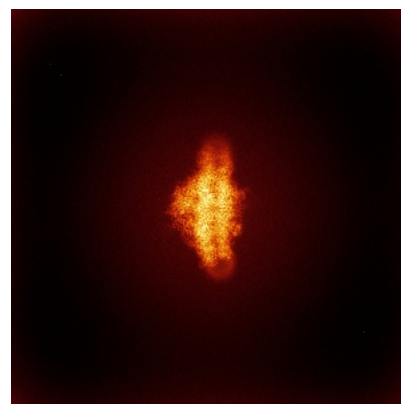
6.4.2 Raw map



X



Y

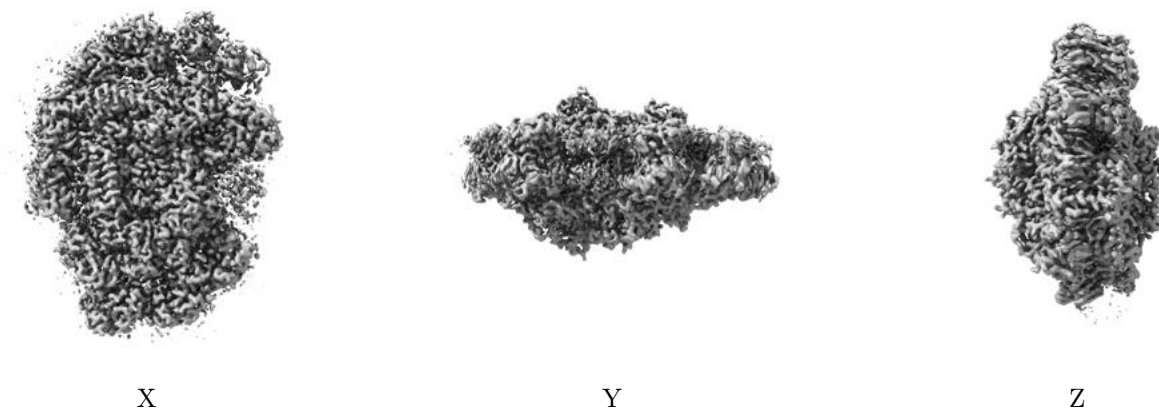


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.215. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

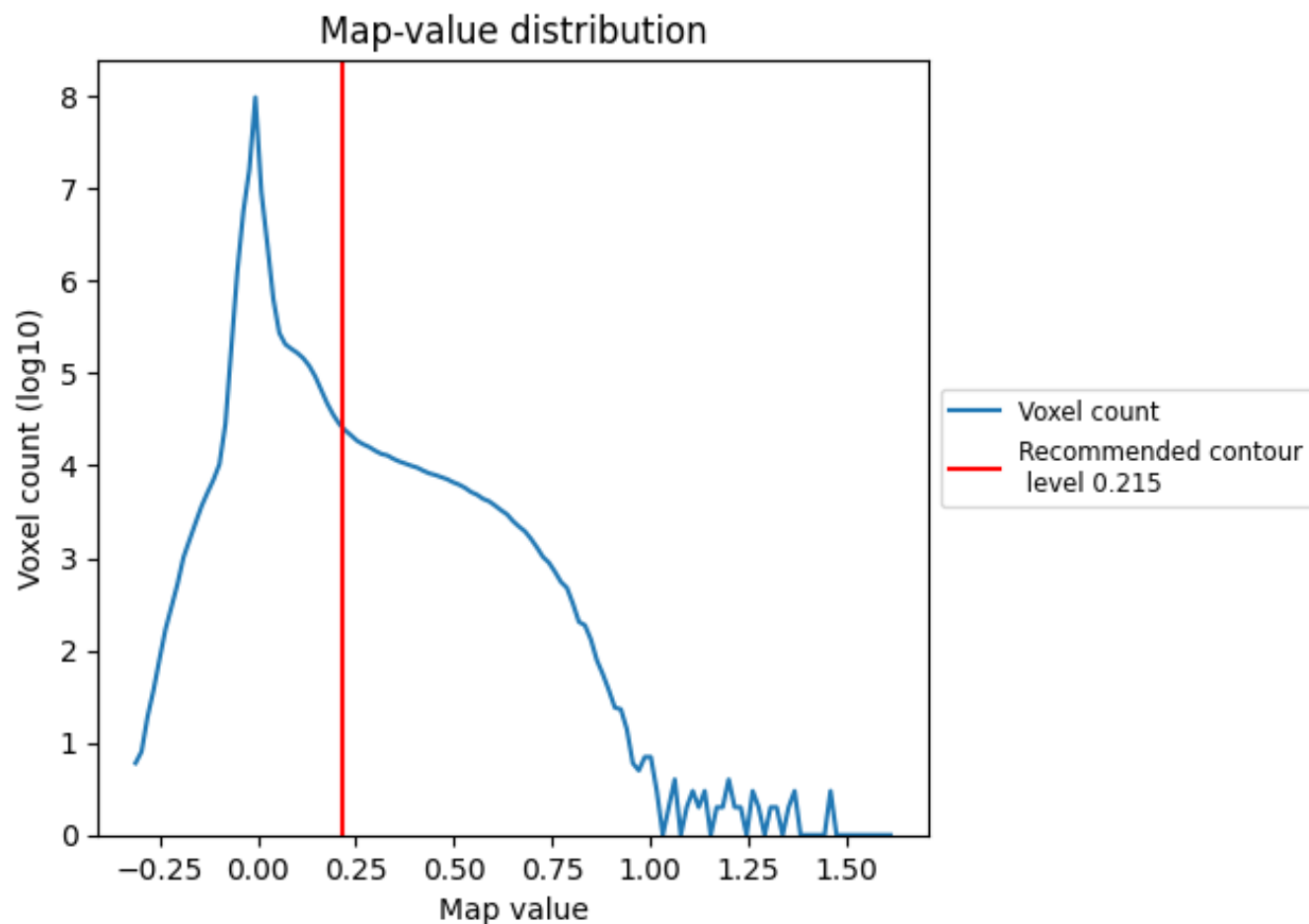
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

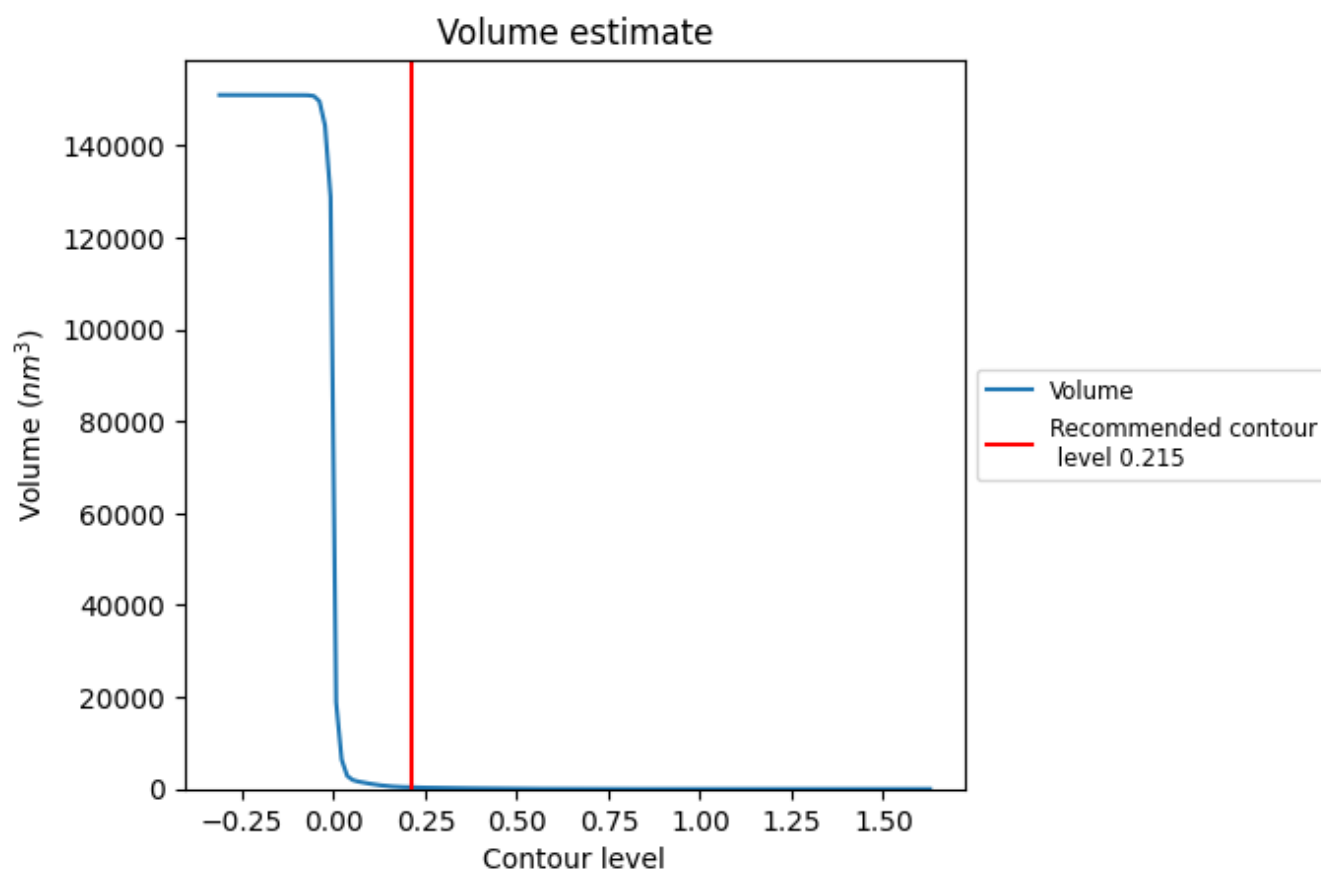
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

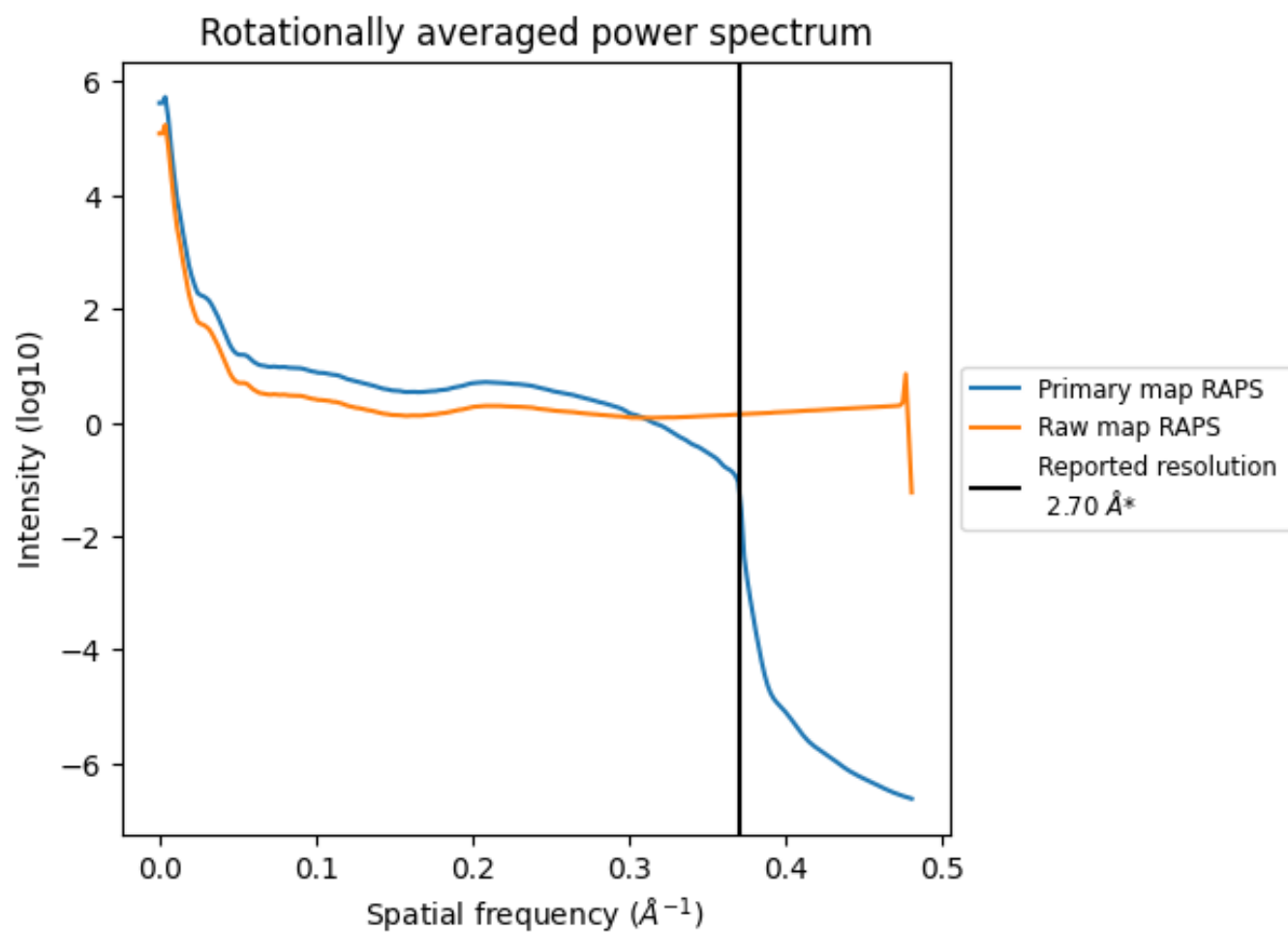
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 344 nm^3 ; this corresponds to an approximate mass of 311 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 ⓘ

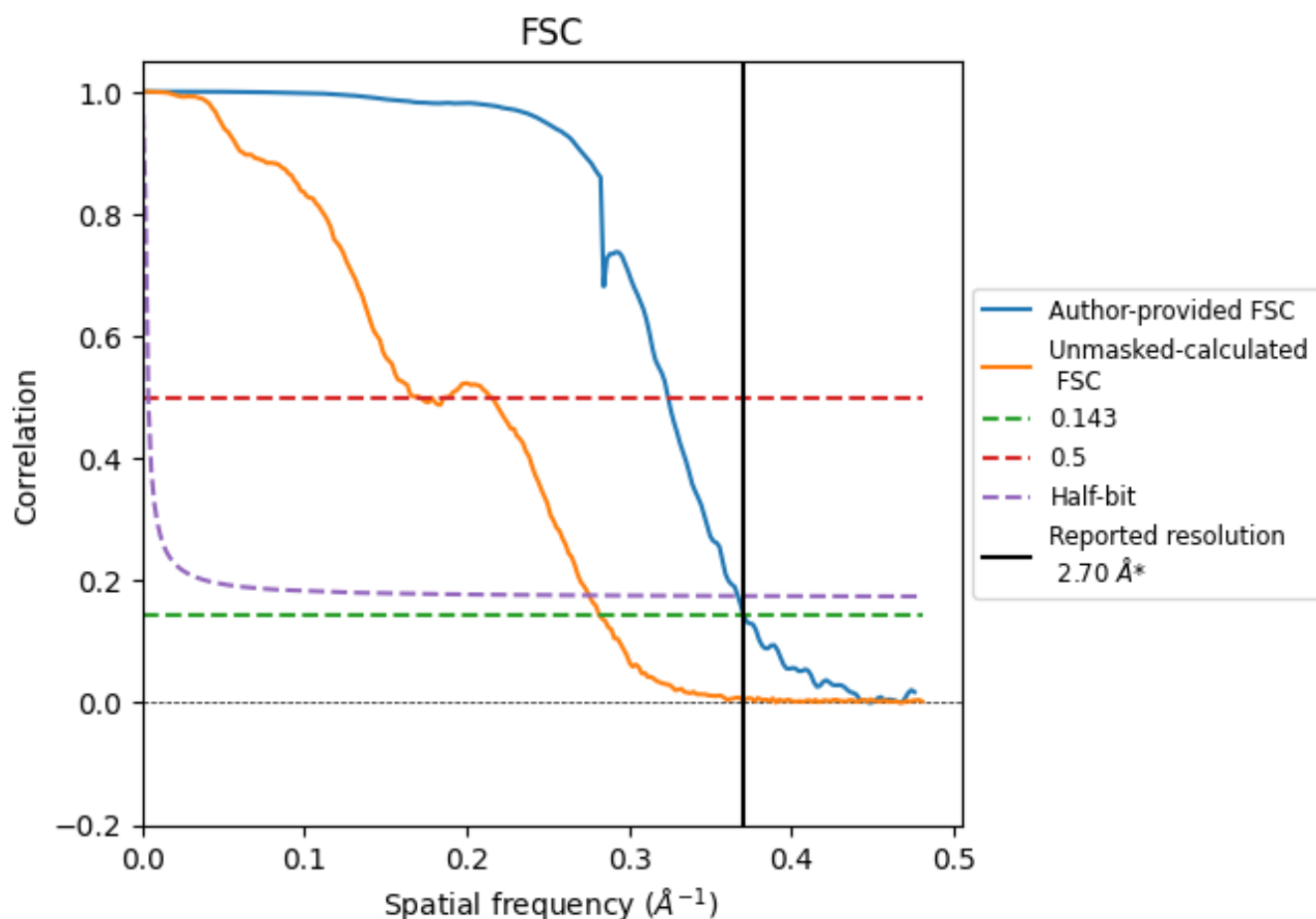


*Reported resolution corresponds to spatial frequency of 0.370 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of $0.370 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.70	-	-
Author-provided FSC curve	2.70	3.09	2.72
Unmasked-calculated*	3.55	5.84	3.63

*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 3.55 differs from the reported value 2.7 by more than 10 %

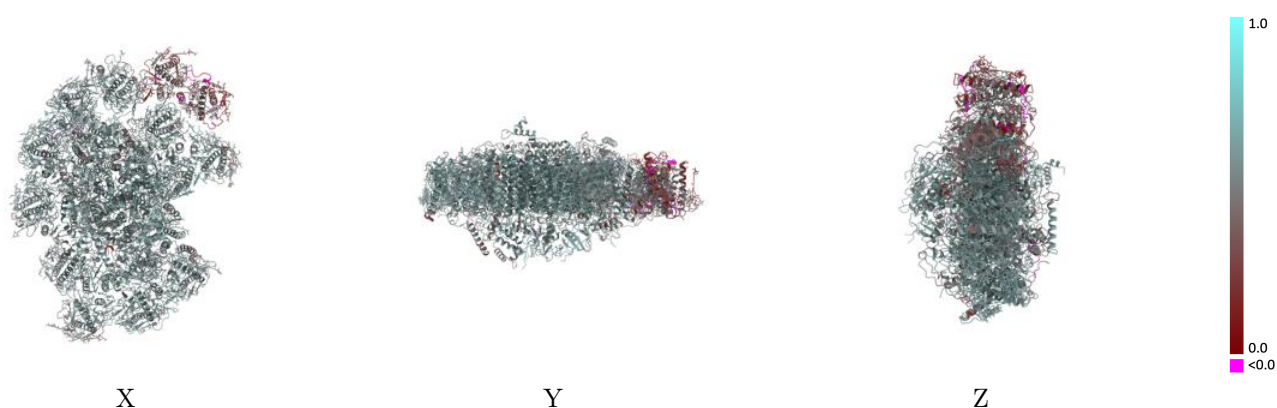
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-36743 and PDB model 8JZF. Per-residue inclusion information can be found in section 3 on page 34.

9.1 Map-model overlay [i](#)

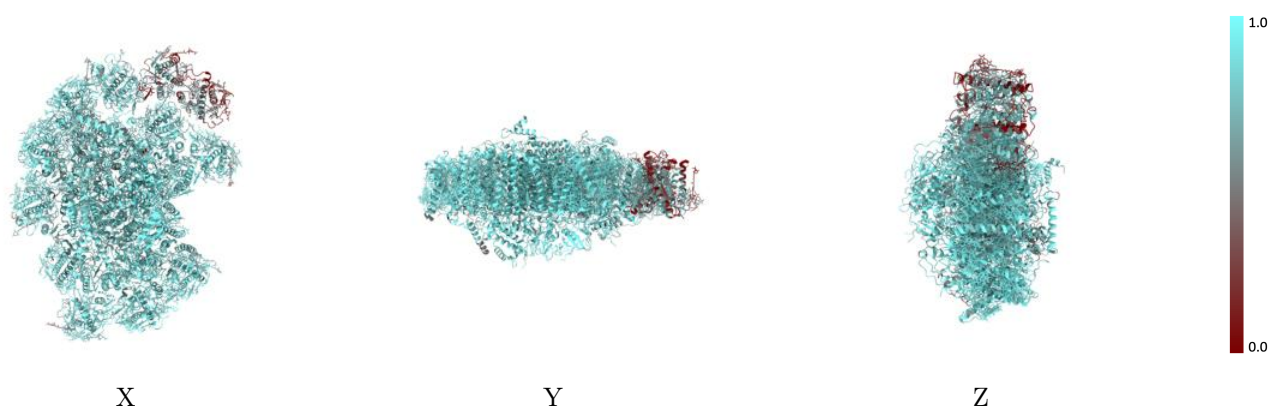
This section was not generated.

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



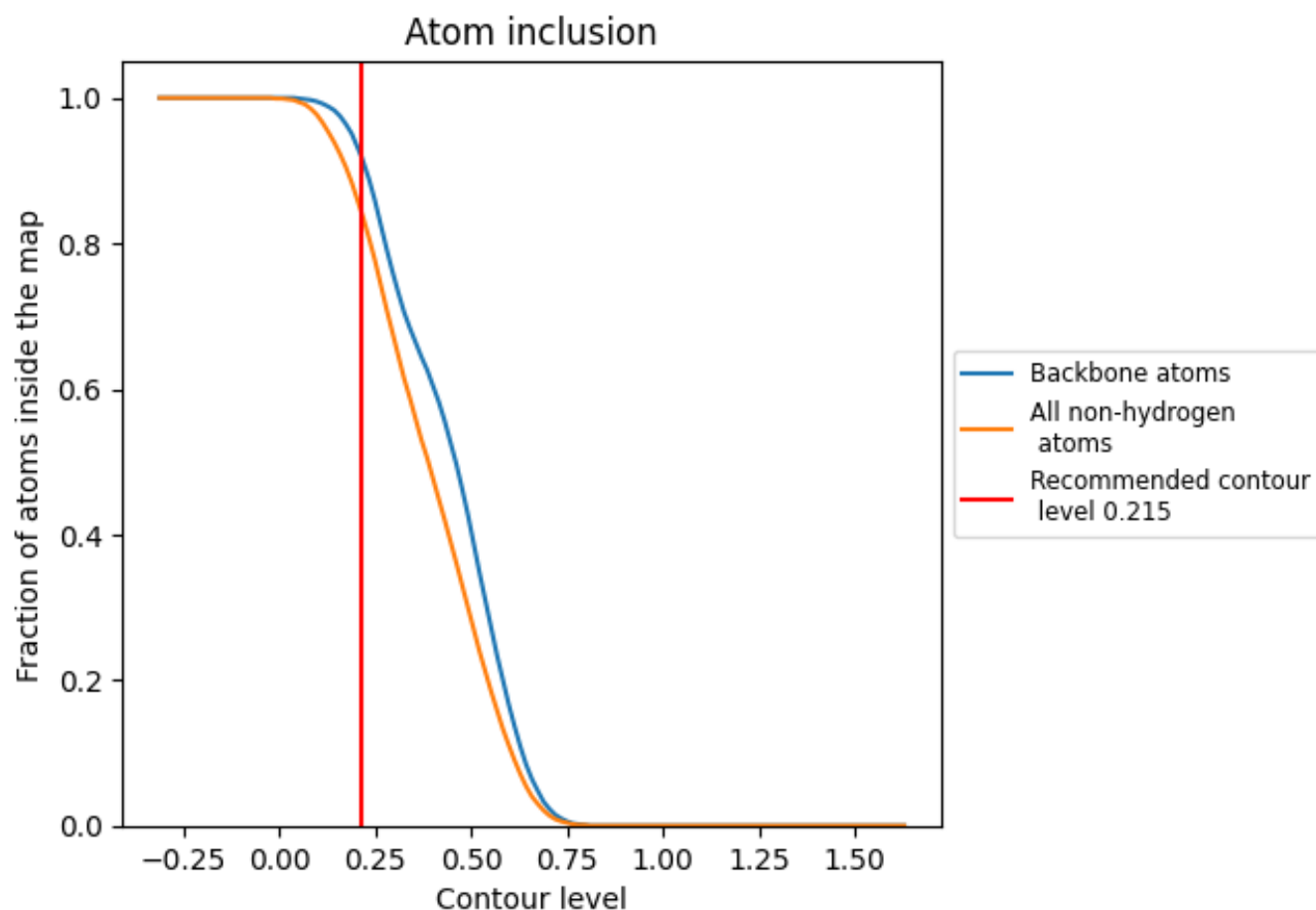
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.215).

9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 84% 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 (0.215) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8420	 0.5370
A	 0.8820	 0.5560
B	 0.8450	 0.5390
D	 0.8150	 0.5140
F	 0.7870	 0.5140
G	 0.8470	 0.5260
H	 0.3050	 0.2360
I	 0.8220	 0.5280
J	 0.8630	 0.5390
K	 0.8900	 0.5620
L	 0.8750	 0.5590
M	 0.8060	 0.5270
N	 0.4790	 0.3450
a	 0.8860	 0.5680
b	 0.9240	 0.5820
c	 0.9440	 0.5790
d	 0.8820	 0.5540
e	 0.9230	 0.5830
f	 0.8710	 0.5580
h	 0.9130	 0.5770
i	 0.8730	 0.5480
j	 0.8130	 0.5390
l	 0.9020	 0.5690
m	 0.8750	 0.5550
y	 0.8730	 0.5410
z	 0.9050	 0.5070

